

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
 Data File : BG057023.D  
 Acq On : 7 Apr 2023 12:31  
 Operator : CG/JU  
 Sample : PB151961BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB151961BL

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057023.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         | 5.429       | 315           | 322         | 329          | rBV      | 139104         | 207325        | 13.47%          | 3.210%        |
| 2         | 5.917       | 398           | 405         | 414          | rBB      | 340971         | 550795        | 35.80%          | 8.528%        |
| 3         | 7.538       | 673           | 681         | 693          | rBB      | 347396         | 600379        | 39.02%          | 9.295%        |
| 4         | 8.408       | 823           | 829         | 837          | rBB      | 55494          | 94436         | 6.14%           | 1.462%        |
| 5         | 9.583       | 1020          | 1029        | 1037         | rBB      | 205156         | 351034        | 22.81%          | 5.435%        |
| 6         | 11.251      | 1306          | 1313        | 1321         | rBB      | 77767          | 134512        | 8.74%           | 2.083%        |
| 7         | 13.648      | 1714          | 1721        | 1729         | rBB      | 579960         | 911708        | 59.25%          | 14.116%       |
| 8         | 15.022      | 1949          | 1955        | 1962         | rVB      | 141842         | 214439        | 13.94%          | 3.320%        |
| 9         | 16.503      | 2201          | 2207        | 2223         | rVB      | 496614         | 748655        | 48.66%          | 11.591%       |
| 10        | 17.766      | 2415          | 2422        | 2428         | rBV      | 188545         | 288047        | 18.72%          | 4.460%        |
| 11        | 20.333      | 2853          | 2859        | 2864         | rBV      | 1210963        | 1538651       | 100.00%         | 23.822%       |
| 12        | 22.083      | 3150          | 3157        | 3165         | rVB      | 170190         | 291120        | 18.92%          | 4.507%        |
| 13        | 23.652      | 3419          | 3424        | 3431         | rVB7     | 11013          | 19922         | 1.29%           | 0.308%        |
| 14        | 24.539      | 3569          | 3575        | 3584         | rVB5     | 16940          | 40089         | 2.61%           | 0.621%        |
