

**Table 3. Metabolite predictions for explanatory ions in *Arabidopsis* mutants**

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| [M+H] <sup>+</sup> | [M+Na] <sup>+</sup> | [M+K] <sup>+</sup> | [M+2Na-H] <sup>+</sup> | [2M+H] <sup>+</sup> | [2M+Na] <sup>+</sup> | [2M+K] <sup>+</sup> |  |
|--------------------|---------------------|--------------------|------------------------|---------------------|----------------------|---------------------|--|
|                    |                     | 207                |                        |                     |                      |                     | <i>homogentisate</i> or phosphoenolpyruvate                                      |
|                    | 207                 | 223                |                        |                     |                      |                     | phosphoryl-choline   |
|                    | 861                 | 877                | 883                    |                     |                      |                     | heme O   |
|                    |                     |                    | 960,961                |                     |                      |                     | hydroxycinnamoyl-CoA   |
|                    |                     | 381, 382, 383      |                        | 685                 |                      |                     | disaccharide (ie. sucrose, lactose, maltose, trehalose, melibiose)               |
| 867                |                     | 905                |                        |                     |                      |                     | dihydrosirohydrochlorin  |
|                    |                     | 867                |                        |                     |                      |                     | uroporphyrin III   |
|                    | 686                 |                    | 708                    |                     |                      |                     | NAD  |
| 617                |                     |                    |                        |                     |                      |                     | protoheme  |
|                    | 617                 |                    |                        |                     |                      |                     | kaempferol-3-glucoside-7-rhamnoside  |
|                    |                     | 617                |                        |                     |                      |                     | kaempferol-3-rhamnoside-7-rhamnoside   |
| 417                |                     |                    |                        |                     |                      |                     | tocopherol, oxo-campestanol, hydroxy-campestanone or dimethyl-phytylbenzoquinone |
|                    |                     | 417                |                        |                     |                      |                     | giberellin A17   |
|                    | 802, 803            |                    |                        |                     |                      |                     | 1-18:3-2-18:3-sn-glycerol-phosphocholine   |
|                    |                     |                    | 802, 803               |                     |                      |                     | 1-18:1-2-16:0-monogalactosyldiacylglycerol                                       |
|                    | 778                 |                    | 800                    |                     |                      |                     | 1-18:1-2-16:1-monogalactosyldiacylglycerol                                       |
|                    | 832                 | 848                |                        |                     |                      |                     | acetyl-CoA   |
|                    |                     | 503                |                        |                     |                      |                     | castasterone, 4-hydroxy-3-indolylmethyl-glucosinolate or quercetin-3-glucoside   |
|                    | 503                 |                    |                        |                     |                      |                     | brassinolide   |
| 912                |                     |                    |                        |                     |                      |                     | carnitiny-CoA or 3-hydroxy-3-methyl-glutaryl-CoA                                 |
|                    |                     | 379                |                        |                     |                      |                     | fructose-1,6-bisphosphate or fructose-2,6-bisphosphate                           |
|                    |                     |                    | 424                    |                     |                      | 797                 | S-lactoyl-glutathione  |
|                    | 424                 |                    |                        |                     |                      |                     | campesterol or campestenol   |
|                    |                     | 619                |                        |                     |                      |                     | UDP-D-glucuronate  |
|                    |                     |                    | 472                    |                     | 877                  |                     | ADP, dGDP, APS or adenosine 3',5'-bisphosphate                                   |
|                    | 400                 | 416                |                        |                     |                      |                     | kinetin-glucoside  |
|                    | 381, 382            | 397, 398, 399      |                        |                     |                      |                     | pantetheine 4'-phosphate   |

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| [M-HCOO] <sup>-</sup> | [M-H] <sup>+</sup> | [M+Na-2H] <sup>+</sup> | [M+K-2H] <sup>+</sup> | [2M+Na-2H] <sup>+</sup> | [fragment] <sup>+</sup> |   |
|-----------------------|--------------------|------------------------|-----------------------|-------------------------|-------------------------|---|
|                       | 164                |                        |                       | 351                     |                         | <i>L-phenylalanine</i>  |
| 149                   |                    |                        |                       |                         |                         | ferulate  |
| 149                   |                    |                        |                       |                         |                         | glucuronate, fructuronate or 5-hydroxy-coniferaldehyde  |
| 179                   | 223                |                        |                       |                         |                         | sinapate  |
| 179                   | 223                |                        |                       |                         |                         | jasmonic acid methyl ester, flavanone or 3-hydroxy-L-kynurenine                                       |
|                       |                    | 380, 381               | 396                   | 739, 740                |                         | 2-propenyl-glucosinolate  |
