

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF020122\  
 Data File : BF126768.D  
 Acq On : 01 Feb 2022 11:52  
 Operator : CG/JU  
 Sample : PB142400BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB142400BL

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126768.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         | 2.357       | 36            | 46          | 52           | rVB      | 137656         | 189779        | 3.56%           | 0.568%        |
| 2         | 5.587       | 589           | 595         | 598          | rBV      | 4016031        | 4341134       | 81.41%          | 12.983%       |
| 3         | 6.575       | 757           | 763         | 766          | rBV      | 3755394        | 4539093       | 85.12%          | 13.575%       |
| 4         | 6.957       | 824           | 828         | 831          | rVB      | 993045         | 867402        | 16.27%          | 2.594%        |
| 5         | 7.522       | 917           | 924         | 927          | rBV      | 2607299        | 3044798       | 57.10%          | 9.106%        |
| 6         | 8.239       | 1041          | 1046        | 1049         | rBV      | 1204864        | 1179109       | 22.11%          | 3.526%        |
| 7         | 9.316       | 1223          | 1229        | 1232         | rBV      | 4807914        | 4894074       | 91.78%          | 14.637%       |
| 8         | 9.998       | 1340          | 1345        | 1348         | rBV      | 1591224        | 1399976       | 26.25%          | 4.187%        |
| 9         | 10.792      | 1473          | 1480        | 1483         | rBV      | 3324572        | 3201460       | 60.03%          | 9.575%        |
| 10        | 11.492      | 1595          | 1599        | 1602         | rBV      | 1713943        | 1447557       | 27.15%          | 4.329%        |
| 11        | 13.086      | 1864          | 1870        | 1873         | rBV      | 5323121        | 5332679       | 100.00%         | 15.949%       |
| 12        | 14.139      | 2045          | 2049        | 2055         | rBV      | 1314788        | 1141928       | 21.41%          | 3.415%        |
| 13        | 14.921      | 2178          | 2182        | 2185         | rVB      | 75481          | 72414         | 1.36%           | 0.217%        |
| 14        | 15.274      | 2237          | 2242        | 2247         | rBV      | 110453         | 121147        | 2.27%           | 0.362%        |
| 15        | 15.662      | 2302          | 2308        | 2319         | rBV      | 634777         | 967932        | 18.15%          | 2.895%        |
| 16        | 16.151      | 2385          | 2391        | 2401         | rBV      | 107212         | 172940        | 3.24%           | 0.517%        |
