

## Barcoding for Isobaric Tagging of Carboxylic Acids and Amines Metabolites

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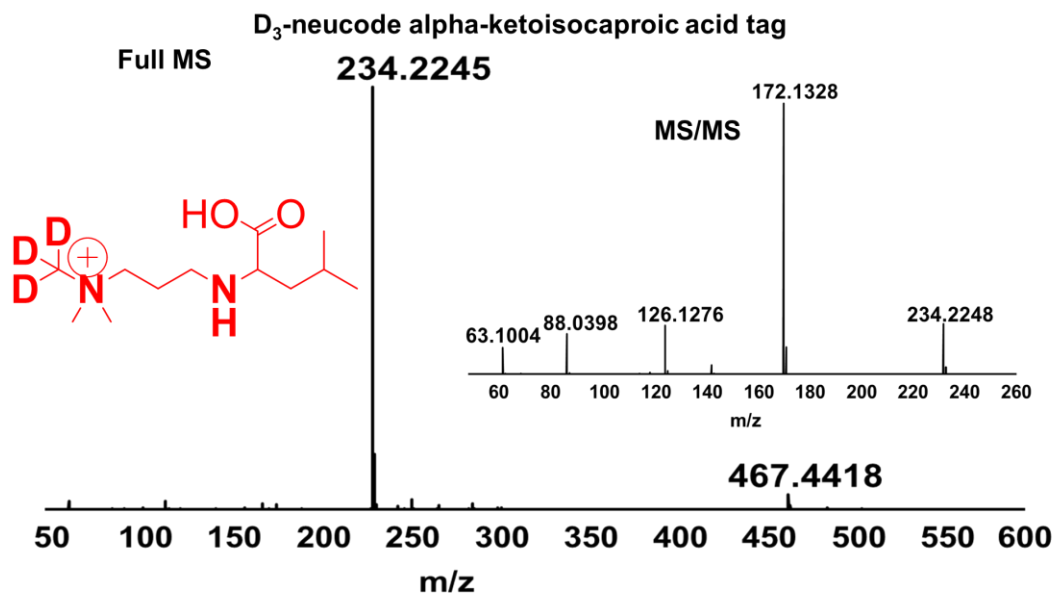
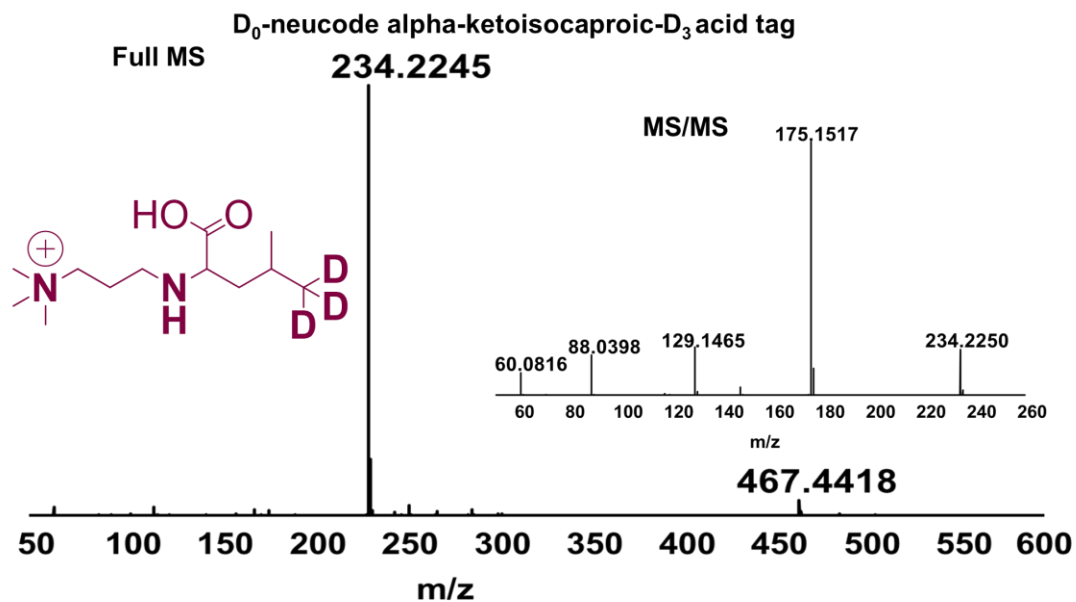
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Table 1: Analytical performance

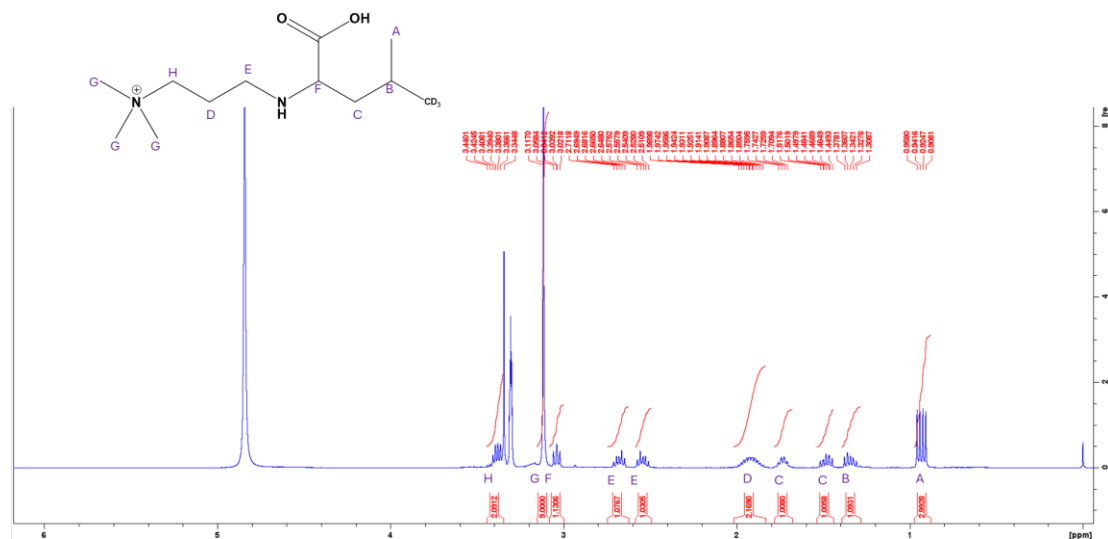
Table 2: HMDB IDs of metabolites and Log<sub>2</sub> fold change

