

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF101018\  
 Data File : BF109748.D  
 Acq On : 10 Oct 2018 17:55  
 Operator : JU/SJ  
 Sample : J5302-05  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-5-(14.5-15)

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\_F\METHODS\8270-BF100818.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         | 4.887       | 472           | 476         | 490          | rVB      | 34860          | 53553         | 2.56%           | 0.325%        |
| 2         | 5.310       | 544           | 548         | 580          | rBV      | 954047         | 1322833       | 63.30%          | 8.038%        |
| 3         | 6.339       | 720           | 723         | 741          | rBV      | 1165206        | 1504604       | 71.99%          | 9.142%        |
| 4         | 6.463       | 741           | 744         | 778          | rVB      | 1438294        | 1667668       | 79.80%          | 10.133%       |
| 5         | 6.692       | 780           | 783         | 794          | rBV      | 231654         | 353713        | 16.92%          | 2.149%        |
| 6         | 6.851       | 806           | 810         | 832          | rBV      | 988209         | 1139904       | 54.54%          | 6.926%        |
| 7         | 7.257       | 875           | 879         | 913          | rBV      | 638220         | 1016473       | 48.64%          | 6.176%        |
| 8         | 7.975       | 998           | 1001        | 1020         | rBV      | 387140         | 512307        | 24.51%          | 3.113%        |
