

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM042221\  
 Data File : BM029600.D  
 Acq On : 22 Apr 2021 18:54  
 Operator : CG/JU  
 Sample : M2106-21  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 SB-28-9.5-10.0

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\_M\Methods\8270-BM042121.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029600.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         | 4.787       | 318           | 323         | 333          | rVB      | 28065          | 45215         | 1.18%           | 0.259%        |
| 2         | 5.228       | 392           | 398         | 412          | rBV      | 1025470        | 1523202       | 39.64%          | 8.726%        |
| 3         | 6.810       | 659           | 667         | 680          | rBV      | 1012178        | 1670234       | 43.46%          | 9.568%        |
| 4         | 7.634       | 800           | 807         | 816          | rBV      | 245582         | 394951        | 10.28%          | 2.263%        |
| 5         | 8.787       | 996           | 1003        | 1024         | rBV      | 621502         | 1052903       | 27.40%          | 6.032%        |
| 6         | 10.410      | 1273          | 1279        | 1293         | rBV      | 289665         | 497817        | 12.95%          | 2.852%        |
| 7         | 12.892      | 1694          | 1701        | 1719         | rBV      | 1807633        | 2617096       | 68.10%          | 14.993%       |
| 8         | 13.739      | 1839          | 1845        | 1852         | rBV      | 31463          | 47777         | 1.24%           | 0.274%        |
| 9         | 14.274      | 1930          | 1936        | 1945         | rBV      | 469098         | 693674        | 18.05%          | 3.974%        |
| 10        | 15.768      | 2184          | 2190        | 2203         | rBV      | 1315982        | 1849228       | 48.12%          | 10.594%       |
| 11        | 17.021      | 2396          | 2403        | 2412         | rBV      | 571286         | 823863        | 21.44%          | 4.720%        |
