

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF020117\  
 Data File : BF092716.D  
 Acq On : 1 Feb 2017 20:41  
 Operator : SJ/MA  
 Sample : I1597-14  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-32-COMP

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 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         | 5.139       | 264           | 267         | 275          | rBV      | 1575903        | 2221119       | 42.51%          | 5.334%        |
| 2         | 5.561       | 301           | 304         | 307          | rBV      | 4050359        | 4363594       | 83.51%          | 10.478%       |
| 3         | 6.590       | 391           | 394         | 397          | rBV2     | 4304611        | 5225535       | 100.00%         | 12.548%       |
| 4         | 6.716       | 402           | 405         | 408          | rBV      | 4199879        | 4371184       | 83.65%          | 10.496%       |
| 5         | 6.944       | 422           | 425         | 427          | rBV      | 1246057        | 1024798       | 19.61%          | 2.461%        |
| 6         | 7.104       | 436           | 439         | 441          | rBV      | 3733765        | 3664661       | 70.13%          | 8.800%        |
| 7         | 7.516       | 472           | 475         | 477          | rBV      | 2803185        | 3389763       | 64.87%          | 8.140%        |
| 8         | 8.236       | 535           | 538         | 540          | rBV      | 1451910        | 1359723       | 26.02%          | 3.265%        |
| 9         | 9.310       | 629           | 632         | 635          | rBV      | 3223286        | 4623777       | 88.48%          | 11.103%       |
| 10        | 9.710       | 664           | 667         | 669          | rBV      | 591940         | 497810        | 9.53%           | 1.195%        |
| 11        | 9.996       | 689           | 692         | 694          | rBV      | 1668860        | 1435805       | 27.48%          | 3.448%        |
| 12        | 10.419      | 728           | 729         | 731          | rVB      | 90236          | 83828         | 1.60%           | 0.201%        |
| 13        | 10.785      | 758           | 761         | 764          | rBV2     | 2074122        | 2517813       | 48.18%          | 6.046%        |
| 14        | 10.899      | 769           | 771         | 775          | rVB      | 117470         | 158110        | 3.03%           | 0.380%        |
| 15        | 11.345      | 808           | 810         | 811          | rBV      | 158411         | 128222        | 2.45%           | 0.308%        |
| 16        | 11.482      | 820           | 822         | 825          | rBV      | 1414345        | 1283858       | 24.57%          | 3.083%        |
| 17        | 11.768      | 845           | 847         | 849          | rVB      | 96499          | 96776         | 1.85%           | 0.232%        |