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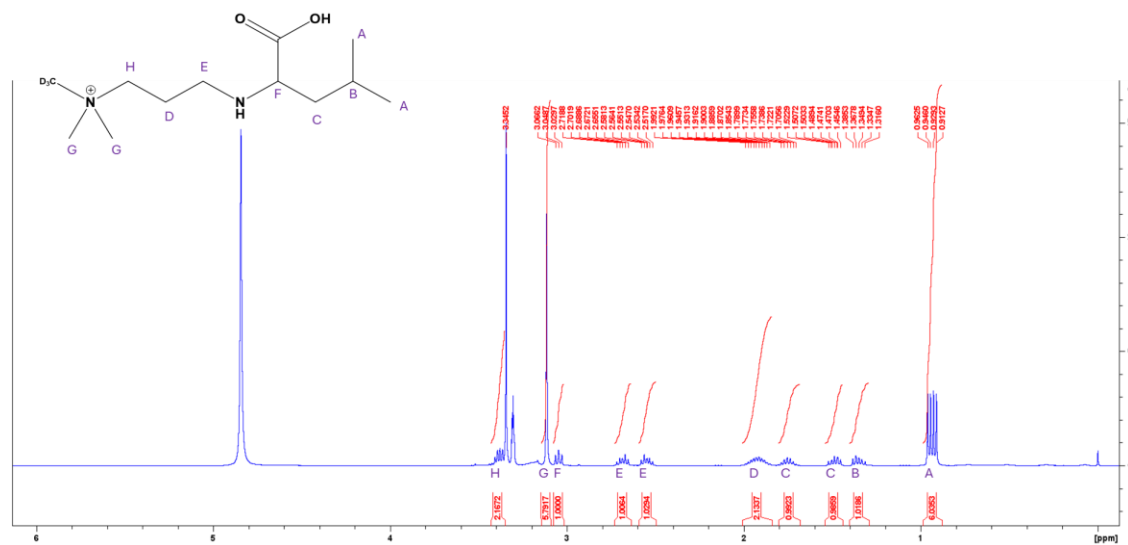


**Figure S1:** HRMS spectra of D<sub>0</sub>-neucode alpha-ketoisocaproic-D<sub>3</sub> and D<sub>3</sub>-neucode alpha-ketoisocaproic acid tags in separate injections. Each tag was characterized by HRMS at a resolution of R = 140K via direct injection.

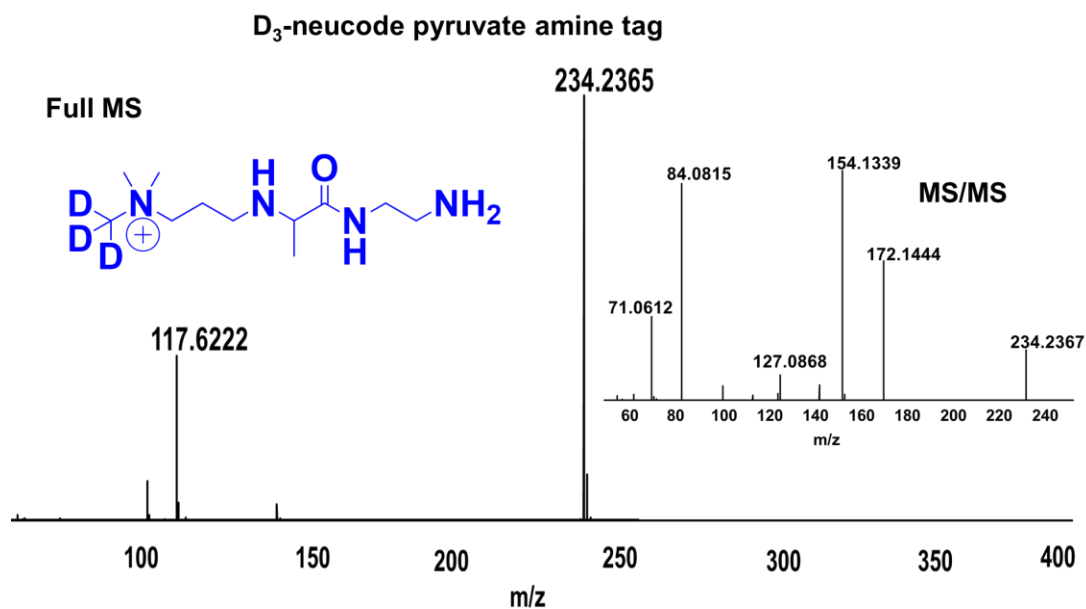
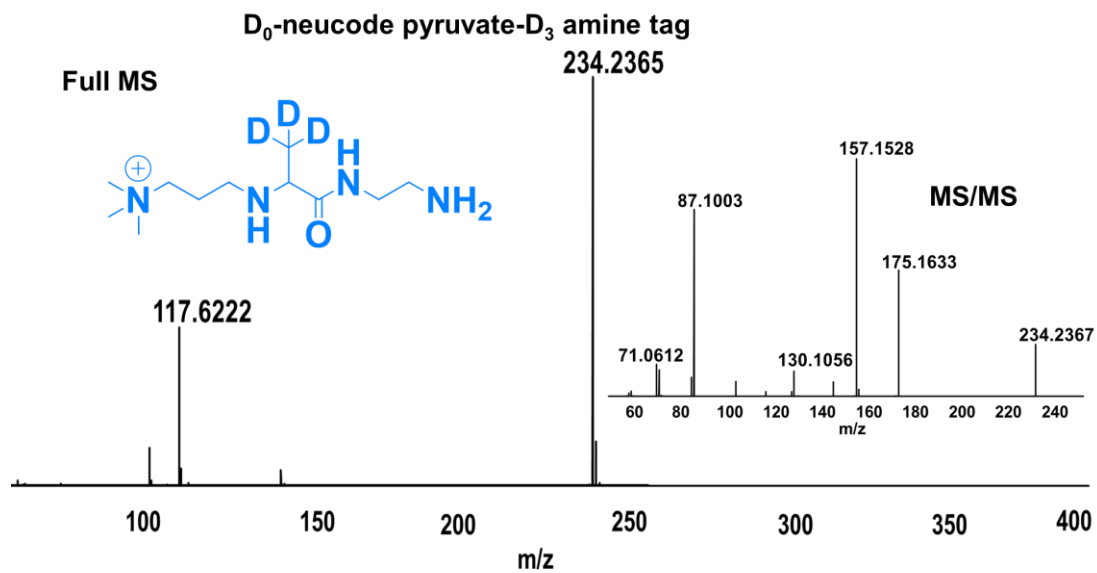
### D<sub>0</sub>-neucode alpha-ketoisocaproic-D<sub>3</sub> acid tag



### D<sub>3</sub>-neucode alpha-ketoisocaproic acid tag

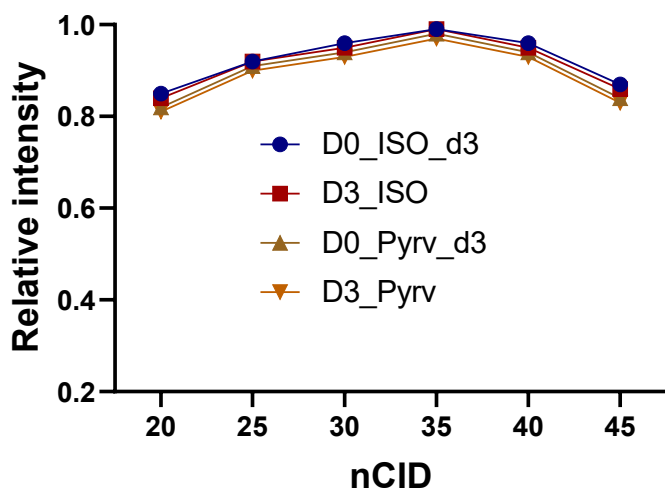


**Figure S2:** NMR spectra of D<sub>0</sub>-neucode alpha-ketoisocaproic-D<sub>3</sub> and D<sub>3</sub>-neucode alpha-ketoisocaproic acid tags.

