

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG012524\  
 Data File : BG060425.D  
 Acq On : 25 Jan 2024 13:00  
 Operator : MA/JU  
 Sample : PB158620BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB158620BL

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\_G\Methods\8270-BG010824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060425.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         | 5.033       | 324           | 331         | 340          | rVB      | 132657         | 224856        | 1.03%           | 0.225%        |
| 2         | 5.509       | 404           | 412         | 429          | rBV      | 4109834        | 6558363       | 30.16%          | 6.575%        |
| 3         | 7.101       | 673           | 683         | 697          | rBV      | 4457073        | 7593898       | 34.93%          | 7.614%        |
| 4         | 7.930       | 817           | 824         | 831          | rBV      | 752952         | 1274759       | 5.86%           | 1.278%        |
| 5         | 9.093       | 1015          | 1022        | 1035         | rBV      | 2716858        | 4912175       | 22.59%          | 4.925%        |
| 6         | 10.732      | 1293          | 1301        | 1310         | rBV      | 1149276        | 2023600       | 9.31%           | 2.029%        |
| 7         | 13.188      | 1710          | 1719        | 1732         | rBV      | 8221493        | 13475852      | 61.98%          | 13.511%       |
| 8         | 14.569      | 1946          | 1954        | 1964         | rBV      | 2130175        | 3386934       | 15.58%          | 3.396%        |
| 9         | 16.055      | 2200          | 2207        | 2220         | rBV      | 6562941        | 10638986      | 48.93%          | 10.667%       |
| 10        | 17.313      | 2414          | 2421        | 2431         | rBV      | 3173358        | 4767286       | 21.93%          | 4.780%        |
| 11        | 19.622      | 2808          | 2814        | 2824         | rVB2     | 228190         | 346464        | 1.59%           | 0.347%        |
| 12        | 19.933      | 2860          | 2867        | 2879         | rBV      | 14750174       | 21743348      | 100.00%         | 21.800%       |
| 13        | 20.662      | 2987          | 2991        | 2995         | rBV      | 197822         | 226485        | 1.04%           | 0.227%        |
| 14        | 21.578      | 3140          | 3147        | 3154         | rBV      | 3161090        | 5236135       | 24.08%          | 5.250%        |
| 15        | 22.354      | 3274          | 3279        | 3284         | rVB2     | 215425         | 325553        | 1.50%           | 0.326%        |
| 16        | 23.029      | 3387          | 3394        | 3402         | rBV      | 484445         | 887208        | 4.08%           | 0.890%        |
| 17        | 23.817      | 3522          | 3528        | 3536         | rVB      | 596406         | 1260916       | 5.80%           | 1.264%        |
| 18        | 24.745      | 3675          | 3686        | 3704         | rBV2     | 2608542        | 7252375       | 33.35%          | 7.271%        |
| 19        | 25.850      | 3865          | 3874        | 3888         | rVB      | 679618         | 2051167       | 9.43%           | 2.056%        |
| 20        | 27.178      | 4090          | 4100        | 4114         | rVB2     | 618616         | 2224240       | 10.23%          | 2.230%        |
| 21        | 28.782      | 4361          | 4373        | 4386         | rVB4     | 422049         | 1708026       | 7.86%           | 1.712%        |
| 22        | 30.720      | 4689          | 4703        | 4715         | rBV6     | 313440         | 1622614       | 7.46%           | 1.627%        |