| 15        | 25.631      | 3746          | 3761        | 3771         | rVB2     | 87394          | 319461        | 20.76%          | 4.946%        |
| 16        | 26.847      | 3959          | 3968        | 3976         | rVB6     | 19373          | 58568         | 3.81%           | 0.907%        |
| 17        | 28.351      | 4216          | 4224        | 4236         | rVB5     | 19787          | 68969         | 4.48%           | 1.068%        |
| 18        | 30.166      | 4526          | 4533        | 4534         | rBV6     | 11742          | 20779         | 1.35%           | 0.322%        |

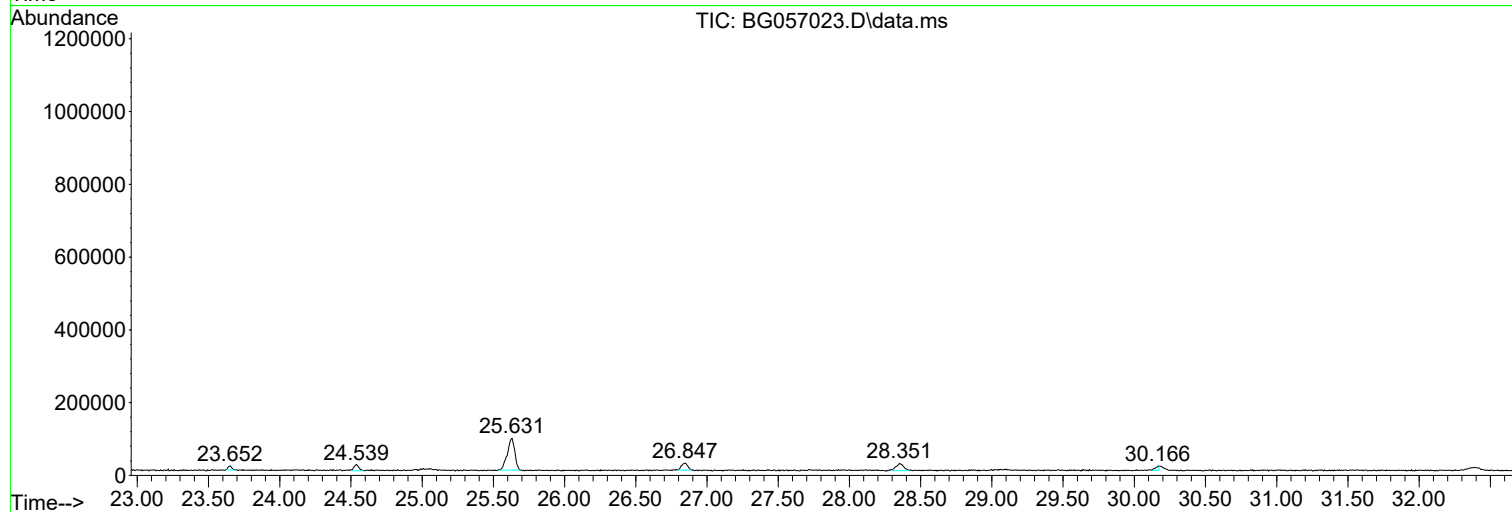
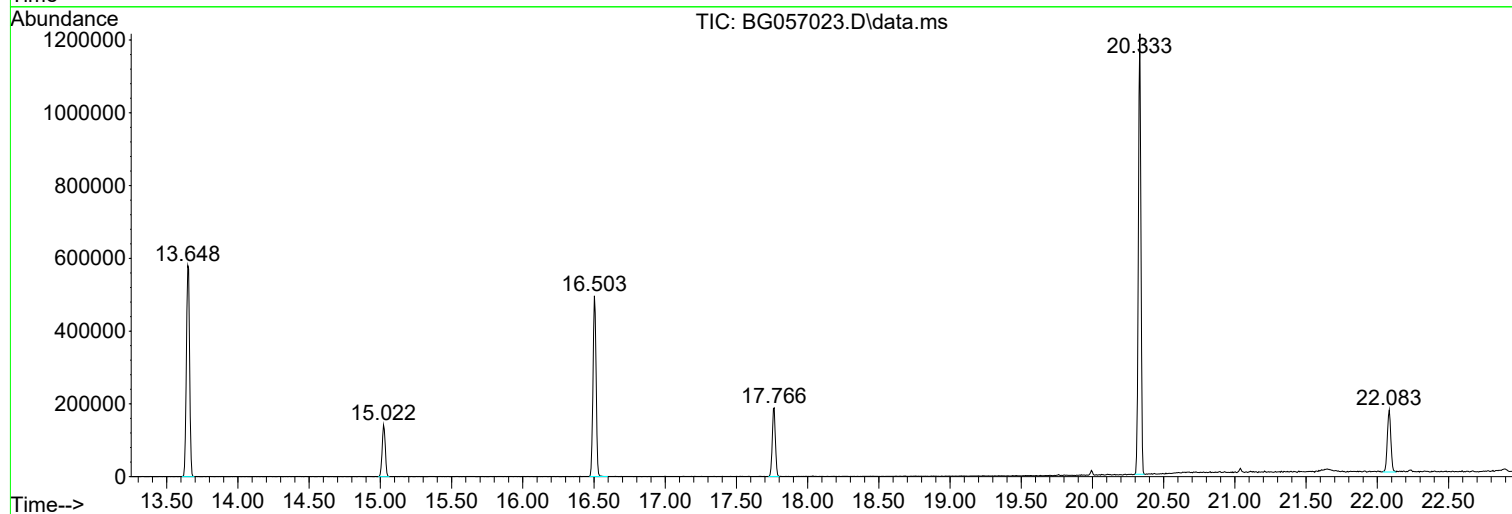
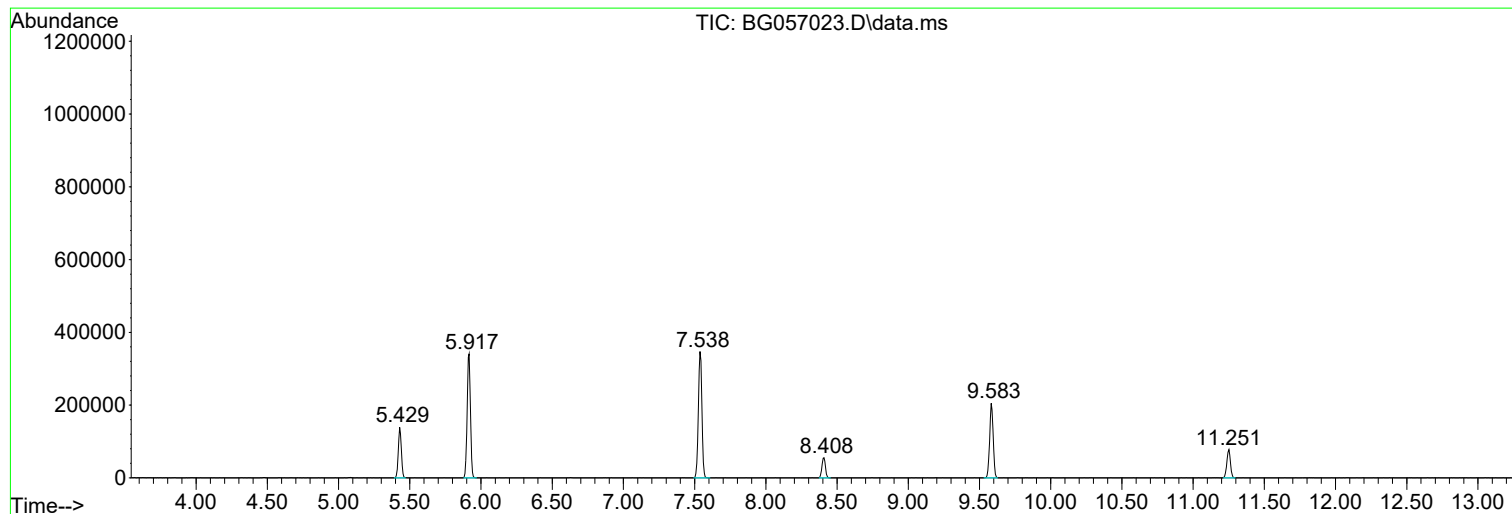
Sum of corrected areas: 6458889

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.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\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

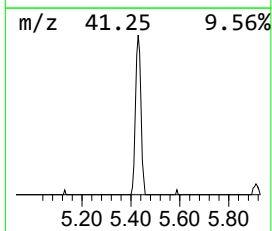
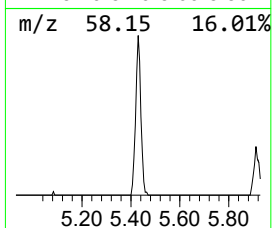
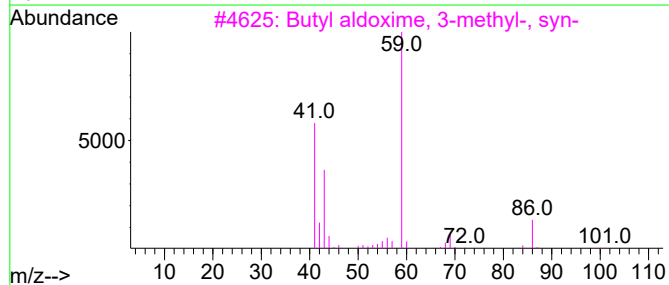
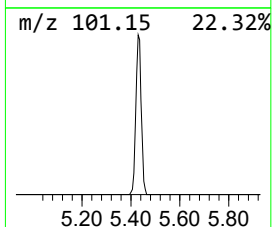
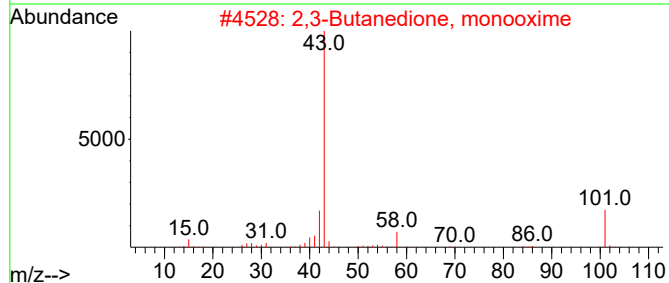
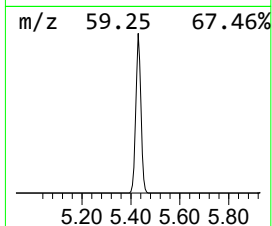
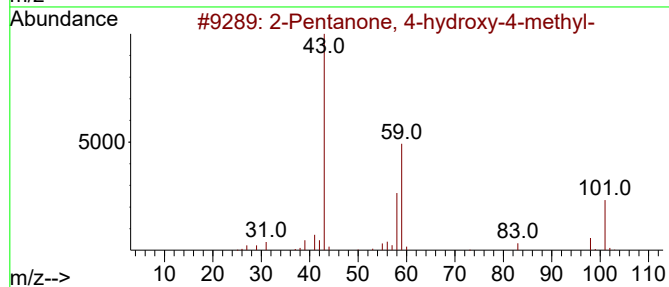