| 18        | 13.071      | 958           | 961         | 964          | rBV      | 3534311        | 3343819       | 63.99%          | 8.029%        |
| 19        | 14.122      | 1050          | 1053        | 1055         | rBV      | 918332         | 922730        | 17.66%          | 2.216%        |
| 20        | 15.231      | 1147          | 1150        | 1153         | rVB      | 47037          | 67265         | 1.29%           | 0.162%        |
| 21        | 15.585      | 1178          | 1181        | 1188         | rVB      | 620610         | 792672        | 15.17%          | 1.903%        |
| 22        | 16.042      | 1218          | 1221        | 1224         | rBV      | 47644          | 71675         | 1.37%           | 0.172%        |

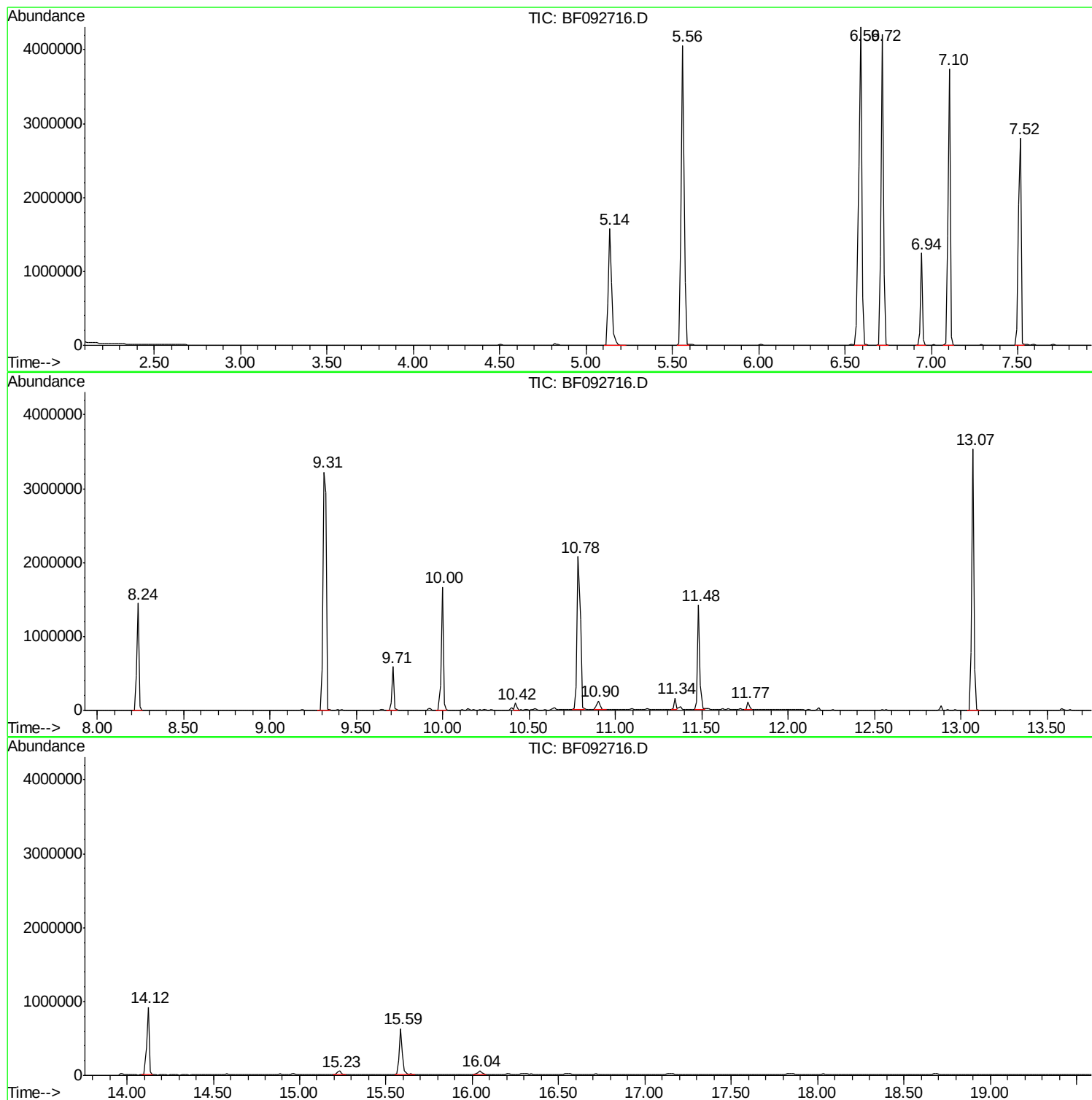
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SB-32-COMP

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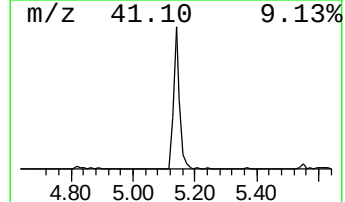
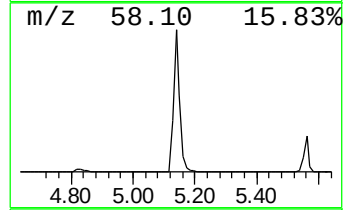
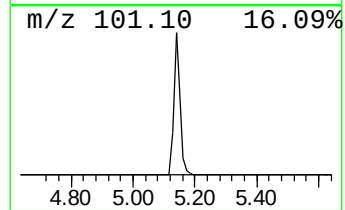
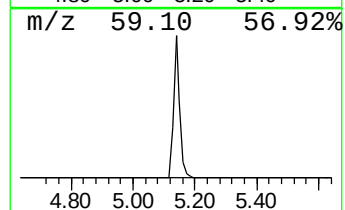
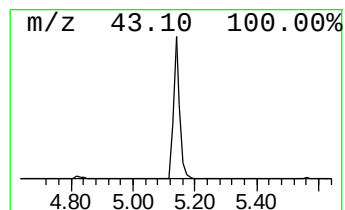
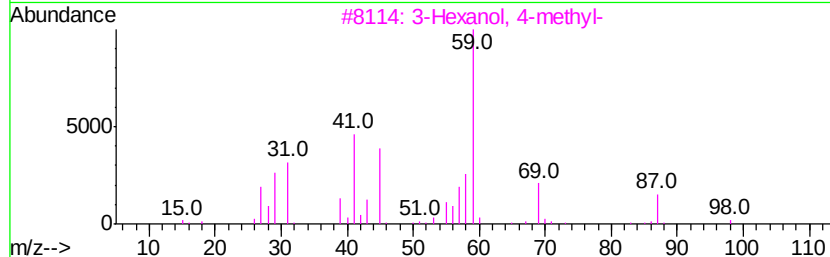
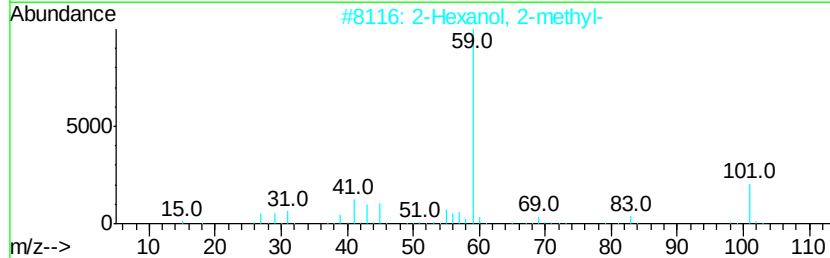
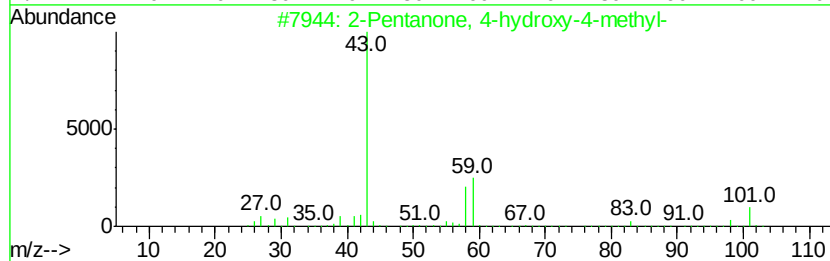
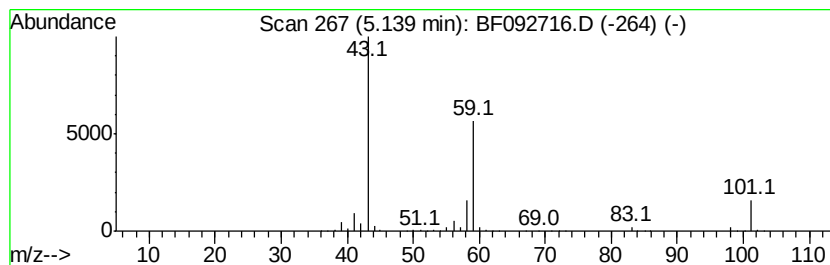
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 5.14 | 43.35 ng | 2221120 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | 2-Hexanol, 2-methyl-                 | 116 | C7H16O   | 000625-23-0 | 33   |
