

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF051223\  
 Data File : BF133367.D  
 Acq On : 12 May 2023 13:47  
 Operator : CG\JU  
 Sample : PB152754BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB152754BL

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133367.D\data.ms

| 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         | 4.922       | 476           | 482         | 497          | rVB      | 2059538        | 3167850       | 47.12%          | 6.549%        |
| 2         | 5.345       | 549           | 554         | 557          | rBV      | 5698966        | 5972075       | 88.82%          | 12.346%       |
| 3         | 6.369       | 722           | 728         | 731          | rBV      | 5284642        | 6043208       | 89.88%          | 12.493%       |
| 4         | 6.716       | 784           | 787         | 791          | rBV      | 1521638        | 1397227       | 20.78%          | 2.889%        |
| 5         | 7.287       | 879           | 884         | 887          | rBV      | 3839480        | 3978374       | 59.17%          | 8.225%        |
| 6         | 8.004       | 1002          | 1006        | 1009         | rBV      | 2351574        | 1909122       | 28.39%          | 3.947%        |
| 7         | 9.081       | 1183          | 1189        | 1192         | rBV      | 6372759        | 6482268       | 96.41%          | 13.401%       |
| 8         | 9.757       | 1300          | 1304        | 1307         | rBV      | 2658986        | 2207219       | 32.83%          | 4.563%        |
| 9         | 10.545      | 1434          | 1438        | 1441         | rBV      | 3846325        | 3861164       | 57.43%          | 7.982%        |
| 10        | 11.233      | 1552          | 1555        | 1559         | rBV      | 2428706        | 2296973       | 34.16%          | 4.749%        |
| 11        | 12.827      | 1821          | 1826        | 1829         | rBV      | 6423164        | 6723573       | 100.00%         | 13.900%       |
| 12        | 13.357      | 1912          | 1916        | 1920         | rBV      | 88439          | 75046         | 1.12%           | 0.155%        |
| 13        | 13.874      | 1999          | 2004        | 2017         | rBV      | 1806776        | 1846487       | 27.46%          | 3.817%        |
| 14        | 14.651      | 2132          | 2136        | 2143         | rVB      | 77059          | 80147         | 1.19%           | 0.166%        |
| 15        | 14.968      | 2186          | 2190        | 2197         | rVB      | 93271          | 102267        | 1.52%           | 0.211%        |
| 16        | 15.292      | 2239          | 2245        | 2249         | rBV      | 1124413        | 1394844       | 20.75%          | 2.884%        |
