

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121818\  
 Data File : BM018282.D  
 Acq On : 18 Dec 2018 21:48  
 Operator : JU/SJ  
 Sample : J6340-11  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 SB-10A

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-BM121518.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         | 4.681       | 301           | 305         | 312          | rBV      | 123432         | 170409        | 2.75%           | 0.345%        |
| 2         | 5.122       | 373           | 380         | 395          | rBV      | 3447275        | 4737820       | 76.36%          | 9.602%        |
| 3         | 6.693       | 638           | 647         | 663          | rBV      | 3126056        | 5216355       | 84.08%          | 10.572%       |
| 4         | 7.028       | 697           | 704         | 714          | rBV      | 3406504        | 5292956       | 85.31%          | 10.728%       |
| 5         | 7.487       | 772           | 782         | 789          | rBV      | 610365         | 933516        | 15.05%          | 1.892%        |
| 6         | 7.798       | 828           | 835         | 850          | rVB      | 2579905        | 3966298       | 63.93%          | 8.039%        |
| 7         | 8.645       | 969           | 979         | 998          | rBV      | 1864374        | 3138278       | 50.58%          | 6.361%        |
| 8         | 10.251      | 1244          | 1252        | 1267         | rBV      | 675902         | 1207172       | 19.46%          | 2.447%        |
