

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF061518\  
 Data File : BF106519.D  
 Acq On : 16 Jun 2018 4:18  
 Operator : JU/SJ  
 Sample : J3447-05  
 Misc :  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 W-22

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-BF061118.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         | 5.195       | 482           | 486         | 498          | rVB      | 64641          | 74425         | 2.90%           | 0.418%        |
| 2         | 5.613       | 553           | 557         | 572          | rVB      | 1214551        | 1212501       | 47.28%          | 6.818%        |
| 3         | 6.607       | 722           | 726         | 740          | rVB      | 886938         | 850835        | 33.17%          | 4.784%        |
| 4         | 6.742       | 745           | 749         | 752          | rBV      | 2221491        | 1927752       | 75.16%          | 10.839%       |
| 5         | 6.966       | 783           | 787         | 790          | rBV      | 802479         | 634962        | 24.76%          | 3.570%        |
| 6         | 7.125       | 809           | 814         | 817          | rBV      | 2039904        | 1876434       | 73.16%          | 10.551%       |
| 7         | 7.530       | 877           | 883         | 886          | rBV      | 1453214        | 1481930       | 57.78%          | 8.332%        |
| 8         | 8.248       | 1001          | 1005        | 1008         | rBV      | 837538         | 685493        | 26.73%          | 3.854%        |
| 9         | 9.319       | 1183          | 1187        | 1197         | rBV      | 2457252        | 2301260       | 89.73%          | 12.939%       |
| 10        | 9.713       | 1250          | 1254        | 1262         | rBV      | 120493         | 108773        | 4.24%           | 0.612%        |
| 11        | 9.919       | 1284          | 1289        | 1293         | rBV      | 36108          | 29283         | 1.14%           | 0.165%        |
| 12        | 10.007      | 1300          | 1304        | 1313         | rVB      | 714738         | 619439        | 24.15%          | 3.483%        |
| 13        | 10.419      | 1372          | 1374        | 1377         | rVB      | 52132          | 37144         | 1.45%           | 0.209%        |
| 14        | 10.801      | 1434          | 1439        | 1442         | rBV      | 1369867        | 1299888       | 50.68%          | 7.309%        |
| 15        | 10.895      | 1452          | 1455        | 1459         | rBV      | 34142          | 36823         | 1.44%           | 0.207%        |
| 16        | 11.495      | 1554          | 1557        | 1561         | rBV      | 726534         | 617827        | 24.09%          | 3.474%        |
| 17        | 13.083      | 1823          | 1827        | 1830         | rBV      | 2751026        | 2564755       | 100.00%         | 14.421%       |
