(S1a Fig) Guanidine derivatives

| No. | Score | Compound score | Molecule | Formula | Mass | SDPPlan (ppm) | Name | Reactions |
|-----|-------|----------------|----------|---------|------|---------------|------|-----------|
| 2   | 3.69E16 | 2.69E16 | Guanidine derivatives | CNH4N2O2 | 127.11390 | 0.17482 | Guanidine (1985) |
| 3   | 0.73E17 | 1.30E13 | guanidine (189) | CNH4N2O | 120.11200 | -4.68E10 | | |
| 1   | 4.02E46 | 4.02E46 | Guanidine derivatives | CNH4N2O | 145.06000 | -4.57E17 | 4-Guanidino-butyric acid (510) |
| 1   | 5.74E25 | 5.74E25 | Guanidine derivatives | CNH4N2O | 153.16100 | -5.55E11 | 4-Nitroguanidino-acetic acid (16446) |
| 2   | 3.67E27 | 3.67E27 | Acetylguanidin | CNH4N2O | 172.13200 | 0.23E17 | Acetylguanidin (435641) |
| 1   | 4.95E24 | 4.95E24 | Guanidine derivatives | CNH4N2O | 174.12900 | -2.46E16 | arginine (232) |
| 3   | 3.63E24 | 3.63E24 | Guanidinobutyric acid | CNH4N2O | 234.18000 | 0.03526 | Brotizolam (405869) |
| 10  | 2.29E23 | 2.29E23 | p-Cyanoguanidine | CNH4N2O | 258.21900 | -0.51E03 | p-Cyanoguanidine (528949) |
| 19  | 2.33E20 | 2.33E20 | Pentylguanidin | CNH4N2O | 366.10900 | 1.04E20 | Pentylguanidin (46173376) |
**(S1b Fig)** Quaternary ammonium compounds (betaines)

| Scan | Assigned | Candidate score | Molecule | Formula | Mass (THM) | pK_a (ppm) | Name | Reactions |
|------|----------|-----------------|----------|---------|------------|------------|------|-----------|
| 2    | no       | 4.99491        | ![Molecule Image](image1) | C5H12NO3 | 127.07000  | 1.52579    | betaine | (S47)     |
| 3    | no       | 6.55339        | ![Molecule Image](image2) | C6H13NO2 | 131.09500  | -2.74773   | Protopetain | (S84646) |
| 1    | no       | 1.04084        | ![Molecule Image](image3) | C7H7NO3 | 137.04600  | -2.02904   | Tropacrine | (S5273)   |
| 27   | no       | 4.88849        | ![Molecule Image](image4) | C7H6NO2 | 140.09500  | -5.04836   | thymidine | (S15246) |
| 1    | no       | 3.13629        | ![Molecule Image](image5) | C7H6NO2 | 146.11000  | -0.02040   | parma-butyrobutane | (L134) |
| 1    | no       | 3.26220        | ![Molecule Image](image6) | C7H7NO2 | 146.11000  | -0.02040   | acetylthalline | (L287) |
| 3    | yes      | 8.25562        | ![Molecule Image](image7) | C9H13NO2 | 157.11940  | 1.85413    | Homosidacrine | (S447045) |
| 22   | no       | 1.57386        | ![Molecule Image](image8) | C7H6NO3 | 169.07594  | -0.77757   | 3-Methylthallididine | (S177375) |
(S1c Fig) Fatty acids and miscellaneous compounds