

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090119\  
 Data File : BG042674.D  
 Acq On : 1 Sep 2019 23:06  
 Operator : HP/JU  
 Sample : K4554-22  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-9-(7-9)

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:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG082219.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         | 3.118       | 3             | 5           | 20           | rVB      | 142790         | 180722        | 7.10%           | 1.528%        |
| 2         | 5.556       | 413           | 420         | 434          | rBV      | 407133         | 677882        | 26.62%          | 5.731%        |
| 3         | 7.160       | 685           | 693         | 712          | rBV      | 417691         | 815855        | 32.04%          | 6.897%        |
| 4         | 7.530       | 748           | 756         | 767          | rBV      | 456376         | 792468        | 31.12%          | 6.699%        |
| 5         | 7.994       | 829           | 835         | 845          | rVB      | 92060          | 152230        | 5.98%           | 1.287%        |
| 6         | 8.323       | 883           | 891         | 903          | rBV      | 371231         | 637285        | 25.03%          | 5.387%        |
| 7         | 9.164       | 1027          | 1034        | 1051         | rBV      | 241907         | 461970        | 18.14%          | 3.905%        |
| 8         | 10.820      | 1307          | 1316        | 1332         | rBV      | 99659          | 204799        | 8.04%           | 1.731%        |
| 9         | 13.276      | 1726          | 1734        | 1752         | rBV      | 835551         | 1335319       | 52.44%          | 11.289%       |
| 10        | 14.111      | 1869          | 1876        | 1890         | rBV      | 34672          | 72007         | 2.83%           | 0.609%        |
| 11        | 14.657      | 1962          | 1969        | 1982         | rBV      | 210267         | 353911        | 13.90%          | 2.992%        |
| 12        | 16.149      | 2216          | 2223        | 2243         | rBV      | 742210         | 1291271       | 50.71%          | 10.916%       |
| 13        | 17.407      | 2431          | 2437        | 2451         | rBV2     | 297607         | 498689        | 19.58%          | 4.216%        |
| 14        | 20.016      | 2875          | 2881        | 2893         | rBV      | 1823523        | 2546400       | 100.00%         | 21.527%       |
| 15        | 21.320      | 3098          | 3103        | 3114         | rBV2     | 56942          | 112307        | 4.41%           | 0.949%        |
