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DANILO ALVES FERREIRA

O PAPEL DO METABOLISMO NO CONTROLE E DESENVOLVIMENTO DAS GEMAS AXILARES DE CANA-DE-AÇÚCAR

THE ROLE OF METABOLISM ON THE CONTROL AND DEVELOPMENT OF SUGARCANE AXILLARY BUDS

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Tese apresentada ao Instituto de Biologia da Universidade Estadual de Campinas como parte dos requisitos exigidos para a obtenção do título de Doutor em Genética e Biologia Molecular, na Área de Genética Vegetal e Melhoramento.

Thesis presented to the Institute of Biology of the University of Campinas in partial fulfillment of the requirements for the degree of Doctor, in the area of Plant Genetics and Breeding.

Orientadora: Dra. Camila Caldana

Este trabalho corresponde à versão final da tese defendida pelo aluno Danilo Alves Ferreira, e orientada pela Dra. Camila Caldana.

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“Temam menos a morte e mais a vida insuficiente” - Bertolt Brecht

RESUMO

O sucesso da produção em larga escala das espécies agrícolas comercialmente cultivadas é em grande parte decorrente da domesticação de suas estruturas propagativas, como sementes, propágulos, tubérculos, dentre outros. Ao contrário do observado para culturas de grãos, propagadas via sementes com alto vigor e taxa de germinação, a cana-de-açúcar é propagada vegetativamente via segmentos de colmo contendo gemas axilares, muitas vezes dormentes ou com baixo vigor de brotação. A dificuldade em desenvolver materiais mais eficientes quanto a sua taxa de brotação é decorrente principalmente por essa não ser uma característica objeto dos programas de melhoramento genético, já que a seleção fenotípica de novos genótipos é intrínseca a brotação da cultura no campo. Além disso, os mecanismos atuantes no controle e desenvolvimento das gemas axilares é complexo e pouco elucidado para a cultura. Com o objetivo de investigar o papel do metabolismo no controle e desenvolvimento das gemas axilares de cana-de-açúcar, foram coletadas amostras desses órgãos e de colmos de diferentes genótipos de cana-de-açúcar e analisadas através de perfis metabólicos em larga escala (GC-TOF-MS), combinadas com a taxa de brotação desses genótipos. Os resultados demonstram diferenças metabólicas, em especial do metabolismo primário entre os genótipos de cana-de-açúcar quando associados ao *trait* brotação. Dentre as via metabólicas identificadas na quebra de dormência e desenvolvimento inicial das gemas axilares, destacam-se as relacionadas à partição de carbono, nitrogênio e produção de energia. Além disso, as poliaminas parecem também exercer papel no desenvolvimento destes órgãos. Estes resultados, em associação ao background genético da cultura, demonstram que os metabólitos podem ser potencialmente utilizados como indicadores para predição de novas variedades.

ABSTRACT

The success of large-scale production of commercial crops is especially due to the domestication of its propagation structures, such as seeds, propagules, tubers, among others. Differently to what is observed for grains crops, propagated by seeds with high vigor and germination rate, sugarcane is vegetatively propagated by stalks segments containing axillary buds, often dormant or with low sprouting vigor. The challenge in developing new varieties more efficient in sprouting rate is mainly due this trait is not a characteristic screened in breeding programs, since the phenotypic selection of new genotypes is intrinsic to the sprouting of the crop in the field. In addition, the mechanisms involved in controlling and development of axillary buds are complex and little elucidated in crop. In order to investigate the role of metabolism in the control and development of sugarcane axillary buds, samples of these tissues and stem from different genotypes were collected and analyzed through large-scale metabolic profiles (GC-TOF-MS), combined with the sprouting rate of these genotypes. Our results demonstrate metabolic differences, especially related to primary metabolism among sugarcane genotypes when associated with the trait sprouting. Among the metabolic pathways, identified in the dormancy break and initial development of the axillary buds, the most relevant are those related to the carbon partitioning, nitrogen and energy production. In addition, the polyamines also figure as candidates in controlling of the development of these tissues. These results, in association with the genetic background of the crop, presents the potentially use of metabolites as indicators to select new sugarcane varieties on breeding programs.

Sumário

1. Introdução geral

A cana-de-açúcar é considerada uma das principais culturas de interesse econômico tanto para indústria alimentícia quanto para fins energéticos por sua alta eficiência em acumulo de biomassa e açúcar. O Brasil é ranqueado como líder mundial em sua produção com 8.7 milhões de hectares plantados e 635 milhões de toneladas produzidas (Companhia Nacional de Abastecimento - CONAB, 2018), e consequentemente, também o maior exportador de açúcar e etanol. Além da produção de açúcar e álcool, o bagaço de cana-de-açúcar pode ser hidrolisado, fermentado e destilado para a produção do etanol de segunda geração, também conhecido como etanol 2G (NAKANISHI et al., 2017), ou, queimado para produção de energia para sustentar as próprias usinas e seu excedente energético ser comercializado ao setor de energia elétrica.

Assim como em outras culturas de interesse agrícola, o sucesso de cultivo da cana-de-açúcar é decorrente de um melhoramento genético bem-sucedido. Apesar disto, o melhoramento genético convencional é extremamente laborioso, demandando um longo período para o lançamento de uma nova variedade dependendo do objetivo do programa: média de 5 anos para cana energia e 15 anos para cana-de-açúcar. Este fato se deve principalmente, ao longo ciclo da cultura, seleção fenotípica da progênie F1, ensaios de competição através da propagação vegetativa desta progênie, resultando geralmente, em uma baixa eficiência na seleção de fenótipos. Dentre os *traits* de difícil seleção, pode-se destacar a brotação da cana-de-açúcar. Uma vez que multiplicada por meio da propagação vegetativa de suas gemas axilares, diferenças genotípicas para tal parâmetro não são exploradas, pois consideram-se todos os eventos que expressaram o fenótipo de “brotação”, ainda que esse possa ser pouco eficiente. A baixa eficiência na taxa de brotação da cultura é evidenciada pelo volume de material empregado no plantio, realizado por meio da distribuição de segmentos de colmo (toletes) contendo de 3 a 4 gemas axilares no sulco de plantio, contabilizando aproximadamente 12 a 15 ou 20 gemas m^{-1} no plantio manual ou mecanizado, respectivamente. Entretanto, em decorrência da competição intraespecífica, apenas 2 a 4 touceiras são perpetuadas em um metro linear. Assim, considerando que uma gema viável é suficiente para formação de uma touceira, apenas 18% das gemas plantadas serão responsáveis pela formação do dossel de um canavial, ou seja, um desperdício de aproximadamente 80%.

Devido à complexidade da maioria das características de interesse agronômico, controlada por inúmeros genes, o uso de métodos de seleção independentes da análise fenotípica, como seleção assistida por marcadores moleculares, tem sido amplamente usado em agricultura para melhoramento de espécies cultivadas. Neste contexto, os adventos das técnicas de biologia molecular somam aos programas de melhoramento da cana-de-açúcar na identificação de novos *traits* de interesse agrícola e industrial, bem como na seleção e desenvolvimento de novas variedades. Desse modo, o melhoramento genético assistido da cana-de-açúcar confere maior eficiência ao processo, resultando em variedades melhores adaptadas aos diferentes ambientes de produção com menor tempo de desenvolvimento e seleção. Entretanto, o complexo genoma da cana-de-açúcar impõe limitações ao uso da técnica, assim, o uso de outras ferramentas moleculares que auxiliem e/ou complementem a técnica já citada, trariam ainda mais eficiência a seleção e desenvolvimento de novas variedades de cana-de-açúcar.

A grande maioria das características de importância agronômica, como aumento do conteúdo de açúcar, ou teor nutricional de frutos é em grande parte controlada pelo metabolismo. Recentemente, foi demonstrado o uso da metabolômica como uma importante ferramenta para seleção de genótipos em programas de melhoramento. Esta técnica constitui-se do estudo em larga escala das pequenas moléculas (aproximadamente < 1000Da) ou metabólitos que fornecem um panorama instantâneo da fisiologia celular, determinando o fenótipo e a intensidade com a qual cada *trait* de interesse esteja sendo expresso.

Assim, por meio do uso da técnica da metabolômica, este trabalho tem como objetivo identificar em diferentes genótipos de cana-de-açúcar, conjuntos de metabolitos que sejam relevantes do ponto de vista bioquímico e fisiológico, em especial, em processos pouco elucidados como o desenvolvimento de meristemas axilares que são cruciais para a propagação vegetativa da cultura bem como para o estabelecimento da arquitetura da planta e o dossel do canavial.

2. Revisão de literatura

2.1 Melhoramento genético da cana-de-açúcar

Saccharum L. é um complexo gênero de plantas poliploides pertencente à família *Poaceae*, da qual cana-de-açúcar faz parte (GUIMARÃES et al., 1999). As variedades atuais de cana-de-açúcar são derivadas da hibridização interespecífica entre espécies deste gênero, sendo elas principalmente *S. officinarum* (2n = 80), *S. spontaneum* (2n = 40-128), *S. sinense* (2n = 81-124), *S. barberi* (2n = 111-120), *S. edule* (2n = 60-80) e *S. robustum* (2n = 60-80), resultando em híbridos poliploides *Saccharum ssp.* (2n = 100-130) (D'HONT et al., 1995, 1996; GRASSL, 1946; GUIMARÃES; SILLS; SOBRAL, 1997), com combinação aleatória e imprevisível do número de cromossomos (GRIVET; ARRUDA, 2002).

Estima-se que as variedades atuais de cana-de-açúcar possuem potencial teórico para acumular 48 g/m^2 dia de massa seca, e produtividade de 381 ton ha^{-1} de colmos (WACLAWOVSKY et al., 2010). Apesar disso, com uma média nacional estimada em 72 ton ha^{-1}, seu rendimento está longe de seu potencial teórico, ou mesmo de sua máxima produtividade experimental (212 ton ha^{-1} (WACLAWOVSKY et al., 2010)), demonstrando que há ainda muito a ser explorado em termos produtivos. Assim, além do acumulo de sacarose, um dos principais objetivos dos programas de melhoramento de cana-de-açúcar é aumentar a produtividade da cultura, uma vez que características do colmo como diâmetro e número de perfilhos estão diretamente associadas à produção e acumulo de açúcar (SCORTECCI, 2012). Além das características diretamente relacionadas à produtividade como biomassa de colmos e açúcar, outras características de interesse agronômico têm sido avaliadas pelos programas de melhoramento, tais como precocidade, resistência a doenças, tolerância à seca, menor florescimento, e mais recentemente, celulose, hemicelulose e lignina em variedades voltadas para geração de energia.

Embora ainda distante de seu potencial produtivo, é atribuído ao melhoramento genético o atual rendimento observado para a cana-de-açúcar, ao qual se considera o principal fator para incrementos de produtividade de aproximadamente 50%, decorrente do continuo lançamento de variedades comerciais mais produtivas (BARBOSA et al., 2012). No Brasil, o melhoramento genético da cultura concentra-se em três principais programas, são eles: Rede Interuniversitária de Desenvolvimento do Setor Sucroalcooleiro (Ridesa), Instituto Agronômico de Campinas (IAC) e Centro de Tecnologia Canavieira (CTC). Desses, as variedades Ridesa tem a maior representatividade nacional, chegando corresponder 64% das variedades cultivadas no país (safra 2016/2017) (**Figura 2.1**) (Ridesa, https://www.ridesa.com.br/censo-varietal; Revista Canavieiros, http://www.revistacanavieiros.com.br/imagens/pdf/09f565a3c66e3938ab965b0e8378b66f.pdf).

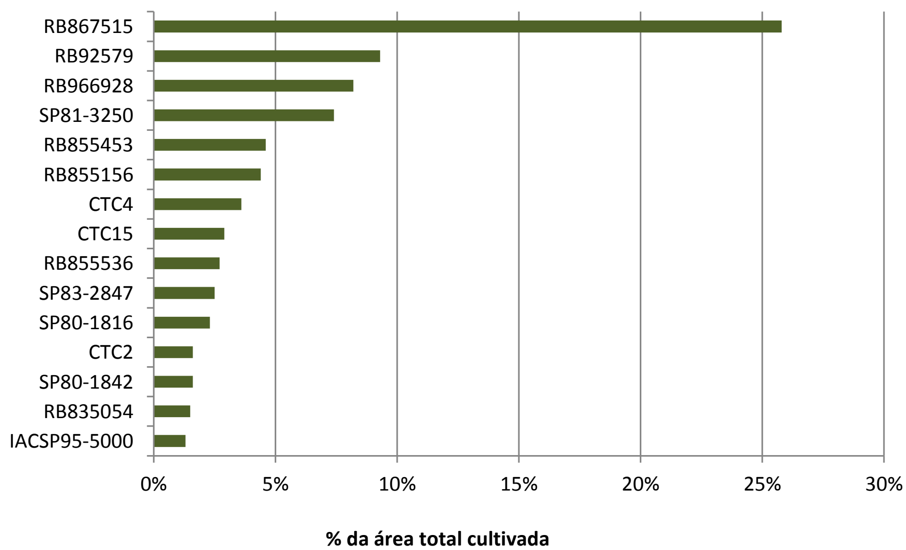

Figura 2.1 - Principais variedades de cana-de-açúcar cultivadas no Brasil na safra de 2016/2017. Adaptado de Revista Canavieiros (http://www.revistacanavieiros.com.br/imagens/pdf/09f565a3c66e3938ab965b0e8378b66f.pdf).

As novas variedades comerciais de cana (*Saccharum ssp.)* vem sendo desenvolvidas a partir seleção massiva de populações segregantes propagadas vegetativamente, provenientes do cruzamento sexuado de híbridos poliploides (BRESSIANI; VENCOVSKY; BURNQUIST, 2002). Esses cruzamentos são realizados de modo biparental, onde os dois genitores são conhecidos, ou por cruzamentos múltiplos, no qual, com objetivo de aumentar a variabilidade genética, apenas a planta mãe é conhecida, e o pólen pode ser proveniente de diversos indivíduos (HEINZ, 2015; SANTOS et al., 2014). Para tal, a escolha dos parentais deve ser muito bem planejada e devem ser considerados fatores como o grau de endogamia entre os parentais e as características de interesse agrícola desejadas. Considera-se que os ganhos em produtividade tanto em açúcar quanto em biomassa de colmos, são atribuídos, principalmente, ao sucesso do uso da seleção recorrente, selecionando clones superiores como genitores (BURNQUIST; REDSHAW; GILMOUR, 2010; E. LINGLE et al., 2010).

Assim, as sementes segregantes obtidas dos cruzamentos, em especial os múltiplos, são distribuídas em diversas localidades e ambientes de produção para que seja feita a seleção fenotípica dos milhares de genótipos obtidos dos cruzamentos. Como consequência, o lançamento de novas variedades de cana-de-açúcar pode demandar longos 15 anos. Nesse sentido, a seleção de clones superiores e a eliminação de grande parte dos clones indesejáveis já nas gerações iniciais é fundamental para que a avaliação dos clones remanescentes seja realizada com maior critério, evitando-se assim o gasto desnecessário de recursos pelos programas de melhoramento. Ainda assim, o melhoramento da cana-de-açúcar é limitado à seleção visual de indivíduos, sendo facilmente descartados materiais promissores, especialmente, nas fases iniciais de seleção. Além disso, e também em consequência do longo período de desenvolvimento de novas variedades, as atuais variedades comerciais apresentam baixa variabilidade genética, uma vez que são provenientes de um germoplasma restrito e possuem poucas gerações de seleção (**Figura 2.2**) (CRESTE et al., 2010; DAL-BIANCO et al., 2012; RABOIN et al., 2008).

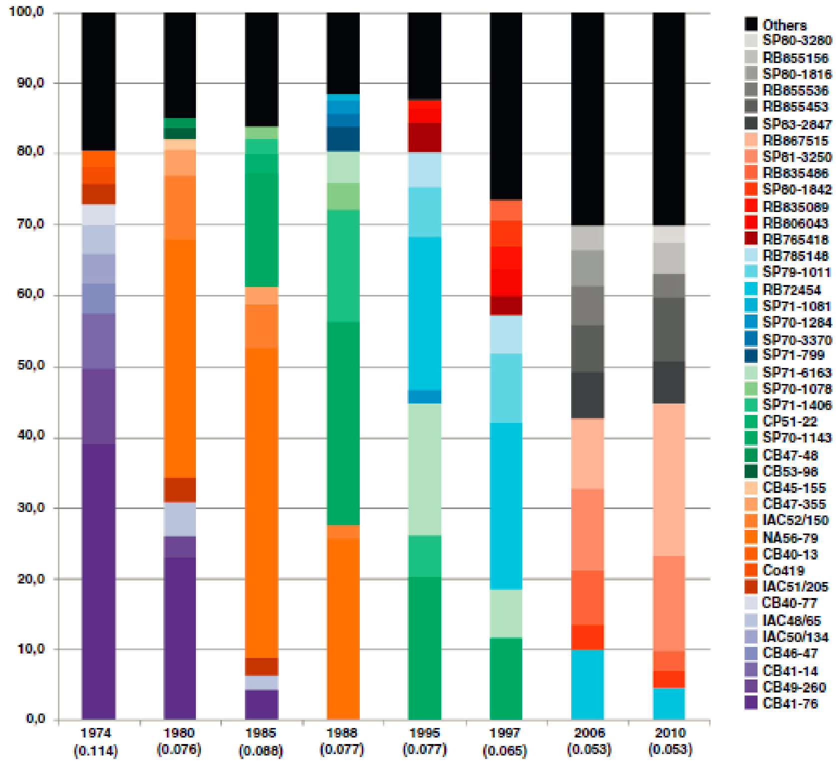

Figura 2.2 - Porcentagem das variedades de cana-de-açúcar em uso no Brasil nas últimas décadas. Os números entre parênteses são a média do coeficiente de parentesco entre as 10 primeiras variedades de um determinado ano. As cores representam as variedades apresentadas, totalizam 100% das mesmas dentro de cada ano, representados pelas colunas. Extraído de: DAL-BIANCO, M. et al. Sugarcane improvement: How far can we go? Current Opinion in Biotechnology, 2012.

Além de sua restrita diversidade genética, o melhoramento genético clássico da cana-de-açúcar não permite explorar variabilidades genotípicas para determinadas características, como é o caso da brotação. Em decorrência de sua multiplicação por propagação vegetativa durante o desenvolvimento de novas variedades, a seleção fenotípica de indivíduos só é possível após a brotação desses, sendo essa, portanto, uma característica considerada inerente ao processo de seleção, e não objetivo deste. Ainda que esta característica não seja adequadamente explorada em programas de melhoramento, as gemas axilares da cana-de-açúcar são também responsáveis pelo perfilhamento da mesma, parâmetro este diretamente relacionado a formação do dossel e rebrota da cultura nas safras subsequentes (MATSUOKA et al., 2014; MATSUOKA; STOLF, 2012) e objeto de seleção pelos programas de melhoramento. Assim, faz-se necessários estudos que elucidam o desenvolvimento das gemas axilares bem como o emprego de tecnologias complementares ao melhoramento genético clássico para seleção de clones propagados vegetativamente ou que identifiquem vias que possam ser manipuladas para aumentar a eficiência deste processo, seja pelo emprego de compostos químicos de efeito fisiológico, ou, pela manipulação genética da cultura.

2.2 O uso de marcadores moleculares em cana-de-açúcar

Assim como em outras culturas, outras abordagens e ferramentas tem sido propostas com objetivo de aumentar a eficiência de seleção de novos genótipos de cana-de-açúcar, como o emprego de regressões logísticas (BRASILEIRO et al., 2016), analises multivariadas (SILVA et al., 2016), mapeamento genético e marcadores moleculares (GARCIA et al., 2013; ZHU; LONG; ORT, 2008). Dentre as ferramentas citadas, o mapeamento genético apresenta o maior potencial de acelerar o melhoramento por meio principalmente da seleção assistida por marcadores moleculares.

O uso de QTLs (*Quantitative Trait Loci*) para mapear regiões cromossômicas associadas à *traits* de interesse tem sido alvo de intensivos estudos, baseado em sua utilização com sucesso em diversas culturas de interesse agrícola. Um QTL é um lócus genético, cujos alelos afetam uma variação fenotípica mensurável devido a influencias genéticas e/ou ambientais (MELCHINGER; UTZ; SCHÖN, 1998; WAN et al., 2008). Em cana-de-açúcar, o uso de QTLs tem grande potencial a ser explorado, uma vez que muitos dos *traits* de interesse para a cultura são de natureza quantitativa (BARBOSA et al., 2012; STRINGER et al., 2011). Entretanto, seu grande genoma (~10 Gb) apresenta complexidades decorrentes de sua elevada ploidia (aneuploidia e poliploidia), resultando em um elevado número de copias de genes (MANCINI et al., 2018; SOUZA et al., 2011) , sendo considerado um dos mais complexos genomas de plantas (BARBOSA et al., 2012). Em espécies de plantas poliploides e com acentuada aneuploidia como a cana-de-açúcar, suposições muitas vezes irrealistas e simplificadas precisam ser feitas, limitando o uso da técnica em questão, pois não permitem uma estimativa direta do número de copias de cada alelo em um determinado lócus polimórfico (GARCIA et al., 2013). Além disso, devido às características já mencionadas de seu genoma, é difícil alocar esses marcadores no número esperado de cromossomos da cana-de-açúcar (SOUZA et al., 2011).

A fim de contornar a complexidade de seu genoma, os primeiros mapas genéticos para a cultura foram elaborados com o uso de RAPD (*random amplified polymorphic DNA*) e RFLPs (*restriction fragment length polymorphisms*) (GUIMARÃES; SILLS; SOBRAL, 1997; MING et al., 1998), entretanto, tais técnicas apresentam limitações como por exemplo a rotina de execução protocolar e reprodutibilidade dos métodos. Assim, na geração de novos mapas, optou-se pela integração de técnicas como SNPs (*single nucleotide polymorphisms*), AFLP (*amplified fragment length polymorphisms*) e principalmente SSRs (*simple sequence repeats* ou microssatélites) (GARCIA et al., 2013; PIPERIDIS et al., 2008), uma vez que essas tecnicas permitem maior reprodutibilidade como os SSRs, ou, permitem detectar um grande número de bandas polimórficas em uma única faixa como os AFLP (GARCIA et al., 2013). Estima-se que os maiores mapas contêm predominantemente marcadores SSR e AFLP (PIPERIDIS et al., 2008; ROSSI et al., 2003).

Com objetivo de impulsionar o mapeamento da cultura e o conhecimento sobre sua estrutura genética, foi realizado um consórcio SUCEST (*Sugarcane Expressed Sequence Tag Project*) para gerar a maior coleção de EST (*Expressed Sequence Tags*) para cana-de-açúcar, com mais de 300.000 ESTs (VETTORE et al., 2001), sendo estes utilizados com sucesso, em ensaios para a geração de QTLs associados principalmente a produção de sacarose e resistência a doenças (BALSALOBRE et al., 2017; BARRETO et al., 2017; ROSSI et al., 2003; SILVA; BRESSIANI, 2005). Mais recentemente, um abrangente mapa genético foi gerado para a variedade australiana Q165 (AITKEN et al., 2014), no qual 2267 marcadores foram gerados a partir da a partir de DArT (*Diversity Array Technology*), AFLP, SSR, SNP, RFLP, e RAPD. O uso de um grande número de diferentes marcadores permitiu que a maioria dos grupos de ligação fossem colocados nos oito grupos de homologia; sendo este número consistente com o número básico de cromossomos das espécies ancestrais de *Saccharum*, que representam até o momento, o menor número cromossômico básico relatado no gênero supracitado.

Embora o uso de marcadores moleculares tenha sido usado com sucesso para seleção de caractere como resistência a doenças e teor de sacarose, caracteres com elevado número de genes associados e com forte interação ambiental, como os associados à produção de colmos, ainda tem apresentado baixa eficiência. Apesar de alguns estudos terem detectado QTLs para as características de peso e o número de colmos, a associação dos marcadores com estes fenótipos foi limitada devido os mapas gerados apresentarem uma baixa cobertura do genoma (MING et al., 1998; SOUZA et al., 2011). Marcadores moleculares associados à produtividade foram encontrados em 27 regiões do genoma da cana-de-açúcar a partir de um cruzamento entre a variedade australiana Q165 e *S. officinarum*, entretanto, nenhuma correlação significativa entre características do caule (peso, diâmetro, altura, número de perfilhos e produtividade) foi encontrada na população analisada (AITKEN et al., 2008). Em relação a *traits* ligados ao desenvolvimento de gemas axilares, marcadores relacionados ao número de colmos de cana-de-açúcar foram identificados em progênies de um cruzamento bi parental entre clones de elite australianos, sendo que estes marcadores puderam ser localizados dentro ou perto de QTLs associados ao perfilhamento de sorgo, sugerindo a utilização dessa espécie como mapa de referência para determinados parâmetros em cana-de-açúcar (JORDAN et al., 2004). O uso de genomas menos complexos e com maior cobertura, de espécies próximas a cana-de-açúcar, tem sido apontado como uma eficiente estratégia para estudos genéticos na cultura (MANCINI et al., 2018).

Recentemente a integração de dados genômicos com resultados experimentais de outras plataformas como, transcriptoma, proteoma e metaboloma tem ajudado a identificar relações biológicas latentes que podem ser evidenciadas apenas pela analise holística de um determinado fenômeno ou característica (WANICHTHANARAK; FAHRMANN; GRAPOV, 2015). Assim, a elucidação do metabolismo das gemas quando no início de seu desenvolvimento em comparação a seu estado dormente pode ajudar na identificação de vias metabólicas associadas a brotação da cana-de-açúcar. Nesse sentido, e considerando a baixa correlação de QTLs com diferentes caracteres de interesse em cana-de-açúcar, a metabolômica pode ser utilizada como uma importante ferramenta na determinação direta de fenótipos, uma vez que está diretamente relacionada com o metabolismo primário e secundário das plantas (OKSMAN-CALDENTEY; SAITO, 2005).

2.3 Gemas axilares e seu desenvolvimento

2.3.1 Desenvolvimento inicial meristemático

Em plantas superiores, o crescimento vegetativo inicia-se na embriogênese com o desenvolvimento de um eixo principal estabelecido pela proliferação de dois grupos de células meristemáticas, as basais ou meristema apical radicular, e apicais ou meristema apical caulinar, originando a raiz primária e a formação dos primórdios foliares e consequente formação da parte aérea das plantas, respectivamente (DE SMET et al., 2010; GRBIĆ; BLEECKER, 2001; MCSTEEN; LEYSER, 2005). Durante o desenvolvimento pós-embrionário, meristemas secundários são desenvolvidos tanto na parte aérea quanto no sistema radicular e podem originar raízes e hastes secundárias (GRBIĆ; BLEECKER, 2001; LEYSER, 2009; MCSTEEN; LEYSER, 2005; SCHMITZ; THERES, 2005). Os meristemas secundários na parte aérea das plantas possuem o mesmo potencial de desenvolvimento dos primários, sendo localizados nas axilas das folhas, e comumente chamados de meristemas axilares, que juntamente aos primórdios foliares constituirão as gemas axilares (SHIMIZU-SATO; MORI, 2001).

Na maioria das espécies vegetais, as gemas axilares encontram-se em estado dormente, no qual, apesar dos meristemas estarem completamente desenvolvidos, não há divisão e crescimento celular (SCHMITZ; THERES, 2005). O estado de dormência pode ocorrer devido a três fatores: i) internos da gema ou endo-dormência; ii) sinalização endógena às gemas, provenientes de outros órgãos, como exemplo a sinalização hormonal, também conhecida como para-dormência; e iii) externos a planta como temperatura, fotoperíodo, disponibilidade de água e nutrientes, conhecido como eco-dormência (DOMAGALSKA; LEYSER, 2011; KEBROM; BURSON; FINLAYSON, 2006). Ainda pouco se conhece sobre como estes fatores interagem e determinam a quebra de dormência das gemas axilares (CHATFIELD et al., 2001; MÜLLER; LEYSER, 2011).

Dentre os mecanismos mencionados, o de para-dormência é o mais conhecido, exercido pelo fenômeno da dominância apical, pelo qual a atividade do meristema apical caulinar reprime o desenvolvimento das gemas axilares, mantendo-as em estado de dormência (CHATFIELD et al., 2001; DOEBLEY; STEC; HUBBARD, 1997; HORVATH et al., 2003; ORTIZ-MOREA et al., 2013; SHIMIZU-SATO; MORI, 2001; WANG; LI, 2008). A dominância apical é um mecanismo natural de sobrevivência de espécies vegetais, garantindo que um meristema secundário possa dar continuidade ao crescimento da planta em decorrência de danos ao meristema apical, além de impedir que outros órgãos compitam por recursos, direcionando e definindo o padrão de crescimento e arquitetura da mesma (SHIMIZU-SATO; MORI, 2001). Assim, a remoção da porção apical ou a perda de funcionalidade de sua zona meristemática, resulta no desenvolvimento das gemas axilares (DOMAGALSKA; LEYSER, 2011).

Dada a importância do desenvolvimento das gemas axilares na definição da arquitetura das plantas, em estudos de genética evolutiva, *TEOSINTE BRANCHED1 (TB1)* foi identificado como gene altamente especifico desses órgãos, agindo na inibição do desenvolvimento dos mesmos (DOEBLEY; STEC; HUBBARD, 1997; KEBROM; SPIELMEYER; FINNEGAN, 2013). *TB1* codifica uma proteína constituinte da família de fatores de transcrição TCP [*TB1, CYCLOIDEA (CYC*) e *PROLIFERATING CELL FACTORS (PCF)]* (LEYSER, 2009). Os fatores da família TCP são do tipo “basic-helix-loop-helix”, específicos de plantas, e atuam regulando positivamente ou negativamente a expressão gênica (GIRAUD et al., 2010). TCP pode ser dividido em duas subfamílias, classe I e II, das quais apenas a segunda exerce função relativamente clara sobre as gemas axilares. Dentro da classe II encontra-se o gene *TB1,* gene inicialmente identificado em milho e responsável pela repressão do desenvolvimento das gemas axilares (DOEBLEY; STEC; HUBBARD, 1997). A subfamília classe I é composta pelos genes *PCF* e codificam proteínas que induzem a expressão de *PROLIFERATING CELL NUCLEAR ANTIGEN (PCNA)* (KOSUGI; OHASHI, 1997), especificamente expresso nas fases G1 e S do ciclo celular e diretamente envolvido na proliferação de células (MÜLLER; LEYSER, 2011).

Além de TCP, outros fatores de transcrição também parecem estar envolvidos na regulação do desenvolvimento das gemas axilares, dentre eles, *GRASSY TILLERS1 (Gt1)* que codifica uma proteína homologa a classe I da família HD-Zip (WHIPPLE et al., 2011). Os autores verificaram expressão de *Gt1* nos primórdios foliares e acumulo de proteínas GT1 nos meristemas de gemas dormentes de gramíneas, indicando que *Gt1* pode contribuir para o processo de dormência nesses órgãos. Foi ainda demonstrado que *Gt1* e *TB1* atuam na mesma via de regulação das gemas axilares, sendo a expressão de *Gt1* controlada por *TB1*.

Em termos dos aspectos moleculares do desenvolvimento vegetal, as gemas dormentes encontram-se predominantemente na fase G1 do ciclo celular (DEVITT; STAFSTROM, 1995; SHIMIZU; MORI, 1998). Neste processo, diversas proteínas reguladoras do ciclo celular têm sido investigadas. Shimizu e Mori (1998) observaram, nas gemas após a quebra da dominância apical, um aumento sequencial no acumulo de mRNA de *PCNA* (*PROLIFERATING CELL NUCLEAR ANTIGEN)* (fases G1 e S – 4horas), histona H4 (fase S – 10horas), Pissa e cycB1;2 (fases G2 e M - 14horas). De maneira oposta, *DRM1 e 2 (DOMAINS REARRANGED METHYLASE 1 e 2)* foram identificadas como expressas preferencialmente em gemas dormentes, e não detectadas 6 horas após decapitação das plantas (STAFSTROM et al., 1998). Do mesmo modo, os mRNAs de *AD1* e 2 *(APICAL DOMINANCE 1 e 2)* foram detectados em níveis elevados em gemas dormentes, enquanto seus níveis foram diminuídos 4 horas após decapitação (MADOKA; MORI, 2000). Interessantemente, após aplicação fito-hormônio auxina (AIA), os níveis *AD1* e *2* foram mantidos até 24 horas da decapitação. Em contrapartida, após 16 horas da aplicação fito-hormônio citocinina (CK), os transcritos de *AD1* e *2* não foram detectados, indicando que a interação hormonal e ciclo celular tem um papel fundamental na determinação do estado dormente das gemas axilares.

2.3.2 Interação hormonal e o desenvolvimento das gemas axilares

Desde a identificação da inibição do desenvolvimento das gemas axilares pela aplicação de um regulador de crescimento na região excisada do meristema apical (THIMANN; SKOOG, 1933), diversos estudos têm apontado AIA como principal mediador do fenômeno da dominância apical (BREWER et al., 2009; CHATFIELD et al., 2001; CLINE; WESSE; IWAMURA, 1997; LEYSER, 2009). A auxina, produzida na região do meristema apical caulinar e em folhas novas (SCHMITZ; THERES, 2005), é redistribuída diretamente pelo floema ou célula a célula por meio do mecanismo denominado transporte polar de auxina (PAT). A interrupção desse transporte pela decapitação do ápice caulinar pode levar ao desenvolvimento das gemas axilares (CLINE; WESSE; IWAMURA, 1997; FRIML, 2003; FRIML; PALME, 2002; SIEBERER; LEYSER, 2006).

Embora a síntese e transporte de AIA sejam fundamentais para o estabelecimento da dominância apical, este hormônio parece não atuar diretamente na supressão das gemas axilares, já que o mesmo não é translocado até seus meristemas (BOOKER; CHATFIELD; LEYSER, 2003; SHIMIZU-SATO; TANAKA; MORI, 2008). Dessa maneira, é sugerido que AIA atue como molécula sinalizadora em outros componentes diretamente ligados a dormência das gemas (BOOKER; CHATFIELD; LEYSER, 2003; BREWER et al., 2009; SCHMITZ; THERES, 2005).

Uma das moléculas reguladas pela sinalização da auxina e capaz de atuar diretamente na quebra de dormência das gemas é CK (FERGUSON; BEVERIDGE, 2009; LEYSER, 2009; WANG; LI, 2008). CK é majoritariamente produzida nas células das raízes e translocada via xilema até as gemas axilares (BANGERTH, 1994; CHEN et al., 1985; PALNI; BURCH; HORGAN, 1988), ou diretamente sintetizada em tecidos próximos as gemas axilares (FERGUSON; BEVERIDGE, 2009; NORDSTRÖM et al., 2004; SHIMIZU-SATO; TANAKA; MORI, 2008). Foi mostrado que a aplicação exógena de CK na gema axilar promove seu desenvolvimento vegetativo, sugerindo que o aumento na concentração deste hormônio em relação à AIA seja um dos fatores determinantes na quebra da dormência (CLINE; WESSE; IWAMURA, 1997; SCHMITZ; THERES, 2005; SHIMIZU-SATO; MORI, 2001).

Embora o exato mecanismo de interação seja ainda desconhecido, a via de síntese e transporte de AIA parece regular diretamente a síntese de CK (BANGERTH, 1994; NORDSTRÖM et al., 2004) pela inibição da expressão dos genes relacionado à biossíntese de CK (*ISOPENTENYL TRANSFERASE 1, IPT1 e IPT2)* (FERGUSON; BEVERIDGE, 2009; SHIMIZU-SATO; TANAKA; MORI, 2008). Ferguson e Beveridge (2009) observaram ainda que a indução da expressão gênica de *IPT1* e *IPT2* tem correlação positiva com a brotação das gemas axilares. Além disso, AIA pode regular a expressão do gene *CKX* (*CYTOKININ OXIDASE),* que codifica uma enzima responsável pela degradação de CK (SHIMIZU-SATO; TANAKA; MORI, 2008).

Recentemente, uma nova classe de hormônios, as estrigolactonas (SL) têm sido propostas como um dos componentes secundários mediados pela ação antagonista de AIA e CK na brotação das gemas axilares (BREWER; KOLTAI; BEVERIDGE, 2013; DUN et al., 2012; DUN; BREWER; BEVERIDGE, 2009; VANSTRAELEN; BENKOVÁ, 2012). SL, derivados do metabolismo de carotenoides, foram, inicialmente, identificados como compostos exsudados pelas raízes, favorecendo a germinação de sementes de certas espécies de plantas daninhas (COOK et al., 1972). Brewer, et al. (2009) verificaram que a inibição no desenvolvimento das gemas laterais de plantas de ervilha através da aplicação direta de SL é independente da interrupção do fluxo de AIA pela decapitação do meristema apical. Assim, a inibição da brotação lateral pelo fluxo de AIA é pelo menos, em parte, devido a promoção de SL. Além disso, foi demonstrado que a expressão de genes envolvidos na biossíntese de SL, como *MORE AXILLARY GROWTH 3 e 4 (MAX3 e MAX4),* é positivamente correlacionado com o fluxo de AIA (HAYWARD et al., 2009).

Apesar do número de resultados que suportam a clássica hipótese de AIA como molécula sinalizadora para componentes secundários, há evidências para uma segunda hipótese, na qual a canalização do transporte de AIA na haste principal iniba o desenvolvimento das gemas axilares. Pela teoria da canalização, inicialmente proposta por Sachs, 1981, o fluxo descendente de AIA do meristema apical em direção ao sistema radicular estabelece uma via principal para seu transporte (DOMAGALSKA; LEYSER, 2011; MÜLLER; LEYSER, 2011). Assim, para que ocorra o desenvolvimento, as gemas precisam, portanto, estabelecer seu próprio transporte de AIA (DOMAGALSKA; LEYSER, 2011), que levará a diferenciação e vascularização de suas células adjacentes, conectando o novo órgão a via principal de transporte em comunicação com o sistema radicular (SACHS, 2000). Assim a exportação de AIA das gemas pode ser considerada um fator chave para o desenvolvimento das mesmas.

Conjuntamente, as hipóteses clássicas de mensageiros secundários e teoria da canalização são de certa maneira convergentes, já que em ambas, a síntese e transporte de AIA regulam a síntese de CK e SL. Além disso, a sinalização hormonal pode ativar para uma rede de regulação transcricional que envolve a expressão diferencial de fatores de transcrição, como *BRANCHED1 (BRC1),* ortólogo de *TB1* em Arabidopsis (DUN et al., 2012) (**Figura 2.3**). É sabido que tanto a aplicação local quanto via vascular de CK reduzem a expressão de *BRC1* nas gemas (DUN et al., 2012). Além disso, os fatores de transcrição TCP e CK podem interagir dentro do ciclo celular na regulação das ciclinas do tipo D, reprimindo ou promovendo respectivamente, sua expressão (MÜLLER; LEYSER, 2011). Entretanto, a superexpressão das ciclinas do tipo D é suficiente apenas para acelerar o ciclo celular, mas não para ativação das gemas, sugerindo que CK seja um sinalizador na ativação da divisão celular (MÜLLER; LEYSER, 2011). De maneira oposta a CK, SL induz a expressão de *BRC1*, sendo este gene portanto, regulador dos sinais desses dois hormônios, embora a maneira como isso ocorra não seja conhecida (DUN et al., 2012). Desse modo, além de integrar sinais hormonais, TCP podem agir também na regulação do ciclo circadiano, agindo tanto pontualmente no início e fim do ciclo quanto em sua oscilação, direcionando e regulando a expressão de genes que codificam componentes do metabolismo energéticos das células (GIRAUD et al., 2010).

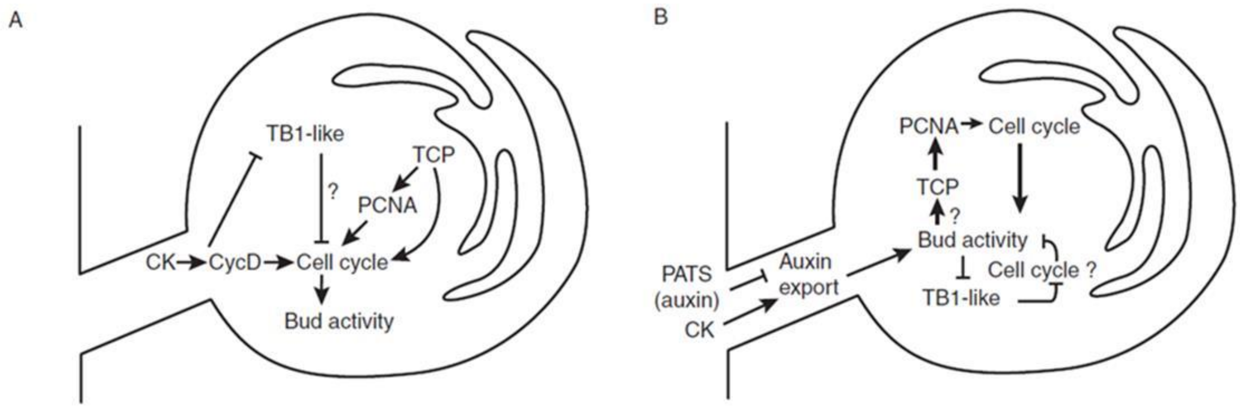

Figura 2.3 – Modelos para quebra de dormência do meristema axilares através da ativação do ciclo celular. (A) A ativação do fator de TCP por CK regula o ciclo celular para controlar a atividade das gemas. (B) A exportação de auxina das gemas é um regulador chave que governa a atividade das mesmas. Neste cenário, a exportação de auxinas é um pré-requisito para ativação de gemas. Extraído de MÜLLER, D.; LEYSER, O. Auxin, cytokinin and the control of shoot branching. Annals of Botany, v. 107, n. 7, p. 1203–1212, 2011.

Mais recentemente, foi reportado um novo fator de transcrição envolvido no desenvolvimento das gemas axilares de *Arabidopsis thaliana* (MEHRNIA et al., 2013). *O ERF BUD ENHANCER (EBE)*, membro da superfamília de fatores de transcrição *APETALA2/ETHYLENE RESPONSE FACTOR (AP2/ERF)*, é fortemente expresso durante a proliferação celular, preferencialmente na fase S do ciclo, sendo essa expressão rapidamente acentuada nas gemas após a quebra da dominância apical. Os autores observaram aumento na formação e crescimento das gemas pela super expressão de *EBE*, enquanto sua repressão resultou na inibição dessas estruturas. Por último, mas não menos importante, linhas transgênicas com expressão constitutiva de EBE (*35S:EBE)* apresentaram neoplasia, indicando que o balanço AIA:CK deve ter sido perturbado, e, portanto, *EBE* também pode atuar na sinalização hormonal.

Pelo exposto, fica evidente a complexidade de interações hormonais conjuntamente a rede transcricional envolvida no processo de desenvolvimento das gemas axilares. Apesar do papel importante destes na ativação do ciclo celular, estudos mostram que há outros fatores essenciais para o desenvolvimento das gemas axilares.

2.3.3 Metabolismo das gemas axilares

Apesar da regulação hormonal ter sido o principal alvo de estudos relacionados ao desenvolvimento das gemas axilares, o metabolismo das plantas pode exercer papel fundamental em tal processo, como por exemplo a sacarose, sugerida como um regulador do crescimento desses órgãos, além de sua interação com as mencionadas vias hormonais (BARBIER; LUNN; BEVERIDGE, 2015). Além da sacarose, outros açúcares, como glicose e frutose, têm sido sugeridos como alguns dos sinalizadores e reguladores do ciclo celular (RIOU-KHAMLICHI et al., 2000; ROLLAND; BAENA-GONZALEZ; SHEEN, 2006), podendo, portanto, impactar no desenvolvimento das gemas axilares. Além de servirem como fonte de energia para processos metabólicos, os açúcares também podem regular ciclinas do tipo D expressas durante a fase G1 do ciclo. Riou-Khamlichi et al. (2000) demonstram aumento na expressão gênica de CyCD2 e CyCD3 na presença de sacarose. Do mesmo modo, CK também aumenta a expressão de CyCD3, entretanto, existe dominância do efeito do açúcar em relação a CK, sugerindo que esse, desempenhe papel central como desencadeador do ciclo celular.

A glicose é um monossacarídeo fruto da hidrolise enzimática da sacarose por meio da atividade das enzimas invertases (INVs) e sucrose synthase (ROITSCH; EHNESS, 2000; ROITSCH; GONZÁLEZ, 2004; ROLLAND; BAENA-GONZALEZ; SHEEN, 2006). Assim, as INVs, consideradas enzimas chave no estabelecimento de órgãos como dreno fisiológico (LECLERE; SCHMELZ; CHOUREY, 2008; ROITSCH et al., 2003; WEIL; RAUSCH, 1990), podem ser classificadas como ácida, com localização no vacúolo (INV-V), e parede celular (INV-CW), ou neutras (INV-N), presentes no citoplasma (ROITSCH; GONZÁLEZ, 2004; ROLLAND; BAENA-GONZALEZ; SHEEN, 2006; WERNER et al., 2008).

A atividade das INVs pode ser regulada por fatores exógenos como o estresse biótico e abiótico, e/ou endógenos como a sinalização hormonal IAA e CK (ROITSCH et al., 2003). AIA pode promover a atividade das INVs (ROITSCH et al., 2003) embora seu efeito possa estar mais relacionado a produção e secreção destas enzimas do que a sua atividade (WEIL; RAUSCH, 1990), sendo importante fator na redistribuição assimétrica das INVs (LONG et al., 2002). Por outro lado, o aumento na concentração de CK impacta positivamente a atividade de INV-CW (EHNESS; ROITSCH, 2003; GUIVARCH et al., 2002; ROITSCH; EHNESS, 2000). Dessa maneira, CK, além de regular diretamente alguns passos do ciclo celular, atua também indiretamente no mesmo por meio da regulação da INV-CW e consequentemente, na formação da sinalização de açúcar proveniente da hidrolise da sacarose (**Figura 2.4**) (ROITSCH; EHNESS, 2000; ROITSCH; GONZÁLEZ, 2004).

Interessantemente, a atividade da INV-CW não é uniformemente distribuída ao longo da haste principal das plantas, sendo sua atividade maior na base das ramificações de *Chenopodium rubrum,* o que pode ser atribuída a indução por meio de CK (ROITSCH; EHNESS, 2000). Corroborando com estes resultados, o aumento de CK, decorrente da superexpressão de *IPT* em plantas transgênicas de tabaco, resultou em um aumento expressivo nos níveis de INV-CW quando comparado às plantas controle, associado ao fenótipo de maior número de brotações laterais (GUIVARCH et al., 2002). Em recente estudo realizado em cana-de-açúcar, foi observado aumento na atividade de INV-CW, bem como na concentração de hexoses durante a brotação das gemas axilares (VERMA et al., 2013). Além dos mecanismos de ação citados, nos quais CK e glicose atuam como ativadores e reguladores do ciclo celular (ROITSCH; GONZÁLEZ, 2004), podendo ainda a quinase TOR (*TARGET OF RAPAMYCIN*) estar envolvida na mediação e tradução da sinalização de açúcar em uma rede transcricional relacionada a ativação e manutenção do ciclo celular bem como proliferação celular (XIONG et al., 2013). Desta forma, além de sinalizadores, acredita-se que estes metabólitos sirvam como fonte de energia e base para biossínteses de componentes estruturais essenciais no crescimento e proliferação celular.

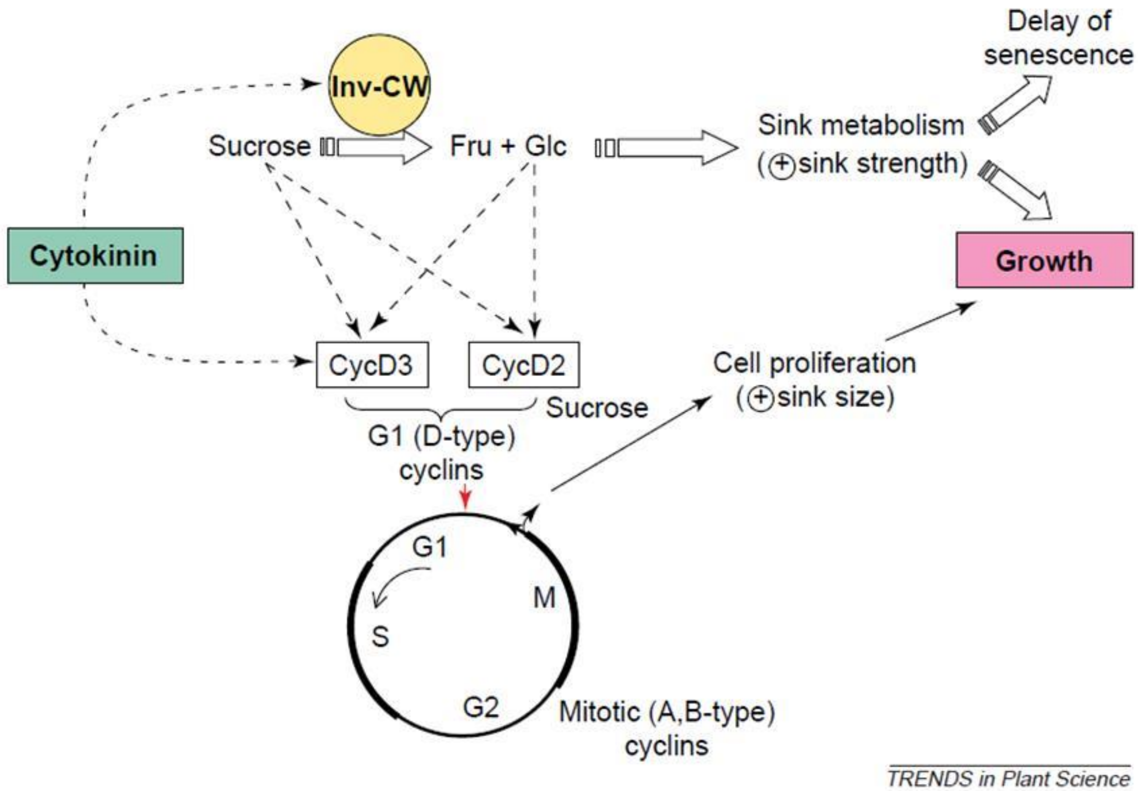

Figura 2.4 – Invertases e regulação do ciclo celular. Este modelo sugere que o crescimento celular induzido por citocinina pode ser regulado pela disponibilidade de carboidratos, sendo essa regulada pela atividade das invertases. Extraído de ROITSCH, T.; GONZA, M. Function and regulation of plant invertases : sweet sensations. v. 9, n. 12, 2004.

Portanto, devido à complexidade dos mecanismos envolvidos na determinação do estado de dormência das gemas de cana-de-açúcar (**Figura 2.5**), são necessários estudos direcionados à elucidação das redes regulatórias envolvidas nesse fenômeno. Neste sentido, como forma de avaliar quais módulos do metabolismo energético são importantes no processo de quebra de dormência em cana-de-açúcar, a metabolômica pode ser utilizada como uma importante ferramenta na definição de novas estratégias voltadas ao aumento do vigor de brotação da cultura.

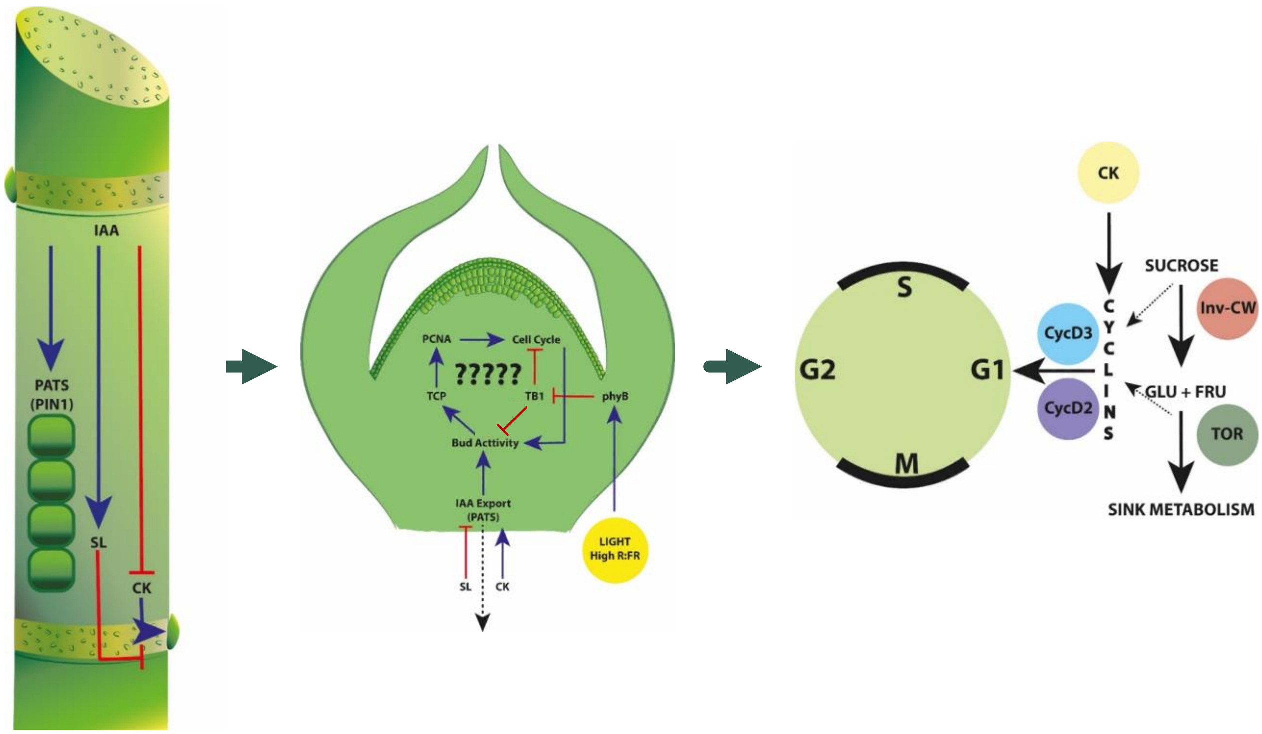

Figura 2.5 – Modelo teórico dos mecanismos moleculares envolvidos na brotação da cana-de-açúcar. O presente modelo integra as teorias clássicas de controle hormonal, fatores de transcrição (TCP), canalização da auxina e metabolismo do ciclo celular.

2.4 A metabolômica empregada a biologia de sistemas

As duas últimas décadas testemunharam enormes desenvolvimentos em diferentes campos denominados comumente de “omicas”, dentre eles a metabolômica. A metabolômica permite detecção de uma vasta gama de pequenas moléculas (metabólitos), desde níveis sub-celulares até analises de uma única célula, figurando-se como uma potente ferramenta para análise de processos fisiológicos (HONG et al., 2016; MISRA; ASSMANN; CHEN, 2014; SWEETLOVE; OBATA; FERNIE, 2014). Apesar da grande quantidade de metabólitos ainda a ser identificada, essa ferramenta tem contribuído significativamente para a compreensão do metabolismo de plantas e seu estado fisiológico a partir da interação dessas pequenas moléculas (KUMAR et al., 2017).

Os metabolitos de plantas apresentam uma enorme diversidade química, estimada em mais 200.000 moléculas, sendo o conjunto dessas moléculas sintetizadas por um organismo, em uma determinada condição, denominado de metaboloma (DIXON; STRACK, 2003; FIEHN, 2002). São considerados metabólitos, moléculas orgânicas de baixo peso molecular (50 – 1500 daltons (Da)), presentes em vias metabólicas como substrato ou produto (FERNIE, 2007; KOSMIDES et al., 2013; WANICHTHANARAK; FAHRMANN; GRAPOV, 2015). Alguns exemplos dessas moléculas são: açúcares, lipídios, aminoácidos, ácidos graxos, compostos fenólicos, alcaloides, dentre outros (D'AURIA; GERSHENZON, 2005; FERNIE, 2007). Esses metabólitos são geralmente classificados em primários e secundários ou especializados (HONG et al., 2016).

