

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
 Data File : BG051158.D  
 Acq On : 20 Nov 2021 22:01  
 Operator : CG/JU  
 Sample : M4758-35  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP18

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: BG051158.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         | 5.263       | 294           | 302         | 309          | rBV      | 11055          | 18709         | 1.34%           | 0.242%        |
| 2         | 5.745       | 375           | 384         | 397          | rBV      | 382049         | 644656        | 46.02%          | 8.352%        |
| 3         | 7.355       | 651           | 658         | 668          | rBV      | 383113         | 698116        | 49.84%          | 9.044%        |
| 4         | 8.201       | 795           | 802         | 815          | rBV      | 95203          | 165052        | 11.78%          | 2.138%        |
| 5         | 9.382       | 995           | 1003        | 1013         | rBV      | 238829         | 450875        | 32.19%          | 5.841%        |
| 6         | 10.780      | 1235          | 1241        | 1252         | rBV2     | 9068           | 18744         | 1.34%           | 0.243%        |
| 7         | 11.033      | 1276          | 1284        | 1296         | rBV      | 123962         | 229585        | 16.39%          | 2.974%        |
| 8         | 13.453      | 1685          | 1696        | 1705         | rBV      | 569613         | 894114        | 63.83%          | 11.583%       |
| 9         | 13.694      | 1729          | 1737        | 1743         | rVB4     | 20829          | 35145         | 2.51%           | 0.455%        |