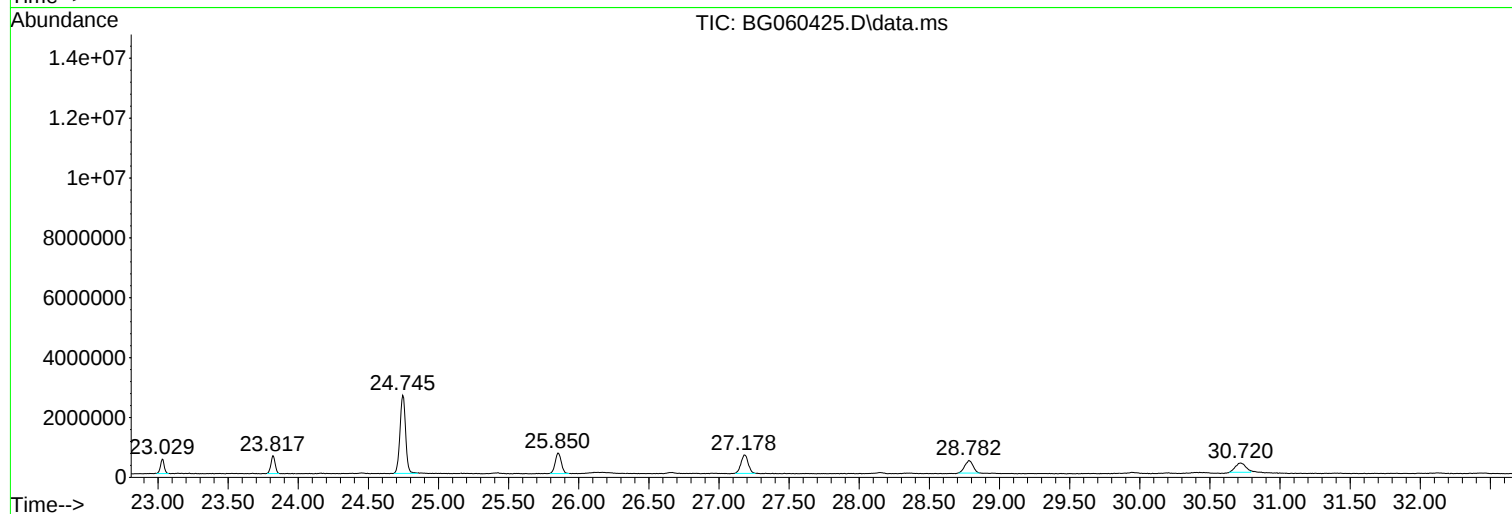
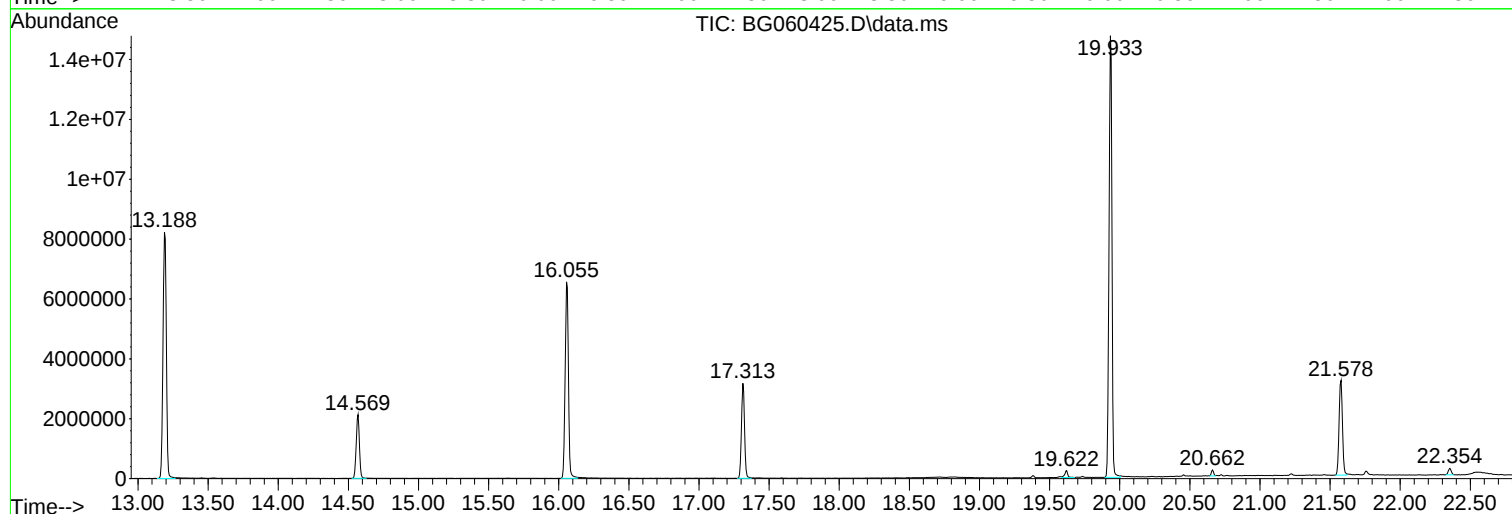
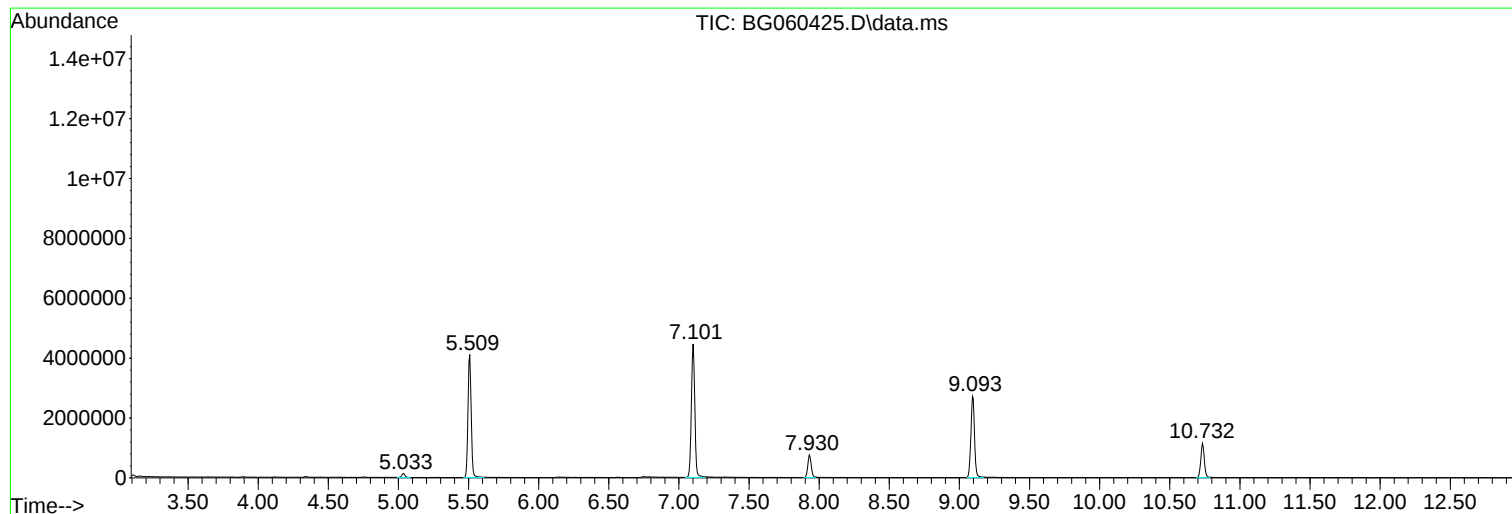
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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.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\_G\Data\BG012524\  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