|                       | 577, 578, 579      |                        |                       |                         |                         | kaempferol-3-rhamnoside-7-rhamnoside  |
|                       | 431, 432, (430?)   |                        |                       |                         |                         | kaempferol-3-rhamnoside   |
|                       |                    | 208, 209?              |                       |                         |                         | 8-amino-7-oxononanoate or N1-acetyl spermidine  |
|                       |                    |                        | 208, 209?             |                         |                         | tetrahydrodipicolinate  |
|                       | 150                |                        |                       |                         |                         | guanine   |
|                       |                    | 150                    |                       |                         |                         | pyrroline-hydroxy-carboxylate   |
|                       |                    |                        | 150                   |                         |                         | pyrroline-5-carboxylate   |
|                       |                    |                        | 205                   |                         |                         | <i>homogentisate</i> or phosphoenolpyruvate   |
|                       |                    | 205                    |                       |                         |                         | 3,4-dihydroxy-2-butanone-4-P or 3-phospho-hydroxypyruvate   |
|                       | 285                |                        |                       |                         |                         | kaempferol, 5-phospho-ribosyl-glycineamide or indolylmethyl glucosinolate aglycone                    |
|                       |                    |                        | 285                   |                         |                         | xanthoxin, pyridoxamine 5'-phosphate or indole carboxyl tetrahydro-thiazole                           |
|                       |                    | 285                    |                       |                         |                         | abscisic acid   |
|                       | 147                |                        |                       |                         |                         | <i>trans-cinnamate</i> or <i>coumaraldehyde</i>   |
|                       | 147                |                        |                       |                         |                         | mevalonate, 2,3-dihydroxy-3-methylvalerate, L-pantoate, p-cumic aldehyde or 2-oxo-4-methylthiobutanoa |
|                       |                    | 147                    |                       |                         |                         | thymine   |
|                       |                    |                        | 147                   |                         |                         | benzosemiquinone  |
|                       |                    | 504                    |                       |                         |                         | CTP   |
|                       |                    |                        | 504                   |                         |                         | dCTP  |
|                       | 401                |                        |                       |                         |                         | dTDP, tocopherol, campestanol or 2-methyl-6-phytyl-1,4-benzoquinone                                   |
|                       |                    |                        | 401                   |                         |                         | xanthosine-5-P or GA44  |
|                       | 472                | 494                    |                       |                         |                         | N10-formyl-THF or N5-formyl-THF   |
|                       | 486                |                        |                       |                         |                         | cyanidin-3-glucoside  |
|                       | 156                |                        |                       |                         |                         | 2-amino-muconate  |
|                       |                    | 156                    |                       |                         |                         | homocysteine or adenine   |
|                       |                    |                        | 156                   |                         |                         | homoserine or threonine   |
|                       | 602                |                        |                       |                         | 150                     | guanosine tetraphosphate  |
|                       | 378                |                        |                       |                         |                         | S-lactoyl-glutathione   |
|                       |                    |                        | 720                   |                         | 150                     | guanosine pentaphosphate  |
|                       | 865                |                        |                       |                         |                         | dihydrosirohdrochlorin  |
|                       |                    | 929                    |                       |                         |                         | precorrin-4B  |
|                       |                    |                        | 929                   |                         |                         | chlorophyll a   |
|                       |                    |                        | 351                   |                         |                         | 7,8-dihydropteroate   |
|                       |                    | 732                    |                       |                         |                         | 2,3-bis(3-hydroxyristoyl)-β-D-glucosaminyl 1-phosphate  |

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| [M+H-NH3] <sup>+</sup> | [M+H-H2O] <sup>+</sup> | [M+H-HCOOH] <sup>+</sup> | [M+H] <sup>+</sup> | [M+Na] <sup>+</sup> | [M+K] <sup>+</sup> | [M+2Na-H] <sup>+</sup> |  |
|------------------------|------------------------|--------------------------|--------------------|---------------------|--------------------|------------------------|--|
| 211                    |                        |                          |                    | 266, 267, 268       | 282                |                        | cytidine   |
|                        |                        |                          |                    |                     | 266, 267, 268      |                        | deoxycytidine  |
|                        |                        | 245                      |                    |                     |                    | 335                    | L-arginino-succinate or N-succinyl-L-2,6-diaminopimelate                 |
|                        |                        |                          |                    | 365                 | 381, 382           |                        | <b>sucrose or other disaccharide</b>                                     |