| 17        | 16.692      | 2477          | 2483        | 2492         | rVB2     | 86800          | 157949        | 2.96%           | 0.472%        |
| 18        | 17.333      | 2585          | 2592        | 2600         | rBV3     | 50443          | 109572        | 2.05%           | 0.328%        |
| 19        | 17.786      | 2656          | 2669        | 2683         | rBV3     | 34642          | 161003        | 3.02%           | 0.482%        |
| 20        | 18.086      | 2712          | 2720        | 2730         | rBV4     | 33221          | 93981         | 1.76%           | 0.281%        |

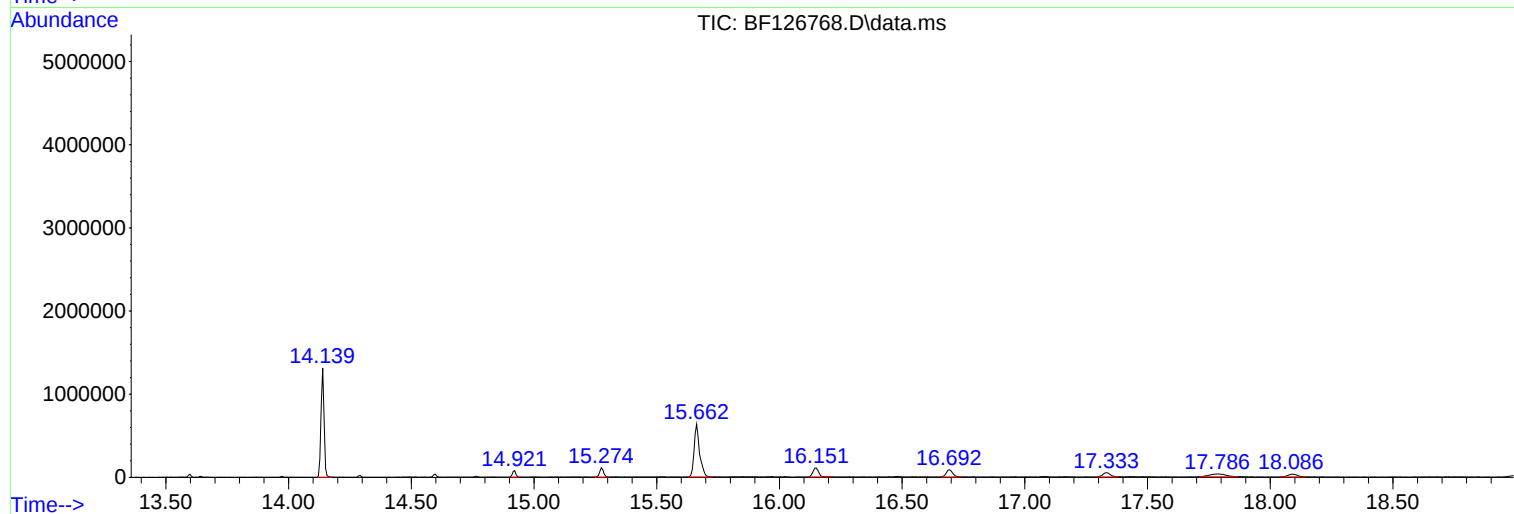
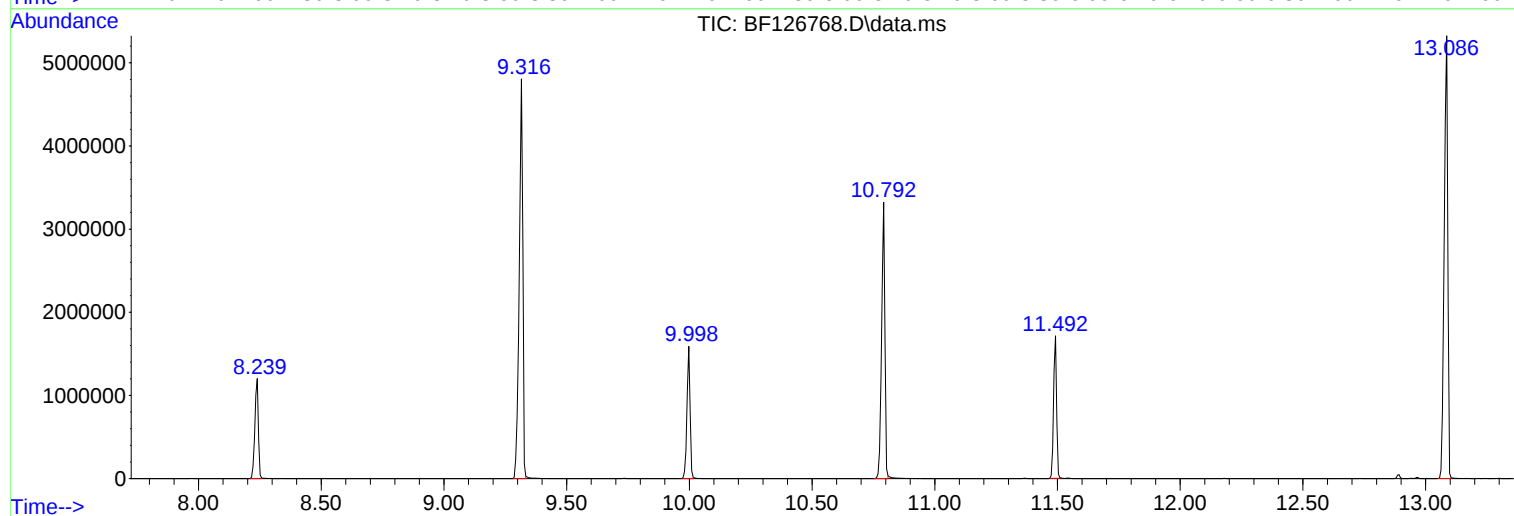
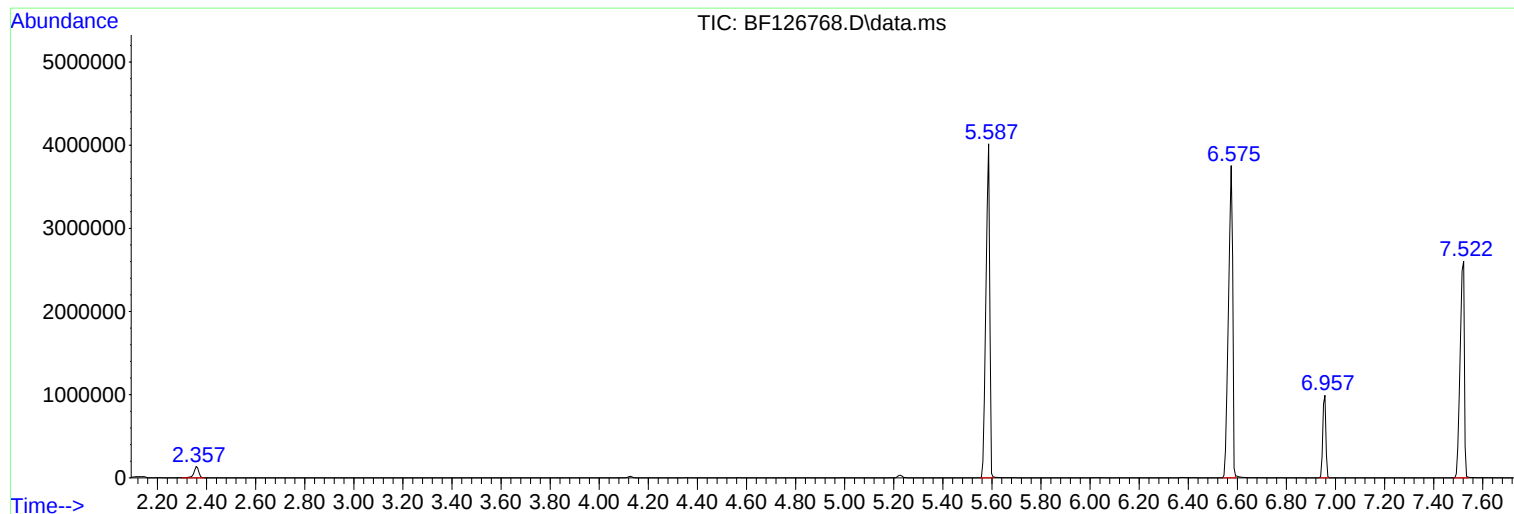
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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF020122\  
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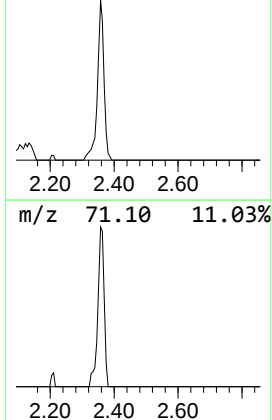
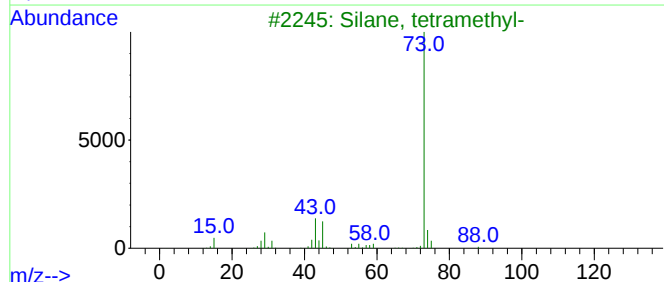
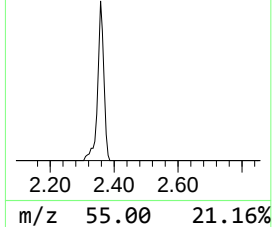
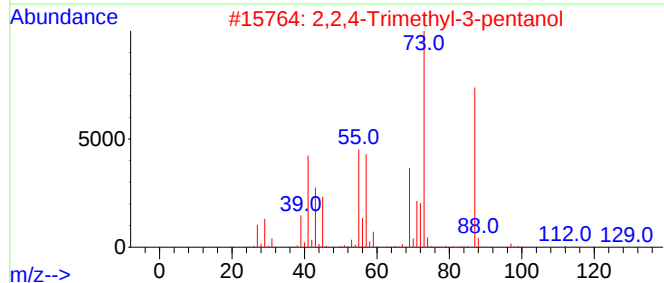
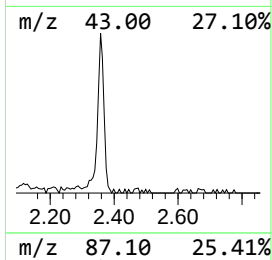
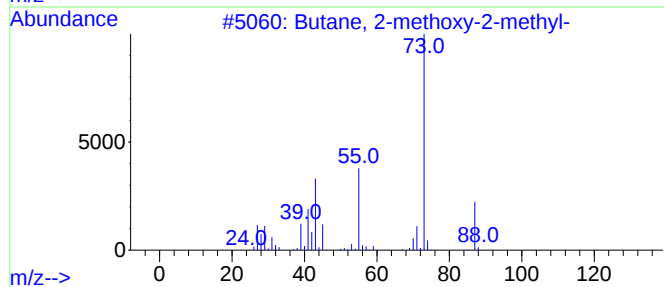
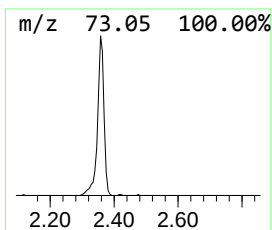
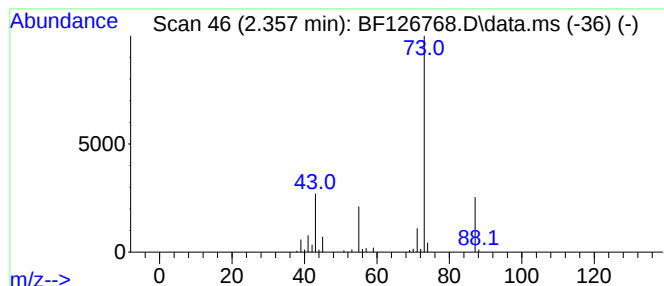