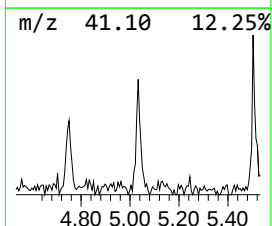
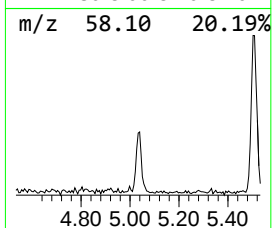
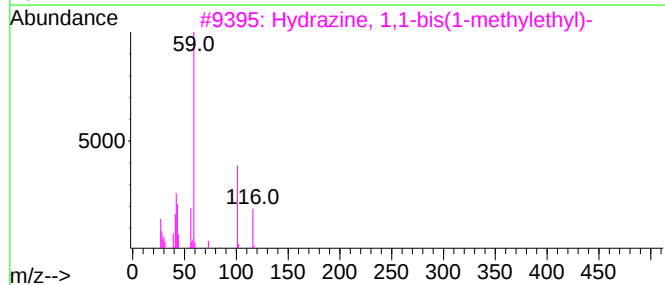
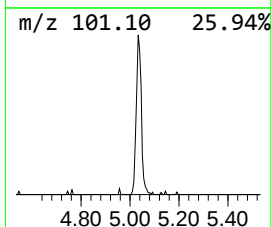
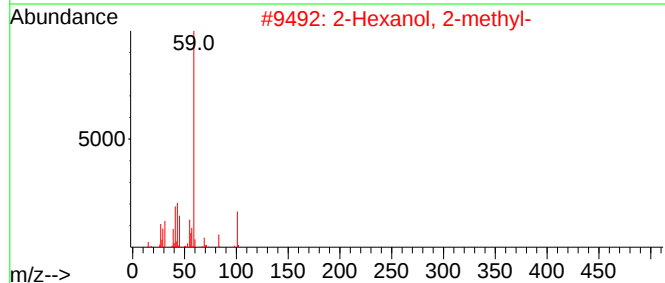
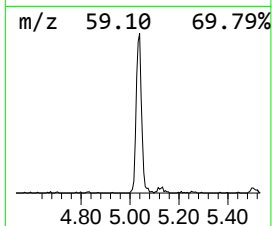
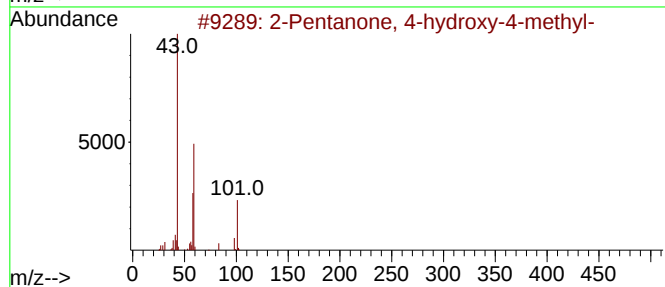
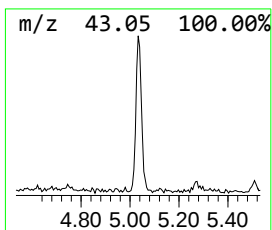
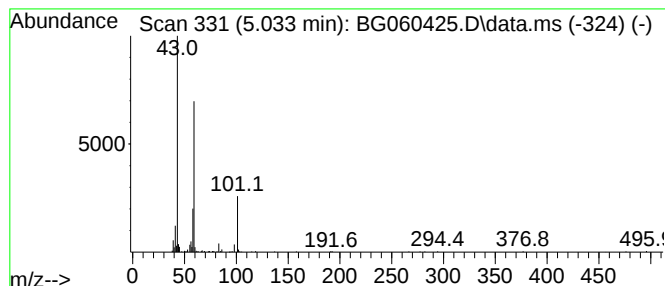
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.033 | 3.53 ng | 224856 | 1,4-Dichlorobenzene-d4 | 7.930 |

| Hit# | of 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|------|------------------------------------|-----|---------|-------------|------|
| 1    |      | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 43   |
| 2    |      | 2-Hexanol, 2-methyl-               | 116 | C7H16O  | 000625-23-0 | 25   |
| 3    |      | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 23   |
| 4    |      | 3-Hexanol, 4-methyl-               | 116 | C7H16O  | 000615-29-2 | 23   |
| 5    |      | Propane, 1-ethoxy-2-methyl-        | 102 | C6H14O  | 000627-02-1 | 22   |



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BNA\_G  
ClientSampleId :  
PB158620BL