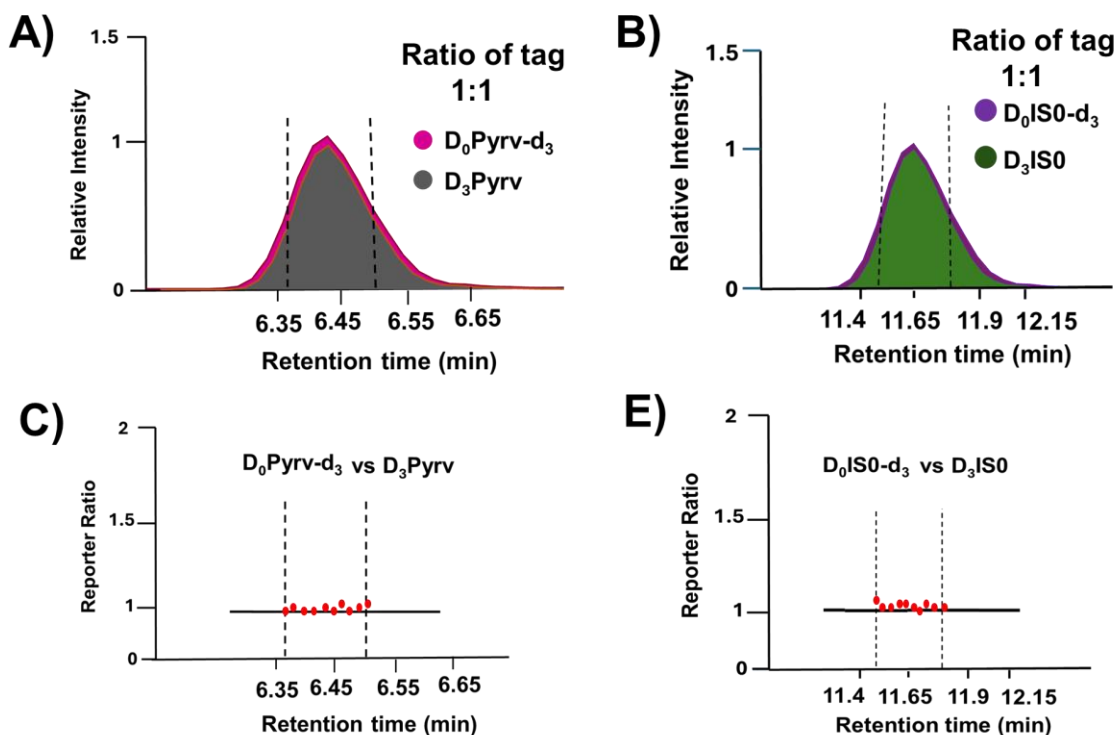


**Figure S3:** HRMS spectra of D<sub>0</sub>-neucode pyruvate-D<sub>3</sub> and D<sub>3</sub>-neucode pyruvate amine tags in separate injections. Each tag was characterized by HRMS at a resolution of R = 140K via direct injection.