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 2.357 | 4.38 ng | 189779 | 1,4-Dichlorobenzene-d4 | 6.957 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 25   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 5    |    |   | 3-Hexanol, 2-methyl-        | 116 | C7H16O  | 000617-29-8 | 17   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

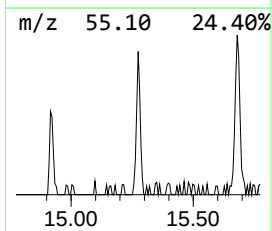
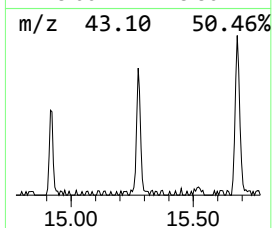
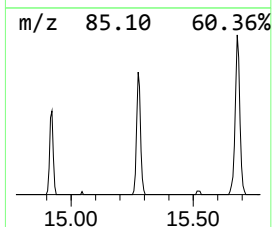
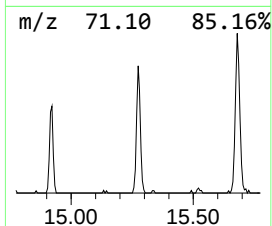
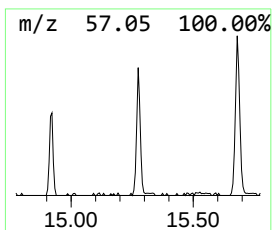
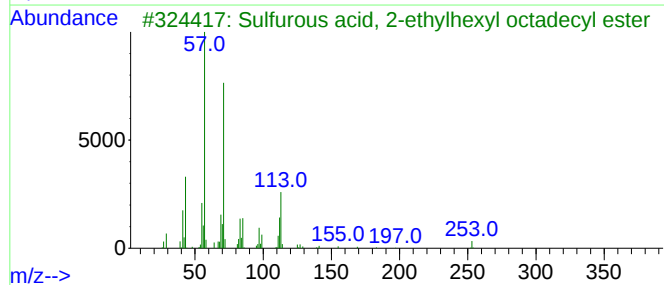
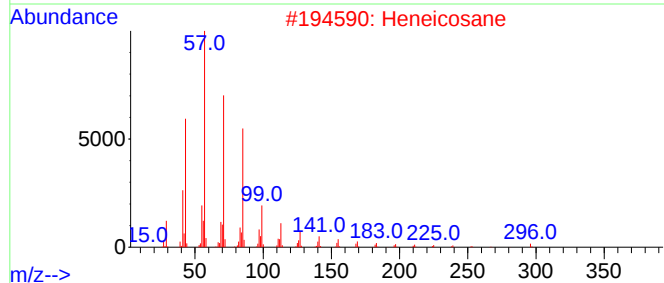
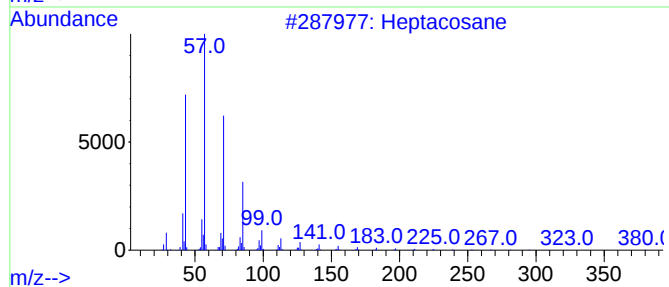
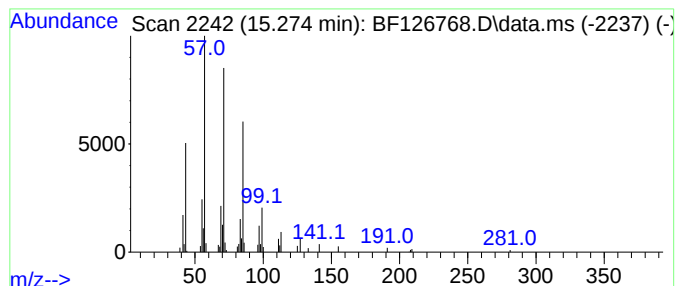
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Heptacosane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.274 | 2.50 ng | 121147 | Perylene-d12     | 15.662 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Heptacosane                         | 380 | C27H56    | 000593-49-7  | 72   |
| 2    |    |   | Heneicosane                         | 296 | C21H44    | 000629-94-7  | 64   |
| 3    |    |   | Sulfurous acid, 2-ethylhexyl oct... | 446 | C26H54O3S | 1000309-20-1 | 52   |
| 4    |    |   | Sulfurous acid, nonyl 2-propyl e... | 250 | C12H26O3S | 1000309-12-0 | 52   |
| 5    |    |   | Sulfurous acid, 2-ethylhexyl tet... | 390 | C22H46O3S | 1000309-19-7 | 50   |