Diferentemente de genes e proteínas, o alto grau de diversidade química entre os pools de metabólitos, bem como a complexidade da distribuição espacial e temporal nos diferentes tecidos vivos, dificulta a caracterização dos mesmos (FIEHN, 2002; HALL et al., 2002). Desse modo, a interação entre essas pequenas moléculas pode ser complexa e de difícil compreensão, e uma vez elucidadas, a análise metabolômica pode contribuir significativamente para o entendimento da relação entre o genótipo e os produtos metabólicos (HONG et al., 2016; TOUBIANA et al., 2013). Avanços significativos no refinamento e desenvolvimento da instrumentação analítica tem possibilitado a detecção cada vez mais precisa de metabólitos de plantas ou qualquer outro organismo vivo. Aliado a isso, a crescente capacidade de processamento de dados tem proporcionado a análise e interpretação de um volume de dados metabólicos cada vez maiores. Assim, a fim de se evitar interpretações errôneas de certas classes de compostos, seja por semelhança de estrutura química ou por aparente abundância no tecido biológico, há uma série de análises que permitem definir a importância dos metabólitos por meio da análise de mudanças relativas a abundância dos mesmos em experimentos comparativos (FIEHN, 2002). Ainda assim, é necessário o contínuo desenvolvimento de ferramentas bioinformáticas ou softwares que possibilitem a análise e interpretação dos dados obtidos, principalmente quando da integração de dados multiplataforma.

Ainda que muitos dos genomas de plantas comercialmente cultivadas tenham sido sequenciados, boa parte dos genes mapeados ainda não foram funcionalmente investigados (CLAROS et al., 2012). Neste contexto, a metabolômica tem se despontado como uma ferramenta cada vez mais útil nos estudos de genômica funcional (CALDANA et al., 2011; FIEHN, 2002; FRANCKI et al., 2015; HALL et al., 2002; WANICHTHANARAK; FAHRMANN; GRAPOV, 2015). A potencial abordagem holística está na possibilidade de explorar comparativamente os metabólitos presentes em plantas de diferentes espécies (FIEHN, 2002), associando-as com a expressão de genes e atividade de proteínas especificas em diferentes substratos ou ambientes (CALDANA et al., 2011; FIEHN, 2002; HALL et al., 2002). Além disso, quando associada a outras plataformas ômicas, permite evidenciar relações biológicas latentes até então difíceis de serem investigadas (WANICHTHANARAK; FAHRMANN; GRAPOV, 2015). Por meio do uso das linhagens mutantes de cevada, *lys3.a* e *lys5.f*, que desencadeiam o aumento de proteínas a base de lisina e acumulo de β-glucano, respectivamente, foram demonstrados padrões metabólicos únicos, principalmente no metabolismo do chiquimato-fenilpropanoide e lipídios, associados a composição das sementes, resultando em um teor proteico e de fibra quase ótimo para a cultura estudada (KHAKIMOV et al., 2017). Assim, a abordagem metabolômica associada ao uso de linhagens mutante-especifica foi capaz de estabelecer uma ligação entre fatores genéticos, ambientais e fenotípicos específicos, contribuindo para o desenvolvimento de linhagens de cevada mais eficientes aos ambientes nos quais é cultivada.

Apesar de geneticamente mais complexas, espécies que apresentam variações cromossômicas naturais, como poliploidia e aneuploidia, podem auxiliar no mapeamento de regiões inteiras relacionadas a uma determinada via metabólica, ao contrário da mutação especifica de genes que nem sempre resulta em variações metabólicas ou em variações do *trait.* Em estudo com linhagens aneuploides de trigo, foi possível correlacionar à função do gene que codifica a trealose-6-fosfato fosfatase (TPP) no cromossomo 3BL, e a aspartato quinase no cromossomo 3AL, alterando a abundância de trealose e aspartato nos grãos, sendo um bom exemplo do uso de linhagens aneuplóides para discriminar os papéis funcionais de genes em cromossomos homólogos no controle da acumulação de metabólitos em grãos maduros (FRANCKI et al., 2015).

Existem hoje diversas ferramentas para integração das informações dos vários domínios bioquímicos, tais como, análise de enriquecimento, análise de network e correlações empíricas como análises multivariadas (PCA e PLS-DA) (WACLAWOVSKY et al., 2010). Apesar do metabolismo ser amplamente influenciado pelo ambiente, estas abordagens tem sido bastante utilizada para a discriminação de genótipos ou classificação de espécies (FIEHN, 2002; FRANCKI et al., 2015; HALL et al., 2002).

Provou-se que é possível por meio da análise multivariada (PCA), a discriminação entre fenótipo selvagem e mutante de plantas de tabaco pelos seus extratos metabólicos (CHOI et al., 2004). Quando aplicada ao desenvolvimento vegetal, a análise de PCA e PLS-DA demostraram clara discriminação entre as classes testadas no desenvolvimento de raízes de rabanete expostas a metais pesados (Pb e Cd) (WANG et al., 2015). Em estudo com plantas medicinais, a analise multivariada do metaboloma possibilitou a discriminação entre espécies de *Ilex* (CHOI et al., 2005), sendo ainda que o metabólito arbutina não havia sido relatado como constituinte das espécies de *Ilex*, servindo como um biomarcador em 8 das 11 espécies investigadas, confirmando o poder desta técnica para classificar e discriminar genótipos.

Como demonstrado a metabolômica é uma valiosa ferramenta na discriminação de genótipos bem como para estudos fenotípicos relacionados a variáveis ambientais. Desse modo, a identificação e uso de metabólitos como biomarcadores (mQTL) apresenta-se como uma abordagem promissora em diagnósticos rápidos, direcionados e de baixo custo que podem ser empregados na predição de genótipos em programas de melhoramento genético. Foi observado em linhagens recombinantes de *Arabidopsis*, correlação significativa entre pelo menos dois QTL e mQTL, suportando a noção de que o perfil metabólico e o acúmulo de biomassa de uma planta estão ligados (JAN et al., 2007). Além da correlação mencionada, este estudo demonstra ainda que pelo menos 33% do mQTL identificados, abrigam provavelmente, genes de funções metabólicas até então desconhecidas. Em espécies cultivadas, a análise de metabólitos extraídos de raízes de híbridos de milho, demonstra padrões específicos quando comparados as suas linhagens parentais, com padrões aditivos para herança metabólica, demonstrando o potencial da abordagem metabólica na predição de híbridos desta espécie (JAN et al., 2007). Além destes, os metabólitos glicose e frutose foram identificados como potenciais biomarcadores para a predição da qualidade da batata chips em diversos genótipos, demonstrando ainda 79% de correlação desses mesmos metabólitos na predição de genótipos com a mesma característica em um intervalo amostral de 59 indivíduos em uma população segregante (STEINFATH et al., 2010).

Desse modo, sua aplicação em estudos exploratórios de sistemas biológicos, tanto em espécies silvestres como cultivadas, permite responder a questões biológicas consideravelmente diversas de natureza científica ou com aplicação industrial (WORLEY; POWERS, 2013), como por exemplo, a brotação de gemas axilares da cana-de-açúcar. Esforços contínuos que elucidam as respostas metabólicas a vários ambientes implicam que o melhoramento assistido por metabolômica pode ser útil na seleção e desenvolvimento de genótipos agronomicamente superiores, adequados a diferentes sistemas de produção (KUMAR et al., 2017; STEINFATH et al., 2010).

Assim, à luz da genética e biologia molecular de plantas, a metabolômica tornou-se uma poderosa ferramenta a explorar aspectos da fisiologia e biologia vegetal, ampliando significativamente o conhecimento sobre os mecanismos moleculares que regulam o crescimento e desenvolvimento das plantas, sua resposta a estresse biótico e abiótico, fatores limitantes relacionados à produtividade, e não menos importante, a melhoria da qualidade das culturas de interesse agrícola. Desse modo, este trabalho hipotetiza a identificação de potenciais metabólitos que possam atuar na regulação e desenvolvimento inicial das gemas axilares de cana-de-açúcar, bem como o emprego da metabolômica na identificação de variedades a partir de características agronômicas desejáveis, tais como, a brotação da cultura.

3. Ojetivos

Considerando a complexidade dos mecanismos envolvidos na quebra da dormência e desenvolvimento inicial das gemas axilares de cana-de-açúcar, e ainda, nas limitações para seleção de genótipos contrastantes quanto a característica de brotação, este trabalho tem como objetivos:

(1) Determinar se a metabolômica pode ser utilizada em cana-de-açúcar como ferramenta para classificação e discriminação de genótipos a partir da taxa de brotação;

(2) Identificar potenciais metabólitos que possam atuar na regulação e desenvolvimento inicial das gemas axilares de cana-de-açúcar, bem como as possíveis vias metabólicas envolvidas em tal processo.

4. Metabolite Profiles of Sugarcane Culm Reveal the Relationship Among Metabolism and Axillary Bud Outgrowth in Genetically Related Sugarcane Commercial Cultivars (Versão *In-press* do artigo publicado na Frontiers in Plant Science Journal)

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Abstract

Metabolic composition is known to exert influence on several important agronomic traits, and metabolomics, which represents the chemical composition in a cell, has long been recognized as a powerful tool for bridging phenotype–genotype interactions. In this work, sixteen truly representative sugarcane Brazilian varieties were selected to explore the metabolic networks in buds and culms, the tissues involved in the vegetative propagation of this species. Due to the fact that bud sprouting is a key trait determining crop establishment in the field, the sprouting potential among the genotypes was evaluated. The use of partial least square discriminant analysis indicated only mild differences on bud outgrowth potential under controlled environmental conditions. However, primary metabolite profiling provided information on the variability of metabolic features even under a narrow genetic background, typical for modern sugarcane cultivars. Metabolite-metabolite correlations within and between tissues revealed more complex patterns for culms in relation to buds, and enabled the recognition of key metabolites (e.g., sucrose, putrescine, glutamate, serine and myo-inositol) affecting sprouting ability. Finally, those results were associated with the genetic background of each cultivar, showing that metabolites can be potentially used as indicators for the genetic background.

Introduction

Plants have an extraordinarily complex metabolism, and a comprehensive understanding on how it operates pose a challenge due to the coordination among various biochemical processes in specialized tissues and subcellular compartments (Lunn 2007; Sweetlove and Fernie 2013). Their sessile nature adds an extra layer of difficult, as there is a constant need to adjust to changes in the surrounding environment (Jaillais and Chory 2010; Kooke and Keurentjes 2012). This significant level of organization allows the production of a plethora of chemical compounds, which differ in their properties (e.g. size, polarity, stability and quantity) and biological functions, representing a readout of the physiological status of a cell. Traditionally, plant metabolomics studies have focused on elucidating the function and regulation of particular biosynthetic routes involving a number of metabolites (Stitt et al. 2010; Fernie and Tohge 2017). However, advances in large-scale automated analytical platforms have increasingly enabled high-throughput detection of metabolites, allowing the elucidation of metabolic networks in terms of structure and connectivity and/or bridging the genotype-to-phenotype gap to elucidate certain biological processes. Although knowledge about the role of specific enzymes was extended by targeted reverse genetics approaches (Alex et al. 2004; Tohge et al. 2005; Zheng et al. 2005; Seki et al. 2011; Goulet et al. 2015), duplication of enzymes and their different subcellular localization hampers metabolic engineering modifications relying on a single transgenic (Huang et al. 2010; Qin et al. 2011; Ren et al. 2014; Fernie and Tohge 2017). Means to surpass this problem include the use of natural/genetic variance to enhance our understanding about the genetic architecture of metabolic traits and monitor gene-phenotype combinations in a wide range of plant species (e.g., Arabidopsis, tomato, and rice) or important agronomic traits such as fruit composition (Bernillon et al. 2013; Monti et al. 2016), grain yield (Obata et al. 2015; Dan et al. 2016), and tolerance to abiotic stresses (Glaubitz et al. 2014; Sprenger et al. 2018; Todaka et al. 2017).

As metabolism is strongly influenced by interactions between the environment and genetic regulation, there is a limitation to extrapolate the complete picture of plant metabolomes by evaluating a single condition (i.e., developmental stage, genetic background and environment) (Soltis and Kliebenstein 2015). Furthermore, apart from having their biosynthesis and accumulation in a tissue-specific manner, metabolites can be produced and transported across tissues and/or organs to mediate certain biological processes. One example of this kind of regulation is the fate of axillary buds, which is governed by a complex interplay among environmental factors, genetic background and endogenous metabolites (Huang et al. 2012). Metabolite signals arising from other parts of the plant such as shoots or stems are sensed prior to trigger systemic responses that will promote bud outgrowth (Dun et al. 2012; Barbier, et al. 2015; Brewer et al. 2015). Several hormones have been long recognized as the main signaling molecules in this process (Umehara et al. 2008; Domagalska and Leyser 2011; Durbak et al. 2012). However, the availability of sugars, especially sucrose, was recently found to be crucial for bud outgrowth release prior to alterations in hormone levels (Mason et al. 2014; Barbier et al. 2015). Manipulation of sucrose supply via decapitation or defoliation was able to promote or suppress bud outgrowth, respectively (Mason et al. 2014; Barbier et al. 2015; Fichtner et al. 2017). Interestingly, dormant buds present a transcriptional response related to carbon starvation that seems to be conserved among different species (Tarancón et al. 2017). Primary metabolites, such as sugars and amino acids, are integral parts of sophisticated signaling networks linking the energetic status and external cues to regulate growth accordingly (Smeekens et al. 2010; Xiong et al. 2013; Chellamuthu et al. 2014; Yadav et al. 2014; Nunes-Nesi et al. 2010). Collectively, this new information placed primary metabolites as essential molecules with more immediate roles in bud development and outgrowth.

The regulation of axillary bud outgrowth is crucial for crops in which either vegetative propagation or tillering are important traits, as it is the case of the perennial C4 grass sugarcane (Saccharum X officinarum). In sugarcane, axillary buds are also naturally in a dormant state (Jain et al. 2009), however, when segments of the culms containing portions of internode and node with embryo roots and at least one viable bud are isolated from the plant body and placed into soil, bud outgrowth is released and a new plant is generated. Sugarcane is capable of accumulating impressive amounts of sucrose in its stems, in a very complex and dynamic process characterized by a continuous cycle of synthesis and degradation (Whittaker and Botha 1997; Zhu et al. 1997; Botha and Black 2000; Rose and Botha 2000), which involves various enzymes and their isoforms. There is a gradient of sucrose accumulation along the stem, with younger internodes containing less sucrose than older internodes (Zhu et al. 1997; Pereira et al. 2017). Interestingly, the stored carbon in the form of sucrose is used for bud outgrowth and formation of a new sugarcane plant (O'Neill et al. 2012). Due to the fact that sucrose was shown to be crucial for bud outgrowth in other species (Mason et al. 2014; Barbier et al. 2015; Kebrom and Mullet 2015), it remains to be elucidated whether the remarkably high levels of sucrose or other components of the primary metabolism are important to promote bud outgrowth release in sugarcane. The complex genetic architecture of sugarcane (e.g., high polyploidy, high heterozygosity, large amount of repetitive sequences, aneuploidy, and large genome size) (Zhang et al. 2012) has hampered the use of genetic information to dissect biological mechanisms in this species (de Setta et al. 2014; Song et al. 2016; Riaño-Pachón and Mattiello 2017; Hoang et al. 2017). All these characteristics make the application of metabolomics a great alternative for investigating complex agronomic traits such as sprouting potential.

In the present study, we assessed the metabolic profile of two tissues involved in the sprouting potential, namely culm and bud, from 16 highly-planted sugarcane varieties from a Brazilian sugarcane breeding program (varietal census 2016/2017 https://www.ridesa.com.br/censo-varietal). The cultivars studied herein rank among the most cultivated genotypes in the world as they cover about 65% of the sugarcane planted area in Brazil, the major sugarcane producer worldwide. These cultivars are therefore a worthy sample of sugarcane commercial genotypes with greater field performance. Our results demonstrate that the culm metabolism plays an important role as primary energy source to provide carbon skeletons and building blocks for protein synthesis for triggering bud outgrowth. Overall, our results suggest that both factors, genetic background and bud sprouting rates, jointly influenced the metabolite profile of sugarcane, opening perspectives for the use of metabolomics to assist sugarcane breeding programs.

Material and Methods

Plant Material

A collection of 16 relevant genotypes was chosen from the leading Brazilian sugarcane-breeding program The Inter-University Network for the Development of Sugarcane Industry (RIDESA) (Supplementary Table 1). Out of 16, the varieties RB867515, RB966928 and RB92579 cover 42% of total sugarcane fields in the country (2016/2017 varieties census: https://www.ridesa.com.br/censo-varietal). Sugarcane breeding programs have been indirect selected genotypes with high sprouting potential by choosing experimental plots with higher density and stalk yield. Consequently, the current commercial cultivars have low variability to this trait and tend to present medium to high sprouting potential under field conditions (Cargnin et al. 2008). The sugarcane breeding programs rely generally on a limited number of elite plant material as parental lines. Therefore, these 16 selected genotypes were also used as a proof of concept to evaluate whether even under a narrow genetic basis metabolic profiles could be used to discriminate their metabolic status. Information on the parents of the selected genotypes was recorded from RIDESA database, the pedigree tree (Figure S1) was drawn using the R packages synbreed (Wimmer et al. 2012) and diagram (Soetaert, 2017). The degree of kinship among the cultivars is represented as the coefficient of relationship between the individuals (Wright 1922) computed using AGHmatrix package (Amadeu et al. 2016) (Figure S2).

Experimental Conditions

Field and greenhouse experiments were conducted at the Federal University of São Carlos (UFSCar)/RIDESA in Araras, São Paulo, Brazil located at 22°21'25'' S, 47°23'03'' W, about 611 m above sea level; in a typic eutroferric red latosol soil. Mature sugarcane plants (approximately 11 month old) were decapitated 24 h before the harvest in the field, to facilitate the loss of apical dominance. After that, three stems of each genotype from independent plants were randomly harvested around 2 h after dawn. For each stem, internodes were counted and divided into three parts. Due to variations in sprouting performance throughout the stem according to bud position, only internodes belonging to the middle portion of the stem were further cut close to the bud, and had their diameter and weight measured to guarantee uniformity. Considering the existence of a sucrose gradient as well as different developmental stages along the sugarcane stem, the selection of the middle third portion of this organ would allow a better comparison among the genotypes. It is worth mentioning that usually entire sugarcane stems are planted in commercial field environments.

This material, also known as setts, was used for both metabolite profiling analysis and sprouting performance evaluation. In case of metabolite profiling, buds and the region of the culm in which they were inserted in were precisely isolated with the help of a scalpel and cork borer, respectively. A total of 3 biological replicates (representing 3 independent stalks), each containing a pool of 3 individual buds or culms, was collected. After the harvesting process, which took approximately 5 min per genotype, tissues were immediately frozen into liquid nitrogen and stored at -80ºC for metabolic profiling analysis.

Setts were planted with buds oriented towards the light into 200 ml pots containing commercial substrate Plantmax® for sprouting evaluation. Since sugarcane initial development is sensitive to soil water content and changes in temperature (Oliveira et al. 2001; Singels and Smit 2002; Smit 2011), the experiment was performed in the greenhouse during May 2016 with automated irrigation system (6 times along the diel cycle) and the temperature was set to 35ºC and 29ºC before and after sprouting, respectively. Each genotype was planted in three completely randomized trays containing 24 individuals each.

Sprouting Rate Evaluation

Sprouting performance was assessed in the greenhouse by monitoring bud outgrowth during the first 14 days after planting. Even considering the lack of synchronization in bud outgrowth release and their potential to be viable over longer terms, dormant buds would hardly become seedlings under field conditions after this period. Sprouting was considered successful when the seedling stem crossed the soil surface (a layer of 2 cm of soil over the bud) and was able to issue the first leaf. In order to classify the genotypes according to the sprouting rate, a descriptive quartile analysis was performed, in which varieties belonging to the top or down 25% of data distribution were considered with high or low sprouting potential, respectively. To further improve the classification of the genotypes belonging to the middle 50% quartile of data distribution, a second quartile analysis was performed to distinguish them as intermediate-low or -high sprouting potential. For assessing the variances, a parametric test (F-test) was applied to all genotypes at 5% of significance levels.

Metabolite Profiling Analysis

Prior to metabolite profiling analyses, sugarcane tissues were ground to a fine powder in liquid nitrogen and aliquots of 20 mg or 50 mg for culms and buds, respectively, were used for metabolite extraction, following the methodology described by Giavalisco et al. 2011. A fraction of 100 µl from the organic phase was dried and derivatized as described in Roessner et al. 2001. Afterwards, 1 µl of the derivatized samples was analyzed on a Combi-PAL autosampler (Agilent Technologies GmbH, Waldbronn, Germany) coupled to an Agilent 7890 gas chromatograph and a Leco Pegasus 2 time-of-flight mass spectrometer (LECO, St. Joseph, MI, USA) in both split (1:40 and 1:65 for buds and culm, respectively) and splitless modes (Weckwerth et al. 2004). Chromatograms were exported from Leco ChromaTOF software (version 3.25) to R software. Peak detection, retention time alignment, and library matching using the Golm Database (http://gmd.mpimp-golm.mpg.de/) were performed using TargetSearch R package (Cuadros-Inostroza et al. 2009). Metabolites were quantified by the peak intensity of a selective mass. Metabolites intensities were normalized by dividing the fresh weight of each biological replicate, followed by the sum of total ion count and log2 transformation.

Statistical Analyses

Statistical analyses and graphical representations were performed using R version 3.2.3 (https://www.r-project.org/). Multivariate analyses, including PCA and PLS-DA, were carried out using mixOmics (Rohart et al. 2017) and pcaMethods (Stacklies et al. 2007) R packages. Correlation analysis, heatmap and network visualization were done using corrplot (Wei and Simko, 2017), d3heatmap (Cheng et al. 2018) and qgraph (Epskamp et al. 2012) packages, respectively.

Results

Commercial sugarcane varieties displayed mild to low variability in bud outgrowth under controlled environmental conditions

During the initial period of seedling establishment (14 days), an overall high sprouting homogeneity was observed among genotypes. The first quartile analysis allowed the classification of 31%, 56% and 13% of the genotypes into low, intermediate and high sprouting potential, respectively. To refine this classification, a second quartile analysis was performed only using the intermediate genotypes. However, due to the fairly homogenous sprouting ability of the genotypes observed in the present study, the subdivision of this group resulted only in 19% and 38% of genotypes with intermediate-low and intermediate–high sprouting potential, respectively. Out of the 16 selected genotypes, RB975375 and RB935744 were classified as high sprouting rate, whereas RB937570, RB975201, RB835486, RB966928, and RB72454 were considered with low sprouting potential (Figure S3). Despite these major groups, the sprouting rate was in the range of 89 to 100% and no statistical differences among the genotypes were observed at level of 5% of significance. Due to the nature of vegetative propagation of this crop, breeding programs have indirectly favored genotypes with high sprouting rates. However, there is still a severe lack of synchronization of the bud outgrowth in the Brazilian field conditions, especially in areas susceptible to drought, leading to massive reduction in sprouting and consequently jeopardizing yield (Cargnin et al. 2008). Furthermore, the sprouting rate estimation was based on the establishment of a new plant, and although this is the measured trait in the field, which indirectly reflects the bud outgrowth performance, it does not enable the assessment of the internal factors involved in the control of bud release.

Metabolite profiling revealed differential metabolic responses of genotypes in distinct tissues

As it is challenging to morphologically and molecularly monitor the factors triggering bud outgrowth release in this crop, we next investigated whether the metabolite profiling could be a great tool to understand the control of bud outgrowth using GC-MS. This platform allows the assessment of molecules involved mainly in central metabolism, which was already reported to be closely linked to plant growth (Meyer et al. 2007; Lisec et al. 2008). Due to the fact that no significant differences were found in water content of the studied genotypes (data not shown), we used fresh weight for normalizing the metabolite levels. A major portion of the metabolites (76.7 %) was found in all samples. Due to the saturation of sucrose levels, the same samples were also injected in a split mode (diluted 1:40 or 1:65 for buds and culms, respectively) to accurately quantify this sugar. We detected a total of 66 metabolites with known structures (e.g., amino acids, sugar, sugar alcohols, organic acids, and polyamines), of which 16 and 15 were specifically identified in bud and culm, respectively (Figure 1A). Figure 1B shows a heatmap including the metabolite abundance of genotypes in each tissue and Supplementary Table S2 summarizes the effect of individual metabolites. By applying ANOVA, we found that most metabolites were significantly affected by the genotype in both tissues (Figure S4), indicating enough variability in metabolic features among genotypes even under a narrow genetic basis (Figure S1 and 2).

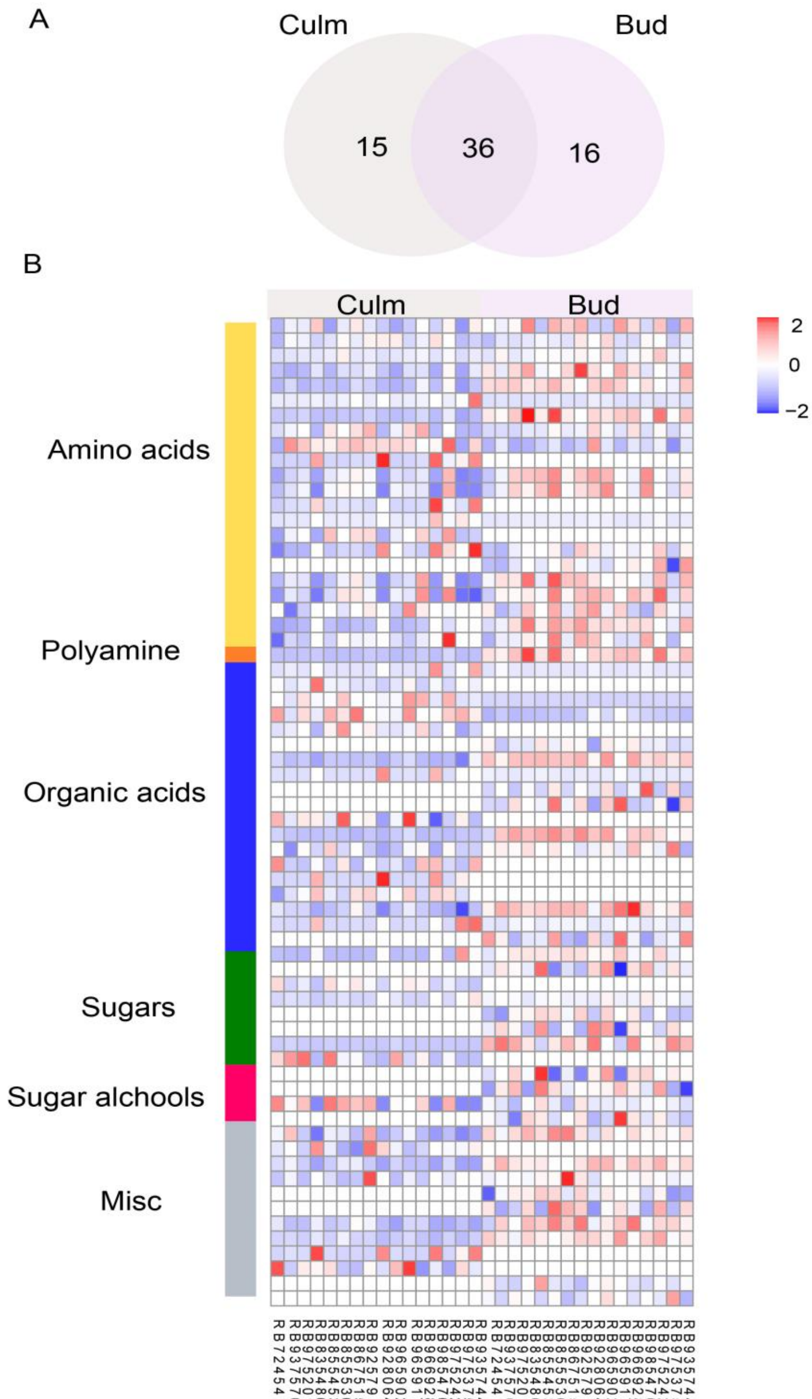

Figure 1. Metabolic composition of buds and culms in different sugarcane commercial cultivars. (A) Number of metabolites identified in culm, bud and common to both tissues; (B) Differential abundance of metabolites in culms and buds according to their compound class. Each column represents the genotype mean, and each row represents a metabolite. Variations in the relative abundance of metabolites are displayed in blue (low) to red (high).

Metabolite-metabolite correlations provide new insights on the regulation of metabolic networks intra- and inter-tissues

To decipher the relationships among metabolites, we performed correlation-based network analysis using significant pairwise correlations ($r \geq 0.5$, $p \leq 0.05$) (Figure 2), which are summarized in Supplementary Table S3. As expected, metabolites belonging to the same biochemical pathway tended to present a high degree of connectivity as it was the case for valine, isoleucine and leucine ($r > 0.8$) in both tissues. In total, there were 148, 414 and 47 significant correlations among metabolites detected in buds, culms and between these two tissues, respectively, suggesting that the metabolite-metabolite correlations were diverse in the different tissues. An exception was a subnetwork containing positive correlations among the branched amino acids leucine, isoleucine and valine, and threonine, conserved in both tissues. Interestingly, those amino acids were only linked to each other and methionine in buds, whereas in culm this network became more complex. Apart from the branched amino acids and threonine, further highly positive connections were built among glutamine, serine and the sugars sucrose, fructose and myo-inositol in culms. This expanded subnetwork was negatively linked to another subnetwork including GABA, putrescine, benzoate, galacturonate, nicotinate and a metabolite with similarity to itaconate, which in turn were all positively correlated to each other. The strongest negative correlation ($r = -0.9679$, $p = 0.05$) was between sucrose and putrescine that is one of the links between these two subnetworks in culms. Remarkably, the role of those two metabolites in controlling bud dormancy have been recently shown (Cui et al. 2010; Mason et al. 2014; Barbier et al. 2015). Interestingly, the compound similar to itaconate, which displayed the strongest positive correlation in culm with galacturonate ($r = 0.977$, $p = 0.05$) presented distinct correlations with amino acids in culms and buds. One example is the connection with glutamate that seems to be the opposite in both tissues. Glutamate and serine are the only metabolites that significant connect the bud and culm network. With respect to the bud, its network is much less interconnected when compared to culm. In addition to the amino acids subnetwork, another highly interconnected subnetwork containing galactose, quinate and sorbose ($r > 0.83$, $p = 0.05$) was identified. Altogether, these results revealed that the metabolic network of culm is more coordinately regulated than that of bud. A logical explanation is that culms constitute more active tissues with pivotal role as strong sinks, not only related to sucrose, but also including amino acids, which will act as primary energy source to provide carbon skeletons and building blocks for protein synthesis during bud outgrowth.

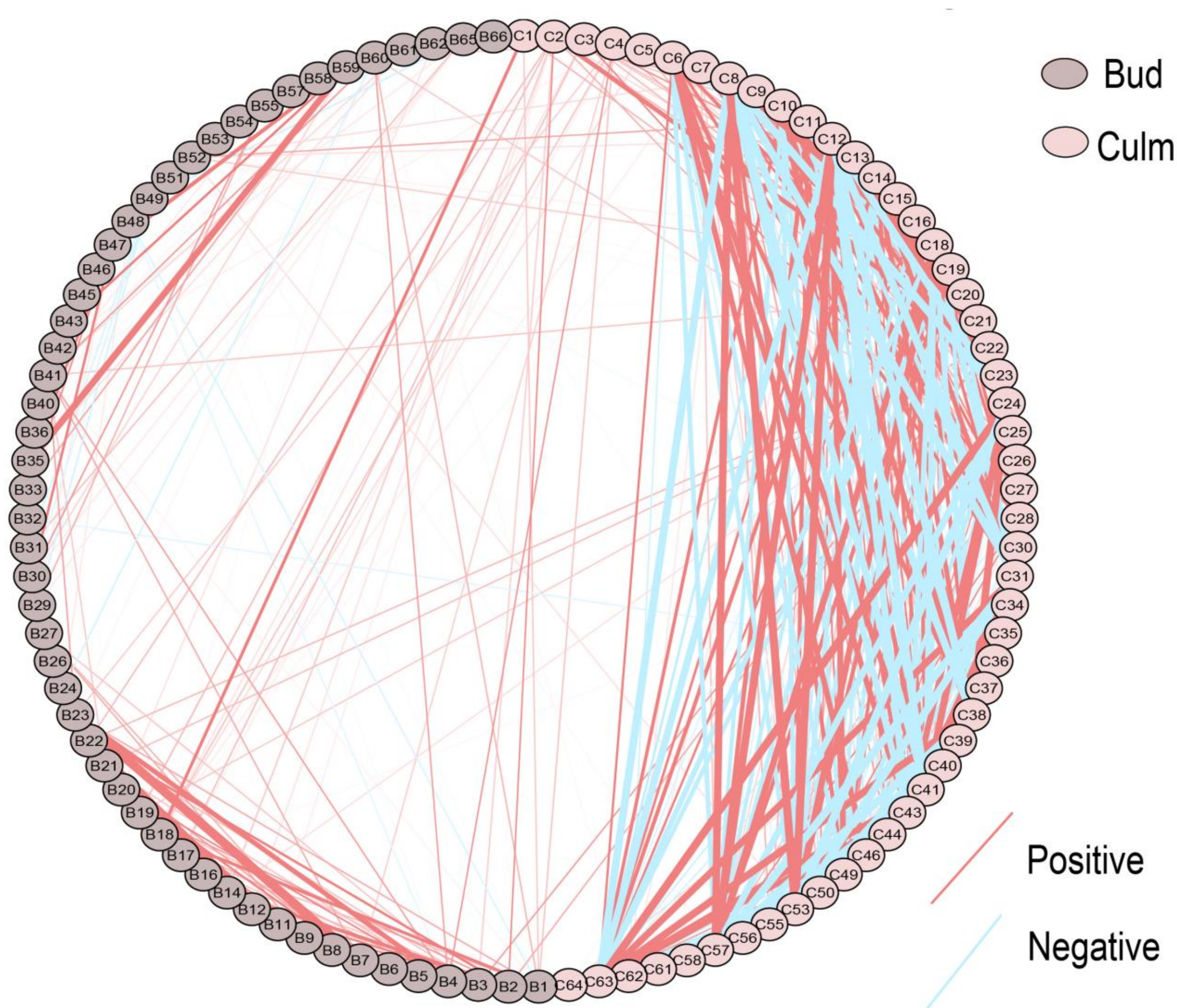

Figure 2. Metabolite-metabolite correlations within and between tissues in different sugarcane commercial cultivars. Metabolites are indicated by codes available at the Supplementary Table S2. Positive and negative correlations are represented in blue and red edges, respectively. Different color of nodes denotes distinct tissues.

Culm metabolic composition is important for bud outgrowth performance

We also investigated whether the metabolic composition of both tissues among the selected commercial cultivars would have an impact on sprouting even under low trait variability. Based on the role of polyamines and sugars controlling axillary meristem dormancy and tillering/branching (Zheng, Rowland, and Kunst 2005; Ge et al. 2006; Purohit et al. 2007; Cui et al. 2010; Mason et al. 2014; Barbier et al. 2015), we hypothesized that the metabolic composition of the culm could be one of the key factors determining bud outgrowth. Although our analysis was restricted to few compounds of the primary metabolism, it covers key metabolites known to play fundamental roles in promoting sink to source transitions and plant growth. A partial least squares discriminant analysis (PLS-DA) was applied in an attempt to understand the role of culms in bud outgrowth (Figure 3). Our results showed that the bud metabolomic data solely did not result in a good separation among genotypes according to the sprouting potential (Figure 3A). One plausible reason is that different genotypes might be at distinct stages of dormancy, which could exert influence on their metabolism hampering the discrimination based on the metabolome. Furthermore, as the metabolic activities of mature culms are committed to sucrose storage and reduced in comparison to fast growing stages of the plant life cycle, we can not exclude the possibility that changes in metabolic contents among cultivars are partially masked at this specific phase. In contrast to bud, the PLS-DA revealed a significant difference in the culm metabolism for low and high sprouting rate at least for the most contrasting genotypes (Figure 3B).

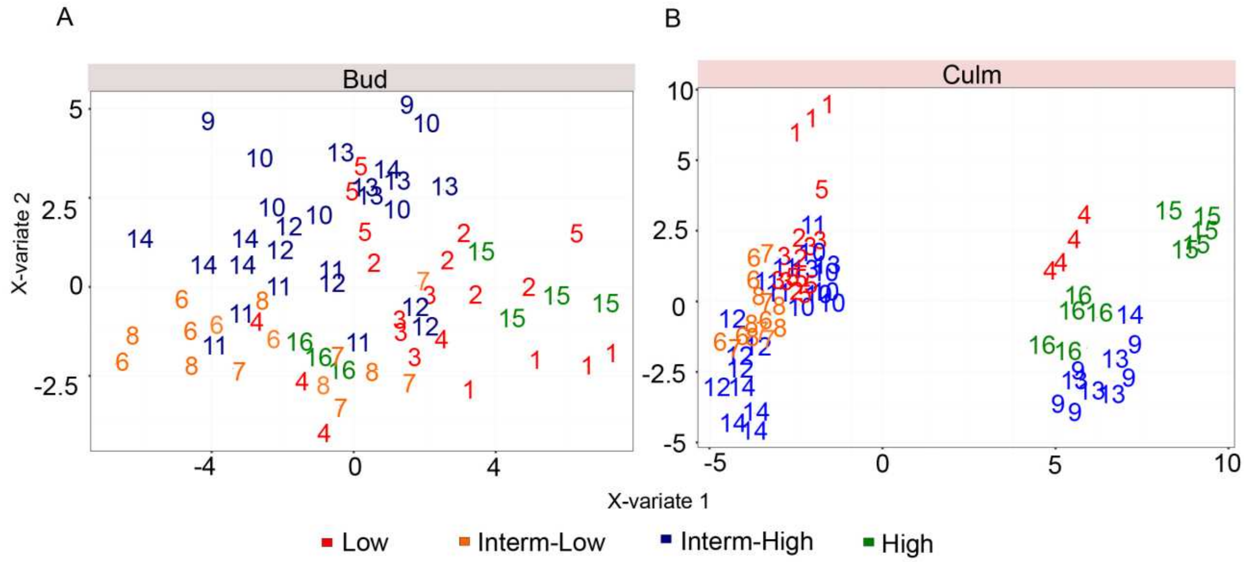

Figure 3. PLS-DA score plots corresponding to a model using genotypes and metabolites as two latent variables. Figures A and B represent the discriminant analysis of bud and culm, respectively. The different genotypes are referred as numbers from 1 to 16, listed in Supplementary Table S1. The color of the numbers denotes its sprouting group.

To identify the metabolites responsible for the separation among genotypes, a cluster image analysis was performed by building a similarity matrix with the PLS-DA results (Figure 4). A total of five well-defined groups was obtained and although there was no clear association in three of the clusters with respect to sprouting rate, two groups presented a very clear trend in relation to bud outgrowth performance. Interestingly, the levels of several metabolites including lysine, histidine, phenylalanine, GABA, methionine, xylose, benzoate, tetradecanoate, putrescine, nicotinate, galacturonate, the compound similar to itaconate, putrescine, nicotinate, benzoate and galacturonate seemed to correlate positively with the high sprouting rate genotypes. In contrast, the levels of glycerol, quinate, fructose, sucrose, myo-inositol, leucine, glutamine, isocitrate, glutamate, ornithine, serine, threonine and isoleucine appeared to have a negative impact on bud outgrowth. Taken together, our results showed that the culm, but not the bud metabolome, enabled the discrimination of the genotypes based on their sprouting performance only among the most contrasting cultivars. Furthermore, the culm metabolism turned up important to determine bud outgrowth efficiency as shown by the correlation of contrasting genotypes with antagonistic metabolites such as sugars and polyamines, this latter suggested as a signaling mediator in bud dormancy, and also by the presence of glutamate and serine, both involved in the connection of culm and bud networks.

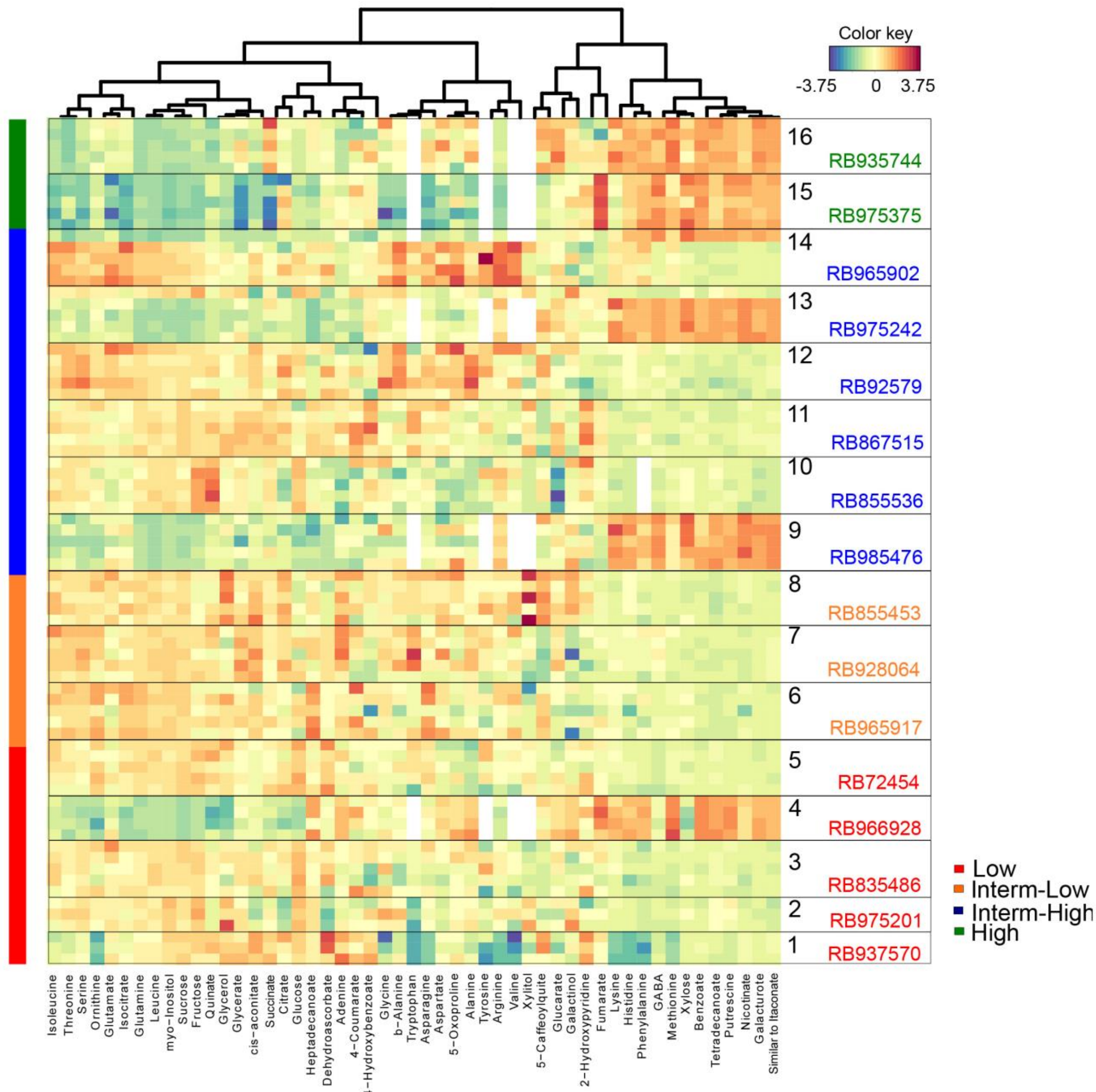

Figure 4. Heat map of metabolites in culms selected by the PLS-DA VIP score. Each row represents a metabolite identified in at least three biological replicates (the number of squares represent the exact number of replicates), whereas columns represent the metabolic abundance among genotypes. Changes in the abundance of metabolites from the overall mean concentration for each genotype are shown in green (low correlation) or red (high correlation).

Sugarcane metabolome reflects sprouting rate and the genetic relatedness of commercial genotypes

As the culm metabolome permitted to rank at some extend the genotypes according to the sprouting rate, we next investigated how central metabolism was influenced by the genetic background of the selected cultivars in the conditions of this experiment. For that, we compared the hierarchical clustering analysis (HCA) considering only the culm metabolome (Figure 5) to numerator relationship matrix (Figure S2) obtained from pedigree information shown in Figure S1.

The HCA analysis revealed the presence of two defined clusters (Figure 5). The first cluster represents a very similar group of eleven genotypes with low to moderate-high sprouting rates. Interestingly, pairs of individuals with a relationship coefficient of 0.5 (parent-offspring or full-sib) in the numerator relationship matrix (Figure S2) tended to be kept in this HCA cluster. This cluster was mainly composed of individuals genetically related to the genotype RB72454, which was used as parental of several crossings of this panel (Figure S1). The mismatch individual, RB975375, displayed 100% of sprouting rate. The other exception was the genotype RB835486, which clustered together with RB72454 despite their complete absence of relatedness as per pedigree information (Figure S1). Interesting to note that RB835486 displayed the third lowest sprouting rate (93.1%), which main explain its placement at this first cluster.

The second cluster represents cultivars with high and moderate-high sprouting rates (RB935744 and RB975375 - high; RB985476 and RB975242 - moderate-high) with the exception of cultivar RB966928 that presents low sprouting rate. All the cultivars located in this cluster tended to display parentage coefficient below 0.25, among themselves and with other cultivars of this panel (Figure S2), according to the information from our pedigree. This fact is reflected in the height of the HCA dendrogram, which confirms their relative weaker genetic relationship.

It is worth to mention that our pedigree estimate is incomplete due the lack of information about the fathers of cultivars obtained from multiparental crosses. Besides, the estimation of the kinship matrix (Figure S2) could also be improved using informative molecular markers, which were out of the scope of this work. Despite this, the numerator relationship matrix (Figure S2) revealed that the parentage coefficient was already high among cultivars (average of 0.114), suggesting a close relationship among cultivars (i.e., such value is almost the coefficient between cousins, 0.125). Apart from RB92579 and RB975242, all the clones share some degree of relatedness with at least one individual in the panel (Figures S1 and S2). Overall, our results suggest that both factors, genetic background and bud sprouting rates, jointly influenced the metabolomic profile of sugarcane revealed by HCA when evaluated under a single environmental condition.

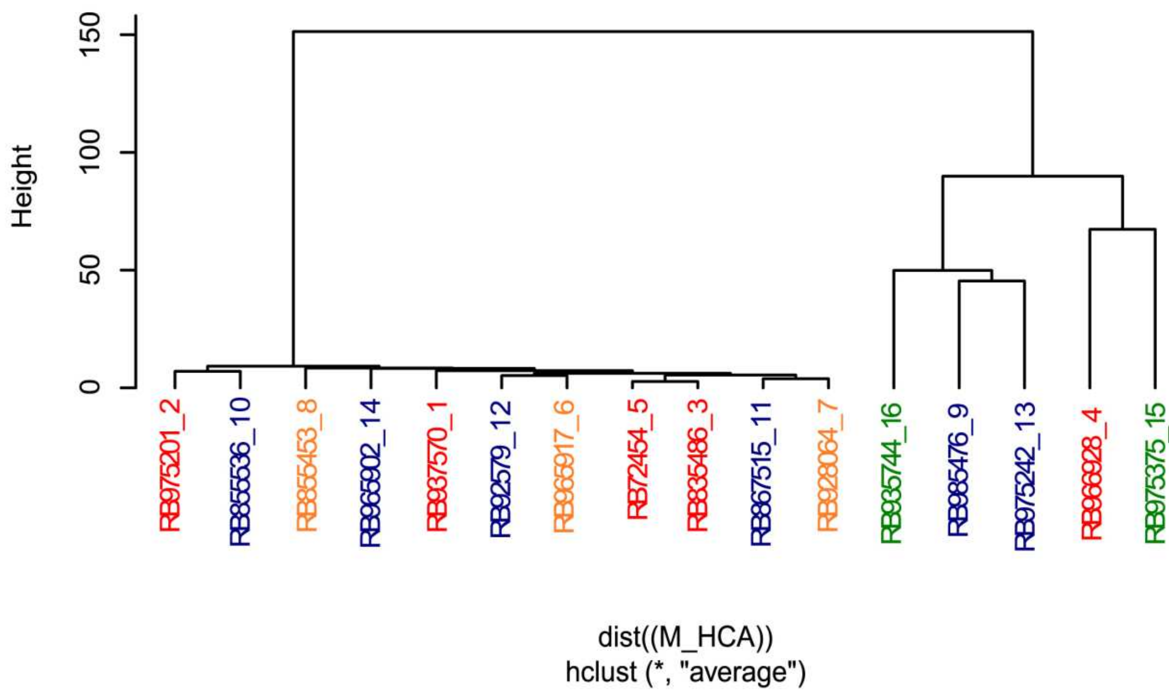

Figure 5. Hierarchical cluster analysis revealed that metabolite profiling from culms discriminates sugarcane commercial cultivars. Genotypes are color-coded as follows: red, orange, blue and green represent low, intermediate-low, intermediate-high and high sprouting groups, respectively.

Discussion

Metabolomics has been widely used as a powerful tool to elucidate mechanisms involved in metabolic regulation as well as bridging the gap between genotype and phenotype (Saito and Matsuda 2010; Kusano et al. 2011; Kumar et al. 2017). Over the last decade, metabolomics has been also used in association with natural variation to unravel the genetic architecture of several agronomic traits controlled by metabolism (Toubiana et al. 2012; Witt et al. 2012; Meyer et al. 2007). Although these studies have provided many insights into biological properties, the complexity of the metabolome and its dependency on the environment, genetics and development, precludes the generation of a full complete picture (Soltis and Kliebenstein 2015). In this study, we minimized this complexity by fixing the environmental conditions to assess whether the primary metabolism of two organs involved in the sprouting potential is regulated to trigger bud outgrowth in 16-highly planted sugarcane cultivars, representing a good sampling of commercial cultivars with overall good field performance, including good sprouting rate. Under our experimental conditions (controlled temperature and water availability), the selected sugarcane genotypes presented low variability in their sprouting rate (about 10%). Optimal sprouting conditions rarely occur in important production areas, when buds are often exposed to several abiotic constraints. One example is the Brazilian central region, in which the impact of limiting environmental conditions resulted in sprouting rates ranging from 29,17 to 76,92% among 8 commercial cultivars. This work evaluated 4 cultivars (RB867515, RB855453, RB835486, RB855536) also studied herein, but only RB8555453 and RB855536 presented sprouting ratios over 70% under those environmental conditions (Cargnin et al. 2008). Furthermore, it is important to mention that a mix of internodes from top, middle and bottom portions of the stem is planted in commercial fields. In our experimental setup, we selected only internodes belonging to the middle part of the stem to minimize the variation in sprouting rate dependent on developmental stage and bud position among the varieties(Manhães et al. 2015; Baracat-Neto et al. 2017).

It is widely known that there is a gradient concentration of sucrose along the sugarcane stem, with mature internodes having higher sucrose levels that decrease towards the top immature internodes. Strikingly, the bud sprouting performance along the stem follows the opposite gradient of sucrose (Whittaker and Botha 1997; Zhu et al. 1997; Vorster and Botha 1999; Uys et al. 2007) and the culm metabolism is apparently essential to determine the dormant status of the axillary meristem and bud outgrowth (Boussiengui-Boussiengui et al. 2016). Although few studies aimed to investigate the mechanisms responsible for successful germination/sprouting in this species (Verma et al. 2013; Singh et al. 2016; Boussiengui-Boussiengui et al. 2016), very little is known about the biochemical and molecular aspects related to this process, especially concerning sink and source interactions of the bud and culm. Plant growth and development is modulated by the balance between source and sink strengths (Paul and Foyer 2001; Dingkuhn et al. 2007; Smith and Stitt 2007; Patrick and Colyvas 2014), namely production of photoassimilates in leaves and their use in non-photosynthetic organs. In sugarcane, sucrose can be quickly metabolized in sink tissues to maintain its levels within a proper range, enabling fast responses to alterations in sucrose supply and demand. However, depending on the carbon demand, the culm starts to act as an additional source tissue, mobilizing sucrose to sustain developmental transitions. In the case of sprouting, sucrose will be used to promote axillary bud outgrowth and seedling establishment (O'Neill et al. 2012). The amino acids leucine and isoleucine seem also to play a later role during this process (O'Neill et al. 2012) and isotopic analysis demonstrated that nitrogen reserves from the culms are important for seedling establishment in the first 50-60 days of development (Carneiro et al. 1995). In this sense, remobilization of carbon and nitrogen mediated by sucrose and amino acids from the culm is crucial for the establishment of a new shoot from the axillary meristem. However, it still remains to be elucidated which key metabolites participate in breaking the axillary meristem dormancy. It is known that bud outgrowth is inhibited by the action of hormones in a phenomenon termed apical dominance, which can be suppressed by excision, developmental transitions or diseases (Botha et al. 2013; Rameau et al. 2015; Barbier et al. 2017). In this work we focused on investigating how primary compounds of central metabolism, rather than hormones, behave and interact in buds and culms during sugarcane bud outgrowth. Unravelling the interaction between hormone and central metabolite signaling will be crucial to dissect the temporal cascade controlling bud outgrowth release.

As plant growth regulation is closed modulated by the primary metabolism, our study used GC-MS-based metabolomics to unravel these relationships in culm and bud among different genotypes. Due to the fact that the modern commercial sugarcane varieties have narrow genetic basis, we first addressed if metabolic features would display any degree of variability among the selected sugarcane cultivars. Statistical tests (ANOVA) on metabolome data did not only confirm metabolic variability, but also unravel differences between the studied organs.

In order to further unravel small molecules involved in this process, metabolite-metabolite correlation analysis was performed within and between tissues. Several studies pinpointed the high connectivity of amino acids in Arabidopsis, tomato and maize (Schauer et al. 2006; Toubiana et al. 2015; Wen et al. 2015), suggesting that their network is controlled by a high degree of metabolic regulation (Galili and Höfgen 2002). Accordingly, our results showed that overall amino acids were highly correlated. Interestingly, glutamate and serine were among the few metabolites presenting correlations between culm and bud. Glutamate, a hub in amino acid metabolism, is substrate of glutamine synthetase (GS) to generate glutamine or is formed by the conversion of glutamine and 2–oxoglutarate in the presence of either reduced ferredoxin (Fd) or NADH by glutamate synthase (GOGAT) during inorganic ammonium assimilation (Lea and Miflin 1974; Yamaya and Oaks 2004b)(Lea and Miflin 1974; Yamaya and Oaks 2004a). In rice, transgenic plants lacking the cytosolic glutamine synthetase 1;2 (GS1;2) exhibited a severe suppression of bud outgrowth (Ohashi et al. 2015), suggesting a role of glutamate as signal molecule for sensing nitrogen status and controlling this process. Furthermore, glutamate is also a precursor of serine biosynthesis in a non-photorespiratory route called phosphorylated pathway, which was the other metabolite linking culm to bud metabolism and has been shown to control cell proliferation (Cascales-Minana et al. 2013; Ros et al. 2014). In this context, metabolomics is a powerful tool for identifying candidate metabolic pathways involved in diverse biological processes.

