

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\  
 Data File : BF106795.D  
 Acq On : 26 Jun 2018 1:52  
 Operator : JU/SJ  
 Sample : J3706-01  
 Misc :  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RO-1-5

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061918.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         | 5.207       | 484           | 488         | 499          | rBB      | 107061         | 144474        | 11.40%          | 1.321%        |
| 2         | 5.607       | 552           | 556         | 560          | rBV      | 1142919        | 1169077       | 92.25%          | 10.687%       |
| 3         | 6.607       | 721           | 726         | 738          | rBV      | 1062052        | 1222259       | 96.45%          | 11.173%       |
| 4         | 6.742       | 744           | 749         | 752          | rBV      | 1230708        | 1184515       | 93.47%          | 10.828%       |
| 5         | 6.960       | 783           | 786         | 790          | rBB      | 349286         | 282067        | 22.26%          | 2.579%        |
| 6         | 7.119       | 809           | 813         | 816          | rBV      | 1061754        | 931306        | 73.49%          | 8.514%        |
| 7         | 7.531       | 877           | 883         | 886          | rBV      | 687420         | 739478        | 58.35%          | 6.760%        |
| 8         | 8.242       | 1000          | 1004        | 1008         | rBV      | 365806         | 320637        | 25.30%          | 2.931%        |
| 9         | 9.319       | 1183          | 1187        | 1190         | rBV      | 1359226        | 1217239       | 96.05%          | 11.128%       |
| 10        | 9.707       | 1249          | 1253        | 1260         | rBV      | 183714         | 147706        | 11.66%          | 1.350%        |
| 11        | 9.913       | 1285          | 1288        | 1292         | rBV      | 18205          | 14768         | 1.17%           | 0.135%        |
| 12        | 10.001      | 1300          | 1303        | 1311         | rVB2     | 366885         | 321337        | 25.36%          | 2.938%        |
| 13        | 10.413      | 1370          | 1373        | 1376         | rVB      | 24444          | 19005         | 1.50%           | 0.174%        |
| 14        | 10.801      | 1434          | 1439        | 1442         | rBV      | 751836         | 742156        | 58.56%          | 6.785%        |
| 15        | 10.883      | 1450          | 1453        | 1457         | rBV      | 21692          | 24493         | 1.93%           | 0.224%        |