| 10        | 14.834      | 1924          | 1931        | 1938         | rVB      | 198316         | 315543        | 22.53%          | 4.088%        |
| 11        | 16.320      | 2178          | 2184        | 2199         | rBV      | 451162         | 708615        | 50.59%          | 9.180%        |
| 12        | 17.454      | 2371          | 2377        | 2382         | rBV3     | 15314          | 19664         | 1.40%           | 0.255%        |
| 13        | 17.584      | 2392          | 2399        | 2405         | rBV      | 263203         | 406213        | 29.00%          | 5.263%        |
| 14        | 18.206      | 2501          | 2505        | 2510         | rVB2     | 15111          | 20061         | 1.43%           | 0.260%        |
| 15        | 18.436      | 2539          | 2544        | 2549         | rBV3     | 11852          | 17835         | 1.27%           | 0.231%        |
| 16        | 19.370      | 2700          | 2703        | 2707         | rVB3     | 16135          | 18886         | 1.35%           | 0.245%        |
| 17        | 19.822      | 2775          | 2780        | 2784         | rBV3     | 10714          | 15399         | 1.10%           | 0.199%        |
| 18        | 20.175      | 2833          | 2840        | 2845         | rBV      | 1030285        | 1400823       | 100.00%         | 18.148%       |
| 19        | 20.944      | 2967          | 2971        | 2975         | rVB3     | 11837          | 15459         | 1.10%           | 0.200%        |