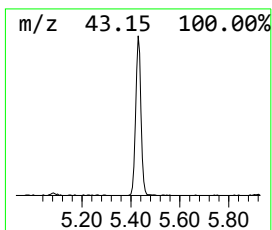
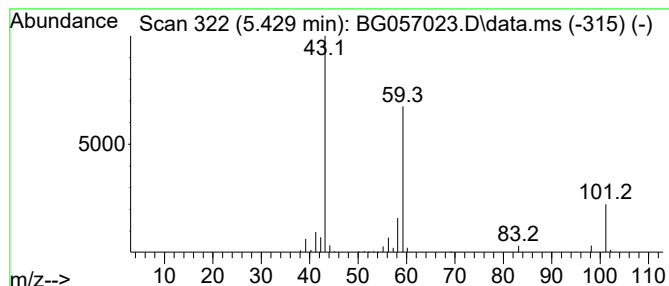
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.429 | 43.91 ng | 207325 | 1,4-Dichlorobenzene-d4 | 8.408 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2      | 000057-71-6 | 35      |      |      |
| 3    | Butyl aldoxime, 3-methyl-, syn-  | 101 | C5H11NO      | 005780-40-5 | 12      |      |      |
| 4    | 1-Propen-2-ol, acetate           | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Acetone                          | 58  | C3H6O        | 000067-64-1 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

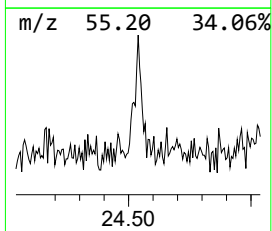
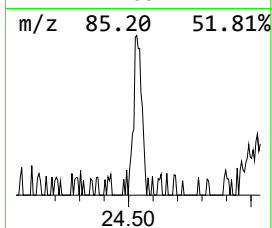
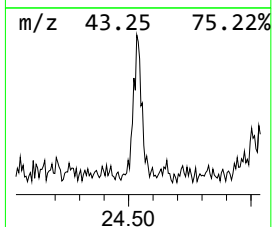
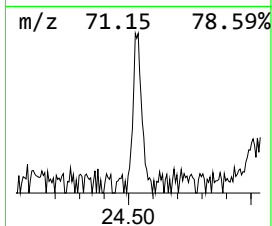
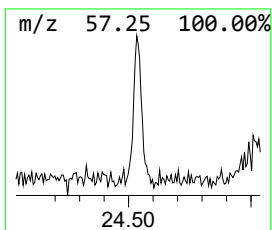
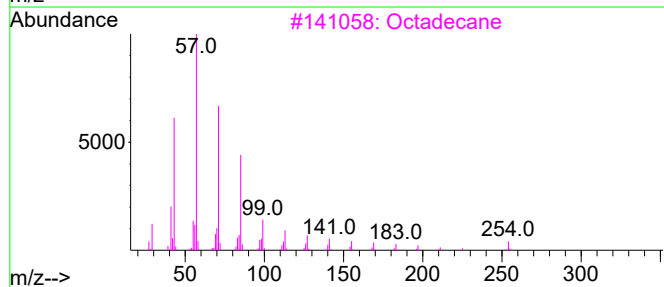
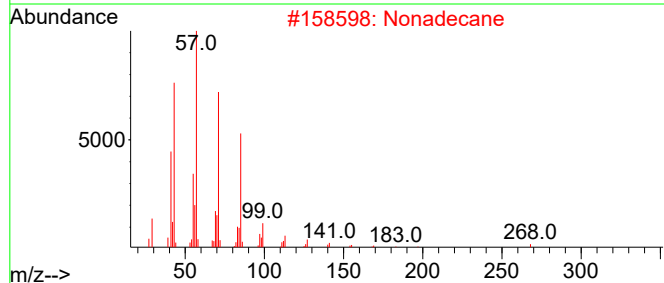
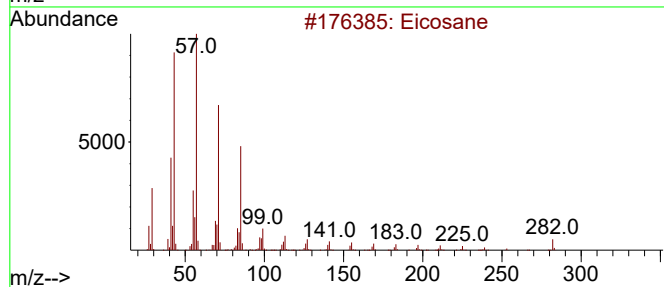
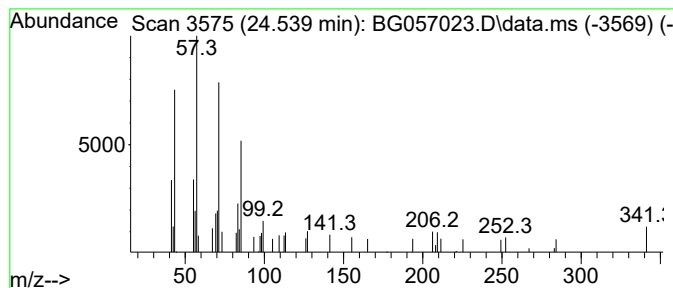
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 Eicosane Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 24.539 | 2.51 ng | 40089 | Perylene-d12     | 25.631 |