|                        |                        |                          |                    | 778, 779            |                    | 800                    | 1-18:1-2-16:1-monogalactosyldiacylglycerol                               |
|                        |                        |                          | 397, 398           |                     |                    |                        | 5-dehydro episterol  |
|                        |                        |                          | 399, 400           |                     |                    |                        | episterol  |
|                        |                        |                          | 428                |                     |                    |                        | ADP, dGDP, APS or adenosine 3',5'-bisphosphate                           |
|                        |                        |                          | 175                |                     |                    |                        | cis-aconitate, shikimate, auxin or dehydroascorbate                      |
| 158                    |                        |                          | 175                |                     |                    |                        | L-arginine   |
|                        |                        |                          |                    | 175                 | 191                |                        | ribitol  |
|                        |                        |                          |                    | 203                 |                    |                        | <b>glucose (or other monosaccharide) or caffeate</b>                     |
|                        |                        |                          |                    | 245                 | 261                |                        | cystathionine or O-succinylbenzoate                                      |
|                        |                        |                          | 187                |                     |                    |                        | 2-phosphoglycerate or 3-phosphoglycerate                                 |
|                        |                        |                          |                    | 187                 | 203                |                        | 4-coumarate, phenylpyruvate or L-fucose                                  |
|                        |                        |                          | 130                | 152                 | 168                | 174                    | pyrroline-hydroxy-carboxylate  |
| 130                    |                        |                          |                    | 169                 |                    | 191                    | L-glutamine or L-lysine  |
|                        | 158                    | 130                      |                    | 198                 |                    |                        | citrulline   |
|                        |                        |                          | 336                |                     |                    |                        | isopentenyl adenosine, dihydroneopterin phosphate or S-Formylglutathione |
|                        |                        |                          |                    | 336                 |                    |                        | N-feruloyltyramine or 5-phosphoribosyl-n-formylglycineamidine            |
|                        |                        |                          | 298                |                     | 336                |                        | 5'-methylthioadenosine   |
|                        |                        |                          | 367                |                     |                    |                        | phosphoribosyl-formamido-carboxamide                                     |
|                        |                        |                          |                    | 282                 | 298                |                        | glucosamine-6-P or glucosamine-1-P                                       |
|                        |                        |                          | 261                |                     |                    |                        | <b>glucose-1-P, glucose-6-P (or other hexose-1-P or hexose-6-P)</b>      |
|                        |                        |                          |                    | 309                 | 335                |                        | 18-oxooleate   |
|                        |                        |                          | 173                |                     | 211                |                        | glycerol-3-P   |
|                        |                        | 127                      | 173                |                     | 211                |                        | 3-dehydroshikimate   |
|                        |                        |                          | 173                |                     |                    |                        | <b>pentose sugar</b>   |
| 298                    |                        |                          |                    | 337                 |                    |                        | 7,8-dihydropteroate  |
|                        |                        |                          | 131                |                     | 169                | 175                    | agmatine, 2-keto-3-methyl-valerate or 2-keto-4-methyl-pentanoate         |
|                        | 131                    |                          |                    |                     | 187                | 193                    | mevalonate, L-pantoate or trans-cinnamate                                |
|                        |                        |                          | 150                |                     |                    |                        | L-methionine   |
| 174                    |                        | 145                      | 191                |                     | 229                |                        | diaminopimelate  |
|                        |                        |                          | 169                | 191                 |                    |                        | phosphoenolpyruvate  |
|                        |                        |                          | 666                |                     |                    |                        | NADH   |
|                        |                        |                          |                    |                     | 234                |                        | 2-amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine                   |
|                        |                        |                          | 152                | 174                 |                    |                        | guanine  |

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| [M-HCOO] <sup>-</sup> | [M-H] <sup>-</sup> | [M+Cl] <sup>-</sup> | [M+Na-2H] <sup>-</sup> | [M+K-2H] <sup>-</sup> | [2M+Na-2H] <sup>-</sup> |  |
