



Supplement Figure 1: Box plots and kernel density plots before and after normalization. The boxplots show at most 50 features due to space limit. The density plots are based on all samples. Selected methods : Row-wise normalization: Normalization to constant sum; Data transformation: N/A; Data scaling: Autoscaling.

Supplementary Table 1. List of annotated metabolite features.

| Label  | Name   | Formula        | mz       | RT [min] | WT1         | WT2         | WT3         | WT4         | WT5         | KO1         | KO2       | KO3         | KO4         | KO5      |
|--------|--|----------------|----------|----------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0001 | (1,5-Cyclohexadien-1-ylsulfonyl)benzene  | C12 H12 O2 S   | 220.0558 | 1.13     | 40444340.2  | 113405983.5 | 151797039.7 | 89526033.07 | 108775746.6 | 188856875.4 | 175767672 | 170306783.4 | 172378635.6 | 50007.86 |
| M_0002 | DA9185000  | C12 H10 O S    | 202.0453 | 1.128    | 40412454.98 | 113308656.3 | 151702034.8 | 89441532.2  | 108673773.6 | 188628583.6 | 175552997 | 170103734.6 | 172108754.9 | 38600.26 |
| M_0003 | 2,4,6-tricyclohexyloxy-1,3,5-triazine  | C21 H33 N3 O3  | 375.2521 | 8.425    | 85108881    | 90951242.43 | 88673366.36 | 115536365.1 | 108656080.5 | 181386461.5 | 179517505 | 159962707   | 99268483.06 | 403904.3 |
| M_0004 | L-Norleucine   | C6 H13 N O2    | 131.0948 | 1.59     | 155470053.4 | 78201487.44 | 100123704.6 | 64201193.34 | 63383558.54 | 71409209.64 | 66849275  | 58698419.06 | 43358853.53 | 105280.1 |
| M_0005 | L-(+)-Valine   | C5 H11 N O2    | 117.0792 | 1.172    | 116489303.1 | 92480191.44 | 128421457.8 | 95474573.22 | 101125335.9 | 141193790.5 | 143380225 | 125830074.4 | 119695185   | 131702.6 |
| M_0006 | DL-Tryptophan  | C11 H12 N2 O2  | 204.0899 | 3.495    | 59243353.82 | 82133981.33 | 85874347.67 | 103435969.8 | 99920639.61 | 113511668.1 | 138858399 | 142076854.2 | 104828365.5 | 15592.77 |
| M_0007 | L-Phenylalanine  | C9 H11 N O2    | 165.0791 | 2.445    | 139531702.5 | 80806957.36 | 139426272   | 84762449.26 | 70366602.52 | 106334813.1 | 88070774  | 80253948.96 | 62591907.01 | 17136.75 |
| M_0008 | trans-3-Indoleacrylic acid   | C11 H9 N O2    | 187.0634 | 3.495    | 58260303.7  | 80521320.23 | 84009008.87 | 101549667.6 | 98012699    | 111492721.8 | 136572646 | 139164254.9 | 102670825.1 | 39339.74 |
| M_0009 | Cinnamic acid  | C9 H8 O2       | 148.0525 | 2.45     | 137466243.2 | 78886961.65 | 135479988.8 | 83084841.82 | 68645615.13 | 103649441.8 | 86658067  | 78530847.74 | 61289294.36 | 12634.73 |
| M_0010 | 1-Linoleoyl-sn-glycero-3-phosphocholine  | C26 H50 N O7 P | 519.3329 | 9.882    | 17667140.76 | 53354407.03 | 37391500.85 | 67080766.84 | 44446251.12 | 60644815.82 | 69411606  | 69368909.95 | 44191997.29 | 169170   |
| M_0011 | 1H-1,2,4-triazolo[4,3-b][1,2,4]triazole-3,6-diamine  | C3 H5 N7       | 139.061  | 1.144    | 32636494.88 | 50093343.44 | 54879857.83 | 49687550.37 | 53605871.53 | 77287235.66 | 84303430  | 71452127.2  | 68638140.64 | 120478.9 |
| M_0012 | (2-Amino-3-hydroxybutanoyl)oxonium   | C4 H10 N O3    | 120.065  | 1.195    | 96073332.59 | 40353173.06 | 29583017.99 | 36897390.2  | 24651536.44 | 12547736.5  | 11378282  | 12057943.58 | 9811476.779 | 53307.76 |
| M_0013 | 1-Stearoylglycerol   | C21 H42 O4     | 358.3083 | 10.464   | 49317997.5  | 60436075.83 | 57805764.82 | 47622311.94 | 66626222.61 | 50805456.85 | 48330770  | 68680436.35 | 47842016.53 | 124995.8 |
| M_0014 | Choline  | C5 H13 N O     | 103.1002 | 1.063    | 45138153.92 | 56823556.34 | 39394279.8  | 59110247.64 | 79561806.41 | 57487982.39 | 54764620  | 85421078.23 | 57695624.13 | 2903.809 |
| M_0015 | Choline  | C5 H13 N O     | 103.1002 | 0.96     | 2926982.18  | 6219810.921 | 1610616.861 | 4612613.289 | 79561806.41 | 4140327.022 | 54764620  | 156276.7737 | 3461618.66  | 90405.45 |
| M_0016 | 2-Hydroxy-3-(palmitoyloxy)propyl 2-(trimethylammonio)ethyl phosphate   | C24 H50 N O7 P | 495.3328 | 10.195   | 34152032.28 | 33205646.04 | 42216764.6  | 53876494.54 | 39110010.85 | 61332023.57 | 42597754  | 57573376.3  | 47053047.79 | 132453.2 |
| M_0017 | g-Butyrobetaine  | C7 H15 N O2    | 145.1104 | 1.121    | 124542.1948 | 146521.1301 | 198332.1293 | 179190.2779 | 141998.2339 | 215937.2169 | 202293.56 | 175040.2832 | 172034.7023 | 3127.13  |
| M_0018 | TRIS(HYDROXYETHYL)AMINOMETHANE   | C7 H17 N O3    | 163.121  | 1.078    | 154567.0033 | 157277.3976 | 258201.7158 | 194028.1464 | 141485.1734 | 258317.6231 | 190779.08 | 244748.1891 | 184337.2185 | 2727.651 |
| M_0019 | N-[[[(8R,9R)-6-[(2S)-1-hydroxypropan-2-yl]-8-methyl-5-oxo-10-oxa-1,6,14,15-tetraabicyclo[10.3.0]pentadeca-12,14-dien-9-yl]methyl]-N-methylcarbamic acid methyl ester | C18 H31 N5 O5  | 397.234  | 8.445    | 16685822.86 | 25368638.72 | 29888356.38 | 35655662.47 | 36761971.86 | 49845552.18 | 70992281  | 34452593.81 | 41628087.17 | 258105.4 |
| M_0020 | D-(+)-Proline  | C5 H9 N O2     | 115.0636 | 1.141    | 22222945.77 | 23800981.46 | 67528411.64 | 29161938.63 | 24128127.88 | 26661402.85 | 30680649  | 28690218.7  | 23270975.06 | 59815.26 |
| M_0021 | N-[[[(8R,9R)-6-[(2S)-1-hydroxypropan-2-yl]-8-methyl-5-oxo-10-oxa-1,6,14,15-tetraabicyclo[10.3.0]pentadeca-12,14-dien-9-yl]methyl]-N-methylcarbamic acid methyl ester | C18 H31 N5 O5  | 397.234  | 8.485    | 16685822.86 | 25368638.72 | 9475952.834 | 35655662.47 | 6456146.146 | 49845552.18 | 9843879.5 | 34452593.81 | 41628087.17 | 9176.502 |
| M_0022 | D-(+)-Proline  | C5 H9 N O2     | 98.03711 | 1.141    | 18348460.21 | 21702091.65 | 60146708.58 | 26059436.64 | 21724208.41 | 24284081    | 27886734  | 25872980.34 | 21070099.91 | 52500.29 |
| M_0023 | Caprylic anhydride   | C16 H30 O3     | 270.2194 | 8.7      | 19257171.4  | 25699699.06 | 15760579.86 | 2408495.265 | 12589761.97 | 11370563.08 | 16728967  | 22341028.67 | 16327214.52 | 479895.9 |
| M_0024 | DA9185000  | C12 H10 O S    | 202.0453 | 1.341    | 4760573.599 | 16058771.64 | 15578801.3  | 4685456.101 | 20640583.72 | 19096043.37 | 44405350  | 38079725.11 | 21704919.92 | 50067.41 |
| M_0025 | Creatine   | C4 H9 N3 O2    | 131.0696 | 1.095    | 27887141.05 | 11393290.95 | 10850521.5  | 12084676.06 | 11022202.99 | 14152021.66 | 18439454  | 16416695.45 | 21475316.96 | 20217.1  |
| M_0026 | Acetophenone   | C8 H8 O        | 120.0578 | 1.333    | 55211.97656 | 35232.20025 | 34852.87462 | 34159.65871 | 28124.17688 | 28707.38116 | 29147.085 | 28174.13615 | 23378.19527 | 9308.971 |
| M_0027 | aloxistatin  | C17 H30 N2 O5  | 342.217  | 9.094    | 32460011.25 | 36018845.87 | 22087351.54 | 42151002.09 | 27591286.5  | 39956685.73 | 29653770  | 39015132.85 | 23608787.58 | 23748.55 |
| M_0028 | quinapyramine  | C17 H22 N6     | 310.1908 | 9.1      | 32026970.83 | 35599435.89 | 21784328.98 | 41584918.48 | 27133584.44 | 39445271.53 | 29005523  | 38434823.16 | 23224544.2  | 15209.73 |
| M_0029 | Anthranilic acid   | C7 H7 N O2     | 137.0478 | 6.119    | 163174.4625 | 74959.10641 | 155686.0952 | 163489.997  | 96814.99265 | 131273.2271 | 107892.22 | 73794.67047 | 89711.83387 | 14174.13 |
| M_0030 | 8-(3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl)octanoic acid   | C18 H28 O3     | 292.2013 | 8.698    | 13886996.01 | 18552892.65 | 11309505.65 | 3241186.072 | 8877551.811 | 8288558.277 | 12063097  | 11891679.09 | 3488859.69  | 122847.8 |
| M_0031 | Phenylacetylene  | C8 H6          | 102.0473 | 2.448    | 32869370.55 | 18607186.58 | 34807822    | 19632948.03 | 16143405.16 | 20671390.83 | 19860147  | 17891887.67 | 14191217.97 | 9748.483 |
| M_0032 | L-(+)-Leucine  | C6 H13 N O2    | 131.0948 | 1.328    | 34688769.99 | 16432724.76 | 8130775.269 | 7548969.225 | 16777047.65 | 16889132.92 | 28921997  | 16590899.04 | 10201026.42 | 63009.73 |
| M_0033 | indoline   | C8 H9 N        | 119.0738 | 2.444    | 30590133.28 | 17291597.41 | 32593245.75 | 18251958.31 | 14974249.63 | 19168481.88 | 18480844  | 16634830.03 | 13207214.57 | 5488.239 |
| M_0034 | γ-Aminobutyric acid (GABA)   | C4 H9 N O2     | 103.0638 | 1.061    | 7912056.488 | 2119579.661 | 1746259.822 | 2086282.726 | 1285093.034 | 873139.9417 | 1018696.8 | 960394.6211 | 985247.1329 | 45239.2  |
| M_0035 | L-(-)-Methionine   | C5 H11 N O2 S  | 149.0511 | 1.223    | 17954358.36 | 14907864.23 | 23703834.52 | 14431549.28 | 10507457.36 | 14561615.15 | 15351990  | 13503484.32 | 15530101.59 | 22906.76 |
| M_0036 | 1-O-Tetradecanoyl-D-glucitol   | C20 H40 O7     | 392.2786 | 8.486    | 5221601.059 | 9820146.469 | 4912743.684 | 1013016.977 | 12147172.48 | 1070988.783 | 30020093  | 10031691.49 | 11282705.23 | 989.6173 |
| M_0037 | Tryptamine   | C10 H12 N2     | 160.1002 | 1.697    | 34710.21292 | 21164.23189 | 23858.92331 | 18746.59024 | 16948.99262 | 19945.71348 | 18054.606 | 18806.41257 | 14216.77383 | 10256.34 |
| M_0038 | 3-Methylsulfolene  | C5 H8 O2 S     | 132.0246 | 1.221    | 17585161.96 | 14586666.79 | 22220634.43 | 13800660.93 | 10400523.9  | 13824002.62 | 14828062  | 12897025.82 | 15079054.38 | 24852.39 |
| M_0039 | 16(R)-HETE   | C20 H32 O3     | 302.2245 | 9.094    | 27497189.35 | 26996754.55 | 16723043.42 | 27983632.55 | 19995893.59 | 28610668.25 | 20854639  | 26580807.31 | 17452103.43 | 36356.63 |
| M_0040 | (2Z,4Z)-6-Amino-2,4-diimino-5-nitro-1,3(2H,4H)-pyrimidinediol  | C4 H6 N6 O4    | 202.0453 | 1.223    | 1346127.16  | 5252215.082 | 9186144.781 | 1003353.233 | 5704681.295 | 2951753.305 | 1409039.4 | 19126543.72 | 1400301.791 | 30104.62 |

|        |  |                  |          |        |             |             |             |             |             |             |           |              |             |          |
|--------|--|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|--------------|-------------|----------|
| M_0041 | 1-arachidonoyl-sn-glycero-3-phosphocholine                       | C28 H50 N O7 P   | 543.3329 | 9.785  | 4847343.13  | 9402470.051 | 12548053.78 | 13678102.45 | 17906824.5  | 21051334.24 | 21602351  | 19424510.44  | 15735290.78 | 36482.99 |
| M_0042 | 8-[3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl]octanoic acid | C18 H28 O3       | 292.2013 | 8.659  | 13886996.01 | 4724883.585 | 2486172.444 | 802585.3959 | 1435429.154 | 8288558.277 | 12063097  | 4196926.415  | 3488859.69  | 25971.09 |
| M_0043 | Choline Alfoscerate  | C8 H20 N O6 P    | 257.1027 | 1.118  | 3738684.3   | 17989576.59 | 8697896.07  | 9559097.444 | 13317436.8  | 21418045.73 | 20872965  | 27151219.92  | 22382886.41 | 5073.605 |
| M_0044 | DL-Glutamine   | C5 H10 N2 O3     | 146.0692 | 1.105  | 22433793.13 | 15099169.95 | 12266192.16 | 16486985.47 | 15769634.43 | 14349474.54 | 23402673  | 16077197.36  | 26278776.97 | 11351.27 |
| M_0045 | D-PANTOTHENIC ACID   | C9 H17 N O5      | 219.1106 | 3.322  | 25521304.51 | 10851434.88 | 25374154.21 | 12758439.3  | 7741726.805 | 5474374.596 | 4723691.7 | 3534373.258  | 2410622.87  | 10718.72 |
| M_0046 | Edaravone  | C10 H10 N2 O     | 174.0793 | 6.032  | 22398.60514 | 21345.55252 | 21218.79722 | 22336.02448 | 21281.02705 | 21391.1113  | 22975.137 | 22144.06008  | 21939.03097 | 21708.37 |
| M_0047 | L-(+)-Valine   | C5 H11 N O2      | 117.0794 | 1.024  | 84128.89989 | 119151.2708 | 93056.8669  | 93127.60304 | 86798.68315 | 77950.65484 | 1021167.3 | 114537.0979  | 104442.3026 | 120799.4 |
| M_0048 | N-methylethanolamine phosphate                                   | C3 H10 N O4 P    | 155.0349 | 1.149  | 4438529.166 | 9257808.463 | 4490825.489 | 5533653.411 | 7064695.505 | 5761202.052 | 6104758.2 | 5914712.515  | 4518009.697 | 4022.809 |
| M_0049 | iodonitrotetrazolium   | C H I N5 O2      | 241.918  | 0.984  | 1329829.8   | 13272401.9  | 10666325.9  | 14044485.02 | 5508558.413 | 7014843.529 | 12323837  | 6477044.514  | 9823305.709 | 4196.741 |
| M_0050 | Benzoxazole  | C7 H5 N O        | 119.0375 | 6.121  | 117917.3551 | 40493.53798 | 110427.6781 | 116070.527  | 78638.67657 | 71380.04693 | 62927.199 | 56509.81425  | 72011.76504 | 4737.781 |
| M_0051 | L-Isoleucine   | C6 H13 N O2      | 131.0947 | 1.41   | 803772.4786 | 11993560.2  | 414686.2049 | 302174.6637 | 2787440.203 | 16889132.92 | 17557146  | 1982012.112  | 16561244.61 | 68504    |
| M_0052 | Paracetamol  | C8 H9 N O2       | 151.0634 | 0.882  | 31211.62145 | 30911.94838 | 30370.92536 | 30587.43713 | 30958.44774 | 30843.32346 | 31434.5   | 29414.93433  | 30441.63312 | 35751.68 |
| M_0053 | DL-Glutamine   | C5 H10 N2 O3     | 105.0427 | 1.108  | 19037446.62 | 12792447.34 | 10891253.48 | 13940897.94 | 13693905.73 | 12759387.1  | 20183423  | 14035861.1   | 22563483    | 23758.23 |
| M_0054 | MNA  | C7 H8 N2 O2      | 152.0586 | 2.337  | 22432855.1  | 6098776.487 | 6673702.064 | 6566370.245 | 5125886.198 | 3503701.749 | 4795318.8 | 3506325.484  | 2217818.779 | 9596.448 |
| M_0055 | Benzene  | C6 H6            | 78.04722 | 2.46   | 1205813.916 | 17292950.26 | 1918644.98  | 18255143.14 | 14976023.54 | 19169966.6  | 999631.64 | 4732728.2675 | 439401.5454 | 5077.342 |
| M_0056 | (R)-3-Hydroxy myristic acid                                      | C14 H28 O3       | 226.1933 | 8.66   | 13331179.15 | 8593596.223 | 1697274.852 | 9515163.066 | 14822409.3  | 18232321.48 | 14196793  | 19368219.41  | 16824165.31 | 1139987  |
| M_0057 | Naphthalen-2-amine   | C10 H9 N         | 143.0737 | 1.737  | 25500.16898 | 16095.4603  | 17143.7266  | 14532.25938 | 12779.14678 | 14376.13124 | 13845.42  | 13776.8016   | 10676.35954 | 6928.458 |
| M_0058 | 5-Chloro-2-pentanone   | C5 H9 Cl O       | 120.0344 | 6.108  | 5029.28735  | 4772.651836 | 4838.055887 | 4863.051138 | 4827.242281 | 4793.828009 | 4861.014  | 4784.807474  | 4877.124075 | 4716.443 |
| M_0059 | Betaine  | C5 H11 N O2      | 117.0793 | 1.401  | 16216729.94 | 8261870.551 | 19673870.99 | 8896916.778 | 7037331.918 | 16531676.42 | 19512611  | 10816636.37  | 2354022.697 | 203244.6 |
| M_0060 | g-Butyrobetaine  | C7 H15 N O2      | 145.1104 | 1.061  | 113555.4171 | 132346.8492 | 270983.3969 | 166523.7331 | 128554.9527 | 197867.3195 | 186194    | 158413.9669  | 155578.9489 | 4982.999 |
| M_0061 | Betaine  | C5 H11 N O2      | 117.0793 | 1.48   | 16208123.31 | 3143507.677 | 5401151.972 | 8989010.624 | 3298157.015 | 5252301.351 | 19500247  | 6615209.972  | 9650106.594 | 2770.624 |
| M_0062 | Betaine  | C5 H11 N O2      | 117.0793 | 1.528  | 16208123.31 | 3143507.677 | 5401151.972 | 8989010.624 | 3298157.015 | 11098339.38 | 19500247  | 6615209.972  | 9650106.594 | 27288.8  |
| M_0063 | Hyoxanthine  | C5 H4 N4 O       | 136.0386 | 1.755  | 3410626.595 | 2864486.644 | 109597.2061 | 2508721.547 | 777145.3831 | 2499374.779 | 1420429.3 | 5656336.674  | 2678125.943 | 16476.32 |
| M_0064 | Serotonin  | C10 H12 N2 O     | 176.095  | 1.497  | 2337374.921 | 2965891.147 | 3212562.134 | 7088210.339 | 3424492.858 | 6889976.747 | 504229.3  | 4482669.698  | 4881409.774 | 14913.07 |
| M_0065 | 6-Methoxyquinoline   | C10 H9 N O       | 159.0684 | 1.528  | 2316705.999 | 2929915.17  | 3150758.048 | 6930221.498 | 3359160.214 | 6782662.797 | 4961302.7 | 4439093.454  | 4776948.455 | 12097.66 |
| M_0066 | Taurine  | C2 H7 N O3 S     | 125.0148 | 1.119  | 17981667.83 | 9212957.85  | 7565692.416 | 14596593.38 | 13634602.42 | 13473059.73 | 17461336  | 14729147.03  | 17062542.12 | 22680.02 |
| M_0067 | Choline  | C5 H13 N O       | 103.1002 | 1.167  | 1723452.055 | 14424353.92 | 1882776.238 | 2780504.582 | 1576923.377 | 2324500.367 | 14422098  | 1339445.351  | 1873895.247 | 71831.36 |
| M_0068 | L-Norleucine   | C6 H13 N O2      | 131.0947 | 1.783  | 12696165.9  | 8455619.388 | 7008507.172 | 6386416.89  | 3014942.029 | 4206216.199 | 5203278.6 | 3275464.803  | 2019954.089 | 10430.17 |
| M_0069 | Choline  | C5 H13 N O       | 71.07415 | 1.337  | 5701679.83  | 17503050.43 | 8055786.987 | 11256952.79 | 1877846.424 | 10194070.4  | 3473735.4 | 2929935.52   | 4637991.22  | 140691.8 |
| M_0070 | 2-Bromo-N-methyl-4-nitrobenzenesulfonamide                       | C7 H7 Br N2 O4 S | 293.9314 | 0.989  | 14558660.39 | 12012022.56 | 15644436.17 | 10173383.41 | 10134862.01 | 15638729.09 | 16034092  | 10933109.89  | 10468928.66 | 4351.84  |
| M_0071 | Tetranor-12(S)-HETE  | C16 H26 O3       | 248.1752 | 8.656  | 10363566.17 | 2065160.093 | 13396086.59 | 7680572     | 11986977.76 | 14930929.68 | 11495569  | 15531097.04  | 13346373.76 | 921519.2 |
| M_0072 | Choline  | C5 H13 N O       | 103.1002 | 10.459 | 253065.4662 | 816460.1313 | 1684798.786 | 2255566.946 | 1139122.956 | 4076294.773 | 5509485.2 | 1510936.032  | 980163.7594 | 211891   |
| M_0073 | 2-Aminonicotinic acid  | C6 H6 N2 O2      | 138.0448 | 6.099  | 2358.662304 | 2238.303997 | 2268.977541 | 2280.699949 | 2263.906118 | 2248.235313 | 2279.7446 | 2244.004814  | 2287.299951 | 2211.943 |
| M_0074 | 1H-1,2,4-triazolo[4,3-b][1,2,4]triazole-3,6-diamine              | C3 H5 N7         | 139.061  | 1.357  | 3021081.442 | 3999337.162 | 1016062.232 | 1255295.961 | 4867953.432 | 7197089.628 | 14812021  | 6681905.218  | 15778249.47 | 19571.88 |
| M_0075 | TM0860000  | C7 H16 N2        | 128.1314 | 0.817  | 2335298.376 | 1819473.65  | 1357478.174 | 1897095.93  | 870359.1587 | 1246786.05  | 598224.51 | 1055700.882  | 597253.1228 | 9474.202 |
| M_0076 | Spermidine   | C7 H19 N3        | 145.158  | 0.817  | 2212192.545 | 1722093.461 | 1288204.826 | 1830651.698 | 828481.0371 | 1184284.098 | 566913.67 | 1006254.152  | 565821.882  | 5247.18  |
| M_0077 | Tryptamine   | C10 H12 N2       | 160.1002 | 2.629  | 13385.8812  | 10529.04531 | 11311.77602 | 10720.76688 | 10075.305   | 10523.65695 | 10117.54  | 9978.424269  | 9927.979694 | 10673.8  |
| M_0078 | Choline  | C5 H13 N O       | 103.1002 | 1.29   | 14153923.84 | 11570948.53 | 9640686.273 | 12256686.71 | 4631229.939 | 10497145.71 | 5447817.8 | 11319522.86  | 6789026.441 | 146071.8 |
| M_0079 | 1H-1,2,4-triazolo[4,3-b][1,2,4]triazole-3,6-diamine              | C3 H5 N7         | 139.0609 | 1.485  | 29712.98905 | 32263.97232 | 175830.0952 | 79914.58062 | 48452.12154 | 153318.3855 | 13855557  | 106539.7301  | 11036454.42 | 1938.042 |
| M_0080 | Acetyl-L-carnitine   | C9 H17 N O4      | 203.1157 | 1.096  | 7742521.909 | 4262844.005 | 4038610.874 | 5579976.984 | 4916802.599 | 6538264.963 | 7768539.4 | 5630082.495  | 6404224.512 | 3756.762 |
| M_0081 | 1962763  | C11 H21 N O4     | 231.147  | 1.766  | 7589212.75  | 9726864.537 | 4830681.442 | 13338580.82 | 7937956.085 | 8621841.628 | 6504514.7 | 5480463.652  | 4136068.487 | 4867.894 |
| M_0082 | N-methylethanolamine phosphate                                   | C3 H10 N O4 P    | 155.0348 | 1.254  | 967372.3818 | 599838.3467 | 407624.7306 | 1927687.885 | 326862.1161 | 5458273.82  | 4184674.2 | 3317988.259  | 7686673.287 | 3954.195 |
| M_0083 | 1-Linoleoyl-sn-glycero-3-phosphocholine                          | C26 H50 N O7 P   | 519.3328 | 9.683  | 696452.7861 | 51575.51815 | 4201349.405 | 1177042.562 | 250990.8694 | 4587530.237 | 7323563.8 | 31671.65162  | 3207089.824 | 34691.65 |
| M_0084 | Hypoxanthine   | C5 H4 N4 O       | 136.0386 | 2.256  | 6747495.061 | 5986107.114 | 2515515.804 | 11112154.29 | 7133915.065 | 4169427.545 | 2182070.2 | 4923464.869  | 2741470.518 | 4859.054 |
| M_0085 | 3-Methylsulfolene  | C5 H8 O2 S       | 132.0246 | 1.368  | 905568.855  | 2781132.713 | 379507.906  | 1544138.468 | 3134304.102 | 4153771.111 | 3480516.4 | 6646504.584  | 4376990.631 | 3530.416 |
| M_0086 | 2-(Phenylthio)-1-[4-(1H-pyrrol-1-yl)piperidino]ethan-1-one       | C17 H20 N2 O S   | 300.1336 | 8.957  | 5879639.626 | 6026815.178 | 8444137.363 | 11752028.24 | 11176770.49 | 11048517.82 | 8370234.8 | 7731034.309  | 9764427.385 | 1780651  |
| M_0087 | Bis(4-ethylbenzylidene)sorbitol                                  | C24 H30 O6       | 414.2043 | 8.535  | 2830054.824 | 3837723.97  | 2858867.965 | 5070866.49  | 7418315.052 | 3893064.595 | 4653524.2 | 12349399.97  | 2906696.497 | 18526.28 |
| M_0088 | DL-Lysine  | C6 H14 N2 O2     | 146.1056 | 0.813  | 12296161.51 | 3976181.33  | 4938355.774 | 3246605.272 | 3267191.675 | 3875799.832 | 4450905.8 | 4249797.66   | 3579158.484 | 70034.56 |
| M_0089 | Pipecolic acid   | C6 H11 N O2      | 129.0791 | 0.809  | 12198282.53 | 3944137.673 | 4893807.001 | 3228509.314 | 3252217.121 | 3480978.333 | 4430606.1 | 4225905.258  | 3551620.707 | 64271.69 |
| M_0090 | L-(-)-Methionine   | C5 H11 N O2 S    | 149.0511 | 1.362  | 1482801.682 | 3420910.591 | 111001.604  | 603551.1275 | 4412171.165 | 4241678.719 | 3573457.8 | 6807003.523  | 4852350.759 | 7563.352 |
| M_0091 | L-(-)-methionine   | C5 H11 N O2 S    | 149.0511 | 1.288  | 917454.1373 | 294853.1455 | 114036.4284 | 178156.5788 | 120025.605  | 412323.4326 | 158618.36 | 194918.9719  | 381193.6391 | 1961.531 |
| M_0092 | Hippuric acid  | C9 H9 N O3       | 179.0582 | 5.331  | 3474232.374 | 5877372.327 | 12002824.3  | 630435.742  | 10382847.72 | 7606960.694 | 4753100.5 | 4004197.519  | 2586974.342 | 26736.32 |
| M_0093 | Octylbenzene   | C14 H22          | 190.1721 | 8.666  | 3645335.477 | 6704863.138 | 8324965.04  | 4277463.713 | 7005251.36  | 7866120.249 | 7041522.3 | 9962387.103  | 8335568.923 | 215755.4 |
| M_0094 | 2-Decylfuran   |                  |          |        |             |             |             |             |             |             |           |              |             |          |

|        |  |                   |          |        |             |             |             |             |             |             |           |              |             |           |
|--------|--|-------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|--------------|-------------|-----------|
| M_0100 | Prolinamide  | C5 H10 N2 O       | 114.0793 | 0.815  | 10443776.72 | 3396225.371 | 4089459.655 | 2747035.187 | 2811564.669 | 3533393.552 | 3868351.3 | 3553895.837  | 3255546.676 | 52699.24  |
| M_0101 | bis(tetrazolyl)amine   | C2 H3 N9          | 153.0514 | 1.099  | 8082300.752 | 3537525.878 | 4377436.194 | 4009353.68  | 3470370.586 | 5077467.685 | 5628002.8 | 5614266.2    | 5526971.281 | 2731.759  |
| M_0102 | DL-Carnitine   | C7 H15 N O3       | 161.1052 | 1.076  | 4160996.709 | 4914893.016 | 6455019.821 | 6054019.3   | 8720267.324 | 7938982.358 | 10034065  | 8104843.976  | 8357307.649 | 3783.911  |
| M_0103 | Hypoxanthine   | C5 H4 N4 O        | 136.0386 | 1.601  | 4420574.698 | 3229385.592 | 114999.7749 | 2467483.87  | 539165.602  | 2049040.347 | 955222.8  | 2668448.905  | 406297.0499 | 16643.5   |
| M_0104 | 2-Ethoxy-4-hydrazino-6-(1-piperidinyl)-1,3,5-triazine  | C10 H18 N6 O      | 238.1545 | 8.621  | 2469145.591 | 2529375.313 | 3580897.879 | 8401753.406 | 1983253.78  | 7563233.827 | 3835496.7 | 6109813.061  | 9889417.058 | 1387796   |
| M_0105 | 1728235  | C19 H38 O4        | 330.2768 | 9.848  | 9046710.057 | 5608977.905 | 7042753.394 | 3669395.909 | 6146426.758 | 4173880.877 | 4661996.7 | 3749198.533  | 3674876.12  | 347362    |
| M_0106 | Betaine  | C5 H11 N O2       | 76.05273 | 1.603  | 2907136.989 | 3143507.677 | 5401151.972 | 1557105.849 | 3298157.015 | 5846038.031 | 4072213.7 | 5449916.057  | 1622469.444 | 218459.2  |
| M_0107 | Hypoxanthine   | C5 H4 N4 O        | 136.0386 | 2.024  | 804026.553  | 3819284.291 | 1583778.732 | 9583699.85  | 62065.80665 | 1987407.562 | 2188202.9 | 3539238.634  | 692845.0241 | 12104.4   |
| M_0108 | Hypoxanthine   | C5 H4 N4 O        | 136.0387 | 2.119  | 6747495.061 | 3819284.291 | 1561962.963 | 426167.2592 | 288628.4641 | 1961278.04  | 2131976   | 3230419.092  | 1165563.535 | 5148.571  |
| M_0109 | D-(+)-Pipicolinic acid   | C6 H11 N O2       | 129.0791 | 1.208  | 9473905.113 | 523118.9306 | 6820314.211 | 5951818.945 | 5226548.253 | 2463604.454 | 2971557.2 | 2850057.306  | 2328895.268 | 18953.79  |
| M_0110 | L-Tyrosine   | C9 H11 N O3       | 181.074  | 1.629  | 9413876.765 | 3358987.82  | 4164708.954 | 5841778.049 | 2437014.506 | 5778818.977 | 4734041.7 | 5822831.794  | 3892019.87  | 10763.13  |
| M_0111 | Naphtho(2,3-b)thiophene-4,9-dione  | C12 H6 O2 S       | 214.0088 | 2.491  | 156908.7892 | 6490261.087 | 5538940.94  | 4198013.29  | 3723092.782 | 8243048.275 | 4247063.8 | 9328854.329  | 4566885.515 | 49425.88  |
| M_0112 | 1792831  | C16 H30 O4        | 286.2143 | 9.224  | 4158352.132 | 2833793.584 | 5057192.822 | 7554128.944 | 9133966.891 | 8887164.334 | 5921207.7 | 6589277.587  | 7395952.198 | 366005.7  |
| M_0113 | nabilone   | C24 H36 O3        | 372.2664 | 8.814  | 407884.2646 | 644010.2082 | 3277737.862 | 9121084.045 | 808531.5361 | 781936.3834 | 1120607.1 | 1728320.254  | 1438803.19  | 8593.71   |
| M_0114 | 4-Morpholinylphosphoric difluoride   | C4 H8 F2 N O2 P   | 171.0254 | 11.317 | 739573.6745 | 766703.9367 | 267896.7498 | 6238466.56  | 9035019.221 | 740196.6752 | 671382.79 | 1141217.602  | 419843.5383 | 694296.8  |
| M_0115 | 4-Indolecarbaldehyde   | C9 H7 N O         | 145.0529 | 7.54   | 6269.550014 | 15609.83716 | 15408.28213 | 15807.98271 | 20179.14223 | 19268.6356  | 2173.9386 | 14752.06138  | 10748.49668 | 3253.461  |
| M_0116 | Betaine  | C5 H11 N O2       | 117.0793 | 1.598  | 8015816.38  | 3143507.677 | 5401151.972 | 3367787.666 | 3298157.015 | 5846038.031 | 3888069.7 | 5449916.057  | 2032459.053 | 335258.5  |
| M_0117 | 4-Hydroxyisoleucine  | C6 H13 N O3       | 147.0897 | 1.206  | 8755159.368 | 5009168.008 | 6555021.172 | 5807863.21  | 5137505.865 | 2593525.46  | 3056148.5 | 2874704.018  | 2447169.343 | 23538.54  |
| M_0118 | Koiganal II  | C18 H32 O         | 264.2451 | 9.947  | 309704.5694 | 360816.7795 | 774844.626  | 294680.409  | 498605.9288 | 988820.9384 | 200312.59 | 296074.3632  | 570884.0111 | 30231.92  |
| M_0119 | 2-Hydroxycinnamic acid   | C9 H8 O3          | 164.0474 | 1.631  | 8645842.836 | 3063526.006 | 3580228.893 | 5373616.22  | 2148398.809 | 5185401.025 | 4222443.2 | 5291404.661  | 3482436.052 | 7967.246  |
| M_0120 | g-Butyrobetaine  | C7 H15 N O2       | 145.1103 | 1.246  | 381583.8025 | 193715.9939 | 759935.9682 | 1063263.255 | 323134.0641 | 309320.7445 | 88814.334 | 245517.9659  | 96200.35677 | 3842.841  |
| M_0121 | DL-Stachydrine   | C7 H13 N O2       | 143.0947 | 1.207  | 6523174.59  | 7939338.528 | 4979990.852 | 7440897.14  | 7140333.357 | 4795108.496 | 4491103.9 | 4299143.392  | 3560225.595 | 12443.96  |
| M_0122 | g-Butyrobetaine  | C7 H15 N O2       | 145.1104 | 1.432  | 391512.3088 | 219779.6828 | 224929.5178 | 267616.7987 | 174343.3799 | 320549.7409 | 159754.61 | 191031.1108  | 92404.8017  | 3580.008  |
| M_0123 | Eicosatetraenoic acid  | C20 H24 O2        | 308.1964 | 9.234  | 3634053.614 | 576274.3822 | 4499361.868 | 6747072.153 | 8181857.643 | 7956790.105 | 5299330.4 | 5934595.758  | 6617067.637 | 310642.1  |
| M_0124 | Nicotinamide   | C6 H6 N2 O        | 122.0483 | 1.386  | 1049143.841 | 1603703.75  | 497121.3398 | 822798.3901 | 1371028.622 | 1309044.768 | 1822536.6 | 1510424.247  | 79811.51708 | 21853.212 |
| M_0125 | Pregabalin   | C8 H17 N O2       | 159.126  | 1.089  | 908529.2258 | 555465.1641 | 763778.8693 | 929095.2173 | 985768.3884 | 1283500.445 | 1152186.6 | 1126377.979  | 1189803.12  | 2140.362  |
| M_0126 | DL-Carnitine   | C7 H15 N O3       | 161.1052 | 1.394  | 2217383.803 | 1990028.908 | 3460083.324 | 4580211.954 | 2737250.804 | 7896159.622 | 1980013   | 3531517.536  | 1361614.136 | 16834.06  |
| M_0127 | Trigonelline   | C7 H7 N O2        | 137.0454 | 1.139  | 3821173.316 | 2065824.813 | 7842462.166 | 3286308.746 | 2416328.517 | 2458714.749 | 2908041.8 | 2905808.344  | 2237864.083 | 9843.127  |
| M_0128 | Phenylacetylglycine  | C10 H11 N O3      | 193.0739 | 5.919  | 6698999.061 | 2203570.141 | 6439348.759 | 7020126.382 | 4048726.184 | 6217798.236 | 4563504   | 4721384.725  | 1699242.448 | 13492.44  |
| M_0129 | 3,3,3-Trifluoropropanol (1R,4aS)-7-(2-Hydroxypropan-2-yl)-1,4a-dimethyl-9-oxo-3,4,10,10a-tetrahydro-2H-phenanthrene-1-carboxylic acid                                  | C3 H5 F3 O        | 114.0297 | 1.201  | 863312.8971 | 1550121.942 | 1034218.628 | 2220947.621 | 1615043.633 | 3429944.263 | 3920163.1 | 4081678.362  | 2721845.056 | 67796.93  |
| M_0130 | 1962763  | C11 H21 N O4      | 231.1471 | 1.66   | 7586135.87  | 2563687.432 | 1246077.736 | 3245210.647 | 1553062.038 | 174745.1655 | 1678132.6 | 925482.0403  | 38090.21264 | 1273.429  |
| M_0131 | CB0700000  | C15 H12           | 192.0947 | 3.412  | 16875.45617 | 20383.44581 | 20838.10975 | 24469.27528 | 23596.07462 | 23166.36595 | 29082.219 | 31505.66419  | 26159.82275 | 1940.93   |
| M_0133 | Octylbenzene   | C14 H22           | 190.1722 | 8.772  | 25254.66327 | 1342790.354 | 263913.8365 | 8111.017428 | 14854.96537 | 193525.9275 | 15179.35  | 25430.47957  | 19958.74046 | 2442.511  |
| M_0134 | 1-((9Z)-hexadecenoyl)-sn-glycero-3-1-Phenyl-1,2,3,4-tetrahydroisoquinoline   | C24 H48 N O7 P    | 493.3171 | 9.701  | 919438.9859 | 2435149.24  | 4141648.935 | 4988170.084 | 2887398.669 | 4019918.298 | 4994359.6 | 4602428.346  | 3972711.165 | 20068.15  |
| M_0135 | DL-TYROSINE  | C9 H11 N O3       | 181.074  | 1.239  | 4054854.509 | 2366438.68  | 2492988.639 | 3641999.982 | 2111483.765 | 5231796.174 | 4177705.2 | 7033824.3754 | 3919100.225 | 6918.713  |
| M_0137 | 2,6-Dioxo(4~14~C)-1,2,3,6-tetrahydro-4-pyrimidinecarboxylic acid   | C4 [14]C H4 N2 O4 | 158.0205 | 1.617  | 1106294.195 | 911264.2931 | 547924.1519 | 1233514.569 | 154269.7268 | 1582875.833 | 461356.56 | 2010980.889  | 1595986.235 | 4518.644  |
| M_0138 | Serotonin  | C10 H12 N2 O      | 176.095  | 1.213  | 5867618.157 | 4384987.309 | 3118396.942 | 7002134.816 | 5649161.925 | 6654705.98  | 5362021.3 | 4093358.249  | 6394125.206 | 6609.741  |
| M_0139 | Caprolactam  | C6 H11 N O        | 113.0844 | 4.426  | 116810.562  | 65761.26188 | 113296.6248 | 97208.00557 | 170406.9737 | 93968.34438 | 78151.845 | 140325.7595  | 79932.97056 | 35821.86  |
| M_0140 | Adenosine 5'-monophosphate (2-Amino-3-hydroxybutanoyl)oxonium  | C10 H14 N5 O7 P   | 347.063  | 1.412  | 16958.56862 | 1144809.335 | 35401.24379 | 2283909.786 | 1895449.865 | 4042791.404 | 6848111.9 | 3582541.306  | 6269368.459 | 3806.664  |
| M_0141 | 6-Methoxyquinoline   | C10 H9 N O        | 159.0685 | 1.212  | 6075521.349 | 5110073.982 | 3175923.082 | 3623189.1   | 5959893.102 | 6801026.774 | 5458827.2 | 4177281.644  | 6338830.893 | 5471.334  |
| M_0143 | quinolizidine  | C9 H17 N          | 139.1362 | 0.79   | 1594047.884 | 1185370.329 | 2763243.787 | 1477423.267 | 2253279.097 | 2045351.863 | 1641369.4 | 4366442.383  | 2555064.307 | 3410.305  |
| M_0144 | L-Methionine sulfoxide   | C5 H11 N O3 S     | 165.046  | 1.577  | 4700141.877 | 1984476.11  | 3561771.018 | 813705.0579 | 1670015.914 | 1870397.8   | 2382903.3 | 1849800.58   | 2034588.939 | 11397.01  |
| M_0145 | Hypoxanthine   | C5 H4 N4 O        | 136.0385 | 1.859  | 2887785.766 | 294864.4662 | 1439207.207 | 2695064.026 | 601304.6084 | 174718.6702 | 824855.63 | 174610.4165  | 1884834.841 | 4483.913  |
| M_0146 | Choline  | C5 H13 N O        | 103.1002 | 10.539 | 81140.28878 | 136310.6065 | 305127.5102 | 464383.6242 | 1139122.956 | 4076294.773 | 5509485.2 | 958734.4425  | 587565.3486 | 60814.96  |
| M_0147 | 2,2,6,6-Tetramethyl-4-piperidinaimine  | C9 H20 N2         | 156.1627 | 0.789  | 1586796.385 | 1178141.414 | 2736957.659 | 1475790.742 | 2233453.174 | 2028627.364 | 1627192   | 4318893.405  | 2531205.169 | 1780.007  |
| M_0148 | Creatine (8S,9S)-6-((2R)-1-hydroxypropan-2-yl)-8-methyl-9-[[methyl(pyridin-4-ylmethyl)amino]methyl]-10-oxa-1,6,14,15-tetraazabicyclo[10.3.0]pentadeca-12,14-dien-5-one | C4 H9 N3 O2       | 131.0696 | 1.594  | 5834962.13  | 1507513.425 | 1452706.135 | 1144839.127 | 1239993.673 | 2623600.105 | 235394.13 | 2847500.724  | 818189.8642 | 3458.785  |
| M_0149 | N,N-Bis(2-hydroxyethyl)dodecanamide  | C22 H34 N6 O3     | 430.2697 | 8.813  | 313432.4258 | 537797.6713 | 1918987.623 | 6606382.368 | 625350.8788 | 709281.209  | 921016.49 | 1505060.277  | 1166367.571 | 12285.57  |
| M_0150 | Choline  | C5 H13 N O        | 103.1002 | 1.401  | 5468834.461 | 6506970.527 | 801540.9565 | 2073637.698 | 1490153.704 | 3468824.352 | 3012398.4 | 2679659.585  | 4296966.039 | 148360.3  |

|        |  |                                    |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|------------------------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0152 | (2S)-2-((N-((2S)-2-Ammonio-4-methylpentanoyl)-L-leucyl)amino)-3-phenylpropanoate       | C21 H33 N3 O4                      | 391.2471 | 8.66   | 4695667.743 | 4683402.694 | 6433753.891 | 5331170.373 | 5415862.787 | 5423439.222 | 6014653.6 | 6291958.678 | 5054978.898 | 62338.03 |
| M_0153 | L-(+)-Citrulline   | C6 H13 N3 O3                       | 175.0957 | 1.108  | 6426022.992 | 3634039.842 | 2038079.034 | 4254765.658 | 4520895.6   | 3084047.552 | 6048320.5 | 3826623.621 | 5423439.701 | 4105.555 |
| M_0154 | (E)-p-coumaric acid  | C9 H8 O3                           | 164.0475 | 1.239  | 3389311.204 | 2093750.68  | 2034491.739 | 3329337.791 | 1728185.978 | 4800992.399 | 3657224.3 | 6298899.838 | 3667545.825 | 4370.551 |
| M_0155 | 1,3-Propanediolate   | C3 H6 O2                           | 74.03756 | 10.614 | 5631666.075 | 5654218.562 | 145750.3149 | 5305789.939 | 6022231.391 | 56250.71971 | 6178418.6 | 5194521.497 | 5055810.672 | 219363.9 |
| M_0156 | 4-Hydrazino-1H-pyrazolo[3,4-d]pyrimidin-6-amine  | C5 H7 N7                           | 165.0766 | 1.202  | 2794307.139 | 5237823.354 | 2969679.884 | 4444721.176 | 4307116.257 | 3108036.513 | 3100640.3 | 3041205.408 | 2416576.137 | 1645.203 |
| M_0157 | Thiomorpholinecarboxylic acid  | C5 H9 N O2 S                       | 147.0354 | 1.566  | 4408469.694 | 1685026.855 | 3366494.446 | 649933.9151 | 1575623.92  | 1689694.445 | 2207553.6 | 1640571.262 | 1923388.094 | 7744.065 |
| M_0158 | Diethoxyethylamine   | C6 H15 N O2                        | 133.1103 | 1.07   | 895757.6914 | 6197563.828 | 163258.0455 | 541177.2995 | 1161446.588 | 69012.72513 | 74383.646 | 37049.16269 | 36540.0177  | 5235.983 |
| M_0159 | Trimethylamine N-oxide   | C3 H9 N O                          | 75.06842 | 1.079  | 864437.732  | 6138680.298 | 154498.3375 | 522331.2909 | 1145566.084 | 44796.5544  | 57363.643 | 20472.47504 | 19072.2453  | 840.2559 |
| M_0160 | Phosphoric acid  | H3 O4 P                            | 97.97737 | 1.461  | 741847.5547 | 204508.1893 | 222328.812  | 312675.8617 | 90819.30127 | 439184.0098 | 4152110.9 | 203914.4259 | 4564711.611 | 22697.75 |
| M_0161 | D-(+)-Pyroglutamic Acid  | C5 H7 N O3                         | 129.0427 | 1.309  | 4461534.351 | 2605272.582 | 1700920.234 | 2403348.777 | 3825008.252 | 2331305.592 | 4733404.7 | 3964611.642 | 2945239.339 | 6977.955 |
| M_0162 | 2,6-Dimethylpyrazine   | C6 H8 N2                           | 108.069  | 0.804  | 2648289.721 | 5067407.368 | 1604870.149 | 6027007.427 | 6063119.043 | 5248120.325 | 5348004.2 | 3698320.729 | 3191307.034 | 5300.173 |
| M_0163 | N-(7-Butyl-8-hydroxy-4,9-dimethyl-2,6-dioxo-1,5-dioxonan-3-yl)-3-formamidosalicylamide | C21 H28 N2 O8<br>C5 [13]C H13 N O2 | 436.1863 | 8.534  | 2039006.321 | 2399579.077 | 1729154.97  | 2798842.065 | 4153502.741 | 1871991.209 | 2595234.8 | 5587712.794 | 1704620.364 | 41600.8  |
| M_0164 | MFC00037583  |                                    | 132.098  | 1.526  | 2066619.818 | 5704500.096 | 900516.3564 | 3265486.589 | 543787.6868 | 3621983.972 | 3033226.4 | 3122249.2   | 2127240.181 | 1721.421 |
| M_0165 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P                    | 309.1071 | 1.402  | 31693.97151 | 910025.0413 | 33695.34194 | 1877159.117 | 1545509.555 | 3415589.533 | 5759884.9 | 3318828.33  | 5295550.259 | 1856.637 |
| M_0166 | 2-Chloro-1,3,2-oxathiaphospholane  | C2 H4 Cl O P S                     | 141.9409 | 1.266  | 5744546.422 | 1540498.587 | 1057628.407 | 1680212.421 | 909884.5005 | 3135335.074 | 1247106.9 | 1779946.757 | 474838.3161 | 8646.241 |
| M_0167 | nabilone   | C24 H36 O3                         | 372.2665 | 8.579  | 228912.3945 | 230865.8722 | 2181641.839 | 5718599.685 | 472106.0803 | 982379.6377 | 688055.76 | 661891.4108 | 769218.1812 | 9977.537 |
| M_0168 | 1,1,2-Trimethylsilane  | C3 H12 Si2                         | 104.0479 | 1.988  | 5267519.082 | 2754099.541 | 1823015.86  | 2002911.674 | 1501883.69  | 3048372.872 | 2266121.9 | 2270371.29  | 1549298.725 | 123564.6 |
| M_0169 | N-Methylhistamine  | C6 H11 N3                          | 125.0955 | 0.806  | 2459228.8   | 4720788.549 | 1505415.951 | 5610583.418 | 5650225.399 | 4857748.03  | 4987974   | 3436616.175 | 3026675.688 | 2920.63  |
| M_0170 | 1-(4-Morpholinyl)-1-dodecanone   | C16 H31 N O2                       | 269.2353 | 8.7    | 2455702.218 | 3048835.795 | 1684204.848 | 552083.3243 | 1391458.165 | 1165736.411 | 1760054   | 2484697.089 | 2243946.449 | 59805.65 |
| M_0171 | DL-Arginine  | C6 H14 N4 O2                       | 174.1117 | 0.863  | 1996707.807 | 3518005.445 | 1648502.461 | 1746723.999 | 2335456.629 | 5630156.862 | 2466252.9 | 4369292.676 | 2453121.658 | 45231.13 |
| M_0172 | DL-Arginine  | C6 H14 N4 O2                       | 174.1117 | 1.059  | 1746320.823 | 3420225.103 | 766233.3694 | 2284236.387 | 5617806.289 | 1217953.389 | 3214817.6 | 2928180.474 | 2433900.768 | 4168.004 |
| M_0173 | 4-Nitro-N-(tetrahydro-2-furanyl)methyl)benzamide                                       | C12 H14 N2 O4                      | 250.0953 | 6.379  | 5607564.564 | 661995.5337 | 2432507.813 | 1255294.177 | 758750.28   | 335702.3849 | 255847.63 | 239636.5655 | 152455.3406 | 6297.888 |
| M_0174 | Cyclopentadecanolid e  | C15 H28 O2                         | 240.2089 | 8.662  | 3688974.238 | 3187503.469 | 3538624.303 | 2433998.415 | 3736152.585 | 4131991.503 | 3077611.4 | 4054988.236 | 4355789.066 | 289085   |
| M_0175 | (2E,6E)-Farnesol   | C15 H26 O                          | 222.1983 | 8.657  | 3646911.788 | 3220299.664 | 4204461.559 | 2373963.831 | 3663039.548 | 4108077.653 | 3517665.2 | 4523206.841 | 4286416.433 | 87161.98 |
| M_0176 | 6-Trifluoromethyloxind ole   | C9 H6 F3 N O                       | 201.0402 | 5.326  | 1580287.551 | 2730700.175 | 5547598.648 | 2945599.389 | 4988791.933 | 3425280.532 | 1845264.5 | 1845959.413 | 1202658.135 | 6534.546 |
| M_0177 | Inosine  | C10 H12 N4 O5                      | 268.0807 | 2.266  | 1558707.351 | 2503379.788 | 1187493.33  | 4725039.115 | 2075052.382 | 1097531.595 | 1342529.7 | 1600374.262 | 847728.2122 | 7056.241 |
| M_0178 | 2515   | C16 H28 O2                         | 252.2088 | 8.699  | 2414004.411 | 3000235.08  | 1659314.862 | 534020.0313 | 1362084.969 | 1132800.866 | 1707354.1 | 2445024.818 | 495717.4201 | 30075.39 |
| M_0179 | Phosphorodifluorido us hydrazide,  | C3 H9 F2 N2 P                      | 142.0467 | 1.193  | 5483028.911 | 2336762.129 | 1409112.286 | 1949901.003 | 1323820.416 | 669214.0097 | 658517.73 | 679978.5517 | 441839.9913 | 1786.454 |
| M_0180 | DC2810000  | C9 H12 O3                          | 168.0787 | 7.913  | 313406.7271 | 89144.38559 | 2345523.594 | 98469.5628  | 5459103.231 | 1790066.223 | 3701777.1 | 336063.2565 | 517361.555  | 453803.8 |
| M_0181 | 5,7-Dihydroxytryptamine  | C10 H12 N2 O2                      | 192.0899 | 1.535  | 4083056.493 | 5405269.307 | 4393606.808 | 4098114.028 | 4802244.701 | 4148465.944 | 3986673.3 | 4499746.675 | 3922622.67  | 7069.545 |
| M_0182 | 144183   | C11 H20 N2 O                       | 196.1572 | 8.598  | 204526.8001 | 305503.1261 | 3285287.318 | 5320618.719 | 23336.91513 | 910458.0127 | 1333812.5 | 1405461.482 | 1178270.548 | 7197.552 |
| M_0183 | Tributyl phosphate   | C12 H27 O4 P                       | 266.1646 | 8.89   | 3316437.232 | 2790865.212 | 4362568.409 | 3573077.279 | 4459478.764 | 4737580.792 | 4007173.7 | 4362312.603 | 4523613.361 | 59213.24 |
| M_0184 | Acetyl-L-carnitine   | C9 H17 N O4                        | 203.1157 | 1.272  | 5295563.686 | 288078.0987 | 2239747.707 | 964477.6017 | 377861.0794 | 738319.9105 | 745872.22 | 400173.1349 | 308689.0117 | 2355.641 |
| M_0185 | DL-Carnitine   | C7 H15 N O3                        | 161.1052 | 1.261  | 5276849.212 | 406144.1453 | 5272944.882 | 2022616.439 | 2582714.64  | 1811989.198 | 1520844.4 | 1527098.035 | 1284646.275 | 10927.46 |
| M_0186 | Edaravone  | C10 H10 N2 O                       | 174.0793 | 1.534  | 4118147.387 | 5275839.639 | 4191940.919 | 4119657.442 | 4724411.116 | 3845727.901 | 3735639.3 | 4332126.342 | 3867143.901 | 6068.373 |
| M_0187 | Creatinine   | C4 H7 N3 O                         | 113.0592 | 1.086  | 5266061.418 | 1898807.34  | 1818660.489 | 2594509.044 | 1838600.118 | 1936171.418 | 2103045.6 | 2007985.326 | 1866948.033 | 15051.02 |
| M_0188 | 2-linoleoyl-sn-glycero-3-phosphoethanolamine   | C23 H44 N O7 P                     | 477.286  | 9.313  | 547702.0163 | 3303671.902 | 2746760.03  | 4888829.104 | 3500092.496 | 3609259.499 | 3423246.8 | 5208715.636 | 3743325.666 | 10722.01 |
| M_0189 | D-(+)-Proline  | C5 H9 N O2                         | 115.0637 | 1.345  | 1651151.964 | 1577480.213 | 2859781.587 | 1924248.461 | 2228685.572 | 2878700.769 | 5185383   | 3070672.662 | 3267082.763 | 114471.7 |
| M_0190 | D-(+)-Proline  | C5 H9 N O2                         | 115.0637 | 1.249  | 903582.974  | 353669.8128 | 911035.2907 | 1924248.461 | 962758.4045 | 2878700.769 | 953759.93 | 3070672.662 | 825748.7906 | 48176.11 |
| M_0191 | VS1150000  | C18 H34 O4                         | 314.2455 | 8.73   | 2006030.055 | 1635526.568 | 966893.9441 | 996527.3628 | 701761.7027 | 1214424.212 | 1173217.1 | 1845217.758 | 1221157.575 | 539570.6 |
| M_0192 | Nicotinamide   | C6 H6 N2 O                         | 122.0483 | 1.431  | 24494.30732 | 48418.19021 | 28234.97555 | 21877.27401 | 34962.41726 | 1309044.768 | 1822536.6 | 20246.00737 | 1659042.515 | 10654.81 |
| M_0193 | L-Phenylalanine  | C9 H11 N O2                        | 165.0793 | 2.616  | 571920.3287 | 320656.1252 | 602230.8534 | 470362.299  | 305465.0887 | 456527.7684 | 380788.74 | 406293.2302 | 292212.5748 | 14045.64 |
| M_0194 | Inosine-5'-monophosphate (IMP)   | C10 H13 N4 O8 P                    | 348.0472 | 2.671  | 12243.41273 | 83704.35077 | 6458.329779 | 92681.14536 | 41550.68628 | 273992.0602 | 135452.75 | 220516.1491 | 147861.6739 | 6208.996 |
| M_0195 | Dimethylphosphoram idocyanidic acid  | C3 H7 N2 O2 P                      | 134.0249 | 0.792  | 3844309.924 | 2188001.952 | 1692408.817 | 3607211.986 | 2019862.976 | 2063171.668 | 1654682.1 | 1758783.541 | 1332989.974 | 41244.8  |
| M_0196 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P                    | 347.063  | 1.222  | 44439.03482 | 1140363.118 | 38697.60489 | 2724491.172 | 1920639.136 | 4599197.51  | 4894062.2 | 3816903.118 | 4041249.903 | 4343.941 |
| M_0197 | DL-Carnitine   | C7 H15 N O3                        | 161.1052 | 1.027  | 572703.1011 | 1079058.47  | 1461194.57  | 85685.42098 | 2063414.214 | 985555.9877 | 2075909.7 | 2367791.313 | 562679.1887 | 249.9974 |
| M_0198 | DL-Carnitine   | C7 H15 N O3                        | 161.1055 | 0.975  | 39957.78919 | 1079058.47  | 1461194.57  | 33551.37546 | 2063414.214 | 72070.02591 | 2075909.7 | 83248.6169  | 2231124.617 | 835.1771 |
| M_0199 | 6-Methyl-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazole-3,7-diamine                          | C4 H7 N7                           | 153.0766 | 1.571  | 4867946.325 | 3189324.588 | 3642856.713 | 2253202.205 | 2748826.426 | 3274600.945 | 2775075.4 | 1940588.152 | 1969799.514 | 6742.19  |
| M_0200 | N-Methyl-2-pyrrolidone   | C5 H9 N O                          | 99.06896 | 2.971  | 1243110.812 | 411547.2939 | 1364452.463 | 949032.3198 | 679022.6143 | 419863.895  | 372337.17 | 553415.8406 | 599681.077  | 77863.51 |
| M_0201 | Embelin  | C17 H26 O4                         | 294.183  | 8.536  | 1625044.49  | 4856631.783 | 2517026.532 | 1997535.751 | 1963954.71  | 2075222.491 | 2807940.6 | 2988533.245 | 2352814.303 | 696622.5 |

