

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
 Data File : BG051155.D  
 Acq On : 20 Nov 2021 19:58  
 Operator : CG/JU  
 Sample : M4758-33  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP17

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-BG111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051155.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         | 5.744       | 377           | 384         | 393          | rBV      | 397576         | 665598        | 40.67%          | 8.411%        |
| 2         | 7.354       | 649           | 658         | 670          | rBV      | 392800         | 733612        | 44.82%          | 9.271%        |
| 3         | 8.200       | 796           | 802         | 814          | rVB      | 94366          | 162530        | 9.93%           | 2.054%        |
| 4         | 9.381       | 995           | 1003        | 1013         | rBV      | 248844         | 467526        | 28.56%          | 5.908%        |
| 5         | 10.779      | 1233          | 1241        | 1256         | rBV2     | 9961           | 20996         | 1.28%           | 0.265%        |
| 6         | 11.032      | 1277          | 1284        | 1295         | rVB      | 124472         | 230505        | 14.08%          | 2.913%        |
| 7         | 13.452      | 1687          | 1696        | 1708         | rBV      | 611514         | 969076        | 59.21%          | 12.246%       |
| 8         | 14.833      | 1924          | 1931        | 1940         | rVB      | 208735         | 325229        | 19.87%          | 4.110%        |
| 9         | 16.184      | 2153          | 2161        | 2168         | rBV5     | 36438          | 58681         | 3.59%           | 0.742%        |
| 10        | 16.325      | 2178          | 2185        | 2197         | rBV      | 480421         | 765954        | 46.80%          | 9.679%        |
| 11        | 17.454      | 2372          | 2377        | 2384         | rVB2     | 15197          | 19878         | 1.21%           | 0.251%        |
| 12        | 17.583      | 2393          | 2399        | 2405         | rBV      | 272068         | 421987        | 25.78%          | 5.333%        |
| 13        | 18.211      | 2501          | 2506        | 2512         | rVB2     | 13507          | 19302         | 1.18%           | 0.244%        |
| 14        | 19.821      | 2775          | 2780        | 2783         | rVB4     | 11798          | 18110         | 1.11%           | 0.229%        |
| 15        | 20.174      | 2834          | 2840        | 2846         | rBV      | 1262861        | 1636775       | 100.00%         | 20.684%       |
| 16        | 21.437      | 3050          | 3055        | 3056         | rBV      | 16650          | 21112         | 1.29%           | 0.267%        |