| Hit# | of          | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------|---|--------------|-----|---------|-------------|------|
| 1    | Eicosane    |   |              | 282 | C20H42  | 000112-95-8 | 58   |
| 2    | Nonadecane  |   |              | 268 | C19H40  | 000629-92-5 | 58   |
| 3    | Octadecane  |   |              | 254 | C18H38  | 000593-45-3 | 52   |
| 4    | Tricosane   |   |              | 324 | C23H48  | 000638-67-5 | 52   |
| 5    | Heptadecane |   |              | 240 | C17H36  | 000629-78-7 | 52   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

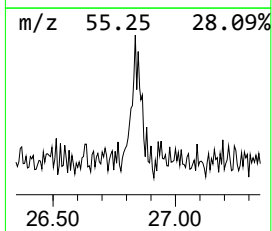
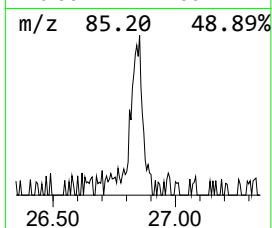
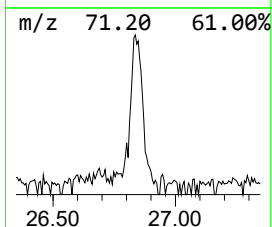
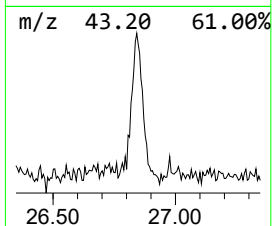
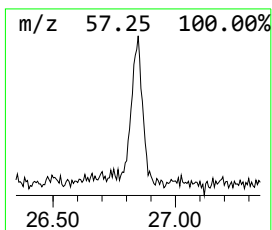
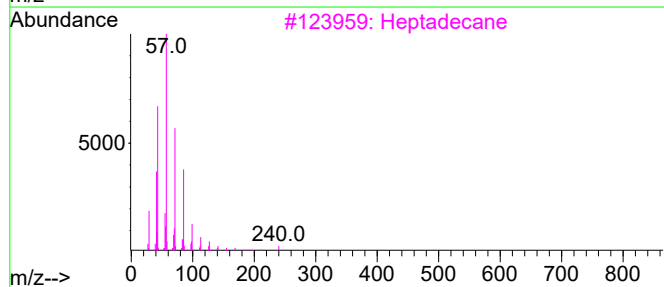
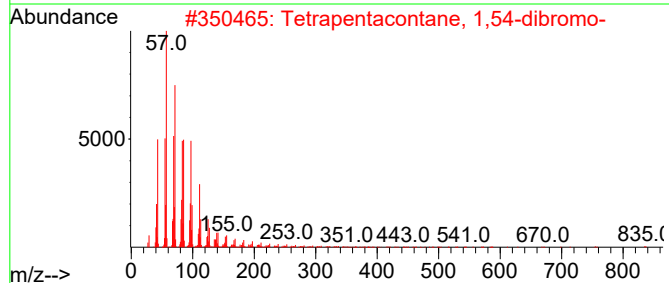
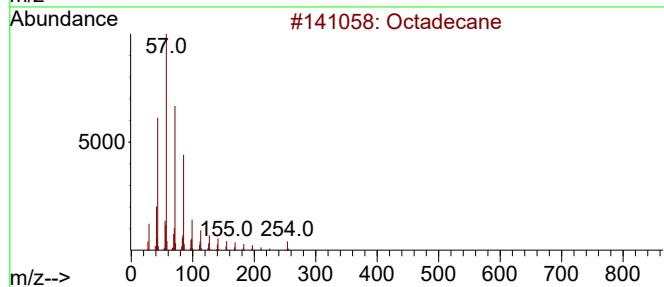
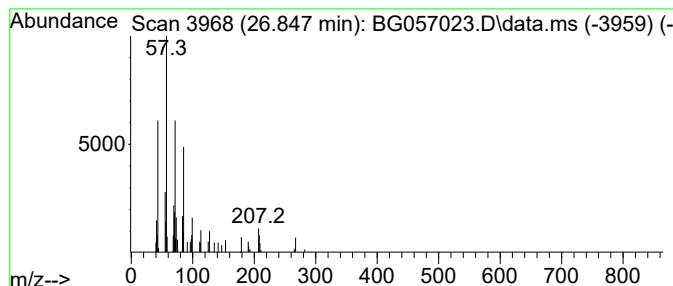
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 Octadecane Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 26.847 | 3.67 ng | 58568 | Perylene-d12     | 25.631 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm    | CAS#         | Qual |