| 18        | 13.971      | 1974          | 1978        | 1988         | rVB3     | 22800          | 34893         | 1.36%           | 0.196%        |
| 19        | 14.148      | 2004          | 2008        | 2012         | rBV      | 842603         | 748801        | 29.20%          | 4.210%        |
| 20        | 15.001      | 2149          | 2153        | 2158         | rBV      | 124627         | 126302        | 4.92%           | 0.710%        |
| 21        | 15.677      | 2263          | 2268        | 2276         | rBV      | 398200         | 515518        | 20.10%          | 2.899%        |

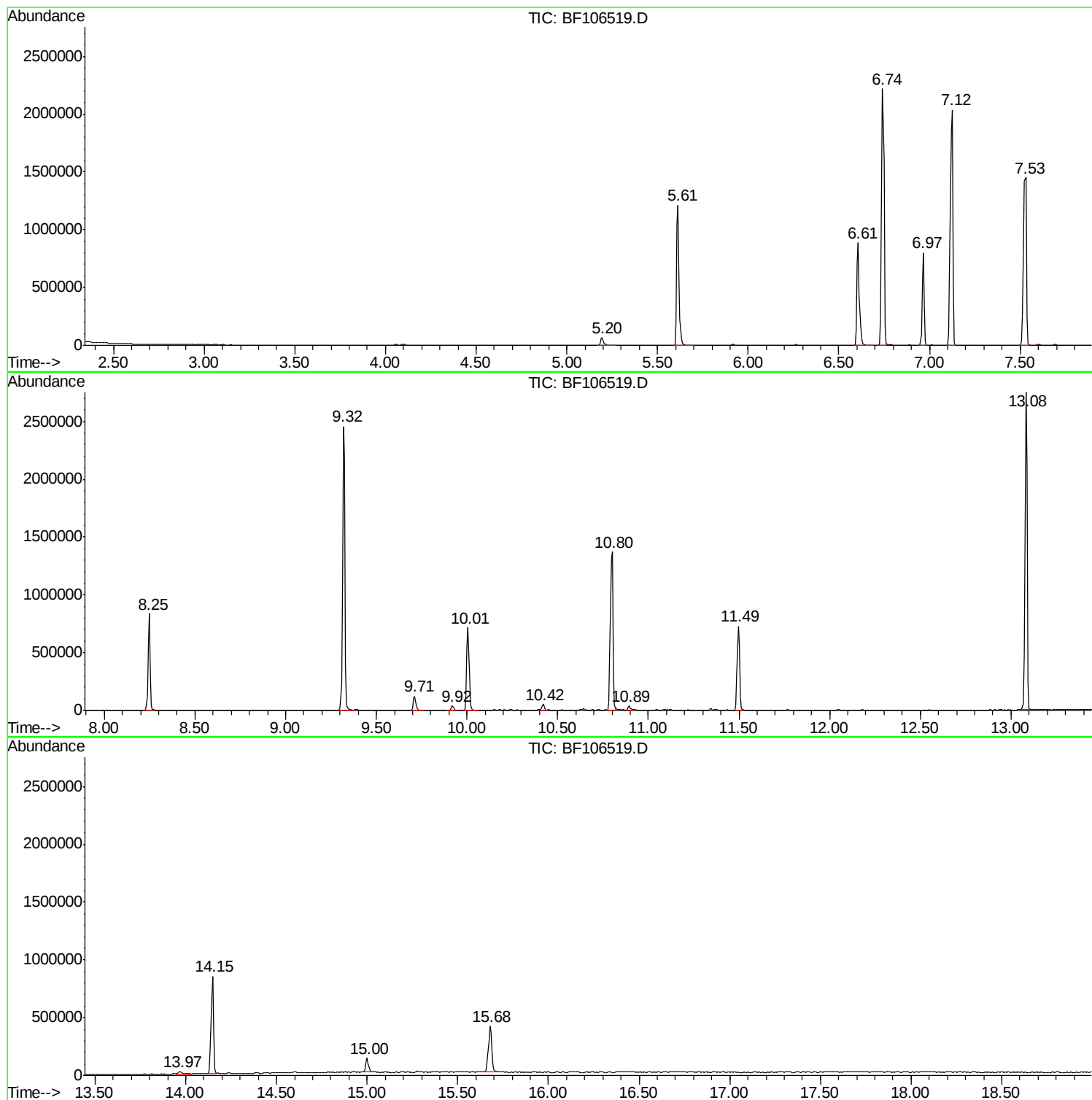
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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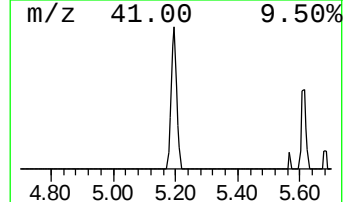
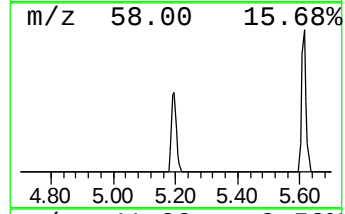
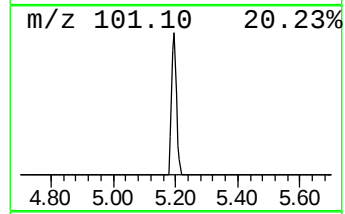
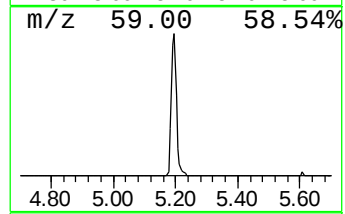
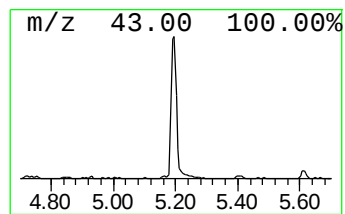
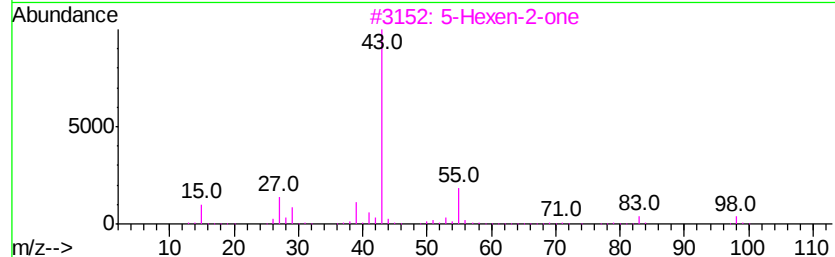
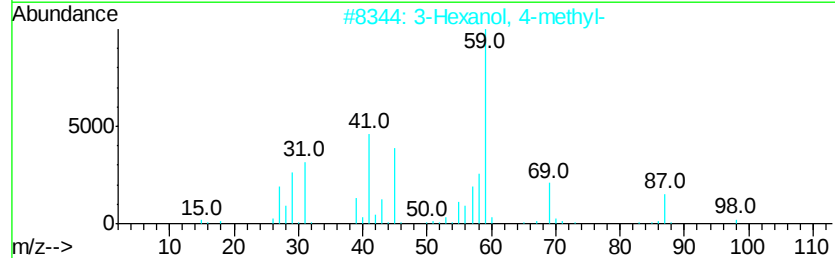
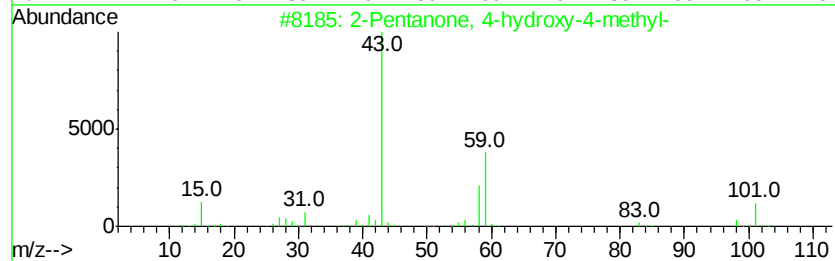
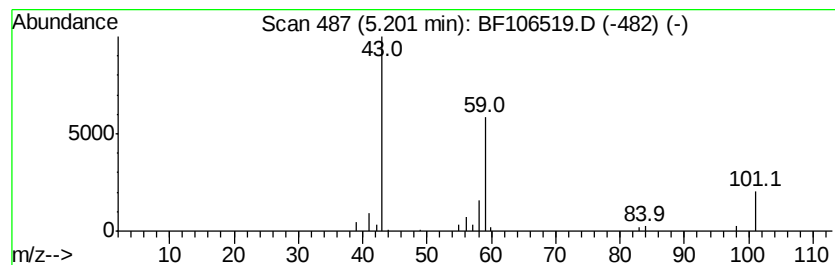
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.20 | 2.34 ng | 74425 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm  | CAS#        | Qual |
|------|----|---|------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    |   | 3-Hexanol, 4-methyl-               | 116 | C7H16O   | 000615-29-2 | 28   |