| 17        | 21.466      | 3056          | 3060        | 3065         | rVV      | 52933          | 91897         | 5.61%           | 1.161%        |
| 18        | 21.572      | 3074          | 3078        | 3085         | rVB      | 52373          | 80933         | 4.94%           | 1.023%        |
| 19        | 21.884      | 3124          | 3131        | 3139         | rBV      | 281002         | 480409        | 29.35%          | 6.071%        |
| 20        | 22.036      | 3154          | 3157        | 3161         | rVB3     | 11846          | 16846         | 1.03%           | 0.213%        |
| 21        | 22.665      | 3260          | 3264        | 3269         | rBV2     | 15229          | 26450         | 1.62%           | 0.334%        |
| 22        | 23.388      | 3384          | 3387        | 3393         | rVB5     | 13512          | 22173         | 1.35%           | 0.280%        |
| 23        | 24.240      | 3524          | 3532        | 3539         | rBV2     | 28985          | 64904         | 3.97%           | 0.820%        |
| 24        | 25.280      | 3698          | 3709        | 3720         | rVB3     | 152907         | 481581        | 29.42%          | 6.086%        |
| 25        | 26.425      | 3896          | 3904        | 3916         | rVB5     | 36875          | 111241        | 6.80%           | 1.406%        |

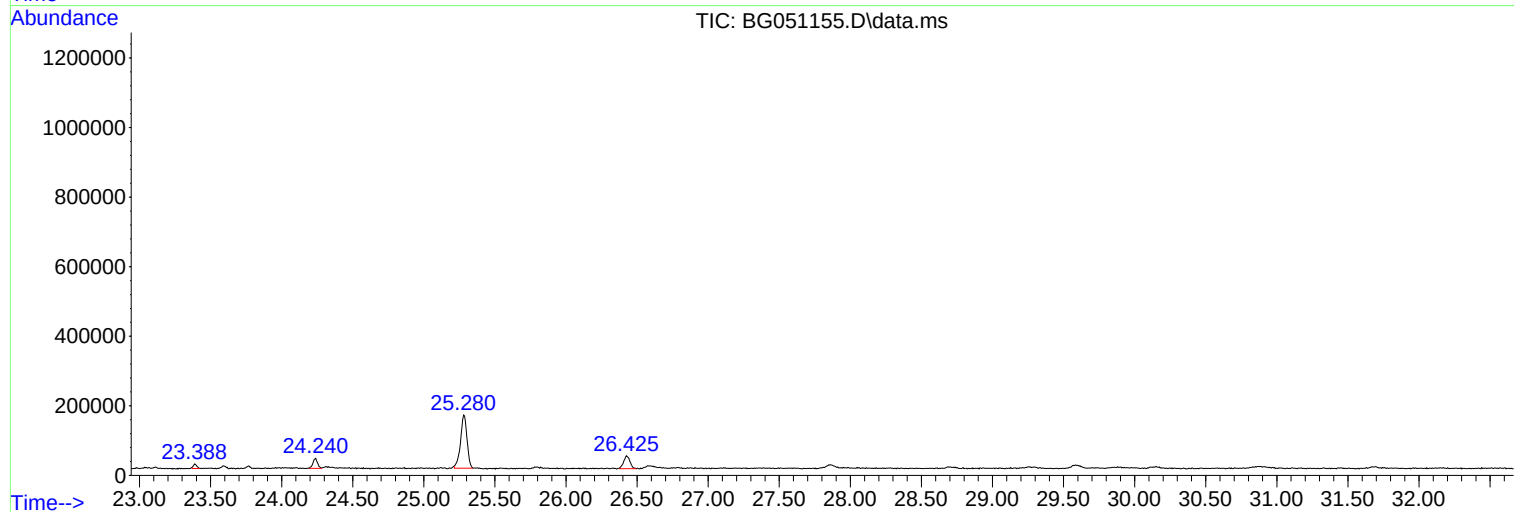
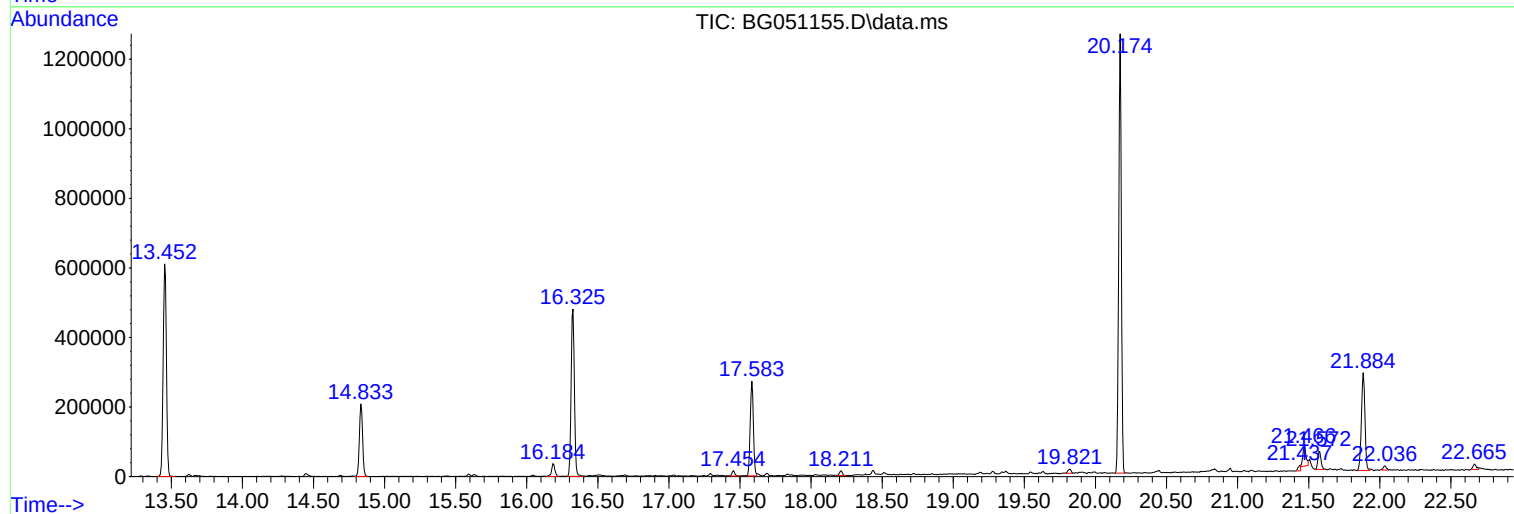
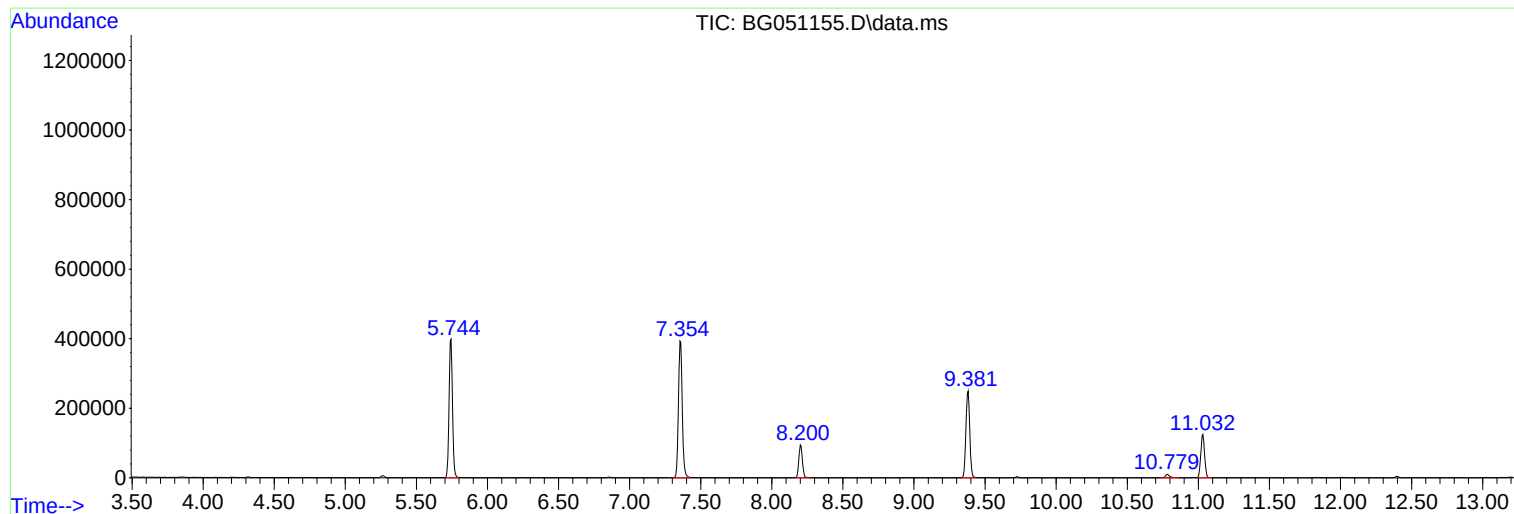
Sum of corrected areas: 7913305

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.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\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

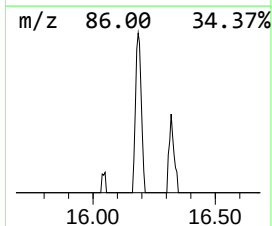
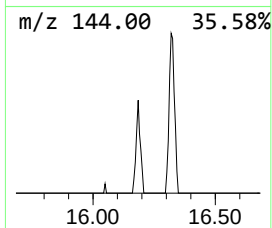
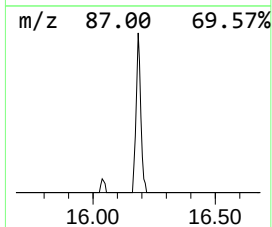
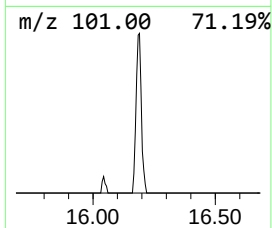
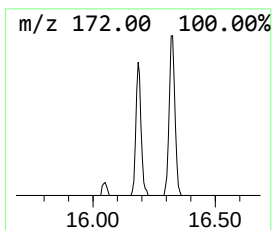
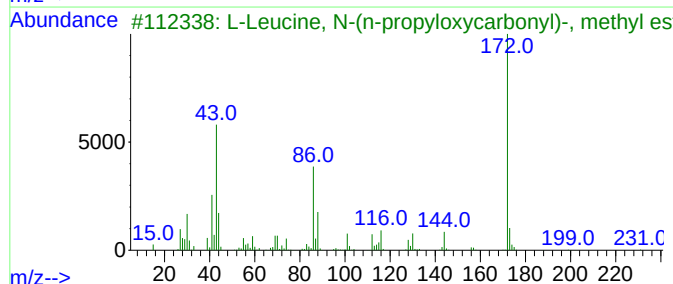
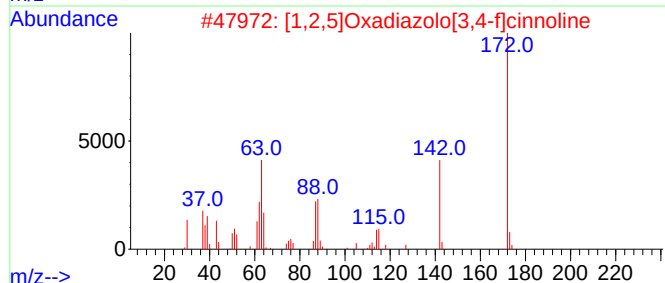
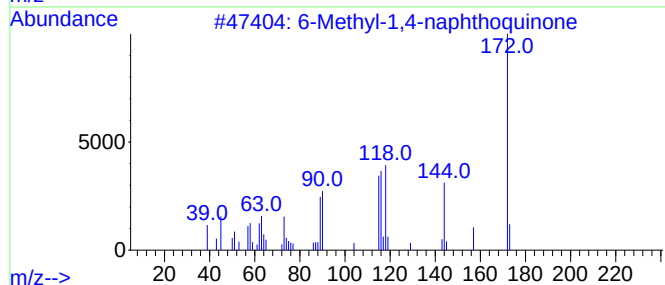
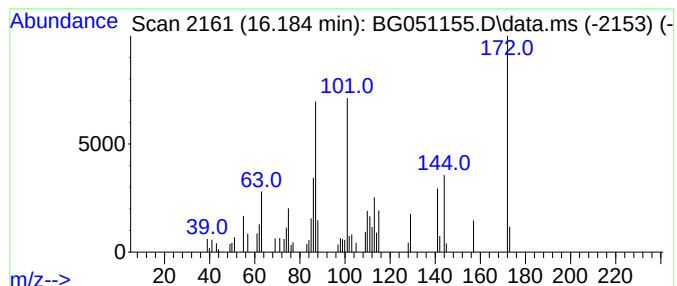
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 1 unknown16.184 Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.184 | 3.61 ng | 58681 | Acenaphthene-d10 | 14.833 |

| Hit# | of | 5 | Tentative ID                                   | MW  | MolForm   | CAS#         | Qual |
|------|----|---|------------------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 6-Methyl-1,4-naphthoquinone                    | 172 | C11H8O2   | 000605-93-6  | 38   |
| 2    |    |   | [1,2,5]Oxadiazolo[3,4-f]cinnoline              | 172 | C8H4N4O   | 217491-04-8  | 35   |
| 3    |    |   | L-Leucine, N-(n-propyloxycarbonyl)-, methyl es | 231 | C11H21NO4 | 1000452-30-4 | 22   |
