

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF082918\  
 Data File : BF108626.D  
 Acq On : 30 Aug 2018 2:05  
 Operator : JU/SJ  
 Sample : J4683-17  
 Misc :  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 082718-TIPC-F-U-B

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-BF080818.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         | 5.631       | 557           | 560         | 586          | rBV      | 311395         | 781780        | 19.95%          | 3.691%        |
| 2         | 6.625       | 726           | 729         | 750          | rBV      | 239616         | 601067        | 15.34%          | 2.838%        |
| 3         | 6.766       | 750           | 753         | 779          | rVV      | 1349841        | 1894413       | 48.34%          | 8.945%        |
| 4         | 7.001       | 789           | 793         | 815          | rVB      | 449492         | 709662        | 18.11%          | 3.351%        |
| 5         | 7.154       | 815           | 819         | 843          | rBV      | 2566832        | 2824747       | 72.08%          | 13.338%       |
| 6         | 7.566       | 884           | 889         | 912          | rBV      | 1640955        | 2327326       | 59.39%          | 10.989%       |
| 7         | 8.283       | 1007          | 1011        | 1041         | rBV      | 541107         | 839432        | 21.42%          | 3.964%        |
| 8         | 9.354       | 1189          | 1193        | 1208         | rBV      | 3906834        | 3918701       | 100.00%         | 18.503%       |
| 9         | 9.742       | 1256          | 1259        | 1274         | rBV      | 187157         | 240787        | 6.14%           | 1.137%        |
| 10        | 10.042      | 1306          | 1310        | 1331         | rVB      | 716652         | 797357        | 20.35%          | 3.765%        |
| 11        | 10.695      | 1418          | 1421        | 1430         | rBV      | 87909          | 80667         | 2.06%           | 0.381%        |
| 12        | 10.836      | 1441          | 1445        | 1462         | rBV      | 931555         | 1233667       | 31.48%          | 5.825%        |
| 13        | 11.536      | 1560          | 1564        | 1583         | rBV      | 564870         | 676648        | 17.27%          | 3.195%        |