| 9         | 12.751      | 1670          | 1677        | 1692         | rBV      | 4326977        | 6204274       | 100.00%         | 12.575%       |
| 10        | 13.621      | 1818          | 1825        | 1836         | rBV      | 331023         | 512512        | 8.26%           | 1.039%        |
| 11        | 14.145      | 1906          | 1914        | 1921         | rBV2     | 858210         | 1320870       | 21.29%          | 2.677%        |
| 12        | 15.651      | 2163          | 2170        | 2180         | rBV      | 2446780        | 3715734       | 59.89%          | 7.531%        |
| 13        | 15.898      | 2205          | 2212        | 2218         | rBV7     | 27422          | 65929         | 1.06%           | 0.134%        |
| 14        | 16.910      | 2378          | 2384        | 2388         | rBV      | 830872         | 1219818       | 19.66%          | 2.472%        |
| 15        | 16.951      | 2388          | 2391        | 2398         | rVV      | 192941         | 281263        | 4.53%           | 0.570%        |
| 16        | 17.045      | 2401          | 2407        | 2413         | rVB      | 66368          | 103336        | 1.67%           | 0.209%        |
| 17        | 17.786      | 2525          | 2533        | 2535         | rBV2     | 47418          | 70236         | 1.13%           | 0.142%        |
| 18        | 17.821      | 2535          | 2539        | 2548         | rVB3     | 194446         | 352730        | 5.69%           | 0.715%        |