| 3    |    |   | 5-Hexen-2-one                      | 98  | C6H10O   | 000109-49-9 | 9    |
| 4    |    |   | Propane, 2-ethoxy-2-methyl-        | 102 | C6H14O   | 000637-92-3 | 9    |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethyl- | 141 | C7H11NO2 | 001116-98-9 | 9    |



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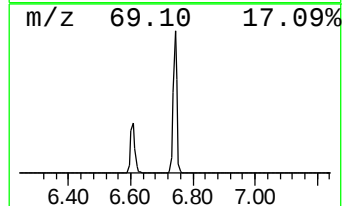
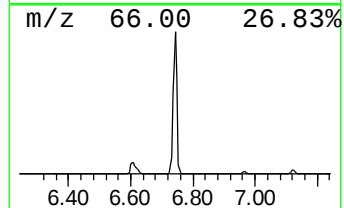
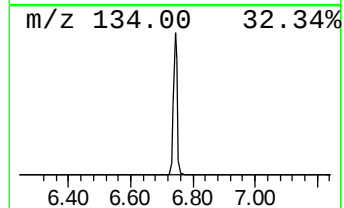
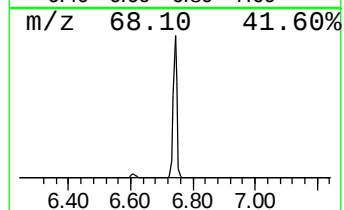
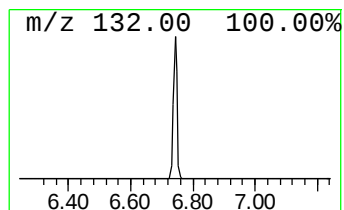
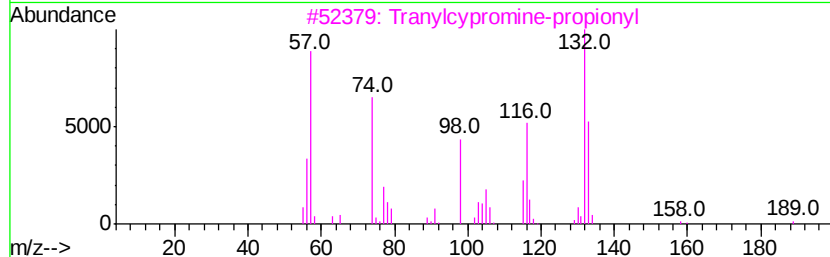
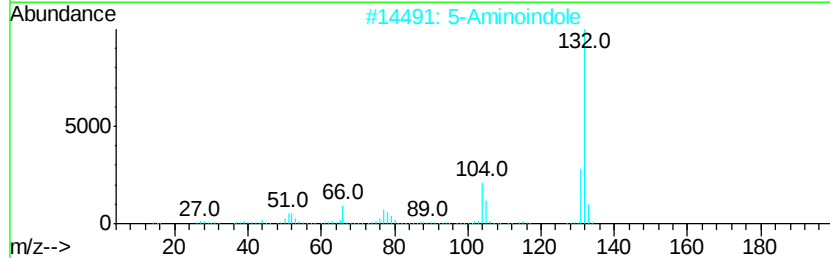
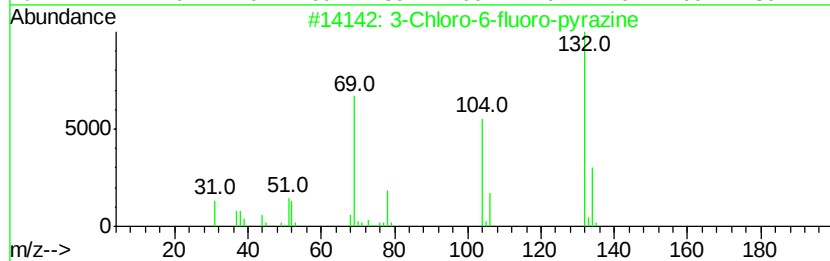
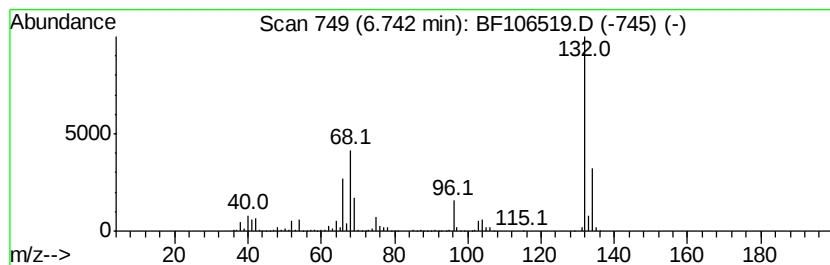
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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 60.72 ng | 1927750 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of                                  | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-----------|--------------|------|------|
| 1    | 3-Chloro-6-fluoro-pyrazine          | 132          | C4H2ClFN2 | 1000146-10-7 | 27   |      |
| 2    | 5-Aminoindole                       | 132          | C8H8N2    | 005192-03-0  | 12   |      |
| 3    | Tranvlcyproline-propionyl           | 189          | C12H15NO  | 1000123-86-3 | 10   |      |
| 4    | 5-Fluoro-2-chloropyrimidine         | 132          | C4H2ClFN2 | 062802-42-0  | 9    |      |