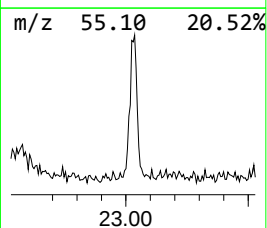
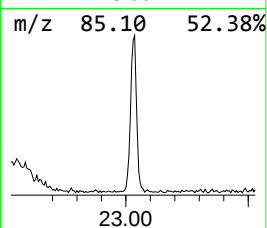
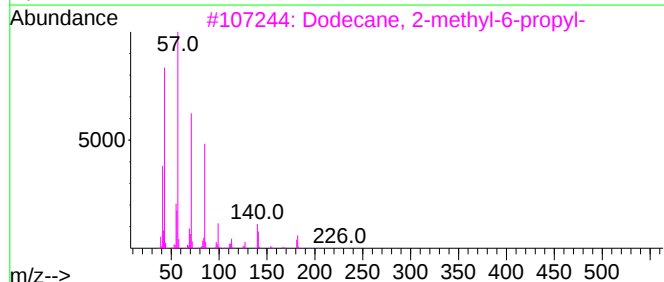
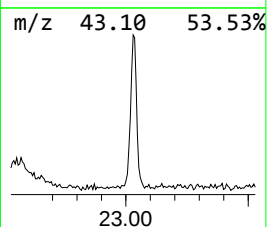
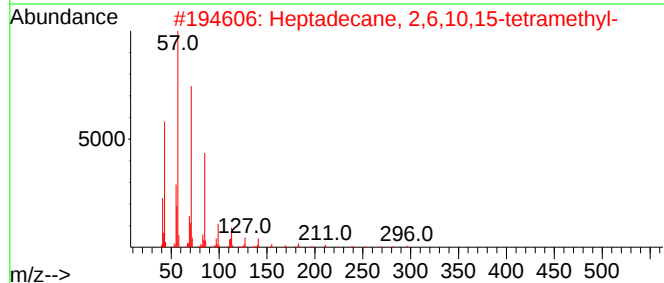
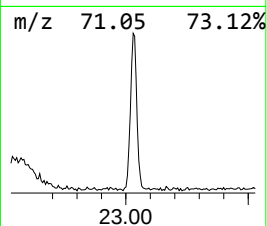
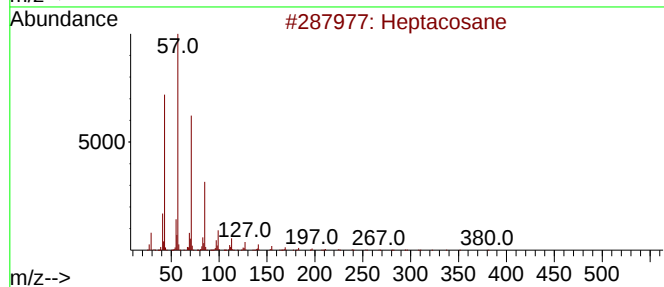
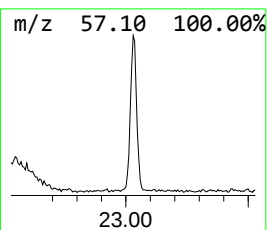
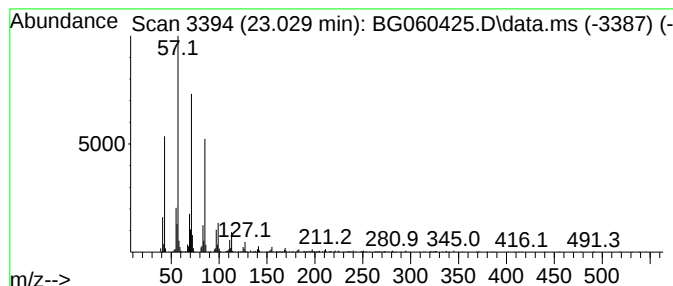
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Heptacosane Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.029 | 3.39 ng | 887208 | Chrysene-d12     | 21.578 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------------------------|-----|---------|-------------|------|
| 1    |      | Heptacosane                         | 380 | C27H56  | 000593-49-7 | 95   |
| 2    |      | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44  | 054833-48-6 | 90   |
| 3    |      | Dodecane, 2-methyl-6-propyl-        | 226 | C16H34  | 055045-08-4 | 87   |
| 4    |      | Hexadecane                          | 226 | C16H34  | 000544-76-3 | 87   |
| 5    |      | Tetradecane, 1-iodo-                | 324 | C14H29I | 019218-94-1 | 87   |



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Sample : PB158620BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

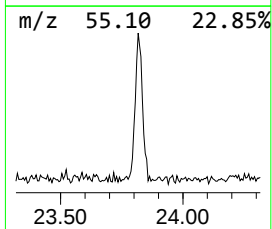
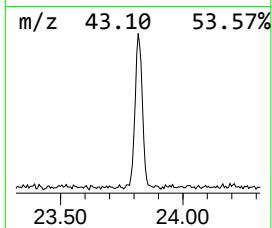
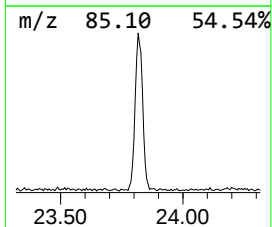
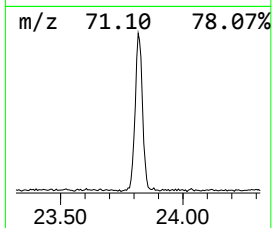
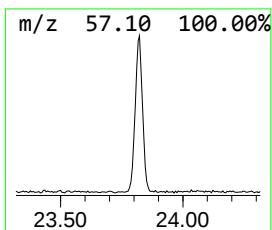
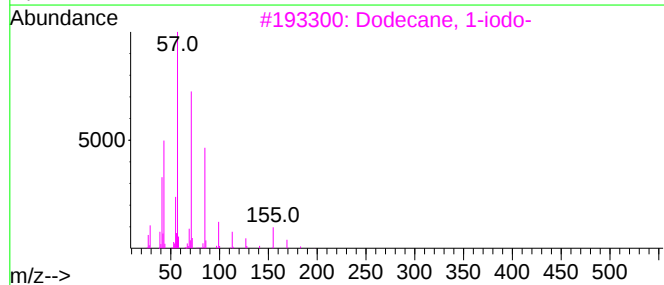
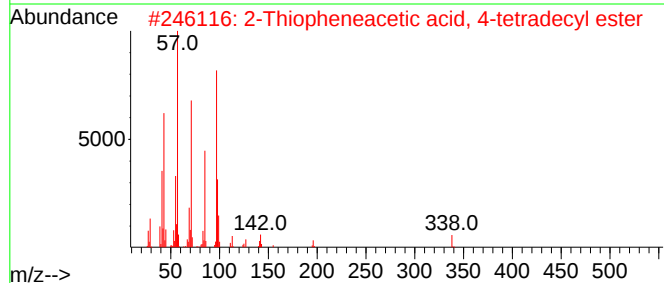
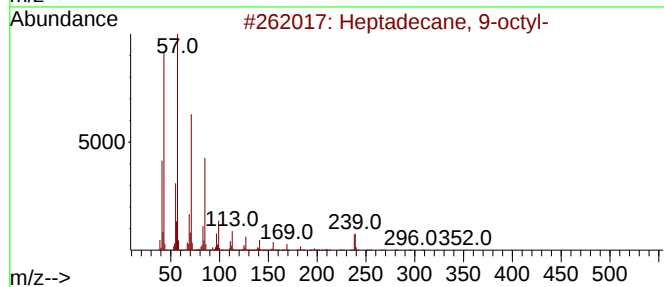
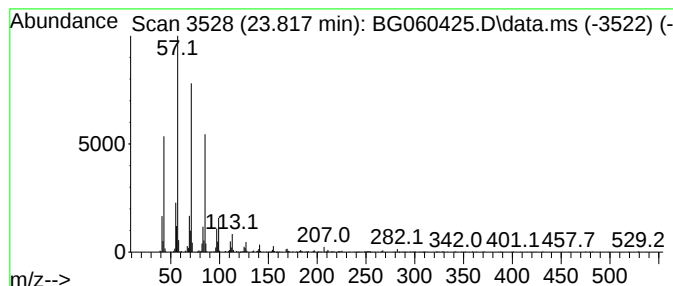
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Heptadecane, 9-octyl- Concentration Rank 6

