

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\  
 Data File : BF117491.D  
 Acq On : 23 Oct 2019 18:58  
 Operator : JU  
 Sample : K5485-11  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-23-S

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\_F\METHODS\8270-BF101819.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         | 5.351       | 552           | 555         | 568          | rBV      | 720391         | 783728        | 75.72%          | 8.806%        |
| 2         | 6.381       | 726           | 730         | 747          | rBV      | 824142         | 902247        | 87.17%          | 10.138%       |
| 3         | 6.504       | 747           | 751         | 766          | rVB      | 1088169        | 933136        | 90.15%          | 10.485%       |
| 4         | 6.733       | 786           | 790         | 799          | rBV      | 231219         | 229582        | 22.18%          | 2.580%        |
| 5         | 6.886       | 812           | 816         | 832          | rBV      | 769844         | 664581        | 64.20%          | 7.467%        |
| 6         | 7.298       | 882           | 886         | 904          | rBV      | 519985         | 540064        | 52.18%          | 6.068%        |
| 7         | 8.010       | 1004          | 1007        | 1020         | rBV      | 291169         | 295486        | 28.55%          | 3.320%        |
| 8         | 9.086       | 1186          | 1190        | 1193         | rBV      | 1252982        | 993383        | 95.97%          | 11.162%       |
| 9         | 9.169       | 1201          | 1204        | 1208         | rVB      | 16667          | 15054         | 1.45%           | 0.169%        |
| 10        | 9.480       | 1254          | 1257        | 1265         | rBV      | 124598         | 111013        | 10.72%          | 1.247%        |
| 11        | 9.698       | 1291          | 1294        | 1298         | rBV      | 17091          | 14959         | 1.45%           | 0.168%        |
| 12        | 9.763       | 1302          | 1305        | 1315         | rVB      | 425210         | 357343        | 34.52%          | 4.015%        |
| 13        | 10.192      | 1375          | 1378        | 1381         | rVB      | 17457          | 14233         | 1.38%           | 0.160%        |
| 14        | 10.551      | 1436          | 1439        | 1452         | rVV      | 583336         | 581844        | 56.21%          | 6.538%        |
| 15        | 10.668      | 1456          | 1459        | 1465         | rVB      | 15006          | 19534         | 1.89%           | 0.219%        |
| 16        | 11.110      | 1531          | 1534        | 1537         | rBV2     | 13894          | 13615         | 1.32%           | 0.153%        |
| 17        | 11.251      | 1554          | 1558        | 1567         | rBV      | 331456         | 354162        | 34.22%          | 3.979%        |
| 18        | 11.774      | 1644          | 1647        | 1655         | rBV      | 53826          | 62875         | 6.07%           | 0.706%        |
| 19        | 12.562      | 1776          | 1781        | 1786         | rBV3     | 9482           | 15407         | 1.49%           | 0.173%        |
| 20        | 12.704      | 1802          | 1805        | 1807         | rBV2     | 13723          | 12538         | 1.21%           | 0.141%        |
| 21        | 12.833      | 1822          | 1827        | 1830         | rBV      | 1059413        | 1035096       | 100.00%         | 11.630%       |
| 22        | 13.057      | 1862          | 1865        | 1869         | rBV      | 16611          | 15503         | 1.50%           | 0.174%        |
| 23        | 13.398      | 1920          | 1923        | 1926         | rBV2     | 18865          | 18640         | 1.80%           | 0.209%        |
| 24        | 13.727      | 1976          | 1979        | 1993         | rBV2     | 95182          | 172693        | 16.68%          | 1.940%        |
| 25        | 13.892      | 2003          | 2007        | 2014         | rBV      | 245693         | 260950        | 25.21%          | 2.932%        |
| 26        | 14.045      | 2029          | 2033        | 2035         | rBV      | 24717          | 22824         | 2.21%           | 0.256%        |
| 27        | 14.345      | 2081          | 2084        | 2087         | rBV      | 31639          | 30150         | 2.91%           | 0.339%        |
| 28        | 14.645      | 2131          | 2135        | 2137         | rVB      | 33877          | 31467         | 3.04%           | 0.354%        |
| 29        | 14.956      | 2184          | 2188        | 2193         | rBV      | 35276          | 40769         | 3.94%           | 0.458%        |
| 30        | 15.315      | 2245          | 2249        | 2263         | rVB      | 207907         | 274576        | 26.53%          | 3.085%        |
| 31        | 15.715      | 2313          | 2317        | 2322         | rVB2     | 23248          | 33919         | 3.28%           | 0.381%        |
| 32        | 15.939      | 2351          | 2355        | 2365         | rVB7     | 10725          | 26097         | 2.52%           | 0.293%        |
| 33        | 16.186      | 2392          | 2397        | 2401         | rBV4     | 15762          | 22542         | 2.18%           | 0.253%        |

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Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 Max Peaks: 100  
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101819.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