|        |  |                   |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0202 | 2,4,7-Pteridinetriamine N-(1-Methyl-4-nitro-1H-pyrazol-3-yl)-4-nitrobenzohydrazide | C6 H7 N7          | 177.076  | 7.465  | 6695.500138 | 5027.271538 | 4314.58604  | 6246.437804 | 8229.729094 | 8113.454591 | 5207.7521 | 5181.430112 | 4609.436151 | 8094.435 |
| M_0203 | Valine   | C11 H10 N6 O5     | 306.0715 | 6.768  | 1703464.054 | 410400.337  | 2400907.476 | 4813198.868 | 499361.1691 | 1123195.692 | 1001177.9 | 590700.573  | 313049.2551 | 4741.113 |
| M_0204 | 1-Adamantanol  | C10 H16 O         | 152.1202 | 8.667  | 2927995.665 | 2657316.659 | 1778869.141 | 1626661.478 | 2705516.717 | 3032306.393 | 2811202.7 | 3755095.5   | 3342027.839 | 32204.62 |
| M_0206 | Allantoin  | C4 H6 N4 O3       | 158.044  | 1.176  | 4800460.35  | 1942867.964 | 2163090.983 | 2284283.436 | 2029573.627 | 984412.6749 | 1312502   | 1106384.496 | 1099641.094 | 18320.25 |
| M_0207 | Indole-3-acetic acid   | C10 H9 N O2       | 175.0634 | 7.47   | 388121.2385 | 327297.712  | 414964.4494 | 452495.9956 | 635823.985  | 456705.1377 | 214197.01 | 154769.0144 | 100398.8246 | 8732.255 |
| M_0208 | Indole-3-lactic acid   | C11 H11 N O3      | 205.0739 | 7.262  | 3624887.213 | 1410019.633 | 2073968.648 | 2370431.457 | 2135162.317 | 1231043.699 | 388086.68 | 351959.1332 | 224998.8831 | 13823.75 |
| M_0209 | hodgkinsine  | C33 H38 N6        | 518.3181 | 10.251 | 1208655.996 | 2174352.1   | 743795.5321 | 2101171.577 | 2598316.839 | 4757780.452 | 2149529.8 | 1505152.136 | 873101.7883 | 1336.337 |
| M_0210 | 2,6-Dioxo(4~14~C)-1,2,3,6-tetrahydro-4-pyrimidinocarboxylic acid                   | C4 [14]C H4 N2 O4 | 158.0205 | 1.744  | 1106294.195 | 942184.0291 | 56517.29278 | 889579.673  | 320563.5542 | 887794.3978 | 398700.78 | 2051973.955 | 12126.85204 | 7783.48  |
| M_0211 | 2H-Pyran-2,4,6(3H,5H)-trione D-(+)-Pyroglutamic Acid                               | C5 H4 O4          | 128.0112 | 2.132  | 4575788.535 | 380358.7773 | 40989.31429 | 4712244.604 | 3670477.451 | 27424.6659  | 2996300.4 | 25329.27685 | 21498.26809 | 15352.46 |
| M_0212 | Pregabalin   | C8 H17 N O2       | 159.1259 | 1.257  | 1419440.709 | 283911.6525 | 1256945.186 | 332944.8892 | 451517.043  | 478538.7331 | 392357.11 | 416944.4894 | 410226.0065 | 1971.84  |
| M_0214 | Muscimol   | C4 H6 N2 O2       | 114.043  | 1.295  | 3661636.256 | 2245791.555 | 1744933.365 | 2144194.572 | 3171911.792 | 1852443.685 | 4376519.9 | 3496502.171 | 2629442.541 | 16639.94 |
| M_0215 | lysophosphatidylethanolamine (0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))                     | C27 H44 N O7 P    | 525.2861 | 9.276  | 378251.4531 | 1469099.899 | 1151929.844 | 2198934.097 | 3514325.5   | 3375430.806 | 3415607.5 | 4116749.012 | 3307787.983 | 23255.2  |
| M_0216 | Drospirenone   | C24 H30 O3        | 366.217  | 9.081  | 4644361.753 | 1759412.247 | 656084.1043 | 1893388.05  | 1178364.296 | 2016573.372 | 1245804.5 | 1235560.192 | 1204419.852 | 6308.035 |
| M_0217 | 3,5-Dimethylpyrazole   | C5 H8 N2          | 96.069   | 0.798  | 3556673.721 | 2049004.524 | 1583003.797 | 3425298.382 | 1895029.506 | 1928317.17  | 1569029.2 | 1677770.727 | 1252775.277 | 3303.655 |
| M_0218 | Octahydro-1,2,8-indolizinetriol  | C8 H15 N O3       | 173.1053 | 6.744  | 4608090.069 | 783261.5987 | 1018062.53  | 1227337.24  | 901078.5169 | 747782.5025 | 662154.09 | 551223.028  | 281314.9645 | 10959.85 |
| M_0219 | 17 $\alpha$ -Methyl-androstan-3-hydroxymine-17 $\beta$ -ol                         | C20 H33 N O2      | 319.2488 | 8.907  | 38807.63034 | 46091.44445 | 59538.9801  | 43745.1226  | 35979.15131 | 88540.63878 | 34816.869 | 81483.30354 | 55420.5637  | 7029.473 |
| M_0220 | DL-Glutamine   | C5 H10 N2 O3      | 146.0692 | 1.316  | 2637488.17  | 750967.2623 | 514729.4365 | 1961955.783 | 3105734.18  | 1841109.39  | 4268885.5 | 3451911.784 | 2611028.388 | 2883.975 |
| M_0221 | DL-1913256   | C18 H30 O         | 262.2296 | 8.913  | 65037.15343 | 79460.95499 | 113742.3169 | 72975.86779 | 77842.39353 | 123868.842  | 65676.169 | 101201.7533 | 82822.19071 | 19612.04 |
| M_0222 | trans,trans-2,4-Heptadienal  | C7 H10 O          | 110.0736 | 8.27   | 220241.955  | 122765.6458 | 164159.7909 | 134570.7832 | 45737.50874 | 58827.18119 | 441831.29 | 468058.1445 | 451243.9272 | 452957.8 |
| M_0223 | 1-(3-Azido-2,3-dideoxypentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione          | C10 H13 N5 O4     | 267.0966 | 1.61   | 24878.58072 | 394235.4582 | 215527.7499 | 895452.2269 | 4522229.423 | 693613.9298 | 3337162.5 | 326642.8479 | 1588224.633 | 2919.396 |
| M_0224 | DL-Homoserine  | C4 H9 N O3        | 87.03226 | 1.104  | 3801870.386 | 2111440.761 | 2787862.597 | 1780368.064 | 1938197.378 | 2702137.443 | 3766415.1 | 2899882.457 | 4427671.459 | 20319.99 |
| M_0225 | Isatin   | C8 H5 N O2        | 147.0321 | 4.898  | 25957.24806 | 26493.69216 | 27136.22351 | 38735.3578  | 25169.49176 | 14313.00111 | 28639.11  | 29850.14751 | 27677.42328 | 24285.93 |
| M_0226 | 3-Decyldihydro-2,5-furandione  | C14 H24 O3        | 240.1725 | 8.811  | 4397402.127 | 476790.7781 | 142713.6175 | 509933.1705 | 352012.9649 | 665705.104  | 708637.36 | 782159.0443 | 628132.2691 | 59164.32 |
| M_0227 | Acetyl-L-carnitine   | C9 H17 N O4       | 203.1157 | 1.422  | 1557799.972 | 1343214.508 | 518892.1075 | 1806128.912 | 1459503.382 | 1671235.466 | 1134514.2 | 2371652.832 | 843050.0918 | 3460.656 |
| M_0228 | Diethylpyrocarbonat  | C6 H10 O5         | 162.0528 | 1.145  | 474158.2488 | 1315135.097 | 2904811.242 | 1004632.288 | 1206489.864 | 2868473.157 | 3279039.3 | 3247008.015 | 1906390.642 | 74955.04 |
| M_0229 | DL-Homoserine  | C4 H9 N O3        | 119.0585 | 1.105  | 3484671.918 | 1809782.146 | 2682485.147 | 1446910.411 | 1748764.102 | 2590166.034 | 3563934.3 | 2728177.368 | 4232311.174 | 27069.64 |
| M_0230 | Linoleamide  | C18 H33 N O       | 279.2562 | 8.913  | 28804.9453  | 40500.46814 | 48366.24374 | 32447.64059 | 26829.03304 | 73438.61674 | 20536.677 | 60608.03604 | 34798.4503  | 6258.97  |
| M_0231 | Choline  | C5 H13 N O        | 103.1002 | 1.531  | 1605231.598 | 2416271.807 | 1441990.493 | 2158269.433 | 2509045.781 | 1943187.116 | 2207870.1 | 2337380.009 | 1064339.743 | 81232.91 |
| M_0232 | DL-Glutamine   | C5 H10 N2 O3      | 146.0691 | 1.23   | 992123.904  | 476906.5296 | 1170138.416 | 1961955.783 | 1034578.556 | 871469.3105 | 4268885.5 | 524967.8092 | 933980.1326 | 2103.588 |
| M_0233 | Vigabatrin   | C6 H11 N O2       | 129.0792 | 1.104  | 201214.1084 | 71418.27073 | 88252.17161 | 75028.43423 | 74713.36951 | 86707.49499 | 83256.497 | 99827.8954  | 75983.48665 | 16301.64 |
| M_0234 | 4-Nonanoylmorpholine   | C13 H25 N O2      | 227.1886 | 8.31   | 1558278.948 | 1897105.026 | 1644833.396 | 1022067.864 | 946817.6753 | 1642436.5   | 1561973.9 | 2647261.532 | 1639017.537 | 812805.1 |
| M_0235 | 2683   | C11 H10 N4 O6     | 294.0589 | 1.682  | 370337.0915 | 599881.7505 | 5735.848265 | 788006.7924 | 27647.48279 | 616812.29   | 100496.44 | 994312.4447 | 249322.3761 | 6153.914 |
| M_0236 | N4-(2,2-DIMETHYL-1-METHYLCARBAMOYL-PROPYL)-2,N1-DIHYDROXY-3-ISOBUTYL-SUCCINAMIDE   | C15 H29 N3 O5     | 331.2107 | 4.266  | 5582.168238 | 5199.009649 | 5120.750656 | 5139.73019  | 4976.066086 | 5108.601316 | 5054.1573 | 5075.89305  | 5085.063532 | 4962.797 |
| M_0237 | Pyridoxamine   | C8 H12 N2 O2      | 168.0875 | 0.983  | 4211250.184 | 1047223.36  | 1155670.959 | 542824.8228 | 867438.3446 | 999254.7013 | 1009825.5 | 846051.4298 | 730976.2926 | 4971.066 |
| M_0238 | 1-arachidonoyl-sn-glycero-3-phosphoethanolamine                                    | C25 H44 N O7 P    | 501.286  | 9.289  | 702646.1063 | 1911429.945 | 1294306.807 | 3314372.934 | 3657460.227 | 3191538.272 | 3940556   | 4210498.587 | 3263757.58  | 8846.715 |
| M_0239 | DL-Arginine  | C6 H14 N4 O2      | 174.1117 | 0.956  | 908463.6319 | 1191569.663 | 128820.4556 | 759138.3836 | 1307768.371 | 207463.1952 | 1835574.7 | 1840062.62  | 867419.5567 | 2646.819 |
| M_0240 | AC-VAL-OH  | C7 H13 N O3       | 159.0896 | 4.577  | 4158497.081 | 451018.5614 | 416553.2395 | 853791.3134 | 450937.5971 | 533542.0951 | 332980.42 | 489472.3011 | 328840.7137 | 15531.85 |
| M_0241 | Trigonelline   | C7 H7 N O2        | 137.0478 | 1.159  | 3609091.881 | 4154909.733 | 4026790.275 | 2401891.77  | 2954027.508 | 1051662.665 | 866704.13 | 1081811.337 | 1094489.939 | 9182.128 |
| M_0242 | 4H-Benzotriazol-4-one  | C6 H3 N3 O        | 133.0282 | 0.79   | 3315254.174 | 1961837.808 | 1397149.322 | 3060197.424 | 1767978.731 | 1780559.385 | 1433683.7 | 1586998.182 | 1116497.994 | 50156.08 |
| M_0243 | 7-ketodeoxycholic acid   | C24 H38 O5        | 406.2722 | 8.507  | 145774.7839 | 132638.1227 | 357354.1896 | 4097283.457 | 196831.1346 | 81130.34273 | 411361.49 | 567591.9196 | 285818.3141 | 9901.364 |
| M_0244 | 5-(Nitroimino)hexahydroimidazo[4,5-d]imidazol-2(1H)-one                            | C4 H6 N6 O3       | 186.0504 | 1.197  | 1038326.571 | 1501555.44  | 846991.1868 | 1791517.456 | 1848284.497 | 1552189.463 | 1750796.8 | 1832491.385 | 1404665.728 | 3853.912 |
| M_0245 | D-(+)-Pyroglutamic Acid  | C5 H7 N O3        | 129.0427 | 1.109  | 2814623.808 | 2288678.681 | 1743421.538 | 2294224.806 | 475579.8399 | 412602.0547 | 3457331.1 | 2272852.64  | 4061214.916 | 2170.208 |
| M_0246 | Methyl indole-3-acetate  | C11 H11 N O2      | 189.079  | 7.817  | 1206481.981 | 3358949.129 | 1424903.053 | 4053992.115 | 3614218.291 | 3867935.06  | 1679029   | 1956570.996 | 1274682.222 | 11565.8  |
| M_0247 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P   | 347.063  | 1.391  | 13436.05692 | 1141870.887 | 33420.91695 | 2281329.471 | 1892677.456 | 4033989.651 | 130309.53 | 995072.842  | 116860.5222 | 2805.267 |
| M_0248 | methoxycinnamate   | C18 H26 O3        | 290.188  | 8.767  | 1623612.401 | 2194770.243 | 1711923.253 | 1866438.755 | 3013492.084 | 3241257.904 | 2003479.9 | 3464115.044 | 1397464.554 | 79128.51 |
| M_0249 | 1-[(8Z,11Z,14Z)-icosatrienoyl]-sn-glycero-3-phosphocholine                         | C28 H52 N O7 P    | 545.3487 | 10.099 | 101818.6916 | 1041003.266 | 697286.7856 | 2112766.715 | 1722868.215 | 2337806.043 | 2271388.8 | 1949995.958 | 2268659.791 | 49816.42 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0250 | N(1)-acetylspermidine  | C9 H21 N3 O     | 187.1684 | 0.804  | 3963143.095 | 216752.7893 | 151747.7955 | 288915.2762 | 231238.0642 | 108877.2986 | 148442.47 | 111265.4034 | 109874.0336 | 2167.115 |
| M_0251 | DC2810000  | C9 H12 O3       | 168.0788 | 7.632  | 121343.7628 | 129344.2218 | 1412255.059 | 1429628.296 | 2466828.586 | 501679.7452 | 71008.08  | 1519832.153 | 1553754.094 | 778180.6 |
| M_0252 | 3b-Hydroxy-5-cholenoic acid  | C24 H38 O3      | 374.2819 | 9.152  | 147608.9802 | 417269.8466 | 1631316.058 | 3913546.766 | 413713.2728 | 524964.5654 | 707577.79 | 1850533.535 | 1250707.016 | 14358.83 |
| M_0253 | Choline  | C5 H13 N O      | 103.1002 | 10.349 | 10926.28433 | 409944.2887 | 211395.2016 | 130042.0164 | 484643.6197 | 957975.7567 | 637280.87 | 762635.026  | 363655.5335 | 64954.55 |
| M_0254 | 3-Thiomorpholinocarboxylic acid  | C5 H9 N O2 S    | 147.0354 | 1.454  | 579319.9211 | 1680888.829 | 1445311.323 | 566542.1701 | 1566944.748 | 3867475.115 | 857009.9  | 1417266.998 | 1026402.794 | 7755.748 |
| M_0255 | 4-Hydroxyindole  | C8 H7 N O       | 133.0529 | 4.883  | 3836.419963 | 4707.565174 | 5514.730038 | 3863.172518 | 3993.367972 | 3766.536123 | 4004.2255 | 4348.053652 | 4262.689801 | 3560.767 |
| M_0256 | 3,3,3-Trifluoropropanol  | C3 H5 F3 O      | 114.0297 | 1.027  | 688649.2457 | 919079.9803 | 618196.4331 | 436190.8669 | 180468.5891 | 484369.0061 | 654948.68 | 200050.3713 | 301349.9367 | 78103.79 |
| M_0257 | MEGA-9   | C16 H33 N O6    | 335.2309 | 8.727  | 1303550.257 | 1176182.385 | 721949.0599 | 823175.2667 | 485453.2829 | 803181.5934 | 783907.82 | 1308294.407 | 800923.5647 | 118363.5 |
| M_0258 | butyl acrylate   | C7 H12 O2       | 128.084  | 7.763  | 116355.6566 | 1320590.607 | 1178192.813 | 1261881.462 | 125026.2922 | 1439038.617 | 120525.78 | 1040819.965 | 160974.1297 | 105023.7 |
| M_0259 | Diethanolamine   | C4 H11 N O2     | 105.0794 | 0.954  | 29584.63862 | 29006.20668 | 30471.96343 | 28657.44289 | 28893.77783 | 19584.23703 | 28818.73  | 30315.81501 | 29267.51514 | 74547.22 |
| M_0260 | L-Glutamic acid  | C5 H9 N O4      | 147.0531 | 1.109  | 876066.5085 | 1852659.327 | 472590.5528 | 903147.8778 | 678513.3523 | 1233607.803 | 1538821.3 | 1321567.152 | 1613373.57  | 2694.539 |
| M_0261 | FZ5600000  | C27 H44         | 368.3443 | 9.277  | 2574131.184 | 653298.6233 | 963092.066  | 1145660.57  | 1921632.794 | 833609.4482 | 949781.92 | 3703882.292 | 1498145.586 | 13965.67 |
| M_0262 | Pregabalin   | C8 H17 N O2     | 159.1259 | 1.432  | 2654635.229 | 1348750.798 | 1915115.843 | 1596018.237 | 1247938.415 | 1553876.413 | 929699.3  | 1389378.997 | 836110.5046 | 4330.559 |
| M_0263 | Xanthine   | C5 H4 N4 O2     | 152.0335 | 2.03   | 3636590.734 | 2282523.112 | 447990.1036 | 2503484.963 | 595724.4634 | 1535870.348 | 1225272.5 | 2437849.123 | 987745.3864 | 9832.143 |
| M_0264 | 1-Allyl-4-((2,5-dimethoxyphenyl)[1-(tetrahydro-2-furanyl)methyl]-1H-tetrazol-5-yl)methyl)piperazine  | C22 H32 N6 O3   | 428.2539 | 8.5    | 78005.62435 | 79808.6015  | 660231.5361 | 3625029.648 | 150338.3577 | 205015.7228 | 304854.14 | 417879.4735 | 287923.288  | 4423.276 |
| M_0265 | 6-Phenoxycotinic acid  | C12 H9 N O3     | 215.0558 | 5.909  | 3010741.068 | 1017535.963 | 3030151.031 | 3241064.963 | 1906937.065 | 2960256.804 | 2130052.6 | 2232809.466 | 799821.092  | 2768.78  |
| M_0266 | Kojic acid   | C6 H6 O4        | 142.0242 | 1.136  | 1386847.628 | 2340193.413 | 2838090.202 | 1436791.756 | 1555245.454 | 2654036.566 | 1667778   | 2500337.389 | 1924739.469 | 5082.053 |
| M_0267 | 2050867  | C12 H23 N O4    | 245.1627 | 2.81   | 3559206.047 | 1521916.206 | 1770929.24  | 2978487.279 | 1145760.572 | 955125.1292 | 1061146.2 | 872478.2457 | 604350.2163 | 5367.167 |
| M_0268 | L-gamma-Glutamyl-L-leucine   | C11 H20 N2 O5   | 260.1372 | 4.342  | 3034719.855 | 2385069.915 | 3142680.247 | 2455892.793 | 1576016.17  | 1565326.846 | 1559257.4 | 2233025.82  | 1117799.696 | 5908.564 |
| M_0269 | Creatine   | C4 H9 N3 O2     | 131.0696 | 1.456  | 534241.5937 | 200700.9169 | 163341.4259 | 281121.1523 | 175536.4287 | 1101705.911 | 2509879   | 1976766.383 | 991863.5116 | 929.09   |
| M_0270 | 1-[2-Hydroxy-3-(phenylthio)propyl]piperidine-4-carboxamide   | C15 H22 N2 O2 S | 294.1443 | 8.327  | 195492.1807 | 42154.16398 | 106285.7119 | 21968.42115 | 797235.5136 | 296557.358  | 516800.23 | 462961.9884 | 752683.0769 | 271125.1 |
| M_0271 | Coenzyme Q1  | C14 H18 O4      | 250.118  | 7.571  | 25744.31453 | 1258935.832 | 17748.64365 | 1462045.389 | 526498.942  | 1271797.368 | 1165300.7 | 11968.55008 | 13711.037   | 384957.4 |
| M_0272 | 4,4'-Methylenebis[2-tert-butyl-6-(.alpha.-methylbenzyl)phenol]   | C37 H44 O2      | 520.3363 | 8.916  | 39408.71702 | 42804.99569 | 35190.96706 | 68845.55769 | 50305.10313 | 56512.85075 | 47181.284 | 52662.75676 | 55706.96122 | 110510.8 |
| M_0273 | 4,4'-Methylenebis[2-tert-butyl-6-(.alpha.-methylbenzyl)phenol]   | C37 H44 O2      | 520.3364 | 8.931  | 10081.87369 | 10761.0011  | 9002.852225 | 6987.676982 | 12869.48001 | 5340.003309 | 4599.5845 | 5074.3793   | 4643.268813 | 25043.37 |
| M_0274 | 2-Ethoxy-4-hydrazino-6-(1-piperidinyl)-1,3,5-triazine  | C10 H18 N6 O    | 238.1552 | 8.559  | 1113731.943 | 46654.99289 | 46078.77216 | 1132638.658 | 601928.7378 | 28030.94542 | 2340023.2 | 500255.671  | 3397415.365 | 1329.468 |
| M_0275 | trans,trans-2,4-Heptadienal  | C7 H10 O        | 110.0736 | 7.772  | 40171.6375  | 838800.8116 | 836036.4765 | 906010.9343 | 21999.80042 | 143496.2198 | 751540.95 | 28589.76039 | 83528.80023 | 118040.4 |
| M_0276 | Adenosine  | C10 H13 N5 O4   | 267.0966 | 1.433  | 11939.36328 | 105690.1569 | 45923.09887 | 627411.6975 | 1152303.674 | 1950330.614 | 3322259.8 | 1326474.798 | 2168820.221 | 1510.106 |
| M_0277 | Choline  | C5 H13 N O      | 103.1002 | 10.08  | 134217.8991 | 768787.9103 | 2073859.649 | 219493.3865 | 571702.6291 | 350780.2876 | 266270.02 | 476298.3643 | 277021.5658 | 11468.08 |
| M_0278 | 4033747  | C26 H52 N O7 P  | 521.3481 | 10.006 | 42548.19618 | 51251.60085 | 204010.8496 | 703947.665  | 821655.6893 | 1119558.812 | 129220.57 | 1327968.599 | 309320.1765 | 11856.87 |
| M_0279 | Ethylidimethylbenzene  | C10 H14         | 134.1097 | 8.667  | 1957178.121 | 1849385.657 | 2182705.279 | 1129867.629 | 1847594.193 | 2113236.767 | 1878473   | 2447624.337 | 2302356.259 | 88128.52 |
| M_0280 | alpha-Ketoglutaric acid  | C5 H6 O5        | 146.0215 | 2.157  | 3192176.283 | 194772.4059 | 470128.2464 | 2047414.09  | 31609.55752 | 39206.40996 | 37364.078 | 196478.3932 | 29810.19951 | 16130.72 |
| M_0281 | N-[(2S,3S)-5-[(2S)-1-hydroxypropan-2-yl]-3-methyl-2-(methylaminomethyl)-6-oxo-2,3,4,7-tetrahydro-1,5-benzoxazin-9-yl]cyclopropanecarboxamide | C21 H31 N3 O4   | 389.2315 | 8.981  | 289047.9102 | 88260.75664 | 38311.76613 | 39241.09571 | 20005.3859  | 396600.2685 | 331322.91 | 618800.7605 | 227716.2846 | 44908.68 |
| M_0282 | DL-Carnitine   | C7 H15 N O3     | 161.1052 | 1.47   | 934075.986  | 1425885.956 | 2923269.068 | 1684565.239 | 2002455.585 | 53149.95527 | 1908231   | 3167990.058 | 1243609.56  | 2485.498 |
| M_0283 | L-Tyrosine   | C9 H11 N O3     | 181.074  | 1.365  | 2080201.45  | 515104.055  | 158376.0134 | 1424724.845 | 890612.816  | 148252.7423 | 3140964.8 | 498575.1746 | 1489863.053 | 2433.388 |
| M_0284 | 2H-Pyran-2,4,6(3H,5H)-trione   | C5 H4 O4        | 128.0111 | 2.277  | 74666.77533 | 1974657.522 | 1099548.686 | 48828.42828 | 3136720.124 | 2551452.838 | 2848049   | 425162.2821 | 2104698.104 | 18794.47 |
| M_0285 | 5-Hydroxyindole-3-acetic acid  | C10 H9 N O3     | 191.0582 | 2.211  | 1431300.164 | 624829.3046 | 3081638.839 | 998297.8053 | 805268.4926 | 608873.7261 | 717985.34 | 670161.0896 | 320532.2057 | 8340.575 |
| M_0286 | 1H-purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-((2E)-2-piperidinylideneamino)propyl]-1,3-dimethyl-  | C15 H22 N6 O3   | 334.1756 | 8.505  | 1143224.924 | 3072523.801 | 1596704.543 | 1359542.084 | 1476535.888 | 2191464.035 | 1962841.4 | 2186518.134 | 1514955.93  | 504199.8 |
| M_0287 | Edaravone  | C10 H10 N2 O    | 174.0794 | 6.107  | 3611.077228 | 3408.967189 | 4307.765733 | 3468.391872 | 3515.012585 | 3490.681594 | 8780.6642 | 3472.671376 | 3529.832417 | 3434.333 |
| M_0288 | 1-[N-Cyano-N-(4,6-dimethyl-2-pyrimidinyl)glycyl]-4-piperidinecarboxamide   | C15 H20 N6 O2   | 316.165  | 8.516  | 1029626.492 | 3048134.102 | 1460382.546 | 1207705.349 | 1325179.257 | 1875677.312 | 1794012.1 | 2156898.316 | 1437415.172 | 322518   |
| M_0289 | 1760709  | C10 H24 N2 O3   | 220.1786 | 1.145  | 652492.9695 | 2064835.347 | 1805019.327 | 2342004.251 | 1760708.096 | 3037774.792 | 2233612.6 | 2578004.649 | 1932742.867 | 2384.538 |
| M_0290 | 5-Hydroxyindole-3-acetic acid  | C10 H9 N O3     | 191.0582 | 5.013  | 819157.0659 | 234087.4767 | 252329.3348 | 408504.0415 | 197456.5985 | 145410.8479 | 135099.04 | 186162.4488 | 120314.987  | 5995.91  |
| M_0291 | (2-Amino-3-hydroxybutanoyl)oxonium   | C4 H10 N O3     | 120.065  | 1.287  | 3032259.661 | 859013.1419 | 312597.3212 | 503270.4577 | 343705.2541 | 139618.8699 | 101462.54 | 133759.965  | 169825.9057 | 27383.48 |
| M_0292 | Creatine   | C4 H9 N3 O2     | 131.0696 | 1.324  | 1474320.035 | 667082.8367 | 396447.6037 | 440056.3748 | 597456.8625 | 177797.5877 | 742453.64 | 76294.05586 | 730544.4141 | 1501.854 |
| M_0293 | Creatine   | C4 H9 N3 O2     | 131.0696 | 1.259  | 3012020.69  | 776114.1634 | 2509946.129 | 1136443.838 | 1003486.245 | 870798.1245 | 419687.57 | 517892.3548 | 936212.5887 | 23170.03 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0294 | N6,N6,N6-Trimethyl-L-lysine   | C9 H20 N2 O2    | 188.1525 | 1.071  | 356159.1748 | 163688.3749 | 100854.1364 | 148479.8521 | 139772.7753 | 86838.53948 | 132681.28 | 147874.4328 | 178310.568  | 2066.876 |
| M_0295 | L-Ergothioneine   | C9 H15 N3 O2 S  | 229.0884 | 1.213  | 61917.90875 | 253960.8935 | 134944.4468 | 282283.9101 | 213754.9336 | 618071.7659 | 471267.81 | 607069.2839 | 396864.3522 | 4073.08  |
| M_0296 | Histamine   | C5 H9 N3        | 94.0535  | 0.796  | 830265.1223 | 2336059.1   | 879032.655  | 2564015.705 | 949611.3145 | 2568689.596 | 1876768.9 | 2300698.407 | 1820271.945 | 4597.254 |
| M_0297 | L-Kynurenine  | C10 H12 N2 O3   | 208.0848 | 2.207  | 1326737.422 | 577523.1696 | 2857567.333 | 927410.452  | 764384.8394 | 577099.9339 | 653654.46 | 630080.7084 | 297847.8098 | 4082.515 |
| M_0298 | Dimethylphosphoramidocyanidic acid  | C3 H7 N2 O2 P   | 134.0249 | 0.896  | 45610.77446 | 29147.78253 | 18874.74384 | 18834.43108 | 31079.75571 | 38868.64903 | 21919.171 | 20506.10769 | 12918.43689 | 4174.58  |
| M_0299 | LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))   | C28 H48 N O7 P  | 541.3146 | 10.653 | 1450.677402 | 120645.9986 | 179603.7479 | 186944.408  | 148140.7107 | 199844.1907 | 179043.46 | 2838020.982 | 154414.3678 | 13696.56 |
| M_0300 | 2-Methoxyestradiol  | C19 H26 O3      | 302.1857 | 8.778  | 1347065.857 | 2479395.97  | 1008353.476 | 896703.722  | 1073013.264 | 2833628.759 | 1374070.6 | 1971709.596 | 1130127.759 | 7144.67  |
| M_0301 | 3,7-Dinitro-1,3,5,7-tetraazabicyclo[3.3.1]nonane  | C5 H10 N6 O4    | 218.0754 | 0.962  | 1066437.783 | 1689661.316 | 449080.7734 | 1649451.805 | 1966097.379 | 1995049.541 | 1407134.4 | 2200866.596 | 1428049.189 | 4035.182 |
| M_0302 | 4-Morpholinylacetic acid  | C6 H11 N O3     | 145.074  | 3.036  | 2796417.667 | 1109143.767 | 457918.6639 | 1285947.966 | 771084.4185 | 922889.9066 | 643367.44 | 567014.726  | 395100.1542 | 37362.06 |
| M_0303 | 2,3-Dimethylbenzothiazol-3-ium 2-(14,15-Epoxyicosatrienoyl) glycerol                    | C9 H10 N S      | 164.0536 | 0.792  | 2193283.935 | 1214854.979 | 941193.7359 | 2117560.379 | 1142727.592 | 1170718.11  | 919488.88 | 1117217.914 | 764976.1707 | 16888.17 |
| M_0304 | tin(ii) hydride   | H2 Sn           | 121.9175 | 1.054  | 238713.2296 | 704356.4864 | 141633.2647 | 330103.7896 | 538558.9579 | 227548.1061 | 225733.02 | 275845.7228 | 158252.1001 | 1227.045 |
| M_0305 | tin(ii) hydride   | H2 Sn           | 121.9175 | 0.991  | 35650.33484 | 60826.33627 | 157373.8552 | 36297.60467 | 142764.3424 | 326582.0465 | 38823.889 | 137026.8028 | 17166.58404 | 3756.215 |
| M_0306 | Glycidyl Stearate   | C21 H40 O3      | 340.2976 | 10.466 | 1705050.092 | 575945.9265 | 1820365.46  | 1212073.54  | 1712709.902 | 276801.0525 | 2317825.2 | 1464435.384 | 1321939.893 | 6090.95  |
| M_0307 | Glycidyl Stearate   | C21 H40 O3      | 340.2977 | 10.522 | 112547.2715 | 82802.79658 | 41293.05968 | 65475.87001 | 153776.7376 | 26956.2578  | 2317825.2 | 442714.1948 | 78665.72828 | 2140.44  |
| M_0308 | MFC022416941  | C25 H47 N O4    | 425.3505 | 8.357  | 2736766.088 | 273184.1965 | 189944.8892 | 1030062.054 | 511994.0345 | 1152427.843 | 1115991.4 | 922045.9616 | 547212.9644 | 4933.188 |
| M_0310 | Glufosinate   | C5 H12 N O4 P   | 181.0506 | 1.22   | 42338.80892 | 1000578.772 | 239216.4341 | 825863.0441 | 672769.7132 | 475140.5133 | 341968.52 | 295859.8716 | 273917.4817 | 1599.96  |
| M_0311 | 1-(3-Aminopropyl)-2-hydroxy-3-oxo-1-propyltriazane                                      | C6 H16 N4 O2    | 176.1273 | 1.373  | 8670.319332 | 5479.774924 | 2701784.231 | 4633.881275 | 370878.9541 | 10829.58645 | 7804.6605 | 37595.72954 | 31044.68416 | 1564.2   |
| M_0312 | 2,1,3-Benzoxadiazol-5-yl(4-phenylpiperazino)methanone                                   | C17 H16 N4 O2   | 308.1234 | 7.907  | 203925.4349 | 179446.1104 | 72006.42668 | 152375.9488 | 1368661.182 | 2692048.445 | 948960.87 | 260115.671  | 226714.0459 | 340730.6 |
| M_0313 | 4-Hydroxybenzotriazole  | C6 H5 N3 O      | 135.0409 | 1.091  | 2691113     | 1089435.937 | 1200204.62  | 1370790.682 | 1032286.646 | 1352112.386 | 1471794.2 | 1541498.143 | 507865.7703 | 2428.977 |
| M_0314 | 2127  | C7 H6 O         | 106.0424 | 9.109  | 10120.22719 | 1106.705038 | 8080.806617 | 11332.64821 | 1775.766493 | 11708.14157 | 9995.3357 | 10777.62311 | 1378.404707 | 6153.919 |
| M_0315 | 1-[N-Cyano-N-(4,6-dimethyl-2-pyrimidinyl)glycyl]-4-piperidinecarboxamide                | C15 H20 N6 O2   | 316.1652 | 8.413  | 1017209.679 | 487321.8899 | 4943.39452  | 920116.972  | 64108.59885 | 121469.8986 | 1766145.7 | 2115.844358 | 1412528.012 | 3708.054 |
| M_0316 | Hydroxycitronellal diethyl acetal   | C14 H30 O3      | 246.2194 | 9.102  | 1189355.334 | 1290046.815 | 769640.7854 | 819939.1514 | 649386.5091 | 601625.568  | 1466359.9 | 1265225.07  | 1391623.016 | 149145.5 |
| M_0317 | Cumene  | C9 H12          | 120.094  | 8.663  | 1720394.239 | 1524779.814 | 1840891.143 | 985012.6643 | 1556476.121 | 1727479.254 | 1702977   | 2111781.094 | 1899672.504 | 167421.5 |
| M_0318 | 2,6-Dimethyl-γ-pyrone   | C7 H8 O2        | 124.0527 | 7.783  | 72007.96598 | 526762.3435 | 332771.6338 | 868930.2625 | 91008.39722 | 544541.6852 | 503922.27 | 28972.99365 | 52416.68319 | 176304.9 |
| M_0319 | Adenosine 5'-monophosphate  | C10 H14 N5 O7 P | 369.0451 | 1.223  | 40375.65987 | 739084.9665 | 38684.705   | 1596264.923 | 1237936.077 | 2406159.606 | 2655989.8 | 2085467.904 | 2150661.612 | 3564.954 |
| M_0320 | Dichloromethane   | C H2 Cl2        | 83.95301 | 0.636  | 1052488.727 | 1099832.274 | 407945.8655 | 605825.3689 | 1491034.764 | 611398.2903 | 274411.77 | 535861.0616 | 1180060.166 | 359755   |
| M_0321 | 1-Boc-3-pyrrolidinol  | C9 H17 N O3     | 187.1209 | 6.905  | 353597.3479 | 245007.9575 | 508585.2757 | 530716.2041 | 391372.7269 | 562135.2635 | 380142.8  | 411568.6706 | 250640.2544 | 19288.43 |
| M_0322 | DL-Glutamine  | C5 H10 N2 O3    | 146.0692 | 1.392  | 2637488.17  | 750967.2623 | 514729.4365 | 226451.2681 | 186603.1713 | 1499600.116 | 410640.95 | 337370.3789 | 119739.5886 | 1379.056 |
| M_0323 | Histamine   | C5 H9 N3        | 111.08   | 0.799  | 774861.2773 | 2097670.305 | 816911.3966 | 2344081.806 | 879562.7107 | 2332508.16  | 1770045.7 | 2138441.618 | 1696490.426 | 2496.941 |
| M_0324 | 2,5,8,11-Tetraoxanonadecane   | C15 H32 O4      | 276.2301 | 8.923  | 1277160.982 | 220553.6929 | 933819.5147 | 2618876.984 | 246919.963  | 949933.8872 | 206115.59 | 1240308.84  | 198107.4974 | 161290.5 |
| M_0325 | 2707  | C8 H14 O        | 126.1047 | 7.747  | 685030.6594 | 35923.86701 | 468196.905  | 287675.882  | 281196.688  | 381140.6875 | 65718.236 | 533058.6703 | 231617.4411 | 194991.3 |
| M_0326 | 3-[4-(Dimethylamino)phenyl]-6,8-dimethylpyrimido[5,4-e][1,2,4]triazine-5,7(6H,8H)-dione | C15 H16 N6 O2   | 312.1333 | 1.536  | 960175.4504 | 1121756.224 | 213974.1243 | 2616655.75  | 386652.2914 | 1701442.562 | 888278.6  | 1886452.57  | 918371.1973 | 2067.543 |
| M_0327 | 1-[3-Hydroxy-2-(2-hydroxy-2-propenyl)-2,3-dihydro-1-benzofuran-5-yl]ethanone            | C13 H16 O4      | 236.1025 | 7.478  | 60554.85348 | 438474.7047 | 570088.3227 | 35912.93238 | 683026.4897 | 623972.6319 | 456444.23 | 473877.6987 | 397121.9597 | 499223.6 |
| M_0328 | MNA   | C7 H8 N2 O2     | 152.0586 | 2.193  | 2593225.665 | 1225524.268 | 1512565.681 | 1469838.74  | 489801.2682 | 839837.5619 | 30244.859 | 932615.8414 | 538780.5878 | 2479.774 |
| M_0329 | 4-Indolecarbaldehyde  | C9 H7 N O       | 145.0529 | 7.397  | 55267.30588 | 28230.50716 | 10433.74685 | 44969.47277 | 72748.58553 | 91770.18863 | 8305.0316 | 32080.92368 | 12299.26086 | 6963.148 |
| M_0330 | 1,1-Dimethyl-3-(2H-tetrazol-5-yl)urea   | C4 H8 N6 O      | 156.0763 | 3.519  | 446860.8656 | 607956.5616 | 833150.8374 | 909720.4679 | 986075.6029 | 1114777.705 | 1081612.2 | 1505151.775 | 1974926.736 | 4218.911 |
| M_0331 | 1-(3-Aminopropyl)-2-hydroxy-3-oxo-1-propyltriazane                                      | C6 H16 N4 O2    | 176.1273 | 1.264  | 13927.63644 | 9070.299375 | 2493234.857 | 9099.69923  | 138150.9423 | 8460.479374 | 6897.9113 | 73404.69393 | 13269.28251 | 1336.683 |
| M_0332 | Inosine-5'-monophosphate (IMP)  | C10 H13 N4 O8 P | 348.0473 | 2.764  | 3037.650884 | 17978.8716  | 2358.39391  | 50739.37571 | 36327.24952 | 73610.40044 | 52227.048 | 40722.00379 | 44906.53344 | 2318.002 |
| M_0333 | 1-O-Tetradecylglycerol  | C17 H36 O3      | 288.2663 | 9.506  | 904952.0938 | 1106679.785 | 785010.9769 | 503377.7653 | 849433.386  | 622813.6217 | 1157127.6 | 1624780.291 | 1140037.443 | 77768.64 |
| M_0334 | 3,5-Diamino-N-carbamimidoyl-2-pyrazinecarboxamide                                       | C6 H9 N7 O      | 195.0872 | 6.746  | 2451059.41  | 262650.3556 | 529819.2724 | 631190.8819 | 476297.9677 | 385059.9506 | 357914.69 | 287013.6419 | 124213.5257 | 2641.854 |
| M_0335 | 2729  | C9 H14 O2       | 154.0994 | 7.651  | 328389.7368 | 314324.375  | 3581.817888 | 249637.0432 | 81343.75163 | 124799.2705 | 34319.916 | 15278.7631  | 44703.25185 | 60376.35 |
| M_0336 | N-Methyl-6-[methyl(propylcarbamoyl)amino]-1,2,4-triazine-5-carboxamide                  | C10 H16 N6 O2   | 252.1337 | 8.172  | 245953.2053 | 489915.0244 | 271972.4953 | 89323.72024 | 318274.9009 | 1564087.932 | 677428.56 | 531080.8478 | 279801.4499 | 485443.3 |
| M_0337 | 14(S)-HDHA  | C22 H32 O3      | 326.2244 | 9.08   | 2427935.827 | 930776.8369 | 350275.7882 | 952448.1348 | 624686.8593 | 1042967.864 | 599131.21 | 870917.9286 | 638806.7704 | 6284.407 |
| M_0338 | CAPROYL SARCOSINE   | C13 H25 N O3    | 243.1834 | 8.289  | 709201.8682 | 826541.847  | 850192.9756 | 602006.6691 | 360729.5557 | 935691.7708 | 789017.36 | 2008484.796 | 756580.1339 | 362779.4 |



|        |  |                  |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0339 | N-[2-(1-Cyclohexen-1-yl)ethyl]-4,6-di(4-morpholinyl)-1,3,5-triazin-2-amine               | C19 H30 N6 O2    | 374.2433 | 9.356  | 239674.9167 | 360128.7055 | 171060.8362 | 399578.2881 | 264642.2145 | 391407.7089 | 230594.24 | 276913.7672 | 207197.5473 | 71385.77 |
| M_0340 | 2-((3-(Dodecyloxy)propyl)(2-(2-hydroxyethoxy)ethyl)amino)ethanol                         | C21 H45 N O4     | 375.335  | 10.461 | 939226.5861 | 1612936.64  | 1294980.659 | 1113169.523 | 1654117.317 | 1216162.28  | 1575103.3 | 1566654.2   | 1340029.18  | 8075.591 |
| M_0341 | hodgekinsine   | C33 H38 N6       | 518.318  | 10.137 | 108526.058  | 647990.3638 | 107591.1706 | 1571429.483 | 703519.9204 | 713523.0761 | 387630.72 | 792079.203  | 895407.8939 | 1336.337 |
| M_0342 | DL-Glutamine   | C5 H10 N2 O3     | 146.0692 | 1.582  | 2397993.388 | 526644.4086 | 621472.1846 | 520800.5182 | 506661.8337 | 608356.4408 | 627137.35 | 204773.2397 | 338269.0941 | 4233.292 |
| M_0343 | Amdoxovir  | C9 H12 N6 O3     | 252.0973 | 7.523  | 88085.44521 | 41339.20362 | 1593634.938 | 26486.65956 | 128216.9183 | 31836.53313 | 90505.299 | 80805.60091 | 1724202.913 | 114075   |
| M_0344 | Heptanoic anhydride  | C14 H26 O3       | 242.1881 | 8.997  | 2386209.981 | 371849.2588 | 45310.69264 | 420962.4583 | 102405.6514 | 532840.8898 | 411389.38 | 474842.4495 | 419665.8879 | 92477.44 |
| M_0345 | p-Decyloxybenzaldehyde   | C17 H26 O2       | 262.1931 | 8.777  | 1192848.968 | 1864557.413 | 857155.682  | 1046469.063 | 901297.1395 | 2368488.504 | 1246463   | 1642204.588 | 964215.8238 | 6932.205 |
| M_0346 | Ethyl 3-isopropyl-1H-pyrazole-5-carboxylate  | C9 H14 N2 O2     | 182.1055 | 2.441  | 2368239.347 | 110414.4008 | 84901.79342 | 177206.8388 | 113388.9002 | 37088.35802 | 22711.106 | 25926.369   | 43816.29388 | 4616.677 |
| M_0347 | (2-Oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)acetic acid                                    | C10 H9 N O4      | 207.0531 | 5.316  | 2349614.757 | 382516.9316 | 571607.6467 | 487087.5144 | 406547.6901 | 520535.3789 | 351854.42 | 425356.3311 | 260194.1207 | 8375.5   |
| M_0348 | 1,1,1-Trifluoroacetone   | C3 H3 F3 O       | 112.0139 | 1.13   | 734697.1036 | 1907673.746 | 1763490.218 | 1922465.909 | 2060037.884 | 1404993.804 | 996310.43 | 1418031.939 | 995493.0721 | 11767.25 |
| M_0349 | Phthalic anhydride   | C8 H4 O3         | 148.0161 | 8.959  | 1100791.12  | 1134521.947 | 1584625.133 | 2076056.383 | 1881695.062 | 1945358.809 | 1542741.4 | 1421479.436 | 1734115.724 | 368663   |
| M_0350 | Inosine 5'-monophosphate (IMP)   | C10 H13 N4 O8 P  | 348.0472 | 2.161  | 6480.789235 | 39597.91894 | 3957.284893 | 50020.52979 | 51994.97036 | 83838.5685  | 68298.101 | 108325.4984 | 74757.68761 | 4207.167 |
| M_0351 | Arachidonoyl amide   | C20 H33 N O      | 303.2537 | 9.96   | 118825.3349 | 144055.2493 | 224590.128  | 51815.73448 | 108117.1665 | 256567.4354 | 69475.708 | 53711.09011 | 110746.2669 | 14932.37 |
| M_0352 | 5-O-methyl embelin   | C18 H28 O4       | 308.1985 | 8.746  | 1191295.478 | 1480018.461 | 1545829.036 | 1314298.437 | 1778207.885 | 2136525.959 | 1310894.5 | 1991455.013 | 1473462.02  | 117842.2 |
| M_0353 | Pregabalin   | C8 H17 N O2      | 159.126  | 5.121  | 798720.3036 | 797188.6123 | 758050.6257 | 849666.9046 | 655819.5825 | 840668.5268 | 686542.64 | 788797.8383 | 537333.4604 | 3454.745 |
| M_0354 | 3H-1,2,3-triazolo[4,5-d]pyrimidine-5,7-diamine   | C4 H5 N7         | 151.061  | 1.099  | 561931.1389 | 856366.0132 | 1301004.907 | 932024.4324 | 1364145.444 | 1968745.504 | 1834251.5 | 1773437.622 | 1486690.536 | 1815.263 |
| M_0355 | FZ5600000  | C27 H44          | 368.3443 | 9.371  | 207754.5737 | 765663.8655 | 7627.235169 | 500340.6995 | 1921632.794 | 91611.38478 | 105684.76 | 221951.4415 | 857537.8388 | 4066.189 |
| M_0356 | 4123225  | C4 H11 Li Si     | 94.07885 | 7.853  | 24406.70426 | 537484.0448 | 49044.53602 | 88170.7648  | 532037.6444 | 475647.2833 | 1483034.2 | 55850.89105 | 220235.782  | 104965.4 |
| M_0357 | Furazano[3,4-b]pyrazine, 5,6-bis(diethylamino)-  | C12 H20 N6 O     | 264.1701 | 8.983  | 2299630.271 | 364166.6383 | 36409.73122 | 403381.2586 | 95236.87668 | 540126.5166 | 419505.17 | 465136.8049 | 405013.8295 | 86144.82 |
| M_0358 | Acetophenone   | C8 H8 O          | 120.058  | 2.451  | 2297578.287 | 1322907.173 | 2323325.172 | 1395650.787 | 1167595.844 | 1514875.871 | 1384353.9 | 1270110.437 | 978648.0603 | 5335.791 |
| M_0359 | Nicotinamide   | C6 H6 N2 O       | 122.0483 | 1.329  | 11169.03092 | 109600.3802 | 14040.2432  | 8746.147088 | 3420.603604 | 11229.18995 | 3383.666  | 22847.52177 | 9678.925531 | 5654.833 |
| M_0360 | N-Methyl-N-(1,2,2,6,6-pentamethylpiperidin-4-yl)-4-tetrazol-1-ylbenzamide                | C19 H28 N6 O     | 356.2327 | 9.402  | 172916.3249 | 301686.9696 | 91289.2064  | 307993.9661 | 102685.4296 | 296457.5563 | 97134.347 | 198663.7078 | 44079.84988 | 5153.75  |
| M_0361 | Phloroglucinol   | C6 H6 O3         | 126.0296 | 1.967  | 1324613.059 | 676323.7093 | 612667.2145 | 583635.8544 | 583169.0792 | 917604.8487 | 1081918.8 | 1074959.359 | 738632.5788 | 50599.93 |
| M_0362 | 172966   | C11 H9 N O3      | 203.0583 | 2.479  | 23511.54479 | 13794.864   | 21441.94933 | 14908.14565 | 12779.41105 | 15139.59268 | 8254.4852 | 14741.18671 | 11333.55404 | 5738.27  |
| M_0363 | fluorophenyl)-3-fluorophenyl)-3-   | C11 H11 Cl F N O | 227.0558 | 7.262  | 1567033.592 | 609648.5417 | 871210.2195 | 1184034.333 | 1016176.045 | 599150.3638 | 146633.7  | 103094.7044 | 56066.82392 | 4841.492 |
| M_0364 | 2080745  | C9 H20 N2 O2     | 188.1525 | 0.885  | 557941.5933 | 260159.3257 | 238944.1056 | 237734.0927 | 298087.1689 | 216938.1981 | 189660.89 | 149510.0018 | 99001.90221 | 3119.56  |
| M_0365 | Rimexolone   | C24 H34 O3       | 370.2507 | 8.488  | 10444.04359 | 9191.477112 | 26266.45677 | 2264775.539 | 20072.47109 | 64235.12362 | 69119.361 | 137227.6982 | 80612.91905 | 6602.076 |
| M_0366 | MFC000216577   | C9 H13 N3 Si     | 191.0885 | 3.416  | 13796.01653 | 15554.58817 | 16552.05061 | 18603.20636 | 18433.59392 | 18521.66161 | 23757.557 | 23390.14411 | 18941.55667 | 7235.943 |
| M_0367 | Octahydro-1,2,8-indolizinetriol  | C8 H15 N O3      | 173.1053 | 7.174  | 148543.0276 | 108748.7528 | 19542.53245 | 442799.7651 | 134579.4704 | 652653.0037 | 177317.11 | 236858.2013 | 143694.5749 | 4800.572 |
| M_0368 | procodazole  | C10 H10 N2 O2    | 190.0742 | 2.414  | 5728.299461 | 13835.07911 | 12695.66916 | 8827.037223 | 7566.62429  | 40534.76299 | 8848.2306 | 22798.44406 | 4898.40189  | 3378.649 |
| M_0369 | monomethyl phosphate   | C H5 O4 P        | 111.9929 | 1.73   | 80969.03434 | 47988.39027 | 53021.0091  | 44472.49894 | 38654.20355 | 45753.52115 | 43813.06  | 40475.69776 | 50446.27593 | 18384.18 |
| M_0370 | 2-[2-(2,6-Dimethylmorpholino)-2-oxoethoxy]phenyl N,N-dimethylcarbamate                   | C17 H24 N2 O5    | 336.17   | 8.972  | 1221265.486 | 940714.795  | 887432.5522 | 2213453.512 | 463284.2318 | 922173.6925 | 662074.42 | 1354286.338 | 858602.9728 | 5173.741 |
| M_0371 | Linoleamide  | C18 H33 N O      | 279.2561 | 9.628  | 28393.1119  | 98212.92913 | 134746.1177 | 65074.15878 | 166162.4028 | 203249.4939 | 50661.039 | 71224.82684 | 106646.7862 | 16766.76 |
| M_0372 | Diethyl N-palmitoylglutamate   | C25 H47 N O5     | 441.3455 | 8.251  | 2199058.009 | 331678.9328 | 255462.9368 | 815053.9106 | 282660.3389 | 895603.6846 | 772681.7  | 955124.1347 | 473842.6437 | 7749.288 |
| M_0373 | Docosahexaenoic acid   | C22 H32 O2       | 328.2401 | 10.018 | 1610809.751 | 655627.7956 | 607565.9454 | 567934.1397 | 1000384.024 | 1349649.68  | 920314.66 | 1392368.184 | 968271.2807 | 17722.85 |
| M_0374 | 2,6-Ditert-butylhexahydro-1H,5H-2,3a,4a,6,7a,8a-hexaazacyclopenta[d]effluorene-4,8-dione | C16 H28 N6 O2    | 336.2278 | 9.009  | 1665402.529 | 1645027.296 | 262072.385  | 1131923.922 | 550105.3287 | 1037574.655 | 667902.85 | 828293.5199 | 874238.4117 | 108290.1 |
| M_0375 | Cafaminol  | C11 H17 N5 O3    | 267.133  | 1.594  | 2195779.353 | 733027.0189 | 39424.45443 | 379693.1964 | 98226.23997 | 407204.1338 | 212907.37 | 635245.1456 | 117392.1413 | 4393.161 |
| M_0376 | Glycidyl Stearate  | C21 H40 O3       | 340.2977 | 10.414 | 102041.5972 | 575945.9265 | 629189.8381 | 1212073.54  | 1712709.902 | 276801.0525 | 239216.02 | 904156.3052 | 1321939.893 | 2042.757 |
| M_0377 | Thromboxane B1   | C20 H36 O6       | 788.4507 | 8.427  | 888989.7026 | 1323697.333 | 795520.6005 | 1430121.798 | 1271628.14  | 1461037.618 | 1919074.8 | 1862810.922 | 747866.4902 | 6038.944 |
| M_0378 | 3-[1,3,3-Tris(allyloxy)propoxy]-1-propene  | C15 H24 O4       | 268.1673 | 8.565  | 752791.1105 | 240925.7049 | 498694.9277 | 558863.1607 | 320548.1698 | 656552.2056 | 648393.71 | 481935.6045 | 371237.8086 | 241454   |
| M_0379 | Bis(4-ethylbenzylidene)sorbitol  | C24 H30 O6       | 414.2042 | 8.675  | 1252357.747 | 915174.5205 | 959376.6341 | 1134587.504 | 1460351.702 | 1397043.285 | 751672.91 | 929700.5714 | 1715237.394 | 14894.53 |
| M_0380 | 5-Nitro-2-thiophenecarboxylic acid   | C5 H3 N O4 S     | 172.9777 | 7.504  | 98448.35816 | 62729.45116 | 271283.7997 | 28133.68824 | 250439.0442 | 595567.0397 | 98579.257 | 154502.0662 | 45975.96288 | 87434.35 |
| M_0381 | Cafestol   | C20 H28 O3       | 316.2014 | 9.055  | 352193.1175 | 330918.2838 | 183753.4288 | 262232.446  | 158532.7335 | 206556.7688 | 387396.08 | 320740.2921 | 382305.4308 | 24764.09 |
| M_0382 | 1-Adamantanol  | C10 H16 O        | 152.1203 | 8.729  | 69377.46983 | 360528.1144 | 8183.49588  | 25370.32105 | 47037.86242 | 15225.81319 | 36840.884 | 17921.81092 | 30322.58146 | 18013.79 |
| M_0383 | Acetyl-L-carnitine   | C9 H17 N O4      | 203.1157 | 1.558  | 2132967.852 | 625008.2505 | 662139.719  | 1254449.447 | 69693.09921 | 1362966.69  | 752437.87 | 323884.315  | 287189.0165 | 3397.722 |

|        |   |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0384 | (1Z,5Z)-1,5-Cyclooctadiene  | C8 H12         | 108.0943 | 8.658 | 850611.1462 | 406366.5167 | 524686.3206 | 317363.8364 | 653438.9292 | 780135.7445 | 402671.65 | 711928.8503 | 552447.3214 | 321538.7 |
| M_0385 | Methyl 8-(8-hexyl-2-methyl-1,3-dioxo-2,3,5,8-tetrahydro-1H-[1,2,4]triazolo[1,2-a]pyridazin-5-yl)octanoate | C22 H37 N3 O4  | 407.2782 | 8.422 | 1174214.763 | 930370.4689 | 936936.6329 | 1131364.533 | 1918883.54  | 1743063.626 | 1700839.2 | 1743102.268 | 1282227.275 | 5567.495 |
| M_0386 | mephenesin  | C10 H14 O3     | 182.0944 | 7.763 | 129202.6692 | 93090.06248 | 9457.435412 | 35230.97073 | 1365021.22  | 424351.7088 | 179095.54 | 88652.07131 | 156848.5438 | 214518.7 |
| M_0387 | 1-Linoleoyl glycerol  | C21 H38 O4     | 354.2769 | 9.644 | 146654.4326 | 938758.1008 | 780316.5728 | 607289.1743 | 2110805.831 | 1118439.571 | 951364.6  | 854252.409  | 984585.7    | 52109.71 |
| M_0388 | halimedin   | C10 H16 N6 O   | 236.1385 | 8.376 | 850228.2581 | 35705.73129 | 64198.79785 | 54120.77704 | 33156.2143  | 69940.2402  | 64544.944 | 67762.37193 | 69655.21543 | 107294.7 |
| M_0389 | Ethyl N-(thioxomethylene)valinate   | C8 H13 N O2 S  | 187.0667 | 5.581 | 1905709.786 | 315292.6607 | 67047.28223 | 2088553.7   | 415367.8241 | 981817.3525 | 608103.12 | 706411.8387 | 263017.2539 | 8723.931 |
| M_0390 | Linoleyl carnitine  | C25 H45 N O4   | 423.335  | 8.254 | 2080489.573 | 318189.1429 | 252898.0511 | 780011.0875 | 268573.2082 | 830953.0181 | 718246.93 | 903497.281  | 455100.997  | 3854.532 |
| M_0391 | L-Tyrosine  | C9 H11 N O3    | 181.074  | 1.312 | 2080201.45  | 1410376.86  | 85744.19945 | 1424724.845 | 890612.816  | 166085.0324 | 127163.52 | 155321.0933 | 860747.1312 | 2286.707 |
| M_0392 | 2,4-Diamino-6-pteridinecarbaldehyde   | C7 H6 N6 O     | 190.0606 | 7.032 | 179973.9079 | 115100.7619 | 1314207.033 | 2069713.47  | 263033.3089 | 310604.8127 | 50741.943 | 38414.7234  | 176281.8842 | 138394.1 |
| M_0393 | butyl acrylate  | C7 H12 O2      | 128.0839 | 8.008 | 83157.16055 | 101605.7346 | 117803.8176 | 86281.1167  | 679656.9417 | 377832.322  | 1149057.7 | 260731.5769 | 430221.8531 | 126310.2 |
| M_0394 | D-PANTOTHENIC ACID  | C9 H17 N O5    | 219.1106 | 3.204 | 2062107.852 | 49067.80437 | 269031.9656 | 59322.24058 | 1346214.302 | 213321.7784 | 23272.295 | 10529.76946 | 619391.4145 | 129.8734 |
| M_0395 | 1-arachidonoyl-sn-glycero-3-phosphocholine  | C28 H50 N O7 P | 543.3345 | 9.916 | 27728.97539 | 83894.37611 | 2061422.226 | 48898.15305 | 153763.705  | 67400.9178  | 163053.53 | 177475.8482 | 141004.8472 | 1405.356 |
| M_0396 | Propionylcarnitine  | C10 H19 N O4   | 217.1313 | 1.196 | 1232346.925 | 1198764.946 | 991034.2403 | 1647383.021 | 1054422.237 | 1519729.254 | 1396623.1 | 1029780.576 | 1083022.51  | 3827.621 |
| M_0397 | (+/-)-12-HpETE  | C20 H32 O4     | 318.2171 | 9.005 | 1558333.226 | 1553731.769 | 196427.4135 | 1083466.201 | 476404.5684 | 992001.2736 | 608632.68 | 759887.7764 | 816296.8436 | 52760.87 |
| M_0398 | Cuminaldehyde   | C10 H12 O      | 148.0889 | 8.534 | 390112.0591 | 823153.5956 | 700386.3091 | 649550.5748 | 946029.4879 | 385224.9352 | 1079267.7 | 2007602.045 | 629952.656  | 214479.8 |
| M_0399 | 3-[[[2-Aminoethoxy](hydroxy)phosphoryloxy]-2-hydroxypropyl]palmitate                                      | C21 H44 N O7 P | 453.2857 | 9.48  | 362388.3721 | 1261016.83  | 1627012.453 | 1644629.232 | 1533726.432 | 1480952.795 | 1482885.8 | 1368679.773 | 972325.0221 | 9224.36  |
| M_0400 | 1-Methyl-1H-purin-1-ium   | C6 H7 N4       | 135.0661 | 4.426 | 20627.75844 | 10439.33941 | 27218.1416  | 39681.16465 | 21919.25783 | 22864.14817 | 21711.943 | 34857.55824 | 25768.98827 | 28814.97 |
| M_0401 | Gramine   | C11 H14 N2     | 129.058  | 6.04  | 2984.821243 | 3673.830868 | 2347.346637 | 2895.369938 | 2393.496078 | 2836.188415 | 3800.3483 | 2430.830173 | 3282.383759 | 2470.67  |
| M_0402 | Creatinine  | C4 H7 N3 O     | 113.0593 | 1.155 | 1986119.592 | 423027.7202 | 453301.3422 | 763572.493  | 650289.9185 | 367597.4443 | 116744.83 | 15596.07897 | 15185.72929 | 8890.844 |
| M_0403 | 1,1-Dimethyl-3-(2H-tetrazol-5-yl)urea   | C4 H8 N6 O     | 156.0763 | 3.593 | 446860.8656 | 607956.5616 | 293852.3721 | 909720.4679 | 986075.6029 | 1114777.705 | 1081612.2 | 1183131.416 | 1974926.736 | 64206.74 |
| M_0404 | 1-carboxy-3-hydroxyadamantane   | C11 H16 O3     | 196.1101 | 7.785 | 281100.2319 | 40787.1446  | 36154.84649 | 22021.54125 | 815751.6523 | 50691.58905 | 24038.735 | 328568.1261 | 359404.3645 | 27500.29 |
| M_0405 | gamma-Aminobutyric acid   | C4 H9 N O2     | 103.0638 | 1.32  | 1966521.646 | 246194.8008 | 238979.6852 | 442106.1283 | 505476.9293 | 343345.3903 | 300060.91 | 324435.786  | 284161.3667 | 72571.34 |
| M_0406 | Sebacic acid  | C10 H18 O4     | 202.1205 | 7.954 | 881297.8199 | 170087.7767 | 362675.0494 | 227495.7453 | 380403.3296 | 444806.2904 | 309263.97 | 352489.841  | 141582.1854 | 218916.6 |
| M_0407 | Dibenzothiophene  | C12 H8 S       | 184.0348 | 1.249 | 167346.4926 | 878506.2018 | 1072210.329 | 478380.6677 | 806735.1018 | 1930116.116 | 51569.785 | 833901.5485 | 1131989.414 | 48639.4  |
| M_0408 | Phosphoramidocyanidic acid  | C H3 N2 O2 P   | 105.9938 | 0.792 | 1609079.792 | 880000.5749 | 682620.9422 | 1443056.656 | 838830.9663 | 861834.5924 | 704435.75 | 740874.4407 | 502477.7386 | 14722.79 |
| M_0409 | Leucylproline   | C11 H20 N2 O3  | 187.1207 | 1.234 | 1904623.153 | 183740.2567 | 855048.6837 | 265057.1895 | 122000.4588 | 196628.7317 | 131096.6  | 161245.1952 | 119768.1036 | 2112.022 |
| M_0410 | 6-(1-Piperidiny)[1,2,5]oxadiazolo[3,4-b]pyrazin-5-amine   | C9 H12 N6 O    | 220.1075 | 8.007 | 140539.3929 | 11222.60561 | 27917.06289 | 221442.7355 | 1898196.595 | 311986.9111 | 267692.73 | 248332.9127 | 234493.8576 | 295850.5 |
| M_0411 | N-Methyl-6-[methyl(propylcarbamoyl)amino]-1,2,4-triazine-5-carboxamide                                    | C10 H16 N6 O2  | 252.1337 | 8.025 | 190303.0279 | 39078.39772 | 127055.2059 | 91683.55264 | 1893052.663 | 202191.9726 | 207420.38 | 140990.7392 | 320716.7542 | 162282.3 |
| M_0412 | Methyl alpha-aspartylphenylalaninate  | C14 H18 N2 O5  | 294.1215 | 4.885 | 930311.2789 | 923952.6626 | 1878028.786 | 1284088.416 | 805687.2629 | 802241.5132 | 709903.24 | 954453.7    | 548042.4887 | 5396.26  |
| M_0413 | DL-Ornithine  | C5 H12 N2 O2   | 132.09   | 0.816 | 1876579.737 | 580103.3683 | 1006342.345 | 465800.0121 | 445360.5959 | 466397.5979 | 509632.27 | 528030.4108 | 558822.0011 | 10610.56 |
| M_0414 | D-(+)-Pyroglutamic Acid   | C5 H7 N O3     | 129.0427 | 1.617 | 1286446.017 | 1298942.659 | 705067.9056 | 1075659.822 | 944954.4463 | 1119851.021 | 1009521.3 | 1795888.28  | 564271.4735 | 18221.85 |
| M_0415 | Benzoxazole   | C7 H5 N O      | 119.0375 | 6.211 | 97035.36959 | 38631.28139 | 88389.48399 | 93898.94663 | 3818.387996 | 69451.94141 | 60972.071 | 39945.03253 | 4838.420724 | 1651.215 |
| M_0416 | LysoPC(18:3(9Z,12Z,15Z))  | C26 H48 N O7 P | 517.3146 | 9.383 | 1837424.34  | 204144.1504 | 213173.0364 | 129769.6066 | 314409.8714 | 412920.1089 | 326327.49 | 1870475.592 | 501234.3692 | 195338.4 |
| M_0417 | Tris(((2-aminoethyl)amino)methyl)phenol   | C15 H30 N6 O   | 310.2483 | 9.428 | 678702.6605 | 848797.2015 | 581816.2258 | 390199.6802 | 711360.7957 | 479940.2869 | 939415.84 | 148765.4179 | 971813.2846 | 4301.152 |
| M_0418 | 5-Hydroxy-DL-tryptophan   | C11 H12 N2 O3  | 220.0847 | 2.519 | 584.7125282 | 1387.721538 | 454.9970781 | 961.2286441 | 351.2355752 | 560.8520971 | 952.70567 | 341.5440783 | 866.810132  | 231.8586 |
| M_0419 | Tris(((2-aminoethyl)amino)methyl)phenol   | C15 H30 N6 O   | 310.2483 | 9.514 | 678702.6605 | 848797.2015 | 581816.2258 | 390199.6802 | 711360.7957 | 479940.2869 | 939415.84 | 1311628.495 | 971813.2846 | 61413.6  |
| M_0420 | Leucylproline   | C11 H20 N2 O3  | 228.1473 | 1.234 | 1847191.906 | 304624.8992 | 911236.0376 | 571204.3654 | 235867.3019 | 258535.6826 | 194483.67 | 250295.9086 | 154356.8512 | 3566.417 |
| M_0421 | Leu-Val   | C11 H22 N2 O3  | 230.1631 | 2.61  | 6302.242279 | 4347.61536  | 4594.477123 | 4917.910303 | 5113.319663 | 4781.675597 | 4818.6823 | 5312.598064 | 4162.854471 | 4441.057 |
| M_0422 | Triacetylspingosine   | C24 H43 N O5   | 425.3142 | 8.815 | 78980.33162 | 137028.6357 | 754914.3447 | 1840701.402 | 181111.0142 | 201184.7214 | 251051.32 | 425834.9853 | 323997.3118 | 4080.434 |
| M_0423 | 4329  | C9 H12 O       | 136.0889 | 7.834 | 167096.3911 | 71453.21798 | 78795.68345 | 35509.92868 | 57906.46849 | 762844.7834 | 158586.51 | 15088.78071 | 24058.36612 | 35553.42 |
| M_0424 | A-134U  | C8 H12 N6 O2   | 224.1024 | 7.983 | 830336.7218 | 143168.6108 | 337540.2999 | 230764.7199 | 350495.5744 | 278395.1008 | 283857.83 | 330813.3174 | 147764.3535 | 215425.3 |
| M_0425 | Creatine  | C4 H9 N3 O2    | 131.0696 | 1.966 | 820230.8939 | 664704.0537 | 310433.3643 | 1111547.788 | 519308.8834 | 1106952.502 | 821146.28 | 831673.2201 | 345384.1566 | 5049.733 |
| M_0426 | Choline   | C5 H13 N O     | 103.1002 | 9.803 | 138104.6806 | 304042.358  | 316775.9456 | 202587.9025 | 173546.8009 | 121848.6904 | 175708.58 | 105497.2404 | 209623.7044 | 7660.545 |
| M_0427 | (E)-di-tert-butyl diazene-1,2-dicarboxylate   | C10 H18 N2 O4  | 230.1266 | 3.166 | 1820044.763 | 295390.7704 | 306438.5423 | 445614.6962 | 209117.054  | 111046.718  | 122443.06 | 87246.05494 | 70974.85639 | 5171.459 |
| M_0428 | 5-Hydroxydecanoic acid  | C10 H20 O3     | 188.1415 | 8.184 | 5740.720512 | 3939.357273 | 3160.107164 | 4652.80408  | 5260.573261 | 4439.190499 | 5948.8455 | 6645.938942 | 8269.745842 | 16862.66 |
| M_0429 | 4,6-Bis(ethylamino)-1,3,5-triazine-2-carboxamide  | C8 H14 N6 O    | 210.1233 | 8.197 | 1842.917181 | 1561.805405 | 1574.700068 | 1399.625519 | 4229.519598 | 9257.317671 | 2141.1386 | 1962.610819 | 2059.122393 | 15174.79 |
| M_0430 | Cuminaldehyde   | C10 H12 O      | 148.0889 | 8.687 | 1506921.392 | 974986.0353 | 887203.3323 | 1315239.653 | 1669639.336 | 1396833.985 | 711639.65 | 1120689.381 | 1807974.067 | 35872.93 |

|        |   |                |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0431 | Leucylproline   | C11 H20 N2 O3  | 228.1473 | 1.616  | 1806792.26  | 657930.5861 | 757665.705  | 817818.773  | 592635.2723 | 546378.3668 | 274540    | 369823.1158 | 297491.2028 | 4099.486 |
| M_0432 | Indole  | C8 H7 N        | 117.0583 | 7.867  | 3249.642756 | 2949.066284 | 2777.247151 | 3121.348786 | 4323.336212 | 4125.008776 | 3280.681  | 3318.626922 | 3420.154585 | 4227.468 |
| M_0433 | Elaidolinolenic acid  | C18 H30 O2     | 278.2245 | 9.005  | 1009597.607 | 920826.265  | 202694.6044 | 675469.8633 | 369324.7947 | 652055.9458 | 416603.56 | 535136.8006 | 451963.8747 | 1503.365 |
| M_0434 | 1-Hexadecanoylpyrrolidine   | C20 H39 N O    | 309.3031 | 10.532 | 71423.3176  | 98270.9501  | 164134.2718 | 129785.757  | 123994.1009 | 315397.6698 | 111820.1  | 121276.2067 | 260879.0683 | 11450.55 |
| M_0435 | Leucylproline   | C11 H20 N2 O3  | 228.1473 | 1.211  | 1786585.498 | 176556.0827 | 144242.2901 | 258296.7069 | 115462.8364 | 189642.1443 | 124978.78 | 155430.0654 | 114210.9389 | 766.2685 |
| M_0436 | DEMP  | C5 H13 O3 P    | 152.0605 | 6.145  | 844.8137318 | 810.6165164 | 902.6596523 | 888.7016509 | 863.6369248 | 865.4607171 | 874.38916 | 872.7335346 | 845.645839  | 852.9047 |
| M_0437 | all-trans-retinal (12,5Z)-1,5-Cyclooctadiene  | C20 H28 O      | 284.2141 | 9.1    | 1370302.692 | 696057.8463 | 402917.2219 | 724569.2867 | 512483.6998 | 727015.1056 | 537009.53 | 673703.9503 | 461758.6646 | 141821.8 |
| M_0438 | (12,5Z)-1,5-Cyclooctadiene  | C8 H12         | 108.0944 | 8.284  | 372121.0881 | 207357.6015 | 858201.701  | 182107.4327 | 147639.2567 | 352913.1214 | 1018121.9 | 1339010.464 | 175544.8342 | 26712.46 |
| M_0439 | Cyclooctadiene  | C8 H12         | 108.0943 | 8.36   | 372121.0881 | 235436.0857 | 242442.9272 | 253271.3908 | 266648.5024 | 292975.8364 | 295379.18 | 286097.3947 | 39882.79266 | 290120.9 |
| M_0440 | DL-Tryptophan   | C11 H12 N2 O2  | 226.0717 | 3.492  | 877998.2734 | 1284089.8   | 1451676.55  | 1395288.42  | 1486443.256 | 1440163.793 | 1181396.2 | 1768512.9   | 1382819.143 | 3891.219 |
| M_0441 | DL-Arginine   | C6 H14 N4 O2   | 174.1117 | 1.263  | 451979.5031 | 209619.9933 | 234382.0918 | 50905.68235 | 222802.3816 | 144549.9944 | 244978.54 | 235563.4768 | 185426.1938 | 1820.155 |
| M_0442 | .alpha.-Amino adipic acid   | C6 H11 N O4    | 161.0688 | 1.125  | 1742789.72  | 634383.3222 | 422866.1165 | 427936.7362 | 377428.4863 | 741502.121  | 833115.33 | 689500.1924 | 636747.1036 | 4867.829 |
| M_0443 | 4253  | C12 H22 O2     | 198.162  | 9.224  | 930325.57   | 698459.2754 | 1006348.907 | 1297146.853 | 1709691.602 | 1637747.083 | 1065241.3 | 1223246.742 | 1485710.289 | 84051.08 |
| M_0444 | 1-Adamantanemethanol  | C11 H18 O      | 166.1358 | 8.661  | 843285.0958 | 836065.0365 | 896515.9105 | 1181853.378 | 1411614.753 | 1419450.729 | 602032.42 | 1229962.429 | 1729433.084 | 206107.3 |
| M_0445 | Indole  | C8 H7 N        | 117.058  | 3.495  | 605042.3077 | 843427.9292 | 919004.743  | 1155697.144 | 1061929.847 | 1359145.408 | 1597804.9 | 1710852.19  | 1236667.191 | 6710.744 |
| M_0446 | 3H-1,2,3-triazolo[4,5-d]pyrimidine-5,7-diamine  | C4 H5 N7       | 151.0609 | 1.205  | 1695383.039 | 687353.402  | 928191.3897 | 735129.3442 | 603665.0574 | 233635.7531 | 257283.66 | 298793.863  | 189130.9379 | 4001.969 |
| M_0447 | 3-Hydroxy-L-proline   | C5 H9 N O3     | 131.0584 | 2.019  | 1604814.156 | 946339.7747 | 1691076.541 | 877556.2615 | 816379.1111 | 544885.6534 | 366949.84 | 746234.6273 | 333981.0721 | 6006.934 |
| M_0448 | FZ5600000   | C27 H44        | 368.3442 | 9.132  | 530537.8932 | 1255120.981 | 107553.2964 | 271770.1791 | 15152.34342 | 171019.4623 | 347133.11 | 240519.363  | 591557.1077 | 6193.143 |
| M_0449 | 2,4-Pyridinedicarboximidamide   | C7 H11 N7      | 193.1077 | 6.904  | 266309.077  | 209409.1758 | 713076.8482 | 142615.5622 | 656535.0871 | 616624.9026 | 153123.14 | 764821.5334 | 285774.9868 | 30199.42 |
| M_0450 | Nicotinamide  | C6 H6 N2 O     | 122.0483 | 1.227  | 17606.11178 | 15164.22604 | 15810.17377 | 14804.61943 | 13786.01553 | 14756.99169 | 13367.425 | 13575.79675 | 12688.03099 | 10783.52 |
| M_0451 | Acetic propanoic anhydride  | C5 H8 O3       | 116.0477 | 1.416  | 38134.385   | 280077.4152 | 590606.4194 | 113837.3997 | 122388.3682 | 484678.0806 | 816661.31 | 318819.6564 | 429333.1144 | 108323.2 |
| M_0452 | bendiocarb  | C11 H13 N O4   | 223.0844 | 4.827  | 1659791.359 | 64038.93592 | 102996.585  | 155206.6775 | 20038.91525 | 72884.23016 | 61367.143 | 64392.927   | 42104.5624  | 6448.037 |
| M_0453 | DEET  | C12 H17 N O    | 191.131  | 8.23   | 809225.1906 | 600018.3139 | 695144.7404 | 686473.3766 | 828447.4071 | 1524921.768 | 1106340.1 | 1260358.893 | 1119983.107 | 111057.6 |
| M_0454 | 1-S-Decyl-1-thiohexitol   | C16 H34 O5 S   | 338.2135 | 10.547 | 589666.1109 | 727674.8178 | 168822.8152 | 342692.349  | 466918.2734 | 645758.023  | 639393.9  | 699156.8304 | 870258.8263 | 22817.67 |
| M_0455 | Cumene  | C9 H12         | 120.0942 | 7.817  | 63090.94416 | 94438.69865 | 162681.6924 | 60802.79555 | 271155.0617 | 17462.20811 | 119479.27 | 297519.8116 | 116853.6498 | 162684.5 |
| M_0456 | 4,4'-di-tert-butylbiphenyl  | C20 H26        | 266.2033 | 9.104  | 742507.6473 | 66206.69044 | 24368.73517 | 73498.66521 | 33932.28608 | 67569.02464 | 57587.967 | 68070.90687 | 49298.01132 | 125772.8 |
| M_0457 | Triethyl Decyl 2-thienylacetate   | C7 H16 O3      | 148.11   | 5.334  | 68793.44225 | 94431.84318 | 297526.3116 | 1640239.735 | 453909.0548 | 456083.9307 | 94756.638 | 1005473.384 | 1220791.636 | 319938.8 |
| M_0458 | Decyl 2-thienylacetate  | C16 H26 O2 S   | 282.1653 | 7.751  | 969684.5073 | 283578.6209 | 513171.7873 | 551030.7531 | 685705.8198 | 1145148.654 | 770988    | 1622633.695 | 945319.8338 | 5049.604 |
| M_0459 | 3-[(2-Aminoethyl)amino]-1-(benzylamino)-7-ethyl-5,6,7,8-tetrahydro-2,7-naphthyridine-4-carbonitrile | C20 H26 N6     | 350.2221 | 10.017 | 1282946.604 | 451278.6266 | 434261.9905 | 395609.681  | 711763.5886 | 970339.1031 | 19269.914 | 970755.4989 | 696914.3165 | 13941.65 |
| M_0460 | 2-Hydroxy-3-(palmitoyloxy)propyl 2-(trimethylammonio)ethyl phosphate                                | C24 H50 N O7 P | 495.3331 | 9.848  | 7073.396439 | 629165.2245 | 712066.3264 | 32279.87938 | 842200.2947 | 525395.4372 | 311169.41 | 439042.3905 | 184798.9271 | 17393.98 |
| M_0461 | Phthalic acid   | C8 H6 O4       | 166.0267 | 8.966  | 756039.3133 | 792568.1351 | 1110486.172 | 1438848.118 | 1348227.537 | 1282097.225 | 1077697.5 | 1021724.888 | 1199771.546 | 284563   |
| M_0462 | CUS250000   | C8 H5 N O      | 131.0373 | 6.627  | 30206.5544  | 12003.66763 | 9029.40948  | 15901.20099 | 6301.829422 | 19535.27867 | 8527.5154 | 15562.08731 | 2463.896974 | 2971.134 |
| M_0463 | Cimaterol   | C12 H17 N3 O   | 219.137  | 6.022  | 2866.485075 | 2711.933419 | 2710.69781  | 2749.856716 | 2731.818848 | 2701.911224 | 2746.6029 | 2824.360697 | 2763.922478 | 2778.152 |
| M_0464 | Trigonelline  | C7 H7 N O2     | 96.02144 | 1.419  | 602587.0997 | 400536.4049 | 1606465.401 | 548874.4038 | 646039.2072 | 356510.1391 | 239253.39 | 257145.0727 | 192674.4117 | 22313.58 |
| M_0465 | quinbolone  | C24 H32 O2     | 352.2401 | 8.485  | 9092.809225 | 7991.287962 | 23627.46062 | 1601600.12  | 18907.99965 | 48241.56628 | 51668.682 | 91511.43335 | 54073.80975 | 9677.618 |
| M_0466 | AU8420000   | C22 H42 O8     | 434.2881 | 8.795  | 967620.3045 | 933732.2949 | 1101715.721 | 1137615.953 | 1082316.872 | 1162637.029 | 1113456.3 | 1153565.642 | 876713.0822 | 20794.56 |
| M_0467 | 1-Fluorosilane  | C5 H11 F Si    | 118.0616 | 7.867  | 11979.32863 | 2869.30337  | 2702.131401 | 3036.926176 | 4206.403645 | 4013.440339 | 3191.949  | 3228.868562 | 4250.597982 | 4108.754 |
| M_0468 | 8-{3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl}octanoic acid                                    | C18 H28 O3     | 292.2012 | 8.771  | 1593515.056 | 284034.0306 | 155261.3312 | 166549.1318 | 189496.6361 | 150924.5354 | 139330.02 | 234563.0515 | 109298.9472 | 95608.49 |
| M_0469 | 1-Dodecyl-2-pyrrolidinone   | C16 H31 N O    | 253.2405 | 9.443  | 7078.07271  | 7554.85624  | 8660.849239 | 10701.8367  | 7621.580741 | 8404.656935 | 8280.2301 | 9431.286672 | 8149.107637 | 9946.557 |
| M_0470 | 3-(imidazol-4-yl)-2-oxopropyl dihydrogen phosphate  | C6 H9 N2 O5 P  | 220.026  | 4.193  | 1575759.542 | 674929.1302 | 867712.7523 | 554955.1556 | 363567.3197 | 299101.3367 | 309589.71 | 456050.1381 | 297845.4685 | 8621.888 |
| M_0471 | procodazole   | C10 H10 N2 O2  | 190.0742 | 1.549  | 334943.3678 | 470785.1923 | 632301.8896 | 710444.7164 | 545630.2867 | 727522.1161 | 646312.83 | 592433.4248 | 545452.9021 | 17851.68 |
| M_0472 | METHOXYMETHYLME LAMINE  | C5 H10 N6 O    | 170.0918 | 5.356  | 61229.27742 | 84255.84473 | 282847.8317 | 1560199.965 | 424848.3161 | 437327.5771 | 86361.188 | 964444.8237 | 1162329.366 | 306155.5 |
| M_0473 | Palmitoylcarnitine  | C23 H45 N O4   | 399.335  | 8.317  | 1364083.182 | 208078.7003 | 243955.9651 | 829009.9507 | 488018.9179 | 968141.2522 | 749828.47 | 609962.627  | 509886.8851 | 5942.164 |
| M_0474 | 3-[1,3,3-Tris(allyloxy)propoxy]-1-propene bis(2-chloro-1-methylethyl) ether                         | C15 H24 O4     | 268.1673 | 8.384  | 348528.4609 | 215153.928  | 112859.5165 | 66747.15553 | 81307.96996 | 138272.1826 | 116171.87 | 202912.6307 | 98473.64923 | 39091.29 |
| M_0475 | methylethyl) ether  | C6 H12 Cl2 O   | 170.0262 | 0.596  | 72913.94085 | 68140.35955 | 72862.58543 | 74619.87811 | 64359.09198 | 1008421.654 | 1552409.8 | 1294604.576 | 968782.0489 | 59592.31 |
| M_0476 | metharbal   | C9 H14 N2 O3   | 198.1005 | 2.792  | 1549665.79  | 171933.0677 | 108565.8128 | 265081.7691 | 242761.3769 | 44805.40663 | 29352.124 | 29865.6851  | 39139.57055 | 5553.536 |
| M_0477 | Cinnamoylglycine N-Methyl-2-pyrrolidone   | C11 H11 N O3   | 205.0739 | 7.497  | 203617.2537 | 85692.56979 | 150517.7506 | 330010.3858 | 320410.4577 | 887095.3451 | 313577.17 | 477745.599  | 163072.6787 | 21235.17 |
| M_0478 | pyrrolidone   | C5 H9 N O      | 99.06893 | 3.253  | 336407.0206 | 331834.6404 | 633495.4746 | 653175.0728 | 357797.567  | 256650.9414 | 247127.9  | 380596.7591 | 433613.4048 | 71274.36 |
| M_0479 | 2729  | C9 H14 O2      | 154.0995 | 8.341  | 29176.5316  | 448198.6496 | 90396.89538 | 1327172.268 | 42319.1274  | 203498.7026 | 520354.9  | 146497.4241 | 118091.6395 | 39515.39 |
| M_0480 | 1913256   | C18 H30 O      | 262.2296 | 9.645  | 24661.88386 | 83233.52974 | 104935.4623 | 60131.28405 | 156355.3644 | 173327.5984 | 50206.731 | 76107.95585 | 103190.2265 | 12003.82 |