| 14        | 13.118      | 1829          | 1833        | 1850         | rBV      | 2547616        | 2605178       | 66.48%          | 12.301%       |
| 15        | 14.042      | 1985          | 1990        | 2001         | rBV4     | 31641          | 99201         | 2.53%           | 0.468%        |
| 16        | 14.189      | 2011          | 2015        | 2026         | rBV      | 647684         | 693877        | 17.71%          | 3.276%        |
| 17        | 15.030      | 2153          | 2158        | 2162         | rBV      | 169945         | 185477        | 4.73%           | 0.876%        |
| 18        | 15.748      | 2275          | 2280        | 2293         | rVB      | 431551         | 668722        | 17.06%          | 3.158%        |

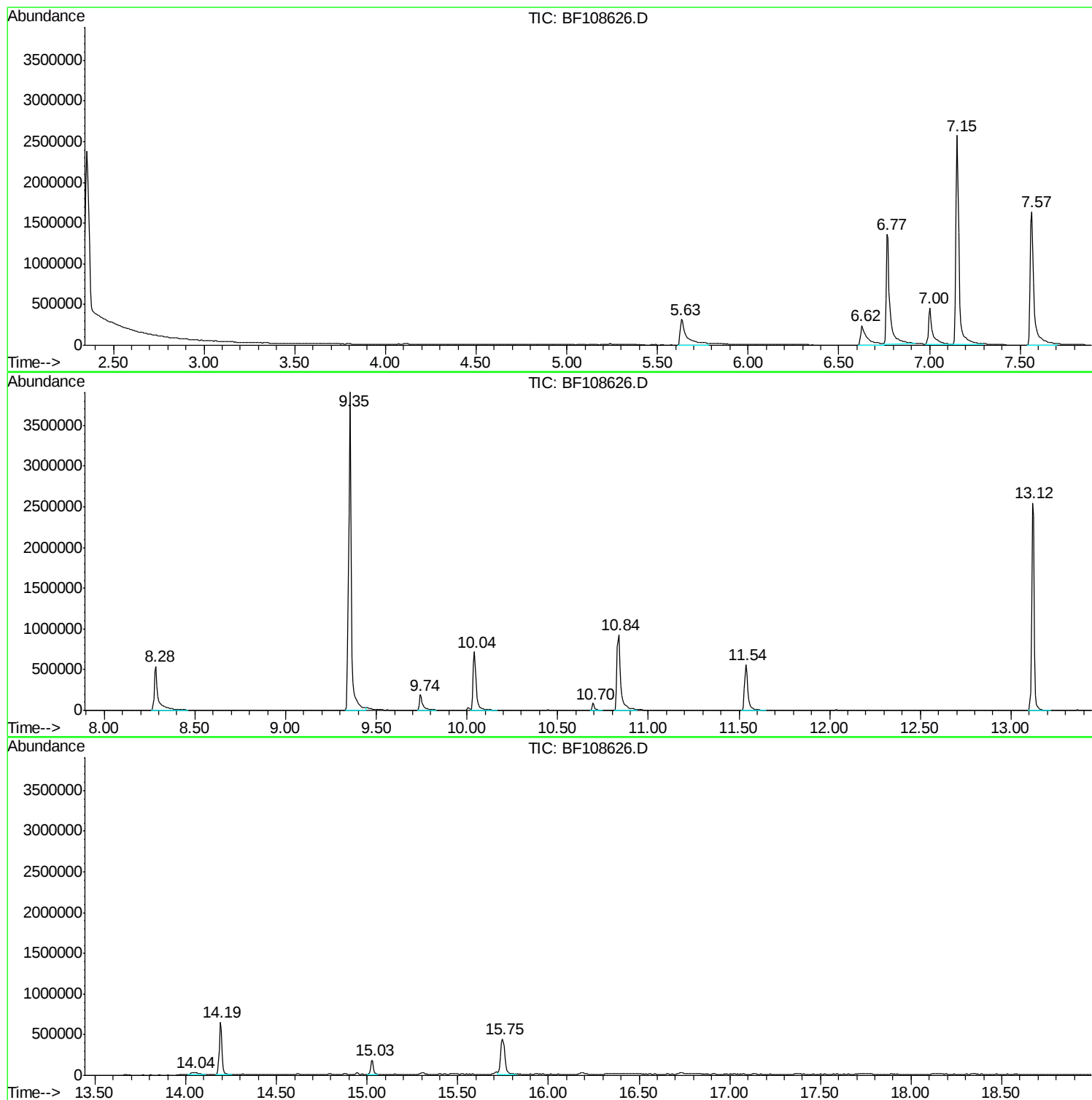
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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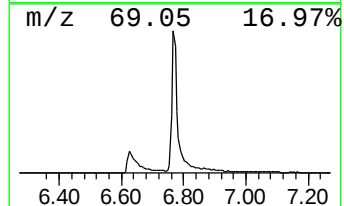
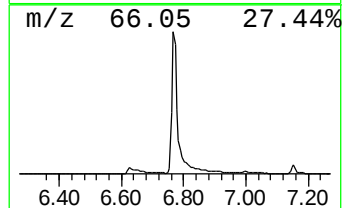
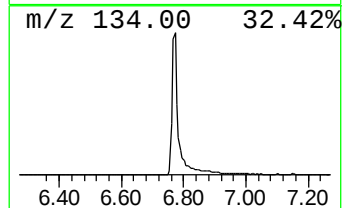
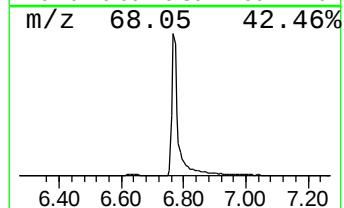
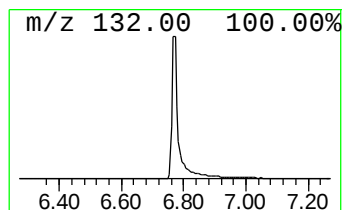
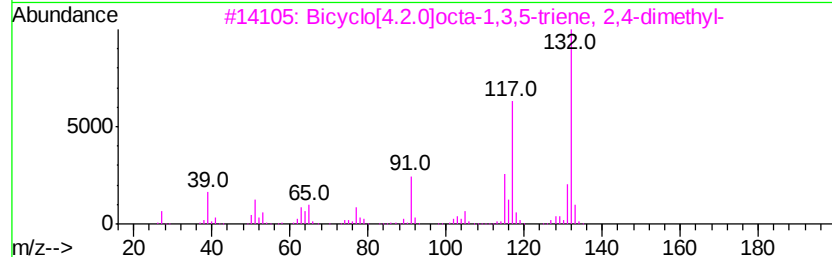