| 4    |    |   | 11-Methyl-2,7-diazatricyclo[6.4.0.0            | 172 | C11H12N2  | 059007-79-3  | 22   |
| 5    |    |   | DL-Norleucine, N-propoxycarbonyl-              | 343 | C19H37NO4 | 1000339-03-2 | 14   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

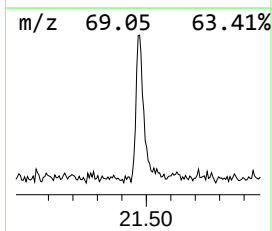
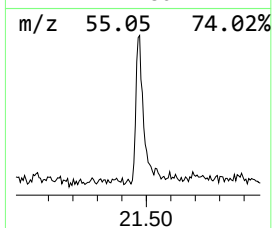
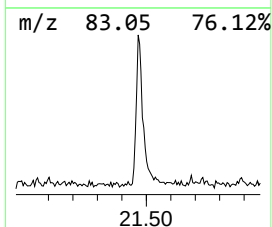
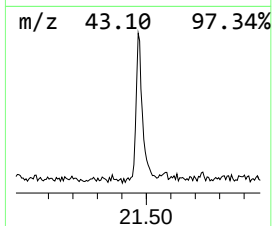
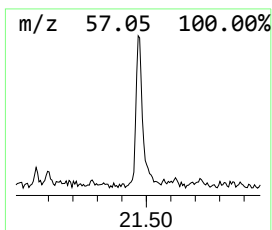
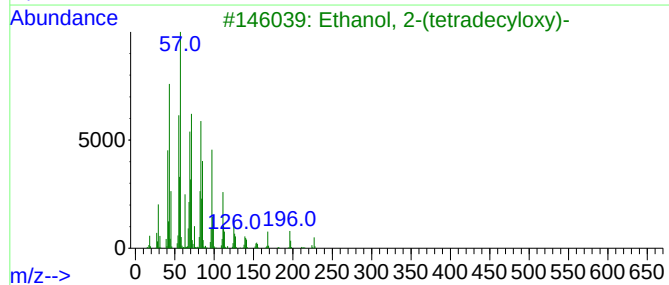
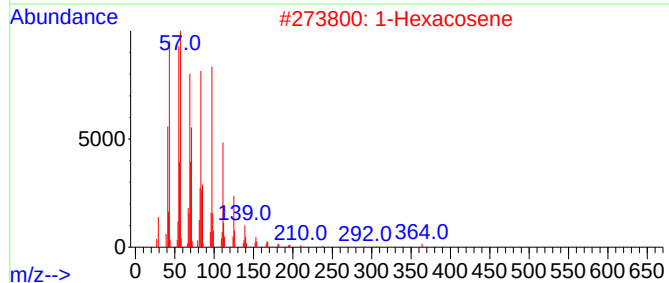
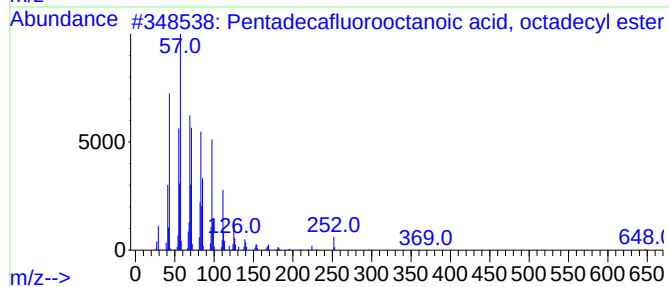
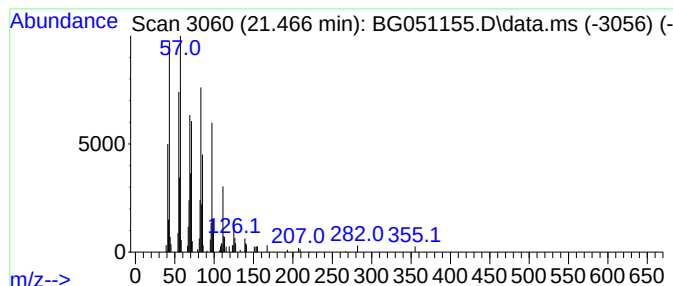
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 2

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 21.467    | 3.83 ng                             | 91897 | Chrysene-d12     | 21.884       |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | Pentadecafluorooctanoic acid, oc... | 666   | C26H37F15O2      | 1000406-04-8 | 93   |
| 2         | 1-Hexacosene                        | 364   | C26H52           | 018835-33-1  | 93   |
| 3         | Ethanol, 2-(tetradecyloxy)-         | 258   | C16H34O2         | 002136-70-1  | 91   |
| 4         | 17-Pentatriacontene                 | 491   | C35H70           | 006971-40-0  | 90   |
| 5         | Dichloroacetic acid, heptadecyl ... | 366   | C19H36Cl2O2      | 1000282-98-2 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