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 23.817 | 3.48 ng | 1260920 | Perylene-d12     | 24.745 |

| Hit# | of | 5 | Tentative ID                               | MW  | MolForm   | CAS#         | Qual |
|------|----|---|--------------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Heptadecane, 9-octyl-                      | 352 | C25H52    | 007225-64-1  | 90   |
| 2    |    |   | 2-Thiopheneacetic acid, 4-tetradecyl ester | 338 | C20H34O2S | 1010280-67-0 | 80   |
| 3    |    |   | Dodecane, 1-iodo-                          | 296 | C12H25I   | 004292-19-7  | 80   |
| 4    |    |   | Heptacosane                                | 380 | C27H56    | 000593-49-7  | 74   |
| 5    |    |   | Sulfurous acid, 2-ethylhexyl hep...        | 432 | C25H52O3S | 1000309-20-0 | 58   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

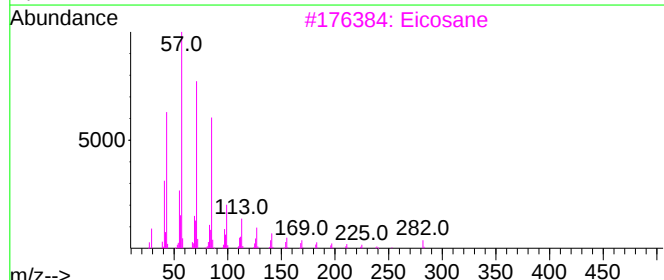
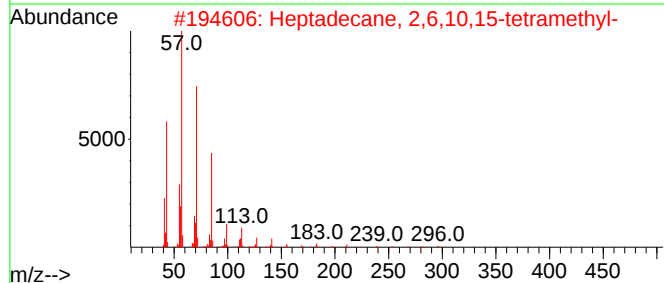
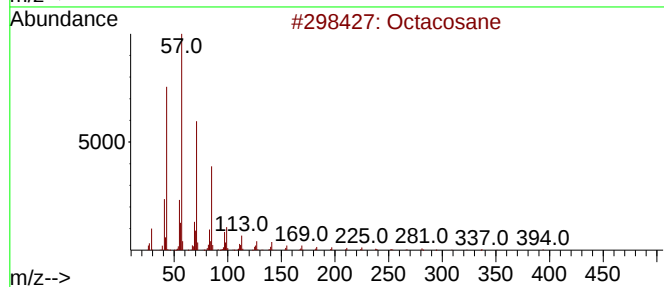
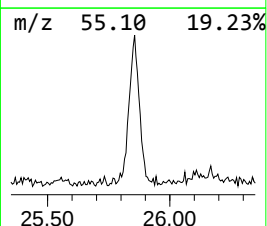
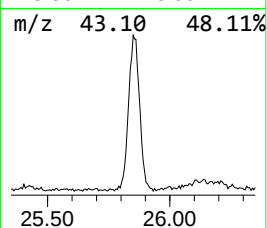
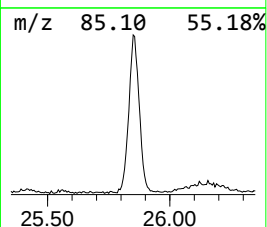
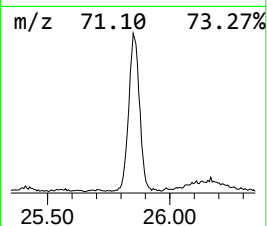
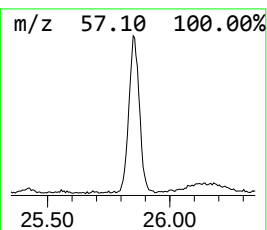
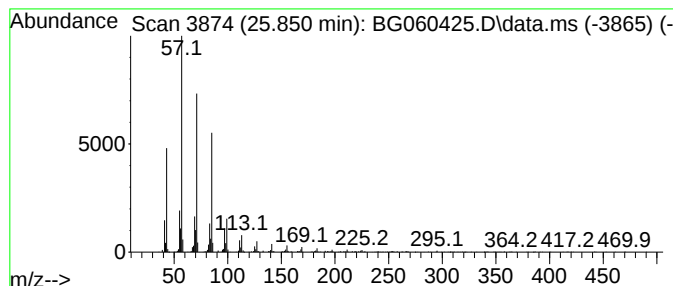
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octacosane Concentration Rank 2

