

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF060322\  
 Data File : BF128685.D  
 Acq On : 03 Jun 2022 18:09  
 Operator : CG\JU  
 Sample : N3025-03  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 EAST-SW

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128685.D\data.ms

| 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         | 5.034       | 464           | 467         | 471          | rVB      | 20932          | 23171         | 1.26%           | 0.188%        |
| 2         | 5.469       | 538           | 541         | 549          | rBV      | 1850057        | 1840611       | 100.00%         | 14.926%       |
| 3         | 6.481       | 710           | 713         | 724          | rVV      | 1867307        | 1770960       | 96.22%          | 14.361%       |
| 4         | 6.563       | 724           | 727         | 730          | rVB      | 29967          | 20602         | 1.12%           | 0.167%        |
| 5         | 6.822       | 767           | 771         | 774          | rBV      | 592178         | 455572        | 24.75%          | 3.694%        |
| 6         | 7.386       | 862           | 867         | 870          | rBV      | 1354740        | 1171344       | 63.64%          | 9.499%        |
| 7         | 8.104       | 985           | 989         | 993          | rBV      | 670887         | 524798        | 28.51%          | 4.256%        |
| 8         | 9.180       | 1168          | 1172        | 1175         | rBV      | 2088707        | 1680065       | 91.28%          | 13.624%       |
| 9         | 9.863       | 1284          | 1288        | 1291         | rBV      | 568519         | 499107        | 27.12%          | 4.047%        |
| 10        | 10.651      | 1418          | 1422        | 1425         | rBV      | 1163190        | 939279        | 51.03%          | 7.617%        |
| 11        | 11.345      | 1537          | 1540        | 1544         | rBV      | 539691         | 446719        | 24.27%          | 3.623%        |
| 12        | 11.880      | 1627          | 1631        | 1638         | rBV      | 78029          | 85224         | 4.63%           | 0.691%        |
| 13        | 12.668      | 1762          | 1765        | 1771         | rBV      | 31675          | 38048         | 2.07%           | 0.309%        |
| 14        | 12.939      | 1807          | 1811        | 1814         | rBV      | 1581983        | 1338574       | 72.72%          | 10.855%       |