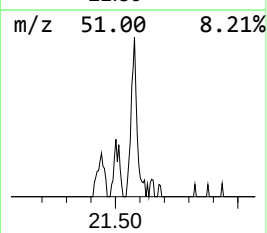
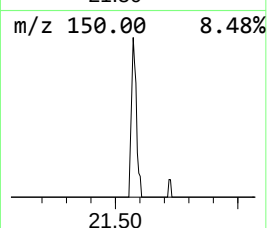
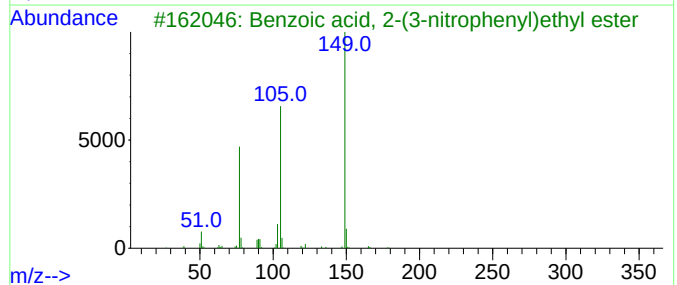
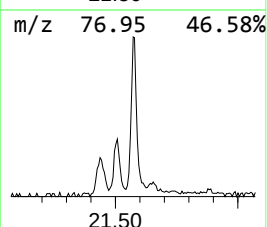
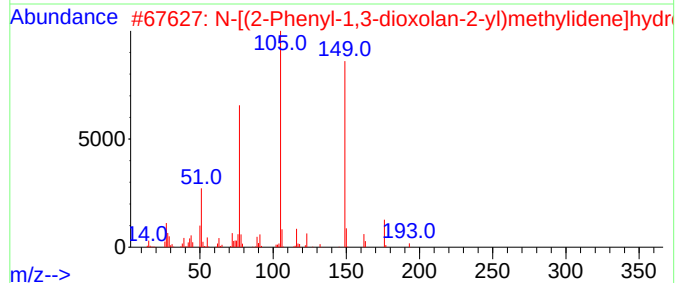
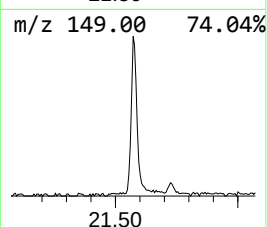
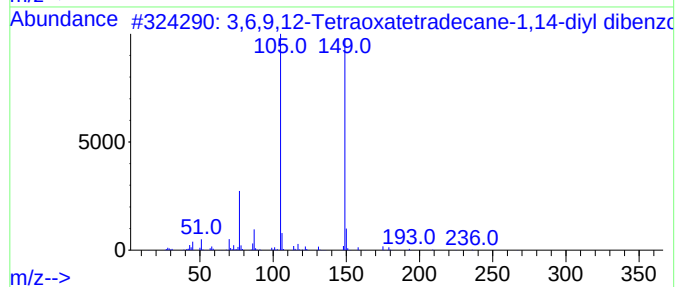
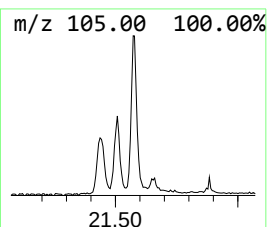
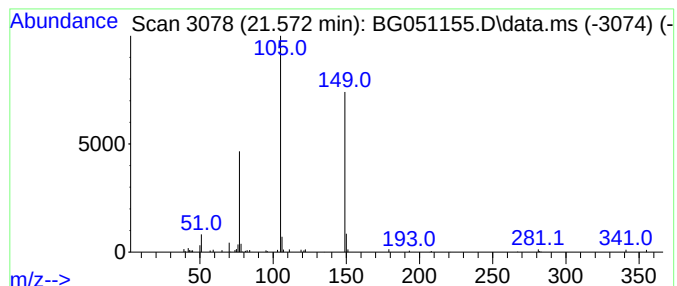
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 3,6,9,12-Tetraoxatetradecan... Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.572 | 3.37 ng | 80933 | Chrysene-d12     | 21.884 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 3,6,9,12-Tetraoxatetradecane-1,1... | 446 | C24H30O8     | 1000366-97-0 | 78      |      |      |
| 2    | N-[(2-Phenyl-1,3-dioxolan-2-yl)m... | 193 | C10H11NO3    | 1000411-48-9 | 78      |      |      |
| 3    | Benzoic acid, 2-(3-nitrophenyl)e... | 271 | C15H13NO4    | 1000368-22-4 | 78      |      |      |
| 4    | Phenyl(2-phenyl-1,3-dioxolan-2-y... | 270 | C17H18O3     | 1000507-07-6 | 78      |      |      |
| 5    | Phenyl(2-phenyl-1,3-dioxolan-2-y... | 256 | C16H16O3     | 005694-69-9  | 78      |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

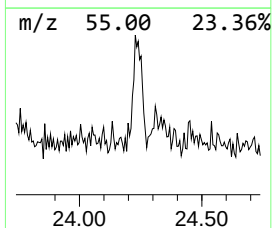
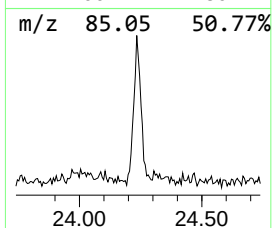
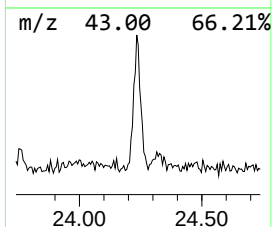
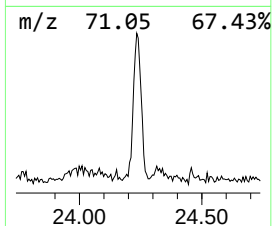