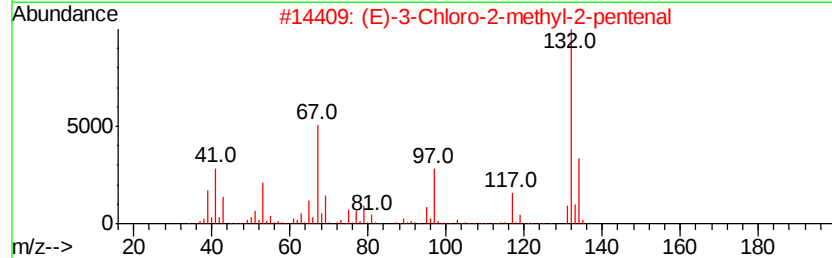
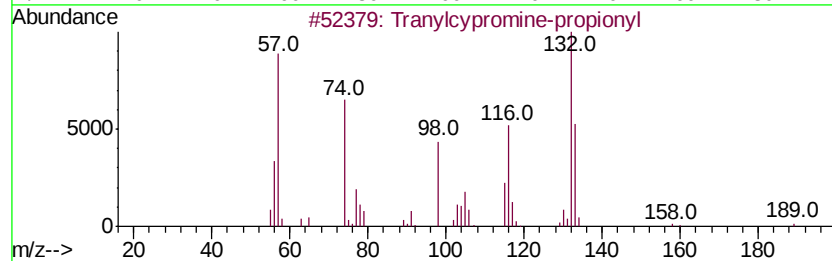
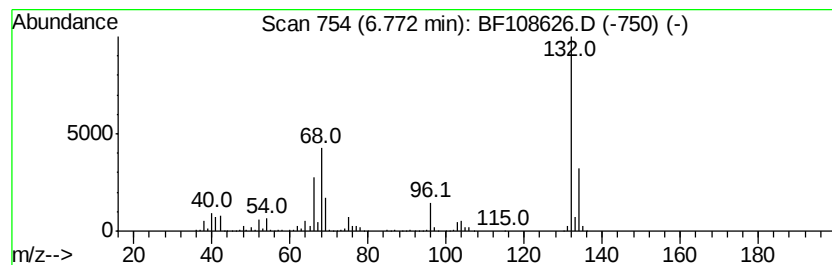
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.77 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.77 | 53.39 ng | 1894410 | 1,4-Dichlorobenzene-d4 | 7.00 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Tranvlcvpromine-propionyl           | 189 | C12H15NO | 1000123-86-3 | 10   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO  | 031357-76-3  | 9    |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12   | 028749-81-7  | 9    |
| 4    |    | 4-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2   | 064608-60-2  | 9    |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5  | 9    |



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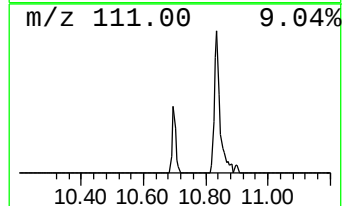
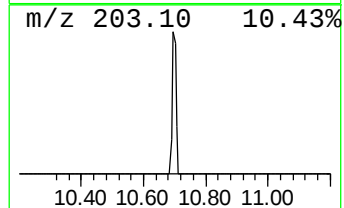
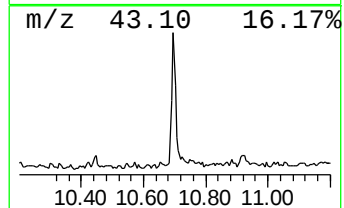
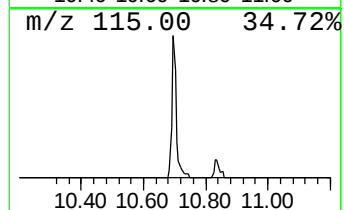
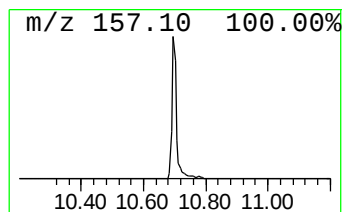
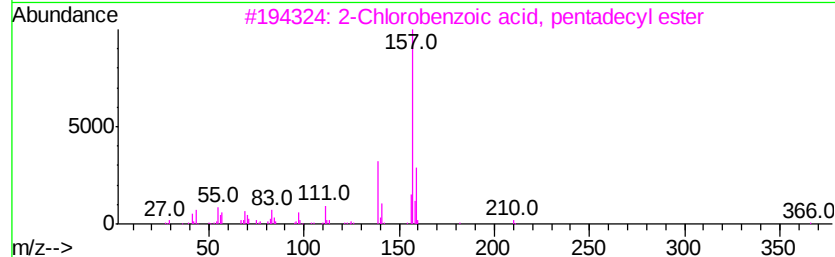
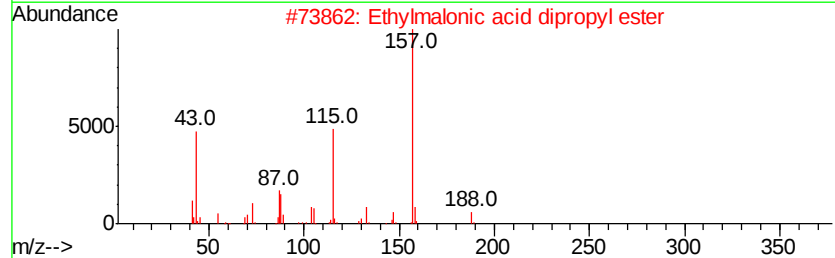
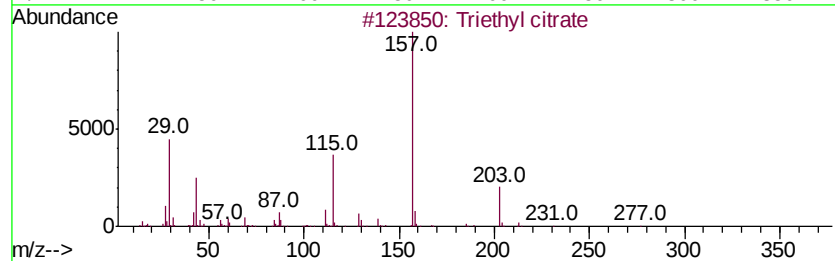
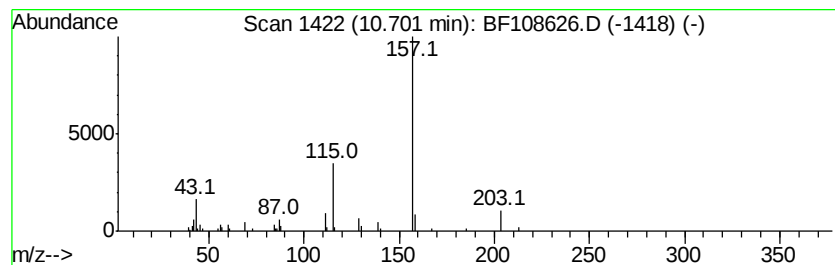