| 16        | 21.684      | 3158          | 3165        | 3176         | rBV      | 375310         | 649294        | 25.50%          | 5.489%        |
| 17        | 22.483      | 3295          | 3301        | 3306         | rBV      | 18076          | 32912         | 1.29%           | 0.278%        |
| 18        | 23.182      | 3413          | 3420        | 3427         | rVB2     | 25117          | 49435         | 1.94%           | 0.418%        |
| 19        | 23.370      | 3445          | 3452        | 3460         | rVB2     | 63918          | 118403        | 4.65%           | 1.001%        |
| 20        | 23.993      | 3550          | 3558        | 3566         | rVB2     | 26060          | 59104         | 2.32%           | 0.500%        |
| 21        | 24.922      | 3704          | 3716        | 3736         | rBV2     | 233574         | 742283        | 29.15%          | 6.275%        |
| 22        | 26.079      | 3903          | 3913        | 3922         | rBV4     | 15528          | 44425         | 1.74%           | 0.376%        |

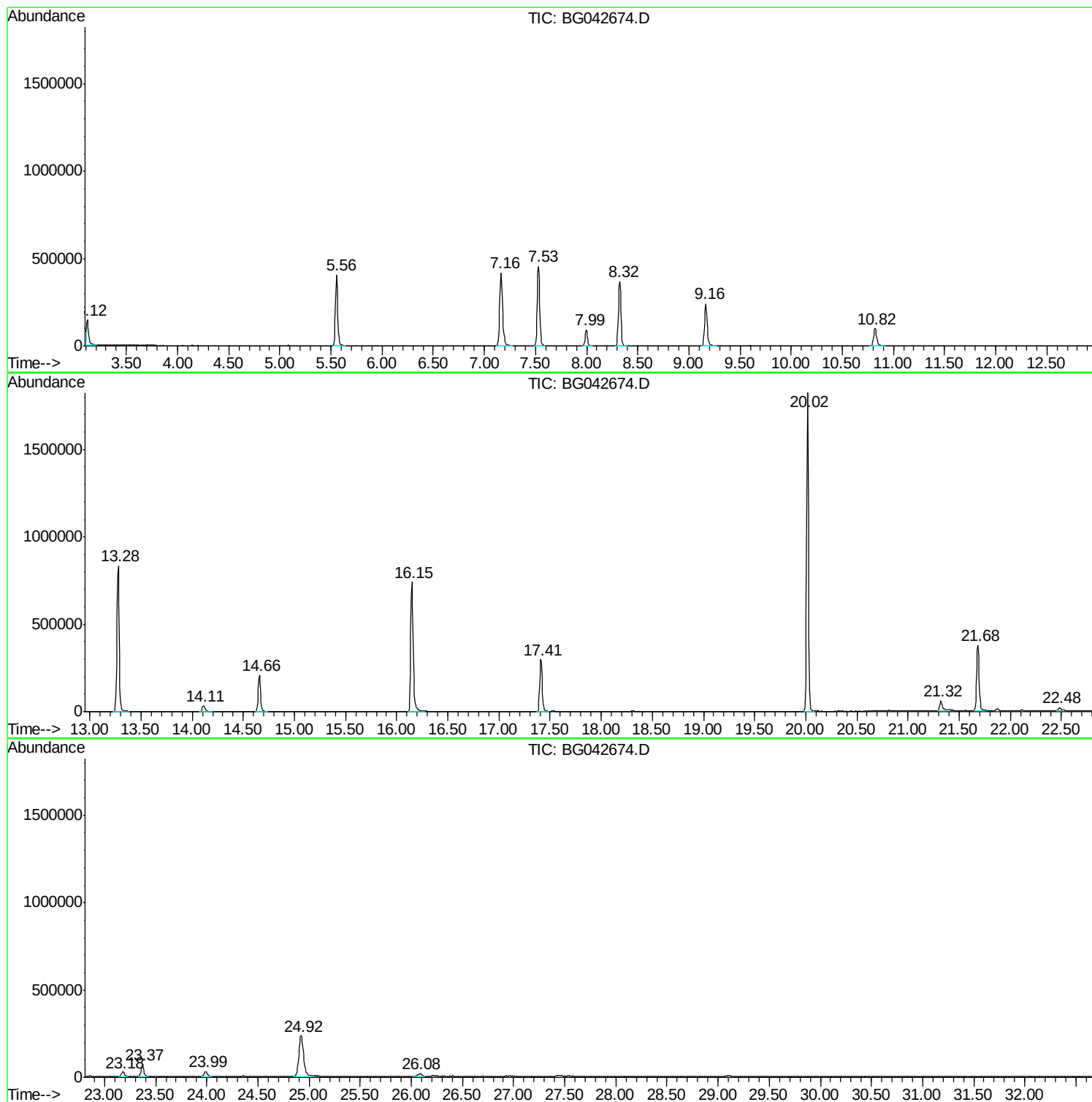
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ClientSampleId :  
SB-9-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082219.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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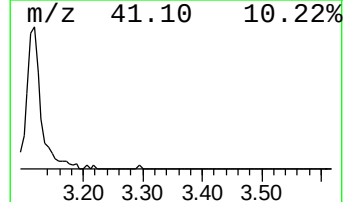