| 9         | 9.051       | 1180          | 1184        | 1203         | rBV      | 1463386        | 1776156       | 84.99%          | 10.792%       |
| 10        | 9.445       | 1248          | 1251        | 1261         | rBV      | 85346          | 103193        | 4.94%           | 0.627%        |
| 11        | 9.722       | 1294          | 1298        | 1320         | rBV      | 609041         | 646006        | 30.91%          | 3.925%        |
| 12        | 10.510      | 1428          | 1432        | 1451         | rBV      | 1004526        | 1270313       | 60.78%          | 7.719%        |
| 13        | 11.198      | 1546          | 1549        | 1570         | rBV      | 529711         | 732396        | 35.04%          | 4.450%        |
| 14        | 11.739      | 1638          | 1641        | 1652         | rBV3     | 15625          | 27478         | 1.31%           | 0.167%        |
| 15        | 12.780      | 1814          | 1818        | 1835         | rBV      | 2081333        | 2089896       | 100.00%         | 12.699%       |
| 16        | 13.686      | 1967          | 1972        | 1988         | rBV      | 81011          | 154416        | 7.39%           | 0.938%        |
| 17        | 13.827      | 1992          | 1996        | 2009         | rVV      | 721998         | 804733        | 38.51%          | 4.890%        |
| 18        | 13.998      | 2021          | 2025        | 2029         | rBV      | 37485          | 35513         | 1.70%           | 0.216%        |
| 19        | 14.304      | 2074          | 2077        | 2080         | rBV      | 41886          | 39058         | 1.87%           | 0.237%        |