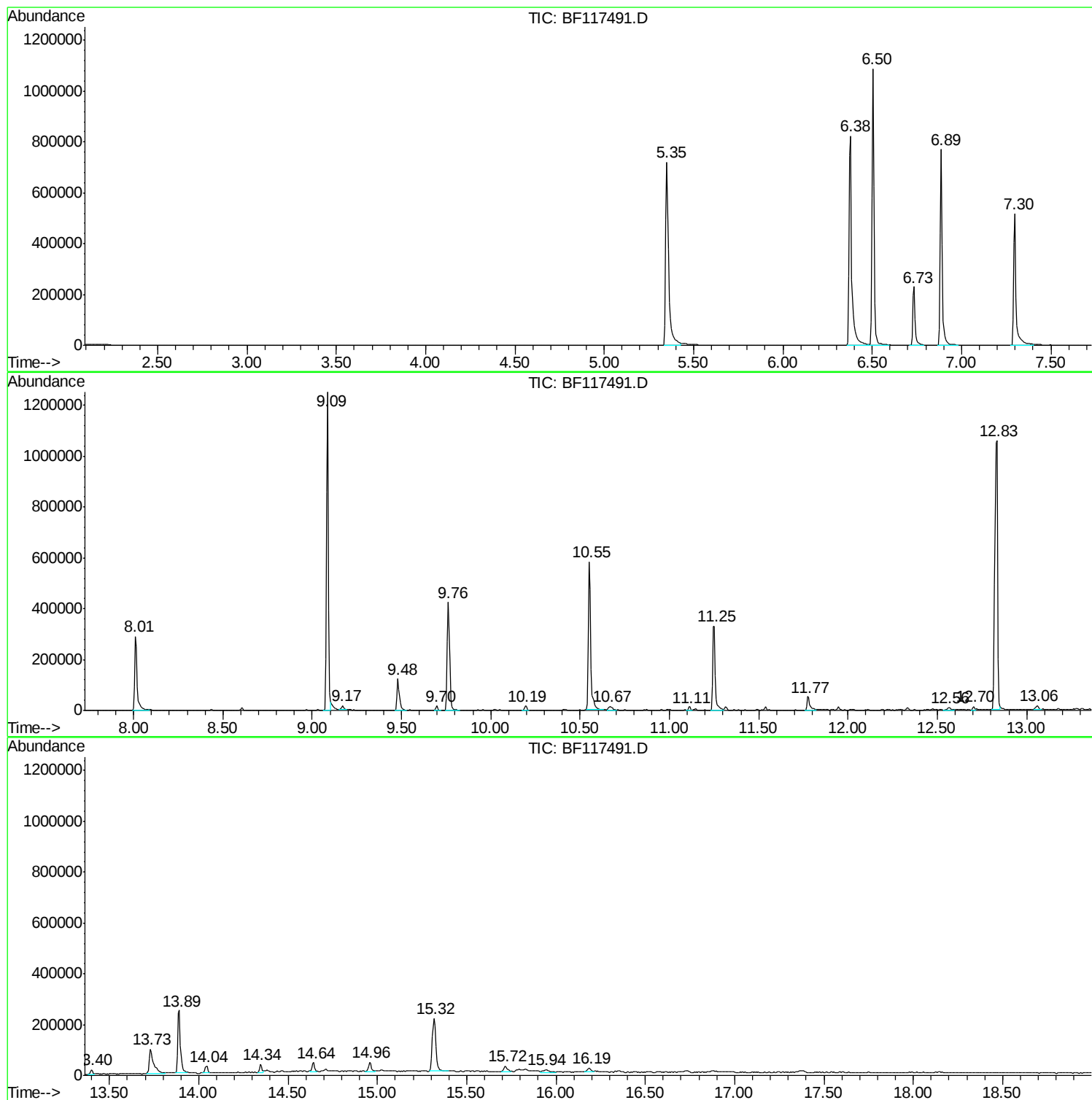
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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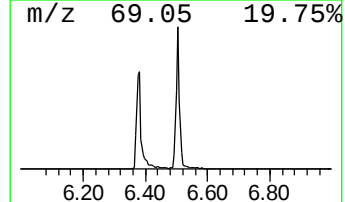
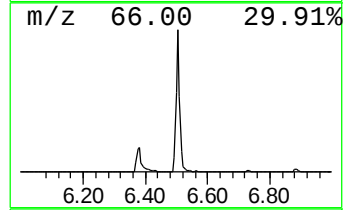
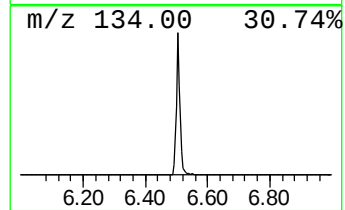
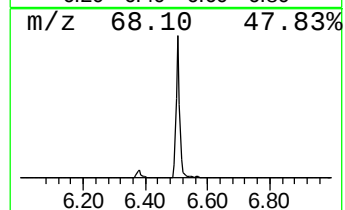
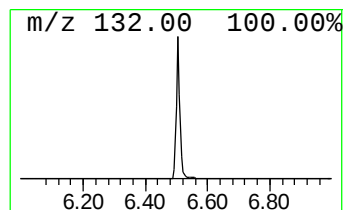
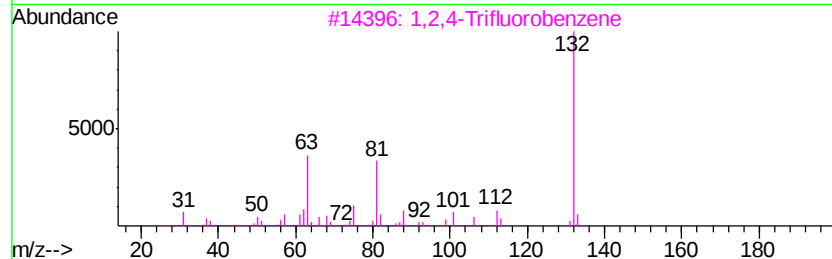
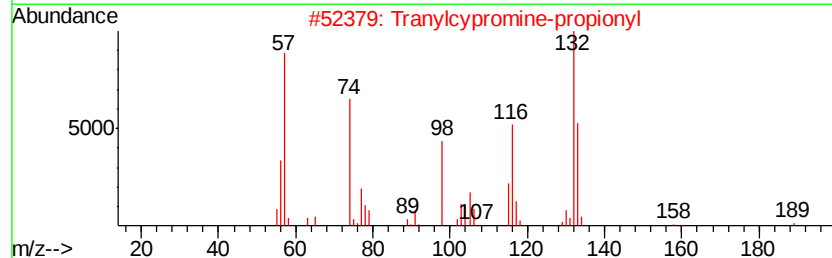
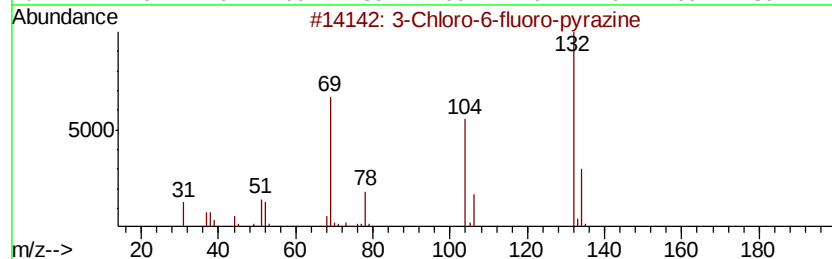
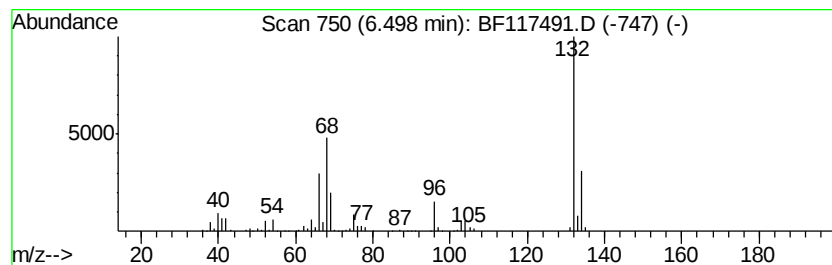
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.50 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.50 | 81.29 ng | 933136 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 3    |    | 1,2,4-Trifluorobenzene           | 132 | C6H3F3    | 000367-23-7  | 9    |
| 4    |    | 1,3,5-Trifluorobenzene           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 9    |