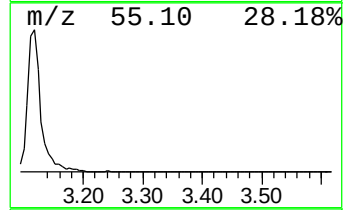
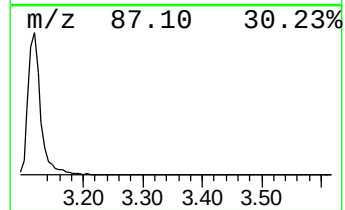
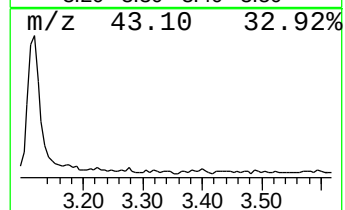
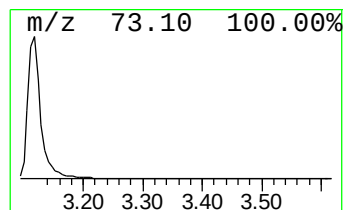
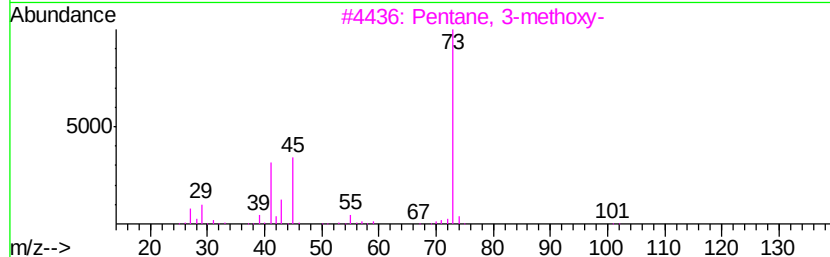
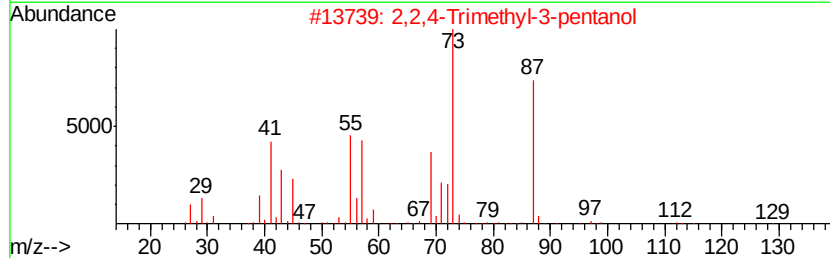
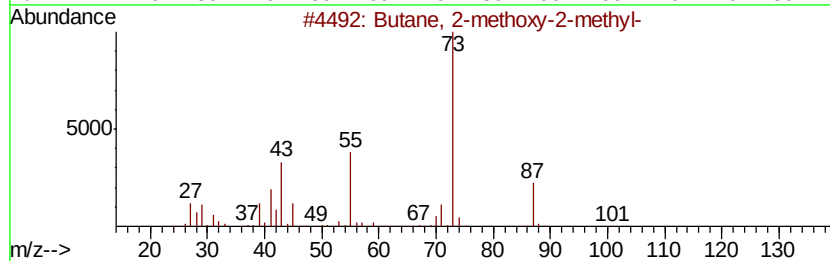
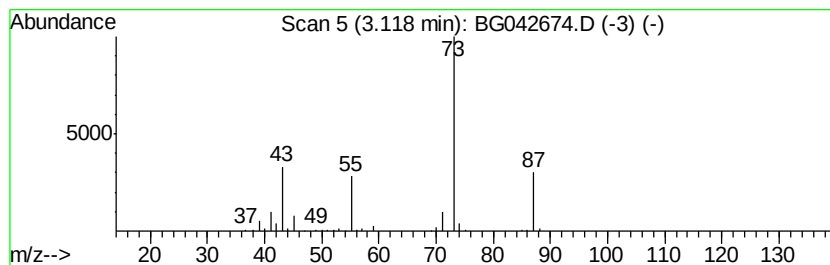
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 3.12 | 23.74 ng | 180722 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 4    |    | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 12   |
| 5    |    | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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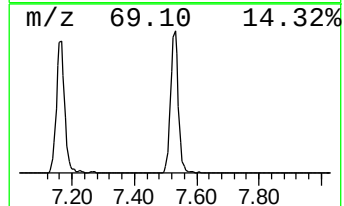
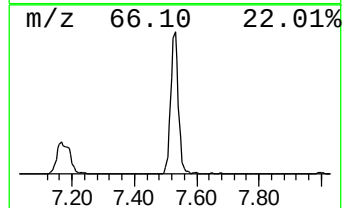
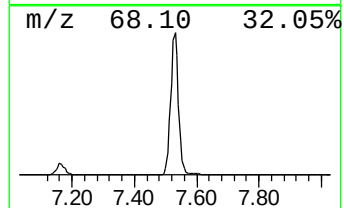
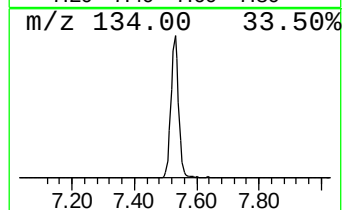
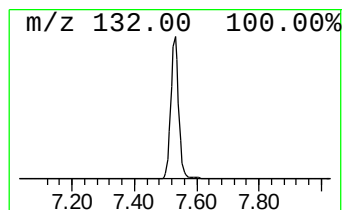
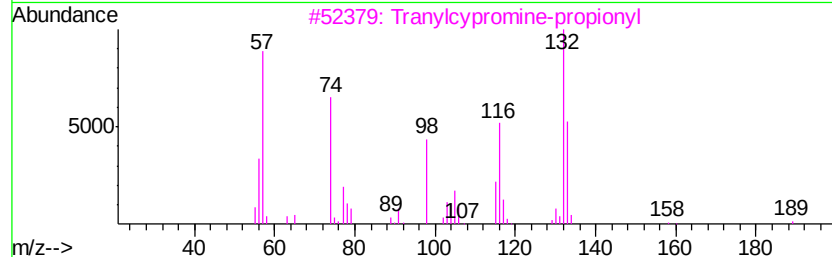
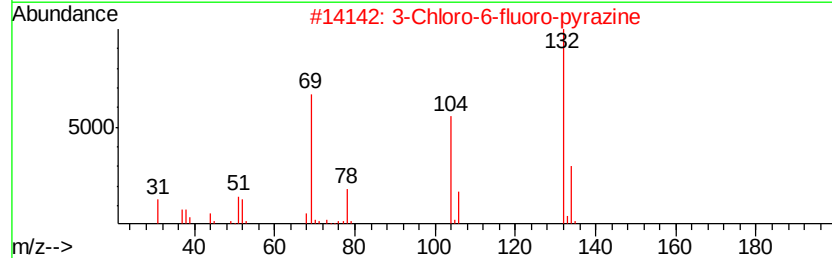
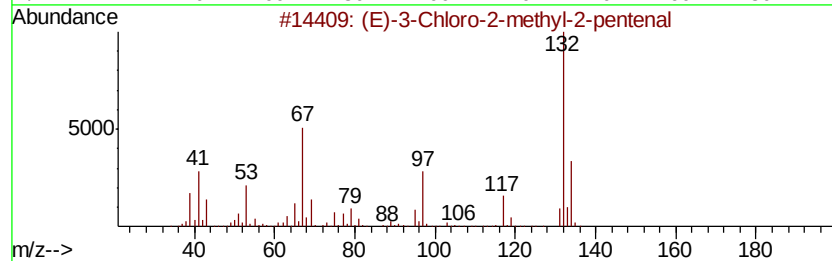
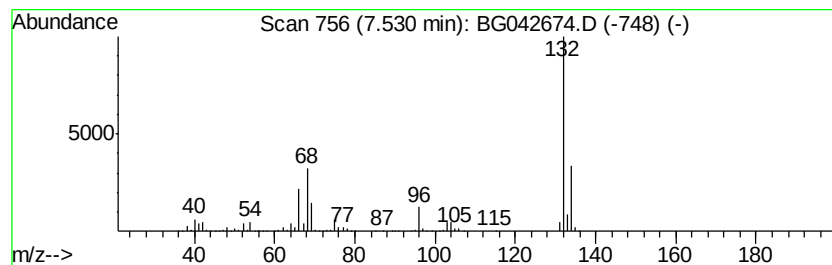
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Peak Number 2 unknown7.53 Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD       | R.T. |
|------|-----------|--------|------------------------|------|
| 7.53 | 104.12 ng | 792468 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 25   |