| 17        | 15.327      | 2249          | 2251        | 2262         | rVB      | 123703         | 161390        | 2.40%           | 0.334%        |
| 18        | 15.733      | 2316          | 2320        | 2327         | rBV      | 90607          | 136547        | 2.03%           | 0.282%        |
| 19        | 16.215      | 2394          | 2402        | 2405         | rBV2     | 133236         | 289654        | 4.31%           | 0.599%        |
| 20        | 16.762      | 2488          | 2495        | 2504         | rVB2     | 63392          | 131752        | 1.96%           | 0.272%        |
| 21        | 17.415      | 2600          | 2606        | 2615         | rVB4     | 45390          | 113762        | 1.69%           | 0.235%        |

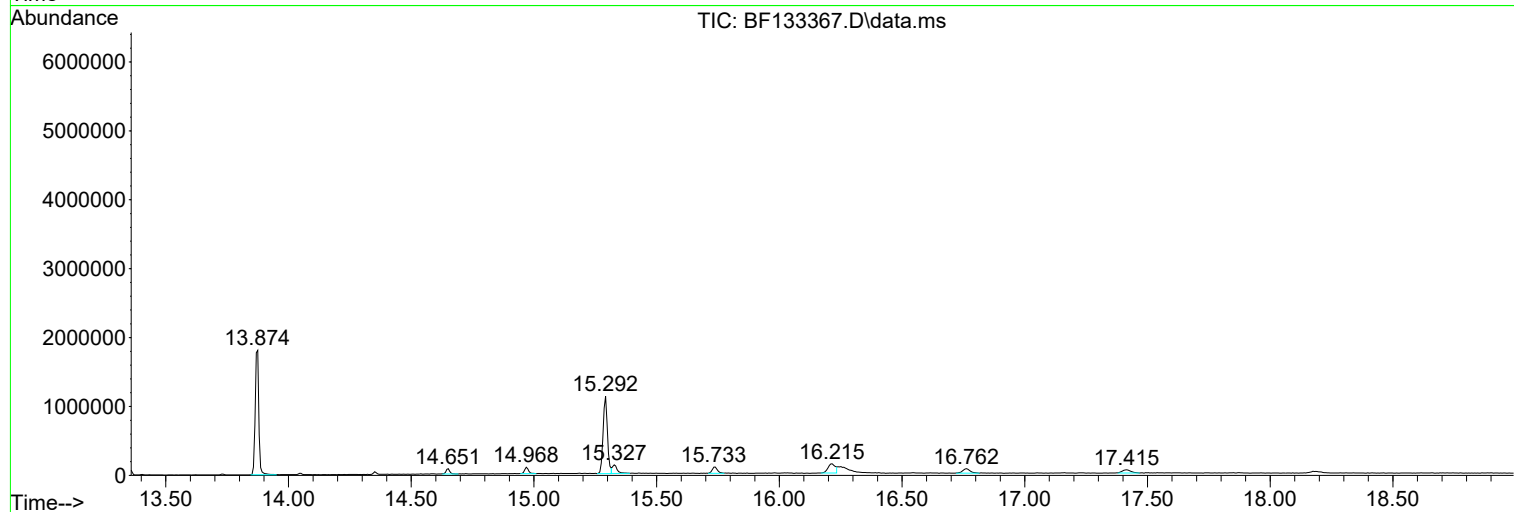
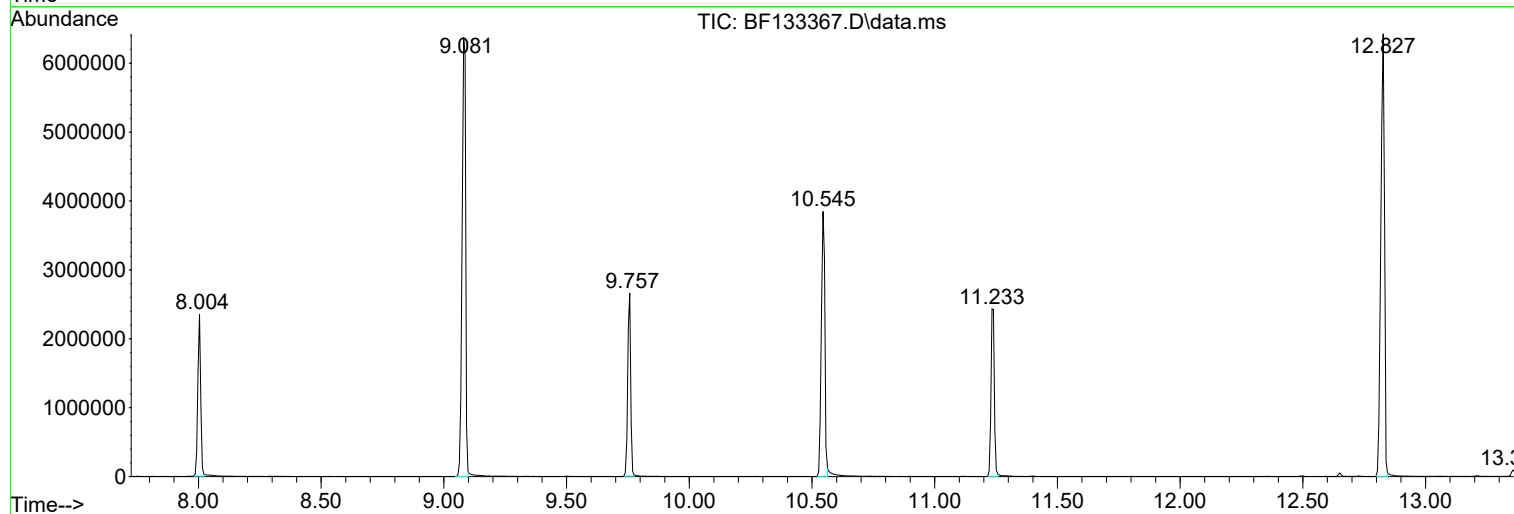
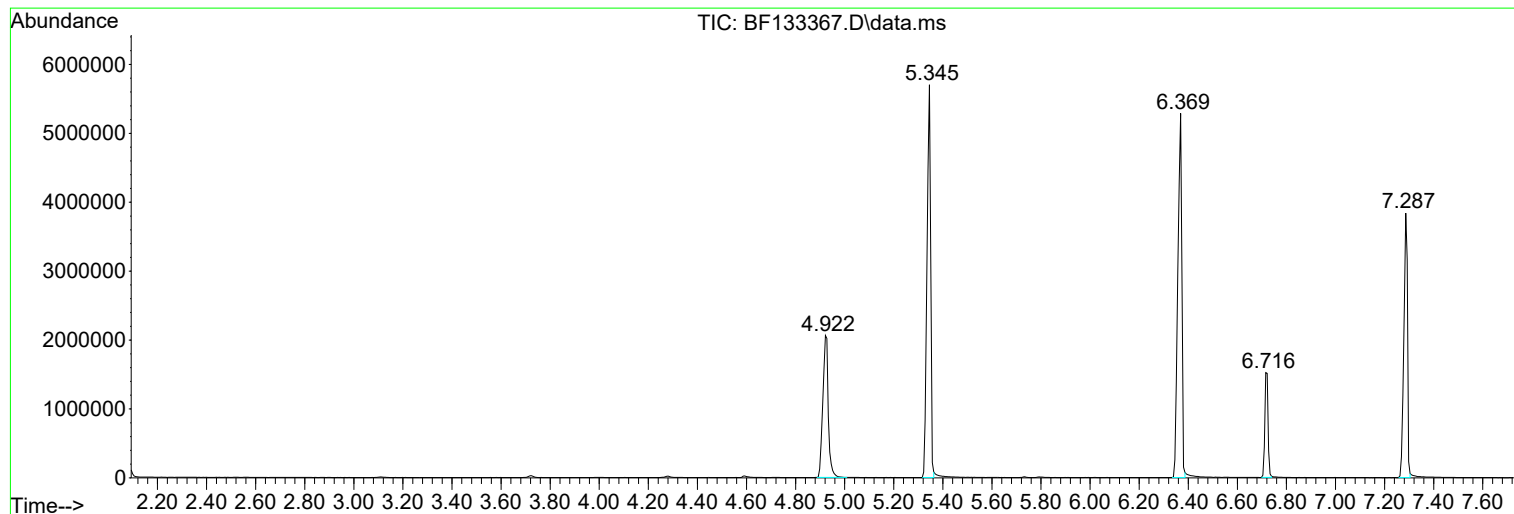
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BNA\_F  
ClientSampleId :  
PB152754BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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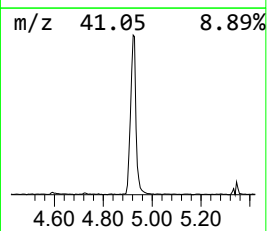
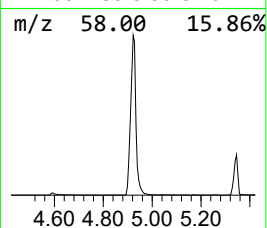
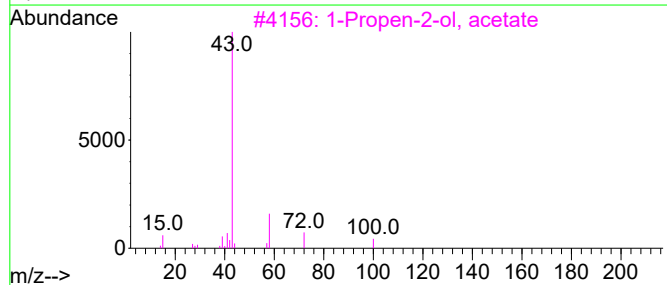
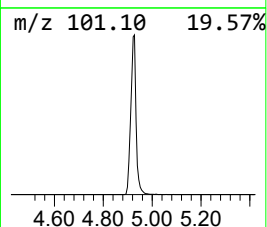
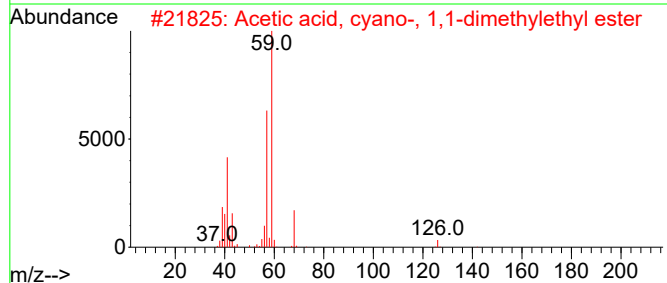
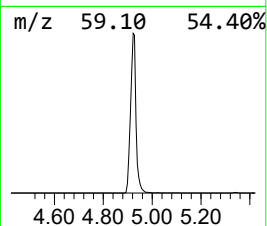
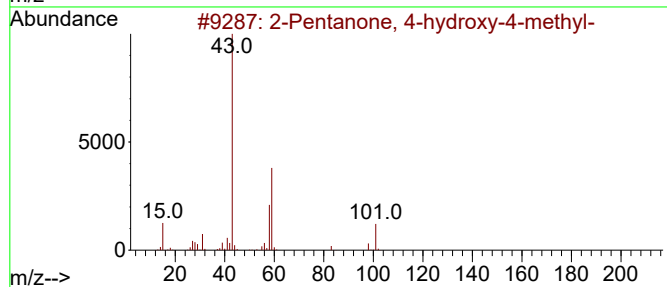