| 16        | 11.495      | 1553          | 1557        | 1560         | rBV      | 378285         | 323329        | 25.51%          | 2.956%        |
| 17        | 12.713      | 1762          | 1764        | 1768         | rBV      | 30628          | 23681         | 1.87%           | 0.216%        |
| 18        | 12.948      | 1801          | 1804        | 1808         | rVB      | 32052          | 35281         | 2.78%           | 0.323%        |
| 19        | 13.083      | 1822          | 1827        | 1830         | rBV      | 1372803        | 1267288       | 100.00%         | 11.585%       |
| 20        | 13.271      | 1855          | 1859        | 1866         | rVB6     | 10890          | 17379         | 1.37%           | 0.159%        |
| 21        | 13.536      | 1901          | 1904        | 1909         | rVB6     | 8420           | 14387         | 1.14%           | 0.132%        |
| 22        | 13.954      | 1972          | 1975        | 1980         | rBV2     | 115631         | 120073        | 9.47%           | 1.098%        |
| 23        | 14.001      | 1980          | 1983        | 1987         | rVB      | 22611          | 24099         | 1.90%           | 0.220%        |
| 24        | 14.148      | 2004          | 2008        | 2012         | rBV      | 366955         | 340937        | 26.90%          | 3.117%        |
| 25        | 14.595      | 2082          | 2084        | 2087         | rBV3     | 22172          | 21092         | 1.66%           | 0.193%        |
| 26        | 14.989      | 2149          | 2151        | 2155         | rVB      | 33697          | 34274         | 2.70%           | 0.313%        |
| 27        | 15.689      | 2265          | 2270        | 2277         | rVB      | 173621         | 236575        | 18.67%          | 2.163%        |

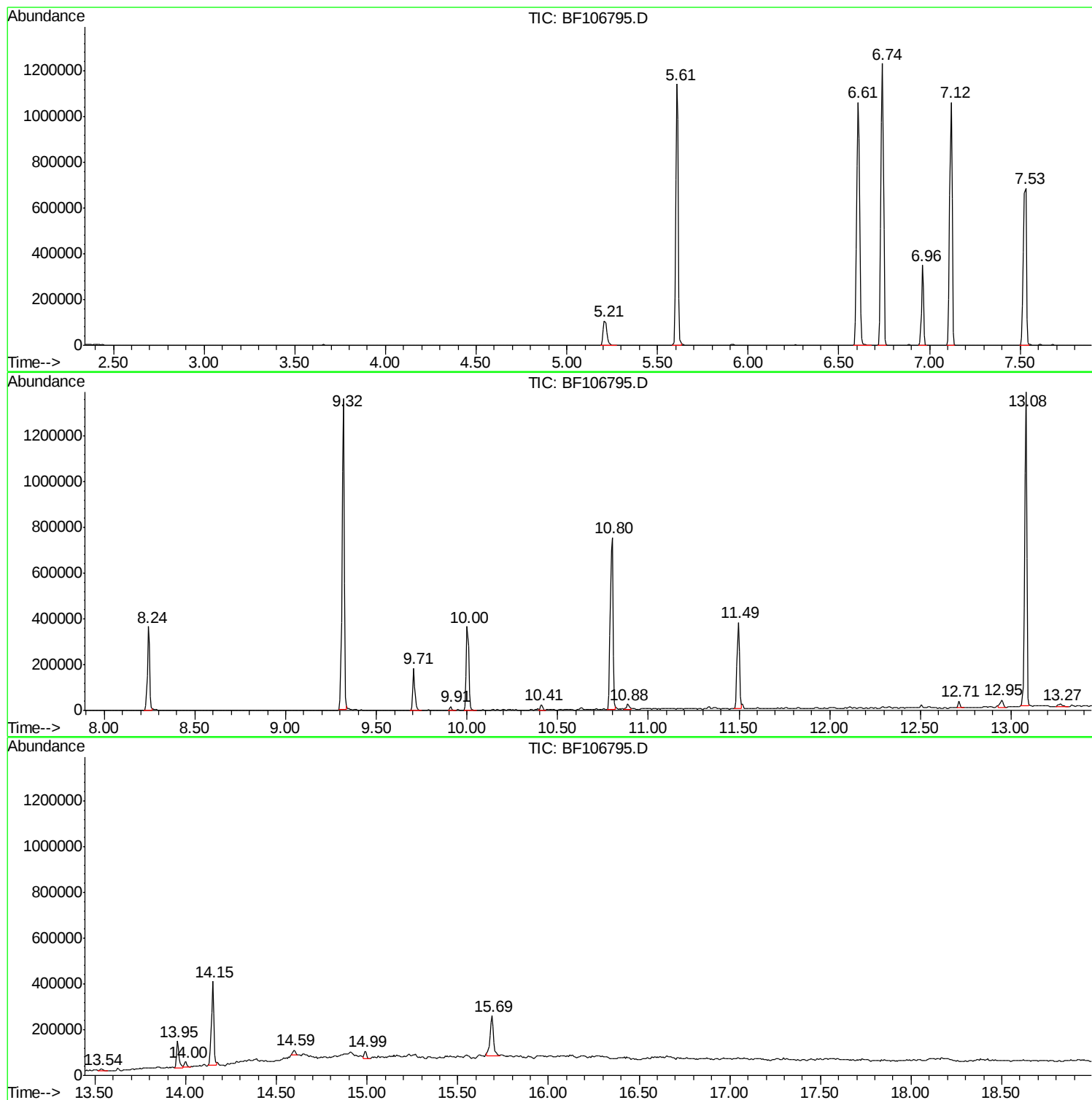
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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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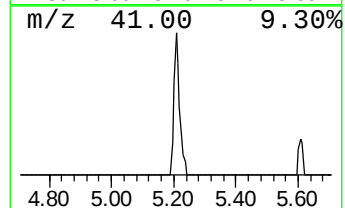
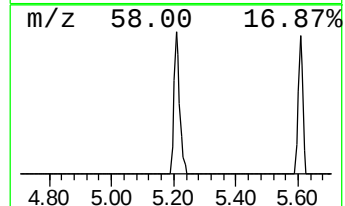
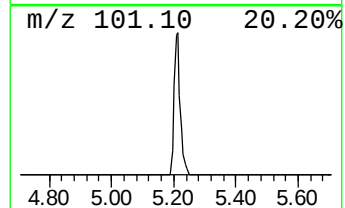
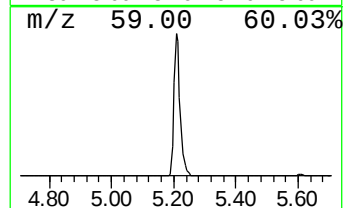
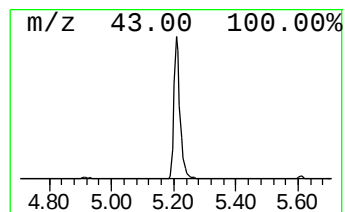
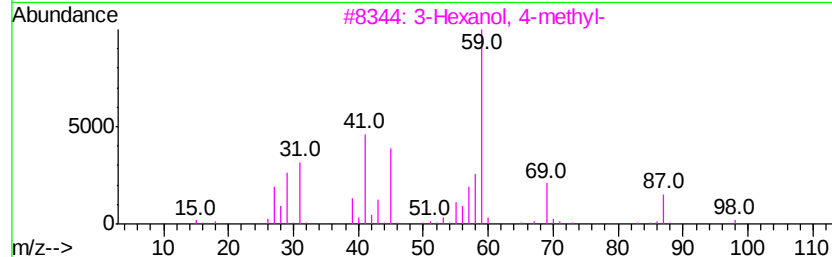
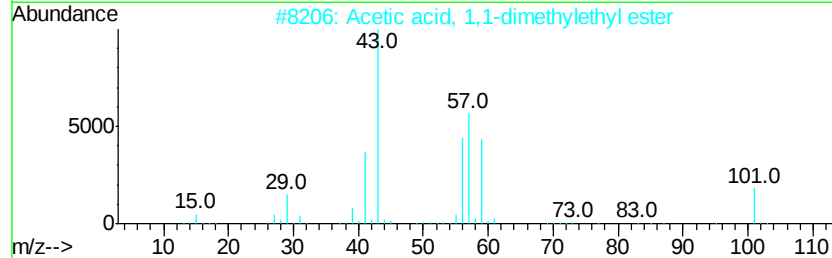
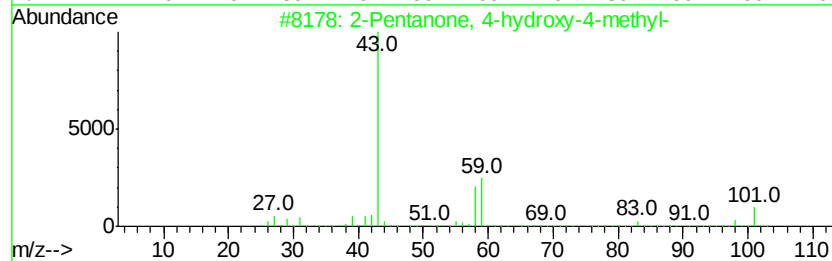
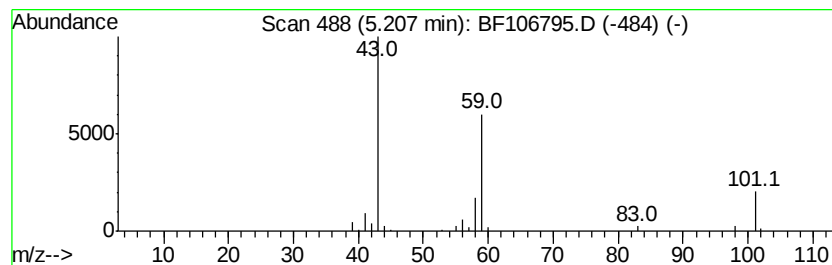
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.21 | 10.24 ng | 144474 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 28   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 5    |    |   | Butane, 1-ethoxy-                   | 102 | C6H14O   | 000628-81-9 | 9    |



