**Amino acid dependent formaldehyde metabolism in mammals**

**Supplementary Information**

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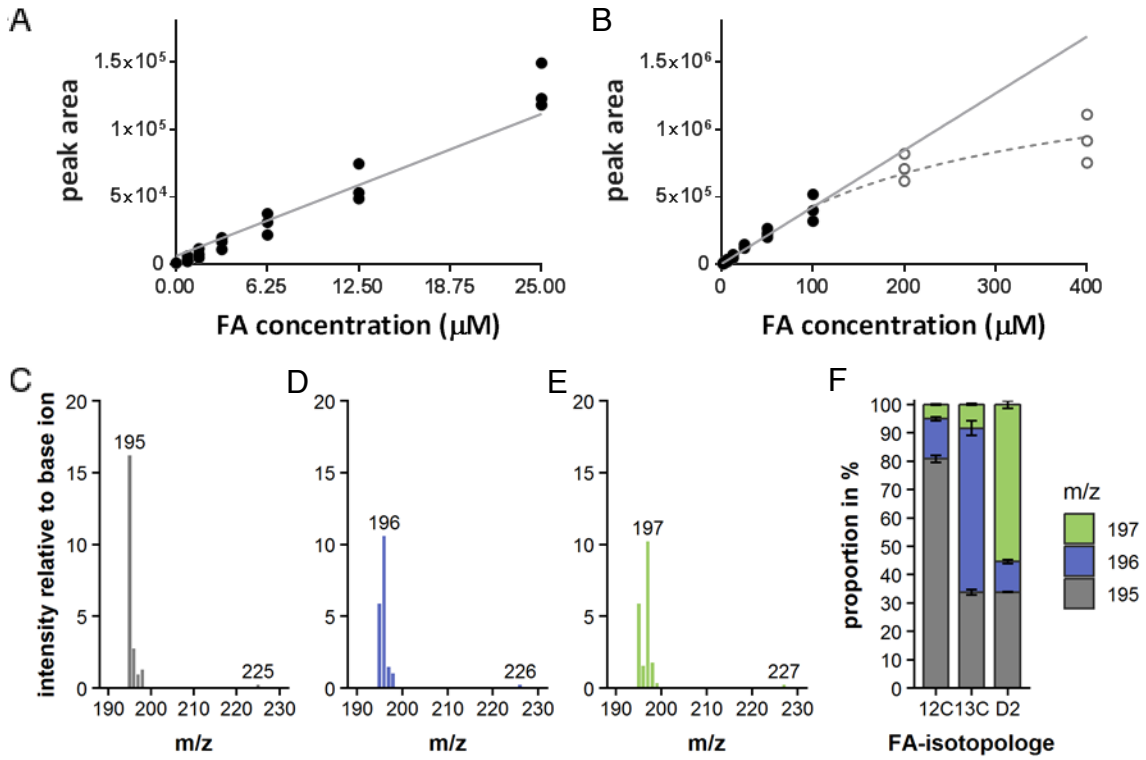


**Supplementary Figure 1**

A,B) Low (A) and high (B) concentration range of figure 1C, emphasizing the linearity up to 100 µM formaldehyde. C-F) Isotopic interference between the formaldehyde-PFBHA fragments containing the formaldehyde backbone in the m/z range from 190 to 230: m/z of $^{12}$C-formaldehyde (C), $^{13}$C-formaldehyde (D) and D2-formaldehyde (E). F) Proportion of each of the fragments within the range of 195 to 197. Evident is a constant fraction of $^{12}$C (m/z = 195) in all cases, indicating an additional fragment that doesn't contain the formaldehyde carbon.