|------|----|---|----------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octadecane                       | 254 | C18H38     | 000593-45-3  | 83   |
| 2    |    |   | Tetrapentacontane, 1,54-dibromo- | 915 | C54H108Br2 | 1000156-09-4 | 80   |
| 3    |    |   | Heptadecane                      | 240 | C17H36     | 000629-78-7  | 80   |
| 4    |    |   | Hexadecane                       | 226 | C16H34     | 000544-76-3  | 80   |
| 5    |    |   | Nonadecane                       | 268 | C19H40     | 000629-92-5  | 80   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

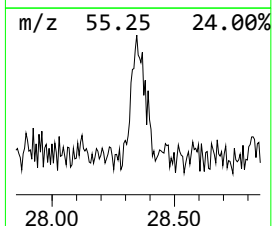
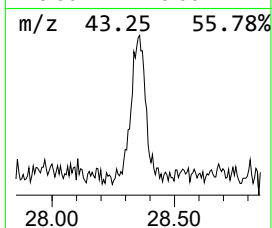
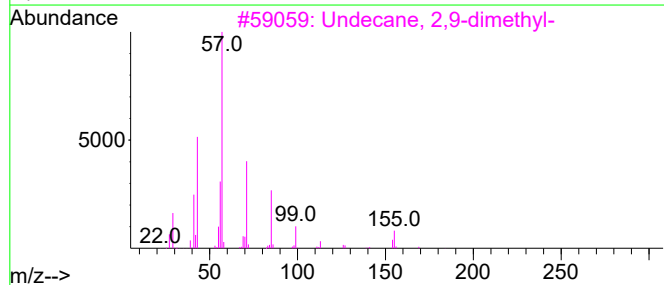
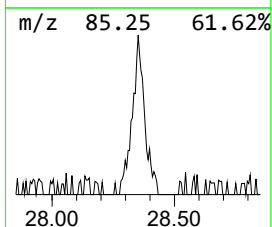
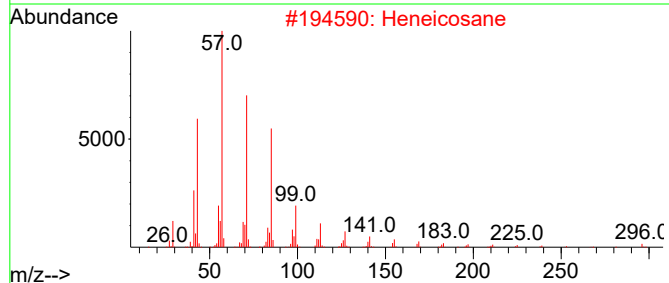
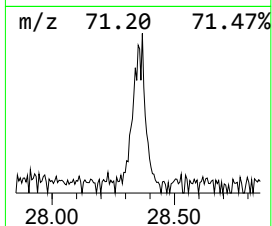
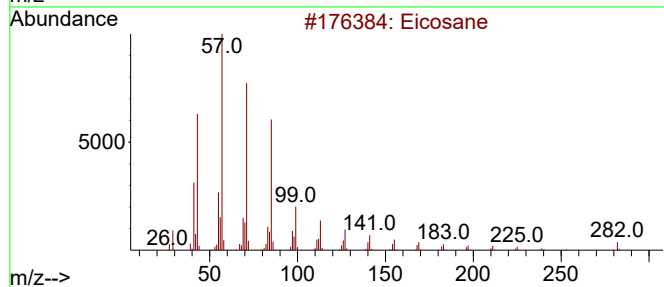
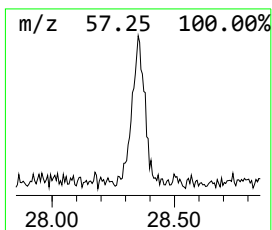
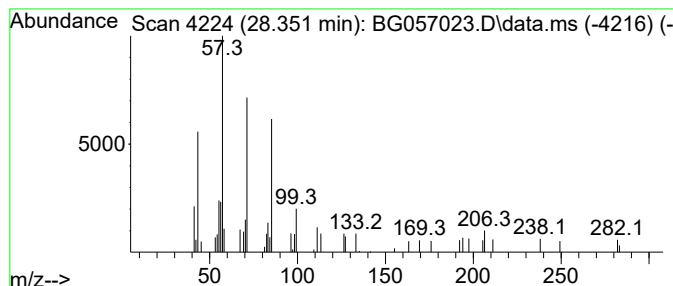
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 Heneicosane Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 28.351 | 4.32 ng | 68969 | Perylene-d12     | 25.631 |

| Hit# | of                      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------------------|---|--------------|-----|---------|-------------|------|
| 1    | Eicosane                |   |              | 282 | C20H42  | 000112-95-8 | 64   |
| 2    | Heneicosane             |   |              | 296 | C21H44  | 000629-94-7 | 53   |
| 3    | Undecane, 2,9-dimethyl- |   |              | 184 | C13H28  | 017301-26-7 | 52   |
| 4    | Octadecane, 2-methyl-   |   |              | 268 | C19H40  | 001560-88-9 | 50   |
| 5    | Decane, 3,8-dimethyl-   |   |              | 170 | C12H26  | 017312-55-9 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG040723\  
Data File : BG057023.D  
Acq On : 7 Apr 2023 12:31  
Operator : CG/JU  
Sample : PB151961BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB151961BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG033023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.429  | 43.9    | ng    | 207325   | 1                     | 8.408  | 94436  | 20.0 |
| Eicosane           | 24.539 | 2.5     | ng    | 40089    | 6                     | 25.631 | 319461 | 20.0 |
| Octadecane         | 26.847 | 3.7     | ng    | 58568    | 6                     | 25.631 | 319461 | 20.0 |
| Heneicosane        | 28.351 | 4.3     | ng    | 68969    | 6                     | 25.631 | 319461 | 20.0 |