| 20        | 14.592      | 2121          | 2126        | 2131         | rBV      | 55833          | 57705         | 2.76%           | 0.351%        |
| 21        | 14.662      | 2134          | 2138        | 2142         | rVV      | 188454         | 173359        | 8.30%           | 1.053%        |
| 22        | 14.904      | 2175          | 2179        | 2184         | rBV      | 54637          | 55286         | 2.65%           | 0.336%        |
| 23        | 15.227      | 2229          | 2234        | 2246         | rBV      | 479698         | 781140        | 37.38%          | 4.746%        |
| 24        | 15.645      | 2301          | 2305        | 2312         | rBV2     | 43474          | 61364         | 2.94%           | 0.373%        |
| 25        | 16.104      | 2377          | 2383        | 2391         | rVB      | 31001          | 51729         | 2.48%           | 0.314%        |
| 26        | 16.633      | 2468          | 2473        | 2479         | rBV3     | 13777          | 26917         | 1.29%           | 0.164%        |

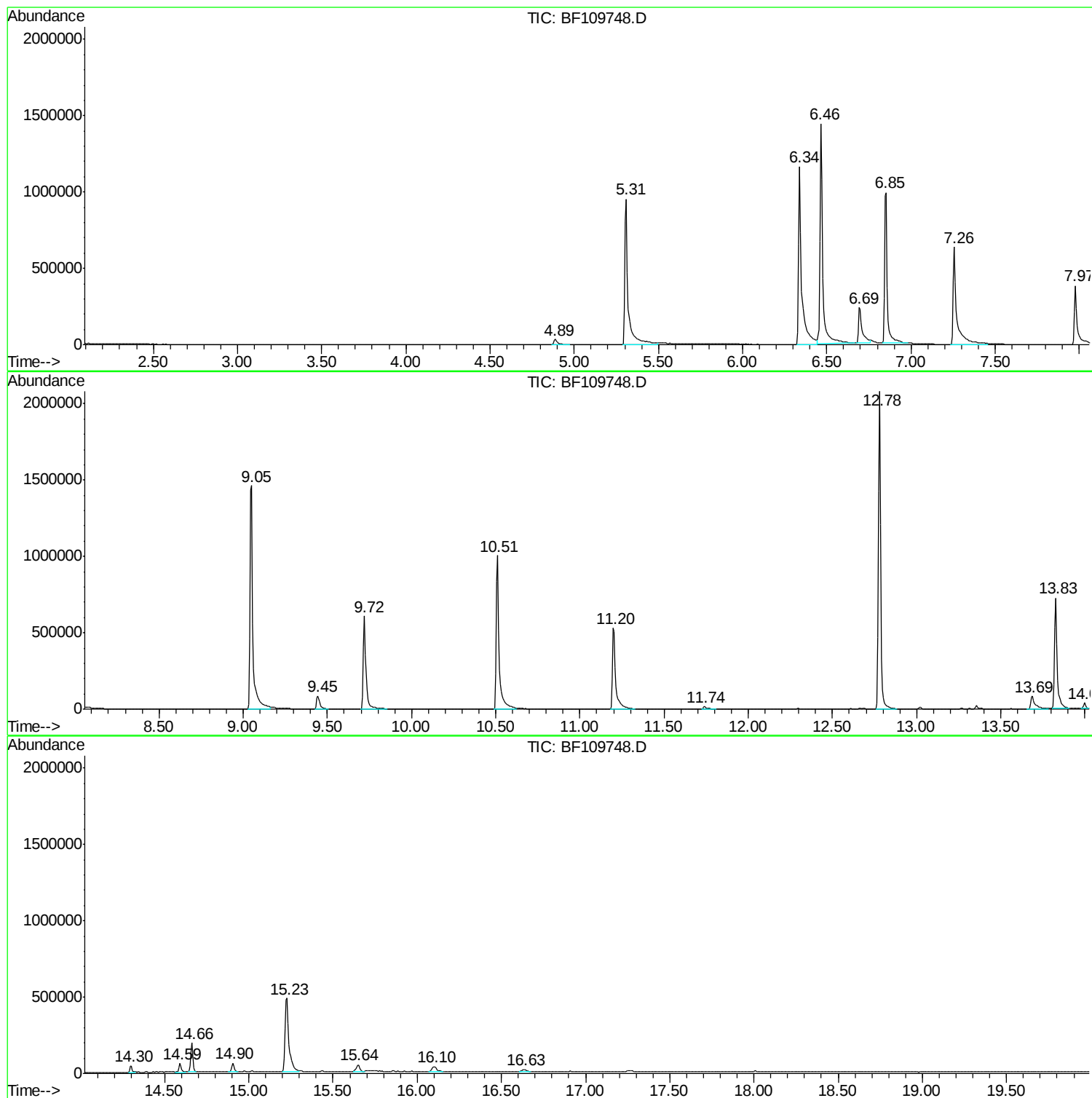
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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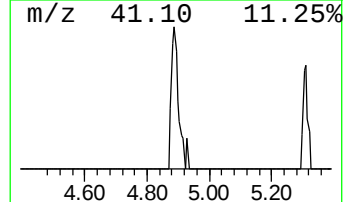
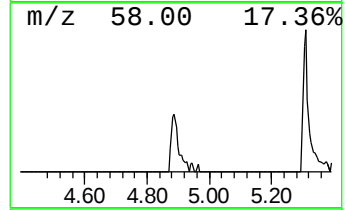
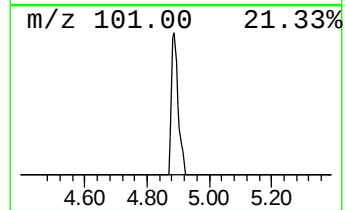
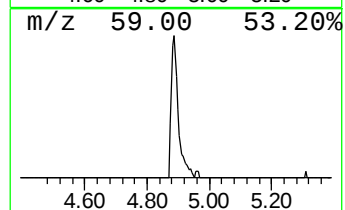
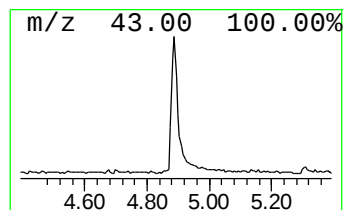
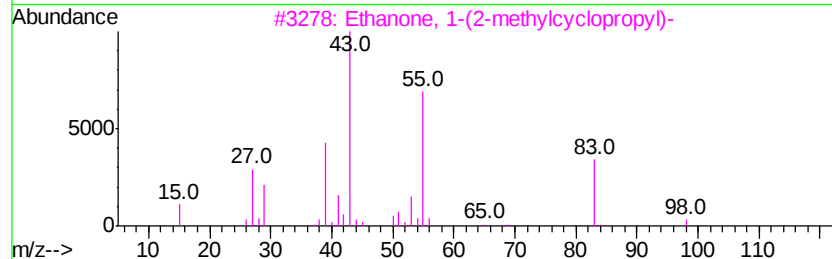
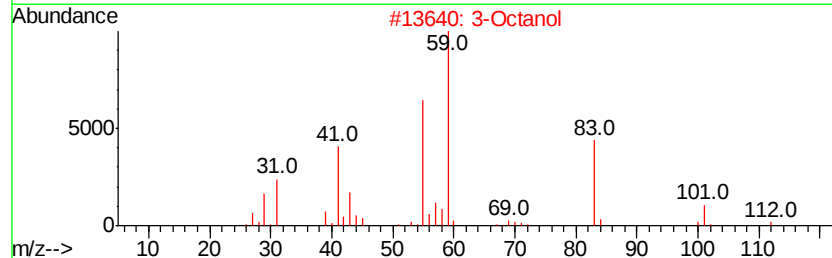
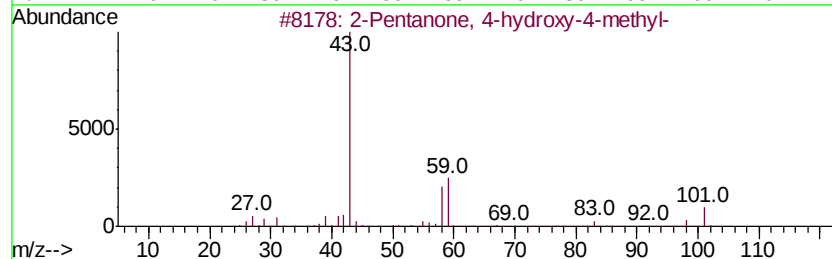
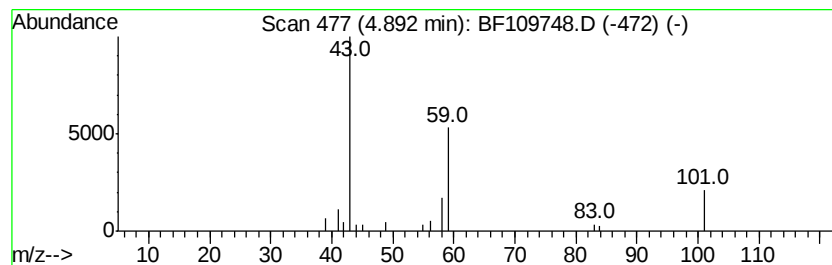