| 15        | 13.421      | 1889          | 1893        | 1899         | rBV      | 114166         | 102680        | 5.58%           | 0.833%        |
| 16        | 13.874      | 1962          | 1970        | 1981         | rBV7     | 34426          | 128098        | 6.96%           | 1.039%        |
| 17        | 13.992      | 1986          | 1990        | 1993         | rBV      | 570444         | 481754        | 26.17%          | 3.907%        |
| 18        | 14.086      | 2002          | 2006        | 2015         | rBV      | 174797         | 203544        | 11.06%          | 1.651%        |
| 19        | 14.774      | 2120          | 2123        | 2128         | rVB3     | 17873          | 20160         | 1.10%           | 0.163%        |
| 20        | 15.109      | 2177          | 2180        | 2187         | rBV3     | 24991          | 33960         | 1.85%           | 0.275%        |
| 21        | 15.456      | 2234          | 2239        | 2243         | rBV      | 360717         | 432440        | 23.49%          | 3.507%        |
| 22        | 15.492      | 2243          | 2245        | 2249         | rVB2     | 29681          | 33842         | 1.84%           | 0.274%        |
| 23        | 15.927      | 2315          | 2319        | 2323         | rVB2     | 22246          | 34478         | 1.87%           | 0.280%        |
| 24        | 16.433      | 2401          | 2405        | 2409         | rVB2     | 18034          | 26339         | 1.43%           | 0.214%        |

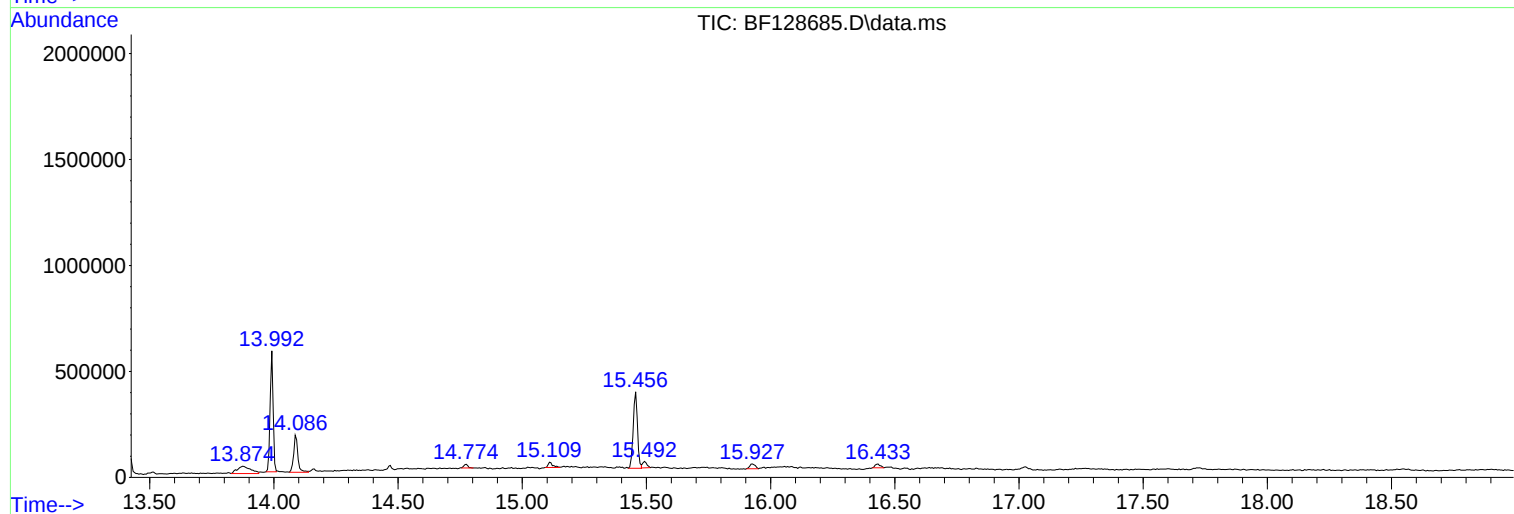
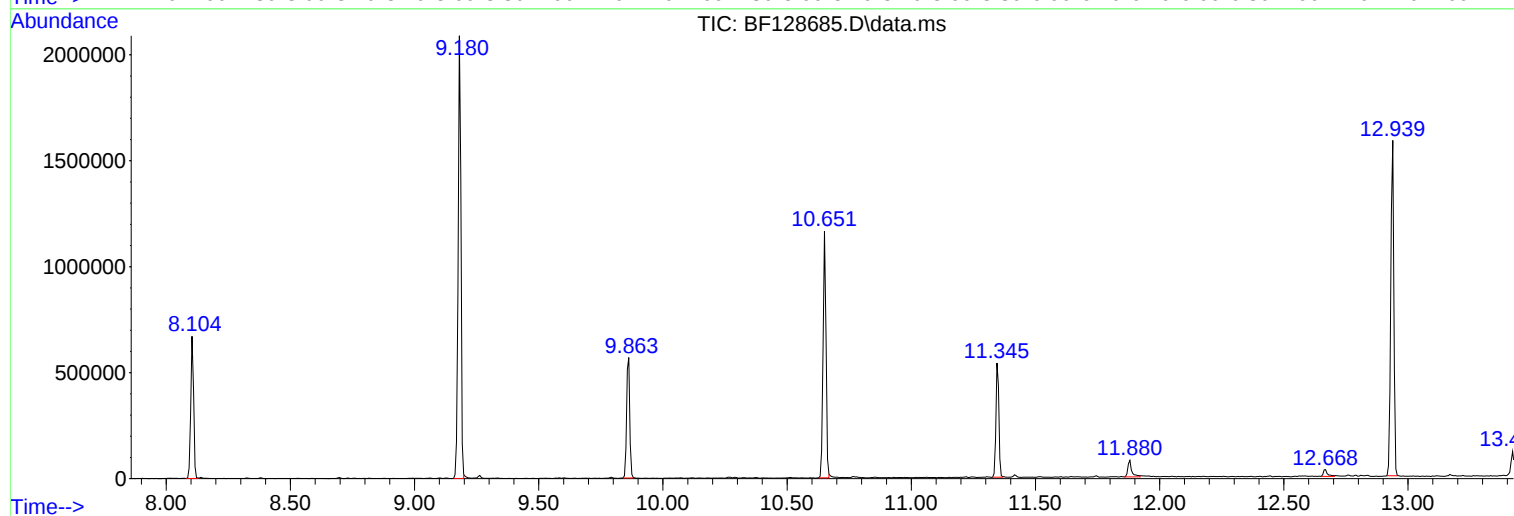
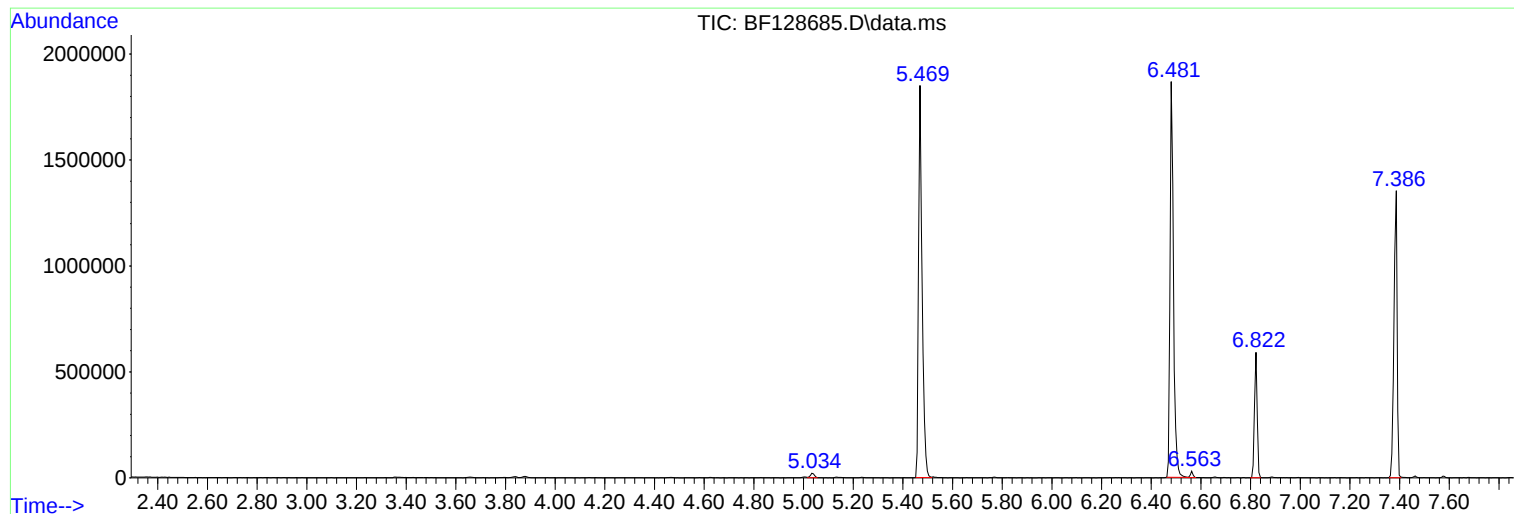
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BNA\_F  
ClientSampleId :  
EAST-SW

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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ClientSampleId :  
EAST-SW

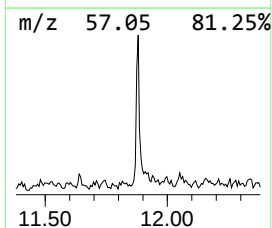
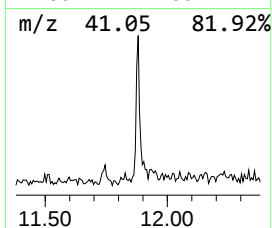
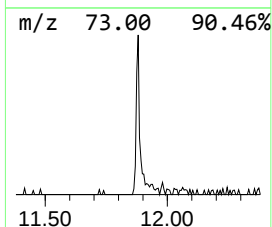
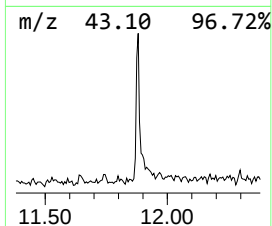
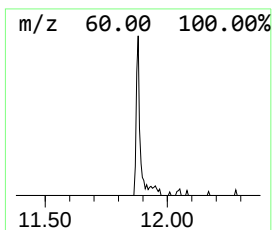
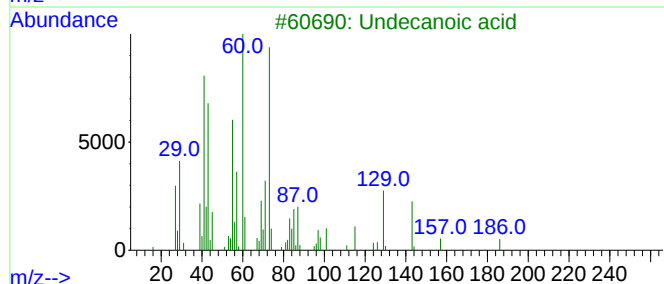
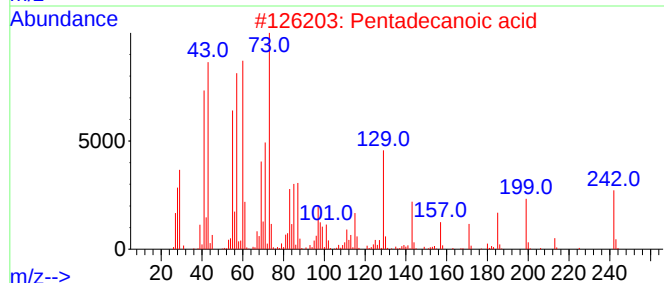
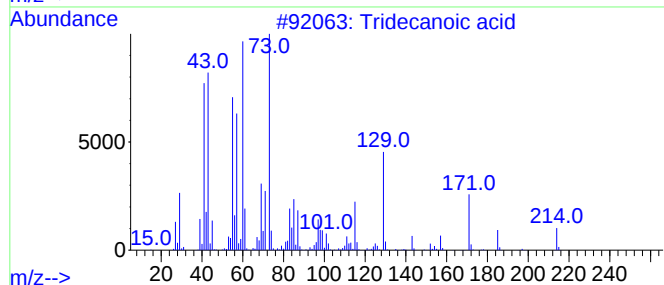
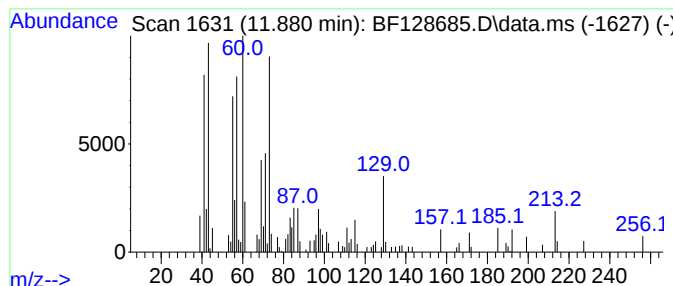
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Tridecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.880 | 3.82 ng | 85224 | Phenanthrene-d10 | 11.345 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 83   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 76   |
| 3    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 64   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 60   |



