

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030419\  
 Data File : BM019017.D  
 Acq On : 04 Mar 2019 19:41  
 Operator : JU/SJ  
 Sample : K1712-19  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 Z-2-4

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\_M\METHODS\8270-BM021119.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         | 5.275       | 366           | 372         | 394          | rBV      | 6494082        | 9302228       | 43.60%          | 8.181%        |
| 2         | 6.863       | 634           | 642         | 658          | rBV      | 6421404        | 10712270      | 50.20%          | 9.421%        |
| 3         | 7.216       | 694           | 702         | 719          | rBV      | 6793160        | 10535601      | 49.38%          | 9.265%        |
| 4         | 7.681       | 773           | 781         | 788          | rBV      | 1087872        | 1742528       | 8.17%           | 1.532%        |
| 5         | 7.999       | 827           | 835         | 846          | rBV      | 4582140        | 7359093       | 34.49%          | 6.472%        |
| 6         | 8.852       | 971           | 980         | 1003         | rBV      | 3655110        | 6137543       | 28.76%          | 5.398%        |
| 7         | 10.463      | 1247          | 1254        | 1273         | rBV      | 1364187        | 2358656       | 11.05%          | 2.074%        |
| 8         | 12.945      | 1669          | 1676        | 1692         | rBV      | 9587242        | 14071751      | 65.95%          | 12.375%       |
| 9         | 13.798      | 1814          | 1821        | 1835         | rBV      | 438610         | 692590        | 3.25%           | 0.609%        |
| 10        | 14.334      | 1905          | 1912        | 1926         | rBV2     | 2048213        | 3189553       | 14.95%          | 2.805%        |
| 11        | 15.833      | 2160          | 2167        | 2185         | rBV      | 8448012        | 12046044      | 56.45%          | 10.594%       |
| 12        | 17.086      | 2373          | 2380        | 2391         | rBV      | 2647705        | 3862520       | 18.10%          | 3.397%        |
| 13        | 17.974      | 2525          | 2531        | 2541         | rBV      | 423742         | 650861        | 3.05%           | 0.572%        |
| 14        | 19.257      | 2745          | 2749        | 2758         | rBV      | 140811         | 236107        | 1.11%           | 0.208%        |
| 15        | 19.721      | 2822          | 2828        | 2833         | rBV      | 17223360       | 21337648      | 100.00%         | 18.765%       |
| 16        | 20.980      | 3038          | 3042        | 3053         | rBV      | 507012         | 692710        | 3.25%           | 0.609%        |