| 19        | 17.980      | 2560          | 2566        | 2570         | rBV2     | 46607          | 96495         | 1.56%           | 0.196%        |
| 20        | 18.715      | 2682          | 2691        | 2695         | rBV2     | 56277          | 96938         | 1.56%           | 0.196%        |
| 21        | 18.980      | 2731          | 2736        | 2743         | rBV      | 368771         | 512653        | 8.26%           | 1.039%        |
| 22        | 19.115      | 2755          | 2759        | 2767         | rVB4     | 76984          | 113073        | 1.82%           | 0.229%        |
| 23        | 19.351      | 2789          | 2799        | 2808         | rBV2     | 291843         | 541016        | 8.72%           | 1.097%        |
| 24        | 19.433      | 2808          | 2813        | 2819         | rVB3     | 34907          | 62769         | 1.01%           | 0.127%        |
| 25        | 19.562      | 2827          | 2835        | 2846         | rVB      | 4265596        | 5268505       | 84.92%          | 10.678%       |
| 26        | 19.680      | 2850          | 2855        | 2864         | rBV7     | 42010          | 117876        | 1.90%           | 0.239%        |
| 27        | 20.009      | 2906          | 2911        | 2915         | rBV3     | 58522          | 101895        | 1.64%           | 0.207%        |
| 28        | 20.615      | 3011          | 3014        | 3020         | rBV      | 63802          | 84080         | 1.36%           | 0.170%        |