| 20        | 21.467      | 3050          | 3060        | 3073         | rBV2     | 78511          | 210759        | 15.05%          | 2.730%        |
| 21        | 21.573      | 3073          | 3078        | 3084         | rVB      | 50821          | 75574         | 5.39%           | 0.979%        |
| 22        | 21.879      | 3123          | 3130        | 3140         | rVB2     | 262658         | 471947        | 33.69%          | 6.114%        |
| 23        | 22.031      | 3152          | 3156        | 3162         | rVB2     | 14335          | 21301         | 1.52%           | 0.276%        |
| 24        | 22.666      | 3259          | 3264        | 3268         | rBV2     | 21560          | 38646         | 2.76%           | 0.501%        |
| 25        | 23.389      | 3382          | 3387        | 3393         | rBV4     | 18969          | 35355         | 2.52%           | 0.458%        |
| 26        | 23.588      | 3416          | 3421        | 3430         | rVB4     | 9105           | 20804         | 1.49%           | 0.270%        |
| 27        | 24.235      | 3524          | 3531        | 3538         | rVB2     | 30664          | 69123         | 4.93%           | 0.896%        |
| 28        | 25.281      | 3695          | 3709        | 3722         | rVB2     | 151556         | 508283        | 36.28%          | 6.585%        |
| 29        | 26.420      | 3894          | 3903        | 3911         | rBV2     | 40547          | 123073        | 8.79%           | 1.594%        |
| 30        | 27.854      | 4141          | 4147        | 4159         | rVB6     | 14472          | 50566         | 3.61%           | 0.655%        |