| 17        | 21.280      | 3088          | 3093        | 3103         | rBV      | 3518752        | 4353594       | 20.40%          | 3.829%        |
| 18        | 22.309      | 3265          | 3268        | 3273         | rVB      | 191990         | 238133        | 1.12%           | 0.209%        |
| 19        | 22.815      | 3350          | 3354        | 3358         | rVB      | 178400         | 236569        | 1.11%           | 0.208%        |
| 20        | 23.380      | 3447          | 3450        | 3460         | rVB2     | 163923         | 260698        | 1.22%           | 0.229%        |
| 21        | 23.527      | 3469          | 3475        | 3487         | rVB      | 2032995        | 3692957       | 17.31%          | 3.248%        |

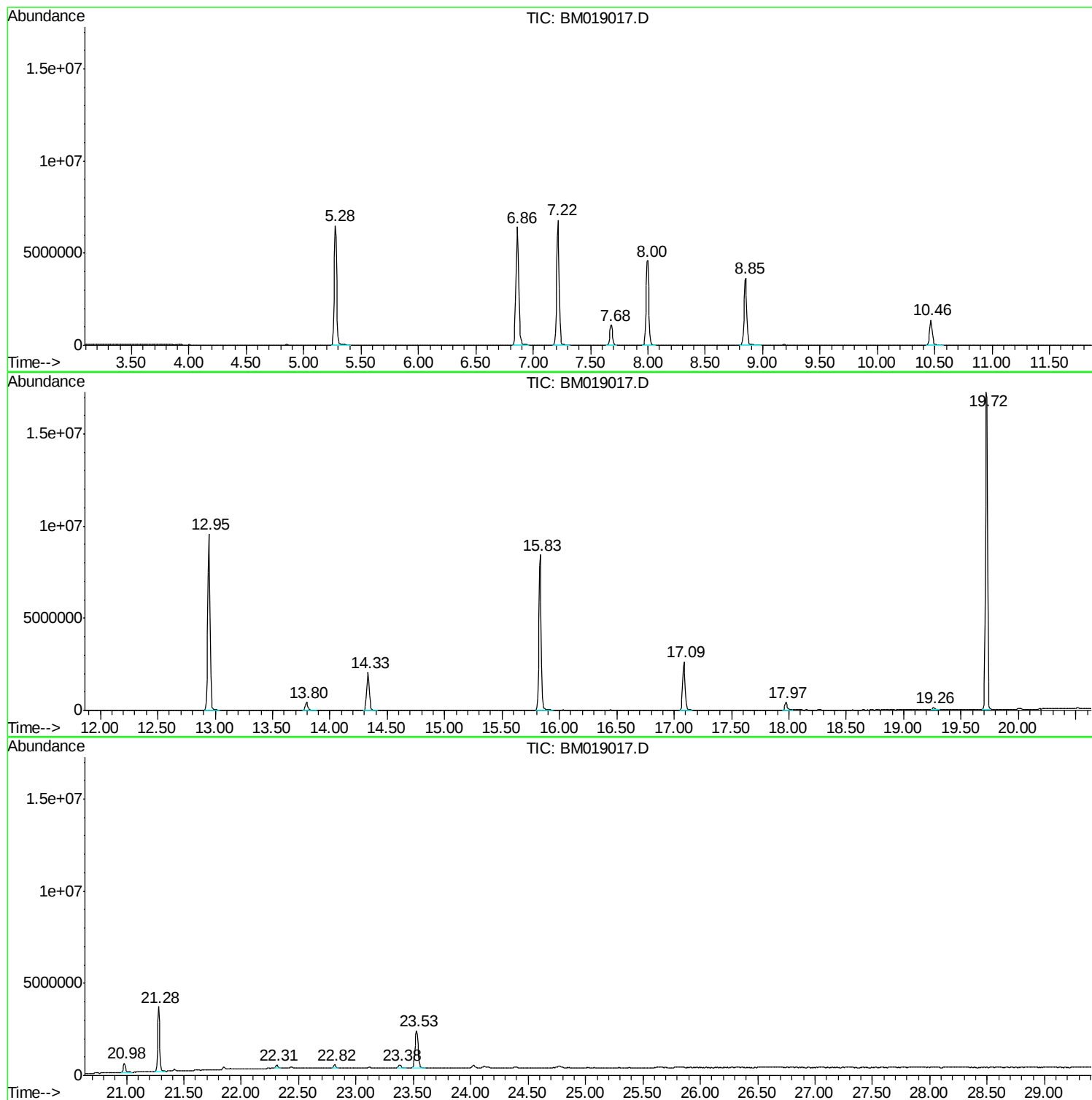
Sum of corrected areas: 113709654

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.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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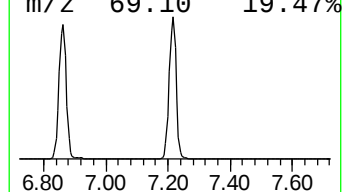
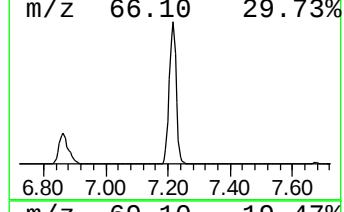
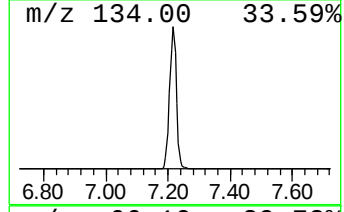
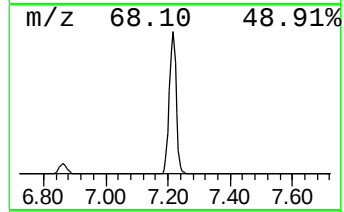
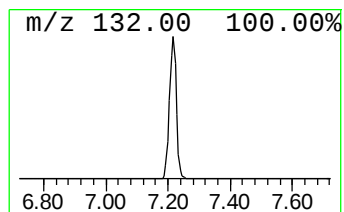
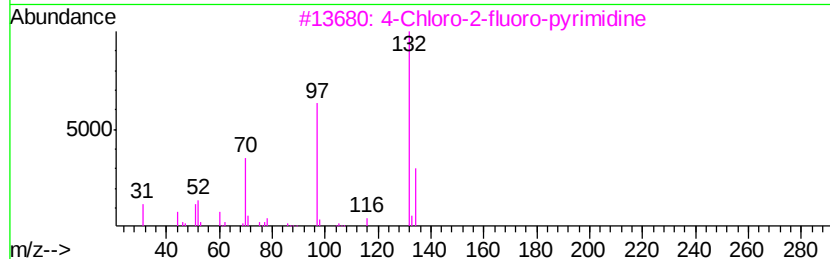
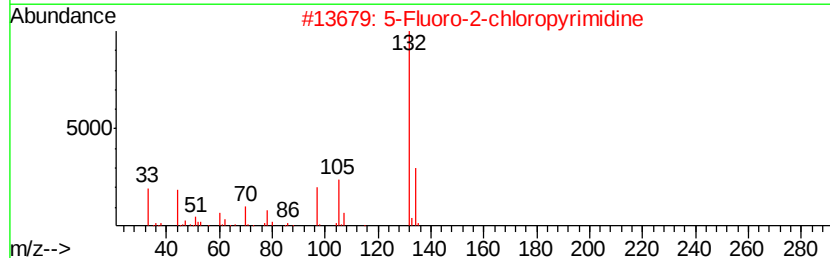