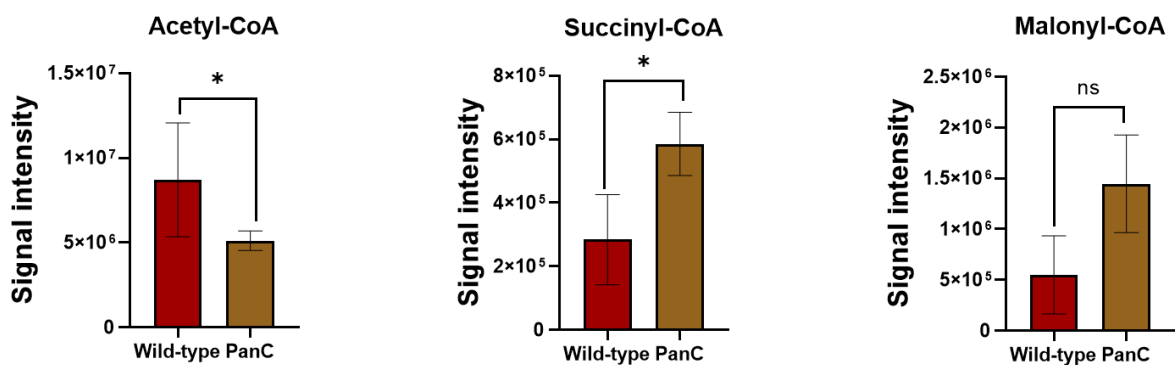




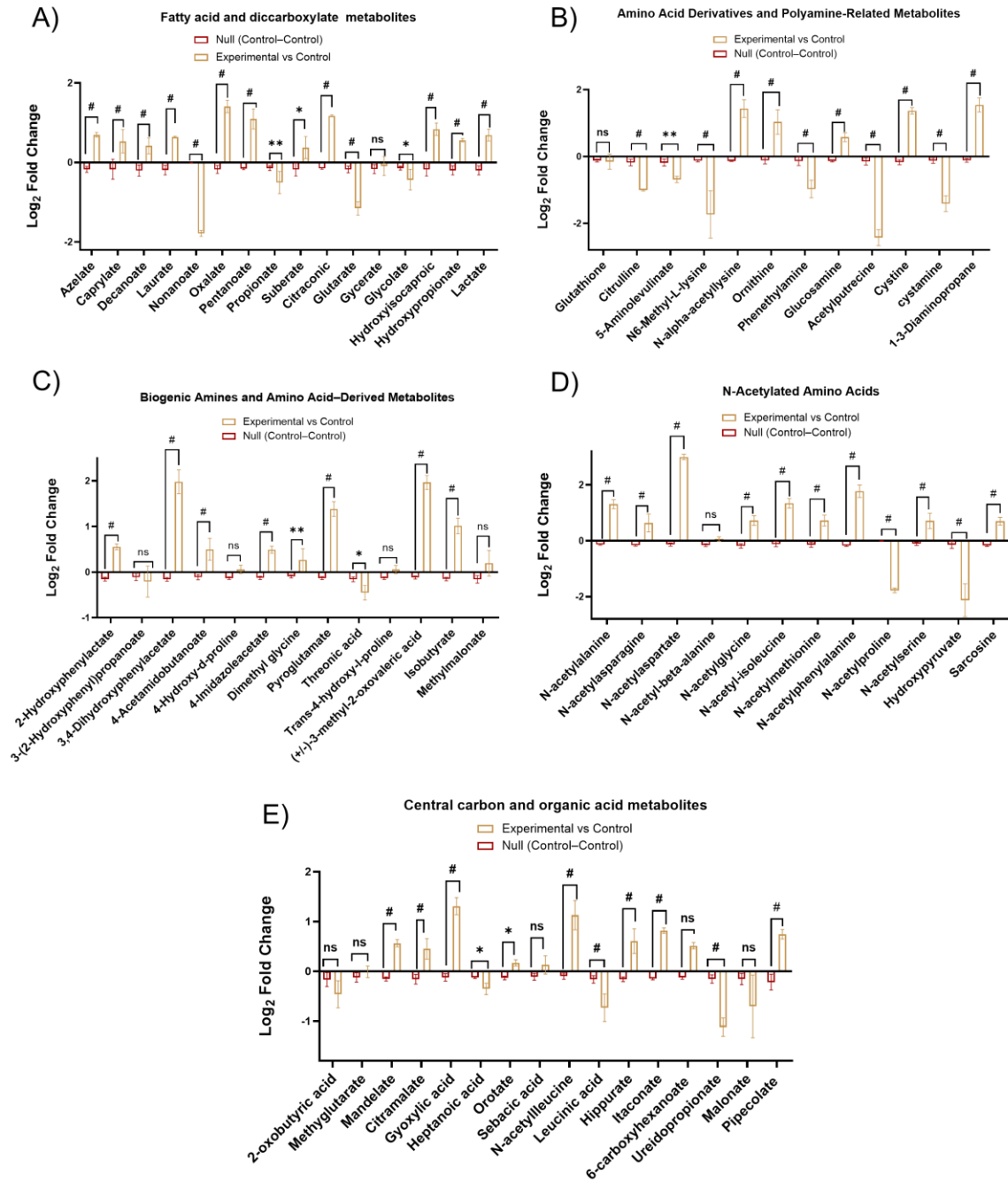
**Figure S5:** Optimizing collision energy fragmentation for both amine and acid tag variants. Tags are characterized at different collision energies to identify the nCID that generated high reporter ion intensity.



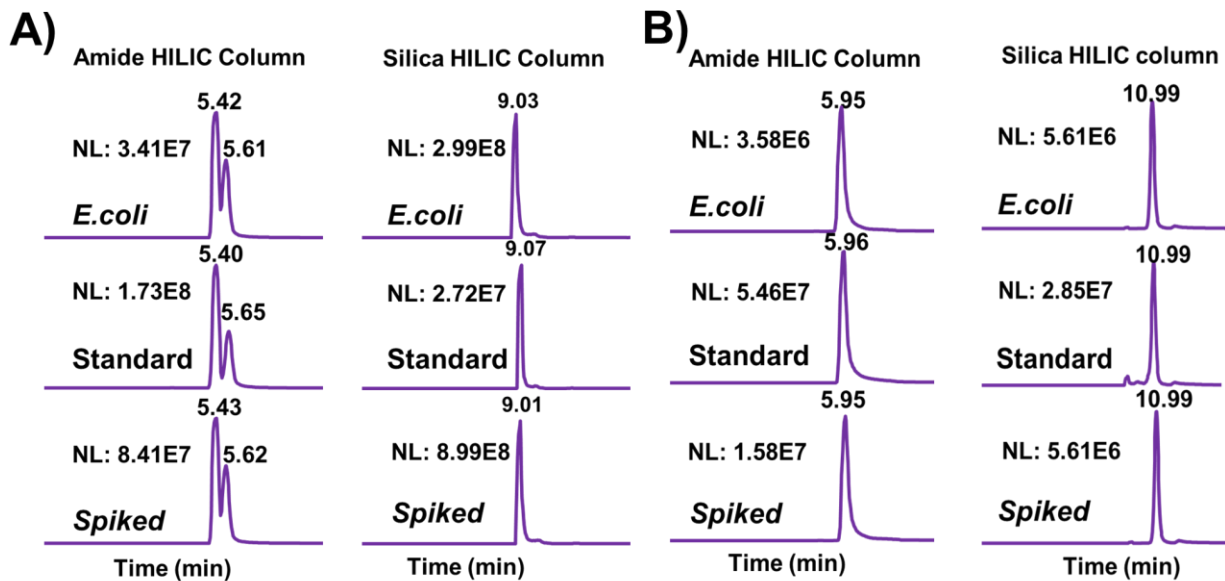
**Figure S6:** Minimal deuterium shifts are observed across each acid and amine tag variant peak (A, B). The lack of deuterium shifts results in consistent reporter intensity across the top 50% of each peak, shown with dotted points (C, D).



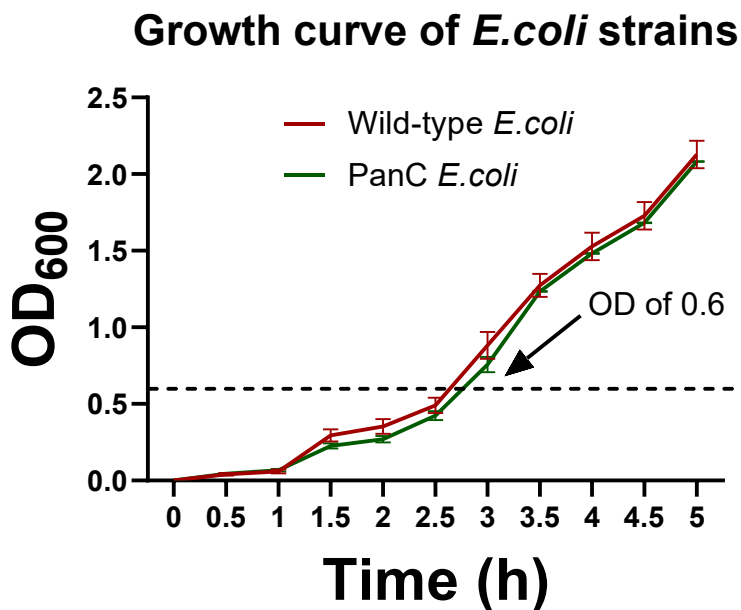
**Figure S7:** Signal intensities of acetyl-CoA, succinyl-CoA, and malonyl-CoA in Wild-type and PanC *E. coli*. Each *E. coli* strain was cultured as n=6. The cell was lysed at an optical density of 0.6. Error bars represent mean values across replicates, and error bars indicate  $\pm$ SD. Ns represent no significant difference and \* ( $p \leq 0.05$ ). Acetyl-CoA (p-value of 0.0273), Succinyl-CoA (p-value of 0.0392), and Malonyl-CoA (p-value of 0.0653). Wild-type and PanC *E. coli* were cultured in LB broth at 37°C in a shaker. Following this, a 1:10 serial dilution of each *E. coli* strain was performed, and at an optical density of 0.6, cells were centrifuged at 6300rpm at 4 °C for 15 minutes to remove media. A 2 mL of a 40:40:20 ratio of ice-cold acetonitrile, methanol, and water was added to the cell pellet and flash-frozen in liquid nitrogen. Cell pellets were freeze-thawed three times. The extract was centrifuged at 6300rpm at 4 °C for 5 min. The supernatant was dried under vacuum using a centrifuge and stored at -80 °C for analysis. Samples were analyzed using an Atlantis™ T3 3 $\mu$ m particle reverse-phase capillary column. The mobile phase A comprised 100% water, supplemented with 8 mM ammonium acetate and 0.05% acetic acid. Mobile phase B was 100% ACN. The gradient used for separating CoAs: 5% B, 0 min; 5% B, 1 min; 70% B, 3 min; 70% B, 13 min; 5% B, 13.1 min; 5% B, 20 min