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 4.89 | 3.03 ng | 53553 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 50   |
| 2    |    | 3-Octanol                          | 130 | C8H18O  | 000589-98-0 | 28   |
| 3    |    | Ethanone, 1-(2-methylcyclopropyl)- | 98  | C6H10O  | 000930-56-3 | 9    |
| 4    |    | 5-Hexen-2-one                      | 98  | C6H10O  | 000109-49-9 | 9    |
| 5    |    | 2,3-Butanedione, monooxime         | 101 | C4H7NO2 | 000057-71-6 | 9    |



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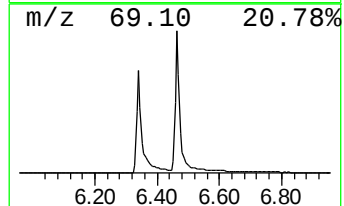
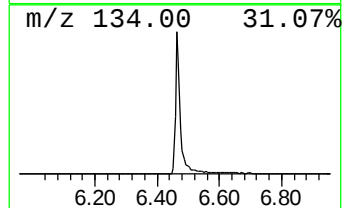
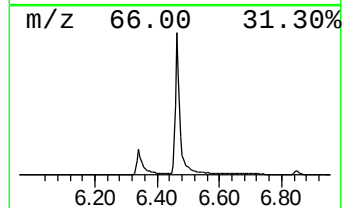
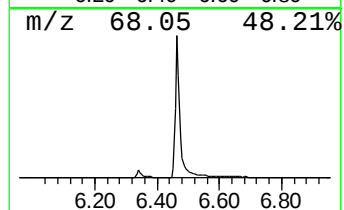
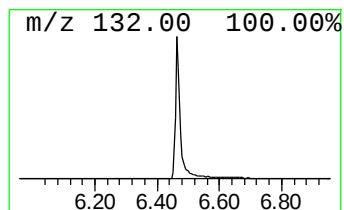
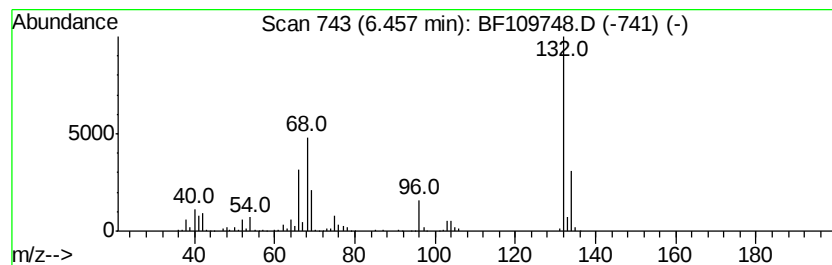
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.46 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.46 | 94.30 ng | 1667670 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of                                  | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-----------|--------------|------|------|
| 1    | 3-Chloro-6-fluoro-pyrazine          | 132          | C4H2ClFN2 | 1000146-10-7 | 27   |      |
| 2    | 5-Fluoro-2-chloropyrimidine         | 132          | C4H2ClFN2 | 062802-42-0  | 16   |      |
| 3    | Tranvlcypropine-propionyl           | 189          | C12H15NO  | 1000123-86-3 | 10   |      |
| 4    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132          | C10H12    | 028749-81-7  | 9    |      |
| 5    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132          | C10H12    | 005379-20-4  | 9    |      |