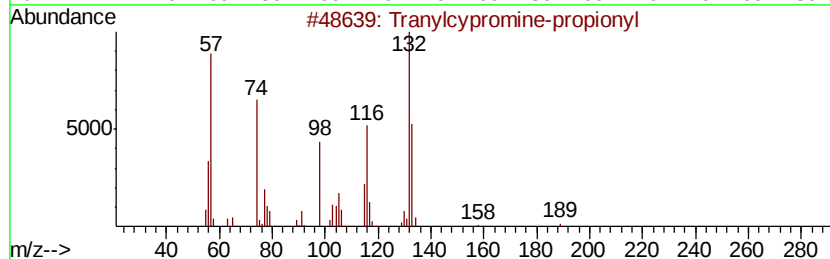
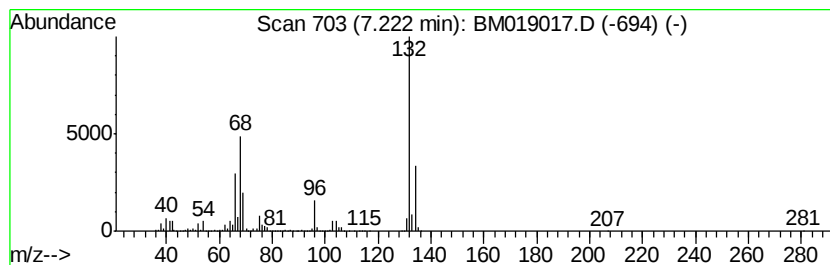
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown7.22 Concentration Rank 1

| R.T. | EstConc   | Area     | Relative to ISTD       | R.T. |
|------|-----------|----------|------------------------|------|
| 7.22 | 120.92 ng | 10535600 | 1,4-Dichlorobenzene-d4 | 7.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | Tranvlcvpromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |
| 5    |    | 2-Cyclohexen-1-one                  | 96  | C6H8O     | 000930-68-7  | 9    |



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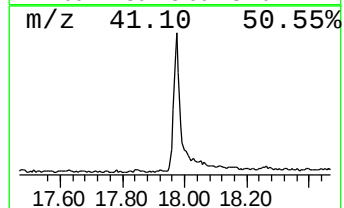
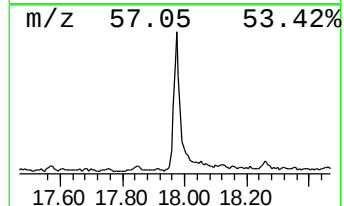
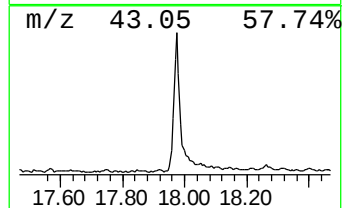
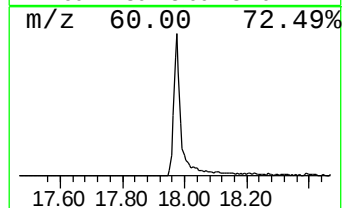
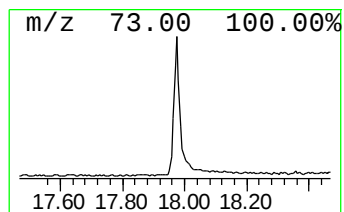
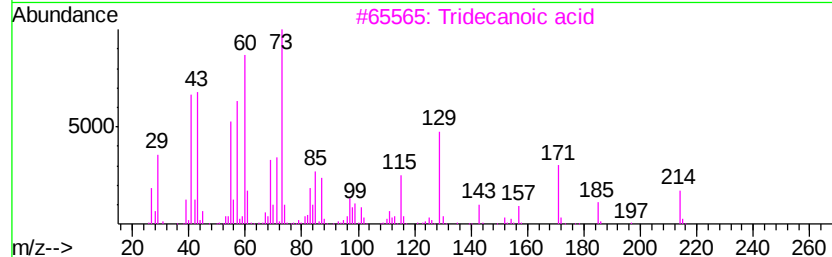
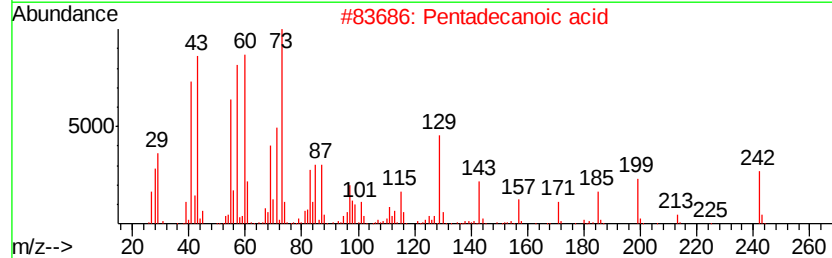
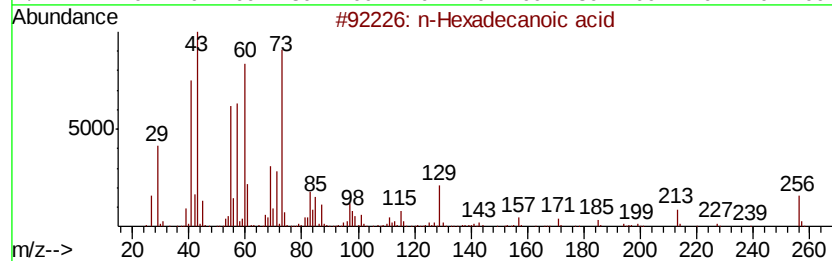
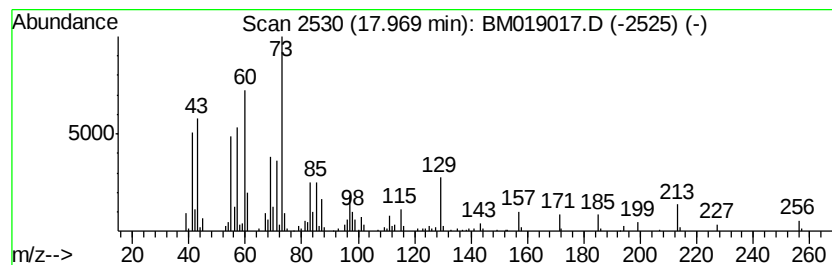
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.97 | 3.37 ng | 650861 | Phenanthrene-d10 | 17.09 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 72   |
| 3       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |
| 4       |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 47   |
| 5       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 47   |