|        |   |                 |          |        |             |             |             |             |             |             |            |              |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|------------|--------------|-------------|----------|
| M_0481 | [4-[1-(1-cyclopentyl-5-tetrazolyl)propyl]-1-piperazinyl]-[2-furanyl]methanone | C18 H26 N6 O2   | 358.2119 | 8.881  | 1044191.033 | 990972.3419 | 762020.5493 | 1520430.427 | 885571.8364 | 1509770.818 | 1057474.6  | 1214172.275  | 880296.5703 | 6044.232 |
| M_0482 | 5-Amino-3-nitro-1H-1,2,4-triazole-1-carboxamide                               | C3 H4 N6 O3     | 172.0348 | 1.244  | 376185.6308 | 581414.6524 | 578338.2448 | 690141.8467 | 613263.5913 | 550530.0323 | 859652.13  | 724322.9095  | 649739.3935 | 3219.533 |
| M_0483 | N-methylethanolamine phosphate  | C3 H10 N O4 P   | 155.0349 | 1.472  | 68304.98262 | 34134.87907 | 29800.80523 | 23149.1881  | 7055.052248 | 23989.98242 | 1505646.5  | 28463.97002  | 1041060.547 | 4285.342 |
| M_0484 | 1-Cyclohexenecarboxylic Acid  | C7 H10 O2       | 126.0683 | 7.73   | 37406.19747 | 16331.65661 | 411560.06   | 491646.3382 | 22576.73707 | 91018.15668 | 382966.46  | 17330.08116  | 382267.9151 | 122335.2 |
| M_0485 | Imidazosagatriazine   | C17 H20 N4 O2   | 290.1729 | 8.169  | 791939.8617 | 666561.9133 | 819524.3018 | 518217.6497 | 884676.5135 | 1312237.505 | 977969.5   | 1169797.922  | 924962.3645 | 110437.2 |
| M_0486 | Thieno[3,4-d]-1,3-dithiol-2-thione  | C5 H2 S4        | 189.9047 | 0.974  | 48783.96738 | 76420.91358 | 13200.34617 | 63824.38537 | 54928.33013 | 11330.30904 | 37442.65   | 22230.46718  | 29435.64858 | 3451.702 |
| M_0487 | 4-Nitroaniline  | C6 H6 N2 O2     | 138.043  | 1.136  | 998612.6011 | 1488485.576 | 51952.60055 | 259077.1831 | 174072.7921 | 704231.6101 | 379262     | 525633.1357  | 438853.721  | 3568.302 |
| M_0488 | 2-(4-Chlorophenyl)-1,3-dithiolane   | C9 H9 Cl S2     | 215.9833 | 8.4    | 38745.5254  | 30078.26095 | 35601.98914 | 34736.71591 | 35059.01773 | 42514.17278 | 41576.822  | 40120.91429  | 39947.8912  | 20129.11 |
| M_0489 | Thymine   | C5 H6 N2 O2     | 126.0432 | 3.003  | 919573.3961 | 706333.995  | 1483273.649 | 1055617.28  | 1102553.908 | 943014.7289 | 942569.57  | 1194704.953  | 997169.0807 | 4199.714 |
| M_0490 | 1,3,9,11-Tetramethyl-5,7-dihydrodibenzo[c,e]thiepine                          | C18 H20 S       | 268.1287 | 7.452  | 18361.28651 | 548962.5879 | 694129.8801 | 30903.69545 | 393174.4354 | 190730.8669 | 553722.76  | 11360.9132   | 569071.6096 | 285387.6 |
| M_0491 | Methylnicotinamide  | C7 H8 N2 O      | 136.0637 | 1.08   | 1463766.161 | 156544.9334 | 128213.776  | 114504.7718 | 141766.5621 | 73571.21772 | 107484.13  | 47559.87654  | 52746.76804 | 2021.091 |
| M_0492 | Trigonelline  | C7 H7 N O2      | 137.0477 | 1.383  | 227245.0276 | 34274.90692 | 1457085.246 | 499490.0202 | 607134.4095 | 20579.00194 | 26362.945  | 20296.8571   | 21310.85884 | 6485.614 |
| M_0493 | Vigabatrin  | C6 H11 N O2     | 129.0791 | 0.849  | 565003.0342 | 15791.38938 | 236907.0192 | 21216.5965  | 195473.0602 | 128886.6079 | 32396.983  | 27581.88404  | 144772.3658 | 13284.7  |
| M_0494 | 1962763   | C11 H21 N O4    | 231.147  | 1.239  | 1438099.38  | 342636.2252 | 401498.1813 | 290543.8859 | 390649.622  | 353522.9068 | 518759.74  | 295393.3746  | 432097.0364 | 6926.134 |
| M_0495 | Gabapentin  | C9 H17 N O2     | 171.126  | 6.905  | 282039.8877 | 184317.1697 | 736129.699  | 185097.7412 | 595825.9278 | 558859.8954 | 132925.33  | 865344.7461  | 344120.015  | 17071.68 |
| M_0496 | N-Acetyl-L-phenylalanine  | C11 H13 N O3    | 207.0896 | 7.194  | 1436691.448 | 543167.2261 | 1139940.468 | 503524.5205 | 837915.5154 | 555053.9041 | 213622.5   | 156741.5092  | 175514.0189 | 9877.865 |
| M_0497 | 25-Hydroxy-24-epi-brassinolide  | C28 H48 O7      | 496.3376 | 9.966  | 428168.5799 | 504917.9111 | 1051297.564 | 477022.3974 | 520243.7285 | 769277.0376 | 655942.55  | 547981.4174  | 728933.8996 | 12651.3  |
| M_0498 | DL-Homoserine   | C4 H9 N O3      | 119.0585 | 1.295  | 758147.3594 | 712716.5574 | 781590.3221 | 520024.9786 | 707063.2061 | 995262.3763 | 1099864.3  | 1087873.568  | 1276335.676 | 3332.224 |
| M_0499 | 4329  | C9 H12 O        | 136.0889 | 8.609  | 98139.76926 | 51732.04334 | 201420.4773 | 761211.7423 | 86128.92528 | 148946.511  | 72511.032  | 85860.47489  | 165724.3719 | 22879.27 |
| M_0500 | Uric acid   | C5 H4 N4 O3     | 168.0284 | 1.723  | 1068966.267 | 1197610.126 | 1098645.223 | 1416865.027 | 1136113.625 | 794711.1936 | 487142.37  | 729922.6691  | 870980.5856 | 3567.804 |
| M_0501 | Dibutyl Fumarate  | C12 H20 O4      | 228.1351 | 8.791  | 829527.8691 | 812031.9308 | 925929.6514 | 993520.9317 | 919261.3695 | 1014938.026 | 960606.56  | 986001.2804  | 736215.8031 | 9448.84  |
| M_0502 | Prolinamide   | C5 H10 N2 O     | 114.0793 | 1.115  | 1394504.082 | 231000.1565 | 239489.1796 | 204743.3901 | 178783.5824 | 164735.3954 | 224981.59  | 146131.2175  | 194384.9006 | 3343.634 |
| M_0503 | DL-Tryptophan   | C11 H12 N2 O2   | 204.0898 | 2.946  | 32636.63487 | 12031.10076 | 3319.555193 | 11326.57919 | 7373.709768 | 90535.06977 | 22183.985  | 46788.45134  | 8756.020878 | 2488.007 |
| M_0504 | 7-ketodeoxycholic acid  | C24 H38 O5      | 406.272  | 8.591  | 163008.8155 | 152520.9211 | 1372904.795 | 874389.7901 | 588801.4563 | 443167.0096 | 640745.95  | 1032626.469  | 720981.7486 | 20578.19 |
| M_0505 | 4-Indolecarbaldehyde  | C9 H7 N O       | 145.0528 | 3.494  | 556923.2689 | 703991.0445 | 798176.6311 | 963610.5391 | 1067601.372 | 1095752.166 | 1232602.3  | 1270501.498  | 961544.6971 | 4050.367 |
| M_0506 | MFC00229832   | C10 H14 O       | 150.1046 | 8.244  | 816167.7479 | 637301.2249 | 558122.9887 | 529425.9298 | 720517.9242 | 1284058.807 | 914715.18  | 1071856.592  | 919033.4724 | 169917.3 |
| M_0507 | 4-Amino-3-hydroxybenzoic acid   | C7 H7 N O3      | 153.0427 | 2.335  | 1359729.122 | 306529.7786 | 272576.7629 | 342618.1946 | 255046.9483 | 135003.118  | 284106.82  | 179525.4017  | 71611.27081 | 8432.135 |
| M_0508 | hydroxybenzoic acid   | C7 H7 N O3      | 153.0427 | 2.335  | 1359729.122 | 306529.7786 | 272576.7629 | 342618.1946 | 255046.9483 | 135003.118  | 284106.82  | 179525.4017  | 71611.27081 | 8432.135 |
| M_0509 | hodgkinsine   | C33 H38 N6      | 518.3183 | 10.005 | 259189.9018 | 325921.6954 | 669222.7891 | 304104.9345 | 569837.8784 | 374338.0303 | 327954.49  | 570152.9121  | 7545.95444  | 7524.666 |
| M_0510 | DL-Lysine   | C6 H14 N2 O2    | 146.1055 | 0.988  | 1346505.013 | 795142.5576 | 969803.953  | 221295.2502 | 654198.2773 | 282184.2407 | 315104.37  | 476873.7344  | 323118.8    | 1796.093 |
| M_0511 | trimethadione   | C6 H9 N O3      | 143.0583 | 2.863  | 1339835.607 | 70314.92373 | 21251.3439  | 108320.7586 | 29750.74352 | 129686.1897 | 63324.734  | 93439.61773  | 51483.81794 | 13112.69 |
| M_0512 | Creatinine  | C4 H7 N3 O      | 113.0593 | 1.581  | 1339301.569 | 548230.3378 | 448275.6097 | 242551.2915 | 449189.9733 | 606280.7419 | 220727.91  | 357518.3636  | 364738.9429 | 63135.04 |
| M_0513 | 3-Hydroxy-L-proline   | C5 H9 N O3      | 131.0584 | 1.88   | 1335950.28  | 184707.5781 | 87389.28117 | 295759.407  | 330028.2289 | 172510.9205 | 185104.17  | 98406.60136  | 72962.96146 | 31453.6  |
| M_0513 | UNII:OUTSYHB7BO   | C18 H35 N O2    | 297.2667 | 9.142  | 95933.77551 | 83756.57524 | 139178.7579 | 98258.5522  | 61248.81109 | 318590.3786 | 61431.814  | 203805.439   | 97183.20967 | 14354.03 |
| M_0514 | 1-Ethoxy-2,3-difluoro-4-(4-pentylcyclohex-1-en-1-yl)benzene                   | C19 H26 F2 O    | 308.1963 | 8.747  | 814048.9079 | 8826.554094 | 9221.96509  | 18238.50522 | 139267.4774 | 143067.3203 | 143983.95  | 7626.023743  | 1044155.738 | 124396.5 |
| M_0515 | Thiomalic acid  | C4 H6 O4 S      | 149.998  | 7.531  | 80877.08015 | 64910.49138 | 15139.30509 | 25201.99411 | 184797.0543 | 167171.2541 | 269881.7   | 236498.8117  | 155998.7798 | 259776.2 |
| M_0516 | LysoPC(18:3(9Z,12Z,15Z))  | C26 H48 N O7 P  | 517.3145 | 9.588  | 153070.5062 | 5036.655779 | 4912.845195 | 5893.982262 | 8724.535837 | 12249.27704 | 1136462.8  | 1323135.29   | 7387.000921 | 59160.9  |
| M_0517 | Bohemine  | C18 H24 N6 O    | 340.2014 | 8.948  | 711833.2785 | 1322659.698 | 214065.6099 | 806612.4319 | 585422.8848 | 1001332.02  | 705123.21  | 874660.3931  | 750651.4826 | 7827.758 |
| M_0518 | DL-Tryptophan   | C11 H12 N2 O2   | 208.1797 | 3.499  | 181949.3024 | 391927.3341 | 523275.6547 | 621841.5182 | 546065.1462 | 734832.9859 | 1272968    | 1322420.574  | 891156.9326 | 2045.193 |
| M_0519 | Taurine   | C2 H7 N O3 S    | 125.0148 | 1.356  | 719638.8284 | 758311.944  | 629327.4728 | 815561.1023 | 698901.678  | 949785.1546 | 1187304.7  | 784202.2888  | 1282791.258 | 2788.058 |
| M_0520 | 5-Hydroxy-DL-tryptophan   | C11 H12 N2 O3   | 220.0847 | 1.548  | 118952.2949 | 123870.3783 | 159916.9434 | 255770.3406 | 180334.8937 | 305395.0562 | 190643.75  | 294615.9216  | 222772.5925 | 3480.844 |
| M_0521 | 3-(Dodecylamino)-2-hydroxy-2-cyclohexen-1-one                                 | C18 H33 N O2    | 295.2511 | 8.927  | 92856.11697 | 111349.7372 | 190707.2583 | 56169.03378 | 105138.9408 | 401733.4335 | 76046.567  | 151887.0213  | 174916.0257 | 14264.84 |
| M_0522 | GB ACID   | C4 H11 O3 P     | 138.0448 | 6.147  | 220.6601155 | 252.9884544 | 287.8182343 | 283.3676451 | 264.3986701 | 266.2548059 | 278.80402  | 478.2761192  | 2762.163535 | 262.1653 |
| M_0523 | 1-Butyrobetaine   | C7 H15 N O2     | 145.1103 | 2.955  | 1295051.832 | 455365.7091 | 586347.6177 | 290057.6501 | 294347.2896 | 418825.2894 | 3228791.68 | 1270511.4282 | 227643.4185 | 8144.288 |
| M_0524 | 1,1,1-Trifluoroacetone  | C3 H3 F3 O      | 112.014  | 1.596  | 143700.7046 | 439675.4871 | 477750.8403 | 622243.1093 | 546814.8281 | 445707.5274 | 420353.08  | 479043.2684  | 1294880.353 | 6501.166 |
| M_0525 | 1,1,1-Trifluoroacetone  | C3 H3 F3 O      | 112.0137 | 1.535  | 101147.1418 | 371812.1479 | 420994.7917 | 694627.698  | 341380.599  | 445707.5274 | 420353.08  | 634035.6401  | 1294880.353 | 4001.268 |
| M_0526 | Piperonylonitrile   | C8 H5 N O2      | 147.0321 | 5.778  | 250217.0325 | 240299.0486 | 547412.3113 | 834427.3901 | 416072.6647 | 888824.9263 | 539589.79  | 1126628.551  | 563889.8721 | 8761.937 |
| M_0527 | Creatinine  | C4 H7 N3 O      | 113.0593 | 1.469  | 44981.33798 | 43346.23967 | 568164.5556 | 162921.4148 | 118267.6515 | 806143.8432 | 533385.84  | 592774.2594  | 548778.2935 | 53566.22 |
| M_0528 | Guanosine monophosphate   | C10 H14 N5 O8 P | 363.058  | 2.252  | 23521.44448 | 340419.8143 | 53573.81077 | 587626.6136 | 368397.203  | 700578.9079 | 692926.62  | 862053.2025  | 486305.7518 | 12417.29 |
| M_0529 | Malondialdehyde   | C3 H4 O2        | 72.02112 | 1.126  | 1279743.848 | 426669.3943 | 129464.7938 | 284335.1543 | 240636.6489 | 317638.3452 | 383900.1   | 257332.1628  | 323638.0778 | 2109.971 |
| M_0530 | 2-Butoxyethanol acetate   | C8 H16 O3       | 160.1099 | 8.12   | 805448.6501 | 341582.2453 | 250166.7588 | 580002.232  | 478271.241  | 638967.5168 | 519672.93  | 307595.3208  | 297381.5885 | 50003.93 |
| M_0531 | 2-Ethoxy-4-hydrazino-6-(1-piperidinyl)-1,3,5-triazine                         | C10 H18 N6 O    | 238.1545 | 8.69   | 24592.50535 | 25711.7971  | 37724.31356 | 96021.37951 | 1276836.227 | 19948.02949 | 15848.723  | 46229.64639  | 102203.0794 | 5484.703 |
| M_0532 | Choline Alfoscerate   | C8 H5 N O6 P    | 257.1027 | 1.419  | 56641.49534 | 46822.48756 | 14371.98836 | 198031.     |             |             |            |              |             |          |

|        |  |                 |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0536 | Octylbenzene   | C14 H22         | 190.1722 | 8.54  | 59442.66361 | 66383.34491 | 9052.221705 | 64675.09543 | 75865.28684 | 13847.75623 | 74363.813 | 52000.88871 | 86300.37683 | 83734.98 |
| M_0537 | glycyclamide   | C14 H20 N2 O3 S | 296.1194 | 4.32  | 4438.731406 | 4180.515018 | 4309.507656 | 4223.126828 | 4197.286785 | 4109.927335 | 4194.9792 | 4310.732914 | 4248.349632 | 4138.807 |
| M_0538 | 1,3'-Dimethyl-1,4':5',1''-terimidazolidine-2,2',2''-trione               | C11 H18 N6 O3   | 282.1445 | 8.121 | 43375.43251 | 74321.27059 | 36942.48043 | 14729.07054 | 743128.2924 | 167325.4704 | 156509.84 | 116866.8437 | 155957.3659 | 183969.1 |
| M_0539 | bis(tetrazolyl)amine   | C2 H3 N9        | 153.0514 | 1.305 | 241027.1627 | 206996.4948 | 176107.6146 | 199045.5321 | 235074.6224 | 571425.2445 | 419899.23 | 487143.2299 | 495617.5165 | 11648.91 |
| M_0540 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P | 369.0448 | 1.396 | 10189.1521  | 301853.1358 | 5860.012726 | 507649.2316 | 457859.6605 | 769618.4792 | 1216440.9 | 781492.1377 | 1126229.401 | 2113.172 |
| M_0541 | Eicosapentaenoic acid methyl ester                                       | C21 H32 O2      | 316.2402 | 9.402 | 125610.9447 | 206483.422  | 58430.5515  | 174119.517  | 46974.38667 | 138079.6651 | 58623.745 | 130970.9999 | 50781.02223 | 3896.303 |
| M_0542 | LysoPC(18:3(9Z,12Z,15Z))   | C26 H48 N O7 P  | 517.3185 | 9.701 | 7907.290957 | 52807.90513 | 58199.50658 | 226275.4042 | 873969.0092 | 1153720.819 | 99277.636 | 24868.3867  | 499335.7809 | 30259.69 |
| M_0543 | Guanylmelamine   | C4 H8 N8        | 168.0875 | 0.846 | 680715.9706 | 1085921.989 | 826383.1846 | 322892.9244 | 497651.1057 | 554809.315  | 540406.06 | 659069.9565 | 585886.8015 | 2230.723 |
| M_0544 | Pyrrolo(2,1,5-cd)indolizine  | C10 H7 N        | 141.0578 | 3.501 | 406201.117  | 563727.2992 | 604300.587  | 764759.8748 | 719857.3141 | 923833.4475 | 1046809.5 | 1194279.973 | 819118.3199 | 5849.42  |
| M_0545 | Hexadecanamide   | C16 H33 N O     | 255.256  | 9.798 | 139009.4732 | 189095.6796 | 216725.5242 | 78850.5525  | 97588.27693 | 276390.1518 | 83978.051 | 82293.66045 | 145445.9852 | 100055.1 |
| M_0546 | 1H-Tetrazolo[1,5':2,3][1,2,4]triazino[5,6-b]indole                       | C9 H5 N7        | 211.0609 | 7.823 | 296276.298  | 898067.3694 | 360357.684  | 1030258.49  | 1114091.196 | 1159061.75  | 447672.18 | 476550.798  | 339570.1439 | 3511.868 |
| M_0547 | 1-carboxy-3-hydroxyadamantane  | C11 H16 O3      | 196.11   | 7.668 | 56296.27683 | 78712.34132 | 107257.3754 | 106962.1247 | 155784.0012 | 162621.9911 | 140516.89 | 77106.96605 | 111138.2743 | 9699.068 |
| M_0548 | N-Oleoyl-L-Serine  | C21 H39 N O4    | 369.288  | 8.012 | 117558.244  | 212984.8032 | 85802.93479 | 325485.2712 | 375194.9121 | 586828.4504 | 478740.86 | 376245.7075 | 236750.1237 | 3550.522 |
| M_0549 | 2878846  | C20 H26 O3      | 314.1881 | 8.629 | 1169469.832 | 201431.8435 | 336671.5434 | 375413.8277 | 248543.1878 | 428010.1416 | 102062.84 | 350247.2386 | 77514.16898 | 58703.43 |
| M_0550 | L-alpha-lysophosphatidylcholine  | C22 H46 N O7 P  | 467.3016 | 9.585 | 189565.4377 | 418965.3469 | 940371.1507 | 1163783.397 | 778443.0198 | 989239.2232 | 769135.54 | 821226.1344 | 620315.2995 | 11036.48 |
| M_0551 | AC-VAL-OH  | C7 H13 N O3     | 159.0896 | 3.26  | 338924.8258 | 295512.1577 | 425827.3637 | 410375.399  | 210272.7282 | 201315.684  | 92738.232 | 167528.7952 | 269923.6388 | 21161.69 |
| M_0552 | (+)-Aphidicolin  | C20 H34 O4      | 320.2327 | 9.147 | 487802.1545 | 380100.6907 | 290959.4736 | 697818.6548 | 558284.9032 | 628067.8814 | 833006.51 | 759745.7428 | 967741.5954 | 140153.6 |
| M_0553 | Arsonate   | H As O3         | 123.9157 | 0.983 | 84699.57191 | 78415.97789 | 22284.84393 | 83696.31616 | 51642.26291 | 56961.65734 | 45643.388 | 29000.06626 | 35358.53601 | 3022.657 |
| M_0554 | 5-Hydroxyindole-3-acetic acid  | C10 H9 N O3     | 191.0582 | 6.326 | 353894.889  | 382243.9352 | 495520.0196 | 776032.9103 | 190333.3575 | 245136.8913 | 287421.04 | 406769.784  | 336573.5966 | 7354.344 |
| M_0555 | Xanthine   | C5 H4 N4 O2     | 152.0335 | 1.904 | 891335.1034 | 897307.522  | 184356.887  | 1152272.243 | 360026.5425 | 842474.0829 | 481825.44 | 765152.9129 | 304288.3603 | 4057.871 |
| M_0556 | Hexylresorcinol  | C12 H18 O2      | 194.1307 | 8.644 | 394739.2931 | 226651.7721 | 835007.5323 | 1037930.504 | 528725.3227 | 508040.0361 | 703069.33 | 1023375.737 | 1143894.944 | 32934.8  |
| M_0557 | 1-benzylimidazole  | C10 H10 N2      | 158.0844 | 3.495 | 380905.9626 | 529192.5099 | 581888.1211 | 721311.2801 | 682134.0814 | 862844.3231 | 1008766   | 1137548.811 | 785717.8021 | 3698.745 |
| M_0558 | 2802   | C8 H16 O        | 128.1205 | 9.226 | 613285.2896 | 452196.8741 | 645229.4986 | 839345.1714 | 1113576.79  | 1092244.167 | 681737.49 | 767625.3589 | 947548.9065 | 56405.37 |
| M_0559 | 2-(5-Benzo[1,3]dioxol-5-yl-tetrazol-2-yl)-1-morpholin-4-yl-ethanone      | C14 H15 N5 O4   | 317.1124 | 1.624 | 1135855.345 | 134668.1234 | 1566.501719 | 152670.6152 | 21530.11725 | 102929.9731 | 186328.91 | 290280.9417 | 36492.32178 | 2283.931 |
| M_0560 | monomethyl phosphate   | C H5 O4 P       | 111.9929 | 1.455 | 8112.682781 | 19611.28962 | 4239.534091 | 21252.02354 | 14712.78278 | 16380.32823 | 19015.892 | 11242.75525 | 14709.64377 | 4098.894 |
| M_0561 | 1-(3-Aminopropyl)-2-hydroxy-3-oxo-1-propyltriazane                       | C6 H16 N4 O2    | 176.1273 | 1.137 | 14286.97522 | 13927.00414 | 1120428.374 | 12941.81831 | 880565.8277 | 17233.58637 | 15354.435 | 52036.96888 | 15694.14815 | 1227.745 |
| M_0562 | Thiomorpholine   | C4 H9 N S       | 103.0461 | 1.223 | 424595.2833 | 510935.3017 | 789775.481  | 428672.3472 | 443754.4134 | 412928.0972 | 365354.54 | 555418.09   | 519724.9004 | 3366.575 |
| M_0563 | DL-Lysine  | C6 H14 N2 O2    | 146.1055 | 1.244 | 1112990.221 | 523759.5769 | 260500.1132 | 281479.8259 | 572088.777  | 376467.6419 | 462776.22 | 595084.8981 | 381930.5858 | 4682.699 |
| M_0564 | 4,4-Dimethyl-1-hexyne  | C8 H14          | 110.11   | 9.224 | 594188.4553 | 430484.6383 | 622578.7763 | 815755.1816 | 1083074.097 | 1065052.828 | 658436.03 | 740277.5411 | 919650.4516 | 41009.44 |
| M_0565 | Diethyl diallylmalonate  | C13 H20 O4      | 240.1359 | 7.845 | 883802.9139 | 136403.5376 | 183664.3451 | 224911.2992 | 498522.9216 | 354486.4203 | 905160.53 | 144968.0489 | 54409.33127 | 220136.8 |
| M_0566 | AD8050000  | C8 H10 N2 O     | 150.0794 | 0.877 | 8043.973084 | 8282.591931 | 8076.143015 | 7512.888143 | 8328.259898 | 8285.746057 | 7902.5058 | 7833.766458 | 7903.656712 | 2721.29  |
| M_0567 | 2-Indolylformic acid   | C9 H7 N O2      | 161.0478 | 4.897 | 6635.2123   | 5719.540556 | 7024.01546  | 3641.797508 | 3465.336221 | 3653.761294 | 4198.5806 | 3639.02522  | 3458.030257 | 3325.025 |
| M_0568 | 2-Chloro-1,3,2-oxathiaphospholane  | C2 H4 Cl O P S  | 141.9408 | 1.385 | 666525.2052 | 272696.1094 | 81566.6839  | 103736.5822 | 303961.0033 | 481340.0077 | 324521.25 | 594865.6057 | 337478.0141 | 2252.069 |
| M_0569 | 4-Morpholino-1,3,5-triazin-2-amine                                       | C7 H11 N5 O     | 181.0964 | 1.742 | 82730.54374 | 170522.8191 | 20327.54184 | 122892.0048 | 44129.38499 | 120068.0921 | 78826.705 | 180733.2429 | 106107.5076 | 3985.453 |
| M_0570 | cyclandelate   | C17 H24 O3      | 276.1724 | 8.499 | 303088.4653 | 1080314.393 | 365140.005  | 340699.4836 | 387526.7369 | 562867.2508 | 505357.58 | 731251.5724 | 453719.4158 | 8192.766 |
| M_0571 | Terazosin impurity n   | C9 H16 N2 O2    | 184.1212 | 3.635 | 1079852.672 | 43680.91168 | 48826.10995 | 44726.09614 | 37641.10911 | 16861.60301 | 20340.065 | 28102.72936 | 20508.92334 | 4675.465 |
| M_0572 | tert-Butyl N-[1-(aminocarbonyl)-3-methylbutyl]carbamate                  | C11 H22 N2 O3   | 230.1632 | 2.31  | 4071.095044 | 3243.320835 | 3436.019777 | 3533.019881 | 2554.69775  | 2489.858737 | 6256.0441 | 2477.907791 | 2237.790912 | 2313.694 |
| M_0573 | 4-Amino-N'-[2-(1-piperidiny)acetoxyl]-1,2,5-oxadiazole-3-carboximidamide | C10 H16 N6 O3   | 268.1285 | 7.096 | 10476.1489  | 13643.62276 | 35496.95023 | 11336.24002 | 30271.99272 | 39642.30365 | 11935.139 | 52669.73203 | 14297.20887 | 3060     |
| M_0574 | Thieno[3,4-d]-1,3-dithiol-2-thione                                       | C5 H2 S4        | 189.9045 | 1.055 | 124764.2086 | 174013.0418 | 30914.54216 | 110293.0189 | 75724.06387 | 83219.17095 | 74908.566 | 77878.24528 | 71876.09801 | 1216.229 |
| M_0575 | 5-Amino-3-nitro-1H-1,2,4-triazole-1-carboxamide                          | C3 H4 N6 O3     | 172.0348 | 1.15  | 331131.3631 | 133409.2146 | 230312.5379 | 295299.4047 | 175281.3237 | 550530.0323 | 311915.33 | 239821.8316 | 207838.8603 | 1662.356 |
| M_0576 | Buifadienolide   | C24 H34 O2      | 354.2558 | 8.57  | 24677.71266 | 39337.9718  | 480406.9682 | 104942.021  | 74662.16216 | 148626.7736 | 192170.03 | 113664.1532 | 128706.3771 | 6109.176 |
| M_0577 | 4-Amino-N'-[2-(1-piperidiny)acetoxyl]-1,2,5-oxadiazole-3-carboximidamide | C10 H16 N6 O3   | 268.1287 | 7.595 | 443512.3346 | 13845.85756 | 291447.984  | 405021.3968 | 209449.3834 | 144364.4146 | 26004.964 | 365799.8183 | 8315.275856 | 80421.88 |
| M_0578 | ACETYL PROLINE   | C7 H11 N O3     | 157.074  | 3.053 | 1048020.596 | 94075.14632 | 194489.8792 | 24558.80888 | 61516.24927 | 22726.72875 | 27992.564 | 21802.7674  | 18854.31374 | 4659.403 |
| M_0579 | OB4520000  | C10 H9 N O      | 159.0686 | 7.462 | 24122.66893 | 18945.60954 | 23750.28237 | 23588.11337 | 10273.00775 | 10351.54135 | 7137.1865 | 19697.23058 | 16832.50914 | 10104.12 |
| M_0580 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P | 331.089  | 1.394 | 10144.29627 | 247840.1646 | 5023.233502 | 401746.5678 | 354642.2398 | 598296.4083 | 1045581.4 | 615421.3415 | 970464.1348 | 1926.386 |
| M_0581 | N-Boc-L-valine   | C10 H19 N O4    | 217.1313 | 1.095 | 318490.4982 | 557966.6079 | 337726.3443 | 2031.883728 | 1789.902473 | 56418.11516 | 1043324.8 | 503581.1398 | 426087.5057 | 344.2748 |
| M_0582 | 5-Hydroxy-DL-tryptophan  | C11 H12 N2 O3   | 220.0848 | 2.783 | 19950.45961 | 44657.2167  | 205064.1452 | 45854.6216  | 49358.71246 | 53974.74887 | 42691.771 | 131217.1128 | 29137.01888 | 3146.574 |
| M_0583 | Gly-Lys  | C8 H17 N3 O3    | 203.1268 | 1.223 | 1040774.763 | 145377.267  | 479211.8942 | 122815.6375 | 117240.8553 | 26640.91567 | 23758.855 | 30444.22344 | 24175.94015 | 2772.062 |
| M_0584 | DL-Stachydrine   | C7 H13 N O2     | 143.0947 | 1.435 | 601935.7036 | 568401.1428 | 734058.8955 | 849099.3936 | 747371.6914 | 368000.2295 | 360662.83 | 368546.6669 | 120661.1487 | 17836.49 |
| M_0585 | MFCDO2123047   | C8 H11 N3 S2    | 213.0402 | 5.007 | 308353.1632 | 76987.89641 | 82614.27036 | 183008.6214 | 66296.82788 | 54769.69713 | 44681.329 | 66044.33529 | 43525.31065 | 3129.543 |

|        |  |                |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0586 | 1-stearoyl-sn-glycero-3-phosphoethanolamine  | C23 H48 N O7 P | 481.3171 | 9.97   | 336638.1398 | 465999.7175 | 1029100.16  | 479648.7503 | 317886.0255 | 707298.899  | 541782.41 | 642173.6585 | 372622.0601 | 12706.49 |
| M_0587 | N-Acetylornithine  | C7 H14 N2 O3   | 174.1005 | 1.144  | 986504.7924 | 1028891.151 | 629592.6861 | 989172.0746 | 872744.6399 | 346902.8552 | 447480.49 | 416755.1587 | 376003.5052 | 2389.152 |
| M_0588 | lactide  | C6 H8 O4       | 144.0424 | 1.149  | 127704.9225 | 298786.856  | 570463.1931 | 252542.9984 | 214521.9218 | 893336.2531 | 800584.46 | 443554.3746 | 618340.428  | 84174.52 |
| M_0589 | D-(+)-Maltose  | C12 H22 O11    | 364.0981 | 1.146  | 901876.1141 | 441112.35   | 462058.0516 | 484466.6143 | 151186.5915 | 136558.621  | 132503.85 | 225646.8436 | 411845.7267 | 1533.808 |
| M_0590 | 3,5-Diamino-N-carbamimidoyl-2-pyrazinecarboxamide  | C6 H9 N7 O     | 195.0872 | 7.157  | 48279.50788 | 64611.53435 | 6127.529122 | 25052.25992 | 57918.72529 | 292198.7088 | 77787.342 | 83643.06146 | 56202.11048 | 361.4237 |
| M_0591 | 3,5-Diamino-N-carbamimidoyl-2-pyrazinecarboxamide N-Acetyl-DL-tryptophan   | C6 H9 N7 O     | 195.0872 | 7.173  | 48279.50788 | 64611.53435 | 6946.769259 | 188557.4221 | 57918.72529 | 292198.7088 | 77787.342 | 83643.06146 | 11279.21892 | 1851.285 |
| M_0592 | Citric acid  | C6 H8 O7       | 192.0271 | 2.124  | 969623.0455 | 48307.42034 | 75086.29728 | 1006610.133 | 44751.46555 | 603996.2867 | 386506.07 | 570152.0634 | 262538.3122 | 29407.12 |
| M_0594 | GV9100000  | C8 H12 O       | 124.0891 | 8.058  | 83127.00277 | 415505.0802 | 428237.5029 | 85534.34997 | 627280.0032 | 42903.4969  | 202922.77 | 732311.4306 | 680499.4335 | 76002.67 |
| M_0595 | 2-[1-Hydroxy-2-(trimethylammonio)ethyl]-3-oxododecanoate   | C17 H33 N O4   | 315.241  | 9.398  | 110108.5612 | 162452.7074 | 59966.20769 | 156607.2847 | 54880.94087 | 127608.78   | 60092.394 | 115226.9256 | 57401.55288 | 11274.72 |
| M_0596 | 2,4-Quinolinediol  | C9 H7 N O2     | 161.0478 | 7.451  | 149124.4993 | 93355.07078 | 190975.591  | 27049.66504 | 427069.0136 | 380464.4652 | 170550.98 | 104109.4747 | 36137.07601 | 23027.45 |
| M_0597 | Boc-Gln-Oh   | C10 H18 N2 O5  | 246.1215 | 2.523  | 999810.1239 | 467062.0142 | 427749.2981 | 472610.0123 | 277256.2897 | 253097.9358 | 215429.85 | 350204.5946 | 231308.1161 | 4340.534 |
| M_0598 | Uracil   | C4 H4 N2 O2    | 112.0277 | 1.531  | 362017.3741 | 494931.6916 | 303292.4763 | 364932.9836 | 429791.4936 | 498640.1601 | 403130.34 | 412948.2354 | 169034.6382 | 121724   |
| M_0599 | L-gamma-Glutamyl-L-leucine   | C11 H20 N2 O5  | 260.1371 | 4.053  | 996407.4491 | 433398.8096 | 489248.5455 | 546198.5233 | 342636.8997 | 576960.8387 | 307873.55 | 473725.3847 | 220621.9613 | 5311.501 |
| M_0600 | 4-(1,4-Dioxaspiro[4.5]dec-8-yl)cyclohexanone Butyl O-phosphonoserinate   | C14 H22 O3     | 238.1568 | 9.041  | 301354.927  | 342597.4477 | 116735.5907 | 441816.528  | 406593.4821 | 574515.7497 | 644595.01 | 958252.6169 | 731187.4284 | 54384.61 |
| M_0601 | phosphoserinate  | C7 H16 N O6 P  | 241.0716 | 1.098  | 113828.582  | 62992.62626 | 57463.0303  | 55330.25136 | 71316.11052 | 126600.6029 | 118823.94 | 70945.58906 | 77514.82931 | 1111.142 |
| M_0602 | [(2-Hydroxytetradecyl)sulfonyl]acetic acid   | C16 H32 O4 S   | 320.2025 | 10.488 | 46873.65797 | 515575.099  | 109226.8464 | 320969.0363 | 315405.6814 | 405870.5537 | 449642.62 | 488028.1774 | 612676.9279 | 1485.79  |
| M_0603 | (2-Dodecen-1-yl)succinic anhydride   | C16 H26 O3     | 266.188  | 8.952  | 620090.2419 | 415022.7254 | 928537.9629 | 864362.9948 | 810853.3593 | 823866.7886 | 719346.61 | 554028.0574 | 983758.6058 | 30879.66 |
| M_0604 | TRIMETHYLALLYL ISOCYANURATE  | C15 H21 N3 O3  | 291.1581 | 1.515  | 384296.224  | 533004.4274 | 982595.1107 | 486295.0272 | 368316.4186 | 609270.034  | 401086.24 | 461534.5921 | 253377.9295 | 2526.378 |
| M_0605 | 2'-Deoxy-5'-O-phosphonocytidine  | C9 H12 N3 O7 P | 305.0404 | 1.163  | 978023.7422 | 214911.4151 | 219353.9292 | 324014.2793 | 231958.8739 | 86764.87183 | 103240.88 | 131582.2739 | 110470.9211 | 2856.675 |
| M_0606 | [1,4-Phenylenebis(methylene)]bis(phosphonic acid)  | C8 H12 O6 P2   | 266.0103 | 4.698  | 975736.0048 | 52136.63548 | 157674.9798 | 178824.1382 | 117798.2144 | 55193.31979 | 55131.712 | 46130.40623 | 26813.89754 | 9268.057 |
| M_0607 | Norethindrone  | C20 H26 O2     | 298.1931 | 8.707  | 478691.3676 | 305594.6263 | 545614.6705 | 973766.4017 | 174545.4658 | 452701.4518 | 202952.15 | 593816.5599 | 426069.6805 | 3303.046 |
| M_0608 | 2-[(6-Amino-7H-purin-8-yl)amino]ethanol  | C7 H10 N6 O    | 194.092  | 8.182  | 96698.39525 | 79142.74333 | 78126.16929 | 82570.7883  | 24478.95151 | 149869.4287 | 121244.75 | 115992.5737 | 118360.2564 | 131212.9 |
| M_0609 | Methyl palmitate   | C17 H34 O2     | 287.2824 | 7.761  | 173584.5893 | 106749.2334 | 141171.5922 | 136066.7764 | 230391.6611 | 237724.2418 | 124645.29 | 160671.3808 | 156904.9215 | 94539.42 |
| M_0610 | 1-(p-Tolylsulfonyl)pyrrole   | C11 H11 N O2 S | 221.0511 | 7.81   | 147444.9504 | 166842.0949 | 43637.90526 | 355880.2715 | 966232.7194 | 484570.9241 | 326108.72 | 213043.4816 | 176360.0766 | 5895.174 |
| M_0611 | L-Glutamic acid  | C5 H9 N O4     | 147.0532 | 1.283  | 280695.6604 | 536219.8605 | 175106.1447 | 314088.8949 | 251482.0086 | 352848.9132 | 287289.51 | 395002.3395 | 338284.1397 | 3193.15  |
| M_0612 | trans-beta-Nitrostyrene  | C8 H7 N O2     | 149.0478 | 4.599  | 60395.12263 | 54708.95593 | 132813.6614 | 241043.9128 | 122514.5251 | 246168.9383 | 314356.1  | 243862.7841 | 233898.9419 | 32039.97 |
| M_0613 | 3408   | C13 H22 O3     | 226.1569 | 8.587  | 580408.6274 | 398198.3688 | 538301.1317 | 491570.6426 | 558426.3607 | 958616.4781 | 593249.11 | 585274.9077 | 556710.7952 | 157163.2 |
| M_0614 | 6-Methyl[1,2,4]triazolo[4,3-b]pyridazin-8-ol 1,1'-(3,6,9,12-Tetraazatetradecane-1,14-diyl)di(2,4-imidazolidinedione) | C6 H6 N4 O     | 150.0544 | 2.325  | 170679.8333 | 59461.55323 | 121383.6943 | 40551.95571 | 71896.80538 | 40523.96723 | 41378.879 | 40479.89312 | 32832.55081 | 7171.566 |
| M_0615 | (2,2,6,6-Tetramethyl-4-piperidinyl)acetic acid   | C16 H30 N8 O4  | 398.2393 | 8.433  | 604147.6983 | 168929.0582 | 178179.2465 | 138334.4704 | 366776.9074 | 407116.2677 | 690.50637 | 394131.4921 | 393083.9528 | 2723.357 |
| M_0616 | L-Histidine  | C6 H9 N3 O2    | 155.0696 | 0.827  | 337097.6948 | 762265.8599 | 792960.4573 | 953169.9179 | 519821.7393 | 563250.8324 | 568132.95 | 569342.2926 | 329767.4523 | 6706.836 |
| M_0617 | 1-(2-Methyl-2-propenyl)-1,3-cyclopentadiene  | C9 H14         | 122.1098 | 7.826  | 53961.02095 | 28992.47795 | 39187.75349 | 25917.89882 | 94778.04665 | 93915.76346 | 60124.847 | 71420.74787 | 33299.61219 | 84435.45 |
| M_0619 | N-Acetyl-L-phenylalanine   | C11 H13 N O3   | 207.0896 | 7.293  | 77900.57889 | 42854.02157 | 46675.00756 | 339155.2689 | 60070.3324  | 498931.2169 | 134428.74 | 81234.81909 | 20874.36322 | 4970.833 |
| M_0620 | Indole   | C8 H7 N        | 117.0583 | 7.536  | 2727.149987 | 2460.528951 | 2272.607695 | 2245.259562 | 3702.3523   | 3512.662076 | 2431.5912 | 2411.528866 | 1964.571397 | 3601.958 |
| M_0621 | PALMITYL 3,5-DI-TERT-BUTYL-4-HYDROXYBENZOATE   | C31 H54 O3     | 474.4077 | 9.122  | 3804.579892 | 3553.929456 | 3010.102146 | 4067.424565 | 3352.152831 | 4250.490715 | 3102.3599 | 3934.222034 | 3082.880163 | 2229.963 |
| M_0622 | N-lauroylethanolamine  | C14 H29 N O2   | 243.2198 | 8.656  | 615800.6062 | 468634.9614 | 760415.2849 | 404926.1472 | 718848.9101 | 846138.9558 | 603443.57 | 875676.0305 | 774284.2837 | 14073.29 |
| M_0623 | Oxprenolol   | C15 H23 N O3   | 265.1654 | 8.291  | 209198.1263 | 278603.4789 | 252260.9777 | 196715.3629 | 126765.8642 | 334723.8089 | 281467.95 | 778614.3989 | 248838.1071 | 110529.7 |
| M_0624 | Methyl isonicotinate   | C7 H7 N O2     | 137.0478 | 1.44   | 408937.1119 | 318129.7279 | 932882.7803 | 499490.0202 | 607134.4095 | 348752.9431 | 133326.72 | 168221.17   | 141067.505  | 10226.46 |
| M_0625 | Sorbic acid  | C6 H8 O2       | 112.0528 | 0.709  | 525180.9855 | 208467.0003 | 364638.9517 | 212089.3888 | 204176.3803 | 119980.8707 | 300043.15 | 289672.8149 | 253131.5201 | 46813.02 |
| M_0626 | PALMITYL 3,5-DI-TERT-BUTYL-4-HYDROXYBENZOATE   | C31 H54 O3     | 474.4077 | 9.224  | 3255.227364 | 3253.637573 | 3237.069102 | 4305.577656 | 3944.50582  | 3996.03593  | 3692.6881 | 3826.975707 | 3903.754008 | 3824.469 |
| M_0627 | Glyphosate   | C3 H8 N O5 P   | 169.014  | 5.783  | 166564.7708 | 177571.197  | 458543.6566 | 545454.2534 | 290359.9285 | 655749.183  | 301172.93 | 794291.2911 | 436876.2245 | 3560.489 |
| M_0628 | MFC000152656   | C18 H37 N O3   | 315.2773 | 6.699  | 93593.33454 | 132426.9574 | 76151.97249 | 31213.15265 | 51949.13354 | 73505.57314 | 85587.298 | 161100.0923 | 91492.16346 | 10508.76 |
| M_0629 | gamma-Glu-gln  | C10 H17 N3 O6  | 275.1115 | 1.156  | 274287.2119 | 846655.9388 | 922175.8388 | 692949.9427 | 670738.4971 | 246908.564  | 52242.39  | 668777.3375 | 486757.9922 | 2821.183 |
| M_0630 | celiprolol   | C20 H33 N3 O4  | 379.2488 | 9.16   | 249655.5609 | 575425.7545 | 784862.2533 | 879499.0765 | 674887.9479 | 567240.2148 | 634812.4  | 478029.6377 | 493668.3992 | 49514.09 |
| M_0631 | cyclandelate   | C17 H24 O3     | 276.1723 | 8.804  | 250145.2726 | 280975.8064 | 404472.2133 | 180052.8558 | 628775.2503 | 355032.8359 | 246153.35 | 417623.8738 | 266704.4113 | 10855.18 |
| M_0632 | dioxanone  | C4 H6 O3       | 102.0322 | 1.347  | 47061.7312  | 135827.2172 | 791368.1486 | 250776.487  | 92854.31177 | 530491.2983 | 117136.12 | 116187.0015 | 55821.71662 | 77251.22 |
| M_0633 | Nithiazide   | C6 H8 N4 O3 S  | 216.0311 | 6.415  | 916004.2726 | 138408.6145 | 446096.2909 | 239555.992  | 111283.7288 | 144199.8711 | 71982.232 | 127371.3671 | 79887.6323  | 7413.129 |
| M_0634 | 2268966  | C13 H25 N O4   | 259.1783 | 4.418  | 586699.5937 | 480467.9721 | 171341.959  | 682841.0088 | 364047.8069 | 523700.3644 | 557160.25 | 391097.1701 | 317798.2621 | 4565.533 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0635 | SSR161421   | C25 H20 N4 O2   | 386.173  | 8.321  | 551116.1331 | 333199.6416 | 510371.2167 | 305606.4969 | 566959.8388 | 882438.4059 | 706853.63 | 597650.424  | 676983.3915 | 92714.63 |
| M_0636 | Ethyl 2-oxocyclohexanecarboxylate   | C9 H14 O3       | 170.0945 | 7.812  | 364082.1258 | 329994.034  | 296047.2552 | 305073.8796 | 88148.84797 | 65701.40938 | 59967.052 | 314687.0601 | 10171.01272 | 26671.5  |
| M_0637 | 2,2,2-Trifluoro-1-phenylethyl azide   | C8 H6 F3 N3     | 201.0512 | 4.467  | 755682.9453 | 75499.52681 | 61432.93382 | 40609.76334 | 9968.469532 | 797103.5469 | 64662.536 | 90514.63114 | 868315.894  | 77094.05 |
| M_0638 | 4,9-Dioxo-3,5,10-trioxo-8-azatridec-12-en-1-yl methacrylate                 | C13 H19 N O7    | 301.1161 | 6.768  | 312496.7133 | 100759.5173 | 248133.1514 | 904185.806  | 83643.10687 | 185471.2615 | 134053.4  | 97129.73392 | 38300.40398 | 2371.216 |
| M_0639 | CU5250000   | C8 H5 N O       | 131.0372 | 8.55   | 900154.8982 | 390602.1264 | 561849.749  | 695933.783  | 194212.1596 | 209118.9761 | 105497.33 | 382076.0217 | 168816.3914 | 24003.67 |
| M_0640 | 4-Vinylpyridine   | C7 H7 N         | 105.0583 | 2.777  | 3643.44968  | 12852.41455 | 11701.5602  | 119980.8862 | 50783.00342 | 340184.5215 | 86399.323 | 158481.0821 | 329355.3761 | 2789.712 |
| M_0641 | 3-Hydroxy-L-proline   | C5 H9 N O3      | 131.0585 | 1.112  | 126196.7228 | 383228.721  | 578221.3556 | 295551.2464 | 526759.9036 | 386693.8089 | 511404.77 | 415847.1731 | 566576.9333 | 6907.622 |
| M_0642 | 7H-Pyrrolo[2,3-d]pyrimidine-2,4-diol  | C6 H5 N3 O2     | 151.0386 | 0.791  | 757082.7925 | 433231.9045 | 305171.6731 | 708453.3171 | 390372.9119 | 403662.6103 | 315251.45 | 344128.4186 | 265500.0451 | 3098.679 |
| M_0643 | lamtidine   | C18 H28 N6 O    | 344.2327 | 9.179  | 551088.981  | 659568.878  | 200221.8573 | 884254.6729 | 359103.7948 | 645835.6323 | 441518.6  | 543837.363  | 468831.136  | 5030.784 |
| M_0644 | DL-Stachydrine  | C7 H13 N O2     | 143.0947 | 1.325  | 470067.7451 | 61469.39378 | 876513.2194 | 155968.2323 | 99729.17289 | 89728.94656 | 55387.93  | 48140.83025 | 48741.71737 | 7550.36  |
| M_0645 | 1-[[4,6-Diamino-1,3,5-triazin-2-yl]amino]-2-propanol                        | C6 H12 N6 O     | 184.1075 | 6.897  | 179048.7203 | 27133.75611 | 319969.5949 | 23023.24505 | 106750.4966 | 136775.5556 | 47993.872 | 149751.8804 | 29940.83776 | 10960.14 |
| M_0646 | N.pi.-Methyl-L-histidine  | C7 H11 N3 O2    | 169.0851 | 1.427  | 857371.5833 | 164647.5704 | 69903.83364 | 306433.8529 | 191126.4773 | 206921.8528 | 329254.97 | 242922.8915 | 285846.7773 | 3148.062 |
| M_0647 | Platelet-activating factor  | C26 H54 N O7 P  | 523.3642 | 10.812 | 7242.091396 | 5681.525835 | 4652.086357 | 402149.0283 | 9389.684291 | 360243.5086 | 4705.2228 | 26146.67985 | 741946.3564 | 1264.522 |
| M_0648 | MFC000467204  | C8 H11 N3 O S2  | 229.0351 | 5.33   | 854920.9462 | 151211.5072 | 196748.0349 | 211031.6382 | 183366.4412 | 240734.8271 | 133185.12 | 190706.2118 | 118073.6996 | 4166.391 |
| M_0649 | AC-VAL-OH   | C7 H13 N O3     | 159.0896 | 5.017  | 206950.0201 | 215659.5283 | 77039.00522 | 286132.4036 | 159627.075  | 296588.24   | 163903.66 | 194590.7613 | 102952.8726 | 8895.977 |
| M_0650 | [4-(Phenylsulfanyl)phenyl]methanol  | C13 H12 O S     | 216.061  | 1.215  | 148983.8913 | 250906.5249 | 142143.0708 | 270161.4214 | 311962.3498 | 282519.7484 | 297785.61 | 306402.2999 | 244236.7947 | 4499.933 |
| M_0651 | 4,6-Bis(dimethylamino)-1,3,5-triazine-2-carbohydrazide                      | C8 H15 N7 O     | 225.1339 | 6.907  | 178391.7447 | 106073.523  | 319085.447  | 81228.11882 | 276130.7455 | 289937.4327 | 114429.36 | 291517.6736 | 86177.37233 | 29081.26 |
| M_0652 | 2,4a,9-Trimethyl-2,3,4,4a,9,9a-hexahydro[1,2]oxazin[6,5-b]indol-6-yl        | C22 H35 N3 O3   | 389.2677 | 8.526  | 430990.502  | 471452.7665 | 525196.87   | 506012.4943 | 594639.4533 | 508454.414  | 761381.91 | 843533.2687 | 640943.0358 | 10287.52 |
| M_0653 | FZ5600000   | C27 H44         | 368.3443 | 9.454  | 33979.25699 | 765663.8655 | 200905.5519 | 851106.0797 | 130250.5952 | 287716.7875 | 441914.53 | 135158.2201 | 512719.611  | 6226.239 |
| M_0654 | 5-(pentylthio)-1,3,4-thiadiazol-2-amine                                     | C7 H13 N3 S2    | 203.0559 | 1.262  | 600268.9833 | 262048.6806 | 445288.2182 | 288649.5366 | 372477.1616 | 408156.0839 | 508080.91 | 729877.5854 | 243324.5818 | 1680.385 |
| M_0655 | 4,4-Dimethyl-1-hexyne   | C8 H14          | 110.11   | 8.627  | 203676.7047 | 214566.3607 | 297872.5124 | 746207.4881 | 608422.2444 | 589807.5321 | 303867.31 | 473828.4919 | 846462.6485 | 130368.3 |
| M_0656 | Trigonelline  | C7 H7 N O2      | 137.0454 | 1.231  | 51678.9236  | 413840.3806 | 841693.4328 | 564124.9387 | 299701.165  | 434997.9199 | 402156.69 | 159736.5763 | 253595.3786 | 4653.053 |
| M_0657 | 2-Isopropyl-5-methylbenzoic acid  | C11 H14 O2      | 178.0995 | 8.426  | 24232.8523  | 13441.55085 | 24174.87795 | 42670.27408 | 23471.78714 | 38012.73103 | 19286.777 | 17929.47107 | 43992.53748 | 146955   |
| M_0658 | Acetyl-L-methionine   | C7 H13 N O3 S   | 191.0616 | 4.534  | 838157.8701 | 374181.0982 | 440304.7105 | 412217.3501 | 252406.0155 | 245511.3944 | 238305.41 | 267841.0848 | 143291.3403 | 6876.309 |
| M_0659 | METHOXYMETHYLME LAMINE  | C5 H10 N O      | 170.0919 | 5.538  | 43729.11621 | 156561.5307 | 221645.2059 | 835134.791  | 301412.6475 | 364590.8901 | 67802.242 | 606370.1189 | 781246.0736 | 125837.4 |
| M_0660 | negamycin   | C9 H20 N4 O4    | 248.1484 | 1.411  | 214320.2085 | 208816.9719 | 31230.9705  | 567167.5187 | 74729.84712 | 832948.3027 | 83141.566 | 481371.7904 | 3711.79814  | 1459.504 |
| M_0661 | 1,3-Dihydro[1,2,5]oxadiazolo[3,4-b]pyrido[2',3':5,6]pyrazino[2,3-e]pyrazine | C9 H5 N7 O      | 227.0558 | 7.495  | 124606.8979 | 46965.86866 | 85758.77507 | 148773.6657 | 175068.9219 | 474360.7201 | 160370.89 | 231605.6431 | 71431.8527  | 7096.613 |
| M_0662 | Bucillamine   | C7 H13 N O3 S2  | 223.0337 | 6.039  | 54410.14095 | 21447.10102 | 404339.9434 | 129482.3772 | 64819.36668 | 29925.87455 | 61460.937 | 63292.03688 | 72520.6289  | 5691.73  |
| M_0663 | AMOZ  | C8 H15 N3 O3    | 201.1113 | 1.452  | 823028.6732 | 439452.6863 | 107792.8291 | 254451.7603 | 321062.0313 | 41157.22187 | 164954.01 | 132742.7071 | 184433.86   | 2374.317 |
| M_0664 | Ethyl hydrogen (2-quinolinylmethyl)phosphonate                              | C12 H14 N O3 P  | 251.0703 | 1.206  | 57469.33847 | 160668.3388 | 114075.1222 | 144373.5102 | 140988.7123 | 331740.2604 | 241936.37 | 312464.643  | 200884.7319 | 3797.211 |
| M_0665 | 80122   | C7 H13 N O      | 127.0999 | 3.292  | 67830.73611 | 59006.5279  | 80712.32868 | 116666.7756 | 80087.53413 | 56344.10348 | 71136.423 | 30080.83468 | 24828.97478 | 12216.31 |
| M_0666 | Acetic propanoic anhydride  | C5 H8 O3        | 116.0477 | 1.534  | 16014.70466 | 145206.5571 | 141321.2842 | 27123.06841 | 146412.6035 | 85538.3951  | 816661.31 | 181571.1783 | 114615.0176 | 64051.76 |
| M_0667 | procodazole   | C10 H10 N2 O2   | 190.0742 | 1.24   | 316591.3442 | 590757.9194 | 240036.7207 | 816372.8468 | 627804.4234 | 601996.2307 | 490848.78 | 406283.5299 | 371652.5488 | 4897.934 |
| M_0668 | (3alpha,5beta,7alpha,12alpha)-N,3,7,12-Tetrahydroxycholan-24-amide          | C24 H41 N O5    | 423.2983 | 8.489  | 5039.552605 | 4578.07253  | 15449.87747 | 815712.767  | 7441.544028 | 20150.10015 | 25774.48  | 29731.36181 | 26742.29438 | 3288.349 |
| M_0669 | Amide C18   | C18 H37 N O     | 283.2874 | 10.411 | 59748.16484 | 129214.3552 | 121080.7388 | 38121.32557 | 51102.48802 | 192948.2006 | 57736.72  | 62786.89402 | 117641.529  | 41654.14 |
| M_0670 | 2-[[2-Cyclohexylethyl]amino]adenosine                                       | C18 H28 N6 O4   | 392.2174 | 8.252  | 313107.2488 | 445528.5831 | 176723.1966 | 290168.4226 | 385660.4652 | 803809.0244 | 330397.1  | 530513.2956 | 369036.7396 | 44463.44 |
| M_0671 | 4-Amino-3-hydroxybenzoic acid   | C7 H7 N O3      | 153.0402 | 2      | 267381.5247 | 324983.7141 | 799452.4959 | 462509.7248 | 402714.3855 | 391918.0028 | 297907.52 | 363355.8915 | 262362.3736 | 6561.392 |
| M_0672 | Tretinoin   | C20 H28 O2      | 300.2088 | 8.945  | 399406.651  | 798963.8007 | 278724.3982 | 601657.7864 | 323205.553  | 542962.524  | 422325.86 | 587551.8568 | 507315.6613 | 14035.21 |
| M_0673 | 1,1'-(1,2-Ethanediylo)bis(1-nitrosourea)                                    | C4 H8 N6 O4     | 204.0608 | 1.127  | 750544.618  | 532028.6262 | 654494.3801 | 626586.7772 | 797874.9006 | 696304.4665 | 630484.66 | 613018.7202 | 660747.3153 | 1520.636 |
| M_0674 | Ethyl lactate   | C5 H10 O3       | 118.0633 | 1.994  | 523757.1083 | 290575.1241 | 290293.7865 | 207349.0927 | 209912.3684 | 371701.2618 | 240155.29 | 257816.0477 | 172515.4723 | 5796.802 |
| M_0675 | Desaminotyrosine  | C9 H10 O3       | 166.0635 | 7.773  | 56438.17413 | 48735.95125 | 53892.26881 | 8899.040623 | 64245.52316 | 26985.91641 | 17179.138 | 47367.26393 | 12910.75077 | 59563.75 |
| M_0676 | 3-hydroxyhexadecanoyl carnitine   | C23 H45 N O5    | 415.33   | 8.187  | 786402.4371 | 162126.464  | 47635.32375 | 398084.5456 | 128994.4867 | 591175.575  | 464102.25 | 493441.0359 | 263096.3804 | 6518.851 |
| M_0677 | Diethylol dimethyl hydantoin  | C9 H16 N2 O4    | 216.1109 | 2.395  | 782143.6144 | 109183.2672 | 45675.8239  | 251475.3373 | 43268.40982 | 17882.6742  | 17432.317 | 18826.5358  | 1198.883468 | 1675.005 |
| M_0678 | [1,2,4]Triazol[4,3-b][1,2,4,5]tetrazin-6-amine                              | C3 H3 N7        | 137.0453 | 1.019  | 319685.8682 | 839.8345687 | 614417.785  | 915.1476532 | 480.0449393 | 486.6184288 | 453.64709 | 675.7337673 | 527.4505525 | 672.4209 |
| M_0679 | L(-)-Asparagine   | C4 H8 N2 O3     | 132.0535 | 1.104  | 357626.9953 | 353308.3352 | 591743.0816 | 330544.7531 | 356143.5845 | 397426.6199 | 685776.51 | 458570.4976 | 778460.2532 | 3242.998 |
| M_0680 | Ethyl L-gamma-glutamyl-L-cysteinyl-L-cysteinate                             | C10 H18 N2 O5 S | 278.0936 | 2.608  | 264963.9625 | 95295.49179 | 777904.601  | 550813.9789 | 325452.4303 | 281703.0122 | 197002.27 | 354187.5357 | 232269.7344 | 4528.971 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0681 | Dimethyl-3,3'-dithiobispropionimide  | C8 H14 N2 O2 S2 | 234.0495 | 0.975  | 168347.1027 | 297075.4858 | 63374.50987 | 320648.6642 | 261021.8461 | 282051.1911 | 317685.61 | 363527.9394 | 310807.3686 | 4252.55  |
| M_0682 | 3,4-Bis(hexyloxy)thiophene   | C16 H28 O2 S    | 284.1809 | 7.859  | 478458.5332 | 128851.7392 | 141874.7362 | 283277.9213 | 299132.1518 | 697314.2821 | 682205.28 | 774390.6821 | 468855.5676 | 4908.83  |
| M_0683 | C10-HSL  | C14 H25 N O3    | 255.1834 | 9.043  | 247678.78   | 280466.7556 | 92841.27703 | 359116.5016 | 335646.2985 | 471794.2086 | 514482.22 | 773973.5746 | 567288.9531 | 41792.63 |
| M_0684 | N'-[(5-methoxy-3-nitro-6-oxo-1-cyclohexa-2,4-dienylidene)methyl]-2-(1,2,4-triazol-1-yl)acetohydrazide          | C12 H12 N6 O5   | 320.0872 | 7.685  | 584279.0633 | 688948.9842 | 612582.7516 | 444991.239  | 770364.2083 | 322597.5411 | 188757.19 | 148462.6953 | 52377.33581 | 5117.649 |
| M_0685 | 5-cyanouracil  | C5 H3 N3 O2     | 137.0231 | 0.793  | 664210.5156 | 374560.8282 | 285430.9043 | 481414.7973 | 342187.5831 | 350631.6243 | 291905.74 | 311373.4707 | 213001.5207 | 10972.76 |
| M_0686 | Boc-Phe(4-NO2)-OH (Hydroxyethyl)methacrylate   | C14 H18 N2 O6   | 310.1164 | 3.268  | 332739.7364 | 184305.3229 | 411700.2863 | 765199.1493 | 163475.5745 | 399609.0692 | 316047.54 | 535542.8279 | 276426.4061 | 5322.527 |
| M_0687 | 2,2'-[[6-Anilino-1,3,5-triazine-2,4-diy]diimino]diethane   | C13 H18 N6 O2   | 290.1492 | 8.513  | 66134.05563 | 103175.7627 | 65549.22322 | 53788.51719 | 162416.6206 | 230832.774  | 273004.72 | 236607.135  | 163325.5788 | 72013.45 |
| M_0689 | Corticosterone   | C21 H30 O4      | 346.2144 | 8.297  | 763495.3535 | 27846.08941 | 95358.54658 | 369800.2691 | 24554.16313 | 243827.0132 | 113919.18 | 92581.43684 | 509519.9517 | 7569.643 |
| M_0690 | Vigabatrin   | C6 H11 N O2     | 129.0791 | 1.334  | 439775.1975 | 583867.9261 | 255656.0321 | 225209.5059 | 761102.415  | 209791.8357 | 305224.54 | 397333.5089 | 182046.5516 | 33865.72 |
| M_0691 | 1,3,6-Thiadiazepane-2,7-dithione   | C4 H6 N2 S3     | 177.9691 | 2.218  | 85739.23978 | 723932.3759 | 121778.2006 | 128584.4283 | 400773.682  | 266263.7857 | 287496.89 | 716694.5763 | 523306.4689 | 21581.53 |
| M_0692 | Melatonin  | C13 H16 N2 O2   | 232.1211 | 6.882  | 6474.198264 | 6988.475862 | 8360.455949 | 17119.27724 | 191381.7816 | 757928.0913 | 198675.45 | 11386.49608 | 6549.101799 | 6116.28  |
| M_0693 | ACPC   | C4 H7 N O2      | 101.0481 | 1.383  | 127848.4527 | 291201.7325 | 756170.339  | 449715.9887 | 268502.814  | 287479.1023 | 224413.28 | 433931.4272 | 244716.5522 | 85378    |
| M_0694 | N-Acetoxy-2-(3-nitro-4,5-dihydro-1H-pyrazol-1-yl)acetamide   | C7 H10 N4 O5    | 230.0653 | 1.919  | 8212.018083 | 5840.505621 | 5307.738528 | 5782.259254 | 4831.375277 | 5054.154646 | 4467.4435 | 4909.092383 | 4070.950035 | 5536.493 |
| M_0695 | (2E)-4,4,4-Trifluoro-2-butenal   | C4 H3 F3 O      | 124.0139 | 1.81   | 537486.1041 | 289138.8619 | 462147.9379 | 149638.3174 | 320397.3056 | 285321.3942 | 753708.3  | 285667.5248 | 564391.9513 | 4499.52  |
| M_0696 | 1-heptadecanoyl-sn-glycero-3-phosphocholine  | C25 H52 N O7 P  | 509.3487 | 10.608 | 274448.9807 | 338494.3837 | 331058.1012 | 307846.7007 | 545650.4414 | 613196.2213 | 426881.78 | 623596.5463 | 407466.1531 | 12842.87 |
| M_0697 | LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))  | C28 H48 N O7 P  | 541.3174 | 9.519  | 24626.87846 | 365101.6532 | 234551.6479 | 694069.7208 | 571447.7666 | 611964.5938 | 748433.57 | 330340.136  | 461609.6854 | 13357.07 |
| M_0698 | Gly-Lys  | C8 H17 N3 O3    | 203.127  | 1.189  | 744823.6217 | 145377.267  | 303041.6196 | 138933.1569 | 117240.8553 | 22528.04072 | 22612.603 | 27495.58318 | 25467.78899 | 2220.17  |
| M_0699 | 3-Oxalomalic acid  | C6 H6 O8        | 206.0069 | 1.08   | 330971.161  | 270326.0705 | 241178.4185 | 315280.3331 | 261917.2489 | 251248.7204 | 219148.03 | 191346.9528 | 227771.9833 | 1160.156 |
| M_0700 | 1',3'-Dimethyl-1,4':5',1''-terimidazolidine-2,2',2''-trione  | C11 H18 N6 O3   | 282.1451 | 8.004  | 8036.903063 | 5500.851928 | 4451.655448 | 5069.418029 | 743128.2924 | 1284.291957 | 8491.3815 | 6962.936139 | 6622.747866 | 10149.74 |
| M_0701 | Icaridin   | C12 H23 N O3    | 229.1678 | 8.112  | 204996.2492 | 260391.3231 | 176501.559  | 172528.9585 | 206261.9181 | 291234.0021 | 287551.73 | 416524.6744 | 213868.0803 | 42865.1  |
| M_0702 | Butoxytriglycol  | C10 H22 O4      | 206.1517 | 7.431  | 65590.73159 | 39610.17606 | 110426.4315 | 93743.4306  | 388990.2231 | 690712.316  | 52086.751 | 33042.10481 | 25805.36718 | 11815.46 |
| M_0703 | Indole-3-acetic acid   | C10 H9 N O2     | 175.0633 | 1.545  | 159692.8559 | 424959.7365 | 427242.6241 | 371921.0566 | 401473.2787 | 741737.8467 | 584167.8  | 525581.8994 | 416981.735  | 4417.912 |
| M_0704 | (3S)-3-Methyl-5-[(1S,8aR)-2,5,5,8a-tetramethyl-4-oxo-1,4,4a,5,6,7,8,8a-octahydro-1-naphthalenyl]pentanoic acid | C20 H32 O3      | 320.2339 | 9.219  | 45149.53725 | 380100.6907 | 23622.41275 | 697818.6548 | 56394.11423 | 628067.8814 | 48638.034 | 68159.34708 | 86826.639   | 14316.05 |
| M_0705 | 4,15,21,32,37,48-Hexaoxa-1,18-diazabicyclo[16.16.16]pentacontane-5,14,22,31,38,47-hexone                       | C42 H72 N2 O12  | 796.5125 | 10.68  | 359782.7559 | 250308.5678 | 239017.1893 | 195012.4888 | 642219.731  | 357073.5991 | 609190.22 | 465683.3682 | 361103.3017 | 103309.7 |
| M_0706 | 1-Allyl-4-((2,5-dimethoxyphenyl)[1-(tetrahydro-2-furanyl)methyl]-1H-tetrazol-5-yl)methylpiperazine             | C22 H32 N6 O3   | 428.2539 | 8.595  | 78005.62435 | 79808.6015  | 660231.5361 | 129616.9049 | 232709.7546 | 205015.7228 | 304854.14 | 417879.4735 | 287923.288  | 3785.007 |
| M_0707 | Hexadecyl N-[(allyloxy)carbonyl]alaninate  | C23 H43 N O4    | 397.3194 | 8.19   | 734064.7344 | 149386.3287 | 45870.07966 | 373364.3992 | 114595.3941 | 563164.2418 | 437923.77 | 464570.0476 | 243017.8515 | 3627.26  |
| M_0708 | 5,7-Dihydroxytryptamine  | C10 H12 N2 O2   | 192.09   | 4.912  | 5619.344012 | 5377.443101 | 5581.891586 | 5498.917935 | 5436.672444 | 5516.982607 | 5421.5646 | 5494.73193  | 5412.310172 | 5410.446 |
| M_0709 | 1,5-Dihydroimidazo[4,5-c][1,2,6]thiadiazin-4(3H)-one 2,2-dioxide   | C4 H4 N4 O3 S   | 187.9999 | 2.499  | 733214.9874 | 77254.98253 | 71999.28135 | 39468.90089 | 80951.72632 | 48720.31174 | 68646.397 | 88003.74744 | 70129.85655 | 3629.732 |
| M_0710 | Eicosatetraynoic acid  | C20 H24 O2      | 314.1881 | 8.389  | 731383.5725 | 248326.5249 | 360405.8822 | 434669.9279 | 138341.3492 | 317336.6876 | 115261.8  | 282566.1767 | 157033.845  | 8329.125 |
| M_0711 | N8720800   | C11 H10 N2 O3 S | 250.0411 | 5.073  | 99610.98141 | 54904.88887 | 24357.41639 | 164243.53   | 20320.77699 | 94667.8639  | 25660.367 | 78501.37374 | 15188.78588 | 3557.614 |
| M_0712 | negamycin  | C9 H20 N4 O4    | 248.1484 | 1.261  | 724759.5049 | 7281.586799 | 134253.5056 | 116982.0461 | 6109.742736 | 25913.15316 | 5537.6055 | 17489.90198 | 5157.426243 | 1057.178 |
| M_0713 | Acetylcholine  | C9 H15 N O2     | 169.1104 | 6.908  | 98758.41552 | 91880.99633 | 139994.5696 | 133990.2532 | 112671.6217 | 171695.3145 | 113639.78 | 149240.953  | 52181.95503 | 13842.89 |
| M_0714 | 12-HHTrE Stearoyl glutamic acid  | C17 H28 O3      | 280.2035 | 8.863  | 80339.1147  | 256647.3475 | 88259.23369 | 720754.9713 | 424310.2156 | 254728.8666 | 201644.75 | 333614.6532 | 295416.3672 | 13726.38 |
| M_0715 | Boc-4-piperidone   | C10 H17 N O3    | 199.1208 | 7.97   | 606221.8904 | 505947.5386 | 241369.0762 | 500371.8801 | 484907.3509 | 715294.3935 | 451111.06 | 524738.103  | 268898.3072 | 8059.786 |
| M_0717 | 3-Hydroxy-L-proline  | C5 H9 N O3      | 131.0584 | 1.792  | 380369.3311 | 184707.5781 | 714898.0342 | 182295.768  | 114728.4475 | 78613.94778 | 62223.944 | 125529.3836 | 101371.2897 | 31001.85 |
| M_0718 | Alphenal   | C13 H12 N2 O3   | 244.0848 | 3.77   | 3270.823584 | 2165.745219 | 2309.441567 | 2198.867478 | 2186.631638 | 2127.044447 | 2186.3364 | 3022.769488 | 2156.885436 | 2276.842 |
| M_0719 | 4-Hydrazino-6-methoxy-1-(piperazin-1-ylmethyl)phthalazine  | C14 H20 N6 O    | 288.17   | 8.95   | 432898.3057 | 312364.8058 | 678574.6797 | 641591.9812 | 597456.928  | 589393.6183 | 522207.74 | 442929.2978 | 712969.899  | 4125.957 |
| M_0720 | Azanidazole  | C10 H10 N6 O2   | 246.0868 | 8.141  | 619668.3714 | 322110.997  | 294905.2047 | 432122.6866 | 567484.7631 | 711149.0711 | 499198.35 | 608029.1444 | 368253.5067 | 13486.69 |