| 3    |    | Tranvlcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 16   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 16   |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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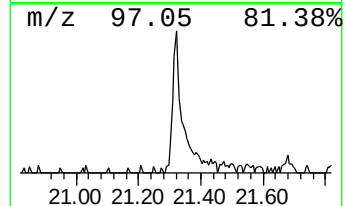
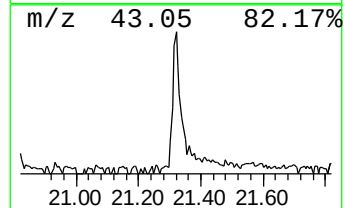
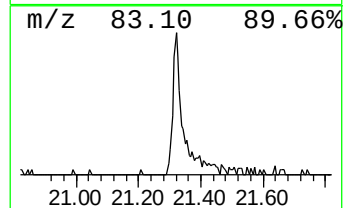
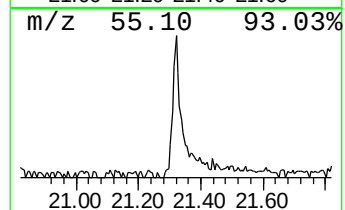
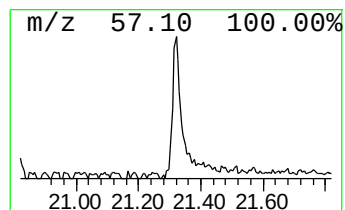
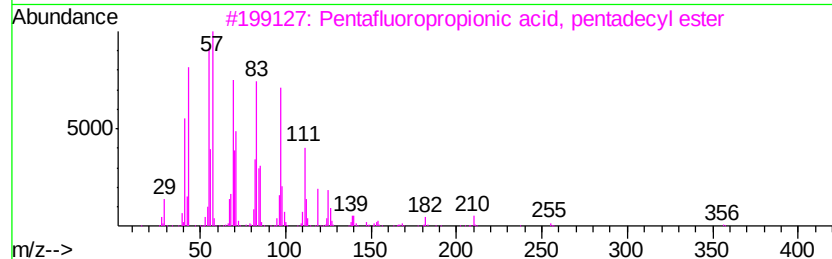
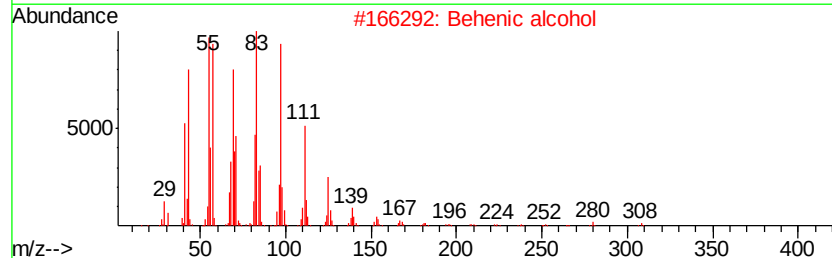
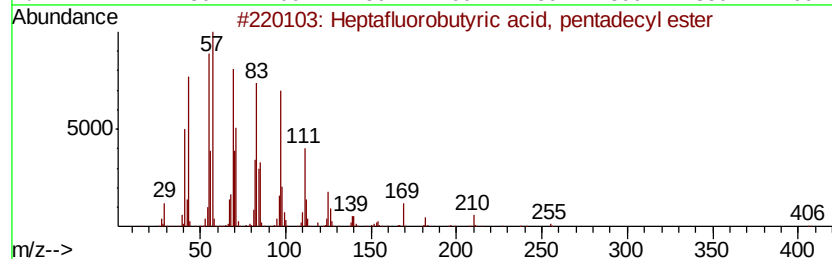
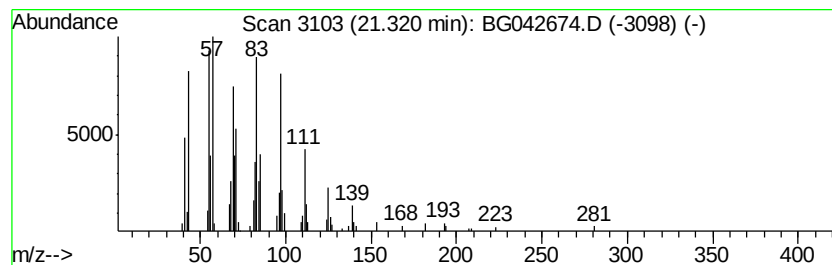
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 21.32 | 3.46 ng | 112307 | Chrysene-d12     | 21.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 95   |
| 2    |    | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 95   |
| 3    |    | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 95   |
| 4    |    | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4 | 95   |
| 5    |    | 1-Heptacosanol                      | 396 | C27H56O    | 002004-39-9 | 95   |



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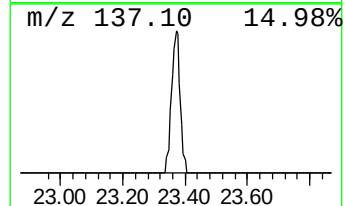
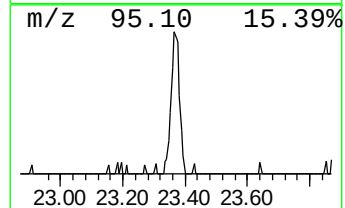
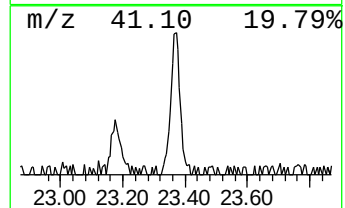
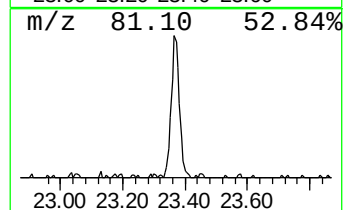
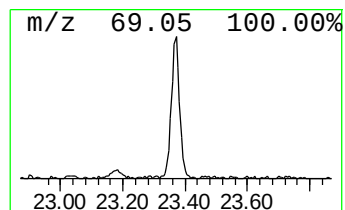
