

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG080223\  
 Data File : BG058580.D  
 Acq On : 2 Aug 2023 16:06  
 Operator : MA/JU  
 Sample : 03686-10  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-29-2-3-20230721

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058580.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         | 5.388       | 384           | 391         | 404          | rBV      | 756089         | 1232249       | 46.40%          | 7.945%        |
| 2         | 6.986       | 652           | 663         | 678          | rBV      | 733064         | 1306895       | 49.21%          | 8.427%        |
| 3         | 7.808       | 796           | 803         | 813          | rVB      | 179688         | 306970        | 11.56%          | 1.979%        |
| 4         | 8.972       | 994           | 1001        | 1016         | rBV      | 423064         | 789730        | 29.74%          | 5.092%        |
| 5         | 10.611      | 1270          | 1280        | 1289         | rBV      | 245075         | 454260        | 17.11%          | 2.929%        |
| 6         | 13.079      | 1692          | 1700        | 1711         | rBV      | 1164674        | 1817724       | 68.45%          | 11.721%       |
| 7         | 13.913      | 1836          | 1842        | 1854         | rBV      | 179117         | 270548        | 10.19%          | 1.744%        |
| 8         | 14.460      | 1927          | 1935        | 1943         | rBV      | 423028         | 650579        | 24.50%          | 4.195%        |