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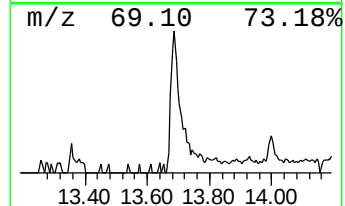
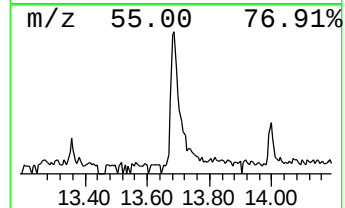
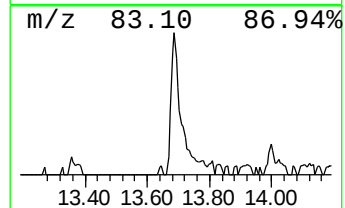
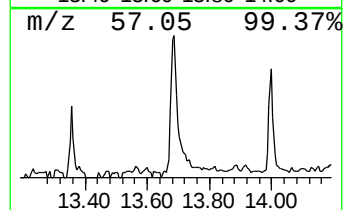
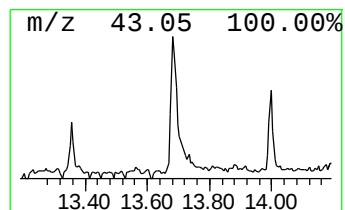
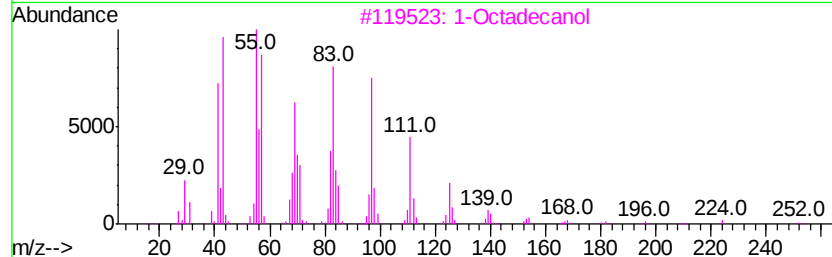
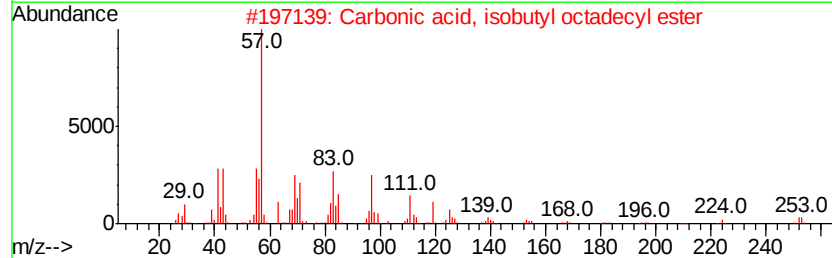
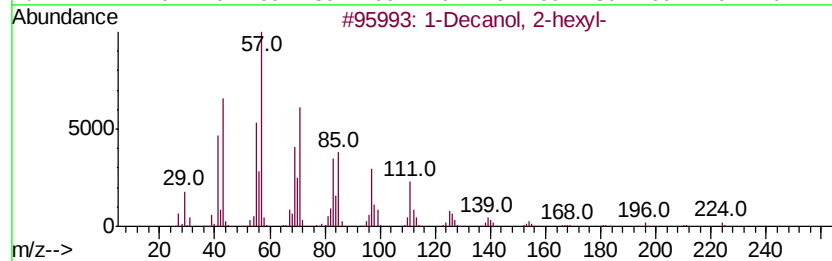
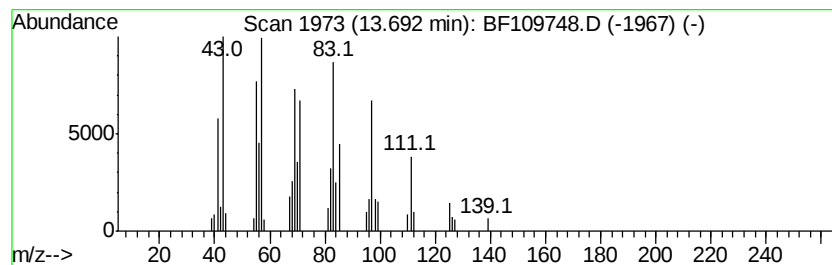
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SB-5-(14.5-15)

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

\*\*\*\*\*  
Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD                     |     | R.T.     |              |      |
|-------|---------|--------|--------------------------------------|-----|----------|--------------|------|
| 13.69 | 3.84 ng | 154416 | Chrysene-d12                         |     | 13.83    |              |      |
| Hit#  | of      | 5      | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
| 1     |         |        | 1-Decanol, 2-hexyl-                  | 242 | C16H34O  | 002425-77-6  | 74   |
| 2     |         |        | Carbonic acid, isobutyl octadecyl... | 370 | C23H46O3 | 1000314-61-5 | 72   |
| 3     |         |        | 1-Octadecanol                        | 270 | C18H38O  | 000112-92-5  | 70   |
| 4     |         |        | n-Heptadecanol-1                     | 256 | C17H36O  | 001454-85-9  | 70   |
| 5     |         |        | 1-Dodecanol, 2-hexyl-                | 270 | C18H38O  | 110225-00-8  | 68   |



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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