|-----------------------|--------------------|---------------------|------------------------|-----------------------|-------------------------|--|
|                       |                    |                     | 436                    |                       | 266                     | isopentenyl adenosine 5'monophosphate  |
|                       | 422                |                     |                        |                       |                         | 3-methylsulfinylpropyl-glucosinolate   |
|                       |                    |                     | 422                    | 438                   |                         | campest-4-en-3-ol or campesterol   |
|                       |                    |                     |                        | 372                   | 266                     | isopentenyl adenosine, S-formylglutathione or dihydroneopterin phosphate   |
|                       |                    |                     | 372                    |                       |                         | zeatin riboside  |
|                       |                    |                     | 377                    |                       |                         | 5-amino-6-(5'-phosphoribitylamino)uracil   |
|                       |                    |                     |                        | 377                   |                         | <b>fructose-1,6-bisphosphate</b> or fructose-2,6-bisphosphate  |
|                       |                    |                     | 231                    | 247                   |                         | sinapyl-alcohol, 5-hydroxyferulate or jasmonate  |
| 231                   | 275                |                     |                        |                       |                         | saccharopine   |
|                       |                    |                     |                        | 231                   |                         | fructuronate, glucuronate, 5-hydroxy-coniferaldehyde or ferulate   |
|                       |                    |                     |                        | 446                   |                         | benzyl-glucosinolate   |
|                       | 563                |                     |                        |                       |                         | dTDP-D-glucose or protoporphyrinogen   |
|                       | 362                | 398, 400            |                        |                       |                         | GMP  |
|                       |                    |                     | 404                    |                       |                         | dihydrozeatin-glucoside  |
|                       | 609                |                     |                        |                       |                         | divinyl protochlorophyllide a  |
|                       |                    |                     |                        | 178                   |                         | carbamoyl-phos, phosphoryl-ethanolamine, 2-aminomuconate semialdehyde or histidinol  |
|                       |                    |                     | 178                    |                       |                         | 2-amino-muconate   |
| 180                   |                    |                     |                        |                       |                         | 4-amino-4-deoxychorismate  |
|                       | 180                |                     |                        |                       |                         | tyrosine   |
|                       |                    |                     | 180                    |                       |                         | indole acetaldehyde  |
|                       |                    |                     |                        | 180                   |                         | 4-methyl-5-(β-hydroxyethyl)thiazole  |
|                       | 421                |                     |                        |                       |                         | <b>sucrose-6-P</b> or trehalose-6-P  |
|                       |                    |                     | 421                    | 421                   |                         | S-adenosyl-homocysteine or C25-allenic-apo-aldehyde  |
|                       |                    |                     | 421                    |                       |                         | 5-campestan-3-one  |
|                       | 593, 594           |                     |                        |                       |                         | kaempferol-3-glucoside-7-rhamnoside  |
|                       |                    |                     |                        | 351                   |                         | 7,8-dihydropteroate, geranyl-PP or 5'-phosphoribosyl-N-formylglycineamide  |
|                       | 341, 342           |                     |                        |                       |                         | <b>sucrose or other disaccharide</b>   |
|                       |                    |                     |                        | 341, 342              |                         | indole-3-acetyl-glu or dihydroquercetin  |
| 128                   | 172                |                     | 341, 342               |                       |                         | 4-coumaroylshikimate   |
|                       |                    |                     | 172                    |                       |                         | N-acetylglutamate semialdehyde   |
|                       |                    |                     |                        | 172                   |                         | guanine  |
|                       |                    |                     | 191                    |                       |                         | adenine or homocysteine  |
|                       | 191                |                     |                        |                       |                         | <b>glyceraldehyde-3-P</b> or dihydroxy-acetone-P   |
|                       | 225                |                     | 247                    |                       |                         | isocitrate or quinate  |
|                       |                    |                     | 225                    |                       |                         | chorismate, isochorismate, prephenate or porphobilinogen   |
|                       |                    |                     |                        | 225                   |                         | tryptophan or 1,4-dihydroxy-2-naphthoate   |
|                       | 266                |                     |                        |                       |                         | 3-carboxyhex-2-enedioate or 7,8-diaminononanoate   |
|                       |                    |                     | 275                    |                       |                         | adenosine [M-H] <sup>-</sup>   |
|                       |                    |                     | 423                    |                       |                         | shikimate-3-P  |
|                       | 195                |                     |                        |                       |                         | dTDP, tocopherol, campestanol or 2-methyl-6-phytyl-1,4-benzoquinone  |