| 9         | 15.952      | 2182          | 2189        | 2204         | rBV      | 956214         | 1526581       | 57.48%          | 9.843%        |
| 10        | 16.957      | 2353          | 2360        | 2363         | rBV      | 21763          | 29631         | 1.12%           | 0.191%        |
| 11        | 17.203      | 2396          | 2402        | 2408         | rBV      | 528293         | 791996        | 29.82%          | 5.107%        |
| 12        | 17.691      | 2481          | 2485        | 2491         | rVB      | 24910          | 30263         | 1.14%           | 0.195%        |
| 13        | 18.091      | 2548          | 2553        | 2563         | rBV      | 138736         | 240159        | 9.04%           | 1.549%        |
| 14        | 19.260      | 2745          | 2752        | 2764         | rVB      | 38935          | 82792         | 3.12%           | 0.534%        |
| 15        | 19.371      | 2764          | 2771        | 2774         | rBV5     | 32318          | 58787         | 2.21%           | 0.379%        |
| 16        | 19.624      | 2811          | 2814        | 2820         | rVB      | 26362          | 36629         | 1.38%           | 0.236%        |
| 17        | 19.824      | 2842          | 2848        | 2855         | rBV      | 2035047        | 2655666       | 100.00%         | 17.124%       |
| 18        | 21.105      | 3062          | 3066        | 3067         | rBV      | 32037          | 35606         | 1.34%           | 0.230%        |
| 19        | 21.445      | 3117          | 3124        | 3131         | rBV2     | 498800         | 880314        | 33.15%          | 5.676%        |