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Triethyl citrate Concentration Rank 5

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 10.70     | 2.02 ng                             | 80667 | Acenaphthene-d10 | 10.04        |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | Triethyl citrate                    | 276   | C12H20O7         | 000077-93-0  | 91   |
| 2         | Ethylmalonic acid dipropyl ester    | 216   | C11H20O4         | 001113-91-3  | 64   |
| 3         | 2-Chlorobenzoic acid, pentadecyl... | 366   | C22H35ClO2       | 1000292-43-0 | 47   |
| 4         | Adipic acid, ethyl 2-methylpent-... | 258   | C14H26O4         | 1000353-55-5 | 38   |
| 5         | O-Methyl-DL-serine, N-dimethylam... | 202   | C9H18N2O3        | 1000375-99-6 | 37   |



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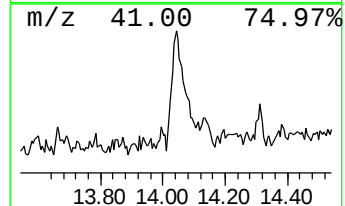
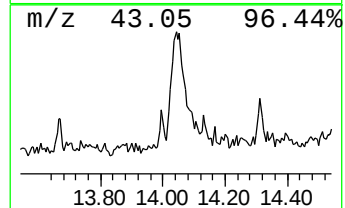
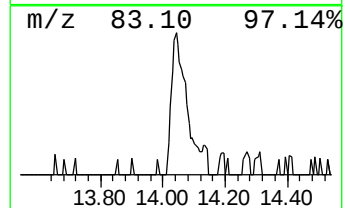
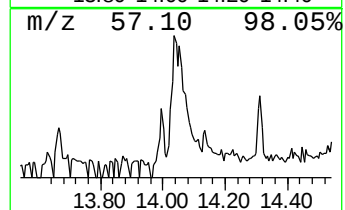
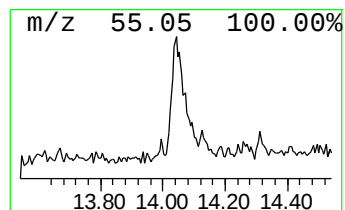
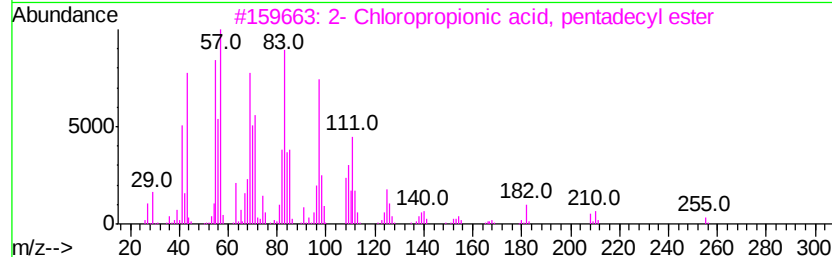
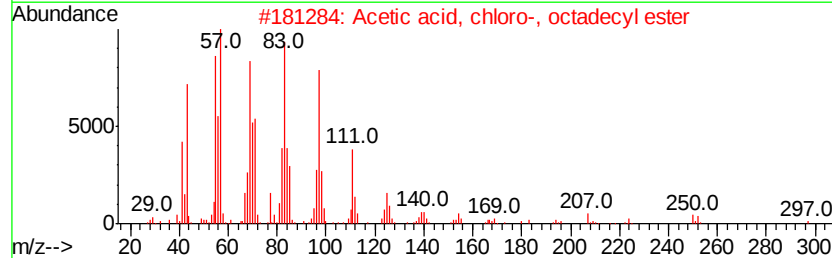
