

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF013017\  
 Data File : BF092644.D  
 Acq On : 30 Jan 2017 20:10  
 Operator : SJ/MA  
 Sample : PB96538BL  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB96538BL

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 4.510       | 210           | 212         | 218          | rVB      | 73151          | 101482        | 1.99%           | 0.248%        |
| 2         | 5.161       | 265           | 269         | 277          | rVB      | 1418390        | 2159114       | 42.28%          | 5.287%        |
| 3         | 5.573       | 302           | 305         | 308          | rBV      | 3119747        | 4320583       | 84.62%          | 10.579%       |
| 4         | 6.602       | 392           | 395         | 397          | rBV      | 3799247        | 3981697       | 77.98%          | 9.750%        |
| 5         | 6.727       | 403           | 406         | 409          | rBV      | 3401606        | 4075922       | 79.82%          | 9.980%        |
| 6         | 6.956       | 424           | 426         | 429          | rVB      | 1019474        | 904418        | 17.71%          | 2.215%        |
| 7         | 7.116       | 437           | 440         | 443          | rBV      | 3512843        | 3203812       | 62.74%          | 7.845%        |
| 8         | 7.527       | 473           | 476         | 478          | rBV      | 2666739        | 2763001       | 54.11%          | 6.765%        |
| 9         | 8.247       | 536           | 539         | 542          | rBV      | 1246188        | 1188018       | 23.27%          | 2.909%        |
| 10        | 9.333       | 630           | 634         | 636          | rBV      | 3931275        | 5106113       | 100.00%         | 12.503%       |
| 11        | 9.928       | 677           | 686         | 690          | rVV      | 158730         | 398758        | 7.81%           | 0.976%        |
| 12        | 10.008      | 690           | 693         | 695          | rVB      | 1537203        | 1429139       | 27.99%          | 3.499%        |
| 13        | 10.796      | 759           | 762         | 765          | rBV      | 2303301        | 2706706       | 53.01%          | 6.628%        |
| 14        | 11.493      | 820           | 823         | 825          | rBV      | 1637940        | 1405319       | 27.52%          | 3.441%        |
| 15        | 13.082      | 959           | 962         | 965          | rBV      | 4303554        | 4498007       | 88.09%          | 11.014%       |