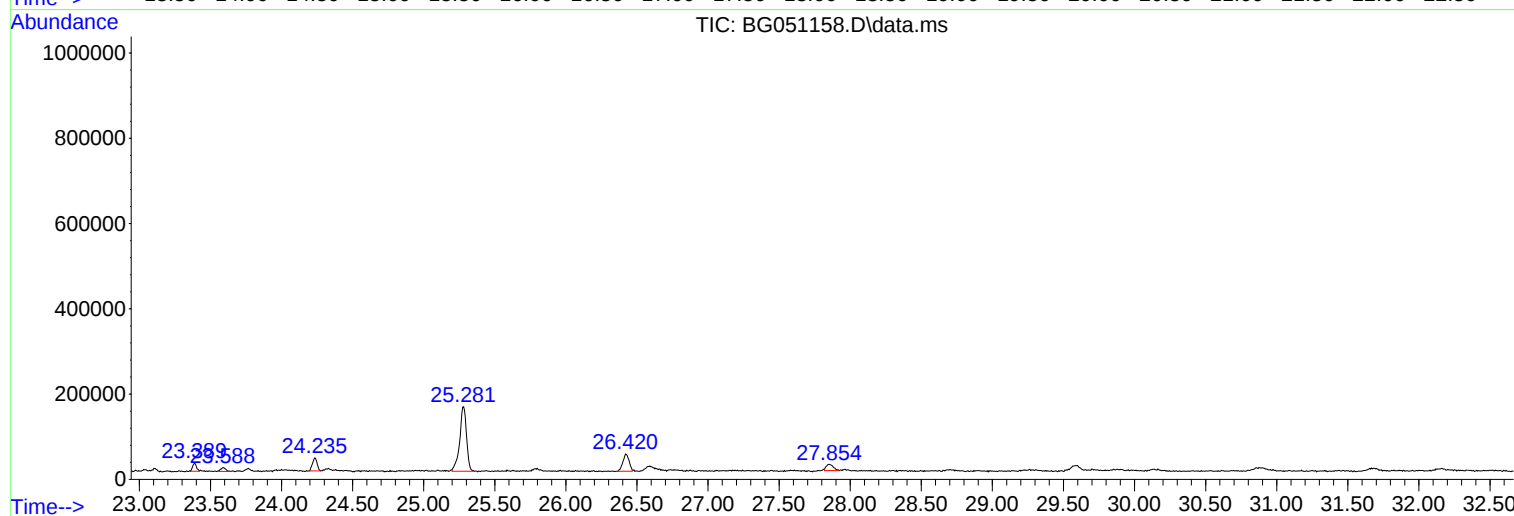
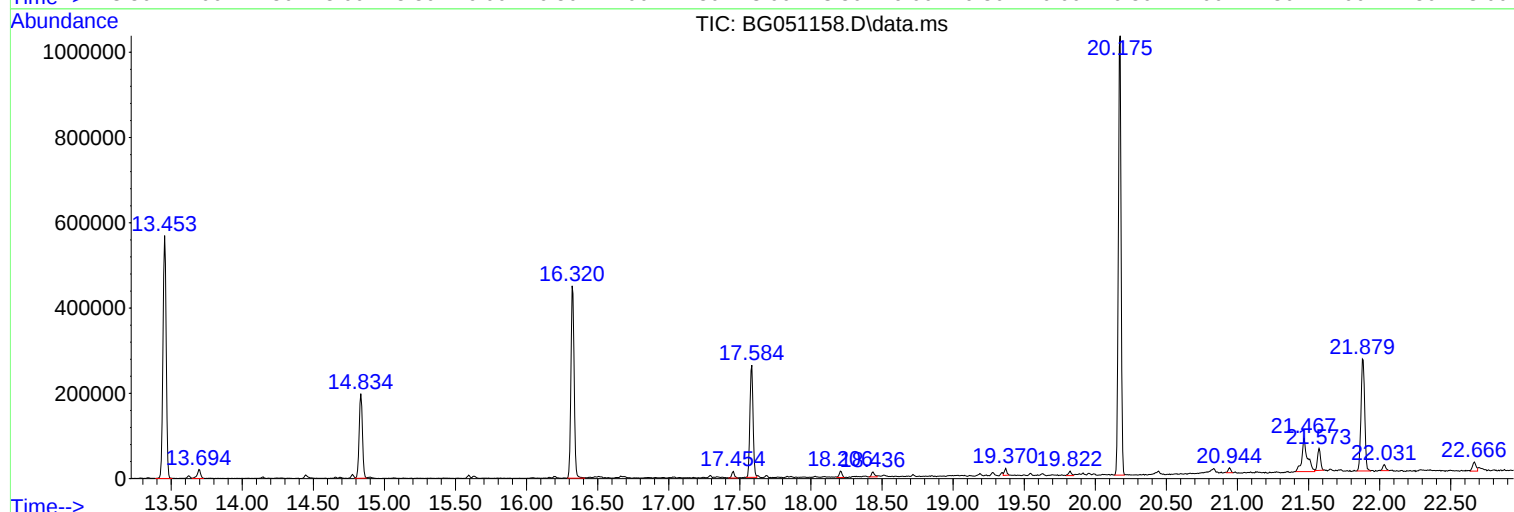
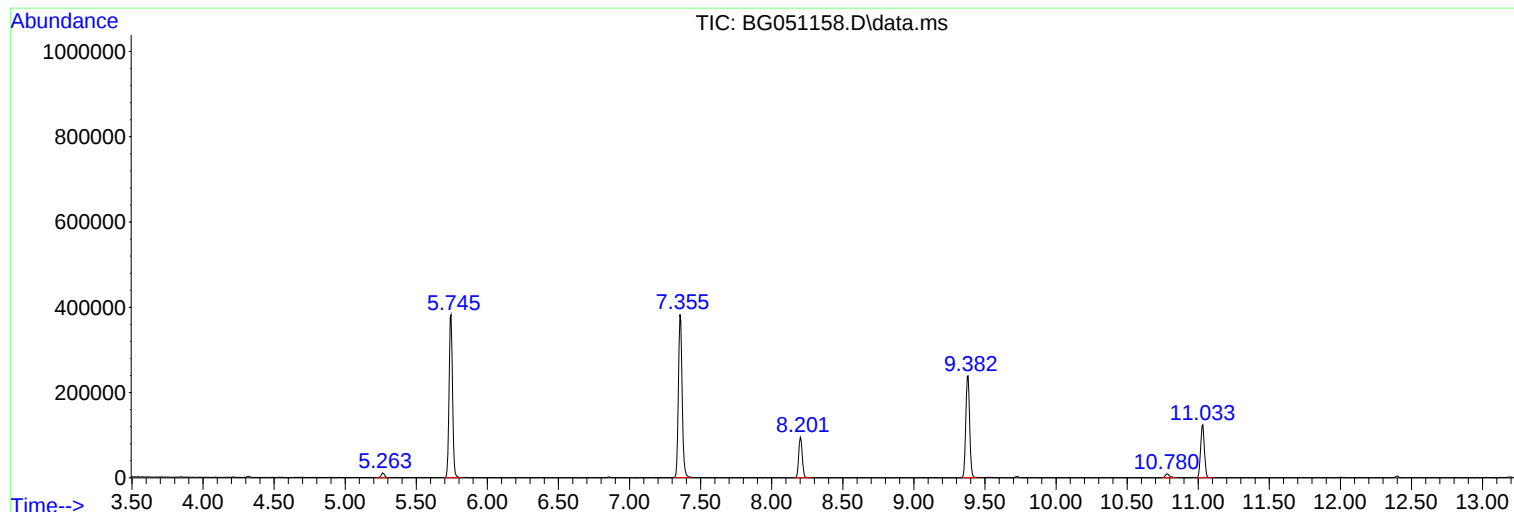
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Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP18

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

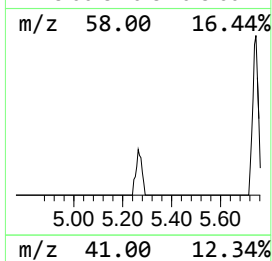
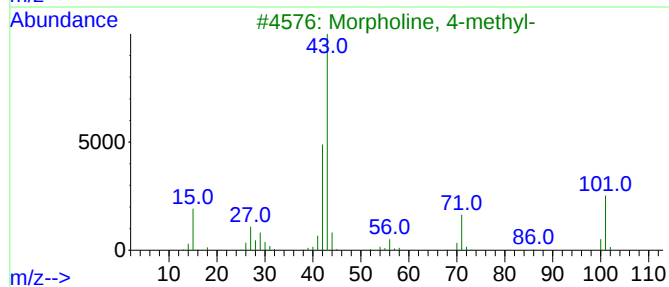
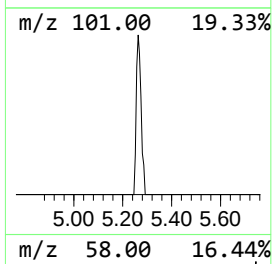
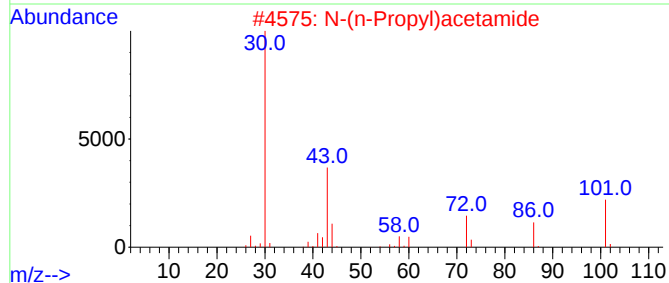
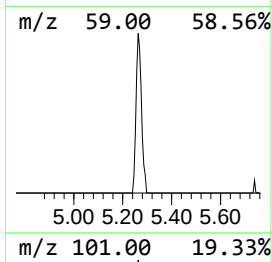
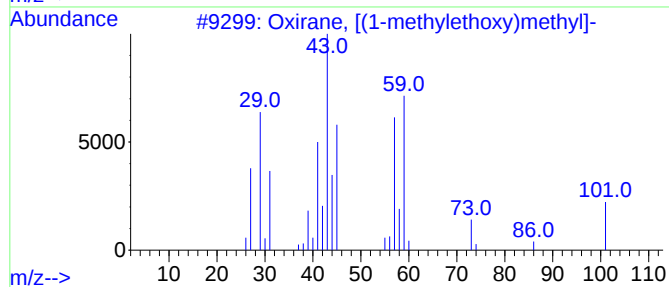
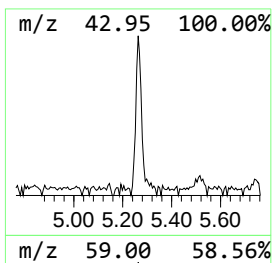
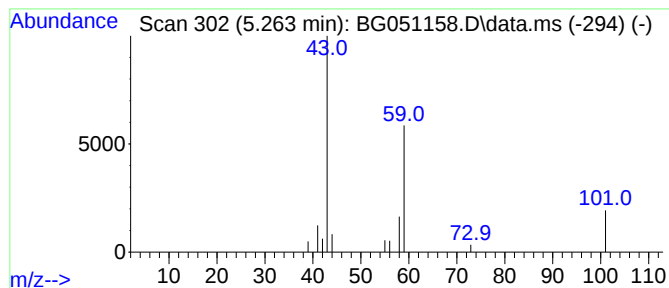
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown5.263 Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.263 | 2.27 ng | 18709 | 1,4-Dichlorobenzene-d4 | 8.201 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Oxirane, [(1-methylethoxy)methyl]- | 116 | C6H12O2 | 004016-14-2 | 40   |
| 2    |    |   | N-(n-Propyl)acetamide              | 101 | C5H11NO | 005331-48-6 | 9    |
| 3    |    |   | Morpholine, 4-methyl-              | 101 | C5H11NO | 000109-02-4 | 9    |
| 4    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 9    |
| 5    |    |   | 2-Methyl-2,3-pentanediol           | 118 | C6H14O2 | 007795-80-4 | 9    |



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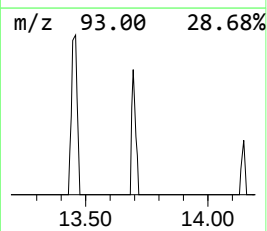
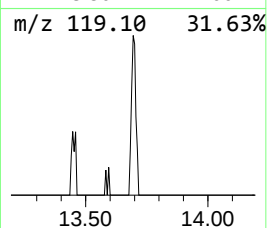
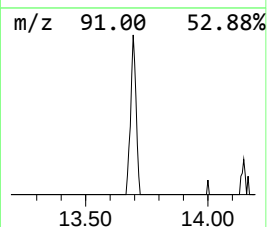
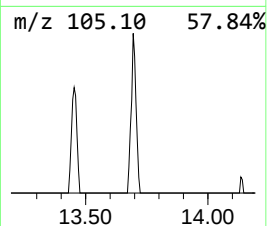
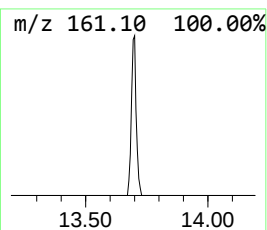
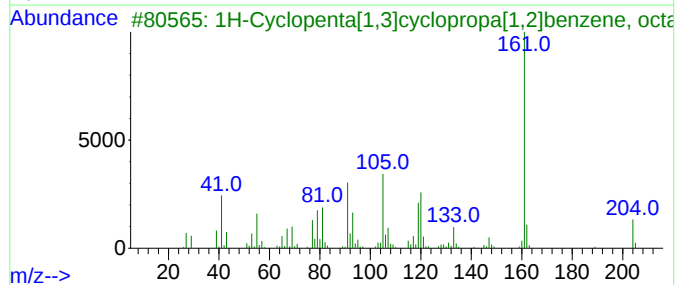
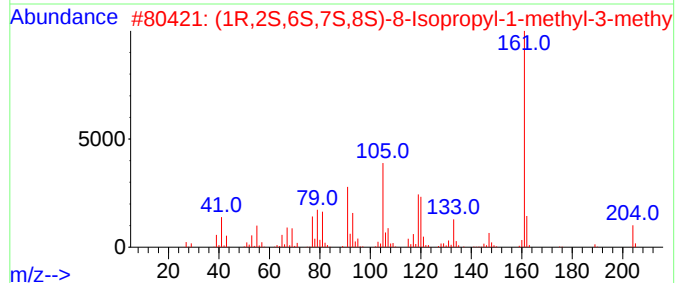