|                       |                    |                     | 195                    |                       |                         | mannonate or gluconate   |
|                       |                    |                     |                        | 195                   |                         | cis-aconitate, dehydroascorbate, shikimate, auxin, acetylmithine or arginine   |
|                       | 175                |                     |                        |                       |                         | dihydroorotate or allantoin  |
|                       |                    |                     |                        | 175                   |                         | ascorbate, carbamoyl-L-aspartate, allantatoate, 2-D-threo-hydroxy-3-carboxy-isocaproate, 3-carboxy-3-hydroxy-isocaproate or N-hydroxyl-tryptan |
|                       |                    |                     | 374                    |                       |                         | salicylate   |
|                       |                    |                     |                        | 374                   |                         | 2,5-diamino-6-(ribosylamino)-4-(3H)-pyrimidinone 5'-phosphate  |
|                       |                    |                     | 370                    | 386                   |                         | indole-3-acetyl-β-1-D-glucose  |
|                       | 353                |                     | 375                    |                       |                         | 1-(o-carboxyphenylamino)-1'-deoxyribulose-5'-phosphate or N-(5'-phosphoribosyl)-anthranilate   |
|                       |                    |                     | 353                    | 369                   |                         | chlorogenate or 5-amino-6-(5'-phosphoribosylamino)uracil   |
|                       |                    |                     |                        |                       |                         | GA20, GA9 or GA4   |

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| [M+H-NH3] <sup>+</sup> | [M+H-H2O] <sup>+</sup> | [M+H-HCOOH] <sup>+</sup> | [M+H] <sup>+</sup> | [M+Na] <sup>+</sup> | [M+K] <sup>+</sup> | [M+2Na-H] <sup>+</sup> | [2M+H] <sup>+</sup> | [2M+Na] <sup>+</sup> | [2M+K] <sup>+</sup> | [2M+2Na-H] <sup>+</sup> |   |
|------------------------|------------------------|--------------------------|--------------------|---------------------|--------------------|------------------------|---------------------|----------------------|---------------------|-------------------------|---|
|                        |                        |                          | 261                |                     | 299                |                        |                     |                      |                     |                         | mannose 1-P, glucose 1-P or fructose 1- |
|                        |                        |                          |                    |                     | 381, 382, 383      |                        | 685                 |                      |                     |                         | sucrose or other disaccharide           |
|                        |                        |                          |                    |                     |                    |                        |                     |                      | 797, 798, 799       |                         | S-lactoyl-glutathione                   |
|                        |                        | 179                      |                    | 247                 |                    |                        |                     |                      |                     |                         | malate                                  |
|                        |                        |                          |                    | 179                 |                    |                        |                     |                      |                     |                         | ornotate                                |
|                        |                        |                          |                    | 179                 |                    |                        |                     |                      |                     |                         | 2-P-glycolate                           |
|                        |                        |                          | 179                |                     |                    |                        |                     |                      |                     |                         | <i>L-galactono-1,4-lactone</i>          |
|                        |                        |                          | 447                |                     | 491                |                        |                     |                      |                     | 937                     | CDP-ethanolamine                        |
|                        | 329                    |                          | 347                |                     | 391                |                        |                     |                      |                     |                         | xanthosine-5-P                          |
|                        |                        |                          | 127                |                     |                    |                        |                     |                      |                     |                         | thymine                                 |
|                        |                        |                          |                    |                     | 127                |                        |                     |                      |                     |                         | pyruvate                                |
|                        |                        | 127                      |                    |                     |                    |                        |                     |                      | 383                 |                         | 3-dehydroshikimate                      |
|                        |                        |                          | 829                |                     |                    | 873                    |                     |                      |                     |                         | uroporphyrin III                        |
|                        |                        | 817, 818, 819            |                    |                     |                    |                        |                     |                      |                     |                         | sirohydrochlorin                        |
| 138                    |                        |                          |                    |                     |                    |                        |                     |                      | 347                 |                         | <i>dopamine</i>                         |