With respect to the tissue-specific metabolic networks, the culm presented a more coordinately regulated metabolism than the bud. Due to its high concentration in parenchyma cells of stem internodes, sucrose was one of the main hubs in the culm network, as expected. This disaccharide was responsible for the most negative correlation in the network with the putrescine, an important precursor for polyamine biosynthesis. Polyamines are aliphatic nitrogen compounds that have been proposed to be involved in many processes during plant growth and development in response to environmental cues (Kusano et al. 2007; Gill and Tuteja 2010) and are crucial for plant survival as blockage of their biosynthesis leads to lethal phenotypes (Urano et al. 2005; Ge et al. 2006). Interestingly, deletion in one of the genes encoding for the enzyme S-adenosylmethionine decarboxylases, involved in both spermidine and spermine biosynthesis, leads to a bushy and dwarf phenotype in Arabidopsis by affecting cytokinin homeostasis (Cui et al. 2010). This mutant, namely bud2-1, has 25% higher levels of putrescine in comparison to the wild-type. Apparently, bud2-1 has also enhanced root growth, supporting previous work that suggests putrescine as a growth promoter (Cui et al. 2010). Cytokinin levels are controlled by auxin (IAA) during bud outgrowth via apical dominance maintenance (Müller and Leyser 2011). In this sense, opposite to putrescine, myo-inositol displays a positive correlation with sucrose. This glycoside conjugates IAA to temporarily control its availability, being hydrolyzed to set free IAA (Kowalczyk et al. 2003). Moreover, IAA conjugates with amino acids in plants, but only few conjugates (e.g., IAA–Ala, –Leu and –Phe) are hydrolyzed to form free IAA. IAA-Asp and -Glu are in the degradation pathway or inhibition of the IAA action as IAA-Trp (Ludwig-Müller 2011). Myo-inositol and galacturonate pathways are interconnected for ascorbate biosynthesis (Shen et al. 2009; Zhang et al. 2009), which is necessary for cell division and elongation (Tullio et al. 1999), biosynthesis of secondary metabolites and phytohormones (Smith et al. 2007). Taken together, our results suggested that the culm metabolism encompasses a complex metabolic network and confirmed the dual function fulfilled by this tissue: its initial sink role is replaced by the novel task as a nutrient source for the emergence of a new organ or seedling during the development of axillary meristem and bud outgrowth.

As the metabolic network of the culm unravel metabolites with putative role on bud outgrowth, we next investigated whether the metabolic composition among the selected commercial cultivars could be associated with sprouting rate. Our data shows that bud metabolome solely cannot explain the differences in the sprouting rate among the genotypes. In contrast, the culm metabolome could be used to classify at least the most contrasting genotypes. Interestingly, genotypes with higher sprouting rates tended to have higher levels of certain metabolites, as it was the case of putrescine, whereas genotypes with low sprouting rates presented higher levels of sugars and amino acids, especially the branched-chain amino acids. These metabolites were positively correlated within their groups but were negatively correlated to each other in the metabolite-metabolite network. These findings suggest that carbon and nitrogen metabolism is not only involved on bud outgrowth but can also regulate this process mediating crosstalk with signaling pathways as, for example, forming conjugated compounds with phytohormones

(Kowalczyk et al. 2003; Ludwig-Müller 2011). Such approach has the potential for selecting metabolic markers and pathways associated to a certain agronomic traits in sugarcane as it was already successfully shown for other crop species (Meyer et al. 2007; Toubiana et al. 2012; Witt et al. 2012).

Our data also demonstrated that the sugarcane metabolome and bud sprouting rate are partially influenced by the genotype at least for the studied cultivars. As these commercial cultivars share part of their genetic background, we considered their genetic relatedness using pedigree information. In breeding programs, sugarcane flowering requires specific environmental conditions and it is highly genotype-dependent. Therefore, synchronization of panicles and flowering time is a challenge, and in many cases, precludes the accomplishment of desirable bi-parental crosses. In order to circumvent this limitation, multi-parental crosses can be performed as an alternative to achieve seed production. In those crosses, only the identity of the mother plant is known, and the pollens come freely from diverse male individuals. Out of the 16 genotypes used in this work, 7 presented an unknown male parental, indicating that these genotypes were obtained from multi-parental crosses. Furthermore, some genotypes, as TUC71-7, SP70-1143, RB855536 and particularly RB72454, are parental of several pedigree crosses leading to an overrepresentation of their genetic background in the selected genotypes, indicating the presence of genetic relatedness (kinship) in this panel.

Despite the incomplete record of both parentals in multi-crosses presented in this pedigree, it was partially possible to correlate bud sprouting and metabolome with the genetic information. We speculate that this correlation would be higher if more contrasting cultivars were analysed. Even so, these results suggest that metabolic profile can be partially conserved at the parent-progeny degree in sugarcane, but not at more distant parentage levels. The use of metabolome as a proxy for genetics is appealing in sugarcane due to the complexity of its genome. Our results indicate that this approach should be feasible, opening the perspective for its application to assist sugarcane breeding programs.

Conclusions

The work presented here clearly shows how metabolomics can be used to enrich the understanding of agronomic traits dependent on metabolic composition focusing on bud sprouting, a crucial process determining yield in sugarcane. Variability in metabolic features were identified even under a narrow genetic background typical for modern sugarcane cultivars. Metabolite-metabolite correlation analysis was performed within and between tissues in order to add information on how the metabolism of buds and culms interact to promote sprouting. Metabolic networks revealed more complex patterns for culms in relation to buds, and enabled the recognition of key metabolites (e.g., sucrose, putrescine, glutamate, serine and myo-inositol) affecting sprouting ability. Finally, those results were associated with the genetic background of each cultivar, showing that metabolites can be potentially used as indicators for the genetic background. Analysis of association panels with broader genetic variability and the use of informative genetic molecular markers could be used in the future to confirm the predictive power of metabolomics.

Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Author Contributions

D.A.F., M.S.C. and C.C. conceived the study. L.G.F.A., J.A.A. and L.D.W. performed experiments. D.A.F., A.C.G., R.R.A., and C.C. analysed the data. M.C.M.M., D.A.F., A.C.G., M.S.C and C.C. wrote the manuscript. M.S.C and H.P.H. provided supportive information.

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5. Interação das vias metabólicas envolvidas na quebra da dormência e desenvolvimento inicial das gemas axilares de cana-de-açúcar

5.1 Introdução

Em consequência de seu estilo de vida séssil, e, frente aos inúmeros desafios impostos por condições ambientais variáveis incluindo mecanismos tanto bióticos como abióticos, as espécies de plantas evoluíram com uma série de adaptações morfológicas, fisiológicas e bioquímicas para suportar seu crescimento. Dentre estas adaptações, podemos citar o desenvolvimento de meristemas auxiliares ou secundários (SHIMIZU-SATO; MORI, 2001) que apresentam o mesmo potencial de desenvolvimento dos meristemas primários ou apicais, contudo, permite dar continuidade ao crescimento das plantas em condições de perda de funcionalidade do meristema apical (SHIMIZU-SATO; MORI, 2001). Assim, juntamente ao desenvolvimento das gemas axilares, as plantas evoluíram o fenômeno da dominância apical, pelo qual a atividade do meristema apical caulinar reprime o desenvolvimento das gemas axilares, mantendo-as em estado de dormência, direcionando e definindo o padrão de crescimento e arquitetura das mesmas (CHATFIELD et al., 2001; DOEBLEY; STEC; HUBBARD, 1997; HORVATH et al., 2003; ORTIZ-MOREA et al., 2013; SHIMIZU-SATO; MORI, 2001; WANG; LI, 2008). Caso contrário, a simples presença de tais meristemas acarretaria no desenvolvimento desordenado da arquitetura das plantas, resultando na competição interna por recursos e energia.

Além da clássica teoria da interação hormonal para o controle do fenômeno da dominância apical e desenvolvimento das gemas axilares (BREWER et al., 2009; CLINE; WESSE; IWAMURA, 1997; LEYSER, 2009), recentemente, tem sido apontado um papel crucial do metabolismo primário neste processo, uma que vez está diretamente envolvido na regulação do crescimento e desenvolvimento celular, fornecendo energia necessária para engatilhar este processo. Alguns compostos pertencentes ao metabolismo primário são sugeridos como reguladores do ciclo celular, como os açúcares, que além de servirem como fonte de energia para processos metabólicos, regulam a expressão dos genes CyCD2 e CyCD3, ciclinas que são ativadas durante a fase G1 do ciclo em resposta a sinais de crescimento (HEALY et al., 2001; RIOU-

KHAMLICHI et al., 2000). Além disso, é reportado, em células de mamíferos, aumento no fluxo de glicose pela via glicolítica guiado, principalmente, pela demanda do ciclo do ácido tricarboxílico (TCA) na fase G1 do ciclo celular (AHN et al., 2017). Este mesmo estudo, demonstra que após a transição da fase G1 para a fase S do ciclo, este açúcar apresenta pouca oscilação, e que a oxidação da glutamina, também crucial para manter as os níveis dos intermediários do TCA, passa então a desempenhar um papel importante na progressão do ciclo e na proliferação celular.

Como mencionado, os açúcares podem exercer papel pivotal no crescimento vegetal e, dentre eles, destaca-se a sacarose, classificada como o principal produto da fotossíntese em plantas. Sua utilização como fonte de carbono e energia depende da sua clivagem em hexoses, glicose e frutose (STURM, 1999). Nas plantas, a sacarose é transportada a partir de órgãos sintetizadores (fonte) para órgãos de armazenamento (dreno), ou ainda metabolizada atuando não só como fonte de esqueletos de carbono, mas também como um vetor de energia (LEMOINE, 2000), sendo, portanto, importante no estabelecimento das relações fonte e dreno na planta. Além disso, este açúcar é proposto como uma molécula sinalizadora, atuando em uma ampla gama de processos de desenvolvimento ao longo do ciclo de vida vegetal, afetando tanto o crescimento como a diferenciação de tecidos (TOGNETTI; PONTIS; MARTÍNEZ-NOËL, 2013). Desta forma, é proposto que a sacarose promova o desenvolvimento das gemas axilares, podendo ser uma das moléculas atuantes na quebra do estado de dormência destes órgãos (ASSUERO; TOGNETTI, 2010). Em sorgo, foi demonstrado que a interrupção do fluxo de fotoassimilados por meio da desfolha parcial das plantas, ocasionou na repressão do desenvolvimento das gemas axilares, sendo verificado o aumento na expressão de genes relacionados a dormência (S*bDRM1*) e a privação de sacarose (Sb*ASN1*), bem como a diminuição daqueles relacionados a resposta do mesmo açúcar no ciclo celular (*SbPFP*), evidenciando a importância desse composto no desenvolvimento desses órgãos. Além disso, a sacarose pode ainda agir na mediação da sinalização hormonal envolvida no processo de quebra da dormência e desenvolvimento inicial das gemas axilares, precedendo a resposta aos hormônios auxina e citocinina, conhecida como hipótese clássica na quebra de dormência axilar. (BARBIER; LUNN; BEVERIDGE, 2015). Mais recentemente, foi demonstrado que a disponibilidade de sacarose em plantas é sensoriada por um açúcar sinal, a Treaolose-6-Fosfato (Tre6P) (FIGUEROA; LUNN, 2016). Em plantas de ervilha decapitadas, foi verificado aumento dos níveis de Tre6P nas primeiras 3 horas após a quebra da dominância apical, indicando a importância da sinalização de açúcares no processo de quebra de dormência no meristema axilar (FRANZISKA et al., 2017).

Pelo pressuposto, o desenvolvimento das gemas axilares em cana-de-açúcar parece ser um grande paradoxo, já que se trata de uma cultura altamente eficiente em acumulo de açúcar, e ainda assim suas gemas axilares apresentam-se em estado dormente. É sabido também que as gemas localizadas nas porções do terço médio superior da planta, têm maior vigor de brotação em relação as basais, sendo que o acumulo de sacarose ocorre primeiramente nos tecidos maduros, localizados na parte basal da planta (UYS et al., 2007; VORSTER; BOTHA, 1999; WHITTAKER; BOTHA, 1997; ZHU; KOMOR; MOORE, 1997). Assim, é esperado que diferentes níveis de certos metabolitos, ou mesmo a variação desses possa estar envolvida na quebra de dormência e desenvolvimento das gemas axilares, bem como toda a rede metabólica envolvida em tal fenômeno.

Além de açúcar, outros compostos do metabolismo primário parecem ser importantes no processo de quebra de dormência. Analisando o desenvolvimento de gemas axilares de ervilhas, a análise dos metabólitos destes órgãos possibilitou distinguir alterações na abundância de aminoácidos e de ácidos orgânicos envolvidos no ciclo do TCA, após a quebra da dominância apical das plantas, sugerindo a formação de esqueleto de carbono para sustentar o crescimento e desenvolvimento do novo órgão (FRANZISKA et al., 2017).

Desta forma, este trabalho teve como objetivo identificar potenciais metabólitos que possam atuar na regulação e desenvolvimento inicial das gemas de cana-de-açúcar, bem como, por meio da análise discriminatória, mapear as possíveis vias metabólicas envolvidas em tal processo.

5.2 Material e métodos

5.2.1 Material vegetal

Para avaliar a influência do metabolismo na brotação em gemas axilares inseridas em diferentes porções do colmo, duas variedades de cana-de-açúcar, RB72454 e RB975375, contrastantes em seu potencial de brotação foram selecionadas com base nos resultados do **capítulo 4**. De forma a induzir a quebra de dominância apical, plantas com aproximadamente 10 meses de idade, cultivadas a campo, foram selecionadas do jardim clonal da RIDESA, e então, decapitadas por meio da remoção de seus ponteiros e consequentemente seus meristemas apicais. Após 24h, gemas axilares do perfilho principal das plantas decapitadas ou intactas foram coletadas. O período de tempo de 24 horas foi estabelecido para que fossem maiores as chances de alterações fisiológicas e metabólicas significativas decorrentes da quebra da dominância apical. Devido à variação da taxa de brotação em diferentes porções do colmo, os mesmos foram divididos em três partes: terço superior (próximo ao meristema apical), médio e basal, e em cada uma das partes, 3 gemas axilares foram coletadas por planta, em um total de 5 réplicas biológicas. As gemas foram precisamente coletadas com auxílio de bisturi e imediatamente congeladas com nitrogênio líquido, e então armazenadas em ultra freezer (-80ºC) até seu processamento para a análise do perfil metabólico que foi realizada conforme descrita no **capítulo 4**.

5.2.3 Análises estatísticas

Foram realizadas análises estatísticas descritivas (ANOVA) na comparação das médias dos metabólitos para cada uma das classes testadas. O teste ANOVA foi realizado com auxílio do software estatístico Minitab, ao nível de 5% de significância, e os resultados foram classificados pelo método Tukey. As análises multivariadas (PLS-DA e *Heatmap*) foram realizadas conforme descrito no **capítulo 4.** Os metabólitos que apresentaram alterações estatisticamente significativas em seus conteúdos foram selecionados e suas nomenclaturas foram padronizadas segundo o banco de dados KEGG (*https://www.genome.jp/kegg/compound/*).Como forma de avaliar as possíveis rotas metabólicas envolvidas no processo de brotação, os compostos selecionados foram mapeados em suas possíveis vias metabólicas por meio do software *Cytoscape* (http://www.cytoscape.org/), com a extensão *MetScape* (http://www.metscape.ncibi.org).

5.3 Resultados

5.3.1 Perfil metabólico de gemas de cana-de-açúcar

A análise de perfil metabólico por GC-MS permitiu a identificação de 56 compostos, principalmente, do metabolismo central como aminoácidos, ácidos orgânicos, açúcares, açúcar-álcool e poliaminas em gemas da cana-de-açúcar dos genótipos selecionados. Devido ao grande número de variáveis abordadas, tais como, genótipos, posições das gemas e condições com e sem dominância apical, foi realizada, inicialmente, uma análise exploratória para reconhecer o padrão de agrupamento das amostras com características semelhantes bem como os compostos que são responsáveis para a separação das mesmas. Para tal, foi realizada uma análise discriminante com calibração multivariada por mínimos quadrados parciais (PLS-DA) (**Figura 5.1 A**) que é um método estatístico para análise multivariada de classes, na qual por meio da regressão dos mínimos quadrados parciais, a máxima separação é obtida, expressando quais variáveis são responsáveis pela separação das classes. Como resultado obtêm-se um ranking das variáveis, neste caso, os metabólitos, com maior peso na discriminação das classes, que estão apresentados na **Figura 5.1 B** em forma de *heatmap*.

A maior discriminação entre as classes analisadas ocorreu entre as variedades, independente da condição com ou sem dominância apical (**Figura 5.1 A**). A variação na abundância dos metabólitos apresentam alta correlação entre as variedades testadas, explicando 40% da discriminação dessas classes. Dentre esses metabólitos, os açúcares apresentaram comportamentos distintos entre as variedades, sendo glicose e frutose discriminantes em favor da variedade com maior potencial de brotação, a RB975375, enquanto a sacarose, trealose e xilulose discriminantes para a RB72454. Tais resultados corroboram com os resultados da análise estatística apresentados nas **tabelas suplementares de 4 a 9,** e indicam que embora a abundância relativa de sacarose em tecidos de reserva seja semelhante para ambos os genótipos, esses se diferenciam quanto aos açúcares provenientes da quebra deste composto, como a glicose e frutose.

Além dos açúcares, os aminoácidos glutamato, aspartato e triptofano foram discriminantes entre as variedades analisadas, com maior tendência a discriminar em favor da variedade de menor taxa de brotação, a RB72454. Glutamato ocupa um papel central no metabolismo de aminoácidos em plantas, atuando principalmente no metabolismo de nitrogênio, servindo de substrato para a síntese de outros aminoácidos como a glutamina e também o aspartato (FORDE; LEA, 2007) e pode sugerir diferenças entre as variedades quanto ao metabolismo de nitrogênio. O triptofano é um precursor na síntese da auxina (FORDE; LEA, 2007; HILDEBRANDT et al., 2015; RADWANSKI; LAST, 1995), e sua maior abundância relativa nas gemas da variedade com menor potencial de brotação podem indicar uma disfunção na conversão deste em auxina, uma vez que a exportação deste hormônio pelas gemas pode ser considerada um fator chave para o desenvolvimento das mesmas.

Além dos açúcares e aminoácidos citados, a poliamina espermidina também foi identificada como variável discriminante entre os dois genótipos. Este metabólito apresentou tendência a discriminar em favor da variedade RB72454 enquanto a putrescina, embora não classificada entre os principais compostos discriminantes, em favor da variedade RB975375. Esses dois compostos apresentam relação direta de produto e substrato respectivamente, sendo a espermidina produzida a partir da conversão da putrescina pela espermidina sintase (TAKAHASHI; KAKEHI, 2010). Além disso, conforme exposto no capítulo anterior, o aumento dos níveis de putrescina causado por uma mutação na via das poliaminas resultou em alta taxa de brotação e alteração do metabolismo de putrescina (CUI et al., 2010). Assim, coletivamente, estes resultados podem sugerir de forma geral que as variedades com maior taxa de brotação apresentam uma maior eficiência na conversão de certos metabólitos que parecem ser importantes para a ativação das gemas axilares como é o caso da sacarose em relação a glicose e frutose e espermidina e putrescina.

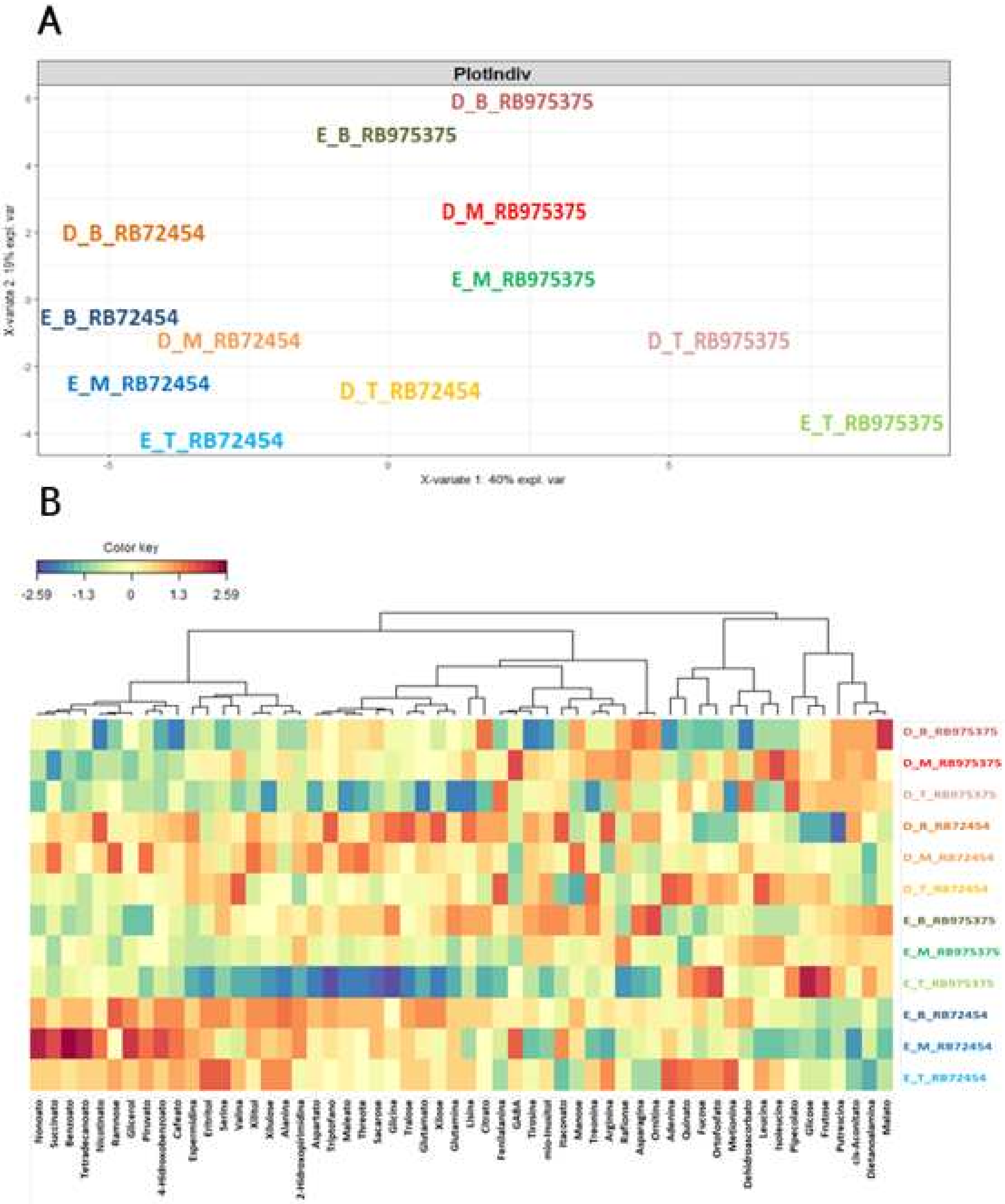

Figura 5.1 – Análise PLS-DA do metaboloma e *de* gemas das variedades RB72454 e RB975375 em ambas as condições, com e sem a dominância apical. As amostras foram codificadas de acordo com as porções do colmo da cana-de-açúcar em que as gemas foram coletadas: terço médio superior (T), mediano (M) e basal B); e inteiras (E) e Decapitadas (D), sendo que cada uma das classes é representada por uma coloração diferente e são o resultado da média de 5 réplicas biológicas. **(A) PLS-DA (B) *Heatmap*** da abundância de cada metabólito representada pelos quadrados dispostos nas linhas que representam a média de 5 réplicas biológicas, enquanto as colunas representam a abundância metabólica entre as classes testadas. Alterações na abundância de metabólitos da concentração média total para cada genótipo são mostradas em azul (baixa correlação) ou vermelho (alta correlação), conforme escala apresentada no canto superior esquerda da figura.

A variação dos componentes do eixo y (**Figura 5.1 A**) foi atribuída, principalmente, as diferentes porções do colmo, seguidas, de forma menos pronunciada, entre as condições com e sem dominância apical, independentemente dos genótipos e de forma menos pronunciada. Estes resultados sugerem que a as diferenças na taxa de brotação entre as gemas das diferentes porções do colmo, podem ser, em partes, explicadas pelas alterações metabólicas ocorridas após a quebra da dominância apical. Curiosamente, os metabólitos adenina, ortofosfato, fucose e quinato parecem contribuir não apenas para a discriminação entre gemas do terço médio superior, porção considerada com maior vigor de brotação, mas também entre as gemas inseridas em diversas porções do colmo independentemente do genótipo de plantas intactas. Desta forma, a presença destes metabólitos sugere importância dos mesmos na classificação das gemas durante o início do desenvolvimento das gemas axilares, uma vez que após a quebra da dominância apical, há uma tendência de redução dos níveis destes metabolitos, indicando um rápido *turnover* em suas respectivas vias metabólicas. Nesta condição, o nucleotídeo adenina está diretamente envolvido transporte energético das células (WANG et al., 2017), enquanto ortofosfato além do transporte energético está também envolvido na sinalização e ativação enzimática (HAFERKAMP; FERNIE; NEUHAUS, 2011), corroborando com a hipótese da disponibilidade e consumo destes dois compostos após o estimulo ao crescimento das gemas axilares. O metabólito fucose, embora não esteja diretamente envolvido no metabolismo energético celular, é um importante composto encontrado principalmente em polissacarídeos de parede celular (EBERT; RAUTENGARTEN; HEAZLEWOOD, 2017). Por sua vez, quinato é classificado como um composto do metabolismo secundário das plantas e que pode servir como substrato para a via do ácido chiquimico (GUO et al., 2014; ZABALZA et al., 2017) e seu papel nos órgãos aqui estudados não está claro.

Devido à complexidade do desenho experimental, contudo, houve um grupo de metabólitos que apareceu associado a grupos de amostras com características supostamente contrastantes, como foi o caso dos intermediários da via do ácido tricarboxílico (TCA), malato e citrato que foram discriminantes em gemas basais de plantas inteiras ou de plantas decapitadas que em teoria apresentam menor e maior taxa de brotação respectivamente. Como as análises apresentadas nesta tese permitem acessar apenas o conteúdo relativo e não o fluxo em relação a uma determinada via, é plausível especular que a variação nos níveis destes compostos possa ser atribuída tanto a uma ativação de uma determinada via, como um bloqueio de passos após este intermediário. No caso do ciclo TCA especificamente, além de atuar na síntese de ATP e na formação de poder redutor a forma de NADH para a cadeia respiratória, este ciclo é altamente dependente de demandas metabólicas e fisiológicas, contribuindo na geração de uma série de precursores para a síntese de lipídeos, aminoácidos e metabólitos secundários (ARAÚJO et al., 2011; POPOV et al., 2010). Assim como estes intermediários do TCA, ornitina e asparagina, marcadores do metabolismo de poliaminas e nitrogênio, respectivamente, também apresentaram mesmas alterações em gemas basais de plantas intactas e em gemas após a decapitação. Desta forma, é possível que o acúmulo destes metabólitos em condições supostamente contrastantes, possa levar a alteração de diferentes rotas metabólicas que possam contribuir diferencialmente neste processo.

5.3.2 Vias metabólicas relacionadas à quebra da dominância apical

Apesar da análise de PLS-DA ter permitido a separação entre plantas expostas a presença ou ausência de dominância apical, as demais variáveis mascararam um pouco estas diferenças e como no caso de malato e citrato, não permitem identificar quais rotas metabólicas são alteradas nas gemas axilares frente a ausência de dominância apical. Assim, considerando que o metabolismo, principalmente, primário é altamente complexo e interconectado, foram selecionados apenas os metabólitos estatisticamente significativos através de ANOVA que apresentaram o mesmo padrão de alterações em ambas as variedades nas condições analisadas. Espera-se com isso, relativizar diferenças ou metabolismos conservados durante o desenvolvimento inicial das gemas axilares, diminuindo a influência dos fatores inferidos como diferenças da atividade metabólica decorrentes de diferentes estádios fisiológicos de desenvolvimento após a quebra da dominância apical. Desta forma, espera-se com esta análise encontrar, primeiramente, os padrões conservados na viabilidade das gemas conforme sua posição no colmo, bem como identificar vias metabólicas chave para a quebra de dormência das gemas axilares em cana de açúcar.

Desse modo, ao todo, foram selecionados 21 metabólitos que foram utilizados na interface *MetScape* da plataforma *Cytoscape*, permitindo a análise de redes de metabólitos com base nas informações de vias metabólicas da plataforma KEGG2. Para tal, foram utilizadas as razões entre as amostras das condições com e sem dominância apical (**Tabela suplementar 10**). Dos metabólitos selecionados, apenas o ácido treônico não foi identificado pelo KEGG2 ID, enquanto os compostos dietanoalamina e maleato apesar de identificados não foram mapeadas pela plataforma. Para apresentação dos mapas das redes, foram selecionados apenas aqueles que representam as gemas do terço médio superior das variedades RB975375 (**Figura 5.2)** e RB72454 **Figura 5.3**), uma vez que essas apresentaram maior discriminação entre as condições testadas de acordo com a análise de PLS-DA.

As redes apresentadas demonstram as variações no metabolismo destas variedades analisadas após a quebra da dominância apical, que podem resultar em diferenças no processo de quebra de dormência axilar. Estas redes evidenciam os metabólitos mais relevantes em cada uma das variedades representados pelo tamanho dos nós, permitindo sua visualização em vias metabólicas mais relevantes neste caso, em resposta a decapitação das gemas para ambas as variedades. Neste sentido, metabólitos como cis-aconitato, glutamato, glutamina, fenilalanina e metionina apresentaram um padrão de alteração de seus níveis comum a ambas variedades após decapitação. Desta forma, enquanto os aminoácidos glutamina e glutamato podem reforçar a importância do metabolismo de nitrogênio no desenvolvimento inicial desses órgãos, estes resultados também apontam a importância do metabolismo energético, mais especificamente o TCA e de poliaminas após a quebra da dominância apical.

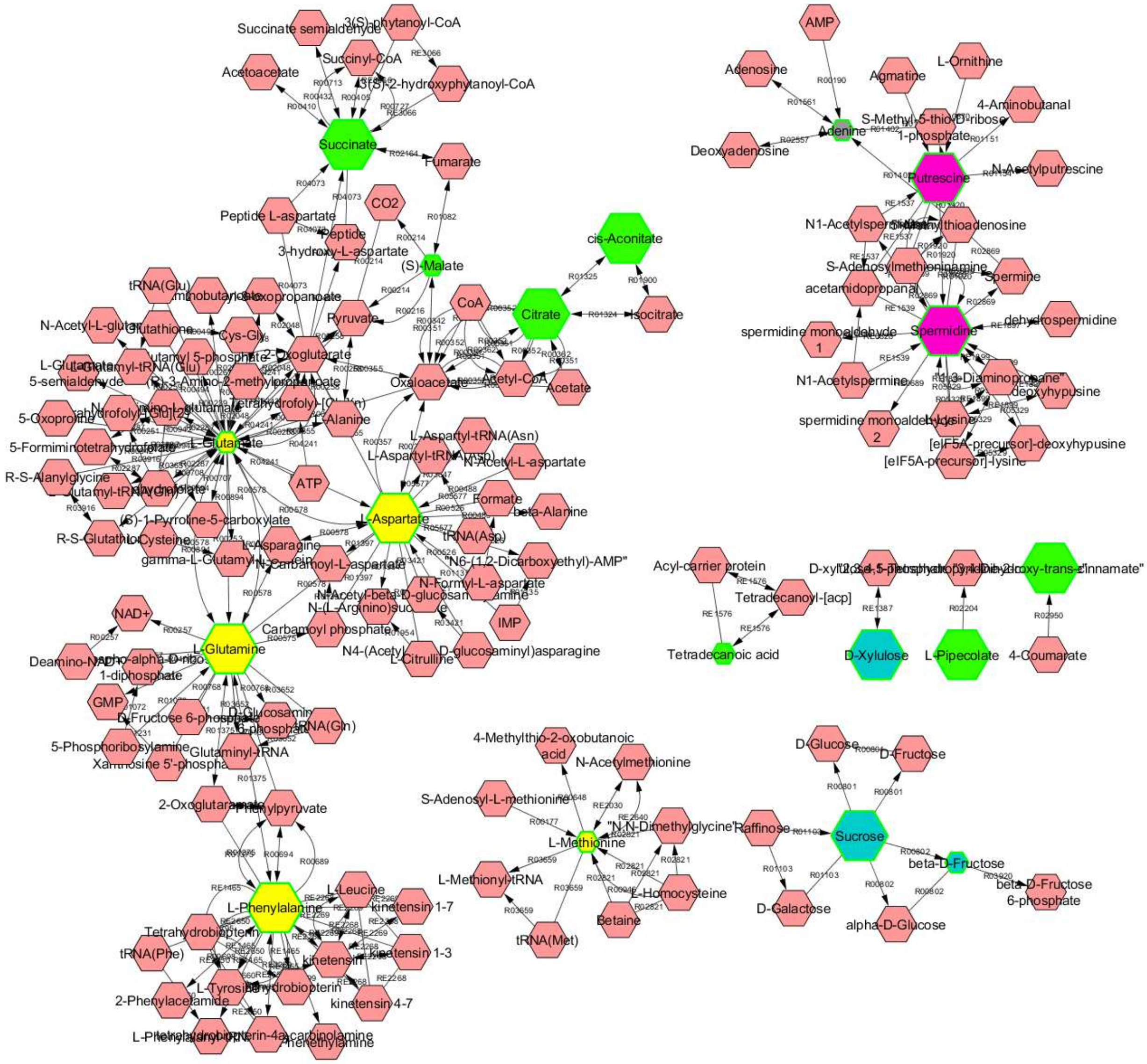

Figura 5.2 – Rede metabólica em gemas do terço médio superior da variedade RB975375, em função da quebra da dominância apical. Os nódulos amarelos, verdes, azuis, rosas e cinza representam os grupos dos aminoácidos, ácidos orgânicos, açucares, poliaminas e outros, respectivamente que foram selecionados como metabolitos estatisticamente significantes na comparação entre gemas de plantas intactas e decapitadas. Os nódulos em vermelho claro são metabólitos envolvidos nas respectivas vias nas quais os metabolitos selecionados estão inseridos, e são associados com base no banco de dados da plataforma KEGG2. Os nódulos maiores e menores representam compostos que tiveram sua abundancia aumentada e diminuída após a decapitação, respectivamente. Setas representam a direção da reação.

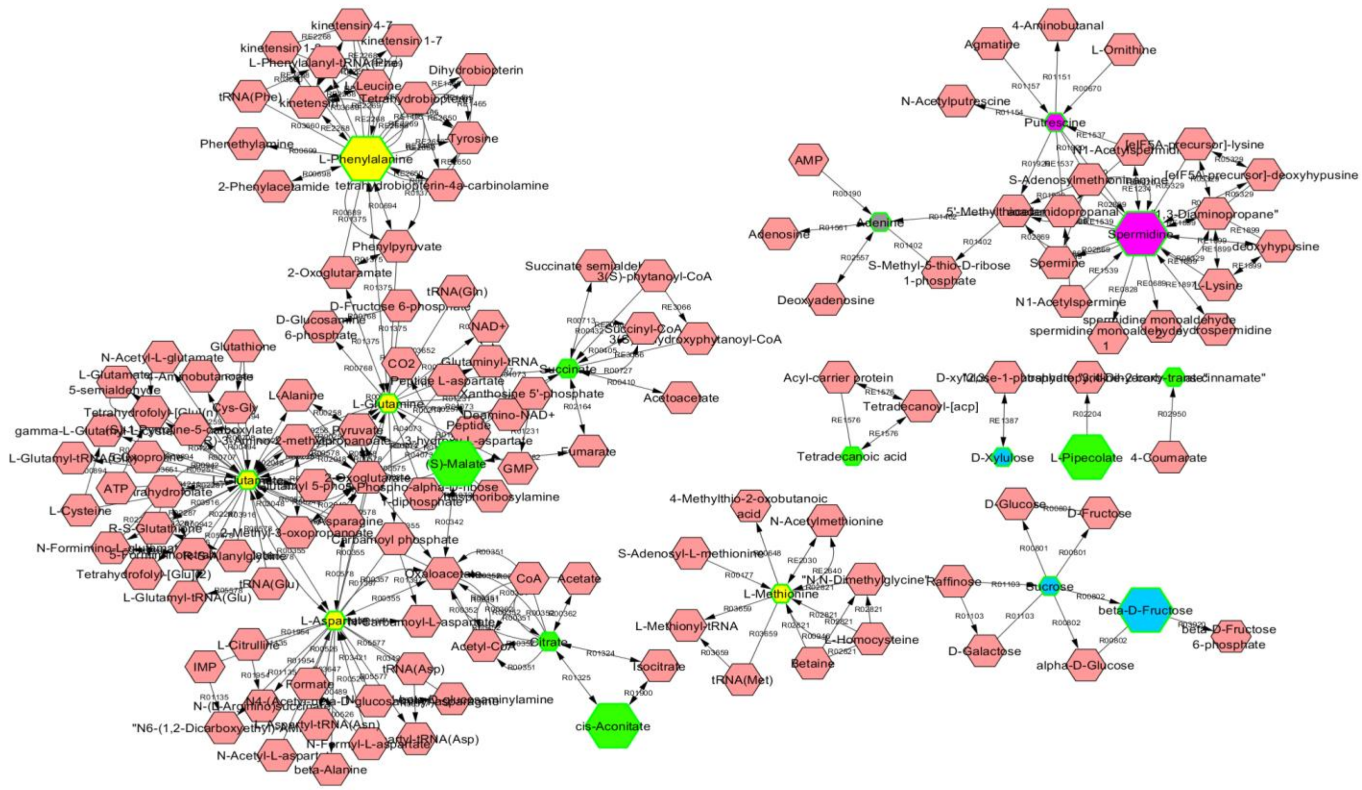

Figura 5.3 – Rede metabólica em gemas do terço médio superior da variedade RB72454, em função da quebra da dominância apical. Os nódulos amarelos, verdes, azuis, rosas e cinza representam os grupos dos aminoácidos, ácidos orgânicos, açucares, poliaminas e outros, respectivamente que foram selecionados como metabolitos estatisticamente significantes na comparação entre gemas de plantas intactas e decapitadas. Os nódulos em vermelho claro são metabólitos envolvidos nas respectivas vias nas quais os metabolitos selecionados estão inseridos, e são associados com base no banco de dados da plataforma KEGG2. Os nódulos maiores e menores representam compostos que tiveram sua abundancia aumentada e diminuída após a decapitação, respectivamente. Setas representam a direção da reação.

Interessantemente, houve uma série de metabólitos que tiveram respostas contrastantes entre as duas variedades, sugerindo que o redirecionamento destas vias pode ter influência na eficiência de brotação. Através desta análise, foi possível verificar que apesar de ambos genótipos apresentaram aumento nos níveis de cis-aconitato após a decapitação, os níveis de outros intermediários do TCA como malato, citrato e succinato foram positivamente correlacionados com o maior vigor de brotação. Desta forma, a variedade com maior taxa de brotação RB975375 apresentou um maior acúmulo destes compostos, enquanto RB2454 apresentou baixos níveis destes metabólitos, sugerindo que o processo de início de quebra de dominância apical induz a uma rápida ativação da geração de ATP através do TCA nas gemas axilares.

Uma tendência similar foi observada para os aminoácidos aspartato e glutamina, mais abundantes na RB975375, e ambos envolvidos na assimilação e metabolismo do nitrogênio, diretamente correlacionados com o glutamato, indicando como esperado a importância do metabolismo de nitrogênio para o estabelecimento de um novo órgão. Corroborando com os resultados anteriores, o metabolismo de poliaminas se mostrou mais uma vez importante neste processo. Apesar dos níveis similares de esperminida, os níveis de seu substrato, a putrescina, foi menos abundante na RB72454. Finalmente, conforme sugerido em literatura, os níveis de sacarose foram maiores em gemas oriundas de plantas decapitadas do genótipo com maior vigor na brotação, RB975375

As principais vias metabólicas mapeadas a partir dos metabólitos selecionados corroboram com os resultados apresentados pela macro-análise de PLS-DA, na qual a discriminação por metabólitos sugere que a partição de carbono, o metabolismo energético e de nitrogênio da cana-de-açúcar como principais atuantes no desenvolvimento inicial das gemas axilares. Esses achados reforçam o pressuposto das diferenças genotípicas quanto a velocidade e eficiência de seu metabolismo em resposta a variáveis de estresse, como a remoção do meristema apical das plantas, podendo ser determinante para o sucesso de sua perpetuação através do desenvolvimento das gemas axilares.

5.4 Discussão

5.4.1 Metabolismo de carbono e o desenvolvimento de gemas axilares de cana-de-açúcar

O desenvolvimento de novas estruturas vegetais envolve uma complexa rede de interações fisiológicas na realocação de recursos para suprir a demanda dos novos órgãos, na qual a sacarose destaca-se como uma das principais fontes de reserva energéticas (PAUL; VAN DIJCK, 2011). Nesse contexto, a cana-de-açúcar apresenta um grande paradoxo ao ser altamente eficiente no acúmulo de sacarose, sendo que a maior concentração deste dissacarídeo é na porção basal do colmo, local onde há menor taxa de brotação entre as gemas axilares. Nas plantas, a sacarose é transportada a partir de órgãos sintetizadores (fonte) para órgãos de armazenamento (dreno), ou ainda metabolizada atuando não só como fonte de esqueletos de carbono, mas também como um vetor de energia (LEMOINE, 2000), sendo, portanto, importante no estabelecimento das relações fonte e dreno na planta. Neste contexto, recentemente, foi mostrado que a sacarose é importante tanto como sinalizador como no estabelecimento do novo dreno em gemas axilares de ervilha (FRANZISKA et al., 2017).

Apesar do gradiente de sacarose em colmos de cana-de-açúcar, e, deste composto ser discriminante com tendência para as gemas da variedade com baixa taxa de brotação, nossos resultados mostraram que os níveis de sacarose também têm uma tendência a aumentar em gemas axilares da variedade com maior potencial de brotação após a decapitação. Além da sacarose, tanto a frutose quanto a glicose, são monossacarídeos fruto da hidrólise enzimática da sacarose por meio da atividade das enzimas invertases (INVs) e sucrose synthase (ROITSCH; EHNESS, 2000; ROITSCH; GONZÁLEZ, 2004; ROLLAND; BAENA-GONZALEZ; SHEEN, 2006), e são descritas como reguladoras do ciclo celular (RIOU-KHAMLICHI et al., 2000; ROLLAND; BAENA-GONZALEZ; SHEEN, 2006). A presença desses monossacarídeos é fundamental para o desenvolvimento das gemas de cana-de-açúcar, nas quais é verificado o aumento na abundância de açúcares redutores bem como da atividade das INVs e ATPase (BOTHA. et al., 2011). Esses resultados, sugerem que a diferença na partição de carbono entre as variedades analisadas pode ser determinante no processo de brotação e podem desempenhar um papel fundamental na alteração das relações de fonte e dreno durante o crescimento vegetal.

O açúcar xilulose também é apresentado como composto discriminante quanto ao processo de crescimento das gemas axilares, com maior concentração em gemas da variedade RB72454 que possui menor taxa de brotação. A xilulose está envolvida na biossíntese de carotenóides em plantas, sendo que a 1-desoxi-D-xilulose 5-fosfato sintase (DXS) é a primeira enzima para a via MEP (2-C-metil-D-eritritol 4-fosfato), catalisando a condensação dos substratos iniciais, gliceraldeído-3-fosfato e piruvato, em 1-desoxi-D-xilulose 5-fosfato (DXP), enzima chave em tal metabolismo (PENG et al., 2013). Os carotenóides e apocarotenóides, produtos da clivagem oxidativa são cruciais para vários processos biológicos em plantas, tais como a formação do aparelho fotossintéticos e a regulação do crescimento e desenvolvimento celular (HAVAUX, 2013).

Além disso, os carotenóides exercem importante papel em plantas como antioxidantes, correlacionando-se com a resposta das plantas às tensões ambientais como a formação de espécies reativas de oxigênio (ROS) (HAVAUX, 2013). Assim, a presença da xilulose está muito provavelmente relacionada a resposta da planta a condição de estresse causada pela decapitação das mesmas.

5.4.2 A contribuição do metabolismo de aminoácidos

Em plantas, os aminoácidos são fundamentais na assimilação do nitrogênio inorgânico proveniente do meio externo, constituindo-se como as principais reservas de nitrogênio orgânico na planta, fundamentais para suprir o crescimento vegetal (LAM et al., 1996; NÄSHOLM; KIELLAND; GANETEG, 2009). Assim como os açúcares, fontes primárias no suprimento de esqueletos de carbono às células, os aminoácidos podem além da biossíntese de proteínas, servir de substrato para várias outras vias de biossíntese, desempenhando papéis cruciais durante os processos de sinalização, bem como na resposta ao estresse da planta (HILDEBRANDT et al., 2015). É estimado que aproximadamente 90% da biomassa vegetal é transportada na forma de açúcares e aminoácidos, via floema, desde os órgãos fonte até os drenos fisiológicos (LALONDE et al., 2003; LOHAUS; MOELLERS, 2000; WINTER; LOHAUS; HELDT, 1992), evidenciando a importância destes compostos no metabolismo desses organismos.

A variação dos metabólitos envolvidos nas vias de síntese e degradação dos aminoácidos alanina, glutamato e aspartato, por meio da seleção de metabólitos conservados em ambas as variedades evidenciam alterações no metabolismo primário dos órgãos analisados, de modo semelhante ao observado em plantas quando sob estresse biótico ou abiótico (FRAIRE-VELÁZQUEZ, 2013; SEIFI et al., 2013; ZHOU et al., 2015), situação a qual as plantas do presente estudo foram submetidas quando da remoção do meristema apical. Em condições de estresse, as plantas reagem em múltiplos níveis de resposta, dentre eles a alteração do ciclo celular e taxa de divisão celular por ajuste metabólico (ATKINSON; URWIN, 2012), podendo esse ser um dos principais mecanismos envolvidos na quebra da dormência e posterior desenvolvimento das gemas axilares. Além disso, como já mencionado, o glutamato ocupa um papel central no metabolismo de nitrogênio, e é substrato para síntese de aspartato e glutamina

(FORDE; LEA, 2007), todos identificados como metabólitos padrão no processo de desenvolvimento das gemas axilares, reforçando o pressuposto que o metabolismo de nitrogênio é tão importante quanto a partição de carbono neste processo, em especial, durante o desenvolvimento inicial de tais estruturas.

O glutamato parece estar também diretamente associado ao desenvolvimento de meristemas axilares. Foi relatado efeito da aplicação externa de glutamato no crescimento e desenvolvimento de raízes de *Arabidopsis thaliana.* Raízes expostas a glutamato, mesmo em baixas concentrações, apresentaram acentuada inibição do crescimento da raiz primária com consequente aumento do crescimento de raízes secundárias. Este efeito na arquitetura das raízes resultou da inibição da atividade meristemática na ponta da raiz primária (WALCH-LIU et al., 2006). Os resultados observados no presente trabalho corroboram com as observações citadas, uma vez que os níveis deste metabólito para a variedade RB975375 foram maiores em gemas da porção basal do colmo em relação à porção superior, nas duas condições testadas, com e sem efeito da dominância apical, ou seja, seus níveis foram naturalmente maiores nas posições onde é observado menor taxa de brotação das gemas. Adicionalmente, quando contrastadas às variedades testadas, os níveis de glutamato foram estatisticamente maiores em gemas do terço médio superior na variedade com baixa brotação, RB72454, em ambas as condições testadas, sendo mais abundante também em gemas basais das plantas decapitadas. Observa-se ainda, embora não seja estatisticamente significante, decréscimo desse mesmo metabólito em gemas do terço médio superior e basal de ambas as variedades após a quebra da dominância apical, decorrente provavelmente da sua metabolização para suprir a demanda de nitrogênio no desenvolvimento inicial dessas estruturas.

Além dos aminoácidos mencionados, a fenilalanina é acumulada nas gemas analisadas, sendo este composto relacionado ao metabolismo de fenilpropanoides e biossíntese de lignina, importante na formação da parede celular (ISHIHARA et al., 2008). O padrão da fenilalanina corrobora em partes com a discriminação das variedades pelo triptofano, sendo ambos os compostos produzidos pela mesma via em comum, a do chiquimato (ISHIHARA et al., 2008). Interessantemente, na variedade RB975375, a fenilalanina aumenta em relação as gemas basais, o que pode indicar o redirecionamento da planta para disponibilização de energia e carbono, ou simplesmente o aumento na produção de compostos fenólicos em reação ao estresse causado pela decapitação (BERNARDS; LEWIS, 1998; ISHIHARA et al., 2008). Esta última hipótese explicaria também o padrão similar do ácido graxo tetradecanoato. A formação de compostos fenólicos em plantas envolve não somente derivados de fenilalanina como também pontes de glicerol de ácidos graxos oxidados (BERNARDS; LEWIS, 1998; GRAÇA; SANTOS, 2006). Desse modo, a fenilalanina desempenha papéis importantes nos sistemas de defesa química e física das plantas em resposta a condições de estresse.

O triptofano, relatado principalmente na via de síntese da auxina em plantas (FORDE; LEA, 2007; HILDEBRANDT et al., 2015; RADWANSKI; LAST, 1995), interessantemente foi discriminante para a variedade com menor taxa de brotação como já citado. Sua maior abundância nas gemas desta variedade pode estar associada ao processo de dominância apical e dormência desses órgãos, entretanto, este hormônio não é transcolado até para dentro das gemas (BOOKER; CHATFIELD; LEYSER, 2003; SHIMIZU-SATO; TANAKA; MORI, 2008). Assim, é possível que a presença deste aminoácido esteja relacionada ao início da quebra do estado de dormência desses órgãos, uma vez que para seu desenvolvimento, as gemas axilares precisam sintetizar e estabelecer seu próprio transporte de auxina (DOMAGALSKA; LEYSER, 2011), indicando diferenças na velocidade de resposta entre as variedades, em função da quebra da dominância apical.

Em conjunto, o comportamento dos aminoácidos sugere que estes podem estar envolvidos tanto na regulação do desenvolvimento de gemas axilares quanto no metabolismo energético desses órgãos, sendo esta última hipótese a mais provável.

5.4.3 Ácidos orgânicos e poliaminas no desenvolvimento de gemas axilares

A via do ácido tricarboxílico, ou TCA, também identificada nas amostras analisadas, pode ser complementar a via já discutida no metabolismo das gemas axilares. O ciclo do TCA em plantas é composto por um conjunto de oito enzimas que oxidam principalmente o piruvato e o malato (MILLAR et al., 2011). Este ciclo, exerce papel fundamental no metabolismo energético das plantas, agindo na metabolização do carbono presente nas mitocôndrias das células (MILLAR et al., 2011).

Em linha com o exposto, o piruvato foi significativamente diferente entre as posições das gemas na RB72454 após a decapitação, que por sua vez são superiores a RB975375 na mesma condição. Embora piruvato não tenha apresentado diferenças significativas dentro das variedades quando comparadas as condições com e sem dominância apical, a variação deste composto entre as variedades após a decapitação é indicativo da diferença na velocidade de resposta destas em relação ao estimulo a brotação. Piruvato está diretamente relacionado ao catabolismo celular por meio de sua descarboxilação pela enzima piruvato desidrogenase, e formação de Acetil-CoA, inicializando a via do TCA (CENTENO et al., 2011; TOVAR-MENDEZ; MIERNYK; RANDALL, 2003). Ao contrário do piruvato, o malato apresentou maior abundância significativa em gemas da variedade RB975375, antes da decapitação das plantas, e de maneira uniforme entre as posições do colmo. A maior disponibilidade de malato em gemas dessa variedade é coerente com a maior disponibilidade de glicose na mesma, especialmente em gemas do topo. Malato apresenta forte correlação com as concentrações de amido celular, e foi demonstrado que este foi mecanisticamente ligado a uma alteração do estado redox da ADP-glucose pirofosforilase (AGPase) (CENTENO et al., 2011; SARIPALLI; GUPTA, 2015). Assim como o amido, o malato pode servir como composto de reserva e utilizado como fonte de carbono para promover o crescimento vegetal. Esses resultados corroboram com o pressuposto quanto as diferenças genotípicas na partição de carbono celular durante o processo de desenvolvimento inicial das gemas axilares em cana-de-açúcar.

Além desses compostos, é observado o acúmulo de cis-Aconitato em ambas as variedades após a decapitação das plantas. Este metabólito é derivado do ciclo do TCA, resultante da conversão do citrato para isocitrato pela enzima aconitase (IGAMBERDIEV; EPRINTSEV, 2016), evidenciando o enriquecimento das vias envolvidas na fosforliaçào oxidativa durante o desenvolvimento inicial das gemas. As alterações nos níveis de compostos associados ao metabolismo da alanina, glutamato e aspartato indicam o fornecimento de fontes de carbono e nitrogênio ao ciclo do TCA para a produção de energia. Comportamento semelhante foi observado para o pipecolato, embora esse resultado deva-se provavelmente a reação das plantas ao estresse decorrente da decapitação, e não ao processo de brotação das gemas axilares, uma vez que este composto tem sido relacionado à resposta ao estresse em plantas (BERNSDORFF et al., 2016; NÁVAROVÁ et al., 2012). Não obstante, é relatado que sob tais condições ocorra o acúmulo de compostos fenólicos, sendo estes sintetizados a partir de ácidos graxos oxidados (BERNARDS; LEWIS, 1998; GRAÇA; SANTOS, 2006), como é o caso do tetradecanoato, composto consumido nas duas variedades.

Ao lado dos compostos discutidos, as poliaminas (putrescina, espermidina e espermina) são um grupo de compostos naturais semelhantes a fito-hormônios, presentes em quase todos os organismos vivos, incluindo plantas (GILL; TUTEJA, 2010). Dentre as poliaminas, a espermidina apresentou enriquecimento de sua via em ambas as variedades após a decapitação, sendo que a variação da putrescina é provavelmente resultado da relação de substrato e produto entres esses dois compostos. Em plantas, as poliaminas têm sido relacionadas em processos como crescimento e desenvolvimento celular, além de desempenhar papel nas respostas de estresse abiótico e biótico (CUI et al., 2010; GILL; TUTEJA, 2010; TAKAHASHI; KAKEHI, 2010) Foi reportado em estudo com bulbos de *Polianthes tuberosa*, alterações nos níveis endógenos de putrescina e espermidina durante os períodos de dormência destes órgãos (SOOD; NAGAR, 2005). Os autores verificaram altos níveis de putrescina e baixos níveis de espermidina associados durante os estágios iniciais de dormência, e quando na quebra desta, altos níveis de espermidina. Adicionalmente, foi demonstrado que o desenvolvimento dos embriões em sementes de *Arabidopsis,* não progride da fase de torpedo em plantas mutantes nos genes *spds1-1e spds2-1* (espermidina sintase), fornecendo evidência genética do papel da espermidina no desenvolvimento embrionário de plantas (IMAI et al., 2004). Embora tenha sido observado o incremento de espermidina em ambas as variedades em função da quebra da dominância apical, quando comparadas, os níveis de espermidina foi maior nas gemas da variedade com baixa taxa de brotação, a RB72454. Esse efeito, entretanto, pode ser simplesmente devido a já comentada diferença metabólica entre as variedades após a decapitação, resultando em diferentes estados de manutenção e quebra de dormência das gemas. Além disso, a putrescina é mais abundante em gemas da RB975375, ao contrário da sacarose, menos abundante nessa variedade, corroborando com o padrão de correlação apresentado no capítulo anterior, o qual demonstra correlação negativa entre esses compostos, suportando a hipótese da maior abundância de espermidina na RB72454, ser decorrente do estádio fisiológico diferente entre os genótipos.

5.5 Conclusão

Os resultados apresentados pelo presente estudo demonstram a alta interação das vias metabólicas envolvidas no mecanismo de quebra da dormência e desenvolvimento inicial das gemas axilares. Sugerem ainda que essas vias metabólicas podem ser flexíveis e com capacidade de fornecer mecanismos compensatórios em resposta ao estimulo de crescimento. É possível concluir que as vias relacionadas ao metabolismo energético, partição de carbono e nitrogênio estão diretamente relacionadas ao desenvolvimento da cana-de-açúcar, e que alguns aminoácidos como o glutamato, e açúcares como sacarose, frutose e glicose podem ser indicadores da eficiência de brotação dessas vias. Por fim, a variação dos níveis de espermidina sugere este composto como um possível regulador na quebra da dormência de gemas axilares.