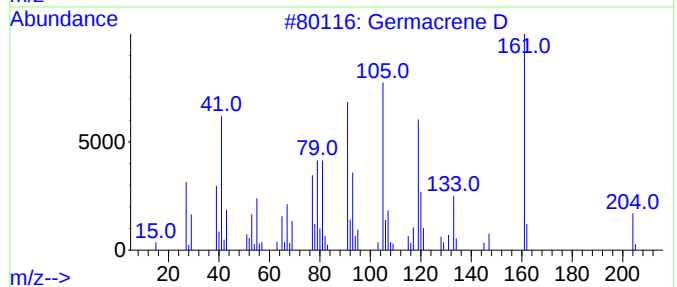
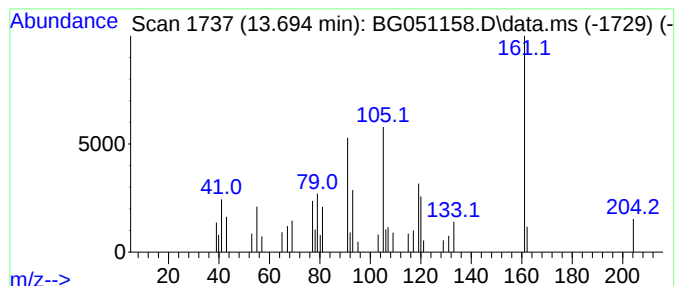
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Germacrene D Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 13.694 | 2.23 ng | 35145 | Acenaphthene-d10 | 14.834 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------------------------|-----|---------|-------------|------|
| 1    |      | Germacrene D                        | 204 | C15H24  | 023986-74-5 | 98   |
| 2    |      | (1R,2S,6S,7S,8S)-8-Isopropyl-1-m... | 204 | C15H24  | 018252-44-3 | 97   |
| 3    |      | 1H-Cyclopenta[1,3]cyclopropa[1,2... | 204 | C15H24  | 013744-15-5 | 97   |
| 4    |      | cis-Muurolo-4(15),5-diene           | 204 | C15H24  | 157477-72-0 | 87   |
| 5    |      | .alpha.-Cubebene                    | 204 | C15H24  | 017699-14-8 | 76   |



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Misc :  
ALS Vial : 13 Sample Multiplier: 1

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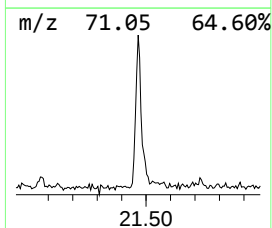
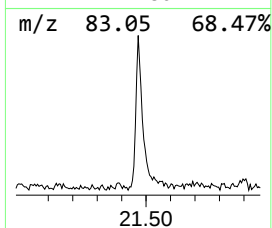
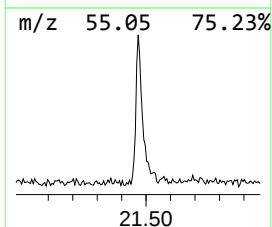
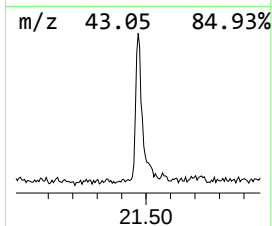
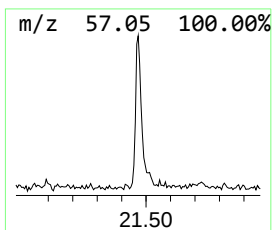
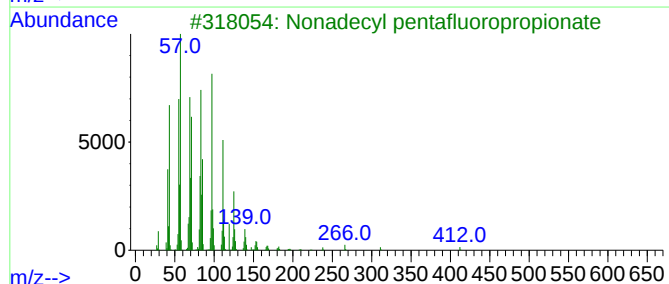
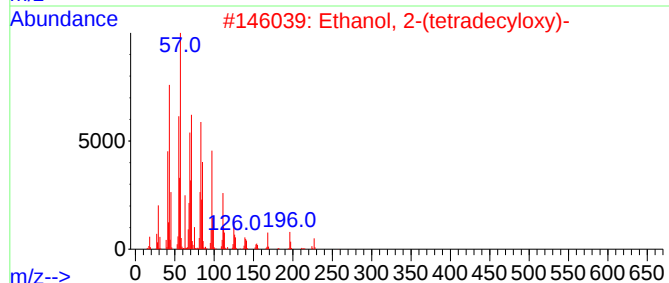
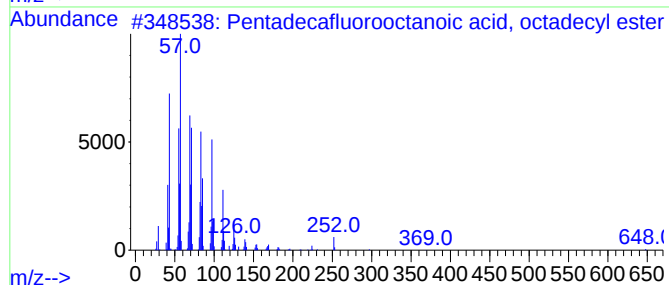
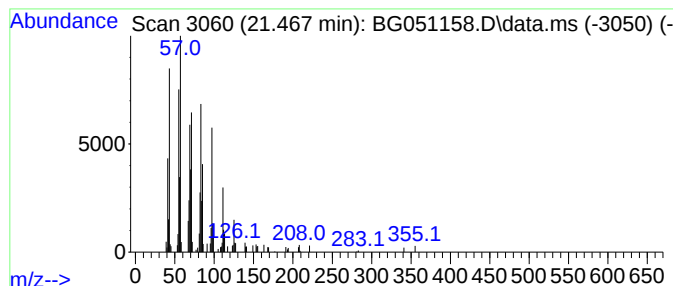
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 1

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 21.467    | 8.93 ng                             | 210759 | Chrysene-d12     | 21.879       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Pentadecafluorooctanoic acid, oc... | 666    | C26H37F15O2      | 1000406-04-8 | 94   |