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Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

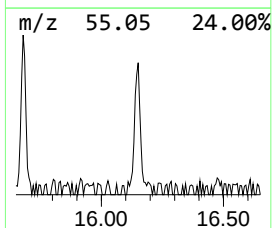
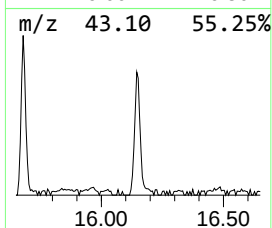
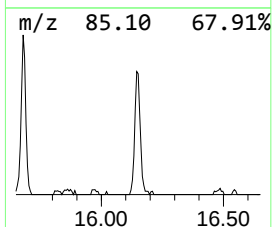
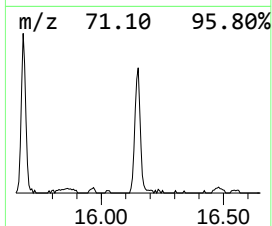
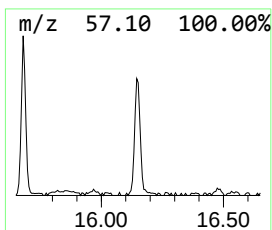
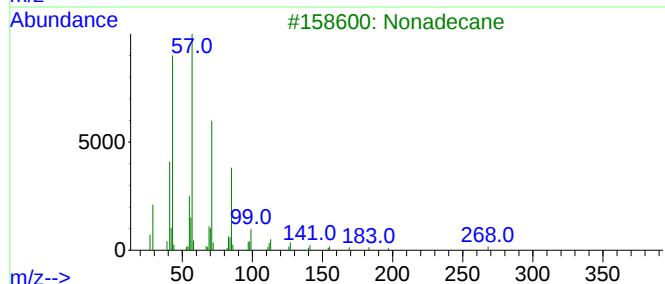
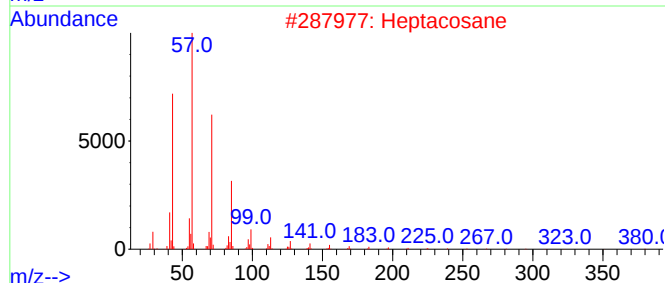
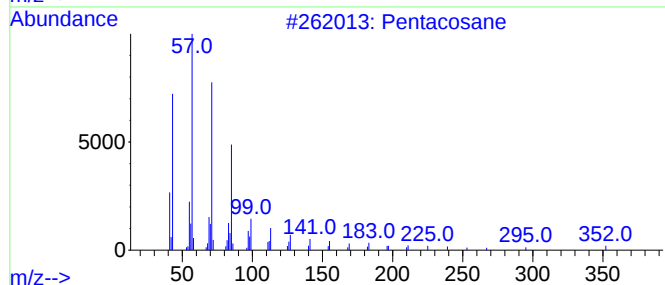
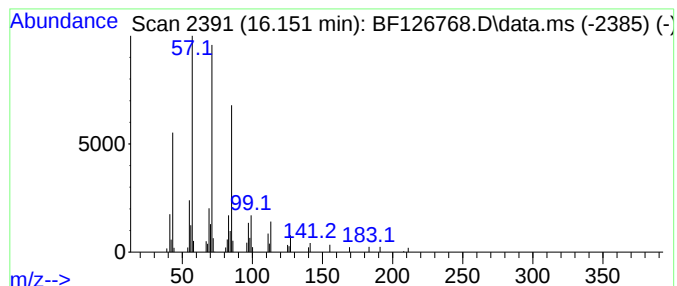
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Pentacosane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.151 | 3.57 ng | 172940 | Perylene-d12     | 15.662 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Pentacosane  | 352 | C25H52  | 000629-99-2 | 90   |
| 2    |    |   | Heptacosane  | 380 | C27H56  | 000593-49-7 | 87   |
| 3    |    |   | Nonadecane   | 268 | C19H40  | 000629-92-5 | 80   |
| 4    |    |   | Heneicosane  | 296 | C21H44  | 000629-94-7 | 80   |
| 5    |    |   | Hexacosane   | 366 | C26H54  | 000630-01-3 | 68   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

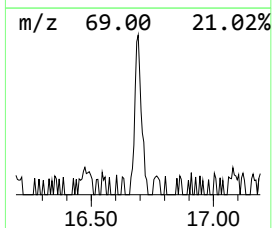
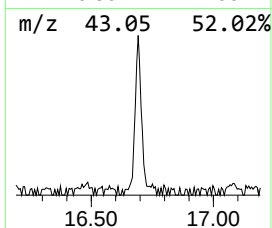
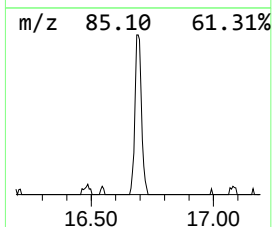
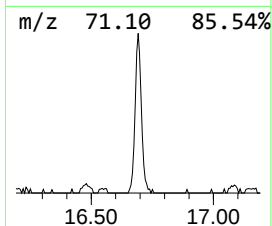
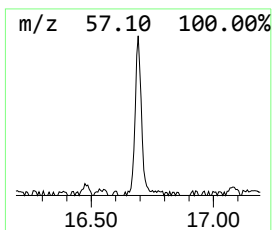
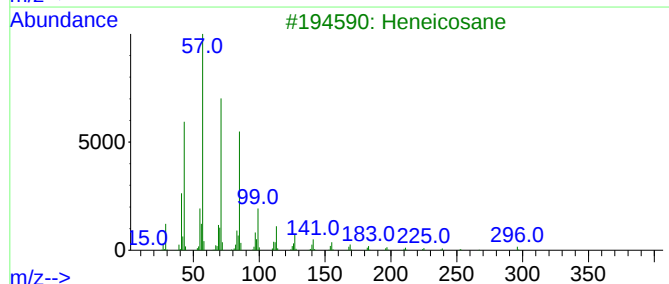