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7. Apêndices

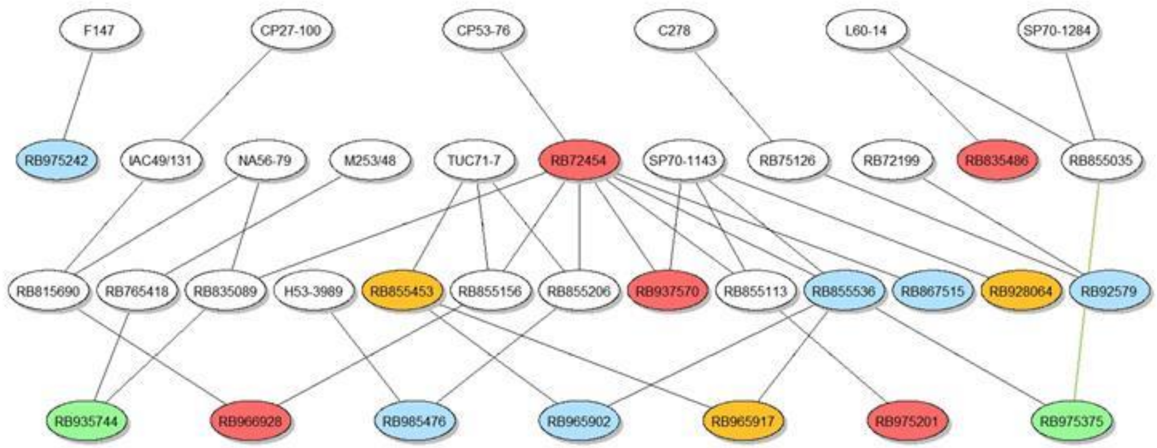

Figure S1. Pedigree of the sixteen selected sugarcane genotypes and their corresponding parentals. Grey circles represent parental genotypes that were not evaluated in this study; red, orange, blue and green circles are genotypes ranked as low, intermediate-low, intermediate-high and high sprouting, respectively. The arrows connecting genotypes are in the same color as their respective relatedness.

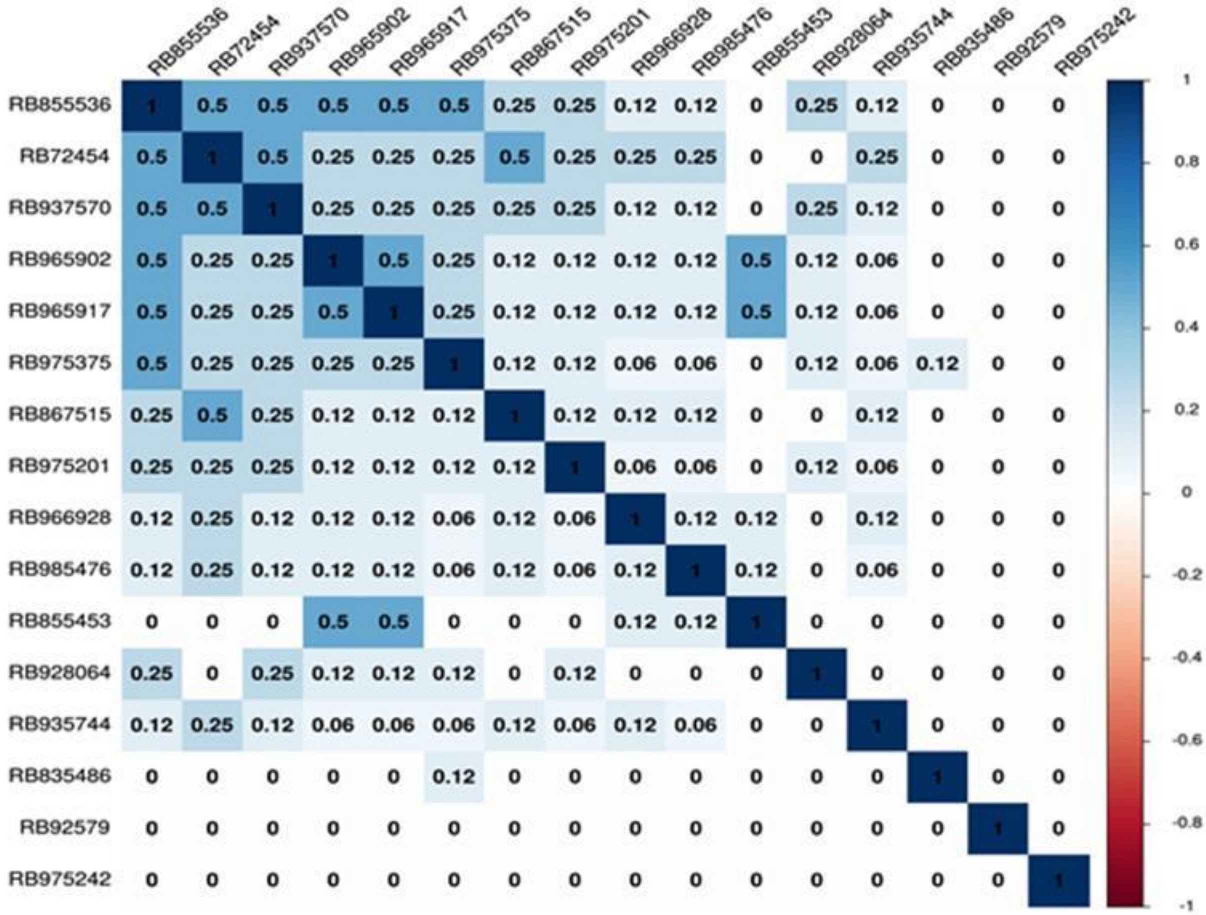

Figure S2. Numerator relationship matrix among selected sugarcane commercial cultivars. The colors indicate the grade of relationship from low (red) to high (blue).

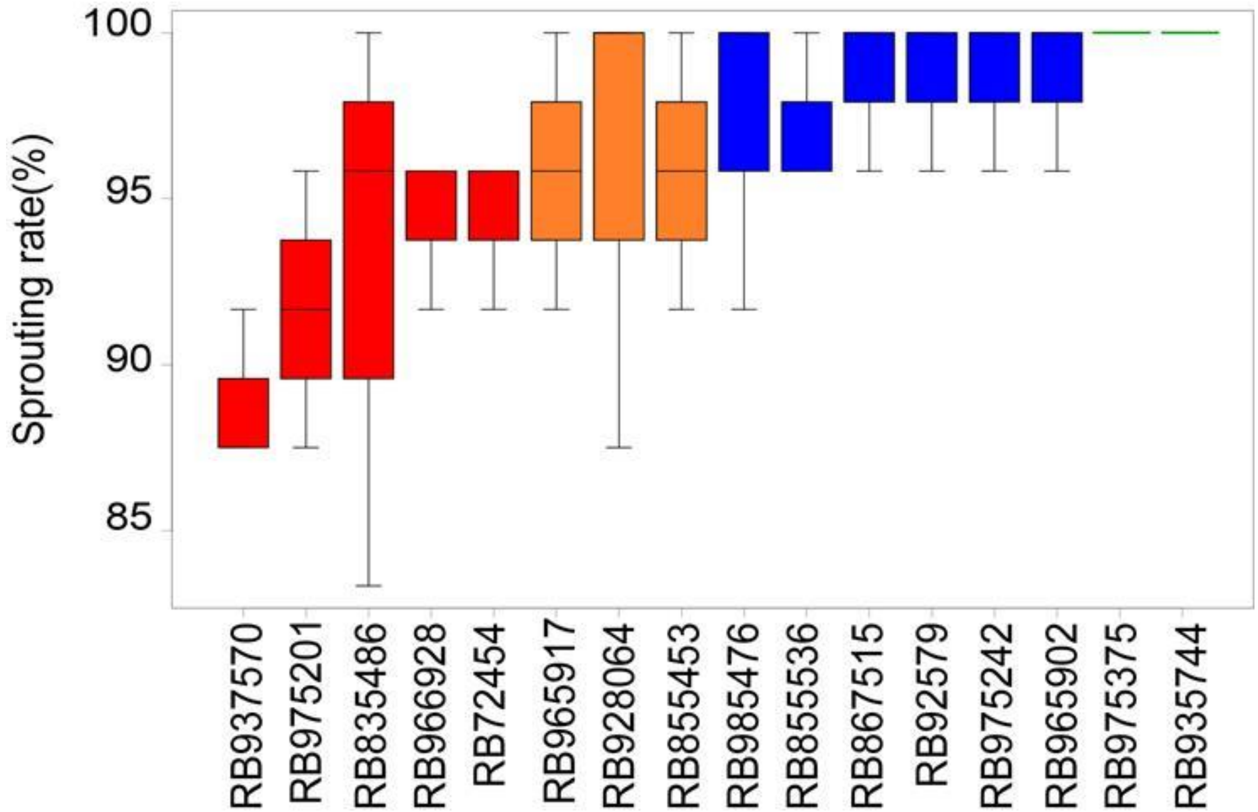

Figure S3. Box plots of sprouting index of the sixteen selected sugarcane genotypes. For comparison among cultivars, the sprouting average considering the quartile analysis to classify them as low, intermediate-low, intermediate-high and high sprouting was plotted. The groups are displayed in red, orange, blue and green, respectively.

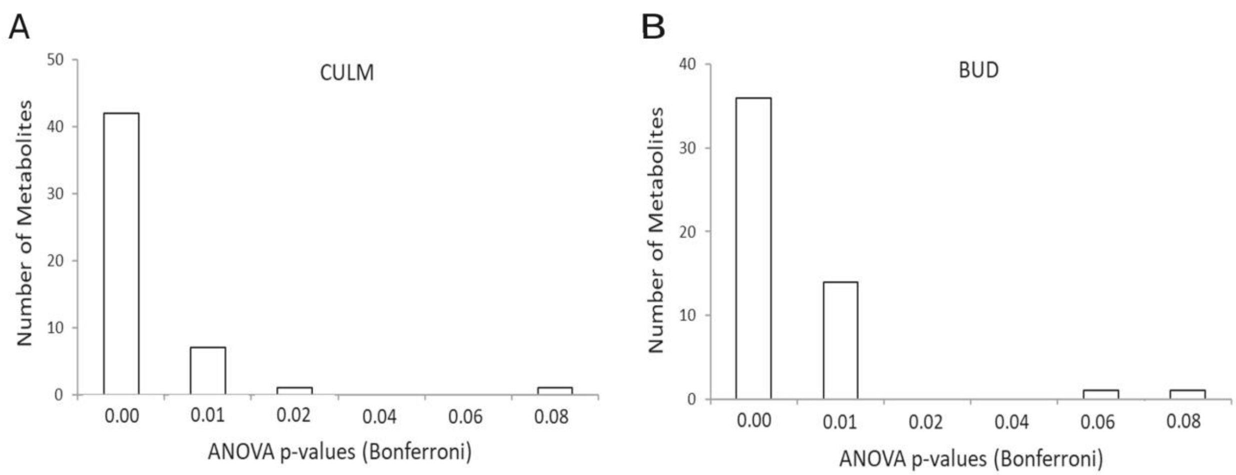

Figure S4. Effect of genotypes on the levels of individual metabolites. Histograms show the number of metabolites whose levels changed according to the significance indicated by P-values. Bonferroni-corrected ANOVA was used to evaluate the effects of genotypes on culm (A) and bud (B).

Supplementary Table 1. Summary of the selected sugarcane genotypes and classification of their agronomical traits.

Variety	ID	Parents[1]	Tillering (First/Second Ratoon)[1]	Sprouting Index (Min - Max %)[2]	POL%*[1]	Flowering[1]
RB937570	1	RB72454 x SP70-1143	Medium/High	87.5 – 91.7	14.5	Frequent
RB975201	2	RB855113 x ?	High/High	87.5 – 91.7	15.9	Rare
RB835486	3	L60-14 x ?	Low/Medium	83.3 - 100	17.2	Eventual
RB966928	4	RB855156 x RB815690	High/High	91.7 – 95.8	16.4	Eventual
RB72454	5	CP53-76 x ?	Medium/Medium	91.7 – 95.8	15.4	Eventual
RB965917	6	RB855453 x RB855536	High/High	91.7 – 100	15.8	Rare
RB928064	7	SP70-1143 x ?	Medium/High	87.5 – 100	15.0	Rare
RB855453	8	TUC71-7 x ?	Medium/Medium	91.7 – 100	16.0	Frequent
RB985476	9	H53-3989 x RB855206	High/High	91.7 – 100	15.5	Eventual
RB855536	10	SP70-1143 x RB72454	Medium/High	95.6 - 100	15.9	Absent
RB867515	11	RB72454 x ?	Medium/Medium	95.6 - 100	15.4	Eventual
RB92579	12	RB75126 x RB72199	High/High	95.6 - 100	15.0	Eventual
RB975242	13	F147 x ?	Medium/High	95.6 - 100	14.5	Absent
RB965902	14	RB855536 x RB855453	High/High	95.6 - 100	15.8	Absent
RB975375	15	RB855035 x RB855536	High/High	100 - 100	16.0	Low
RB935744	16	RB835089 x RB765418	Medium/Medium	100 – 100	14.5	Rare

Genotypes are coded from 1 to 16 and ranked as low (red), median-low (orange), intermediate-high (blue) and high sprouting (green) ability.

* POL: percentage by weight of apparent sucrose;
[1] Data obtained from RIDESA breeding program (Carneiro, personal communication)
[2] Data obtained from greenhouse experiments performed in this study

Supplementary Table 2. Levels of all detected metabolites in culm of the selected sugarcane cultivars

Genotypes	Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Histidine	Isoleucine	Leucine	Lysine	Methionine	Ornithine	Phenylalanine	Serine
	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C18
RB937570	13.29804	4.054864	6.350087	12.90644	6.797646	11.12881	11.30654	11.23289	9.823106	2.111218	8.914593	8.95398	6.243917	6.400369	8.555299	4.433628	10.44514
RB937570	12.44747	3.963227	6.370634	12.51277	6.306501	10.63227	10.83686	11.46889	9.336851	2.282985	8.968803	9.148624	6.708999	6.783	8.991439	4.125069	9.974987
RB937570	12.604	4.37617	6.32954	12.78243	6.21147	10.69127	11.07965	10.99688	8.439357	2.197102	8.199684	8.550872	6.835031	6.324386	8.11916	4.742188	9.916269
RB975201	13.75459	6.491674	8.307751	12.22911	7.173114	10.40256	11.18624	11.57043	10.78322	5.348763	10.02342	9.90159	8.748621	7.944771	12.24817	5.722745	11.177
RB975201	14.08996	6.150858	8.879476	12.18562	6.956413	10.67338	11.21801	12.29239	10.50926	5.204315	9.103417	9.169172	8.744543	7.619848	11.69069	5.626384	11.24342
RB975201	13.72115	6.941636	8.775791	12.408	7.300119	10.89383	11.16668	11.79626	11.21759	5.599588	10.36323	10.24938	8.538749	8.657141	12.05165	5.674565	11.39596
RB975201	13.43488	6.382529	9.140146	12.15377	6.732862	10.89383	11.05741	12.35015	10.5524	5.749616	9.591879	9.431367	8.996577	7.940561	12.2161	5.674565	11.09071
RB835486	13.86139	5.59554	9.520438	12.49716	6.750013	10.51519	11.11356	12.86213	10.84525	4.908227	9.124067	9.166986	8.71024	7.365143	13.05461	5.640505	11.13994
RB835486	12.90617	5.989824	7.84162	12.0824	5.921735	10.32183	11.15411	11.42082	9.873059	2.810946	10.47374	10.34116	8.695159	7.690542	10.46423	5.48859	10.56457
RB835486	13.17448	6.674439	8.251327	12.3553	5.886591	10.74192	10.95187	11.80118	11.00705	5.566239	10.60472	10.61133	9.37474	8.040868	11.16586	5.966005	11.34775
RB835486	13.86728	6.644636	9.520005	12.84144	6.441901	11.05237	11.5597	11.95774	10.37957	4.626609	10.40881	10.30345	9.180373	8.321552	12.15802	5.802806	11.09589
RB835486	14.22522	6.33198	10.21923	12.82209	6.93584	11.48367	11.95961	12.99264	10.52535	5.221024	9.741551	9.680755	8.844913	8.02934	13.16087	5.30462	11.2623
RB966928	14.90572	5.453405	8.585472	13.23897	6.791242	11.35621	11.22716	6.035672	10.7316	10.49898	8.794711	4.917055	11.1599	14.58115	9.557531	7.782044	9.155014
RB966928	14.43025	5.359232	9.273813	13.60912	6.622569	10.656	10.78958	6.655727	10.14457	9.526277	8.458749	4.600479	11.80907	13.67781	8.158984	7.853933	8.702711
RB966928	14.13015	5.011179	9.37137	13.36897	6.714022	11.25394	10.3211	6.672842	10.01932	9.324906	8.38436	4.741437	11.34305	12.98638	9.426107	8.092341	8.320911
RB966928	14.25224	5.989804	8.190935	13.47542	6.839626	11.52274	10.62661	6.198753	10.33667	9.742695	8.90104	4.706776	10.21138	12.88378	10.10617	7.834282	8.65855
RB72454	12.35068	5.256096	9.463404	12.47181	6.22435	10.2494	10.7281	12.85382	10.16101	4.447325	9.053653	8.957861	8.224428	7.881725	13.01888	5.575591	10.08444
RB72454	12.36773	6.101388	10.23685	12.51729	6.590044	10.57341	11.30241	12.59859	10.24811	6.096844	9.984621	9.913873	8.5631	8.766238	13.69907	6.095073	10.44213
RB72454	12.82121	6.104971	9.938467	12.77459	7.062431	10.58266	10.68699	13.38196	10.41232	6.056954	10.26758	10.15569	9.197288	8.935641	13.13023	6.14229	10.95459
RB72454	12.41274	5.935054	9.505796	12.55137	6.431951	10.51002	10.91862	12.34582	10.14919	5.711225	10.70402	10.88695	9.370182	8.980084	11.93106	5.969737	10.60932
RB72454	12.08903	6.277762	9.905315	12.02806	6.751499	10.415	10.55498	12.61872	10.43957	5.582238	10.42172	10.29699	9.073935	8.631953	12.87919	5.922849	10.40332
RB965917	14.08504	6.698912	11.51112	13.99971	6.850451	11.33162	11.30246	14.23505	9.934466	4.803658	10.73105	10.6193	9.634215	9.598654	13.86971	6.550157	11.52506
RB965917	13.56418	6.18505	11.32439	12.91856	6.452181	11.42818	10.52832	13.60371	10.45976	5.556465	9.584939	9.783277	8.998566	8.945496	13.53263	5.427982	11.05748
RB965917	13.17076	6.28929	8.657286	12.76419	5.822595	10.98435	10.45648	13.53936	10.69087	1.960429	10.40486	10.25	9.012976	8.409627	12.24817	5.950167	11.09131
RB965917	13.75272	7.084468	11.67283	13.2725	6.885226	11.19296	10.87536	14.17775	10.7749	4.803658	10.82874	10.85135	9.515637	9.157735	14.00544	6.793465	11.44548
RB965917	13.69566	7.236838	12.25364	13.32222	6.763643	11.02447	11.60748	14.55625	10.57431	6.894081	10.22828	10.2531	9.361174	9.262906	14.10681	6.180443	11.51755
RB928064	13.70861	5.526426	8.382783	12.3455	6.49488	11.37534	11.01498	12.58196	10.17869	5.287899	10.36534	10.29181	8.610495	8.060634	11.32641	5.398844	11.13384
RB928064	14.44963	6.383794	9.404588	13.03983	7.577808	12.04269	11.53166	13.13407	10.80759	6.296401	10.62703	10.59018	9.423767	8.706592	12.08756	6.212782	11.94985
RB928064	14.5727	6.072232	9.202342	14.14445	7.107573	12.17936	10.63228	12.87626	10.92237	6.471021	10.56544	10.39978	8.847722	8.68774	13.05102	6.365202	12.26589
RB928064	13.93407	6.582667	9.819655	12.82209	6.933926	11.98603	10.97663	12.92064	10.65644	6.459756	10.20761	10.0546	8.89106	8.497507	13.22124	6.378296	11.5826
RB928064	14.14915	6.179358	9.202342	13.43126	7.260394	12.42379	10.75852	12.97504	10.47886	6.96693	11.49338	10.33409	9.129923	9.48759	13.38422	6.803631	12.06516
RB855453	13.54249	7.047791	8.86984	13.79651	6.538667	10.84946	11.48255	12.32139	10.53957	5.556465	9.527427	9.452097	8.739747	7.619973	12.31778	5.406412	11.2346
RB855453	13.73401	7.087778	10.00105	13.48833	7.021753	10.85903	11.15523	14.02919	10.56213	6.677661	10.80068	10.26795	8.51836	8.672251	12.69115	6.286272	11.25591
RB855453	13.59386	6.696985	9.351541	13.10965	7.026412	10.87775	11.32898	12.93627	10.23742	6.715657	11.03042	10.8122	8.748621	8.206598	12.05397	5.787213	10.81378
RB855453	13.57653	6.288303	9.717657	13.15349	6.918658	10.88249	11.37523	13.8004	10.61097	6.531551	10.02418	9.742519	8.048944	8.549413	13.47012	5.965243	11.16018
RB855453	13.77004	7.031342	10.6482	13.99888	7.190589	10.88033	11.80199	13.04543	10.51519	6.623924	10.53582	10.46701	8.721045	8.727034	13.12351	6.381075	11.35029

Genotypes	Threonine	Tryptophar	Tyrosine	Valine	-Oxoprolin	Putrescine	Fumarate	s-Aconitat	Citrate	Isocitrate	Succinate	Benzoate	-Coumarat	droxybenz	ydroascorb	ffeoylqui	alacturona
	C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C30	C31	C34	C35	C36	C37	C38
RB937570	7.931255	6.098567	7.440997	10.75206	8.361413	6.992132	5.308226	13.99063	10.72651	9.276041	8.211448	6.928217	6.418771	5.927832	7.046738	5.695649	5.676334
RB937570	7.399736	6.122294	7.524369	10.47052	7.943232	6.875375	5.228168	14.43048	11.05828	8.999438	7.864894	7.405109	5.930731	5.680271	7.246564	8.280898	5.517013
RB937570	7.109476	6.110431	8.07936	10.01135	8.108855	7.124856	5.629966	14.68005	11.85078	8.595004	8.085328	7.050193	6.309859	5.568988	7.53685	8.144568	5.585761
RB975201	8.797391	7.545151	7.998041	12.06126	8.205042	10.37688	5.416808	9.517427	9.538498	8.64418	7.714334	6.703862	6.241263	5.623252	4.417313	5.488264	5.174079
RB975201	8.584504	6.19496	7.995993	11.20393	8.244043	9.005637	4.895482	11.3999	9.98427	9.519126	7.640107	6.854023	5.947041	5.357483	4.392874	5.12132	5.214749
RB975201	9.357681	6.715847	8.250615	12.37083	8.18171	10.05902	5.193264	10.32011	9.695629	8.77067	7.699272	7.218461	5.834564	5.671173	4.13023	4.136742	4.723053
RB975201	8.691777	6.407429	8.006701	11.81732	8.144277	10.25037	4.669687	10.72591	9.564119	9.598927	7.092649	6.628033	5.659901	4.833531	4.63108	5.257843	5.399549
RB835486	8.412493	7.730704	7.535336	11.0741	8.176684	7.301374	5.2957	11.27076	10.05206	9.908005	8.103047	7.265679	6.592816	5.896475	4.440972	4.290557	5.282968
RB835486	8.429837	7.419632	8.377934	11.71003	8.171175	8.617905	4.839394	13.60782	10.65181	9.54297	7.707182	6.827477	5.63423	4.341901	6.651351	4.513478	5.612931
RB835486	8.885719	7.559559	8.802886	11.95545	7.976797	7.71833	5.076188	13.41722	11.11247	9.086441	7.434694	6.481792	5.897404	4.524697	6.253049	4.513478	5.525679
RB835486	8.655007	7.559559	8.538065	11.97164	8.557425	7.945328	5.551451	13.37806	11.18454	9.224376	7.57176	7.110235	6.127654	5.532966	5.892696	4.783523	5.746903
RB835486	8.686607	7.528341	7.819742	11.76471	8.22052	8.495373	5.398259	10.92978	11.01925	9.953058	7.897722	7.24781	6.063026	5.56076	6.225411	4.466355	5.896173
RB966928	6.408969	NA	NA	NA	8.767116	14.3169	5.826666	12.00185	10.26056	7.675311	6.978595	11.71999	5.686453	5.077052	5.364553	6.748111	12.87381
RB966928	7.249171	NA	NA	NA	8.384464	14.8302	6.265325	12.09333	9.510354	7.637743	6.729378	11.75545	6.191356	5.344386	5.443614	5.207052	12.351
RB966928	6.879278	NA	NA	NA	8.335679	15.10916	6.600376	11.55238	9.865928	7.213426	7.252245	11.78125	6.467557	5.284076	5.672149	6.406675	12.00318
RB966928	6.979694	NA	NA	NA	8.394484	14.54107	6.368935	11.78969	10.09457	8.174764	6.954161	11.73941	5.838168	5.43079	5.390112	7.114331	11.84767
RB72454	7.877625	6.473008	7.718432	11.13046	7.831985	7.593148	5.286377	11.98143	11.65012	9.688777	8.133757	7.034458	6.128216	5.780252	6.799287	5.468885	6.092606
RB72454	8.575153	8.065233	8.538241	11.8872	8.405245	8.031296	5.265235	11.81344	11.26207	9.582501	7.826789	7.214693	6.097134	5.443411	6.314671	5.1123	5.980013
RB72454	8.983723	8.290124	8.224461	12.03034	7.791225	7.84645	5.171889	11.7461	11.20164	10.25222	7.588149	6.714616	5.552546	5.241637	6.172329	4.942447	5.697877
RB72454	8.857447	8.195715	8.681888	12.12953	7.949904	8.06842	5.16796	11.84699	10.30955	9.406108	7.601894	7.000219	5.914234	5.371948	5.967933	5.165434	4.659971
RB72454	8.742335	8.323577	8.736144	12.0581	7.602478	8.060676	5.434712	12.40233	11.19636	9.724038	7.69717	6.693101	5.930731	5.379809	6.794044	5.138104	5.153727
RB965917	9.651855	8.380735	8.357392	12.75955	8.41887	7.153124	5.202711	13.61093	10.72133	10.4214	7.630346	6.547379	6.329723	5.815307	5.446089	7.12534	5.965545
RB965917	8.980248	7.316679	7.860982	11.7354	7.875001	7.421968	5.566163	13.247	11.08838	10.12462	8.032966	7.038654	6.589885	5.257031	5.521673	7.437767	6.106681
RB965917	9.223211	7.678516	8.044629	12.25676	7.670846	7.640828	4.730653	13.68108	10.27513	10.18237	7.55494	6.838279	5.81063	4.136683	5.620526	7.026798	5.346091
RB965917	9.55141	7.675694	8.377984	12.69771	7.962101	7.508584	5.025065	13.61181	10.83068	10.69736	7.66921	6.658406	6.03381	5.619811	5.498403	7.282329	5.733397
RB965917	9.741197	7.506029	7.964147	12.56076	7.981705	6.919341	5.274281	10.78111	10.72888	10.94791	7.729285	6.814641	6.800205	5.456322	5.521673	5.191695	5.63176
RB928064	8.772806	7.494297	8.017863	11.9275	8.031636	8.029614	4.892336	14.31146	11.47729	9.34823	7.565384	7.272069	5.569412	4.828648	5.996017	3.672263	5.175499
RB928064	9.546712	9.134252	8.381071	12.39354	8.501891	7.98633	4.746225	14.02281	11.89859	9.92552	7.467688	6.51192	5.701289	4.751619	6.077061	3.672263	5.292969
RB928064	9.587572	9.707557	8.43133	12.08063	7.758118	7.287473	4.963191	15.13314	11.27508	9.194034	7.766214	7.075115	6.124083	5.00385	6.0292	3.320622	5.656217
RB928064	9.301952	8.550296	8.597847	11.76884	8.010745	8.191732	5.249025	13.72011	11.28126	9.764647	7.642622	6.315294	6.218081	4.990612	6.014522	3.895543	5.298307
RB928064	9.787371	8.721601	8.485829	12.8673	7.920413	8.121434	5.156021	13.6841	11.24035	9.528631	7.690826	6.827477	6.394294	5.444523	6.0292	3.800624	5.423385
RB855453	8.562027	7.279603	8.335071	11.28767	8.485971	7.538527	5.065541	15.16766	11.77707	9.3651	7.664238	6.731802	5.537288	5.250267	5.259814	8.512563	5.910308
RB855453	9.493277	8.094224	8.845592	12.70224	8.170138	7.844554	5.050904	14.07828	11.82051	10.37493	7.837468	6.901515	6.253008	5.17796	5.259814	7.946665	5.947763
RB855453	8.789826	8.180716	8.478251	12.65759	8.358626	7.406486	5.169926	14.19622	11.3414	9.16874	7.7632	7.257623	6.11499	5.557845	5.064203	8.374065	5.577184
RB855453	9.221306	8.258317	8.308774	12.04797	8.396488	7.531868	4.975795	13.6538	11.74899	10.04527	7.667594	6.674398	5.773364	5.617787	4.776191	7.370049	5.37777
RB855453	9.154848	8.675888	8.40347	12.39272	8.890117	7.580359	5.065541	13.33611	11.79976	9.54416	7.883499	6.942238	6.473787	5.577862	5.939047	7.79033	5.811834

Genotypes	Glucarate	Glycerate	lar to Itaco	Nicotinate	Quinate	Xylose	Fructose	Glucose	Sucrose	Glycerol	Galactinol	hyo-Inosito	Xylitol	Adenine	ptadecano	tradecano	droxypyrid
	C39	C40	C41	C43	C44	C46	C49	C50	C53	C55	C56	C57	C58	C61	C62	C63	C64
RB937570	4.630726	5.939104	5.488438	5.060205	9.926007	9.07791	9.617341	13.41701	14.92981	11.37007	10.48469	11.17828	7.797493	5.573494	6.180174	6.827149	8.912629
RB937570	4.265471	5.903579	6.988555	5.016736	11.16364	9.019278	11.01159	14.11014	13.82426	11.06065	10.78464	11.71211	6.394719	5.618937	6.175094	7.553654	8.726171
RB937570	4.701	5.387168	6.391372	5.05659	10.72303	9.048594	11.11991	13.93928	14.36033	10.75123	10.48469	12.61519	7.096106	6.010948	6.185253	7.812604	9.032214
RB975201	4.808043	5.75091	4.830696	4.711048	8.976857	9.609848	12.5317	14.31169	13.56111	10.75123	12.10525	12.63839	8.494012	5.058061	6.538844	8.882319	8.582788
RB975201	5.214096	5.605067	4.658041	4.824734	8.558886	9.052084	11.41106	14.48347	13.01378	12.78986	11.95904	12.47585	9.163687	5.435236	6.318028	8.6616	8.272664
RB975201	4.559837	5.485641	4.685856	4.65092	8.685669	9.532146	12.61402	13.93677	13.89244	10.98293	11.43255	12.10943	7.84111	4.839939	6.23068	8.826246	8.435056
RB975201	5.394907	5.100946	4.45757	3.96298	8.521265	8.966308	11.80025	14.62397	13.63574	11.508	10.88665	12.87413	8.477239	4.918435	6.320736	8.934818	7.82418
RB835486	5.121627	5.151714	5.463303	4.320472	9.501573	9.042046	9.838993	14.2929	13.33336	10.69327	10.25817	10.9666	7.170336	5.151899	6.200693	7.883806	8.945693
RB835486	4.89616	5.695646	5.677804	3.710932	9.501573	9.557061	10.50301	14.93908	13.58224	9.117249	10.43284	11.69623	7.000241	5.045442	5.841263	8.634938	8.505672
RB835486	5.316931	5.686197	5.319269	4.152565	9.93393	9.119802	10.92946	14.45286	13.98964	10.34462	9.960999	11.29087	7.085288	4.876642	5.890792	8.183495	8.17145
RB835486	5.498267	5.514243	5.794296	4.769865	9.86611	9.064468	10.96076	14.67924	14.68834	10.85208	9.488459	11.93278	6.913002	5.107881	6.051319	8.449636	8.506786
RB835486	5.242814	5.435002	5.061844	4.648526	8.704679	9.370202	10.28284	14.09933	14.61636	10.71589	11.15037	11.28163	6.396143	5.14393	5.996017	7.935146	8.692962
RB966928	5.738418	4.770596	10.93511	6.82873	8.56696	8.668984	5.242814	10.81335	8.43883	9.179446	11.75086	6.302294	NA	5.842482	7.025251	12.67787	8.411136
RB966928	5.55323	4.332357	10.78381	6.800008	6.647861	7.44769	5.334983	9.330093	8.318554	8.708821	11.37445	6.111256	NA	5.936128	6.008187	12.07393	8.482335
RB966928	5.511219	5.088289	11.14556	6.988617	6.418782	8.010217	5.308731	9.428268	8.224471	8.392625	11.33178	6.048907	NA	5.982473	6.91458	11.96101	8.811831
RB966928	5.55337	4.891143	11.04317	7.488687	7.415929	9.068134	4.856261	9.857237	8.377984	8.531332	11.36256	6.018221	NA	5.770865	6.846603	12.16352	8.435056
RB72454	5.353344	4.972431	6.008367	5.118006	9.679134	8.891531	10.71553	14.35466	14.74224	10.94085	11.15834	11.35806	7.991836	4.865114	6.287643	7.719644	8.817393
RB72454	5.500312	5.443454	4.838745	4.675087	10.81047	9.338008	12.00311	14.82153	14.6672	10.82746	10.23053	11.75574	8.356057	5.296571	6.010797	8.13231	8.837744
RB72454	5.250652	5.034169	5.643799	4.462184	9.700506	8.716075	10.44542	14.07441	14.73487	10.13624	10.07185	11.50285	7.795295	5.20354	6.218081	7.984721	8.228868
RB72454	4.67914	5.027192	5.787142	4.807917	11.41145	9.324365	11.73295	14.01642	14.07285	10.90647	10.73646	11.07104	7.799687	5.65416	5.657493	8.214371	8.502954
RB72454	4.575302	5.365677	5.464379	4.764121	10.72303	9.003324	11.20253	14.90759	14.12938	11.72132	10.84683	11.54452	8.016304	4.774312	6.141152	8.610506	8.679867
RB965917	4.918707	5.209445	5.763848	5.119896	8.904783	8.93111	7.873669	10.03748	14.15727	10.58943	8.393023	12.13283	7.228352	5.502758	7.279592	6.94637	8.165069
RB965917	4.918707	5.800248	5.52454	4.487091	10.72303	9.633095	10.26122	13.51833	14.01816	10.78023	10.3771	12.52878	7.095481	5.739041	7.117417	7.052062	8.54692
RB965917	4.511178	5.603864	5.97133	2.747794	9.885941	9.143386	8.881409	14.04397	14.37474	10.82708	9.406307	11.89656	7.195778	5.267844	6.468226	7.25228	7.996185
RB965917	5.110691	5.373213	5.49727	4.746559	10.79923	9.752652	9.54685	13.22303	14.49444	11.61186	10.01012	12.49812	6.715536	5.278105	6.915461	6.990785	8.303646
RB965917	5.134251	5.143145	4.680369	5.334116	9.116716	9.512587	7.843895	9.637149	14.36018	10.18795	10.81412	12.47195	5.342535	5.159208	7.117706	7.018812	8.321566
RB928064	5.138169	6.137413	6.61315	4.124644	10.32578	8.894508	10.88013	13.71499	13.52634	10.52581	9.66438	12.67043	5.958771	5.443097	6.017549	7.885843	8.286787
RB928064	5.748224	6.512138	6.522395	4.33258	10.40826	8.923639	10.57105	13.42635	13.53578	10.14782	10.26559	12.66005	6.655931	5.983218	5.62607	7.386702	7.953479
RB928064	5.431356	5.850411	6.552747	4.340869	9.082835	8.71691	8.377521	10.34681	14.89854	10.47235	8.021093	12.03424	7.821938	6.501403	6.435005	7.046243	8.31829
RB928064	5.327859	6.331023	6.726481	4.514685	10.77073	9.039825	10.29015	13.8706	13.86617	9.247388	9.666151	12.67429	7.683352	6.337653	6.526105	7.595736	8.192363
RB928064	5.511174	5.85608	6.197201	4.391565	11.04128	8.997674	10.04272	11.98641	14.25084	10.42375	9.708096	11.8811	7.235478	6.325769	6.136279	7.516717	8.443674
RB855453	5.4956	5.902864	5.838571	4.628228	10.63105	9.624414	8.260803	11.23107	14.15488	12.01434	11.06433	11.75233	11.02553	6.197467	5.990272	7.31593	8.304852
RB855453	5.656925	5.484705	6.002481	4.06892	10.12	8.874243	8.722251	12.00782	14.78198	11.02345	11.72513	10.77646	7.704144	5.749198	6.254212	6.591072	8.620204
RB855453	5.401173	5.10269	5.838571	5.117937	8.909501	8.775805	7.548058	10.6156	13.77202	12.22821	11.53273	11.17553	10.5621	6.031455	6.350809	6.775308	8.705344
RB855453	5.242814	5.278927	5.439873	5.022506	9.216512	8.667963	7.618567	10.64247	13.89116	11.85102	11.53273	10.92704	8.133978	5.560824	6.007475	6.814814	8.360469
RB855453	5.780653	5.66876	6.073358	5.222414	9.912461	8.985606	9.154335	11.65838	14.4635	12.13809	11.80874	11.82476	10.33899	6.097935	6.399313	6.812118	8.656181

Genotypes	Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Histidine	Isoleucine	Leucine	Lysine	Methionine	Ornithine	Phenylalanine	Serine
	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C18
RB985476	12.46069	5.534199	7.167266	12.24733	6.279625	14.57687	10.50095	5.57827	10.27164	9.921353	8.321552	3.602487	10.1311	11.01669	9.883105	7.768337	8.714858
RB985476	13.64995	7.609324	8.283444	13.19244	7.06316	14.04571	11.2589	6.536185	10.47963	10.38161	8.926385	4.106976	11.89121	10.18763	10.586	7.320823	8.575301
RB985476	13.31311	6.987525	9.172293	12.86807	6.508577	14.76427	10.99912	6.372186	10.26553	10.25493	8.026225	3.924228	12.40082	10.2941	9.515096	7.815163	8.591047
RB985476	12.59685	7.044376	8.510773	12.01934	5.990315	14.74859	10.29382	6.314093	9.608016	9.192506	7.668281	3.924228	11.61351	9.891528	9.576659	7.884301	8.42
RB985476	13.56519	6.793856	8.283444	13.47117	6.460419	14.04571	11.16089	6.235262	11.2182	11.04327	8.235611	4.063221	13.4194	10.08055	9.854671	7.33358	8.575301
RB855536	12.35718	6.032482	8.448812	11.52671	6.018911	10.36358	10.82635	12.19358	10.33024	4.589734	9.9565	9.959225	7.891537	8.27106	12.30806	NA	10.27473
RB855536	12.69943	6.975373	9.179776	12.2876	6.752983	11.05644	10.4767	11.81762	10.5211	4.576579	10.72481	10.71529	8.412656	8.943164	11.56721	NA	11.04098
RB855536	12.51003	7.279304	9.428841	11.7833	6.496561	10.64879	10.30934	12.41154	10.48631	4.668934	9.880641	9.833336	7.838314	8.589845	12.37616	NA	10.71457
RB855536	12.52454	7.461053	7.626586	12.34262	5.622302	10.52841	10.74873	11.16978	9.631321	4.668934	10.06424	10.05692	8.242451	9.165531	10.64392	NA	10.70393
RB855536	12.52279	6.544026	9.298703	11.83357	6.537417	11.28038	10.82199	11.89813	11.15006	4.840489	9.695022	9.719829	8.674486	8.476845	12.28571	NA	11.07752
RB867515	13.33653	5.529272	9.590449	13.41559	6.777546	11.39638	11.09768	13.52874	10.77747	5.580255	9.850407	9.462192	8.166766	8.191492	12.65215	6.018083	11.12979
RB867515	13.12158	5.453419	8.54712	12.82209	6.377162	10.45331	10.82559	12.13774	10.42455	4.507603	9.475042	9.777848	8.256407	7.419271	11.4785	6.646789	10.7428
RB867515	13.38365	5.567394	9.936131	13.39017	7.102975	11.0435	10.87852	13.15353	10.34615	5.610671	10.57592	10.64101	8.680722	8.694382	12.14447	6.777564	11.0784
RB867515	12.80038	5.658732	9.074522	13.08498	6.2759	10.87261	10.75864	12.59859	9.78707	4.929428	10.07734	10.12937	8.657932	8.152241	11.33424	5.730582	10.90746
RB867515	13.41511	6.084841	10.47071	13.77043	6.751499	10.7949	11.1265	13.00194	10.62768	5.461918	9.221461	9.168375	7.680731	7.926195	13.15698	6.293255	11.17108
RB92579	14.68927	6.477166	9.29921	12.86339	7.09389	11.34082	11.50066	13.49173	10.823	6.478021	10.2366	10.06762	8.73312	7.999741	12.39269	6.056188	11.67181
RB92579	15.80779	6.186613	10.20457	13.82386	7.719476	11.03385	11.605	13.92835	11.83663	6.727362	10.67859	10.0966	8.449835	8.798654	13.35991	6.351678	13.05734
RB92579	15.27283	6.554994	10.96104	13.52102	7.691248	11.92402	11.5566	13.13465	10.88779	6.595907	10.14727	9.885608	9.158796	8.370177	12.85609	5.930327	12.27646
RB92579	15.11504	6.08343	10.46791	13.11152	7.509373	10.89833	11.51911	12.80682	10.9024	6.678969	9.720921	9.056559	8.03607	7.89018	12.84727	6.117946	12.24884
RB975242	12.87128	7.195543	7.903421	11.39717	6.212816	14.68552	10.76835	5.932448	10.22257	10.18252	8.743424	4.382423	11.38448	11.12999	11.45942	7.729285	8.760749
RB975242	13.58556	7.349882	9.226266	12.52584	6.631	14.3883	10.82757	6.13644	10.41016	10.35458	8.891474	4.348931	12.16423	12.19081	10.73556	7.513256	9.112474
RB975242	13.31618	6.715042	9.295741	12.68495	6.738635	14.15163	10.33546	6.149033	10.02936	9.930943	8.408692	4.576124	12.17505	12.10384	11.41007	7.779146	8.713282
RB975242	13.00036	6.628906	8.020404	11.90565	6.579197	14.42288	10.0532	5.946789	10.0244	9.779406	8.271232	4.535961	10.4914	12.10476	11.84888	7.79392	8.639497
RB975242	13.60826	7.42921	8.611458	12.14474	6.80719	14.14853	10.87974	6.408132	10.45513	10.41012	9.150281	4.068678	13.07084	12.20511	11.39902	7.691386	9.091457
RB965902	14.0588	7.996588	9.537197	14.12356	7.751544	10.78041	12.17534	14.81334	10.8522	6.868761	11.0098	10.87689	9.686234	9.555756	12.50037	6.800869	11.5102
RB965902	14.37287	8.842218	11.18112	13.82066	7.850539	11.40899	12.18943	14.47793	11.29144	7.780637	11.24921	11.29018	10.25097	10.14766	13.78199	7.556788	11.83594
RB965902	13.93122	8.664589	10.2765	14.3255	7.41045	10.92351	12.05844	13.93123	10.47135	7.54067	11.23337	11.06537	10.41047	9.921383	12.72726	6.231499	11.64068
RB965902	13.63408	8.526996	11.06561	13.18065	7.644269	10.98971	11.68914	13.5382	10.91936	8.11717	11.04789	10.79176	9.87873	9.586411	13.72909	7.166924	11.35843
RB965902	14.25225	8.608575	10.51511	14.08604	7.931064	10.88138	11.49452	15.10599	10.8912	8.408139	11.64702	11.3736	10.18498	10.60302	13.18468	7.775195	12.12463
RB975375	12.45201	4.72433	5.75448	11.43279	5.875951	14.92429	9.837207	6.444149	9.351631	8.90415	7.272403	4.274654	8.792142	11.99969	10.74099	8.273447	7.9125
RB975375	11.62718	4.552823	6.455727	11.8917	5.408488	14.72044	8.883137	5.956712	8.280388	8.085668	6.695902	4.522972	9.060773	11.78666	10.58787	7.774434	7.027462
RB975375	12.70863	4.42692	5.851764	11.93263	5.770645	13.75512	9.787771	6.353315	9.21224	9.0477	7.327481	4.261089	8.053754	11.14358	11.4354	7.909814	7.829064
RB975375	11.97298	4.384788	6.020657	11.66556	5.88835	15.21022	10.05568	6.042023	9.425867	8.919595	7.196774	4.098027	9.699477	10.33733	10.5199	7.911999	7.815199
RB975375	12.02919	4.522215	6.020657	12.74048	5.909792	14.80668	9.147557	5.765028	9.543067	9.10477	7.45909	4.148705	8.901536	10.45062	10.42078	7.53305	7.810839
RB935744	13.48332	5.369667	9.531308	12.95077	6.764546	14.21349	10.51519	5.439477	9.779675	9.472631	8.063799	5.06533	11.86917	13.34224	11.61952	7.955203	8.868541
RB935744	14.79381	5.756879	10.42415	13.163	6.656149	13.44519	10.67097	5.525728	10.41668	10.57333	8.037539	4.955629	12.77722	13.86442	9.841481	7.946033	9.285512
RB935744	13.94829	5.354787	10.1775	14.1531	6.916288	13.38449	10.4745	5.525728	9.737943	9.561231	8.080879	4.869225	11.45536	13.48646	10.93816	8.040569	8.864435
RB935744	13.56418	5.263736	7.792443	13.08787	6.685186	14.60089	10.61786	5.520205	10.48525	10.12893	7.880711	4.262053	9.985738	12.56838	11.68258	7.78018	8.970576
RB935744	14.49703	5.436267	9.690838	13.85216	6.755542	13.5821	11.07633	5.617502	11.3757	9.934032	8.015732	4.569976	12.27956	13.45989	11.21788	7.445608	8.997266

Genotypes	Threonine	ryptophar	Tyrosine	Valine	-Oxoprolin	Putrescine	Fumarate	s-Aconitat	Citrate	Isocitrate	Succinate	Benzoate	-Coumarat	droxybenz	ydroascorb	affeoylqui	alacturona
	C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C30	C31	C34	C35	C36	C37	C38
RB985476	6.174973	NA	NA	NA	7.90385	14.19937	4.745214	10.82644	10.44543	7.343636	6.822391	11.02661	5.502794	4.47755	4.886131	5.500841	12.26246
RB985476	7.980082	NA	NA	NA	8.849681	13.48458	4.505445	11.65118	10.3683	9.543945	7.224783	11.33767	5.492746	5.444523	4.781194	5.192917	12.81627
RB985476	7.493886	NA	NA	NA	8.147252	14.51927	4.745214	12.07306	10.27482	9.324844	8.004994	11.34884	5.70833	4.977228	4.781194	4.635095	12.87459
RB985476	6.461253	NA	NA	NA	7.49987	13.94232	4.813893	11.41252	10.40478	8.240132	6.846964	10.14483	5.973029	4.784111	4.625463	4.665422	12.46583
RB985476	7.797493	NA	NA	NA	8.50498	13.73026	4.916304	11.89855	9.461791	9.889026	7.224783	9.416017	5.864752	5.202727	4.831987	5.970312	13.6622
RB855536	8.599028	7.762936	7.947944	11.78624	7.844255	8.240726	4.913809	11.62094	10.47547	9.203541	7.665079	6.922801	6.18368	5.294114	5.422331	4.594774	4.313863
RB855536	9.272113	7.540143	8.182648	12.12701	7.538569	8.564449	5.061732	11.79656	9.780275	8.995967	7.846841	6.814175	5.900253	5.646091	5.184246	6.634265	4.156298
RB855536	8.963011	7.705968	8.109847	11.74171	7.523599	7.477741	5.219646	12.14515	9.471932	9.24497	7.848914	6.75228	5.832557	5.709778	5.520031	6.716485	4.549215
RB855536	9.098951	7.540143	8.757062	12.45293	7.827337	7.844554	5.096097	11.79656	9.858849	8.578166	7.717796	6.863345	5.39931	5.148135	4.979329	5.692961	4.032311
RB855536	8.95858	7.151527	7.866985	11.91107	7.995757	7.636456	5.017376	11.62359	10.67042	9.005661	7.960727	7.174479	6.406989	5.784803	4.815293	4.826318	4.517628
RB867515	8.940477	8.619549	8.442224	11.91523	8.187823	7.396351	5.469489	13.71557	11.52171	9.826613	8.142411	7.22588	6.408614	5.48316	6.133363	3.316373	6.050999
RB867515	8.352027	8.053233	8.129827	11.2337	7.915251	7.688064	5.568079	13.68756	11.1417	8.484688	8.33814	7.369743	6.6292	5.907025	5.920385	4.956158	6.259298
RB867515	9.075542	8.888789	8.59525	12.12795	8.027438	7.561079	5.531864	14.06606	11.67454	9.582629	8.103322	7.174216	6.591533	6.393509	6.075205	4.136265	6.034456
RB867515	8.900323	8.857633	8.424778	11.75636	7.911306	7.389759	5.440571	13.75057	11.0078	9.154619	7.861161	7.854458	5.990988	5.843382	5.376778	4.154173	5.350995
RB867515	8.782996	8.416547	8.113168	11.55124	8.286624	7.002524	5.658635	12.74807	11.33644	9.349762	8.016043	7.267421	6.177073	5.987792	6.096194	4.207895	5.663299
RB92579	9.640665	7.897993	8.377984	12.15558	8.510278	6.821823	4.604708	13.18419	11.58742	10.13542	7.569388	6.536257	6.093457	4.520879	6.384812	6.80204	5.185593
RB92579	10.41403	8.624326	8.454425	12.64946	8.589256	6.275881	4.689077	13.58071	11.23828	10.45326	7.260879	6.479028	5.684023	5.037584	5.819208	6.372735	5.455322
RB92579	9.81546	7.990539	8.852937	11.97957	8.542376	7.033818	4.915729	13.45059	12.05981	9.970786	7.651288	6.582596	6.285359	5.436865	6.551329	8.014782	5.399549
RB92579	9.76295	8.014526	8.57739	11.83174	8.500162	7.437318	4.736439	13.58688	11.72495	9.611358	7.592613	6.542784	5.739357	5.253968	5.18425	7.931539	5.160944
RB975242	6.256477	NA	NA	NA	7.733286	13.23328	5.549361	10.53173	10.61308	8.932883	7.217209	9.752513	5.806547	4.405762	5.135194	8.038204	12.59542
RB975242	7.257143	NA	NA	NA	8.192953	13.62348	5.312535	10.75289	10.42282	8.71458	7.235521	11.03119	5.329873	5.444979	4.817635	6.613159	13.12395
RB975242	8.382653	NA	NA	NA	7.955424	14.03622	4.869103	11.07446	10.04094	8.354791	6.763842	10.41562	5.520413	5.543905	4.872045	8.122092	12.03019
RB975242	7.774217	NA	NA	NA	7.570256	13.03701	5.363076	10.93794	10.45791	8.193472	7.288575	10.54345	5.665303	5.50989	4.436506	7.591152	11.84834
RB975242	7.417623	NA	NA	NA	8.052549	13.9372	5.468602	11.15128	10.51591	9.377175	7.847851	10.74541	5.580534	5.444066	4.983582	5.552659	12.54207
RB965902	9.724567	6.784856	8.57648	13.15349	9.201016	7.807631	5.187628	14.06024	11.07261	11.26518	7.699457	6.827477	5.611773	4.071787	6.07	5.258875	5.735569
RB965902	10.13162	7.481844	8.774685	13.4726	9.22305	7.669329	4.740267	13.54623	11.11072	11.18179	7.385721	6.282143	5.823432	5.189433	6.098751	5.920103	5.468936
RB965902	9.569938	8.297642	8.787399	13.01336	9.027041	7.298662	4.704098	13.40237	11.59215	10.49222	7.507302	7.134419	6.026014	5.439209	6.589938	4.597646	5.949232
RB965902	9.742711	7.956065	9.541797	13.1013	8.70188	7.568238	4.938614	13.45896	11.05154	10.46525	7.479978	6.154213	5.853324	5.500492	5.300047	5.454839	5.535293
RB965902	10.47775	8.62341	8.660438	13.62497	8.719362	7.497331	4.75517	12.54405	9.368612	11.7265	7.24924	6.603879	5.902893	5.362689	6.030862	6.042731	5.196552
RB975375	5.52028	NA	NA	NA	7.874387	14.31647	6.812497	10.92392	11.5517	6.69824	5.492341	11.01085	5.949309	5.625601	5.302949	4.354178	11.33542
RB975375	7.180357	NA	NA	NA	7.186812	14.31507	6.707436	10.05647	11.2798	7.085925	5.720021	11.16519	5.84726	5.457735	5.11954	4.806729	10.9335
RB975375	7.518768	NA	NA	NA	8.351923	12.58712	6.909717	10.06512	11.66812	7.142943	5.606181	11.9706	6.067254	5.398449	5.762046	4.354178	11.22107
RB975375	5.96347	NA	NA	NA	7.612269	14.18345	6.666724	10.07428	11.32796	6.765045	6.561872	11.14173	6.401997	5.444523	5.180631	4.607624	11.51869
RB975375	6.545719	NA	NA	NA	7.665491	14.81482	6.774094	10.39582	8.628062	6.923038	5.845104	11.73576	6.024814	5.170195	5.585351	3.648181	11.74768
RB935744	6.656633	NA	NA	NA	7.407916	13.28488	5.483112	10.25397	10.68258	8.5587	8.454944	11.20308	5.930731	5.349267	5.399549	8.0932	12.3158
RB935744	6.23735	NA	NA	NA	8.069407	14.10342	5.706284	11.5512	10.58044	8.752686	7.863091	10.87173	5.747218	5.805657	5.527932	4.88581	13.49046
RB935744	6.295771	NA	NA	NA	8.231668	13.37802	5.594698	10.82552	10.39622	8.542733	8.409928	11.74455	6.343936	5.655103	5.399584	7.413087	12.60797
RB935744	6.295771	NA	NA	NA	7.965755	13.04994	3.851244	11.02209	10.79083	8.868428	8.111907	11.41797	5.437278	4.652144	5.448511	8.009303	12.23171
RB935744	5.99333	NA	NA	NA	8.359189	13.07386	4.799578	11.42923	10.64328	8.748621	9.209772	11.31061	5.276926	5.284165	5.222342	7.59144	13.45409