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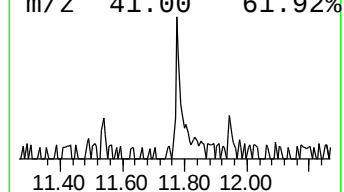
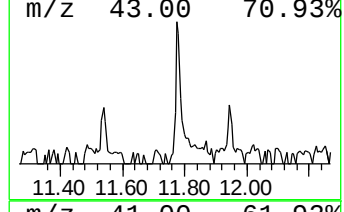
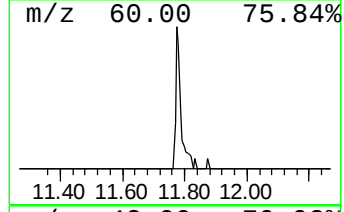
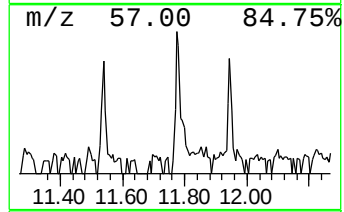
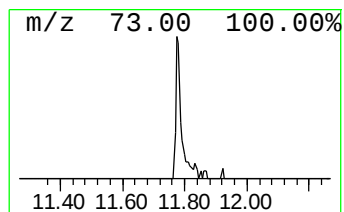
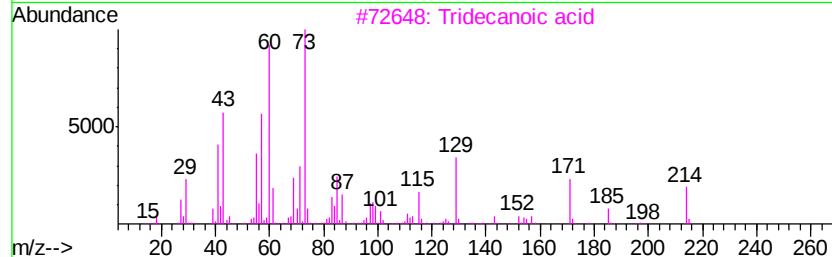
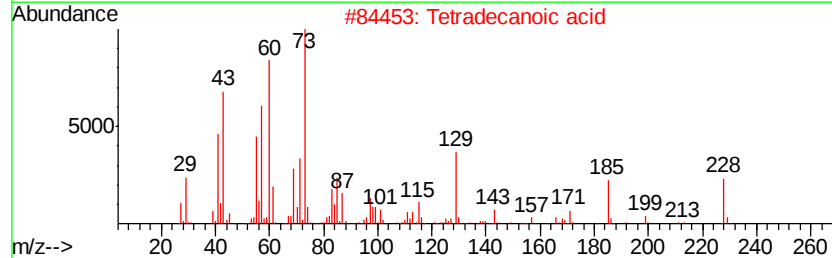
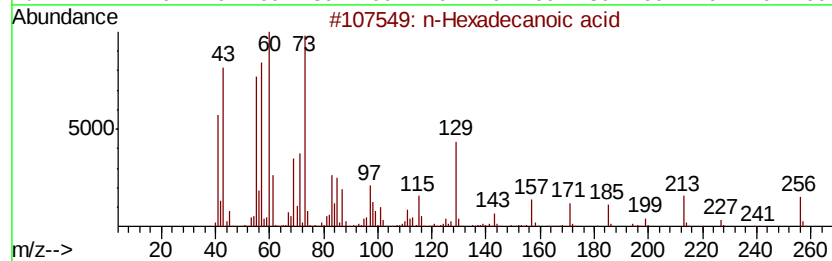
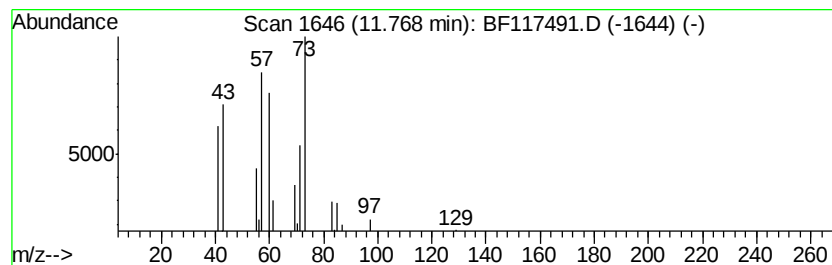
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 11.77 | 3.55 ng | 62875 | Phenanthrene-d10 | 11.25 |