| 16        | 14.134      | 1051          | 1054        | 1056         | rBV      | 1412365        | 1388597       | 27.19%          | 3.400%        |
| 17        | 14.980      | 1125          | 1128        | 1130         | rBV      | 71942          | 86285         | 1.69%           | 0.211%        |
| 18        | 15.608      | 1180          | 1183        | 1190         | rVB      | 810816         | 1122960       | 21.99%          | 2.750%        |

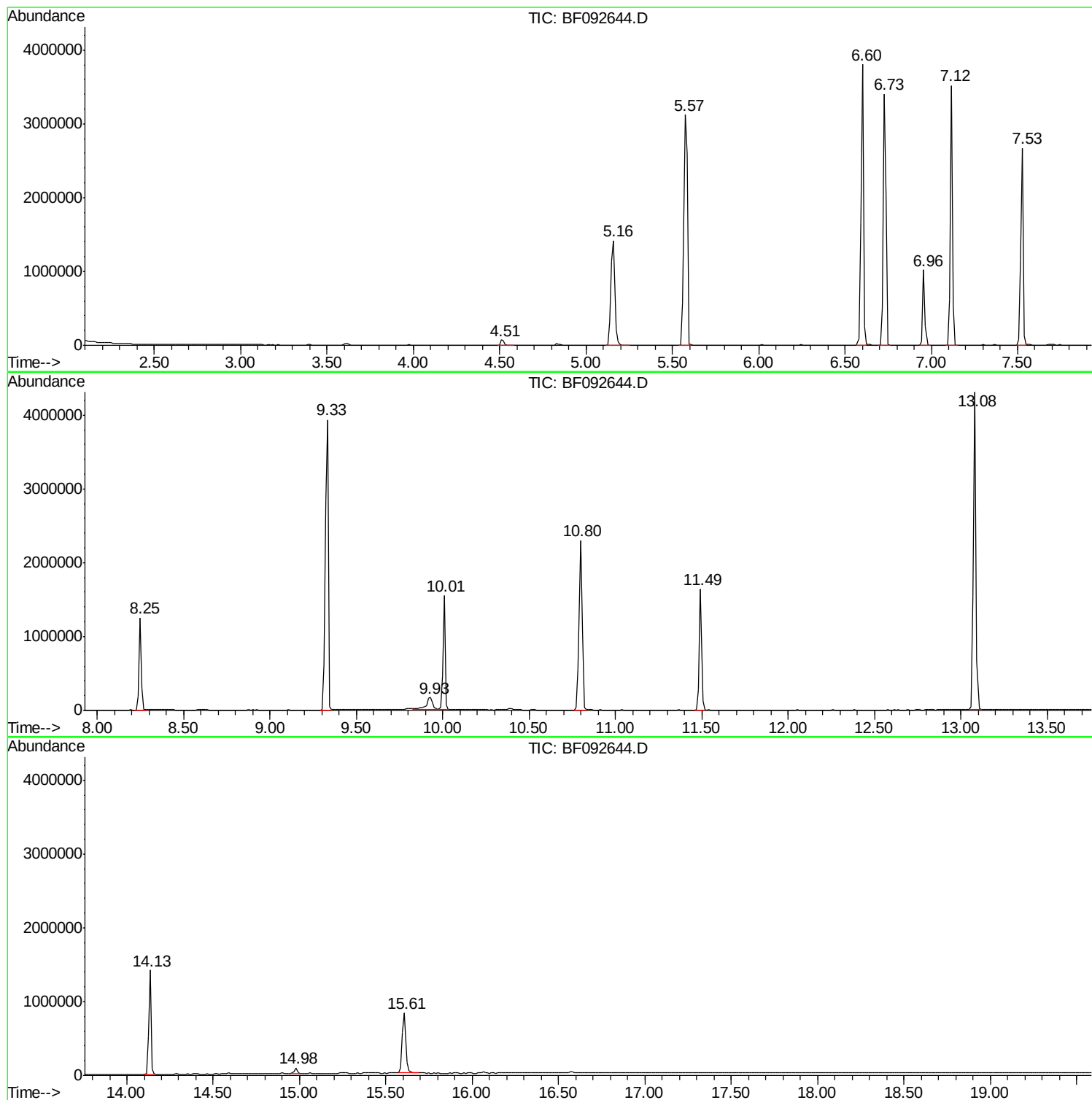
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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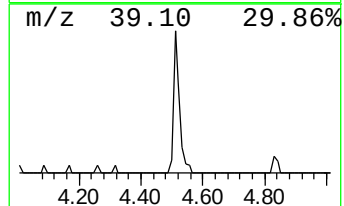
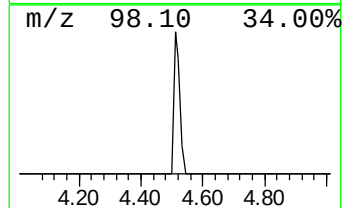
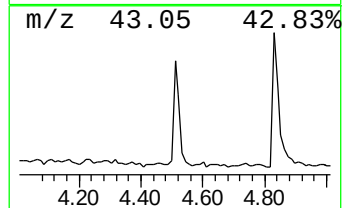
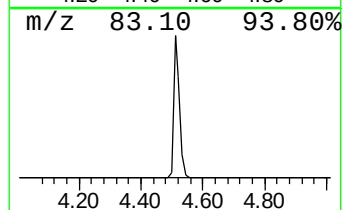
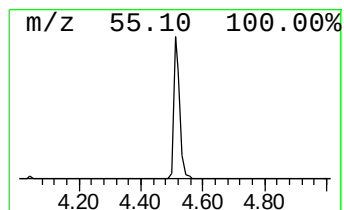
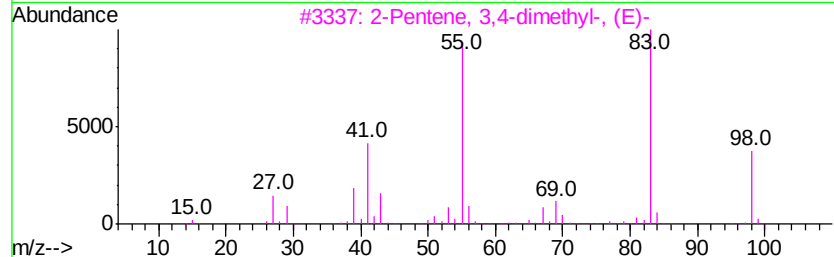
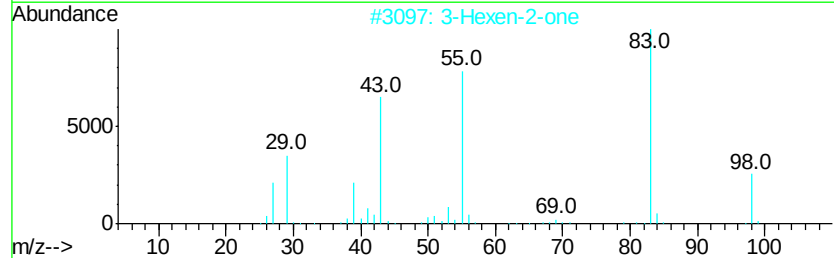
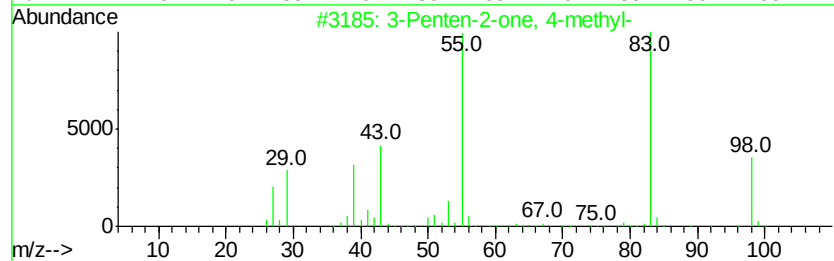
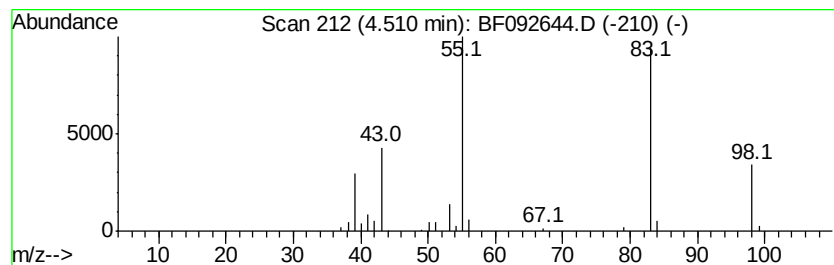
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.51 | 2.24 ng | 101482 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|--------------------------------|----|---------|-------------|------|
| 1    | 5  | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 95   |