| 29        | 20.815      | 3045          | 3048        | 3051         | rVV2     | 78549          | 100227        | 1.62%           | 0.203%        |
| 30        | 20.856      | 3051          | 3055        | 3061         | rVV2     | 155103         | 237102        | 3.82%           | 0.481%        |
| 31        | 21.127      | 3095          | 3101        | 3106         | rBV2     | 1053934        | 1650787       | 26.61%          | 3.346%        |
| 32        | 21.168      | 3106          | 3108        | 3113         | rVB      | 167782         | 189157        | 3.05%           | 0.383%        |
| 33        | 22.656      | 3356          | 3361        | 3366         | rBV      | 136695         | 308659        | 4.97%           | 0.626%        |
| 34        | 23.291      | 3463          | 3469        | 3475         | rVB      | 759684         | 1348965       | 21.74%          | 2.734%        |

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ALS Vial : 13 Sample Multiplier: 1

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BNA\_M  
ClientSampleId :  
SB-10A

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-BM121518.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

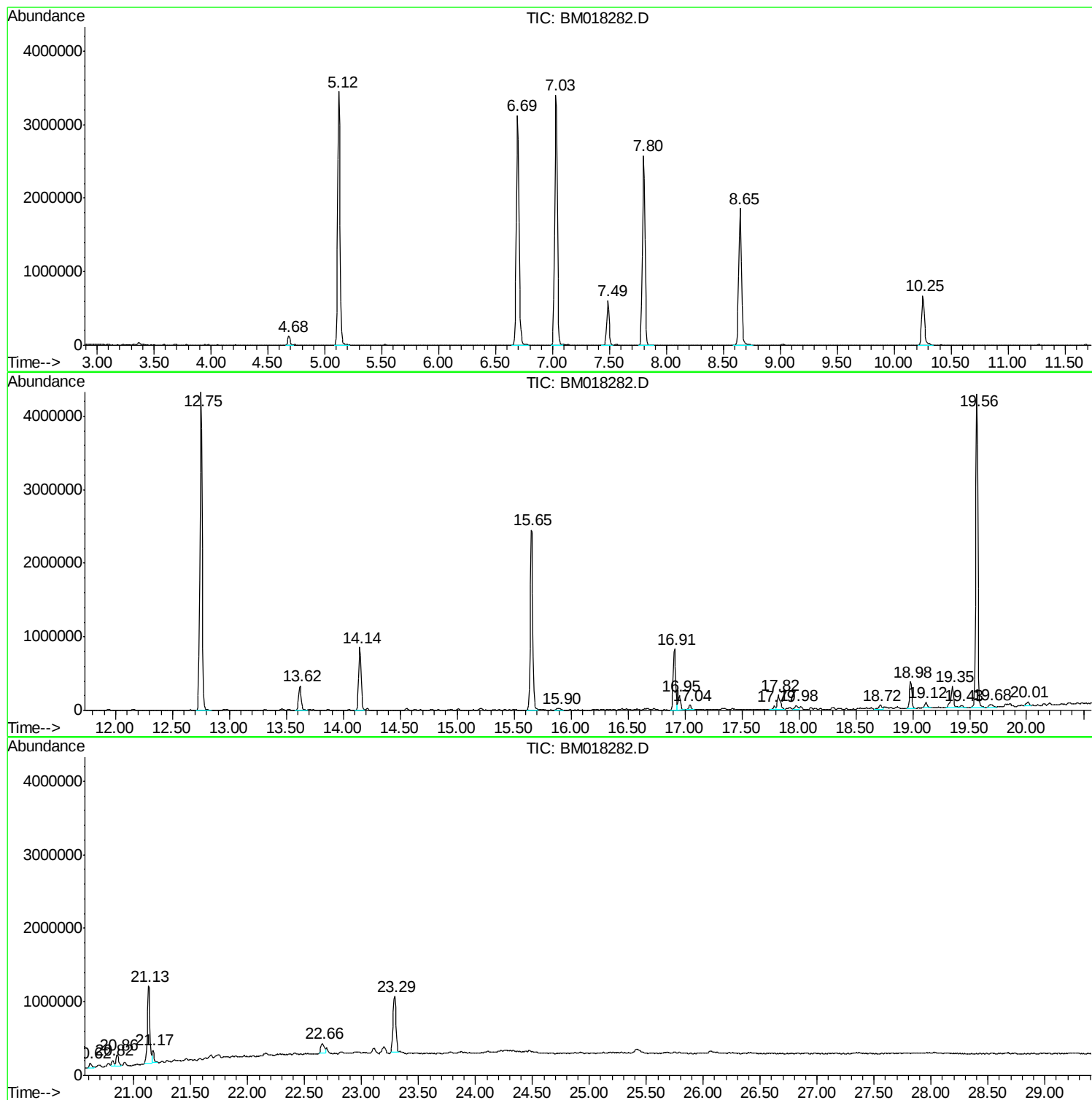
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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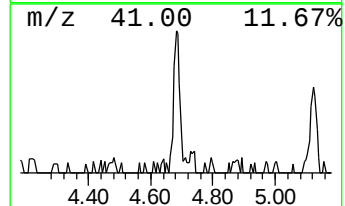
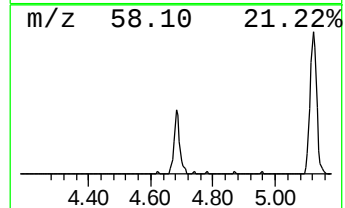
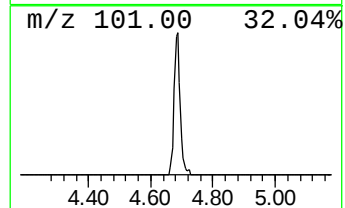
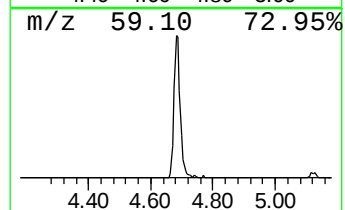
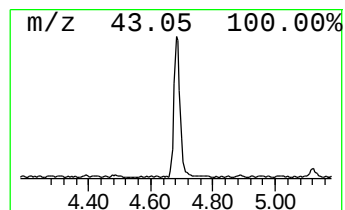