| 12        | 17.927      | 2552          | 2557        | 2567         | rBV      | 50451          | 85924         | 2.24%           | 0.492%        |
| 13        | 19.651      | 2845          | 2850        | 2860         | rBV      | 3141152        | 3843012       | 100.00%         | 22.016%       |
| 14        | 20.927      | 3063          | 3067        | 3074         | rBV3     | 101465         | 152931        | 3.98%           | 0.876%        |
| 15        | 21.203      | 3109          | 3114        | 3126         | rBV      | 778995         | 1037439       | 27.00%          | 5.943%        |
| 16        | 23.392      | 3480          | 3486        | 3496         | rVB2     | 594917         | 1120338       | 29.15%          | 6.418%        |

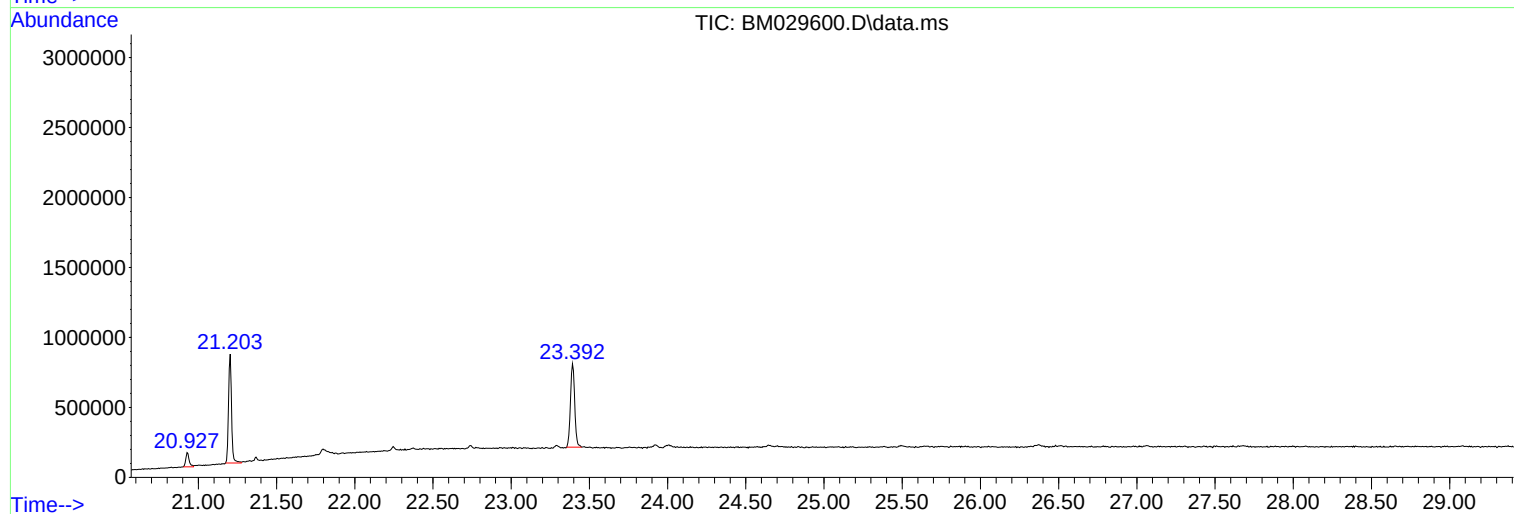
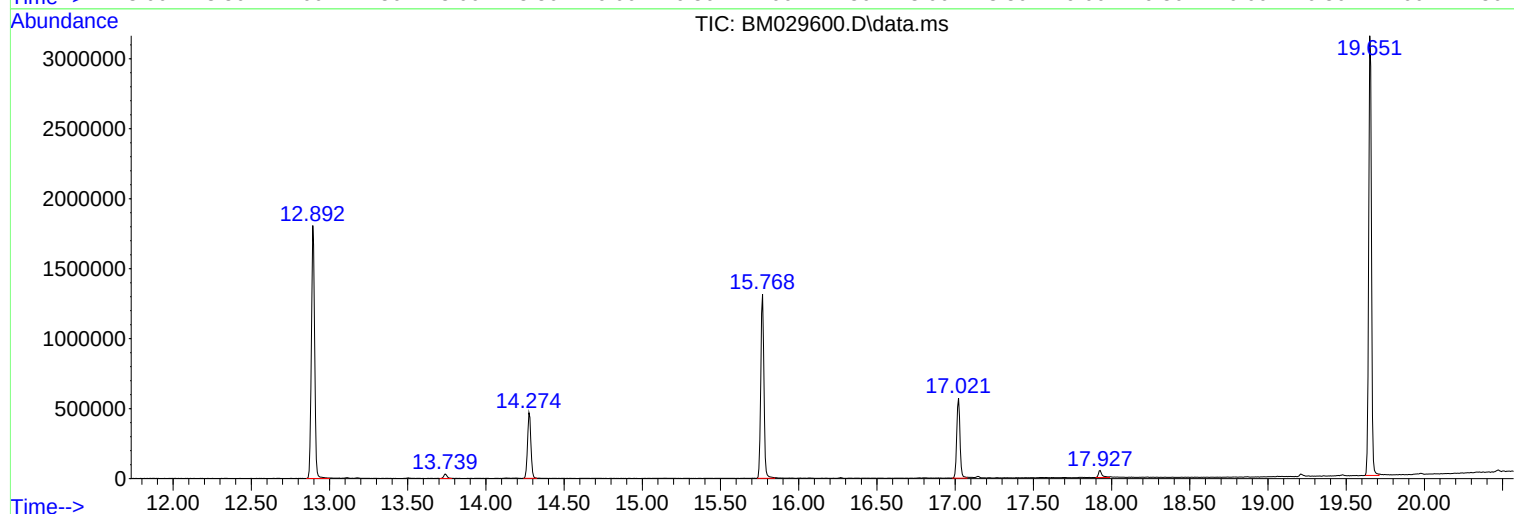
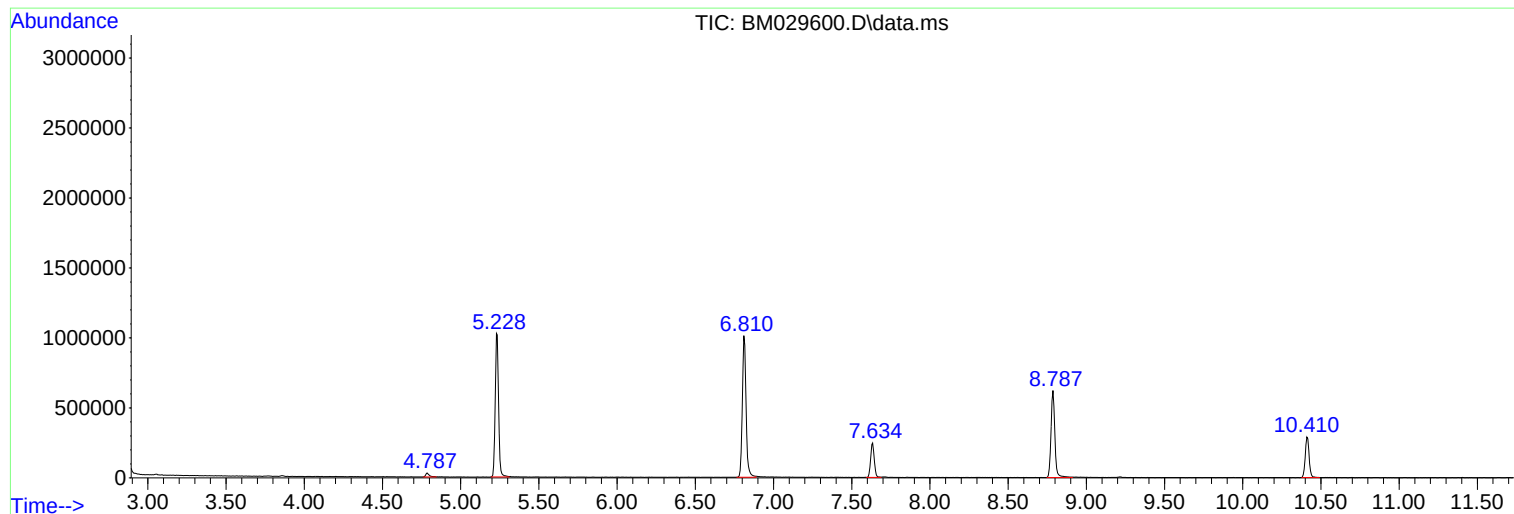
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042121.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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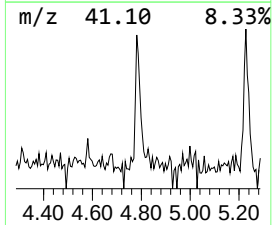