Genotypes	Glucarate	Glycerate	lar to Itaco	Nicotinate	Quinate	Xylose	Fructose	Glucose	Sucrose	Glycerol	Galactinol	hyo-Inosit	Xylitol	Adenine	ptadecano	tradecano	droxypyri
	C39	C40	C41	C43	C44	C46	C49	C50	C53	C55	C56	C57	C58	C61	C62	C63	C64
RB985476	5.024615	4.004429	11.50636	7.893167	8.741027	12.19565	4.201965	10.47357	8.421215	9.348006	10.87996	5.618845	NA	5.21453	5.396453	11.95545	8.458586
RB985476	5.087746	4.005946	12.42874	8.397183	8.655911	10.97715	5.022495	10.24783	9.02797	9.901737	11.79709	6.142096	NA	4.522991	5.053736	12.48413	8.061112
RB985476	5.146884	4.971352	12.58292	9.65449	8.930741	11.48573	5.578294	10.86319	8.455535	10.12222	11.14692	6.368571	NA	5.001802	5.305036	11.93127	8.654073
RB985476	5.488268	3.042058	12.67273	8.730854	8.642291	12.16616	5.287227	9.281196	8.211862	9.401055	10.40671	6.438873	NA	5.248123	4.910533	11.55214	8.545412
RB985476	4.986907	4.005946	12.72134	8.978576	8.271187	12.43841	5.022495	9.690182	9.076476	10.73566	11.29134	6.142096	NA	5.021566	4.32645	11.98075	8.047772
RB855536	3.894671	5.37344	4.744221	3.598741	11.33787	9.350313	12.50295	14.56274	14.21142	10.69238	10.68196	12.00222	6.851459	3.978925	6.175094	8.29202	8.482873
RB855536	3.292944	5.330602	4.903802	4.882114	13.02184	9.751576	12.48307	13.75771	13.36921	10.45488	10.51098	11.48774	6.851459	4.623149	5.649011	7.869023	8.738917
RB855536	4.13271	5.329673	4.8549	4.800225	12.17295	9.72845	12.43969	14.11377	13.75622	10.45488	10.34134	11.41779	6.875408	3.959739	5.815435	8.140826	8.599202
RB855536	3.821188	5.55323	4.903802	4.416389	11.85624	9.826039	13.32444	14.26907	12.68702	10.10114	10.1101	11.86134	6.739265	4.402171	5.254555	8.862174	8.676857
RB855536	4.331844	5.066065	5.112285	4.807832	10.89229	8.984552	10.92946	14.52751	13.01048	10.57111	11.50239	11.59841	6.939705	4.461123	6.010383	8.296054	9.08147
RB867515	5.812128	5.803586	6.92082	4.877192	10.2723	8.872823	10.30704	12.25285	14.83266	11.46676	9.782809	11.32117	8.862341	5.622711	6.545261	7.438304	8.691241
RB867515	5.583866	6.019707	6.565953	5.275507	10.3071	8.863158	9.966141	11.67038	14.98828	11.49198	10.15496	11.02035	8.009529	5.083908	6.472004	7.222224	9.112277
RB867515	5.814003	6.081356	6.030722	5.439335	10.9175	9.252669	9.989303	12.84524	14.52655	10.92234	10.48469	11.3612	8.365685	5.875113	6.234589	7.616154	8.986831
RB867515	5.015183	5.751919	6.464371	4.627532	10.36039	8.626118	10.04902	12.36983	14.45186	10.71919	9.854057	10.45922	7.607104	5.413504	6.113589	7.394813	8.730592
RB867515	5.283011	5.30625	5.763848	5.298849	9.944683	8.791254	8.351646	9.721314	15.04937	10.53233	10.47218	10.2575	8.994072	5.34883	6.482837	7.302569	8.993827
RB92579	4.830833	5.326208	4.892252	3.860001	10.4789	8.939553	10.80834	13.81567	14.00528	10.2033	10.36213	10.94629	7.630487	5.803317	5.59871	7.585905	8.057451
RB92579	5.260062	4.838498	6.392218	4.26328	9.13405	8.199542	8.942216	12.25137	14.24942	9.979514	9.436368	10.47655	6.274193	5.292654	5.481594	5.62155	7.868644
RB92579	5.122949	5.555584	6.491053	4.820882	10.72303	9.143105	10.55634	13.35315	14.18959	10.21749	10.68614	11.49221	7.929272	5.42655	5.530581	7.079168	8.268146
RB92579	4.539672	5.622095	5.994307	4.627532	10.112	9.055503	10.20475	13.91869	13.21892	10.46964	10.89185	10.91821	6.873444	5.18368	5.195335	7.471795	8.268801
RB975242	5.55323	5.193471	12.03045	9.225478	9.02678	12.58204	4.676748	10.65752	8.371335	9.54416	10.64373	6.114703	NA	3.674907	4.479531	12.25363	8.338647
RB975242	5.139967	5.672003	12.37994	8.810462	8.471497	11.05737	4.762387	10.60645	8.468309	10.21357	11.13508	6.603348	NA	4.838731	4.821815	12.23753	8.433807
RB975242	5.668546	4.918009	12.11238	9.038736	8.255756	12.22926	5.095887	10.56176	8.19086	9.213823	10.93311	5.822215	NA	4.507039	4.681964	11.96054	8.307496
RB975242	5.468848	4.153342	11.72183	8.877295	8.465286	12.11401	3.91304	10.60007	8.367164	9.369625	10.44312	5.731399	NA	4.901117	4.681964	11.74559	8.597841
RB975242	5.660658	4.984206	11.90955	8.78261	8.223451	12.06425	5.363872	10.60645	8.282522	9.54416	10.95856	6.252087	NA	4.666209	4.744547	12.19708	8.435056
RB965902	5.704971	4.953485	5.806058	3.965704	9.95657	9.377603	9.828896	13.14834	14.22048	10.49383	11.34692	12.20707	8.820809	4.27066	6.181104	7.715134	8.354964
RB965902	5.468555	4.715946	6.204117	4.578356	9.454231	9.132317	9.604313	12.60067	13.83684	9.942923	10.99739	11.57633	8.631165	4.656638	5.958236	7.533462	8.038487
RB965902	5.608532	4.714634	5.740171	4.566838	9.93361	9.127275	10.05875	13.09947	14.71456	10.20999	9.302009	12.34242	7.247421	4.714338	6.296533	7.029711	8.396474
RB965902	5.124406	5.158594	5.987728	4.811492	9.609825	9.354289	10.48246	14.04571	14.20113	10.62321	11.37632	12.02187	7.2336	4.73627	5.662706	7.837312	8.091301
RB965902	5.236289	4.012222	5.099916	4.628404	9.094888	8.545101	9.170057	11.59688	14.12938	9.744422	9.709268	11.40331	8.660858	4.62236	6.296226	7.205614	7.931555
RB975375	5.022267	2.51346	11.59023	8.291114	8.314086	12.83561	3.859944	10.89238	8.227173	9.066289	10.83267	4.980815	NA	5.393875	5.154673	10.99293	8.63334
RB975375	5.012958	2.83478	11.21848	8.054742	8.604006	11.89787	3.778025	10.4639	7.546143	9.162442	10.17035	4.003147	NA	5.235112	5.303416	10.04697	8.590018
RB975375	5.116131	2.83478	11.45734	7.269415	7.024468	10.09088	3.797448	10.87511	8.388723	8.977311	11.37474	4.502744	NA	5.08693	5.038463	10.44006	8.778502
RB975375	5.154576	2.76089	11.4645	8.287737	8.830912	11.40956	3.359587	9.601091	8.300621	9.243493	10.59025	4.871088	NA	4.716552	4.819773	11.0964	8.824699
RB975375	4.805405	3.22999	11.55613	8.914178	8.79696	12.19532	4.192236	10.45812	8.16637	9.362676	10.60356	4.589449	NA	5.002179	4.875989	11.10663	8.340142
RB935744	5.88316	5.030544	11.14016	7.055746	7.936087	11.14488	5.2389	10.69467	8.103354	9.306249	10.17731	5.529715	NA	4.428878	5.816399	11.65784	8.594527
RB935744	6.249269	5.494627	11.66278	6.745117	7.356936	9.549045	5.543605	10.62843	8.609997	10.18076	10.99898	6.063024	NA	4.528967	5.720534	11.95035	8.610703
RB935744	5.947092	5.774975	11.54722	7.358218	7.287509	10.31478	5.711835	10.54348	8.549726	9.543175	11.16894	5.886501	NA	4.427678	6.197096	11.41813	8.568422
RB935744	6.022998	4.072323	11.75441	7.381692	8.026764	11.10331	4.804128	10.75123	8.699284	9.473679	10.92673	5.882485	NA	4.2041	6.056728	11.82352	8.176369
RB935744	5.627762	5.093117	11.69261	7.424021	7.088084	10.54457	5.740932	11.52351	8.834927	10.28006	11.30923	6.312736	NA	4.548766	6.195088	12.93188	8.049576

Supplementary Table 2. Levels of all detected metabolites in bud of the selected sugarcane cultivars

Genotypes	Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Isoleucine	Leucine	Methionin	enylalanin	Proline	Serine	Threonine	Tryptophan
	B1	B2	B3	B4	B5	B6	B7	B8	B9	B11	B12	B14	B16	B17	B18	B19	B20
RB937570	13.88301	3.96424	9.035629	14.24508	7.781324	9.284143	12.58466	11.16973	9.324467	9.870799	9.474213	7.923124	5.996189	10.14581	11.21	8.439199	8.276925
RB937570	14.78699	4.983506	8.505497	14.19075	7.401822	9.06403	12.88421	11.57236	9.670455	9.911892	9.385277	7.673415	6.217869	10.94848	12.06316	8.85926	8.249243
RB937570	12.87302	4.146379	7.406368	13.82754	8.591948	8.341038	12.15486	10.68195	8.995685	9.155391	8.907902	7.726795	5.597313	10.13699	11.06125	8.284202	7.964725
RB937570	13.73127	4.364708	9.074495	14.33037	8.059327	8.896404	12.87078	11.03667	9.293578	9.216216	9.38664	7.370326	5.958122	10.17514	11.21383	8.235477	8.011808
RB975201	13.82995	6.424101	11.36695	13.35666	7.960143	10.55711	12.21271	11.67345	10.37586	10.34496	10.08254	8.1597	5.748213	10.33574	12.05864	9.393215	6.896662
RB975201	13.91686	6.230346	11.45483	14.24827	8.503473	9.752303	12.77648	11.80346	10.06505	10.89748	10.54163	8.468915	5.681658	10.93846	12.19286	9.67024	7.807012
RB975201	13.65922	5.972015	11.46193	13.48281	8.057174	9.703903	12.25748	11.23159	9.87932	10.57115	10.13553	8.243252	5.8388	10.21018	11.86794	9.324706	7.431953
RB975201	13.91035	5.917616	11.54073	13.26596	7.892176	9.513482	12.53628	10.21033	9.78467	10.41429	9.993418	8.071795	5.668677	10.18301	11.94184	9.082007	7.224291
RB975201	13.45036	5.717635	10.60866	13.00084	7.958193	9.108622	12.26631	10.59911	9.500477	9.530305	9.167112	7.382912	5.470942	9.482863	11.69197	8.842901	7.270451
RB835486	13.70146	5.85411	9.366457	14.2863	8.124294	9.296971	12.84094	10.75256	9.527487	11.54053	11.38657	8.987244	6.715957	11.18267	11.6532	9.300567	7.248245
RB835486	14.68068	6.165817	9.705786	14.22363	7.987248	9.736118	12.74092	11.30419	8.913197	11.60816	11.43536	8.962557	6.949343	10.93757	12.36596	9.687467	7.636528
RB835486	14.00104	5.288169	9.504712	14.42295	8.575819	8.022093	13.06703	10.99687	9.50606	9.108651	9.040617	7.67282	6.16132	10.68041	11.92455	9.061211	7.654665
RB835486	13.3376	6.108343	8.888874	14.22363	7.803454	9.932338	13.2471	10.93386	8.988517	11.06811	10.45368	8.561497	6.533513	9.879931	11.56108	8.759377	8.011808
RB966928	14.89505	6.467	10.01978	14.62842	7.835398	9.988281	13.49056	12.14403	9.391082	11.45627	10.81238	9.367352	6.961259	11.3422	12.69975	9.399088	8.293594
RB966928	15.34122	6.217944	10.47617	15.15235	7.161974	8.754614	14.09158	11.38461	9.391471	10.54669	9.878535	8.536227	6.696039	11.08971	12.85833	9.169515	8.82131
RB966928	14.22026	5.335405	9.67326	14.11428	7.929623	8.798217	12.58361	11.58946	9.1919	10.43477	9.053573	8.926438	6.176445	10.13825	12.13149	8.782478	7.60354
RB966928	14.34948	6.006783	10.54365	14.50173	8.435852	9.767505	13.75946	11.61863	9.324818	11.80556	11.21396	9.455112	7.398589	11.09883	12.56992	9.904578	8.529124
RB72454	12.40819	5.186167	8.114142	13.19534	7.890402	9.169082	11.97788	11.61289	9.316025	10.36542	10.04859	8.279894	6.439361	10.12599	11.06344	8.703062	7.531337
RB72454	13.26218	6.634658	11.32915	14.00426	8.04898	9.530927	13.17872	11.68744	9.374169	11.01186	10.68368	9.075391	7.088678	10.49589	11.28773	9.033596	8.446758
RB72454	12.99465	6.536253	10.9299	13.71364	8.322298	9.388257	12.49125	11.75003	9.538656	11.25221	11.01278	9.009709	6.853007	10.92323	11.36338	9.298138	7.849981
RB72454	13.4898	6.912679	11.64292	13.85566	7.769923	10.33148	12.52709	11.54198	10.18613	11.91464	11.56503	9.305358	6.891722	11.26376	11.2149	9.335606	8.050998
RB965917	14.90473	6.199127	11.01488	15.28393	8.058594	9.767505	13.84695	12.31998	9.839734	11.99804	11.84331	9.689786	7.258314	12.42858	12.95402	10.40306	8.521967
RB965917	14.69755	6.127952	10.74324	14.7642	8.622038	9.155754	13.19399	12.59101	9.856637	11.42326	11.28222	8.92413	6.455995	11.74251	12.59501	9.893188	8.121495
RB965917	14.3636	6.088297	10.42641	14.66259	8.076624	10.90558	12.87078	11.81063	9.68228	10.65207	10.41575	8.432921	6.688724	10.99949	12.15512	9.299088	8.308785
RB965917	14.65027	6.381133	11.71004	15.26284	8.527026	11.67188	13.92766	13.03777	9.846898	10.95025	10.75873	9.178638	7.454193	11.88053	12.93135	10.02314	8.850183
RB965917	14.2794	6.199127	11.17984	14.95976	8.058594	10.88717	13.55682	12.20282	10.18785	11.88559	11.6491	9.602851	6.901314	11.82523	12.46626	10.10665	8.560276
RB928064	13.97105	4.826258	9.644639	13.90078	7.899657	9.584133	12.44056	12.10577	9.59719	9.493486	9.531354	7.743368	6.190024	11.3799	11.99464	8.86653	7.760539
RB928064	15.22842	6.381133	10.89558	14.79111	7.617592	9.442517	12.59752	11.55561	9.374855	10.91303	10.35204	9.130022	5.956432	10.97114	12.62137	9.230375	8.451194
RB928064	13.46315	4.767039	10.17643	13.88605	8.127375	9.701551	12.39944	11.5808	8.872045	9.90913	9.230222	7.772528	5.815482	11.01982	11.92467	8.828189	7.722251
RB928064	14.20493	6.438963	11.07499	13.71772	7.954005	9.608332	12.43709	11.7049	9.084662	11.4195	10.99905	9.19141	5.86379	11.24054	11.83031	9.556555	6.67966
RB928064	14.52645	6.418781	10.91397	14.85442	7.899657	9.584133	13.11297	12.01023	9.783605	11.01094	10.72747	8.776682	5.956432	11.4465	12.52898	9.685506	7.892166
RB855453	14.30274	7.053729	11.46796	14.41726	8.270295	9.744224	13.10768	11.94639	9.723911	11.07738	10.92976	9.041948	6.844115	11.34733	12.15661	9.915078	8.11722
RB855453	14.18314	7.267392	12.03999	14.31063	6.191998	8.330811	13.81681	11.63751	8.410446	11.57007	11.12222	9.278019	7.694404	10.70198	11.88703	9.513115	8.291844
RB855453	14.52763	6.483637	10.47858	15.23117	7.894804	10.04985	13.80036	11.8122	9.760998	11.25957	10.81548	9.016601	7.420826	11.03358	12.05064	9.471643	8.398214
RB855453	14.90805	6.187159	10.00831	14.72879	7.631065	9.946632	13.56883	11.51174	9.595753	10.52258	9.683181	8.820372	6.629835	10.4857	12.52961	8.934343	8.344488
RB855453	14.89705	7.604448	11.74494	15.5708	7.49704	8.265163	13.99509	12.82413	10.15179	11.1074	10.63766	9.039235	7.794382	10.89215	12.46325	10.38418	8.748499

Genotypes	Tyrosine	Valine	-Oxoprolin	Putrescine	s-Aconitat	Citrate	Pyruvate	Succinate	Benzoate	etoglucon	Caffeate	droxybenz	ydroascorl	Glycerate	lar to Itaco	Lactate	Nicotinate
	B21	B22	B23	B24	B26	B27	B29	B30	B31	B32	B33	B35	B36	B40	B41	B42	B43
RB937570	8.943107	11.34337	10.3639	7.456502	8.594782	8.310576	6.121126	9.09447	7.874489	9.709045	8.90132	5.559731	6.003173	6.267012	7.881118	11.96306	5.899251
RB937570	8.966291	12.19978	10.72566	7.541228	8.009767	8.132466	6.896454	9.376263	8.750474	9.315881	9.250011	6.049143	6.325133	6.258472	7.984599	12.59124	6.170143
RB937570	8.824708	10.73283	10.01961	8.025044	7.557655	7.905825	6.364001	9.136136	8.422871	9.554941	10.05339	5.804437	6.020859	5.656331	8.284411	11.54103	6.034697
RB937570	8.795515	11.03599	10.6983	7.397761	7.876865	8.180999	6.345739	9.162454	8.789384	9.524682	10.02161	5.92679	5.885335	6.452271	8.987516	13.02687	7.384162
RB975201	9.094157	12.08236	10.04707	11.392	9.248021	9.109002	5.969677	8.590741	7.776685	11.19684	9.301458	6.744678	6.342808	6.659132	7.570255	12.29471	6.862827
RB975201	9.705251	12.48039	10.58898	11.39108	9.330302	9.406644	6.290433	9.05608	8.384242	11.59753	9.378053	7.282802	6.803126	6.916003	8.209101	12.31786	7.205132
RB975201	9.156929	12.17011	10.09203	10.80839	9.043933	8.939868	6.011852	8.75098	8.062624	11.14122	9.747426	7.331569	6.24994	6.456075	7.746316	11.76062	7.52935
RB975201	8.970136	12.39979	10.37251	11.77091	9.893173	8.743859	6.266824	8.717147	8.770346	11.32619	9.978786	6.755719	5.03469	6.856571	7.815894	11.54882	7.06521
RB975201	8.938333	11.74886	10.18567	11.13988	7.476645	9.154229	6.059044	8.788279	8.192734	11.23836	9.553143	7.540944	5.928445	6.463871	7.924728	11.58763	7.245921
RB835486	9.672711	12.57202	10.59858	9.599955	7.837591	7.92699	6.23672	9.022857	7.812362	9.526119	9.997183	7.452806	5.588475	6.32405	9.000728	11.93165	7.545453
RB835486	10.10677	12.52958	10.6103	9.70849	7.806321	8.418046	6.295098	8.851305	7.846839	9.344212	10.08414	6.131925	6.392009	6.728489	8.930866	10.37142	7.037238
RB835486	9.734096	11.75844	10.90048	9.115454	7.54921	8.974876	6.288341	9.421977	8.220774	9.002029	9.885323	7.779303	6.208081	6.894318	9.05148	10.95445	7.533921
RB835486	9.459657	11.73787	11.02989	9.490385	8.032162	8.352271	6.333205	9.438501	8.086462	9.290786	10.18254	7.700332	6.062855	6.346305	9.716708	10.56027	7.88412
RB966928	10.6792	12.64611	11.18348	7.245598	8.815082	8.529789	6.034531	9.026312	8.085904	9.69712	9.744106	7.152243	5.82865	6.156859	9.454368	11.91905	7.563098
RB966928	9.545185	12.40951	11.865	5.921356	8.716638	8.665272	6.275456	9.45089	8.17268	9.866833	9.418437	6.77514	6.572861	6.110163	9.677705	11.0719	7.716787
RB966928	9.743132	12.10679	10.42332	8.374599	8.205107	8.804843	6.51638	9.015301	8.314792	9.744551	9.855509	7.136381	6.38499	6.542571	9.024416	11.65177	7.525344
RB966928	10.78141	13.01186	11.49261	7.180518	9.129725	8.800755	6.275456	9.411103	8.806108	10.60709	10.32006	7.765499	6.407791	6.673159	9.82459	11.54757	7.601743
RB72454	9.070062	11.49367	9.929893	9.025235	6.516462	8.527162	6.523279	9.153347	8.704886	9.064583	8.844587	5.859228	6.962702	5.897214	8.208588	11.91487	7.010027
RB72454	9.770073	12.11326	10.94819	9.819026	6.447732	8.572585	6.426915	9.407244	8.276351	9.93069	10.09573	7.718906	7.636976	6.505522	8.67716	11.11129	7.602563
RB72454	9.799226	12.43691	10.32861	9.533745	6.336345	8.863325	6.49709	9.325567	8.744433	9.493779	10.10918	7.905055	7.353363	6.564418	8.993309	11.50858	7.990273
RB72454	9.538314	13.04045	10.39016	9.837768	6.044843	9.116384	6.645833	9.162454	8.48696	9.498292	9.826225	7.24484	6.126813	6.854051	8.235711	11.78063	7.658352
RB965917	10.1095	13.86257	11.58334	8.52235	9.188098	8.81331	6.395449	9.237039	8.438528	10.1458	10.90453	7.478574	6.251851	6.576818	9.600446	12.3953	7.732946
RB965917	9.743132	13.20661	11.04822	8.734169	6.901084	9.117534	6.30608	9.428024	8.841742	9.788929	10.1646	7.958329	6.204756	6.775912	9.204533	13.04162	7.758666
RB965917	9.971061	12.20175	10.6983	9.507071	8.720922	8.875332	6.553522	9.265425	7.970468	10.35855	10.28194	7.589047	6.24856	6.587437	9.154141	11.39919	7.533921
RB965917	10.6579	12.76924	11.48917	8.875257	8.297962	8.992606	5.905486	8.720155	7.148054	10.70276	9.860328	6.759474	6.24856	6.7739	9.045527	11.61372	7.059068
RB965917	10.13401	13.20078	11.25935	8.737437	8.381744	9.16425	6.369865	9.333467	8.509425	10.61124	10.30979	7.522485	6.289073	6.509489	9.002955	12.78708	7.50597
RB928064	9.600274	11.40701	10.31394	9.046649	8.291308	8.63315	6.775186	9.630642	7.996689	9.375812	9.920683	7.693807	NA	6.863067	9.63541	11.24315	7.993979
RB928064	9.930809	12.67029	10.43338	7.213865	8.568458	8.367113	6.291456	8.964164	7.92495	9.526285	9.920923	6.490222	NA	6.047773	9.163638	11.06098	8.074184
RB928064	9.929744	11.43011	10.23578	9.54323	9.00236	8.760829	6.506707	9.041172	8.327325	9.845612	9.90152	7.233433	NA	6.667515	9.157068	10.73994	7.56897
RB928064	9.589289	12.54493	10.26476	9.327895	8.277274	9.047197	6.016925	8.703431	7.766896	9.097522	9.140763	6.983072	NA	6.621218	8.580306	10.32936	7.031143
RB928064	10.32978	12.40951	10.91903	9.804158	8.702888	8.995855	6.572249	9.396879	7.967583	9.837361	10.00606	7.493665	NA	6.782495	9.61901	11.93149	7.644515
RB855453	10.41831	12.59784	10.86117	9.127223	8.681853	9.349856	5.940146	9.252806	7.986616	9.656064	10.12086	7.845867	5.390464	6.731996	9.464577	10.95684	7.91698
RB855453	10.09328	12.76148	11.47052	7.801397	8.464414	8.446284	6.296201	9.056404	7.488858	10.48542	9.578979	6.546536	5.72444	6.210032	8.646775	10.91548	6.878205
RB855453	10.3815	12.89894	11.56623	8.398979	9.163092	8.89807	6.918042	9.604449	8.643109	9.872957	10.22012	7.817997	5.557452	6.77852	9.390589	10.91548	7.903775
RB855453	9.647274	12.02399	11.27509	7.881142	9.470507	9.123593	6.370126	9.262426	8.221542	10.28529	9.787328	7.25913	6.004468	6.466305	9.42413	11.0418	7.619442
RB855453	10.13509	13.94156	11.6911	8.786154	9.389259	9.800165	6.46483	9.305796	8.450774	10.31334	10.429	7.678972	5.669206	6.711107	9.373394	10.7478	7.737848

Genotypes	Quinate	Xylose	Fucose	Sorbose	Fructose	Galactose	lar to Ribu	Sucrose	Trehalose	Glycerol	ıyo-Inosit	Xylitol	Uracil	:hophosph	Adenine	ptadecano	Decanoate	:thanolami
	B45	B46	B47	B48	B49	B51	B52	B53	B54	B55	B57	B58	B59	B60	B61	B62	B65	B66
RB937570	14.83241	9.778143	6.885096	15.89163	16.11734	14.46783	3.367315	13.92842	7.698702	11.66511	13.31047	8.388943	5.649527	14.08286	5.302036	7.247462	5.061691	8.375951
RB937570	12.29179	9.937871	7.16684	13.65224	13.35454	12.38995	3.931191	13.25626	8.156456	12.11416	12.23619	8.210344	6.554388	13.84836	5.366544	7.764725	5.049286	7.355958
RB937570	14.86428	9.937871	7.593559	15.95605	16.40206	14.52563	3.649253	12.58106	7.286947	11.02388	13.36276	8.774855	6.627275	13.90008	5.33429	8.656737	4.6259	8.797468
RB937570	14.55613	10.0976	7.561914	15.89145	16.153	14.36822	3.649253	13.25929	8.419633	11.50501	12.9762	8.458048	7.677912	14.69019	5.350417	8.095423	5.147154	9.013132
RB975201	14.74811	10.09812	6.888871	15.94985	16.08102	14.26681	4.660137	13.04606	7.759349	10.95923	13.49667	8.619999	7.035872	11.48823	6.356631	7.372567	4.479348	7.950927
RB975201	15.11051	10.35301	7.277053	16.00271	16.38607	14.36995	3.344668	13.25603	8.028952	11.34423	14.11461	8.87033	7.679221	12.09625	6.938645	7.921864	4.797958	7.924128
RB975201	14.72626	10.12061	7.085553	15.96564	16.03383	14.31107	4.986524	12.98805	7.56693	11.05955	13.61019	8.942373	7.536406	11.88147	6.678984	7.57888	4.598282	7.992353
RB975201	14.7868	10.22446	7.206717	16.04382	16.43366	14.36995	4.724134	13.35353	7.777761	11.28281	13.57938	8.479672	7.237156	11.52939	6.624923	7.926587	4.507068	7.064288
RB975201	14.90659	9.94064	7.538177	16.05154	16.31003	14.53198	4.427575	11.989	7.788039	10.72894	13.55148	8.796842	7.97293	12.01858	6.406636	7.585868	4.595664	5.860329
RB835486	14.8616	10.06635	7.707988	15.90286	16.19292	14.56694	3.853128	12.27115	6.855538	11.26348	12.37968	9.075358	7.64706	12.26521	6.724499	6.531881	4.318894	8.929386
RB835486	14.66814	10.08849	6.663245	15.80446	15.82191	14.5975	5.034857	11.81732	6.063247	11.41819	13.11114	8.259302	6.188004	12.41227	7.728313	6.853585	4.339878	9.302759
RB835486	14.32476	9.949908	7.727013	15.6282	15.86592	14.4406	4.731217	11.70824	7.274034	12.00958	13.67199	8.819994	8.053035	12.81148	7.818121	7.329522	4.842769	7.273038
RB835486	14.94981	10.24922	8.029094	15.85985	16.04655	14.8527	5.125812	11.93224	6.73094	11.50863	13.40387	8.799635	8.06211	13.75698	6.910477	7.420092	4.500514	9.036645
RB966928	14.56525	9.143929	7.115128	15.26815	15.35956	14.39569	3.664405	13.13061	8.555698	11.44596	13.384	8.930941	7.57129	14.7281	7.164275	8.027229	4.716633	8.933693
RB966928	13.32229	9.534986	7.698655	13.88984	13.49344	13.55278	3.718155	13.95084	8.288476	12.1373	12.33674	8.630314	7.188589	14.75454	6.485624	7.914475	5.12379	8.173485
RB966928	15.1888	9.394742	7.581197	15.94462	16.12886	14.91112	3.610654	13.16209	7.880938	12.35221	13.13226	8.445929	7.578381	13.93554	6.520375	7.760979	4.877046	8.39063
RB966928	14.21178	10.06629	7.959977	15.40063	14.99395	14.17226	3.664405	13.27241	8.428792	11.08285	13.28036	8.514071	8.120319	13.53694	6.723425	8.051656	4.905823	8.788921
RB72454	15.41591	9.66244	7.300689	16.20213	11.88941	15.06836	3.925409	13.70807	8.2681	11.76842	12.69346	8.697721	6.770594	11.58852	5.897662	7.315842	5.670228	7.605118
RB72454	15.24268	10.02942	7.803901	16.05684	12.21863	14.88705	5.346748	14.04188	7.983946	11.23369	13.60877	8.697721	8.141533	11.77236	7.071774	8.109938	5.367993	7.884166
RB72454	15.27963	10.22472	7.864713	16.41403	12.30355	14.83578	5.390369	14.14019	8.172228	11.76125	13.33143	9.365064	8.326008	12.26668	6.988412	7.451498	5.340338	7.59452
RB72454	15.59627	10.0972	7.854982	16.39776	12.80261	15.14261	4.693269	13.66476	8.255463	11.50501	12.87585	9.022861	7.53206	12.05025	6.221001	7.496199	5.175173	7.336668
RB965917	12.53879	10.19521	7.682986	14.3159	14.39347	12.79237	4.903454	13.34808	8.006625	12.44298	14.18699	8.888617	7.666952	14.89271	7.244539	9.795326	4.711317	9.277312
RB965917	13.24911	10.00076	7.958431	14.89729	15.08491	13.48354	3.40895	12.06411	7.88452	11.75613	14.19011	8.808087	8.397669	15.13154	7.007732	9.354932	4.650271	7.77174
RB965917	13.45918	9.974445	7.479267	15.39725	15.37705	13.45212	4.7743	12.80643	7.526553	12.11562	14.75503	8.653781	7.689557	15.00077	6.679548	9.252542	4.633607	8.83119
RB965917	14.0982	10.61043	7.494434	15.57728	15.72608	13.99035	4.732874	13.86053	6.773696	11.62422	14.57951	8.888617	6.904824	14.95832	7.00371	9.276801	4.109315	8.316845
RB965917	13.29843	10.19521	7.787661	15.12728	15.14538	13.2977	4.785306	13.02818	7.859919	11.98474	14.44063	9.203984	7.755521	14.46388	7.095866	9.318845	5.146845	8.982194
RB928064	13.65308	10.33124	7.897706	15.13821	15.27574	13.72239	4.194047	12.29012	9.155996	12.07586	14.26805	10.85196	7.386285	14.83001	6.961519	7.576678	4.796378	6.504819
RB928064	14.20349	9.317814	7.130057	14.95641	14.86645	14.33614	4.334978	11.89666	9.390703	11.81759	12.86317	10.69179	6.812304	14.19306	6.280354	7.812724	4.179869	6.547938
RB928064	14.69228	9.76448	7.470539	15.97229	16.01547	14.6075	4.217969	11.34807	8.524832	11.45726	14.95259	8.902263	7.510824	14.99864	6.675654	7.667663	4.599512	6.044991
RB928064	15.05084	9.610196	7.298072	16.46408	16.76408	14.6555	4.266415	12.0518	6.971194	11.41967	13.54825	8.847292	7.292089	13.64161	6.074802	7.1218	4.812598	6.77977
RB928064	13.67039	10.06207	7.805846	15.43551	15.67385	13.66315	4.253352	11.89666	8.985899	12.90321	14.58974	10.15936	7.929922	14.93872	7.046271	7.704524	4.597089	6.646576
RB855453	14.34047	9.597138	7.825458	15.60294	15.86215	14.32617	3.843088	13.22553	7.487972	11.51287	13.30493	9.431364	8.221421	14.47261	6.958939	7.674388	4.219068	8.133325
RB855453	14.78557	9.844803	7.127649	15.92188	16.02678	13.38801	4.369557	13.36799	8.063068	11.3249	12.78437	8.101376	6.559231	12.13142	6.057999	7.335112	4.394476	7.502804
RB855453	12.50187	10.04199	8.016282	13.76305	13.51148	12.49686	4.369557	14.2834	8.501511	11.88887	13.5691	8.894598	8.023645	14.37407	7.35871	8.174593	4.306772	7.779692
RB855453	14.29338	9.582629	7.675647	15.01426	14.93377	14.23307	4.608664	14.08771	8.156721	11.49588	13.16749	9.477511	7.696323	14.98478	7.005602	8.187731	4.448871	7.83371
RB855453	12.49606	10.13785	7.895095	14.13751	14.02109	12.49593	4.656919	13.71516	8.574333	11.25685	13.35796	9.649061	7.919098	14.81349	7.413444	8.278476	4.342297	7.919018

Genotypes	Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Isoleucine	Leucine	Methionine	enylalanin	Proline	Serine	Threonine	Tryptophan
	B1	B2	B3	B4	B5	B6	B7	B8	B9	B11	B12	B14	B16	B17	B18	B19	B20
RB985476	12.86074	7.415243	14.8784	14.1629	7.989759	10.61622	12.67869	11.96519	9.912799	11.08613	10.70366	9.346865	6.773636	10.68183	11.33886	9.359338	8.769395
RB985476	13.32355	8.548825	12.46336	13.55491	7.679035	10.91433	11.63828	13.19434	11.22466	10.9558	10.82034	9.247581	6.93055	10.74366	11.91042	9.698391	7.200739
RB985476	13.51426	8.284822	14.51734	14.78058	8.534796	11.29281	13.59148	13.52866	10.8737	11.86002	11.20754	9.95301	7.489134	11.03119	12.29152	10.25655	9.077841
RB855536	13.55381	6.82424	9.927362	14.23335	8.841265	10.3999	13.36548	11.86644	9.448718	11.72271	11.76017	9.314439	6.596845	11.07135	11.69417	9.783545	8.557075
RB855536	13.4522	6.862917	11.58842	14.17153	8.361959	10.74799	12.96611	12.47199	10.04046	10.42343	10.14785	8.873589	6.418305	10.22366	11.75709	9.545153	8.063925
RB855536	12.52422	7.087795	11.97504	13.832	7.675533	10.19372	12.44609	11.3988	9.538775	11.14929	11.09047	9.488338	6.840964	10.62061	11.22776	9.502733	7.872845
RB855536	12.90236	7.627154	11.76329	13.69127	8.296008	11.03776	12.61991	11.81063	9.932565	11.91428	11.98474	9.712944	7.152791	11.00643	11.6651	10.10391	7.855385
RB855536	13.36147	7.447115	12.5882	13.15014	7.940677	10.63876	11.41493	12.83463	10.35387	10.48434	10.43208	8.926438	5.97532	10.11024	11.42328	9.415144	6.241746
RB867515	14.54898	5.280251	8.708981	14.21385	7.804466	8.868995	12.32021	11.31429	9.792152	9.675833	9.805745	7.607006	6.165583	10.8218	11.68977	8.577548	8.5042
RB867515	14.92463	5.782537	9.097032	14.58957	8.135394	9.782547	12.97479	11.69203	9.042292	10.84384	10.86736	8.397495	7.082726	11.22137	11.76545	9.3747	8.010161
RB867515	15.61597	6.194762	8.961849	14.75032	8.060012	9.660244	13.67871	11.8124	9.662341	11.07847	10.52718	8.977419	7.258702	11.46289	11.67606	9.545838	8.662116
RB867515	13.35308	6.08492	9.062552	14.21415	8.013337	9.210252	12.33573	11.03229	9.239026	9.596468	9.333203	7.801368	6.747365	10.15977	11.52057	8.57499	7.953742
RB867515	13.98724	5.480502	8.978831	15.03463	8.494921	8.920409	13.06511	11.51736	9.17804	10.92975	10.38633	8.395598	6.934088	11.00643	11.72847	9.517969	8.375724
RB92579	14.34857	5.635273	10.86043	14.42542	8.539218	8.713186	12.97608	13.41042	9.955351	9.666116	9.161201	7.370477	6.171378	11.56612	12.83993	9.86144	7.241255
RB92579	14.66727	6.031675	10.68378	14.20171	9.131099	8.939261	13.24161	12.72647	10.15801	10.91295	10.75089	8.205779	7.014477	11.09349	12.98081	9.982735	7.838484
RB92579	14.03029	4.737098	9.958372	14.35169	9.135946	9.039948	13.21181	12.87537	9.795789	10.37171	9.638562	8.271445	6.725417	11.06215	12.72139	9.556947	7.586519
RB92579	14.29624	5.629404	10.53365	14.02629	8.79827	9.119509	12.92179	13.2364	10.25052	10.18664	10.06268	7.677894	6.764291	11.18648	13.12229	9.934252	7.674283
RB92579	14.10183	6.11357	10.89558	14.1272	8.125328	8.884401	12.7189	11.87433	9.007787	10.58199	9.873671	7.884995	6.23678	10.5592	12.39443	9.415336	7.477747
RB975242	13.4077	6.401149	10.36568	13.11175	7.655763	10.14095	11.8024	11.80886	9.511843	10.887	10.76997	9.030768	6.534853	10.4804	11.20399	9.359363	6.971512
RB975242	13.19739	6.360836	10.36547	13.09858	8.047209	10.39138	12.05219	11.2103	9.503351	11.29144	11.10982	8.858139	6.64873	11.46897	11.14189	9.492789	7.013171
RB975242	13.58751	7.204364	12.01978	13.50847	7.943009	10.21722	12.57372	11.04923	9.903487	12.04802	11.73664	9.262985	7.157085	11.01229	11.46142	9.471643	7.403651
RB975242	13.59432	6.692175	11.05299	13.70182	8.04587	10.27022	12.33684	11.43141	9.979749	11.55166	11.44609	9.40047	7.102838	11.10413	11.24032	9.674769	7.628563
RB975242	13.3482	6.802352	11.46103	13.6303	8.111908	10.94405	12.276	11.40205	9.813136	11.30916	10.78726	9.340027	6.749728	10.76201	11.20376	9.514061	7.323133
RB965902	14.08058	8.145188	11.65428	14.7957	8.502527	8.733456	13.19463	12.14785	9.701947	11.95391	11.99526	10.00619	7.514522	11.34838	12.01214	10.18788	8.013453
RB965902	14.90974	8.604423	12.57143	15.03689	9.217254	10.02942	13.74025	12.97194	10.17469	11.97691	11.94327	10.57515	7.434443	11.52112	12.68124	10.32164	8.456728
RB965902	14.76646	8.141369	12.66398	15.47197	9.107062	9.389767	13.47948	12.55847	10.25859	11.5254	11.23434	9.802927	7.210996	11.44986	12.43104	9.693281	8.571025
RB965902	14.00104	7.284841	11.74818	15.07725	8.663573	9.219863	13.18894	11.96495	9.744432	12.0525	11.48254	10.0255	7.039557	11.57973	11.94184	9.94429	8.075885
RB975375	12.338	4.294757	8.791714	13.58326	7.610874	9.890472	12.23082	10.52833	8.856383	9.737136	9.250368	7.674711	5.913709	9.308904	10.78222	8.569563	8.262227
RB975375	12.56883	5.819318	9.877211	13.58599	6.975856	10.30219	12.56684	10.99537	8.658226	10.29197	9.828679	8.263279	6.298851	9.339441	10.63746	8.54916	8.026193
RB975375	12.81342	5.470189	11.47854	13.58924	7.646886	10.56885	12.36882	11.49646	9.263187	10.52934	9.886523	8.449549	5.946042	9.655113	11.03556	9.27358	7.331798
RB935744	14.38519	5.535978	11.36282	14.33211	7.653392	9.859219	12.29636	12.40637	10.33953	10.48192	10.29155	8.201406	5.993069	10.93743	12.01471	9.450183	7.310159
RB935744	14.60533	6.021583	9.85242	14.63509	8.728173	8.716738	12.84068	11.99325	9.978732	10.82876	10.6711	9.361628	7.382102	12.25103	12.76366	9.596614	7.533642
RB935744	14.41349	6.504413	10.69819	14.70284	7.617501	9.749878	13.39159	11.5367	9.694008	10.98197	10.80565	8.862956	7.187465	11.40917	12.01034	9.439868	8.057404
RB935744	14.88133	6.545373	10.26886	14.9513	8.400203	8.928724	13.3852	11.88797	9.527136	11.02238	10.9161	8.948681	7.017351	11.21966	12.27113	9.899792	8.055196

Genotypes	Tyrosine	Valine	-Oxoprolin	Putrescine	s-Aconitat	Citrate	Pyruvate	Succinate	Benzoate	etoglucon	Caffeate	droxybenz	ydroascorl	Glycerate	lar to Itaco	Lactate	Nicotinate
	B21	B22	B23	B24	B26	B27	B29	B30	B31	B32	B33	B35	B36	B40	B41	B42	B43
RB985476	9.458494	12.67107	10.469	11.28551	7.049081	9.083575	5.921729	8.766557	8.197956	9.717549	9.417543	7.250443	5.872529	5.89361	8.501919	11.98617	7.480032
RB985476	9.327606	12.55319	9.600223	9.348189	7.074367	10.60956	5.816941	8.319088	7.930415	9.792191	8.82085	6.83818	5.842662	5.896344	7.587143	12.33128	6.599665
RB985476	10.27107	13.28246	11.29988	10.567	7.099653	10.64814	6.161834	9.067182	7.662874	9.866833	9.694671	7.443162	5.857595	6.028322	8.783706	12.06692	7.51447
RB855536	10.47259	12.59353	11.14025	9.794466	7.52	9.543609	6.673979	9.714018	8.051445	10.7387	9.957659	7.076864	6.120535	6.699463	9.205233	11.49013	7.234806
RB855536	9.663635	11.9338	10.7933	9.580319	7.52	9.344374	6.475431	9.438801	8.2993	10.14815	10.30314	7.350171	6.427548	6.675989	9.278827	11.68486	7.538478
RB855536	9.832254	12.31976	10.2423	9.569358	7.669395	9.133989	5.763629	9.12883	7.423335	10.51892	9.797337	6.826902	6.252089	6.522987	8.157941	11.1054	6.979815
RB855536	10.02405	12.83671	10.52091	9.651866	7.749883	9.512772	6.46409	9.424741	8.314792	10.54624	10.64599	7.70719	6.289073	7.018737	8.825451	11.4268	7.685689
RB855536	8.74665	12.22981	9.484645	8.991319	7.140722	10.01997	6.801678	9.334099	8.406736	10.1114	9.701676	7.864207	5.513431	6.405347	8.50789	11.4268	7.357978
RB867515	9.17607	11.41411	10.28249	8.214311	7.745628	NA	7.299166	9.972847	9.314388	9.004721	10.11376	7.259518	5.987206	6.589113	9.416926	12.74263	7.877104
RB867515	9.715793	12.15127	10.84229	7.997574	8.088683	NA	7.078835	9.716512	9.387782	9.210584	9.973222	7.167768	4.535392	6.889379	9.536885	11.53888	7.548019
RB867515	9.989422	12.42714	11.43845	6.969906	8.445279	NA	6.726896	9.690618	8.605525	9.800018	10.40962	8.127971	6.034189	6.628841	9.742098	12.86398	7.955812
RB867515	9.509143	11.58364	10.25872	8.920618	6.650663	NA	7.44855	9.827995	8.742468	9.655604	10.58725	7.883273	5.665094	7.266679	9.236387	12.17477	8.190251
RB867515	9.707945	12.28779	10.91401	8.680344	8.28587	NA	7.027287	9.71208	8.857561	9.568297	10.71159	8.0304	6.103587	6.975703	9.416758	12.8725	7.95447
RB92579	9.454654	11.53566	10.72783	9.050182	8.896483	9.603492	5.807277	8.747494	7.762827	9.566598	8.395311	5.713326	5.921379	6.309832	9.095922	11.30823	6.240165
RB92579	10.14748	12.494	11.0423	9.968986	8.619203	9.484964	6.705577	9.91432	7.922056	10.03912	9.981748	7.328057	6.199807	7.393194	9.275106	12.40616	6.240165
RB92579	9.810274	11.87775	10.94821	9.492679	8.530854	9.755092	6.837504	9.318295	7.809928	10.0763	9.602225	7.291676	6.757463	7.011752	9.377902	11.44189	7.533165
RB92579	10.00452	12.17837	10.81865	9.992941	6.718504	10.09757	6.766102	9.624464	8.328648	10.25416	9.813978	7.729437	7.008703	7.604879	9.052923	12.31812	7.297788
RB92579	9.273873	12.02326	10.51754	8.76454	8.312696	9.045924	6.012799	8.886998	7.786821	9.586694	9.458176	6.938101	6.519092	6.139527	8.700584	9.699097	7.079457
RB975242	9.769962	12.39166	9.715277	10.18713	8.579641	9.365738	6.295169	8.941214	7.976069	11.10504	9.506351	6.774976	6.327172	6.274971	8.336127	10.67223	6.972933
RB975242	9.665887	12.45797	9.94707	10.13444	7.981161	9.147221	6.395327	9.12414	8.051194	10.74909	9.755953	7.648082	4.725976	6.420993	8.83648	11.26023	7.34799
RB975242	9.907799	13.53227	10.44244	10.83019	9.092148	9.05283	6.294065	8.880763	8.084239	11.16433	9.380324	6.815737	6.339216	6.60777	8.371449	11.0226	6.812428
RB975242	9.528349	13.31381	10.22824	10.91551	7.843125	9.093231	5.997438	8.869376	7.756516	10.36287	9.860328	7.178106	6.453042	6.131654	8.525225	10.47644	7.297596
RB975242	9.858045	12.9667	10.1356	11.14297	8.919252	9.928794	6.513205	8.978654	8.387954	11.55017	9.57675	7.271207	5.961352	6.576818	8.193292	10.85788	7.18766
RB965902	10.55492	13.19396	10.95694	8.218509	8.023207	8.46007	5.977842	9.147174	8.239936	9.006692	10.10094	6.917098	4.831355	6.058355	9.301705	11.14975	7.915747
RB965902	11.15516	13.78279	11.48952	8.628037	8.475643	9.780323	6.449006	9.115595	7.730453	9.799844	9.774502	6.569474	5.723435	6.330962	9.243811	11.97057	7.667224
RB965902	10.05791	13.66024	11.29113	8.752202	9.248857	9.10042	6.403019	9.083512	8.50901	9.139674	9.563856	6.755811	6.337918	5.854074	9.4286	11.63935	7.59624
RB965902	10.00642	13.47227	10.98447	8.913399	8.154866	8.937165	6.420336	9.210835	8.578514	8.989559	10.18302	7.42601	6.001031	6.159491	9.14437	11.39595	7.913426
RB975375	9.087845	10.89806	10.07158	9.547993	8.188954	8.863331	6.086498	9.171504	8.36047	10.7477	9.539767	7.250259	7.122371	6.282748	8.831842	12.08295	7.245898
RB975375	8.899097	11.58715	10.43919	9.181643	8.98299	8.999648	6.364377	8.622205	7.778004	10.25129	8.608115	5.30604	6.679085	5.962829	7.987081	12.1609	6.216414
RB975375	9.322722	11.99473	10.28421	9.327895	8.505054	9.338133	6.190164	8.924151	7.776964	10.58216	8.63413	6.588829	6.548864	6.48009	8.664237	10.15108	6.848213
RB935744	9.427454	11.80139	10.1455	7.765088	8.056722	8.850301	5.970771	8.7539	7.911425	8.966548	8.444813	5.624435	4.931548	6.020783	7.625103	12.21358	5.978309
RB935744	10.36888	13.03561	10.67662	8.541123	8.145936	8.357581	6.579858	9.382896	8.33012	9.276752	10.48511	6.602714	3.825979	7.209499	9.494676	12.11145	7.713936
RB935744	10.17608	12.05689	11.11773	8.561598	8.617697	8.603941	6.281614	9.173714	8.162383	9.452601	10.50766	6.912501	4.833691	6.628713	9.210488	13.2084	6.846123
RB935744	10.02625	12.35092	11.16125	8.797518	8.89188	8.603941	6.107649	9.196316	8.096749	9.191197	10.27708	7.271207	5.743547	6.790743	9.362577	11.84007	7.571267

Genotypes	Quinate	Xylose	Fucose	Sorbose	Fructose	Galactose	lar to Ribu	Sucrose	Trehalose	Glycerol	yo-Inosito	Xylitol	Uracil	hophosph	Adenine	ptadecano	Decanoate	thanolami
	B45	B46	B47	B48	B49	B51	B52	B53	B54	B55	B57	B58	B59	B60	B61	B62	B65	B66
RB985476	14.75577	9.602949	7.436993	15.90904	16.11616	14.33203	4.736012	13.14177	7.609106	10.5163	13.39839	7.500523	7.686573	10.32389	5.807969	8.055355	4.633701	9.128574
RB985476	14.96911	9.521742	7.027319	16.31695	16.36534	14.35693	3.796517	13.03838	7.112084	10.73308	13.30213	8.402227	6.843187	11.10138	5.682584	7.687267	4.894785	8.148342
RB985476	15.19186	10.05088	7.591515	16.64364	16.24075	14.68326	4.606033	13.03645	7.08894	10.94986	14.17241	8.103204	7.666952	11.31262	6.205287	8.056454	5.069544	8.638458
RB855536	15.58989	10.81228	7.859814	16.23092	NA	15.15916	4.432591	13.47581	7.794695	12.17296	14.39278	9.314048	7.452456	13.94321	6.446757	7.459398	4.990286	9.590889
RB855536	15.26855	10.35699	7.697098	16.39623	NA	14.87777	4.653694	13.62407	8.134086	11.50501	14.06298	8.734521	7.513503	14.21724	6.50351	8.273016	4.705459	9.818689
RB855536	14.79757	10.33232	7.589468	15.90751	NA	14.34589	4.647643	12.76952	7.498229	10.96631	13.27962	8.685642	7.076263	13.11706	5.539114	7.086649	5.077602	8.269105
RB855536	15.32493	10.55561	7.887068	16.38901	NA	14.79427	4.656919	13.09864	7.415974	11.57977	13.56437	9.192692	7.929447	13.87755	6.672364	7.672954	5.046449	9.301843
RB855536	15.36182	9.72777	7.593227	16.23092	NA	14.79427	3.772106	12.19061	6.713073	11.11514	12.34066	7.549741	8.14658	14.13377	6.413497	6.804972	5.118717	8.368088
RB867515	7.925035	9.439995	7.702382	13.78462	11.68694	12.52691	4.918602	13.31669	8.313121	12.63938	12.56358	9.098991	7.913545	14.06174	6.346113	8.454452	6.127462	NA
RB867515	11.72832	9.849293	7.946002	14.29782	11.59929	13.29482	5.061962	13.12998	8.8209	12.69666	13.26907	10.60729	7.74065	14.10794	6.376364	8.97112	5.568387	NA
RB867515	13.55316	9.644644	7.977998	14.3153	11.86009	13.67103	4.281141	13.74651	8.731815	12.35694	12.95833	11.09807	8.628037	14.80087	7.100151	8.079826	6.000364	NA
RB867515	11.72832	10.22219	8.4001	14.34854	11.86009	14.06233	4.449416	12.32803	8.731815	12.19952	13.13803	11.52414	8.344041	13.59405	6.693697	7.76076	5.542696	NA
RB867515	13.70677	9.789031	8.380676	14.99642	12.29404	13.70695	4.808778	13.54388	9.061423	11.89221	12.96334	10.01595	8.35515	14.2018	6.706735	8.316539	6.238286	NA
RB92579	14.52371	9.816608	6.640819	15.63473	16.01547	14.26912	4.499145	13.36348	8.439069	11.4773	13.07175	8.185804	6.265843	13.79705	6.724646	7.335892	4.625823	7.710493
RB92579	15.41681	10.17009	8.083398	15.89548	16.12507	15.02216	4.409462	13.19171	8.428422	12.02956	13.61869	8.783214	7.97745	13.79641	7.447402	7.92989	4.988106	8.368088
RB92579	14.69721	9.816608	7.677605	15.58705	15.74003	14.2705	4.544651	13.63342	7.89152	11.08341	13.28773	9.153972	7.910344	13.32934	6.905271	7.137333	4.732268	6.510236
RB92579	14.8915	9.863682	7.972868	15.92394	15.99708	14.49454	4.668779	12.03723	8.25465	12.08008	14.28826	7.933833	7.898117	13.75698	7.021171	7.349279	4.912682	8.230344
RB92579	14.92828	9.416057	7.55779	16.43622	16.7477	14.63793	4.373687	12.63238	7.834141	10.71614	13.40872	8.936668	7.283809	13.38766	7.007365	7.089186	3.676176	8.345187
RB975242	15.13795	10.38473	6.856182	NA	16.43402	14.73814	3.925509	13.14168	7.658304	11.18794	13.2115	8.673231	7.287586	12.24718	5.758452	7.37864	4.566459	10.08357
RB975242	15.32552	10.40585	7.367792	NA	16.46717	14.897	4.058447	13.0669	7.887001	11.38954	13.16935	9.181608	7.330676	11.49635	6.410369	8.284243	4.857497	10.95312
RB975242	14.66007	10.7148	7.430261	NA	16.34494	14.34666	4.399474	13.28893	7.538501	11.35522	13.30611	8.748212	7.080026	12.20669	5.940917	7.32137	4.368809	10.17955
RB975242	14.84285	10.3067	7.591515	NA	16.02411	14.38675	4.195429	13.2992	7.703844	11.15626	13.0925	8.936668	7.390868	11.60633	6.055593	8.216182	4.267929	10.33113
RB975242	15.65642	10.52996	7.49366	NA	17.05701	14.59214	4.398286	13.77802	7.971057	11.44441	13.69386	9.312519	7.564224	12.21545	5.919706	8.362086	4.771601	10.29638
RB965902	14.49075	9.548526	7.574508	15.38109	15.62501	14.45333	4.758259	13.26255	7.798454	11.44944	13.51286	8.181984	8.139014	14.24007	6.758663	7.979183	5.006352	8.368088
RB965902	14.9174	10.36247	7.367883	15.27207	15.00831	14.61065	4.691162	13.5248	8.135698	11.61209	14.38506	8.818894	7.057209	14.94769	6.679548	7.92983	4.022117	8.138164
RB965902	13.34915	9.968889	7.517257	14.40583	14.3916	13.57631	4.838636	13.67401	8.12641	11.11158	13.40161	9.125643	7.288912	14.92986	6.316687	8.829342	5.218694	8.229967
RB965902	14.63779	10.10684	7.818443	16.02931	15.00831	14.5708	5.066488	13.43167	8.383378	11.24461	13.27011	8.70884	7.775621	14.2354	6.329416	8.333113	4.995594	7.890529
RB975375	14.84173	9.98009	7.676291	16.01609	16.0289	14.43486	4.173849	12.89187	7.56539	11.2104	13.22711	8.357416	7.654577	12.40308	6.57218	7.694647	4.82637	9.98815
RB975375	14.92852	10.12526	6.723926	15.88962	16.25089	14.53122	2.670606	13.24945	7.735588	11.01687	12.77098	8.479289	5.784503	11.85429	6.434424	7.181162	4.995594	9.465486
RB975375	14.89224	10.33919	7.496653	16.01405	16.20732	14.50904	4.046744	13.42626	7.662628	11.23386	12.96643	8.594682	7.006508	12.78617	6.73841	6.778632	3.930411	9.563184
RB935744	14.78796	9.659243	6.262339	15.90286	16.10613	14.48218	2.830573	13.24396	7.712845	11.19371	12.74436	8.36814	6.062656	13.58942	5.53837	7.449244	4.271282	6.051905
RB935744	14.45944	9.827453	7.608324	15.85509	15.81642	14.5121	3.155981	11.76218	6.447762	11.99745	13.71354	8.424162	6.989809	14.76205	6.680113	7.426414	5.000883	6.768926
RB935744	14.21995	9.491033	7.385433	15.33885	15.33637	14.22094	3.155981	12.77473	7.947883	11.3003	13.65839	9.076027	7.181134	14.64174	5.84619	7.915868	5.003043	5.449914
RB935744	14.43497	9.659243	7.75787	15.8184	16.00677	14.40507	3.481389	13.23008	7.369497	11.47559	13.31429	8.622776	7.725637	13.93759	6.6874	7.630407	5.094987	5.936876

Supplementary Table 3. Metabolite-metabolite correlations for culm. Significant pairwise correlations within and between tissues (r ≥ 0.5, p ≤ 0.05) were highlighted in blue and yellow, representing positive and negative correlations, respectively.