| Hit# of | 5 | Tentative ID                   | MW  | MolForm    | CAS#        | Qual |
|---------|---|--------------------------------|-----|------------|-------------|------|
| 1       |   | n-Hexadecanoic acid            | 256 | C16H32O2   | 000057-10-3 | 96   |
| 2       |   | Tetradecanoic acid             | 228 | C14H28O2   | 000544-63-8 | 80   |
| 3       |   | Tridecanoic acid               | 214 | C13H26O2   | 000638-53-9 | 64   |
| 4       |   | Pentadecanoic acid             | 242 | C15H30O2   | 001002-84-2 | 58   |
| 5       |   | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 53   |



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Instrument :  
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TP-23-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

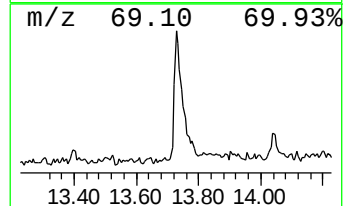
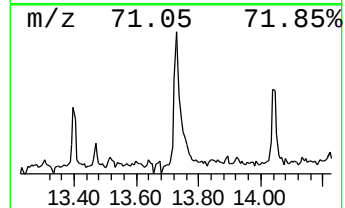
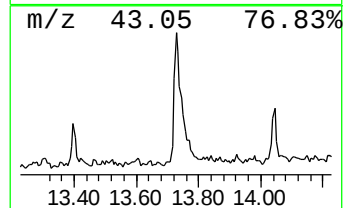
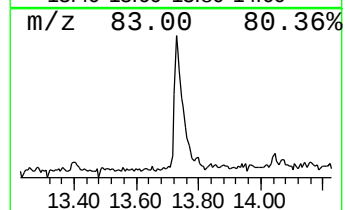
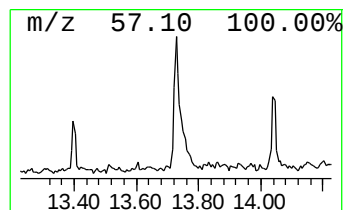
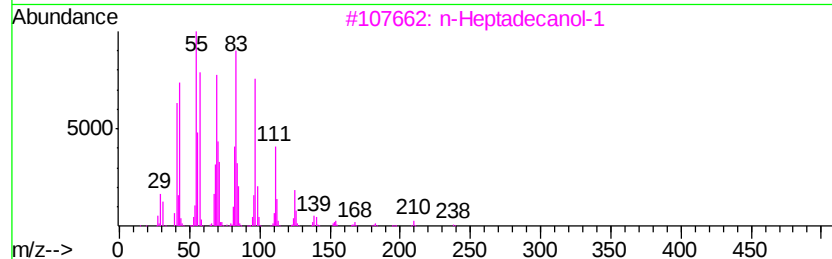
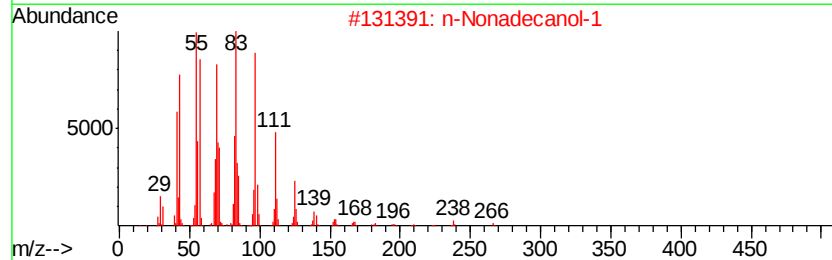
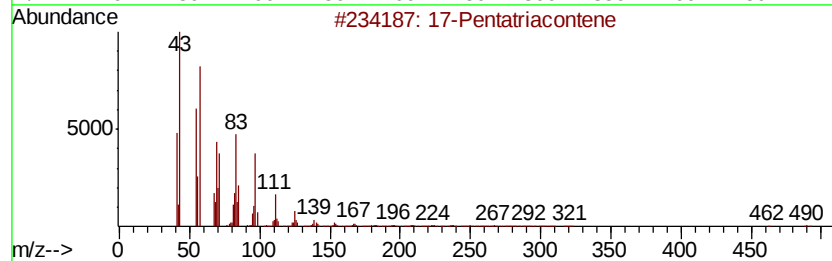
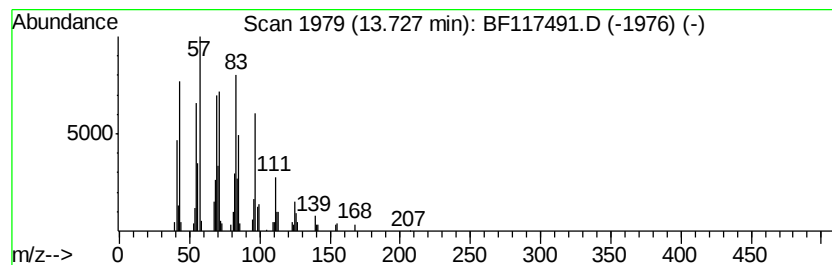
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 17-Pentatriacontene Concentration Rank 3