**Figure S8:** Log<sub>2</sub> fold change of metabolites relative to control compared with a control/control null distribution. Log<sub>2</sub> fold change (Log<sub>2</sub> FC) values for the null distribution were calculated by comparing control samples against other control replicates to estimate baseline variability under no biological change. Experimental Log<sub>2</sub> FC values were calculated relative to the control condition. Bars represent mean values across replicates, and error bars indicate  $\pm$ SD. The horizontal line at Log<sub>2</sub> FC = 0 denotes 1:1 and no change relative to control. Ns represent no significant difference, \* ( $p \leq 0.05$ ), \*\* ( $p \leq 0.01$ ), \*\*\* ( $p \leq 0.001$ ), # ( $p \leq 0.0001$ ).



**Figure S9:** Level one confirmation of methionine sulfoxide and gamma-aminobutyric acid. (A) Retention time match of unlabeled methionine sulfoxide in *E. coli* lysate, standard, and spiked *E. coli* lysate. (B) Retention time match of unlabeled gamma-aminobutyric acid in *E. coli* lysate, standard, and spiked *E. coli* lysate



**Figure S10:** Growth curve of Wild-type and PanC *E. coli* using LB Broth. The optical density (OD) of the two strains was measured at timed intervals to determine the time at which the cells would be lysed. Subsequent culture growth was consistent with the predetermined growth curve. At an OD of 0.6, cells are lysed and metabolites extracted.

**Table 1:** Targeted analytes, linearity, retention time, relative standard deviation of standards

Analyte	R <sup>2</sup> (n=3)	RT (min)	RT RSD (n=3) %	Reaction RSD (n=3) %
(+/-)-3-methyl-2-oxovaleric acid sodium salt	0.9981	10.71	0.18	4.62
1,3_diaminopropane	0.9976	12.26	0.05	3.45
2-hydroxyphenylactate	0.9934	11.67	0.26	3.75
2-oxobutyric acid	0.9951	10.01	0.12	2.61
3-(2-Hydroxyphenyl) propanoate	0.9973	11.71	0.33	2.42
3,4-dihydroxyphenylacetate	0.9924	14.47	0.06	1.87
4-acetamidobutanoate	0.9927	11.43	0.23	3.52
4-hydroxy-d-proline	0.9998	10.22	0.25	3.49
4-imidazoleacetate	0.9932	13.67	0.18	3.13
5-aminolevulinate	0.9952	9.28	0.13	1.91
6-carboxyhexanoate	0.9935	9.02	0.11	1.51
Acetylputrecine	1	9.89	0.35	2.33
Alanine	0.9992	10.3	0.13	1.51
Alpha ketoisovalerate`	0.9961	9.83	0.25	1.58
Alpha-ketopantoate	1	10.22	0.61	1.28
Arginine	0.9953	14.41	0.17	3.26
Asparagine	0.9965	9.83	0.19	2.17
Aspartic acid	0.9931	9.85	0.21	1.92
Azelate	1	10.39	0.18	1.48
Beta-alanine	0.9992	9.8	0.06	1.67
Caprylate	0.9971	9.5	0.18	2.59
Citraconic	1	10.24	0.44	2.78
Citramalate	0.9953	10.42	0.16	1.89