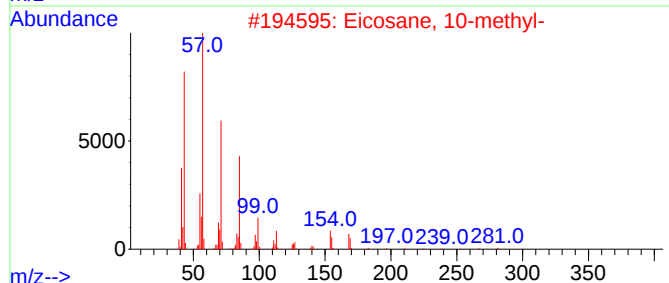
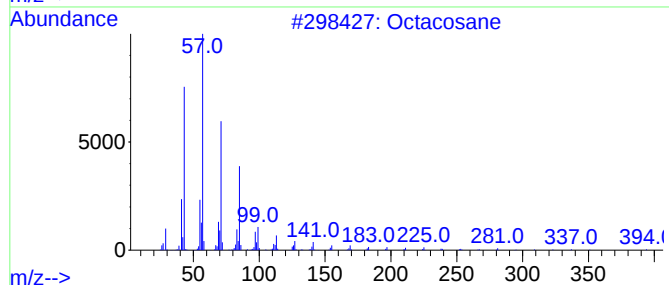
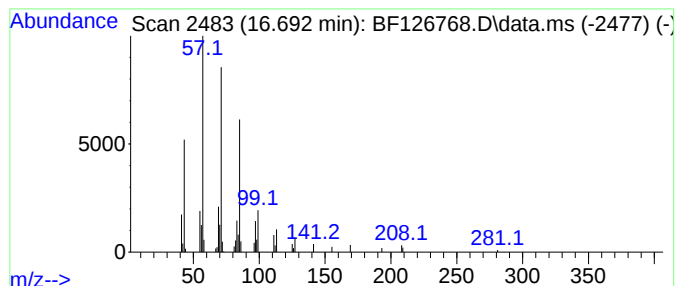
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Octacosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.692 | 3.26 ng | 157949 | Perylene-d12     | 15.662 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane           | 394 | C28H58  | 000630-02-4 | 86   |
| 2    |    |   | Eicosane, 10-methyl- | 296 | C21H44  | 054833-23-7 | 86   |
| 3    |    |   | Heneicosane          | 296 | C21H44  | 000629-94-7 | 86   |
| 4    |    |   | Octadecane, 1-iodo-  | 380 | C18H37I | 000629-93-6 | 86   |
| 5    |    |   | Nonadecane           | 268 | C19H40  | 000629-92-5 | 80   |



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ClientSampleId :  
PB142400BL

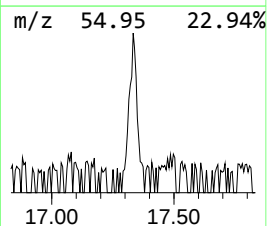
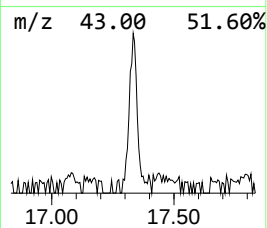
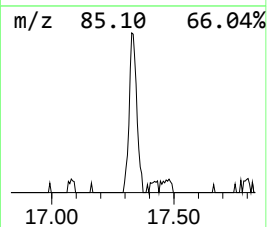
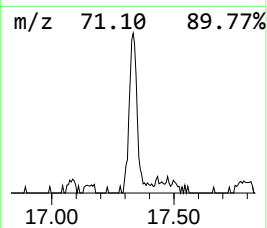
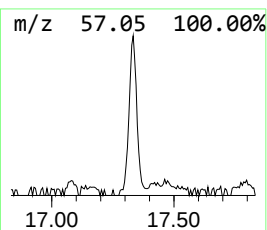
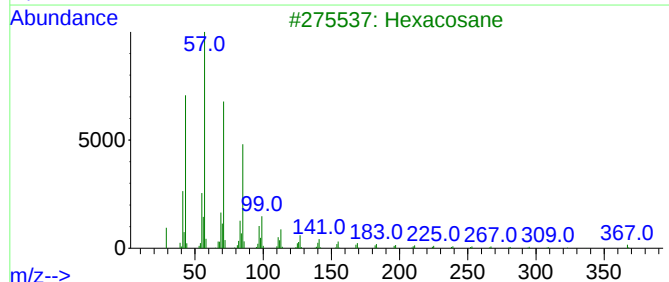
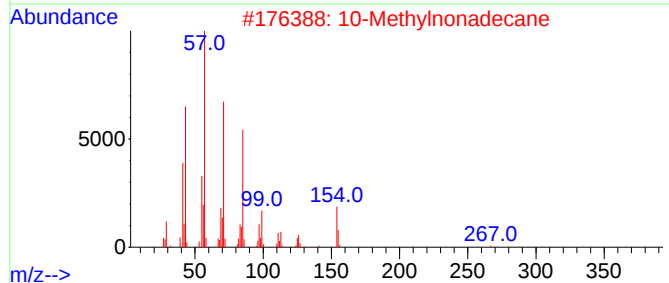
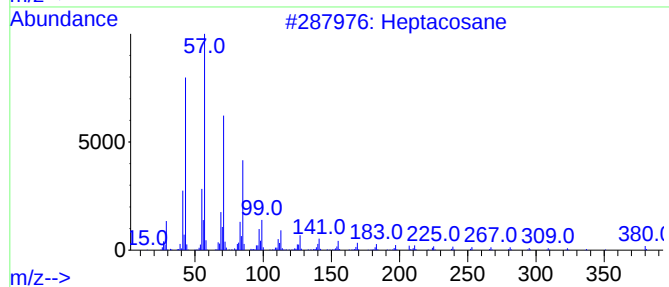
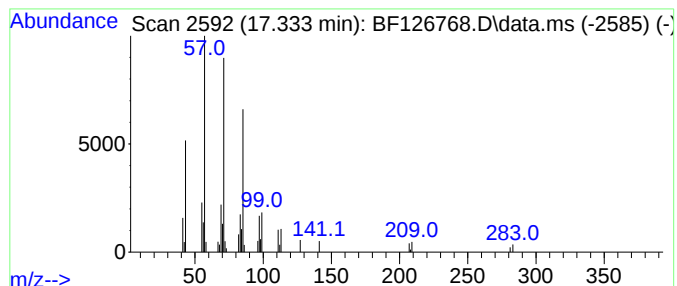
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 5 10-Methylnonadecane Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.333 | 2.26 ng | 109572 | Perylene-d12     | 15.662 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------|-----|---------|-------------|------|