| 5    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132          | C8H8N2    | 022291-85-6  | 9    |      |



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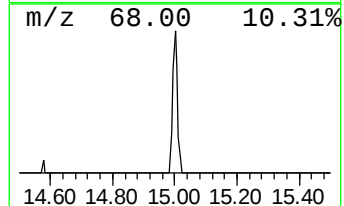
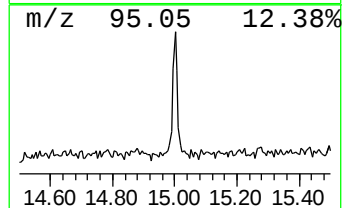
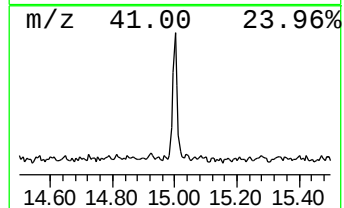
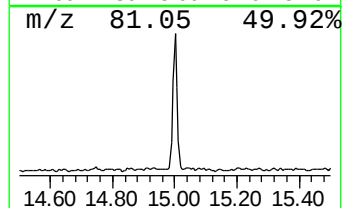
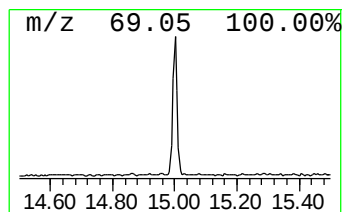
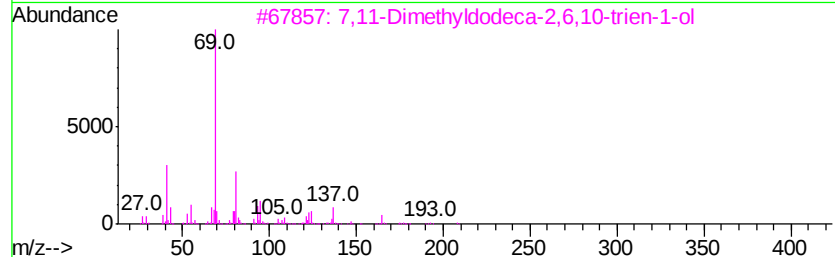
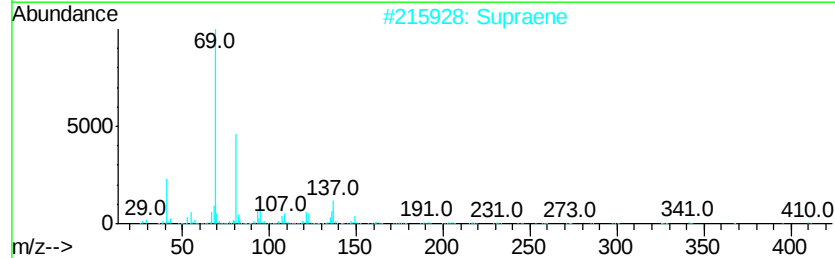
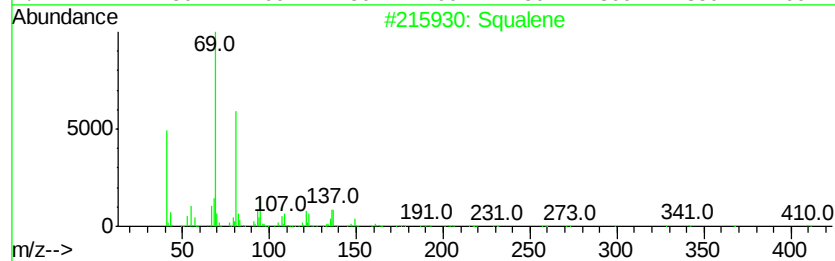
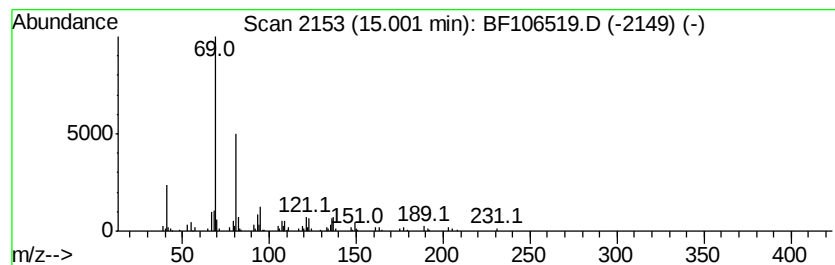
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Squalene Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.00 | 4.90 ng | 126302 | Perylene-d12     | 15.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50  | 000111-02-4 | 91   |
| 2    |    | Supraene                            | 410 | C30H50  | 007683-64-9 | 90   |
| 3    |    | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 80   |
| 4    |    | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 64   |
| 5    |    | 1,6-Octadiene, 3,5-dimethyl-, tr... | 138 | C10H18  | 074630-87-8 | 59   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.20  | 2.3     | ng    | 74425    | 1                     | 6.97  | 634962 | 20.0 |
| unknown6.74          | 6.74  | 60.7    | ng    | 1927750  | 1                     | 6.97  | 634962 | 20.0 |
| Squalene             | 15.00 | 4.9     | ng    | 126302   | 6                     | 15.68 | 515518 | 20.0 |