| Gene annotation | Compound name | InChI Key | MAGI score | GT5  | MRT5 | Reaction ID |
|-----------------|---------------|-----------|------------|------|------|-------------|
| Abhydrolase domain-containing protein 4 | Isobutyric acid | KQNPFQTWMSNSAP-UHFFFAOYSA-N | 5.129376 | UP   | UP   | RXN-668    |
| Alcohol dehydrogenase [NADP(+)] | 5alpha-Androstane-3beta,17beta-diol | CBMYJHJOYEBBS-YSZC3XEEOSA-N | 9.052214 | UP   | DOWN | RHEA:16300 |
| Alcohol dehydrogenase [NADP(+)] | 2-Hexenal | MDJOYVRWFFCHM-SNAWJCMRSA-N | 8.730280 | NA   | NA   | RXN-12299  |
| Alcohol dehydrogenase [NADP(+)] | Acrolein | HGINCLSHVWDNT-UHFFFAOYSA-N | 8.676901 | UP   | UP   | RHEA:12170 |
| Alcohol dehydrogenase [NADP(+)] | (1R,2R)-Cyclohexa-3,5-diene-1,2-diol | YDROQRPHLEPTP-HIDIMXHHSA-N | 8.592966 | UP   | NA   | RXN-12299  |
| Alcohol dehydrogenase [NADP(+)] | 1-Butanone | LRPDLIYGMMRGKHI-UHFFFAOYSA-N | 8.548746 | NA   | NA   | ENZRXN-201-RXN |
| Alcohol dehydrogenase [NADP(+)] | L-Gulonic acid | RGHNNJXZEOKBD-YSZC3XEEOSA-N | 7.707037 | UP   | UP   | GLUCURONATE-REDUCTASE-RXN |
| Alcohol dehydrogenase [NADP(+)] | N,N-Dimethylaniline N-oxide | LUQDAATMKBQKQ-UHFFFAOYSA-N | 10.270345 | NA   | NA   | RHEA:22339 |
| Cytochrome P450 1A1 | 4-Hydroxymelatonin | YRFQPVLFPCONSP-UHFFFAOYSA-N | 6.959443 | UP   | UP   | RXN-9844   |
| Cytochrome P450 1A1 | Progesterone | LTPDQVLPLFTMPN-UHFFFAOYSA-N | 6.312111 | UP   | NA   | RXN66-355  |
| Cytochrome P450 1A1 | T October 2014 | LTPDQVLPLFTMPN-UHFFFAOYSA-N | 6.312111 | UP   | NA   | RXN66-355  |
| Dimethylamine monoxygenase [N-oxide-forming] | 4-Methyl-2-pentenal | USFJGINJGUIFSA-UHFFFAOYSA-N | 6.595443 | NA   | NA   | RXN-9844   |
| DLH domain-containing protein | 4-Carbomethoxyen-but-2-en-4-olide | AYFXPGXAZMFWNH-UHFFFAOYSA-N | 5.990086 | UP   | UP   | RXN-9844   |
| FAD-linked oxidase | (R)-6-Hydroxynicotinic acid | AIJLQKETJEXLJ-UHFFFAOYSA-N | 7.305923 | NA   | NA   | RXN-9844   |
| Glutamine amidotransferase type-1 domain-containing protein | cis-4-Hydroxy-D-proline | PPMYEEVMWASQN-QWZSWWVQMSA-N | 6.306699 | DOWN | NA   | RXN-8003   |
| Glutamine amidotransferase type-1 domain-containing protein | 1-Aminocyclohexa-3,5-diene-1,2-diol | PWIWIJBHJCRSC-UHFFFAOYSA-N | 6.051894 | UP   | UP   | RXN-15250  |
| Glutamine amidotransferase type-1 domain-containing protein | N(5)-Phenyl-L-glutamine | VMNURJGLOBEPK-VIIPVBQESA-N | 5.977851 | UP   | UP   | RXN-15250  |
| Guanulate cyclase (Fragment) | Pyrophosphoric acid | XPPKVPQAPFPLU-UHFFFAOYSA-N | 10.689955 | DOWN | UP   | RHEA:13655 |
| Inositol oxygenase | D-Glucuronate Acid | AEMOLEFQBMNLQ-AQKNRBDQSA-N | 7.260806 | NA   | NA   | RXN-32697  |
| L-tyrosine decarboxylase | Tyramine | DZGWFCCGJZKUFP-UHFFFAOYSA-N | 5.953216 | NA   | NA   | RXN-14346  |
| 1-pyrroline-5-carboxylate synthase | D-Glutamic acid | WHUJTBXJRMK-GSVOUGTGSA-N | 11.232582 | UP   | UP   | RXN-24889  |
| Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial | 4-Hydroxyglutamate semialdehyde | XOCXUZPXXFRQGGP-DMTCNVIQSA-N | 11.232582 | NA   | NA   | RXN-14472  |
| Phenylalanine | Tyrosine | OUYCCCAQQFSEME-QMMPGOBPSA-N | 11.494889 | NA   | NA   | RHEA:20273 |
| S-(hydroxymethyl)glutathione dehydrogenase | Phenylalanine | COLNVLHDKAWLRT-QMMPGOBPSA-N | 10.804993 | NA   | NA   | RHEA:25290 |
| Glyceraldehyde | D-Glyceric acid | RBNPOMFGQHSH-UWTATZPHSA-N | 9.742343 | DOWN | DOWN | RHEA:18658 |

**Table S3.** MAGI output at TP5, showing the highest scoring gene-metabolite interactions with a MAGI score ≥ 5. The gene annotations, analyte identifications, MAGI scores, and reaction IDs are shown for both genes (GRT5) and metabolites (MRT5) at TP5. Rows highlighted in blue indicate redox reactions. Entries in the bold text take part in the same biochemical reaction.