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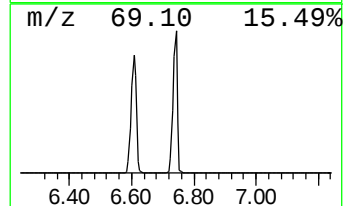
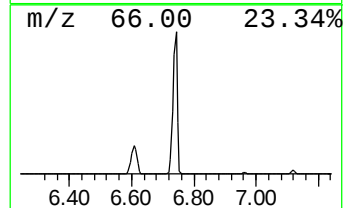
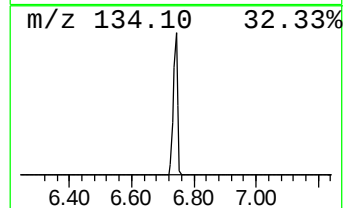
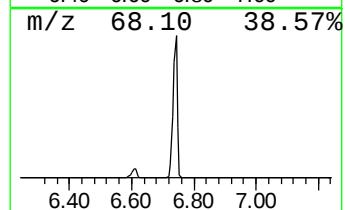
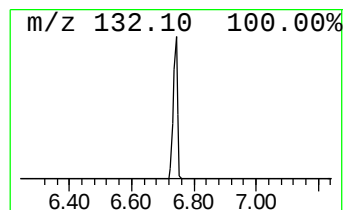
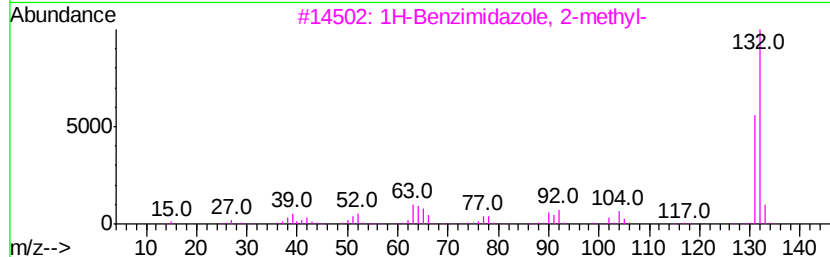
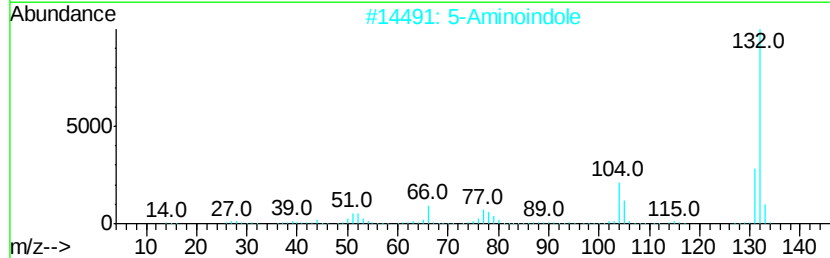
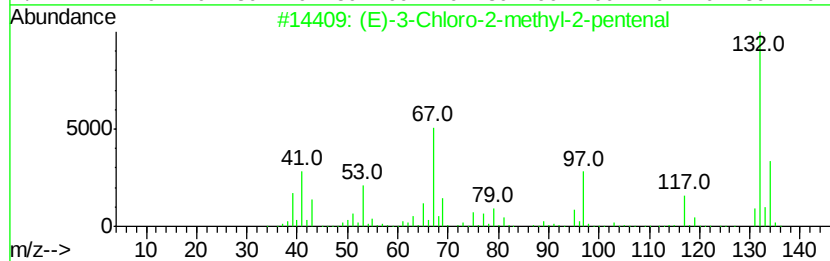
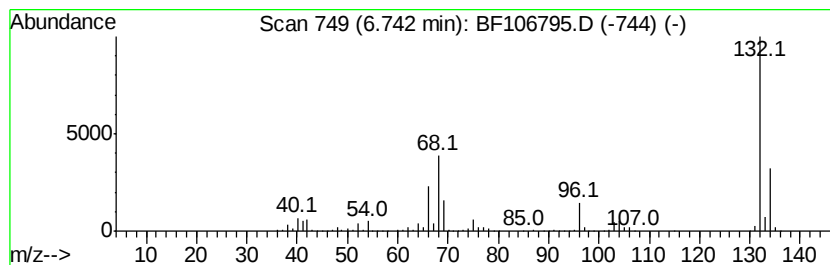
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 83.99 ng | 1184520 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|----------------------------------|-----|-----------|-------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3 | 12   |
| 2    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0 | 12   |
| 3    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6 | 9    |
| 4    |    | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6 | 9    |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2 | 9    |



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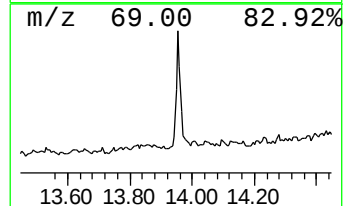
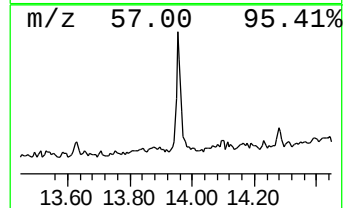
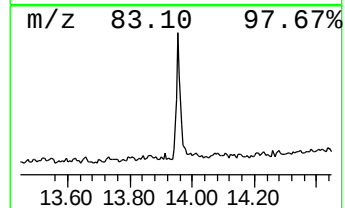
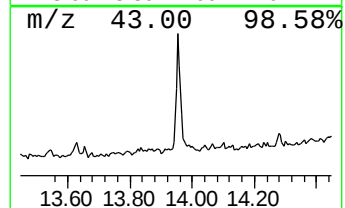