| 20        | 21.622      | 3151          | 3154        | 3160         | rVB      | 29425          | 41368         | 1.56%           | 0.267%        |
| 21        | 22.198      | 3247          | 3252        | 3256         | rBV      | 49495          | 82737         | 3.12%           | 0.533%        |
| 22        | 22.685      | 3329          | 3335        | 3350         | rBV2     | 85609          | 257517        | 9.70%           | 1.660%        |
| 23        | 22.850      | 3360          | 3363        | 3370         | rVB2     | 29969          | 51650         | 1.94%           | 0.333%        |
| 24        | 23.185      | 3414          | 3420        | 3430         | rVB      | 166638         | 332685        | 12.53%          | 2.145%        |
| 25        | 23.608      | 3487          | 3492        | 3499         | rVB2     | 85957          | 180156        | 6.78%           | 1.162%        |
| 26        | 24.512      | 3636          | 3646        | 3657         | rBV      | 356673         | 1004278       | 37.82%          | 6.476%        |
| 27        | 24.994      | 3723          | 3728        | 3739         | rVB5     | 63250          | 152882        | 5.76%           | 0.986%        |
| 28        | 25.564      | 3818          | 3825        | 3835         | rVB2     | 71254          | 208164        | 7.84%           | 1.342%        |

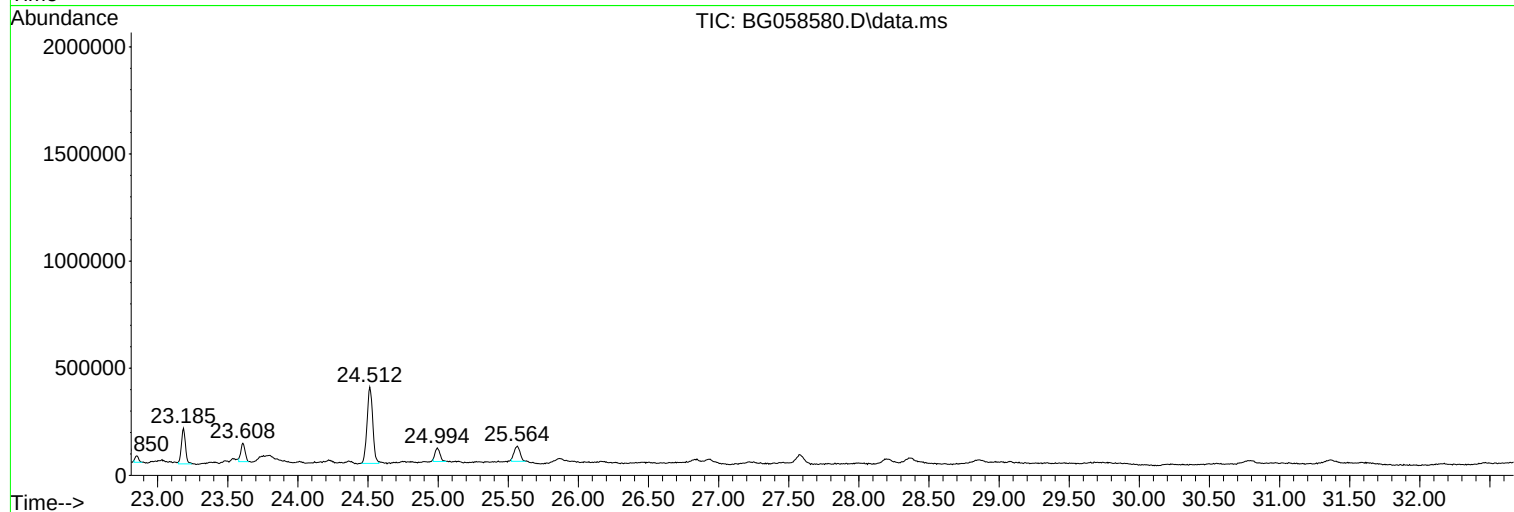
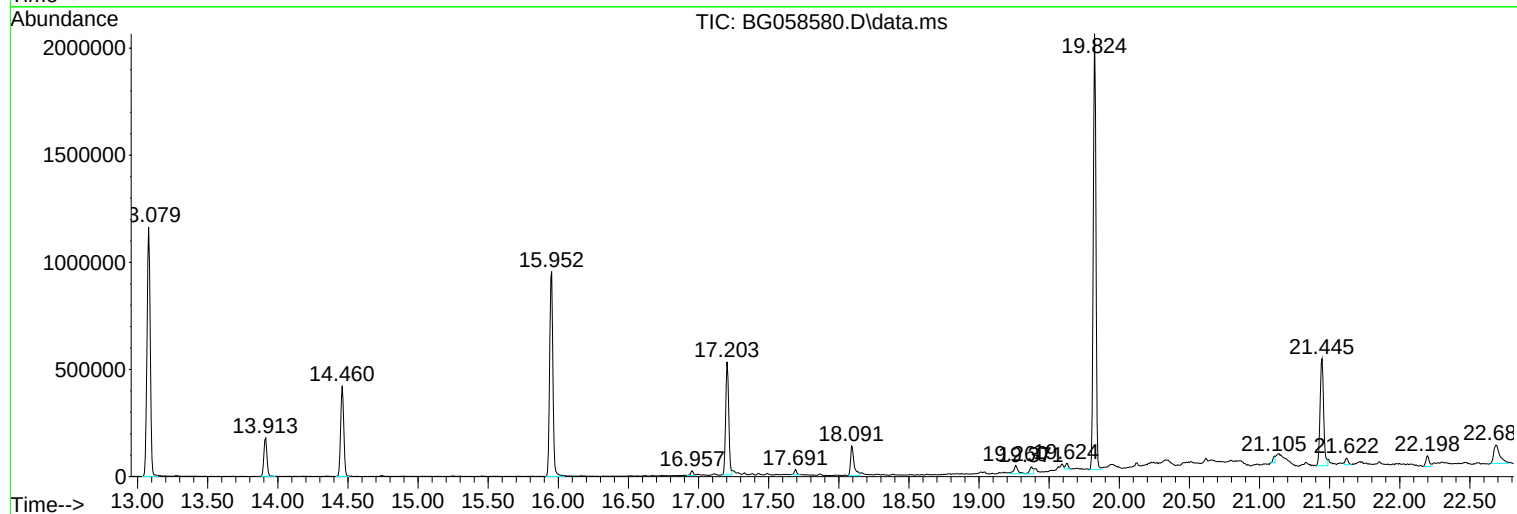
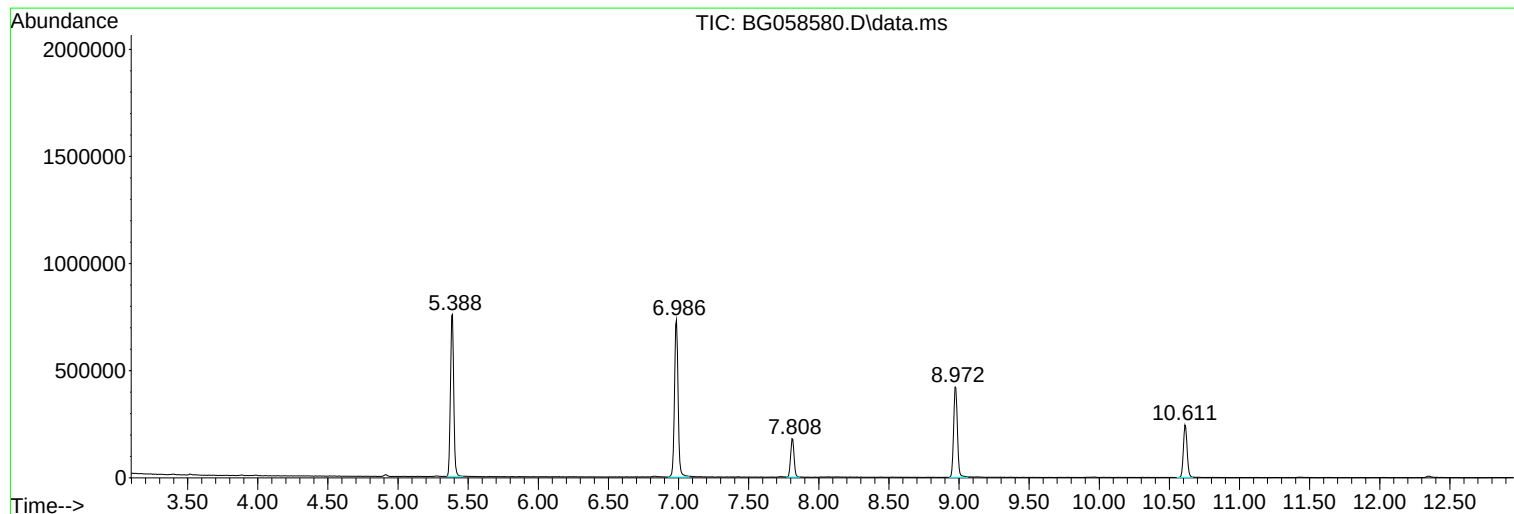
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Instrument :  
BNA\_G  
ClientSampleId :  