<b>Citrate</b>	<b>0.9972</b>	<b>9.61</b>	<b>0.55</b>	<b>3.57</b>
<b>Citrulline</b>	<b>1</b>	<b>9.7</b>	<b>0.36</b>	<b>2.34</b>
<b>Cysteamine</b>	<b>0.9927</b>	<b>9.82</b>	<b>0.35</b>	<b>3.13</b>
<b>Cysteine</b>	<b>0.9915</b>	<b>13.59</b>	<b>0.24</b>	<b>1.78</b>
<b>Cystine</b>	<b>0.9953</b>	<b>6.51</b>	<b>0.15</b>	<b>3.81</b>
<b>Decanoate</b>	<b>0.9982</b>	<b>9.33</b>	<b>0.47</b>	<b>3.23</b>
<b>Dimethyl glycine</b>	<b>0.9995</b>	<b>12.29</b>	<b>0.55</b>	<b>2.58</b>
<b>Fumarate</b>	<b>0.9973</b>	<b>9.73</b>	<b>0.26</b>	<b>3.33</b>
<b>Glucosamine</b>	<b>1</b>	<b>9.69</b>	<b>0.11</b>	<b>2.78</b>
<b>Glutamic acid</b>	<b>0.9956</b>	<b>10.87</b>	<b>0.26</b>	<b>2.56</b>
<b>Glutamine</b>	<b>1</b>	<b>10.19</b>	<b>0.08</b>	<b>1.68</b>
<b>Glutarate</b>	<b>0.9967</b>	<b>10.32</b>	<b>0.25</b>	<b>3.44</b>
<b>Glutathione</b>	<b>1</b>	<b>10.22</b>	<b>0.15</b>	<b>3.4</b>
<b>Glycerate</b>	<b>0.9967</b>	<b>9.92</b>	<b>0.59</b>	<b>3.21</b>
<b>Glycine</b>	<b>0.9977</b>	<b>10.24</b>	<b>2.3</b>	<b>2.89</b>
<b>Glycolic acid</b>	<b>0.9979</b>	<b>10.44</b>	<b>0.08</b>	<b>3.67</b>
<b>Glyoxylic acid</b>	<b>0.9995</b>	<b>9.76</b>	<b>0.18</b>	<b>2.37</b>
<b>Heptanoic acid</b>	<b>0.9938</b>	<b>9.55</b>	<b>0.13</b>	<b>1.86</b>
<b>Hippurate</b>	<b>0.9919</b>	<b>8.29</b>	<b>0.22</b>	<b>1.98</b>
<b>Histidine</b>	<b>0.9998</b>	<b>11.07</b>	<b>0.15</b>	<b>3.41</b>
<b>Hydroxy isocaproic</b>	<b>0.9947</b>	<b>9.52</b>	<b>0.1</b>	<b>2.52</b>
<b>Hydroxyl propionic acid</b>	<b>1</b>	<b>10.41</b>	<b>0.03</b>	<b>1.75</b>
<b>Hydroxy pyruvate</b>	<b>0.9965</b>	<b>10.47</b>	<b>0.2</b>	<b>2.57</b>
<b>Isobuyrate</b>	<b>1</b>	<b>10.29</b>	<b>0.8</b>	<b>3.89</b>
<b>Isoleucine</b>	<b>0.9968</b>	<b>9.34</b>	<b>0.1</b>	<b>2.78</b>
<b>Itaconate</b>	<b>0.9938</b>	<b>10.24</b>	<b>0.13</b>	<b>2.56</b>
<b>Lactate</b>	<b>1</b>	<b>10.34</b>	<b>0.37</b>	<b>1.97</b>
<b>Laurate</b>	<b>0.9973</b>	<b>8.9</b>	<b>0.05</b>	<b>2.57</b>
<b>Leucine</b>	<b>0.9993</b>	<b>9.76</b>	<b>0.24</b>	<b>3.67</b>
<b>Leucinic acid</b>	<b>1</b>	<b>10.32</b>	<b>0.17</b>	<b>2.95</b>
<b>Lysine</b>	<b>0.9954</b>	<b>10.06</b>	<b>0.06</b>	<b>4.5</b>
<b>Malate</b>	<b>1</b>	<b>14.77</b>	<b>0.08</b>	<b>5.78</b>
<b>Malonate</b>	<b>0.9959</b>	<b>10.47</b>	<b>0.13</b>	<b>2.58</b>
<b>Mandelate</b>	<b>0.9992</b>	<b>9.77</b>	<b>0.48</b>	<b>1.53</b>

<b>Methionine</b>	<b>0.9944</b>	<b>9.82</b>	<b>0.19</b>	<b>3.08</b>
<b>Methylglutarate</b>	<b>0.9915</b>	<b>10.22</b>	<b>0.43</b>	<b>1.48</b>
<b>Methylmalonate</b>	<b>0.9933</b>	<b>10</b>	<b>0.1</b>	<b>2.27</b>
<b>N6-methyl_L_lysine</b>	<b>0.998</b>	<b>10.32</b>	<b>0.38</b>	<b>2.73</b>
<b>N-acetyl alanine</b>	<b>0.9935</b>	<b>12.24</b>	<b>0.11</b>	<b>2.46</b>
<b>N-acetyl asparagine</b>	<b>0.9974</b>	<b>10.11</b>	<b>0.2</b>	<b>2.96</b>
<b>N-acetyl aspartate</b>	<b>1</b>	<b>13.16</b>	<b>0.08</b>	<b>2.45</b>
<b>N-acetyl-beta-alanine</b>	<b>0.9956</b>	<b>11.02</b>	<b>0.33</b>	<b>1.99</b>
<b>N-acetyl glycine</b>	<b>1</b>	<b>10.52</b>	<b>0.06</b>	<b>2.38</b>
<b>N-acetyl-isoleucine</b>	<b>0.9953</b>	<b>12.91</b>	<b>0.05</b>	<b>2.57</b>
<b>N-acetyl leucine</b>	<b>0.999</b>	<b>11.27</b>	<b>0.11</b>	<b>1.87</b>
<b>N-acetylmethionine</b>	<b>0.9976</b>	<b>9.79</b>	<b>0.08</b>	<b>2.09</b>
<b>N-acetyl phenylalanine</b>	<b>0.9986</b>	<b>9.89</b>	<b>0.38</b>	<b>2.58</b>
<b>N-acetyl proline</b>	<b>1</b>	<b>10.39</b>	<b>0.12</b>	<b>3.15</b>
<b>N-acetyl serine</b>	<b>0.9953</b>	<b>11.43</b>	<b>0.15</b>	<b>3.47</b>
<b>N-alpha_acetyllysine</b>	<b>0.9958</b>	<b>9.92</b>	<b>0.45</b>	<b>2.5</b>
<b>Nonanoate</b>	<b>0.9891</b>	<b>9.4</b>	<b>0.27</b>	<b>2.18</b>
<b>Ornithine</b>	<b>0.9919</b>	<b>9.89</b>	<b>0.09</b>	<b>1.84</b>
<b>Orotate</b>	<b>0.9982</b>	<b>9.41</b>	<b>0.21</b>	<b>3.39</b>
<b>Oxalate</b>	<b>1</b>	<b>12.26</b>	<b>0.26</b>	<b>2.24</b>
<b>Oxaloacetate</b>	<b>0.9982</b>	<b>10.65</b>	<b>0.17</b>	<b>2.06</b>
<b>Pantoate</b>	<b>1</b>	<b>9.8</b>	<b>0.19</b>	<b>3.17</b>
<b>Pantothenate</b>	<b>0.9983</b>	<b>10.25</b>	<b>0.22</b>	<b>2.08</b>
<b>Pentanoate</b>	<b>0.9963</b>	<b>10.32</b>	<b>0.16</b>	<b>1.97</b>
<b>Phenethylamine</b>	<b>0.9928</b>	<b>7.86</b>	<b>0.17</b>	<b>2.68</b>
<b>Phenylalanine</b>	<b>1</b>	<b>9.04</b>	<b>0.14</b>	<b>2.97</b>
<b>Pipecolate</b>	<b>0.9918</b>	<b>10.41</b>	<b>0.12</b>	<b>1.43</b>
<b>Proline</b>	<b>1</b>	<b>11.35</b>	<b>0.36</b>	<b>2.58</b>
<b>Propionate</b>	<b>0.9975</b>	<b>10.49</b>	<b>0.46</b>	<b>1.79</b>
<b>Pyroglutamate</b>	<b>0.9969</b>	<b>10.95</b>	<b>0.19</b>	<b>1.94</b>
<b>Pyruvate</b>	<b>0.9957</b>	<b>10.37</b>	<b>0.27</b>	<b>2.45</b>
<b>Sarcosine</b>	<b>0.9982</b>	<b>11.8</b>	<b>0.22</b>	<b>3.21</b>
<b>Sebacic acid</b>	<b>0.9949</b>	<b>8.93</b>	<b>0.18</b>	<b>4.07</b>
<b>Serine</b>	<b>0.9925</b>	<b>9.25</b>	<b>0.14</b>	<b>1.39</b>