| 2    |    | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |    | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 86   |
| 4    |    | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 86   |
| 5    |    | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |



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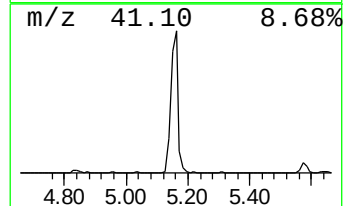
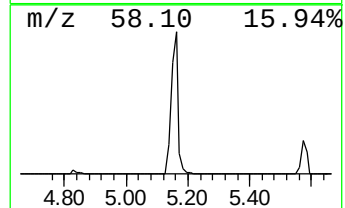
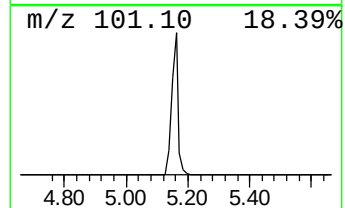
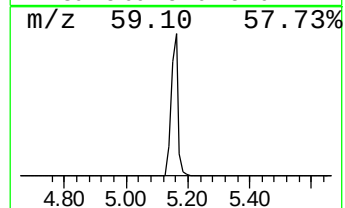
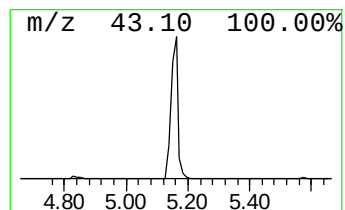
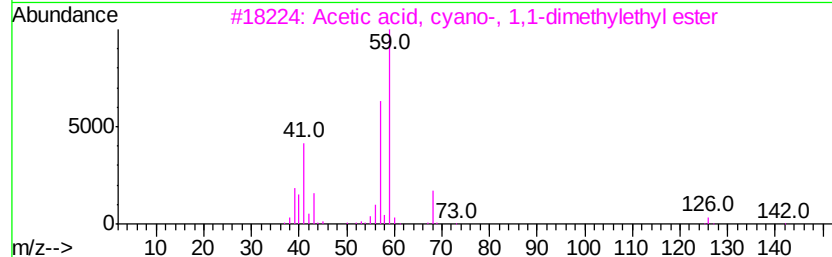
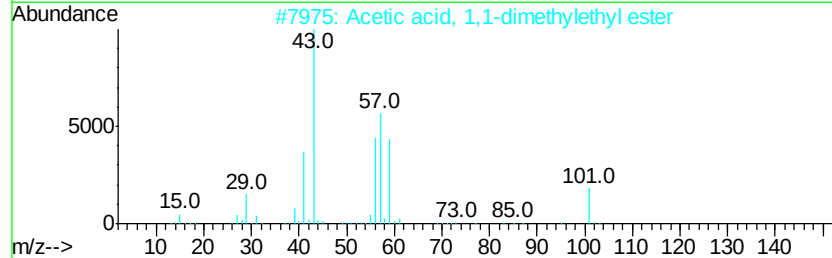
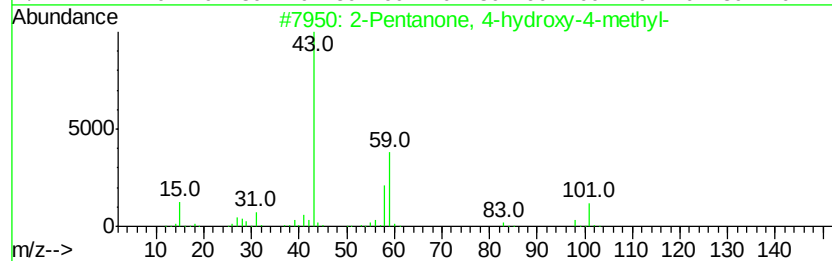
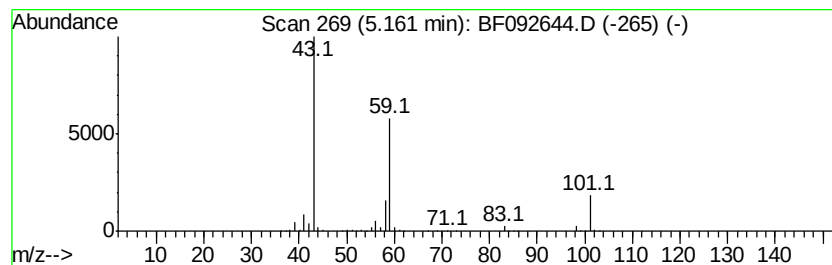
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 5.16 | 47.75 ng | 2159110 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e...  | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    | Ethanol, pentamethyl-                | 116 | C7H16O   | 000594-83-2 | 9    |
| 5    |    | 3-Hydroxy-3-methyl-2-butanone        | 102 | C5H10O2  | 000115-22-0 | 9    |



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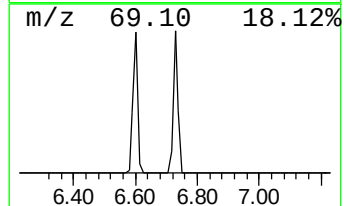
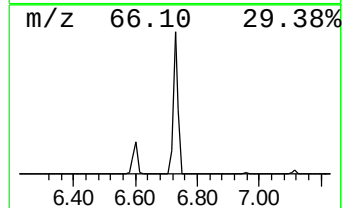