| 2         | Ethanol, 2-(tetradecyloxy)-         | 258    | C16H34O2         | 002136-70-1  | 91   |
| 3         | Nonadecyl pentafluoropropionate     | 430    | C22H39F5O2       | 1000351-88-8 | 91   |
| 4         | 1-Hexacosene                        | 364    | C26H52           | 018835-33-1  | 90   |
| 5         | Trifluoroacetoxy hexadecane         | 338    | C18H33F3O2       | 006222-03-3  | 87   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

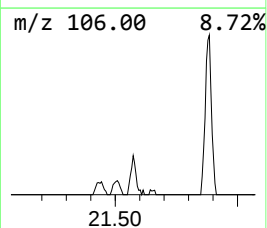
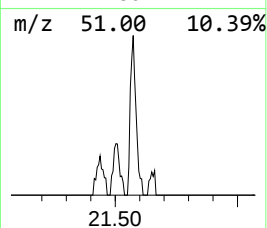
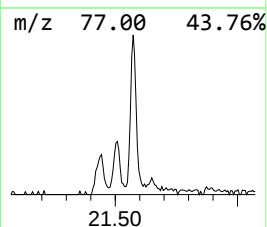
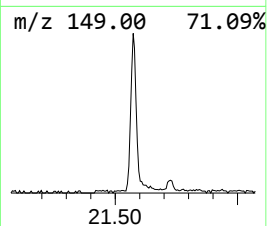
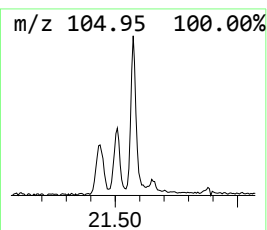
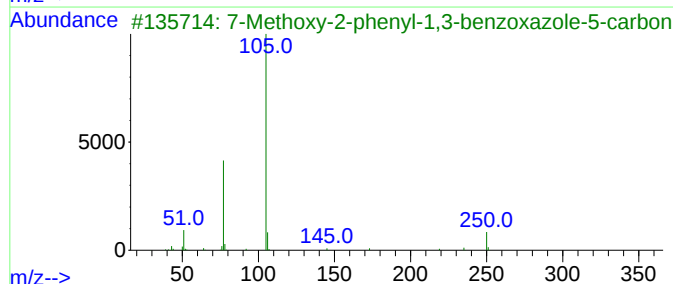
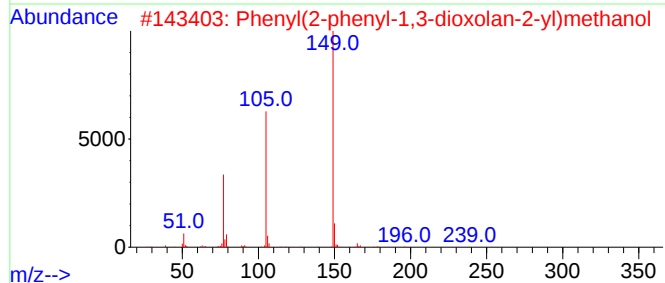
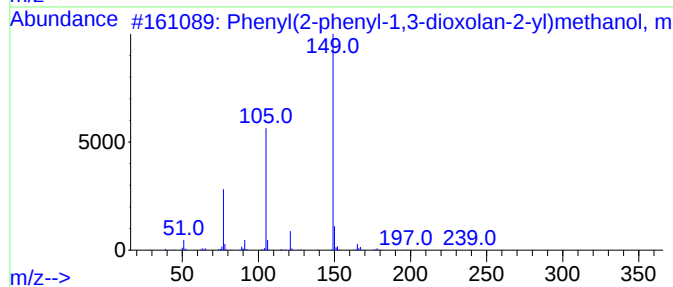
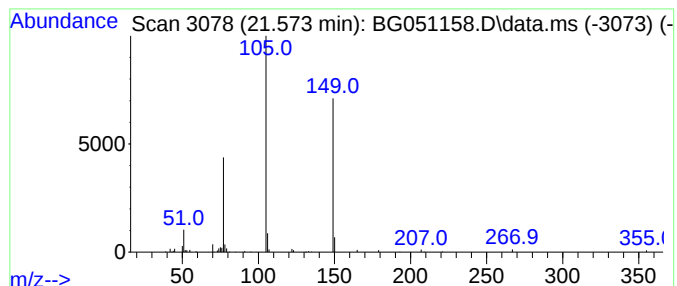
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.573 | 3.20 ng | 75574 | Chrysene-d12     | 21.879 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Phenyl(2-phenyl-1,3-dioxolan-2-y... | 270 | C17H18O3   | 1000507-07-6 | 72   |
| 2    |    |   | Phenyl(2-phenyl-1,3-dioxolan-2-y... | 256 | C16H16O3   | 005694-69-9  | 72   |
| 3    |    |   | 7-Methoxy-2-phenyl-1,3-benzoxazo... | 250 | C15H10N2O2 | 1000436-00-1 | 43   |
| 4    |    |   | 2-Benzoyloxyacetophenone            | 240 | C15H12O3   | 004010-33-7  | 43   |
| 5    |    |   | 1-Phenylpent-4-en-1-one             | 160 | C11H12O    | 003240-29-7  | 43   |



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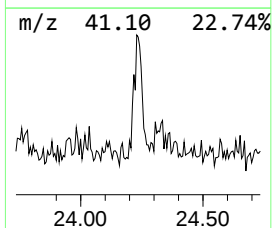