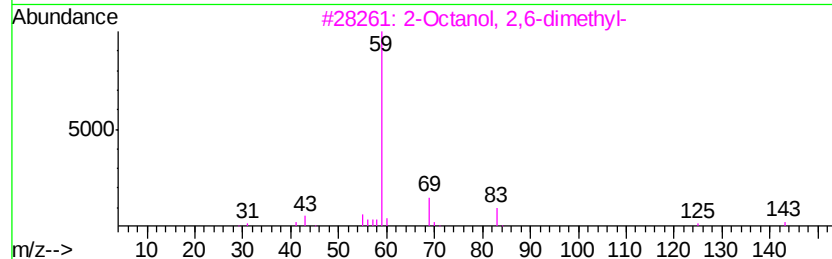
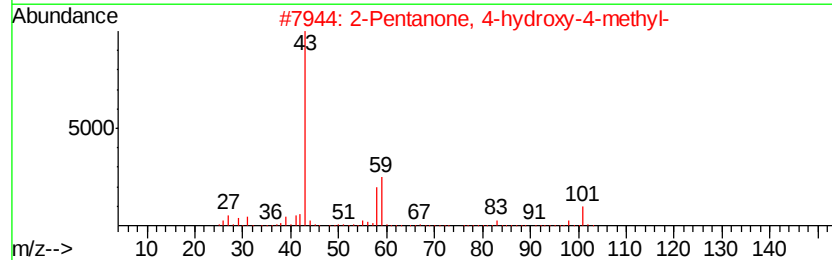
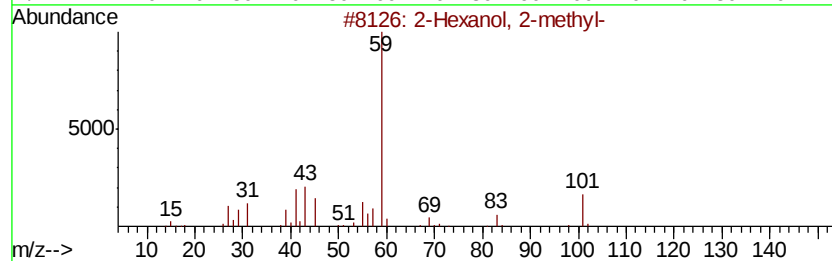
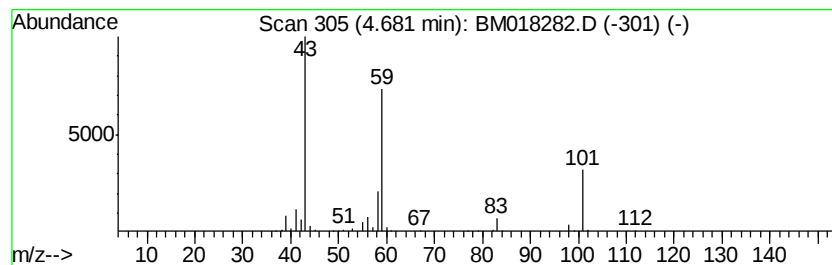
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Hexanol, 2-methyl- Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.68 | 3.65 ng | 170409 | 1,4-Dichlorobenzene-d4 | 7.49 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Hexanol, 2-methyl-             | 116 | C7H16O  | 000625-23-0 | 50   |
| 2    |    |   | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45   |
| 3    |    |   | 2-Octanol, 2,6-dimethyl-         | 158 | C10H22O | 018479-57-7 | 17   |
| 4    |    |   | 3-Hydroxy-3-methyl-2-butanone    | 102 | C5H10O2 | 000115-22-0 | 12   |
| 5    |    |   | 2-Nonanone                       | 142 | C9H18O  | 000821-55-6 | 12   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

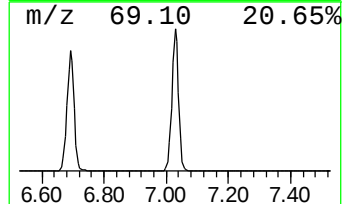
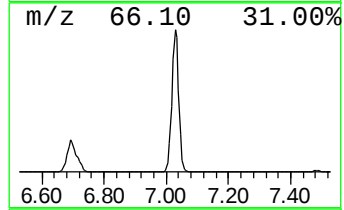
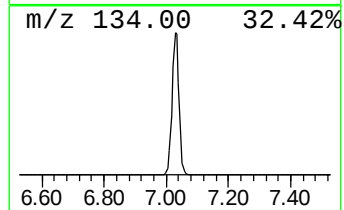
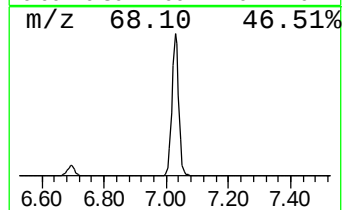
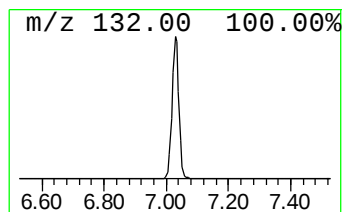
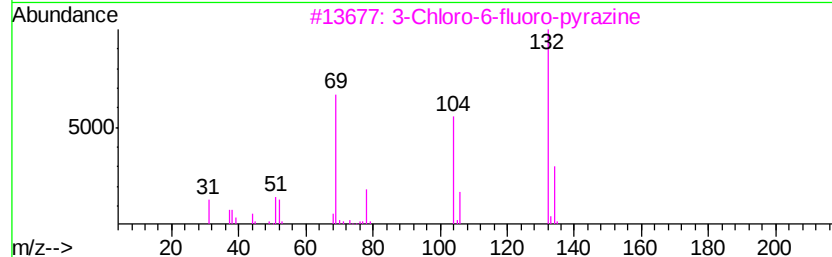
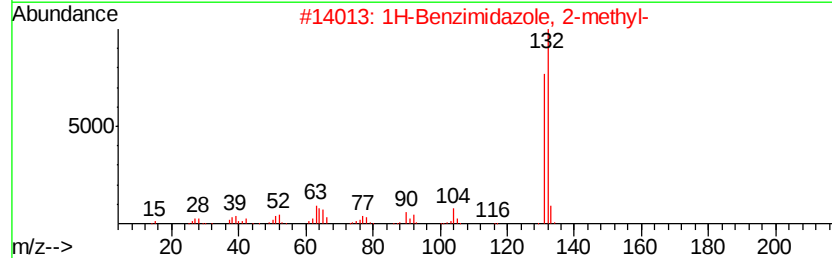
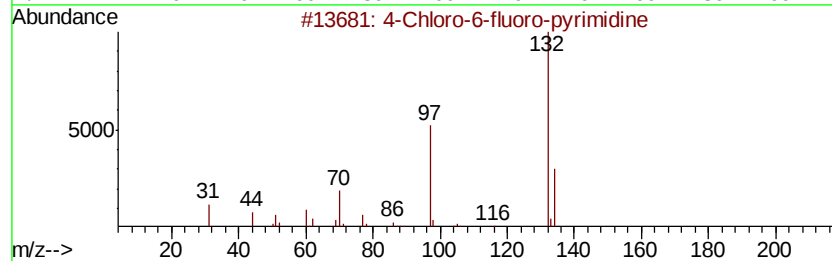
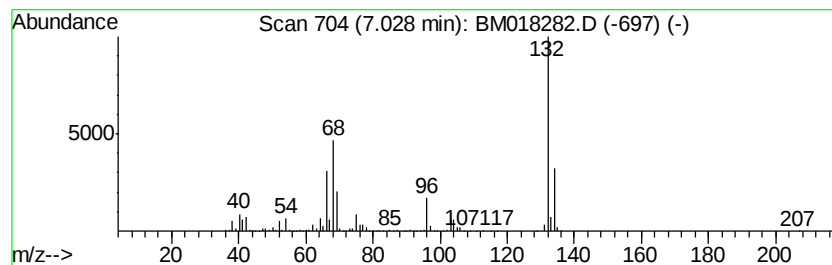
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.03 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.03 | 113.40 ng | 5292960 | 1,4-Dichlorobenzene-d4 | 7.49 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6  | 27   |
| 2    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 22   |