Metabolites		Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Histidine	Isoleucine	Leucine	Lysine	Methionine	Ornithine	Phenylalanine	Serine
		C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C18
Alanine	C1	0	0.28370354	0.53498847	0.66382756	0.73100185	-0.16821626	0.59253625	0.19071976	0.62108019	0.18980212	0.3213509	0.14871465	0.24262094	0.15030752	0.222998	0.01170645	0.45573889
Arginine	C2	0.28370354	0	0.57474414	0.26365789	0.50672543	-0.15963246	0.54934811	0.35833288	0.54321931	0.12267332	0.59783578	0.34328362	0.29154195	-0.04086042	0.48327853	0.08887135	0.43233495
Asparagine	C3	0.53498847	0.57474414	0	0.55528627	0.63537886	-0.40597815	0.5697216	0.53391772	0.60253685	-0.05050577	0.5974521	0.48546198	0.15003554	-0.05899274	0.68875212	-0.10251881	0.60729645
Aspartate	C4	0.66382756	0.26365789	0.55528627	0	0.63093708	-0.22572617	0.52213489	0.27857991	0.38459481	0.10448625	0.3553618	0.23019816	0.15760081	0.10061829	0.23494047	-0.00463407	0.38229878
b-Alanine	C5	0.73100185	0.50672543	0.63537886	0.63093708	0	-0.28945197	0.69408227	0.44052826	0.64930874	0.08007193	0.57238018	0.39563946	0.07491348	-0.05472748	0.47676209	-0.0856336	0.60239558
GABA	C6	-0.16821626	-0.15963246	-0.40597815	-0.22572617	-0.28945197	0	-0.53116539	-0.81311236	-0.30904515	0.75035689	-0.71240852	-0.84026166	0.59945302	0.62588779	-0.36655326	0.72204737	-0.73669167
Glutamate	C7	0.59253625	0.54934811	0.5697216	0.52213489	0.69408227	-0.53116539	0	0.59728918	0.60642665	-0.23153331	0.6552939	0.56578161	-0.07192823	-0.36594455	0.3887039	-0.4310424	0.69571123
Glutamine	C8	0.19071976	0.35833288	0.53391772	0.27857991	0.44052826	-0.81311236	0.59728918	0	0.40410807	-0.7402414	0.86001296	0.96877458	-0.63498785	-0.76761576	0.69606186	-0.71313107	0.92096391
Glycine	C9	0.62108019	0.54321931	0.60253685	0.38459481	0.64930874	-0.30904515	0.60642665	0.40410807	0	0.02637861	0.55846746	0.374303	0.13594596	-0.11632637	0.52042563	-0.10152578	0.6036229
Histidine	C10	0.18980212	0.12267332	-0.05050577	0.10448625	0.08007193	0.75035689	-0.23153331	-0.7402414	0.02637861	0	-0.49660685	-0.77745014	0.82338376	0.85185282	-0.24903325	0.88844097	-0.61026898
Isoleucine	C11	0.3213509	0.59783578	0.5974521	0.3553618	0.57238018	-0.71240852	0.6552939	0.86001296	0.55846746	-0.49660685	0	0.89095113	-0.32958604	-0.51234461	0.65008911	-0.48692181	0.88512031
Leucine	C12	0.14871465	0.34328362	0.48546198	0.23019816	0.39563946	-0.84026166	0.56578161	0.96877458	0.374303	-0.77745014	0.89095113	0	-0.6396209	-0.74883253	0.6375196	-0.73154262	0.91442738
Lysine	C13	0.24262094	0.29154195	0.15003554	0.15760081	0.07491348	0.59945302	-0.07192823	-0.63498785	0.13594596	0.82338376	-0.32958604	-0.6396209	0	0.7730851	-0.26536228	0.73640449	-0.48828427
Methionine	C14	0.15030752	-0.04086042	-0.05899274	0.10061829	-0.05472748	0.62588779	-0.36594455	-0.76761576	-0.11632637	0.85185282	-0.51234461	-0.74883253	0.7730851	0	-0.33379868	0.87739324	-0.65791415
Ornithine	C15	0.222998	0.48327853	0.68875212	0.23494047	0.47676209	-0.36655326	0.3887039	0.69606186	0.52042563	-0.24903325	0.65008911	0.6375196	-0.26536228	-0.33379868	0	-0.23794674	0.68336283
Phenylalanir	C16	0.01170645	0.08887135	-0.10251881	-0.00463407	-0.0856336	0.72204737	-0.4310424	-0.71313107	-0.10152578	0.88844097	-0.48692181	-0.73154262	0.73640449	0.87739324	-0.23794674	0	-0.63998504
Serine	C18	0.45573889	0.43233495	0.60729645	0.38229878	0.60239558	-0.73669167	0.69571123	0.92096391	0.6036229	-0.61026898	0.88512031	0.91442738	-0.48828427	-0.65791415	0.68336283	-0.63998504	0
Threonine	C19	0.32705094	0.557735	0.59414134	0.34093048	0.56192849	-0.66550318	0.57669519	0.89170399	0.52151359	-0.51891587	0.8830818	0.86780016	-0.41794633	-0.60481085	0.71591476	-0.50909909	0.8922287
Tryptophan	C20	0.29579439	0.2372861	0.45913069	0.44698197	0.3097856	0.39095987	-0.00863048	0.41897976	0.33450175	0.52015331	0.56054925	0.48097165	0.38036296	0.47724336	0.51588331	0.58581278	0.49610755
Tyrosine	C21	0.24152614	0.62015385	0.38418704	0.3900582	0.37711059	0.16207131	0.29916001	0.33063946	0.26669398	0.62449541	0.68353645	0.62514584	0.56940932	0.59124656	0.32393768	0.66425451	0.40019652
Valine	C22	0.39513348	0.83008455	0.61386292	0.47528327	0.56362824	0.27350983	0.38500598	0.69327648	0.55136242	0.72605641	0.92443701	0.85905068	0.77962303	0.91693057	0.61858769	0.81490062	0.59967282
5-Oxoprolin	C23	0.62527949	0.41155047	0.35004152	0.62839888	0.64800079	-0.294652	0.78114741	0.27808186	0.45514094	0.10246151	0.36889647	0.2270536	0.09669256	-0.02176886	0.16151977	-0.07863923	0.35355158
Putrescine	C24	-0.1226277	-0.23917436	-0.43132752	-0.22929317	-0.33516241	0.79129076	-0.55667533	-0.95220447	-0.32154104	0.812678	-0.78630026	-0.94536017	0.71469088	0.82119925	-0.61406491	0.79528121	-0.89125259
Fumarate	C25	-0.29766643	-0.52285894	-0.40287884	-0.22259983	-0.4281999	0.21905523	-0.57489677	-0.39503849	-0.55839959	0.18329145	-0.50324194	-0.39476305	-0.02507464	0.33087001	-0.33426278	0.3088433	-0.54005131
cis-Aconitate	C26	0.30087722	0.13993459	0.27174422	0.49201057	0.31363605	-0.52631025	0.48326983	0.63521323	0.21455025	-0.51175776	0.59583823	0.62184912	-0.39610926	-0.52632719	0.20456199	-0.53245658	0.62912551
Citrate	C27	0.10415427	-0.09721656	0.14315173	0.17577793	0.14533514	-0.14159654	0.27974431	0.36455567	-0.04505247	-0.23843634	0.2084877	0.31647392	-0.36372475	-0.31919382	0.32582056	-0.32626151	0.31792891
Isocitrate	C28	0.39612322	0.63141918	0.71310973	0.45896197	0.62417803	-0.52095547	0.74177953	0.77102263	0.58976985	-0.3540647	0.77274851	0.70541219	-0.1291296	-0.45364763	0.66729851	-0.43723267	0.77625815
Succinate	C30	0.24369807	0.13187888	0.48041135	0.32914943	0.32172677	-0.42024305	0.48566777	0.37486635	0.38192547	-0.37370332	0.37196219	0.41407141	-0.0940266	-0.30344052	0.24535998	-0.43871641	0.4663776
Benzoate	C31	-0.11321955	-0.35514133	-0.43830469	-0.12857351	-0.35935769	0.78128592	-0.57322162	-0.95291273	-0.38754215	0.78893925	-0.82475737	-0.9561721	0.6434407	0.83818452	-0.62267819	0.77946408	-0.90675509
4-Coumarate	C34	-0.024552	-0.23738347	0.19573153	0.12136383	0.02328487	-0.29936785	0.0235239	0.32894784	-0.10217179	-0.3365716	0.11747826	0.29124662	-0.36056845	-0.31510768	0.19028944	-0.24195357	0.20959754
4-Hydroxybe	C35	-0.08527221	-0.18061686	0.14988547	0.07503657	0.08579716	-0.15612992	-0.06417439	0.07223464	-0.15099528	-0.13695456	-0.05768833	0.07648659	-0.18347378	-0.07204485	0.08164503	-0.09895137	0.0023851
Dehydroascc	C36	-0.01032262	-0.22856784	0.02616612	0.24346742	0.07659451	-0.38065939	0.22448393	0.38462206	-0.14942442	-0.4535667	0.27438902	0.39804038	-0.41820896	-0.3445828	0.02828585	-0.43986304	0.28965766
5-Caffeoylqu	C37	0.17781504	0.07581028	0.12828207	0.17910692	0.12548289	0.02302419	0.0985826	-0.11565731	-0.0147153	0.0920814	-0.07389169	-0.1206689	0.11340463	0.17247354	-0.03703109	0.01955599	-0.06220025
Galacturonat	C38	-0.02583617	-0.22321513	-0.33516848	-0.06510069	-0.27674384	0.83176034	-0.45927178	-0.94301512	-0.27027586	0.85576117	-0.78658156	-0.96433493	0.77588619	0.83870389	-0.57715904	0.81081348	-0.865136
Glucarate	C39	0.41136771	0.02061345	0.23312698	0.44474038	0.28730129	0.27522117	0.15584733	-0.2311031	0.11642305	0.50558211	-0.13666814	-0.27535992	0.47017946	0.44030575	0.04929174	0.47275139	-0.12885619
Glycerate	C40	0.3360046	0.14887737	0.45330937	0.25707469	0.33334532	-0.60905237	0.4948608	0.54899056	0.37325418	-0.54162295	0.58781457	0.61230814	-0.27980686	-0.46316697	0.27647934	-0.61490613	0.6590532
Similar to Ita	C41	-0.07533732	-0.24596461	-0.40640672	-0.10281144	-0.30314838	0.87561155	-0.51314626	-0.93875234	-0.32337629	0.8324469	-0.78898848	-0.95997661	0.72699514	0.7922984	-0.59252326	0.80294291	-0.86713885
Nicotinate	C43	-0.19954206	-0.16736376	-0.38887019	-0.19681134	-0.30499189	0.87264193	-0.50731088	-0.89894889	-0.34945234	0.80430174	-0.78137776	-0.92990814	0.67301969	0.69894789	-0.52952549	0.75146326	-0.86255905
Quinate	C44	-0.26028148	0.19301364	0.1463367	-0.12965514	0.02596234	-0.51411445	0.20721178	0.65964914	0.09535873	-0.68817715	0.57442099	0.7008295	-0.61153346	-0.69813221	0.35071421	-0.66813814	0.57724849
Xylose	C46	-0.40814371	-0.03160448	-0.44579962	-0.42224232	-0.40856627	0.87067239	-0.50547548	-0.70556419	-0.33056686	0.56637545	-0.63095732	-0.71465611	0.48105555	0.43087094	-0.30538933	0.55415747	-0.69608858
Fructose	C49	0.01911689	0.23359229	0.3255339	-0.01921865	0.25088602	-0.82490407	0.47098778	0.8176969	0.30397055	-0.80533678	0.72167776	0.87907394	-0.6277202	-0.76416572	0.42689219	-0.81753675	0.78302581
Glucose	C50	-0.10168729	0.09602716	0.11796161	-0.26507699	0.08723755	-0.63825149	0.31330947	0.6152093	0.20225044	-0.72690115	0.51413667	0.68703711	-0.55937908	-0.65566817	0.31228043	-0.71939345	0.56939254
Sucrose	C53	0.114955	0.24347995	0.43974408	0.23873333	0.3520564	-0.83501693	0.5754748	0.96386506	0.35201256	-0.82388991	0.81336388	0.96259141	-0.70123038	-0.8358923	0.60371925	-0.81134483	0.89279506
Glycerol	C55	-0.00304729	0.14660761	0.29327989	0.11186619	0.19733146	-0.54411376	0.43202936	0.62959578	0.27700893	-0.58650985	0.46811681	0.62262765	-0.45823319	-0.68565564	0.38542908	-0.69023177	0.56472253
Galactinol	C56	-0.0099802	0.00282919	-0.10746605	-0.13448077	0.06883033	0.0808158	0.07368056	-0.32048833	0.04364159	0.32274323	-0.29673401	-0.33314395	0.20443295	0.22613693	-0.26146639	0.16710819	-0.33767703
myo-Inositol	C57	0.14997586	0.32328052	0.45467845	0.1744544	0.36754427	-0.83664433	0.60277431	0.9410296	0.36927787	-0.81169992	0.82921011	0.95728129	-0.62796619	-0.80552413	0.56551734	-0.81485574	0.90062551
Xylitol	C58	0.01222951	0.1423183	0.0309527	0.30660039	0.22077844	-0.13782631	0.20107468	0.07026118	0.08027902	0.24503892	0.01788285	0.01098109	0.05920381	-0.02541697	0.09522575	0.14845342	-0.03525543
Adenine	C61	0.26098816	-0.277244	0.05067524	0.33463356	0.12386861	-0.27002204	0.10015908	0.27316848	-0.05626705	-0.23284636	0.17601271	0.23371018	-0.29895106	-0.25702931	-0.00199998	-0.37387394	0.25713154
Heptadecan	C62	0.26348792	-0.04098739	0.45243005	0.42584403	0.25578994	-0.66287645	0.31645826	0.53478561	0.20138553	-0.4660241	0.4369842	0.53611709	-0.35769559	-0.22985444	0.32395469	-0.40679036	0.47721909
Tetradecano	C63	-0.11793877	-0.18196058	-0.39682241	-0.25405115	-0.33163634	0.74494895	-0.47113399	-0.95190422	-0.2500115	0.78939853	-0.75170474	-0.9283247	0.75364118	0.80834997	-0.62039213	0.74439638	-0.86408052
2-Hydroxypy	C64	-0.46774969	-0.43506848	-0.24674975	-0.27242257	-0.37356865	-0.09697956	-0.27297571	-0.08765084	-0.46578261	-0.25313764	-0.26229182	-0.0552525	-0.31631642	-0.14721175	-0.25083459	-0.1227018	-0.23284507

Metabolites		Threonine	Tryptophan	Tyrosine	Valine	5-Oxoproline	Putrescine	Fumarate	cis-Aconitate	Citrate	Isocitrate	Succinate	Benzoate	4-Coumarate	ydroxybenzo	hydroascorb	Caffeoylquin	Galacturonat
		C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C30	C31	C34	C35	C36	C37	C38
Alanine	C1	0.32705094	0.29579439	0.24152614	0.39513348	0.62527949	-0.1226277	-0.29766643	0.30087722	0.10415427	0.39612322	0.24369807	-0.11321955	-0.024552	-0.08527221	-0.01032262	0.17781504	-0.02583617
Arginine	C2	0.557735	0.2372861	0.62015385	0.83008455	0.41155047	-0.23917436	-0.52285894	0.13993459	-0.09721656	0.63141918	0.13187888	-0.35514133	-0.23738347	-0.18061686	-0.22856784	0.07581028	-0.22321513
Asparagine	C3	0.59414134	0.45913069	0.38418704	0.61386292	0.35004152	-0.43132752	-0.40287884	0.27174422	0.14315173	0.71310973	0.48041135	-0.43830469	0.19573153	0.14988547	0.02616612	0.12828207	-0.33516848
Aspartate	C4	0.34093048	0.44698197	0.3900582	0.47528327	0.62839888	-0.22929317	-0.22259983	0.49201057	0.17577793	0.45896197	0.32914943	-0.12857351	0.12136383	0.07503657	0.24346742	0.17910692	-0.06510069
b-Alanine	C5	0.56192849	0.3097856	0.37711059	0.56362824	0.64800079	-0.33516241	-0.4281999	0.31363605	0.14533514	0.62417803	0.32172677	-0.35935769	0.02328487	0.08579716	0.07659451	0.12548289	-0.27674384
GABA	C6	-0.66550318	0.39095987	0.16207131	0.27350983	-0.294652	0.79129076	0.21905523	-0.52631025	-0.14159654	-0.52095547	-0.42024305	0.78128592	-0.29936785	-0.15612992	-0.38065939	0.02302419	0.83176034
Glutamate	C7	0.57669519	-0.00863048	0.29916001	0.38500598	0.78114741	-0.55667533	-0.57489677	0.48326983	0.27974431	0.74177953	0.48566777	-0.57322162	0.0235239	-0.06417439	0.22448393	0.0985826	-0.45927178
Glutamine	C8	0.89170399	0.41897976	0.33063946	0.69327648	0.27808186	-0.95220447	-0.39503849	0.63521323	0.36455567	0.77102263	0.37486635	-0.95291273	0.32894784	0.07223464	0.38462206	-0.11565731	-0.94301512
Glycine	C9	0.52151359	0.33450175	0.26669398	0.55136242	0.45514094	-0.32154104	-0.55839959	0.21455025	-0.04505247	0.58976985	0.38192547	-0.38754215	-0.10217179	-0.15099528	-0.14942442	-0.0147153	-0.27027586
Histidine	C10	-0.51891587	0.52015331	0.62449541	0.72605641	0.10246151	0.812678	0.18329145	-0.51175776	-0.23843634	-0.3540647	-0.37370332	0.78893925	-0.3365716	-0.13695456	-0.4535667	0.0920814	0.85576117
Isoleucine	C11	0.8830818	0.56054925	0.68353645	0.92443701	0.36889647	-0.78630026	-0.50324194	0.59583823	0.2084877	0.77274851	0.37196219	-0.82475737	0.11747826	-0.05768833	0.27438902	-0.07389169	-0.78658156
Leucine	C12	0.86780016	0.48097165	0.62514584	0.85905068	0.2270536	-0.94536017	-0.39476305	0.62184912	0.31647392	0.70541219	0.41407141	-0.9561721	0.29124602	0.07648659	0.39804038	-0.1206689	-0.96433493
Lysine	C13	-0.41794633	0.38036296	0.56940932	0.77962303	0.09669256	0.71469088	-0.02507464	-0.39610926	-0.36372475	-0.1291296	-0.0940266	0.6434407	-0.36056845	-0.18347378	-0.41820896	0.11340463	0.77588619
Methionine	C14	-0.60481085	0.47724336	0.59124656	0.91693057	-0.02176886	0.82119925	0.33087001	-0.52632719	-0.31919382	-0.45364763	-0.30344052	0.83818452	-0.31510768	-0.07204485	-0.3445828	0.17247354	0.83870389
Ornithine	C15	0.71591476	0.51588331	0.32393768	0.61858769	0.16151977	-0.61406491	-0.33426278	0.20456199	0.32582056	0.66729851	0.24535998	-0.62267819	0.19028944	0.08164503	0.02828585	-0.03703109	-0.57715904
Phenylalanir	C16	-0.50909909	0.58581278	0.66425451	0.81490062	-0.07863923	0.79528121	0.3088433	-0.53245658	-0.32626151	-0.43723267	-0.43871641	0.77946408	-0.24195357	-0.09895137	-0.43986304	0.01955599	0.81081348
Serine	C18	0.8922287	0.49610755	0.40019652	0.59967282	0.35355158	-0.89125259	-0.54005131	0.62912551	0.31792891	0.77625815	0.4663776	-0.90675509	0.20959754	0.0023851	0.28965766	-0.06220025	-0.865136
Threonine	C19	0	0.55793074	0.58354031	0.87426956	0.33661542	-0.81794085	-0.47374201	0.54503982	0.22890042	0.78171998	0.2570872	-0.84961984	0.17858483	0.01982462	0.19615296	-0.10099416	-0.82173924
Tryptophan	C20	0.55793074	0	0.50144269	0.47896849	0.03166436	-0.25973964	-0.07207938	0.25418165	0.28938898	0.19780259	-0.12936879	-0.06376147	0.10231055	0.03237592	-0.00166641	-0.2641515	0.09664704
Tyrosine	C21	0.58354031	0.50144269	0	0.64584391	0.36792226	-0.07116196	-0.2564295	0.28210858	0.25508043	0.29675902	-0.45011081	-0.43770984	-0.26917763	-0.22613716	0.02911431	0.00184487	0.01645968
Valine	C22	0.87426956	0.47896849	0.64584391	0	0.42411367	0.02735404	-0.43907234	-0.01778252	-0.08655747	0.63835778	-0.56803659	-0.41523647	-0.19155156	-0.25841544	-0.23135454	-0.07052621	-0.06170025
5-Oxoprolin	C23	0.33661542	0.03166436	0.36792226	0.42411367	0	-0.20365185	-0.25109589	0.34471518	0.17659584	0.44097698	0.09218056	-0.17948549	-0.05018207	-0.05035465	0.14756069	0.09228406	-0.11594034
Putrescine	C24	-0.81794085	-0.25973964	-0.07116196	0.02735404	-0.20365185	0	0.42066707	-0.68530627	-0.44718153	-0.70950554	-0.4733125	0.94663214	-0.3232644	-0.12032847	-0.47762664	0.03572284	0.94269602
Fumarate	C25	-0.47374201	-0.07207938	-0.2564295	-0.43907234	-0.25109589	0.42066707	0	-0.33947522	-0.06043833	-0.65546085	-0.51578146	0.47181407	0.33092626	0.31522631	0.02307	-0.19659289	0.34125869
cis-Aconitate	C26	0.54503982	0.25418165	0.28210858	-0.01778252	0.34471518	-0.68530627	-0.33947522	0	0.53952997	0.5130728	0.35744261	-0.60612867	0.1437055	-0.05823406	0.54171579	0.08632201	-0.55204753
Citrate	C27	0.22890042	0.28938898	0.25508043	-0.08655747	0.17659584	-0.44718153	-0.06043833	0.53952997	0	0.21854063	0.1516704	-0.32357999	0.18981055	0.04873778	0.48940512	0.04824933	-0.29798125
Isocitrate	C28	0.78171998	0.19780259	0.29675902	0.63835778	0.44097698	-0.70950554	-0.65546085	0.5130728	0.21854063	0	0.4990906	-0.72822967	0.0538744	-0.08847458	0.25690023	0.06810876	-0.59417784
Succinate	C30	0.2570872	-0.12936879	-0.45011081	-0.56803659	0.09218056	-0.4733125	-0.51578146	0.35744261	0.1516704	0.4990906	0	-0.40672558	0.15822082	0.18571584	0.20473162	0.20760889	-0.34836196
Benzoate	C31	-0.84961984	-0.06376147	-0.43770984	-0.41523647	-0.17948549	0.94663214	0.47181407	-0.60612867	-0.32357999	-0.72822967	-0.40672558	0	-0.25388885	-0.03354711	-0.35740101	0.07839696	0.95423924
4-Coumarate	C34	0.17858483	0.10231055	-0.26917763	-0.19155156	-0.05018207	-0.3232644	0.33092626	0.1437055	0.18981055	0.0538744	0.15822082	-0.25388885	0	0.45193488	0.25288718	-0.16408228	-0.30508561
4-Hydroxybe	C35	0.01982462	0.03237592	-0.22613716	-0.25841544	-0.05035465	-0.12032847	0.31522631	-0.05823406	0.04873778	-0.08847458	0.18571584	-0.03354711	0.45193488	0	-0.01209146	-0.02364674	-0.10068701
Dehydroascc	C36	0.19615296	-0.00166641	0.02911431	-0.23135454	0.14756069	-0.47762664	0.02307	0.54171579	0.48940512	0.25690023	0.20473162	-0.35740101	0.25288718	-0.01209146	0	-0.06164001	-0.36525672
5-Caffeoylqu	C37	-0.10099416	-0.2641515	0.00184487	-0.07052621	0.09228406	0.03572284	-0.19659289	0.08632201	0.04824933	0.06810876	0.20760889	0.07839696	-0.16408228	-0.02364674	-0.06164001	0	0.1441984
Galacturonat	C38	-0.82173924	0.09664704	0.01645968	-0.06170025	-0.11594034	0.94269602	0.34125869	-0.55204753	-0.29798125	-0.59417784	-0.34836196	0.95423924	-0.30508561	-0.10068701	-0.36525672	0.1441984	0
Glucarate	C39	-0.22591934	0.34048478	0.27519575	0.23381408	0.29805695	0.28947926	0.05402736	0.0302805	0.25880031	0.01968233	0.05882383	0.32672481	0.00531271	-0.06355863	0.00905098	0.01496753	0.4257067
Glycerate	C40	0.48367082	0.08545462	-0.15601427	-0.43718182	0.13949203	-0.59942951	-0.39810755	0.55416007	0.21362886	0.47967581	0.72845025	-0.59871914	0.15630334	0.0751114	0.28301088	0.07954006	-0.55789688
Similar to Ita	C41	-0.80122619	0.33336373	0.18770704	-0.10137742	-0.16083544	0.92186879	0.34062321	-0.49459621	-0.23806579	-0.62135542	-0.40037546	0.94179796	-0.32147762	-0.11508548	-0.3374616	0.11662377	0.97709266
Nicotinate	C43	-0.75789296	0.0102698	-0.04912998	-0.18218921	-0.20749573	0.88770165	0.3582759	-0.58764995	-0.30182469	-0.60552398	-0.40792398	0.88082334	-0.25317801	0.04173239	-0.41509111	0.11702029	0.92232673
Quinate	C44	0.56693487	0.04705208	0.06177572	-0.17265539	-0.13346197	-0.73337472	-0.32175462	0.49777842	0.27202653	0.40309778	0.31300611	-0.73237555	0.17304973	0.07332346	0.35837955	-0.05841047	-0.75202496
Xylose	C46	-0.5937588	-0.35928315	-0.02642573	-0.01677076	-0.38134516	0.67470584	0.1372345	-0.56760803	-0.24388652	-0.44503125	-0.38518363	0.60375325	-0.34455668	-0.15065101	-0.43099254	0.08021582	0.67552845
Fructose	C49	0.70414178	-0.35175863	-0.05837761	-0.22606874	0.10346283	-0.82693775	-0.40506631	0.42890897	0.1346771	0.54553023	0.47705109	-0.87982597	0.20213582	0.08688875	0.34335029	-0.16737036	-0.9083972
Glucose	C50	0.48739513	-0.45050742	-0.09698199	-0.28928048	0.02277027	-0.64919913	-0.33853098	0.26037634	0.1306427	0.40485637	0.33661957	-0.7074581	0.02694171	-0.05355595	0.33290878	-0.14789796	-0.74017925
Sucrose	C53	0.81466152	0.26098035	0.05993469	-0.01203834	0.21849918	-0.96723034	-0.394012	0.65433182	0.38299884	0.69767875	0.47200332	-0.95486808	0.34876334	0.13105305	0.46879234	-0.12944931	-0.94885147
Glycerol	C55	0.46864728	-0.23129457	-0.21018804	-0.26887433	0.13160989	-0.65470097	-0.38016889	0.44162998	0.24866573	0.48429718	0.48841055	-0.66741915	0.1941184	0.2558664	0.08152138	0.08049071	-0.6204612
Galactinol	C56	-0.31224963	-0.44616748	-0.09276467	-0.09823583	0.24953782	0.37189136	0.10831386	-0.38138606	-0.17198703	-0.21560916	-0.05748545	0.31433919	-0.122928	0.09661801	-0.3490823	0.26215903	0.30281032
myo-Inositol	C57	0.81034784	-0.27988064	-0.06550455	0.05642673	0.21970987	-0.92493947	-0.4624916	0.6126746	0.28064773	0.70272387	0.48316789	-0.96026927	0.27746724	0.04667808	0.36926311	-0.10477009	-0.94614074
Xylitol	C58	-0.05373666	0.07222774	0.16380739	0.04608759	0.35005815	0.13466284	0.07976216	0.13290328	0.12325112	-0.02460672	0.0763489	0.03393138	-0.00692014	0.09653497	-0.12824397	0.20057309	0.26515115
Adenine	C61	0.1958817	0.30866671	-0.00623427	-0.20892263	0.13372244	-0.24538889	0.14842875	0.52668907	0.37413887	-0.00605566	-0.03692984	-0.20323913	0.35795119	0.08775043	0.2671499	-0.06168243	-0.22711588
Heptadecanc	C62	0.33252185	-0.02033379	-0.32828945	0.00203535	0.19029296	-0.47260747	-0.04665764	0.36966367	0.11746133	0.3441503	0.43924291	-0.40501823	0.45555724	0.17483633	0.28569336	0.01467074	-0.47064945
Tetradecano	C63	-0.82485232	-0.38781058	-0.07154714	-0.20630145	-0.17717711	0.95667061	0.29950837	-0.67311665	-0.46710258	-0.64628305	-0.32241638	0.91699035	-0.40580313	-0.13850684	-0.44651147	0.07783875	0.93031483
2-Hydroxypy	C64	-0.27218309	-0.15918569	-0.36434268	-0.53054401	-0.31466678	-0.01776768	0.47363088	-0.07653753	0.14255648	-0.39336887	0.16329701	0.09557849	0.50622635	0.55496323	0.14576953	-0.12330228	-0.03305286

Metabolites		Glucarate	Glycerate	ilar to Itacon	Nicotinate	Quinate	Xylose	Fructose	Glucose	Sucrose	Glycerol	Galactinol	myo-Inositol	Xylitol	Adenine	eptadecanoa	etradecanoat	ydroxypyridi
		C39	C40	C41	C43	C44	C46	C49	C50	C53	C55	C56	C57	C58	C61	C62	C63	C64
Alanine	C1	0.41136771	0.3360046	-0.07533732	-0.19954206	-0.26028148	-0.40814371	0.01911689	-0.10168729	0.114955	-0.00304729	-0.0099802	0.14997586	0.01222951	0.26098816	0.26348792	-0.11793877	-0.46774969
Arginine	C2	0.02061345	0.14887737	-0.24596461	-0.16736376	0.19301364	-0.03160448	0.23359229	0.09602716	0.24347995	0.14660761	0.00282919	0.32328052	0.1423183	-0.277244	-0.04098739	-0.18196058	-0.43506848
Asparagine	C3	0.23312698	0.45330937	-0.40640672	-0.38887019	0.1463367	-0.44579962	0.3255339	0.11796161	0.43974408	0.29327989	-0.10746605	0.45467845	0.0309527	0.05067524	0.45243005	-0.39682241	-0.24674975
Aspartate	C4	0.44474038	0.25707469	-0.10281144	-0.19681134	-0.12965514	-0.42224232	-0.01921865	-0.26507699	0.23873333	0.11186619	-0.13448077	0.1744544	0.30660039	0.33463356	0.42584403	-0.25405115	-0.27242257
b-Alanine	C5	0.28730129	0.33334532	-0.30314838	-0.30499189	0.02596234	-0.40856627	0.25088602	0.08723755	0.3520564	0.19733146	0.06883033	0.36754427	0.22077844	0.12386861	0.25578994	-0.33163634	-0.37356865
GABA	C6	0.27522117	-0.60905237	0.87561155	0.87264193	-0.51411445	0.87067239	-0.82490407	-0.63825149	-0.83501693	-0.54411376	0.0808158	-0.83664433	-0.13782631	-0.27002204	-0.66287645	0.74494895	-0.09697956
Glutamate	C7	0.15584733	0.4948608	-0.51314626	-0.50731088	0.20721178	-0.50547548	0.47098778	0.31330947	0.5754748	0.43202936	0.07368056	0.60277431	0.20107468	0.10015908	0.31645826	-0.47113399	-0.27297571
Glutamine	C8	-0.2311031	0.54899056	-0.93875234	-0.89894889	0.65964914	-0.70556419	0.8176969	0.6152093	0.96386506	0.62959578	-0.32048833	0.9410296	0.07026118	0.27316848	0.53478561	-0.95190422	-0.08765084
Glycine	C9	0.11642305	0.37325418	-0.32337629	-0.34945234	0.09535873	-0.33056686	0.30397055	0.20225044	0.35201256	0.27700893	0.04364159	0.36927787	0.08027902	-0.05626705	0.20138583	-0.2500115	-0.46578261
Histidine	C10	0.50558211	-0.54162295	0.8324469	0.80430174	-0.68817715	0.56637545	-0.80533678	-0.72690115	-0.82388991	-0.58650985	0.32274323	-0.81169992	0.24503892	-0.23284636	-0.4660241	0.78939853	-0.25313764
Isoleucine	C11	-0.13666814	0.58781457	-0.78898848	-0.78137776	0.57442099	-0.63095732	0.72167776	0.51413667	0.81336388	0.46811681	-0.29673401	0.82921011	0.01788285	0.17601271	0.4369842	-0.75170474	-0.26229182
Leucine	C12	-0.27535992	0.61230814	-0.95997661	-0.92990814	0.7008295	-0.71465611	0.87907394	0.68703711	0.96259141	0.62262765	-0.33314395	0.95728129	0.01098109	0.23371018	0.53611709	-0.9283247	-0.0552525
Lysine	C13	0.47017946	-0.27980686	0.72699514	0.67301969	-0.61153346	0.48105555	-0.6277202	-0.55937908	-0.70123038	-0.45823319	0.20443295	-0.62796619	0.05920381	-0.29895106	-0.35769559	0.75364118	-0.31631642
Methionine	C14	0.44030575	-0.46316697	0.7922984	0.69894789	-0.69813221	0.43087094	-0.76416572	-0.65566817	-0.8358923	-0.68565564	0.22613693	-0.80552413	-0.02541697	-0.25702931	-0.22985444	0.80834997	-0.14721175
Ornithine	C15	0.04929174	0.27647934	-0.59252326	-0.52952549	0.35071421	-0.30538933	0.42689219	0.31228043	0.60371925	0.38542908	-0.26146639	0.56551734	0.09522575	-0.00199998	0.32395469	-0.62039213	-0.25083459
Phenylalanir	C16	0.47275139	-0.61490613	0.80294291	0.75146326	-0.66813814	0.55415747	-0.81753675	-0.71939345	-0.81134483	-0.69023177	0.16710819	-0.81485574	0.14845342	-0.37387394	-0.40679036	0.74439638	-0.1227018
Serine	C18	-0.12885619	0.6590532	-0.86713885	-0.86255905	0.57724849	-0.69608858	0.78302581	0.56939254	0.89279506	0.56472253	-0.33767703	0.90062551	-0.03525543	0.25713154	0.47721909	-0.86408052	-0.23284507
Threonine	C19	-0.22591934	0.48367082	-0.80122619	-0.75789296	0.56693487	-0.5937588	0.70414178	0.48739513	0.81466152	0.46864728	-0.31224963	0.81034784	-0.05373666	0.1958817	0.33252185	-0.82485232	-0.27218309
Tryptophan	C20	0.34048478	0.08545462	0.33336373	0.0102698	0.04705208	-0.35928315	-0.35175863	-0.45050742	0.26098035	-0.23129457	-0.44616748	-0.27988064	0.07222774	0.30866671	-0.02033379	-0.38781058	-0.15918569
Tyrosine	C21	0.27519575	-0.15601427	0.18770704	-0.04912998	0.06177572	-0.02642573	-0.05837761	-0.09698199	0.05993469	-0.21018804	-0.09276467	-0.06550455	0.16380739	-0.00623427	-0.32828945	-0.07154714	-0.36434268
Valine	C22	0.23381408	-0.43718182	-0.10137742	-0.18218921	-0.17265539	-0.01677076	-0.22606874	-0.28928048	-0.01203834	-0.26887433	-0.09823583	0.05642673	0.04608759	-0.20892263	0.00203535	-0.20630145	-0.53054401
5-Oxoprolin	C23	0.29805695	0.13949203	-0.16083544	-0.20749573	-0.13346197	-0.38134516	0.10346283	0.02277027	0.21849918	0.13160989	0.24953782	0.21970987	0.35005815	0.13372244	0.19029296	-0.17717711	-0.31466678
Putrescine	C24	0.28947926	-0.59942951	0.92186879	0.88770165	-0.73337472	0.67470584	-0.82693775	-0.64919913	-0.96723034	-0.65470097	0.37189136	-0.92493947	0.13466284	-0.24538889	-0.47260747	0.95667061	-0.01776768
Fumarate	C25	0.05402736	-0.39810755	0.34062321	0.3582759	-0.32175462	0.1372345	-0.40506631	-0.33853098	-0.394012	-0.38016889	0.10831386	-0.4624916	0.07976216	0.14842875	-0.04665764	0.29950837	0.47363088
cis-Aconitate	C26	0.0302805	0.55416007	-0.49459621	-0.58764995	0.49777842	-0.56760803	0.42890897	0.26037634	0.65433182	0.44162998	-0.38138606	0.6126746	0.13290328	0.52668907	0.36966367	-0.67311665	-0.07653753
Citrate	C27	0.25880031	0.21362886	-0.23806579	-0.30182469	0.27202653	-0.24388652	0.1346771	0.1306427	0.38299884	0.24866573	-0.17198703	0.28064773	0.12325112	0.37413887	0.11746133	-0.46710258	0.14255648
Isocitrate	C28	0.01968233	0.47967581	-0.62135542	-0.60552398	0.40309778	-0.44503125	0.54553023	0.40485637	0.69767875	0.48429718	-0.21560916	0.70272387	-0.02460672	-0.00605566	0.3441503	-0.64628305	-0.39336887
Succinate	C30	0.05882383	0.72845025	-0.40037546	-0.40792398	0.31300611	-0.38518363	0.47705109	0.33661957	0.47200332	0.48841055	-0.05748545	0.48316789	0.0763489	-0.03692984	0.43924291	-0.32241638	0.16329701
Benzoate	C31	0.32672481	-0.59871914	0.94179796	0.88082334	-0.73237555	0.60375325	-0.87982597	-0.7074581	-0.95486808	-0.66741915	0.31433919	-0.96026927	0.03393138	-0.20323913	-0.40501823	0.91699035	0.09557849
4-Coumarate	C34	0.00531271	0.15630334	-0.32147762	-0.25317801	0.17304973	-0.34455668	0.20213582	0.02694171	0.34876334	0.1941184	-0.122928	0.27746724	-0.00692014	0.35795119	0.45555724	-0.40580313	0.50622635
4-Hydroxybe	C35	-0.06355863	0.0751114	-0.11508548	0.04173239	0.07332346	-0.15065101	0.08688875	-0.05355595	0.13105305	0.2558664	0.09661801	0.04667808	0.09653497	0.08775043	0.17483633	-0.13850684	0.55496323
Dehydroascc	C36	0.00905098	0.28301088	-0.3374616	-0.41509111	0.35837955	-0.43099254	0.34335029	0.33290878	0.46879234	0.08152138	-0.3490823	0.36926311	-0.12824397	0.2671499	0.28569336	-0.44651147	0.14576953
5-Caffeoylqu	C37	0.01496753	0.07954006	0.11662377	0.11702029	-0.05841047	0.08021582	-0.16737036	-0.14789796	-0.12944931	0.08049071	0.26215903	-0.10477009	0.20057309	-0.06168243	0.01467074	0.07783875	-0.12330228
Galacturonat	C38	0.4257067	-0.55789688	0.97709266	0.92232673	-0.75202496	0.67552845	-0.9083972	-0.74017925	-0.94885147	-0.6204612	0.30281032	-0.94614074	0.26515115	-0.22711588	-0.47064945	0.93031483	-0.03305286
Glucarate	C39	0	-0.02125456	0.37480955	0.27292164	-0.55179395	0.04156988	-0.44460914	-0.44492579	-0.25361308	-0.15080861	0.06669994	-0.29624977	0.41444424	0.16454236	0.08118214	0.25611705	-0.12830362
Glycerate	C40	-0.02125456	0	-0.57806213	-0.60994929	0.46123638	-0.57837944	0.6521883	0.50099276	0.62637425	0.51692335	-0.15810982	0.68684258	-0.06910964	0.25750202	0.47742366	-0.50282595	0.03020935
Similar to Ita	C41	0.37480955	-0.57806213	0	0.93437295	-0.685141	0.71100497	-0.90952708	-0.738549	-0.9476705	-0.64822731	0.2419111	-0.9497908	0.02741774	-0.1993219	-0.55213746	0.89976768	-0.02406826
Nicotinate	C43	0.27292164	-0.60994929	0.93437295	0	-0.60717215	0.80116275	-0.86394437	-0.73012745	-0.90738697	-0.54246287	0.30255418	-0.90931244	0.21607782	-0.2589637	-0.60452227	0.86484294	0.07082636
Quinate	C44	-0.55179395	0.46123638	-0.685141	-0.60717215	0	-0.29455264	0.7505951	0.64385591	0.7024636	0.47516686	-0.31743437	0.69911337	-0.21993284	0.07906339	0.14339703	-0.67584148	0.17361871
Xylose	C46	0.04156988	-0.57837944	0.71100497	0.80116275	-0.29455264	0	-0.63058024	-0.42536697	-0.70720972	-0.38853445	0.14217412	-0.68990221	-0.13631098	-0.43087213	-0.72053873	0.66135721	-0.03630125
Fructose	C49	-0.44460914	0.6521883	-0.90952708	-0.86394437	0.7505951	-0.63058024	0	0.87200063	0.86725752	0.5944022	-0.19756049	0.91534459	-0.25365722	0.07835253	0.41855967	-0.75164347	0.04675037
Glucose	C50	-0.44492579	0.50099276	-0.738549	-0.73012745	0.64385591	-0.42536697	0.87200063	0	0.67209103	0.45607604	-0.10997579	0.73208182	-0.2939082	-0.07147008	0.22611871	-0.55460213	0.0174805
Sucrose	C53	-0.25361308	0.62637425	-0.9476705	-0.90738697	0.7024636	-0.70720972	0.86725752	0.67209103	0	0.6912635	-0.33013728	0.95541047	0.14961896	0.27993022	0.54144579	-0.94258701	0.02393933
Glycerol	C55	-0.15080861	0.51692335	-0.64822731	-0.54246287	0.47516686	-0.38853445	0.5944022	0.45607604	0.6912635	0	0.05173869	0.67582713	0.53210756	0.18906879	0.33519571	-0.62612748	0.08950982
Galactinol	C56	0.06669994	-0.15810982	0.2419111	0.30255418	-0.31743437	0.14217412	-0.19756049	-0.10997579	-0.33013728	0.05173869	0	-0.28463939	0.35498154	-0.15231622	-0.14192007	0.38255013	0.13313247
myo-Inositol	C57	-0.29624977	0.68684258	-0.9497908	-0.90931244	0.69911337	-0.68990221	0.91534459	0.73208182	0.95541047	0.67582713	-0.28463939	0	-0.137605	0.25231778	0.55407507	-0.88128227	-0.0575494
Xylitol	C58	0.41444424	-0.06910964	0.02741774	0.21607782	-0.21993284	-0.13631098	-0.25365722	-0.2939082	0.14961896	0.53210756	0.35498154	-0.137605	0	0.265576	0.11899873	-0.05589707	0.08329325
Adenine	C61	0.16454236	0.25750202	-0.1993219	-0.2589637	0.07906339	-0.43087213	0.07835253	-0.07147008	0.27993022	0.18906879	-0.15231622	0.25231778	0.265576	0	0.38945612	-0.35075523	0.07389139
Heptadecano	C62	0.08118214	0.47742366	-0.55213746	-0.60452227	0.14339703	-0.72053873	0.41855967	0.22611871	0.54144579	0.33519571	-0.14192007	0.55407507	0.11899873	0.38945612	0	-0.48420143	0.08870697
Tetradecano	C63	0.25611705	-0.50282595	0.89976768	0.86484294	-0.67584148	0.66135721	-0.75164347	-0.55460213	-0.94258701	-0.62612748	0.38255013	-0.88128227	-0.05589707	-0.35075523	-0.48420143	0	-0.0238072
2-Hydroxypy	C64	-0.12830362	0.03020935	-0.02406826	0.07082636	0.17361871	-0.03630125	0.04675037	0.0174805	0.02393933	0.08950982	0.13313247	-0.0575494	0.08329325	0.07389139	0.08870697	-0.0238072	0

Supplementary Table 3. Metabolite-metabolite correlations for bud. Significant pairwise correlations within and between tissues (r ≥ 0.5, p ≤ 0.05) were highlighted in blue and yellow, representing positive and negative correlations, respectively.

Metabolites		Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Isoleucine	Leucine	Methionine	henylalanine	Proline	Serine	Threonine	Tryptophan
		B1	B2	B3	B4	B5	B6	B7	B8	B9	B11	B12	B14	B16	B17	B18	B19	B20
Alanine	B1	0	0.07659767	-0.05693692	0.71265928	0.11944811	-0.28879295	0.63388884	0.32489711	0.13574717	0.16682354	0.13161652	0.13204473	0.29481327	0.60702674	0.77636085	0.37034718	0.34567999
Arginine	B2	0.07659767	0	0.77766946	0.19760987	0.08936461	0.37986824	0.21745813	0.44669802	0.50348478	0.71992298	0.72538465	0.79670981	0.58930076	0.30627129	0.15978644	0.67367868	0.12032656
Asparagine	B3	-0.05693692	0.77766946	0	0.06742811	0.07087532	0.46060988	0.10590299	0.48725392	0.56770219	0.51966358	0.49340395	0.58352844	0.30217878	0.19765095	0.1724535	0.6014445	0.03656528
Aspartate	B4	0.71265928	0.19760987	0.06742811	0	0.23153366	-0.20006613	0.84268747	0.39555299	0.10642194	0.29466189	0.25094052	0.34163258	0.53285589	0.59246038	0.62900914	0.43721048	0.718579
b-Alanine	B5	0.11944811	0.08936461	0.07087532	0.23153366	0	-0.02767521	0.15287676	0.40025991	0.36160057	0.12115876	0.18140056	0.14907628	0.12960383	0.39136397	0.3578614	0.39687315	0.03145631
GABA	B6	-0.28879295	0.37986824	0.46060988	-0.20006613	-0.02767521	0	-0.15092228	0.18928845	0.3616227	0.37578551	0.38237768	0.39636309	0.11179681	0.00800091	-0.18319604	0.23585862	-0.00415695
Glutamate	B7	0.63388884	0.21745813	0.10590299	0.84268747	0.15287676	-0.15092228	0	0.30285372	-0.01084676	0.38033072	0.30356127	0.35617487	0.60885643	0.49442499	0.60701538	0.46643589	0.7369898
Glutamine	B8	0.32489711	0.44669802	0.48725392	0.39555299	0.40025991	0.18928845	0.30285372	0	0.6280861	0.27204337	0.27823656	0.33671802	0.40583382	0.51043896	0.58889255	0.68159481	0.14406272
Glycine	B9	0.13574717	0.50348478	0.56770219	0.10642194	0.36160057	0.3616227	-0.01084676	0.6280861	0	0.23635754	0.30057656	0.29987084	0.19569374	0.34994349	0.32651209	0.52675179	-0.0468159
Isoleucine	B11	0.16682354	0.71992298	0.51966358	0.29466189	0.12115876	0.37578551	0.38033072	0.27204337	0.23635754	0	0.94677822	0.90128311	0.67401293	0.52479616	0.18498301	0.72611199	0.21540244
Leucine	B12	0.13161652	0.72538465	0.49340395	0.25094052	0.18140056	0.38237768	0.30356127	0.27823656	0.30057656	0.94677822	0	0.85737044	0.66806332	0.5694892	0.13487409	0.73475376	0.16898087
Methionine	B14	0.13204473	0.79670981	0.58352844	0.34163258	0.14907628	0.39636309	0.35617487	0.33671802	0.29987084	0.90128311	0.85737044	0	0.68510586	0.48013969	0.1518834	0.66817965	0.26854727
Phenylalanir	B16	0.29481327	0.58930076	0.30217878	0.53285589	0.12960383	0.11179681	0.60885643	0.40583382	0.19569374	0.67401293	0.66806332	0.68510586	0	0.54153074	0.28113556	0.61555664	0.48697471
Proline	B17	0.60702674	0.30627129	0.19765095	0.59246038	0.39136397	0.00800091	0.49442499	0.51043896	0.34994349	0.52479616	0.5694892	0.48013969	0.54153074	0	0.62688186	0.68043379	0.2563283
Serine	B18	0.77636085	0.15978644	0.1724535	0.62900914	0.3578614	-0.18319604	0.60701538	0.58889255	0.32651209	0.18498301	0.13487409	0.1518834	0.28113556	0.62688186	0	0.56936325	0.25617571
Threonine	B19	0.37034718	0.67367868	0.6014445	0.43721048	0.39687315	0.23585862	0.46643589	0.68159481	0.52675179	0.72611199	0.73475376	0.66817965	0.61555664	0.68043379	0.56936325	0	0.15163482
Tryptophan	B20	0.34567999	0.12032656	0.03656528	0.718579	0.03145631	-0.00415695	0.7369898	0.14406272	-0.0468159	0.21540244	0.16898087	0.26854727	0.48697471	0.2563283	0.25617571	0.15163482	0
Tyrosine	B21	0.45679327	0.49325447	0.29292043	0.59867867	0.36820736	0.13275503	0.65653535	0.44434992	0.15021144	0.64866495	0.62533556	0.66947687	0.71280388	0.67800934	0.55722526	0.70783169	0.43257795
Valine	B22	0.36383713	0.75181208	0.60567438	0.43242138	0.20004143	0.21870497	0.45453307	0.39972749	0.44061818	0.85752436	0.81738559	0.83359794	0.68375523	0.61535353	0.39115805	0.80324858	0.24806142
5-Oxoprolin	B23	0.6458472	0.22222068	0.09218526	0.84571303	0.16202884	-0.16586593	0.99648131	0.3041127	-0.00354154	0.37647314	0.30580726	0.34968846	0.61204846	0.49300961	0.6081312	0.46554948	0.73624934
Putrescine	B24	-0.51769865	0.20410369	0.39737671	-0.53407846	0.19607696	0.37657565	-0.41360947	-0.07272568	0.28762654	0.09709088	0.12980099	0.00249269	-0.19586342	-0.20010207	-0.24906048	0.12926715	-0.41436329
cis-Aconitate	B26	0.42239869	-0.05812925	0.01437984	0.27430157	-0.10036347	-0.03388922	0.32048278	-0.08410437	-0.0867293	0.05443542	-0.04066606	0.01127749	-0.0283106	0.11045304	0.32702861	0.14574377	0.04187328
Citrate	B27	-0.1112845	0.49970813	0.59488625	-0.09373371	0.27443124	0.43169466	-0.07108259	0.63011677	0.64178817	0.19117003	0.18309899	0.22193419	0.16809921	0.05069987	0.15050079	0.52330646	-0.11727515
Pyruvate	B29	0.15547988	-0.21373694	-0.4186047	0.12268296	0.11847357	-0.18331697	0.04108947	-0.03738953	-0.09882996	-0.1560127	-0.12434707	-0.19159455	0.09668951	0.05660817	-0.01332143	-0.19615755	0.1460741
Succinate	B30	0.25207839	-0.16737252	-0.39458061	0.33855821	0.25275766	-0.27537722	0.33292777	0.04250805	-0.09442138	-0.05966997	0.00769791	-0.09497677	0.24762202	0.2097724	0.13656254	-0.0024518	0.38736026
Benzoate	B31	0.10004951	-0.21114664	-0.35733908	0.08679666	0.10048381	-0.27584373	-0.02020288	-0.21674995	-0.04350071	-0.13370515	-0.09945729	-0.18039193	-0.03015517	0.00720004	-0.11749541	-0.22161791	0.15687161
2-Ketoglucor	B32	-0.26881168	0.08115785	0.26230161	-0.39098134	-0.11325817	0.43555803	-0.12266159	-0.14593224	0.11102485	0.09209884	0.0572364	0.02085074	-0.12702594	-0.24901622	-0.11507988	0.11477161	-0.16647629
Caffeate	B33	0.27032491	0.12227784	-0.12412866	0.41182639	0.26994451	-0.09105918	0.39260626	-0.06952604	-0.04156397	0.2652393	0.31380126	0.27372125	0.42186341	0.36825571	0.2176869	0.24435443	0.37817591
4-Hydroxybe	B35	0.08660455	0.24726398	0.14341353	0.13948342	0.25135505	0.10898057	0.19691049	0.10275459	0.17504403	0.25638768	0.24264658	0.20526604	0.26790298	0.22633655	0.14087585	0.31088549	0.12254172
Dehydroascc	B36	-0.2914867	-0.1778331	-0.05483283	-0.17456929	0.005729	0.06490596	-0.03145243	-0.00767814	-0.13435311	-0.0882955	-0.16298295	-0.14377344	-0.18476798	-0.31652474	-0.11744348	-0.14890254	0.1395509
Glycerate	B40	0.21348552	-0.14665278	-0.13904766	0.06888903	0.3297901	-0.07188735	0.14890715	0.08355955	0.07676545	-0.04228081	0.01960714	-0.16736928	0.11081493	0.24611113	0.3142778	0.21261211	-0.07906143
Similar to Ita	B41	0.51726707	0.03307555	-0.19168611	0.66458098	0.30388604	-0.22455791	0.64033918	0.22643523	-0.16462234	0.17869492	0.15991171	0.19493106	0.44530809	0.48306198	0.47055469	0.2635163	0.4823975
Lactate	B42	0.14629763	-0.14285194	-0.14606419	0.18555702	0.14947456	-0.01635487	0.09101026	0.13399988	0.32498431	-0.11173864	-0.03092584	-0.1120308	0.00052957	0.16830265	0.10536037	-0.02708589	0.25501514
Nicotinate	B43	0.22314419	0.26376947	0.06856225	0.36684788	0.19588123	-0.02793517	0.30615627	0.02681012	0.00635131	0.27405616	0.25615888	0.32754531	0.31732434	0.29038507	0.18660677	0.19744067	0.32069491
Quinate	B45	-0.46387876	0.1434295	0.27814512	-0.43770985	0.12096213	0.23829299	-0.24499277	0.01530399	0.01282271	0.17081682	0.10796562	0.18598529	-0.11928599	-0.23322422	-0.21632757	0.0780659	-0.38884964
Xylose	B46	-0.35196203	0.13042896	0.14696478	-0.1924222	0.2038177	0.40729895	-0.01800576	-0.07386298	0.10951047	0.22545253	0.31351192	0.16310572	0.11021644	-0.00070561	-0.23203095	0.19557014	-0.04842234
Fucose	B47	0.05404027	0.04238094	-0.14341387	0.30055146	0.33877667	-0.12527927	0.33054693	-0.00332588	-0.03074967	0.11558274	0.12599002	0.09757693	0.32601769	0.17090487	0.06988161	0.11549732	0.34981522
Sorbose	B48	-0.62212568	0.06928661	0.27801726	-0.58808218	0.13279737	0.25237405	-0.44581982	-0.00664058	0.02386702	0.04069621	0.03634875	0.03895165	-0.26562953	-0.31938677	-0.31094857	-0.01498321	-0.47292958
Fructose	B49	-0.20723715	0.01185401	0.2940782	-0.27958675	0.04936208	0.17623058	-0.20633857	0.00843816	0.0637325	-0.01909971	-0.04308081	-0.00635631	-0.29038217	-0.13616442	0.05623916	0.10562913	-0.44355305
Galactose	B51	-0.52436857	0.05983617	0.11162456	-0.52839781	0.25267213	0.18749995	-0.41516308	-0.09277	-0.04671595	0.03779291	0.02162732	0.07424018	-0.21980108	-0.30472155	-0.30829897	-0.10235329	-0.42910501
Similar to Ril	B52	-0.00126012	0.26763261	0.21355657	0.10514641	0.22604295	0.09838043	0.17149122	0.07643679	0.07222341	0.22124481	0.22492888	0.16843352	0.23837051	0.09940069	0.08609074	0.22838697	0.1938957
Sucrose	B53	0.04359682	0.17686917	0.14383535	0.19055375	-0.04619947	0.15100512	0.31324884	0.13382467	0.15475462	0.22949183	0.16746789	0.24355903	0.36170463	0.00914402	-0.10353868	0.12071735	0.36588235
Trehalose	B54	0.275541	-0.14687267	-0.16229631	0.25502088	-0.05599906	-0.26213683	0.2095279	0.05439496	-0.08932801	-0.1288629	-0.17019086	-0.17323392	-0.00684053	0.11226357	0.12884733	-0.07589824	0.31542344
Glycerol	B55	0.4735944	-0.25207139	-0.45344962	0.36518681	0.07104445	-0.20851834	0.27345095	0.02528589	-0.10653524	-0.0715705	-0.02522698	-0.11021335	0.07902132	0.36884211	0.28138177	-0.01384334	0.27161738
myo-Inositol	B57	0.07138888	0.11966623	0.24009155	0.21669925	0.447496	0.30316005	0.2510704	0.32181264	0.20831894	0.14351341	0.18138612	0.160293	0.07332193	0.34099159	0.35351021	0.3630542	0.19707308
Xylitol	B58	0.25650023	-0.08265802	-0.32045681	0.21917182	0.03458978	-0.06619193	0.10728648	-0.13521211	-0.14746642	-0.03147168	-0.01860226	-0.04876854	0.06400998	0.18542449	0.0247581	-0.06028875	0.1879276
Uracil	B59	0.08837147	0.17193081	0.03912785	0.17772653	0.34699357	-0.05176451	0.21834147	0.06059909	0.12527407	0.1615861	0.1669366	0.13154775	0.21522187	0.15112365	0.10296296	0.21173375	0.16033854
Orthophospl	B60	0.62569396	-0.1176952	-0.26489586	0.66670931	0.22474347	-0.217443	0.4974072	0.2705515	-0.06232897	-0.03637295	-0.02109689	0.03782843	0.15089172	0.4398868	0.51079581	0.14832874	0.35510166
Adenine	B61	0.35713835	0.06343689	-0.02323005	0.35186914	0.28998716	-0.11529516	0.44956756	0.19407731	-0.02065496	0.15180837	0.11538993	0.05697784	0.23543469	0.26963995	0.49660457	0.37079302	0.15766382
Heptadecan	B62	0.3474315	0.09078921	0.04551748	0.50395692	0.20821939	0.15445256	0.40661018	0.18749749	0.18021098	0.18225069	0.20214095	0.21984805	0.28905801	0.4184559	0.26963946	0.24111812	0.54405156
Decanoate	B65	-0.04416328	-0.11922283	-0.3177547	0.03161413	0.08311236	-0.1597455	-0.04511953	-0.06128925	-0.00871668	-0.10590771	-0.04883455	-0.09143674	0.10597719	0.03557473	-0.22483095	-0.19495996	0.20121379
Diethanolam	B66	-0.36568593	0.14224173	0.04768126	-0.20645028	0.00192519	0.42399828	-0.11022928	-0.11121998	-0.04591556	0.26864997	0.27097405	0.24054835	0.17693218	-0.16386668	-0.35837597	0.05836159	0.0369847