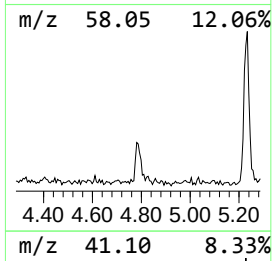
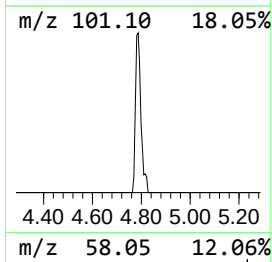
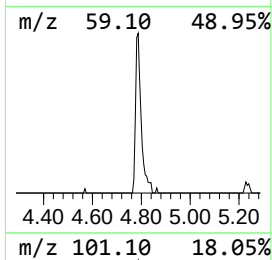
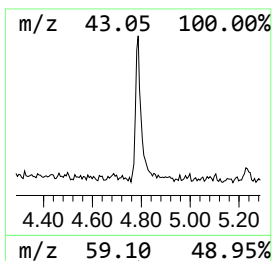
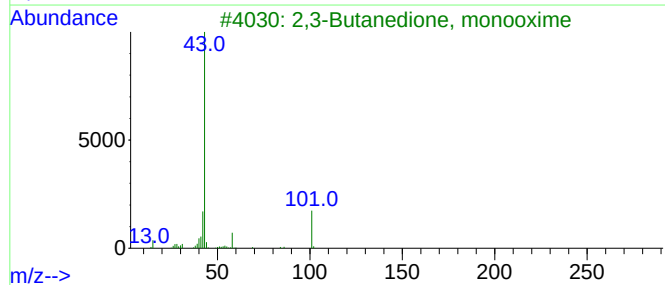
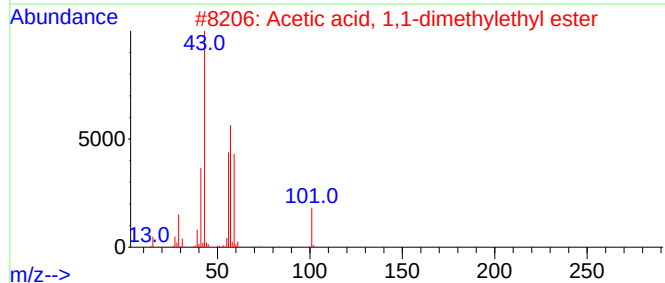
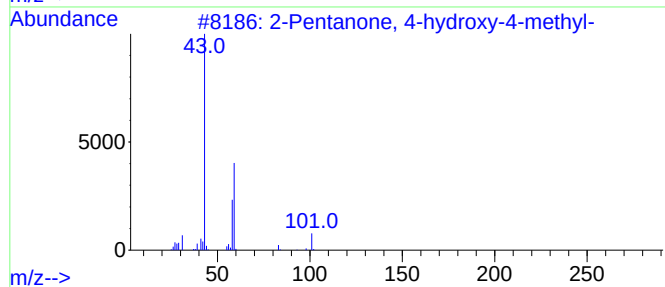
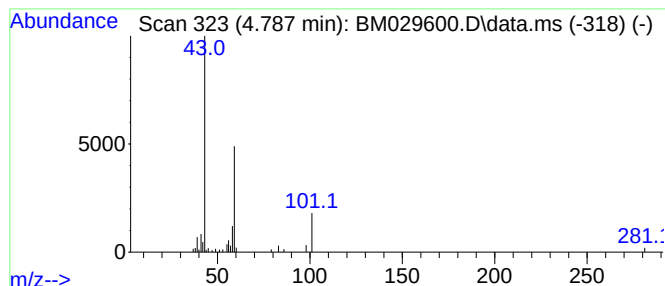
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.787 | 2.29 ng | 45215 | 1,4-Dichlorobenzene-d4 | 7.634 |

| 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 | 38      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 16      |      |      |
| 4    | 5-Hexen-2-one                       | 98  | C6H10O       | 000109-49-9 | 9       |      |      |
| 5    | n-Octanoic acid isopropyl ester     | 186 | C11H22O2     | 005458-59-3 | 9       |      |      |



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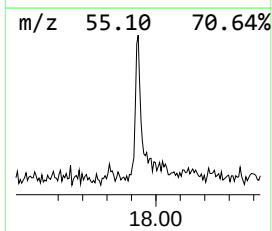
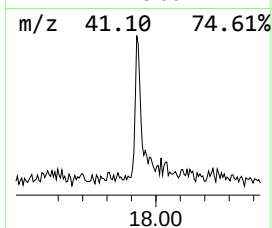
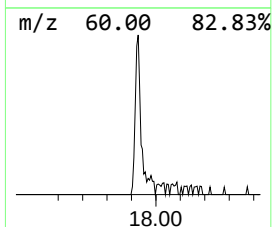
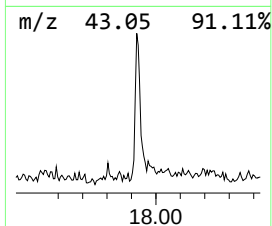