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 13.73 | 13.24 ng | 172693 | Chrysene-d12     | 13.89 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|---------|---|-------------------------------------|-----|------------|--------------|------|
| 1       |   | 17-Pentatriacontene                 | 491 | C35H70     | 006971-40-0  | 83   |
| 2       |   | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8  | 76   |
| 3       |   | n-Heptadecanol-1                    | 256 | C17H36O    | 001454-85-9  | 76   |
| 4       |   | 1-Dodecanol, 2-octyl-               | 298 | C20H42O    | 005333-42-6  | 74   |
| 5       |   | Octatriacontyl pentafluoropropio... | 697 | C41H77F5O2 | 1000351-89-1 | 74   |



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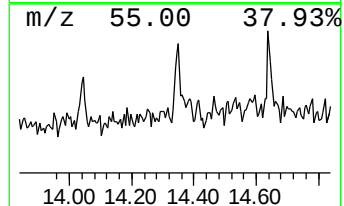
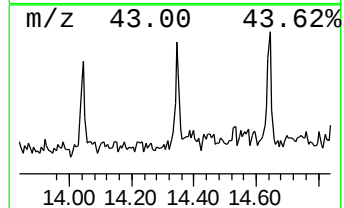
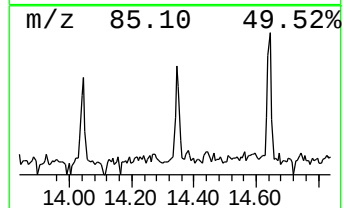
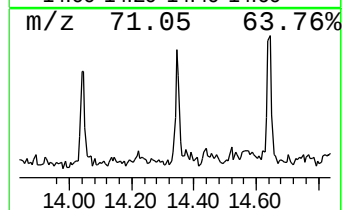
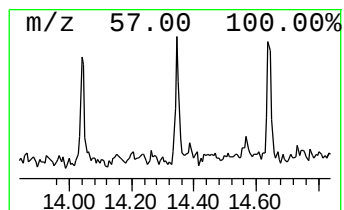
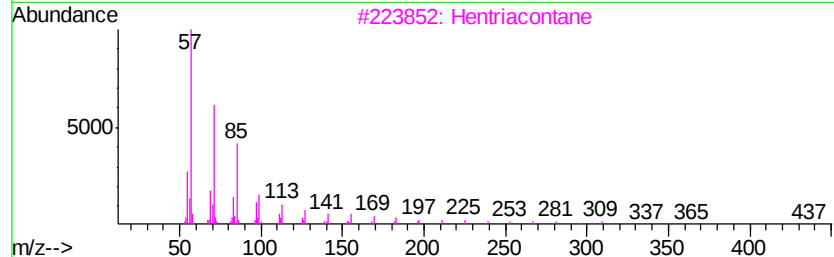
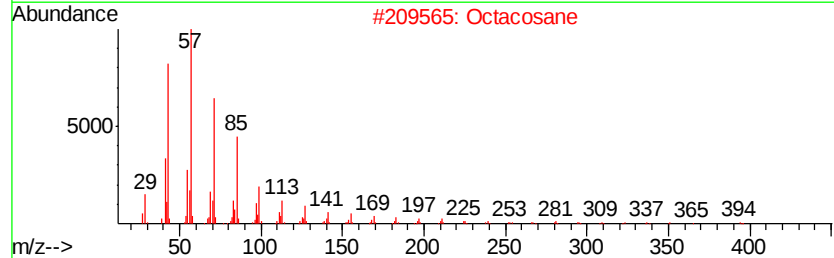
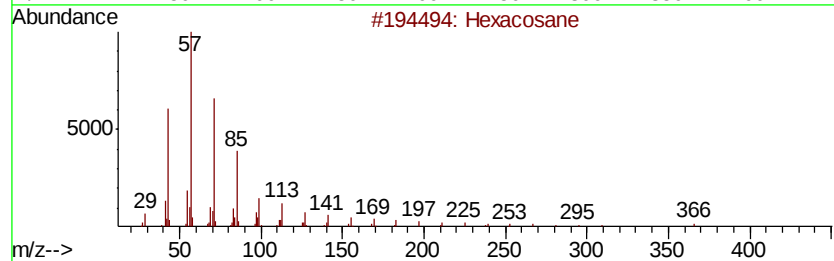
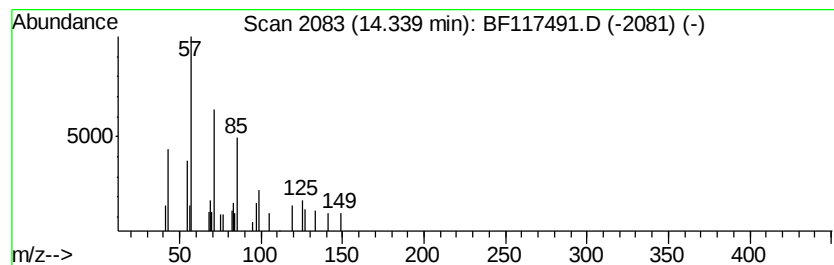
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexacosane Concentration Rank 7

| R.T.      | EstConc        | Area  | Relative to ISTD |             | R.T.  |
|-----------|----------------|-------|------------------|-------------|-------|
| 14.34     | 2.31 ng        | 30150 | Chrysene-d12     |             | 13.89 |
| Hit# of 5 | Tentative ID   | MW    | MolForm          | CAS#        | Qual  |
| 1         | Hexacosane     | 366   | C26H54           | 000630-01-3 | 86    |
| 2         | Octacosane     | 394   | C28H58           | 000630-02-4 | 86    |
| 3         | Hentriacontane | 437   | C31H64           | 000630-04-6 | 86    |
| 4         | Pentacosane    | 352   | C25H52           | 000629-99-2 | 86    |
| 5         | Heneicosane    | 296   | C21H44           | 000629-94-7 | 86    |