SB-29-2-3-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.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\BG080223\  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

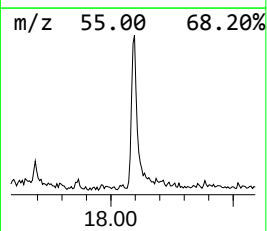
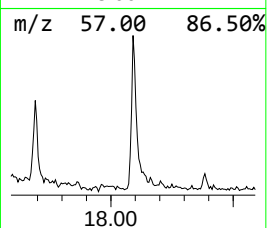
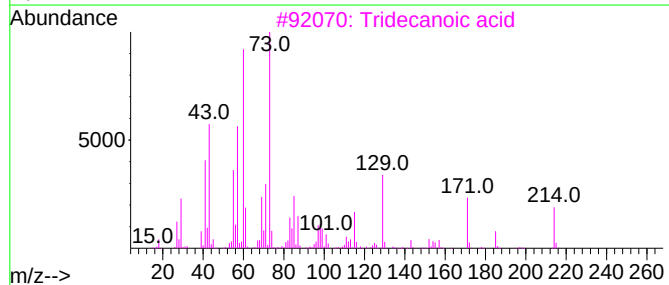
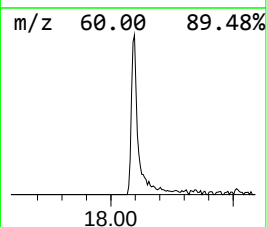
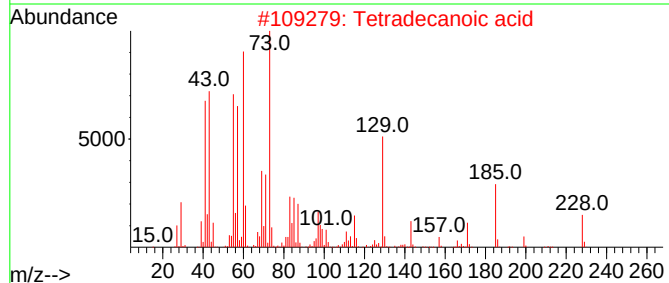
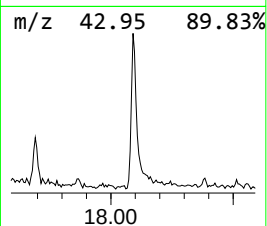
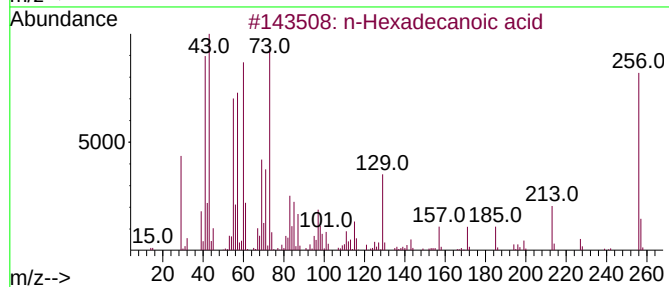
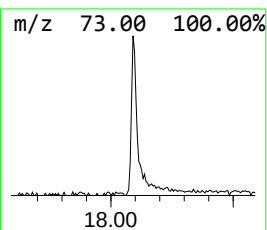
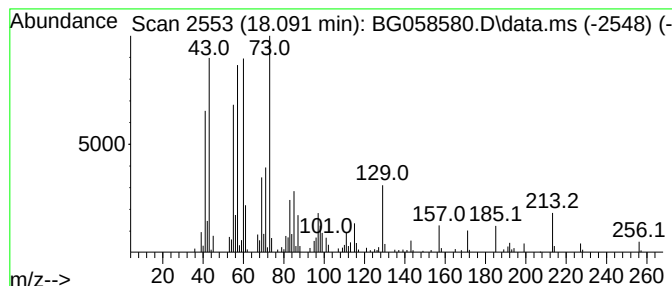
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.091 | 6.06 ng | 240159 | Phenanthrene-d10 | 17.203 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 93   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 87   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 80   |
| 5    |    |   | Nonanoic acid       | 158 | C9H18O2  | 000112-05-0 | 46   |



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Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-29-2-3-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

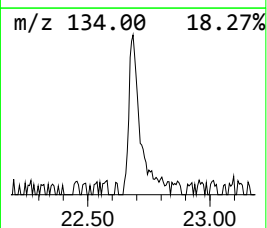
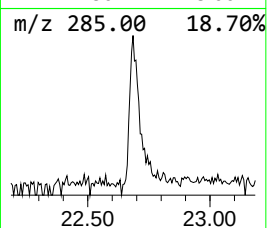
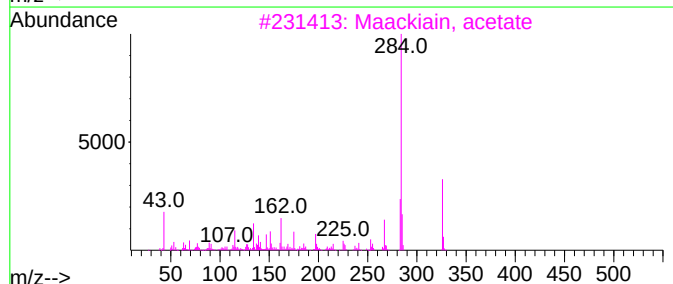
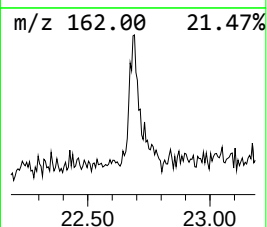
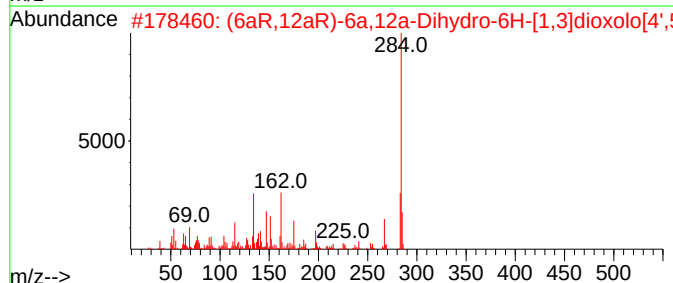
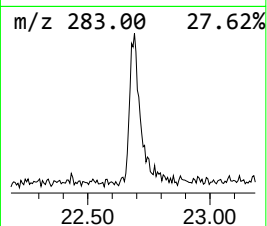
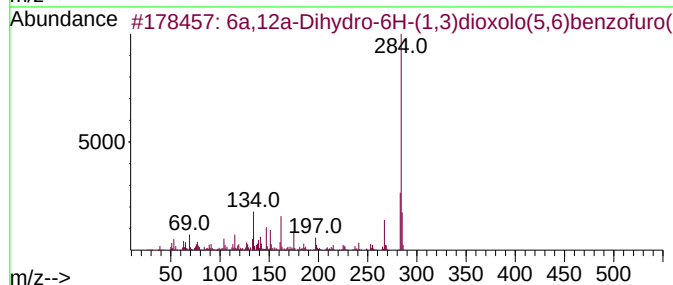
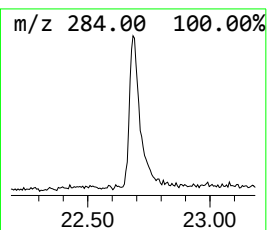
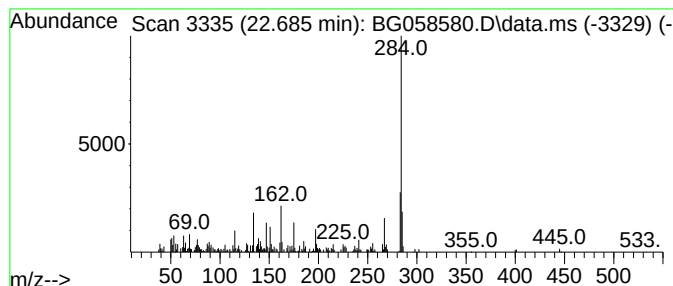
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.685 | 5.85 ng | 257517 | Chrysene-d12     | 21.445 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 6a,12a-Dihydro-6H-(1,3)dioxolo(5... | 284 | C16H12O5 | 076496-57-6  | 96   |