|        |  |                |          |        |             |             |             |             |             |             |            |             |             |            |
|--------|--|----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|------------|-------------|-------------|------------|
| M_0721 | 16-Heptadecyne-1,2,4-triol   | C17 H32 O3     | 306.2169 | 8.956  | 492271.6368 | 419669.5388 | 460217.1794 | 169335.5509 | 498859.6277 | 530567.046  | 343274.95  | 490280.5232 | 620696.889  | 5152.418   |
| M_0722 | (9aR,9bS)-9a-Hydroxy-6,9-dimethyl-3-methylene-3,3a,4,5,9a,9b-hexahydroazuleno[4,5-b]furan-2,7-dione  | C15 H16 O4     | 238.1203 | 8.187  | 260062.8038 | 219753.6264 | 244413.3395 | 488576.3124 | 468913.9733 | 600490.7953 | 473350.88  | 662421.6145 | 519621.6833 | 78017.9    |
| M_0723 | cealylin   | C6 H12 N6 O3   | 216.0974 | 3.032  | 293558.1264 | 278802.0391 | 304172.2417 | 186951.9566 | 509260.3143 | 324696.8951 | 303300.27  | 707848.6292 | 186935.4026 | 44028.99   |
| M_0724 | hodgkinsine  | C33 H38 N6     | 518.318  | 9.59   | 20240.0759  | 5348.000008 | 5216.53599  | 6258.322697 | 5361.539183 | 6046.199389 | 199052.81  | 706903.8667 | 5034.164359 | 6540.529   |
| M_0725 | Trigonelline   | C7 H7 N O2     | 137.0477 | 5.129  | 705948.2383 | 239949.5263 | 153272.5245 | 63453.3902  | 63418.55228 | 35417.92616 | 17141.947  | 30782.62493 | 75856.86342 | 3780.841   |
| M_0726 | L-Aspartic acid β-benzyl ester   | C11 H13 N O4   | 245.0664 | 4.828  | 700114.027  | 30803.90316 | 41254.04118 | 55782.10931 | 15428.72522 | 28920.98954 | 26829.27   | 28542.52658 | 17924.6343  | 3608.264   |
| M_0727 | Methyl palmitate   | C17 H34 O2     | 255.2561 | 7.693  | 178475.6586 | 68293.61562 | 144388.0649 | 137674.5169 | 135830.4158 | 245565.0919 | 128398.36  | 54273.13206 | 159933.2856 | 101543.4   |
| M_0728 | N-Desmethyltramadol  | C15 H23 N O2   | 232.1438 | 8.316  | 194322.3359 | 206542.2626 | 264511.2995 | 222763.7574 | 168152.6386 | 342852.0717 | 319715.06  | 328841.1316 | 324684.7955 | 123594.6   |
| M_0729 | Gramine  | C11 H14 N2     | 129.058  | 7.817  | 222920.9995 | 538346.047  | 231641.8035 | 671685.0869 | 562024.5748 | 593208.4568 | 278740.66  | 325933.7339 | 215783.9503 | 5667.958   |
| M_0730 | YQ3683000  | C11 H18 O2     | 182.1308 | 7.843  | 22180.13391 | 9321.613691 | 11667.66075 | 173592.2662 | 143063.1878 | 35196.70184 | 77383.797  | 38624.52429 | 29259.61132 | 41033.78   |
| M_0731 | Methyl palmitate   | C17 H34 O2     | 287.2824 | 7.707  | 72809.37618 | 62982.82034 | 141171.5922 | 31358.37582 | 130939.586  | 237724.2418 | 72763.767  | 52297.35892 | 156904.9215 | 47319.19   |
| M_0732 | 4-Aminobenzoic acid  | C7 H7 N O2     | 137.0479 | 6.219  | 10243.39381 | 6017.380196 | 7035.307838 | 9794.08548  | 6933.166665 | 5419.946871 | 960.73076  | 6258.795639 | 5438.030112 | 3528.936   |
| M_0733 | Dimethylguanosine  | C12 H19 N5 O5  | 313.1385 | 2.258  | 22519.38624 | 175975.8671 | 99915.50599 | 209376.9512 | 306330.6605 | 118213.5754 | 105455.55  | 233452.0141 | 130523.6607 | 2949.893   |
| M_0734 | Trihexyphenidyl  | C20 H31 N O    | 301.2381 | 9.626  | 2976.34231  | 18168.08161 | 31923.27622 | 7931.7179   | 18147.25382 | 36187.24991 | 3022.3109  | 1084.960446 | 1534.14814  | 3736.744   |
| M_0735 | (3S)-3-((2S,3R,5S)-5-((2R)-3-((2S,4aS,5aR,6R,6aS,7aR,8R,9Z,11aS,12aR,13aS,14aR,17S,18R,19aS,20aR,21aS,23aR,24aS,25aS,26aS,27aR)-6,17-Dihydroxy-2-((2E,4R)-5-hydroxy-2,4-dimethyl-2-penten-1-yl)-6a,8,12a,13a,17,27a-hexamethyl-3-methylene-2,3,4,4a,5a,6,6a,7a,8,11,11a,12a,13,13a,14a,15,16,17,18,19a,20,20a,21a,22,23,23a,24a,25,25a,26a,27,27a-dotriacontahydrooxepino[2''',3''':5'',6''']pyrano[2'',3''':5'',6''']pyrano[2'',3''':6,7]oxepino[3,2-b]pyrano[2''', | C60 H94 O16    | 1070.656 | 8.853  | 25870.89506 | 186773.6716 | 37943.77859 | 139717.0595 | 28815.49375 | 41182.08659 | 59273.808  | 70400.62089 | 4814.318909 | 3716.329   |
| M_0736 | O24400000  | C10 H14 O4     | 198.0894 | 7.728  | 86390.11942 | 6870.979311 | 69728.17335 | 5773.150701 | 111775.8017 | 17036.09076 | 7623.0833  | 78538.2714  | 94354.61563 | 8808.511   |
| M_0737 | 2-Oxindole   | C8 H7 N O      | 133.0529 | 5.098  | 175752.6764 | 129518.2048 | 81676.25843 | 676203.3075 | 43340.06842 | 118251.1493 | 71809.569  | 70976.72136 | 71129.33735 | 3811.479   |
| M_0738 | Arachidonic acid   | C20 H32 O2     | 304.2401 | 10.049 | 249915.7207 | 180851.2983 | 276178.7576 | 322521.1099 | 389167.0613 | 465083.0798 | 437106.99  | 491928.3872 | 444441.7066 | 12995.2    |
| M_0739 | Ethyl 4-fluoro-3-nitrobenzoate   | C9 H8 F N O4   | 213.0441 | 1.118  | 120530.4421 | 94754.6424  | 52740.13108 | 59792.7245  | 108383.4205 | 173730.9166 | 258326.46  | 179095.3251 | 394747.474  | 3327.286   |
| M_0740 | (9aR,9bS)-9a-Hydroxy-6,9-dimethyl-3-methylene-3,3a,4,5,9a,9b-hexahydroazuleno[4,5-b]furan-2,7-dione  | C15 H16 O4     | 260.1025 | 8.188  | 182423.8147 | 185271.6175 | 67630.67226 | 320247.5439 | 348078.5225 | 490888.777  | 409404.36  | 487637.5846 | 431422.4165 | 80139.04   |
| M_0741 | L-(-)-Asparagine   | C4 H8 N2 O3    | 132.0536 | 1.348  | 230633.631  | 622303.5839 | 337648.0094 | 590418.338  | 373095.9067 | 367131.955  | 235402.37  | 321040.0377 | 261874.454  | 12282.47   |
| M_0742 | 2,2,4-Trimethyl-1,3-pentadienol  | C6 H12 O       | 98.1462  | 5.205  | 22223.2499  | 10589.7446  | 17195.2585  | 13212.5992  | 11417.8377  | 10538.0411  | 10538.0411 | 10538.0411  | 10538.0411  | 10538.0411 |
| M_0743 | diisobutyrate  | C16 H30 O4     | 303.241  | 9.228  | 368606.5118 | 224272.322  | 362181.096  | 553876.0026 | 652026.7895 | 604503.5688 | 403422.21  | 423343.4811 | 6164.776856 | 30260.77   |
| M_0744 | Glycidyl Stearate  | C21 H40 O3     | 340.2976 | 10.312 | 127449.1715 | 518282.628  | 99286.6743  | 311908.9457 | 516801.7344 | 364159.7895 | 482989.96  | 471773.1954 | 202137.9048 | 5918.851   |
| M_0745 | 1H-Inden-1-ylidene   | C9 H6          | 114.047  | 3.496  | 272412.0205 | 315265.5317 | 405400.8833 | 505666.7814 | 462720.2121 | 563643.2973 | 659412.67  | 667138.5648 | 482066.2349 | 5206.509   |
| M_0746 | Metalaxyl  | C15 H21 N O4   | 279.147  | 3.304  | 572452.4929 | 147773.9073 | 665732.1426 | 259692.1969 | 240299.2774 | 118584.4001 | 128315.55  | 54466.6026  | 28112.97114 | 2575.73    |
| M_0747 | Triethanolamine  | C6 H15 N O3    | 149.1053 | 0.965  | 21814.02469 | 21053.79144 | 21946.44498 | 20428.00989 | 21141.74695 | 20115.1167  | 21171.671  | 21866.68024 | 21879.3999  | 7677.994   |
| M_0748 | LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))  | C28 H48 N O7 P | 541.3147 | 10.129 | 64572.69132 | 252954.3925 | 179412.3001 | 305353.5502 | 176082.1206 | 484806.6305 | 309872.18  | 341959.4922 | 347297.8997 | 3061.724   |
| M_0749 | MTIC   | C5 H8 N6 O     | 168.0761 | 5.003  | 1801.784936 | 4651.478195 | 1689.308864 | 1835.658766 | 4590.846234 | 4773.200836 | 6077.8112  | 7526.262389 | 8343.257556 | 3546.797   |
| M_0750 | Phosphocholine   | C5 H14 N O4 P  | 183.0659 | 1.122  | 114846.6348 | 209045.9203 | 47203.87445 | 85734.52872 | 99710.46477 | 158770.7282 | 172817.27  | 140800.4309 | 206190.1304 | 2588.922   |
| M_0751 | Lauramide  | C12 H25 N O    | 199.1936 | 8.934  | 125097.0144 | 240837.8863 | 254363.9813 | 172180.1944 | 654002.0961 | 467730.1985 | 161897.8   | 638300.6282 | 170319.6556 | 29069.95   |
| M_0752 | leucoline  | C9 H7 N        | 129.0579 | 3.501  | 284508.3196 | 444637.9434 | 341173.5941 | 310754.759  | 382961.7517 | 362793.1248 | 503066.93  | 269602.8085 | 405398.7927 | 6026.295   |
| M_0753 | dimethyl-L-arginine  | C8 H18 N4 O2   | 202.1429 | 1.229  | 93470.62306 | 15525.32946 | 652920.5004 | 17929.43941 | 317573.3301 | 15768.52138 | 14335.758  | 3634.442997 | 13142.73331 | 1615.536   |
| M_0754 | 4149853  | C21 H41 N O4   | 371.3037 | 8.13   | 652447.9086 | 161172.3746 | 78773.91942 | 262265.8132 | 167282.2704 | 378491.7313 | 285303.97  | 320191.7647 | 135161.8189 | 3250.47    |
| M_0755 | S-(2-Methyl-2-propanyl) 2-(2-methyl-3-oxocyclohexyl)propa nethioate  | C14 H24 O2 S   | 256.1496 | 7.618  | 463219.4288 | 133374.7449 | 75331.91537 | 293727.5989 | 225547.2996 | 597627.7046 | 438492.56  | 573797.0382 | 183819.402  | 5826.4     |
| M_0756 | Pro-Leu  | C11 H20 N2 O3  | 228.1473 | 1.478  | 650827.2849 | 406720.9598 | 142728.9909 | 365474.745  | 308481.9333 | 253991.8108 | 17013.64   | 292460.3107 | 57063.37009 | 4713.199   |
| M_0757 | O24400000  | C10 H14 O4     | 198.0893 | 7.627  | 35503.31409 | 2078.714348 | 5426.240525 | 2058.081163 | 44516.3179  | 43539.09549 | 38031.964  | 2305.517297 | 28115.02305 | 3449.601   |
| M_0758 | 4-Aminobenzoic acid  | C7 H7 N O2     | 137.0477 | 1.247  | 647595.2996 | 27798.35236 | 518060.0924 | 33659.798   | 37815.27554 | 70710.66974 | 15797.059  | 17388.02355 | 22476.21715 | 3879.123   |
| M_0759 | N <sup>4</sup> -(1,3-Dimethyl-1H-pyrazolo[3,4-b]quinolin-4-yl)-N <sup>1</sup> ,N <sup>1</sup> -diethyl-1,4-pentanediamine  | C21 H31 N5     | 353.2564 | 8.877  | 140038.2653 | 98573.74438 | 84334.64133 | 139403.6436 | 108738.4246 | 161927.7365 | 97065.738  | 159427.256  | 82386.42108 | 4253.757   |
| M_0760 | Propofol   | C12 H18 O      | 178.1358 | 8.948  | 22075.35681 | 5298.643548 | 20311.99146 | 19451.48727 | 5662.209076 | 21123.2806  | 21944.066  | 5713.541586 | 16253.31922 | 17843.28   |
| M_0760 | Dihydrothymine   | C5 H8 N2 O2    | 128.0587 | 1.102  | 645529.4272 | 471215.4899 | 413942.1447 | 494829.466  | 458291.0707 | 366092.3198 | 501985.72  | 392802.1187 | 551620.4541 | 6749.628   |

|        |  |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|--|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0761 | OB4520000  | C10 H9 N O     | 159.0685 | 7.91  | 1132.20474  | 2023.152246 | 1777.845539 | 6826.952818 | 3705.85113  | 2786.508356 | 2970.9225 | 1954.588706 | 2263.278158 | 2860.579 |
| M_0762 | Bohemine   | C18 H24 N6 O   | 340.2012 | 9.13  | 287985.6672 | 640404.8167 | 134861.3727 | 334866.3621 | 244503.1557 | 349372.2893 | 292374.28 | 355643.3032 | 220515.888  | 4831.965 |
| M_0763 | Andrographolide  | C20 H30 O5     | 332.1963 | 8.938 | 640261.8753 | 136459.2952 | 203646.9828 | 197758.7074 | 156372.0923 | 122015.2455 | 105401.17 | 87634.21753 | 96208.06568 | 35517.53 |
| M_0764 | N-Arachidonoyl taurine   | C22 H37 N O4 S | 411.2498 | 8.529 | 321258.2501 | 346787.936  | 497809.5826 | 469666.5511 | 463742.0818 | 46541.96781 | 574909.8  | 638655.0055 | 503554.9546 | 9792.542 |
| M_0765 | Laurixamine  | C15 H33 N O    | 243.2563 | 7.757 | 15008.87384 | 8215.559012 | 3423.962394 | 7827.401105 | 24316.69678 | 23483.36624 | 13748.176 | 11430.44563 | 13583.80976 | 24178.63 |
| M_0766 | tert-Butyl hydrazodiformate  | C10 H20 N2 O4  | 232.1423 | 1.922 | 5634.718985 | 3548.047558 | 3535.455668 | 3946.644911 | 3178.597437 | 3361.200332 | 3166.1123 | 3150.79068  | 2712.772353 | 3923.756 |
| M_0767 | (Dodecylsulfonyl)acet onitrile   | C14 H27 N O2 S | 273.1761 | 7.619 | 458881.7313 | 132847.8815 | 73090.04928 | 287663.5614 | 217147.6845 | 563682.4674 | 424479.34 | 538763.6066 | 171650.0782 | 20207.97 |
| M_0768 | 5-Indolol  | C8 H7 N O      | 133.0529 | 8.521 | 634045.8235 | 377649.8649 | 455033.1977 | 409451.2462 | 149313.0132 | 166850.5586 | 121335.5  | 156621.521  | 92165.47452 | 24844.81 |
| M_0769 | SSR161421  | C25 H20 N4 O2  | 408.155  | 8.325 | 330216.8478 | 203404.8712 | 299229.2499 | 147978.8282 | 350348.3844 | 567404.1782 | 449853.07 | 363593.7867 | 434091.5746 | 66953.81 |
| M_0770 | Leu-Leu  | C12 H24 N2 O3  | 244.1787 | 3.947 | 2019.275405 | 818.5804773 | 3061.313941 | 3817.229949 | 764.1142989 | 4797.747676 | 3046.3931 | 7299.512377 | 1951.763909 | 1986.788 |
| M_0771 | N4-(2,2-DIMETHYL-1-METHYLCARBAMOYL-PROPYL)-2,N1-DIHYDROXY-3-ISOBUTYL-SUCCINAMIDE           | C15 H29 N3 O5  | 331.2107 | 2.415 | 11705.57352 | 7083.238134 | 11009.78112 | 7654.873999 | 6561.834291 | 7773.714924 | 7673.253  | 6896.070665 | 5819.431215 | 2929.99  |
| M_0772 | (4Z)-4-[Nitroso(1H-triaziren-1-yl)methylene]-4,5-dihydro-1,2,5-oxadiazol-3-amine           | C3 H3 N7 O2    | 169.0351 | 1.101 | 209936.7996 | 428710.7489 | 118233.7192 | 232967.7071 | 168753.2191 | 323891.5902 | 283626.77 | 342961.752  | 264531.7317 | 2252.368 |
| M_0773 | 1099281  | C9 H6 O        | 130.0421 | 7.498 | 26280.96851 | 16790.85653 | 19093.71292 | 120564.1616 | 86051.3205  | 330200.0723 | 110482.17 | 223300.0959 | 75918.30699 | 2921.793 |
| M_0774 | benzzyne   | C6 H4          | 76.03155 | 3.496 | 233298.4669 | 326132.6562 | 357644.2065 | 462944.1481 | 395728.6781 | 521055.4098 | 621229.98 | 588390.8235 | 473138.1455 | 5481.309 |
| M_0775 | ACETYL PROLINE   | C7 H11 N O3    | 157.074  | 4.242 | 620295.032  | 31471.18854 | 35672.76136 | 57982.37544 | 46202.19534 | 130544.0454 | 61773.039 | 61046.98614 | 37342.24495 | 8099.406 |
| M_0776 | 6-Methylindole   | C9 H9 N        | 131.0736 | 3.494 | 248614.5552 | 304406.1555 | 371967.419  | 452662.3885 | 422593.2953 | 523027.8841 | 599307.87 | 618748.4514 | 432648.6199 | 3147.494 |
| M_0777 | Acetic propanoic anhydride   | C5 H8 O3       | 116.0476 | 1.245 | 30384.81361 | 69186.83096 | 590606.4194 | 25549.96853 | 69703.6153  | 112933.0102 | 198829.43 | 174038.9499 | 66703.79622 | 2691.648 |
| M_0778 | 11343172   | C11 H21 N O3   | 215.1522 | 7.887 | 110896.3905 | 95829.32534 | 88641.67004 | 104469.6713 | 152237.6383 | 231687.1522 | 147821.11 | 224531.3256 | 115889.3525 | 25951.95 |
| M_0779 | all-trans-retinal  | C20 H28 O      | 284.2139 | 9.503 | 287764.798  | 17145.31743 | 58921.70475 | 125574.4887 | 47051.04107 | 150606.1507 | 234565.01 | 129252.8585 | 159994.8096 | 8778.051 |
| M_0780 | 6-Methoxyquinaldine  | C11 H11 N O    | 173.0842 | 7.459 | 3821.462296 | 2869.319429 | 3232.322561 | 4305.261136 | 4697.124754 | 4733.032654 | 2972.3289 | 3236.651033 | 2925.697977 | 4619.906 |
| M_0781 | 1-Allyl 2-tetradecyl 1,2-pyrrolidinedicarboxylate  | C23 H41 N O4   | 395.3038 | 8.08  | 612441.5282 | 57918.61229 | 38987.85815 | 96995.71685 | 114858.5834 | 182897.8694 | 135305.07 | 112590.0607 | 80874.6586  | 3531.63  |
| M_0782 | 4129939  | C5 H11 N O3 S  | 165.046  | 1.114 | 164623.2985 | 179611.0218 | 107668.7429 | 122235.783  | 81537.10673 | 139948.4184 | 148136.32 | 124829.6401 | 142477.6687 | 2822.383 |
| M_0783 | Creatinine   | C4 H7 N3 O     | 113.0593 | 1.226 | 610478.6394 | 358506.9778 | 452674.5262 | 318850.932  | 221718.4219 | 228813.2728 | 116744.83 | 272683.9604 | 103768.1673 | 28904.8  |
| M_0784 | N-[3-(Acetyl(2-cyanoethyl)amino)propyl]-N-[3-(13-oxoazacyclotridecan-2-yl)propyl]acetamide | C25 H44 N4 O3  | 448.3414 | 8.441 | 359120.6049 | 109838.1276 | 264045.1588 | 164174.9773 | 360345.681  | 386936.755  | 234993.37 | 407307.853  | 408402.8428 | 6557.124 |
| M_0785 | (2,6-Diethyltetrahydro[1,3,2]dioxaborolo[4,5-e][1,3,2]dioxaborepin-4-yl)methanol           | C9 H18 B2 O5   | 228.1348 | 7.444 | 55446.54468 | 30748.51965 | 5108.528204 | 14815.22818 | 39455.10186 | 159649.7193 | 8461.1652 | 47390.70737 | 6944.451655 | 52832.26 |
| M_0786 | 2,3-Dihydroxypropyl 3-sulfanyloxypropanoate  | C6 H12 O4 S    | 180.0456 | 1.586 | 96223.56829 | 126100.1338 | 118666.6548 | 97038.90733 | 91857.08348 | 98616.48798 | 125040.99 | 246450.0493 | 152214.1666 | 4975.34  |
| M_0787 | N-[5-(1H-Benzimidazol-2-yl)-1,3-thiazol-2-yl]formamide                                     | C11 H8 N4 O S  | 244.0425 | 2.508 | 600955.4747 | 92258.65616 | 72941.16329 | 58116.2441  | 64111.60386 | 84128.00327 | 83627.067 | 76858.8065  | 56981.25451 | 4719.209 |
| M_0788 | FZ5600000  | C27 H44        | 368.3443 | 8.991 | 1500.287247 | 28034.17801 | 1469.476288 | 18388.84788 | 13568.24259 | 12990.89454 | 3503.9937 | 11786.62984 | 591557.1077 | 1114.372 |
| M_0789 | 2-(Bis(2-hydroxyethyl)amino)ethyl laurate  | C18 H37 N O4   | 331.2722 | 8.72  | 168457.2102 | 147794.1029 | 111109.1718 | 90620.16294 | 68897.16226 | 115736.2607 | 119957.27 | 205267.4619 | 110657.8273 | 57093.34 |
| M_0790 | 6-Methylquinoline  | C10 H9 N       | 143.0736 | 3.495 | 216850.8774 | 204930.5363 | 306064.9393 | 441490.4212 | 355505.9535 | 496837.4631 | 556001.73 | 586254.301  | 396514.225  | 3199.109 |
| M_0791 | BOC-ARG-OH   | C11 H22 N4 O4  | 274.1638 | 1.258 | 189056.6232 | 18210.13203 | 17312.99203 | 28514.79715 | 27095.24013 | 40070.79009 | 38801.257 | 27496.9162  | 12836.25516 | 2329.321 |
| M_0792 | 2-Methyl-4-isothiazolin-3-one  | C4 H5 N O S    | 115.0095 | 2.583 | 7229.170939 | 4881.788579 | 6053.328604 | 4860.1013   | 4744.659126 | 4837.234935 | 4879.6564 | 4791.614663 | 4459.991411 | 56754.08 |
| M_0793 | 1,2-Dioxin   | C4 H4 O2       | 84.02136 | 1.131 | 18174.7496  | 69186.83096 | 208169.9746 | 42665.17879 | 55865.42394 | 212526.648  | 280820.4  | 283803.445  | 192689.3803 | 898.8736 |
| M_0794 | Acetic propanoic anhydride   | C5 H8 O3       | 116.0477 | 1.143 | 18174.7496  | 69186.83096 | 208169.9746 | 42665.17879 | 55865.42394 | 212526.648  | 280820.4  | 283803.445  | 192689.3803 | 1405.645 |
| M_0795 | Pro-Leu  | C11 H20 N2 O3  | 228.1473 | 1.139 | 576065.2837 | 210711.5185 | 179745.6507 | 220820.0515 | 119643.3216 | 91463.20741 | 80199.115 | 78656.29957 | 110920.8718 | 2128.87  |
| M_0796 | fMet   | C6 H11 N O3 S  | 177.046  | 3.377 | 575593.3245 | 150141.548  | 127408.2755 | 191370.6096 | 155151.1721 | 96623.68921 | 94808.464 | 97022.92986 | 63934.61574 | 4912.227 |
| M_0797 | Rabenzazole  | C12 H12 N4     | 212.1023 | 7.669 | 16816.16563 | 107337.1064 | 61687.27236 | 399872.474  | 575284.3495 | 508291.3436 | 67456.248 | 250363.1284 | 302976.7287 | 68834.61 |
| M_0798 | 1-O-palmitoyl-2-O-(5-oxovaleryl)-sn-glycero-3-phosphocholine                               | C29 H56 N O9 P | 593.3698 | 9.976 | 2330.165526 | 7684.97179  | 2728.586381 | 2594.098703 | 2687.277426 | 2804.211009 | 2661.3122 | 2696.649406 | 3354.434385 | 2919.653 |
| M_0799 | 1099281  | C9 H6 O        | 130.042  | 2.446 | 573349.7686 | 368751.1438 | 453531.7797 | 337978.3081 | 303429.6812 | 393784.6793 | 396693.32 | 349053.2194 | 305073.3417 | 3417.562 |
| M_0800 | Cafestol   | C20 H28 O3     | 316.203  | 8.913 | 553287.7499 | 393643.5522 | 327261.9008 | 572221.5025 | 100611.8144 | 343831.6283 | 99679.802 | 223471.1065 | 202097.0932 | 20483.36 |
| M_0801 | CU5250000  | C8 H5 N O      | 131.0373 | 4.601 | 47948.07185 | 30927.55024 | 75464.13538 | 144411.1174 | 62390.16896 | 146533.4276 | 147384.91 | 130032.6464 | 116883.7379 | 3596.335 |
| M_0802 | A-134U   | C8 H12 N6 O2   | 224.1024 | 6.972 | 567669.6736 | 217313.1263 | 445329.2882 | 372856.2765 | 229643.7755 | 220690.5955 | 142863.11 | 169233.0599 | 62810.11219 | 87175.85 |
| M_0803 | TBHQ   | C10 H14 O2     | 166.0996 | 7.83  | 35116.89171 | 245804.8145 | 233723.8556 | 252257.0445 | 75700.26103 | 94889.15607 | 278814.84 | 14555.04497 | 35664.12487 | 110826.5 |
| M_0804 | 1-Hydroxycyclohexyl Phenyl Ketone (2E)-4,4,4-Trifluoro-2-butenal                           | C13 H16 O2     | 204.1151 | 8.452 | 564477.3329 | 124165.7804 | 71325.92825 | 154901.1251 | 91190.62813 | 35842.55713 | 53272.264 | 81841.51714 | 39777.91769 | 47193.46 |
| M_0805 | TFMAA  | C4 H3 F3 O     | 124.0139 | 1.885 | 254983.4919 | 289138.8619 | 462147.9379 | 149638.3174 | 320397.3056 | 151013.2553 | 452287.09 | 285667.5248 | 564391.9513 | 3863.912 |
| M_0806 | Cyclohexylamine  | C6 H13 N       | 99.10534 | 1.218 | 13095.68416 | 10670.23566 | 11124.75371 | 5669.561499 | 12010.05479 | 10695.75182 | 6997.1904 | 9552.544931 | 8927.872769 | 5204.157 |
| M_0807 | 1-(4,6-Dimethyl-2-pyrimidinyl)-3-[3-(2-oxo-1-pyrrolidinyl)propyl]guanidine                 | C14 H22 N6 O   | 290.1857 | 8.818 | 40731.48453 | 54685.67744 | 71004.43581 | 119353.2954 | 15402.69868 | 60484.0184  | 49071.371 | 49685.81163 | 90224.91661 | 67436.68 |

|        |   |                 |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0809 | RZ2670000   | C10 H22 O6      | 238.1416 | 3.857 | 172201.2711 | 184074.484  | 216822.3309 | 295558.4761 | 178915.1443 | 215184.6455 | 157721.63 | 225623.6065 | 192476.015  | 7947.501 |
| M_0810 | L-(+)-Citrulline  | C6 H13 N3 O3    | 197.0776 | 1.312 | 228771.5285 | 308982.7721 | 281333.3116 | 555803.8925 | 357637.9452 | 112757.211  | 140413.25 | 539567.5245 | 355472.9223 | 2369.749 |
| M_0811 | N-Benzoyl-DL-alanine  | C10 H11 N O3    | 193.074  | 6.501 | 555767.9595 | 46934.16842 | 192389.7459 | 115870.2259 | 132754.9533 | 40316.39291 | 19022.478 | 15091.67036 | 5731.380468 | 12228.47 |
| M_0812 | 2,3,4,9-Tetrahydro-1H- $\beta$ -carboline-3-carboxylic acid                 | C12 H12 N2 O2   | 216.0899 | 4.515 | 194869.1655 | 223902.7684 | 257464.8127 | 211117.8139 | 117745.106  | 43514.03011 | 47240.762 | 59679.93286 | 22160.64545 | 3104.864 |
| M_0813 | DL-Arginine   | C6 H14 N4 O2    | 174.1117 | 1.387 | 22910.95741 | 110625.0732 | 23968.69426 | 115473.6453 | 12790.89371 | 122599.695  | 67473.773 | 56946.58107 | 42105.33736 | 528.7802 |
| M_0814 | N-[3-(3,5-Dimethyl-1H-pyrazol-1-yl)-5-ethyl-4H-1,2,4-triazol-4-yl]acetamide | C11 H16 N6 O    | 248.1388 | 8.588 | 271016.4404 | 211655.458  | 271496.0116 | 272133.4607 | 321370.3595 | 532879.6753 | 367482.17 | 344323.2842 | 308455.2342 | 22289.25 |
| M_0815 | Gramine   | C11 H14 N2      | 129.058  | 7.474 | 45043.50847 | 34977.67185 | 48459.64177 | 51110.52397 | 73360.42782 | 67727.41514 | 23123.822 | 20361.42623 | 14514.37006 | 3060.577 |
| M_0816 | Isophorone  | C9 H14 O        | 138.1046 | 7.817 | 15625.27493 | 176133.0624 | 161133.5199 | 235303.9159 | 232678.9969 | 35603.79743 | 53166.087 | 23300.60847 | 45897.86649 | 13702.52 |
| M_0817 | 1-Methyladamantane triolinoleyl 2-monolysocardiolipin                       | C11 H18         | 150.1409 | 8.663 | 308809.5688 | 249927.9787 | 337730.0537 | 158482.5154 | 218191.331  | 357374.2557 | 207524.02 | 439260.08   | 340726.2556 | 41575.06 |
| M_0818 | Resorufin   | C12 H7 N O3     | 213.0401 | 6.325 | 137323.8613 | 162754.4945 | 221725.3995 | 369504.2525 | 96729.33533 | 118622.6065 | 157004.12 | 199429.0536 | 162187.3417 | 2429.817 |
| M_0820 | 1,3-Dinitro-1,2,3,4-tetrahydro-1,3,5-triazine                               | C3 H5 N5 O4     | 175.0334 | 1.074 | 546015.7806 | 201311.8827 | 251856.9297 | 264359.3599 | 217135.8775 | 294564.1975 | 309667.68 | 356462.3866 | 338160.4672 | 1114.047 |
| M_0821 | pyrrolizidine   | C7 H13 N        | 111.1051 | 0.812 | 123105.8308 | 97380.18881 | 69273.34861 | 65967.42621 | 41878.1216  | 62501.95215 | 32777.284 | 49446.72996 | 31528.51364 | 4365.757 |
| M_0822 | 4-Aminobenzoic acid   | C7 H7 N O2      | 137.0479 | 6.252 | 7636.827936 | 5879.194592 | 7184.505123 | 6459.645349 | 5936.316428 | 5782.351557 | 5307.7946 | 5853.47992  | 5194.393624 | 3150.528 |
| M_0823 | 3-AB  | C7 H8 N2 O      | 136.0637 | 1.042 | 544203.6373 | 74512.51838 | 6500.520368 | 4963.826618 | 65059.58532 | 73571.21772 | 107484.13 | 47559.87654 | 3387.633117 | 191.5516 |
| M_0824 | Chromic acid  | H2 Cr O4        | 117.9355 | 0.652 | 194054.8061 | 179647.0599 | 65153.89274 | 192167.8065 | 543787.349  | 228132.6554 | 215371.1  | 46715.458   | 202725.536  | 77539.75 |
| M_0825 | Tamsulosin  | C20 H28 N2 O5 S | 408.1673 | 8.604 | 121204.7347 | 162277.9524 | 123913.0726 | 163077.146  | 191071.9374 | 224871.8907 | 198180.81 | 168547.9664 | 156566.5394 | 4227.567 |
| M_0826 | Cimaterol   | C12 H17 N3 O    | 219.1373 | 6.109 | 1039.539192 | 1004.278458 | 1032.177659 | 1033.149928 | 1047.03711  | 1039.789497 | 1054.3623 | 1034.424689 | 1051.451578 | 1023.005 |
| M_0827 | 1-[(2-Hydroxyethoxy)methyl]-5-methyl-2,4(1H,3H)-pyrimidinedione             | C8 H12 N2 O4    | 200.0797 | 1.559 | 537696.7152 | 34883.08131 | 7369.648613 | 31040.85355 | 38057.02937 | 12495.37266 | 15600.566 | 10937.95368 | 7007.863644 | 3979.767 |
| M_0828 | Arachidonic acid  | C20 H32 O2      | 304.2397 | 9.173 | 308224.5158 | 537036.0878 | 99912.04139 | 468657.0008 | 250571.6945 | 384908.6334 | 244888.42 | 363421.2639 | 335088.3197 | 9305.646 |
| M_0829 | 1,1-Dimethyl-3-(2H-tetrazol-5-yl)urea                                       | C4 H8 N6 O      | 156.0763 | 3.892 | 66531.73072 | 64379.53012 | 105339.3964 | 132560.2993 | 145141.5134 | 152299.462  | 96856.093 | 219976.7865 | 169140.9962 | 88417.91 |
| M_0830 | 6132055   | C19 H36 O3      | 312.2663 | 9.85  | 449563.1215 | 321597.1638 | 415275.3628 | 229430.1593 | 40993.64514 | 246860.9831 | 138312.28 | 254041.3156 | 207879.9851 | 70373.63 |
| M_0831 | Nonylthiol  | C9 H20 S        | 160.1292 | 1.101 | 40247.44674 | 20714.5123  | 28723.94234 | 71004.07229 | 40337.6393  | 105570.807  | 78696.861 | 67303.21131 | 82486.50582 | 852.2005 |
| M_0832 | Aminomethyl dihydrogen phosphate  | C H6 N O4 P     | 127.0037 | 1.071 | 54503.37488 | 86279.50546 | 212138.3944 | 81307.66799 | 83840.89719 | 100311.7559 | 91563.404 | 81014.78931 | 72931.44078 | 2259.576 |
| M_0833 | 5-(2-phenyl-4-triazolyl)-2H-tetrazole                                       | C9 H7 N7        | 213.0766 | 7.457 | 2145.363914 | 1610.832159 | 2833.086808 | 2001.475914 | 3269.277507 | 2599.703135 | 1668.6615 | 1660.22746  | 1464.288003 | 2593.609 |
| M_0834 | 1-Allyl 2-dodecyl 1,2-pyrrolidinedicarboxylate                              | C21 H37 N O4    | 367.2724 | 7.899 | 531859.2727 | 82436.23807 | 54918.60831 | 147477.5895 | 153335.484  | 248624.7329 | 152060.21 | 148228.9389 | 78978.58811 | 3448.504 |
| M_0835 | 5-(1-Phenyl-1H-tetrazol-5-yl)-1,3,4-oxadiazol-2-amine                       | C9 H7 N7 O      | 229.0715 | 7.159 | 411220.525  | 260288.5417 | 530508.5521 | 211508.0718 | 400623.1983 | 215647.9851 | 26667.617 | 58900.73289 | 53723.56595 | 2239.513 |
| M_0836 | 2-Benzylthiophene   | C11 H10 S       | 174.0503 | 1.131 | 529857.5786 | 391989.7954 | 263535.384  | 362225.5822 | 242816.2303 | 130129.4048 | 142088.19 | 123261.2349 | 101574.3918 | 1289.792 |
| M_0837 | tranexamic acid   | C8 H15 N O2     | 157.1103 | 1.225 | 285961.7906 | 373698.9373 | 258010.6863 | 410292.6017 | 529679.7555 | 460480.6019 | 367569.6  | 349961.9947 | 325474.818  | 3829.175 |
| M_0838 | Trigonelline  | C7 H7 N O2      | 137.0478 | 1.51  | 411776.8143 | 528662.2016 | 303484.7655 | 278443.6234 | 265607.2885 | 236161.5653 | 136456.84 | 124629.9389 | 59239.29524 | 16490.68 |
| M_0839 | Aceturic acid   | C4 H7 N O3      | 117.0429 | 1.424 | 180779.49   | 110923.6283 | 172705.5431 | 194400.6888 | 153647.0255 | 197359.3851 | 218255.58 | 303719.6162 | 207111.424  | 7672.087 |
| M_0840 | 2127  | C7 H6 O         | 106.0423 | 2.444 | 525066.0836 | 336077.5684 | 505687.7579 | 323346.7027 | 244119.0467 | 331432.0618 | 344352.26 | 247013.426  | 240685.1037 | 9818.19  |
| M_0841 | AJ3278000   | C2 H5 O5 P      | 139.9876 | 1.434 | 129508.0907 | 271724.1633 | 30702.47325 | 135315.7919 | 132831.7484 | 167704.0024 | 155333.96 | 227025.8411 | 186813.9582 | 1857.705 |
| M_0842 | 2-(14,15-Epoxyicosatrienoyl) glycerol                                       | C23 H38 O5      | 416.2539 | 8.372 | 84856.35197 | 12071.39547 | 86108.26448 | 523325.4221 | 34122.9307  | 132984.7653 | 55536.035 | 87463.54931 | 27228.24477 | 2837.22  |
| M_0843 | 9-(2-Azido-2,3-dideoxypentofuranos-yl)-9H-purin-6-amine                     | C10 H12 N8 O2   | 276.1083 | 1.161 | 492080.2459 | 520059.5628 | 509075.4413 | 395408.2337 | 365945.3544 | 150245.3649 | 125893.33 | 138568.9065 | 139775.5154 | 981.1763 |
| M_0844 | Glycerol 3-phosphate  | C3 H9 O6 P      | 172.0137 | 1.418 | 127207.3408 | 270395.164  | 29500.70645 | 134036.6811 | 131707.8332 | 166367.229  | 153227.4  | 225701.0726 | 185145.4574 | 39198.46 |
| M_0845 | Osthol  | C15 H16 O3      | 244.11   | 8.329 | 7069.77344  | 14810.82976 | 11230.7249  | 46891.16899 | 18729.74493 | 76737.35151 | 49380.948 | 68937.65101 | 61666.10628 | 7637.377 |
| M_0846 | 2-Arachidonoyl glycerol   | C23 H38 O4      | 356.2924 | 9.981 | 37572.43257 | 337394.0159 | 168235.3482 | 104138.3764 | 515527.5364 | 217157.8315 | 234502.6  | 252254.4466 | 328236.7429 | 28227.53 |
| M_0847 | Creatine  | C4 H9 N3 O2     | 131.0706 | 7.468 | 2604.594593 | 1955.642446 | 1856.141249 | 2429.906324 | 3201.419977 | 3156.188413 | 2025.8506 | 2015.611168 | 1799.259973 | 3148.79  |
| M_0848 | D-(+)-Pyroglutamic Acid   | C5 H7 N O3      | 129.0428 | 2.13  | 514191.7394 | 64138.39397 | 97052.44639 | 88818.90539 | 129392.7359 | 206292.7234 | 154037.92 | 57174.39875 | 93142.59039 | 18809.17 |
| M_0849 | 1-Methyl-4-nitro-1H-imidazole-5-sulfonamide                                 | C4 H6 N4 O4 S   | 206.0104 | 2.504 | 513441.3188 | 72399.84681 | 58469.21436 | 46631.05613 | 66142.21394 | 53806.7297  | 68253.445 | 38216.42721 | 35849.47907 | 5761.041 |
| M_0850 | GX1529000   | C7 H15 N        | 113.1208 | 5.119 | 216985.1858 | 170879.1339 | 168879.1699 | 193039.3682 | 148176.1988 | 205562.5742 | 164410.75 | 179253.2493 | 120707.9003 | 3436.983 |
| M_0851 | (1,4,8,11-Tetraazacyclotetradecan-1-ylmethyl)phosphonic acid                | C11 H27 N4 O3 P | 294.183  | 9.147 | 6779.861153 | 6669.652631 | 21693.17812 | 7678.506316 | 512699.4228 | 8177.83278  | 6365.0043 | 6939.983516 | 365727.8633 | 4188.136 |
| M_0852 | negamycin   | C9 H20 N4 O     | 248.1484 | 1.452 | 26107.96233 | 214942.86   | 33332.43833 | 36972.07832 | 75728.15283 | 175031.679  | 56974.103 | 23536.16846 | 109479.8907 | 2067.769 |
| M_0853 | Nitrosobis(2-Oxopropyl)amine  | C6 H10 N2 O3    | 158.0692 | 1.139 | 499811.3058 | 290805.5568 | 177531.0312 | 323459.0188 | 389669.4301 | 31303.81465 | 510618.19 | 309120.1418 | 470258.0855 | 443.1671 |
| M_0854 | Andrographolide   | C20 H30 O5      | 332.1964 | 8.757 | 74078.84393 | 21440.16961 | 46102.69803 | 56748.22034 | 42195.31971 | 59088.89058 | 61794.548 | 53589.83879 | 44897.66454 | 33145.94 |
| M_0855 | cealylin  | C6 H12 N6 O3    | 216.0974 | 2.929 | 52554.12658 | 57469.14565 | 304172.2417 | 186951.9566 | 509260.3143 | 91788.99012 | 57656.845 | 176888.2822 | 40249.58347 | 10460.61 |
| M_0856 | ipA   | C11 H11 N O2    | 189.079  | 1.534 | 218796.7819 | 339540.3534 | 267827.2549 | 449234.0837 | 358947.3467 | 509134.1137 | 397279.57 | 424917.8079 | 417164.7965 | 3956.761 |
| M_0857 | 8-Azaguanine  | C4 H4 N6 O      | 152.045  | 3.966 | 213964.0854 | 173232.113  | 266067.1446 | 258617.2937 | 399749.7912 | 303732.5161 | 461361.59 | 509003.4881 | 192179.4459 | 58861.89 |
| M_0858 | Sulcatol  | C8 H16 O        | 128.1203 | 8.614 | 135411.6363 | 133664.1174 | 183880.839  | 451940.8843 | 368961.2826 | 359032.7689 | 202133.37 | 298097.9206 | 508667.3308 | 52601.76 |
| M_0859 | Diaveridine   | C13 H16 N4 O2   | 260.1235 | 3.844 | 139504.9668 | 159645.7695 | 177886.1958 | 274860.6268 | 156559.9001 | 185062.37   | 144112.29 | 187786.2125 | 168730.5622 | 3891.105 |
| M_0860 | dimethyl-L-arginine   | C8 H18 N4 O2    | 202.1428 | 1.084 | 506533.262  | 187377.9119 | 277737.8985 | 144908.9794 | 195235.0357 | 126954.3464 | 148429.02 | 160744.7385 | 128831.3131 | 1764.108 |
| M_0861 | Ti0889000   | C20 H26 O4      | 330.1832 | 8.36  | 506219.3166 | 88981.27774 | 313814.9222 | 402396.2942 | 41375.27826 | 129000.3243 | 91212.965 | 190523.0747 | 142841.179  | 11041.99 |
| M_0862 | Methyl 1-(sulfanylmethyl)cyclopropylacetate                                 | C7 H12 O2 S     | 160.0555 | 0.598 | 18308.09878 | 7301.668012 | 7992.060606 | 11375.71584 | 7425.17866  | 7898.253461 | 13666.449 | 7421.898831 | 393329.853  | 9591.538 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0863 | Gly-Phe   | C11 H14 N2 O3   | 222.1004 | 1.548  | 221821.2749 | 342542.9623 | 353929.4876 | 332119.1195 | 319886.6807 | 271769.4552 | 237519.59 | 204719.8207 | 232836.9423 | 5212.883 |
| M_0864 | 4-(4-Morpholinyl)-6-(4-morpholinylmethyl)-1,3,5-triazin-2-amine   | C12 H20 N6 O2   | 280.1651 | 8.088  | 142847.1435 | 75769.04638 | 60743.03691 | 85791.29551 | 105132.6785 | 32907.13541 | 42440.439 | 108726.4162 | 104201.8614 | 71590.32 |
| M_0865 | U-44069   | C21 H34 O4      | 332.2327 | 9.333  | 20825.10024 | 93764.8412  | 21052.48626 | 96995.88708 | 14324.445   | 31734.71128 | 16520.16  | 29405.6317  | 15588.07503 | 3708.576 |
| M_0866 | 3,6-Dinitro-1,4-dihydropyrazolo[4,3-c]pyrazole  | C4 H2 N6 O4     | 198.0139 | 1.326  | 46216.90851 | 59322.95374 | 46350.68417 | 260435.2232 | 222886.0406 | 215341.6431 | 443919.85 | 88280.78754 | 501872.131  | 4853.939 |
| M_0867 | Coumarone   | C8 H6 O         | 118.042  | 1.631  | 500928.9011 | 204020.7493 | 312057.5882 | 389683.4175 | 178072.3122 | 328697.9283 | 386330.26 | 358068.7035 | 228558.9107 | 15973.13 |
| M_0868 | Nonyl N-[(allyloxy)carbonyl]-N-methylglycyl-N-methylglycinate   | C19 H34 N2 O5   | 370.2485 | 9.327  | 499191.3779 | 259473.0696 | 139762.5261 | 403370.7668 | 181596.1954 | 307931.4779 | 182575.95 | 230019.7548 | 162445.816  | 4065.157 |
| M_0869 | 1,2-  | C2 H10 Si2      | 90.03227 | 1.606  | 122213.8703 | 278094.3571 | 282794.4945 | 473563.5329 | 243393.6493 | 311683.3657 | 195937.15 | 498094.305  | 326672.4516 | 87826.58 |
| M_0870 | N,N-Dimethylaniline   | C8 H11 N        | 121.0894 | 1.488  | 10569.91332 | 17319.99032 | 11454.78781 | 14230.61711 | 12238.28983 | 15670.29487 | 12767.135 | 13779.96687 | 12529.69568 | 18649.97 |
| M_0871 | N-[1-[4-Amino-6-(dimethylamino)-1,3,5-triazin-2-yl]-3-methylbutyl]leucina mide  | C16 H31 N7 O    | 337.259  | 8.705  | 9421.265853 | 4462.86904  | 3093.631778 | 2663.77226  | 3812.68277  | 11631.20188 | 4713.3181 | 17326.35824 | 7830.097337 | 1203.338 |
| M_0872 | 2-O-Phosphonohexose   | C6 H13 O9 P     | 260.0296 | 1.404  | 55904.54113 | 47035.61437 | 16288.20083 | 14654.88831 | 20492.17994 | 65870.4985  | 63924.513 | 59978.0815  | 86549.14999 | 3784.629 |
| M_0873 | 4-Morpholinylacetic acid  | C6 H11 N O3     | 145.074  | 2.844  | 493773.6645 | 65869.62703 | 3798.400984 | 94009.34853 | 52500.04479 | 57414.05991 | 63209.314 | 61139.86005 | 58468.39433 | 30327.92 |
| M_0874 | 1,17'-Dihydroxy-10',11a,13',13a-tetramethyl-2,3,3a,3b,4,4',5,5',5a,6,6',7',8',9,9',10,10',11,11',11a,11b,12,12',13,13',13a,14',15',16',17'-triacontahydro-1H-spiro[cyclopenta[5,6]naphtho[1,2-g]chromene-8,2'-cyclopenta[a]phenanthren]-3'(1'H)-one | C40 H60 O4      | 604.4495 | 9.093  | 489503.8709 | 283776.8978 | 167689.2732 | 474937.0851 | 216047.9363 | 491276.7171 | 235773.48 | 447347.3079 | 175173.5193 | 1705.221 |
| M_0875 | Eicosapentaenoic acid   | C20 H30 O2      | 302.226  | 9.09   | 489503.8709 | 283776.8978 | 167689.2732 | 474937.0851 | 216047.9363 | 491276.7171 | 235773.48 | 447347.3079 | 175173.5193 | 2039.123 |
| M_0876 | 2-Amino-9-(2-deoxypentofuranosyl)-7,9-dihydro-3H-purine-6,8-dione   | C10 H13 N5 O5   | 283.0915 | 2.269  | 315102.4469 | 146292.8706 | 376092.506  | 490661.2748 | 491270.6746 | 123618.8062 | 102915.55 | 130873.1057 | 69800.09969 | 3866.28  |
| M_0877 | MFC00037215   | C8 H14 N2 O5    | 218.0901 | 1.267  | 15005.93857 | 41310.52374 | 10639.78629 | 25776.12134 | 18312.46613 | 4869.356541 | 37864.169 | 22014.64085 | 7734.702092 | 1464.572 |
| M_0878 | Rabenzazole   | C12 H12 N4      | 212.105  | 7.806  | 57935.58565 | 20720.93658 | 16905.9405  | 24270.58582 | 40254.91085 | 32944.4232  | 52238.187 | 28117.63948 | 31714.4756  | 36646.6  |
| M_0879 | Precocene II  | C13 H16 O3      | 220.1101 | 8.726  | 225296.7147 | 297183.3925 | 311064.6957 | 302695.2905 | 367456.4444 | 432693.0133 | 349384.29 | 412767.4986 | 319040.8136 | 58506.76 |
| M_0880 | Dibutyl itaconate   | C13 H22 O4      | 242.152  | 8.211  | 170954.3615 | 60573.09852 | 92530.31118 | 177336.4949 | 34625.23693 | 409803.3739 | 44811.563 | 76693.72866 | 70508.33021 | 70385.47 |
| M_0881 | Docosahexaenoic acid  | C22 H32 O2      | 306.2555 | 9.676  | 381907.0458 | 207684.8781 | 428210.8838 | 343728.2826 | 320517.0658 | 188580.1527 | 211845.04 | 191847.1428 | 301104.0443 | 17358.64 |
| M_0882 | 7-(2,3-Dihydroxypropyl)the ophylline  | C10 H14 N4 O4   | 254.103  | 6.889  | 1694.902391 | 1668.594474 | 1814.507341 | 10620.64445 | 130563.4055 | 479174.6627 | 144126.23 | 6100.459043 | 1714.511642 | 1601.202 |
| M_0883 | Inosine-5'-monophosphate (IMP)  | C10 H13 N4 O8 P | 348.047  | 3.456  | 28787.93591 | 33041.01497 | 34792.64468 | 41308.52216 | 38913.62687 | 44323.70888 | 48631.929 | 50726.29301 | 41759.06288 | 13840.66 |
| M_0884 | AM9627000   | C8 H7 N O3      | 165.0428 | 7.463  | 12156.79766 | 9734.645568 | 13349.06191 | 15289.29688 | 12619.72885 | 11042.6107  | 11180.228 | 12801.74203 | 13085.96214 | 6839.832 |
| M_0885 | N6,N6,N6-Trimethyl-L-lysine   | C9 H20 N2 O2    | 188.1525 | 1.293  | 152461.6214 | 7500.283667 | 18364.50819 | 39510.11254 | 6616.194199 | 44166.34903 | 10873.413 | 25098.34646 | 5339.325641 | 1423.931 |
| M_0886 | Maraniol  | C12 H12 O3      | 204.0788 | 8.961  | 227034.5019 | 232182.5523 | 333504.4796 | 450884.404  | 423214.1019 | 386637.9608 | 325022.59 | 294116.7817 | 362346.5315 | 70562.74 |
| M_0887 | (4,6-Di-piperidin-1-yl-[1,3,5]triazin-2-yloxy)-acetonitrile   | C15 H22 N6 O    | 302.1855 | 8.952  | 1959.242899 | 2347.363651 | 932.630601  | 476972.6144 | 1352.607319 | 2449.238519 | 2082.6937 | 2432.469936 | 1756.290878 | 428.5447 |
| M_0888 | DL-Citrulline   | C6 H13 N3 O3    | 175.096  | 1.24   | 108890.5179 | 335099.3596 | 120880.7453 | 256087.6953 | 476690.8162 | 342591.0566 | 257652.98 | 48151.57538 | 118782.377  | 1745.098 |
| M_0889 | 1-arachidonoyl-sn-glycero-3-phosphocholine  | C28 H50 N O7 P  | 543.3328 | 10.029 | 8777.834773 | 150083.6613 | 80731.76752 | 48898.15305 | 117726.7012 | 67400.9178  | 131387.53 | 174545.1224 | 148788.4062 | 1563.231 |
| M_0890 | Temozolomide  | C6 H6 N6 O2     | 194.0556 | 7.418  | 48949.72873 | 100006.0455 | 55865.54055 | 93588.33444 | 292360.8712 | 262402.0595 | 116423.79 | 118297.0753 | 63221.71795 | 72931.22 |
| M_0891 | Docosahexaenoic acid  | C22 H32 O2      | 328.2377 | 9.664  | 382703.1628 | 192131.4522 | 421334.4014 | 337425.0478 | 314110.7733 | 183583.3811 | 209807.72 | 189658.7741 | 299023.9965 | 5310.449 |
| M_0892 | 2,6-Ditert-butylhexahydro-1H,5H-2,3a,4a,6,7a,8a-hexaazacyclopenta[deffluorene-4,8-dione   | C16 H28 N6 O2   | 336.2275 | 9.34   | 475030.238  | 35241.88802 | 49097.63522 | 30490.37357 | 15184.84813 | 88291.60253 | 92221.967 | 4148.505803 | 58049.65935 | 55458.86 |
| M_0893 | 1-carboxy-3-hydroxyadamantane   | C11 H16 O3      | 196.1099 | 8.395  | 29062.67154 | 28331.55467 | 11744.46333 | 26187.43931 | 32067.7624  | 36109.56262 | 18328.792 | 37265.23621 | 15645.11007 | 54050.71 |
| M_0894 | negamycin   | C9 H20 N4 O4    | 248.1483 | 1.117  | 473476.3887 | 111172.1057 | 117209.224  | 192584.0121 | 116980.9531 | 222761.156  | 212542.26 | 214748.4381 | 210029.1832 | 1644.052 |
| M_0895 | 1-(2-Deoxypentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione   | C10 H14 N2 O5   | 242.0903 | 3.011  | 355100.434  | 325186.74   | 393117.1644 | 297068.9495 | 407348.5595 | 405091.1131 | 344832.5  | 418221.3532 | 472908.7595 | 9348.647 |
| M_0896 | Fluperlapine  | C19 H20 F N3    | 309.1633 | 8.331  | 40614.06933 | 60302.83014 | 37318.93271 | 36411.93076 | 36749.77593 | 46794.68805 | 43581.908 | 44830.60324 | 470791.3167 | 93117.85 |
| M_0897 | Myristamide   | C14 H29 N O     | 227.225  | 9.322  | 24543.95981 | 29330.55613 | 30104.36381 | 42507.07765 | 41424.53683 | 52213.2051  | 31360.764 | 39592.7294  | 30417.20034 | 17668.82 |
| M_0898 | DA9185000   | C12 H10 O S     | 202.0453 | 1.6    | 39559.56631 | 179829.425  | 340233.3371 | 147447.6673 | 25524.86563 | 131247.5806 | 310626.81 | 319564.7996 | 314370.5502 | 14169.31 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0899 | 1-(2-[[1-Ethoxy-1-oxo-2-pentanyl]amino]prop-1-en-1-yl)indole-2-carboxylic acid   | C19 H32 N2 O5   | 368.2328 | 9.178  | 467756.5564 | 263900.2663 | 162977.1614 | 358123.657  | 194856.6852 | 342516.7628 | 266746.41 | 328291.9546 | 256154.2114 | 4588.056 |
| M_0900 | N4-(2,2-DIMETHYL-1-METHYLCARBAMOYL-PROPYL)-2,N1-DIHYDROXY-3-ISOBUTYL-SUCCINAMIDE   | C15 H29 N3 O5   | 331.2108 | 3.544  | 4449.015173 | 12299.49912 | 4912.752526 | 5405.933959 | 5664.126321 | 6596.646966 | 7200.4349 | 7007.25204  | 3167.977305 | 2138.997 |
| M_0901 | Indoline   | C8 H9 N         | 119.0738 | 7.174  | 464492.8307 | 101821.2857 | 131910.5862 | 94602.77389 | 92271.33966 | 80074.4062  | 35220.07  | 22370.66606 | 15986.26178 | 2754.68  |
| M_0902 | SL4860000  | C13 H20 O2      | 208.146  | 8.438  | 2609.949926 | 1611.300157 | 1992.73866  | 2641.132453 | 1261.027934 | 29189.65609 | 346105.75 | 1991.810146 | 5063.424808 | 9264.164 |
| M_0903 | Midodrine  | C12 H18 N2 O4   | 254.1265 | 3.26   | 5628.654423 | 26131.0938  | 23269.89351 | 23589.83153 | 14368.78312 | 6774.307858 | 6290.1133 | 10086.68244 | 6133.885021 | 6486.981 |
| M_0904 | 2062850  | C23 H34 O3      | 358.2504 | 8.367  | 128518.909  | 15072.81417 | 75097.07746 | 461623.2894 | 20515.05614 | 92547.32559 | 38389.126 | 65164.7192  | 22510.80341 | 5691.998 |
| M_0905 | Allantoinic acid   | C4 H8 N4 O4     | 176.0537 | 0.964  | 459866.427  | 122362.1676 | 222685.8783 | 113690.0522 | 220649.9131 | 124520.7655 | 113240.53 | 231193.2876 | 120235.0854 | 4796.109 |
| M_0906 | Resorufin  | C12 H7 N O3     | 213.0435 | 4.536  | 459740.8704 | 208705.6215 | 229719.9158 | 229493.2924 | 128027.3056 | 150199.7894 | 137175.43 | 148020.2617 | 86163.25032 | 3171.599 |
| M_0907 | 4-Morpholinylacetic acid   | C6 H11 N O3     | 145.0739 | 2.256  | 429079.3153 | 119869.9405 | 459133.0545 | 152493.376  | 126164.844  | 58259.20555 | 17169.131 | 34972.44284 | 49507.33204 | 6328.238 |
| M_0908 | 3-Phenylpyrazole-4-carbaldehyde  | C10 H8 N2 O     | 172.0637 | 1.543  | 246055.6474 | 344255.0063 | 356644.815  | 329564.4599 | 312631.5475 | 257189.1541 | 241979.4  | 185211.8091 | 222193.6602 | 4397.914 |
| M_0909 | Creatinine   | C4 H7 N3 O      | 113.0592 | 1.318  | 307424.8687 | 301144.7546 | 452674.5262 | 345130.9577 | 122476.0188 | 119838.4075 | 142934.13 | 62977.41157 | 74687.60194 | 23359.77 |
| M_0910 | 2-Arachidonoyl glycerol  | C23 H38 O4      | 378.2745 | 9.986  | 31936.94204 | 291889.6393 | 154551.7069 | 88664.06875 | 452372.2984 | 183195.2595 | 197347.66 | 221591.4402 | 214638.1501 | 25566.75 |
| M_0911 | AMOZ   | C8 H15 N3 O3    | 201.1113 | 1.236  | 451918.2145 | 101391.9965 | 101197.3125 | 91225.15811 | 92940.28571 | 25709.83987 | 20032.899 | 26500.35469 | 24565.61689 | 2637.146 |
| M_0912 | Diethyl formamidomalonate  | C8 H13 N O5     | 203.0794 | 2.721  | 451779.7295 | 57069.8865  | 6754.888324 | 15907.56453 | 19429.38922 | 8892.947085 | 8122.787  | 11271.15675 | 4574.83582  | 4854.896 |
| M_0913 | 2509   | C12 H20 O2      | 196.1464 | 8.628  | 161657.4802 | 383584.7797 | 141439.7659 | 133195.2748 | 135323.7474 | 160070.7237 | 131179.24 | 307187.9797 | 163449.3409 | 39968.9  |
| M_0914 | 2210856  | C18 H32 O2      | 280.2401 | 10.103 | 220373.9447 | 295243.9855 | 71502.77842 | 156082.3509 | 155960.1431 | 164071.4597 | 169269.12 | 216159.7317 | 221669.6087 | 14192.32 |
| M_0915 | (1R)-N1'-(3-fluorophenyl)-1-(hydroxymethyl)-7-methoxy-9-methyl-N2-propylspiro[1,3-dihydropyrido[3,4-b]indole-4,4'-piperidine]-1',2-dicarboxamide | C29 H36 F N5 O4 | 537.2742 | 8.722  | 22790.05011 | 23996.35805 | 45945.92736 | 21836.96447 | 24681.04712 | 74796.22016 | 448664.04 | 219561.0434 | 27547.9084  | 51953.93 |
| M_0916 | 1,4-Diphenyl-1,4-diphosphinane   | C16 H18 P2      | 272.0884 | 8.643  | 186157.5561 | 868.0008063 | 1658.46043  | 158956.0231 | 256369.2975 | 323502.9525 | 234907.32 | 289370.693  | 255200.9747 | 6587.309 |
| M_0917 | 5-(2-Methyl-2-propanyl) 2,3-dimethyl-5-oxohexanethioate  | C12 H22 O2 S    | 230.134  | 7.434  | 448175.9127 | 72171.19153 | 43403.39987 | 53633.02835 | 91090.12523 | 211104.7055 | 109320.66 | 145554.4505 | 52602.37046 | 4640.619 |
| M_0918 | 2,6-Dimethyl-γ-pyrone  | C7 H8 O2        | 124.0527 | 7.626  | 6792.368489 | 199460.8642 | 176025.879  | 195400.0012 | 293494.9912 | 8396.694636 | 214761.33 | 5574.553383 | 217044.6496 | 8569.451 |
| M_0919 | N-[3-(3,5-Dimethyl-1H-pyrazol-1-yl)-5-ethyl-4H-1,2,4-triazol-4-yl]acetamide  | C11 H16 N6 O    | 248.1387 | 8.491  | 95079.75101 | 47389.31742 | 64781.0266  | 8477.673996 | 56280.64549 | 25663.22932 | 9949.7197 | 73164.13348 | 72720.13263 | 63342.91 |
| M_0920 | 2-Oxo-4-pentenoate   | C5 H5 O3        | 113.0246 | 1.065  | 133959.6968 | 445088.371  | 25546.49176 | 95900.57062 | 130220.7969 | 28763.74708 | 26421.191 | 14928.16939 | 6530.327515 | 1022.822 |
| M_0921 | 1886839  | C20 H30 O4      | 334.2141 | 8.255  | 156638.3242 | 254039.4517 | 110686.9669 | 135775.6008 | 131628.1262 | 444657.1919 | 246403.03 | 432652.8892 | 226277.4804 | 33694.71 |
| M_0922 | Acetanilide  | C8 H9 N O       | 135.0685 | 1.629  | 443659.6737 | 185431.4215 | 280433.5312 | 334700.9591 | 157735.4108 | 302627.4809 | 349181.74 | 310361.8597 | 204756.9222 | 12101.18 |
| M_0923 | leucaline  | C9 H7 N         | 129.0581 | 6.105  | 1976.563794 | 1680.948962 | 1703.984557 | 2282.610588 | 1700.175957 | 1688.407304 | 1731.3945 | 1685.230232 | 1717.744545 | 1661.152 |
| M_0924 | Glycerol (1-(12-Hydroxystearate))  | C21 H42 O5      | 374.3037 | 9.067  | 223007.6982 | 215122.7915 | 168686.9305 | 278225.7987 | 308729.9318 | 240393.4082 | 275385.78 | 235560.0647 | 258453.1921 | 23433.77 |
| M_0925 | NL8513000  | C11 H13 N O2    | 191.0946 | 1.665  | 41026.04806 | 24315.1474  | 26865.1156  | 22533.68703 | 19585.62586 | 24006.0784  | 21183.525 | 20508.55534 | 16093.93032 | 9139.746 |
| M_0926 | Coumarone  | C8 H6 O         | 118.042  | 1.25   | 274627.9044 | 135679.4954 | 127707.4609 | 270502.8672 | 121483.7764 | 179007.9685 | 231982.21 | 346994.5915 | 254274.3223 | 10587.18 |
| M_0927 | n-Amylbenzene  | C11 H16         | 148.1253 | 8.668  | 250326.2742 | 201823.1473 | 211180.3474 | 99255.92899 | 259573.761  | 287349.9122 | 179295.26 | 336083.2398 | 252129.5742 | 47794.95 |
| M_0928 | D-Serine   | C3 H7 N O3      | 105.0431 | 1.259  | 193102.5993 | 279611.985  | 202012.6719 | 213283.5513 | 232768.238  | 365706.1698 | 333637.25 | 354895.5538 | 281503.154  | 3140.827 |
| M_0929 | Epitestosterone  | C19 H28 O2      | 288.2087 | 8.59   | 7095.877828 | 5802.673328 | 6963.95549  | 7978.74732  | 6482.570118 | 8358.785227 | 7503.7266 | 8199.2313   | 8187.614478 | 7238.39  |
| M_0930 | 1-(4-Nitrophenyl)piperidine  | C11 H14 N2 O2   | 206.1055 | 1.542  | 189483.7231 | 292336.3028 | 222178.0548 | 389953.0094 | 320744.7845 | 434768.405  | 330391.48 | 355302.7176 | 358569.019  | 2217.151 |
| M_0931 | Adenosine 5'-monophosphate   | C10 H14 N5 O7 P | 347.063  | 1.505  | 8437.20441  | 110146.0308 | 6663.507167 | 432843.5022 | 117934.9821 | 220570.3991 | 434568.66 | 125088.7371 | 341769.3171 | 2151.348 |
| M_0932 | Thymine  | C5 H6 N2 O2     | 126.0432 | 2.903  | 183996.933  | 194817.1705 | 434113.3248 | 264824.9088 | 214252.9685 | 123498.9588 | 39613.693 | 34580.46724 | 261337.73   | 2353.524 |
| M_0933 | 3,4-Dihydroxyphenylglycol O-sulfate  | C8 H10 O7 S     | 250.0155 | 7.123  | 38256.28187 | 38671.6281  | 32994.26966 | 53251.72124 | 49633.51794 | 31268.81841 | 6966.1214 | 9453.304608 | 7579.461101 | 2584.649 |
| M_0934 | L-(+)-Valine   | C5 H11 N O2     | 117.0793 | 0.598  | 32407.04096 | 36890.31112 | 30411.09421 | 217389.4143 | 26376.22022 | 36799.32276 | 337783.52 | 36625.36995 | 376107.1448 | 39986.17 |
| M_0935 | Azelaic acid   | C9 H16 O4       | 188.1051 | 8.503  | 432922.204  | 37798.83801 | 36931.924   | 53781.72136 | 70992.26886 | 291531.9812 | 375037.72 | 52318.95337 | 48858.80377 | 66113.31 |
| M_0936 | 3-Methoxy-5-(methylsulfonyl)-4-isothiazolecarbonitrile   | C6 H6 N2 O3 S2  | 217.9819 | 1.179  | 431366.6875 | 182828.0326 | 138490.2866 | 192556.8492 | 161101.6106 | 71862.05126 | 49385.564 | 63552.39907 | 44507.31942 | 959.133  |
| M_0937 | 2-Pyrrolidone  | C4 H7 N O       | 85.05321 | 0.598  | 22188.64112 | 22775.3121  | 22074.39593 | 24457.56929 | 19152.14952 | 23493.70977 | 25592.745 | 114365.6645 | 362272.947  | 23563.19 |
| M_0938 | Cafestol   | C20 H28 O3      | 316.2015 | 8.884  | 363393.8753 | 232143.6579 | 19874.13371 | 428984.6035 | 90166.22376 | 257440.9699 | 69224.884 | 133944.719  | 93699.01656 | 18291.35 |
| M_0939 | N-Benzoyl-DL-alanine   | C10 H11 N O3    | 193.0743 | 5.788  | 9263.647128 | 129520.299  | 404256.4711 | 356212.5974 | 1102.012079 | 2028.020806 | 1309.3786 | 2589.675256 | 136744.3269 | 324.8704 |
| M_0940 | (2E)-3-[3-(Cyanomethyl)-7,8,12,13,17,18-hexaethyl-2-porphyrinyl]acrylonitrile  | C37 H40 N6      | 568.3341 | 10.101 | 2440.711991 | 138667.5658 | 32819.38906 | 138686.6856 | 97078.3161  | 201703.7406 | 133455.44 | 158895.3023 | 147420.9279 | 3096.494 |
| M_0941 | AMOZ   | C8 H15 N3 O3    | 201.1112 | 1.545  | 428007.973  | 312802.2447 | 113234.7727 | 281600.5432 | 321062.0313 | 142273.5199 | 108005.82 | 139651.89   | 4337.499478 | 2478.828 |
| M_0942 | 2,3-Dihydroxypropyl 2-(methylamino)ethyl hydrogen phosphate  | C6 H16 N O6 P   | 229.0715 | 7.294  | 13528.75924 | 8334.243345 | 13191.04965 | 100792.4217 | 6323.642764 | 225546.8931 | 43874.671 | 31629.90344 | 19254.53155 | 2025.839 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0943 | N-(2-Hydroxyethyl)-N-[2-(octanoylamino)ethyl]-beta-alanine   | C15 H30 N2 O4   | 302.2221 | 10.094 | 208775.9741 | 266503.5089 | 130796.446  | 190401.4423 | 213569.0516 | 225702.7946 | 194582.9  | 178045.1099 | 268341.8075 | 11320.32 |
| M_0944 | Tetrahydrogestrinon  | C21 H28 O2      | 312.2064 | 9.622  | 137631.3938 | 134404.8969 | 42502.66369 | 74614.17483 | 30342.83934 | 61278.27568 | 154944.86 | 141425.1843 | 98316.96348 | 5778.974 |
| M_0945 | Olomoucine   | C15 H18 N6 O    | 298.1544 | 8.611  | 41588.58489 | 42935.63354 | 39079.64408 | 39166.28686 | 41067.05707 | 43096.08867 | 55336.532 | 45849.80315 | 44743.00137 | 49029.97 |
| M_0946 | Guanosine monophosphate  | C10 H14 N5 O8 P | 363.0582 | 2.143  | 941.587506  | 15023.43762 | 3056.515625 | 28883.6289  | 16827.17326 | 3635.782406 | 2170.4995 | 1663.21542  | 2660.157994 | 362.338  |
| M_0947 | Butyl O-phosphoserinate  | C7 H16 N O6 P   | 241.0713 | 1.305  | 15683.67046 | 12832.21567 | 10796.78052 | 8984.411068 | 19205.52258 | 17461.86482 | 44356.268 | 13942.64392 | 15793.32178 | 1873.302 |
| M_0948 | 1-Allyl-3-(7H-purin-6-yl)urea  | C9 H10 N6 O     | 218.0919 | 7.54   | 58536.99591 | 48882.44056 | 39731.81092 | 34163.34326 | 44264.5439  | 422465.6014 | 50466.832 | 33977.81247 | 35658.8367  | 78331.27 |
| M_0949 | 2-(Dimethylamino)-1,3,5-triazine   | C13 H22 N6 O2   | 294.1807 | 9.143  | 287240.8766 | 108930.7779 | 174285.8188 | 390947.1811 | 402672.4897 | 385917.9138 | 193649.58 | 293631.3791 | 315109.9619 | 61216.15 |
| M_0950 | Eicosatetraynoic acid  | C20 H24 O2      | 296.1774 | 8.39   | 419735.5786 | 145942.9928 | 217498.9897 | 276346.1508 | 85800.73836 | 197880.0293 | 71168.083 | 161030.8032 | 83985.36925 | 6786.847 |
| M_0951 | Methyl 3,3,3-trifluoropyruvate   | C4 H3 F3 O3     | 156.0035 | 1.436  | 63754.95446 | 34003.53347 | 3578.455887 | 44090.61751 | 55577.70969 | 175689.6573 | 373950.42 | 183846.104  | 418632.1906 | 823.6551 |
| M_0952 | 3H-1,2,4-Triazol-3-one   | C2 H N3 O       | 83.01202 | 1.197  | 418124.7369 | 301010.6827 | 234529.9117 | 283424.5147 | 272529.6671 | 228566.7836 | 212473.52 | 245898.0355 | 212327.3629 | 2277.094 |
| M_0953 | D00750000  | C15 H24 O2      | 236.1776 | 8.622  | 82475.28047 | 65344.80288 | 127957.9556 | 88142.0972  | 98787.83923 | 11828.06719 | 117018.12 | 136032.7929 | 98413.37013 | 47626.81 |
| M_0954 | Z-ORN-OH   | C13 H18 N2 O4   | 266.1267 | 2.636  | 5005.299757 | 3942.099752 | 4085.612954 | 4001.69974  | 3749.750185 | 3775.512444 | 3766.1069 | 3746.892094 | 3654.114553 | 3879.914 |
| M_0955 | negamycin  | C9 H20 N4 O4    | 248.1483 | 1.29   | 176285.0631 | 4483.827162 | 134253.5056 | 116982.0461 | 3736.007227 | 10507.20991 | 3424.3515 | 6565.630317 | 3101.220177 | 855.5388 |
| M_0956 | Glucosylurea   | C7 H14 N2 O6    | 222.0851 | 1.17   | 21297.4274  | 114022.7259 | 268075.599  | 137234.1621 | 148424.5808 | 337436.7819 | 286757.36 | 373586.2812 | 175239.8726 | 1881.14  |
| M_0957 | FZ5600000  | C27 H44         | 368.3443 | 9.565  | 6011.103866 | 338754.2309 | 138249.1564 | 278220.3791 | 270666.3262 | 204041.4268 | 182924.41 | 279760.6867 | 262144.1618 | 5390.141 |
| M_0958 | ACPC   | C4 H7 N O2      | 101.0482 | 1.277  | 324974.4986 | 292102.2947 | 312373.9954 | 315395.3389 | 412652.5465 | 171680.5331 | 80653.945 | 108986.3416 | 99364.9295  | 62043.19 |
| M_0959 | 4-(3-Aminopropyl)-1-methylpiperazine   | C8 H19 N3       | 157.1579 | 0.799  | 100441.7834 | 60294.40845 | 24483.61871 | 12883.58082 | 22587.1681  | 26524.72145 | 23052.455 | 12553.4663  | 18888.55674 | 1645.114 |
| M_0960 | 4-(3-Aminopropyl)-1-methylpiperazine   | C8 H19 N3       | 157.1578 | 0.895  | 753.5838744 | 60294.40845 | 1852.610854 | 655.9876745 | 825.0570949 | 26524.72145 | 851.52495 | 1066.267772 | 18888.55674 | 244.9171 |
| M_0961 | PTA  | C6 H12 N3 P     | 157.0767 | 3.549  | 349481.2342 | 373335.2879 | 400075.1295 | 215778.5914 | 312641.0691 | 302494.7149 | 319414.17 | 277274.567  | 187462.741  | 6094.69  |
| M_0962 | L-Histidine  | C6 H9 N3 O2     | 155.0696 | 0.92   | 213877.8572 | 43408.97164 | 409420.4339 | 47747.87956 | 7800.946054 | 356857.5637 | 268221.01 | 270425.4359 | 348464.5616 | 2585.12  |
| M_0963 | 4,4'-Methylenebis[2-tert-butyl-6-(alpha-methylbenzyl)phenol]   | C37 H44 O2      | 520.3362 | 8.975  | 16731.35146 | 17743.80627 | 10417.43993 | 27593.44279 | 21357.51743 | 8861.990824 | 20029.123 | 8421.17508  | 8186.917045 | 46918.43 |
| M_0964 | 4-Morpholinylacetic acid   | C6 H11 N O3     | 145.074  | 1.244  | 206431.5966 | 167729.2212 | 406072.5004 | 217195.0396 | 222743.9121 | 123275.1714 | 264004.16 | 258604.1194 | 132052.574  | 30136.33 |
| M_0965 | Rhodamine 6G   | C28 H30 N2 O3   | 442.2262 | 7.721  | 32122.03406 | 34437.47413 | 321111.9221 | 261745.9336 | 216502.182  | 3371.894972 | 3161.8898 | 42748.08303 | 66553.17323 | 3635.307 |
| M_0966 | (+)-Alantolactone  | C15 H20 O2      | 232.1465 | 8.575  | 92753.01647 | 16163.42065 | 4795.594815 | 5003.514084 | 3365.814434 | 13508.37845 | 10672.372 | 4310.172504 | 13135.33601 | 4841.833 |
| M_0967 | N-Boc-L-valine   | C10 H19 N O4    | 217.1314 | 1.317  | 404912.1247 | 40084.10634 | 55153.24697 | 2478.978696 | 4629.603965 | 5614.272009 | 8707.9501 | 5511.649845 | 7762.65853  | 335.5479 |
| M_0968 | N-Boc-L-valine   | C10 H19 N O4    | 217.1314 | 1.256  | 404912.1247 | 20018.93619 | 302803.6235 | 55823.64195 | 23617.85632 | 20276.02699 | 5053.5079 | 13694.65687 | 14527.08739 | 845.6637 |
| M_0969 | ACETYL PROLINE   | C7 H11 N O3     | 157.074  | 3.254  | 131710.0209 | 404485.8308 | 214763.5101 | 85578.90193 | 66423.66005 | 51800.02641 | 46394.176 | 33204.48953 | 40963.41755 | 6111.201 |
| M_0970 | phenacetin   | C10 H13 N O2    | 179.0947 | 2.669  | 14905.80095 | 11650.254   | 4386.255094 | 4190.047947 | 11743.14492 | 3189.871364 | 4518.9456 | 4232.556888 | 3809.34863  | 3279.284 |
| M_0971 | DL-Lysine  | C6 H14 N2 O2    | 146.1056 | 1.6    | 401565.9936 | 69991.74239 | 96807.91164 | 82350.69539 | 66310.15426 | 101428.618  | 101702.81 | 88695.75239 | 26250.88963 | 4928.419 |
| M_0972 | 1-[(9E)-9-Octadecenoyl]pyrroli dine  | C22 H41 N O     | 335.3187 | 9.462  | 134807.4532 | 256562.0672 | 213154.3403 | 255282.999  | 92908.86211 | 109515.4513 | 217552.98 | 235118.0194 | 178584.8933 | 29149.77 |
| M_0973 | Phenol   | C6 H6 O         | 94.04203 | 1.244  | 266331.2319 | 70796.46115 | 121185.6885 | 119416.9829 | 117129.6608 | 162105.2819 | 209248.68 | 306936.7872 | 218853.189  | 10510.15 |
| M_0974 | Hydroxymethylfurfural  | C6 H6 O3        | 126.0319 | 1.234  | 26196.16438 | 38269.38643 | 123526.0551 | 90682.16315 | 38214.71662 | 216758.0745 | 132432.84 | 178701.161  | 183634.6931 | 55600.59 |
| M_0975 | DL-Tryptophan  | C11 H12 N2 O2   | 204.0899 | 1.543  | 208451.3815 | 296081.0877 | 312474.7369 | 266015.1532 | 258872.9482 | 204667.8709 | 193977.63 | 145876.7066 | 175897.7089 | 2237.644 |
| M_0976 | Acetanilide  | C8 H9 N O       | 135.0685 | 1.243  | 261169.0387 | 66865.36679 | 117453.4982 | 260715.9897 | 112963.3596 | 158877.204  | 206127.5  | 303891.722  | 224102.0059 | 9512.585 |
| M_0977 | Isopropyl N,S-diisopropylcysteinate  | C12 H25 N O2 S  | 247.1606 | 7.433  | 396328.7533 | 64944.82668 | 41187.58216 | 86157.5007  | 81555.4545  | 192123.0678 | 97879.056 | 134496.46   | 49291.156   | 2193.547 |
| M_0978 | Docosahexaenoic acid   | C22 H32 O2      | 328.2402 | 9.663  | 238929.5748 | 4041.692767 | 4155.4246   | 4735.592628 | 4396.619444 | 4585.795366 | 3897.5688 | 3927.142926 | 3979.313217 | 5266.538 |
| M_0979 | 611459   | C16 H29 N O     | 251.2249 | 8.631  | 4434.33015  | 4888.614244 | 5042.345301 | 5036.974503 | 5669.403008 | 6136.921863 | 5566.8394 | 6555.903059 | 5363.75351  | 4043.579 |
| M_0980 | 12,12,23,23-Tetramethyl-2,5,8,11,13,16,19,22,24,27,30,33-dodecaoxa-12,23-disilatetratricontane   | C24 H54 O12 Si2 | 590.3165 | 9.869  | 41046.64163 | 12045.94072 | 18874.03031 | 33952.27391 | 62360.91742 | 9908.984835 | 320858.7  | 13792.99373 | 19635.42947 | 1547.728 |
| M_0981 | 4-(5-Amino-1,3,4-oxadiazol-2-yl)-1,2,5-oxadiazol-3-amine   | C4 H4 N6 O2     | 168.0399 | 5.24   | 78346.67539 | 286390.0206 | 46123.41508 | 394072.7503 | 109856.4035 | 90956.45947 | 33792.743 | 85576.04832 | 89105.23965 | 3500.954 |
| M_0982 | 2127   | C7 H6 O         | 106.0424 | 8.768  | 7232.487686 | 4062.038609 | 2690.772049 | 4016.041205 | 4022.219148 | 4857.082132 | 4007.5676 | 784.5288288 | 3892.997525 | 3614.178 |
| M_0983 | 3-[[4-(2-Furolylamino)-3-hydroxyphenyl]carbamoyl]-5-nonadecenoic acid  | C31 H44 N2 O6   | 540.3218 | 10.324 | 7598.715206 | 44037.99406 | 130214.9269 | 185494.7093 | 123078.725  | 162829.9802 | 159469.02 | 391928.7942 | 135642.7295 | 3852.738 |
| M_0984 | 3-Acetyl-4-thiazolidinecarboxylic acid   | C6 H9 N O3 S    | 175.0304 | 6.038  | 38897.79364 | 13198.03845 | 181373.8422 | 48818.29301 | 31384.05474 | 16279.13583 | 23147.077 | 28656.03055 | 29483.27268 | 3004.714 |
| M_0985 | 1H-1,2,4-triazolo[4,3-b][1,2,4]triazole-3,6-diamine  | C3 H5 N7        | 139.0611 | 1.008  | 7047.742134 | 15013.13088 | 5903.855619 | 14162.8463  | 7746.443263 | 6707.312727 | 13926.836 | 12784.60493 | 15575.39353 | 46789.82 |
| M_0986 | (2S,8R,14Z,17Z,20Z,32)-2-Ammonio-8-[[heptadecanoyloxy)methyl]-5-oxido-10-oxo-4,6,9-trioxa-5-phosphanonacos-14,17,20,23-tetraen-1-olate 5-oxide | C43 H75 N O10 P | 796.5129 | 10.805 | 25307.39163 | 16551.92747 | 4000.558082 | 3766.191442 | 5303.040496 | 33323.736   | 12084.677 | 20989.34498 | 17556.29601 | 2134.582 |
| M_0987 | Fluoroacetophenone   | C8 H7 F O       | 138.0487 | 1.151  | 116036.4407 | 70381.95068 | 388645.4236 | 115767.6585 | 89669.80012 | 72554.25101 | 89594.267 | 121351.9807 | 58572.53155 | 1559.844 |
| M_0988 | 7936339  | C10 H11 N5 O3   | 249.0861 | 2.565  | 51327.41018 | 64531.75494 | 25066.97505 | 45688.46007 | 26918.02876 | 84045.8174  | 31232.219 | 53355.2437  | 28957.34036 | 2713.836 |
| M_0989 | MFC00037215  | C8 H14 N2 O5    | 218.0902 | 1.216  | 25218.42469 | 46424.91083 | 388213.6382 | 66158.13984 | 87072.64629 | 122683.9128 | 128714.89 | 104981.1631 | 93190.19327 | 2037.287 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_0990 | 2,4,6-tricyclohexyloxy<br>1,3,5-triazine  | C21 H33 N3 O3   | 375.2521 | 10.797 | 35943.42414 | 267494.7885 | 256531.0096 | 70635.46071 | 43567.99531 | 29852.66511 | 40769.924 | 27619.89602 | 36538.38748 | 4759.073 |
| M_0991 | DL-Stachydrine  | C7 H13 N O2     | 143.0947 | 1.553  | 325638.7727 | 192260.7079 | 92412.41747 | 387447.4212 | 306805.2439 | 172694.3653 | 125811.6  | 194967.8855 | 78313.63442 | 12785.13 |
| M_0992 | ACPC  | C4 H7 N O2      | 101.0482 | 1      | 1274.824099 | 1190.049503 | 1359.510386 | 4001.0252   | 1401.500219 | 2701.138456 | 1782.4801 | 1986.531833 | 1554.494034 | 8687.643 |
| M_0993 | 2-(Methylsulfonyl)-N-<br>phenylbenzamide  | C14 H13 N O S   | 243.0718 | 1.177  | 192374.1174 | 273860.189  | 185351.5829 | 219555.4951 | 218125.0766 | 197799.2813 | 232973.39 | 240794.3601 | 175461.3234 | 1820.263 |
| M_0994 | Thiamine  | C12 H16 N4 O S  | 264.1044 | 0.813  | 50099.57162 | 59197.7203  | 39574.93339 | 80600.91885 | 70611.84112 | 92594.90367 | 120069.77 | 88541.92928 | 130352.8524 | 1639.432 |
| M_0995 | alpha-D-<br>Galactopyranose, 1-O-<br>[hydroxy[[[hydroxy[[[<br>2E,6E,10E,14E,18E,22<br>E,26E,30E,34E,38E]-<br>3,7,11,15,19,23,27,31<br>,35,39,43-<br>undecamethyl-<br>2,6,10,14,18,22,26,30<br>,34,38,42-<br>tetratetracontaundec<br>aen-1-yl]oxy]phos<br>phinyloxy]phosphiny<br>l-, ion(2-) | C61 H100 O12 P2 | 1086.667 | 9.999  | 37225.76174 | 63501.65105 | 139423.3535 | 227213.7102 | 63794.35273 | 188851.5769 | 141482.43 | 293286.9916 | 176710.382  | 2277.068 |
| M_0996 | Myristyl nicotinate   | C20 H33 N O2    | 319.2508 | 9.072  | 276336.3197 | 228429.8532 | 77043.87665 | 102242.3665 | 251823.2855 | 191879.4913 | 103894.93 | 381461.614  | 225703.8221 | 3908.427 |
| M_0997 | Myristyl nicotinate   | C20 H33 N O2    | 319.2504 | 9.114  | 276336.3197 | 321781.869  | 101166.7068 | 264628.3461 | 274649.5531 | 222458.7397 | 205318.52 | 379482.8999 | 225703.8221 | 7432.977 |
| M_0998 | 17alpha-Methyl-<br>androstan-3-<br>hydroxylimine-17beta-ol  | C20 H33 N O2    | 319.2488 | 9.153  | 34954.67889 | 26656.14859 | 56728.74052 | 54170.66255 | 47984.90118 | 178557.2692 | 31621.804 | 68889.37723 | 11879.62205 | 1760.746 |
| M_0999 | 2707  | C8 H14 O        | 126.1047 | 9.258  | 298202.9119 | 234979.4053 | 57014.39474 | 79957.86922 | 65425.02098 | 79772.35814 | 70522.417 | 76041.87152 | 69530.76257 | 46176.91 |
| M_1000 | Hydroxyacetylaminof<br>luorene  | C15 H13 N O2    | 239.0946 | 2.706  | 46971.83663 | 50214.52008 | 30435.97112 | 68570.83368 | 38335.44157 | 76896.4386  | 68116.982 | 54572.09925 | 35490.37693 | 4841.935 |
| M_1001 | N-(4H-1,2,4-Triazol-4-<br>yl)-1H-1,2,4-triazole-<br>5-carboxamide   | C5 H5 N7 O      | 179.0558 | 4.233  | 376887.987  | 25985.26646 | 17627.11537 | 40619.66997 | 24846.52944 | 100520.2616 | 37813.417 | 41196.59166 | 28534.19074 | 4405.775 |
| M_1002 | 2,4,6-Triamino-1,3,5-<br>cyclohexanetriol   | C6 H15 N3 O3    | 177.1114 | 1.194  | 374497.6193 | 125834.2913 | 131692.0572 | 120588.6384 | 87321.21036 | 84950.48241 | 49313.003 | 63290.98061 | 41482.27731 | 1163.913 |
| M_1003 | Tetrafluoro(selenoxo)<br>molybdenum   | F4 Mo Se        | 253.8162 | 1.354  | 26906.1916  | 89510.37928 | 141475.6358 | 374204.1916 | 39792.39931 | 87636.21285 | 2743.5408 | 46943.2109  | 2319.209997 | 902.0693 |
| M_1004 | tris(3,5-dimethyl-1-<br>pyrazolyl)methane   | C16 H22 N6      | 298.1908 | 9.045  | 214225.4729 | 98514.4994  | 97321.81875 | 95206.50604 | 93588.60952 | 109425.2706 | 191066.83 | 213786.4352 | 214111.5908 | 4173.353 |
| M_1005 | Aceglutamide  | C7 H12 N2 O4    | 188.0797 | 1.517  | 373262.8319 | 34916.37467 | 31924.73828 | 52543.44434 | 47493.95851 | 48230.93603 | 23413.148 | 39332.61584 | 26932.34415 | 1948.74  |
| M_1006 | 5-Hydroxy-3,3,6,6-<br>tetramethyl-4-<br>thiepanone  | C10 H18 O2 S    | 202.1028 | 6.327  | 373132.3892 | 70469.23395 | 61347.4113  | 104060.7901 | 42792.98887 | 96677.24289 | 112233.12 | 152765.8561 | 50698.71225 | 4048.554 |
| M_1007 | 4,5-Difluoro-1,2-<br>benzenediol  | C6 H4 F2 O2     | 146.0178 | 0.787  | 285573.6636 | 282183.6975 | 182114.433  | 372902.8352 | 238552.7368 | 247248.7528 | 194669.16 | 196211.7564 | 130561.8695 | 4594.233 |
| M_1008 | 1-(4,6-<br>Diaminopyrimidin-5-<br>yl)guanidine  | C5 H9 N7        | 167.0921 | 1.219  | 96230.10364 | 81655.61582 | 131739.5938 | 370771.2298 | 170376.1792 | 95762.69432 | 40096.334 | 113455.2751 | 50646.08447 | 1095.276 |
| M_1009 | 172966  | C11 H9 N O3     | 203.0582 | 1.58   | 19272.09387 | 11422.10438 | 12619.95864 | 10585.25869 | 9200.399205 | 10890.16513 | 9951.0166 | 9633.947756 | 7560.166052 | 4293.42  |
| M_1010 | hexahydropyridazine-<br>3-phosphonic acid   | C4 H11 N2 O3 P  | 166.0511 | 0.793  | 295543.7459 | 160201.8503 | 115505.2208 | 214230.1554 | 153547.0499 | 159283.7322 | 110733.22 | 92400.7169  | 96205.14635 | 2747.559 |
| M_1011 | all-cis-4,7,10,13,16-<br>Docosapentaenoic<br>acid   | C22 H34 O2      | 330.2557 | 9.328  | 367714.9914 | 212454.4614 | 109373.5235 | 257011.9026 | 133855.3373 | 202583.5314 | 129462.74 | 156858.3087 | 123828.1142 | 3631.544 |
| M_1012 | 1-<br>(4Z,7Z,10Z,13Z,16Z,19<br>Z-docosahexaenoyl)-<br>sn-glycero-3-<br>phosphocholine   | C30 H50 N O7 P  | 567.3307 | 10.069 | 1486.826354 | 10205.77833 | 15290.15221 | 34302.51847 | 26173.21223 | 14307.72707 | 40218.471 | 367034.5229 | 3726.57498  | 360.9286 |
| M_1013 | 1H-1,2,4-triazolo[4,3-<br>b][1,2,4]triazole-3,6-<br>diamine   | C3 H5 N7        | 139.0609 | 0.681  | 223327.1752 | 228548.2984 | 320485.983  | 180619.7221 | 210299.8198 | 239895.5237 | 297418.78 | 274696.5413 | 250711.3778 | 33808.36 |
| M_1014 | (E)-Dacarbazine   | C6 H10 N6 O     | 182.0916 | 4.696  | 124526.3063 | 220255.9923 | 277873.6907 | 182682.2333 | 292323.082  | 349659.8205 | 184386.49 | 352988.906  | 365476.769  | 8702.402 |
| M_1015 | 1,6-cleve's acid  | C10 H9 N O3 S   | 223.0303 | 6.424  | 85575.47337 | 97939.44987 | 115504.3426 | 16066.91774 | 82265.92025 | 207705.1892 | 169577.06 | 133183.1233 | 59650.66068 | 6505.955 |
| M_1016 | Cyclamic acid   | C6 H13 N O3 S   | 179.0616 | 1.571  | 139293.4345 | 79608.43939 | 239192.5118 | 70585.47254 | 68498.7972  | 78476.43842 | 137445.43 | 83261.65352 | 155158.7173 | 3943.181 |
| M_1017 | 2-Isopropyl-5-<br>methylbenzoic acid  | C11 H14 O2      | 178.0994 | 7.623  | 92938.9503  | 98681.35389 | 73924.20311 | 77942.24061 | 114033.6216 | 110889.6987 | 98600.43  | 82200.60248 | 81548.02713 | 9996.771 |
| M_1018 | Dodecyl 2,6-dioxo-<br>1,2,3,6-tetrahydro-4-<br>pyrimidinecarboxylat<br>e  | C17 H28 N2 O4   | 324.2039 | 10.096 | 175350.5416 | 202941.6614 | 112462.9812 | 155634.3569 | 177850.8464 | 190168.2925 | 156299.03 | 172168.4674 | 212980.29   | 8209.347 |
| M_1019 | Olomoucine  | C15 H18 N6 O    | 298.1544 | 8.801  | 24216.8941  | 27926.4366  | 19630.4041  | 22167.16105 | 36303.86202 | 121922.5756 | 24017.576 | 136204.8205 | 31649.4144  | 21451.22 |
| M_1020 | 4-Methyl-2,6,7-trioxa-<br>1-<br>phosphabicyclo[2.2.2]<br>octane 1-sulfide   | C5 H9 O3 P S    | 180.001  | 1.213  | 62312.28757 | 151207.2356 | 99319.92415 | 80322.70247 | 84677.62593 | 87549.18638 | 63953.199 | 117806.8714 | 88416.54156 | 1092.75  |
| M_1021 | 7-Deazaguanine  | C6 H6 N4 O      | 150.0544 | 1.341  | 297250.4288 | 309519.8644 | 13697.52584 | 66621.5622  | 54243.25184 | 184226.0113 | 287875.93 | 99633.22725 | 208442.6588 | 4463.161 |
| M_1022 | Phenobarbital   | C12 H12 N2 O3   | 232.0848 | 6.621  | 202520.4437 | 112078.3927 | 195681.2092 | 360914.0839 | 159294.8559 | 124584.4399 | 79457.728 | 56573.98664 | 27741.24147 | 4920.676 |
| M_1023 | Vorinostat  | C14 H20 N2 O3   | 264.1474 | 3.515  | 3134.433842 | 3352.601596 | 3788.227237 | 4297.297417 | 3990.507682 | 4825.970626 | 5295.0501 | 5523.084737 | 4546.731668 | 1506.973 |
| M_1024 | Bis[(2-isopropyl-5-<br>methylcyclohexyl)oxy<br>](2-<br>methoxyphenyl)phen<br>ylsilane   | C33 H50 O3 Si   | 522.3517 | 10.35  | 56786.79675 | 150912.6434 | 148370.9244 | 215480.5204 | 153170.8329 | 202586.7293 | 275057.47 | 298012.9186 | 197719.1039 | 1837.701 |
| M_1025 | Trisopropanolamine  | C9 H21 N O3     | 191.1522 | 1.069  | 25981.47088 | 12455.77754 | 25579.04899 | 25246.64876 | 21222.02529 | 36887.6464  | 20729.525 | 33703.05184 | 51773.45463 | 2074.642 |
| M_1026 | Embelin   | C17 H26 O4      | 294.1827 | 8.415  | 25609.493   | 22005.22471 | 27600.93365 | 24489.41981 | 18183.40298 | 210452.2216 | 44783.432 | 39679.78981 | 18675.32661 | 39547.66 |
| M_1027 | Cyclohexylamine   | C6 H13 N        | 99.10534 | 1.474  | 9094.271771 | 15225.77926 | 6452.463007 | 21598.22097 | 4365.746626 | 7464.636814 | 6947.4212 | 4688.006568 | 7041.921912 | 15857.33 |
| M_1028 | bis(tetrazolyl)amine  | C2 H3 N9        | 153.0514 | 1.462  | 17072.27786 | 4940.246492 | 17421.32482 | 5567.265817 | 19619.7346  | 29101.22172 | 43791.883 | 25743.78047 | 34084.20604 | 2272.735 |
| M_1029 | BOC-GLU-OTBU  | C14 H25 N O6    | 303.1679 | 2.452  | 354750.6226 | 65139.22974 | 10559.84638 | 88638.91223 | 10420.01965 | 11602.22306 | 7359.6716 | 11326.7654  | 5581.609569 | 2806.866 |
| M_1030 | Divinyl sulfone   | C4 H6 O2 S      | 118.0091 | 1.185  | 45303.99849 | 39648.10577 | 114439.9052 | 109076.2029 | 57831.91766 | 72553.38446 | 97090.939 | 67600.34632 | 90151.12372 | 5404.171 |