Metabolites		Tyrosine	Valine	5-Oxoproline	Putrescine	cis-Aconitate	Citrate	Pyruvate	Succinate	Benzoate	Ketogluconat	Caffeate	ydroxybenzo	hydroascorba	Glycerate	ilar to Itacon	Lactate	Nicotinate
		B21	B22	B23	B24	B26	B27	B29	B30	B31	B32	B33	B35	B36	B40	B41	B42	B43
Alanine	B1	0.45679327	0.36383713	0.6458472	-0.51769865	0.42239869	-0.1112845	0.15547988	0.25207839	0.10004951	-0.26881168	0.27032491	0.08660455	-0.2914867	0.21348552	0.51726707	0.14629763	0.22314419
Arginine	B2	0.49325447	0.75181208	0.22222068	0.20410369	-0.05812925	0.49970813	-0.21373694	-0.16737252	-0.21114664	0.08115785	0.12227784	0.24726398	-0.1778331	-0.14665278	0.03307555	-0.14285194	0.26376947
Asparagine	B3	0.29292043	0.60567438	0.09218526	0.39737671	0.01437984	0.59488625	-0.4186047	-0.39458061	-0.35733908	0.26230161	-0.12412866	0.14341353	-0.05483283	-0.13904766	-0.19168611	-0.14606419	0.06856225
Aspartate	B4	0.59867867	0.43242138	0.84571303	-0.53407846	0.27430157	-0.09373371	0.12268296	0.33855821	0.08679666	-0.39098134	0.41182639	0.13948342	-0.17456929	0.06888903	0.66458098	0.18555702	0.36684788
b-Alanine	B5	0.36820736	0.20004143	0.16202884	0.19607696	-0.10036347	0.27443124	0.11847357	0.25275766	0.10048381	-0.11325817	0.26994451	0.25135505	0.005729	0.3297901	0.30388604	0.14947456	0.19588123
GABA	B6	0.13275503	0.21870497	-0.16586593	0.37657565	-0.03388922	0.43169466	-0.18331697	-0.27537722	-0.27584373	0.43555803	-0.09105918	0.10898057	0.06490596	-0.07188735	-0.22455791	-0.01635487	-0.02793517
Glutamate	B7	0.65653535	0.45453307	0.99648131	-0.41360947	0.32048278	-0.07108259	0.04108947	0.33292777	-0.02020288	-0.12266159	0.39260626	0.19691049	-0.03145243	0.14890715	0.64033918	0.09101026	0.30615627
Glutamine	B8	0.44434992	0.39972749	0.3041127	-0.07272568	-0.08410437	0.63011677	-0.03738953	0.04250805	-0.21674995	-0.14593224	-0.06952604	0.10275459	-0.00767814	0.08355955	0.22643523	0.13399988	0.02681012
Glycine	B9	0.15021144	0.44061818	-0.00354154	0.28762654	-0.0867293	0.64178817	-0.09882996	-0.09442138	-0.04350071	0.11102485	-0.04156397	0.17504403	-0.13435311	0.07676545	-0.16462234	0.32498431	0.00635131
Isoleucine	B11	0.64866495	0.85752436	0.37647314	0.09709088	0.05443542	0.19117003	-0.1560127	-0.05966997	-0.13370515	0.09209884	0.2652393	0.25638768	-0.0882955	-0.04228081	0.17869492	-0.11173864	0.27405616
Leucine	B12	0.62533556	0.81738559	0.30580726	0.12980099	-0.04066606	0.18309899	-0.12434707	0.00769791	-0.09945729	0.0572364	0.31380126	0.24264658	-0.16298295	0.01960714	0.15991171	-0.03092584	0.25615888
Methionine	B14	0.66947687	0.83359794	0.34968846	0.00249269	0.01127749	0.22193419	-0.19159455	-0.09497677	-0.18039193	0.02085074	0.27372125	0.20526604	-0.14377344	-0.16736928	0.19493106	-0.1120308	0.32754531
Phenylalanir	B16	0.71280388	0.68375523	0.61204846	-0.19586342	-0.0283106	0.16809921	0.09668951	0.24762202	-0.03015517	-0.12702594	0.42186341	0.26790298	-0.18476798	0.11081493	0.44530809	0.00052957	0.31732434
Proline	B17	0.67800934	0.61535353	0.49300961	-0.20010207	0.11045304	0.05069987	0.05660817	0.2097724	0.00720004	-0.24901622	0.36825571	0.22633655	-0.31652474	0.24611113	0.48306198	0.16830265	0.29038507
Serine	B18	0.55722526	0.39115805	0.6081312	-0.24906048	0.32702861	0.15050079	-0.01332143	0.13656254	-0.11749541	-0.11507988	0.2176869	0.14087585	-0.11744348	0.3142778	0.47055469	0.10536037	0.18660677
Threonine	B19	0.70783169	0.80324858	0.46554948	0.12926715	0.14574377	0.52330646	-0.19615755	-0.0024518	-0.22161791	0.11477161	0.24435443	0.31088549	-0.14890254	0.21261211	0.2635163	-0.02708589	0.19744067
Tryptophan	B20	0.43257795	0.24806142	0.73624934	-0.41436329	0.04187328	-0.11727515	0.1460741	0.38736026	0.15687161	-0.16647629	0.37817591	0.12254172	0.1395509	-0.07906143	0.4823975	0.25501514	0.32069491
Tyrosine	B21	0	0.64480606	0.64863628	-0.14173754	0.1835912	0.15581056	0.00553494	0.23502363	-0.17495901	-0.04001228	0.43990232	0.32652252	-0.17005334	0.27212208	0.59067585	-0.06725217	0.40275199
Valine	B22	0.64480606	0	0.46115673	0.09314328	0.15888985	0.30131862	-0.09865255	-0.05281699	-0.05921253	0.12413638	0.29129026	0.28676667	-0.16085473	0.03835148	0.19199657	-0.07656836	0.32098036
5-Oxoprolin	B23	0.64863628	0.46115673	0	-0.42541113	0.30210464	-0.0572956	0.09058251	0.37606338	0.02670167	-0.14014802	0.40976915	0.21711716	-0.02879645	0.16895743	0.66234804	0.10175689	0.32976816
Putrescine	B24	-0.14173754	0.09314328	-0.42541113	0	-0.07627583	0.41006266	-0.17731274	-0.32664153	-0.20334355	0.54485967	-0.09874998	0.2009384	0.15898354	0.19991359	-0.4533353	-0.14413829	-0.07634167
cis-Aconitat	B26	0.1835912	0.15888985	0.30210464	-0.07627583	0	-0.09448937	-0.17136803	-0.19261792	-0.14556476	0.32900853	-0.03192655	-0.14499758	-0.18709153	0.01421218	0.12957504	-0.14101628	-0.10157957
Citrate	B27	0.15581056	0.30131862	-0.0572956	0.41006266	-0.09448937	0	0.00820362	-0.05637995	-0.17053756	0.35134775	-0.17589989	0.30891316	0.09984103	0.19123753	-0.10226814	-0.00974739	0.01698995
Pyruvate	B29	0.00553494	-0.09865255	0.09058251	-0.17731274	-0.17136803	0.00820362	0	0.77242963	0.61607662	-0.18349197	0.41295402	0.32051649	-0.02910059	0.47561758	0.37990415	0.24868753	0.34547504
Succinate	B30	0.23502363	-0.05281699	0.37606338	-0.32664153	-0.19261792	-0.05637995	0.77242963	0	0.53475029	-0.25834541	0.59182437	0.50496381	-0.00547661	0.52263877	0.655306	0.23898078	0.45546215
Benzoate	B31	-0.17495901	-0.05921253	0.02670167	-0.20334355	-0.14556476	-0.17053756	0.61607662	0.53475029	0	-0.20401773	0.38634091	0.28695729	-0.07907728	0.19758302	0.23050676	0.37434223	0.35948557
2-Ketogluco	B32	-0.04001228	0.12413638	-0.14014802	0.54485967	0.32900853	0.35134775	-0.18349197	-0.25834541	-0.20401773	0	-0.07161641	0.13148813	0.22330464	0.16732585	-0.36679007	-0.08761601	-0.14851808
Caffeate	B33	0.43990232	0.29129026	0.40976915	-0.09874998	-0.03192655	-0.17589989	0.41295402	0.59182437	0.38634091	-0.07161641	0	0.64215966	-0.17092572	0.46866545	0.60946144	0.16567732	0.67712727
4-Hydroxybe	B35	0.32652252	0.28676667	0.21711716	0.2009384	-0.14499758	0.30891316	0.32051649	0.50496381	0.28695729	0.13148813	0.64215966	0	0.06374145	0.49003729	0.46703125	0.00230025	0.73331982
Dehydroasc	B36	-0.17005334	-0.16085473	-0.02879645	0.15898354	-0.18709153	0.09984103	-0.02910059	-0.00547661	-0.07907728	0.22330464	-0.17092572	0.06374145	0	-0.05176392	-0.11602269	-0.09975843	-0.04088454
Glycerate	B40	0.27212208	0.03835148	0.16895743	0.19991359	0.01421218	0.19123753	0.47561758	0.52263877	0.19758302	0.16732585	0.46866545	0.49003729	-0.05176392	0	0.32333858	0.14189627	0.2861341
Similar to Ita	B41	0.59067585	0.19199657	0.66234804	-0.4533353	0.12957504	-0.10226814	0.37990415	0.655306	0.23050676	-0.36679007	0.60946144	0.46703125	-0.11602269	0.32333858	0	-0.00614535	0.65052619
Lactate	B42	-0.06725217	-0.07656836	0.10175689	-0.14413829	-0.14101628	-0.00974739	0.24868753	0.23898078	0.37434223	-0.08761601	0.16567732	0.00230025	-0.09975843	0.14189627	-0.00614535	0	-0.04593111
Nicotinate	B43	0.40275199	0.32098036	0.32976816	-0.07634167	-0.10157957	0.01698995	0.34547504	0.45546215	0.35948557	-0.14851808	0.67712727	0.73331982	-0.04088454	0.2861341	0.65052619	-0.04593111	0
Quinate	B45	-0.02089941	-0.01077086	-0.27460315	0.38650784	-0.13540466	0.22272075	-0.50682006	-0.47096045	-0.50740117	0.28003491	-0.30245248	-0.15662111	0.17021046	-0.14496734	-0.38552154	-0.2685837	-0.29800711
Xylose	B46	0.1152074	0.22821351	-0.01784664	0.50290678	0.005985	0.20577835	0.08318987	0.05504661	-0.11958011	0.54714353	0.12447244	0.10812571	0.18974047	0.2780121	-0.1255214	-0.11408742	-0.04630365
Fucose	B47	0.26076368	0.14515936	0.36210868	-0.06950466	-0.24250636	0.0831576	0.53272287	0.75498624	0.44084485	-0.10217724	0.69944189	0.75456625	0.07203577	0.49503849	0.61725546	0.08857142	0.65207979
Sorbose	B48	-0.16447926	-0.19416695	-0.47843209	0.53397915	-0.31608812	0.20952267	-0.47094201	-0.46316934	-0.43529978	0.19613515	-0.27889701	-0.13733739	0.17527631	-0.07632495	-0.45906067	-0.20188499	-0.29018309
Fructose	B49	-0.04047566	-0.02401851	-0.24293482	0.38163601	0.32834572	0.1932449	-0.65648301	-0.61834456	-0.63774455	0.36409411	-0.33525942	-0.26027339	-0.11509418	-0.14467822	-0.33267703	-0.26144898	-0.42388193
Galactose	B51	-0.08419242	-0.20093839	-0.4327764	0.36998519	-0.33684681	0.12087018	-0.32154837	-0.29662064	-0.3418687	0.08376397	-0.23105461	-0.12424277	0.12017303	-0.06083869	-0.28145819	-0.22188551	-0.1708682
Similar to Ril	B52	0.17602665	0.2344086	0.17368462	0.28733034	-0.14881169	0.17051965	0.17417296	0.20522131	0.11186895	0.04009753	0.33930016	0.40862139	0.24550093	0.1777841	0.19471132	-0.25755869	0.42151518
Sucrose	B53	0.07699608	0.20574821	0.30376714	-0.1422688	0.15419224	0.13213965	0.02400296	0.04017021	0.11087922	0.16235461	-0.11533181	-0.09610538	0.22812232	-0.1739202	-0.04166219	0.07348019	-0.06687966
Trehalose	B54	0.08919754	-0.04098193	0.22677258	-0.2971359	0.15066983	-0.02905796	0.42433233	0.40729942	0.40333764	-0.07193821	0.12015791	0.15096465	0.10971719	0.118209	0.31455265	0.20699654	0.27331621
Glycerol	B55	0.24134764	-0.01429088	0.30702863	-0.36979182	-0.00407565	-0.19044188	0.63269862	0.67883459	0.3998484	-0.2672725	0.38031605	0.20978922	-0.08134916	0.45837211	0.53275875	0.26905157	0.3172627
myo-Inositol	B57	0.47872119	0.19424267	0.23715736	0.32853353	0.11445396	0.26108622	-0.05176202	0.06225016	-0.15477908	0.25226137	0.30401926	0.29570924	0.05362309	0.34511162	0.20707496	0.03782583	0.18459395
Xylitol	B58	0.16501234	-0.01573695	0.11755675	-0.17862186	0.07619078	-0.08905853	0.46490524	0.43133027	0.24624613	-0.08898007	0.39088542	0.36101341	-0.1007505	0.30063295	0.40312179	0.04445345	0.46663829
Uracil	B59	0.26226447	0.19492483	0.24361605	0.10238221	-0.17840847	0.21891588	0.36269465	0.57014425	0.45838785	0.02181452	0.65122686	0.90363739	0.06417559	0.43975442	0.51344109	0.10877831	0.75010696
Orthophospl	B60	0.38675912	0.06804771	0.51300576	-0.64362472	0.28134834	-0.17650257	0.29667433	0.48968451	0.18301721	-0.35410589	0.42027202	0.11712185	-0.22111545	0.23776541	0.67660323	0.13654976	0.28619283
Adenine	B61	0.44769571	0.22270061	0.46295188	0.04123908	0.15770091	0.10934881	0.17405177	0.33668954	0.02773672	0.00734539	0.41657315	0.5492734	0.14263756	0.50813146	0.56126982	-0.15636053	0.4913356
Heptadecan	B62	0.25983314	0.31880494	0.4127917	-0.16417382	0.13569994	0.00603061	0.15697695	0.23437538	0.37859967	0.0469015	0.45145192	0.24469928	-0.07517599	-0.00283306	0.31929205	0.33165779	0.26369094
Decanoate	B65	-0.14138452	-0.17641466	-0.01261639	-0.20825659	-0.3405254	-0.0205693	0.53100156	0.53461903	0.60443488	-0.27898442	0.24408644	0.192868	0.04520368	0.16303678	0.16064697	0.53328773	0.20788672
Diethanolam	B66	-0.01238879	0.16121337	-0.10644959	0.1924266	-0.03436512	0.16491862	-0.06881802	-0.02755691	-0.04651519	0.39123563	0.0011335	0.02572472	0.23761443	-0.1900436	-0.03993301	-0.16352978	-0.06208412

Metabolites		Quinate	Xylose	Fucose	Sorbose	Fructose	Galactose	nilar to Ribul	Sucrose	Trehalose	Glycerol	myo-Inositol	Xylitol	Uracil	rthophospha	Adenine	eptadecanoa	Decanoate	iethanolamin
		B45	B46	B47	B48	B49	B51	B52	B53	B54	B55	B57	B58	B59	B60	B61	B62	B65	B66
Alanine	B1	-0.46387876	-0.35196203	0.05404027	-0.62212568	-0.20723715	-0.52436857	-0.00126012	0.04359682	0.275541	0.4735944	0.07138888	0.25650023	0.08837147	0.62569396	0.35713835	0.3474315	-0.04416328	-0.36568593
Arginine	B2	0.1434295	0.13042896	0.04238094	0.06928661	0.01185401	0.05983617	0.26763261	0.17686917	-0.14687267	-0.25207139	0.11966623	-0.08265802	0.17193081	-0.1176952	0.06343689	0.09078921	-0.11922283	0.14224173
Asparagine	B3	0.27814512	0.14696478	-0.14341387	0.27801726	0.2940782	0.11162456	0.21355657	0.14383535	-0.16229631	-0.45344962	0.24009155	-0.32045681	0.03912785	-0.26489586	-0.02323005	0.04551748	-0.3177547	0.04768126
Aspartate	B4	-0.43770985	-0.1924222	0.30055146	-0.58808218	-0.27958675	-0.52839781	0.10514641	0.19055375	0.25502088	0.36518681	0.21669925	0.21917182	0.17772653	0.66670931	0.35186914	0.50395692	0.03161413	-0.20645028
b-Alanine	B5	0.12096213	0.2038177	0.33877667	0.13279737	0.04936208	0.25267213	0.22604295	-0.04619947	-0.05599906	0.07104445	0.447496	0.03458978	0.34699357	0.22474347	0.28998716	0.20821939	0.08311236	0.00192519
GABA	B6	0.23829299	0.40729895	-0.12527927	0.25237405	0.17623058	0.18749995	0.09838043	0.15100512	-0.26213683	-0.20851834	0.30316005	-0.06619193	-0.05176451	-0.217443	-0.11529516	0.15445256	-0.1597455	0.42399828
Glutamate	B7	-0.24499277	-0.01800576	0.33054693	-0.44581982	-0.20633857	-0.41516308	0.17149122	0.31324884	0.2095279	0.27345095	0.2510704	0.10728648	0.21834147	0.4974072	0.44956756	0.40661018	-0.04511953	-0.11022928
Glutamine	B8	0.01530399	-0.07386298	-0.00332588	-0.00664058	0.00843816	-0.09277	0.07643679	0.13382467	0.05439496	0.02528589	0.32181264	-0.13521211	0.06059909	0.2705515	0.19407731	0.18749749	-0.06128925	-0.11121998
Glycine	B9	0.01282271	0.10951047	-0.03074967	0.02386702	0.0637325	-0.04671595	0.07222341	0.15475462	-0.08932801	-0.10653524	0.20831894	-0.14746642	0.12527407	-0.06232897	-0.02065496	0.18021098	-0.00871668	-0.04591556
Isoleucine	B11	0.17081682	0.22545253	0.11558274	0.04069621	-0.01909971	0.03779296	0.22124481	0.22949183	-0.1288629	-0.0715705	0.14351341	-0.03147168	0.1615861	-0.03637295	0.15180837	0.18225069	-0.10590771	0.26864997
Leucine	B12	0.10796562	0.31351192	0.12599002	0.03634875	-0.04308081	0.02162732	0.22492888	0.16746789	-0.17019086	-0.02522698	0.18138612	-0.01860226	0.1669366	-0.02109689	0.11538993	0.20214095	-0.04883455	0.27097405
Methionine	B14	0.18598529	0.16310572	0.09757693	0.03895165	-0.00635631	0.07424018	0.16843352	0.24355903	-0.17323392	-0.11021335	0.160293	-0.04876854	0.13154775	0.03782843	0.05697784	0.21984805	-0.09143674	0.24054835
Phenylalanir	B16	-0.11928599	0.11021644	0.32601769	-0.26562953	-0.29038217	-0.21980108	0.23837051	0.36170463	-0.00684053	0.07902132	0.07332193	0.06400998	0.21522187	0.15089172	0.23543469	0.28905801	0.10597719	0.17693218
Proline	B17	-0.23322422	-0.00070561	0.17090487	-0.31938677	-0.13616442	-0.30472155	0.09940069	0.00914402	0.11226357	0.36884211	0.34099159	0.18542449	0.15112365	0.4398868	0.26963995	0.4184559	0.03557473	-0.16386668
Serine	B18	-0.21632757	-0.23203095	0.06988161	-0.31094857	0.05623916	-0.30829897	0.08609074	-0.10353868	0.12884733	0.28138177	0.35351021	0.0247581	0.10296296	0.51079581	0.49660457	0.26963946	-0.22483095	-0.35837597
Threonine	B19	0.0780659	0.19557014	0.11549732	-0.01498321	0.10562913	-0.10235329	0.22838697	0.12071735	-0.07589824	-0.01384334	0.3630542	-0.06028875	0.21173375	0.14832874	0.37079302	0.24111812	-0.19495996	0.05836159
Tryptophan	B20	-0.38884964	-0.04842234	0.34981522	-0.47292958	-0.44355305	-0.42910501	0.1938957	0.36588235	0.31542344	0.27161738	0.19707308	0.1879276	0.16033854	0.35510166	0.15766382	0.54405156	0.20121379	0.0369847
Tyrosine	B21	-0.02089941	0.1152074	0.26076368	-0.16447926	-0.04047566	-0.08419242	0.17602665	0.07699608	0.08919754	0.24134764	0.47872119	0.16501234	0.26226447	0.38675912	0.44769571	0.25983314	-0.14138452	-0.01238879
Valine	B22	-0.01077086	0.22821351	0.14515936	-0.19416695	-0.02401851	-0.20093839	0.2344086	0.20574821	-0.04098193	-0.01429088	0.19424267	-0.01573695	0.19492483	0.06804771	0.22270061	0.31880494	-0.17641466	0.16121337
5-Oxoproline	B23	-0.27460315	-0.01784664	0.36210868	-0.47843209	-0.24293482	-0.4327764	0.17368462	0.30376714	0.22677258	0.30702863	0.23715736	0.11755675	0.24361605	0.51300576	0.46295188	0.4127917	-0.01261639	-0.10644959
Putrescine	B24	0.38650784	0.50290678	-0.06950466	0.53397915	0.38163601	0.36998519	0.28733034	-0.1422688	-0.2971359	-0.36979182	0.32853353	-0.17862186	0.10238221	-0.64362472	0.04123908	-0.16417382	-0.20825659	0.1924266
cis-Aconitate	B26	-0.13540466	0.005985	-0.24250636	-0.31608812	0.32834572	-0.33684681	-0.14881169	0.15419224	0.15066983	-0.00407565	0.11445396	0.07619078	-0.17840847	0.28134834	0.15770091	0.13569994	-0.3405254	-0.03436512
Citrate	B27	0.22272075	0.20577835	0.0831576	0.20952267	0.1932449	0.12087018	0.17051965	0.13213965	-0.02905796	-0.19044188	0.26108622	-0.08905853	0.21891588	-0.17650257	0.10934881	0.00603061	-0.0205693	0.16491862
Pyruvate	B29	-0.50682006	0.08318987	0.53272287	-0.47094201	-0.65648301	-0.32154837	0.17417296	0.02400296	0.42433233	0.63269862	-0.05176202	0.46490524	0.36269465	0.29667433	0.17405177	0.15697695	0.53100156	-0.06881802
Succinate	B30	-0.47096045	0.05504661	0.75498624	-0.46316934	-0.61834456	-0.29662064	0.20522131	0.04017021	0.40729942	0.67883459	0.06225016	0.43133027	0.57014425	0.48968451	0.33668954	0.23437538	0.53461903	-0.02755691
Benzoate	B31	-0.50740117	-0.11958011	0.44084485	-0.43529978	-0.63774455	-0.3418687	0.11186895	0.11087922	0.40333764	0.3998484	-0.15477908	0.24624613	0.45838785	0.18301721	0.02773672	0.37859967	0.60443488	-0.04651519
2-Ketoglucoı	B32	0.28003491	0.54714353	-0.10217724	0.19613515	0.36409411	0.08376397	0.04009753	0.16235461	-0.07193821	-0.2672725	0.25226137	-0.08898007	0.02181452	-0.35410589	0.00734539	0.0469015	-0.27898442	0.39123563
Caffeate	B33	-0.30245248	0.12447244	0.69944189	-0.27889701	-0.33525942	-0.23105461	0.33930016	-0.11533181	0.12015791	0.38031605	0.30401926	0.39088542	0.65122686	0.42027202	0.41657315	0.45145192	0.24408644	0.0011335
4-Hydroxybe	B35	-0.15662111	0.10812571	0.75456625	-0.13733739	-0.26027339	-0.12424277	0.40862139	-0.09610538	0.15096465	0.20978922	0.29570924	0.36101341	0.90363739	0.11712185	0.5492734	0.24469928	0.192868	0.02572472
Dehydroascc	B36	0.17021046	0.18974047	0.07203577	0.17527631	-0.11509418	0.12017303	0.24550093	0.22812232	0.10971719	-0.08134916	0.05362309	-0.1007505	0.06417559	-0.22111545	0.14263756	-0.07517599	0.04520368	0.23761443
Glycerate	B40	-0.14496734	0.2780121	0.49503849	-0.07632495	-0.14467822	-0.06083869	0.1777841	-0.1739202	0.118209	0.45837211	0.34511162	0.30063295	0.43975442	0.23776541	0.50813146	-0.00283306	0.16303678	-0.1900436
Similar to Ita	B41	-0.38552154	-0.1255214	0.61725546	-0.45906067	-0.33267703	-0.28145819	0.19471132	-0.04166219	0.31455265	0.53275875	0.20707496	0.40312179	0.51344109	0.67660323	0.56126982	0.31929205	0.16064697	-0.03993301
Lactate	B42	-0.2685837	-0.11408742	0.08857142	-0.20188499	-0.26144898	-0.22188551	-0.25755869	0.07348019	0.20699654	0.26905157	0.03782583	0.04445345	0.10877831	0.13654976	-0.15636053	0.33165779	0.53328773	-0.16352978
Nicotinate	B43	-0.29800711	-0.04630365	0.65207979	-0.29018309	-0.42388193	-0.1708682	0.42151518	-0.06687966	0.27331621	0.3172627	0.18459395	0.46663829	0.75010696	0.28619283	0.4913356	0.26369094	0.20788672	-0.06208412
Quinate	B45	0	0.20138072	-0.2601869	0.84304685	0.57481702	0.83582405	-0.15476948	-0.03587026	-0.34329054	-0.53530014	0.09205034	-0.3723566	-0.19882164	-0.41318515	-0.13545876	-0.44397771	-0.32913589	0.21055162
Xylose	B46	0.20138072	0	0.15169882	0.1627772	0.14288441	0.11996123	0.25884026	0.128029	-0.14194507	-0.01663821	0.3422779	0.07045006	0.01810997	-0.18537013	0.05090895	0.07947467	-0.15052044	0.46919953
Fucose	B47	-0.2601869	0.15169882	0	-0.24481922	-0.44375098	-0.15627045	0.33920877	0.01007269	0.27704069	0.39094498	0.19015934	0.43886659	0.80748285	0.32594231	0.38894002	0.29450253	0.36149827	0.03818386
Sorbose	B48	0.84304685	0.1627772	-0.24481922	0	0.5797738	0.8516963	-0.06562822	-0.19662521	-0.46620873	-0.52535815	0.15914339	-0.42897083	-0.16832695	-0.51530649	-0.17212653	-0.477618	-0.22560852	0.09552896
Fructose	B49	0.57481702	0.14288441	-0.44375098	0.5797738	0	0.40810082	-0.32694431	-0.35088387	-0.50028031	-0.51629006	0.26703994	-0.49128425	-0.33842809	-0.21196254	-0.13366037	-0.27139431	-0.66268627	0.2059842
Galactose	B51	0.83582405	0.11996123	-0.15627045	0.8516963	0.40810082	0	-0.10327923	-0.15252862	-0.33930313	-0.40139336	0.01836643	-0.23445382	-0.10221766	-0.39740746	-0.12791933	-0.49539834	-0.11535548	0.14966229
Similar to Ril	B52	-0.15476948	0.25884026	0.33920877	-0.06562822	-0.32694431	-0.10327923	0	0.11981397	0.09449294	0.11835351	0.23347272	0.17473267	0.38025404	-0.07405783	0.35337823	0.21780339	0.08802501	0.13270849
Sucrose	B53	-0.03587026	0.128029	0.01007269	-0.19662521	-0.35088387	-0.15252862	0.11981397	0	0.24990765	-0.03433714	-0.21498856	-0.02709037	-0.03379108	-0.06567346	-0.11645181	0.25485097	0.17536681	0.25183694
Trehalose	B54	-0.34329054	-0.14194507	0.27704069	-0.46620873	-0.50028031	-0.33930313	0.09449294	0.24990765	0	0.40083264	0.011366	0.56331741	0.22862784	0.29919671	0.05993233	0.26590903	0.27785059	-0.22510909
Glycerol	B55	-0.53530014	-0.01663821	0.39094498	-0.52535815	-0.51629006	-0.40139336	0.11835351	-0.03433714	0.40083264	0	0.16294453	0.47315615	0.23882001	0.5428896	0.30120723	0.30976742	0.39496372	-0.10603646
myo-Inositol	B57	0.09205034	0.3422779	0.19015934	0.15914339	0.26703994	0.01836643	0.23347272	-0.21498856	0.011366	0.16294453	0	0.08106014	0.20515994	0.26447713	0.33720875	0.40440518	-0.21203553	-0.07071838
Xylitol	B58	-0.3723566	0.07045006	0.43886659	-0.42897083	-0.49128425	-0.23445382	0.17473267	-0.02709037	0.56331741	0.47315615	0.08106014	0	0.33417856	0.31996191	0.24627757	0.2029363	0.24067992	-0.19448555
Uracil	B59	-0.19882164	0.01810997	0.80748285	-0.16832695	-0.33842809	-0.10221766	0.38025404	-0.03379108	0.22862784	0.23882001	0.20515994	0.33417856	0	0.18699637	0.48013481	0.27606455	0.31135394	-0.00270494
Orthophospl	B60	-0.41318515	-0.18537013	0.32594231	-0.51530649	-0.21196254	-0.39740746	-0.07405783	-0.06567346	0.29919671	0.5428896	0.26447713	0.31996191	0.18699637	0	0.25630117	0.38086953	0.05842602	-0.25681439
Adenine	B61	-0.13545876	0.05090895	0.38894002	-0.17212653	-0.13366037	-0.12791933	0.35337823	-0.11645181	0.05993233	0.30120723	0.33720875	0.24627757	0.48013481	0.25630117	0	0.10473356	-0.11871654	-0.05314403
Heptadecanc	B62	-0.44397771	0.07947467	0.29450253	-0.477618	-0.27139431	-0.49539834	0.21780339	0.25485097	0.26590903	0.30976742	0.40440518	0.2029363	0.27606455	0.38086953	0.10473356	0	0.1722102	0.15578867
Decanoate	B65	-0.32913589	-0.15052044	0.36149827	-0.22560852	-0.66268627	-0.11535548	0.08802501	0.17536681	0.27785059	0.39496372	-0.21203553	0.24067992	0.31135394	0.05842602	-0.11871654	0.1722102	0	-0.07086319
Diethanolam	B66	0.21055162	0.46919953	0.03818386	0.09552896	0.2059842	0.14966229	0.13270849	0.25183694	-0.22510909	-0.10603646	-0.07071838	-0.19448555	-0.00270494	-0.25681439	-0.05314403	0.15578867	-0.07086319	0

Supplementary Table 3. Metabolite-metabolite correlations common to both tissues. Significant pairwise correlations within and between tissues (r ≥ 0.5, p ≤ 0.05) were highlighted in blue and yellow, representing positive and negative correlations, respectively.

Metabolites		Alanine	Arginine	Asparagine	Aspartate	b-Alanine	GABA	Glutamate	Glutamine	Glycine	Histidine	Isoleucine	Leucine	Lysine	Methionine	Ornithine	Phenylalanine	Serine
		C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C18
Alanine	B1	0.590873	0.066077	0.430255	0.600427	0.484782	-0.26856	0.458451	0.254489	0.377874	-0.02172	0.350616	0.250497	0.077632	0.029747	0.135314	-0.06612	0.35648
Arginine	B2	-0.02923	0.706285	0.281907	0.12378	0.218221	0.103009	0.247951	-0.02675	0.287818	0.314044	0.231403	-0.02445	0.405848	0.199944	0.191335	0.343042	-0.01118
Asparagine	B3	0.045659	0.581714	0.210076	0.031449	0.251709	0.261253	0.123385	-0.10261	0.29512	0.374179	0.117751	-0.11707	0.384116	0.218416	0.165265	0.360724	-0.02089
Aspartate	B4	0.404343	0.166565	0.474418	0.684058	0.355025	-0.23723	0.432587	0.298965	0.206838	-0.03318	0.338135	0.274314	0.029385	0.026758	0.192236	0.010535	0.298927
b-Alanine	B5	0.347975	0.305807	0.287213	0.198615	0.322174	-0.16182	0.389043	0.250756	0.402828	-0.07635	0.245819	0.232821	0.006491	-0.14741	0.220446	-0.0816	0.375508
GABA	B6	-0.31045	0.272363	-0.10047	-0.35308	-0.22703	0.307137	-0.24965	-0.21324	-0.06368	0.137134	-0.07335	-0.19777	0.238264	0.168564	0.035184	0.310883	-0.25245
Glutamate	B7	0.381021	0.165071	0.447313	0.577139	0.294192	-0.28835	0.361508	0.259475	0.186128	0.012337	0.313545	0.231574	0.005862	0.063405	0.18798	0.040453	0.238867
Glutamine	B8	0.392807	0.385375	0.443741	0.346168	0.440922	0.017979	0.376337	0.167602	0.409963	0.144516	0.262952	0.113529	0.165242	0.014406	0.268767	0.119986	0.260534
Glycine	B9	0.207601	0.431937	0.300924	0.104841	0.374875	0.115556	0.323854	-0.00661	0.370118	0.203996	0.126697	-0.02493	0.320695	0.050531	0.135184	0.093962	0.114581
Isoleucine	B11	0.074441	0.524966	0.373685	0.17749	0.179028	0.051819	0.188329	-0.02038	0.166626	0.271933	0.174497	-0.03639	0.366661	0.268564	0.25787	0.306661	-0.02588
Leucine	B12	-0.0056	0.544134	0.35365	0.094406	0.114476	0.034715	0.183587	0.031875	0.185207	0.176383	0.206024	0.029032	0.297424	0.17874	0.305002	0.239574	0.033531
Methionine	B14	0.013323	0.589173	0.332562	0.188122	0.179002	0.105133	0.194746	-0.0754	0.138192	0.335709	0.153099	-0.08347	0.442226	0.340088	0.147808	0.400224	-0.09896
Phenylalanine	B16	0.129953	0.400009	0.420857	0.412151	0.166218	0.001833	0.226231	-0.00979	0.140049	0.253603	0.161388	-0.03469	0.309276	0.243272	0.145209	0.29387	-0.0302
Proline	B17	0.507612	0.363408	0.609875	0.528394	0.405738	-0.10913	0.40564	0.218476	0.376917	0.100381	0.363872	0.19433	0.291814	0.100725	0.285907	0.032888	0.346582
Serine	B18	0.779459	0.243599	0.548448	0.600442	0.557023	-0.27693	0.527529	0.286296	0.510863	0.033409	0.387515	0.251491	0.129155	0.029393	0.216503	-0.04821	0.456366
Threonine	B19	0.360684	0.61581	0.485679	0.314623	0.367816	0.010027	0.361729	0.117945	0.408387	0.220502	0.300805	0.093155	0.276679	0.131584	0.366031	0.22736	0.236716
Tryptophan	B20	-0.00649	-0.03766	0.161096	0.403086	0.0447	-0.1693	0.166112	0.17355	-0.08535	-0.08025	0.139445	0.129524	-0.11518	0.002241	-0.02221	0.010924	0.04088
Tyrosine	B21	0.441208	0.43408	0.442099	0.480724	0.325845	-0.08207	0.31989	0.098262	0.344181	0.236891	0.344282	0.094618	0.30422	0.248007	0.235476	0.282306	0.192398
Valine	B22	0.221096	0.612589	0.470529	0.306352	0.330606	0.022993	0.326761	0.051208	0.289568	0.290639	0.263549	0.025883	0.412499	0.238654	0.265849	0.252621	0.083146
5-Oxoproline	B23	0.373049	0.162	0.447302	0.580993	0.282696	-0.29837	0.358593	0.263526	0.182902	0.00813	0.316914	0.236718	0.001565	0.062	0.185386	0.041689	0.239649
Putrescine	B24	-0.15996	0.303758	-0.08313	-0.471	-0.07242	0.247249	-0.10969	-0.07354	0.146415	0.082281	-0.01493	-0.07243	0.108938	-0.10122	0.215945	0.02319	0.016402
cis-Aconitate	B26	0.426007	0.109787	-0.00729	0.245729	0.283804	0.081547	0.130125	-0.03319	0.113192	0.1469	0.029108	-0.03756	0.087244	0.163001	0.04683	0.129749	0.059714
Citrate	B27	0.079863	0.492334	0.155578	-0.02445	0.182543	0.228193	0.128548	-0.03439	0.296995	0.286499	0.067273	-0.10032	0.234715	0.030976	0.185291	0.275564	0.029495
Pyruvate	B29	-0.02716	-0.15871	0.166262	0.177986	0.011569	-0.31365	0.10104	0.332796	0.02123	-0.29146	0.250424	0.324106	-0.25541	-0.28217	0.109222	-0.2722	0.282676
Succinate	B30	0.074391	-0.12476	0.228112	0.23942	0.006088	-0.40646	0.171916	0.355667	0.148626	-0.28672	0.283751	0.349132	-0.32183	-0.23821	0.132542	-0.24268	0.346825
Benzoate	B31	-0.1251	-0.16413	0.091738	0.151984	-0.04406	-0.26041	0.068735	0.152154	-0.04178	-0.13836	0.046014	0.136899	-0.14654	-0.12812	0.013564	-0.17992	0.079015
2-Ketoglucona	B32	-0.06045	0.214646	-0.09678	-0.38921	-0.04146	0.147916	-0.18278	-0.13988	0.012713	0.134078	-0.1014	-0.17675	0.083665	0.092105	0.059651	0.155808	-0.12985
Caffeate	B33	0.103123	0.213118	0.391098	0.339189	0.06216	-0.32104	0.212734	0.286734	0.173055	-0.19468	0.371045	0.32728	-0.0608	-0.08958	0.213637	-0.11571	0.33331
4-Hydroxyben:	B35	0.12998	0.330113	0.369373	0.169796	0.118616	-0.17035	0.172267	0.217272	0.417575	0.03228	0.347077	0.20649	0.035459	-0.06227	0.350036	-0.00112	0.299658
Dehydroascort	B36	-0.19339	-0.06184	-0.09712	-0.231	-0.06204	-0.16811	-0.09156	0.189417	-0.0964	-0.18265	0.084897	0.134668	-0.31044	-0.17666	0.173155	-0.14058	0.049133
Glycerate	B40	0.29588	0.029981	0.298266	0.111913	0.102782	-0.28929	0.078007	0.276886	0.322152	-0.17668	0.301183	0.313598	-0.17773	-0.19474	0.293709	-0.18442	0.425482
Similar to Itaco	B41	0.414885	0.0944	0.390712	0.520725	0.186358	-0.21968	0.249406	0.243603	0.266353	0.021589	0.330448	0.227152	0.010456	0.074931	0.21211	0.101411	0.296103
Lactate	B42	0.082624	-0.23048	0.206873	0.252682	0.150009	-0.02773	0.004445	0.044553	-0.00807	-0.03929	-0.13215	-0.01903	-0.03757	0.0178	0.002628	-0.03953	0.027644
Nicotinate	B43	0.128205	0.328577	0.404475	0.266504	0.140082	-0.22716	0.23053	0.2601	0.345465	0.039165	0.396564	0.266815	0.102051	0.008435	0.305145	0.031218	0.280104
Quinate	B45	-0.05447	0.12345	-0.17696	-0.3455	-0.04693	0.195994	-0.12592	-0.26763	-0.01964	0.201859	-0.184	-0.23018	0.190148	0.171231	-0.10606	0.195928	-0.19316
Xylose	B46	-0.27582	0.330869	-0.0259	-0.38497	-0.19192	0.000205	-0.09702	0.103373	-0.10475	-0.13661	0.16005	0.135159	-0.0378	-0.12953	0.191458	-0.04692	0.0384
Fucose	B47	0.054381	0.088821	0.306428	0.266671	0.041032	-0.29484	0.128846	0.298106	0.17098	-0.11713	0.261716	0.2622	-0.18275	-0.15903	0.254007	-0.0906	0.280453
Sorbose	B48	-0.16314	0.080794	-0.19458	-0.40333	-0.15696	0.221976	-0.21275	-0.21521	-0.00583	0.099587	-0.18815	-0.18121	0.084488	0.04268	-0.03227	0.115878	-0.14326
Fructose	B49	0.259607	0.145883	-0.2475	-0.2391	-0.00079	0.467891	-0.11321	-0.37415	0.001693	0.317033	-0.26865	-0.37098	0.303345	0.247837	-0.19116	0.231371	-0.19499
Galactose	B51	-0.10603	0.032126	-0.20101	-0.35654	-0.12861	0.18113	-0.16772	-0.27909	0.004384	0.182322	-0.21775	-0.2308	0.184743	0.168137	-0.12829	0.212979	-0.1937
Similar to Ribu	B52	-0.03497	0.474274	0.305181	0.053105	0.186404	-0.40457	0.435856	0.556243	0.395022	-0.3207	0.649654	0.548277	-0.23766	-0.434	0.465202	-0.27665	0.520972
Sucrose	B53	-0.16737	0.068344	0.05272	0.077701	0.134701	-0.0691	0.092177	-0.00103	-0.08568	0.098408	-0.03375	-0.06662	-0.0037	0.086322	0.044813	0.094305	-0.16888
Trehalose	B54	0.219071	-0.05855	0.152348	0.356173	0.366372	-0.20332	0.171574	0.263208	0.115702	0.005444	0.277771	0.219183	-0.16935	-0.06974	0.181888	-0.08583	0.258839
Glycerol	B55	0.17372	-0.21848	0.236958	0.268747	0.016492	-0.37292	0.072062	0.357892	0.100019	-0.30277	0.323304	0.342958	-0.19381	-0.18227	0.136762	-0.2128	0.329595
myo-Inositol	B57	0.248202	0.308271	0.270245	0.159982	0.147033	-0.03654	0.13844	0.240057	0.240891	-0.08189	0.344652	0.236917	0.033431	-0.08844	0.295529	-0.03145	0.324754
Xylitol	B58	0.057614	0.026591	0.19382	0.208432	0.128261	-0.22011	0.13291	0.311927	0.052445	-0.1789	0.330011	0.334249	-0.137	-0.19921	0.234766	-0.1654	0.302024
Uracil	B59	0.125481	0.247301	0.365996	0.201801	0.132202	-0.20913	0.17745	0.244602	0.398721	0.019698	0.307158	0.215605	-0.0189	-0.07745	0.369981	-0.00739	0.308779
Orthophospha	B60	0.3896	0.007053	0.361636	0.572497	0.245054	-0.35267	0.279504	0.380234	0.162202	-0.24516	0.366403	0.395927	-0.17832	-0.05649	0.183683	-0.12833	0.408009
Adenine	B61	0.332752	0.162873	0.359721	0.219059	0.10515	-0.34303	0.248715	0.368885	0.361352	-0.10955	0.430055	0.382888	-0.11651	-0.12124	0.406885	-0.11427	0.418739
Heptadecanoa	B62	0.101178	0.234535	0.385142	0.37628	0.118734	-0.08672	0.191292	0.21341	0.063898	-0.06258	0.215713	0.142159	0.089289	0.02676	0.203929	0.011078	0.148948
Decanoate	B65	-0.18062	-0.17786	0.132036	0.093082	-0.07739	-0.17737	-0.03526	0.102224	0.015183	-0.11777	-0.02887	0.067368	-0.13687	-0.09638	-0.01541	-0.0495	0.027205
Diethanolamin	B66	-0.34088	0.139398	-0.28275	-0.44466	-0.38317	0.199564	-0.22102	-0.25876	-0.22924	0.099933	-0.22722	-0.29742	0.107535	0.141698	-0.18233	0.246368	-0.36436

Metabolites		Threonine	ryptophar	Tyrosine	Valine	-Oxoprolir	Putrescine	Fumarate	s-Aconitat	Citrate	Isocitrate	Succinate	Benzoate	-Coumarat	droxybenz	ydroascorl	ffeoylquir	alacturona
		C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C30	C31	C34	C35	C36	C37	C38
Alanine	B1	0.256861	0.271505	0.187844	0.339525	0.41027	-0.18533	-0.20375	0.443525	0.141829	0.367491	0.321447	-0.16284	0.222259	-0.09041	0.147247	0.171697	-0.09824
Arginine	B2	0.17864	0.152013	0.388748	0.639462	0.275201	0.133163	-0.3667	-0.14675	-0.26716	0.260185	0.043439	0.065334	-0.32523	-0.19759	-0.40985	0.06087	0.103459
Asparagine	B3	0.15548	0.071192	0.332737	0.668605	0.153637	0.220113	-0.35	-0.27449	-0.31659	0.139711	-0.1145	0.119828	-0.33227	-0.30557	-0.47377	0.070082	0.148926
Aspartate	B4	0.250799	0.31872	0.275304	0.456008	0.422502	-0.24496	-0.15036	0.459304	0.227544	0.383276	0.26688	-0.15132	0.285475	-0.00718	0.232347	0.134716	-0.12613
b-Alanine	B5	0.294622	-0.08446	0.147019	0.130815	0.291985	-0.2529	-0.32542	0.16884	0.045738	0.371799	0.208836	-0.26244	-0.12127	-0.1587	0.14329	-0.01003	-0.21119
GABA	B6	-0.05696	-0.0618	-0.12555	0.254776	-0.26467	0.25348	-0.02162	-0.37952	-0.41039	-0.08778	-0.18455	0.198591	-0.2735	-0.02251	-0.48755	-0.05808	0.169855
Glutamate	B7	0.24405	0.239744	0.366912	0.485615	0.384226	-0.16696	-0.07479	0.347763	0.136721	0.308677	0.111088	-0.12198	0.217562	-0.01489	0.101248	0.245554	-0.10617
Glutamine	B8	0.320367	0.16758	0.234152	0.464779	0.32363	-0.13523	-0.38913	0.179925	0.158606	0.409353	0.223626	-0.09473	-0.01541	-0.18501	0.0031	0.232548	-0.04217
Glycine	B9	0.187514	-0.13792	-0.01142	0.36499	0.235112	0.044545	-0.44279	-0.19715	-0.28198	0.293234	0.207613	0.001828	-0.18528	-0.0291	-0.33304	0.137952	0.050018
Isoleucine	B11	0.119854	0.166985	0.223377	0.490825	0.19951	0.115859	-0.15695	-0.1696	-0.25835	0.255309	0.034197	0.078902	-0.1236	-0.03907	-0.28433	0.102295	0.128177
Leucine	B12	0.153613	0.106953	0.169883	0.456225	0.108709	0.025635	-0.25664	-0.15898	-0.26279	0.320301	0.125891	-0.00893	-0.16202	-0.06735	-0.29061	0.094486	0.051706
Methionine	B14	0.045502	0.112771	0.279045	0.549121	0.245361	0.177782	-0.13027	-0.13472	-0.24592	0.235634	0.037961	0.139439	-0.17193	-0.08626	-0.24112	0.08156	0.191969
Phenylalanine	B16	0.066982	0.30857	0.404619	0.467529	0.277773	0.04077	-0.15792	0.124653	0.030523	0.262728	0.148618	0.112482	-0.11896	0.054305	-0.07337	0.319923	0.173339
Proline	B17	0.276631	0.317334	0.228997	0.427802	0.244472	-0.18403	-0.38346	0.299709	0.016793	0.511	0.388185	-0.15037	0.024635	-0.09092	0.064924	0.158551	-0.03565
Serine	B18	0.373804	0.212102	0.267894	0.492734	0.48002	-0.18116	-0.32571	0.365371	0.046294	0.437722	0.212117	-0.19637	0.050776	-0.23784	0.022651	0.217112	-0.13493
Threonine	B19	0.315873	0.178626	0.308717	0.584399	0.301293	-0.048	-0.38759	-0.01718	-0.11503	0.408162	0.154505	-0.07454	-0.11954	-0.18408	-0.25785	0.253236	-0.00424
Tryptophan	B20	0.060697	0.184067	0.166188	0.245331	0.187973	-0.11527	0.018513	0.349231	0.168671	0.140596	0.030317	-0.043	0.114109	0.028391	0.218058	0.052314	-0.06025
Tyrosine	B21	0.188394	0.38446	0.466928	0.608258	0.323877	-0.0123	-0.17634	0.252013	0.013747	0.332871	0.128536	-0.00251	-0.14229	-0.25586	-0.04776	0.17691	0.06013
Valine	B22	0.223508	0.155191	0.263277	0.615042	0.348914	0.067596	-0.2508	-0.04419	-0.20614	0.352409	0.043717	0.014261	-0.13149	-0.09565	-0.26998	0.192646	0.099575
5-Oxoproline	B23	0.253093	0.251356	0.380686	0.495342	0.388977	-0.17398	-0.06847	0.357984	0.145399	0.304173	0.109335	-0.12312	0.219849	-0.01191	0.110189	0.232057	-0.11154
Putrescine	B24	0.073962	-0.1815	-0.01065	0.071733	-0.20236	0.116255	-0.29374	-0.43587	-0.32247	-0.01456	-0.15653	-0.05428	-0.35764	-0.20884	-0.46859	-0.10621	-0.01453
cis-Aconitate	B26	0.049881	-0.00188	0.036964	0.284934	0.250275	0.125483	0.041474	0.014708	-0.06274	-0.00703	-0.19315	0.047317	0.01769	-0.06869	-0.19549	0.177084	0.081784
Citrate	B27	0.23053	0.181559	0.324558	0.409839	0.163945	0.087925	-0.23076	-0.13661	-0.03429	0.136616	-0.07925	0.054019	-0.20704	-0.13611	-0.35821	0.022899	0.073012
Pyruvate	B29	0.243787	0.28748	0.061998	-0.05619	-0.01057	-0.37198	0.043266	0.35559	0.307914	0.148656	0.256758	-0.26653	0.261067	0.24702	0.27722	-0.20155	-0.31247
Succinate	B30	0.23535	0.304817	0.082316	-0.0353	0.036114	-0.42111	0.029561	0.424853	0.288305	0.158603	0.28865	-0.28911	0.261108	0.241853	0.280488	-0.08905	-0.33249
Benzoate	B31	-0.02458	0.04512	-0.11965	-0.20532	0.024709	-0.16309	0.130169	0.116812	0.120359	-0.01518	0.188306	-0.10395	0.252912	0.301978	0.191649	-0.1411	-0.12856
2-Ketoglucona	B32	0.00559	-0.218	-0.14954	0.131166	-0.14542	0.243527	0.098034	-0.44859	-0.40681	-0.1377	-0.34428	0.091659	-0.15537	0.046188	-0.60354	0.160024	0.089505
Caffeate	B33	0.212603	0.38741	0.234029	0.245089	0.078914	-0.27517	-0.12773	0.273971	-0.03046	0.235586	0.335707	-0.24859	0.106027	0.131247	-0.01112	-0.02081	-0.24771
4-Hydroxyben:	B35	0.264848	0.454718	0.276949	0.291252	0.11038	-0.16884	-0.12166	0.114003	-0.00887	0.139251	0.112589	-0.14818	0.034871	0.117212	-0.29127	-0.12817	-0.16559
Dehydroascorl	B36	0.203666	-0.02918	0.087787	0.023026	-0.04928	-0.13867	0.115787	-0.03551	0.104169	0.010203	-0.34471	-0.18065	-0.01056	-0.07033	0.170612	-0.0703	-0.22557
Glycerate	B40	0.336265	0.316594	0.211535	0.099825	-0.04352	-0.28988	-0.1465	0.162181	-0.00336	0.157014	0.177685	-0.29772	0.00695	0.060138	-0.09352	-0.02119	-0.31018
Similar to Itaco	B41	0.219084	0.595946	0.41341	0.39777	0.306975	-0.21003	0.022592	0.483481	0.335189	0.19313	0.077809	-0.11064	0.177435	-0.02621	0.201396	-0.05345	-0.10648
Lactate	B42	-0.06317	-0.139	-0.34014	-0.09026	-0.02255	-0.02878	0.032438	-0.10365	-0.09385	0.100071	0.246282	0.033251	0.258406	0.317793	-0.02235	-0.03699	0.011011
Nicotinate	B43	0.246617	0.505949	0.3701	0.422187	0.194204	-0.14837	-0.06469	0.205347	0.069656	0.172988	0.099994	-0.15683	0.011676	0.009061	-0.13657	-0.315	-0.16811
Quinate	B45	-0.15816	-0.25301	0.00048	-0.03243	-0.08103	0.263111	-0.05275	-0.39159	-0.23059	-0.14585	-0.21242	0.160499	-0.36725	-0.18221	-0.1955	0.052092	0.164715
Xylose	B46	0.21169	-0.22827	-0.04035	0.21544	-0.22026	-0.09197	-0.06555	-0.2088	-0.2439	0.13562	-0.14318	-0.16695	-0.20102	-0.00335	-0.20776	0.019466	-0.16982
Fucose	B47	0.259248	0.410176	0.21452	0.10143	0.115079	-0.30741	0.014917	0.300002	0.18804	0.125412	0.110815	-0.20121	0.171957	0.301719	0.051082	-0.11535	-0.25317
Sorbose	B48	-0.10773	-0.21224	0.001986	-0.09226	-0.22694	0.202221	-0.11496	-0.42395	-0.23156	-0.11879	-0.13161	0.089592	-0.31515	-0.20045	-0.19473	-0.15046	0.076463
Fructose	B49	-0.1923	-0.2725	-0.00552	0.042191	-0.01622	0.382737	-0.082	-0.27401	-0.25289	-0.17129	-0.30121	0.271529	-0.31149	-0.36738	-0.36281	0.197237	0.325773
Galactose	B51	-0.18683	-0.12764	0.050956	-0.11532	-0.12559	0.254293	-0.00011	-0.38054	-0.21531	-0.19141	-0.16342	0.175225	-0.37943	-0.17863	-0.12227	-0.19074	0.162133
Similar to Ribu	B52	0.586075	0.376779	0.508846	0.510669	0.220691	-0.46887	-0.35339	0.241481	0.098314	0.43936	0.094447	-0.53984	-0.04268	-0.12914	0.108842	-0.2337	-0.50374
Sucrose	B53	-0.02676	-0.14546	0.002283	0.129978	0.166801	0.057631	0.055665	-0.16566	-0.02712	0.059399	-0.06411	0.076566	-0.03027	0.215315	-0.02132	0.327409	0.070796
Trehalose	B54	0.255093	0.428433	0.113274	0.199598	0.166675	-0.21435	0.033524	0.276388	0.309902	0.098205	0.040174	-0.14848	0.136115	0.098818	0.198136	-0.0756	-0.17995
Glycerol	B55	0.273186	0.318333	-0.02944	0.050271	-0.05771	-0.34997	0.058982	0.44025	0.194542	0.196082	0.250683	-0.28037	0.339641	0.128806	0.307393	-0.19027	-0.27995
myo-Inositol	B57	0.319191	0.078447	0.113112	0.351382	-0.00925	-0.15936	-0.28581	0.179128	-0.07301	0.317079	0.103392	-0.23116	-0.05696	-0.28867	-0.09078	-0.0402	-0.1817
Xylitol	B58	0.287043	0.455099	0.117276	0.062596	0.011337	-0.30845	0.005151	0.322872	0.268883	0.184336	0.228709	-0.25519	0.151012	0.26175	0.12649	-0.30495	-0.2704
Uracil	B59	0.242694	0.43698	0.287395	0.222638	0.123166	-0.20153	-0.06412	0.130994	0.079224	0.129098	0.119196	-0.16939	0.114631	0.141898	-0.18479	-0.12009	-0.18504
Orthophospha	B60	0.3088	0.301584	0.096632	0.281667	0.231364	-0.39681	0.004704	0.58887	0.28841	0.298751	0.293577	-0.28199	0.348989	0.07258	0.358154	0.102296	-0.29483
Adenine	B61	0.404097	0.368613	0.379364	0.440584	0.243852	-0.28086	-0.06515	0.220844	0.197045	0.229928	-0.09356	-0.29531	0.057771	-0.14669	-0.05414	-0.15287	-0.29789
Heptadecanoa	B62	0.163232	0.070834	0.028826	0.258246	0.112053	-0.13201	-0.06171	0.224825	0.025788	0.298945	0.16304	-0.10383	0.168628	0.065151	0.029804	0.199847	-0.03936
Decanoate	B65	-0.01312	0.147386	-0.06071	-0.19975	-0.11043	-0.13581	0.068385	0.037291	0.048994	0.028948	0.26005	-0.05339	0.228922	0.382551	0.264256	-0.3412	-0.08386
Diethanolamin	B66	-0.17429	-0.29393	-0.19955	-0.03895	-0.0963	0.265909	0.301798	-0.31057	-0.25593	-0.26454	-0.45032	0.224886	-0.18109	0.087086	-0.29914	0.068879	0.227899