| 3    |    | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 4    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 5    |    | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2    | 1000241-93-9 | 10   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

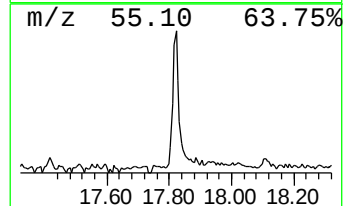
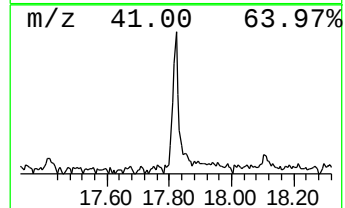
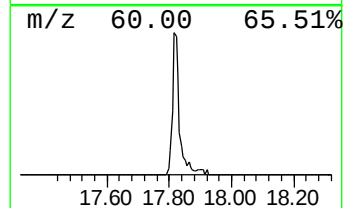
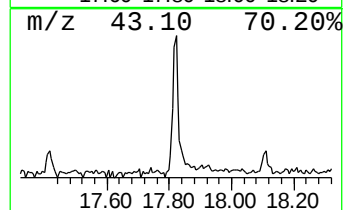
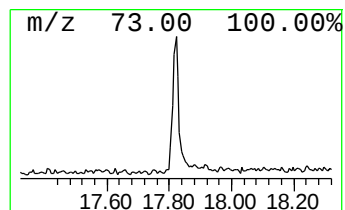
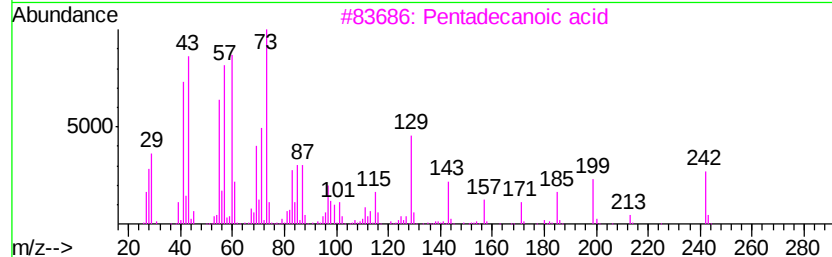
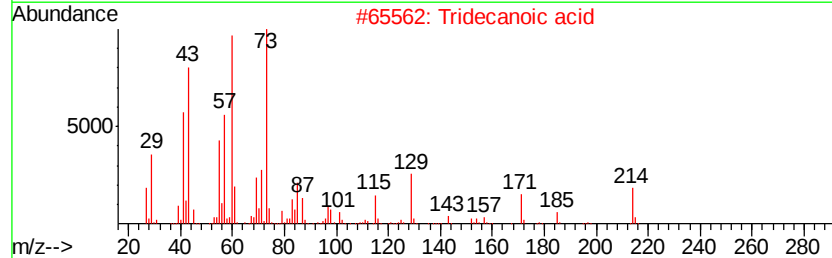
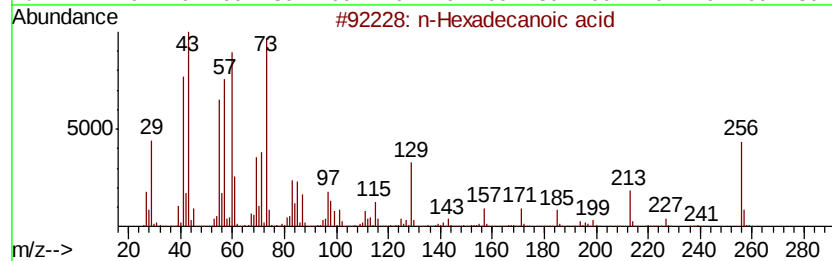
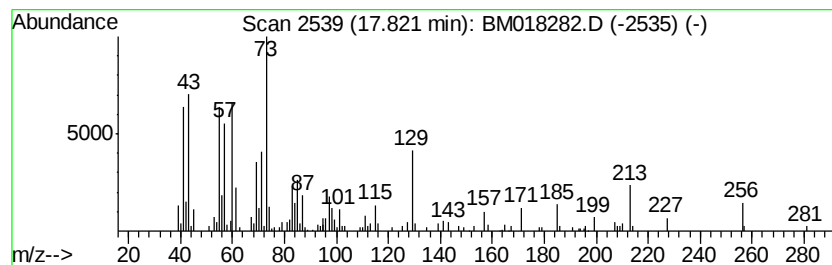
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.82 | 5.78 ng | 352730 | Phenanthrene-d10 | 16.91 |

| Hit# of | 5 | Tentative ID                       | MW  | MolForm  | CAS#         | Qual |
|---------|---|------------------------------------|-----|----------|--------------|------|
| 1       |   | n-Hexadecanoic acid                | 256 | C16H32O2 | 000057-10-3  | 98   |
| 2       |   | Tridecanoic acid                   | 214 | C13H26O2 | 000638-53-9  | 58   |
| 3       |   | Pentadecanoic acid                 | 242 | C15H30O2 | 001002-84-2  | 52   |
| 4       |   | 3,7-Dimethyl-8-oxo-1,5-dioxaspi... | 256 | C13H20O5 | 1000193-79-8 | 44   |
| 5       |   | Dodecanoic acid                    | 200 | C12H24O2 | 000143-07-7  | 38   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

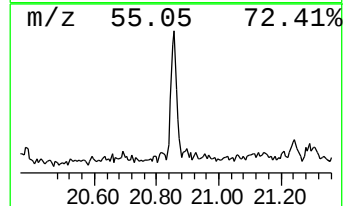
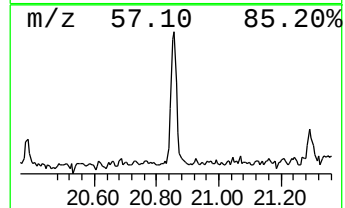