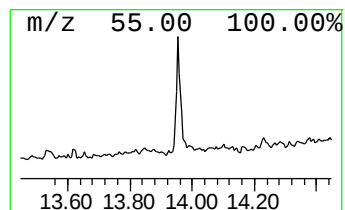
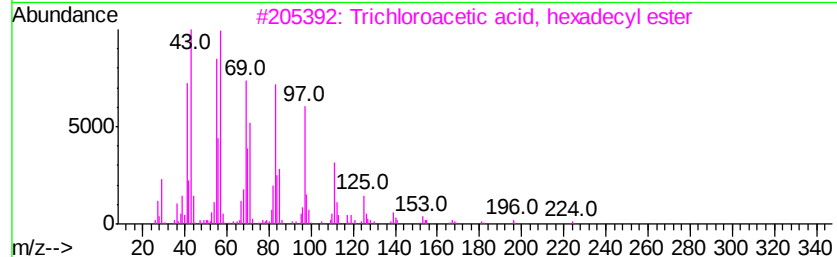
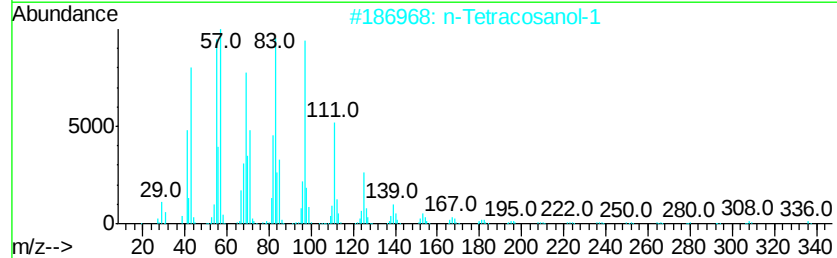
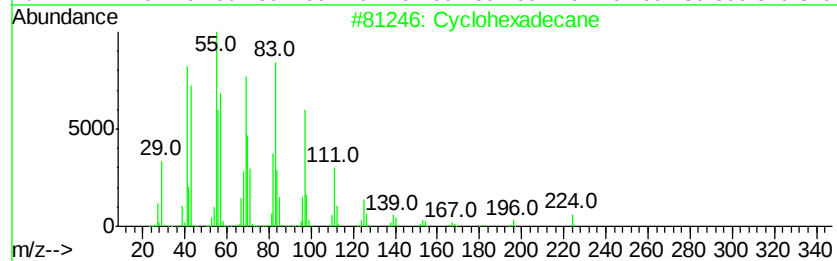
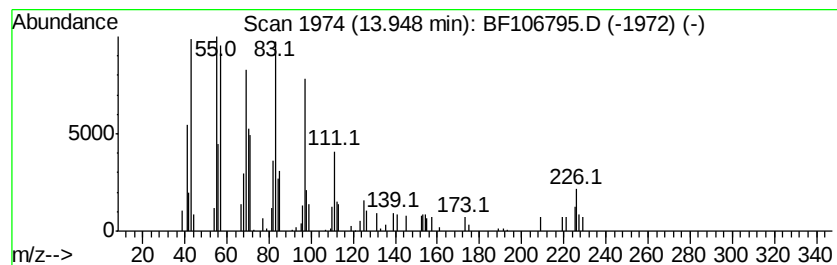
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 Cyclohexadecane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.95 | 7.04 ng | 120073 | Chrysene-d12     | 14.15 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Cyclohexadecane                     | 224 | C16H32      | 000295-65-8 | 97   |
| 2    |    | n-Tetracosanol-1                    | 354 | C24H50O     | 000506-51-4 | 95   |
| 3    |    | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94   |
| 4    |    | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2  | 959092-08-1 | 94   |
| 5    |    | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2  | 959010-23-2 | 94   |



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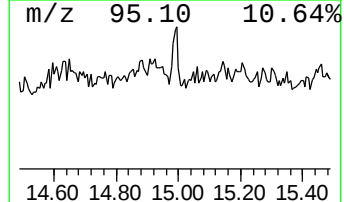
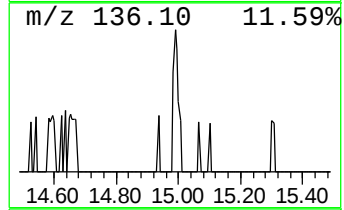
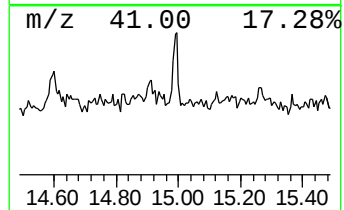
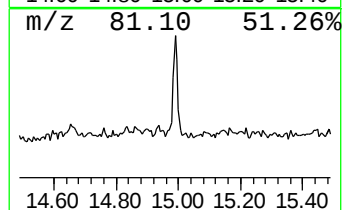
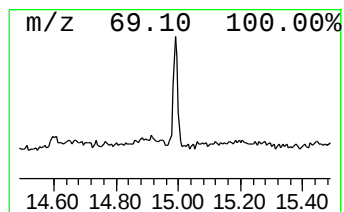
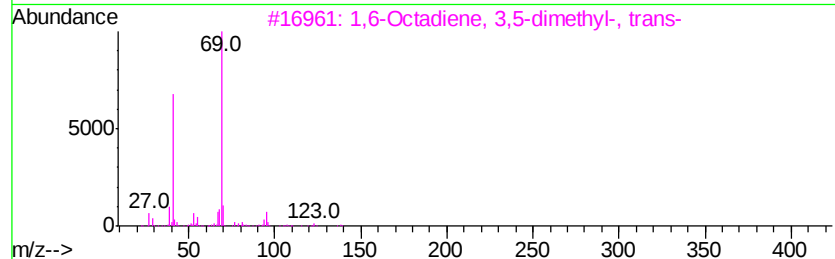
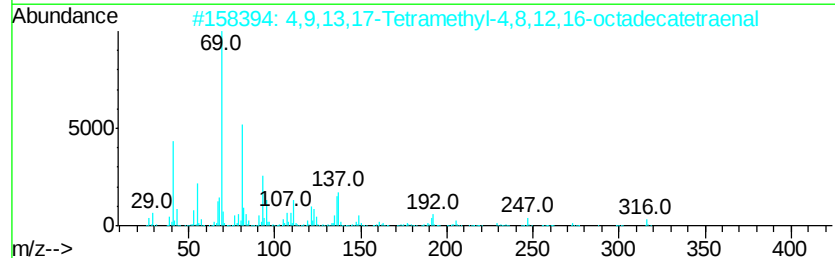
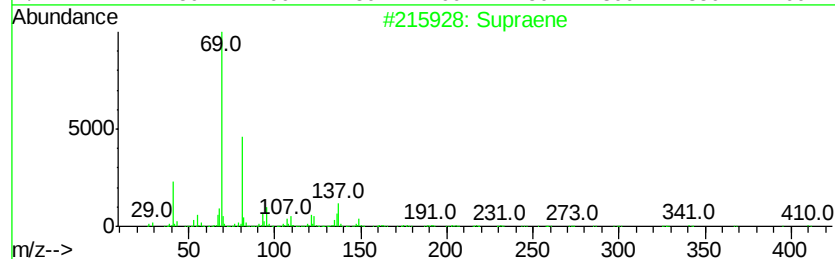
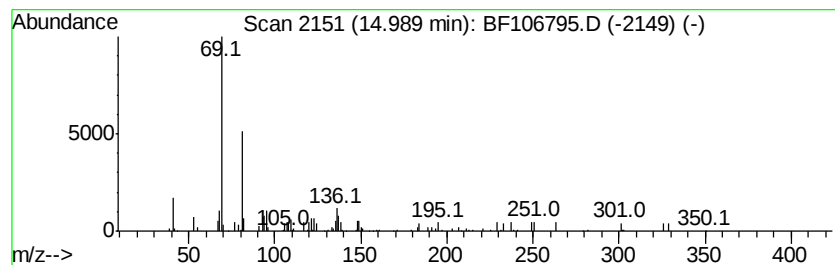