Metabolites		Glucarate	Glycerate	ilar to Itaco	Nicotinate	Quinate	Xylose	Fructose	Glucose	Sucrose	Glycerol	Galactinol	yo-Inosit	Xylitol	Adenine	ptadecano	radecano	droxypyri
		C39	C40	C41	C43	C44	C46	C49	C50	C53	C55	C56	C57	C58	C61	C62	C63	C64
Alanine	**B1**	0.401998	0.413092	-0.14093	-0.26185	-0.0655	-0.44627	0.028787	-0.13904	0.189825	0.153759	0.016484	0.211216	0.160082	0.318168	0.446792	-0.22279	-0.22377
Arginine	**B2**	0.034434	-0.09329	0.082817	0.137183	0.087416	0.205283	-0.0464	-0.06746	-0.12146	-0.01503	0.297367	-0.05507	0.219948	-0.36123	-0.17097	0.170346	-0.19374
Asparagine	**B3**	-0.05392	-0.19062	0.124499	0.1871	-0.04293	0.306029	-0.11921	-0.10525	-0.21369	-0.09351	0.240629	-0.11782	0.119389	-0.24978	-0.21716	0.202819	-0.31566
Aspartate	**B4**	0.298158	0.165385	-0.17291	-0.23929	0.022498	-0.3628	-0.01597	-0.22451	0.232991	0.190747	-0.08842	0.188034	0.204037	0.277807	0.493254	-0.30028	-0.08805
b-Alanine	**B5**	-0.09952	0.141989	-0.22113	-0.22258	0.170619	-0.12605	0.253266	0.227508	0.221321	0.062496	-0.1687	0.261835	-0.03556	-0.19324	0.052443	-0.18046	-0.22523
GABA	**B6**	-0.33491	-0.23113	0.181995	0.301212	0.038296	0.480214	-0.16409	-0.08968	-0.26575	-0.08876	0.066115	-0.1732	-0.20501	-0.35249	-0.23913	0.271058	-0.04008
Glutamate	**B7**	0.23281	0.100959	-0.17475	-0.19963	-0.00283	-0.34399	-0.0074	-0.17748	0.18443	0.161103	0.029178	0.14777	0.188451	0.263673	0.440549	-0.24696	-0.1207
Glutamine	**B8**	-0.06961	0.078643	-0.04386	-0.05219	0.187902	-0.06337	0.02597	-0.0402	0.065373	0.052822	0.091989	0.088921	-0.03225	-0.05841	0.031011	-0.1181	-0.22161
Glycine	**B9**	-0.11137	0.008131	0.03096	0.119541	0.024148	0.149023	0.041057	0.006433	-0.08368	0.135732	0.259625	0.017778	0.063476	-0.30727	-0.16328	0.113483	-0.25801
Isoleucine	**B11**	0.129581	-0.06193	0.085032	0.148653	-0.04404	0.159131	-0.13501	-0.16711	-0.11175	-0.13085	0.107353	-0.05887	0.054249	-0.21843	0.032014	0.136895	-0.11639
Leucine	**B12**	0.055901	-0.00443	0.015955	0.078104	0.076049	0.202872	-0.03921	-0.05534	-0.04266	-0.05112	0.0388	0.016024	-0.00326	-0.35575	-0.00581	0.080274	-0.12273
Methionine	**B14**	0.140657	-0.10436	0.146485	0.201092	-0.02241	0.181586	-0.17457	-0.20665	-0.17514	-0.16656	0.175403	-0.10066	0.059524	-0.2944	0.0134	0.204272	-0.07129
Phenylalanine	**B16**	0.257146	-0.04252	0.141437	0.15737	-0.01814	0.058812	-0.22382	-0.29766	-0.06225	-0.00026	0.11763	-0.1443	0.189588	-0.16639	0.007591	0.045019	0.020631
Proline	**B17**	0.249493	0.393473	-0.08203	-0.14899	0.070923	-0.19415	0.02468	-0.13396	0.142297	0.093495	-0.20449	0.19904	-0.07573	0.068889	0.285124	-0.12477	-0.3081
Serine	**B18**	0.183805	0.319383	-0.18783	-0.31063	-0.06523	-0.46313	0.091196	-0.07386	0.173499	0.085895	0.010309	0.24454	-0.05915	0.241669	0.397488	-0.21171	-0.46907
Threonine	**B19**	0.026485	0.060821	-0.04828	-0.00644	0.060433	0.062488	-0.01844	-0.11317	0.000679	0.007154	0.10841	0.075757	0.062749	-0.19872	0.042438	-0.0219	-0.31782
Tryptophan	**B20**	0.088586	-0.02537	-0.08162	-0.07573	0.096644	-0.15174	-0.0433	-0.20382	0.153089	0.181356	-0.05861	0.077388	0.138964	0.26824	0.335316	-0.19468	0.041086
Tyrosine	**B21**	0.289066	0.181487	0.017355	-0.0663	-0.01235	-0.11405	-0.10931	-0.22104	0.008166	-0.03245	-0.0092	0.028881	0.122263	-0.00713	0.201636	-0.0148	-0.27408
Valine	**B22**	0.201179	0.003449	0.057306	0.10886	-0.08324	0.077318	-0.12905	-0.20566	-0.07479	-0.01184	0.168169	0.002989	0.17266	-0.14817	0.061165	0.069482	-0.24607
5-Oxoproline	**B23**	0.230112	0.097148	-0.17576	-0.20476	-0.00086	-0.36015	-0.00327	-0.17825	0.187136	0.155458	0.024475	0.147697	0.193747	0.256808	0.434038	-0.25165	-0.10716
Putrescine	**B24**	-0.23481	-0.13084	-0.00255	0.119106	0.00327	0.45611	0.097188	0.233401	-0.07996	0.055927	0.011835	0.004521	0.031339	-0.35066	-0.41901	0.140671	-0.2535
cis-Aconitate	**B26**	0.311301	-0.01154	0.052889	0.034514	-0.38147	-0.0388	-0.21051	-0.31829	-0.10372	0.054333	0.117692	-0.04424	0.317385	0.162763	0.146072	0.018145	-0.3271
Citrate	**B27**	-0.19389	-0.15684	0.106747	0.21711	0.092472	0.264541	-0.07318	-0.11514	-0.13007	0.015107	0.246692	-0.10616	0.187162	-0.26106	-0.37503	0.100868	-0.21075
Pyruvate	**B29**	-0.00734	0.294532	-0.23676	-0.27062	0.236728	-0.38653	0.248058	0.060639	0.356584	0.271344	-0.2152	0.256431	0.033488	0.12904	0.140699	-0.37706	0.302177
Succinate	**B30**	-0.04067	0.312839	-0.30455	-0.32514	0.31182	-0.44925	0.274727	0.0677	0.386957	0.278339	-0.24832	0.284394	-0.03441	0.130537	0.224363	-0.40481	0.258594
Benzoate	**B31**	0.10162	0.129608	-0.13918	-0.0909	0.015697	-0.2623	0.130884	-0.06057	0.204334	0.216465	-0.06326	0.148612	0.216666	0.152461	0.305887	-0.14362	0.256527
2-Ketogluconа	**B32**	-0.2433	-0.17559	0.058913	0.226969	-0.16275	0.327591	-0.0858	-0.07215	-0.21009	0.068068	0.336615	-0.10715	0.037569	-0.19775	-0.23899	0.198206	-0.14825
Caffeate	**B33**	0.036346	0.357151	-0.27076	-0.26068	0.194992	-0.27974	0.215846	-0.01104	0.303038	0.223971	-0.26386	0.314475	0.007337	0.054805	0.365619	-0.24547	0.069578
4-Hydroxybenz	**B35**	0.00653	0.19904	-0.1713	-0.1059	0.146277	-0.15325	0.112583	-0.03661	0.184835	0.19162	-0.10076	0.194036	0.134135	0.108936	0.160323	-0.13046	-0.00699
Dehydroascorb	**B36**	-0.31788	-0.26687	-0.1904	-0.10026	0.160294	-0.01016	0.174975	0.250447	0.13632	-0.15096	-0.0951	0.129967	-0.2327	0.143117	-0.0519	-0.15678	-0.08936
Glycerate	**B40**	-0.07546	0.362745	-0.30261	-0.33414	0.161754	-0.29362	0.288946	0.146973	0.278759	0.24656	-0.16494	0.264566	0.01134	0.042539	0.109249	-0.29539	-0.12306
Similar to Itaco	**B41**	0.267926	0.201049	-0.10538	-0.2209	0.068652	-0.40851	-0.02283	-0.19523	0.189	0.016987	-0.26475	0.131781	0.056038	0.303405	0.315496	-0.23045	-0.05049
Lactate	**B42**	-0.03655	0.023449	-0.02437	0.008655	-0.00663	-0.04072	0.027768	-0.09059	0.030774	0.107354	0.048539	-0.00147	-0.12095	-0.04523	0.320716	-0.04967	0.125297
Nicotinate	**B43**	0.195887	0.211597	-0.18188	-0.18736	0.108565	-0.2653	0.128821	-0.0525	0.211292	0.163551	-0.11195	0.228055	0.240421	0.158515	0.25674	-0.13476	-0.01526
Quinate	**B45**	-0.20879	-0.25025	0.138452	0.180193	-0.07916	0.283822	-0.0621	0.161409	-0.26969	-0.30582	0.188377	-0.1938	-0.21145	-0.30831	-0.40197	0.295557	-0.12167
Xylose	**B46**	-0.36516	-0.07748	-0.1497	-0.01221	0.193338	0.274101	0.189781	0.234785	0.072159	0.113457	-0.12942	0.131984	-0.26639	-0.4211	-0.26835	-0.06597	-0.0668
Fucose	**B47**	-0.01687	0.103705	-0.22169	-0.18255	0.229817	-0.31091	0.160649	-0.04125	0.296857	0.212202	-0.19896	0.220827	0.045902	0.165899	0.191678	-0.29868	0.176767
Sorbose	**B48**	-0.28622	-0.22399	0.066359	0.09877	0.037892	0.354311	0.06662	0.286883	-0.17738	-0.24229	0.022703	-0.11791	-0.26858	-0.3392	-0.37711	0.243483	-0.08973
Fructose	**B49**	-0.09088	-0.20431	0.324607	0.280966	-0.35174	0.418231	-0.32038	-0.09161	-0.42193	-0.30627	0.106859	-0.28243	-0.235	-0.18535	-0.34189	0.358187	-0.39175
Galactose	**B51**	-0.15945	-0.19841	0.153177	0.158329	-0.03928	0.235288	-0.00254	0.21916	-0.24551	-0.35045	0.012852	-0.20671	-0.23916	-0.37239	-0.4156	0.313281	-0.06037
Similar to Ribu	**B52**	-0.18691	0.209137	-0.49585	-0.40703	0.405024	-0.20249	0.472571	0.336801	0.54714	0.254258	-0.26249	0.510073	-0.03273	-0.02251	0.066968	-0.43669	-0.16351
Sucrose	**B53**	0.013901	-0.2877	0.023591	0.161076	-0.06785	0.041065	-0.11338	-0.18341	-0.03463	0.159576	0.351251	-0.11496	0.429745	-0.07418	-0.00949	0.015055	0.091438
Trehalose	**B54**	0.169068	0.185062	-0.14714	-0.15378	0.109453	-0.3306	0.088492	-0.17503	0.226748	0.154796	-0.08769	0.153413	0.174144	0.380774	0.17182	-0.27593	-0.04015
Glycerol	**B55**	0.080191	0.407149	-0.26652	-0.3623	0.162663	-0.50249	0.210791	-0.00503	0.357619	0.207742	-0.36832	0.293802	-0.15562	0.288424	0.371126	-0.36848	0.059106
myo-Inositol	**B57**	-0.13495	0.221141	-0.20312	-0.21629	0.124327	-0.01187	0.148345	0.052578	0.20054	0.176884	-0.29386	0.286038	-0.16405	-0.00243	0.211371	-0.18617	-0.38159
Xylitol	**B58**	0.196981	0.410452	-0.22346	-0.21799	0.255575	-0.25573	0.220279	-0.00632	0.327989	0.258344	-0.23919	0.285348	0.089403	0.225395	0.150082	-0.30649	0.071059
Uracil	**B59**	0.073547	0.154545	-0.19302	-0.12732	0.151026	-0.2023	0.137646	-0.02373	0.219234	0.193852	-0.10611	0.20183	0.20462	0.137425	0.203558	-0.16658	0.031962
Orthophospha	**B60**	0.084605	0.363654	-0.29409	-0.41629	0.202397	-0.52383	0.157011	-0.07977	0.339402	0.174913	-0.28945	0.334657	-0.05302	0.289205	0.510498	-0.41764	-0.01096
Adenine	**B61**	0.109806	0.101407	-0.34953	-0.37966	0.018912	-0.3784	0.167249	0.083873	0.291429	0.180323	-0.13189	0.289441	0.122237	0.276942	0.30146	-0.32381	-0.23544
Heptadecanoa	**B62**	0.069547	0.109785	-0.08377	-0.02677	0.029023	-0.06794	-0.05153	-0.26022	0.157589	0.230476	-0.19579	0.174465	0.011862	0.162029	0.409613	-0.17242	-0.11825
Decanoate	**B65**	-0.01138	0.105385	-0.08082	-0.02104	0.169713	-0.2001	0.156951	-0.00114	0.173415	0.04357	-0.13115	0.047001	-0.01671	-0.03671	0.163223	-0.09177	0.324815
Diethanolamin	**B66**	-0.33417	-0.39027	0.234195	0.387253	-0.05624	0.432012	-0.26512	-0.15127	-0.29973	-0.21189	0.109125	-0.28814	-0.17338	-0.25198	-0.38188	0.282197	0.203872

Tabela Suplementar 4 – Efeito dos genótipos nos níveis de cada metabólito na condição sob a dominância apical. A abundancia relativa de cada metabólito é comparada em cada variedade, entre os terços médios superior, mediano e basal. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	INTEIRA											
	RB72454						RB975375					
	TOPO		MEIO		BASE		TOPO		MEIO		BASE	
2-Hidroxipirimidina	8.6	a	8.8	a	8.8	a	8.3	a	8.8	a	8.6	a
Alanina	11.0	a	10.8	a	11.0	a	9.5	a	10.2	a	10.6	a
Piruvato	4.8	a	4.9	a	4.7	a	4.3	a	4.6	a	4.2	a
Valina	9.7	a	9.3	a	9.7	a	9.1	a	9.4	a	9.5	a
Glicerol	11.0	a	11.4	a	11.2	a	10.8	a	10.8	a	10.5	a
Leucina	8.1	a	7.3	a	7.7	a	7.6	a	8.1	a	7.4	a
Isoleucina	8.0	a	7.4	a	7.7	a	7.9	a	8.2	a	7.6	a
Glicina	7.0	a	7.1	a	7.0	a	5.9	a	7.1	a	7.4	a
Ortofosfato	9.9	a	9.3	a	9.3	a	10.2	a	9.5	a	9.2	a
Benzoato	7.8	a	8.3	a	7.9	a	7.6	a	7.7	a	7.5	a
Serina	9.3	a	8.9	a	9.2	a	8.7	a	8.9	a	9.1	a
Succinato	7.0	a	7.3	a	7.0	a	6.8	a	6.7	a	6.9	a
Treonina	6.9	a	6.5	a	6.7	a	6.7	a	6.8	a	7.0	a
Pipecolato	8.0	a	7.1	a	7.7	a	8.9	a	8.1	a	7.5	a
Nonoato	6.9	a	7.4	a	7.0	a	6.7	a	6.8	a	6.6	a
Nicotinato	6.3	a	6.6	a	6.1	a	6.0	a	5.8	a	5.9	a
Itaconato	6.6	a	7.0	a	6.7	a	6.7	a	6.7	a	6.9	a
Eritritol	7.1	a	6.4	a	6.8	a	4.4	a	5.2	a	5.6	a
Malato	9.2	a	9.0	a	9.1	a	9.5	a	9.6	a	9.8	a
GABA	7.5	a	8.0	a	7.5	a	7.3	a	7.0	a	7.6	a
Aspartato	11.6	a	11.7	a	11.9	a	10.9	b	11.4	ab	11.8	a
Maleato	5.1	a	5.1	a	5.3	a	4.4	b	4.9	ab	5.2	a
Threote	5.3	a	5.3	a	5.6	a	4.6	b	5.1	ab	5.5	a
Metionina	6.2	a	5.7	a	5.9	a	5.6	a	5.8	a	5.5	a
Dietanoalamina	3.0	b	4.8	a	5.4	a	7.7	a	6.7	a	7.7	a
Arginina	5.0	a	3.9	b	4.7	ab	4.5	a	4.7	a	4.7	a
Ornitina	7.3	a	8.1	a	8.4	a	7.1	a	7.9	ab	9.8	a
Xilose	7.6	a	7.5	a	8.0	a	6.9	a	7.5	a	7.8	a
Xilitol	7.8	a	8.5	a	8.7	a	6.0	a	6.9	a	7.5	a
Glutamato	11.7	a	11.6	a	11.9	a	10.8	b	11.4	ab	11.6	a
Xilulose	4.9	a	4.7	a	5.0	a	3.8	b	4.4	ab	4.5	a
Ramnose	5.9	a	5.6	a	6.1	a	5.5	a	5.3	a	5.4	a
Putrescina	7.3	a	7.1	a	7.1	a	8.0	a	7.7	a	7.9	a
Fucose	6.0	a	5.5	a	5.9	a	6.1	a	5.8	ab	5.4	b
Fenilalanina	4.6	a	4.8	a	5.1	a	4.5	a	4.8	a	5.1	a

4-Hidroxibenzoato	5.9	a	6.3	a	6.1	a	5.6	a	5.8	a	5.8	a
Asparagina	9.9	a	10.4	a	11.0	a	9.2	b	10.6	ab	12.0	a
Quinato	9.7	a	9.0	a	9.2	a	9.5	a	8.6	b	8.9	b
Frutose	13.0	a	12.1	a	12.5	a	15.2	a	13.6	b	13.9	ab
cis-Aconitato	12.8	a	12.5	a	12.9	a	13.2	a	13.6	a	13.7	a
Manose	9.8	a	10.1	a	10.2	a	9.9	a	9.9	a	10.2	a
Citrato	10.8	a	10.8	a	11.0	a	10.2	b	10.5	ab	11.1	a
Glicose	9.4	a	9.0	a	9.2	a	11.7	a	9.5	b	10.1	b
Glutamina	9.2	a	9.1	a	9.2	a	8.3	a	8.5	a	9.4	a
Lisina	6.6	a	6.0	a	6.6	a	6.0	a	6.4	a	6.7	a
Tetradecanoato	8.8	a	9.2	a	8.8	a	8.6	a	8.7	a	8.5	a
Dehidroascorbato	6.8	a	6.6	a	7.2	a	6.7	a	7.1	a	6.7	a
mio-Inositol	11.4	a	10.9	a	11.3	a	10.9	b	11.4	ab	11.6	a
Tirosina	7.7	a	7.5	a	7.8	a	7.6	a	7.9	a	7.9	a
Adenina	5.2	a	4.9	ab	4.6	b	4.8	a	4.6	a	4.4	a
Espermidina	6.9	a	7.2	a	6.7	a	4.2	a	5.0	a	5.1	a
Cafeato	9.3	a	9.4	a	9.4	a	8.7	a	8.8	a	8.9	a
Triptofano	7.7	a	8.0	a	8.2	a	6.6	b	7.6	a	7.8	a
Trealose	7.2	a	7.3	a	7.8	a	3.6	a	5.9	a	6.4	a
Rafinose	9.2	a	9.1	a	9.3	a	8.6	b	9.6	a	8.9	b
Sacarose	13.9	a	14.6	a	14.5	a	12.8	b	14.0	a	14.4	a

Tabela Suplementar 5 – Comparação dos níveis de cada metabólito entre as variedades RB72454 e RB975375 na condição sob a dominância apical. A abundancia relativa de cada metabólito é comparada em cada porção do colmo, terços médios superior, mediano e basal, entre as variedades testadas. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	INTEIRA											
	TOPO				MEIO				BASE			
	RB72454		RB975375		RB72454		RB975375		RB72454		RB975375	
2-Hidroxipirimidina	8.6	a	8.3	a	8.8	a	8.8	a	8.8	a	8.6	a
Alanina	11.0	a	9.5	b	10.8	a	10.2	a	11.0	a	10.6	a
Piruvato	4.8	a	4.3	a	4.9	a	4.6	a	4.7	a	4.2	b
Valina	9.7	a	9.1	a	9.3	a	9.4	a	9.7	a	9.5	a
Glicerol	11.0	a	10.8	a	11.4	a	10.8	a	11.2	a	10.5	b
Leucina	8.1	a	7.6	a	7.3	a	8.1	a	7.7	a	7.4	a
Isoleucina	8.0	a	7.9	a	7.4	a	8.2	a	7.7	a	7.6	a
Glicina	7.0	a	5.9	a	7.1	a	7.1	a	7.0	a	7.4	a
Ortofosfato	9.9	a	10.2	a	9.3	a	9.5	a	9.3	a	9.2	a
Benzoato	7.8	a	7.6	a	8.3	a	7.7	b	7.9	a	7.5	b
Serina	9.3	a	8.7	b	8.9	a	8.9	a	9.2	a	9.1	a

Succinato	7.0	a	6.8	a	7.3	a	6.7	b	7.0	a	6.9	a
Treonina	6.9	a	6.7	a	6.5	a	6.8	a	6.7	a	7.0	a
Pipecolato	8.0	a	8.9	a	7.1	a	8.1	a	7.7	a	7.5	a
Nonoato	6.9	a	6.7	a	7.4	a	6.8	b	7.0	a	6.6	b
Nicotinato	6.3	a	6.0	a	6.6	a	5.8	b	6.1	a	5.9	a
Itaconato	6.6	a	6.7	a	7.0	a	6.7	a	6.7	a	6.9	a
Eritritol	7.1	a	4.4	b	6.4	a	5.2	b	6.8	a	5.6	a
Malato	9.2	b	9.5	a	9.0	b	9.6	a	9.1	b	9.8	a
GABA	7.5	a	7.3	a	8.0	a	7.0	a	7.5	a	7.6	a
Aspartato	11.6	a	10.9	b	11.7	a	11.4	a	11.9	a	11.8	a
Maleato	5.1	a	4.4	b	5.1	a	4.9	a	5.3	a	5.2	a
Threote	5.3	a	4.6	b	5.3	a	5.1	a	5.6	a	5.5	a
Metionina	6.2	a	5.6	b	5.7	a	5.8	a	5.9	a	5.5	a
Dietanoalamina	3.0	b	7.7	a	4.8	a	6.7	a	5.4	b	7.7	a
Arginina	5.0	a	4.5	b	3.9	a	4.7	a	4.7	a	4.7	a
Ornitina	7.3	a	7.1	a	8.1	a	7.9	a	8.4	b	9.8	a
Xilose	7.6	a	6.9	b	7.5	a	7.5	a	8.0	a	7.8	a
Xilitol	7.8	a	6.0	b	8.5	a	6.9	a	8.7	a	7.5	a
Glutamato	11.7	a	10.8	b	11.6	a	11.4	a	11.9	a	11.6	a
Xilulose	4.9	a	3.8	b	4.7	a	4.4	a	5.0	a	4.5	a
Ramnose	5.9	a	5.5	a	5.6	a	5.3	a	6.1	a	5.4	a
Putrescina	7.3	b	8.0	a	7.1	a	7.7	a	7.1	a	7.9	a
Fucose	6.0	a	6.1	a	5.5	a	5.8	a	5.9	a	5.4	b
Fenilalanina	4.6	a	4.5	a	4.8	a	4.8	a	5.1	a	5.1	a
4-Hidroxibenzoato	5.9	a	5.6	a	6.3	a	5.8	a	6.1	a	5.8	b
Asparagina	9.9	a	9.2	a	10.4	a	10.6	a	11.0	b	12.0	a
Quinato	9.7	a	9.5	a	9.0	a	8.6	a	9.2	a	8.9	a
Frutose	13.0	b	15.2	a	12.1	a	13.6	a	12.5	b	13.9	a
cis-Aconitato	12.8	a	13.2	a	12.5	b	13.6	a	12.9	b	13.7	a
Manose	9.8	a	9.9	a	10.1	a	9.9	a	10.2	a	10.2	a
Citrato	10.8	a	10.2	b	10.8	a	10.5	a	11.0	a	11.1	a
Glicose	9.4	b	11.7	a	9.0	a	9.5	a	9.2	a	10.1	a
Glutamina	9.2	a	8.3	b	9.1	a	8.5	a	9.2	a	9.4	a
Lisina	6.6	a	6.0	a	6.0	a	6.4	a	6.6	a	6.7	a
Tetradecanoato	8.8	a	8.6	a	9.2	a	8.7	b	8.8	a	8.5	b
Dehidroascorbato	6.8	a	6.7	a	6.6	a	7.1	a	7.2	a	6.7	a
mio-Inositol	11.4	a	10.9	a	10.9	a	11.4	a	11.3	a	11.6	a
Tirosina	7.7	a	7.6	a	7.5	a	7.9	a	7.8	a	7.9	a
Adenina	5.2	a	4.8	b	4.9	a	4.6	a	4.6	a	4.4	a
Espermidina	6.9	a	4.2	b	7.2	a	5.0	b	6.7	a	5.1	b
Cafeato	9.3	a	8.7	a	9.4	a	8.8	a	9.4	a	8.9	b

Triptofano	7.7	a	6.6	b	8.0	a	7.6	a	8.2	a	7.8	a
Trealose	7.2	a	3.6	b	7.3	a	5.9	a	7.8	a	6.4	a
Rafinose	9.2	a	8.6	a	9.1	a	9.6	a	9.3	a	8.9	a
Sacarose	13.9	a	12.8	b	14.6	a	14.0	a	14.5	a	14.4	a

Tabela Suplementar 6 - Efeito dos genótipos nos níveis de cada metabólito na condição sem a dominância apical. A abundancia relativa de cada metabólito é comparada em cada variedade, entre os terços médios superior, mediano e basal. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	DECAPITADA											
	RB72454						RB975375					
	TOPO		MEIO		BASE		TOPO		MEIO		BASE	
2-Hidroxipirimidina	8.4	a	8.8	a	8.7	a	8.5	a	8.5	a	8.4	a
Alanina	10.4	a	10.1	a	10.5	a	10.1	a	10.6	a	10.0	a
Piruvato	4.6	b	5.0	a	4.7	ab	4.4	a	4.4	a	4.4	a
Valina	9.8	a	9.6	a	9.5	a	9.2	a	9.7	a	9.3	a
Glicerol	10.9	a	10.9	a	10.9	a	10.7	a	10.6	a	10.9	a
Leucina	8.3	a	7.8	a	7.8	a	7.3	b	8.2	ab	7.4	a
Isoleucina	8.2	a	7.9	a	7.7	a	7.5	b	8.4	a	7.5	b
Glicina	7.0	a	7.2	a	7.5	a	6.8	a	6.8	a	6.9	a
Ortofosfato	9.8	a	9.4	ab	9.0	b	9.7	a	9.3	a	8.9	a
Benzoato	7.6	a	7.8	a	7.8	a	7.4	a	7.4	a	7.6	a
Serina	9.1	a	8.9	a	9.1	a	8.8	a	9.0	a	8.7	a
Succinato	6.9	a	7.2	a	7.0	a	6.9	a	6.6	a	6.9	a
Treonina	7.1	a	6.8	a	6.7	a	6.4	a	7.0	a	6.7	a
Pipecolato	8.4	a	7.7	ab	7.4	b	9.2	a	8.9	ab	7.2	b
Nonoato	6.7	a	6.9	a	6.8	a	6.4	a	6.6	a	6.8	a
Nicotinato	5.9	b	6.3	ab	6.7	a	5.8	a	5.7	a	5.2	a
Itaconato	6.6	b	6.7	ab	7.0	a	6.8	a	6.8	a	6.7	a
Eritritol	6.3	a	6.2	a	5.4	a	5.3	a	6.0	a	5.3	a
Malato	9.3	a	9.3	a	9.2	a	9.5	a	9.4	a	10.0	a
GABA	7.0	a	6.9	a	7.1	a	7.1	a	8.0	a	7.2	a
Aspartato	11.6	a	12.0	a	11.8	a	11.0	b	11.6	a	11.7	a
Maleato	5.1	a	5.5	a	5.2	a	4.4	b	5.2	a	5.2	a
Threote	5.4	a	5.7	a	5.4	a	4.7	b	5.3	a	5.4	a
Metionina	5.9	a	5.5	a	5.1	a	4.9	b	6.0	a	5.2	ab
Dietanoalamina	3.8	b	3.4	b	5.8	a	7.1	a	7.6	a	7.7	a
Arginina	4.4	a	4.1	a	5.2	a	4.2	a	4.9	a	4.5	a
Ornitina	7.8	a	7.6	a	9.1	a	7.8	a	8.7	a	9.3	a
Xilose	7.7	a	7.7	a	8.1	a	7.3	a	7.6	a	7.4	a
Xilitol	7.0	b	8.9	ab	8.5	a	6.8	a	7.0	a	6.8	a
Glutamato	11.4	a	11.7	a	11.9	a	10.7	b	11.5	a	11.5	a

Xilulose	4.5	a	4.8	a	4.6	a	3.9	b	4.4	a	4.4	a
Ramnose	5.5	a	6.0	a	5.7	a	5.6	a	5.4	a	5.3	a
Putrescina	7.2	a	7.2	a	6.2	b	8.0	a	8.1	a	8.1	a
Fucose	5.9	a	5.8	a	5.4	a	5.7	a	5.9	a	5.4	a
Fenilalanina	5.6	a	5.1	a	5.4	a	5.5	a	5.1	ab	4.5	b
4-Hidroxibenzoato	5.7	a	5.9	a	5.9	a	5.5	a	5.5	a	5.4	a
Asparagina	10.5	ab	10.1	b	11.7	a	10.2	b	11.3	ab	12.0	a
Quinato	9.7	a	9.0	a	9.2	a	9.5	a	8.8	a	8.7	a
Frutose	14.3	a	13.6	a	12.0	b	14.3	a	13.7	a	13.8	a
cis-Aconitato	13.0	b	13.1	ab	13.7	a	13.7	a	13.6	a	13.7	a
Manose	9.6	b	10.4	a	9.8	b	9.7	b	10.2	ab	10.3	a
Citrato	10.5	b	10.9	ab	11.1	a	10.2	b	10.7	ab	11.3	a
Glicose	10.4	a	10.0	a	8.4	b	10.4	a	10.2	a	9.7	a
Glutamina	9.1	a	9.0	a	9.1	a	8.2	a	9.0	a	9.0	a
Lisina	6.3	a	6.3	a	6.9	a	5.6	b	6.7	a	6.2	ab
Tetradecanoato	8.5	a	8.6	a	8.8	a	8.5	a	8.3	a	8.6	a
Dehidroascorbato	6.9	a	7.1	a	6.9	a	7.3	a	6.7	a	6.2	a
mio-Inositol	11.5	a	11.4	a	11.4	a	11.3	a	11.4	a	10.8	a
Tirosina	7.9	a	7.9	a	7.9	a	7.7	a	7.9	a	7.4	a
Adenina	5.2	a	4.7	a	4.7	a	4.7	a	4.5	ab	4.1	b
Espermidina	6.9	a	6.8	a	7.3	a	4.8	a	5.9	a	5.2	a
Cafeato	9.0	a	9.0	a	9.2	a	8.9	a	8.7	a	8.3	a
Triptofano	7.5	b	8.0	ab	8.6	a	7.5	a	7.8	a	7.8	a
Trealose	6.0	b	6.5	ab	8.6	a	5.1	a	6.1	a	6.1	a
Rafinose	9.0	a	9.4	a	9.0	a	9.5	a	9.6	a	9.5	a
Sacarose	13.7	b	14.6	a	14.6	a	13.5	b	13.9	b	14.4	a

Tabela Suplementar 7 - Comparação dos níveis de cada metabólito entre as variedades RB72454 e RB975375 na condição sem a dominância apical (DECAPITATED). A abundancia relativa de cada metabólito é comparada em cada porção do colmo, terços médios superior, mediano e basal, entre as variedades testadas. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	DECAPITADA											
	TOPO				MEIO				BASE			
	RB72454		RB975375		RB72454		RB975375		RB72454		RB975375	
2-Hidroxipirimidina	8.4	a	8.5	a	8.8	a	8.5	a	8.7	a	8.4	a
Alanina	10.4	a	10.1	a	10.1	a	10.6	a	10.5	a	10.0	a
Piruvato	4.6	a	4.4	b	5.0	a	4.4	b	4.7	a	4.4	a
Valina	9.8	a	9.2	b	9.6	a	9.7	a	9.5	a	9.3	a
Glicerol	10.9	a	10.7	a	10.9	a	10.6	a	10.9	a	10.9	a
Leucina	8.3	a	7.3	b	7.8	a	8.2	a	7.8	a	7.4	a

Isoleucina	8.2	a	7.5	a	7.9	a	8.4	a	7.7	a	7.5	a
Glicina	7.0	a	6.8	a	7.2	a	6.8	a	7.5	a	6.9	b
Ortofosfato	9.8	a	9.7	a	9.4	a	9.3	a	9.0	a	8.9	a
Benzoato	7.6	a	7.4	b	7.8	a	7.4	a	7.8	a	7.6	a
Serina	9.1	a	8.8	a	8.9	a	9.0	a	9.1	a	8.7	b
Succinato	6.9	a	6.9	a	7.2	a	6.6	b	7.0	a	6.9	a
Treonina	7.1	a	6.4	a	6.8	a	7.0	a	6.7	a	6.7	a
Pipecolato	8.4	b	9.2	a	7.7	a	8.9	a	7.4	a	7.2	a
Nonoato	6.7	a	6.4	b	6.9	a	6.6	a	6.8	a	6.8	a
Nicotinato	5.9	a	5.8	a	6.3	a	5.7	a	6.7	a	5.2	b
Itaconato	6.6	a	6.8	a	6.7	a	6.8	a	7.0	a	6.7	a
Eritritol	6.3	a	5.3	a	6.2	a	6.0	a	5.4	a	5.3	a
Malato	9.3	a	9.5	a	9.3	a	9.4	a	9.2	b	10.0	a
GABA	7.0	a	7.1	a	6.9	a	8.0	a	7.1	a	7.2	a
Aspartato	11.6	a	11.0	b	12.0	a	11.6	b	11.8	a	11.7	a
Maleato	5.1	a	4.4	b	5.5	a	5.2	b	5.2	a	5.2	a
Threote	5.4	a	4.7	b	5.7	a	5.3	b	5.4	a	5.4	a
Metionina	5.9	a	4.9	b	5.5	a	6.0	a	5.1	a	5.2	a
Dietanoalamina	3.8	b	7.1	a	3.4	b	7.6	a	5.8	b	7.7	a
Arginina	4.4	a	4.2	a	4.1	a	4.9	a	5.2	a	4.5	a
Ornitina	7.8	a	7.8	a	7.6	a	8.7	a	9.1	a	9.3	a
Xilose	7.7	a	7.3	a	7.7	a	7.6	a	8.1	a	7.4	b
Xilitol	7.0	a	6.8	a	8.9	a	7.0	b	8.5	a	6.8	a
Glutamato	11.4	a	10.7	b	11.7	a	11.5	a	11.9	a	11.5	b
Xilulose	4.5	a	3.9	b	4.8	a	4.4	b	4.6	a	4.4	a
Ramnose	5.5	a	5.6	a	6.0	a	5.4	b	5.7	a	5.3	b
Putrescina	7.2	b	8.0	a	7.2	a	8.1	a	6.2	b	8.1	a
Fucose	5.9	a	5.7	a	5.8	a	5.9	a	5.4	a	5.4	a
Fenilalanina	5.6	a	5.5	a	5.1	a	5.1	a	5.4	a	4.5	b
4-Hidroxibenzoato	5.7	a	5.5	a	5.9	a	5.5	a	5.9	a	5.4	a
Asparagina	10.5	a	10.2	a	10.1	a	11.3	a	11.7	a	12.0	a
Quinato	9.7	a	9.5	a	9.0	a	8.8	a	9.2	a	8.7	b
Frutose	14.3	a	14.3	a	13.6	a	13.7	a	12.0	b	13.8	a
cis-Aconitato	13.0	a	13.7	a	13.1	b	13.6	a	13.7	a	13.7	a
Manose	9.6	a	9.7	a	10.4	a	10.2	a	9.8	b	10.3	a
Citrato	10.5	a	10.2	a	10.9	a	10.7	a	11.1	a	11.3	a
Glicose	10.4	a	10.4	a	10.0	a	10.2	a	8.4	b	9.7	a
Glutamina	9.1	a	8.2	b	9.0	a	9.0	a	9.1	a	9.0	a
Lisina	6.3	a	5.6	a	6.3	a	6.7	a	6.9	a	6.2	b
Tetradecanoato	8.5	a	8.5	a	8.6	a	8.3	a	8.8	a	8.6	a
Dehidroascorbato	6.9	a	7.3	a	7.1	a	6.7	a	6.9	a	6.2	a

mio-Inositol	11.5	a	11.3	a	11.4	a	11.4	a	11.4	a	10.8	a
Tirosina	7.9	a	7.7	a	7.9	a	7.9	a	7.9	a	7.4	b
Adenina	5.2	a	4.7	b	4.7	a	4.5	a	4.7	a	4.1	b
Espermidina	6.9	a	4.8	b	6.8	a	5.9	b	7.3	a	5.2	b
Cafeato	9.0	a	8.9	a	9.0	a	8.7	a	9.2	a	8.3	b
Triptofano	7.5	a	7.5	a	8.0	a	7.8	a	8.6	a	7.8	b
Trealose	6.0	a	5.1	a	6.5	a	6.1	a	8.6	a	6.1	a
Rafinose	9.0	b	9.5	a	9.4	a	9.6	a	9.0	a	9.5	a
Sacarose	13.7	a	13.5	a	14.6	a	13.9	b	14.6	a	14.4	a

Tabela Suplementar 8 - Comparação dos níveis de cada metabólito entre as condições com e sem a dominância apical na variedade RB72454. A abundancia relativa de cada metabólito é comparada entre as condições inteira e dacpitada em cada porção do colmo, terços médios superior, mediano e basal. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	RB72454											
	TOPO				MEIO				BASE			
	INTEIRA		DECAP.		INTEIRA		DECAP.		INTEIRA		DECAP.	
2-Hidroxipirimidina	8.6	a	8.4	a	8.8	a	8.8	a	8.8	a	8.7	a
Alanina	11.0	a	10.4	b	10.8	a	10.1	a	11.0	a	10.5	a
Piruvato	4.8	a	4.6	a	4.9	a	5.0	a	4.7	a	4.7	a
Valina	9.7	a	9.8	a	9.3	a	9.6	a	9.7	a	9.5	a
Glicerol	11.0	a	10.9	a	11.4	a	10.9	a	11.2	a	10.9	a
Leucina	8.1	a	8.3	a	7.3	a	7.8	a	7.7	a	7.8	a
Isoleucina	8.0	a	8.2	a	7.4	a	7.9	a	7.7	a	7.7	a
Glicina	7.0	a	7.0	a	7.1	a	7.2	a	7.0	a	7.5	a
Ortofosfato	9.9	a	9.8	a	9.3	a	9.4	a	9.3	a	9.0	a
Benzoato	7.8	a	7.6	a	8.3	a	7.8	b	7.9	a	7.8	a
Serina	9.3	a	9.1	a	8.9	a	8.9	a	9.2	a	9.1	a
Succinato	7.0	a	6.9	a	7.3	a	7.2	a	7.0	a	7.0	a
Treonina	6.9	a	7.1	a	6.5	a	6.8	a	6.7	a	6.7	a
Pipecolato	8.0	a	8.4	a	7.1	a	7.7	a	7.7	a	7.4	a
Nonoato	6.9	a	6.7	a	7.4	a	6.9	a	7.0	a	6.8	b
Nicotinato	6.3	a	5.9	a	6.6	a	6.3	a	6.1	b	6.7	a
Itaconato	6.6	a	6.6	a	7.0	a	6.7	a	6.7	b	7.0	a
Eritritol	7.1	a	6.3	a	6.4	a	6.2	a	6.8	a	5.4	b
Malato	9.2	a	9.3	a	9.0	a	9.3	a	9.1	a	9.2	a
GABA	7.5	a	7.0	a	8.0	a	6.9	b	7.5	a	7.1	a
Aspartato	11.6	a	11.6	a	11.7	a	12.0	a	11.9	a	11.8	a
Maleato	5.1	a	5.1	a	5.1	a	5.5	a	5.3	a	5.2	a
Threote	5.3	a	5.4	a	5.3	a	5.7	a	5.6	a	5.4	a
Metionina	6.2	a	5.9	a	5.7	a	5.5	a	5.9	a	5.1	a

Dietanoalamina	3.0	a	3.8	a	4.8	a	3.4	b	5.4	a	5.8	a
Arginina	5.0	a	4.4	b	3.9	a	4.1	a	4.7	a	5.2	a
Ornitina	7.3	a	7.8	a	8.1	a	7.6	a	8.4	a	9.1	a
Xilose	7.6	a	7.7	a	7.5	a	7.7	a	8.0	a	8.1	a
Xilitol	7.8	a	7.0	a	8.5	a	8.9	a	8.7	a	8.5	a
Glutamato	11.7	a	11.4	a	11.6	a	11.7	a	11.9	a	11.9	a
Xilulose	4.9	a	4.5	b	4.7	a	4.8	a	5.0	a	4.6	a
Ramnose	5.9	a	5.5	a	5.6	a	6.0	a	6.1	a	5.7	a
Putrescina	7.3	a	7.2	a	7.1	a	7.2	a	7.1	a	6.2	a
Fucose	6.0	a	5.9	a	5.5	a	5.8	a	5.9	a	5.4	b
Fenilalanina	4.6	b	5.6	a	4.8	a	5.1	a	5.1	b	5.4	a
4-Hidroxibenzoato	5.9	a	5.7	a	6.3	a	5.9	a	6.1	a	5.9	a
Asparagina	9.9	a	10.5	a	10.4	a	10.1	a	11.0	a	11.7	a
Quinato	9.7	a	9.7	a	9.0	a	9.0	a	9.2	a	9.2	a
Frutose	13.0	a	14.3	a	12.1	a	13.6	a	12.5	a	12.0	a
cis-Aconitato	12.8	a	13.0	a	12.5	a	13.1	a	12.9	b	13.7	a
Manose	9.8	a	9.6	a	10.1	a	10.4	a	10.2	a	9.8	b
Citrato	10.8	a	10.5	a	10.8	a	10.9	a	11.0	a	11.1	a
Glicose	9.4	a	10.4	a	9.0	a	10.0	a	9.2	a	8.4	a
Glutamina	9.2	a	9.1	a	9.1	a	9.0	a	9.2	a	9.1	a
Lisina	6.6	a	6.3	a	6.0	a	6.3	a	6.6	a	6.9	a
Tetradecanoato	8.8	a	8.5	a	9.2	a	8.6	b	8.8	a	8.8	a
Dehidroascorbato	6.8	a	6.9	a	6.6	a	7.1	a	7.2	a	6.9	a
mio-Inositol	11.4	a	11.5	a	10.9	a	11.4	a	11.3	a	11.4	a
Tirosina	7.7	a	7.9	a	7.5	a	7.9	a	7.8	a	7.9	a
Adenina	5.2	a	5.2	a	4.9	a	4.7	a	4.6	a	4.7	a
Espermidina	6.9	a	6.9	a	7.2	a	6.8	a	6.7	a	7.3	a
Cafeato	9.3	a	9.0	a	9.4	a	9.0	a	9.4	a	9.2	a
Triptofano	7.7	a	7.5	a	8.0	a	8.0	a	8.2	a	8.6	a
Trealose	7.2	a	6.0	a	7.3	a	6.5	a	7.8	a	8.6	a
Rafinose	9.2	a	9.0	a	9.1	a	9.4	a	9.3	a	9.0	a
Sacarose	13.9	a	13.7	a	14.6	a	14.6	a	14.5	a	14.6	a

Tabela Suplementar 9 - Comparação dos níveis de cada metabólito entre as condições com e sem a dominância apical na variedade RB975375. A abundancia relativa de cada metabólito é comparada entre as condições inteira e dacpitada em cada porção do colmo, terços médios superior, mediano e basal. Valores seguidos da mesma letra não diferem estatisticamente entre si ao nível de 5% de significância.

METABÓLITOS	RB975375											
	TOPO				MEIO				BASE			
	INTEIRA		DECAP.		INTEIRA		DECAP.		INTEIRA		DECAP.	
2-Hidroxipirimidina	8.3	a	8.5	a	8.8	a	8.5	a	8.6	a	8.4	a

Alanina	9.5	a	10.1	a	10.2	a	10.6	a	10.6	a	10.0	a
Piruvato	4.3	a	4.4	a	4.6	a	4.4	a	4.2	a	4.4	a
Valina	9.1	a	9.2	a	9.4	a	9.7	a	9.5	a	9.3	a
Glicerol	10.8	a	10.7	a	10.8	a	10.6	a	10.5	a	10.9	a
Leucina	7.6	a	7.3	a	8.1	a	8.2	a	7.4	a	7.4	a
Isoleucina	7.9	a	7.5	a	8.2	a	8.4	a	7.6	a	7.5	a
Glicina	5.9	a	6.8	a	7.1	a	6.8	a	7.4	a	6.9	a
Ortofosfato	10.2	a	9.7	a	9.5	a	9.3	a	9.2	a	8.9	a
Benzoato	7.6	a	7.4	a	7.7	a	7.4	a	7.5	a	7.6	a
Serina	8.7	a	8.8	a	8.9	a	9.0	a	9.1	a	8.7	a
Succinato	6.8	a	6.9	a	6.7	a	6.6	a	6.9	a	6.9	a
Treonina	6.7	a	6.4	a	6.8	a	7.0	a	7.0	a	6.7	a
Pipecolato	8.9	a	9.2	a	8.1	a	8.9	a	7.5	a	7.2	a
Nonoato	6.7	a	6.4	a	6.8	a	6.6	a	6.6	a	6.8	a
Nicotinato	6.0	a	5.8	a	5.8	a	5.7	a	5.9	a	5.2	a
Itaconato	6.7	a	6.8	a	6.7	a	6.8	a	6.9	a	6.7	a
Eritritol	4.4	a	5.3	a	5.2	a	6.0	a	5.6	a	5.3	a
Malato	9.5	a	9.5	a	9.6	a	9.4	a	9.8	a	10.0	a
GABA	7.3	a	7.1	a	7.0	a	8.0	a	7.6	a	7.2	a
Aspartato	10.9	a	11.0	a	11.4	a	11.6	a	11.8	a	11.7	a
Maleato	4.4	a	4.4	a	4.9	a	5.2	a	5.2	a	5.2	a
Threote	4.6	a	4.7	a	5.1	a	5.3	a	5.5	a	5.4	a
Metionina	5.6	a	4.9	b	5.8	a	6.0	a	5.5	a	5.2	a
Dietanoalamina	7.7	a	7.1	a	6.7	a	7.6	a	7.7	a	7.7	a
Arginina	4.5	a	4.2	a	4.7	a	4.9	a	4.7	a	4.5	a
Ornitina	7.1	a	7.8	a	7.9	a	8.7	a	9.8	a	9.3	a
Xilose	6.9	a	7.3	a	7.5	a	7.6	a	7.8	a	7.4	a
Xilitol	6.0	a	6.8	a	6.9	a	7.0	a	7.5	a	6.8	a
Glutamato	10.8	a	10.7	a	11.4	a	11.5	a	11.6	a	11.5	a
Xilulose	3.8	a	3.9	a	4.4	a	4.4	a	4.5	a	4.4	a
Ramnose	5.5	a	5.6	a	5.3	a	5.4	a	5.4	a	5.3	a
Putrescina	8.0	a	8.0	a	7.7	a	8.1	a	7.9	a	8.1	a
Fucose	6.1	a	5.7	b	5.8	a	5.9	a	5.4	a	5.4	a
Fenilalanina	4.5	b	5.5	a	4.8	a	5.1	a	5.1	a	4.5	a
4-Hidroxibenzoato	5.6	a	5.5	a	5.8	a	5.5	a	5.8	a	5.4	a
Asparagina	9.2	a	10.2	a	10.6	a	11.3	a	12.0	a	12.0	a
Quinato	9.5	a	9.5	a	8.6	a	8.8	a	8.9	a	8.7	a
Frutose	15.2	a	14.3	b	13.6	a	13.7	a	13.9	a	13.8	a
cis-Aconitato	13.2	a	13.7	a	13.6	a	13.6	a	13.7	a	13.7	a
Manose	9.9	a	9.7	a	9.9	a	10.2	a	10.2	a	10.3	a
Citrato	10.2	a	10.2	a	10.5	a	10.7	a	11.1	a	11.3	a

Glicose	11.7	a	10.4	b	9.5	a	10.2	a	10.1	a	9.7	a
Glutamina	8.3	a	8.2	a	8.5	a	9.0	a	9.4	a	9.0	a
Lisina	6.0	a	5.6	a	6.4	a	6.7	a	6.7	a	6.2	a
Tetradecanoato	8.6	a	8.5	a	8.7	a	8.3	b	8.5	a	8.6	a
Dehidroascorbato	6.7	a	7.3	a	7.1	a	6.7	a	6.7	a	6.2	a
mio-Inositol	10.9	b	11.3	a	11.4	a	11.4	a	11.6	a	10.8	a
Tirosina	7.6	a	7.7	a	7.9	a	7.9	a	7.9	a	7.4	a
Adenina	4.8	a	4.7	a	4.6	a	4.5	a	4.4	a	4.1	a
Espermidina	4.2	a	4.8	a	5.0	a	5.9	a	5.1	a	5.2	a
Cafeato	8.7	a	8.9	a	8.8	a	8.7	a	8.9	a	8.3	a
Triptofano	6.6	b	7.5	a	7.6	a	7.8	a	7.8	a	7.8	a
Trealose	3.6	b	5.1	a	5.9	a	6.1	a	6.4	a	6.1	a
Rafinose	8.6	b	9.5	a	9.6	a	9.6	a	8.9	a	9.5	a
Sacarose	12.8	b	13.5	a	14.0	a	13.9	a	14.4	a	14.4	a

Tabela Suplementar 10 – Analise de Fold Change (FC). Os valores representam o FC médio de cada metabólito após a decapitação.

Metabólitos	**FOLD CHANGE (FC)**					
	RB72454			**RB975375**		
	TOPO	**MEIO**	**BASE**	**TOPO**	**MEIO**	**BASE**
Aspartato	-0.02	0.34	-0.14	0.18	0.21	-0.12
Fenilalanina	0.95	0.24	0.29	1.04	0.27	-0.58
Glutamato	-0.39	0.13	-0.07	-0.15	0.10	-0.10
Glutamina	-0.05	-0.13	-0.13	0.13	0.51	-0.45
Metionina	-0.32	-0.17	-0.84	-0.67	0.22	-0.32
Cafeato	-0.28	-0.40	-0.11	0.21	-0.07	-0.52
cis-Aconitato	0.24	0.62	0.75	0.44	0.03	0.07
Citrato	-0.24	0.17	0.11	0.04	0.19	0.12
Malato	0.12	0.33	0.10	0.00	-0.13	0.26
Maleato	-0.03	0.38	-0.11	0.03	0.29	-0.05
Pipecolato	0.41	0.91	-0.29	0.25	0.81	-0.27
Succinato	-0.12	0.02	0.01	0.12	-0.19	0.04
Tetradecanoato	-0.32	-0.53	-0.05	-0.12	-0.38	0.12
Frutose	1.27	1.45	-0.51	-0.89	0.13	-0.11
Sacarose	-0.21	0.00	0.12	0.73	-0.06	0.01
Xilulose	-0.46	0.13	-0.31	0.02	0.03	-0.07
Espermidina	0.02	-0.34	0.62	0.60	0.84	0.12
Putrescina	-0.12	0.17	-0.87	0.00	0.41	0.17
Adenina	0.00	-0.15	0.06	-0.11	-0.12	-0.25
Dietanoalamina	1.41	-1.57	0.46	-0.55	1.15	0.00

8. **Anexos**

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