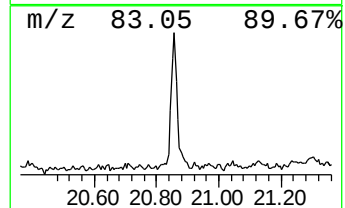
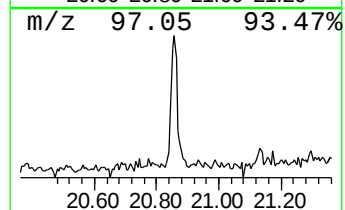
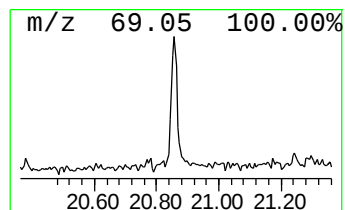
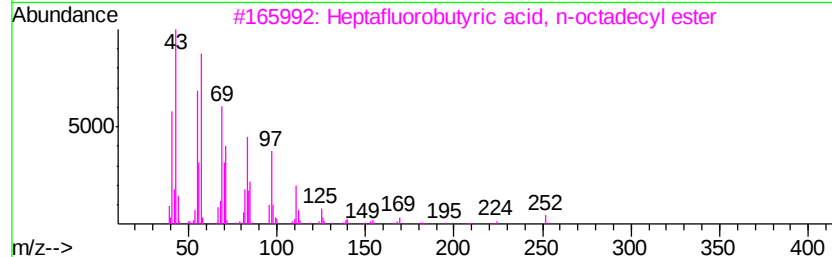
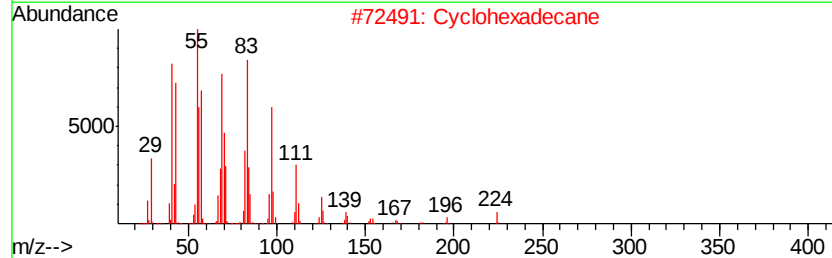
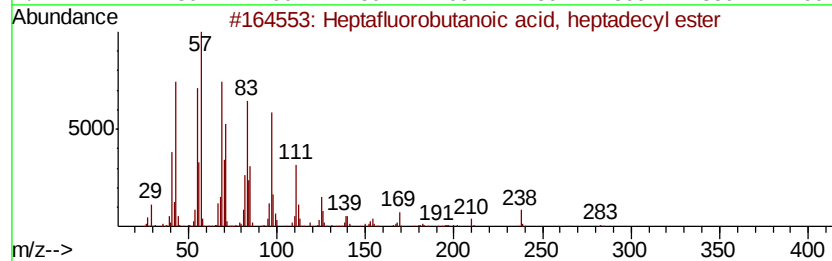
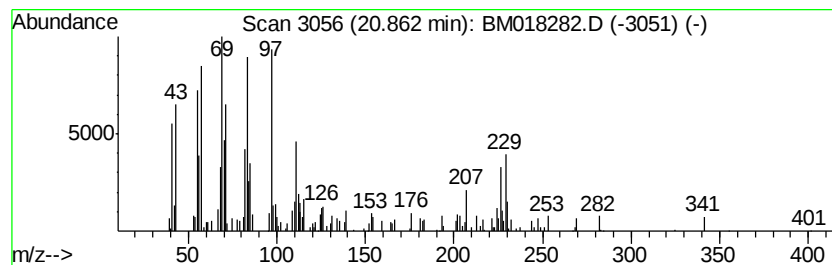
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.86 | 2.87 ng | 237102 | Chrysene-d12     | 21.13 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|---------|---|-------------------------------------|-----|-------------|--------------|------|
| 1       |   | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2  | 1000282-97-3 | 90   |
| 2       |   | Cyclohexadecane                     | 224 | C16H32      | 000295-65-8  | 86   |
| 3       |   | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2  | 000400-57-7  | 81   |
| 4       |   | 3-Octadecene, (E)-                  | 252 | C18H36      | 007206-19-1  | 80   |
| 5       |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1  | 76   |



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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Hexanol, 2-methyl- | 4.68  | 3.6     | ng    | 170409   | 1                     | 7.49  | 933516  | 20.0 |
| unknown7.03          | 7.03  | 113.4   | ng    | 5292960  | 1                     | 7.49  | 933516  | 20.0 |
| n-Hexadecanoic acid  | 17.82 | 5.8     | ng    | 352730   | 4                     | 16.91 | 1219820 | 20.0 |
| Heptafluorobutano... | 20.86 | 2.9     | ng    | 237102   | 5                     | 21.13 | 1650790 | 20.0 |