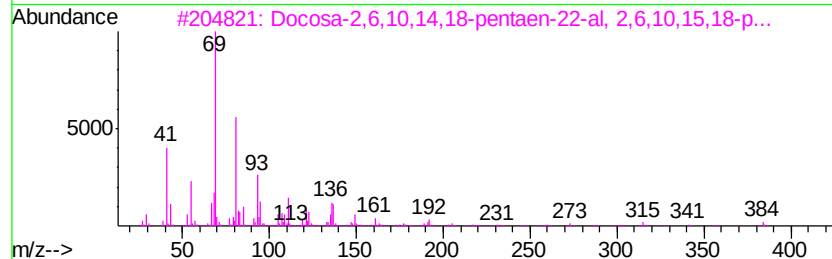
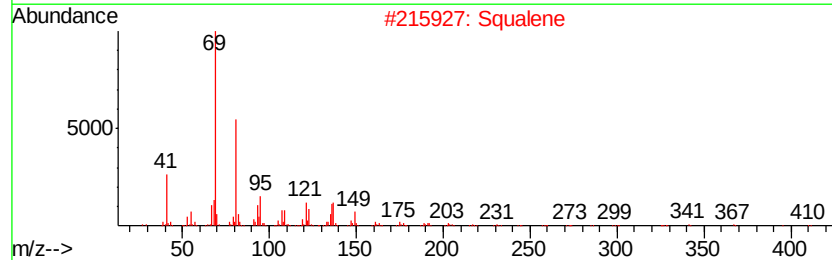
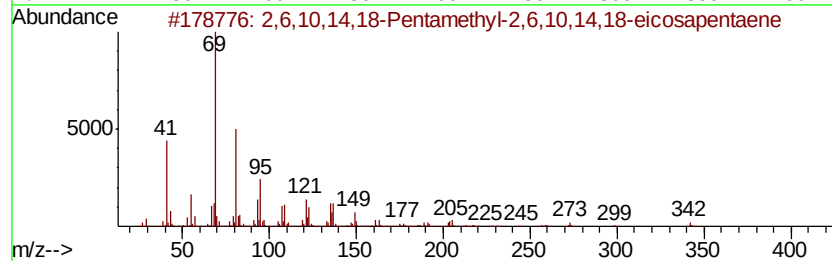
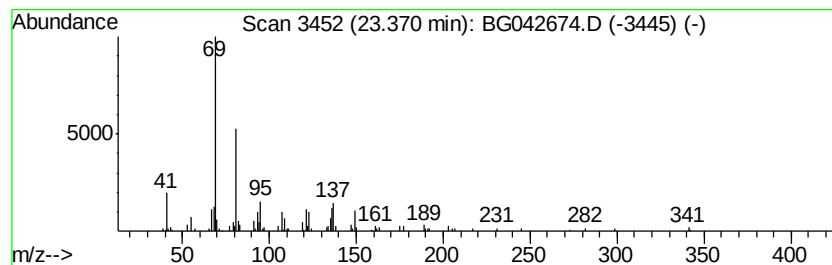
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Peak Number 5 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 23.37 | 3.19 ng | 118403 | Perylene-d12     | 24.92 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42       | 075581-03-2  | 91      |      |      |
| 2    | Squalene                            | 410 | C30H50       | 000111-02-4  | 91      |      |      |
| 3    | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O      | 1000163-04-7 | 90      |      |      |
| 4    | Supraene                            | 410 | C30H50       | 007683-64-9  | 86      |      |      |
| 5    | 4,9,13,17-Tetramethyl-4,8,12,16-... | 316 | C22H36O      | 056882-09-8  | 78      |      |      |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| Butane, 2-methoxy... | 3.12  | 23.7    | ng    | 180722   | 1                     | 7.99  | 152230 | 20.0 |
| unknown7.53          | 7.53  | 104.1   | ng    | 792468   | 1                     | 7.99  | 152230 | 20.0 |
| Heptafluorobutyri... | 21.32 | 3.5     | ng    | 112307   | 5                     | 21.68 | 649294 | 20.0 |
| 2,6,10,14,18-Pent... | 23.37 | 3.2     | ng    | 118403   | 6                     | 24.92 | 742283 | 20.0 |