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Peak Number 6 Supraene Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.99 | 2.90 ng | 34274 | Perylene-d12     | 15.69 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Supraene                            | 410 | C30H50  | 007683-64-9 | 47   |
| 2    |    | 4,9,13,17-Tetramethyl-4,8,12,16-... | 316 | C22H36O | 056882-09-8 | 47   |
| 3    |    | 1,6-Octadiene, 3,5-dimethyl-, tr... | 138 | C10H18  | 074630-87-8 | 47   |
| 4    |    | Squalene                            | 410 | C30H50  | 000111-02-4 | 47   |
| 5    |    | 3,7-Nonadien-2-ol, 4,8-dimethyl-    | 168 | C11H20O | 067845-50-5 | 38   |



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TIC Library : C:\DATABASE\NIST11.L  
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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.21  | 10.2    | ng    | 144474   | 1                     | 6.96  | 282067 | 20.0 |
| unknown6.74          | 6.74  | 84.0    | ng    | 1184520  | 1                     | 6.96  | 282067 | 20.0 |
| Cyclohexadecane      | 13.95 | 7.0     | ng    | 120073   | 5                     | 14.15 | 340937 | 20.0 |
| Supraene             | 14.99 | 2.9     | ng    | 34274    | 6                     | 15.69 | 236575 | 20.0 |