|        |  |                |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1031 | 2-Bromo-3-methylthiophene  | C5 H5 Br S     | 175.9287 | 0.997  | 101704.2742 | 142291.0118 | 78986.19469 | 71557.76578 | 113873.2172 | 120602.0659 | 100547.8  | 101023.7865 | 94461.34142 | 4133.501 |
| M_1032 | Eugenol  | C10 H12 O2     | 164.0839 | 7.812  | 68159.84641 | 13541.96907 | 8289.035043 | 119086.2301 | 42305.90266 | 38160.9569  | 19601.827 | 18401.63347 | 22724.95378 | 36672.49 |
| M_1033 | (4Z)-4-[Nitroso(1H-triaziren-1-yl)methylene]-4,5-dihydro-1,2,5-oxadiazol-3-amine   | C3 H3 N7 O2    | 169.0351 | 1.318  | 188929.3393 | 125404.0148 | 73502.8565  | 224611.9898 | 216785.9325 | 133556.5979 | 110960.22 | 207932.8463 | 137320.8794 | 4373.597 |
| M_1034 | 2210856  | C18 H32 O2     | 280.2401 | 9.18   | 143838.2427 | 185922.2418 | 70318.6775  | 211678.6482 | 204357.6521 | 286397.8943 | 149007.3  | 350870.5099 | 228263.0815 | 41496.14 |
| M_1035 | Nicotinamide   | C6 H6 N2 O     | 122.0483 | 1.495  | 51939.62125 | 166469.7705 | 40162.28043 | 76991.4126  | 83148.41576 | 41472.92828 | 32648.807 | 89575.89198 | 45536.54989 | 12716.22 |
| M_1036 | (Chloromethyl)phosphonic acid  | C H4 Cl O3 P   | 129.958  | 0.645  | 9665.539443 | 23500.55409 | 221961.1777 | 25567.01845 | 22222.25847 | 22530.80466 | 25706.281 | 24901.0498  | 14265.81091 | 36249.76 |
| M_1037 | 1422990  | C9 H19 N O2    | 173.1417 | 2.034  | 348605.1242 | 263184.8598 | 230003.1138 | 202358.0909 | 177340.8177 | 86094.59569 | 57324.068 | 106854.586  | 154877.9514 | 7122.446 |
| M_1038 | tert-Butyl (4R,6R)-6-cyanomethyl-2,2-dimethyl-1,3-dioxane-4-acetate  | C14 H23 N O4   | 269.1627 | 7.784  | 29317.99821 | 133609.7605 | 59330.35691 | 97653.59504 | 150164.3751 | 142514.2829 | 71203.566 | 74357.50613 | 31331.75338 | 8963.581 |
| M_1039 | Amphetamine  | C9 H13 N       | 135.1049 | 1.499  | 15807.54271 | 25258.8862  | 30484.65521 | 31145.30731 | 26793.05309 | 28215.22635 | 24846.792 | 25492.55853 | 18848.06171 | 20694.71 |
| M_1040 | 2-(2-(2-(4-nonylphenoxy)ethoxy)ethoxy)ethanol  | C23 H40 O5     | 396.2856 | 9.062  | 160891.9076 | 155012.8499 | 113125.9318 | 216571.4174 | 218581.6937 | 180955.0236 | 191400.98 | 173912.191  | 201311.5451 | 4557.979 |
| M_1041 | Disperse red 11  | C15 H12 N2 O3  | 268.0823 | 7.292  | 321113.6534 | 198434.6151 | 2298.594385 | 343783.9361 | 294525.7293 | 251256.6577 | 112796.58 | 59266.29127 | 42006.59768 | 1754.321 |
| M_1042 | 1,11-Diamino-3,6,9-trioxadecane  | C8 H20 N2 O3   | 192.1475 | 1.131  | 131497.8888 | 343338.2359 | 39884.60093 | 167562.9485 | 144613.6377 | 39790.65137 | 10757.303 | 15998.47593 | 12604.322   | 919.1739 |
| M_1043 | MFC03701570  | C8 H7 B O4     | 178.044  | 0.789  | 182464.9282 | 319407.1227 | 180221.6905 | 343206.0878 | 262968.7593 | 266430.1275 | 216601.21 | 238132.0917 | 114858.303  | 10020.54 |
| M_1044 | DA9185000  | C12 H10 O S    | 202.0453 | 1.513  | 30231.89226 | 116425.6404 | 295383.7275 | 14364.6936  | 120930.3104 | 241299.5617 | 263928.82 | 266439.4311 | 223197.4154 | 9047.309 |
| M_1045 | Roxatidine   | C17 H26 N2 O3  | 306.1958 | 9.503  | 144827.1268 | 26605.61197 | 28987.16419 | 67899.89805 | 20598.52792 | 70699.20445 | 119063.23 | 127902.6011 | 89658.79431 | 3735.128 |
| M_1046 | 2127   | C7 H6 O        | 106.0423 | 2.365  | 87535.88394 | 332737.854  | 122613.4008 | 60126.21181 | 240085.9909 | 113250.8232 | 340770.51 | 49332.91643 | 237968.6862 | 1377.652 |
| M_1047 | 5,5-Dimethyl-3-[2-(2-oxiranylmethoxy)propyl]-1-(2-oxiranylmethyl)-2,4-imidazolidinedione   | C14 H22 N2 O5  | 298.1533 | 8.874  | 1384.24477  | 2481.933718 | 1100.530389 | 4966.031019 | 1596.73167  | 1291.636261 | 2803.4725 | 1674.290355 | 1082.335205 | 1461.354 |
| M_1048 | 1,1'-Octahydropentalene-2,5-diylbis(4-phenylpiperazine)  | C28 H38 N4     | 430.3084 | 9.191  | 115386.0913 | 181212.7174 | 232406.9479 | 339953.0954 | 187891.0416 | 147257.7115 | 163777.72 | 97176.37347 | 145995.465  | 7883.645 |
| M_1049 | MFC01656717  | C6 H10 O6 S2   | 241.9926 | 7.769  | 8180.123703 | 6887.151791 | 6498.974788 | 5786.739181 | 9376.02951  | 9371.673128 | 7775.1997 | 6993.867596 | 7004.036505 | 9214.151 |
| M_1050 | (8S,9S)-6-[(2R)-1-hydroxypropan-2-yl]-8-methyl-9-[[methyl(pyridin-4-ylmethyl)amino]methyl]-10-oxa-1,6,14,15-tetrazabicyclo[10.3.0]pentadeca-12,14-dien-5-one | C22 H34 N6 O3  | 430.27   | 8.521  | 25398.86673 | 31082.72706 | 11008.1674  | 97856.51402 | 41890.36156 | 92983.1201  | 128825.94 | 86613.91231 | 185133.5435 | 1469.87  |
| M_1051 | 1-[1-(4-Amino-1,2,5-oxadiazol-3-yl)-5-methyl-1H-1,2,3-triazol-4-yl]ethanol   | C7 H10 N6 O2   | 210.0867 | 11.364 | 32896.06624 | 35424.79347 | 32754.08731 | 30620.12199 | 27468.40098 | 26770.96893 | 29959.806 | 33597.29306 | 28633.0429  | 31584.52 |
| M_1052 | MFC01656717  | C6 H10 O6 S2   | 241.9926 | 7.899  | 5337.757201 | 4911.09313  | 4561.815587 | 5229.666518 | 7101.371053 | 6803.505497 | 6113.0578 | 5451.068342 | 5493.98585  | 7096.069 |
| M_1053 | MFC00266981  | C18 H11 N O3   | 289.0739 | 8.41   | 15874.41321 | 10626.13141 | 14586.47627 | 13191.67601 | 13542.67094 | 17418.46417 | 17034.422 | 16437.92322 | 15873.47182 | 8020.531 |
| M_1054 | Hexyl N-(methoxycarbonyl)methionine  | C13 H25 N O4 S | 291.1503 | 8.277  | 334220.6918 | 64657.1198  | 164107.4841 | 118377.1339 | 14377.43304 | 42706.7216  | 33888.952 | 26897.16246 | 7442.335064 | 7047.687 |
| M_1055 | D-Sphingosine  | C18 H37 N O2   | 299.2825 | 7.998  | 27140.39997 | 70110.03747 | 23655.63902 | 36602.57459 | 61103.02301 | 74805.81113 | 34129.939 | 39433.98754 | 35098.39389 | 7682.486 |
| M_1056 | L-Histidine  | C6 H9 N3 O2    | 155.0695 | 1.015  | 34229.11014 | 193797.9345 | 333427.2478 | 53080.06507 | 34410.06746 | 109697.0752 | 76809.67  | 64170.49244 | 44915.35873 | 2417.622 |
| M_1057 | 1,8-Diazabicyclo[5.4.0]undec-7-ene   | C9 H16 N2      | 152.1315 | 1.502  | 33947.0822  | 22141.64468 | 27045.18894 | 28179.15906 | 24256.19361 | 25340.90573 | 22251.692 | 22621.47044 | 16481.32985 | 19426.04 |
| M_1058 | L-(+)-Aspartic acid  | C4 H7 N O4     | 133.0376 | 1.116  | 93494.93567 | 280848.2965 | 69128.51281 | 130985.398  | 154390.9115 | 200639.41   | 279950.51 | 276096.0069 | 282760.1182 | 2643.755 |
| M_1059 | DO0750000  | C15 H24 O2     | 236.1775 | 9.096  | 180912.6222 | 184043.3585 | 145327.5685 | 288010.9044 | 123559.442  | 329837.247  | 177927.24 | 241644.5387 | 146923.4703 | 19472.34 |
| M_1060 | Methyl [(1-methyl-1H-tetrazol-5-yl)sulfonyl]acetate N.pi.-Methyl-L-histidine   | C5 H8 N4 O4 S  | 220.026  | 2.508  | 329779.0061 | 36430.29436 | 36843.585   | 26478.81352 | 35642.58791 | 35844.73684 | 28710.074 | 30407.58057 | 32141.79187 | 6048.906 |
| M_1061 | Triethylamine  | C6 H15 N       | 101.121  | 0.73   | 147581.5293 | 258486.2717 | 222476.932  | 220386.192  | 245953.8191 | 171701.6477 | 205415.85 | 283206.5387 | 155281.0676 | 64279.8  |
| M_1062 | Avocadyne 1-acetate  | C19 H34 O4     | 348.2276 | 8.914  | 59618.67976 | 13203.18604 | 5921.636902 | 66750.66356 | 72268.82367 | 51062.78506 | 6539.2071 | 14326.00714 | 61073.66355 | 36499.87 |
| M_1063 | Heptyl (9Z)-12-hydroxy-9-octadecenoate   | C25 H48 O3     | 396.3605 | 10.376 | 13783.64362 | 16758.88018 | 19702.62677 | 13480.55895 | 16982.83302 | 17881.62058 | 17551.374 | 14326.43506 | 15768.11025 | 10975.26 |
| M_1064 | Acetyl-L-carnitine   | C9 H17 N O4    | 203.1155 | 2.557  | 266473.99   | 187454.9057 | 145848.9914 | 211443.2259 | 167968.8161 | 241915.8953 | 219214.58 | 175223.2815 | 127802.673  | 15627.39 |
| M_1065 | S-(4-Pentylphenyl) 4-(tetradecyloxy)benzenecarbothioate  | C32 H48 O2 S   | 496.337  | 9.838  | 88400.46377 | 193103.9858 | 243140.8578 | 12621.55611 | 255275.7426 | 204612.3946 | 166665.38 | 2484.006338 | 12208.45457 | 8518.853 |
| M_1066 | MFC01318414  | C8 H13 N O4    | 187.0845 | 3.185  | 326013.9085 | 45076.64741 | 58984.73162 | 42806.40397 | 32841.26399 | 36732.46423 | 23142.055 | 21111.21143 | 14376.01879 | 15348.38 |
| M_1067 | Docosahexaenoic acid   | C22 H32 O2     | 328.2402 | 9.198  | 325277.6781 | 278314.3297 | 111780.4673 | 303855.9348 | 169019.9462 | 238612.4568 | 155079.16 | 194845.973  | 162447.4864 | 6827.026 |
| M_1068 | Trigonelline   | C7 H7 N O2     | 137.0478 | 1.591  | 324255.2224 | 74407.62662 | 167821.0854 | 86500.37029 | 62938.76373 | 129630.8927 | 74440.747 | 34872.78905 | 54862.47181 | 12169.34 |
| M_1069 | L-Alanyl-L-glutamine   | C8 H15 N3 O4   | 217.1063 | 1.572  | 324067.265  | 23950.14482 | 7122.428577 | 32519.49606 | 20649.42779 | 5465.141853 | 8515.7463 | 4768.998478 | 3146.085886 | 1786.663 |
| M_1070 | Tretinoin  | C20 H28 O2     | 300.2088 | 9.205  | 205243.4261 | 156131.8054 | 199074.6041 | 232309.4841 | 190501.5694 | 116649.1112 | 217555.59 | 160819.3525 | 239213.077  | 8762.094 |
| M_1071 | 1,11-Diamino-3,6,9-trioxadecane  | C8 H20 N2 O3   | 192.1474 | 1.517  | 181491.0033 | 322091.2239 | 57235.35833 | 16798.57419 | 61718.31079 | 56420.58157 | 23799.291 | 19730.57152 | 4985.169671 | 2957.239 |
| M_1072 | Avocadyne 1-acetate  | C19 H34 O4     | 348.23   | 8.216  | 321958.7912 | 53963.97248 | 65348.92753 | 63001.3509  | 20750.22384 | 91335.35531 | 83425.351 | 76265.68777 | 61256.47441 | 6761.506 |
| M_1073 | Uracil   | C4 H4 N2 O2    | 112.0277 | 1.4    | 109913.7746 | 116544.7127 | 96152.58247 | 240666.3653 | 59879.28556 | 172624.9784 | 30838.695 | 53443.80321 | 19810.14145 | 34868.42 |



|        |   |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1075 | N-(5-Fluorotricyclo[2.2.1.0~2,6~]hept-3-yl)acetamide  | C9 H12 F N O   | 169.0909 | 0.977 | 321176.9292 | 58698.73837 | 56464.51731 | 27036.35777 | 37840.71831 | 61256.12621 | 58354.254 | 41472.0459  | 2941.612289 | 1901.843 |
| M_1076 | 1-LAURYL GLYCERYL ETHER   | C15 H32 O3     | 260.235  | 9.212 | 76929.82644 | 32939.69211 | 226616.4812 | 206991.825  | 261083.9884 | 222297.227  | 145321.17 | 180748.8969 | 88973.68996 | 16840.78 |
| M_1077 | N,N'-Diheptyl-2-hydroxy-N,N'-dimethylmalonamide   | C19 H38 N2 O3  | 342.2882 | 8.715 | 44472.52449 | 47931.68581 | 41517.72808 | 37771.39651 | 42031.86684 | 34130.6758  | 41752.334 | 192113.4294 | 41347.53086 | 28270.1  |
| M_1078 | 4-Nitro-2,1,3-benzoxadiazole (2Z,4E)-2-   | C6 H3 N3 O3    | 165.0179 | 0.795 | 253375.0041 | 131218.6597 | 97372.80417 | 225995.4244 | 106471.267  | 126912.3283 | 103998.03 | 110949.8644 | 79041.30473 | 2851.504 |
| M_1079 | hydroxymuconic acid (13E)-1,11,16-Trihydroxy-16-methylprost-13-en-9-one   | C6 H6 O5       | 158.0215 | 2.873 | 318796.4118 | 6882.370966 | 17819.92666 | 1591.676915 | 1937.670186 | 1970.714236 | 1964.6672 | 1943.45557  | 1937.461909 | 1960.711 |
| M_1080 | 4-Acetamidobenzoic acid   | C9 H9 N O3     | 179.0583 | 6.337 | 224562.5563 | 161792.2831 | 317563.6313 | 81212.82937 | 80545.80375 | 59273.79443 | 45014.919 | 47481.08198 | 21079.83942 | 2311.331 |
| M_1082 | negamycin   | C9 H20 N4 O4   | 248.1484 | 1.336 | 317270.248  | 3584.578331 | 51125.18266 | 9427.175176 | 2701.295406 | 115985.8655 | 2733.1132 | 9389.651232 | 2421.910844 | 869.0476 |
| M_1083 | DL-Histidine  | C6 H9 N3 O2    | 155.0696 | 1.103 | 211085.0833 | 299364.4889 | 317135.1756 | 238043.2592 | 151016.6512 | 105567.705  | 164955.63 | 153206.8921 | 195257.7315 | 1445.409 |
| M_1084 | pentahomomethionine   | C10 H21 N O2 S | 219.1293 | 6.33  | 317092.8818 | 62892.51053 | 50503.59647 | 87727.06756 | 37294.38897 | 87792.99043 | 92819.116 | 129763.7985 | 45338.00661 | 2420.597 |
| M_1085 | Dihydroxyphenylglycine  | C8 H9 N O4     | 183.0532 | 4.926 | 5361.32133  | 5068.335939 | 4700.620893 | 8827.494183 | 4965.195127 | 2704.754679 | 5361.7605 | 4683.636286 | 4618.859565 | 4509.955 |
| M_1086 | 4-Nitro-2H-benzimidazol-2-one   | C7 H3 N3 O3    | 177.0168 | 1.188 | 316336.1321 | 189294.2467 | 120226.2087 | 127890.1018 | 108131.2298 | 96060.42054 | 78176.684 | 69909.95186 | 49474.77522 | 1087.388 |
| M_1087 | Propyl dibutylcarbomodithioate  | C12 H25 N S2   | 247.1417 | 1.136 | 142525.5974 | 26264.99751 | 38340.98691 | 65543.4661  | 61200.27034 | 73305.06435 | 99743.181 | 99378.04317 | 73288.99399 | 1862.823 |
| M_1088 | Dimethyl N-octanoylglutamate 1-Methyl-4-(2-methyl-2H-tetrazol-5-yl)-1H-pyrazol-5-amine                                      | C15 H27 N O5   | 301.1888 | 3.684 | 315388.3602 | 33846.86392 | 27454.5591  | 23198.94818 | 10140.13378 | 5820.105017 | 3522.3383 | 3491.128456 | 3375.256333 | 3538     |
| M_1089 | Imidocarb   | C6 H9 N7       | 179.0921 | 1.223 | 68714.02287 | 255441.4917 | 78953.19441 | 225827.9019 | 313208.89   | 315342.056  | 262327.78 | 243409.8568 | 225131.6304 | 1325.301 |
| M_1090 | 4-Nitrobenzoate   | C9 H20 N6 O    | 326.194  | 5.192 | 66120.76658 | 74771.3317  | 91784.40269 | 99668.83023 | 55517.40163 | 48418.2911  | 63515.557 | 121328.8039 | 55210.44823 | 14864.62 |
| M_1091 | MFC00055819   | C5 H9 N3 O4    | 175.0585 | 1.307 | 197539.6974 | 270047.8922 | 94267.82374 | 70614.88662 | 209913.4587 | 161399.8503 | 313702.5  | 194287.635  | 221480.5582 | 2145.895 |
| M_1092 | ACPC  | C4 H7 N O2     | 101.0482 | 1.23  | 153281.2081 | 65930.57417 | 312373.9954 | 206088.5803 | 144149.7325 | 171680.5331 | 80653.945 | 108986.3416 | 99364.9295  | 49392.28 |
| M_1094 | 2,3-Dihydroxypropyl 3-sulfanylpropanoate 1,2-di-O-methyl-4-[(2R)-2,4-dihydrobutyramido]-4,6-dideoxy-alpha-D-mannopyranoside | C6 H12 O4 S    | 180.0456 | 1.633 | 96223.56829 | 126100.1338 | 118666.6548 | 97038.90733 | 91857.08348 | 98616.48798 | 125040.99 | 246450.0493 | 152214.1666 | 4681.416 |
| M_1095 | 2,2'-(Dodecanoylimino)diacetic acid   | C16 H29 N O5   | 315.2046 | 2.939 | 255122.918  | 209571.3615 | 167417.8037 | 257273.5313 | 205847.9786 | 288981.5046 | 207235.55 | 240917.4599 | 224473.1181 | 22319.92 |
| M_1097 | 3-Oxoestra-4,9,11-trien-17-yl acetate   | C20 H24 O3     | 312.1728 | 8.363 | 309000.9313 | 53332.18619 | 186136.6114 | 266159.9797 | 16518.57686 | 77335.45038 | 41988.892 | 103919.2107 | 65832.57587 | 5553.087 |
| M_1098 | Norepinephrine sulfate  | C8 H11 N O6 S  | 249.0313 | 5.33  | 79691.84817 | 120076.4909 | 272533.8876 | 145498.1122 | 306811.3721 | 192479.6161 | 172900.35 | 99682.46576 | 79554.73195 | 6826.4   |
| M_1099 | Diphenyl sulfone  | C12 H10 O2 S   | 218.0402 | 1.206 | 128926.1877 | 163132.4174 | 166308.7768 | 233399.8317 | 207889.2919 | 107713.4105 | 90725.657 | 135394.7446 | 107433.3777 | 1464.967 |
| M_1100 | Octahydro-1,2,8-indolizinetriol   | C8 H15 N O3    | 173.1053 | 5.274 | 64986.26592 | 67134.41758 | 91752.07116 | 88411.24334 | 94677.18384 | 89986.06244 | 84801.331 | 152211.8578 | 71449.33503 | 11179.29 |
| M_1101 | Nicotinamide  | C6 H6 N2 O     | 122.0483 | 1.808 | 81901.7216  | 93118.08779 | 62351.80514 | 80487.69345 | 81224.43353 | 64214.55633 | 18123.74  | 91518.21368 | 68158.60435 | 20528.37 |
| M_1102 | methylpyron   | C10 H17 N O2   | 183.126  | 7.884 | 51086.02315 | 45001.34327 | 36257.50009 | 39628.12231 | 58750.56433 | 94102.0044  | 56207.747 | 84955.337   | 46911.76846 | 19734.95 |
| M_1103 | [[[2,5-Dioxo-1-pyrrolidinyl]oxy]carbonyl]oxidanide  | C5 H4 N O5     | 158.0093 | 1.411 | 303338.6189 | 20728.77559 | 13418.40555 | 15941.94892 | 7917.270198 | 23594.39205 | 17213.033 | 14713.9595  | 12410.72543 | 1174.574 |
| M_1104 | tert-Butyl 3-[(methylsulfonyl)oxy]-1-piperidinecarboxylate  | C11 H21 N O5 S | 279.114  | 6.877 | 302720.056  | 35270.23941 | 121991.5225 | 44602.59045 | 10586.59785 | 14821.87879 | 9767.938  | 4252.401303 | 3369.856548 | 2248.275 |
| M_1105 | 4-Pteridinol  | C6 H4 N4 O     | 148.0389 | 1.499 | 203253.7881 | 129828.3341 | 101746.8212 | 59647.54776 | 52550.08581 | 105952.598  | 97893.755 | 109730.0938 | 50979.15544 | 4248.962 |
| M_1106 | 5-[[3-Methoxyphenoxy)methyl]-2-furoic acid  | C13 H12 O5     | 248.0685 | 6.769 | 94602.06472 | 48791.31608 | 136606.2426 | 300450.5383 | 13573.09297 | 87065.27798 | 35772.58  | 38891.56295 | 11291.67112 | 3558.573 |
| M_1107 | 3-[Dodecyl(2-hydroxyethyl)amino]-1,2-propanediol  | C17 H37 N O3   | 303.2774 | 7.818 | 2398.388767 | 1920.067903 | 2022.315708 | 2246.875442 | 2917.581983 | 7138.562389 | 3136.7949 | 2831.830593 | 1040.953976 | 2867.21  |
| M_1108 | Nevirapine  | C15 H14 N4 O   | 234.0867 | 7.073 | 11691.68151 | 13703.74549 | 298647.7108 | 17843.88612 | 8863.346926 | 21102.30714 | 20723.943 | 8425.034191 | 10309.52931 | 9149.676 |
| M_1109 | Norepinephrine sulfate  | C8 H11 N O6 S  | 249.0313 | 2.43  | 298339.7091 | 187728.877  | 259971.4238 | 152852.4436 | 137525.8865 | 128271.9461 | 129215.39 | 154902.76   | 126975.0165 | 3357.275 |
| M_1110 | 1,11-Diamino-3,6,9-trioxaundecane   | C8 H20 N2 O3   | 192.1473 | 1.376 | 37291.67139 | 298309.5938 | 4351.685948 | 48319.39099 | 42639.85245 | 36644.30663 | 26335.819 | 26154.94738 | 3965.807459 | 1542.522 |
| M_1111 | 2-Ethoxy-4-hydrazino-6-(1-piperidinyl)-1,3,5-triazine   | C10 H18 N6 O   | 238.1544 | 8.784 | 70127.18408 | 65675.47352 | 22314.88515 | 46291.83334 | 34583.81954 | 38802.9291  | 39443.686 | 32267.40361 | 51813.09157 | 1685.9   |
| M_1112 | Acetic acid   | C4 H7 N O3     | 117.0429 | 1.478 | 20902.66742 | 29692.3731  | 134151.4268 | 15165.50726 | 116792.2774 | 194900.8199 | 126459.09 | 224064.3164 | 102656.4483 | 4657.64  |
| M_1113 | MFC00674100   | C7 H7 N3 O2    | 165.0542 | 0.793 | 230416.7518 | 103457.8361 | 72819.95783 | 162688.7775 | 120361.3564 | 123898.8688 | 104534.79 | 117127.4511 | 78068.2472  | 1891.867 |
| M_1114 | 3,6-Difluoro-2-methoxyphenol  | C7 H6 F2 O2    | 160.0335 | 0.786 | 144490.7752 | 285458.4303 | 59156.78049 | 297499.4241 | 237062.5975 | 244629.0814 | 195266.01 | 34575.81573 | 101207.8469 | 10206.77 |
| M_1115 | AC-VAL-OH   | C7 H13 N O3    | 159.0896 | 4.28  | 297305.6623 | 26249.77539 | 24808.65929 | 29530.95683 | 24045.50679 | 26282.28809 | 25638.212 | 26386.08938 | 20412.6104  | 12803.74 |
| M_1116 | Cyclamic acid   | C6 H13 N O3 S  | 179.0616 | 1.467 | 44515.39578 | 68904.71956 | 149636.4365 | 48299.59187 | 89452.67578 | 71450.35455 | 70637.154 | 108169.3545 | 17261.09885 | 7409.023 |
| M_1117 | 2-[Bis(2-chloroethyl)amino]ethanol  | C6 H13 Cl2 N O | 185.0382 | 1.211 | 38770.1897  | 66485.05632 | 296323.0799 | 45343.68537 | 86931.7546  | 245661.1819 | 184374.93 | 212827.251  | 161042.2538 | 3490.78  |
| M_1118 | Gly-Leu   | C8 H16 N2 O3   | 188.1161 | 1.193 | 295868.7972 | 154052.7214 | 137893.6241 | 141888.655  | 134661.6166 | 103908.9248 | 103916.05 | 97368.90362 | 81501.35158 | 2368.741 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1119 | MFC00083078  | C22 H45 N O3    | 371.34   | 9      | 118831.788  | 162236.1735 | 108916.83   | 184814.3854 | 83575.72137 | 102030.7935 | 168463    | 181545.0911 | 149523.3694 | 21536.01 |
| M_1120 | Guanylmelamine   | C4 H8 N8        | 168.0874 | 1.286  | 293649.2879 | 75241.83502 | 52377.26337 | 31020.01673 | 36562.35031 | 48756.26819 | 62142.393 | 49069.64472 | 41488.2568  | 3538.547 |
| M_1121 | Leu-Val  | C11 H22 N2 O3   | 230.1632 | 8.011  | 4759.301265 | 3997.685247 | 4222.668018 | 4382.89274  | 5762.596846 | 5560.156539 | 5050.1024 | 4963.19035  | 4666.009236 | 5867.175 |
| M_1122 | 2,2'-Thiobis(3,6-dicyclopentyl-p-cresol)   | C34 H46 O2 S    | 518.3207 | 9.599  | 17731.86968 | 189217.885  | 157380.0003 | 292975.4546 | 174596.4876 | 236056.1026 | 239527.79 | 205614.0065 | 175296.8561 | 8057.632 |
| M_1123 | Gly-Lys  | C8 H17 N3 O3    | 203.1268 | 1.307  | 290941.0528 | 9821.879617 | 74264.4477  | 21329.55148 | 8528.716964 | 5072.991249 | 4325.1334 | 4703.554895 | 3644.763465 | 1189.286 |
| M_1124 | NPPB   | C16 H16 N2 O4   | 300.1111 | 7.757  | 11076.71295 | 14056.08507 | 9084.596615 | 8349.578455 | 20655.93444 | 18246.82188 | 6608.5228 | 9018.253183 | 10818.85982 | 11885.17 |
| M_1125 | 7-Methylguanosine  | C11 H15 N5 O5   | 297.1073 | 2.741  | 289910.845  | 107416.9184 | 183871.5526 | 192724.8348 | 108717.9104 | 82407.26581 | 63671.977 | 72758.12904 | 46226.65032 | 6191.624 |
| M_1126 | 2-Oxindole   | C8 H7 N O       | 133.0529 | 6.733  | 67823.16402 | 17732.53271 | 70320.04902 | 289569.5726 | 21318.18113 | 51557.05429 | 19806.855 | 24302.48975 | 36112.42049 | 3407.97  |
| M_1127 | Pipecolic acid   | C6 H11 N O2     | 129.0791 | 0.939  | 277378.9101 | 133197.5653 | 41900.47294 | 109246.7459 | 90511.33354 | 128886.6079 | 177333    | 61101.25397 | 105665.0585 | 28673.29 |
| M_1128 | N-Acetylthranilic acid   | C9 H9 N O3      | 179.0583 | 7.711  | 21860.47896 | 8012.784819 | 8225.587688 | 11142.32845 | 8348.552845 | 21609.35743 | 7517.6128 | 6856.511861 | 4411.373547 | 5937.322 |
| M_1129 | OB4520000  | C10 H9 N O      | 159.0685 | 1.642  | 288391.7817 | 72279.86317 | 18654.08953 | 86527.34919 | 109371.2355 | 103817.172  | 123318.38 | 58942.68013 | 61517.35969 | 10690.36 |
| M_1130 | 2-Amino-2-propanyl 5'-S-Methyl-5'-thioadenosine  | C3 H8 N         | 58.06589 | 1.422  | 60587.4603  | 41027.66155 | 59492.81173 | 32975.56366 | 18761.28185 | 104937.7325 | 51849.91  | 71980.2477  | 43315.24423 | 11542.43 |
| M_1131 | MA4000000  | C5 H7 N O2      | 113.048  | 1.648  | 286284.9342 | 181159.6838 | 210324.0665 | 85746.05577 | 98676.05815 | 161748.9439 | 16198.781 | 6106.719129 | 7827.085501 | 45270.49 |
| M_1133 | Cyclo(leucylprolyl)  | C11 H18 N2 O2   | 210.1368 | 6.834  | 22252.38911 | 39859.73391 | 53506.63667 | 47888.93625 | 23706.99251 | 43808.04569 | 26070.506 | 19916.3498  | 27857.30225 | 5795.646 |
| M_1134 | Amide C18  | C18 H37 N O     | 283.2874 | 10.515 | 406.5020213 | 701.1838786 | 453.300686  | 338.3284404 | 42943.68755 | 538.5373151 | 47434.968 | 57417.55233 | 2346.389329 | 34956.58 |
| M_1135 | Indane   | C9 H10          | 118.0785 | 8.68   | 170120.5086 | 185220.1674 | 279935.4008 | 131880.5608 | 138317.2446 | 160325.665  | 178187.86 | 102193.827  | 227423.0161 | 7926.464 |
| M_1136 | Methyl 5-chloro-1H-pyrrole-2-carboxylate   | C6 H6 Cl N O2   | 159.0092 | 0.687  | 115851.5087 | 142019.0063 | 7969.625101 | 121226.2614 | 128667.3048 | 6621.554176 | 229106.87 | 187879.4371 | 98149.32861 | 10361.69 |
| M_1137 | 2-Amino-N-(3-aminopropyl)-4-oxo-4,7-dihydro-1H-pyrrolo[2,3-d]pyrimidine-5-carboxamide  | C10 H14 N6 O2   | 250.1179 | 11.104 | 285042.4101 | 46888.29011 | 41760.22702 | 42824.30012 | 60376.40912 | 42975.96908 | 40295.791 | 47032.18258 | 44272.59954 | 53265.01 |
| M_1138 | Fludrocortisone acetate  | C23 H31 F O6    | 422.2129 | 5.323  | 4734.424772 | 3006.31135  | 3276.32285  | 3173.232863 | 3195.357974 | 3085.642288 | 2932.9734 | 4175.163766 | 3001.61585  | 2743.111 |
| M_1139 | 2,2'-(Dodecanoylimino)diacetic acid  | C16 H29 N O5    | 315.2045 | 9.055  | 10576.58432 | 12918.24423 | 12388.63722 | 28418.82307 | 18802.37319 | 26370.85699 | 12842.486 | 15961.17624 | 17233.16064 | 6203.513 |
| M_1140 | Boc-Phe(4-NO2)-OH  | C14 H18 N2 O6   | 310.1177 | 1.549  | 201885.1877 | 284364.4334 | 13576.64721 | 142330.6957 | 36629.47919 | 77301.83969 | 38872.222 | 152483.9051 | 33708.18952 | 3455.943 |
| M_1141 | MFC00083078  | C22 H45 N O3    | 371.3401 | 9.136  | 125331.9532 | 155049.0289 | 133799.3098 | 202485.2492 | 86942.96916 | 114307.782  | 195983.12 | 169058.7257 | 142756.2423 | 16946.3  |
| M_1142 | 4'-Dimethylamino-3,4,5-Trimethoxy Benzanilide  | C18 H22 N2 O4   | 330.1579 | 2.435  | 191279.4201 | 62871.9121  | 284027.1917 | 76019.33928 | 64071.46714 | 97663.21909 | 64956.548 | 75993.46552 | 24965.91021 | 2272.215 |
| M_1143 | 18-acetoxy-1alpha,25-dihydroxyvitamin D3   | C29 H46 O5      | 474.335  | 8.719  | 85327.40207 | 49605.05715 | 74490.87428 | 283248.7788 | 109637.8572 | 159471.1638 | 112356.94 | 106067.8602 | 49662.93289 | 11832.92 |
| M_1144 | (+/-)-12-HpETE   | C20 H32 O4      | 318.219  | 8.89   | 221992.5987 | 282796.5568 | 124950.6344 | 228415.4427 | 84271.25024 | 248454.5211 | 211130.6  | 78550.28945 | 162468.6749 | 4781.131 |
| M_1145 | FAB-144  | C20 H27 F N2 O  | 330.2168 | 9.425  | 6907.307389 | 7357.715351 | 3320.752042 | 13962.40584 | 12398.08555 | 17093.19415 | 13264.173 | 14465.33268 | 10724.45321 | 4887.208 |
| M_1146 | Linoleyl alcohol   | C18 H34 O       | 266.2608 | 10.467 | 139060.9874 | 170328.6364 | 186625.1342 | 111762.6988 | 176907.6373 | 118430.2738 | 188021.44 | 145633.7854 | 128357.6794 | 12234.3  |
| M_1147 | 1-stearoyl-sn-glycero-3-phosphoethanolamine  | C23 H48 N O7 P  | 481.3171 | 9.843  | 102964.8072 | 148376.4754 | 281314.676  | 256821.4957 | 94223.29529 | 117387.4179 | 100934.36 | 90097.1856  | 14422.17701 | 2662.577 |
| M_1148 | MFC00025173  | C18 H31 N O     | 277.2406 | 8.78   | 2834.66448  | 3153.652793 | 3010.613218 | 3231.326925 | 3500.552076 | 3908.032679 | 3224.509  | 3443.101549 | 3299.245424 | 2822.263 |
| M_1149 | Avocadylne 1-acetate   | C19 H34 O4      | 316.2039 | 8.25   | 66131.36662 | 166182.4848 | 49564.98191 | 47148.56393 | 49230.63135 | 280502.6185 | 117642.42 | 208475.3769 | 57777.10897 | 6660.194 |
| M_1150 | Xanthurenic acid   | C10 H7 N O4     | 205.0374 | 5.034  | 106063.5111 | 21798.03168 | 21244.52224 | 41721.02296 | 20293.33265 | 15442.96618 | 9786.4733 | 19801.81281 | 11419.7317  | 8122.096 |
| M_1151 | CAPROYL SARCOSINE  | C13 H25 N O3    | 243.1835 | 7.563  | 1344.455043 | 1207.530667 | 1008.716272 | 1101.884932 | 1717.16215  | 3747.115369 | 1180.1148 | 2646.246365 | 1071.889046 | 1767.699 |
| M_1152 | Valerophenone  | C11 H14 O       | 162.1045 | 8.232  | 102064.7107 | 65760.97794 | 87322.827   | 88041.19444 | 77206.63242 | 96091.2128  | 72546.021 | 113405.6984 | 116493.7905 | 30824.45 |
| M_1153 | 1-(tert-Butylamino)-3-((5,6,7,8-tetrahydrocis-6,7-dihydroxy-1-naphthyl)oxy)-2-propanol | C17 H27 N O4    | 309.1939 | 7.096  | 182704.4662 | 106442.8465 | 163229.2161 | 162734.4256 | 278894.2968 | 137126.7233 | 38641.921 | 31842.43716 | 34004.92216 | 1909.28  |
| M_1154 | 1,5-Dihydroimidazo[4,5-c][1,2,6]thiadiazin-4(3H)-one 2,2-dioxide                       | C4 H4 N4 O3 S   | 187.9999 | 1.995  | 222466.8891 | 126068.4968 | 148721.5271 | 164734.9788 | 101396.9399 | 234265.8107 | 221736.81 | 171084.3334 | 161271.1831 | 5324.958 |
| M_1155 | Phosphorazidothioic difluoride   | F2 N3 P S       | 142.9518 | 0.628  | 55793.56485 | 75615.99596 | 200085.56   | 18697.79476 | 117688.6182 | 6554.920151 | 8670.2054 | 164103.2804 | 93503.18179 | 16625.2  |
| M_1156 | MFC005664229   | C13 H14 O2 S    | 234.0713 | 1.16   | 7752.587229 | 102225.9651 | 225677.5701 | 41426.30546 | 47419.11931 | 134877.2073 | 179001.76 | 165342.8845 | 156603.5771 | 1608.239 |
| M_1157 | Boc-Gln-OH   | C10 H18 N2 O5   | 246.1215 | 2.415  | 275854.3537 | 97738.90414 | 61930.4359  | 87130.9401  | 32572.83153 | 87647.61481 | 67682.725 | 43238.07929 | 48879.72074 | 1640.681 |
| M_1158 | 2-Indolylformic acid   | C9 H7 N O2      | 161.0478 | 6.495  | 275331.4276 | 56027.3196  | 121882.7333 | 56791.60504 | 66560.46297 | 16568.4688  | 16305.108 | 17111.99412 | 7950.195337 | 4327.56  |
| M_1159 | Palmitoyl ethanolamide   | C18 H37 N O2    | 299.2823 | 9.686  | 6393.88504  | 15766.88191 | 10861.79809 | 18947.50735 | 11545.43099 | 9839.78339  | 12964.649 | 8349.217758 | 10552.72177 | 7180.075 |
| M_1160 | 4,6-Bis(dimethylamino)-1,3,5-triazin-2-yl(methoxymethyl)cy anamide                     | C10 H17 N7 O    | 251.1497 | 8.112  | 62083.44813 | 96925.52585 | 50487.82895 | 54174.58631 | 75743.32698 | 114968.2013 | 102732.87 | 132484.5609 | 73932.5293  | 19982.59 |
| M_1161 | 2-amino-3-(((R)-2-amino-2-carboxylethyl)disulfan yl)propanoic acid                     | C6 H12 N2 O4 S2 | 240.0238 | 1.107  | 274286.8633 | 13956.6285  | 75841.62317 | 16777.93351 | 48606.1686  | 39419.0268  | 107323.56 | 23960.64482 | 72395.99354 | 1849.498 |
| M_1162 | tranexamic acid  | C8 H15 N O2     | 157.1104 | 3.794  | 180212.4424 | 143641.209  | 209283.0329 | 130456.4134 | 127685.8327 | 162166.3213 | 112553.14 | 135278.9407 | 48368.2879  | 3280.96  |
| M_1163 | L-(-)-Asparagine   | C4 H8 N2 O3     | 132.0538 | 1.224  | 260470.6846 | 132220.3911 | 125258.1898 | 181094.2757 | 43835.7493  | 131078.1665 | 114466.26 | 166606.3282 | 178085.2416 | 2495.354 |
| M_1164 | N-[(3-nitrophenyl)methylid eneamino]-4-oxo-1H-quinazoline-2-carboxamide                | C16 H11 N5 O4   | 337.0796 | 4.75   | 273234.7631 | 42680.02278 | 187607.5883 | 4210.9108   | 103815.7865 | 25278.40984 | 28140.39  | 19428.38281 | 4940.809473 | 3630.766 |
| M_1165 | Rosoxacin  | C17 H14 N2 O3   | 294.1006 | 3.807  | 2595.051087 | 2394.693644 | 2567.82792  | 2501.223595 | 2431.277695 | 2379.915362 | 2430.9495 | 2408.08364  | 2398.203411 | 2531.581 |
| M_1166 | Diethylene glycol  | C4 H10 O3       | 106.0635 | 7.54   | 36691.59893 | 35277.56185 | 52445.11731 | 38343.71066 | 122477.1903 | 122425.2308 | 68466.409 | 53318.90223 | 38226.39846 | 38768.35 |
| M_1167 | Propylparaben  | C10 H12 O3      | 180.0788 | 7.792  | 25181.30899 | 8184.429126 | 16472.42337 | 9169.985058 | 6427.804179 | 6424.817631 | 12383.752 | 4794.696019 | 6421.254712 | 6316.827 |

|        |   |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1168 | Disulfane, bis(2-diisopropylaminoethyl)-  | C16 H36 N2 S2  | 320.2327 | 8.642 | 38236.80655 | 33200.61314 | 37667.35517 | 49223.76176 | 24507.03356 | 22382.82448 | 13864.489 | 47310.66304 | 29930.33873 | 11510.79 |
| M_1169 | N-Boc-3-Pyrrolidinone   | C9 H15 N O3    | 185.1053 | 7.282 | 1761.163631 | 13877.81074 | 15309.22819 | 12795.53843 | 12077.08536 | 16256.95005 | 1445.6754 | 7544.668285 | 6725.847155 | 14095.46 |
| M_1170 | 1,3-diguanidino-2,4,5,6-cyclohexanetetrol   | C8 H18 N6 O4   | 262.1388 | 1.1   | 61052.6135  | 9007.593593 | 9694.238518 | 8278.572219 | 8369.734775 | 11390.54087 | 21322.577 | 16067.19059 | 69270.78209 | 1115.229 |
| M_1171 | procadazole   | C10 H10 N2 O2  | 190.0741 | 1.191 | 167378.9278 | 225664.2912 | 215832.0928 | 191148.8337 | 272215.0836 | 138023.6975 | 132943.97 | 158242.556  | 137608.7402 | 1182.532 |
| M_1172 | 3,4,5-Trifluorobenzonitrile   | C7 H2 F3 N     | 157.0141 | 1.078 | 118656.0001 | 51915.62807 | 88521.65532 | 58522.60269 | 42471.35721 | 74434.79497 | 57951.76  | 67769.95141 | 49546.41284 | 2016.944 |
| M_1173 | Homocitric acid   | C7 H10 O7      | 206.0432 | 0.96  | 236315.7295 | 54610.91073 | 58899.87099 | 57865.96866 | 48803.35489 | 82480.12148 | 62179.724 | 43050.88366 | 50076.18775 | 4289.343 |
| M_1174 | GSK-2816126   | C31 H38 N6 O2  | 526.3063 | 9.938 | 78796.43194 | 189376.0697 | 256458.6448 | 189365.0915 | 219123.5393 | 213605.6659 | 214437.71 | 223987.1131 | 184236.7163 | 3159.695 |
| M_1175 | Tetrahydroisoquinoline-3-carboxylic acid  | C10 H11 N O2   | 177.0791 | 7.311 | 15008.83497 | 2630.086981 | 4545.75705  | 3047.34634  | 3638.509583 | 6616.829864 | 4451.1765 | 5850.244319 | 2409.06124  | 3523.047 |
| M_1176 | 2050867   | C12 H23 N O4   | 245.1627 | 6.976 | 17463.85325 | 31839.28665 | 19575.17235 | 22809.59257 | 4097.11359  | 1679.694482 | 3948.4962 | 9855.579088 | 33620.58315 | 821.9419 |
| M_1177 | Di(2-ethylhexyl)adipate   | C22 H40 O4     | 368.2927 | 9.15  | 9789.543374 | 32749.28354 | 173432.7523 | 269296.8044 | 48959.99585 | 48353.93078 | 79141.66  | 182469.3557 | 142799.6072 | 9425.122 |
| M_1178 | 2-((2R,4aS,6S,8aS)-6-(beta-D-Glucopyranosyloxy)-4a-methyl-8-methylenedecahydro-2-naphthalenyl)-2-propanyl beta-D-glucopyranoside  | C27 H46 O12    | 562.2969 | 9.518 | 2527.50623  | 103447.7807 | 72956.80889 | 269040.1765 | 135752.3906 | 231142.6632 | 202323.25 | 117847.7455 | 149374.1565 | 3088.32  |
| M_1179 | 2-(Amidinoamidino)Hydrazide Isonicotinic Acid   | C8 H11 N7 O    | 221.1027 | 7.974 | 156477.1087 | 227207.2554 | 80707.69972 | 179659.617  | 114243.8769 | 268251.6011 | 182880.7  | 118927.0489 | 66456.44473 | 2652.88  |
| M_1180 | Hypotaourine  | C2 H7 N O2 S   | 109.0202 | 1.122 | 36531.44351 | 34345.88271 | 16850.53864 | 88275.53521 | 29405.74257 | 53625.52561 | 96884.064 | 136692.5775 | 86049.38332 | 1166.02  |
| M_1181 | 2-(Dicyclohexylamino)ethanol  | C14 H27 N O    | 225.2092 | 8.664 | 117952.6731 | 82397.0079  | 190283.5198 | 63401.71685 | 151880.9449 | 248954.1744 | 218278.9  | 208052.7822 | 190242.77   | 17393.08 |
| M_1182 | 2-EHTG  | C10 H20 O2 S   | 204.1191 | 1.427 | 233340.0246 | 119217.6661 | 42027.79643 | 118990.7761 | 135717.3729 | 187727.8345 | 96841.737 | 132676.7693 | 27791.21509 | 2042.726 |
| M_1183 | Methyl 2-((2,2,3,3,4,4,4-heptafluorobutanoyloxy)docosanoate   | C27 H45 F7 O4  | 566.3183 | 9.634 | 21651.89075 | 35104.23213 | 95966.49497 | 105002.1097 | 162469.437  | 251213.8253 | 122233.02 | 131972.3225 | 248461.2377 | 2896.704 |
| M_1184 | 3-((3-Hydroxynonanoyloxy)-4-(trimethylammonio)butanoate   | C16 H31 N O5   | 317.22   | 9.016 | 206624.0252 | 215818.5893 | 32141.96808 | 131859.6264 | 62958.90515 | 142794.7892 | 74827.561 | 92237.89049 | 91920.90449 | 2508.263 |
| M_1185 | 1-Allyl 2-pentadecyl 1,2-pyrrolidinedicarboxylate   | C24 H43 N O4   | 409.3192 | 9.156 | 5779.102042 | 29157.65166 | 163801.647  | 263268.5691 | 44175.6297  | 45996.05252 | 70271.709 | 172736.2318 | 130117.555  | 3543.494 |
| M_1186 | Phosphocholine  | C5 H14 N O4 P  | 183.0654 | 9.662 | 25568.73471 | 49905.45326 | 40676.97741 | 72166.81297 | 74111.78386 | 91008.49913 | 78377.421 | 36291.20061 | 76134.24162 | 4087.844 |
| M_1187 | 6-Azabenz(a)pyrene N-oxide  | C19 H11 N O    | 269.084  | 2.127 | 170403.7699 | 81906.07226 | 85682.56418 | 262445.8437 | 212115.3182 | 14468.3859  | 62504.793 | 93502.39681 | 28874.28212 | 5985.733 |
| M_1188 | N-(((2-Methyl-2-propanyl)oxy)carbonyl)phenylalanine-N-((Z)-1-ethoxy-6-methyl-1-oxo-2-hepten-4-yl)alaninamide  | C27 H41 N3 O6  | 503.2988 | 9.972 | 40645.50272 | 135624.8322 | 262236.7186 | 115804.6849 | 102320.1041 | 75606.64643 | 108078.67 | 123931.3386 | 65868.14794 | 5500.743 |
| M_1189 | Rhodamine 6G  | C28 H30 N2 O3  | 442.2252 | 7.692 | 3686.391066 | 34437.47413 | 13538.69294 | 261745.9336 | 216502.182  | 494.5651127 | 5624.1588 | 42748.08303 | 66553.17323 | 495.5094 |
| M_1190 | alpha-Aspartylphenylalanine   | C13 H16 N2 O5  | 280.1058 | 4.337 | 261651.8709 | 21114.31468 | 16088.60606 | 9170.298644 | 8773.079976 | 4414.476333 | 4000.2616 | 2781.624181 | 3544.175491 | 2593.615 |
| M_1191 | 1,4-Dinitrotetrahydroimidazo[4,5-d]imidazole-2,5(1H,3H)-dione   | C4 H4 N6 O6    | 232.0195 | 1.401 | 19651.77394 | 26184.23362 | 29057.24197 | 26522.88775 | 44180.41872 | 29000.14547 | 56405.816 | 39158.14934 | 9916.688669 | 2184.269 |
| M_1192 | 3-Phosphonopropanoic acid   | C3 H7 O5 P     | 154.0032 | 1.78  | 61649.15168 | 261186.9901 | 40369.75689 | 97949.61486 | 65822.25416 | 78251.03362 | 117114.24 | 110876.1234 | 82334.21275 | 13866.87 |
| M_1193 | 1-Linoleoyl-sn-glycero-3-phosphocholine   | C26 H50 N O7 P | 519.3338 | 9.589 | 10484.3076  | 51575.51815 | 4080.167892 | 12275.40409 | 3731.18403  | 4167.952225 | 33009.048 | 31671.65162 | 8239.319573 | 9232.125 |
| M_1194 | N-Palmitoyl-L-serine  | C19 H37 N O4   | 343.2723 | 7.914 | 257286.4399 | 57719.37121 | 23301.91503 | 74934.56315 | 98375.91832 | 152667.6613 | 103706.01 | 81978.10294 | 60992.25838 | 2921.145 |
| M_1195 | 2-O-((2E)-3-[4-(beta-D-Glucopyranosyloxy)-3-methoxyphenyl]-2-propenoyl)-1-O-((3beta,5xi,9xi,16alpha)-3-(beta-D-glucopyranuronosyloxy)-16-hydroxy-28-oxoolean-12-en-28-yl)-alpha-L-arabinopyranose | C57 H82 O22    | 1118.529 | 4.014 | 11027.98081 | 10694.80096 | 10529.81748 | 10916.53071 | 10541.08205 | 11296.97485 | 10449.724 | 10498.94946 | 10404.14275 | 10758.4  |
| M_1196 | Spirosolane-3,7,11-triol  | C27 H45 N O4   | 447.3351 | 8.249 | 259332.8573 | 83898.49603 | 70260.71239 | 122132.6193 | 56577.20842 | 214922.7161 | 197883.35 | 251820.315  | 112355.1132 | 3718.057 |
| M_1197 | 3,4-Diethoxyphenylacetic acid   | C12 H16 O4     | 224.1044 | 7.764 | 2369.262192 | 1895.566764 | 1784.538883 | 4880.914293 | 2519.801084 | 2558.154634 | 2213.1198 | 5856.44406  | 6272.014357 | 2546.741 |