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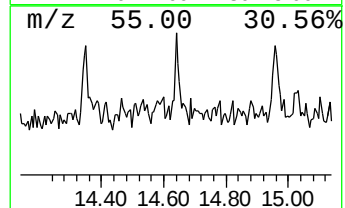
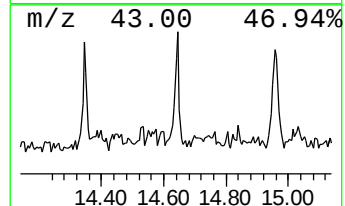
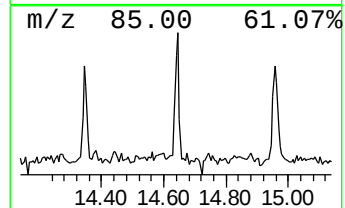
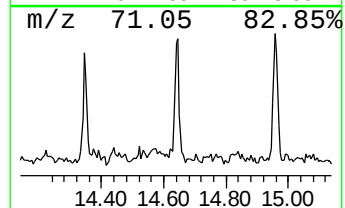
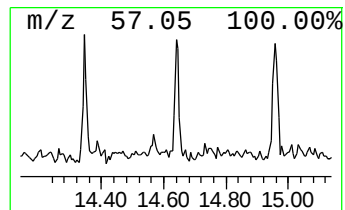
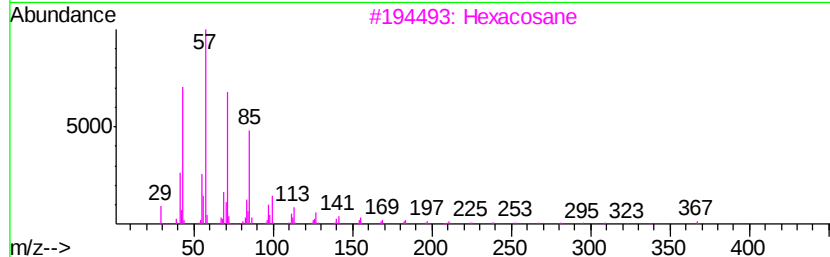
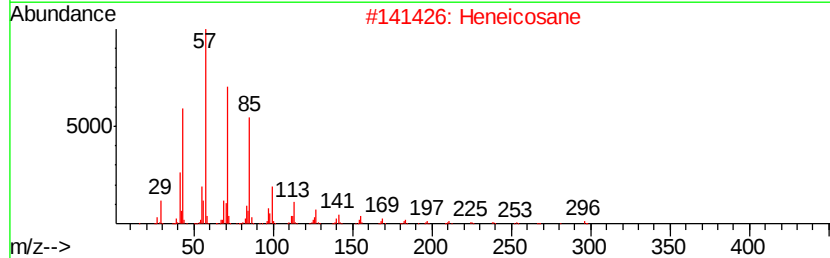
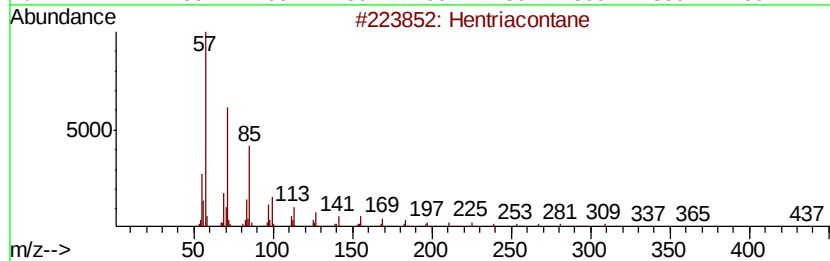
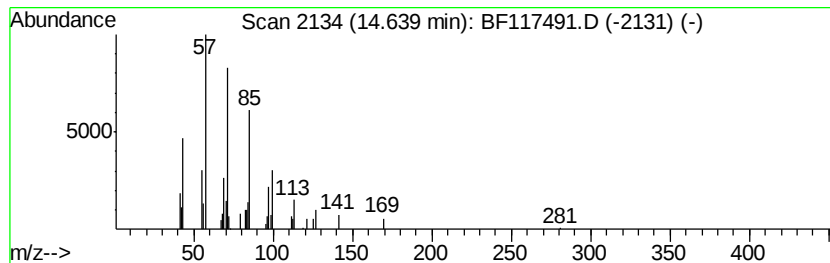
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Hentriacontane Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.64 | 2.29 ng | 31467 | Perylene-d12     | 15.32 |

| Hit# of | 5                 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------------|--------------|-----|---------|-------------|------|
| 1       | Hentriacontane    |              | 437 | C31H64  | 000630-04-6 | 87   |
| 2       | Heneicosane       |              | 296 | C21H44  | 000629-94-7 | 86   |
| 3       | Hexacosane        |              | 366 | C26H54  | 000630-01-3 | 86   |
| 4       | Tetratetracontane |              | 619 | C44H90  | 007098-22-8 | 86   |
| 5       | Heptacosane       |              | 380 | C27H56  | 000593-49-7 | 86   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\  
Data File : BF117491.D  
Acq On : 23 Oct 2019 18:58  
Operator : JU  
Sample : K5485-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-23-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