| 1    |    |   | Heptacosane         | 380 | C27H56  | 000593-49-7 | 90   |
| 2    |    |   | 10-Methylnonadecane | 282 | C20H42  | 056862-62-5 | 90   |
| 3    |    |   | Hexacosane          | 366 | C26H54  | 000630-01-3 | 87   |
| 4    |    |   | Heneicosane         | 296 | C21H44  | 000629-94-7 | 86   |
| 5    |    |   | Nonadecane          | 268 | C19H40  | 000629-92-5 | 80   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF020122\  
Data File : BF126768.D  
Acq On : 01 Feb 2022 11:52  
Operator : CG/JU  
Sample : PB142400BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

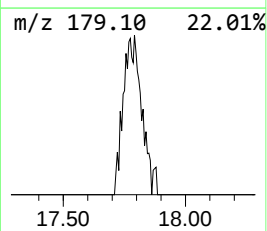
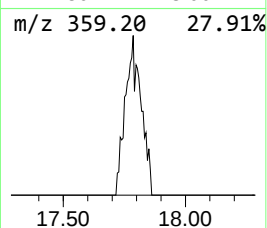
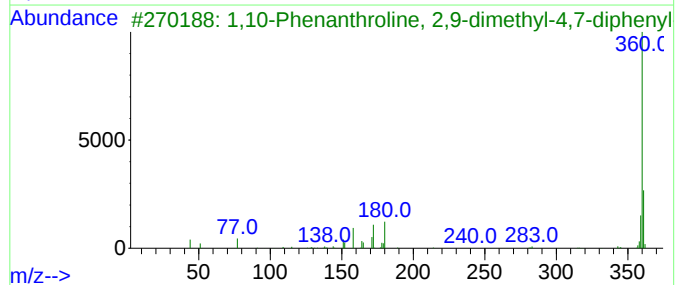
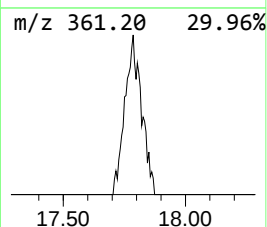
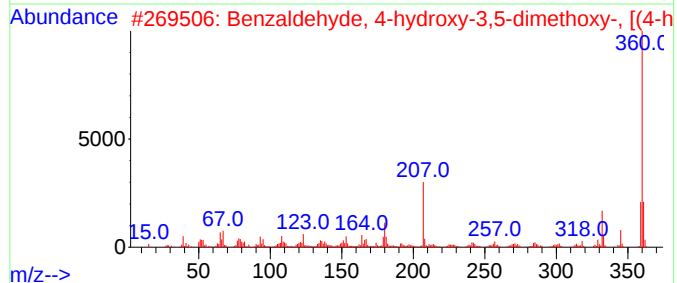
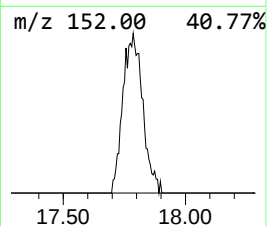
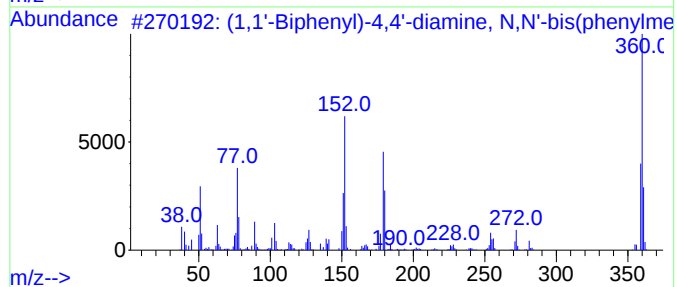
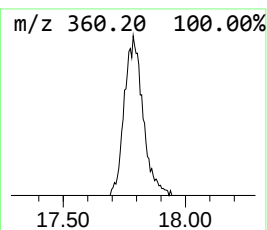
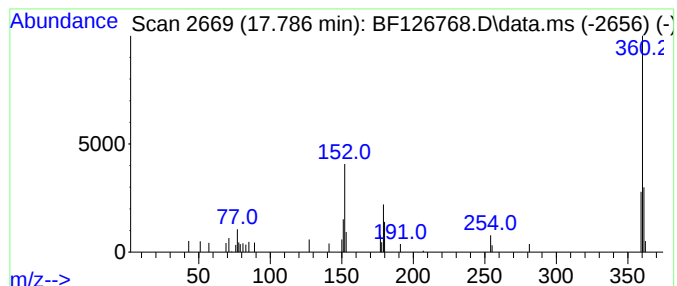
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.786 | 3.33 ng | 161003 | Perylene-d12     | 15.662 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|------|-------------------------------------|-----|------------|-------------|------|