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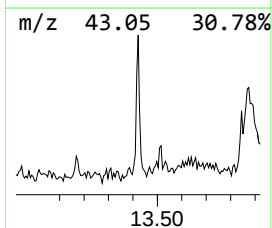
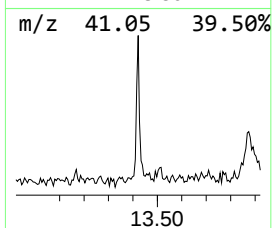
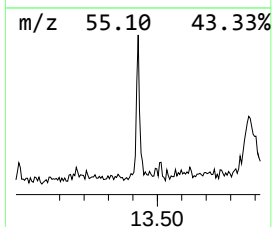
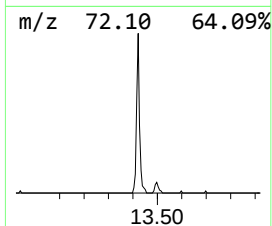
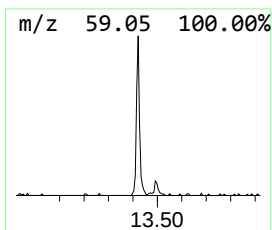
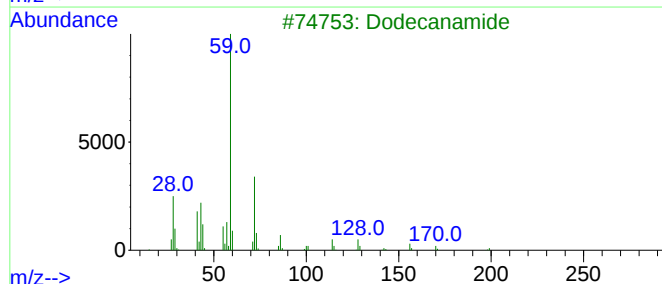
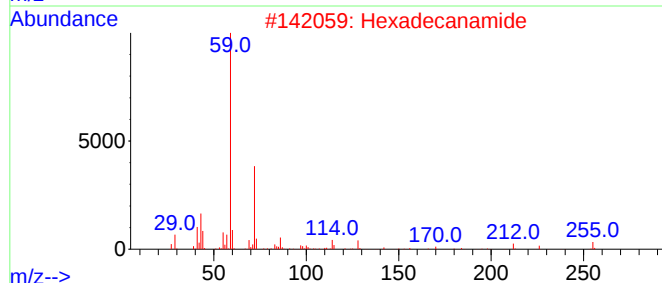
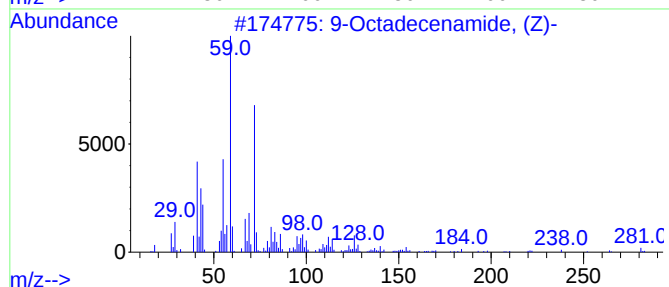
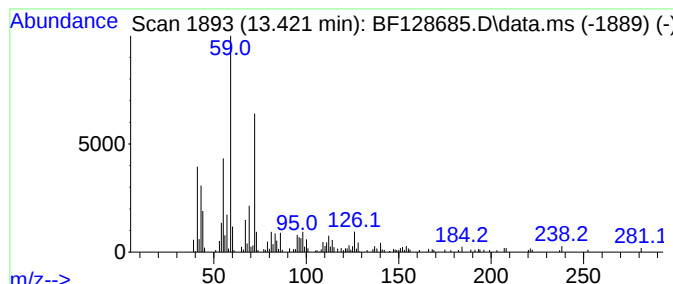
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TIC Integration Parameters: LSCINT.P

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Peak Number 2 9-Octadecenamide, (Z)- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.421 | 4.26 ng | 102680 | Chrysene-d12     | 13.992 |

| Hit# | of 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|------|------|------------------------|-----|----------|-------------|------|
| 1    |      | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 99   |
| 2    |      | Hexadecanamide         | 255 | C16H33NO | 000629-54-9 | 72   |
| 3    |      | Dodecanamide           | 199 | C12H25NO | 001120-16-7 | 70   |
| 4    |      | Pentanamide, 4-methyl- | 115 | C6H13NO  | 001119-29-5 | 59   |
| 5    |      | 7-Nonenamide           | 155 | C9H17NO  | 090949-53-4 | 58   |