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 25.850 | 5.66 ng | 2051170 | Perylene-d12     | 24.745 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane                          | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    |   | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44  | 054833-48-6 | 90   |
| 3    |    |   | Eicosane                            | 282 | C20H42  | 000112-95-8 | 90   |
| 4    |    |   | Hexacosane                          | 366 | C26H54  | 000630-01-3 | 87   |
| 5    |    |   | Octadecane, 1-iodo-                 | 380 | C18H37I | 000629-93-6 | 86   |



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BNA\_G  
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PB158620BL

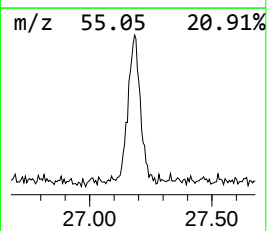
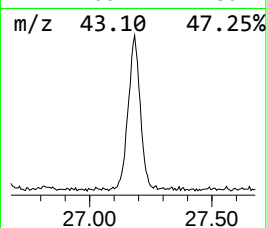
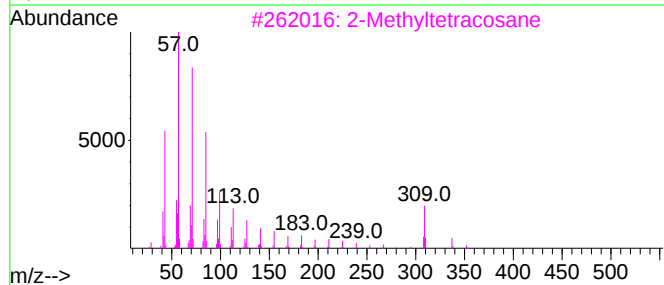
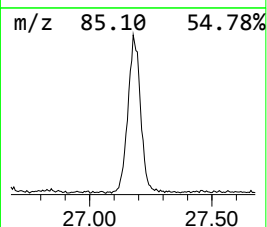
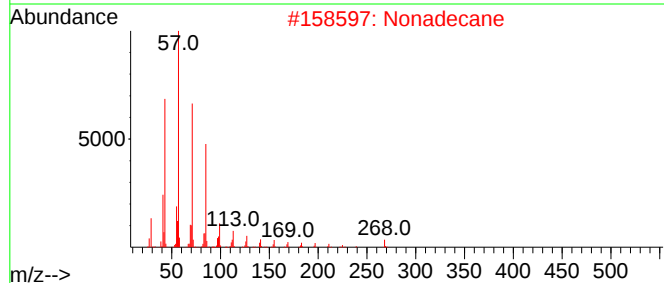
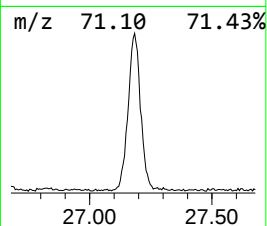
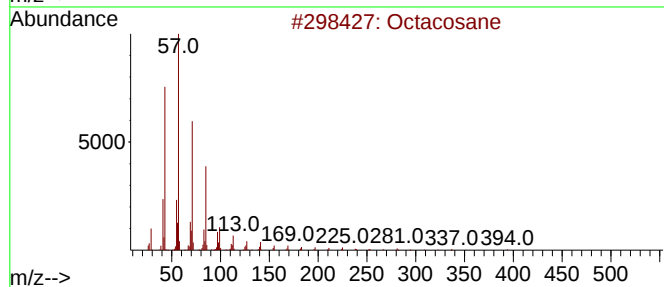
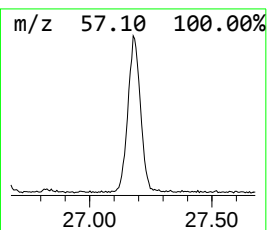
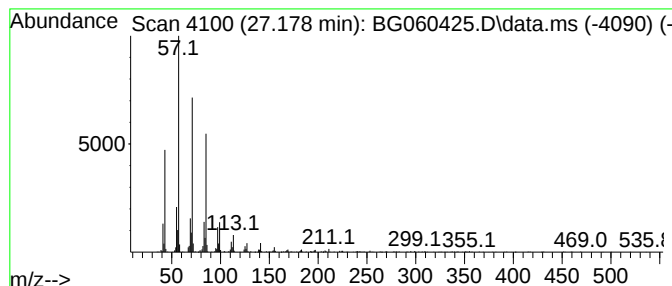
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Nonadecane Concentration Rank 1