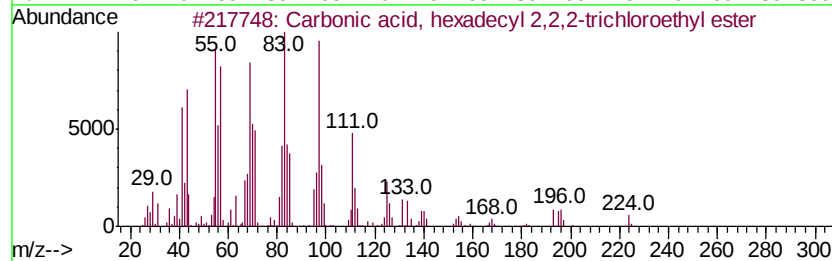
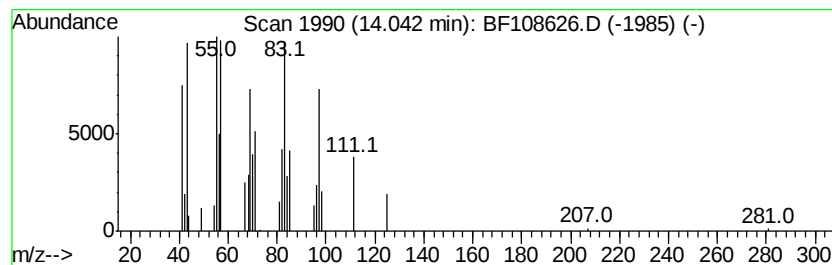
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Carbonic acid, hexadecyl 2,... Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.04 | 2.86 ng | 99201 | Chrysene-d12     | 14.19 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | Carbonic acid, hexadecyl 2,2,2-t... | 416 | C19H35Cl3O3 | 1000314-56-2 | 91   |
| 2    |    | Acetic acid, chloro-, octadecyl ... | 346 | C20H39ClO2  | 005348-82-3  | 91   |
| 3    |    | 2- Chloropropionic acid, pentade... | 318 | C18H35ClO2  | 1000292-44-1 | 91   |
| 4    |    | n-Tetracosanol-1                    | 354 | C24H50O     | 000506-51-4  | 91   |
| 5    |    | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 91   |



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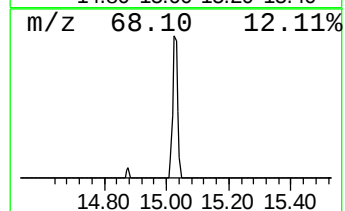
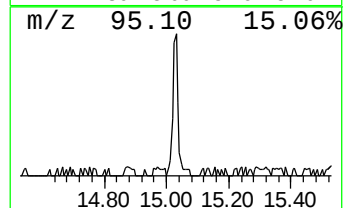
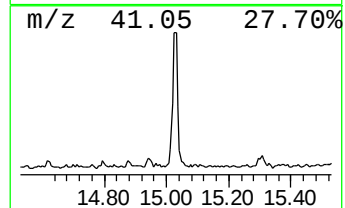
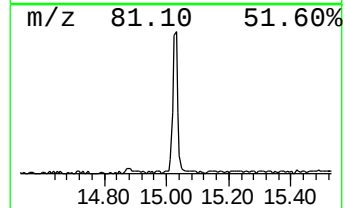
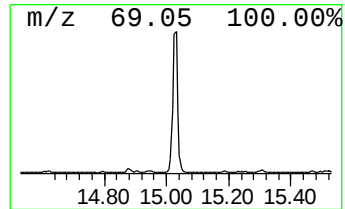
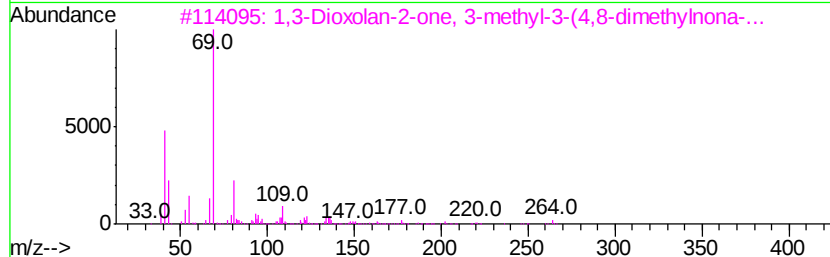
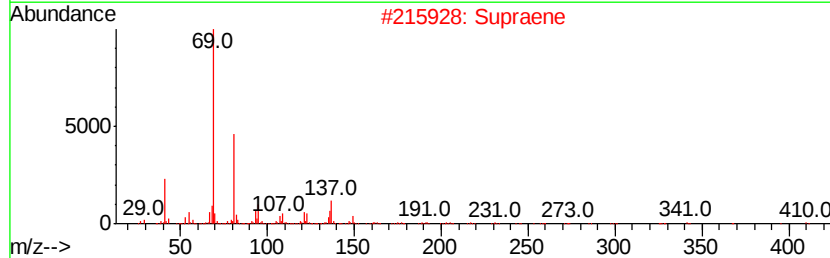
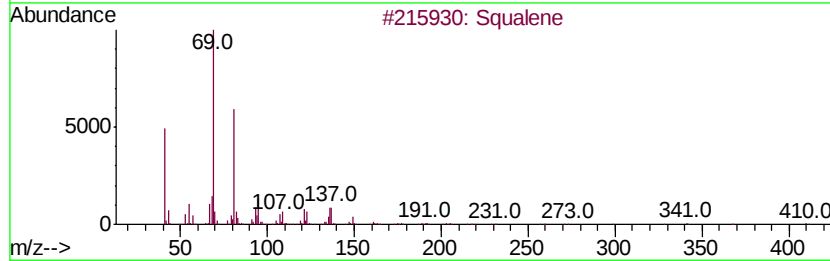
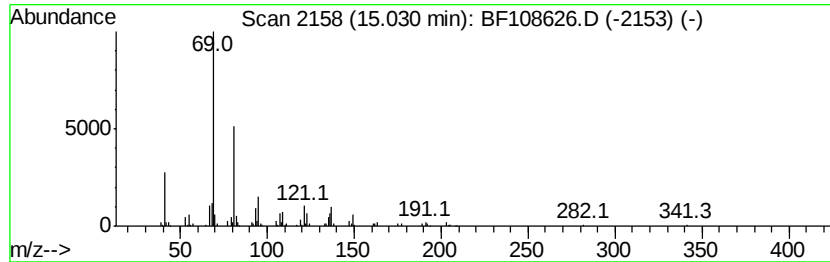
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TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Squalene Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.03 | 5.55 ng | 185477 | Perylene-d12     | 15.75 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50   | 000111-02-4 | 91   |
| 2    |    | Supraene                            | 410 | C30H50   | 007683-64-9 | 91   |
| 3    |    | 1,3-Dioxolan-2-one, 3-methyl-3-(... | 264 | C16H24O3 | 336879-76-6 | 64   |
| 4    |    | 1,5-Heptadiene, 3,3,6-trimethyl-    | 138 | C10H18   | 035387-63-4 | 52   |
| 5    |    | 4-Methyl-1,5-Heptadiene             | 110 | C8H14    | 000998-94-7 | 50   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown6.77          | 6.77  | 53.4    | ng    | 1894410  | 1                     | 7.00  | 709662 | 20.0 |
| Triethyl citrate     | 10.70 | 2.0     | ng    | 80667    | 3                     | 10.04 | 797357 | 20.0 |
| Carbonic acid, he... | 14.04 | 2.9     | ng    | 99201    | 5                     | 14.19 | 693877 | 20.0 |
| Squalene             | 15.03 | 5.5     | ng    | 185477   | 6                     | 15.75 | 668722 | 20.0 |