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Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
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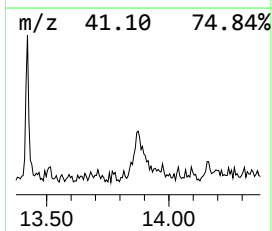
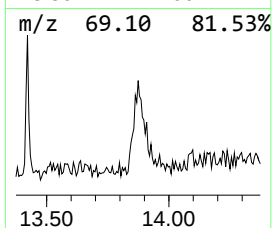
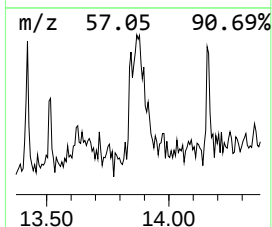
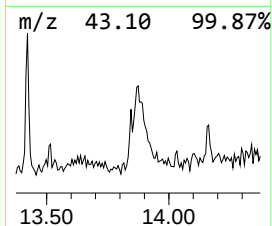
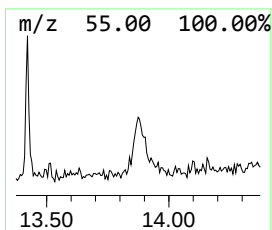
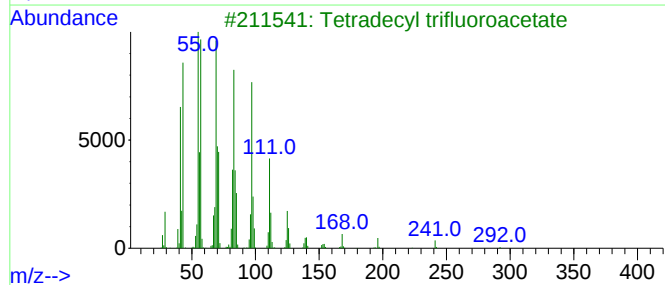
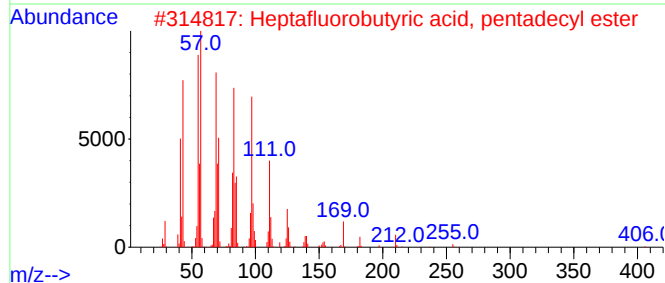
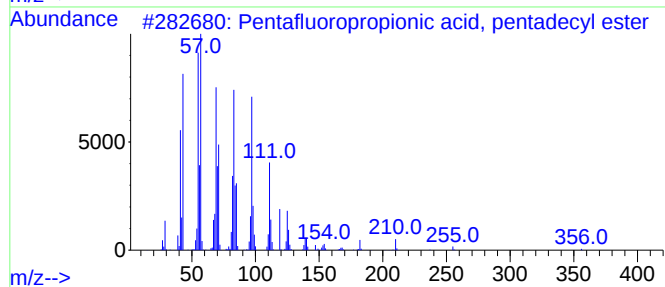
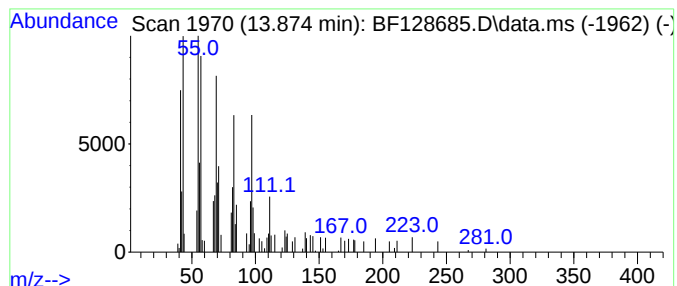
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.874 | 5.32 ng | 128098 | Chrysene-d12     | 13.992 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 87   |
| 2    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 87   |
| 3    |    |   | Tetradecyl trifluoroacetate         | 310 | C16H29F3O2 | 006222-02-2 | 87   |
| 4    |    |   | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 87   |
| 5    |    |   | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 87   |



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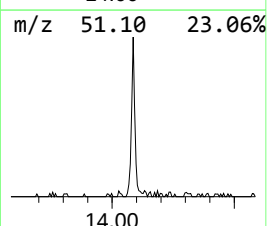
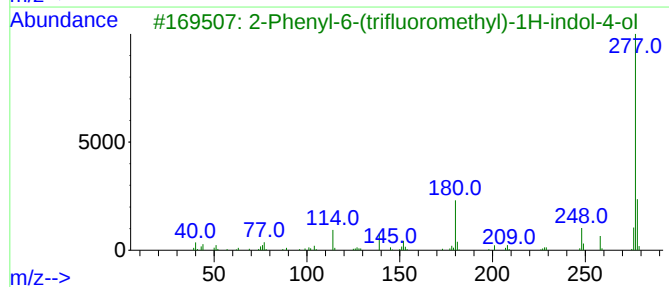
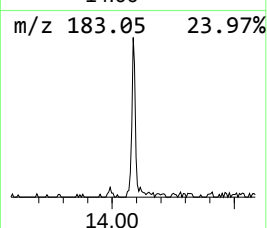
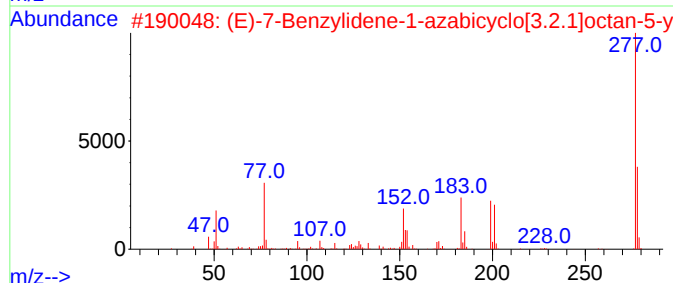