|        |   |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1198 | ethylestrenol   | C20 H32 O      | 288.2451 | 9.666 | 170457.3345 | 62145.44363 | 258569.2439 | 173142.9231 | 166802.1744 | 157748.7209 | 132369.01 | 97833.54611 | 198165.7542 | 5494.994 |
| M_1199 | trimethadione   | C6 H9 N O3     | 143.0583 | 2.588 | 258257.3145 | 48810.32039 | 55221.53171 | 33607.02417 | 27761.90903 | 37913.96426 | 35190.611 | 30965.18297 | 27234.12059 | 23230.91 |
| M_1200 | 4-Nitrobenzyl (5-phenyl-2H-tetrazol-2-yl)acetate  | C16 H13 N5 O4  | 339.0955 | 6.375 | 160927.8803 | 52453.54142 | 258217.9866 | 8722.605326 | 190993.9691 | 58933.93916 | 57038.679 | 19827.54901 | 5909.531084 | 5055.894 |
| M_1201 | [Amino(4-hydroxyphenyl)methyl]phosphonic acid   | C7 H10 N O4 P  | 203.0349 | 2.438 | 21437.78025 | 38770.69405 | 96822.88587 | 33500.85131 | 38265.62912 | 52067.72583 | 41725.844 | 44455.21047 | 37499.13154 | 2631.739 |
| M_1202 | imidocarb   | C19 H20 N6 O   | 348.176  | 5.187 | 61298.42642 | 65973.83974 | 75853.86136 | 88739.73796 | 54384.99424 | 40524.56224 | 55917.385 | 97624.476   | 59494.88206 | 14935.47 |
| M_1203 | Succinyladenosine   | C14 H17 N5 O8  | 383.1077 | 4.195 | 256774.2393 | 137231.2515 | 70137.42973 | 171924.1321 | 66349.52944 | 84930.94532 | 95600.944 | 150239.469  | 40091.9301  | 4460.841 |
| M_1204 | Dihydrothymine  | C5 H8 N2 O2    | 128.0588 | 2.029 | 252959.1003 | 103097.0448 | 198724.0117 | 256247.4165 | 100468.4869 | 101866.1908 | 150770.52 | 125003.8022 | 116166.6475 | 6021.635 |
| M_1205 | 2,5-Dioxo-2,5-dihydro-1H-pyrrole-3,4-dicarbonitrile   | C6 H N3 O2     | 147.0073 | 0.789 | 173101.3084 | 104377.4066 | 83433.32553 | 179559.2594 | 96309.17772 | 97112.7835  | 81683.204 | 77060.40354 | 52516.41369 | 2766.788 |
| M_1206 | MFCDD0091818  | C7 H5 N3 O3    | 179.0334 | 0.791 | 103061.9874 | 84107.0814  | 66629.27079 | 114730.6598 | 67326.54683 | 67203.05758 | 52425.243 | 46979.90404 | 37257.12481 | 2456.489 |
| M_1207 | (1-Hydroxy-4-oxido-2,3,5,7a-tetrahydro-1H-pyrrolizin-7-yl)methyl 2,3-dihydroxy-2-isopropylbutanoate (+/-)-cis-3-Methylthiofentanyll | C15 H25 N O6   | 315.168  | 8.971 | 255328.9416 | 819.6827552 | 2151.527198 | 1503.005833 | 1507.452385 | 1624.514611 | 2299.777  | 870.8814936 | 1221.828987 | 815.9142 |
| M_1208 | N <sup>6</sup> -Cycloheptyl-N <sup>2</sup> -phenyl-7H-purine-2,6-diamine  | C21 H28 N2 O S | 356.1961 | 8.967 | 254981.9212 | 10560.18652 | 18669.97472 | 19973.62128 | 9534.895547 | 10491.46139 | 3975.5452 | 8753.385    | 8439.969189 | 2839.952 |
| M_1209 | Nitrosoimino-diacetic acid  | C4 H6 N2 O5    | 162.0269 | 4.198 | 254213.8293 | 90127.73494 | 119360.5788 | 79526.2838  | 70251.07271 | 57343.87411 | 59505.728 | 72408.36041 | 41525.75151 | 4674.348 |
| M_1210 | (E)-Dacarbazine   | C6 H10 N6 O    | 182.0916 | 4.571 | 46979.59402 | 57257.06718 | 16965.32927 | 163238.2074 | 26257.33009 | 105109.4963 | 5257.4348 | 52411.44368 | 97627.1248  | 28952.27 |
| M_1211 | 5-Hydroxy-DL-tryptophan   | C11 H12 N2 O3  | 220.0847 | 1.996 | 151899.5798 | 47892.74954 | 80786.28591 | 58278.74368 | 38859.28819 | 37724.80912 | 26086.461 | 27859.36527 | 7642.181658 | 4304.254 |
| M_1212 | Corticosterone  | C21 H30 O4     | 346.212  | 9.03  | 38827.24814 | 18597.52915 | 21801.13994 | 8268.657084 | 25744.78708 | 10688.55959 | 5460.7385 | 17036.08371 | 9243.867402 | 5178.176 |
| M_1213 | PTA   | C6 H12 N3 P    | 157.0767 | 3.425 | 251801.6094 | 175838.9748 | 175041.2222 | 158147.3986 | 204433.6762 | 155975.8137 | 166093.8  | 176008.3744 | 160360.4807 | 2497.89  |
| M_1214 | N,N'-[(2-Bromo-1,3-phenylene)bis(methylene)]bis(N-cyclohexylcyclohexanamine)  | C32 H51 Br N2  | 542.321  | 9.513 | 9905.301554 | 124245.3446 | 59039.07232 | 251579.997  | 119697.3147 | 194305.788  | 227288.73 | 143170.2544 | 168395.6689 | 15467.4  |
| M_1215 | MFCDD0005448  | C9 H9 N O6 S   | 259.0158 | 7.471 | 15318.44866 | 14688.22723 | 17660.33182 | 13863.00924 | 25332.22751 | 16166.1892  | 7175.7381 | 5635.132574 | 3472.456739 | 5239.888 |
| M_1216 | gaboxadol   | C6 H8 N2 O2    | 140.0585 | 1.121 | 217084.0954 | 137700.1779 | 226386.3423 | 41904.89831 | 157685.5229 | 53149.6577  | 186440.6  | 113198.8781 | 197617.9012 | 1274.904 |
| M_1217 | Gly-Lys   | C8 H17 N3 O3   | 203.1268 | 1.418 | 248991.3879 | 78323.62027 | 67430.16928 | 22613.31883 | 84522.05363 | 12847.44039 | 7231.914  | 9841.016177 | 3034.925932 | 843.1043 |
| M_1218 | Dodecyl N-[[allyloxy]carbonyl]alaninate   | C19 H35 N O4   | 341.2567 | 7.776 | 235556.3005 | 60543.79589 | 47131.16472 | 83253.09724 | 114749.3736 | 114819.5208 | 80101.485 | 47088.4734  | 45081.33609 | 3732.614 |
| M_1219 | MFCDD20642996   | C3 H4 O6 S     | 167.973  | 0.635 | 77104.55259 | 8983.008968 | 15635.16161 | 44652.14418 | 37353.27713 | 9063.155398 | 47911.965 | 15909.06106 | 2726.463988 | 12260.87 |
| M_1220 | Bis(2-aminoethyl)hydrogen phosphate   | C4 H13 N2 O4 P | 184.0614 | 0.976 | 246881.7178 | 29023.05033 | 20446.57051 | 24210.58263 | 12239.35147 | 22655.27235 | 22036.347 | 4047.435639 | 9475.575344 | 2223.839 |
| M_1221 | 4-tert-Butylphenylacetic acid   | C12 H16 O2     | 192.1155 | 8.176 | 30426.53639 | 6708.713226 | 31851.04623 | 30827.50602 | 31855.82821 | 33994.54564 | 32957.167 | 10255.27852 | 34984.03165 | 37229.99 |
| M_1222 | EK5700000   | C8 H18 O S     | 162.1085 | 1.438 | 69958.45283 | 123746.4416 | 105133.7194 | 218444.9299 | 183750.327  | 245946.2674 | 155568.64 | 167051.1981 | 90793.88813 | 2250.935 |
| M_1223 | 1-Boc-4-piperidinol   | C10 H19 N O3   | 201.1364 | 7.569 | 55095.18451 | 51739.01698 | 46041.7687  | 42996.37783 | 97283.67724 | 113114.4009 | 59609.672 | 78799.25411 | 43986.17856 | 8534.943 |
| M_1224 | 1-[[[8Z,11Z,14Z]-icosatrienoyl]-sn-glycero-3-phosphocholine   | C28 H52 N O7 P | 545.3465 | 9.876 | 1572.309763 | 23361.58571 | 13507.41128 | 30603.41558 | 19521.52065 | 60806.51925 | 31983.224 | 50572.21214 | 51285.24841 | 30660.42 |
| M_1225 | (2-PHENYL-1,3-THIAZOL-4-YL)METHANOL   | C10 H9 N O S   | 191.0405 | 4.026 | 5468.821624 | 6721.654279 | 5091.782146 | 16303.75678 | 5256.287794 | 49294.72837 | 5193.2592 | 17755.20795 | 5176.988785 | 5184.227 |
| M_1226 | 1-(Phenylthioxomethyl)piperidine  | C12 H15 N S    | 205.0934 | 3.304 | 393.8868425 | 328.6451696 | 26902.76309 | 342.4323068 | 317.8964468 | 286.0354282 | 5939.9519 | 1842.078389 | 244725.1615 | 313.3724 |
| M_1227 | Batrachotoxin   | C31 H42 N2 O6  | 538.3067 | 9.666 | 7661.284161 | 30045.82588 | 41656.45124 | 79829.20491 | 58431.73345 | 96267.64115 | 64485.144 | 134818.8444 | 84543.08371 | 3561.874 |
| M_1228 | Benzoxazole   | C7 H5 N O      | 119.0375 | 7.711 | 22575.44809 | 4088.761539 | 4572.666942 | 9081.429485 | 5615.068776 | 14601.22366 | 3359.1385 | 10159.76372 | 1749.703865 | 2997.432 |
| M_1229 | Tanaproget  | C16 H15 N3 O S | 297.0936 | 1.161 | 96879.28854 | 109976.2452 | 138692.9222 | 243656.4349 | 146671.6599 | 88528.27045 | 103393.88 | 213174.8456 | 150787.9272 | 1262.694 |
| M_1230 | 1,3-Adamantanedi-acetic acid  | C14 H20 O4     | 252.1355 | 8.766 | 70910.55636 | 143637.9666 | 20215.23603 | 143719.7148 | 192940.9048 | 243276.3094 | 109679.4  | 195405.1853 | 41931.73855 | 10963.4  |
| M_1231 | Adenine   | C5 H5 N5       | 135.0546 | 0.6   | 7511.936109 | 5214.894088 | 18142.51663 | 4223.406596 | 3630.013641 | 9558.049487 | 18885.004 | 33300.88757 | 17836.99305 | 13149.53 |
| M_1232 | Dimethyl N-octanoylglutamate  | C15 H27 N O5   | 301.1889 | 3.895 | 242090.8501 | 41832.53489 | 50529.33419 | 25559.43784 | 22967.21666 | 17720.07142 | 10735.03  | 4727.860721 | 3700.153373 | 1898.16  |
| M_1233 | Methyl N-[[[2-methyl-2-propanyl]oxy]carbonyl]alanylvalinate   | C14 H26 N2 O5  | 302.1841 | 8.02  | 10261.48782 | 8006.170446 | 9137.104589 | 9254.663593 | 12469.23743 | 12031.19251 | 10927.526 | 10478.66564 | 10096.41635 | 12695.53 |
| M_1234 | Guvacine  | C6 H9 N O2     | 127.0635 | 1.235 | 241240.5147 | 101824.1989 | 94331.98597 | 68891.93903 | 79785.40991 | 83905.18465 | 98537.322 | 69588.93141 | 55304.82205 | 36889.95 |
| M_1235 | 5,8-Dimethoxy-6-[4-diethylamino-1-methylbutylamino]quinazoline  | C19 H30 N4 O2  | 346.2354 | 8.257 | 241125.2215 | 61120.25151 | 175838.776  | 100591.8253 | 35884.85761 | 89364.51132 | 38413.161 | 66259.72186 | 95136.44148 | 41198.72 |
| M_1236 | dihydroxyphenylalanine  | C9 H11 N O4    | 197.0688 | 6.694 | 5737.29178  | 4911.198167 | 5208.707131 | 5220.099242 | 5096.886598 | 6463.78869  | 5192.639  | 5511.1249   | 4988.196677 | 5035.464 |
| M_1237 | 6-(1-Piperidinyll)[1,2,5]oxadiazolo[3,4-b]pyrazin-5-amine   | C9 H12 N6 O    | 220.1075 | 8.241 | 35908.95787 | 8452.006716 | 30056.78159 | 2326.392938 | 28422.29264 | 15017.42434 | 19946.219 | 20281.42217 | 42192.76771 | 11823.85 |
| M_1238 | MFCDD0055819  | C5 H9 N3 O4    | 175.0586 | 1.562 | 149835.5855 | 160600.9561 | 141260.429  | 112056.175  | 133141.6735 | 93206.34807 | 115482.07 | 65464.34489 | 155315.2108 | 3453.711 |
| M_1239 | 6-Methylnicotinamide  | C7 H8 N2 O     | 136.0613 | 1.017 | 239895.0841 | 83329.90931 | 141821.4813 | 93598.13652 | 68439.58662 | 77259.87618 | 68001.022 | 143920.1061 | 64662.26522 | 4203.144 |
| M_1240 | 2207  | C9 H16 O3      | 172.1101 | 7.764 | 21881.02459 | 9080.952855 | 6547.235274 | 5829.710704 | 34179.67006 | 16386.83906 | 78140.521 | 84269.5074  | 14015.49901 | 9390.77  |

|        |  |                  |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1242 | Diethyl (2-(2,2,3-trimethylcyclopentyl)ethyl)malonate                          | C17 H30 O4       | 298.2141 | 8.227  | 5961.52095  | 3797.699842 | 3718.133485 | 4503.998285 | 6930.826009 | 4276.276887 | 5126.4265 | 18804.13121 | 4669.374057 | 3141.777 |
| M_1243 | 5-[Fluoro(dimethyl)silyl]-1,3-2-(2-(4-Nonylphenoxy)ethoxy)ethanol              | C8 H13 F O2 Si   | 188.067  | 3.344  | 1180.571667 | 36835.4876  | 174.3734734 | 87532.88103 | 556.3752325 | 245.0495421 | 238647.2  | 75524.26506 | 77008.91969 | 147.5233 |
| M_1244 | 4-[[6-Hydroxyhexyl]oxy]benzoic acid  | C19 H32 O3       | 308.2342 | 9.438  | 4346.420815 | 8297.605883 | 6298.242786 | 6622.839044 | 6560.046477 | 4364.607933 | 6094.3098 | 2312.909423 | 6971.974583 | 4765.711 |
| M_1245 | 1-[[4-Hydroxy-6-(methoxymethyl)pyrimidin-2-yl]thio]-3,3-dimethylbutan-2-one    | C12 H18 N2 O3 S  | 238.0816 | 7.073  | 17681.13183 | 11610.98574 | 238282.9618 | 146237.1223 | 20547.2885  | 17901.52278 | 10837.596 | 7216.058833 | 8470.218666 | 21385.45 |
| M_1247 | Ethyl L-methioninate   | C7 H15 N O2 S    | 177.0824 | 3.157  | 238077.3541 | 183113.2648 | 56629.44257 | 135423.1997 | 139394.7601 | 69836.45759 | 55531.109 | 97712.56227 | 144338.9299 | 6470.425 |
| M_1248 | 1-[7-(1-Hydroxyethyl)-1-benzofuran-2-yl]-2-[[2-methyl-2-propanyl)amino]ethanol | C16 H23 N O3     | 277.1678 | 7.84   | 2149.082733 | 1844.160447 | 1976.368878 | 2090.340495 | 2895.301159 | 2849.969988 | 2364.4749 | 2096.026778 | 2239.446744 | 2802.067 |
| M_1249 | N-hydroxyhexahomothionine  | C11 H23 N O3 S   | 249.1398 | 7.47   | 237971.6772 | 52389.25679 | 74707.21857 | 45257.96621 | 56661.67628 | 70099.13285 | 27850.967 | 48875.82749 | 15290.79835 | 4970.146 |
| M_1250 | N-Methylmorpholine   | C5 H11 N O       | 101.0842 | 1.073  | 29433.4998  | 59444.91767 | 8251.491728 | 12487.31325 | 19555.3042  | 15919.85227 | 14644.19  | 14022.63855 | 14682.76845 | 22635.8  |
| M_1251 | L-Threonyl-L-seryl-L-lysine  | C13 H26 N4 O6    | 334.1854 | 0.799  | 5384.700687 | 3415.522849 | 2879.447848 | 4599.283802 | 3288.297492 | 3377.987432 | 3153.73   | 2998.905854 | 2635.960388 | 1158.887 |
| M_1252 | 4,4'-Methylenebis[2-tert-butyl-6-(alpha-methylbenzyl)phenol]                   | C37 H44 O2       | 520.3363 | 9.139  | 5271.144471 | 5939.705085 | 3965.129331 | 6291.822846 | 15202.21568 | 7416.712618 | 9252.6417 | 5368.680522 | 4169.169419 | 22655.59 |
| M_1253 | Oglufanide   | C16 H19 N3 O5    | 333.1324 | 5.665  | 59162.5457  | 116496.0089 | 200983.4791 | 236840.7309 | 142516.6369 | 104425.059  | 126432.58 | 120361.0714 | 63577.24549 | 2921.514 |
| M_1254 | CUS250000  | C8 H5 N O        | 131.0373 | 4.476  | 3952.052702 | 3704.974677 | 11567.70966 | 1450.989789 | 1921.554156 | 2277.276386 | 5101.5151 | 4244.796659 | 2777.646785 | 1724.388 |
| M_1255 | Trimethoprim   | C14 H18 N4 O3    | 580.268  | 3.403  | 8445.45964  | 8757.722683 | 9092.287561 | 9931.885695 | 9643.459444 | 9889.789822 | 12524.275 | 13075.95408 | 10186.22724 | 4329.322 |
| M_1256 | 2361   | C10 H18 O2       | 170.1308 | 7.954  | 65994.14414 | 7057.3516   | 10739.57243 | 19112.09995 | 47296.69779 | 16759.74208 | 23990.249 | 13304.5733  | 17300.29225 | 5383.99  |
| M_1257 | Paracetamol  | C8 H9 N O2       | 151.0634 | 6.175  | 11161.19673 | 1096.250544 | 1047.705692 | 10300.84808 | 9218.543377 | 12085.16337 | 8676.9443 | 1103.474671 | 9904.229353 | 9773.206 |
| M_1258 | Glycylglycylglycine  | C6 H11 N3 O4     | 189.075  | 1.762  | 141750.3361 | 234991.7938 | 1842.60278  | 76499.19021 | 36112.21007 | 58763.553   | 49966.959 | 70642.71638 | 56698.66513 | 4717.944 |
| M_1259 | negamycin  | C9 H20 N4 O4     | 248.1483 | 1.586  | 146378.5844 | 16773.13726 | 24827.13621 | 21277.69182 | 30270.02906 | 11528.4237  | 42537.715 | 15118.74353 | 15662.65031 | 3796.742 |
| M_1260 | 2,3-Dideoxy-3-nitropentarate   | C5 H5 N O7       | 191.0073 | 1.071  | 103095.478  | 35822.81862 | 23018.54531 | 51577.74897 | 26820.9808  | 44197.86386 | 46258.202 | 29743.79427 | 35340.45936 | 1088.603 |
| M_1261 | 3,3'-Sulfanediyldipropylhydrazide  | C6 H14 N4 O2 S   | 206.0837 | 1.441  | 3722.106828 | 2150.028388 | 233865.0995 | 2069.319855 | 14301.98756 | 2162.605016 | 3407.9458 | 2143.183841 | 2864.887546 | 1015.85  |
| M_1262 | 1-(4,6-Diaminopyrimidin-5-yl)guanidine   | C5 H9 N7         | 167.0922 | 3.289  | 3772.064965 | 3140.651168 | 3447.178732 | 3248.995382 | 3120.842468 | 2859.456911 | 2883.0414 | 3683.759579 | 2837.812606 | 2973.275 |
| M_1263 | S-(2-[[4-(2,6-Dioxo-1-piperidinyl)butyl]amino]ethyl) hydrogen sulfurothioate   | C11 H20 N2 O5 S2 | 324.0812 | 4.008  | 233307.788  | 1709.305153 | 1572.259214 | 1638.307951 | 1653.714672 | 1649.110137 | 1633.8848 | 1988.086954 | 1628.765898 | 1631.043 |
| M_1264 | p-Hexyloxybenzoic Acid   | C13 H18 O3       | 222.1258 | 7.787  | 3650.195422 | 2920.398236 | 2749.343524 | 2582.201643 | 3952.113066 | 4070.260107 | 3469.5073 | 3120.855431 | 2930.235384 | 4111.607 |
| M_1265 | 1-Benzenesulfinylpiperidine  | C11 H15 N O S    | 209.0882 | 2.163  | 117201.2535 | 66298.8417  | 232274.0723 | 105243.7953 | 64528.32633 | 60397.53448 | 69313.792 | 49815.9599  | 28333.07397 | 4807.968 |
| M_1266 | 1,4-Dimethyl-N-nitro-1,4-dihydro-5H-tetrazol-5-imine                           | C3 H6 N6 O2      | 158.0555 | 1.21   | 178993.9773 | 133266.2746 | 129117.3297 | 231731.5849 | 198643.5397 | 99473.04682 | 56666.483 | 104205.038  | 63878.85657 | 1616.351 |
| M_1267 | 3,5-Diamino-N-carbamimidoyl-2-pyrazinecarboxamide                              | C6 H9 N7 O       | 195.0872 | 6.431  | 231132.7537 | 56011.7918  | 59121.36498 | 87795.68961 | 51449.85984 | 47112.67934 | 49996.976 | 26570.75571 | 14728.29117 | 2664.856 |
| M_1268 | 80122  | C7 H13 N O       | 127.0999 | 6.747  | 231124.6374 | 40535.91712 | 45365.53976 | 64847.54611 | 46933.51202 | 31570.17085 | 32179.61  | 24883.81563 | 10371.71913 | 8235.961 |
| M_1269 | 1-(4,6-Dimethyl-2-pyrimidinyl)-3-[3-(2-oxo-1-pyrrolidinyl)propyl]guanidine     | C14 H22 N6 O     | 290.186  | 8.872  | 74882.9513  | 92136.95355 | 110976.9199 | 75509.95175 | 83744.59274 | 112807.761  | 79723.298 | 97116.66066 | 122071.0253 | 38260.09 |
| M_1270 | secoverine   | C22 H35 N O2     | 345.2668 | 10.018 | 182279.6715 | 66152.56141 | 44113.65848 | 53387.91262 | 101852.3594 | 93913.46156 | 70480.538 | 136577.2413 | 104569.4027 | 3967.692 |
| M_1271 | aldehydo-D-glucosamine 6-phosphate   | C6 H14 N O8 P    | 259.0459 | 1.184  | 10401.7286  | 41883.47858 | 16092.68839 | 27978.4625  | 9349.820124 | 20284.18542 | 9580.8278 | 13511.24982 | 8990.006145 | 936.5481 |
| M_1272 | 8-Hydrazino-7-(2-hydroxyethyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione    | C9 H14 N6 O3     | 254.1131 | 7.673  | 139408.7441 | 23170.70466 | 67122.47866 | 85261.51644 | 137314.3849 | 177608.0989 | 14342.487 | 87184.50579 | 2943.584181 | 18906.68 |
| M_1273 | Gallic acid  | C7 H6 O5         | 170.0218 | 2.214  | 226395.3824 | 199261.4067 | 85351.78673 | 177053.7606 | 221411.5523 | 117940.4715 | 128548.53 | 62454.15317 | 64133.75201 | 7242.452 |
| M_1274 | 1-Adamantanemethanol   | C11 H18 O        | 166.1358 | 8.799  | 32939.67194 | 41725.85357 | 31807.95842 | 35071.71167 | 35156.04558 | 37045.03606 | 39516.152 | 40770.02022 | 32056.80721 | 5138.347 |
| M_1275 | aloin A  | C21 H22 O9       | 418.1267 | 7.704  | 205603.8787 | 212567.5406 | 226015.4978 | 187878.3463 | 141224.7614 | 114891.357  | 68030.697 | 66259.59181 | 42031.43159 | 7024.886 |
| M_1276 | Indane   | C9 H10           | 118.0785 | 8.536  | 51169.96703 | 97686.90365 | 58628.25499 | 60993.80694 | 114921.3993 | 69214.84651 | 112328.22 | 225446.2972 | 65947.25257 | 32046.48 |
| M_1277 | N <sup>2</sup> -,N <sup>6</sup> -Diocanoyl-L-lysine                            | C22 H42 N2 O4    | 398.3148 | 9.278  | 53441.95476 | 33231.14626 | 31494.7196  | 35415.23985 | 7698.264397 | 48133.12549 | 53277.927 | 87511.26811 | 40334.16008 | 9068.478 |
| M_1278 | Pentahydroxyphosphorane  | H5 O5 P          | 115.9878 | 1.413  | 136519.2813 | 14057.0194  | 10221.89734 | 26873.00359 | 15139.79586 | 49099.53439 | 39976.54  | 39550.8582  | 43988.46411 | 1076.688 |
| M_1279 | Testosterone   | C19 H28 O2       | 288.2085 | 9.022  | 97853.384   | 76710.39617 | 88603.62593 | 91506.30233 | 58307.95133 | 62558.79955 | 93905.726 | 103601.8474 | 135271.9621 | 9478.795 |
| M_1280 | Benzylsodium   | C7 H7 Na         | 114.0441 | 0.597  | 4839.178378 | 3595.983387 | 6210.207406 | 1739.125644 | 5376.310587 | 2198.128533 | 6238.5871 | 4209.078826 | 2230.123199 | 14261.17 |
| M_1281 | Piperonylonitrile  | C8 H5 N O2       | 147.0322 | 7.458  | 8722.749203 | 4834.814739 | 9780.512251 | 6214.144423 | 6505.55446  | 7628.845361 | 8501.8891 | 1644.339213 | 8507.695699 | 2568.788 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1282 | 3-(Allylsulfanyl)[1,2,4]triazino[5,6-d][3,1]benzoxazepine                                       | C13 H10 N4 O S  | 270.0576 | 1.942  | 12320.05017 | 8485.167979 | 7780.103831 | 8529.534787 | 7251.516434 | 7231.300329 | 6694.737  | 7234.962005 | 5926.294936 | 8174.44  |
| M_1283 | 1957290   | C14 H22 O4      | 254.1507 | 8.622  | 2637.07536  | 2753.041841 | 1758.183522 | 9885.027389 | 11211.66674 | 14060.17734 | 13665.23  | 16085.85599 | 10239.40513 | 11962.4  |
| M_1284 | 2,2,2-Trifluoroethyl Benzyl 2-acetamido-3,4,6-tri-O-benzyl-2-deoxyhexopyranoside                | C2 H2 F3        | 83.0109  | 1.193  | 116898.3638 | 222555.3462 | 216501.9869 | 166927.9796 | 218002.2792 | 113472.8302 | 105113.53 | 166369.3842 | 111837.2154 | 1257.369 |
| M_1285 | 6-(1-Azepanyl)-N-(2,3-dimethylphenyl)[1,2,5]oxadiazolo[3,4-b]pyrazin-5-amine                    | C18 H22 N6 O    | 338.1855 | 8.842  | 192278.2394 | 157973.5377 | 160382.7227 | 221210.9912 | 59613.99491 | 137312.3049 | 100055.23 | 145319.7315 | 130114.0387 | 6390.58  |
| M_1286 | N-Cyclohexyl-N'-(5-methyl-1,2-oxazol-3-yl)sulfuric diamide                                      | C10 H17 N3 O3 S | 259.099  | 1.484  | 9864.699369 | 26398.33286 | 6078.097615 | 5597.254929 | 16512.40112 | 23700.83435 | 46524.438 | 69707.89318 | 30640.65401 | 2542.73  |
| M_1288 | gamma-Aminobutyric acid   | C4 H9 N O2      | 103.0638 | 1.195  | 220629.4752 | 90408.18504 | 84075.46364 | 216811.0459 | 69690.76772 | 53893.3975  | 43638.452 | 57350.94951 | 41914.05613 | 16093.46 |
| M_1289 | g-Butyrobetaine   | C7 H15 N O2     | 145.1104 | 2.005  | 27759.59524 | 20296.85299 | 18761.5198  | 25778.38927 | 1840.102378 | 1897.368865 | 17322.73  | 18785.21534 | 11655.17525 | 2140.507 |
| M_1290 | 2,5-TBHQ  | C14 H22 O2      | 222.162  | 8.809  | 220461.0953 | 2326.779096 | 28203.02    | 34285.10255 | 29831.16661 | 13798.95836 | 29521.492 | 31640.61071 | 34414.96816 | 20148.83 |
| M_1291 | Methyl N-acetyl-S-(2-hydroxycyclohexyl)-L-cysteinate  | C12 H21 N O4 S  | 275.1191 | 4.542  | 220443.7697 | 12120.92668 | 4633.520523 | 28363.30284 | 9031.95048  | 8381.790061 | 6581.1762 | 15161.89927 | 11301.14393 | 2281.382 |
| M_1292 | 4-(2H-Tetrazol-5-yl)-1,2,5-oxadiazolo-3-amine   | C3 H3 N7 O      | 153.0404 | 1.102  | 102738.2315 | 70190.90372 | 219436.4278 | 83728.55196 | 126836.4019 | 95773.83429 | 92251.127 | 104308.8757 | 71685.47466 | 3439.113 |
| M_1293 | g-Butyrobetaine   | C7 H15 N O2     | 145.1104 | 3.264  | 12598.73956 | 8288.284814 | 55423.83563 | 16675.94965 | 8539.605919 | 18760.11015 | 17534.552 | 10253.3664  | 14181.27134 | 5194.269 |
| M_1294 | Gly-Lys   | C8 H17 N3 O3    | 203.1268 | 1.446  | 219208.2219 | 14785.5471  | 44932.29275 | 23443.81496 | 14891.07605 | 8272.847429 | 7231.914  | 2987.394902 | 7601.197564 | 802.7397 |
| M_1295 | N-methylethanolamine phosphate  | C3 H10 N O4 P   | 155.0349 | 1.6    | 13287.68084 | 8235.113108 | 29413.33202 | 48299.6286  | 19568.24276 | 72599.82038 | 17253.467 | 33312.39711 | 43457.69876 | 5073.283 |
| M_1296 | Butyl O-phosphoserinate   | C7 H16 N O6 P   | 241.0714 | 1.242  | 20944.1832  | 94578.865   | 21383.89516 | 100608.0372 | 68487.51198 | 103280.5616 | 61029.473 | 66334.13855 | 73847.07882 | 1907.982 |
| M_1297 | 2,3-Dihydroxypropyl nonanoate   | C12 H24 O4      | 232.1676 | 8.083  | 116168.615  | 24833.86313 | 91661.64968 | 80341.57486 | 117973.228  | 147700.3332 | 218183.26 | 182143.2896 | 162477.9625 | 5129.667 |
| M_1298 | Ethyl 4-acetamido-5-amino-3-(3-pentanyloxy)-1-cyclohexene-1-carboxylate                         | C16 H28 N2 O4   | 312.2062 | 9.142  | 32819.55172 | 18739.09365 | 14032.84018 | 17422.29548 | 29368.77819 | 16704.13647 | 21066.148 | 32202.65348 | 30531.5327  | 3456.49  |
| M_1299 | Homocitrulline  | C7 H15 N3 O3    | 189.1113 | 1.119  | 216818.7247 | 87728.36625 | 42673.5877  | 108975.9244 | 127793.5058 | 44542.24696 | 55770.139 | 37533.67299 | 26529.71268 | 1482.715 |
| M_1300 | 2,2'-Thenil   | C10 H6 O2 S2    | 221.9808 | 1.077  | 19903.69305 | 14937.1086  | 3423.8602   | 18843.57858 | 5038.23838  | 9234.317582 | 8791.5042 | 4065.176477 | 13036.27433 | 723.1513 |
| M_1301 | 4-[[6-Hydroxyhexyl]oxy]benzoic acid   | C13 H18 O4      | 238.1202 | 7.709  | 1219.089491 | 13697.18115 | 24666.15035 | 989.3733742 | 1596.788499 | 1514.929288 | 1147.8484 | 1113.893905 | 977.5703207 | 1587.951 |
| M_1302 | Propylparaben   | C10 H12 O3      | 180.0793 | 7.827  | 3633.027102 | 3443.989638 | 15286.05036 | 5064.18429  | 5261.865837 | 5179.48182  | 9983.3838 | 12236.76928 | 20108.62058 | 5092.424 |
| M_1303 | BOC-L-PHENYLALANINOL  | C14 H21 N O3    | 251.152  | 8.518  | 214289.3534 | 64509.82147 | 40615.46698 | 186137.0953 | 67452.93963 | 88615.16393 | 83575.985 | 167231.2661 | 70262.39245 | 9274.738 |
| M_1304 | LysoPC(18:3(9Z,12Z,15Z))  | C26 H48 N O7 P  | 517.3145 | 9.699  | 72114.06179 | 2715.28723  | 2722.009969 | 2998.715427 | 2875.847075 | 3003.597086 | 2876.1714 | 213806.7711 | 2520.828228 | 32508.39 |
| M_1305 | VS1150000   | C18 H34 O4      | 314.2457 | 8.992  | 213794.4784 | 26473.04173 | 23580.88258 | 28714.76865 | 12314.38744 | 26322.24537 | 20833.469 | 20762.26314 | 13867.16782 | 11564.77 |
| M_1306 | L-Glutamic acid 5-benzyl ester  | C12 H15 N O4    | 237.1001 | 7.495  | 28500.62265 | 20361.2863  | 97906.14231 | 25527.61104 | 39995.20347 | 52453.88129 | 33985.431 | 31315.91303 | 18583.14422 | 8050.627 |
| M_1307 | N-Hydroxyphthalimide  | C8 H5 N O3      | 163.027  | 2.743  | 31049.35497 | 101802.4006 | 66444.46776 | 213314.5619 | 116310.9698 | 24498.44625 | 58245.732 | 104533.5289 | 77275.7281  | 13643.49 |
| M_1308 | 2-Hydroxy-3-(palmitoyloxy)propyl 2-(trimethylammonio)ethyl phosphate                            | C24 H50 N O7 P  | 495.3327 | 10.787 | 56858.7808  | 79307.47216 | 119766.2349 | 129316.2888 | 119269.0574 | 193660.1865 | 143109.41 | 178802.2864 | 128965.4589 | 5156.526 |
| M_1309 | 2-O-(Methylsulfonyl)pentose   | C6 H12 O7 S     | 228.0303 | 1.237  | 11686.50678 | 79491.32111 | 5917.543947 | 112752.247  | 67115.55736 | 90790.15505 | 32873.812 | 42222.01566 | 137608.7402 | 1354.887 |
| M_1310 | (4S)-4-Cyclohexyl-L-proline   | C11 H19 N O2    | 197.1417 | 7.889  | 30689.83847 | 23399.96083 | 25390.33153 | 26535.07855 | 31657.75727 | 53536.52953 | 39675.94  | 50053.71664 | 879.3072421 | 1952.007 |
| M_1311 | L-Proline   | C5 H9 N O2      | 115.0635 | 0.757  | 3917.671769 | 21336.83762 | 66734.64371 | 210656.5529 | 3225.735854 | 14028.31682 | 3518.771  | 25076.89327 | 2993.575716 | 4081.296 |
| M_1312 | Falcalcitriol   | C27 H38 F6 O3   | 524.2715 | 9.285  | 23428.23772 | 109375.6384 | 64892.25266 | 148174.5503 | 141567.7512 | 128680.5369 | 191941.1  | 202418.5498 | 161656.3041 | 3584.974 |
| M_1313 | OB4520000   | C10 H9 N O      | 159.0685 | 7.263  | 82028.69484 | 23691.59029 | 44461.95543 | 36491.9066  | 25690.71226 | 18977.10287 | 15662.64  | 17911.73828 | 13414.59442 | 4084.013 |
| M_1314 | L-(+)-Leucine   | C6 H13 N O2     | 131.0947 | 1.095  | 5383.818649 | 6030.237162 | 5958.660048 | 6015.8886   | 5133.900574 | 6289.33258  | 6925.3717 | 6548.171474 | 6021.930322 | 18236.26 |
| M_1315 | Phenolate   | C6 H5 O         | 93.03463 | 5.332  | 49606.8587  | 98983.77229 | 209279.6733 | 70651.13812 | 183838.1074 | 122402.0283 | 55891.406 | 51651.041   | 46289.08907 | 4200.506 |
| M_1316 | protocatechuic acid   | C7 H6 O4        | 154.0271 | 4.852  | 3459.800795 | 3241.293105 | 3420.135795 | 3431.053273 | 3280.739391 | 3180.034793 | 3322.5435 | 3323.550198 | 3776.873346 | 3196.312 |
| M_1317 | 2,5-TBHQ  | C14 H22 O2      | 222.1621 | 9.634  | 33036.80435 | 28600.08726 | 31485.22419 | 35149.92609 | 32323.3769  | 207516.6784 | 7188.8065 | 27303.63033 | 26760.38044 | 34718.97 |
| M_1318 | Muscimol  | C4 H6 N2 O2     | 114.0433 | 1.36   | 34744.57305 | 107368.3251 | 34461.97512 | 182238.7891 | 85356.27972 | 73220.54298 | 107634.35 | 65428.12577 | 28304.35333 | 5635.767 |
| M_1319 | Loratadine impurity   | C8 H13 N O3     | 171.0896 | 3.644  | 9953.235309 | 15513.21351 | 16664.89214 | 21943.69726 | 15693.5319  | 11199.77336 | 10832.203 | 13343.2589  | 9668.405386 | 6864.674 |
| M_1320 | [[Dicyclohexylamino)sulfanyl](dimethylamino)methanethione                                       | C15 H28 N2 S2   | 300.1701 | 8.783  | 33856.88082 | 156195.567  | 44922.20057 | 100769.6624 | 98293.42659 | 205888.6803 | 124278.05 | 151198.3789 | 99937.49707 | 8097.749 |
| M_1321 | (2E)-2-[(1E)-1-[[[Amino(hydrazono)methyl]hydrazono]-2-propanylidene]hydrazinecarbohydrazonamide | C5 H14 N10      | 214.1407 | 10.475 | 60007.74218 | 69291.67633 | 158630.9595 | 64576.02988 | 64682.55844 | 60574.47421 | 146383.41 | 56928.78271 | 87286.93931 | 4738.069 |
| M_1322 | Linoleamide   | C18 H33 N O     | 279.2561 | 9.15   | 13723.65352 | 9405.653096 | 33452.45175 | 6453.727262 | 11952.68058 | 34411.59375 | 7396.761  | 22350.45854 | 27530.31865 | 4044.333 |
| M_1323 | 4-ethyl-2,3-dioxiperazin-1-carbonylchlorid  | C7 H9 Cl N2 O3  | 204.0305 | 0.784  | 205108.8056 | 116721.9459 | 106909.711  | 161971.4727 | 137523.5457 | 104662.124  | 129416.16 | 51921.33662 | 103964.5558 | 5649.355 |

|        |   |                   |          |       |             |             |             |             |             |             |            |             |             |            |
|--------|---|-------------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|------------|-------------|-------------|------------|
| M_1324 | [4-(Phenylsulfanyl)phenyl]methanol  | C13 H12 O S       | 216.061  | 1.127 | 205088.351  | 66172.31652 | 20680.63253 | 61408.43432 | 49362.79754 | 22029.87741 | 29438.77   | 25756.61408 | 21442.62533 | 754.8909   |
| M_1325 | 5-Hydroxyindole-3-acetic acid   | C10 H9 N O3       | 191.0583 | 6.08  | 65021.84944 | 62125.04712 | 179337.1983 | 16755.58403 | 85166.05339 | 53102.75579 | 60460.271  | 60055.0809  | 19288.79903 | 4666.016   |
| M_1326 | carisoprodol  | C12 H24 N2 O4     | 260.1733 | 8.655 | 75179.85802 | 150642.3225 | 83023.53569 | 77676.3123  | 17973.01229 | 45973.77578 | 105788.25  | 99623.51886 | 107043.8495 | 12748.01   |
| M_1327 | 4-Fluorobenzaldehyde  | C7 H5 F O         | 124.0318 | 0.596 | 9958.269174 | 7622.34095  | 12896.58452 | 11203.48763 | 6507.710097 | 9151.20524  | 173222.59  | 189765.5664 | 149591.0761 | 6225.737   |
| M_1328 | (1-Oxido-2,6,7-trioxaphosphabicyclo[2.2.0]oct-4-yl)methanol   | C5 H9 O5 P        | 180.0188 | 1.845 | 24380.0209  | 50156.15667 | 53887.3955  | 43886.88155 | 47840.8436  | 136842.9596 | 46292.351  | 59927.3667  | 36904.81195 | 9568.373   |
| M_1329 | tioxolone   | C7 H4 O3 S        | 167.9885 | 0.837 | 191378.8781 | 68697.28198 | 95127.53479 | 175023.1531 | 112346.1399 | 108593.9622 | 76168.864  | 88878.83097 | 63267.11299 | 1112.774   |
| M_1330 | Docosahexaenoic acid  | C22 H32 O2        | 328.2399 | 9.955 | 110035.6214 | 64502.19533 | 8291.498291 | 2695.916765 | 46066.66128 | 12623.21533 | 11482.695  | 65530.48645 | 56017.58858 | 1285.425   |
| M_1331 | Asarone   | C12 H16 O3        | 208.1101 | 7.737 | 20125.33505 | 3279.562603 | 5074.583263 | 15807.14095 | 19094.87739 | 30301.68071 | 2775.6371  | 11591.69598 | 17158.53322 | 21716.44   |
| M_1332 | N-Acetylphenylalanine   | C12 H15 N O2      | 207.2323 | 6.737 | 10000.0000  | 10000.0000  | 10000.0000  | 10000.0000  | 10000.0000  | 10000.0000  | 10000.0000 | 10000.0000  | 10000.0000  | 10000.0000 |
| M_1333 | octylphenol   | C14 H22 O         | 206.1671 | 8.954 | 150058.3787 | 95577.26708 | 200774.145  | 178103.2009 | 178257.1034 | 162735.8164 | 140975.05  | 129255.9869 | 191135.6861 | 17358.43   |
| M_1334 | fMet  | C6 H11 N O3 S     | 177.0459 | 3.285 | 7460.691354 | 28739.69275 | 37013.67975 | 191370.6096 | 6102.468666 | 96623.68921 | 94808.464  | 79315.10031 | 63934.61574 | 5857.682   |
| M_1335 | methylthiomethylithium  | C2 H5 Li S        | 68.02686 | 0.597 | 12575.32471 | 9455.247195 | 7876.604537 | 13964.4041  | 7513.320092 | 10801.7144  | 18566.103  | 15798.99407 | 16155.36928 | 16319.8    |
| M_1336 | 2,5-Furandicarboxylic acid  | C6 H4 O5          | 156.006  | 2.85  | 37210.36278 | 20271.01681 | 108328.9177 | 52389.13013 | 12100.8915  | 23267.35042 | 12379.226  | 13329.32642 | 11926.84416 | 12958.62   |
| M_1337 | beta-Carotene-3,3'-diene  | C40 H56 O2        | 568.4272 | 9.192 | 35924.92963 | 36767.62984 | 28685.36481 | 40228.79939 | 32916.96077 | 40135.46414 | 35481.588  | 38258.56322 | 34982.66182 | 22378.77   |
| M_1338 | (2-Amino-3-hydroxybutanoyl)oxonium  | C4 H10 N O3       | 120.065  | 2.234 | 200982.6294 | 3454.042909 | 21609.8203  | 109794.0902 | 11057.27696 | 77809.45164 | 91035.562  | 80655.42356 | 81455.94058 | 1699.042   |
| M_1339 | metharbital   | C9 H14 N2 O3      | 198.1005 | 2.898 | 200624.9954 | 34022.25532 | 6349.14153  | 51479.85045 | 167236.4931 | 5514.969296 | 6349.7577  | 33339.89936 | 39139.57505 | 5486.285   |
| M_1340 | N,N',N''-triethyl-1,3,5-triazine-2,4,6-triamine   | C13 H26 N6        | 266.2222 | 9.517 | 147887.5987 | 82564.91371 | 155560.5911 | 132843.2738 | 115389.8179 | 185372.2468 | 123731.99  | 131460.8816 | 130476.3639 | 19401.41   |
| M_1341 | MFC00037048   | C17 H33 N O       | 267.2561 | 9.669 | 6435.058424 | 6924.255274 | 7119.101416 | 7940.180743 | 7532.318049 | 7753.681774 | 7044.5632  | 6598.908502 | 6817.386209 | 8800.952   |
| M_1342 | Elaidolinolenic acid  | C18 H30 O2        | 278.2244 | 9.792 | 63201.74003 | 149521.6292 | 44929.63988 | 133478.0492 | 107397.1363 | 103469.4176 | 91378.025  | 132397.9675 | 122302.7315 | 7020.948   |
| M_1343 | 1-Naphthylisocyanate  | C11 H7 N O        | 169.0529 | 3.497 | 84032.78947 | 74253.01794 | 112444.0424 | 152933.5474 | 127774.7812 | 171988.1804 | 172994.6   | 189964.4855 | 124223.4611 | 15866.41   |
| M_1344 | Diethyl(methyl)malonate   | C15 H20 O5        | 280.1304 | 8.543 | 5298.606211 | 73935.64571 | 52653.65788 | 54098.83831 | 131159.7372 | 13667.14849 | 57763.832  | 92190.68982 | 23447.50827 | 7804.237   |
| M_1345 | Temozolomide  | C6 H6 N6 O2       | 194.0555 | 6.866 | 199225.2509 | 39035.08143 | 51433.74324 | 27136.84463 | 17843.19493 | 23077.19248 | 43905.963  | 11496.05771 | 37987.98798 | 1594.304   |
| M_1346 | 1-Butyl-4-isothiocyanatobenzene   | C11 H13 N S       | 191.0773 | 2.42  | 16879.66485 | 10214.16726 | 15876.31866 | 11038.4773  | 9462.292765 | 11209.84823 | 11064.98   | 9944.268123 | 8391.733079 | 4225.103   |
| M_1347 | Demethylphosphinotricin   | C4 H10 N O4 P     | 167.0349 | 7.392 | 1105.771459 | 1093.688402 | 1445.971323 | 1279.688878 | 1679.480557 | 4152.194523 | 1042.0021  | 1526.683117 | 911.2080937 | 1681.331   |
| M_1348 | Bufadienolide   | C24 H34 O2        | 354.2567 | 8.755 | 9039.533048 | 5140.473155 | 52953.31517 | 197939.0644 | 462.7806092 | 17904.27332 | 17514.273  | 182168.0819 | 27450.19999 | 309.0169   |
| M_1349 | C8-HSL  | C12 H21 N O3      | 227.1521 | 8.507 | 71269.0298  | 82780.77039 | 58894.50914 | 197892.6792 | 63820.36717 | 106612.255  | 68591.957  | 166577.76   | 96958.38778 | 8869.88    |
| M_1350 | C7-HSL  | C11 H19 N O3      | 213.1366 | 7.931 | 4637.865244 | 4896.092626 | 3899.614292 | 4560.023551 | 3817.891986 | 6049.044158 | 5448.5821  | 4644.545668 | 5520.032331 | 6324.742   |
| M_1351 | 8-Azaguanine  | C4 H4 N6 O        | 152.0449 | 5.067 | 196533.6141 | 62794.261   | 45625.48785 | 59288.03246 | 31928.21872 | 78874.15543 | 96747.74   | 81683.49832 | 58083.68657 | 37208.78   |
| M_1352 | 1-BOC-Piperazine  | C9 H18 N2 O2      | 186.1368 | 4.767 | 41748.37333 | 51211.13124 | 40365.52098 | 49065.75606 | 35356.63211 | 81549.69147 | 31514.833  | 48360.23786 | 43026.98262 | 4955.301   |
| M_1353 | Methohexital  | C14 H18 N2 O3     | 262.1317 | 5.21  | 21115.10764 | 39085.00976 | 55823.23962 | 73328.97071 | 18845.20149 | 31114.67335 | 51200.228  | 54330.93542 | 30394.02314 | 3261.996   |
| M_1354 | 8-Hydroxyquinoline  | C9 H7 N O         | 145.0529 | 5.014 | 62324.76687 | 12798.9977  | 13888.07435 | 22671.05794 | 22525.02905 | 22470.39391 | 21832.963  | 24652.74155 | 11302.39807 | 3280.074   |
| M_1355 | 2'-Hydroxy-4,4',6'-trimethoxychalcone   | C18 H18 O5        | 314.1153 | 8.605 | 56677.35739 | 37580.79026 | 195680.7405 | 47033.51442 | 39285.68427 | 37761.57766 | 66099.017  | 49558.1292  | 82539.98847 | 16087.07   |
| M_1356 | 3796  | C12 H18 O3        | 210.1253 | 8.132 | 195148.6216 | 929.1145175 | 13039.9815  | 12212.65565 | 20070.35129 | 20169.45928 | 15966.234  | 16287.62424 | 21351.64443 | 18760.64   |
| M_1357 | 2,4-Bis(dimethylamino)-6-nitro-1,3,5-triazine   | C7 H12 N6 O2      | 212.1027 | 7.37  | 7250.849144 | 10825.75182 | 1936.536384 | 16542.18442 | 5626.422212 | 4880.803012 | 5788.2831  | 8629.989458 | 10018.61582 | 17148.99   |
| M_1358 | o-Toluidine   | C7 H9 N           | 107.0739 | 1.518 | 1908.929172 | 9043.19678  | 3754.881824 | 10281.81202 | 6145.670371 | 3334.258599 | 3486.2413  | 2889.736312 | 2650.898761 | 4389.383   |
| M_1359 | Dimethyl(2-methyl-2-propanyl)silyl N,1-bis(dimethyl(2-methyl-2-propanyl)silyl)tryptophanate   | C29 H54 N2 O2 Si3 | 546.351  | 9.934 | 1101.303254 | 6089.88165  | 1563.275944 | 10168.94496 | 8620.676538 | 3313.624625 | 3698.0093  | 8225.0158   | 5024.161897 | 5210.696   |
| M_1360 | (6Z)-5-Methyl-6-((2E)-(5-methyl-1,3-diazatricyclo[3.3.1.1 <sup>3,7</sup> ]-dec-6-ylidene)hydrazono)-1,3-diazatricyclo[3.3.1.1 <sup>3,7</sup> ]-decane | C18 H28 N6        | 328.2375 | 9.547 | 740.1754512 | 748.1934848 | 1878.240078 | 194355.6165 | 3616.835644 | 1115.2611   | 1194.2415  | 198.3878321 | 275.3104722 | 252.1948   |
| M_1361 | Acetanilide   | C8 H9 N O         | 135.0685 | 1.392 | 120768.5709 | 47024.65785 | 17650.05214 | 37269.29977 | 14634.34405 | 111326.3548 | 79617.569  | 36243.17487 | 106762.274  | 6298.874   |
| M_1362 | Acetanilide   | C8 H9 N O         | 135.0685 | 1.326 | 120768.5709 | 106110.0707 | 43629.16484 | 145012.6809 | 18709.92388 | 111326.3548 | 145119.71  | 36243.17487 | 61338.90017 | 8675.731   |
| M_1363 | D-Erythritol 4-phosphate  | C4 H11 O7 P       | 202.0244 | 1.196 | 12398.76161 | 36230.87191 | 7905.725502 | 28885.51881 | 6583.123548 | 7251.036058 | 7166.6982  | 7415.197476 | 6192.966196 | 738.7183   |
| M_1364 | Trimethylphosphoran ylidene cyanamide   | C4 H9 N2 P        | 116.0498 | 3.496 | 74784.77935 | 100311.7852 | 137613.0273 | 130006.5217 | 128865.1737 | 145828.1382 | 193285.21  | 181443.5989 | 135176.7267 | 2980.536   |
| M_1365 | 1-BOC-3-pyrrolidinol  | C9 H17 N O3       | 187.1209 | 7.797 | 174274.9395 | 23588.22836 | 16541.72356 | 63989.20894 | 26806.80093 | 91374.6365  | 40480.434  | 61317.42284 | 44986.88918 | 19233.58   |
| M_1366 | 2475675   | C23 H34 O2        | 342.2558 | 8.97  | 153974.2752 | 28101.66749 | 27350.41746 | 9688.526542 | 20174.29547 | 22011.62285 | 10460.517  | 24586.64149 | 8456.175117 | 16263.38   |

|        |  |                  |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1367 | AS8925000  | C11 H16 O4       | 212.1054 | 7.497  | 24442.6496  | 8379.558515 | 9511.990585 | 10414.22339 | 2268.335532 | 18847.46511 | 12373.507 | 74206.59938 | 10358.14171 | 7550.845 |
| M_1368 | 2-Amino-6-propoxybenzothiazole   | C10 H12 N2 O S   | 208.0669 | 4.024  | 3639.540584 | 8213.342469 | 3397.147185 | 12651.41826 | 3498.097773 | 39200.79208 | 3456.1518 | 14489.21289 | 3445.323706 | 3450.141 |
| M_1369 | Glufosinate  | C5 H12 N O4 P    | 181.0505 | 7.887  | 5563.806377 | 5119.073469 | 4755.00434  | 5344.150599 | 7402.107675 | 7062.545596 | 5789.5988 | 5681.916142 | 5726.651167 | 7282.521 |
| M_1370 | 6132055  | C19 H36 O3       | 312.2662 | 9.736  | 59283.952   | 138469.6527 | 61295.53225 | 81389.6725  | 84205.73381 | 122256.5924 | 102998.3  | 99837.36385 | 97624.11659 | 25058.43 |
| M_1371 | (2-Heptadecyl-4-methyl-4,5-dihydro-1,3-oxazol-4-yl)methanol                  | C22 H43 N O2     | 353.3289 | 9.923  | 113379.3139 | 181450.9782 | 85726.22028 | 56447.46689 | 17227.8116  | 18964.65823 | 53258.335 | 60605.93756 | 32469.47884 | 11089.35 |
| M_1372 | 907502   | C12 H25 N O2     | 215.1886 | 8.166  | 48049.85759 | 66529.71964 | 78052.35098 | 47125.00543 | 37729.21217 | 66863.75075 | 73107.677 | 153488.428  | 45350.34742 | 13554.65 |
| M_1373 | 6-(1-Azepanyl)-N-(2,3-dimethylphenyl)[1,2,5]oxadiazolo[3,4-b]pyrazin-5-amine | C18 H22 N6 O     | 338.1858 | 8.933  | 189893.8746 | 41325.15094 | 61899.66263 | 61321.63514 | 13169.46352 | 26496.11002 | 20002.541 | 26057.0759  | 35741.84139 | 1633.321 |
| M_1374 | MFC001667459   | C12 H17 N O5     | 255.1105 | 1.585  | 189361.5076 | 23945.84367 | 25665.58692 | 44332.53156 | 21452.28182 | 30951.14643 | 32151.835 | 33808.62835 | 16471.8334  | 2202.686 |
| M_1375 | abacavir 5'-carboxylate  | C14 H16 N6 O2    | 300.1337 | 8.527  | 189097.9598 | 27408.75904 | 31107.50399 | 28388.99279 | 27435.89747 | 38265.14001 | 30167.712 | 33499.33843 | 15133.19543 | 28960.95 |
| M_1376 | Phenoxathiin   | C12 H8 O S       | 200.0296 | 1.141  | 119024.3541 | 119122.9181 | 185147.547  | 117151.6841 | 111447.8766 | 96741.57514 | 68816.512 | 90369.42761 | 100537.1855 | 2055.617 |
| M_1377 | N-Dodecanoyl-L-serine  | C15 H29 N O4     | 287.2096 | 7.123  | 13462.0492  | 31566.06553 | 27261.82244 | 109411.0878 | 76882.9577  | 108753.4853 | 43559.189 | 22862.72087 | 19392.70145 | 1719.44  |
| M_1378 | Octahydro-1,6,7,8-indolizinetetrol   | C8 H15 N O4      | 189.1001 | 1.456  | 6245.234136 | 3424.846884 | 3149.403737 | 3270.409712 | 3010.444112 | 3626.584996 | 5718.1108 | 4357.222806 | 4806.92638  | 1751.792 |
| M_1379 | 3,6-Difluoro-2-methoxyphenol   | C7 H6 F2 O2      | 160.0331 | 1.175  | 185211.0206 | 187870.3329 | 160205.4069 | 78638.59829 | 99475.26116 | 9077.397238 | 11497.154 | 36555.95441 | 28644.99129 | 733.0489 |
| M_1380 | 1792084  | C15 H29 N O3     | 271.2147 | 8.593  | 56061.91708 | 63270.98909 | 75430.21586 | 49643.53944 | 35363.07334 | 62606.99374 | 77780.518 | 105273.2529 | 44488.56947 | 34037.24 |
| M_1381 | Benzyl phenyl sulfide  | C13 H12 S        | 200.0659 | 2.511  | 16527.99107 | 187601.0997 | 36797.07639 | 10719.28357 | 15848.059   | 13327.97018 | 15803.787 | 21718.10639 | 17996.04337 | 2237.777 |
| M_1382 | Arachidonic acid   | C20 H32 O2       | 304.2401 | 10.006 | 166351.5312 | 98368.92784 | 67926.7153  | 88821.26556 | 44056.17026 | 81687.6997  | 56319.072 | 176330.7896 | 60177.4271  | 2144.391 |
| M_1383 | Phenyl N,N'-dibutyl-N,N'-dimethylphosphorodiamidate                          | C16 H29 N2 O2 P  | 312.1978 | 10.385 | 72975.16486 | 87455.64175 | 39275.73565 | 87661.63083 | 51489.45681 | 83834.58323 | 75457.303 | 72242.85449 | 79354.48338 | 18483.54 |
| M_1384 | 3,5-Diamino-N-carbamimidoyl-2-pyrazinecarboxamide                            | C6 H9 N7 O       | 195.0872 | 5.272  | 41104.94827 | 41846.25379 | 60680.40562 | 53292.93646 | 52182.68765 | 57022.29627 | 58191.907 | 91180.27025 | 45339.52847 | 3265.26  |
| M_1385 | 1-(4,6-Diaminopyrimidin-5-yl)guanidine                                       | C5 H9 N7         | 167.0927 | 0.798  | 2934.677564 | 1861.469905 | 1569.307467 | 2506.623073 | 1792.131714 | 1841.012993 | 1718.792  | 1620.234813 | 1436.606092 | 622.3471 |
| M_1386 | 2-Hydroxyquinoline   | C9 H7 N O        | 145.0528 | 7.132  | 22982.44953 | 21730.52928 | 185882.4482 | 23356.77334 | 138188.7121 | 144974.1971 | 42077.31  | 20656.48045 | 2849.095649 | 9777.073 |
| M_1387 | Eicosapentaenoic acid methyl ester   | C21 H32 O2       | 316.2396 | 9.344  | 13560.60797 | 2509.377588 | 58430.5515  | 1847.224868 | 1007.257871 | 138079.6651 | 6387.6915 | 8431.814449 | 15239.8498  | 979.2583 |
| M_1388 | 3-Nitro-1H-1,2,4-triazole-1,5-diamine  | C2 H4 N6 O2      | 144.0398 | 1.142  | 170666.3916 | 102558.3578 | 167631.9777 | 184820.9179 | 110994.0811 | 52371.94789 | 78400.713 | 49151.6765  | 38970.02566 | 5196.349 |
| M_1389 | Dimethyl(pentafluorophenyl)silyl nonadecanoate                               | C27 H43 F5 O2 Si | 522.2948 | 10.212 | 9665.07609  | 93934.86447 | 84495.64067 | 146356.8059 | 12521.00495 | 37473.90965 | 140878.68 | 82607.47977 | 4124.5973   | 2969.864 |
| M_1390 | Nonylthiol   | C9 H20 S         | 160.1292 | 1.415  | 184580.0747 | 96661.38833 | 127871.2089 | 96618.05179 | 52436.68327 | 69611.08914 | 45087.569 | 53015.24648 | 36858.81613 | 3016.727 |
| M_1391 | 2,2'-Bipyridine  | C10 H8 N2        | 156.069  | 3.518  | 150401.2748 | 137404.8305 | 184309.9109 | 105179.442  | 87963.14803 | 79438.6975  | 80006.235 | 88639.36456 | 37088.4964  | 3700.312 |
| M_1392 | 11-Deoxy prostaglandin F1α   | C20 H36 O4       | 362.2453 | 10.118 | 19786.47085 | 10757.8015  | 93961.92857 | 9105.83238  | 105097.0976 | 75574.08352 | 13184.976 | 18214.5816  | 18682.11236 | 8447.352 |
| M_1393 | Uracil   | C4 H4 N2 O2      | 112.0277 | 0.728  | 113253.6089 | 132787.2423 | 129192.8435 | 106188.2175 | 109440.5573 | 118274.0497 | 137005.99 | 146332.2428 | 86148.16449 | 28465.22 |
| M_1394 | Leu-Leu  | C12 H24 N2 O3    | 244.1789 | 3.574  | 3525.678388 | 3888.249396 | 4406.829951 | 6584.269832 | 4847.645652 | 5518.452238 | 6123.1618 | 6043.74391  | 5242.414232 | 2289.588 |
| M_1395 | 2512   | C14 H24 O2       | 224.1768 | 8.743  | 183400.9106 | 5219.418763 | 3532.278731 | 2706.432274 | 4030.494627 | 4249.245649 | 4137.4667 | 4547.530957 | 5318.91844  | 4647.135 |
| M_1396 | Isopentyl cinnamate  | C14 H18 O2       | 218.1306 | 9.096  | 109699.508  | 165519.5731 | 69530.58078 | 152547.5354 | 113132.2684 | 161778.6207 | 166872.98 | 183361.7243 | 126552.0803 | 19743.7  |
| M_1397 | Isothiazole-4-carbonitrile, 5-ethylsulfanyl-3-methoxy-                       | C7 H8 N2 O S2    | 200.0087 | 1.148  | 10628.12775 | 11151.90504 | 42125.51476 | 13405.17998 | 10694.2913  | 10119.38877 | 14711.731 | 15472.95574 | 21782.3344  | 1016.171 |
| M_1398 | Safingol   | C18 H39 N O2     | 301.2981 | 8.046  | 10822.08617 | 30561.4396  | 9477.984063 | 9583.392543 | 29816.87802 | 31729.90528 | 21818.045 | 12851.28577 | 13832.57994 | 3298.202 |
| M_1399 | 2-Butoxy-5-(2,4,4-trimethyl-2-pentanyl)benzenesulfonic acid                  | C18 H30 O4 S     | 342.1872 | 10.045 | 59873.28025 | 71236.72761 | 93970.89351 | 51639.70605 | 100006.2588 | 73443.98971 | 78958.511 | 138244.6095 | 80323.90186 | 3935.677 |
| M_1400 | 2,1,3-Benzoxadiazole-5-carbonitrile 3-oxide                                  | C7 H3 N3 O2      | 161.0229 | 0.789  | 69817.05462 | 52458.42102 | 41013.38067 | 63850.143   | 38152.0839  | 41091.128   | 29302.008 | 30998.35316 | 25051.36416 | 1266.973 |
| M_1401 | O-suberoylcarnitine  | C15 H27 N O6     | 317.1838 | 3.735  | 182507.5445 | 55068.17973 | 37428.44515 | 73598.07702 | 40953.8687  | 26954.57081 | 28640.743 | 31243.21802 | 19794.64892 | 2527.254 |
| M_1402 | 2,2'-Thiobis(3,6-dicyclopentyl-p-cresol)                                     | C34 H46 O2 S     | 518.3209 | 9.877  | 21504.83244 | 133236.5716 | 54403.81524 | 21104.5756  | 84740.12174 | 31829.82732 | 48683.432 | 119808.436  | 7545.95444  | 1790.526 |
| M_1403 | Clofilium  | C21 H36 Cl N     | 337.259  | 8.621  | 7654.992607 | 2337.697066 | 6322.763794 | 3845.988565 | 5906.141277 | 7632.977475 | 5420.7643 | 17326.25635 | 2330.298535 | 2058.974 |
| M_1404 | 2-Nitro-1,3-propanediyl bis(2,2-dimethylpropanoate)                          | C13 H23 N O6     | 289.1524 | 2.266  | 6418.797724 | 133271.7326 | 25793.80366 | 173184.0597 | 53112.68401 | 3401.003873 | 24938.633 | 3019.651018 | 36805.52691 | 3248.459 |
| M_1405 | Glutaric acid  | C5 H8 O4         | 132.0423 | 1.414  | 51031.36976 | 78706.09116 | 33927.74465 | 38475.49971 | 36136.75311 | 80210.72714 | 69609.834 | 49694.5852  | 35224.91874 | 12975.76 |
| M_1406 | 1498   | C10 H21 N O      | 171.1624 | 8.59   | 47100.43712 | 37031.77274 | 50317.16957 | 74080.90819 | 68013.98928 | 89285.27415 | 85591.443 | 181845.4754 | 51042.12647 | 30329.9  |
| M_1407 | 1-(4-tert-butylcyclohex-1-en-1-yl)pyrrolidine                                | C14 H25 N        | 207.1987 | 8.665  | 62630.34969 | 43790.12744 | 98598.53115 | 34562.48726 | 71613.3032  | 146321.6955 | 136173.46 | 103981.3051 | 106104.5472 | 20821.05 |
| M_1408 | 2,2'-Methylenebis(4,6-bis(1,1-dimethylpropyl)phenyl)                         | C33 H52 O2       | 480.3949 | 10.45  | 7764.679419 | 8661.629131 | 8943.418803 | 7360.730557 | 9884.359943 | 8116.827444 | 8249.1696 | 8859.471186 | 7625.70892  | 5260.474 |
| M_1409 | OB4520000  | C10 H9 N O       | 159.0685 | 3.503  | 71754.74293 | 80442.16648 | 59493.4566  | 98018.36093 | 93953.8172  | 134492.8723 | 103431.09 | 160242.464  | 85693.83791 | 4689.092 |
| M_1410 | 3854   | C5 H12 O S       | 120.0613 | 0.807  | 89643.17243 | 29969.60411 | 45621.73703 | 57878.01033 | 56115.77017 | 62872.11758 | 60380.39  | 61828.0069  | 41365.75684 | 1976.792 |
| M_1411 | 2-Methyl-2-propanyl(2,4,6-triamino-5-pyrimidinyl)carbamate                   | C9 H16 N6 O2     | 240.1341 | 8.17   | 7852.330528 | 2160.247217 | 2217.995666 | 7106.425194 | 6148.078858 | 80352.1626  | 9968.3897 | 4819.579805 | 2868.755958 | 2906.975 |
| M_1412 | N-Boc-3-Pyrrolidinone  | C9 H15 N O3      | 185.1052 | 7.007  | 13130.76311 | 114522.1084 | 66860.44947 | 33190.86989 | 44716.43865 | 52894.43752 | 22680.236 | 31513.82065 | 17284.82671 | 11178.09 |



|        |   |                    |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|--------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1413 | 3,4-Diethoxyphenylacetic acid   | C12 H16 O4         | 224.1052 | 7.799  | 6019.733727 | 4816.185909 | 4782.580209 | 5058.378117 | 7006.288239 | 6896.592137 | 5721.7511 | 5146.770658 | 5419.1977   | 6780.672 |
| M_1414 | DO0750000   | C15 H24 O2         | 236.1776 | 9.192  | 32566.99101 | 18476.52367 | 26795.85277 | 23947.98214 | 20239.07791 | 24901.17286 | 47829.27  | 30831.15397 | 38247.10417 | 20614.7  |
| M_1415 | Pyrazine, (chloromethyl)-   | C4 H3 Cl N4 O2     | 173.9945 | 2.433  | 23659.86984 | 14316.98259 | 22253.50067 | 15472.40058 | 13263.09599 | 15712.60759 | 15509.549 | 13938.67068 | 11762.51509 | 5955.456 |
| M_1416 | 1-Benzosuberone   | C11 H12 O          | 160.0889 | 8.766  | 112280.128  | 91546.74455 | 70395.60587 | 73221.04211 | 85205.04064 | 145775.5942 | 97230.385 | 125195.8866 | 82932.99817 | 17097.68 |
| M_1417 | BRD32048  | C16 H22 N6 O       | 314.1855 | 8.922  | 7209.807677 | 10805.2184  | 5357.652864 | 15361.64178 | 16963.42823 | 12076.22612 | 8339.9015 | 24111.39755 | 5696.361492 | 5427.726 |
| M_1418 | 13-Hydroxyoctadecadienoic acid  | C18 H32 O3         | 296.2349 | 9.146  | 42879.31437 | 57064.92702 | 27276.87418 | 65934.53836 | 48660.26473 | 47947.65429 | 52676.963 | 32757.45423 | 44508.00176 | 5605.519 |
| M_1419 | 4149853   | C21 H41 N O4       | 371.3034 | 9.645  | 3955.846824 | 70824.33543 | 56609.10113 | 41114.26566 | 179664.1034 | 91446.69594 | 62614.763 | 951.7586222 | 79186.96538 | 3403.355 |
| M_1420 | 4-Aminopyrazolo[5,1-c][1,2,4]triazine-3-carbonitrile  | C6 H4 N6           | 160.0494 | 10.656 | 179506.5915 | 28623.15685 | 9338.692768 | 14245.60441 | 7962.192957 | 6140.343853 | 6983.9899 | 96522.33545 | 5578.481744 | 9385.894 |
| M_1421 | 3,6-Dihydro-1H-[1,2,5]oxadiazolo[3,4-b][1,2,3]triazolo[4,5-e]pyrazine   | C4 H3 N7 O         | 165.0403 | 2.872  | 110221.2723 | 3552.354266 | 4009.891696 | 850.1285926 | 3510.853696 | 23039.28379 | 8972.4276 | 19713.72608 | 10339.40597 | 5052.798 |
| M_1422 | Paracetamol   | C8 H9 N O2         | 151.0634 | 7.25   | 18007.94649 | 30284.67747 | 26768.77951 | 30402.79407 | 6018.001806 | 30974.30213 | 3692.2904 | 3155.602615 | 24044.07601 | 6940.414 |
| M_1423 | 2616  | C12 H19 N O3       | 225.1365 | 6.58   | 6891.707502 | 13628.70745 | 2482.35633  | 26209.09643 | 8050.691045 | 22105.09686 | 16082.136 | 13754.91195 | 11092.94327 | 2440.54  |
| M_1424 | Decanoylcarnitine   | C17 H33 N O4       | 315.241  | 7.635  | 89677.40252 | 17547.95564 | 9325.183422 | 49522.52723 | 45891.70376 | 93437.37152 | 30171.703 | 31623.94169 | 18127.19957 | 2711.013 |
| M_1425 | 5-Hydroxy-DL-tryptophan   | C11 H12 N2 O3      | 220.0847 | 1.238  | 82031.33657 | 96137.23426 | 65827.11543 | 178075.514  | 116937.5914 | 151200.5535 | 117426.66 | 89048.16959 | 139023.5598 | 2563.091 |
| M_1426 | n-hexyl-1h-purin-6-amine  | C11 H17 N5         | 219.149  | 7.952  | 177989.2534 | 12955.61453 | 24984.2233  | 29899.13347 | 21820.22846 | 24337.17334 | 21544.295 | 30911.97932 | 24306.56174 | 1807.449 |
| M_1427 | DL-Glutamine  | C5 H10 N2 O3       | 146.0691 | 1.012  | 6713.202984 | 54218.19787 | 4312.114971 | 4359.018822 | 4329.717287 | 61675.88112 | 4264.7684 | 58533.27792 | 4928.770037 | 9988.62  |
| M_1428 | Trimethoprim  | C14 H18 N4 O3      | 290.1341 | 3.397  | 7685.826225 | 6973.97796  | 7895.364807 | 8516.781989 | 7215.010315 | 7853.562252 | 9757.8569 | 11899.82726 | 8333.89586  | 3707.621 |
| M_1429 | DL-Carbidopa  | C10 H14 N2 O4      | 226.0954 | 2.975  | 176714.2846 | 64934.5516  | 103893.453  | 47261.05455 | 40642.7364  | 18380.99222 | 10416.957 | 9634.286821 | 6539.919177 | 7105.679 |
| M_1430 | 2,2'-(1H-1,2,4-Triazole-3,5-diyl)dipyrazine   | C10 H7 N7          | 225.0766 | 1.859  | 11625.32835 | 39717.19239 | 41715.17047 | 27400.76698 | 23842.04545 | 78526.95664 | 37885.513 | 38089.93312 | 26601.87364 | 7643.32  |
| M_1431 | Boc-Pro-Pro   | C15 H24 N2 O5      | 312.1672 | 8.453  | 39073.02125 | 54037.9189  | 53141.31266 | 66512.46147 | 68891.5385  | 84504.65332 | 63034.699 | 83675.03101 | 67121.67564 | 3952.743 |
| M_1432 | 1',3'-Dimethyl-1,4':5',1''-terimidazolidine-2,2',2''-trione   | C11 H18 N6 O3      | 282.145  | 7.443  | 13433.32582 | 1665.784419 | 9799.271319 | 2166.011257 | 30893.74115 | 32043.00858 | 13243.486 | 16876.89957 | 12312.58152 | 27949.25 |
| M_1433 | 2,7-Dimethoxynaphthalene  | C12 H12 O2         | 188.0838 | 8.141  | 153521.2494 | 71207.75299 | 52717.51527 | 106758.4565 | 129500.2229 | 175996.3589 | 129079.94 | 150364.3733 | 96924.66074 | 5489.846 |
| M_1434 | N-1H-Tetrazol-5-yl-Guanidine  | C2 H5 N7           | 127.0613 | 0.952  | 6724.302623 | 6694.002562 | 6748.313886 | 6571.563644 | 6705.550725 | 6572.770414 | 6621.6653 | 6677.600563 | 6724.890147 | 3124.064 |
| M_1435 | L-Histidine   | C6 H9 N3 O2        | 155.0696 | 1.4    | 32197.77641 | 38244.59925 | 15996.70258 | 33846.16296 | 37007.48801 | 27334.36587 | 32608.392 | 60517.16237 | 35411.5204  | 881.145  |
| M_1436 | [[[2R,3R,4R,5S,6R]-3-acetamido-5-[[[2S,3R,4R,5S,6R]-3-acetamido-4-hydroxy-6-(hydroxymethyl)-5-[[[(2R)-2-hydroxy-3-oxido-[[2S,3R,4R)-2,3,4,5-tetrahydroxypentoxyl]phosphoryl]oxypropoxy]-oxido-phosphoryl]oxytetrahydropyran-2-yl]oxy-4-hydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxido-[[[2Z,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetrate tracontane-2,6,10,14,18,22,26,30,34,38,42-undecaenoxy]phosphoryl] phosphate | C79 H132 N2 O29 P4 | 1696.783 | 4.617  | 17857.99828 | 21828.95314 | 10247.7559  | 38346.38369 | 34459.85051 | 122727.7191 | 52331.323 | 102766.5093 | 53585.91862 | 1760.863 |
| M_1437 | PYRIDOXAMINE  | C8 H12 N2 O2       | 168.09   | 2.91   | 37652.53482 | 75581.71206 | 78102.58761 | 46628.99588 | 44037.29651 | 55071.07781 | 31419.012 | 20605.82488 | 29027.34627 | 4673.194 |
| M_1438 | Oleic acid  | C18 H34 O2         | 282.2558 | 10.535 | 53021.84648 | 49240.48914 | 6108.060019 | 22342.79907 | 29051.25507 | 51043.37662 | 46339.995 | 56379.53023 | 70029.777   | 5393.997 |
| M_1439 | 6132055   | C19 H36 O3         | 312.2665 | 8.889  | 34230.26844 | 2679.553025 | 29834.34508 | 27366.8635  | 33513.89842 | 173946.189  | 37738.402 | 37661.96539 | 42380.40595 | 30005.78 |
| M_1440 | DL-Cerulenin  | C12 H17 N O3       | 223.1198 | 1.56   | 42818.97005 | 27779.26286 | 26882.26659 | 25502.48466 | 24667.51288 | 29471.12618 | 32589.708 | 32539.59055 | 173089.1861 | 16064.32 |
| M_1441 | Capsi-amide   | C17 H35 N O        | 269.2717 | 9.283  | 125539.1944 | 111455.8745 | 156432.2773 | 100613.8943 | 152624.2503 | 122200.9342 | 111874.79 | 140526.0851 | 154925.7673 | 6892.812 |
| M_1442 | 1,2-Diphosphocine   | C6 H6 P2           | 139.995  | 0.813  | 12309.32609 | 14126.86828 | 172631.5752 | 1871.704952 | 9497.293617 | 9546.284287 | 161251.08 | 15182.4303  | 4744.660352 | 16629.36 |
| M_1443 | hodgkinsine   | C33 H38 N6         | 518.3177 | 10.75  | 14765.34772 | 22920.82595 | 34272.40421 | 24425.87468 | 30057.23375 | 172563.5946 | 5504.0139 | 7588.616113 | 6047.035963 | 5995.76  |
| M_1444 | 7098783   | C14 H18 N2 O4      | 278.1266 | 6.371  | 2489.140596 | 7234.68941  | 11796.37537 | 5317.476109 | 2168.765849 | 2798.901722 | 3654.344  | 2264.188974 | 2394.713048 | 2146.603 |
| M_1445 | 1,1-Dichloro-4-methyl-1,3-pentadiene  | C6 H8 Cl2          | 150.0009 | 10.909 | 5823.248519 | 45862.01934 | 44394.57306 | 45512.33738 | 38181.92981 | 15189.31647 | 48207.368 | 43608.52248 | 10221.67821 | 14032.85 |
| M_1446 | 7,8,9,10-Tetrahydrobenzo[b]naphtho[2,3-d]thiophene  | C16 H14 S          | 238.0817 | 11.471 | 157899.4644 | 11303.21079 | 11663.39604 | 15827.18735 | 13660.23352 | 12074.22926 | 13674.473 | 11934.49792 | 14877.61296 | 12457.44 |
| M_1447 | Octahydro-1,2,8-indolizinetriol   | C8 H15 N O3        | 173.1053 | 6.433  | 170910.6266 | 57692.10529 | 57457.25919 | 62634.73651 | 43646.79911 | 42978.67761 | 33890.984 | 35632.89349 | 26818.6603  | 2151.567 |
| M_1448 | val-val-ile-ala   | C19 H36 N4 O5      | 400.2687 | 6.502  | 1593.488709 | 1559.414667 | 1512.535737 | 1499.351194 | 1514.53546  | 1576.589473 | 1655.7749 | 1598.24289  | 1531.090147 | 1453.941 |