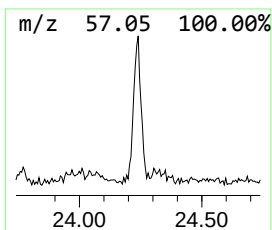
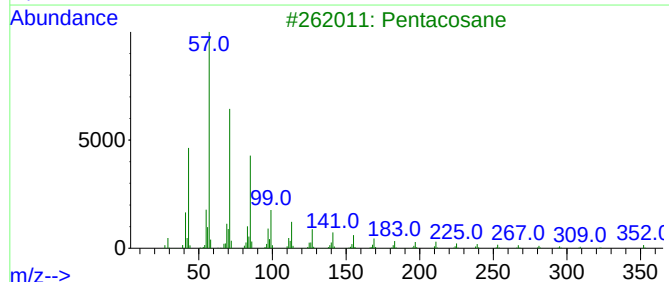
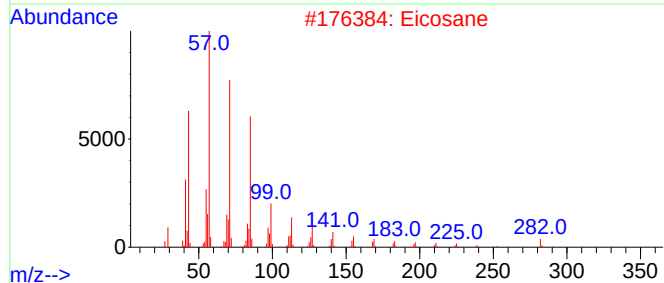
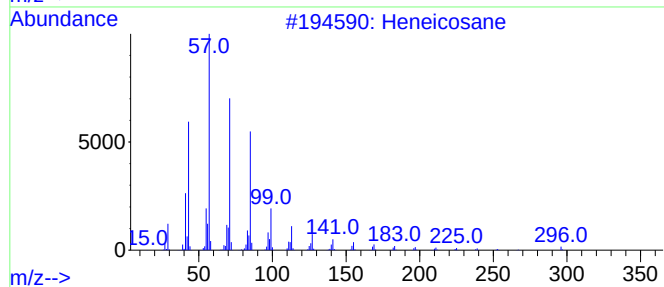
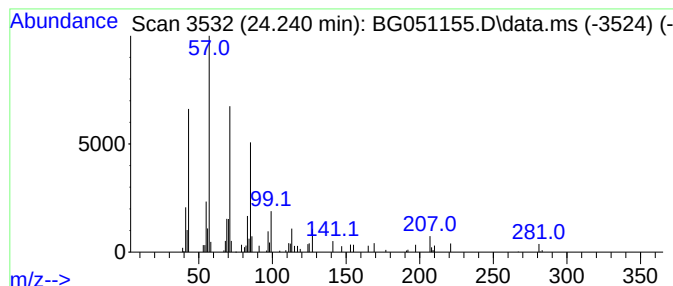
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 4 Heneicosane Concentration Rank 5

| R.T.      | EstConc           | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------|-------|------------------|--------------|------|
| 24.240    | 2.70 ng           | 64904 | Perylene-d12     | 25.280       |      |
| Hit# of 5 | Tentative ID      | MW    | MolForm          | CAS#         | Qual |
| 1         | Heneicosane       | 296   | C21H44           | 000629-94-7  | 90   |
| 2         | Eicosane          | 282   | C20H42           | 000112-95-8  | 87   |
| 3         | Pentacosane       | 352   | C25H52           | 000629-99-2  | 86   |
| 4         | Eicosane, 1-iodo- | 408   | C20H41I          | 1000406-31-8 | 86   |
| 5         | Docosane          | 310   | C22H46           | 000629-97-0  | 86   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

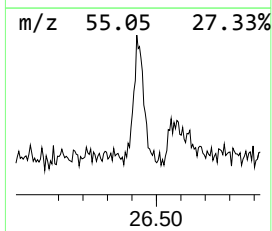
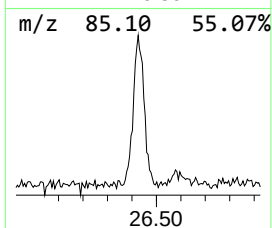
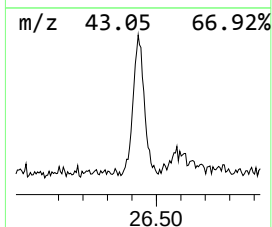
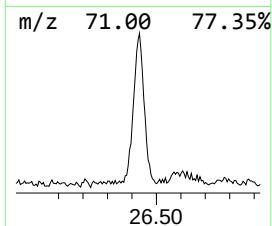
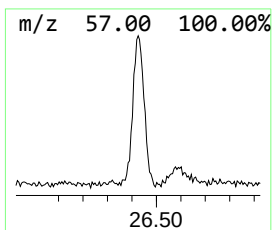
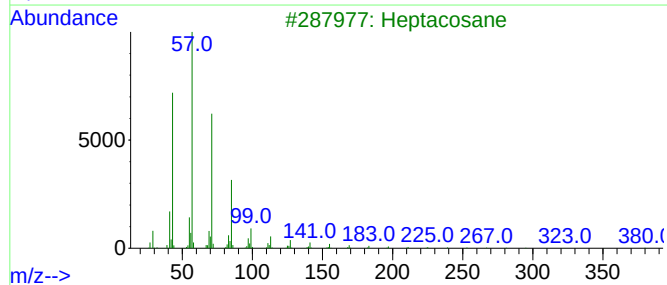
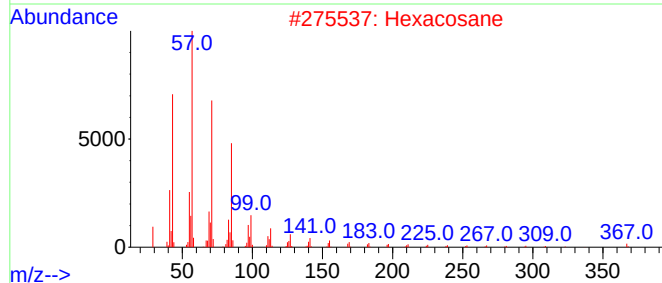
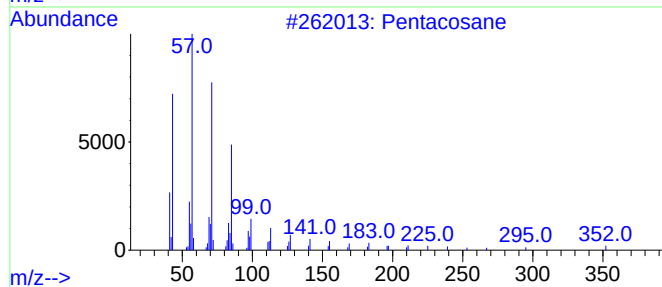