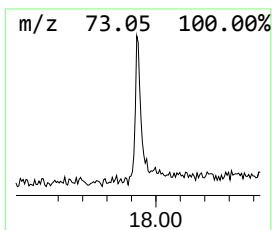
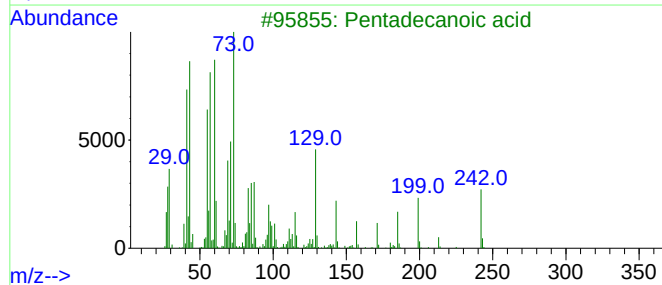
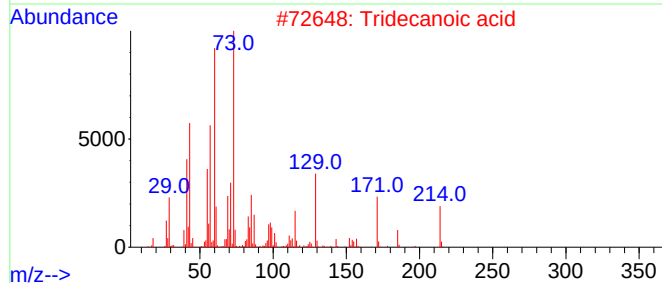
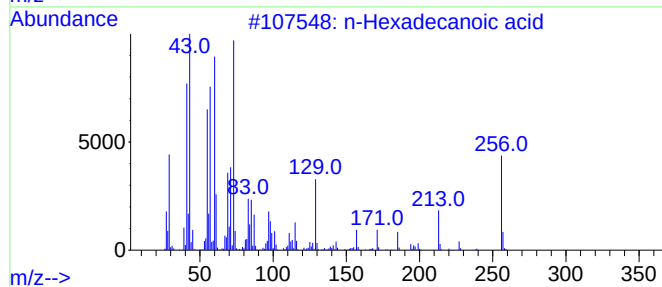
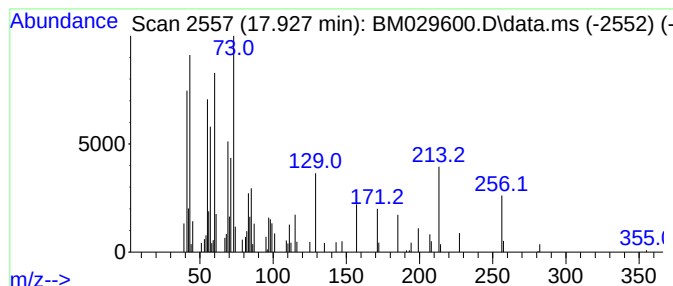
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TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 17.927 | 2.09 ng | 85924 | Phenanthrene-d10 | 17.021 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91   |
| 2    |      | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 53   |
| 3    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 52   |
| 4    |      | Isopropyl palmitate | 298 | C19H38O2 | 000142-91-6 | 50   |
| 5    |      | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 43   |



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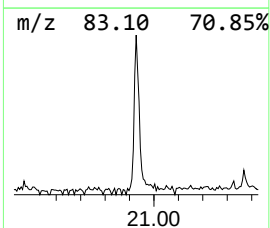
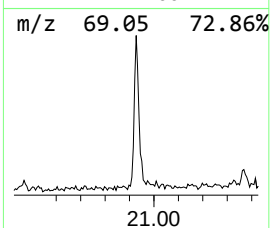
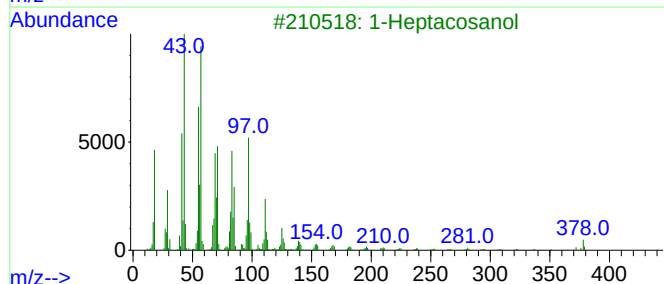
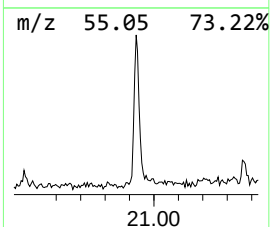
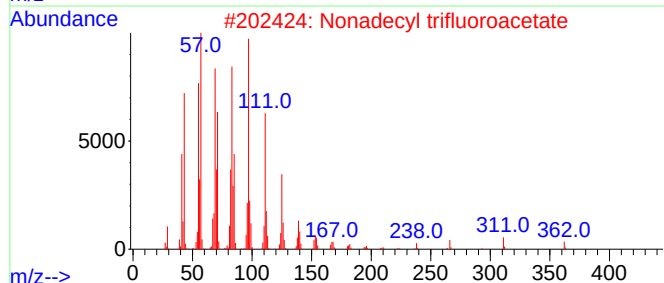
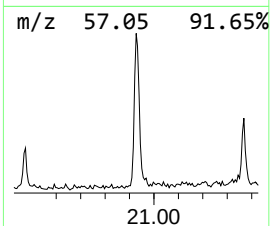
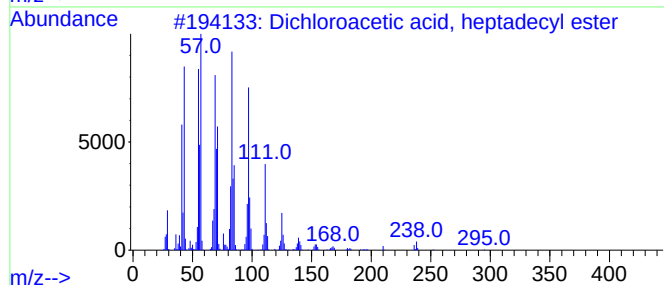