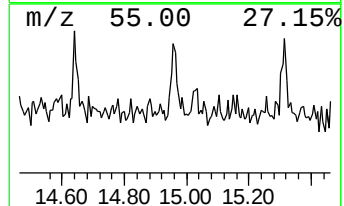
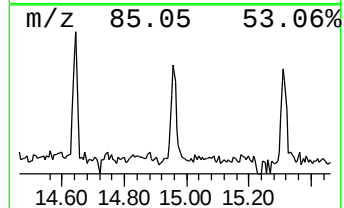
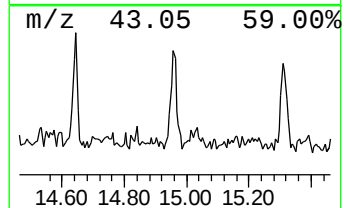
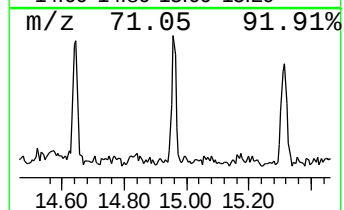
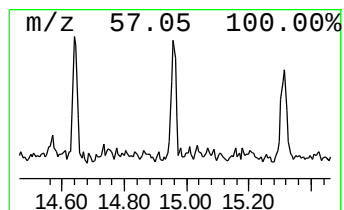
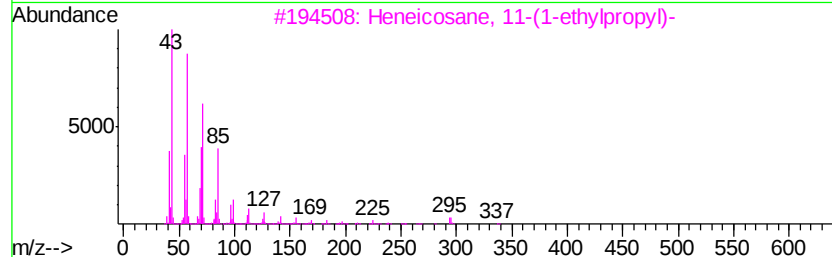
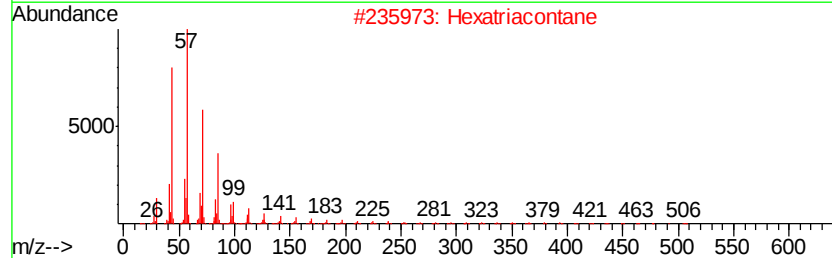
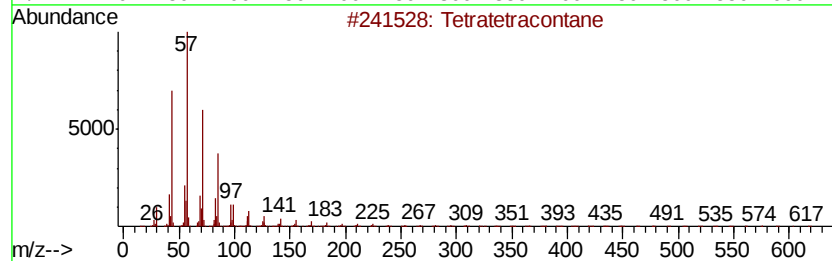
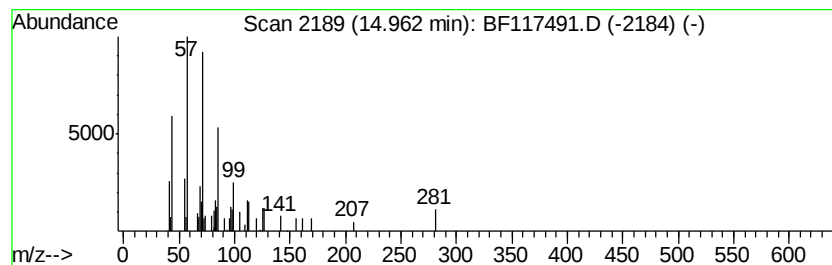
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Tetratetracontane Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.96 | 2.97 ng | 40769 | Perylene-d12     | 15.32 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|---------|---|-------------------------------------|-----|-----------|--------------|------|
| 1       |   | Tetratetracontane                   | 619 | C44H90    | 007098-22-8  | 90   |
| 2       |   | Hexatriacontane                     | 507 | C36H74    | 000630-06-8  | 90   |
| 3       |   | Heneicosane, 11-(1-ethylpropyl)-    | 366 | C26H54    | 055282-11-6  | 86   |
| 4       |   | Octacosane                          | 394 | C28H58    | 000630-02-4  | 86   |
| 5       |   | Sulfurous acid, dodecyl 2-propyl... | 292 | C15H32O3S | 1000309-12-3 | 86   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\  
Data File : BF117491.D  
Acq On : 23 Oct 2019 18:58  
Operator : JU  
Sample : K5485-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-23-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