| 2    |    |   | (6aR,12aR)-6a,12a-Dihydro-6H-[1,... | 284 | C16H12O5 | 002035-15-6  | 95   |
| 3    |    |   | Maackiain, acetate                  | 326 | C18H14O6 | 002035-16-7  | 91   |
| 4    |    |   | Dibenz[a,c]cycloheptane, 2,3,7-t... | 284 | C18H20O3 | 054705-02-1  | 55   |
| 5    |    |   | Coumaran-5,6-diol-3-one, 2-[4-me... | 284 | C16H12O5 | 1000129-33-0 | 50   |



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Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-29-2-3-20230721

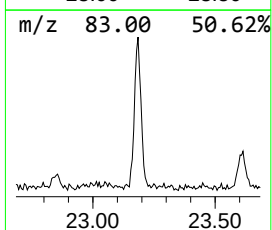
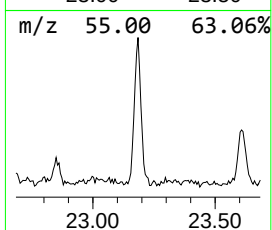
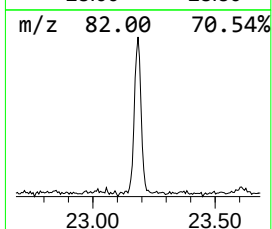
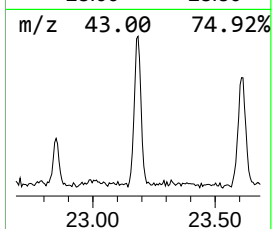
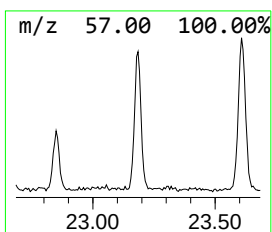
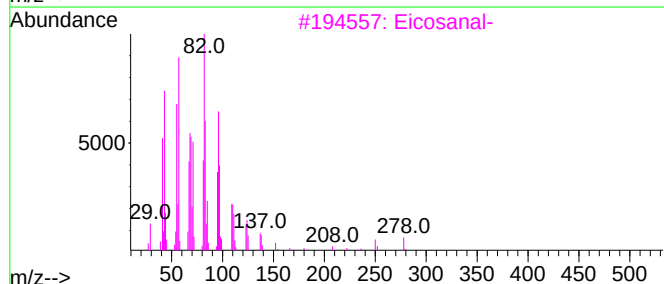
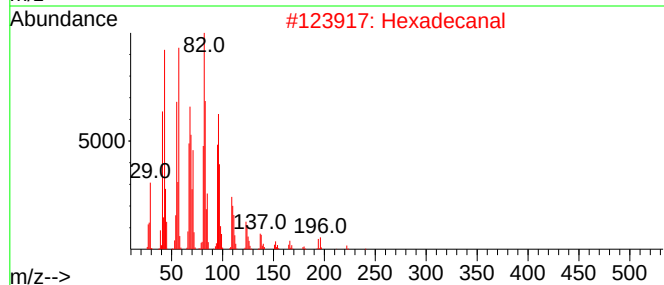
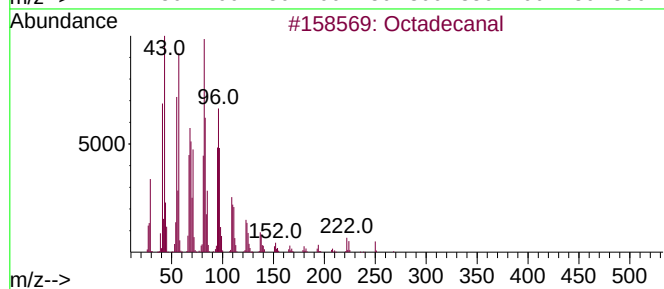
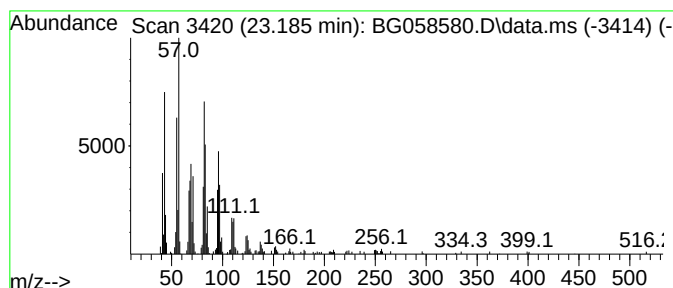
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Octadecanal Concentration Rank 1

| R.T.      | EstConc          | Area   | Relative to ISTD |         | R.T.        |      |
|-----------|------------------|--------|------------------|---------|-------------|------|
| 23.185    | 6.63 ng          | 332685 | Perylene-d12     |         | 24.512      |      |
| Hit# of 5 | Tentative ID     |        | MW               | MolForm | CAS#        | Qual |
| 1         | Octadecanal      |        | 268              | C18H36O | 000638-66-4 | 91   |
| 2         | Hexadecanal      |        | 240              | C16H32O | 000629-80-1 | 90   |