| m/z 195 (Peak area) | m/z 196 (Peak area) | mz/197 (Peak area) | $F_0$ (mM) | $F_1$ (mM) | $F_2$ (mM) |
|---|---|---|---|---|---|
| 50022.0112 | 11486.75889 | 84305.68527 | 0 | 0 | 0.01 |
| 67369.21804 | 13476.80554 | 79063.73855 | 0.001 | 0 | 0.01 |
| 88591.57913 | 14845.47327 | 80406.57654 | 0.003 | 0 | 0.01 |
| 118436.0286 | 18691.82262 | 76580.53826 | 0.006 | 0 | 0.01 |
| 178219.3993 | 26251.11177 | 77465.08001 | 0.012 | 0 | 0.01 |
| 344824.8688 | 45413.88982 | 94706.31722 | 0.025 | 0 | 0.01 |
| 610068.1277 | 72793.02112 | 104234.4871 | 0.05 | 0 | 0.01 |
| 1166748.891 | 138147.9644 | 125521.4035 | 0.1 | 0 | 0.01 |
| 57097.82014 | 22599.72822 | 81744.69495 | 0 | 0.001 | 0.01 |
| 61827.10108 | 35192.92003 | 82000.37224 | 0 | 0.003 | 0.01 |
| 73427.09768 | 60033.15332 | 88396.43395 | 0 | 0.006 | 0.01 |
| 95533.70968 | 110621.1491 | 95946.38733 | 0 | 0.012 | 0.01 |
| 159262.0484 | 229627.5876 | 121690.6415 | 0 | 0.025 | 0.01 |
| 252020.2936 | 429709.2193 | 132336.6509 | 0 | 0.05 | 0.01 |
| 509136.1414 | 955266.9226 | 209248.586 | 0 | 0.1 | 0.01 |
| 54239.56108 | 11096.08687 | 89094.8986 | 0 | 0 | 0.01 |
| 80067.76302 | 14982.0862 | 95708.224 | 0.001 | 0 | 0.01 |
| 86940.89952 | 15693.203 | 85870.54207 | 0.003 | 0 | 0.01 |
| 133712.8038 | 19758.57228 | 90335.71983 | 0.006 | 0 | 0.01 |
| 192915.7721 | 26685.84261 | 89471.26188 | 0.012 | 0 | 0.01 |
| 360336.3492 | 47477.16199 | 106263.0843 | 0.025 | 0 | 0.01 |
| 710946.5161 | 86073.05134 | 123796.8851 | 0.05 | 0 | 0.01 |
| 1242834.645 | 140025.7089 | 138803.6856 | 0.1 | 0 | 0.01 |
| 59243.73696 | 25716.50016 | 93119.38244 | 0 | 0.001 | 0.01 |
| 64634.37403 | 39993.51315 | 94488.53158 | 0 | 0.003 | 0.01 |
| 80821.45506 | 64618.79223 | 103494.651 | 0 | 0.006 | 0.01 |
| 103314.1851 | 119191.9921 | 103329.0836 | 0 | 0.012 | 0.01 |
| 147883.1333 | 217449.5561 | 109493.5828 | 0 | 0.025 | 0.01 |
| 265667.4009 | 448600.2819 | 145191.608 | 0 | 0.05 | 0.01 |
| 500684.9384 | 933911.3867 | 214067.7842 | 0 | 0.1 | 0.01 |
| 52137.68543 | 11390.75128 | 89863.84098 | 0 | 0 | 0.01 |
| 73312.09223 | 14818.61165 | 90201.17776 | 0.001 | 0 | 0.01 |
| 98866.15264 | 16801.5797 | 95371.96103 | 0.003 | 0 | 0.01 |
| 132255.1796 | 21283.84233 | 94091.42805 | 0.006 | 0 | 0.01 |
| 218905.7898 | 30477.11722 | 100843.3232 | 0.012 | 0 | 0.01 |
| 344588.1321 | 44912.28766 | 101251.8323 | 0.025 | 0 | 0.01 |
| 643304.7357 | 77833.66983 | 112937.9941 | 0.05 | 0 | 0.01 |
| 1242574.765 | 137117.4354 | 137546.864 | 0.1 | 0 | 0.01 |
| 57365.81475 | 23314.0875 | 85178.03193 | 0 | 0.001 | 0.01 |
| 68419.47312 | 38400.65767 | 99142.89642 | 0 | 0.003 | 0.01 |
| 78457.25626 | 63535.70559 | 98130.51581 | 0 | 0.006 | 0.01 |
| 92997.68031 | 107079.2725 | 98253.55779 | 0 | 0.012 | 0.01 |
| 153709.1975 | 222578.709 | 107895.1161 | 0 | 0.025 | 0.01 |
| 257049.6529 | 423045.7406 | 149233.0386 | 0 | 0.05 | 0.01 |
| 438415.5227 | 824217.5172 | 191300.0782 | 0 | 0.1 | 0.01 |

**Supplementary Table 1**. Data used to train the formaldehyde quantification model.

| **Compound** | **IUPAC name** | **PubChem -ID** | **Sum formula** | **measured m/z** | **polarity** | **retent ion time** | **validated with authentic standard?** | **M+1 when 13C was supplied?** |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Timonacic | thiazolidine-4-carboxylic acid | 9934 | C4H7NO2S | 132.0125 (M-H), 134.0271 (M+H) | neg / pos | 2.6 | yes | yes |
| N-formyl-Cysteine | N-formyl-L-cysteine | 29649 | C4H7NO3S | 148.0074 (M-H) , 149.0109 (M+H) | neg / pos | 2.6 | | yes |
| Spinacine | (6*S*)-4,5,6,7-tetrahydro-3*H*-imidazo[4,5-c]pyridine-6-carboxylic acid | 162899 | C7H9N3O2 | 168.0767 (M+H) | neg / pos | 7.3 | | yes |
| N-methyl-Glutamate | N-methyl-L-glutamic acid | 439377 | C6H11NO4 | … | … | … | | … |

**Supplementary Table 2.** Parameters for the identification of previous unknown compounds by LC-MS.