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 27.178 | 6.13 ng | 2224240 | Perylene-d12     | 24.745 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm  | CAS#         | Qual |
|------|----|---|----------------------------|-----|----------|--------------|------|
| 1    |    |   | Octacosane                 | 394 | C28H58   | 000630-02-4  | 91   |
| 2    |    |   | Nonadecane                 | 268 | C19H40   | 000629-92-5  | 86   |
| 3    |    |   | 2-Methyltetracosane        | 352 | C25H52   | 001560-78-7  | 76   |
| 4    |    |   | Borane, diethyl(decyloxy)- | 226 | C14H31BO | 1000152-34-3 | 76   |
| 5    |    |   | Triacontane, 1-bromo-      | 500 | C30H61Br | 004209-22-7  | 74   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG012524\  
Data File : BG060425.D  
Acq On : 25 Jan 2024 13:00  
Operator : MA/JU  
Sample : PB158620BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

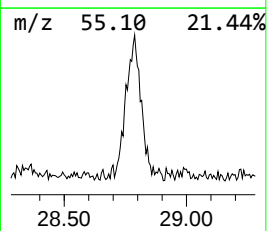
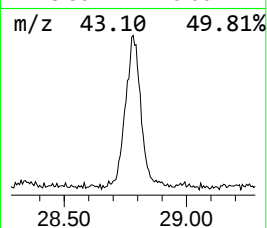
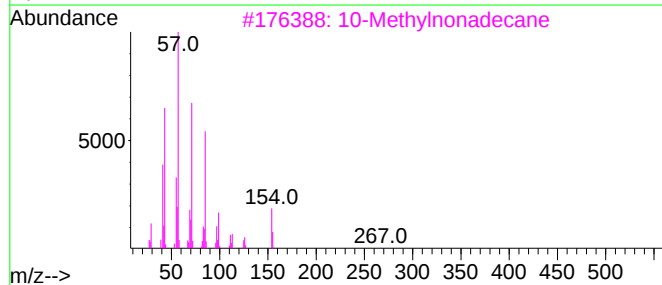
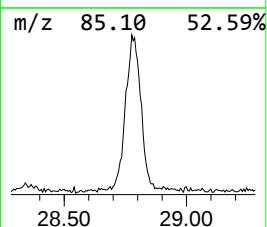
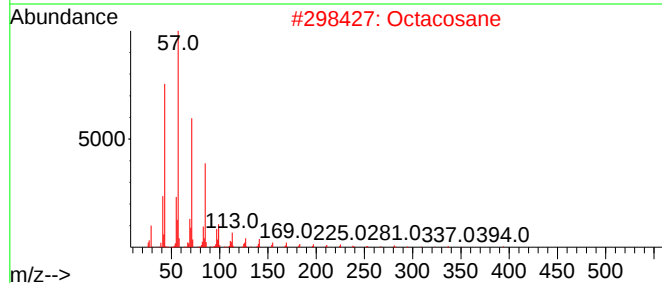
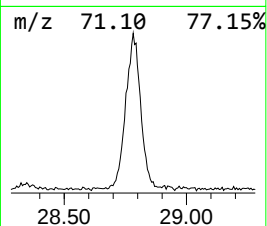
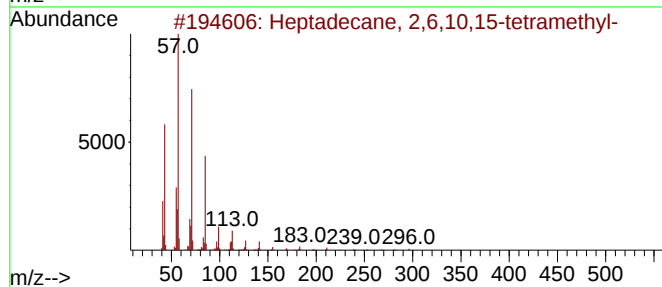
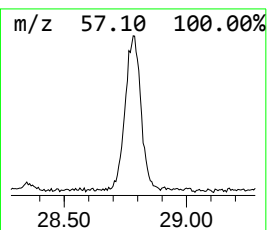
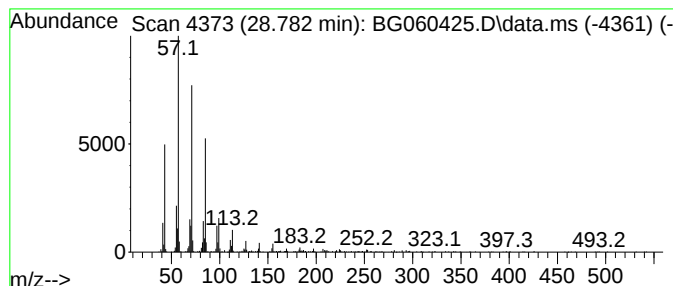
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 3

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 28.782 | 4.71 ng | 1708030 | Perylene-d12     | 24.745 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44  | 054833-48-6  | 93   |
| 2    |    |   | Octacosane                          | 394 | C28H58  | 000630-02-4  | 91   |
| 3    |    |   | 10-Methylnonadecane                 | 282 | C20H42  | 056862-62-5  | 90   |
| 4    |    |   | Heptadecane                         | 240 | C17H36  | 000629-78-7  | 86   |
| 5    |    |   | Tetracosane, 1-iodo-                | 464 | C24H49I | 1000406-32-0 | 86   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG012524\  
Data File : BG060425.D  
Acq On : 25 Jan 2024 13:00  
Operator : MA/JU  
Sample : PB158620BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