| 3         | Eicosanal-       |        | 296              | C20H40O | 002400-66-0 | 90   |
| 4         | 17-Octadecenal   |        | 266              | C18H34O | 056554-86-0 | 90   |
| 5         | 1,19-Eicosadiene |        | 278              | C20H38  | 014811-95-1 | 87   |



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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

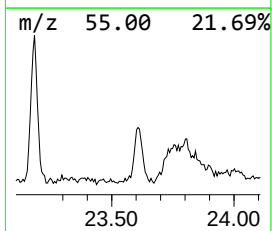
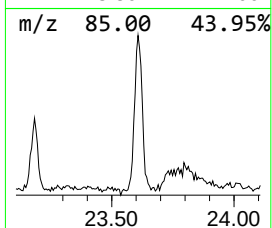
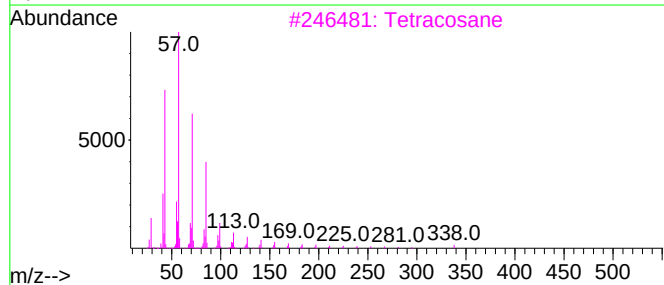
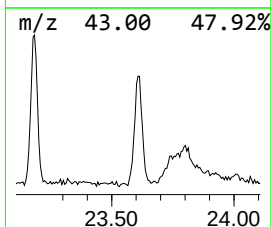
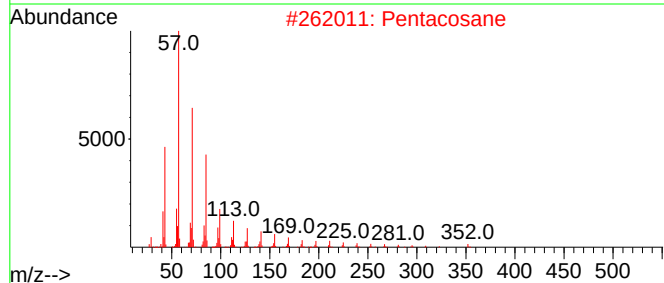
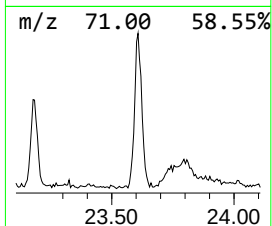
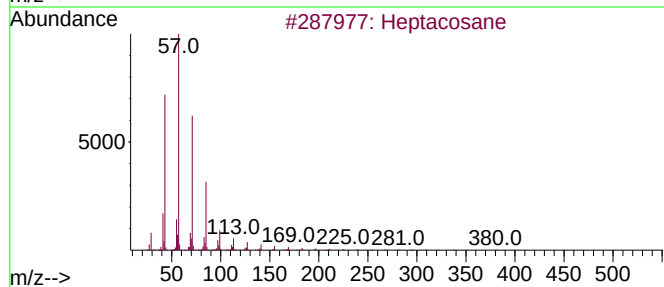
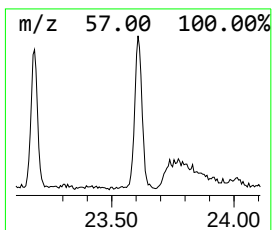
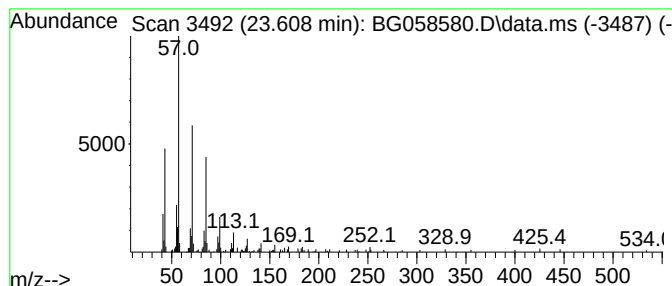
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heptacosane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.608 | 3.59 ng | 180156 | Perylene-d12     | 24.512 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Heptacosane  | 380 | C27H56  | 000593-49-7 | 90   |
| 2    |    |   | Pentacosane  | 352 | C25H52  | 000629-99-2 | 87   |
| 3    |    |   | Tetracosane  | 338 | C24H50  | 000646-31-1 | 87   |
| 4    |    |   | Eicosane     | 282 | C20H42  | 000112-95-8 | 87   |
| 5    |    |   | Docosane     | 310 | C22H46  | 000629-97-0 | 87   |



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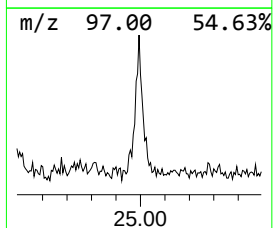
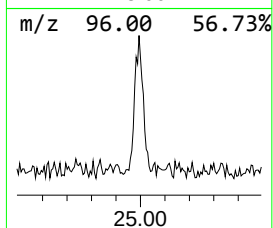
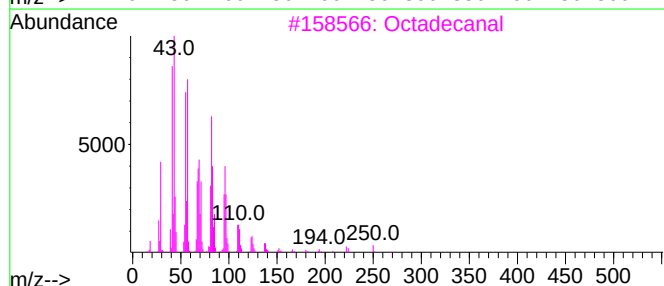
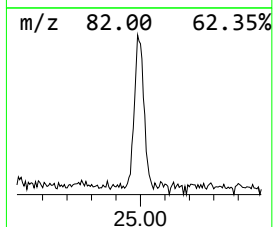
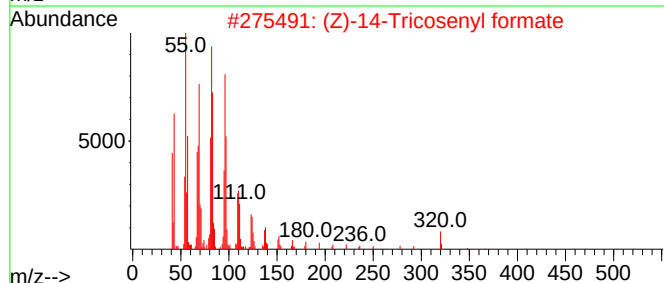
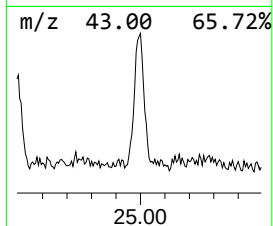