<b>Suberate</b>	<b>1</b>	<b>9.52</b>	<b>0.28</b>	<b>2.05</b>
<b>Succinate</b>	<b>0.9982</b>	<b>9.9</b>	<b>0.19</b>	<b>3.45</b>
<b>Threonic acid</b>	<b>1</b>	<b>15.66</b>	<b>0.21</b>	<b>2.78</b>
<b>Threonine</b>	<b>0.9964</b>	<b>9.86</b>	<b>0.37</b>	<b>1.79</b>
<b>Trans-4-hydroxy-l-proline</b>	<b>0.9954</b>	<b>8.43</b>	<b>0.23</b>	<b>1.76</b>
<b>Tryptophan</b>	<b>0.9991</b>	<b>9.38</b>	<b>0.17</b>	<b>3.51</b>
<b>Tyrosine</b>	<b>0.9945</b>	<b>9.03</b>	<b>0.38</b>	<b>2.86</b>
<b>Ureidopropionate</b>	<b>0.9939</b>	<b>10.28</b>	<b>0.39</b>	<b>1.76</b>
<b>Valine</b>	<b>1</b>	<b>10.02</b>	<b>0.45</b>	<b>2.02</b>
<b>Average</b>	<b>0.9968 ± 0.0027</b>	<b>10.42</b>	<b>0.25</b>	<b>2.63 ± 0.8082</b>

**Table 2:** Metabolites with HMDB IDs and fold change

<b>Analyte</b>	<b>HMDB</b>	<b>Log2 Fold change (n=3)</b>		
		<b>1</b>	<b>2</b>	<b>3</b>
(+/-)-3-methyl-2-oxovaleric acid sodium salt	HMDB0000491	2.027593	1.789169	2.076828
1,3_diaminopropane	HMDB0000002	1.508083	1.76354	1.345414
2-hydroxyphenylactate	HMDB0000669	0.494886	0.621172	0.544303
2-oxobutyric acid	HMDB0000005	-0.404214	-0.23023	-0.76142
3-(2-Hydroxyphenyl) propanoate	HMDB0033752	-0.31839	0.17565	-0.4791
3,4-dihydroxyphenylacetate	HMDB0001336	1.795222	2.275815	1.861533
4-acetamidobutanoate	HMDB0003681	0.430834	0.763963	0.296994
4-hydroxy-d-proline	HMDB0060460	0.138971	0.075317	-0.04248
4-imidazoleacetate	HMDB0002024	0.546028	0.521676	0.39954
5-aminolevulinate	HMDB0001149	-0.62236	-0.6473	-0.7964
6-carboxyhexanoate	HMDB0000857	0.500486	0.453355	0.580817
Acetylputrecine	HMDB0002064	-2.65381	-2.17719	-2.45093
Alanine	HMDB0000161	-1.2823	-1.60268	-0.74072
Alpha ketoisovalerate	HMDB0000019	0.692521	0.509586	0.059026
Alpha-ketopantoate	HMDB0304068	0.061308	0.187535	0.051241
Arginine	HMDB0000517	1.397977	1.551345	1.292265
Asparagine	HMDB0000168	-0.76852	-1.3763	-0.95658
Aspartic acid	HMDB0000191	-0.16048	-0.32657	-0.23549
Azelate	HMDB0000784	0.635894	0.753212	0.694047
Beta-alanine	HMDB0000056	0.931286	0.893071	0.68083
Caprylate	HMDB0000482	0.412132	0.313365	0.863817
Citraconic	HMDB0000634	1.163462	1.15302	1.200071

Citramalate	HMDB0000426	0.628595	0.224122	0.499124
Citrate	HMDB0000094	0.615852	0.591759	0.375574
Citrulline	HMDB0000904	-0.96504	-1.02035	-1.02668
Cysteamine	HMDB0250701	-1.31056	-1.68248	-1.24177
Cysteine	HMDB0251515	1.415702	1.369356	1.264413
Cystine	HMDB0000192	1.478332	1.306039	1.308777
Decanoate	HMDB0000511	0.240999	0.373297	0.638919
Dimethyl glycine	HMDB0000092	0.549215	0.167065	0.085578
Fumarate	HMDB0000134	-0.20381	-0.36995	-0.487386
Glucosamine	HMDB0001514	0.428657	0.694288	0.613728
Glutamic acid	HMDB0000148	2.51654	2.227166	2.363606
Glutamine	HMDB0000641	1.413681	1.513485	1.448873
Glutarate	HMDB0000661	-0.97334	-1.31282	-1.18039
Glutathione	HMDB0000125	-0.4069	-0.08876	0.031172
Glycerate	HMDB0000139	-0.27229	-0.17843	0.182331
Glycine	HMDB0000123	-0.46108	-0.88901	0.053441
Glycolic acid	HMDB0000115	-0.61075	-0.56207	-0.13672
Glyoxylic acid	HMDB0000119	1.204004	1.506333	1.212586
Heptanoic acid	HMDB0000666	-0.30269	-0.48636	-0.2768
Hippurate	HMDB0000714	0.591843	0.363429	0.858754
Histidine	HMDB0000177	2.442213	2.737674	2.21475
Hydroxy isocaproic	HMDB0000746	0.979427	0.85347	0.667027
Hydroxyl propionic acid	HMDB0000700	0.548082	0.524097	0.604182
Hydroxy pyruvate	HMDB0001352	-2.30693	-1.47566	-2.61239
Isobutyrate	HMDB0001873	0.903262	0.925054	1.20914
Isoleucine	HMDB0000172	-1.1744	-1.6913	-1.32208
Itaconate	HMDB0002092	0.858427	0.753392	0.836536
Lactate	HMDB0000190	0.60313	0.857047	0.597099
Laurate	HMDB0000638	0.663145	0.633212	0.612412
Leucine	HMDB0000687	-0.66009	-1.33215	-0.93321
Leucinic acid	HMDB0000665	-0.85613	-0.92866	-0.41588