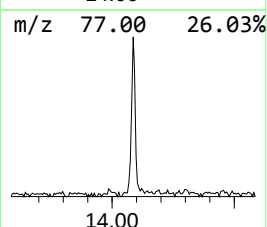
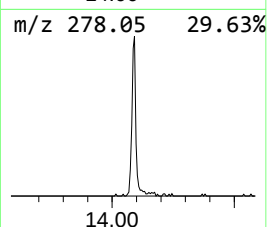
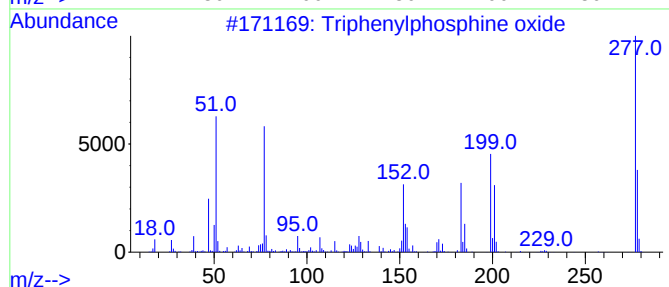
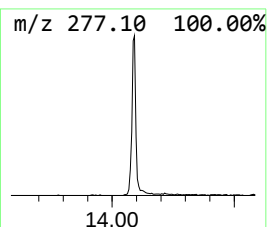
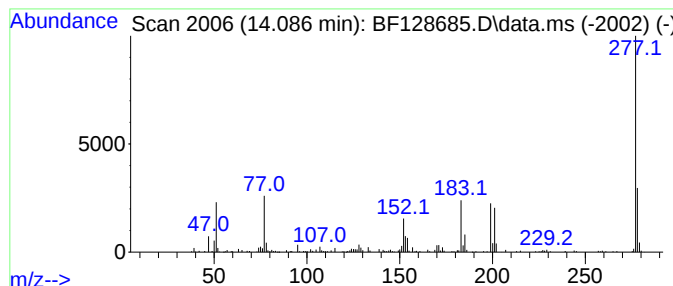
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.086 | 8.45 ng | 203544 | Chrysene-d12     | 13.992 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide            | 278 | C18H15OP   | 000791-28-6  | 98   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 90   |
| 3    |    |   | 2-Phenyl-6-(trifluoromethyl)-1H...  | 277 | C15H10F3NO | 1000387-59-3 | 38   |
| 4    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd... | 277 | C18H15NO2  | 299962-12-2  | 37   |
| 5    |    |   | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P  | 015990-54-2  | 36   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Tridecanoic acid   | 11.880 | 3.8     | ng    | 85224    | 4                     | 11.345 | 446719 | 20.0 |
| 9-Octadecenamid... | 13.421 | 4.3     | ng    | 102680   | 5                     | 13.992 | 481754 | 20.0 |
| Pentafluoroprop... | 13.874 | 5.3     | ng    | 128098   | 5                     | 13.992 | 481754 | 20.0 |
| Triphenylphosph... | 14.086 | 8.4     | ng    | 203544   | 5                     | 13.992 | 481754 | 20.0 |