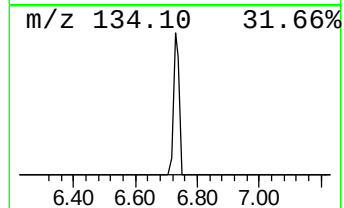
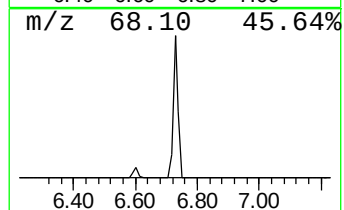
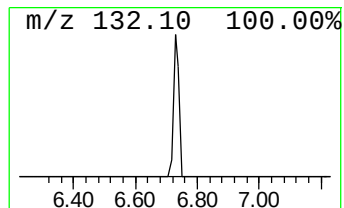
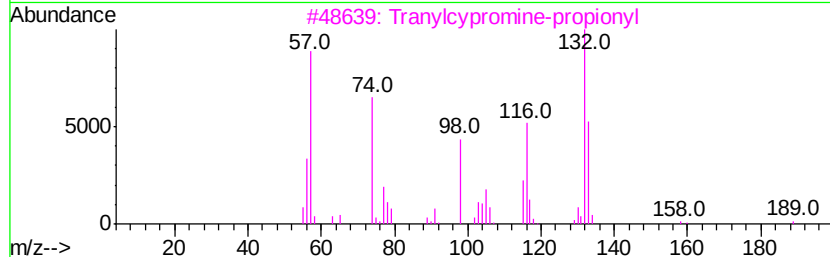
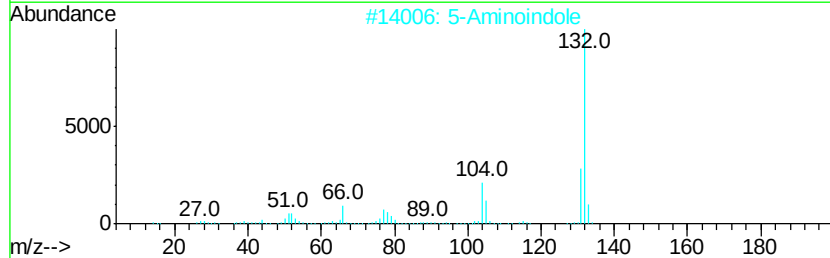
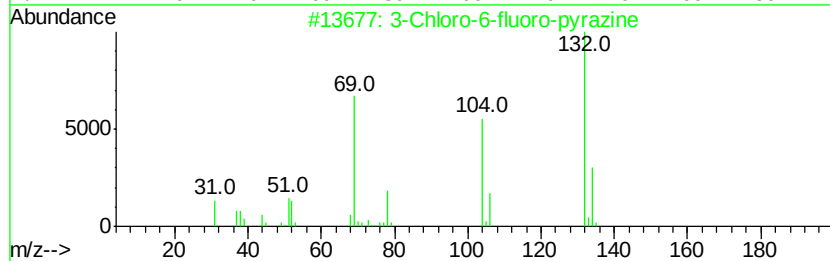
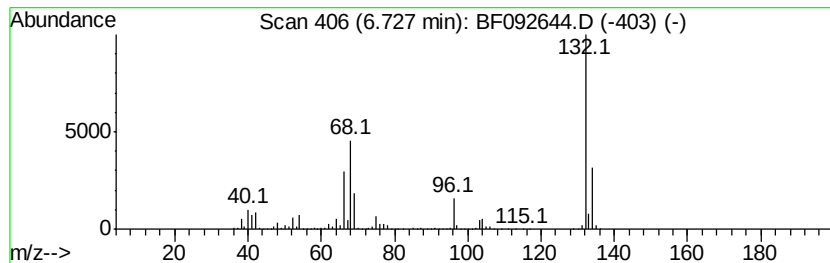
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.73 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.73 | 90.13 ng | 4075920 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 3    |    | Tranvlcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4  | 9    |



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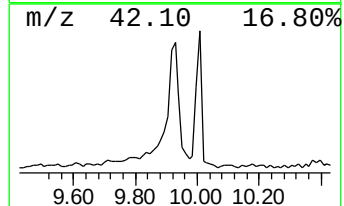
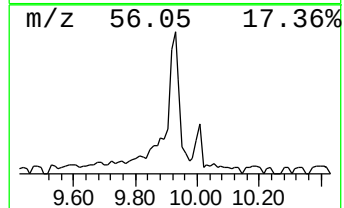
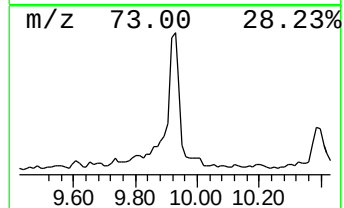
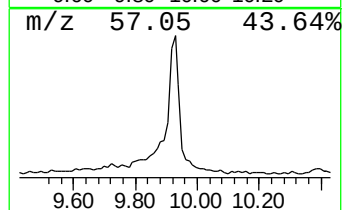
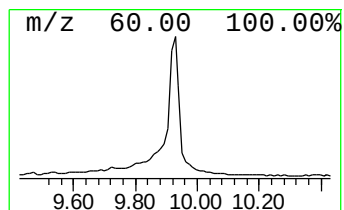
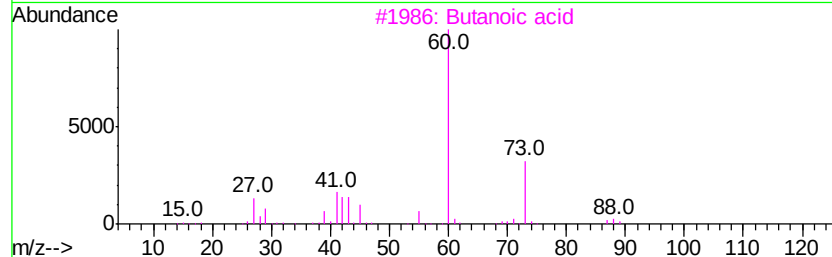
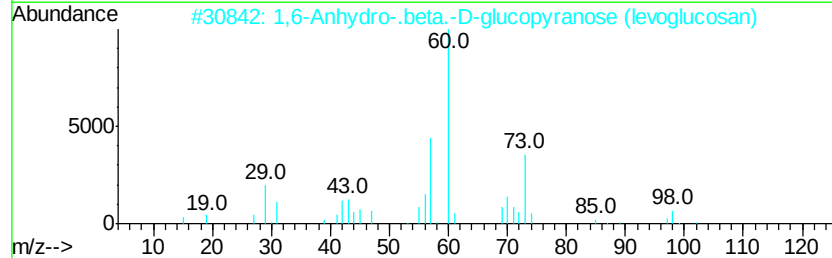
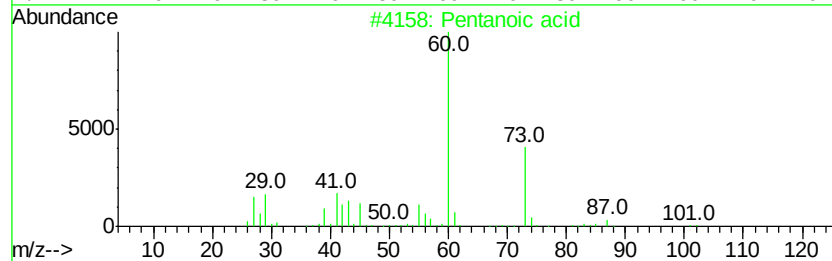
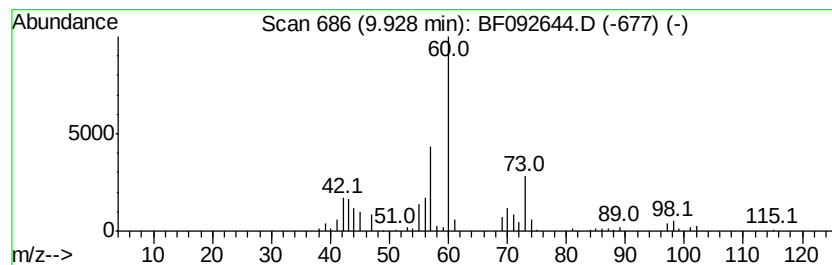
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Peak Number 5 Pentanoic acid Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD | R.T.  |
|------|---------|--------|------------------|-------|
| 9.93 | 5.58 ng | 398758 | Acenaphthene-d10 | 10.01 |