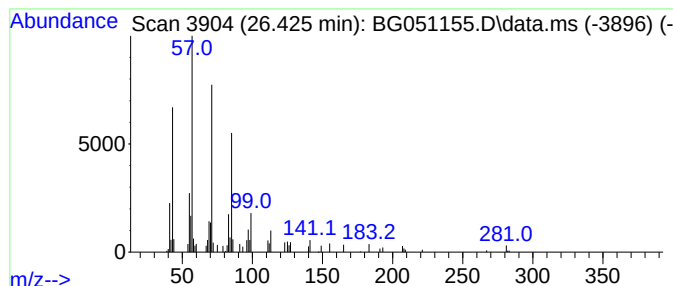
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 Pentacosane Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 26.425 | 4.62 ng | 111241 | Perylene-d12     | 25.280 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Pentacosane  | 352 | C25H52  | 000629-99-2 | 91   |
| 2    |    |   | Hexacosane   | 366 | C26H54  | 000630-01-3 | 91   |
| 3    |    |   | Heptacosane  | 380 | C27H56  | 000593-49-7 | 90   |
| 4    |    |   | Eicosane     | 282 | C20H42  | 000112-95-8 | 87   |
| 5    |    |   | Heneicosane  | 296 | C21H44  | 000629-94-7 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051155.D  
Acq On : 20 Nov 2021 19:58  
Operator : CG/JU  
Sample : M4758-33  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.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 |
| unknown16.184      | 16.184 | 3.6     | ng    | 58681    | 3                     | 14.833 | 325229 | 20.0 |
| Pentadecafluoro... | 21.467 | 3.8     | ng    | 91897    | 5                     | 21.884 | 480409 | 20.0 |
| 3,6,9,12-Tetrao... | 21.572 | 3.4     | ng    | 80933    | 5                     | 21.884 | 480409 | 20.0 |
| Heneicosane        | 24.240 | 2.7     | ng    | 64904    | 6                     | 25.280 | 481581 | 20.0 |
| Pentacosane        | 26.425 | 4.6     | ng    | 111241   | 6                     | 25.280 | 481581 | 20.0 |