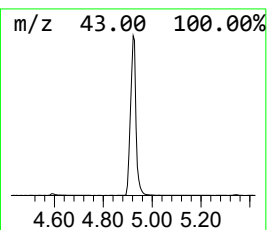
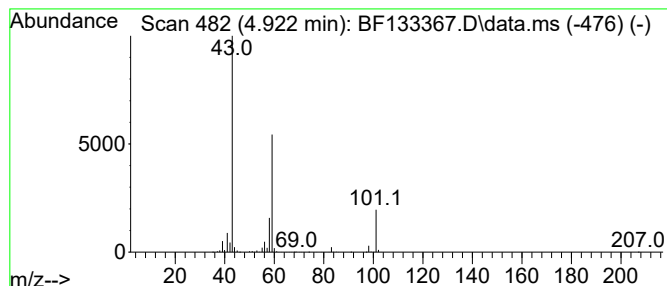
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.      | EstConc                             | Area    | Relative to ISTD       |          |             | R.T.  |
|-----------|-------------------------------------|---------|------------------------|----------|-------------|-------|
| 4.922     | 45.34 ng                            | 3167850 | 1,4-Dichlorobenzene-d4 |          |             | 6.722 |
| Hit# of 5 | Tentative ID                        |         | MW                     | MolForm  | CAS#        | Qual  |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    |         | 116                    | C6H12O2  | 000123-42-2 | 53    |
| 2         | Acetic acid, cyano-, 1,1-dimethy... |         | 141                    | C7H11NO2 | 001116-98-9 | 25    |
| 3         | 1-Propen-2-ol, acetate              |         | 100                    | C5H8O2   | 000108-22-5 | 10    |
| 4         | Morpholine, 4-methyl-               |         | 101                    | C5H11NO  | 000109-02-4 | 9     |
| 5         | 1,2-Butanediol                      |         | 90                     | C4H10O2  | 000584-03-2 | 9     |



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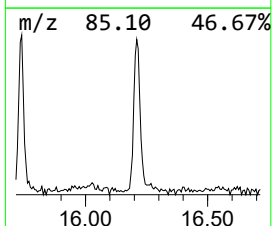
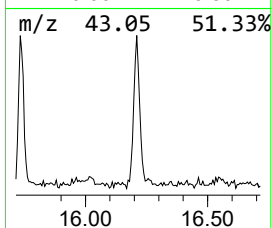