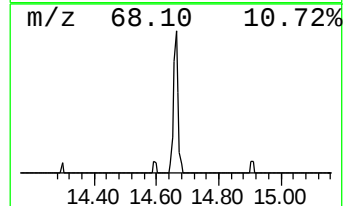
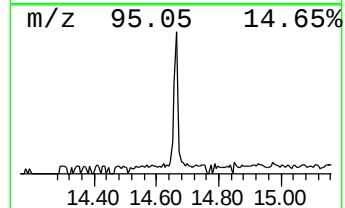
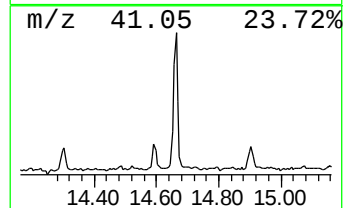
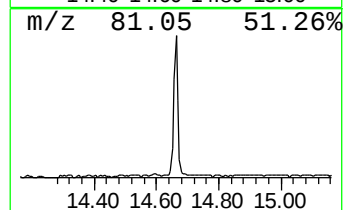
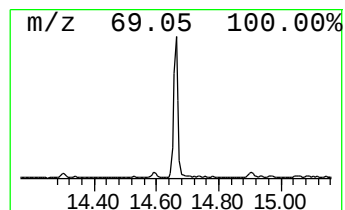
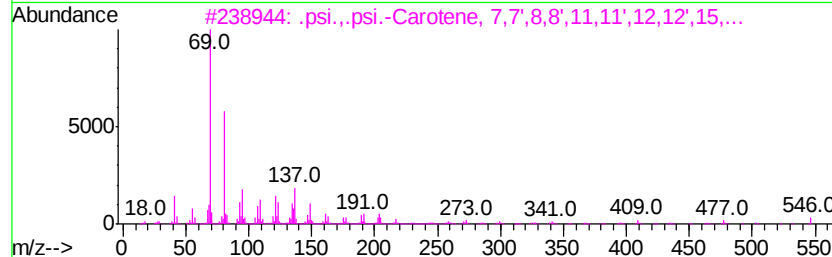
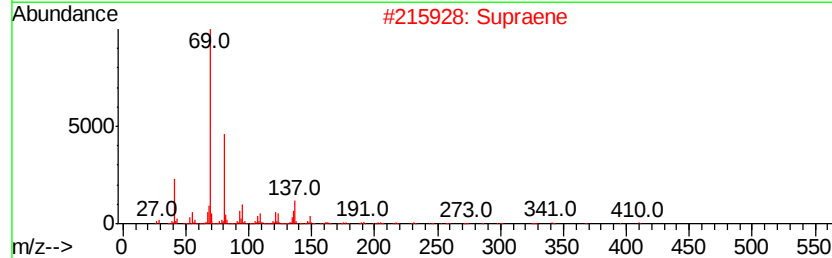
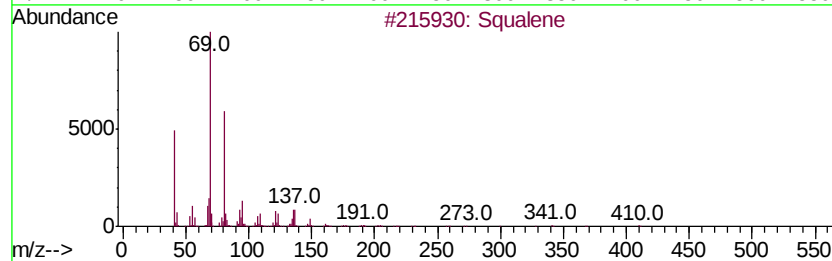
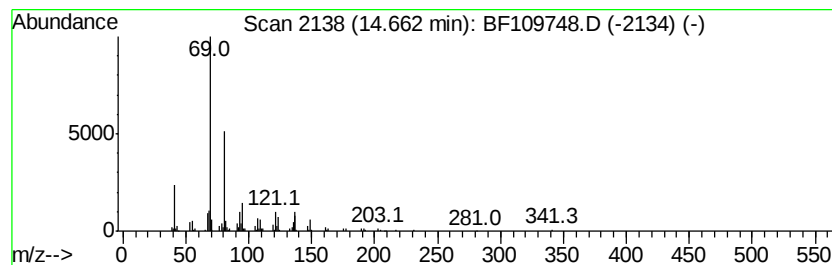
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Squalene Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.66 | 4.44 ng | 173359 | Perylene-d12     | 15.23 |

| 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    |    | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66   | 000502-62-5 | 83   |
| 4    |    | 2,6,10,14-Hexadecatetraen-1-ol, ... | 332 | C22H36O2 | 061691-98-3 | 72   |
| 5    |    | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 72   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | ---Internal Standard--- |       |        |      |
|----------------------|-------|---------|-------|----------|-------------------------|-------|--------|------|
|                      |       |         |       |          | #                       | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.89  | 3.0     | ng    | 53553    | 1                       | 6.70  | 353713 | 20.0 |
| unknown6.46          | 6.46  | 94.3    | ng    | 1667670  | 1                       | 6.70  | 353713 | 20.0 |
| 1-Decanol, 2-hexyl-  | 13.69 | 3.8     | ng    | 154416   | 5                       | 13.83 | 804733 | 20.0 |
| Squalene             | 14.66 | 4.4     | ng    | 173359   | 6                       | 15.23 | 781140 | 20.0 |