| 3    |    | 3-Hexanol, 4-methyl-                 | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 32   |
| 5    |    | Acetic acid, 1,1-dimethylethyl e...  | 116 | C6H12O2  | 000540-88-5 | 9    |



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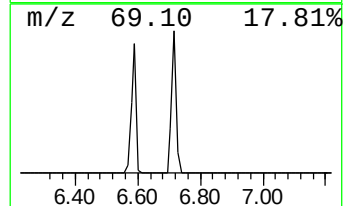
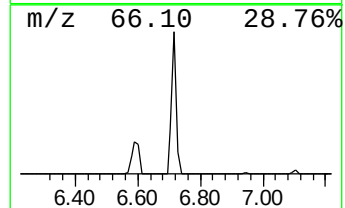
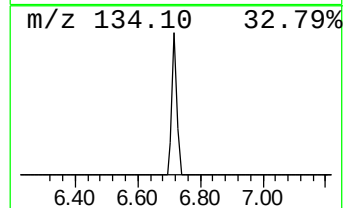
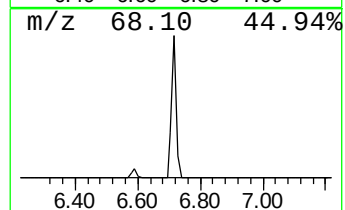
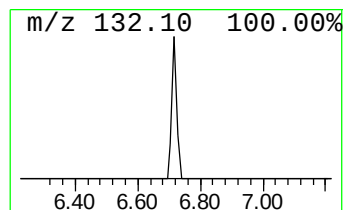
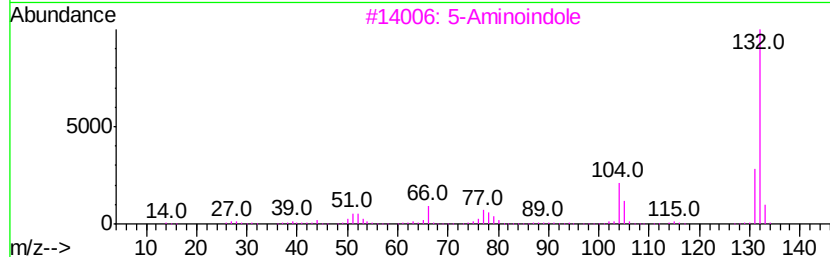
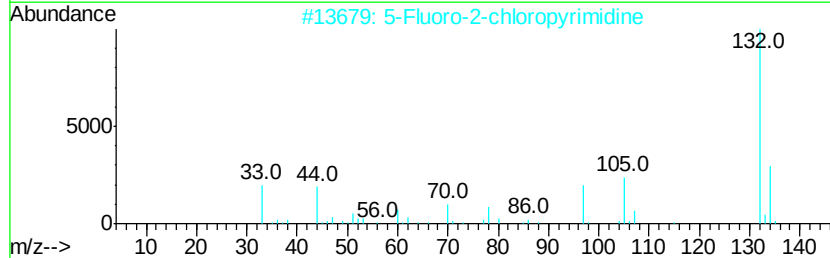
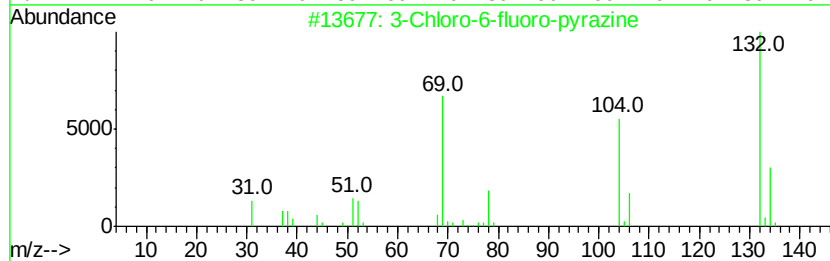
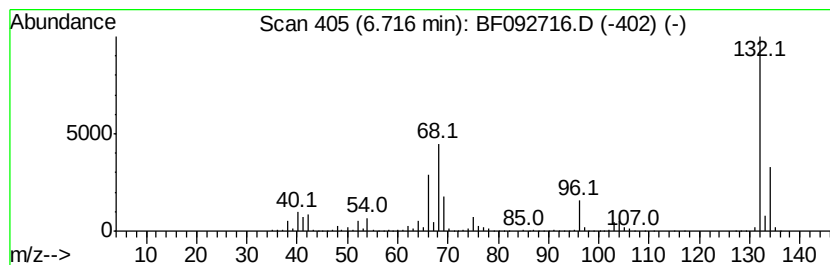
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Peak Number 2 unknown6.72 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.72 | 85.31 ng | 4371180 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# | of | Tentative ID                | MW  | MolForm   | CAS#         | Qual |
|------|----|-----------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | 5-Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl   | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Benzene, 1,2,4-trifluoro-   | 132 | C6H3F3    | 000367-23-7  | 9    |



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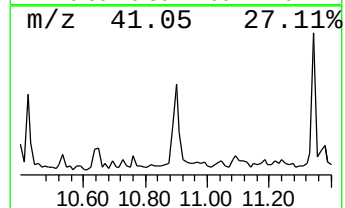
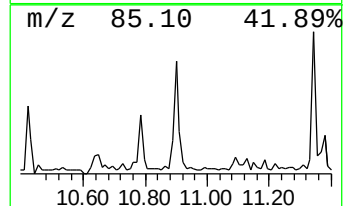
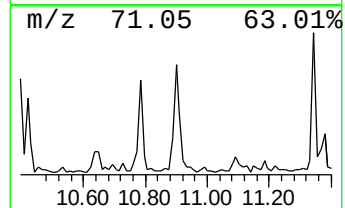
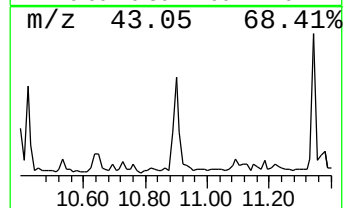