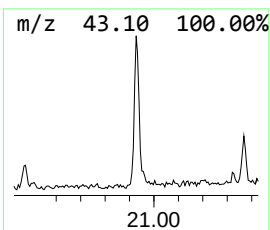
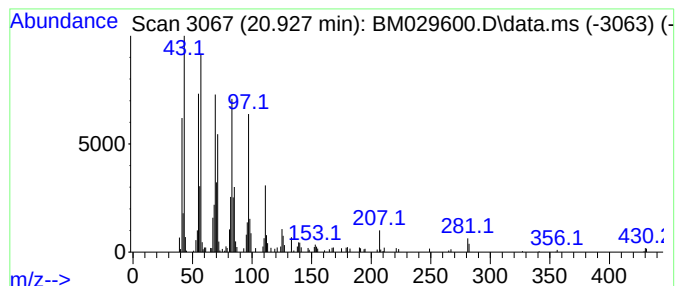
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Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.927 | 2.95 ng | 152931 | Chrysene-d12     | 21.203 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 90   |
| 2    |    |   | Nonadecyl trifluoroacetate          | 380 | C21H39F3O2  | 1000351-76-3 | 87   |
| 3    |    |   | 1-Heptacosanol                      | 396 | C27H56O     | 002004-39-9  | 87   |
| 4    |    |   | 5-Eicosene, (E)-                    | 280 | C20H40      | 074685-30-6  | 87   |
| 5    |    |   | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2  | 006385-15-5  | 81   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.787  | 2.3     | ng    | 45215    | 1                     | 7.634  | 394951  | 20.0 |
| n-Hexadecanoic ... | 17.927 | 2.1     | ng    | 85924    | 4                     | 17.021 | 823863  | 20.0 |
| Dichloroacetic ... | 20.927 | 3.0     | ng    | 152931   | 5                     | 21.203 | 1037440 | 20.0 |