Lysine	HMDB0000182	0.50297	0.353946	0.057205
Malate	HMDB0000156	-0.49478	-0.75073	-0.65344
Malonate	HMDB0000691	-0.28047	-1.43016	-0.40662
Mandelate	HMDB0000703	0.49757	0.639278	0.547313
Methionine	HMDB0000696	1.011912	1.16984	0.766716
Methylglutarate	HMDB0000752	0.043314	0.068682	-0.14515
Methylmalonate	HMDB0000202	0.422608	-0.12009	0.280477
N6-methyl_L_lysine	HMDB0002038	-1.93378	-0.95225	-2.32483
N-acetyl alanine	HMDB0000766	1.388861	1.407228	1.123128
N-acetyl asparagine	HMDB0006028	0.843058	0.261877	0.796764
N-acetyl aspartate	HMDB0000812	2.886989	3.028711	3.069507
N-acetyl-beta-alanine	HMDB0061880	0.131721	0.073198	-0.03156
N-acetyl glycine	HMDB0000532	0.906773	0.563773	0.695071
N-acetyl-isoleucine	HMDB0061684	1.190309	1.300058	1.530755
N-acetyl leucine	HMDB0011756	1.459115	1.007873	0.910437
N-acetylmethionine	HMDB0011745	0.825802	0.496408	0.837791
N-acetyl phenylalanine	HMDB0000512	2.026182	1.679616	1.606752
N-acetyl proline	HMDB0094701	-1.68571	-1.86178	-1.78471
N-acetyl serine	HMDB0002931	0.409905	0.772297	0.947796
N-alpha_acetyllysine	HMDB0000446	1.315469	1.249071	1.729039
Nonanoate	HMDB0000847	-1.70332	-1.829	-1.83244
Ornithine	HMDB0000214	1.453618	0.79141	0.850795
Orotate	HMDB0000226	0.146812	0.240677	0.117872
Oxalate	HMDB0002329	1.301893	1.329961	1.58582
Oxaloacetate	HMDB0000223	1.732596	1.20649	1.093424
Pantoic acid	HMDB0240389	2.315777	1.395684	1.528525
Pantothenate	HMDB0000210	1.56007	1.763134	1.428973
Pentanoate	HMDB0000892	1.244044	1.233708	0.799521
Phenethylamine	HMDB0012275	-0.75972	-1.26999	-0.89077
Phenylalanine	HMDB0000159	-1.02947	-0.99361	-1.34837
Pipecolate	HMDB0000070	0.849634	0.708988	0.667795

Proline	HMDB0000162	2.325456	2.345727	2.346504
Propionate	HMDB0000237	-0.7068	-0.18717	-0.62831
Pyroglutamate	HMDB0000267	1.462421	1.195168	1.486451
Pyruvate	HMDB0000243	1.58582	1.300846	1.337192
Sarcosine	HMDB0000271	0.847683	0.664808	0.576155
Sebacic acid	HMDB0000792	0.013407	0.337548	0.028664
Serine	HMDB0000187	0.049489	0.049836	0.064559
Suberate	HMDB0000893	0.10999	0.663591	0.345964
Succinate	HMDB0000254	0.435715	0.831707	0.285045
Threonic acid	HMDB0000943	-0.4014	-0.3272	-0.63251
Threonine	HMDB0000167	0.636414	0.658178	0.402117
Trans-4-hydroxy-l-proline	HMDB0000725	0.136241	0.075641	-0.04501
Tryptophan	HMDB0000929	0.248047	-0.09437	-0.08867
Tyrosine	HMDB0250803	-0.40468	0.035555	-0.30754
Ureidopropionate	HMDB0000026	-0.94252	-1.31149	-1.11568
Valine	HMDB0000883	-1.48092	-1.76706	-1.97091

**Table 3:** Ratio of reporter ions to cyclized products of tagged analyte

<b>Analyte</b>	<b>Ratio of single to double fragmentation</b>	
	<b>Cyclized product</b>	<b>Reporter ion</b>
(+/-)-3-methyl-2-oxovaleric acid sodium salt	1	3.4
1,3_diaminopropane	1	4
2-hydroxyphenylactate	1	3.5
2-oxobutyric acid	1	4.3
3-(2-Hydroxyphenyl) propanoate	1	2.9
3,4-dihydroxyphenylacetate	1	3.7
4-acetamidobutanoate	1	4.3
4-hydroxy-d-proline	1	2.8
4-imidazoleacetate	1	4.3
5-aminolevulinate	1	4
6-carboxyhexanoate	1	3
Acetylputrecine	1	3.3
Alanine	1	3.6
Alpha ketoisovalerate	1	3.2
Alpha-ketopantoate	1	3.7
Arginine	1	3.1
Asparagine	1	2.9
Aspartic acid	1	3.4
Azelate	1	4.5
Beta-alanine	1	3.5
Caprylate	1	3.8
Citraconic	1	3.3
Citramalate	1	3.1
Citrate	1	3.6
Citrulline	1	2.9
Cysteamine	1	2.8

Cysteine	1	3.4
Cystine	1	3.1
Decanoate	1	4
Dimethyl glycine	1	4.2
Fumarate	1	3.9
Glucosamine	1	3.7
Glutamic acid	1	3.5
Glutamine	1	3.8
Glutarate	1	2.9
Glutathione	1	3.3
Glycerate	1	3.1
Glycine	1	3.5
Glycolic acid	1	4.1
Glyoxylic acid	1	3.3
Heptanoic acid	1	3.7
Hippurate	1	4.2
Histidine	1	4.4
Hydroxy isocaproic	1	3.5
Hydroxyl propionic acid	1	3.3
Hydroxy pyruvate	1	3.9
Isobutyrate	1	3.6
Isoleucine	1	3.2
Itaconate	1	3.7
Lactate	1	4.2
Laurate	1	3.3
Leucine	1	2.8
Leucinic acid	1	3.7
Lysine	1	3.5
Malate	1	3.9
Malonate	1	3.3
Mandelate	1	4.2
Methionine	1	3.5
Methylglutarate	1	4.3
Methylmalonate	1	2.9

N6-methyl_L_lysine	1	3.8
N-acetyl alanine	1	3.6
N-acetyl asparagine	1	4
N-acetyl aspartate	1	3.3
N-acetyl-beta-alanine	1	3.5
N-acetyl glycine	1	3.7
N-acetyl-isoleucine	1	2.9
N-acetyl leucine	1	3.7
N-acetylmethionine	1	3
N-acetyl phenylalanine	1	3.6
N-acetyl proline	1	3.8
N-acetyl serine	1	3.3
N-alpha_acetyllysine	1	3.5
Nonanoate	1	4.2
Ornithine	1	3.2
Orotate	1	2.7
Oxalate	1	3.1
Oxaloacetate	1	3.8
Pantoic acid	1	4.2
Pantothenate	1	3.3
Pentanoate	1	3.6
Phenethylamine	1	2.9
Phenylalanine	1	4.1
Pipecolate	1	3.1
Proline	1	3.5
Propionate	1	3.8
Pyroglutamate	1	3.3
Pyruvate	1	4.1
Sarcosine	1	3.1
Sebacic acid	1	3.6
Serine	1	3.3
Suberate	1	4.4
Succinate	1	4.2
Threonic acid	1	3.7

Threonine	1	3.1
Trans-4-hydroxy-L-proline	1	3.8
Tryptophan	1	4.3
Tyrosine	1	2.8
Ureidopropionate	1	3.6
Valine	1	3.3