|        |  |                     |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|---------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1449 | 2-(2-(4-Nonylphenoxy)ethoxy)ethanol  | C19 H32 O3          | 308.2348 | 8.993  | 2859.79115  | 8245.708047 | 9114.228441 | 12499.99625 | 4658.874085 | 7969.079482 | 11245.457 | 9620.437375 | 3658.290268 | 10283.77 |
| M_1450 | (Dimethylamino)methyl dimethylcarbamodithioate   | C6 H14 N2 S2        | 178.0606 | 3.864  | 32362.1972  | 22203.6604  | 45425.08975 | 37772.53538 | 34374.54083 | 32970.56262 | 65501.97  | 33414.73403 | 52949.66041 | 5007.214 |
| M_1451 | LysoPC(22:1(13Z))  | C30 H60 N O7 P      | 577.4108 | 10.507 | 170165.1442 | 20293.76356 | 2393.851531 | 28794.48896 | 70703.97281 | 77703.34373 | 98103.531 | 118577.8233 | 65104.40261 | 3096.01  |
| M_1452 | Benzyl vinyl ether   | C9 H10 O            | 134.0733 | 8.714  | 22779.73389 | 37476.04938 | 36202.76592 | 44339.62555 | 41871.69529 | 42706.88013 | 4570.5965 | 37450.77608 | 51411.34559 | 16681.85 |
| M_1453 | 2,2,2-Trichloroethyl 3-[2-(bromomethyl)-4-chloro-1,3-oxazol-5-yl]-2-chloro-1H-indole-1-carboxylate | C15 H8 Br Cl5 N2 O3 | 517.8164 | 10.207 | 51597.88114 | 96596.76414 | 114355.0295 | 56880.2862  | 112599.7894 | 109354.3008 | 103160.36 | 99042.83622 | 85187.56835 | 6247.515 |
| M_1454 | DIETHYLENE GLYCOL PALMITATE  | C20 H40 O4          | 344.2926 | 10.125 | 169431.0046 | 127277.2749 | 87606.88976 | 78566.53666 | 141456.2388 | 99848.70472 | 106127.31 | 94927.9445  | 72381.51453 | 6692.888 |
| M_1455 | Phenolate  | C6 H5 O             | 93.03463 | 8.664  | 34126.84465 | 23004.0613  | 45981.22223 | 49975.82664 | 12240.84928 | 59189.56878 | 51356.084 | 49054.79087 | 29331.61752 | 26492.28 |
| M_1456 | 1,1,1-Trifluoroacetone   | C3 H3 F3 O          | 112.0141 | 1.245  | 6066.8281   | 4619.988615 | 16357.78868 | 5972.647006 | 5740.79126  | 18464.77562 | 12114.213 | 58903.90669 | 12678.21253 | 643.4109 |
| M_1457 | Norharman  | C11 H8 N2           | 168.0689 | 4.009  | 3262.725989 | 2374.064375 | 2393.406882 | 2447.046334 | 2470.058467 | 2463.180938 | 2440.4398 | 2416.027073 | 2432.793919 | 2436.195 |
| M_1458 | Nonanoylmorpholine   | C13 H25 N O2        | 227.1886 | 10.229 | 56798.93048 | 83642.74036 | 62880.3743  | 55520.85764 | 27341.03967 | 34470.46813 | 27212.736 | 94536.0468  | 29874.50783 | 3355.118 |
| M_1459 | TX-1041  | C4 H6 N6 O          | 154.0605 | 5.511  | 159661.0231 | 130975.1473 | 78195.86676 | 167902.4948 | 69993.56547 | 99759.34455 | 110734.58 | 102944.2273 | 101654.8679 | 3036.617 |
| M_1460 | ARECOLINE  | C8 H13 N O2         | 155.0947 | 6.743  | 167614.0812 | 6469.657147 | 7462.040516 | 44404.97579 | 30460.31077 | 36293.24308 | 39837.777 | 13115.79726 | 11102.80469 | 2700.464 |
| M_1461 | 2-(((Acetylcarbamoyloxy)methyl)-2,3-dimethylbutyl acetylcarbamate                                  | C13 H22 N2 O6       | 302.1493 | 8.583  | 167380.8145 | 20997.21371 | 50313.47936 | 19489.07691 | 41042.04387 | 64203.63563 | 28792.321 | 35892.6289  | 34094.47325 | 21290.15 |
| M_1462 | Ethyl 4-Quinazoline-2-carboxylate  | C11 H10 N2 O3       | 218.0691 | 1.549  | 58742.05293 | 112538.8937 | 124126.849  | 92567.68163 | 96853.95208 | 99410.1243  | 66690.914 | 92534.74271 | 74368.74714 | 3671.384 |
| M_1463 | 2616   | C12 H19 N O3        | 225.1364 | 6.881  | 2192.650004 | 2234.551449 | 2347.379737 | 3537.62642  | 2300.121151 | 2198.411569 | 2228.3458 | 2604.081177 | 2218.017969 | 2071.432 |
| M_1464 | Triethylamine  | C6 H15 N            | 101.121  | 0.598  | 8882.895409 | 10084.43123 | 9716.155242 | 11827.25229 | 8731.413645 | 11217.25613 | 9166.8042 | 8529.747641 | 5738.371352 | 4482.333 |
| M_1465 | 4,6-Di(1-piperidinyl)-1,3,5-triazine-2-carbonitrile  | C14 H20 N6          | 272.1752 | 9.079  | 17895.53231 | 59415.68201 | 102885.7578 | 97403.14709 | 79889.95969 | 61941.74743 | 65323.011 | 19330.71643 | 135020.7167 | 5984.427 |
| M_1466 | MFCD00041564   | C11 H22 O3          | 202.1566 | 8.797  | 47487.20781 | 110192.9819 | 97277.30238 | 113349.2857 | 72523.50214 | 138253.3816 | 110744.06 | 112133.2051 | 166954.4465 | 6377.768 |
| M_1467 | 2512   | C14 H24 O2          | 224.1775 | 8.979  | 166752.1224 | 39306.77645 | 31799.14443 | 44109.68819 | 44515.3483  | 44611.74288 | 4241.7755 | 43980.63062 | 41659.52729 | 3564.763 |
| M_1468 | 5-(4-Methylphenyl)-1,3-cyclohexanedione  | C13 H14 O2          | 202.0994 | 8.763  | 44459.23017 | 85971.06765 | 90863.22946 | 87815.78115 | 107495.8751 | 150640.8525 | 155528.07 | 123819.9887 | 98823.43139 | 6919.706 |
| M_1469 | MFCD00029794   | C22 H41 N O3        | 367.3084 | 9.312  | 29901.43263 | 116864.4249 | 40025.4418  | 54044.30601 | 11679.23392 | 46042.52567 | 85926.341 | 53418.52084 | 38008.21482 | 7162.118 |
| M_1470 | 3-Methoxy-23,26-epoxylanosta-7,24-dien-26-one  | C31 H48 O3          | 468.3583 | 9.6    | 24740.08603 | 4960.717217 | 4838.773346 | 5861.109898 | 4973.275933 | 5608.355527 | 5018.6729 | 4707.677829 | 4902.964254 | 6066.887 |
| M_1471 | 1422990  | C9 H19 N O2         | 173.1417 | 1.207  | 13852.55673 | 13225.61202 | 13404.12265 | 14022.12382 | 11161.65688 | 12294.09959 | 12151.105 | 12572.43455 | 10500.14682 | 1252.494 |
| M_1472 | 2-Hydroxyquinoline   | C9 H7 N O           | 145.0528 | 6.338  | 140749.0602 | 46699.30101 | 79210.53959 | 111142.9842 | 24927.72492 | 29634.88009 | 18075.848 | 40673.14589 | 36371.27756 | 3435.852 |
| M_1473 | 1-(4-Nitrophenyl)piperidine  | C11 H14 N2 O2       | 206.1055 | 2.163  | 28221.5138  | 20659.21619 | 4091.782764 | 3269.565566 | 5610.480583 | 131071.5742 | 34385.298 | 43175.463   | 22656.66177 | 3055.975 |
| M_1474 | 5,5'-(1,3-Propanediyl)bis(1H-1,2,4-triazol-3-amine)  | C7 H12 N8           | 208.1187 | 4.767  | 34676.60322 | 44364.98483 | 37279.5706  | 44531.27967 | 32976.94482 | 69932.33745 | 29131.214 | 44801.73767 | 35930.59035 | 2683.672 |
| M_1475 | benzyl phenyl sulfone  | C13 H12 O2 S        | 232.0559 | 1.137  | 112234.3129 | 110864.1047 | 157651.0046 | 97315.75614 | 84632.87495 | 56604.89957 | 52036.021 | 66670.67202 | 91230.44303 | 1468.645 |
| M_1476 | DL-Lysine  | C6 H14 N2 O2        | 146.1055 | 1.865  | 163200.7155 | 32462.96719 | 32955.46453 | 51056.92112 | 27463.92214 | 31271.2791  | 29776.934 | 28326.50101 | 19698.6549  | 4638.06  |
| M_1477 | Indole-3-lactic acid   | C11 H11 N O3        | 205.0739 | 5.127  | 7248.123074 | 8932.29552  | 12667.8395  | 8273.846186 | 5011.911987 | 6082.389604 | 6442.4876 | 13039.36318 | 6425.008529 | 6377.247 |
| M_1478 | 4-Nitrophenyl caprate  | C16 H23 N O4        | 293.1627 | 4.45   | 3569.455409 | 13111.06242 | 11578.2236  | 28420.77792 | 18273.66778 | 33634.54443 | 28680.058 | 2606.236846 | 2509.348356 | 2237.638 |
| M_1479 | 2-Asn-OH   | C12 H14 N2 O5       | 266.0902 | 5.158  | 162342.8937 | 4457.521146 | 20027.56944 | 8059.868608 | 1856.999334 | 1810.252419 | 1814.8502 | 1972.108583 | 1845.975337 | 1864.455 |
| M_1480 | Nicotinic acid   | C8 H8 N2 O3         | 180.0535 | 4.603  | 162188.9733 | 11790.52576 | 49709.56247 | 7324.264656 | 904.4428619 | 1907.812219 | 916.54461 | 2807.585245 | 2103.895912 | 2032.468 |
| M_1481 | 4,4'-Methylenebis[2-tert-butyl-6-(alpha-methylbenzyl)phenol  | C37 H44 O2          | 520.3363 | 9.271  | 736.5134663 | 3536.588366 | 4838.372919 | 4270.133664 | 5313.227942 | 10532.11752 | 13379.197 | 8903.34272  | 3959.314005 | 24915.04 |
| M_1482 | Desmethylmisonidazole  | C6 H9 N3 O4         | 187.0595 | 1.92   | 11817.55647 | 7904.300326 | 7240.150362 | 7952.792718 | 6662.227644 | 6887.382574 | 6150.6945 | 6780.046338 | 5683.849628 | 7510.151 |
| M_1483 | Ethyl [2-methyl-4-(1-piperidinylmethyl)-1,3-dioxolan-2-yl]acetate                                  | C14 H25 N O4        | 271.1783 | 8.668  | 153256.1821 | 95717.70504 | 52799.09952 | 161794.806  | 35214.34134 | 50538.31129 | 41553.894 | 67176.58261 | 31778.17771 | 6602.88  |
| M_1484 | Clofilium  | C21 H36 Cl N        | 337.2593 | 8.639  | 7654.992607 | 2001.702055 | 6322.763794 | 3845.988565 | 5486.807573 | 7632.977475 | 5420.7643 | 7633.127522 | 2537.287434 | 1855.923 |
| M_1485 | 2491   | C5 H6 O2            | 98.03728 | 0.597  | 16358.64675 | 11523.81228 | 131590.048  | 16906.99088 | 7681.522719 | 11673.94978 | 21734.141 | 26184.8119  | 17121.67097 | 27731.78 |
| M_1486 | MFCD00002731   | C12 H21 N O2        | 211.1572 | 8.108  | 38096.23051 | 43267.48964 | 36623.43942 | 33929.15433 | 33718.59938 | 6405.980776 | 50422.473 | 90892.24733 | 37951.96914 | 8773.45  |
| M_1487 | methylthiomethyl lithium   | C2 H5 Li S          | 68.02703 | 1.152  | 14116.04814 | 5031.979219 | 45506.67958 | 13222.72713 | 20185.92802 | 116183.2229 | 80549.638 | 61971.51219 | 11597.86535 | 3886.408 |
| M_1488 | DPTH   | C15 H12 N2 O S      | 268.0671 | 1.219  | 160084.871  | 49990.61014 | 83856.99739 | 46624.33386 | 88057.1644  | 28689.1892  | 29266.327 | 35566.36518 | 30627.07778 | 1027.674 |
| M_1489 | Deferiprone  | C7 H9 N O2          | 139.0634 | 3.041  | 159910.0468 | 15427.68522 | 21394.31209 | 2240.131386 | 2083.093513 | 13085.37954 | 11186.544 | 10932.888   | 9991.326518 | 2233.701 |
| M_1490 | 1-Carboxy-4-aminopiperidine  | C8 H16 N2 O2        | 172.1212 | 2.83   | 22777.43491 | 47746.61419 | 41474.91838 | 81513.91103 | 26154.49712 | 54738.46168 | 32762.187 | 35605.90853 | 55689.86938 | 4655.215 |
| M_1491 | Indole-3-carbidol  | C9 H9 N O           | 147.0685 | 7.404  | 3033.33393  | 4577.670911 | 37762.08291 | 6580.515776 | 13648.43518 | 26106.26607 | 17176.751 | 7813.577829 | 3515.643545 | 4612.199 |
| M_1492 | Bis[(2-isopropyl-5-methylcyclohexyl)oxy][2-methoxyphenyl]phenylsilane                              | C33 H50 O3 Si       | 522.3517 | 10.333 | 25743.54762 | 70901.54102 | 35849.10884 | 23881.77448 | 75698.10475 | 105290.8873 | 143689.27 | 116272.0044 | 77641.62    | 1004.06  |
| M_1493 | GX1529000  | C7 H15 N            | 113.1209 | 8.125  | 103234.7584 | 35174.93209 | 28871.77095 | 74311.1249  | 53157.01158 | 69039.8312  | 48707.146 | 54340.44969 | 23964.13348 | 3408.029 |
| M_1494 | 5-Hydroxy-DL-tryptophan  | C11 H12 N2 O3       | 220.0848 | 3.514  | 69720.86317 | 63886.58444 | 110852.874  | 122300.0001 | 95503.16948 | 152339.8961 | 158212.84 | 148367.7857 | 133222.2895 | 3366.987 |
| M_1495 | 4-Morpholinylacetic acid   | C6 H11 N O3         | 145.074  | 1.132  | 157987.2819 | 86403.72775 | 64473.10127 | 80769.97268 | 75685.37042 | 53853.75111 | 51194.449 | 52912.26249 | 31372.28231 | 10183.53 |

|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1496 | 2-Methyl-2-propanyl N-((benzyloxy)carbonyl)leucyl-O-benzilyltyrosinate               | C34 H42 N2 O6   | 574.3044 | 9.828  | 1167.167014 | 6232.376821 | 5894.861609 | 2252.147744 | 4415.024485 | 11150.82528 | 10167.615 | 5997.272075 | 6685.351972 | 1084.107 |
| M_1497 | butanethiol  | C4 H10 S        | 90.05069 | 0.74   | 107174.0953 | 86669.11003 | 132862.2117 | 132519.414  | 81533.42511 | 76006.72567 | 107565.08 | 104506.0599 | 102569.8803 | 14687.89 |
| M_1498 | 1-Boc-4-piperidinol  | C10 H19 N O3    | 201.1365 | 6.906  | 18043.03214 | 14443.80222 | 26080.7554  | 23422.39352 | 20493.80815 | 30490.98273 | 24153.006 | 29315.37468 | 16645.40411 | 10308.03 |
| M_1499 | 2,4-Bis(dimethylamino)-6-nitro-1,3,5-triazine  | C7 H12 N6 O2    | 212.1028 | 7.55   | 520.7869404 | 550.6333377 | 13704.55221 | 502.4589392 | 47353.05496 | 44759.2284  | 6475.4831 | 30474.93532 | 439.6446971 | 25478.07 |
| M_1500 | 1-[(Boc)amino]cyclopanecarboxylic acid   | C9 H15 N O4     | 201.1    | 3.316  | 157187.2097 | 137025.7177 | 138929.9341 | 106525.0141 | 65689.59615 | 56214.56445 | 42747.484 | 29684.17893 | 24045.77968 | 3442.186 |
| M_1501 | 3-Phenylpyrazole-4-carbaldehyde  | C10 H8 N2 O     | 172.0637 | 2.005  | 9347.766073 | 5965.909708 | 5700.114502 | 6679.646756 | 5220.116147 | 6390.748511 | 6307.4403 | 7017.241236 | 4646.502313 | 6072.322 |
| M_1502 | 2-Heptadecyl 1-isobutyl 1,2-pyrrolidinedicarboxylate                                 | C27 H51 N O4    | 453.382  | 8.513  | 119514.3819 | 23449.18911 | 4636.51658  | 156743.9559 | 27235.26635 | 65804.19765 | 54354.356 | 35539.97589 | 15474.60891 | 4026.505 |
| M_1503 | TRIS(HYDROXYETHYL)AMINOMETHANE   | C7 H17 N O3     | 163.121  | 0.955  | 28278.17603 | 156020.9203 | 87732.86166 | 42076.11821 | 56931.91827 | 58859.20479 | 5540.6137 | 116010.3632 | 65504.61536 | 1737.378 |
| M_1504 | 4-Aminopyrazolo[5,1-c][1,2,4]triazine-3-carboxohydrazide                             | C6 H7 N7 O      | 193.0715 | 3.66   | 3406.529915 | 4150.158188 | 5209.459888 | 3373.761949 | 3702.271728 | 3345.100236 | 3294.9738 | 3228.599926 | 3088.071289 | 3124.77  |
| M_1505 | 4-((2-oxohexadecanoyl)amino)butanoic acid  | C20 H37 N O4    | 355.2722 | 7.905  | 155503.3048 | 6778.350916 | 3817.188568 | 11118.48639 | 9013.319033 | 17016.34172 | 13830.763 | 16718.2355  | 6640.372734 | 2521.659 |
| M_1506 | Ethosuximide   | C7 H11 N O2     | 141.0791 | 1.457  | 81881.64445 | 59313.98005 | 45430.23169 | 82538.88338 | 104614.015  | 47310.51233 | 39498.087 | 66505.53032 | 15168.67765 | 9016.494 |
| M_1507 | Icaridin   | C12 H23 N O3    | 229.1679 | 6.781  | 10249.22306 | 14722.94363 | 9231.057117 | 2671.325271 | 10426.75288 | 11340.72206 | 9502.0441 | 2803.043933 | 9925.112223 | 11727.76 |
| M_1508 | uronium  | C H5 N2 O       | 61.0395  | 1.204  | 98956.76749 | 153623.5143 | 98927.33695 | 31096.61444 | 154312.0285 | 76815.03079 | 45284.786 | 63606.06971 | 100300.1259 | 1671.194 |
| M_1509 | N,N'-Diheptyl-3-hydroxy-N,N'-dimethylpentanediamide                                  | C21 H42 N2 O3   | 370.3195 | 9.07   | 6626.273474 | 7012.706883 | 10337.97108 | 10667.58365 | 13320.33069 | 7099.621171 | 4440.6835 | 81035.74433 | 5902.479279 | 6732.57  |
| M_1510 | N,pi.-Methyl-L-histidine   | C7 H11 N3 O2    | 169.0852 | 1.396  | 25406.22903 | 37817.12879 | 12048.47852 | 51982.09259 | 39816.47622 | 152279.7104 | 9320.9551 | 110180.1844 | 5138.948973 | 639.8196 |
| M_1511 | Glycylglycylglycine  | C6 H11 N3 O4    | 189.0749 | 1.818  | 95699.39428 | 106266.8296 | 40614.83632 | 66513.80264 | 41184.38692 | 54206.09814 | 46296.898 | 53654.54771 | 48322.92644 | 4464.794 |
| M_1512 | 5L4860000  | C13 H20 O2      | 208.1467 | 8.097  | 29579.33036 | 8579.157817 | 10539.27676 | 7558.150182 | 13745.42352 | 22971.95228 | 10520.922 | 32996.52033 | 17126.33695 | 12274.91 |
| M_1513 | 4,4'-(1-Methyl-1H-1,2,4-triazole-3,5-diyl)bis(1,2,5-oxadiazol-3-amine)               | C7 H7 N9 O2     | 249.0725 | 1.104  | 72932.21813 | 59569.13049 | 153137.2449 | 67174.58282 | 99923.64611 | 60743.33637 | 59822.423 | 92348.5579  | 58478.39292 | 928.3493 |
| M_1514 | (E)-Dacarbazine  | C6 H10 N6 O     | 182.0916 | 5.508  | 4455.151714 | 21145.22945 | 152665.8408 | 51618.61622 | 18526.63326 | 26995.44602 | 24583.663 | 25948.47183 | 23912.41409 | 2427.148 |
| M_1515 | 7-Methoxy-3-(tetrahydro-2H-pyran-2-yloxy)crinan-1-ol                                 | C22 H29 N O6    | 403.1997 | 8.325  | 89082.59584 | 56651.01118 | 93728.69135 | 72088.08404 | 98666.48974 | 129719.5036 | 130938.96 | 113467.445  | 110300.1199 | 13222.73 |
| M_1516 | CM0120000  | C9 H15 N O      | 153.1154 | 4.701  | 4468.47413  | 3186.125676 | 3038.192811 | 3031.795347 | 2941.78063  | 3492.021    | 2952.6644 | 4108.451739 | 3440.770247 | 2904.526 |
| M_1517 | 3420   | C13 H18 O       | 190.1358 | 8.568  | 37024.85382 | 29732.21792 | 28259.80381 | 21952.67288 | 34488.39711 | 38496.40139 | 24239.678 | 36700.15472 | 35397.77072 | 14590.92 |
| M_1518 | 3-Carboxylato-1,3,5-trideoxy-5-(trimethylammonio)pent-2-ulose                        | C9 H17 N O4     | 203.1158 | 7.222  | 35303.03941 | 40831.56778 | 84918.46206 | 55658.08598 | 24640.57558 | 60195.79568 | 10807.928 | 7825.142477 | 8593.303076 | 2582.832 |
| M_1519 | 5-Indolol  | C8 H7 N O       | 133.0529 | 8.33   | 151684.9975 | 38203.00154 | 81780.85495 | 78242.32573 | 40040.93982 | 33439.02507 | 29485.885 | 10479.44361 | 7237.61083  | 5560.533 |
| M_1520 | 3-(5,6-Dimethoxy-2-methyl-1,3-benzothiazol-3-ium-3-yl)-1-propanesulfonate            | C13 H17 N O5 S2 | 331.0536 | 5.012  | 28453.34214 | 6542.491321 | 4317.155254 | 8508.817949 | 3713.38903  | 1749.04161  | 1681.5043 | 1078.844127 | 1746.626155 | 1676.876 |
| M_1521 | S-(2-Hydroxyethyl)glutathione  | C12 H21 N3 O7 S | 351.1115 | 8.564  | 151475.9673 | 33836.12058 | 87363.81508 | 7648.763376 | 16359.66014 | 19689.10754 | 25253.782 | 28223.56009 | 12635.02795 | 11384.33 |
| M_1522 | Lauro lactam   | C12 H23 N O     | 197.178  | 8.754  | 63949.30943 | 38586.3929  | 104922.3071 | 109924.9503 | 78434.15048 | 122060.6232 | 108929.41 | 150970.9581 | 104507.1434 | 6686.375 |
| M_1523 | Elaidolinolenic acid   | C18 H30 O2      | 278.2244 | 9.748  | 51343.64213 | 8775.156112 | 41041.56527 | 19705.41869 | 19217.64389 | 22830.61238 | 48951.423 | 49764.39603 | 23794.30511 | 1867.532 |
| M_1524 | S-(tert-Butyl) 2-tert-butyl-4-(1-hydroxy-1-phenylethyl)-1,3-dioxolane-4-carbothioate | C20 H30 O4 S    | 366.1871 | 10.019 | 143223.1499 | 61878.88319 | 39414.68138 | 44427.64247 | 74090.29581 | 76101.76362 | 61347.558 | 95778.72129 | 70869.69458 | 4486.315 |
| M_1525 | 5,5'-methylenebis(1H-benzotriazole)  | C13 H10 N6      | 250.0953 | 1.551  | 51866.10289 | 90643.2773  | 70473.80524 | 78531.01753 | 75314.96164 | 83584.35315 | 53124.007 | 60658.27345 | 58912.10527 | 2234.087 |
| M_1526 | leu-leu-asp  | C16 H29 N3 O6   | 359.2055 | 5.909  | 875.1971626 | 853.0707897 | 854.1059641 | 1049.779786 | 834.4206334 | 893.5778137 | 818.19559 | 1716.398707 | 771.6789601 | 772.6529 |
| M_1527 | N,pi.-Methyl-L-histidine   | C7 H11 N3 O2    | 169.085  | 1.254  | 149093.6662 | 4130.679411 | 22609.76522 | 4776.898198 | 12618.41458 | 4778.708532 | 3141.3583 | 3282.25828  | 7889.360812 | 599.7129 |
| M_1528 | Gly-Lys  | C8 H17 N3 O3    | 203.1263 | 1.527  | 148936.5838 | 20301.02912 | 32077.73791 | 13673.08809 | 16707.91261 | 7046.472769 | 7958.2681 | 6965.00872  | 4360.15466  | 1068.188 |
| M_1529 | 3-Amino-3-[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]-1-propanol                  | C8 H16 N6 O     | 212.1386 | 7.343  | 26903.53683 | 39709.36561 | 42965.95024 | 48092.22499 | 135396.5785 | 113718.711  | 58484.109 | 46272.28171 | 36783.83371 | 4724.298 |
| M_1530 | 2-(Dibutylamino)ethanethiol  | C10 H23 N S     | 189.1557 | 0.863  | 31622.99408 | 9448.335908 | 6278.10367  | 9815.351922 | 11360.64498 | 5255.812818 | 6845.12   | 6150.321155 | 6908.554684 | 1852.02  |
| M_1531 | trans-3-Indoleacrylic acid   | C11 H9 N O2     | 187.0634 | 7.244  | 148557.0077 | 46504.95046 | 56102.81444 | 60940.32184 | 59243.95249 | 36197.62599 | 13965.617 | 12207.01671 | 9759.785405 | 6240.293 |
| M_1532 | 1-t-butyl-4-ethylbenzene   | C12 H18         | 162.1409 | 8.811  | 148156.6753 | 27271.25758 | 21106.46229 | 33018.28492 | 20959.63537 | 28251.975   | 29726.082 | 29498.31342 | 4003.894988 | 15418.73 |
| M_1533 | (4Z)-4-[Nitroso(1H-triaziren-1-yl)methylene]-4,5-dihydro-1,2,5-oxadiazol-3-amine     | C3 H3 N7 O2     | 169.0351 | 1.418  | 23670.19746 | 51125.50072 | 2822.27874  | 8955.239936 | 14856.30747 | 119284.3908 | 67702.413 | 101249.8799 | 81455.28106 | 1051.423 |

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|--------|---|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1534 | 5-Methyl-1H-pyrrole-2-carboxylate   | C6 H6 N O2       | 124.0409 | 0.793  | 100051.6433 | 52589.86423 | 35789.84974 | 88961.34663 | 58661.22637 | 55908.56732 | 42362.316 | 50014.74233 | 28747.60765 | 2350.023 |
| M_1535 | AZA-21-CROWN-7  | C14 H29 N O6     | 307.1994 | 8.181  | 65553.53274 | 60838.89063 | 54083.78521 | 54197.35859 | 76540.72006 | 109225.0227 | 79020.6   | 87113.49207 | 1759.819609 | 3394.538 |
| M_1536 | dimethyl itosonate  | C7 H10 O4        | 158.0581 | 7.054  | 13336.73183 | 13560.00146 | 20208.04542 | 5438.041468 | 24444.33541 | 18815.08097 | 15607.858 | 2040.314084 | 15126.07227 | 18859.37 |
| M_1537 | 2-Indolinecarboxylic acid   | C9 H9 N O2       | 163.0634 | 4.738  | 36497.98831 | 19053.45339 | 104405.8147 | 3443.131895 | 58110.55236 | 51777.43145 | 37074.836 | 32567.88477 | 5283.764912 | 5081.024 |
| M_1538 | melamine  | C3 H6 N6         | 126.066  | 2.681  | 11943.10075 | 25802.61135 | 7082.936208 | 5264.815552 | 6998.668047 | 18263.42033 | 18940.609 | 40926.93016 | 7755.506192 | 6330.312 |
| M_1539 | .alpha.-Amino adipic acid   | C6 H11 N O4      | 161.0689 | 1.202  | 15523.69603 | 42287.135   | 15622.9438  | 40533.18998 | 13137.34713 | 16628.09928 | 24582.871 | 41824.3083  | 12580.48972 | 1708.901 |
| M_1540 | 9-Hydroxy-5,6-dimethyl-3-[(5-phenyl-2-pentanyloxy]-5,6,6a,7,8,9,10,10a-octahydro-1-phenanthridinyl 1-[(3R,6R,7S)-4-(N,N-Dimethylglycyl)-7-methoxy-3,6,9-trimethyl-10-oxo-3,4,5,6,7,8,9,10-octahydro-2H-1,4,9-benzoxadiazacyclodecin-12-yl]-3-phenylurea | C28 H37 N O4     | 451.2699 | 9.183  | 6524.959107 | 54870.24524 | 37471.74588 | 89256.57596 | 44441.14302 | 70954.70771 | 72845.224 | 71368.70047 | 56684.23146 | 6276.685 |
| M_1541 | phenylurea  | C28 H39 N5 O5    | 525.2971 | 10.243 | 35866.45065 | 44162.72255 | 10953.11364 | 35169.7468  | 54590.10165 | 99207.05931 | 43381.487 | 65201.30737 | 44426.66125 | 4476.144 |
| M_1542 | CU5250000   | C8 H5 N O        | 131.0373 | 6.538  | 210.4502742 | 783.5853161 | 212.6587071 | 562.9293895 | 200.9971011 | 227.5878114 | 208.07245 | 410.3041132 | 195.5754441 | 185.2772 |
| M_1543 | N.pi.-Methyl-L-histidine  | C7 H11 N3 O2     | 169.0851 | 1.548  | 48858.11173 | 43270.7707  | 85116.69361 | 91554.23933 | 146622.9522 | 103237.0368 | 30856.38  | 42818.04946 | 33197.68338 | 5788.72  |
| M_1544 | Valyllysine   | C11 H23 N3 O3    | 245.1738 | 0.834  | 65637.96532 | 31195.73959 | 23502.72821 | 34547.27537 | 37679.7136  | 35728.72662 | 32728.697 | 41053.06833 | 36898.1287  | 2822.16  |
| M_1545 | trimethadione   | C6 H9 N O3       | 143.0582 | 2.504  | 34091.10589 | 24140.19864 | 16520.56046 | 2129.915464 | 14485.10812 | 8248.939034 | 18553.889 | 13761.66346 | 17764.87899 | 6194.319 |
| M_1546 | MNA   | C7 H8 N2 O2      | 152.0586 | 3.413  | 130432.8812 | 49240.72406 | 50842.17233 | 46747.84191 | 48962.74469 | 39763.71649 | 34842.578 | 146423.7568 | 32564.04028 | 8715.128 |
| M_1547 | 2-Hydroxy-3-(palmitoyloxy)propyl 2-(trimethylammonio)ethyl phosphate  | C24 H50 N O7 P   | 495.3329 | 10.586 | 23133.80277 | 38668.77676 | 8855.432603 | 61650.12627 | 79974.72152 | 66713.01227 | 86078.617 | 85482.96248 | 77879.15504 | 2118.64  |
| M_1548 | Phenylphosphanide   | C6 H6 P          | 109.0209 | 1.107  | 146278.9137 | 4832.042552 | 38733.45703 | 1340.614557 | 38172.66337 | 28432.15048 | 72791.476 | 6831.458478 | 45864.5365  | 164.379  |
| M_1549 | MTDA  | C8 H18 O2 Si     | 174.1085 | 6.749  | 145887.7984 | 34253.73784 | 35840.07158 | 35007.34118 | 25725.18947 | 21668.68419 | 16342.618 | 16299.11514 | 8126.059748 | 1456.342 |
| M_1550 | stearyl carnitine   | C25 H49 N O4     | 427.3664 | 8.221  | 34540.70017 | 28891.94571 | 53634.19308 | 41141.1026  | 44141.47823 | 25340.82698 | 2970.6768 | 116926.0089 | 26546.73197 | 3261.739 |
| M_1551 | methylthiomethyl lithium  | C2 H5 Li S       | 68.02698 | 0.975  | 11310.27978 | 10934.42611 | 11040.95994 | 10619.32326 | 11086.02982 | 10493.70492 | 10919.731 | 11457.69409 | 11609.83668 | 11271.07 |
| M_1552 | 1-Boc-4-piperidinol   | C10 H19 N O3     | 201.1365 | 8.24   | 48371.7499  | 9294.461792 | 6274.104094 | 39424.00779 | 9805.241901 | 52953.06865 | 29656.259 | 44073.05942 | 31739.57802 | 5874.895 |
| M_1553 | 1-Boc-3-pyrrolidinol  | C9 H17 N O3      | 187.1209 | 7.565  | 145623.6609 | 12327.21006 | 12649.78559 | 44582.71971 | 25134.18591 | 18052.66504 | 12716.403 | 11822.04569 | 10818.72724 | 19037.61 |
| M_1554 | 2127  | C7 H6 O          | 106.0424 | 9.403  | 4433.100445 | 4357.826562 | 4388.738903 | 5414.591936 | 4665.880771 | 5287.398543 | 4558.2343 | 4605.286428 | 4478.55678  | 5474.223 |
| M_1555 | Methyl 8-[2-(2-acetamidophenyl)-2-oxoethyl]-3-isopropyl-6a,7,10b-trimethyldodecahydro-1H-benzo[f]chromene-7-carboxylate   | C31 H45 N O5     | 511.3279 | 9.595  | 27930.41534 | 28357.62486 | 34037.22236 | 114575.8635 | 71544.40475 | 73880.34819 | 77774.571 | 61355.13158 | 47567.54802 | 9929.144 |
| M_1556 | 24FC717FE5  | C4 H8 N6         | 140.0813 | 4.7    | 28311.84023 | 15875.12657 | 21751.00718 | 23655.38507 | 16679.73317 | 20969.9758  | 13640.202 | 19356.42867 | 31914.24678 | 2864.229 |
| M_1557 | [[chloro(sulfido)phosphoryl]-ethyl-oxidanuidyl]benzene  | C8 H10 Cl O2 P S | 235.9831 | 0.598  | 8267.379395 | 6904.454162 | 95797.27375 | 9255.921145 | 5199.940637 | 8697.127275 | 8170.6649 | 4701.1191   | 6594.934066 | 3663.343 |
| M_1558 | N-[1-(4-Amino-6-(dimethylamino)-1,3,5-triazin-2-yl)-3-methylbutyl]leucinamide   | C16 H31 N7 O     | 337.2595 | 8.726  | 1379.68019  | 4462.86904  | 3399.657405 | 2663.77226  | 3812.68277  | 6324.841473 | 1198.5139 | 4835.328604 | 7830.097337 | 937.8775 |
| M_1559 | Dihexyl cyanocarbonodithioimidate   | C14 H26 N2 S2    | 286.1544 | 8.855  | 69233.98118 | 37782.38014 | 104110.2924 | 87931.71265 | 88942.87117 | 86509.35143 | 93681.661 | 67177.81852 | 121167.7574 | 4989.764 |
| M_1560 | 4-Nitroaniline  | C6 H6 N2 O2      | 138.0431 | 1.233  | 86887.46576 | 52529.13385 | 9857.050599 | 23156.77735 | 30313.40655 | 27769.49521 | 35117.16  | 93077.33022 | 37612.84887 | 2136.014 |
| M_1561 | hexobarbital  | C12 H16 N2 O3    | 236.116  | 3.251  | 3534.423576 | 2972.942928 | 3150.98658  | 2966.476025 | 4018.67246  | 3085.411739 | 2729.0893 | 3014.570461 | 2661.306643 | 2786.476 |
| M_1562 | Phenethylamine  | C8 H11 N         | 121.0893 | 0.874  | 8356.937133 | 7590.693134 | 9299.540782 | 7423.287553 | 6123.755154 | 5271.050115 | 7313.1265 | 7837.18202  | 7683.586835 | 23184.67 |
| M_1563 | N-Benzoyl-DL-alanine  | C10 H11 N O3     | 193.074  | 8.268  | 4232.344719 | 3713.870031 | 3792.328476 | 4301.516042 | 4109.599233 | 5269.655189 | 4518.468  | 4886.534956 | 4767.471365 | 5231.705 |
| M_1564 | 4-Hydroxyisoleucine   | C6 H13 N O3      | 147.0896 | 0.956  | 17647.59425 | 17205.80484 | 18000.37159 | 17974.8703  | 17235.48744 | 16894.19804 | 17154.45  | 17889.1514  | 17421.65013 | 5336.946 |
| M_1565 | 4-(4-Morpholinyl)-6-(4-morpholinylmethyl)-1,3,5-triazin-2-amine   | C12 H20 N6 O2    | 280.165  | 8.584  | 4515.688275 | 17387.67492 | 20358.63402 | 18091.19909 | 17336.84943 | 13682.22986 | 5558.8781 | 20587.94924 | 11433.77963 | 17493.89 |
| M_1566 | Benzoic acid  | C7 H6 O2         | 122.0371 | 6.062  | 32342.00047 | 12187.98535 | 16529.6521  | 11242.3309  | 13859.01585 | 7321.578173 | 24203.486 | 7764.291643 | 5227.44116  | 8858.455 |
| M_1567 | Decyl N-((allyloxy)carbonyl)alaninate   | C17 H31 N O4     | 313.2252 | 7.473  | 84685.72774 | 36476.73173 | 30888.16771 | 12846.48178 | 83491.44325 | 108072.0669 | 32910.881 | 42278.37189 | 30763.08008 | 2979.984 |
| M_1568 | 6-Amino-1-ethyl-3-propyl-2,4(1H,3H)-pyrimidinedione   | C9 H15 N3 O2     | 197.1165 | 1.453  | 4431.131027 | 14810.5165  | 2248.012574 | 3277.554737 | 2793.74287  | 23015.11644 | 5258.869  | 11125.54289 | 5077.715704 | 1250.412 |
| M_1569 | N-(2,1,3-Benzothiadiazol-4-yl)-2-thiophenecarboxamide   | C11 H7 N3 O S2   | 261.0023 | 1.215  | 13831.8105  | 132441.7133 | 92166.70813 | 33911.40653 | 74698.37099 | 31045.63285 | 77753.594 | 59051.20079 | 89019.06963 | 1224.444 |
| M_1570 | 2-[[2-[[[4,6-Diamino-1,3,5-triazin-2-yl)amino]ethoxy]ethanol  | C7 H14 N6 O2     | 214.118  | 5.804  | 91004.62188 | 43555.55837 | 129418.5777 | 94875.29951 | 94071.56732 | 74609.10111 | 100047.67 | 124127.2514 | 92853.77745 | 22296.61 |
| M_1571 | 3854  | C5 H12 O S       | 120.0613 | 0.906  | 951.5327449 | 1869.642209 | 625.094644  | 534.2362402 | 47762.57628 | 1050.850034 | 1783.7867 | 7459.029961 | 36066.04487 | 193.9328 |

|        |   |                  |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1572 | Crocetin  | C20 H24 O4       | 328.1672 | 8.424  | 110484.6543 | 29436.40999 | 115385.4117 | 60010.4508  | 5423.082969 | 109968.663  | 52758.029 | 141466.5105 | 46290.63109 | 2818.311 |
| M_1573 | argininamide  | C6 H15 N5 O      | 173.1277 | 0.812  | 141194.2884 | 57422.99923 | 12631.41343 | 50649.09818 | 14298.59672 | 23885.69199 | 34065.562 | 31586.35393 | 39268.98083 | 1495.406 |
| M_1574 | Aniracetam  | C12 H13 N O3     | 219.0897 | 7.494  | 1218.496183 | 1008.842409 | 1309.626619 | 988.7488952 | 1763.745158 | 1778.886488 | 1226.5076 | 1272.054746 | 1099.608851 | 1711.242 |
| M_1575 | Acetylglutamide   | C7 H12 N2 O4     | 188.0797 | 1.41   | 79604.02621 | 29457.98077 | 17416.8545  | 72627.29281 | 27651.57066 | 83473.82605 | 72261.543 | 97815.48284 | 94299.77757 | 3139.03  |
| M_1576 | terpendole E  | C28 H39 N O3     | 437.2907 | 9.685  | 84644.59092 | 140920.417  | 87046.64251 | 117536.2087 | 65942.2015  | 95915.91625 | 67603.266 | 67168.5765  | 46036.92306 | 6819.623 |
| M_1577 | Paracetamol   | C8 H9 N O2       | 151.0634 | 7.377  | 12305.66272 | 12096.86275 | 14486.3391  | 18515.93702 | 22215.43693 | 21875.64786 | 1459.7502 | 12477.22045 | 11476.70869 | 2355.392 |
| M_1578 | Hypusine  | C10 H23 N3 O3    | 233.174  | 0.792  | 5258.696609 | 3932.359382 | 3315.165573 | 5295.24691  | 3785.882299 | 4441.910157 | 3630.9521 | 4304.382639 | 3034.833618 | 1334.25  |
| M_1579 | Maraniol  | C12 H12 O3       | 204.0786 | 9.024  | 5664.22721  | 2405.196578 | 695.7592318 | 2737.373411 | 1771.276144 | 7446.323349 | 1061.4917 | 6014.92157  | 2742.94853  | 1685.006 |
| M_1580 | Guanine   | C5 H5 N5 O       | 151.0494 | 2.252  | 103211.6031 | 104423.0971 | 96729.03267 | 140286.4835 | 95505.87979 | 69077.04401 | 107542.9  | 89331.8496  | 44901.24011 | 5648.33  |
| M_1581 | Itaconic acid   | C5 H6 O4         | 130.0268 | 1.608  | 4274.602259 | 16874.14655 | 12158.40666 | 60085.00886 | 27252.01662 | 39748.24297 | 30879.304 | 35007.38775 | 15272.69379 | 4136.396 |
| M_1582 | 4-(Heptyloxy)benzoic acid   | C14 H20 O3       | 236.141  | 8.467  | 26725.37965 | 111290.5828 | 9458.497367 | 8598.262282 | 24924.77765 | 954.928911  | 21718.027 | 10324.0148  | 28456.26843 | 512.4629 |
| M_1583 | LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))   | C28 H48 N O7 P   | 541.3146 | 10.151 | 24463.1534  | 70689.01292 | 41528.42583 | 77877.39244 | 82771.79192 | 79413.94168 | 73757.37  | 67373.22099 | 91375.4854  | 2889.442 |
| M_1584 | Gly-Lys   | C8 H17 N3 O3     | 203.1266 | 1.399  | 139478.7275 | 78323.62027 | 48152.58166 | 9623.543975 | 6108.155481 | 9316.773024 | 1364.0311 | 7027.877887 | 1213.817069 | 451.1545 |
| M_1585 | 6844478   | C6 H13 N3 O2 S   | 191.0728 | 0.933  | 139421.015  | 20099.6304  | 42174.0593  | 22594.33258 | 15635.56283 | 19065.22842 | 30419.398 | 46604.07673 | 26158.95241 | 2136.463 |
| M_1586 | 2595  | C13 H20 O        | 192.1515 | 8.311  | 55705.48991 | 60904.27423 | 49337.6959  | 44718.50886 | 15487.90026 | 50300.49404 | 69277.42  | 82024.47397 | 98919.21154 | 10591.97 |
| M_1587 | 106330  | C3 H4 S3         | 135.9468 | 0.588  | 102869.4399 | 42905.40588 | 61113.62756 | 36881.44323 | 6972.977001 | 41690.81349 | 44655.166 | 18462.04416 | 47476.91311 | 3902.763 |
| M_1588 | (+)-Nootkatone  | C15 H22 O        | 218.167  | 9.326  | 3672.30429  | 4256.167443 | 4339.333038 | 5530.221389 | 4605.390411 | 4460.781812 | 4539.2796 | 4039.729535 | 4161.415578 | 5131.202 |
| M_1589 | 1H-Imidazole-4,5-dicarbohydrazide   | C5 H8 N6 O2      | 184.071  | 3.118  | 22898.1603  | 15812.51995 | 21933.59186 | 22722.29362 | 13513.04918 | 19435.43075 | 8604.4367 | 15607.10333 | 8960.681195 | 22279.88 |
| M_1590 | quinapyramine   | C17 H22 N6       | 310.1906 | 9.025  | 69905.7031  | 50819.7593  | 52153.56127 | 58230.2839  | 53897.85652 | 40391.88935 | 52911.559 | 64331.14745 | 86974.1434  | 4309.338 |
| M_1591 | (20Z)-20-(Methoxyimino)-3,21-bis(trimethylsilyloxy)pregnan-11-one   | C28 H51 N O4 Si2 | 521.3375 | 9.973  | 22761.8012  | 61780.82234 | 21662.87296 | 80359.63144 | 14344.60365 | 79419.31447 | 74245.8   | 92066.58018 | 79175.28882 | 806.1748 |
| M_1592 | 3652038   | C11 H19 N O4     | 229.1312 | 1.424  | 46611.28792 | 62660.13314 | 48502.08935 | 137748.7758 | 65635.96922 | 35154.26093 | 20328.766 | 20120.19414 | 10919.23105 | 2063.254 |
| M_1593 | 3-O-Carbamoyl-2-deoxy-2-((3,6-diaminohexanoyl)amino)-N-(5-methyl-4-oxo-3a,4,5,6,7,7a-hexahydro-1H-imidazo[4,5-c]pyridin-2-yl)hexopyranosylamine | C20 H36 N8 O7    | 500.2716 | 9.335  | 9610.164761 | 94591.67078 | 43915.40646 | 76109.47131 | 95341.47339 | 53958.41667 | 48765.238 | 137729.4331 | 55697.25574 | 1847.343 |
| M_1594 | 6-aminohexyl phosphate  | C6 H16 N O4 P    | 197.0818 | 1.237  | 16177.72932 | 76193.64366 | 14707.08369 | 35397.66831 | 25263.96672 | 31999.45618 | 12603.558 | 13958.19681 | 20021.47854 | 1012.1   |
| M_1595 | 5-Nitroxystearic acid   | C18 H35 N O5     | 345.2513 | 8.667  | 3903.646419 | 2923.696734 | 4342.136997 | 4853.547394 | 4354.323515 | 6153.592924 | 9394.9536 | 6416.344168 | 4860.106006 | 3175.781 |
| M_1596 | FOSAMINE  | C3 H8 N O4 P     | 153.0192 | 1.139  | 35810.02048 | 20583.11104 | 68159.75872 | 22939.85107 | 12047.44775 | 7504.946699 | 8187.9503 | 10170.86419 | 8369.106549 | 654.711  |
| M_1597 | FOSAMINE  | C3 H8 N O4 P     | 153.0192 | 1.159  | 35810.02048 | 20583.11104 | 68159.75872 | 22939.85107 | 12047.44775 | 13619.48184 | 11236.487 | 11915.12358 | 10733.75517 | 960.5086 |
| M_1598 | 1-arachidonoyl-sn-glycero-3-phosphoethanolamine   | C25 H44 N O7 P   | 501.2837 | 9.568  | 3946.335676 | 18198.53202 | 16048.21932 | 51573.03011 | 34528.0875  | 29763.68032 | 18829.023 | 24676.53878 | 16566.60074 | 701.0253 |
| M_1599 | DL-Histidine  | C6 H9 N3 O2      | 155.0696 | 1.258  | 75304.16934 | 56268.95266 | 53130.67805 | 72654.02075 | 46227.60796 | 8774.820041 | 58446.393 | 71679.1468  | 50139.46849 | 1236.135 |
| M_1600 | 4-((4-((5-Aminopentyl)(hydroxy)amino)-4-oxobutanoyl)amino)pentyl((hydroxy)amino)-4-oxobutanoic acid   | C18 H34 N4 O7    | 418.2429 | 2.296  | 3866.699828 | 2692.887882 | 3095.527087 | 2889.230149 | 2430.76994  | 2398.748746 | 2423.6776 | 2493.746457 | 2252.218721 | 2543.181 |
| M_1601 | 7-Deazaguanine  | C6 H6 N4 O       | 150.0545 | 1.56   | 22053.22208 | 14189.96548 | 20858.27615 | 19725.50307 | 10674.71412 | 15318.47226 | 7228.6575 | 18898.24228 | 11127.08137 | 2561.284 |
| M_1602 | Timonacic   | C4 H7 N O2 S     | 133.0199 | 6.043  | 7772.062826 | 2558.229743 | 68580.48468 | 15703.6965  | 8387.517835 | 3437.275506 | 7792.5407 | 11890.14791 | 9524.95214  | 2615.828 |
| M_1603 | Norepinephrine sulfate  | C8 H11 N O6 S    | 249.0313 | 5.921  | 125268.5545 | 25108.13901 | 113590.1034 | 124021.5182 | 71728.69407 | 96579.41079 | 92427.256 | 66855.69522 | 24054.68481 | 6124.192 |
| M_1604 | Piperonylonitrile   | C8 H5 N O2       | 147.0321 | 5.657  | 34916.69776 | 42762.15908 | 22355.67324 | 91028.45885 | 24615.92525 | 66488.88209 | 32435.816 | 47425.621   | 22884.43478 | 14847.05 |
| M_1605 | 5-Amino-5-oxo-2-((2,3,4,5,6-pentahydroxyhexyl)amino)pentanoic acid  | C11 H22 N2 O8    | 310.1374 | 8.635  | 23509.62024 | 23895.97324 | 19328.56202 | 25770.29305 | 39067.62854 | 14170.34915 | 26394.754 | 23003.42498 | 27213.98507 | 1282.263 |
| M_1606 | 1,10-Dimethyl-4,7,13-trioxo-1,10-diazacyclotetradecane  | C12 H26 N2 O3    | 246.1943 | 1.194  | 87068.13261 | 135038.051  | 55003.25758 | 120709.1552 | 76315.75339 | 65340.99448 | 42940.903 | 61604.0407  | 35539.48721 | 985.7774 |
| M_1607 | 1H-Imidazole-4-carboxamide, 5-(3-butyl-3-methyl-1-triazenyl)-   | C9 H16 N6 O      | 224.1386 | 8.795  | 44937.23713 | 97802.18874 | 82592.19248 | 93773.84908 | 61406.48359 | 117544.5422 | 91786.913 | 98518.90952 | 134805.4885 | 10348.26 |
| M_1608 | Bis(4-chlorophenyl)hydrogen phosphate   | C12 H9 Cl2 O4 P  | 317.9625 | 1.338  | 13978.58292 | 24356.91948 | 30757.37305 | 134516.3569 | 7175.633495 | 25983.45807 | 6929.5686 | 7445.953491 | 5869.553121 | 2034.148 |
| M_1609 | TX-1041   | C4 H6 N6 O       | 154.0605 | 4.03   | 92935.74557 | 62993.24784 | 48568.62015 | 73939.67723 | 44724.50704 | 51676.79921 | 32279.489 | 43882.89513 | 27256.10772 | 25025.72 |
| M_1610 | 4-(2,3-dihydroindol-1-yl)-N-[3-(N-ethyl-3-methylanyllo)propyl]-3-(1-imidazolyl)-4-oxobutanamide   | C27 H33 N5 O2    | 459.2626 | 8.537  | 17528.67637 | 20521.17009 | 17351.65743 | 17364.90704 | 54861.57294 | 19780.87757 | 42228.825 | 88683.15968 | 31346.53756 | 3763.338 |
| M_1611 | tranexamic acid   | C8 H15 N O2      | 157.1103 | 1.151  | 133703.7297 | 35008.56666 | 24598.01401 | 57898.14654 | 18369.93088 | 11553.38302 | 10293.602 | 11076.37425 | 11154.37569 | 1044.758 |
| M_1612 | 4-(1,1-Dioxido-2,3-dihydro-3-thiophenyl)morpholine  | C8 H13 N O3 S    | 203.0617 | 3.788  | 133703.0636 | 14401.6019  | 4709.981992 | 46452.76966 | 18977.88103 | 46025.76948 | 24967.693 | 56245.15199 | 4756.504239 | 3166.217 |
| M_1613 | 1,1-Bis(cyclohexyloxy)-N,N-dimethylmethanamine  | C15 H29 N O2     | 255.2197 | 8.615  | 59309.98394 | 60875.85738 | 64079.68611 | 44374.46953 | 35348.75406 | 55570.82241 | 53224.659 | 70282.73089 | 50727.63622 | 13511.24 |
| M_1614 | Diethyl (E)-azodicarboxylate  | C6 H10 N2 O4     | 174.064  | 1.116  | 132987.182  | 8997.399498 | 12043.2956  | 8879.859712 | 9065.065405 | 12222.17411 | 11251.479 | 11477.28335 | 10673.90833 | 902.2755 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1615 | N-Methylmorpholine  | C5 H11 N O      | 101.0846 | 0.599  | 18619.18355 | 18208.2467  | 14435.74949 | 21025.4007  | 13820.71917 | 15824.72115 | 22265.004 | 18810.36462 | 18200.78558 | 22370.57 |
| M_1616 | (±)-Equol   | C15 H14 O3      | 242.0944 | 7.697  | 84163.92715 | 86338.31327 | 132648.6392 | 84865.65842 | 52788.37999 | 47529.09239 | 22623.681 | 32215.79557 | 27826.16996 | 3411.659 |
| M_1617 | Glycylglycyl-L-valine   | C9 H17 N3 O4    | 231.1218 | 2.42   | 132606.4962 | 6039.949805 | 5714.938873 | 19527.39187 | 3406.106032 | 3702.34296  | 3912.8649 | 3579.600893 | 3020.740678 | 1520.894 |
| M_1618 | 4-[3-(Diphenylmethylene)cyclopentyl]-2-butanone                                   | C22 H24 O       | 304.1818 | 7.762  | 9127.2817   | 7684.599499 | 7251.47636  | 6456.772605 | 10623.12211 | 10456.79793 | 8675.4725 | 7803.671686 | 8076.817824 | 10281.04 |
| M_1619 | amino-(3,4-dihydroxyphenyl)methylphosphonic acid                                  | C7 H10 N O5 P   | 219.0297 | 1.235  | 65274.32172 | 7454.598274 | 9254.86067  | 24012.65444 | 7581.632742 | 16717.30513 | 12399.956 | 5046.984314 | 5766.345607 | 848.0085 |
| M_1620 | octylphenol   | C14 H22 O       | 206.1671 | 9.185  | 20536.47919 | 25764.32449 | 18744.76396 | 20098.83743 | 28710.06037 | 18255.19477 | 3998.54   | 21447.26635 | 16777.22373 | 11371.5  |
| M_1621 | US1836000   | C6 H8 N2 O      | 124.0639 | 1.145  | 10944.27906 | 10505.4353  | 12905.67604 | 9762.288683 | 9671.227647 | 12999.66057 | 11582.177 | 11961.13425 | 11838.42959 | 2778.369 |
| M_1622 | Propane-1,2,3-triyl tris((3-isocyanatomethylphenyl)carbamate)                     | C30 H26 N6 O9   | 614.1783 | 7.857  | 2079.620232 | 2075.270131 | 1862.572855 | 2196.50604  | 3042.349559 | 13433.18819 | 2622.3612 | 9205.133168 | 3936.044744 | 2971.723 |
| M_1623 | 5,6-Diphenyl-1,2,4-triazine-3(2H)-thione  | C15 H11 N3 S    | 265.0673 | 1.101  | 53864.35511 | 50099.90713 | 131143.7918 | 66668.32939 | 91725.76098 | 79641.27831 | 63801.511 | 91917.4973  | 71416.41645 | 1698.778 |
| M_1624 | Ribose 5-phosphate  | C5 H11 O8 P     | 230.0191 | 1.421  | 12013.90103 | 20575.47023 | 3905.835005 | 3903.552895 | 4081.764252 | 7229.033843 | 8312.0958 | 14947.67684 | 9723.824484 | 1786.391 |
| M_1625 | 1-[(4-Nitrobenzyl)sulfonyl]pyrrolidine  | C11 H14 N2 O4 S | 270.0673 | 1.93   | 70278.86046 | 32968.01741 | 49615.24061 | 131123.2198 | 48788.59484 | 42215.08563 | 38053.518 | 56111.63591 | 34903.11896 | 3847.448 |
| M_1626 | DA9380000   | C6 H7 N O2 S    | 157.0198 | 3.369  | 62613.65777 | 64144.31977 | 130803.7711 | 19415.81274 | 40105.66133 | 72399.04508 | 60345.866 | 28998.21786 | 57375.03878 | 2685.393 |
| M_1627 | 2-Hydroxyquinoline  | C9 H7 N O       | 145.0529 | 4.741  | 36379.43614 | 16331.30453 | 63989.61912 | 17326.88095 | 32397.91204 | 31067.64561 | 22513.442 | 27169.37305 | 16833.05539 | 3067.81  |
| M_1628 | CHEIROLIN   | C5 H9 N O2 S2   | 179.0075 | 1.647  | 10288.92392 | 5994.242397 | 16859.73554 | 5465.842252 | 6870.348179 | 5820.701272 | 5360.2419 | 5120.67336  | 4138.045204 | 2457.984 |
| M_1629 | DL-Tryptophan   | C11 H12 N2 O2   | 204.0899 | 1.993  | 3602.148326 | 2106.878456 | 2226.507965 | 2345.277396 | 1940.783867 | 2728.688988 | 2760.8684 | 3029.687365 | 1875.866728 | 2257.625 |
| M_1630 | (2,5-Dimethyl-1,4-phenylene)bis(methylene) bis(N-carbamimidoylcarbamimidothioate) | C14 H22 N8 S2   | 366.1427 | 2.177  | 75370.32108 | 24994.65511 | 129372.6561 | 34044.81551 | 38884.80858 | 21357.10713 | 16502.54  | 18205.07357 | 12903.21028 | 3224.058 |
| M_1631 | Prolinamide   | C5 H10 N2 O     | 132.09   | 1.111  | 129337.4479 | 23273.48624 | 49260.92967 | 57046.72725 | 45226.99455 | 36098.22933 | 70636.878 | 51065.75988 | 41750.30286 | 2086.146 |
| M_1632 | 2-trimethylammonioethyl methylphosphonofluoridate                                 | C6 H16 F N O2 P | 184.0906 | 1.309  | 17267.15959 | 52718.5524  | 7076.803418 | 12312.92635 | 65330.23759 | 73527.37549 | 63238.127 | 129335.1649 | 79253.70984 | 2062.439 |
| M_1633 | 4,4'-Methylenebis[2-tert-butyl-6-(alpha-methylbenzyl)phenol]                      | C37 H44 O2      | 520.3363 | 10.379 | 91039.59619 | 96973.8195  | 56036.30413 | 109886.5026 | 91558.9212  | 100551.7243 | 102803.4  | 113935.9399 | 95929.42003 | 5098.35  |
| M_1634 | Nonanoylmorpholine  | C13 H25 N O2    | 227.1885 | 10.39  | 27253.50559 | 41455.76647 | 33734.41135 | 31937.20062 | 10953.92227 | 22049.2211  | 12690.949 | 57539.04332 | 11915.5074  | 3221.986 |
| M_1635 | 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycerol-3-phosphocholine            | C30 H50 N O7 P  | 567.3328 | 10.584 | 5765.675649 | 5295.358415 | 5075.555181 | 20025.5379  | 31247.17728 | 19924.60679 | 5346.0206 | 26894.37786 | 17315.32931 | 5225.943 |
| M_1636 | Paracetamol   | C8 H9 N O2      | 151.0634 | 6.217  | 9972.981444 | 8438.484756 | 9259.82915  | 8998.044799 | 7894.046085 | 9163.859635 | 9435.1618 | 8141.761573 | 10392.92015 | 7945.458 |
| M_1637 | 2-Methyl-2-propanyl (2,4,6-triamino-5-pyrimidinyl)carbamate                       | C9 H16 N6 O2    | 240.1343 | 7.419  | 4133.340488 | 4734.167692 | 12048.80034 | 10444.26261 | 11762.52634 | 16783.60946 | 15162.974 | 11799.88991 | 15456.45565 | 12078.86 |
| M_1638 | 9-Butyl-6-  | C9 H15 N5 S     | 225.1055 | 7.973  | 6773.387567 | 10332.63504 | 10050.15077 | 10638.19661 | 13829.74454 | 1612.333231 | 1420.23   | 9860.965642 | 10871.54414 | 5943.051 |
| M_1639 | Jasmonic acid   | C12 H18 O3      | 210.123  | 8.439  | 2953.286993 | 2509.957875 | 2621.622654 | 11088.75914 | 4841.251714 | 10202.62324 | 9127.3044 | 14615.26159 | 17499.35426 | 1595.797 |
| M_1640 | Glycerate   | C3 H5 O4        | 105.0195 | 1.301  | 31263.21964 | 74749.09482 | 12679.64781 | 72905.78228 | 113867.1925 | 103329.2433 | 6367.6616 | 92933.76886 | 68887.07387 | 21960.22 |
| M_1641 | 4,6-Bis(ethylamino)-1,3,5-triazine-2-carboxamide                                  | C8 H14 N6 O     | 210.1238 | 8.082  | 991.9071295 | 802.6748036 | 806.5140118 | 813.0968912 | 1444.03485  | 9319.612293 | 21027.31  | 1282.188417 | 1218.512473 | 15174.79 |
| M_1642 | 1-Tetradecylamine   | C14 H31 N       | 213.2457 | 7.694  | 17315.41802 | 127778.7087 | 13658.46052 | 25869.3636  | 29245.90905 | 31361.36438 | 35039.715 | 20641.70745 | 11756.67074 | 16731.05 |
| M_1643 | Valpromide  | C8 H17 N O      | 143.1311 | 8.158  | 27422.41469 | 30290.69923 | 26160.74408 | 24287.53639 | 28679.08201 | 51146.10671 | 34578.422 | 38631.92569 | 40227.47011 | 18837.42 |
| M_1644 | 1-(Phenylthioxomethyl)piperidine  | C12 H15 N S     | 205.0933 | 2.949  | 4393.19978  | 2431.798805 | 2399.045512 | 2482.549617 | 3106.021706 | 6503.278915 | 2428.2721 | 4361.244315 | 2556.026354 | 2382.395 |
| M_1645 | D-Erythrose 4-phosphate   | C4 H9 O7 P      | 200.0088 | 1.219  | 6994.998604 | 4507.768748 | 4600.875553 | 4250.916702 | 4199.555918 | 5493.801845 | 5623.4318 | 5248.154368 | 3599.87071  | 482.2342 |
| M_1646 | L-Methionine sulfoxide  | C5 H11 N O3 S   | 165.046  | 1.442  | 39483.39859 | 24983.24057 | 40322.50334 | 14241.10417 | 17101.50811 | 46429.1591  | 48392.703 | 12814.67659 | 73935.10985 | 1264.792 |
| M_1647 | Bis[(2-isopropyl-5-methylcyclohexyl)oxy](2-methoxyphenyl)phenylsilane             | C33 H50 O3 Si   | 522.3526 | 10.084 | 13196.17159 | 20127.73448 | 37948.44673 | 75227.31378 | 49732.50042 | 76189.74407 | 65642.952 | 90436.1363  | 76780.38834 | 4264.298 |
| M_1648 | Nitrosobis(2-oxopropyl)amine  | C6 H10 N2 O3    | 158.0692 | 1.31   | 91163.41496 | 72985.13731 | 22542.35998 | 83144.79998 | 126848.6092 | 107590.39   | 69859.407 | 84804.44417 | 69909.33713 | 2407.248 |
| M_1649 | Precocene II  | C13 H16 O3      | 220.11   | 8.609  | 9117.491427 | 11104.99752 | 9470.093234 | 12775.02698 | 4986.350458 | 20550.02449 | 8298.7064 | 16049.00136 | 14521.80776 | 14378.03 |
| M_1650 | tranexamic acid   | C8 H15 N O2     | 157.1103 | 1.414  | 78509.97669 | 46310.73087 | 39139.23065 | 109959.7154 | 96260.30446 | 121359.9122 | 66539.702 | 126256.9337 | 19911.31402 | 2138.862 |
| M_1651 | 2-Phenylimidazo[2,1-b][1,3]benzothiazole  | C15 H10 N2 S    | 250.0564 | 2.067  | 11904.27492 | 62474.68556 | 126095.1548 | 56703.28172 | 87949.84703 | 65028.82025 | 76660.408 | 111694.187  | 67185.94779 | 6355.909 |
| M_1652 | 2,2'-Bipyridine   | C10 H8 N2       | 156.0689 | 7.67   | 5880.138028 | 5559.786634 | 4010.507108 | 4122.244414 | 7225.334744 | 7268.999543 | 5375.6314 | 4921.040069 | 4679.501369 | 7418.554 |
| M_1653 | Lys-Trp   | C17 H24 N4 O3   | 332.1862 | 8.777  | 52490.13514 | 70416.06767 | 62226.07913 | 52466.43893 | 96907.31494 | 112539.8267 | 60929.975 | 113409.1515 | 67763.1887  | 2917.806 |
| M_1654 | trans-3-Indoleacrylic acid  | C11 H9 N O2     | 187.0632 | 7.306  | 125597.634  | 37669.82267 | 52764.30744 | 39008.44715 | 46085.4984  | 26239.51772 | 9314.1456 | 8753.977803 | 2623.073471 | 1651.991 |
| M_1655 | 1-Benzosuberone   | C11 H12 O       | 160.0889 | 8.143  | 110461.9862 | 57629.21856 | 58549.04396 | 79712.7545  | 94966.43287 | 125557.0066 | 116599.6  | 121589.0956 | 83936.74787 | 11212.01 |
| M_1656 | 4-Hydrazino-6-methoxy-N,N-dipropyl-1,3,5-triazin-2-amine                          | C10 H20 N6 O    | 240.1707 | 8.79   | 4651.519962 | 8971.392395 | 26977.69336 | 8749.350168 | 9272.279194 | 6252.421166 | 105539.86 | 7463.972394 | 125470.9301 | 7859.24  |