| 1    |      | (1,1'-Biphenyl)-4,4'-diamine, N,... | 360 | C26H20N2   | 006311-48-4 | 95   |
| 2    |      | Benzaldehyde, 4-hydroxy-3,5-dime... | 360 | C18H20N2O6 | 014414-32-5 | 49   |
| 3    |      | 1,10-Phenanthroline, 2,9-dimethy... | 360 | C26H20N2   | 004733-39-5 | 49   |
| 4    |      | N,N'-di-2-Naphthyl-p-phenylenedi... | 360 | C26H20N2   | 000093-46-9 | 43   |
| 5    |      | Androst-4-ene-3,17-dione, 12-hyd... | 360 | C21H32N2O3 | 069688-31-9 | 43   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF020122\  
Data File : BF126768.D  
Acq On : 01 Feb 2022 11:52  
Operator : CG/JU  
Sample : PB142400BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB142400BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.357  | 4.4     | ng    | 189779   | 1                     | 6.957  | 867402 | 20.0 |
| Heptacosane        | 15.274 | 2.5     | ng    | 121147   | 6                     | 15.662 | 967932 | 20.0 |
| Pentacosane        | 16.151 | 3.6     | ng    | 172940   | 6                     | 15.662 | 967932 | 20.0 |
| Octacosane         | 16.692 | 3.3     | ng    | 157949   | 6                     | 15.662 | 967932 | 20.0 |
| 10-Methylnonade... | 17.333 | 2.3     | ng    | 109572   | 6                     | 15.662 | 967932 | 20.0 |
| (1,1'-Biphenyl)... | 17.786 | 3.3     | ng    | 161003   | 6                     | 15.662 | 967932 | 20.0 |