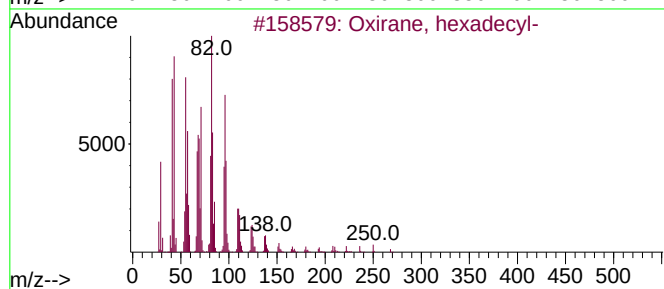
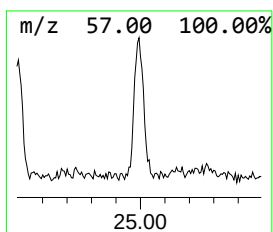
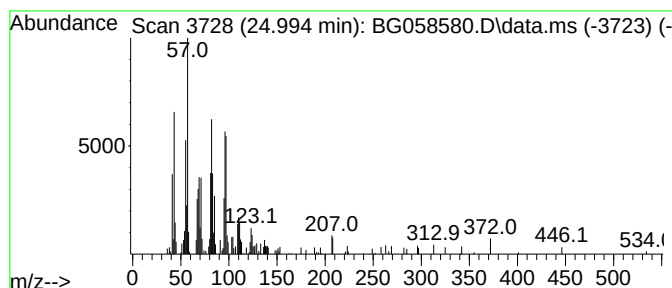
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Oxirane, hexadecyl- Concentration Rank 6

| R.T.      | EstConc                   | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------------|--------|------------------|-------------|------|
| 24.994    | 3.04 ng                   | 152882 | Perylene-d12     | 24.512      |      |
| Hit# of 5 | Tentative ID              | MW     | MolForm          | CAS#        | Qual |
| 1         | Oxirane, hexadecyl-       | 268    | C18H36O          | 007390-81-0 | 62   |
| 2         | (Z)-14-Tricosenyl formate | 366    | C24H46O2         | 077899-10-6 | 58   |
| 3         | Octadecanal               | 268    | C18H36O          | 000638-66-4 | 53   |
| 4         | Oxirane, heptadecyl-      | 282    | C19H38O          | 067860-04-2 | 53   |
| 5         | Eicosanal-                | 296    | C20H40O          | 002400-66-0 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG080223\  
Data File : BG058580.D  
Acq On : 2 Aug 2023 16:06  
Operator : MA/JU  
Sample : 03686-10  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-29-2-3-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

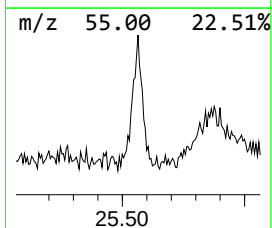
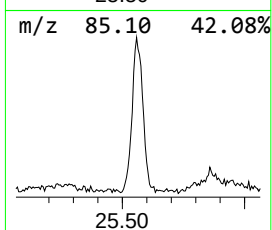
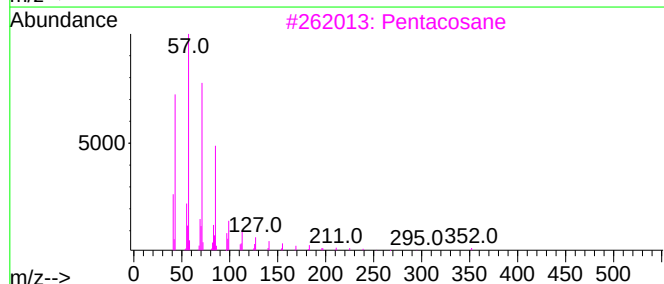
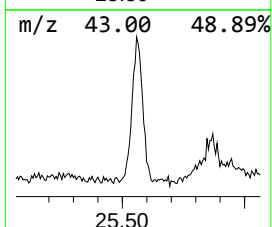
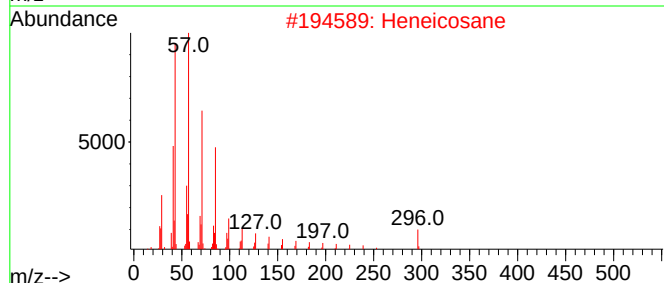
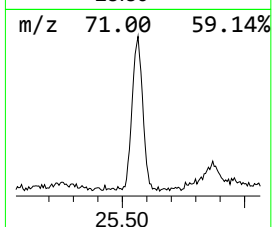
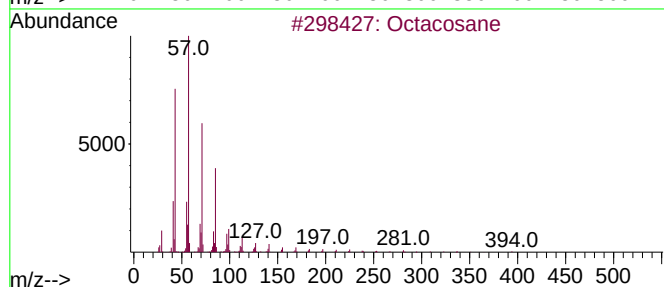
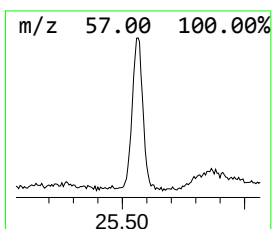