|        |   |                    |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|--------------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1657 | 5,5-dimethyl-2-(6-methyl-2-(methylsulfanyl)pyrimidin-4-yloxy)-1,3,2-dioxaphosphorinane-2-thione | C11 H17 N2 O3 P S2 | 320.0422 | 2.868  | 125369.3317 | 4701.118486 | 3554.436457 | 3946.45912  | 3731.683728 | 4974.318011 | 4257.4741 | 4354.591949 | 3485.349129 | 3527.173 |
| M_1658 | 4-Acetamido-1,2,3-cyclohexanetriyl triacetate   | C14 H21 N O7       | 315.1317 | 7.686  | 114877.181  | 125297.8373 | 100429.4981 | 59740.69054 | 118796.0162 | 54944.42025 | 42422.538 | 16116.79813 | 3898.644906 | 2859.737 |
| M_1659 | benzoquinone  | C6 H4 O2           | 108.0216 | 1.411  | 10088.99121 | 11699.52396 | 18618.63345 | 2714.284281 | 2841.311139 | 21424.50028 | 14385.987 | 3313.997107 | 8709.819373 | 1891.847 |
| M_1660 | Ethyl 4-[(2-(benzoylamino)ethyl)amino]-1-piperidinecarboxylate                                  | C17 H25 N3 O3      | 319.1894 | 8.042  | 5650.527475 | 1737.339055 | 1938.050351 | 4747.065373 | 11616.81631 | 14663.79907 | 12468.189 | 3258.895059 | 3410.823449 | 2819.33  |
| M_1661 | 6-Amino-9-methyl-7H-purin-9-ium   | C6 H8 N5           | 150.0768 | 1.028  | 124893.4343 | 19821.05061 | 28282.93024 | 12118.68817 | 15575.52166 | 2632.474078 | 23459.705 | 11923.63201 | 2992.97393  | 2639.962 |
| M_1662 | noradrenaline   | C8 H11 N O3        | 169.074  | 3.726  | 11409.27397 | 11567.87117 | 16292.29458 | 9035.021494 | 5425.277178 | 4804.997655 | 4959.8167 | 4939.65738  | 4775.707931 | 6189.676 |
| M_1663 | Gly-Lys   | C8 H17 N3 O3       | 203.1262 | 1.482  | 124644.5511 | 22266.8616  | 28267.13811 | 18840.64126 | 12808.76542 | 6423.457666 | 5830.0182 | 5953.167863 | 8267.173332 | 758.3109 |
| M_1664 | P,P-Bis(1-aziridinyl)-N,N-dimethylphosphinic amide  | C6 H14 N3 O P      | 175.0872 | 1.502  | 25697.20705 | 14787.34812 | 30964.8164  | 72948.32456 | 26762.07573 | 58295.40951 | 44218.617 | 27477.09226 | 45357.56632 | 6397.484 |
| M_1665 | 1-Methyl-4-(2-methyl-2H-tetrazol-5-yl)-1H-pyrazol-5-amine                                       | C6 H9 N7           | 179.092  | 5.226  | 18068.72836 | 12266.17098 | 19371.04272 | 12506.75184 | 17939.73958 | 19702.93342 | 20269.033 | 62656.54874 | 22378.03153 | 11821.85 |
| M_1666 | Phenol  | C6 H6 O            | 94.04242 | 0.681  | 29918.76248 | 28390.11668 | 38530.43589 | 54328.509   | 76942.69428 | 26414.31597 | 29228.192 | 29107.0447  | 25648.71627 | 9582.08  |
| M_1667 | 4-Nitroaniline  | C6 H6 N2 O2        | 138.0431 | 1.482  | 38861.07143 | 37927.93615 | 45270.59844 | 27518.25849 | 37685.71351 | 41288.91782 | 39493.411 | 26454.50004 | 32084.70001 | 5846.386 |
| M_1668 | 1,4-Butanesultone   | C4 H8 O3 S         | 136.0193 | 0.596  | 3582.598059 | 122791.829  | 4795.102593 | 3101.898245 | 2316.993881 | 3395.894035 | 5220.4625 | 3864.057684 | 3831.63768  | 4717.426 |
| M_1669 | Procaine  | C13 H20 N2 O2      | 236.1521 | 8.343  | 5628.212136 | 4416.504915 | 4719.285758 | 4404.619479 | 4677.207648 | 5886.075718 | 5476.2532 | 5489.967291 | 5494.974262 | 5799.778 |
| M_1670 | 235BBF3K97  | C20 H28            | 268.2189 | 9.943  | 48125.69428 | 67091.68539 | 44711.23112 | 122752.9899 | 99221.76382 | 85965.04541 | 48669.467 | 76120.4161  | 61362.4173  | 4634.319 |
| M_1671 | Pyridoxal   | C8 H9 N O3         | 167.0586 | 2.359  | 122144.0978 | 28257.04353 | 17887.48905 | 26590.23318 | 24058.65967 | 18311.15963 | 23787.821 | 19000.301   | 7523.400368 | 2731.9   |
| M_1672 | trimethadione   | C6 H9 N O3         | 143.0583 | 1.123  | 121736.728  | 99682.2288  | 21861.23022 | 51070.90775 | 42938.67288 | 30145.87144 | 30129.417 | 28081.74474 | 26743.05144 | 6589.501 |
| M_1673 | Loratadine impurity   | C8 H13 N O3        | 171.0897 | 5.441  | 121434.8089 | 9951.907084 | 8093.87199  | 7399.133408 | 6248.553277 | 7838.2635   | 2293.4281 | 7741.085868 | 6027.280225 | 5355.745 |
| M_1674 | MFCDD0056730  | C11 H19 N3 O6 S    | 321.0995 | 1.235  | 18864.25486 | 15079.20586 | 15592.1292  | 14164.00716 | 13722.12775 | 13530.60143 | 13042.993 | 12211.11619 | 11453.56499 | 1715.357 |
| M_1675 | 8-Azaguanine  | C4 H4 N6 O         | 152.0452 | 0.916  | 48633.48893 | 49224.05239 | 55421.40267 | 43634.23644 | 48400.7261  | 63432.256   | 71417.619 | 39334.58487 | 48777.59814 | 3989.981 |
| M_1676 | 6-Amino-1-ethyl-3-propyl-2,4(1H,3H)-pyrimidinedione   | C9 H15 N3 O2       | 197.1165 | 1.42   | 3000.92732  | 1805.725164 | 1601.93454  | 3277.554737 | 1625.306326 | 23015.11644 | 2468.1069 | 5811.594498 | 1908.240741 | 732.6682 |
| M_1677 | Tetrahydrodibenzothioophene   | C12 H12 S          | 188.0661 | 1.211  | 111175.3098 | 113866.9689 | 47646.93002 | 32744.05693 | 21572.65491 | 15485.12777 | 9427.441  | 10076.47483 | 25142.29384 | 1063.655 |
| M_1678 | Arsenic acid  | H3 As O4           | 141.9249 | 1.932  | 3058.675308 | 1945.817549 | 1906.359377 | 2142.34381  | 1706.716457 | 1824.548924 | 1647.741  | 1697.542127 | 1472.564973 | 2129.919 |
| M_1679 | thiodiglycol  | C4 H10 O2 S        | 122.0401 | 0.802  | 14138.82544 | 120428.24   | 7161.547904 | 1363.322415 | 7195.802816 | 1661.287103 | 2279.7878 | 7288.754178 | 84682.27275 | 9846.916 |
| M_1680 | DO0750000   | C15 H24 O2         | 236.1769 | 8.825  | 34896.7753  | 9038.335705 | 29784.46215 | 24830.02239 | 13226.56664 | 10804.48261 | 15756.888 | 28120.58465 | 20912.73397 | 13131.6  |
| M_1681 | 1,3-Dicyclohexylurea  | C13 H24 N2 O       | 224.1889 | 8.251  | 29822.84281 | 68110.0589  | 26272.20686 | 34205.64318 | 5080.849434 | 23480.29046 | 52134.889 | 74642.1237  | 43537.42363 | 6651.682 |
| M_1682 | 4,6-Di(1-piperidinyl)-1,3,5-triazine-2-carbonitrile   | C14 H20 N6         | 272.1754 | 9.104  | 7066.881044 | 47079.21832 | 60145.09005 | 9334.047498 | 11728.26543 | 41647.38267 | 8527.9333 | 22821.83923 | 12164.55314 | 2004.05  |
| M_1683 | 3-Phthalimidopropionic acid   | C11 H9 N O4        | 219.0531 | 5.033  | 37938.46343 | 5662.903902 | 8424.572334 | 10345.72492 | 7156.238713 | 7117.055784 | 5840.1033 | 6717.175269 | 7073.804639 | 5652.941 |
| M_1684 | L-(+)-Leucine   | C6 H13 N O2        | 131.0948 | 0.721  | 88614.642   | 5178.224286 | 65084.79292 | 41099.93841 | 54307.07388 | 119566.9739 | 86078.959 | 85631.42174 | 63364.84    | 18656.66 |
| M_1685 | AM9627000   | C8 H7 N O3         | 165.0428 | 4.917  | 4325.177004 | 4186.032071 | 4345.181661 | 4280.591445 | 4476.940241 | 4294.653753 | 4148.5281 | 6303.587721 | 8644.475432 | 4760.16  |
| M_1686 | ANDROSTENONE  | C19 H28 O          | 272.2138 | 10.092 | 31253.12953 | 5805.994917 | 3798.08235  | 5471.484566 | 4347.222092 | 10156.84709 | 18945.854 | 21885.73138 | 16033.45263 | 4445.354 |
| M_1687 | (2R)-3-[[[2-Aminoethoxy](hydroxy)phosphoryl]oxy]-2-(hexanoyloxy)propyl hexanoate                | C17 H34 N O8 P     | 411.2025 | 7.035  | 9784.139262 | 25281.20162 | 30980.61863 | 63301.31465 | 57727.68428 | 75921.18191 | 32004.109 | 45142.16342 | 25852.58596 | 4401.021 |
| M_1688 | HM1650000   | C12 H26 N2 O4      | 262.1892 | 1.568  | 118791.2692 | 40852.19824 | 47315.03332 | 6528.572191 | 13382.40374 | 24451.83486 | 16258.363 | 26067.92647 | 7545.482394 | 2159.289 |
| M_1689 | Diethyl 4-dodecyl-2,6-dimethyl-1,4-dihydro-3,5-pyridinedicarboxylate                            | C25 H43 N O4       | 421.3193 | 8.166  | 118775.9624 | 32766.6326  | 30113.78923 | 59859.69113 | 41589.54126 | 99170.52425 | 75840.69  | 100387.7965 | 33449.6439  | 3208.215 |
| M_1690 | 4-Hydrazino-6-methoxy-N,N-dipropyl-1,3,5-triazin-2-amine  | C10 H20 N6 O       | 240.1705 | 8.695  | 7448.474905 | 92776.25607 | 10633.69277 | 118400.8161 | 7295.244476 | 16952.44695 | 18699.955 | 118359.6808 | 23465.6967  | 12758.53 |
| M_1691 | Butylphthalide  | C12 H14 O2         | 190.0996 | 8.139  | 118387.3943 | 10875.17276 | 7724.436119 | 1891.916051 | 2767.959138 | 3118.062299 | 9680.4676 | 9657.649195 | 2592.324464 | 1149.255 |
| M_1692 | 4-[(2-Methyl-4,6-dinitro-1H-benzimidazol-5-yl)amino]phenol                                      | C14 H11 N5 O5      | 329.0744 | 4.7    | 118330.9105 | 9123.166015 | 21834.92281 | 13707.55358 | 2358.753252 | 2672.067263 | 2367.48   | 2317.85077  | 2296.488182 | 2328.882 |
| M_1693 | C8-HSL  | C12 H21 N O3       | 227.1521 | 8.373  | 12760.50289 | 12027.57095 | 7686.781234 | 27330.28858 | 6646.521854 | 17784.71213 | 10431.241 | 20528.43846 | 14828.988   | 6033.628 |
| M_1694 | 2,2'-(Dodecanoylimino)diacetic acid   | C16 H29 N O5       | 315.2047 | 4.653  | 68444.82837 | 23073.84623 | 29546.16199 | 46553.24063 | 30217.48847 | 20031.57463 | 15148.331 | 7441.159765 | 15627.80891 | 2898.196 |
| M_1695 | 2-Ethylhexyl maleate  | C20 H36 O4         | 340.2617 | 8.966  | 107156.6894 | 15130.92552 | 15160.25481 | 14969.87932 | 13669.26852 | 16356.2257  | 2360.87   | 8521.879982 | 13096.66651 | 16181.56 |
| M_1696 | Benzoazole  | C7 H5 N O          | 119.0374 | 4.629  | 118185.8024 | 21071.05727 | 41221.41859 | 45582.78657 | 22599.80274 | 11236.89323 | 6068.5866 | 6138.14199  | 12309.20059 | 3637.777 |
| M_1697 | 1-[N-Cyano-N-(4,6-dimethyl-2-pyrimidinyl)glycyl]-4-piperidinecarboxamide                        | C15 H20 N6 O2      | 316.1649 | 8.03   | 9395.149114 | 2925.244309 | 3493.381196 | 2736.55208  | 12126.62437 | 10487.55875 | 3201.4665 | 3175.599098 | 1459.644123 | 3753.996 |
| M_1698 | glu-thr   | C9 H16 N2 O6       | 248.1008 | 1.216  | 25944.10931 | 25412.85344 | 69750.97665 | 35883.36313 | 25143.98755 | 62242.68861 | 45684.491 | 77908.46895 | 54282.83329 | 2296.671 |
| M_1699 | [5-(3,5-Dinitrophenyl)-1,3,4-oxadiazol-2-yl]methyl  | C11 H8 N4 O7       | 308.0393 | 1.181  | 117334.1805 | 59854.33152 | 56615.91113 | 63022.28005 | 59378.48118 | 59965.0939  | 95596.446 | 76579.26154 | 63640.43724 | 922.8516 |

|        |   |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1700 | 2-Amino-3-hydroxypropyl dihydrogen phosphate  | C3 H10 N O5 P   | 171.0296 | 4.481  | 12200.68398 | 14233.1019  | 13286.43287 | 13750.55296 | 8613.99978  | 11029.64493 | 8561.6545 | 14499.47888 | 2131.226988 | 12285.63 |
| M_1701 | (2E)-2-[(1E)-1-[[[(Z)-Amino(hydrazono)methyl]hydrazono]-2-propanylidene]hydrazinocarbohydrazonamide   | C5 H14 N10      | 214.1407 | 10.596 | 444.7484286 | 857.143329  | 3118.566061 | 1458.606042 | 1005.463312 | 431.6794084 | 1212.2881 | 2052.960279 | 737.7717844 | 1288.81  |
| M_1702 | methylthiomethylithium  | C2 H5 Li S      | 68.02703 | 2.884  | 116598.708  | 5044.112099 | 27698.39483 | 28236.81778 | 4923.549646 | 4955.481494 | 5572.8189 | 32022.81846 | 26424.32113 | 4941.636 |
| M_1703 | Octyl 5-oxo-L-prolinate   | C13 H23 N O3    | 241.1678 | 8.677  | 116352.808  | 8310.735703 | 7498.990188 | 37841.16349 | 8539.327787 | 24973.80038 | 31703.207 | 73695.4934  | 15418.56531 | 3871.417 |
| M_1704 | TAA   | C9 H15 N        | 137.1205 | 1.489  | 8474.85323  | 5789.381093 | 5221.749115 | 6041.638017 | 4877.194734 | 4436.759739 | 4233.9852 | 4999.492293 | 5670.823649 | 6772.01  |
| M_1705 | 2'-Deoxyadenosine   | C10 H13 N5 O3   | 251.1018 | 1.607  | 15835.58885 | 8798.887296 | 5157.64644  | 5770.44975  | 3619.398586 | 6479.576716 | 1627.2747 | 41576.51856 | 3089.761594 | 1694.992 |
| M_1706 | TRANS-3'-METHOXY-4-(METHYLTHIO)CHALCONE   | C17 H16 O2 S    | 284.0871 | 8.617  | 10245.22251 | 12297.70368 | 18573.03573 | 12126.82441 | 13782.97589 | 20199.26828 | 24901.471 | 24359.53992 | 17718.18015 | 17797.01 |
| M_1707 | Leu-ala   | C9 H18 N2 O3    | 202.1318 | 1.877  | 5008.889651 | 2975.751481 | 2874.197941 | 3189.620291 | 2560.243142 | 2718.185364 | 2497.1862 | 2594.364688 | 2197.178463 | 3039.945 |
| M_1708 | Loratadine impurity 3,11,17,21-Tetrahydroxypregnan-20-one   | C21 H34 O5      | 366.2405 | 8.259  | 51043.00233 | 75867.92827 | 18502.03101 | 33002.67478 | 26384.59906 | 115113.9969 | 51615.482 | 87498.0043  | 44722.3158  | 3911.623 |
| M_1710 | OZ4150000   | C10 H19 N O2    | 185.1416 | 7.278  | 2239.987868 | 7765.444748 | 32974.20955 | 14727.95681 | 114895.0697 | 47717.70988 | 7929.6748 | 27800.84359 | 7672.334806 | 4154.73  |
| M_1711 | 5,5',5'-Tetraallyl-1,1'-dicyclohexyl-3,3'-bipiperidine-2,2',4,4',6,6'-hexone  | C34 H44 N2 O6   | 576.3172 | 10.477 | 42427.51241 | 37988.80929 | 1596.653849 | 13624.58901 | 8251.757428 | 61370.12243 | 2108.1467 | 51624.00947 | 35415.70517 | 4271.509 |
| M_1712 | 1H-1,2,4-triazole-3-sulfonic acid   | C2 H3 N3 O3 S   | 148.9901 | 0.597  | 60435.23255 | 49270.73718 | 52554.80556 | 58497.53968 | 49910.05222 | 64231.6302  | 59571.846 | 40434.53557 | 22525.75893 | 4058.069 |
| M_1713 | benzyne   | C6 H4           | 76.03155 | 2.442  | 73625.08953 | 57257.061   | 114684.2453 | 64796.91564 | 40887.65385 | 33357.25354 | 46687.759 | 40472.56967 | 44123.7624  | 2709.533 |
| M_1714 | 2,4,6-Triisopropylbenzophenone  | C22 H28 O       | 308.214  | 9.382  | 46939.13829 | 114358.7895 | 46966.74749 | 91511.37559 | 29505.42106 | 94175.20099 | 42867.376 | 78907.05855 | 24652.39696 | 9447.052 |
| M_1715 | 2,2'-[[1-(4-Piperidiny)-1,3-propanediyl]di-4,1-piperidinediyl]diethanol   | C22 H43 N3 O2   | 381.3356 | 7.179  | 1849.707509 | 2039.610526 | 21239.51575 | 2246.440373 | 2898.661927 | 9218.019324 | 3016.2903 | 24591.71021 | 1722.049323 | 2288.012 |
| M_1716 | 3-(2-Thioxo-2,3-dihydro-1H-imidazol-4-yl)-2-(trimethylammonio)propanoate  | C9 H15 N3 O2 S  | 229.0884 | 1.422  | 3562.536699 | 2143.658103 | 1901.729025 | 2476.402656 | 1998.311664 | 31247.68301 | 21096.401 | 20535.23142 | 22555.27555 | 869.7836 |
| M_1717 | 7,13-Dimethyl-1,4,10-trioxa-7,13-diazacyclopentadecane-2,6,14-trione  | C12 H20 N2 O6   | 288.132  | 6.285  | 113863.0399 | 26962.83342 | 60890.47911 | 22557.89816 | 15603.34659 | 6162.675865 | 4724.2199 | 4914.144451 | 6380.872923 | 4129.757 |
| M_1718 | 3748  | C13 H24 O3      | 228.1726 | 8.196  | 5209.785838 | 20614.19836 | 9911.793072 | 10993.67698 | 18239.97238 | 11774.05642 | 12245.173 | 17064.36511 | 12839.34585 | 11600.52 |
| M_1719 | Pivaloylacetoneitrile   | C7 H11 N O      | 125.0842 | 1.111  | 113775.4343 | 24329.09684 | 30874.49201 | 17325.55188 | 23934.55394 | 30979.71427 | 28939.651 | 29918.66806 | 27112.92699 | 2389.475 |
| M_1720 | 1,5,9-Trimethyl-10-[[2-methyl-2-propanyl)peroxy]-11,14,15,16-tetraoxatetracyclo[3.3.1.0 <sup>-4</sup> .13 <sup>-0</sup> .0 <sup>-8</sup> .13 <sup>-</sup> ]hexadecane | C19 H32 O6      | 356.2196 | 10.531 | 3143.60261  | 64699.23762 | 9925.210054 | 39412.89575 | 35306.17611 | 72101.4173  | 30305.871 | 37834.60589 | 51817.41994 | 15806.86 |
| M_1721 | 1-Cyano-3-(2-[[[3-methoxy-2-pyridinyl)methyl]sulfanyl]ethyl)-2-methylguanidine  | C12 H17 N5 O S  | 279.1149 | 6.837  | 113635.0417 | 16638.26614 | 20715.74721 | 10066.5432  | 4931.3222   | 4337.621841 | 6476.4859 | 4893.883813 | 4662.434936 | 5105.2   |
| M_1722 | MFC00083078   | C22 H45 N O3    | 371.34   | 8.103  | 4769.777454 | 3500.598289 | 2091.249226 | 15475.27545 | 21462.48383 | 2068.474724 | 3787.8956 | 4206.260013 | 1573.68683  | 2287.162 |
| M_1723 | MFC00041564   | C11 H22 O3      | 202.1577 | 8.798  | 46471.7614  | 27029.70188 | 36779.39264 | 113349.2857 | 17542.85771 | 40676.12549 | 36046.355 | 25675.14378 | 46236.29868 | 9538.838 |
| M_1724 | Dimethyl 4-morpholinylphosphonate   | C6 H14 N O4 P   | 195.0662 | 1.236  | 13654.3158  | 31729.16901 | 9887.008502 | 23552.41555 | 27176.30125 | 32339.10835 | 12941.423 | 20769.12364 | 15682.15401 | 1087.712 |
| M_1725 | N-Boc-3-Pyrrolidinone   | C9 H15 N O3     | 185.1053 | 7.128  | 15293.23202 | 13985.4326  | 13868.61434 | 13544.75719 | 12766.79084 | 16710.5152  | 2270.2003 | 1971.193277 | 8670.161922 | 2582.723 |
| M_1726 | N-(2-oxolanylmethyl)-2-[7-oxo-3-(phenylmethyl)-6-triazolo[4,5-d]pyrimidinyl]acetamide   | C18 H20 N6 O3   | 368.1598 | 8.423  | 48746.60092 | 18313.84618 | 93153.43165 | 54485.26054 | 29961.18637 | 112526.9416 | 49511.292 | 83548.97242 | 45932.70454 | 3132.908 |
| M_1727 | 4-(2,2-Dimethylhydrazino)-2,6-dimethyl-1,1,3,3-cyclohexanetetraconitrile  | C14 H18 N6      | 270.1594 | 8.899  | 65474.3401  | 59189.27991 | 87939.85526 | 91442.34783 | 97578.12779 | 99132.31981 | 71145.634 | 112440.0313 | 97645.79774 | 1341.06  |
| M_1728 | MFC001580212  | C10 H13 N O2 S2 | 243.0388 | 6.687  | 2723.69918  | 2333.983901 | 2435.68206  | 2442.150814 | 2463.749125 | 2429.160859 | 2401.8749 | 2616.329611 | 2383.056538 | 2390.516 |
| M_1729 | 4-(4-nitrobenzoyl)morpholine  | C11 H12 N2 O4   | 236.0796 | 1.557  | 17627.88051 | 55246.31512 | 84691.67049 | 60230.69976 | 61938.61691 | 60082.9455  | 53431.78  | 72399.88931 | 62772.96425 | 3497.979 |



|        |  |                 |          |        |             |             |             |             |             |             |           |             |             |          |
|--------|--|-----------------|----------|--------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1730 | (2R)-2-[(7-Oxoheptanoyloxy)-3-(palmitoyloxy)propyl 2-(trimethylammonio)ethyl phosphate                                   | C31 H60 N O9 P  | 621.4011 | 10.674 | 7371.688932 | 6753.635889 | 6954.503445 | 7239.931275 | 6894.112435 | 6426.025615 | 7249.6465 | 7205.614794 | 6733.575827 | 6582.767 |
| M_1731 | 2-(4-Thiomorpholinyl)ethanol   | C6 H13 N O S    | 147.0725 | 1.391  | 25246.54817 | 11836.92869 | 15669.28666 | 11960.29914 | 86035.77092 | 8421.083911 | 2852.6511 | 30116.96326 | 2858.223995 | 1006.298 |
| M_1732 | 3-AB   | C7 H8 N2 O      | 136.0638 | 0.936  | 111793.1448 | 14932.87965 | 10955.24107 | 7098.743069 | 9825.867368 | 4692.286961 | 4977.214  | 4770.93177  | 4690.884664 | 1599.429 |
| M_1733 | 1,3-Dioxolane, 2-(2,4,6-trimethylcyclohex-3-enyl)-4-(1-piperidylmethyl)-   | C18 H31 N O2    | 293.2354 | 8.801  | 3641.397046 | 5979.6975   | 3844.164481 | 4360.904021 | 3978.134244 | 3923.857219 | 3830.6285 | 4479.821041 | 3664.57261  | 3696.856 |
| M_1734 | Ethyl 7-[3-(3-cyclohexyl-3-hydroxypropyl)-2,5-dioxo-4-imidazolidinyl]heptanoate  | C21 H36 N2 O5   | 396.2624 | 7.719  | 1817.350062 | 1681.966398 | 1209.560208 | 1337.596084 | 2070.033063 | 2003.340997 | 1422.2134 | 1444.02168  | 1268.924186 | 2079.615 |
| M_1735 | O-Cyclododecyl O-methyl carbonothioate   | C14 H26 O2 S    | 258.1653 | 7.727  | 110705.8573 | 20319.55119 | 13582.07828 | 46680.24866 | 33164.9717  | 88468.61078 | 35780.1   | 51354.23824 | 41125.40644 | 3243.903 |
| M_1736 | 2,2,5,5-Tetramethyl-3-pyrroline-3-carboxamide  | C9 H16 N2 O     | 168.1263 | 6.585  | 26030.84945 | 28704.97691 | 65356.32964 | 24176.7453  | 63478.78445 | 49400.19246 | 22988.73  | 110587.8879 | 28837.64651 | 3514.697 |
| M_1737 | ANDROSTENONE   | C19 H28 O       | 272.2138 | 9.626  | 60663.77364 | 41914.8013  | 12853.60358 | 24747.926   | 9105.807493 | 27254.91243 | 56032.576 | 39816.78111 | 38363.95559 | 10209.96 |
| M_1738 | 4'-tert-Butylacetophenone  | C12 H16 O       | 176.1203 | 8.148  | 5199.215094 | 15459.27074 | 13806.07555 | 41161.83513 | 35217.92583 | 12313.57603 | 12690.828 | 24602.75271 | 9605.879108 | 19820.54 |
| M_1739 | 1-(4-Nitrophenyl)piperidine  | C11 H14 N2 O2   | 206.1055 | 1.237  | 110291.2034 | 37955.55771 | 24962.17575 | 78587.74274 | 38602.4659  | 76509.9282  | 48273.525 | 29909.85828 | 51743.89038 | 732.6014 |
| M_1740 | [4-[1-(1-cyclopentyl-5-tetrazolyl)propyl]-1-piperazinyl]-[2-furanyl]methanone  | C18 H26 N6 O2   | 358.2118 | 8.501  | 34933.03251 | 61079.17285 | 25358.35376 | 110218.7558 | 28265.88097 | 50430.65925 | 38155.313 | 55803.5654  | 11010.83264 | 3635.485 |
| M_1741 | MFCD03100412   | C16 H29 N O3    | 283.2147 | 8.954  | 59289.93518 | 34803.5779  | 92154.35164 | 83386.98606 | 77366.66277 | 92579.2537  | 74181.986 | 38071.25752 | 110134.0997 | 3884.566 |
| M_1742 | Dehydrothiotoluidine   | C14 H12 N2 S    | 240.0722 | 1.208  | 6420.086861 | 8190.226894 | 110116.2892 | 13014.80381 | 15321.9261  | 14980.13007 | 14222.944 | 10704.86792 | 13859.95306 | 568.3304 |
| M_1743 | PA3500000  | C23 H32 O2      | 340.2402 | 9.382  | 45702.44725 | 110087.2853 | 43777.27246 | 86569.31356 | 28246.72161 | 90061.36979 | 41135.588 | 77683.24636 | 23404.79268 | 8204.032 |
| M_1744 | D-Erythrose 4-phosphate  | C4 H9 O7 P      | 200.0087 | 1.133  | 1235.802381 | 1685.827289 | 2099.532986 | 1573.064648 | 1466.186707 | 2776.258855 | 1909.125  | 5416.379324 | 1893.040024 | 149.776  |
| M_1745 | 4-Nitrophenyl (2E)-3-(2-thienyl)acrylate   | C13 H9 N O4 S   | 275.0244 | 7.817  | 19056.68281 | 71309.90847 | 31022.41173 | 98839.60754 | 92830.67789 | 109966.9764 | 47754.865 | 43065.91508 | 44266.39685 | 4198.694 |
| M_1746 | Strophanthidin, 3-((dipropylamino)acetate)   | C31 H47 N O7    | 545.3356 | 10.287 | 3044.787926 | 10080.2706  | 65452.63911 | 8652.773781 | 8612.563829 | 7568.920045 | 17935.589 | 21173.3695  | 11374.91707 | 749.352  |
| M_1747 | Phenyl N,N'-dibutyl-N,N'-dimethylphosphorodiamidate  | C16 H29 N2 O2 P | 312.1978 | 10.369 | 72975.16486 | 87455.64175 | 38943.00841 | 86390.29712 | 56048.1809  | 81314.39893 | 75457.303 | 69748.46587 | 79354.48338 | 18153.58 |
| M_1748 | 2,4-Diamino-6-pteridinecarboxylic acid   | C7 H6 N6 O2     | 206.0554 | 5.533  | 109456.9593 | 21961.17603 | 43108.14087 | 12466.53675 | 10610.73508 | 11063.3898  | 19300.422 | 32872.65116 | 6996.349991 | 20624.84 |
| M_1749 | 3,18-diethyl-2,7,13,17-tetramethyl-1,19-dioxo-1,2,3,4,5,15,16,17,18,19,22,24-dodecahydro-21H-bilin-8,12-dipropanoic acid | C33 H46 N4 O6   | 594.341  | 10.723 | 10040.97333 | 33588.35645 | 30945.8132  | 20453.39743 | 41883.51028 | 47198.57525 | 50496.034 | 49398.40538 | 50112.13276 | 9040.905 |
| M_1750 | 3-hydroxylinoleoylcarnitine  | C25 H45 N O5    | 439.33   | 8.136  | 109390.5879 | 7355.371871 | 920.1511782 | 15403.97841 | 14999.49753 | 35926.57869 | 25110.33  | 28239.33597 | 8416.74154  | 2976.469 |
| M_1751 | Ethyl 4-isothiocyanatobutanoate  | C7 H11 N O2 S   | 173.051  | 3.551  | 29100.27123 | 9037.372608 | 10211.65805 | 109213.3673 | 13784.51511 | 49758.06918 | 1387.0373 | 61731.40907 | 12256.30516 | 4062.241 |
| M_1752 | 9-Fluorononanal  | C9 H17 F O      | 160.126  | 9.099  | 8047.012326 | 12526.67512 | 13829.46662 | 9011.058557 | 7373.241695 | 25814.42669 | 8080.2058 | 6463.280218 | 14583.29162 | 4652.245 |
| M_1753 | 141551   | C4 H4 N6        | 136.0502 | 4.626  | 8518.84639  | 14790.35133 | 9556.115047 | 20392.96968 | 3877.958513 | 11238.36579 | 12887.254 | 6732.665398 | 9038.78231  | 12940.86 |
| M_1754 | N-(Phosphonomethyl)-D-glutamine  | C6 H13 N2 O6 P  | 240.051  | 1.843  | 44205.96009 | 37269.68273 | 53017.43013 | 55362.03134 | 41757.26406 | 40600.47488 | 30726.794 | 54349.76618 | 22444.59893 | 4146.112 |
| M_1755 | 5-[3-(4-Aminophenoxy)propyl]-2,4,6-pyrimidinotriamine  | C13 H18 N6 O    | 274.1544 | 8.424  | 1971.846667 | 5278.953189 | 108637.7459 | 4851.449725 | 1448.328107 | 5511.071014 | 4104.5899 | 1673.990941 | 4433.505155 | 6172.805 |
| M_1756 | Precocene II   | C13 H16 O3      | 220.1101 | 8.519  | 2055.766234 | 22687.9533  | 11108.42587 | 7576.751042 | 2919.22686  | 2428.615683 | 4925.6405 | 6477.316077 | 2111.993722 | 2073.531 |
| M_1757 | Tetrahydroisoquinoline-3-carboxylic acid   | C10 H11 N O2    | 177.0791 | 6.987  | 31951.3795  | 10086.03664 | 108365.9623 | 13646.28036 | 41930.26464 | 39619.44417 | 13950.31  | 41279.20662 | 19404.76119 | 3215.822 |
| M_1758 | Loratadine impurity ((4,6-Bis[(hydroxymethyl)amino]-1,3,5-triazin-2-yl)imino)dimethanol                                  | C8 H13 N O3     | 171.0896 | 2.652  | 107910.3189 | 26150.39244 | 13356.2059  | 33949.10592 | 19908.6432  | 23995.76862 | 26472.316 | 3648.533409 | 3671.059206 | 4305.647 |
| M_1759 | Ethyl 7-nitro-1H-indole-2-carboxylate  | C11 H10 N2 O4   | 234.064  | 2.502  | 8515.196995 | 5578.723363 | 7929.191433 | 6051.53559  | 5174.387656 | 5716.95852  | 5567.0387 | 5538.080911 | 4389.311556 | 2395.101 |
| M_1761 | Nitrosobis(2-oxopropyl)amine   | C6 H10 N2 O3    | 158.0692 | 1.393  | 30364.00928 | 14681.54168 | 22542.35998 | 19008.53457 | 13474.91698 | 107590.39   | 70622.231 | 66967.18432 | 89399.72755 | 4203.178 |

|        |   |                 |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|---|-----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1762 | 2,4-dihydroxyheptadec-16-ynyl acetate   | C19 H34 O4      | 326.2448 | 9.117 | 66494.93234 | 7829.828179 | 7517.47469  | 6576.013592 | 107534.9906 | 9125.172213 | 7623.8835 | 6551.585648 | 2969.095381 | 3901.89  |
| M_1763 | GW7000000   | C6 H8 O         | 96.05794 | 0.598 | 12097.91755 | 11381.26327 | 9333.090306 | 66978.2179  | 7927.343881 | 107459.9151 | 15301.033 | 14292.24665 | 42253.90927 | 10147.08 |
| M_1764 | QU1920000   | C10 H20 N2 O    | 184.1577 | 1.139 | 23588.87414 | 16718.31424 | 13451.49589 | 26700.04772 | 35209.82109 | 20051.1227  | 21338.805 | 73372.17727 | 18367.96196 | 748.9209 |
| M_1765 | Isatin<br>Thiosemicarbazone<br>3,4',5-Tri-tert-butylbiphenyl-4-ol   | C9 H8 N4 O S    | 220.0413 | 7.913 | 4098.748892 | 6672.943526 | 18077.53529 | 53667.6306  | 54893.2404  | 53759.06765 | 41969.869 | 18785.9548  | 21847.79913 | 5332.073 |
| M_1766 | fosclic acid  | C24 H34 O       | 338.2611 | 9.154 | 7290.102852 | 12035.43103 | 36614.90066 | 107404.0493 | 9925.987496 | 31150.11848 | 15678.879 | 43305.25862 | 32422.1073  | 3476.667 |
| M_1767 | Loratadine impurity (+/-)-C75   | C8 H13 N O3     | 171.0895 | 3.037 | 23327.92117 | 5895.043897 | 5751.484472 | 58534.40701 | 11444.59359 | 24629.88836 | 26601.366 | 16896.264   | 10524.0172  | 10486.34 |
| M_1768 | MFC00053351   | C14 H22 O4      | 236.141  | 8.542 | 266.5781043 | 4547.847445 | 330.2280804 | 367.2288549 | 333.3784336 | 438.8407213 | 16756.233 | 428.7595985 | 364.096239  | 386.195  |
| M_1770 | hodgkinsine   | C22 H43 N O3    | 369.3247 | 9.074 | 6227.523741 | 4267.250603 | 5816.880164 | 2823.950482 | 3113.330018 | 9179.138335 | 2026.5244 | 48943.86269 | 2163.042351 | 2582.91  |
| M_1771 | 1-Butyl-N-(3-pyridinylmethyl)-1H-tetrazol-5-amine (9Z)-9-   | C33 H38 N6      | 518.3179 | 9.764 | 1667.924966 | 1723.516002 | 6898.156931 | 1840.342138 | 6955.03827  | 3249.584191 | 6247.2129 | 45635.07331 | 1862.128334 | 2095.034 |
| M_1772 | Octadecenamide  | C11 H16 N6      | 232.1435 | 8.705 | 4472.599392 | 62957.41298 | 7471.632633 | 25758.06124 | 57874.38588 | 36071.00422 | 56094.505 | 13472.66684 | 106928.9246 | 7853.239 |
| M_1773 | 2-(Dicyclohexylamino)ethanol  | C18 H35 N O     | 281.2719 | 9.077 | 4542.940529 | 4813.214985 | 3755.17346  | 6383.527161 | 4053.738629 | 4609.89505  | 4644.8605 | 4879.811333 | 4243.066187 | 2977.756 |
| M_1774 | DO0750000   | C14 H27 N O     | 225.2093 | 9.057 | 3458.927462 | 3572.752123 | 2654.45581  | 4055.76746  | 3107.463858 | 3945.318921 | 2993.3208 | 3447.224965 | 3290.727914 | 2559.798 |
| M_1775 | 1,3-Dioxolane, 2-(2,4,6-trimethylcyclohex-3-enyl)-4-(1-piperidylmethyl)-  | C15 H24 O2      | 236.1775 | 8.985 | 22119.43294 | 106839.6265 | 8956.788127 | 13482.05996 | 16538.83395 | 10574.84491 | 10417.728 | 10484.92446 | 8675.859896 | 8863.032 |
| M_1776 | adrenaline  | C18 H31 N O2    | 293.2353 | 8.76  | 3495.1002   | 3458.866568 | 2068.163159 | 8298.961716 | 3927.749672 | 10303.90874 | 3769.188  | 3798.807901 | 4869.51402  | 6409.342 |
| M_1777 | adrenaline  | C9 H13 N O3     | 183.0896 | 3.32  | 106476.7069 | 47927.76655 | 74857.74487 | 44676.97621 | 23357.88291 | 17516.83076 | 18748.527 | 15823.41281 | 8929.550575 | 5117.643 |
| M_1778 | 1,2,3,4,7-Pentahydroxy-1,3,4,4a,5,11b-hexahydro[1,3]dioxol[4,5- <i>j</i> ]phenanthridin-6(2H)-one   | C14 H15 N O8    | 325.0799 | 2.617 | 53287.39931 | 19434.80912 | 26255.23939 | 106356.2725 | 42853.9436  | 20504.59899 | 19268.803 | 18435.805   | 15759.58521 | 8880.509 |
| M_1779 | epsilon-Caprolactone  | C6 H10 O2       | 114.0685 | 0.594 | 79807.07597 | 6489.451127 | 4285.900006 | 6057.024788 | 3797.792468 | 3412.875925 | 8735.0424 | 9053.952659 | 7577.741885 | 6445.893 |
| M_1780 | LYSINOALANINE,  | C9 H19 N3 O4    | 233.1375 | 0.802 | 5036.308424 | 3194.537171 | 2693.146434 | 4301.708322 | 3075.543345 | 3159.43031  | 2949.6824 | 2804.87546  | 2465.412709 | 1083.907 |
| M_1781 | (E)-p-coumaric acid   | C9 H8 O3        | 164.0473 | 4.014 | 35987.84195 | 105978.7245 | 39535.89142 | 47790.35511 | 66760.11622 | 23742.38313 | 16771.742 | 24404.87354 | 14416.72693 | 4925.378 |
| M_1782 | MFC00093639   | C12 H8 O3 S     | 232.0195 | 1.258 | 18883.17493 | 12951.02622 | 14910.51954 | 16434.36965 | 27918.48575 | 21130.89159 | 24739.422 | 11949.53152 | 12239.86838 | 1796.344 |
| M_1783 | NL3680000   | C11 H9 N O2     | 187.0634 | 8.099 | 30885.54463 | 28618.02472 | 37089.91141 | 33285.08087 | 38891.11406 | 22212.73062 | 9131.4722 | 12165.35401 | 12366.15823 | 8523.892 |
| M_1784 | 2,2'-(5,5',10,10'-Tetrahydroxy-1,1'-dimethyl-6,6',9,9'-tetraoxo-3,3',4,4',6,6',9,9'-octahydro-1H,1'H-8,8'-bibenzo[ <i>g</i> ]isochromene-3,3'-diyl)diacetic acid                      | C32 H26 O14     | 634.1341 | 1.208 | 10709.72626 | 9371.577398 | 9934.610257 | 9033.647606 | 8382.743909 | 13642.23883 | 8141.7541 | 8252.756781 | 10757.64039 | 949.2786 |
| M_1785 | 4-Chloro-3-methoxy-2-methylpyridine 1-oxide   | C7 H8 Cl N O2   | 173.025  | 1.291 | 1644.962938 | 3383.597413 | 1044.363398 | 1042.547626 | 1843.652388 | 1399.537147 | 1880.2879 | 6401.777136 | 1799.292609 | 13289    |
| M_1786 | 2,4-Bis(dimethylamino)-6-nitro-1,3,5-triazine   | C7 H12 N6 O2    | 212.1027 | 7.86  | 2220.330215 | 2215.68578  | 2086.595019 | 2345.124678 | 3248.19914  | 3099.192222 | 2464.8338 | 2493.343239 | 2512.404958 | 3172.794 |
| M_1787 | 2-[4-[(2 <i>R</i> ,4 <i>S</i> )-2-Benzyl-4-piperidinyl]-1-piperazinyl]-N-(2,6-dimethylphenyl)acetamide  | C26 H36 N4 O    | 420.2875 | 8.505 | 2394.675575 | 2112.789501 | 2826.42869  | 105114.8365 | 2875.090814 | 5328.391592 | 2869.6352 | 7999.942791 | 1675.879884 | 2261.801 |
| M_1788 | 1732026   | C D3 I          | 144.9472 | 0.598 | 51312.48122 | 47769.78702 | 65100.37828 | 55621.78937 | 53195.20018 | 42784.86302 | 65078.273 | 36054.51932 | 33387.86628 | 3567.841 |
| M_1789 | 6-Phosphononorleucine   | C6 H14 N O5 P   | 211.061  | 7.978 | 30544.32387 | 43546.38791 | 38287.07864 | 41618.6888  | 39696.43488 | 25333.65284 | 18403.816 | 15297.15559 | 17942.16991 | 2856.103 |
| M_1790 | S-(3-Amino-2-hydroxypropyl)dihydrogen phosphorothioate  | C3 H10 N O4 P S | 187.007  | 1.325 | 10080.82373 | 6060.342635 | 5857.958513 | 5392.081777 | 10470.12231 | 2745.508906 | 4916.2505 | 6495.960428 | 10097.34807 | 1354.243 |
| M_1791 | N-[(3 <i>R</i> ,6 <i>R</i> ,7 <i>S</i> )-4-(4-Fluorobenzyl)-7-methoxy-3,6,9-trimethyl-10-oxo-3,4,5,6,7,8,9,10-octahydro-2H-1,4,9-benzoxadiazacyclodecin-12-yl]cyclopentanecarboxamide | C30 H40 F N3 O4 | 525.2988 | 9.691 | 2447.11048  | 31575.07394 | 34551.92721 | 83377.56956 | 23559.77244 | 37964.30946 | 65548.492 | 73357.69206 | 40251.87445 | 3431.121 |
| M_1792 | Gly-Lys   | C8 H17 N3 O3    | 203.1262 | 1.349 | 104773.4583 | 4495.366777 | 22338.3761  | 7850.534066 | 3196.259051 | 2626.839778 | 1243.4833 | 1271.2024   | 1494.167046 | 412.6538 |
| M_1793 | 1,1,1-Trifluoroacetylacetone  | C5 H5 F3 O2     | 154.0246 | 2.773 | 89893.40903 | 9096.442155 | 2571.963903 | 47911.83277 | 8866.958306 | 90838.04818 | 24230.13  | 37801.80309 | 1675.296035 | 2960.987 |
| M_1794 | 3-Vinyl-1,2,3-dioxaborolane   | C4 H7 B O2      | 98.05418 | 1.068 | 25853.16918 | 104299.6315 | 3507.49704  | 7491.715744 | 40221.42084 | 4125.073762 | 4503.9338 | 3972.818835 | 4245.036857 | 835.6629 |
| M_1795 | Ritipenem   | C10 H12 N2 O6 S | 288.0421 | 3.497 | 17481.86215 | 26637.56755 | 38562.2352  | 44674.0153  | 59468.88475 | 78992.84592 | 92349.226 | 85496.19543 | 84640.17962 | 2234.191 |
| M_1796 | Leu-Val   | C11 H22 N2 O3   | 230.163  | 2.933 | 2569.666281 | 2111.042099 | 2082.608999 | 2150.749284 | 2060.584772 | 2073.948764 | 2107.9806 | 2026.207466 | 1984.528787 | 2068.154 |
| M_1797 | N <sup>2</sup> ~,N <sup>2</sup> ~,N <sup>4</sup> ~,N <sup>4</sup> ~,N <sup>6</sup> ~-Pentaethyl-1,3,5-triazine-2,4,6-triamine   | C13 H26 N6      | 266.2222 | 9.633 | 4214.408397 | 2342.598493 | 692.3473569 | 4619.745359 | 1409.417931 | 1621.987814 | 3327.0512 | 943.0756276 | 3524.557071 | 1602.077 |

|        |  |                |          |       |             |             |             |             |             |             |           |             |             |          |
|--------|--|----------------|----------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|-------------|-------------|----------|
| M_1798 | N,N-Bis(aminomethyl)metanediamine  | C3 H12 N4      | 104.1064 | 1.077 | 55953.19725 | 103813.9113 | 56511.04101 | 71291.98609 | 62329.89947 | 80032.94322 | 58190.509 | 60699.20055 | 52539.22219 | 1819.228 |
| M_1799 | Indole   | C8 H7 N        | 117.0582 | 7.392 | 3775.76062  | 1131.8078   | 3077.693073 | 1198.699    | 1573.188373 | 1535.113673 | 976.05515 | 1379.853293 | 1088.717641 | 1574.922 |
| M_1800 | 2-Hydroxy-3-(phosphonoxy)propyl myristate  | C17 H35 O7 P   | 382.2117 | 8.898 | 103794.0831 | 3719.034143 | 682.9070054 | 2250.58106  | 17083.52669 | 41355.25108 | 30039.107 | 46178.1446  | 29620.91736 | 321.085  |
| M_1801 | 1-Cyclohexyl-3-(2-hydroxyethyl)thiourea  | C9 H18 N2 O S  | 202.1147 | 1.479 | 103748.7822 | 34810.97185 | 3874.763567 | 25706.11056 | 30046.28497 | 9351.698211 | 5432.6896 | 4995.469332 | 7831.768646 | 1833.808 |
| M_1802 | 1-[[[8Z,11Z,14Z]-icosatrienoyl]-sn-glycero-3-phosphocholine  | C28 H52 N O7 P | 545.3462 | 9.856 | 1130.826315 | 37731.43688 | 2967.202886 | 30603.41558 | 19521.52065 | 60806.51925 | 31983.224 | 50572.21214 | 31846.72367 | 2730.582 |
| M_1803 | p-Cresol   | C7 H8 O        | 108.0579 | 0.67  | 7677.724849 | 6766.897501 | 30044.89094 | 20803.76594 | 25663.33957 | 21536.03488 | 27294.442 | 17847.95116 | 23005.49119 | 6596.844 |
| M_1804 | 2-Chloro-1,3,2-oxathiaphospholane  | C2 H4 Cl O P S | 141.9408 | 1.906 | 82636.27749 | 21744.29689 | 19599.10921 | 20294.21087 | 16156.32244 | 38731.55824 | 48852.946 | 32600.25205 | 23387.97433 | 4794.916 |
| M_1805 | 2-(4-Chlorophenyl)-2-oxoethyl 3-methoxybenzoate  | C16 H13 Cl O4  | 304.0497 | 0.83  | 102699.3673 | 18902.28273 | 25892.35846 | 17264.30427 | 22877.17477 | 22111.92899 | 22438.473 | 19185.8405  | 13199.21715 | 670.5982 |
| M_1806 | SKF-91488  | C7 H17 N3 S    | 175.1147 | 1.253 | 45685.94122 | 67515.5998  | 25409.99844 | 54807.904   | 50387.81954 | 69086.65538 | 102313.33 | 69501.64057 | 90654.38879 | 2870.395 |
| M_1807 | 3-Methyl-N~7~-nitro[1,2,4]triazolo[4,3-a][1,3,5]triazine-5,7-diamine   | C5 H6 N8 O2    | 210.0615 | 1.507 | 7772.066118 | 6129.408476 | 9215.579833 | 28029.99379 | 3683.021979 | 24431.68265 | 13197.406 | 4560.579847 | 32078.12211 | 1903.802 |
| M_1808 | N-(2-Hydroxypropyl) methacrylamide   | C7 H13 N O2    | 143.0946 | 1.077 | 2821.605979 | 1998.643041 | 102205.17   | 14097.53175 | 1888.284339 | 2449.530139 | 1852.9123 | 1996.683145 | 2157.073376 | 2190.716 |
| M_1809 | N-(Phosphonomethyl)-D-glutamine  | C6 H13 N2 O6 P | 240.0512 | 1.764 | 44205.96009 | 2968.708923 | 5796.20732  | 2980.701399 | 41757.26406 | 40600.47488 | 30726.794 | 4739.761182 | 22444.59893 | 700.2718 |
| M_1810 | Spirostan-3-yl   | C29 H46 O4     | 458.3392 | 9.064 | 18911.72969 | 24669.75059 | 52945.81302 | 102099.7098 | 36589.49597 | 21522.92094 | 19461.723 | 30130.89361 | 7607.247404 | 5417.403 |
| M_1811 | g-Butyrobetaine  | C7 H15 N O2    | 145.1104 | 2.74  | 29949.60928 | 40250.95848 | 29654.35635 | 78611.55544 | 30198.41196 | 76071.65705 | 36430.342 | 51217.97064 | 66542.52585 | 2542.571 |
| M_1812 | glas#16  | C22 H40 O11    | 480.255  | 6.573 | 40884.79625 | 21302.84169 | 48208.31659 | 39223.24362 | 33082.14654 | 26544.88094 | 28316.906 | 79345.37047 | 38099.339   | 18715.63 |
| M_1813 | 2450705  | C8 H15 N O4 S  | 221.0721 | 3.397 | 101031.6347 | 22626.83059 | 55651.07739 | 61830.55806 | 24993.96978 | 22276.63712 | 13552.123 | 18101.31532 | 8016.247577 | 3633.992 |
| M_1814 | Phenolate  | C6 H5 O        | 93.03462 | 2.445 | 67014.37083 | 57461.70661 | 65794.80436 | 90294.46454 | 77189.42037 | 94573.82317 | 49999.748 | 51661.87658 | 25776.36216 | 2759.837 |
| M_1815 | N~2~-((tert-Butoxycarbonyl)-N~6~-formyl-L-lysine   | C12 H22 N2 O5  | 274.1527 | 5.273 | 2866.000349 | 2771.643007 | 2903.265754 | 2838.24491  | 2879.802348 | 2839.540737 | 2691.0937 | 2768.3963   | 2635.268377 | 2564.398 |
| M_1816 | 4-(2,5-Diethoxy-4-nitrophenyl)morpholine   | C14 H20 N2 O5  | 296.1369 | 2.161 | 49194.64159 | 100646.2414 | 2719.989016 | 3107.621087 | 2704.617548 | 3680.845942 | 3172.6405 | 6026.110813 | 2659.186702 | 2904.61  |
| M_1817 | (2R)-3-Hydroxy-2-(((5Z,8Z,11R,12E,14Z)-11-hydroxy-5,8,12,14-icosatetraenoyl)oxy)propyl 2-(trimethylammonio)ethyl phosphate | C28 H50 N O8 P | 559.3278 | 8.843 | 4434.406398 | 29340.16483 | 10924.6678  | 17023.53836 | 1524.7682   | 8381.407597 | 3808.3406 | 15386.46043 | 5916.442244 | 2211.415 |
| M_1818 | (2-Amino-3-hydroxybutanoyl)oxonium   | C4 H10 N O3    | 120.065  | 2.392 | 14167.36826 | 100481.3592 | 39755.21857 | 66331.49694 | 83808.70175 | 50219.88957 | 47839.12  | 57261.90045 | 58824.91491 | 1552.622 |
| M_1819 | (2S)-2-((N-((2S)-Ammoniopropanoyl)-L-leucyl)amino)propanoate   | C12 H23 N3 O4  | 273.1688 | 2.4   | 9524.514747 | 6143.116336 | 9835.275126 | 6673.405405 | 5422.254757 | 6604.855523 | 6409.3762 | 6105.924021 | 5113.59566  | 2762.746 |
| M_1820 | (2E)-2-(methylthiomethyl)-3-phenyl-2-propenal  | C11 H12 O S    | 192.0614 | 5.023 | 11161.91597 | 2837.08322  | 1623.076817 | 1891.210017 | 862.0102017 | 2348.516297 | 2991.7938 | 5430.653943 | 1558.854754 | 527.8268 |

**Supplementary Table 2. List of metabolite features that were significantly altered between WT and ghrelin KO mice.**

| Label  | m.z      | RT [min] | t.score | p.value  | FDR      |
|--------|----------|----------|---------|----------|----------|
| M_0843 | 276.1083 | 5.0311   | -9.877  | 9.31E-06 | 0.016942 |
| M_0241 | 137.0478 | 4.0646   | -7.2722 | 8.62E-05 | 0.07842  |
| M_0117 | 147.0897 | 3.8033   | -6.6714 | 0.000157 | 0.095415 |
| M_0587 | 174.1005 | 3.6442   | -6.324  | 0.000227 | 0.10168  |
| M_0539 | 153.0514 | 3.5227   | 6.0672  | 0.0003   | 0.10168  |
| M_0684 | 320.0872 | 3.4747   | -5.9678 | 0.000335 | 0.10168  |
| M_0129 | 114.0297 | 3.3762   | 5.7674  | 0.000421 | 0.10934  |
| M_0836 | 174.0503 | 3.1126   | -5.2524 | 0.000772 | 0.162    |
| M_1379 | 160.0331 | 3.0533   | -5.1405 | 0.000885 | 0.162    |
| M_0363 | 227.0558 | 3.0215   | -5.0811 | 0.000952 | 0.162    |
| M_0208 | 205.0739 | 3.0092   | -5.0583 | 0.000979 | 0.162    |
| M_0975 | 204.0899 | 2.9652   | -4.9771 | 0.001083 | 0.16432  |
| M_1716 | 229.0884 | 2.8933   | 4.8459  | 0.001279 | 0.17899  |
| M_1266 | 158.0555 | 2.8385   | -4.7472 | 0.00145  | 0.18856  |
| M_0835 | 229.0715 | 2.774    | -4.6325 | 0.001683 | 0.20415  |
| M_0908 | 172.0637 | 2.7004   | -4.5032 | 0.001994 | 0.21744  |
| M_0500 | 168.0284 | 2.6923   | -4.4891 | 0.002031 | 0.21744  |
| M_0447 | 131.0584 | 2.5991   | -4.3285 | 0.002517 | 0.25449  |
| M_0812 | 216.0899 | 2.5655   | -4.2712 | 0.00272  | 0.25671  |
| M_1533 | 169.0351 | 2.5496   | 4.2443  | 0.002821 | 0.25671  |
| M_0121 | 143.0947 | 2.5079   | -4.1739 | 0.003105 | 0.26914  |
| M_1795 | 288.0421 | 2.4656   | 4.1031  | 0.003423 | 0.27951  |
| M_1099 | 218.0402 | 2.4287   | -4.0418 | 0.003726 | 0.27951  |
| M_1171 | 190.0741 | 2.4223   | -4.0312 | 0.003782 | 0.27951  |
| M_1436 | 1696.783 | 2.4157   | 4.0203  | 0.003839 | 0.27951  |
| M_0446 | 151.0609 | 2.3925   | -3.982  | 0.00405  | 0.28352  |
| M_0194 | 348.0472 | 2.3201   | 3.8634  | 0.004786 | 0.32259  |
| M_0045 | 219.1106 | 2.3013   | -3.8329 | 0.004997 | 0.32481  |
| M_1131 | 297.0895 | 2.2415   | -3.7364 | 0.005735 | 0.34975  |
| M_0664 | 251.0703 | 2.2337   | 3.7239  | 0.005838 | 0.34975  |
| M_0268 | 260.1372 | 2.225    | -3.7099 | 0.005957 | 0.34975  |
| M_0941 | 201.1112 | 2.1981   | -3.667  | 0.006337 | 0.3584   |
| M_0876 | 283.0915 | 2.1834   | -3.6435 | 0.006556 | 0.3584   |
| M_1332 | 803.4254 | 2.1742   | 3.6289  | 0.006695 | 0.3584   |
| M_0076 | 145.158  | 2.1416   | -3.5772 | 0.007218 | 0.35933  |
| M_0075 | 128.1314 | 2.1403   | -3.5752 | 0.007239 | 0.35933  |
| M_0952 | 83.01202 | 2.1364   | -3.5689 | 0.007305 | 0.35933  |
| M_0475 | 170.0262 | 2.1012   | 3.5134  | 0.007922 | 0.37943  |
| M_0936 | 217.9819 | 2.0762   | -3.4741 | 0.008392 | 0.37981  |
| M_1475 | 232.0559 | 2.0694   | -3.4636 | 0.008523 | 0.37981  |
| M_0267 | 245.1627 | 2.0677   | -3.4609 | 0.008556 | 0.37981  |
| M_1153 | 309.1939 | 2.0265   | -3.3966 | 0.009408 | 0.39728  |
| M_0699 | 206.0069 | 2.0257   | -3.3952 | 0.009427 | 0.39728  |
| M_1494 | 220.0848 | 2.0175   | 3.3826  | 0.009605 | 0.39728  |

|        |          |        |         |          |         |
|--------|----------|--------|---------|----------|---------|
| M_0206 | 158.044  | 2.0045 | -3.3624 | 0.009897 | 0.39975 |
| M_1284 | 83.0109  | 1.9955 | -3.3484 | 0.010104 | 0.39975 |
| M_0496 | 207.0896 | 1.9838 | -3.3302 | 0.010381 | 0.40197 |
| M_1297 | 232.1676 | 1.9661 | 3.3029  | 0.010811 | 0.40993 |
| M_0532 | 257.1027 | 1.9085 | 3.2142  | 0.012346 | 0.45855 |
| M_1214 | 157.0767 | 1.8686 | -3.1532 | 0.013534 | 0.48297 |
| M_0592 | 246.1004 | 1.8606 | -3.141  | 0.013784 | 0.48297 |
| M_1083 | 155.0696 | 1.8588 | -3.1382 | 0.013842 | 0.48297 |
| M_0863 | 222.1004 | 1.8519 | -3.1277 | 0.014064 | 0.48297 |
| M_1376 | 200.0296 | 1.8295 | -3.0936 | 0.014808 | 0.49222 |
| M_1327 | 124.0318 | 1.7904 | 3.0343  | 0.016203 | 0.49222 |
| M_0364 | 188.1525 | 1.7889 | -3.032  | 0.016259 | 0.49222 |
| M_0012 | 120.065  | 1.7878 | -3.0304 | 0.016301 | 0.49222 |
| M_0262 | 159.1259 | 1.7855 | -3.0269 | 0.016386 | 0.49222 |
| M_0745 | 279.147  | 1.7842 | -3.0249 | 0.016436 | 0.49222 |
| M_0192 | 122.0483 | 1.7824 | 3.0221  | 0.016506 | 0.49222 |
| M_1606 | 246.1943 | 1.7764 | -3.0131 | 0.016734 | 0.49222 |
| M_1086 | 177.0168 | 1.7755 | -3.0118 | 0.016768 | 0.49222 |
| M_0068 | 131.0947 | 1.759  | -2.9868 | 0.017419 | 0.5032  |
| M_0295 | 229.0884 | 1.746  | 2.9673  | 0.017946 | 0.50634 |
| M_1632 | 184.0906 | 1.7267 | 2.9382  | 0.018761 | 0.51735 |
| M_0509 | 146.1055 | 1.711  | -2.9145 | 0.019454 | 0.52844 |
| M_1761 | 158.0692 | 1.6982 | 2.8954  | 0.020034 | 0.5299  |
| M_0217 | 96.069   | 1.6946 | -2.8899 | 0.020201 | 0.5299  |
| M_0412 | 294.1215 | 1.6846 | -2.8749 | 0.020672 | 0.5299  |
| M_0642 | 151.0386 | 1.6502 | -2.8233 | 0.022379 | 0.54925 |
| M_0179 | 142.0467 | 1.6494 | -2.8221 | 0.02242  | 0.54925 |
| M_1118 | 188.1161 | 1.6471 | -2.8187 | 0.022538 | 0.54925 |
| M_0640 | 105.0583 | 1.6452 | 2.816   | 0.022634 | 0.54925 |
| M_0528 | 363.058  | 1.6359 | 2.802   | 0.023128 | 0.55385 |
| M_0228 | 162.0528 | 1.5943 | 2.74    | 0.02545  | 0.60154 |
| M_0084 | 136.0386 | 1.5835 | -2.7239 | 0.026093 | 0.60531 |
| M_0738 | 304.2401 | 1.5778 | 2.7154  | 0.026437 | 0.60531 |
| M_1488 | 268.0671 | 1.5746 | -2.7107 | 0.02663  | 0.60531 |
| M_1042 | 192.1475 | 1.5663 | -2.6983 | 0.027147 | 0.60531 |
| M_1112 | 117.0429 | 1.5632 | 2.6936  | 0.027343 | 0.60531 |
| M_0004 | 131.0948 | 1.5542 | -2.6803 | 0.027913 | 0.60531 |
| M_0199 | 153.0766 | 1.5538 | -2.6797 | 0.027937 | 0.60531 |
| M_0358 | 120.058  | 1.5289 | -2.6427 | 0.02959  | 0.60805 |
| M_1109 | 249.0313 | 1.5204 | -2.6301 | 0.030175 | 0.60805 |
| M_1081 | 179.0583 | 1.514  | -2.6206 | 0.03062  | 0.60805 |
| M_0156 | 165.0766 | 1.5106 | -2.6156 | 0.03086  | 0.60805 |
| M_0303 | 164.0536 | 1.5036 | -2.6052 | 0.031362 | 0.60805 |
| M_1299 | 189.1113 | 1.496  | -2.594  | 0.031914 | 0.60805 |
| M_0682 | 284.1809 | 1.4953 | 2.5929  | 0.031968 | 0.60805 |
| M_0146 | 103.1002 | 1.4953 | 2.5929  | 0.031969 | 0.60805 |
| M_0597 | 246.1215 | 1.4912 | -2.5869 | 0.032267 | 0.60805 |

|        |          |        |         |          |         |
|--------|----------|--------|---------|----------|---------|
| M_0739 | 213.0441 | 1.4867 | 2.5802  | 0.032606 | 0.60805 |
| M_1010 | 166.0511 | 1.4846 | -2.5772 | 0.032761 | 0.60805 |
| M_0408 | 105.9938 | 1.4828 | -2.5744 | 0.032904 | 0.60805 |
| M_0801 | 131.0373 | 1.4762 | 2.5646  | 0.033405 | 0.60805 |
| M_0348 | 112.0139 | 1.4738 | -2.5611 | 0.033591 | 0.60805 |
| M_0391 | 181.074  | 1.4733 | -2.5604 | 0.033624 | 0.60805 |
| M_1007 | 146.0178 | 1.4718 | -2.5582 | 0.033744 | 0.60805 |
| M_0891 | 328.2377 | 1.4635 | -2.5459 | 0.034396 | 0.61373 |
| M_0189 | 115.0637 | 1.4579 | 2.5376  | 0.034842 | 0.61565 |
| M_1329 | 167.9885 | 1.4532 | -2.5307 | 0.035219 | 0.61628 |
| M_0097 | 114.0431 | 1.4491 | 2.5246  | 0.035555 | 0.61628 |
| M_0624 | 137.0478 | 1.426  | -2.4905 | 0.037494 | 0.62361 |
| M_0269 | 131.0696 | 1.4242 | 2.4878  | 0.037652 | 0.62361 |
| M_0994 | 264.1044 | 1.4219 | 2.4844  | 0.037852 | 0.62361 |
| M_0131 | 231.1471 | 1.4123 | -2.4702 | 0.038698 | 0.62361 |
| M_0031 | 102.0473 | 1.4122 | -2.4701 | 0.038706 | 0.62361 |
| M_0658 | 191.0616 | 1.4099 | -2.4667 | 0.038911 | 0.62361 |
| M_0916 | 272.0884 | 1.4098 | 2.4665  | 0.038925 | 0.62361 |
| M_0033 | 119.0738 | 1.4051 | -2.4596 | 0.039344 | 0.62361 |
| M_0195 | 134.0249 | 1.4027 | -2.456  | 0.039565 | 0.62361 |
| M_0176 | 201.0402 | 1.4005 | -2.4528 | 0.039763 | 0.62361 |
| M_0906 | 213.0435 | 1.3973 | -2.4481 | 0.040055 | 0.62361 |
| M_0109 | 129.0791 | 1.397  | -2.4476 | 0.040089 | 0.62361 |
| M_0932 | 126.0432 | 1.3919 | -2.44   | 0.040563 | 0.62564 |
| M_0773 | 130.0421 | 1.3818 | 2.4252  | 0.041513 | 0.63491 |
| M_0470 | 220.026  | 1.3774 | -2.4187 | 0.041935 | 0.63602 |
| M_0141 | 120.065  | 1.3638 | -2.3986 | 0.043269 | 0.64233 |
| M_0755 | 228.1473 | 1.3583 | -2.3905 | 0.043824 | 0.64233 |
| M_1228 | 538.3067 | 1.3575 | 2.3893  | 0.0439   | 0.64233 |
| M_0860 | 202.1428 | 1.3571 | -2.3888 | 0.04394  | 0.64233 |
| M_0794 | 116.0477 | 1.3554 | 2.3862  | 0.044116 | 0.64233 |
| M_1492 | 522.3517 | 1.3494 | 2.3773  | 0.044733 | 0.64503 |
| M_0353 | 159.126  | 1.3439 | -2.3693 | 0.045296 | 0.64503 |
| M_0402 | 113.0593 | 1.3433 | -2.3683 | 0.045365 | 0.64503 |
| M_0081 | 231.147  | 1.3396 | -2.3629 | 0.045754 | 0.64552 |
| M_0589 | 364.0981 | 1.3323 | -2.3522 | 0.046525 | 0.64859 |
| M_0350 | 348.0472 | 1.3247 | 2.3409  | 0.047351 | 0.64859 |
| M_1050 | 430.27   | 1.3241 | 2.34    | 0.047417 | 0.64859 |
| M_0799 | 130.042  | 1.3213 | -2.3358 | 0.047724 | 0.64859 |
| M_0092 | 179.0582 | 1.3182 | -2.3313 | 0.048062 | 0.64859 |
| M_1002 | 177.1114 | 1.3103 | -2.3196 | 0.048948 | 0.64859 |
| M_0120 | 145.1103 | 1.3059 | -2.3132 | 0.049444 | 0.64859 |
| M_1575 | 188.0797 | 1.3052 | 2.3122  | 0.049521 | 0.64859 |
| M_0177 | 268.0807 | 1.3044 | -2.311  | 0.049615 | 0.64859 |
| M_0663 | 201.1113 | 1.3007 | -2.3055 | 0.05004  | 0.64859 |
| M_0082 | 155.0348 | 1.2999 | 2.3044  | 0.050128 | 0.64859 |
| M_1218 | 203.1268 | 1.2989 | -2.3028 | 0.050248 | 0.64859 |

|        |          |        |         |          |         |
|--------|----------|--------|---------|----------|---------|
| M_0249 | 545.3487 | 1.2905 | 2.2904  | 0.05123  | 0.65058 |
| M_0795 | 228.1473 | 1.2894 | -2.2888 | 0.05136  | 0.65058 |
| M_0165 | 309.1071 | 1.2861 | 2.2839  | 0.051751 | 0.65058 |
| M_0831 | 160.1292 | 1.2828 | 2.2791  | 0.052147 | 0.65058 |
| M_0276 | 267.0966 | 1.2746 | 2.2671  | 0.053134 | 0.65058 |
| M_0186 | 174.0793 | 1.2736 | -2.2655 | 0.053262 | 0.65058 |
| M_1147 | 481.3171 | 1.2664 | -2.255  | 0.054145 | 0.65058 |
| M_0207 | 175.0634 | 1.263  | -2.2499 | 0.054575 | 0.65058 |
| M_1044 | 202.0453 | 1.2576 | 2.242   | 0.055255 | 0.65058 |
| M_0584 | 143.0947 | 1.2543 | -2.2371 | 0.055674 | 0.65058 |
| M_0535 | 312.1549 | 1.2529 | 2.2351  | 0.055854 | 0.65058 |
| M_1308 | 495.3327 | 1.2512 | 2.2325  | 0.05608  | 0.65058 |
| M_0140 | 347.063  | 1.2395 | 2.2152  | 0.057614 | 0.65058 |
| M_1806 | 175.1147 | 1.2344 | 2.2077  | 0.058287 | 0.65058 |
| M_0617 | 155.0696 | 1.2335 | -2.2063 | 0.058413 | 0.65058 |
| M_1473 | 206.1055 | 1.2249 | 2.1936  | 0.059585 | 0.65058 |
| M_0961 | 157.0767 | 1.2234 | -2.1914 | 0.059786 | 0.65058 |
| M_0297 | 208.0848 | 1.2223 | -2.1898 | 0.059943 | 0.65058 |
| M_0629 | 275.1115 | 1.2162 | -2.1807 | 0.060791 | 0.65058 |
| M_0698 | 203.127  | 1.2153 | -2.1795 | 0.060914 | 0.65058 |
| M_1364 | 116.0498 | 1.211  | 2.1732  | 0.061516 | 0.65058 |
| M_0054 | 152.0586 | 1.2107 | -2.1727 | 0.061563 | 0.65058 |
| M_0332 | 348.0473 | 1.2059 | 2.1656  | 0.062241 | 0.65058 |
| M_0007 | 165.0791 | 1.2015 | -2.1591 | 0.062874 | 0.65058 |
| M_0009 | 148.0525 | 1.1977 | -2.1535 | 0.063425 | 0.65058 |
| M_1287 | 259.099  | 1.1975 | 2.1531  | 0.063463 | 0.65058 |
| M_1547 | 495.3329 | 1.1964 | 2.1516  | 0.063619 | 0.65058 |
| M_0173 | 250.0953 | 1.1936 | -2.1474 | 0.064036 | 0.65058 |
| M_0793 | 84.02136 | 1.1682 | 2.1098  | 0.06789  | 0.65058 |
| M_0285 | 191.0582 | 1.1639 | -2.1035 | 0.068563 | 0.65058 |
| M_0181 | 192.0899 | 1.1624 | -2.1012 | 0.068809 | 0.65058 |
| M_1456 | 112.0141 | 1.1576 | 2.0942  | 0.069563 | 0.65058 |
| M_0196 | 347.063  | 1.1551 | 2.0905  | 0.069968 | 0.65058 |
| M_1487 | 68.02703 | 1.1514 | 2.085   | 0.070561 | 0.65058 |
| M_0420 | 228.1473 | 1.1488 | -2.0812 | 0.070983 | 0.65058 |
| M_0955 | 248.1483 | 1.1456 | -2.0765 | 0.071508 | 0.65058 |
| M_0049 | 241.918  | 1.1446 | -2.0749 | 0.071685 | 0.65058 |
| M_1180 | 109.0202 | 1.142  | 2.0711  | 0.072104 | 0.65058 |
| M_1312 | 524.2715 | 1.1344 | 2.0598  | 0.073384 | 0.65058 |
| M_0850 | 113.1208 | 1.1343 | -2.0597 | 0.073393 | 0.65058 |
| M_0605 | 305.0404 | 1.1282 | -2.0506 | 0.074444 | 0.65058 |
| M_0185 | 161.1052 | 1.1235 | -2.0436 | 0.075248 | 0.65058 |
| M_0872 | 260.0296 | 1.1225 | 2.0421  | 0.075431 | 0.65058 |
| M_0403 | 156.0763 | 1.1143 | 2.03    | 0.076855 | 0.65058 |
| M_1183 | 566.3183 | 1.1085 | 2.0213  | 0.077902 | 0.65058 |
| M_1677 | 188.0661 | 1.1082 | -2.0209 | 0.077944 | 0.65058 |
| M_1658 | 315.1317 | 1.105  | -2.0161 | 0.07853  | 0.65058 |

|        |          |        |         |          |         |
|--------|----------|--------|---------|----------|---------|
| M_0599 | 260.1371 | 1.1028 | -2.0129 | 0.078925 | 0.65058 |
| M_0305 | 121.9175 | 1.1003 | -2.0092 | 0.079377 | 0.65058 |
| M_1008 | 167.0921 | 1.087  | -1.9894 | 0.081851 | 0.65058 |
| M_1584 | 203.1266 | 1.0857 | -1.9874 | 0.0821   | 0.65058 |
| M_1041 | 268.0823 | 1.0845 | -1.9858 | 0.08231  | 0.65058 |
| M_0122 | 145.1104 | 1.0817 | -1.9815 | 0.082859 | 0.65058 |
| M_0501 | 228.1351 | 1.0765 | -1.9737 | 0.083859 | 0.65058 |
| M_1162 | 157.1104 | 1.0689 | -1.9626 | 0.08532  | 0.65058 |
| M_0492 | 137.0477 | 1.0679 | -1.961  | 0.085526 | 0.65058 |
| M_1400 | 161.0229 | 1.0646 | -1.956  | 0.086188 | 0.65058 |
| M_0940 | 568.3341 | 1.0643 | 1.9557  | 0.086235 | 0.65058 |
| M_1513 | 249.0725 | 1.0496 | -1.9337 | 0.089212 | 0.65058 |
| M_1028 | 153.0514 | 1.0434 | 1.9245  | 0.090487 | 0.65058 |
| M_0074 | 139.061  | 1.0404 | 1.92    | 0.091114 | 0.65058 |
| M_0583 | 203.1268 | 1.0385 | -1.9171 | 0.091518 | 0.65058 |
| M_0839 | 117.0429 | 1.0261 | 1.8986  | 0.094173 | 0.65058 |
| M_1698 | 248.1008 | 1.026  | 1.8984  | 0.094193 | 0.65058 |
| M_1022 | 232.0848 | 1.0206 | -1.8904 | 0.095369 | 0.65058 |
| M_1205 | 147.0073 | 1.0201 | -1.8897 | 0.095468 | 0.65058 |
| M_0920 | 113.0246 | 1.0198 | -1.8892 | 0.095546 | 0.65058 |
| M_1149 | 316.2039 | 1.0157 | 1.8831  | 0.096448 | 0.65058 |
| M_1500 | 201.1    | 1.0152 | -1.8823 | 0.096568 | 0.65058 |
| M_0724 | 518.318  | 1.0133 | 1.8795  | 0.096986 | 0.65058 |
| M_1078 | 165.0179 | 1.0115 | -1.8767 | 0.097393 | 0.65058 |
| M_0503 | 204.0898 | 1.004  | 1.8656  | 0.099072 | 0.65058 |
| M_0319 | 369.0451 | 1.0019 | 1.8623  | 0.099574 | 0.65058 |