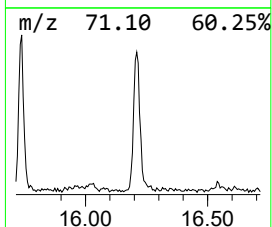
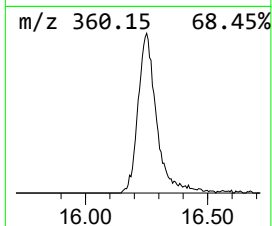
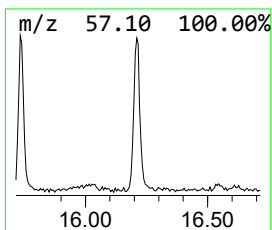
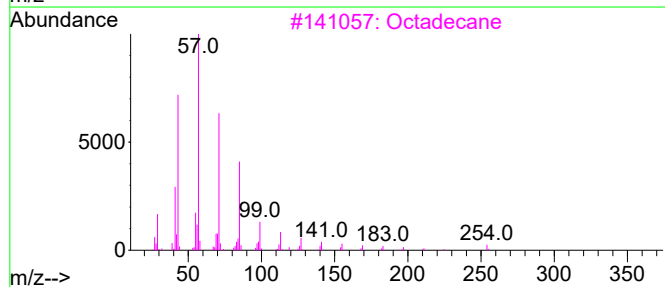
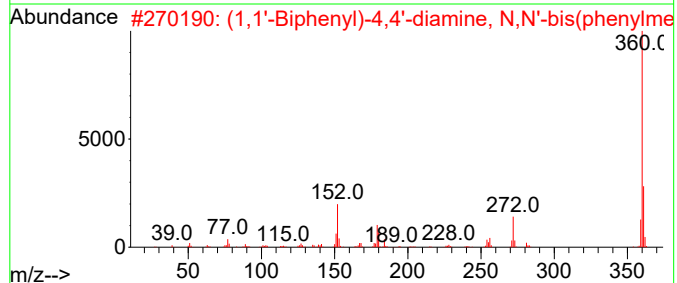
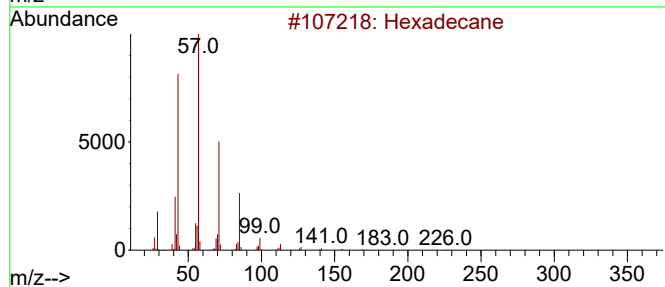
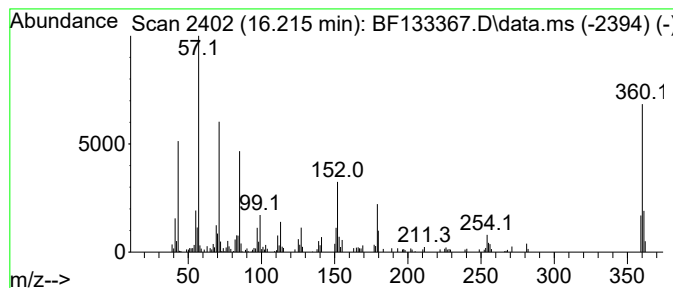
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Peak Number 2 Hexadecane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.215 | 4.15 ng | 289654 | Perylene-d12     | 15.292 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm  | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|----------|-------------|------|
| 1    | Hexadecane                          |   |              | 226 | C16H34   | 000544-76-3 | 81   |
| 2    | (1,1'-Biphenyl)-4,4'-diamine, N,... |   |              | 360 | C26H20N2 | 006311-48-4 | 64   |
| 3    | Octadecane                          |   |              | 254 | C18H38   | 000593-45-3 | 59   |
| 4    | Nonadecane                          |   |              | 268 | C19H40   | 000629-92-5 | 42   |
| 5    | Docosane                            |   |              | 310 | C22H46   | 000629-97-0 | 42   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.922  | 45.3    | ng    | 3167850  | 1                     | 6.722  | 1397230 | 20.0 |
| Hexadecane         | 16.215 | 4.2     | ng    | 289654   | 6                     | 15.292 | 1394840 | 20.0 |