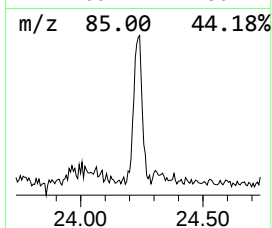
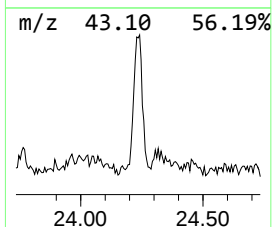
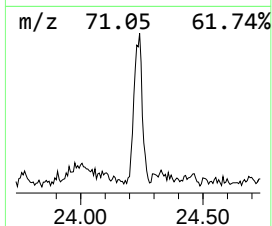
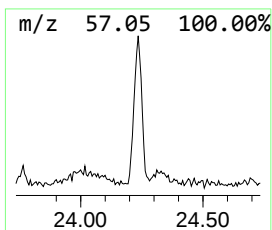
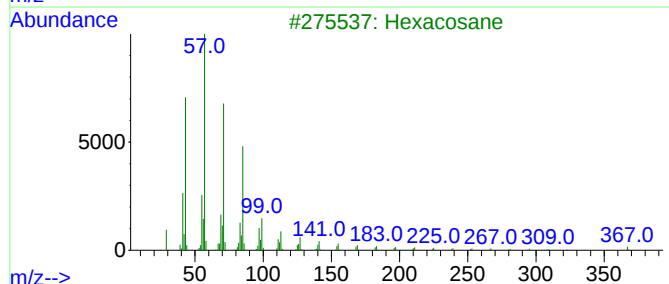
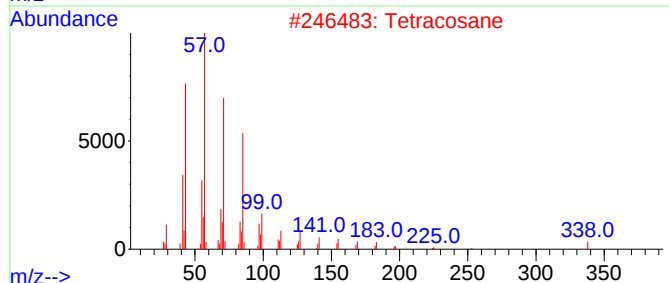
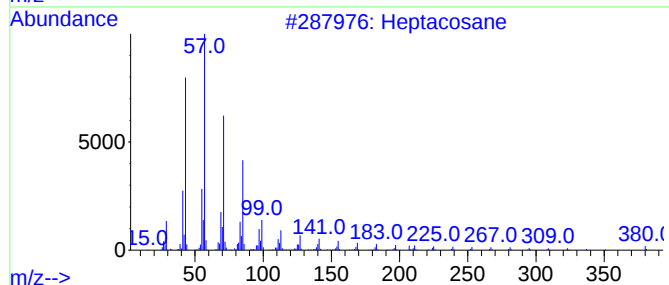
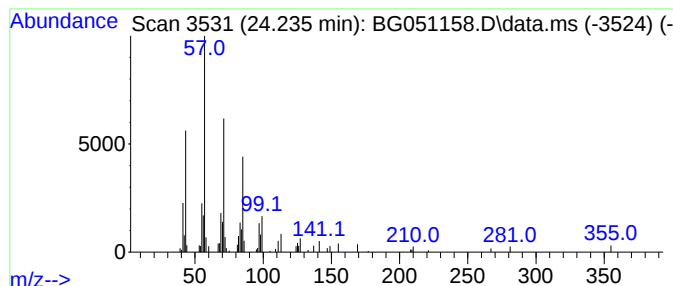
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heptacosane Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 24.235 | 2.72 ng | 69123 | Perylene-d12     | 25.281 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Heptacosane           | 380 | C27H56  | 000593-49-7 | 91   |
| 2    |    |   | Tetracosane           | 338 | C24H50  | 000646-31-1 | 90   |
| 3    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 90   |
| 4    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 87   |
| 5    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051158.D  
Acq On : 20 Nov 2021 22:01  
Operator : CG/JU  
Sample : M4758-35  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP18

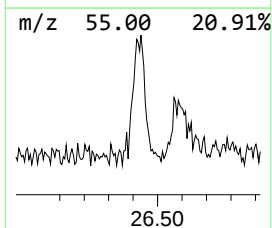
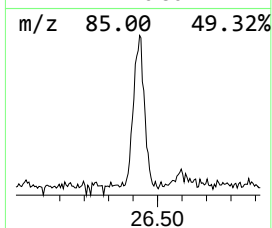
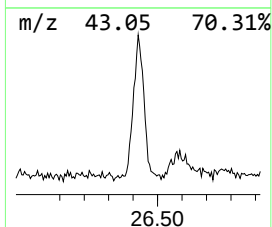
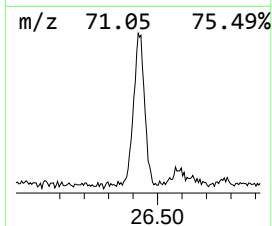
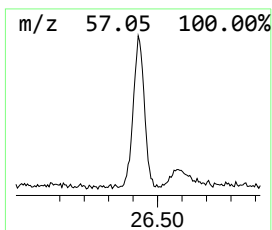
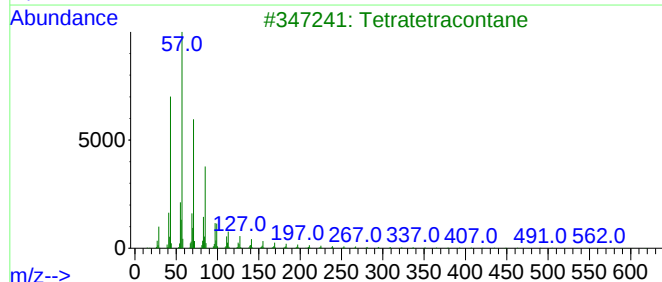
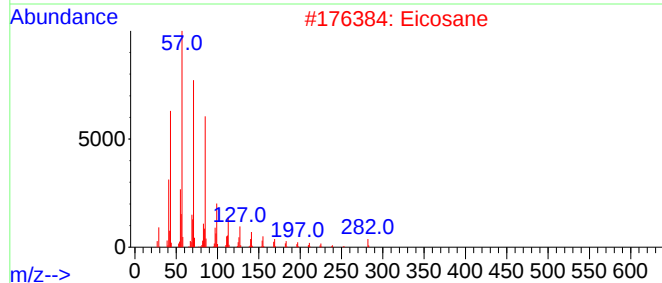
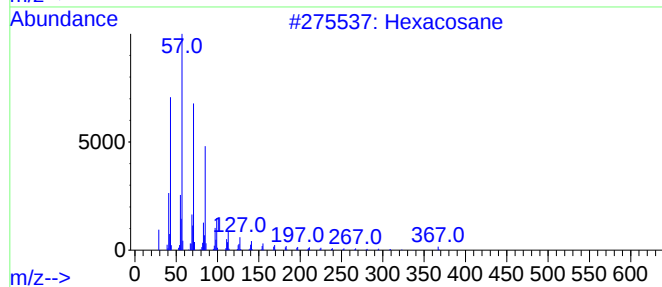
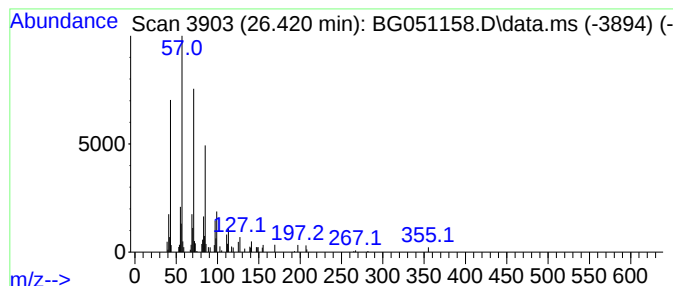
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Hexacosane Concentration Rank 2

| R.T.      | EstConc           | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------|--------|------------------|-------------|------|