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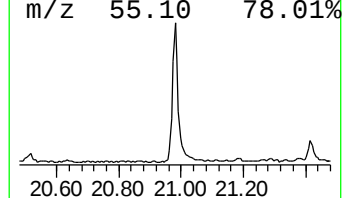
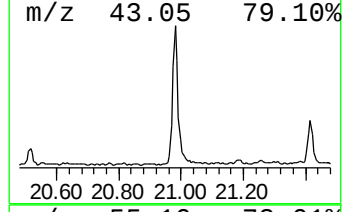
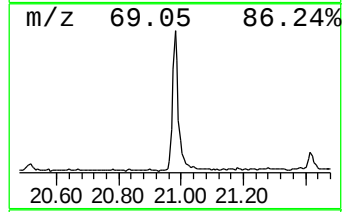
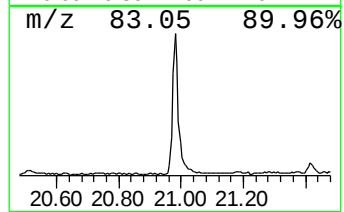
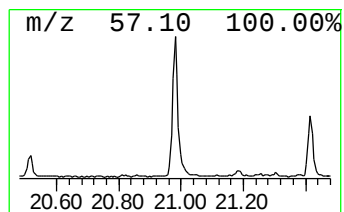
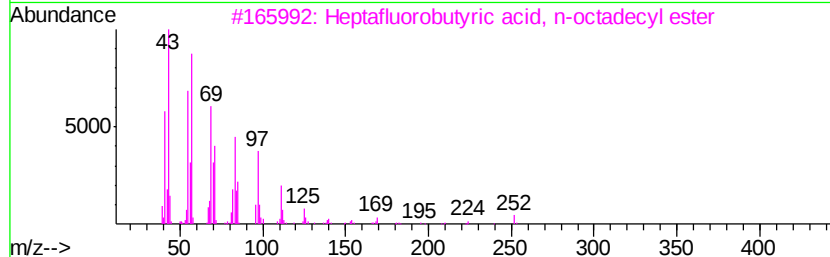
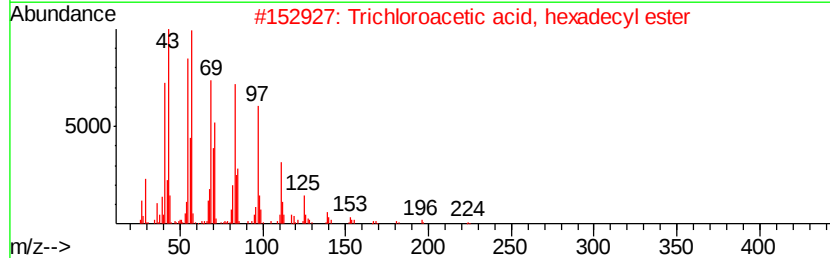
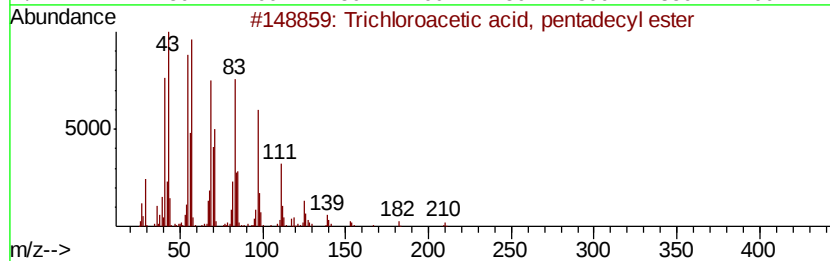
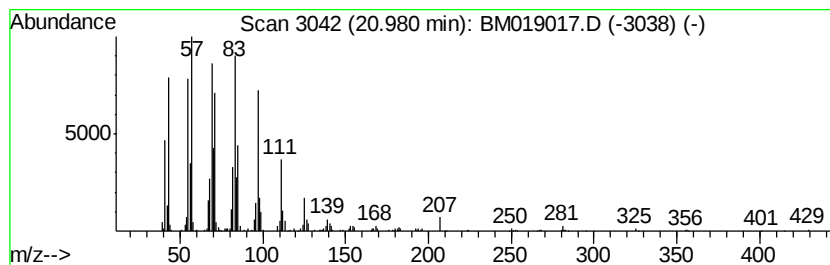
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.98 | 3.18 ng | 692710 | Chrysene-d12     | 21.28 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91   |
| 2    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91   |
| 3    |    |   | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2  | 000400-57-7 | 91   |
| 4    |    |   | 1-Tetracosanol                      | 354 | C24H50O     | 000506-51-4 | 91   |
| 5    |    |   | 1-Heneicosyl formate                | 340 | C22H44O2    | 077899-03-7 | 90   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown7.22          | 7.22  | 120.9   | ng    | 10535600 | 1                     | 7.68  | 1742530 | 20.0 |
| n-Hexadecanoic acid  | 17.97 | 3.4     | ng    | 650861   | 4                     | 17.09 | 3862520 | 20.0 |
| Trichloroacetic a... | 20.98 | 3.2     | ng    | 692710   | 5                     | 21.28 | 4353590 | 20.0 |