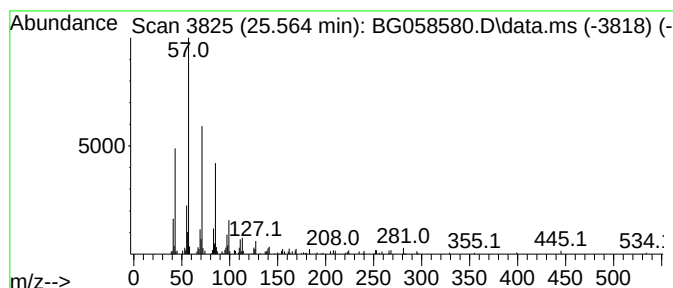
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Octacosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 25.564 | 4.15 ng | 208164 | Perylene-d12     | 24.512 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane           | 394 | C28H58  | 000630-02-4 | 90   |
| 2    |    |   | Heneicosane          | 296 | C21H44  | 000629-94-7 | 90   |
| 3    |    |   | Pentacosane          | 352 | C25H52  | 000629-99-2 | 87   |
| 4    |    |   | Nonadecane           | 268 | C19H40  | 000629-92-5 | 81   |
| 5    |    |   | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 80   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG080223\  
Data File : BG058580.D  
Acq On : 2 Aug 2023 16:06  
Operator : MA/JU  
Sample : 03686-10  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-29-2-3-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.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 |
| n-Hexadecanoic ... | 18.091 | 6.1     | ng    | 240159   | 4                     | 17.203 | 791996  | 20.0 |
| 6a,12a-Dihydro-... | 22.685 | 5.8     | ng    | 257517   | 5                     | 21.445 | 880314  | 20.0 |
| Octadecanal        | 23.185 | 6.6     | ng    | 332685   | 6                     | 24.512 | 1004280 | 20.0 |
| Heptacosane        | 23.608 | 3.6     | ng    | 180156   | 6                     | 24.512 | 1004280 | 20.0 |
| Oxirane, hexade... | 24.994 | 3.0     | ng    | 152882   | 6                     | 24.512 | 1004280 | 20.0 |
| Octacosane         | 25.564 | 4.2     | ng    | 208164   | 6                     | 24.512 | 1004280 | 20.0 |