| 26.420    | 4.84 ng           | 123073 | Perylene-d12     | 25.281      |      |
| Hit# of 5 | Tentative ID      | MW     | MolForm          | CAS#        | Qual |
| 1         | Hexacosane        | 366    | C26H54           | 000630-01-3 | 91   |
| 2         | Eicosane          | 282    | C20H42           | 000112-95-8 | 91   |
| 3         | Tetratetracontane | 619    | C44H90           | 007098-22-8 | 91   |
| 4         | Heneicosane       | 296    | C21H44           | 000629-94-7 | 91   |
| 5         | Heptacosane       | 380    | C27H56           | 000593-49-7 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112021\  
Data File : BG051158.D  
Acq On : 20 Nov 2021 22:01  
Operator : CG/JU  
Sample : M4758-35  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP18

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111921.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 |
| unknown5.263       | 5.263  | 2.3     | ng    | 18709    | 1                     | 8.201  | 165052 | 20.0 |
| Germacrene D       | 13.694 | 2.2     | ng    | 35145    | 3                     | 14.834 | 315543 | 20.0 |
| Pentadecafluoro... | 21.467 | 8.9     | ng    | 210759   | 5                     | 21.879 | 471947 | 20.0 |
| Phenyl(2-phenyl... | 21.573 | 3.2     | ng    | 75574    | 5                     | 21.879 | 471947 | 20.0 |
| Heptacosane        | 24.235 | 2.7     | ng    | 69123    | 6                     | 25.281 | 508283 | 20.0 |
| Hexacosane         | 26.420 | 4.8     | ng    | 123073   | 6                     | 25.281 | 508283 | 20.0 |