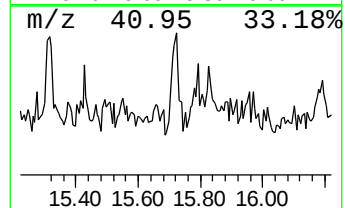
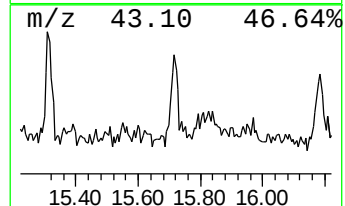
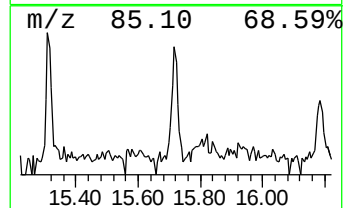
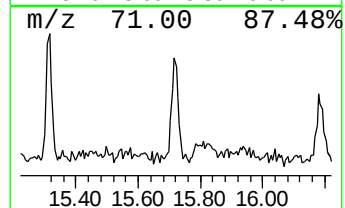
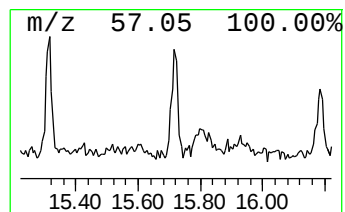
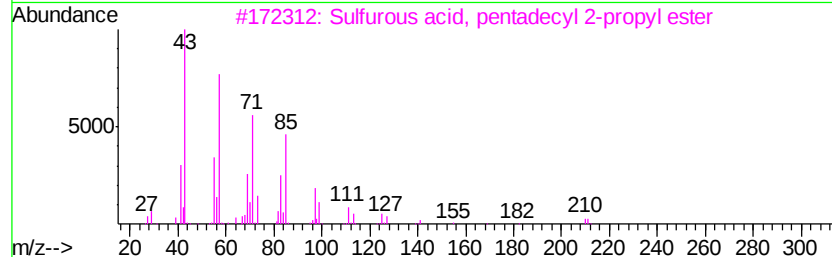
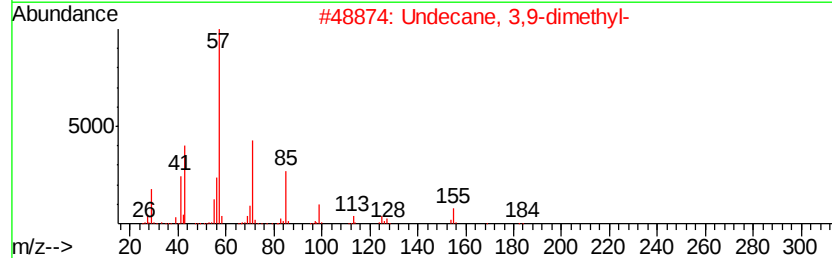
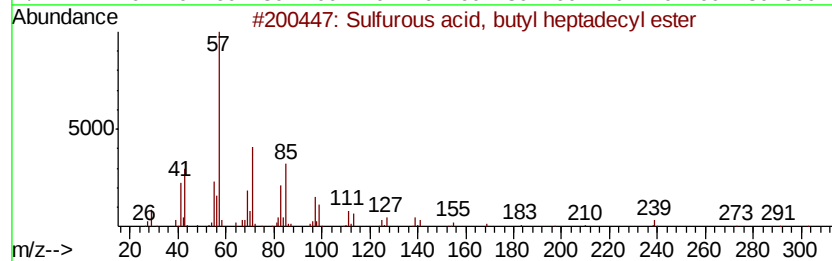
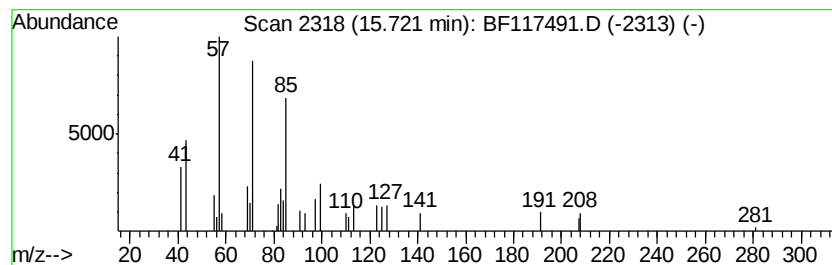
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Sulfurous acid, butyl hepta... Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 15.72 | 2.47 ng | 33919 | Perylene-d12     | 15.32 |

| Hit# | of | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|--------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | Sulfurous acid, butyl heptadecyl...  | 376 | C21H44O3S   | 1000309-18-4 | 64   |
| 2    |    | Undecane, 3,9-dimethyl-              | 184 | C13H28      | 017301-31-4  | 59   |
| 3    |    | Sulfurous acid, pentadecyl 2-pro...  | 334 | C18H38O3S   | 1000309-12-6 | 59   |
| 4    |    | Sulfurous acid, 2-propyl tridecyl... | 306 | C16H34O3S   | 1000309-12-4 | 59   |
| 5    |    | Silane, trichlorooctadecyl-          | 386 | C18H37Cl3Si | 000112-04-9  | 53   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF102319\  
Data File : BF117491.D  
Acq On : 23 Oct 2019 18:58  
Operator : JU  
Sample : K5485-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-23-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101819.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown6.50          | 6.50  | 81.3    | ng    | 933136   | 1                     | 6.73  | 229582 | 20.0 |
| n-Hexadecanoic acid  | 11.77 | 3.5     | ng    | 62875    | 4                     | 11.25 | 354162 | 20.0 |
| 17-Pentatriacontene  | 13.73 | 13.2    | ng    | 172693   | 5                     | 13.89 | 260950 | 20.0 |
| Hexacosane           | 14.34 | 2.3     | ng    | 30150    | 5                     | 13.89 | 260950 | 20.0 |
| Hentriacontane       | 14.64 | 2.3     | ng    | 31467    | 6                     | 15.32 | 274576 | 20.0 |
| Tetratetracontane    | 14.96 | 3.0     | ng    | 40769    | 6                     | 15.32 | 274576 | 20.0 |
| Sulfurous acid, b... | 15.72 | 2.5     | ng    | 33919    | 6                     | 15.32 | 274576 | 20.0 |