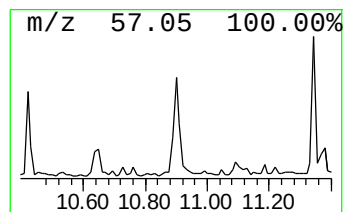
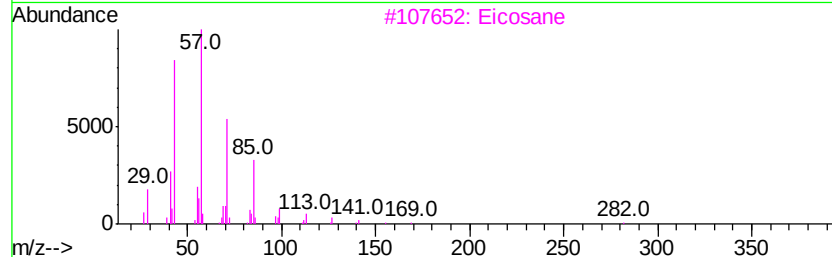
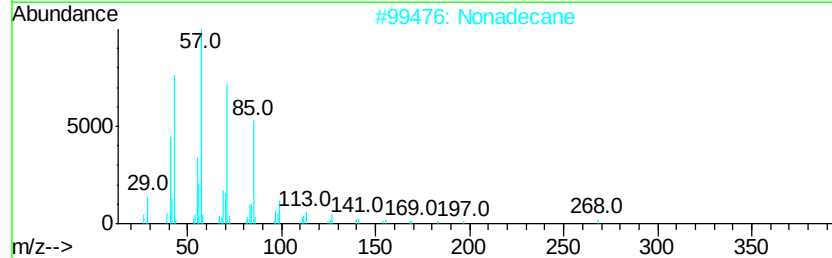
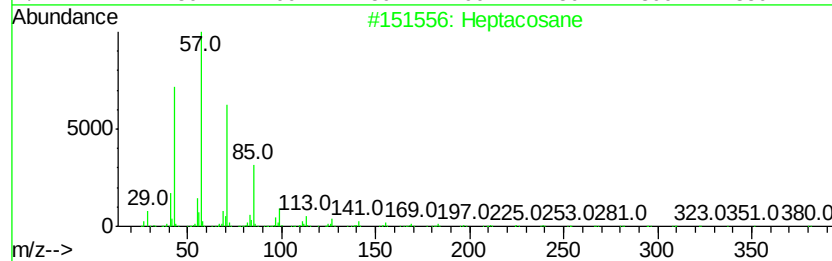
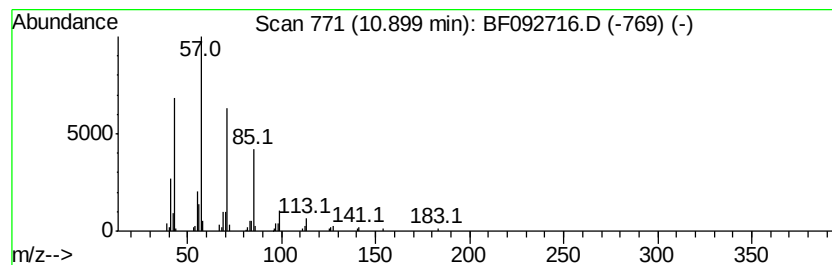
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Peak Number 4 Heptacosane Concentration Rank 4

| R.T.      | EstConc                  | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------------|--------|------------------|-------------|------|
| 10.90     | 2.46 ng                  | 158110 | Phenanthrene-d10 | 11.48       |      |
| Hit# of 5 | Tentative ID             | MW     | MolForm          | CAS#        | Qual |
| 1         | Heptacosane              | 380    | C27H56           | 000593-49-7 | 90   |
| 2         | Nonadecane               | 268    | C19H40           | 000629-92-5 | 87   |
| 3         | Eicosane                 | 282    | C20H42           | 000112-95-8 | 83   |
| 4         | Decane, 2,3,5-trimethyl- | 184    | C13H28           | 062238-11-3 | 83   |
| 5         | Octacosane               | 394    | C28H58           | 000630-02-4 | 83   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.14  | 43.4    | ng    | 2221120  | 1                     | 6.94  | 1024800 | 20.0 |
| unknown6.72          | 6.72  | 85.3    | ng    | 4371180  | 1                     | 6.94  | 1024800 | 20.0 |
| Heptacosane          | 10.90 | 2.5     | ng    | 158110   | 4                     | 11.48 | 1283860 | 20.0 |