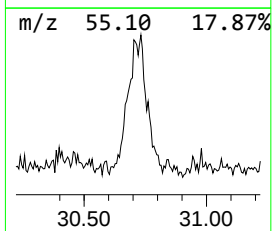
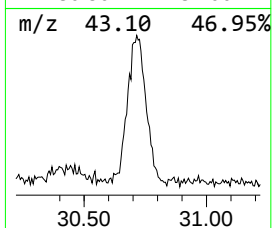
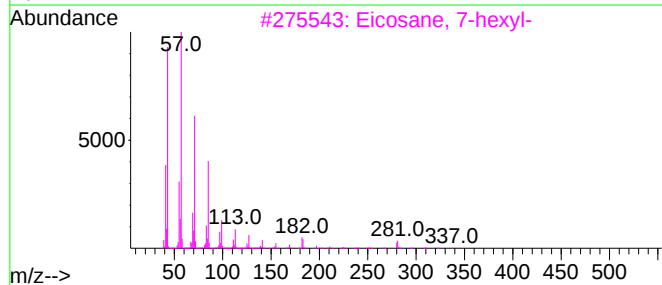
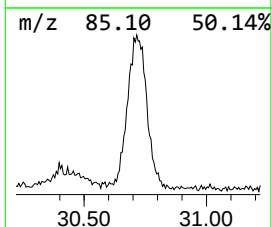
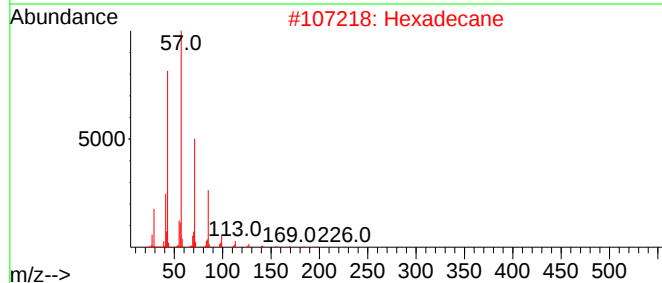
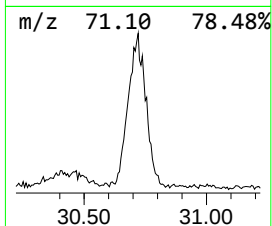
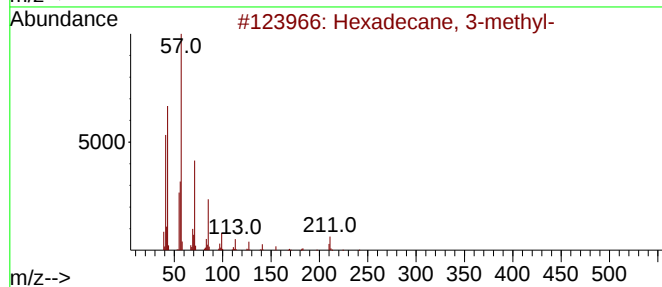
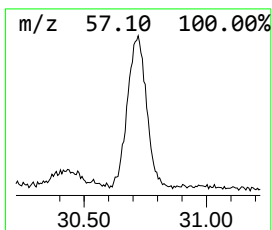
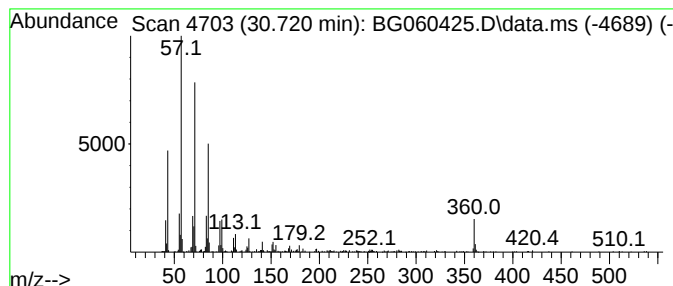
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Hexadecane, 3-methyl- Concentration Rank 4

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 30.721 | 4.47 ng | 1622610 | Perylene-d12     | 24.745 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Hexadecane, 3-methyl- | 240 | C17H36  | 006418-43-5 | 81   |
| 2    |    |   | Hexadecane            | 226 | C16H34  | 000544-76-3 | 74   |
| 3    |    |   | Eicosane, 7-hexyl-    | 366 | C26H54  | 055333-99-8 | 72   |
| 4    |    |   | Heptacosane           | 380 | C27H56  | 000593-49-7 | 72   |
| 5    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG012524\  
Data File : BG060425.D  
Acq On : 25 Jan 2024 13:00  
Operator : MA/JU  
Sample : PB158620BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB158620BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG010824.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 |
| 2-Pentanone, 4-... | 5.033  | 3.5     | ng    | 224856   | 1                     | 7.930  | 1274760 | 20.0 |
| Heptacosane        | 23.029 | 3.4     | ng    | 887208   | 5                     | 21.578 | 5236140 | 20.0 |
| Heptadecane, 9-... | 23.817 | 3.5     | ng    | 1260920  | 6                     | 24.745 | 7252380 | 20.0 |
| Octacosane         | 25.850 | 5.7     | ng    | 2051170  | 6                     | 24.745 | 7252380 | 20.0 |
| Nonadecane         | 27.178 | 6.1     | ng    | 2224240  | 6                     | 24.745 | 7252380 | 20.0 |
| Heptadecane, 2,... | 28.782 | 4.7     | ng    | 1708030  | 6                     | 24.745 | 7252380 | 20.0 |
| Hexadecane, 3-m... | 30.721 | 4.5     | ng    | 1622610  | 6                     | 24.745 | 7252380 | 20.0 |