|                        |                        |                          | 852                |                     |                    |                        |                     |                      |                     |                         | acetoacetyl-CoA                         |
|                        | 329                    | 301                      | 347                |                     | 391                |                        |                     |                      |                     |                         | gibberellin A24                         |
|                        |                        |                          |                    |                     | 301                |                        |                     |                      |                     |                         | <i>mannitol-1-P</i>                     |
|                        |                        |                          | 447                |                     | 491                |                        |                     |                      |                     | 937                     | 3-dehydroteasterone                     |
|                        |                        |                          |                    |                     |                    |                        |                     | 937                  |                     |                         | 5,10-methylenetetrahydrofolate          |
|                        |                        |                          |                    |                     |                    |                        | 803                 |                      | 841, 842            |                         | campesterol, campest-4-en-3beta-ol      |
|                        |                        |                          |                    |                     |                    |                        | 799                 | 821                  |                     | 843                     | S-adenosylmethionine                    |
|                        |                        |                          | 460                |                     |                    |                        |                     |                      |                     |                         | 5-methyl-THF                            |

*vtc* ESI -ve

| [M-HCOO] <sup>-</sup> | [M-H] <sup>-</sup> | [M+Cl] <sup>-</sup> | [M+Na-2H] <sup>-</sup> | [M+K-2H] <sup>-</sup> |  |
|-----------------------|--------------------|---------------------|------------------------|-----------------------|--|
| 569                   | 613                |                     |                        |                       | CMP-N-acetylneuraminate or chlorophyllide a                          |
|                       |                    |                     | 599                    |                       | kaempferol-3-rhamnoside-7-rhamnoside                                 |
|                       | 483                |                     |                        | 521                   | UTP  |
|                       |                    |                     | 469                    |                       | kaempferol-3-glucoside   |
|                       | 445                |                     |                        | 483                   | CDP-ethanolamine   |
|                       |                    |                     |                        | 200, 201              | homomethionine   |
|                       | 313                |                     |                        | 351                   | 7,8-dihydropteroate  |
|                       | 449                |                     | 471                    |                       | geranylgeranyl-PP or 6-deoxocastasterone                             |
|                       |                    |                     | 433                    | 449                   | various sterols (ie. stigmasterol)                                   |
|                       | 433                | 469, 471            |                        |                       | 6-deoxoteasterone or 6-deoxytyphasterol                              |
|                       | 574                |                     |                        |                       | isopentenyladenosine-5'-triphosphate                                 |
|                       |                    |                     |                        | 532                   | dihydroneopterin triphosphate or isopentenyl-adenosine diphosphate   |
|                       | 341                |                     |                        |                       | sucrose or other disaccharide  |
|                       |                    |                     |                        | 263                   | chorismate, isochorismate, prephenate or porphobilinogen             |
|                       | 152                |                     |                        |                       | <i>dopamine</i>  |
|                       | 147                |                     |                        |                       | trans-cinnamate or mevalonate  |
|                       |                    |                     | 147                    |                       | thymine  |
|                       | 362                |                     |                        |                       | GMP  |
|                       | 542                |                     |                        |                       | CMP-3-deoxy-D-manno-octulosonate                                     |
|                       |                    | 542, 544            |                        |                       | ATP, dGTP or PAPS  |
|                       |                    |                     | 152                    | 168                   | leucine or isoleucine  |
|                       |                    |                     |                        | 517                   | brassinolide   |
|                       |                    |                     |                        | 573                   | UDP-D-xylose, r UDP-L-arabinose, carotene or lycopene                |
|                       |                    |                     | 201                    |                       | various hexose   |
|                       |                    |                     |                        | 649                   | <i>GSH (oxidized glutathione)</i> or monovinyl protochlorophyllide a |

The metabolites predicted to be explanatory of metabolome differences between three well known *Arabidopsis* biochemical pathway mutants (*fah1-2*, *pgm1-1* and *vtc1-2*) and a wild

type progenitor are presented. The metabolite predictions are based upon interpretative associations between (de)protonated nominal mass, adduct, neutral loss and isotope  $m/z$  of the top 30 ions ranked by RF analysis of FIE-MS data in both ionization modes. Bold lettering indicates metabolite predictions directly associated with the respective biochemical pathway lesions while metabolites potentially "upstream or downstream" of the affected pathway are indicated in italics. Metabolite predictions linking to signals found in both ESI +ve and -ve modes are designated by blue lettering.