| Hit# of | 5                                   | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------------------------------|--------------|-----|---------|-------------|------|
| 1       | Pentanoic acid                      |              | 102 | C5H10O2 | 000109-52-4 | 59   |
| 2       | 1,6-Anhydro-.beta.-D-glucopyrano... |              | 162 | C6H10O5 | 000498-07-7 | 53   |
| 3       | Butanoic acid                       |              | 88  | C4H8O2  | 000107-92-6 | 52   |
| 4       | 5-Hexenoic acid                     |              | 114 | C6H10O2 | 001577-22-6 | 42   |
| 5       | Heptanoic acid                      |              | 130 | C7H14O2 | 000111-14-8 | 42   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |      |         |       |          | #                     | RT    | Resp    | Conc |
| 3-Penten-2-one, 4... | 4.51 | 2.2     | ng    | 101482   | 1                     | 6.96  | 904418  | 20.0 |
| 2-Pentanone, 4-hy... | 5.16 | 47.8    | ng    | 2159110  | 1                     | 6.96  | 904418  | 20.0 |
| unknown6.73          | 6.73 | 90.1    | ng    | 4075920  | 1                     | 6.96  | 904418  | 20.0 |
| Pentanoic acid       | 9.93 | 5.6     | ng    | 398758   | 3                     | 10.01 | 1429140 | 20.0 |