

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG051923\  
 Data File : BG057477.D  
 Acq On : 19 May 2023 21:36  
 Operator : CG/JU  
 Sample : 02845-21  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP3

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057477.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         | 5.389       | 308           | 315         | 321          | rBV      | 13879          | 21733         | 2.84%           | 0.462%        |
| 2         | 5.870       | 390           | 397         | 410          | rBV      | 152981         | 252697        | 33.01%          | 5.368%        |
| 3         | 7.497       | 666           | 674         | 689          | rBV      | 163534         | 289916        | 37.87%          | 6.158%        |
| 4         | 8.355       | 814           | 820         | 827          | rBB2     | 64822          | 108753        | 14.21%          | 2.310%        |
| 5         | 9.530       | 1013          | 1020        | 1029         | rBV      | 99064          | 177323        | 23.16%          | 3.767%        |
| 6         | 11.192      | 1295          | 1303        | 1311         | rBV      | 84393          | 148038        | 19.34%          | 3.145%        |
| 7         | 13.589      | 1705          | 1711        | 1720         | rBV      | 313726         | 469071        | 61.28%          | 9.964%        |
| 8         | 14.282      | 1824          | 1829        | 1834         | rVB2     | 22998          | 31921         | 4.17%           | 0.678%        |
| 9         | 14.911      | 1928          | 1936        | 1940         | rBV      | 74769          | 103221        | 13.48%          | 2.193%        |
| 10        | 14.970      | 1940          | 1946        | 1952         | rVV      | 147465         | 228923        | 29.90%          | 4.863%        |
| 11        | 15.193      | 1980          | 1984        | 1988         | rVB      | 13469          | 14336         | 1.87%           | 0.305%        |
| 12        | 15.263      | 1988          | 1996        | 2002         | rBV4     | 6923           | 9659          | 1.26%           | 0.205%        |
| 13        | 16.303      | 2169          | 2173        | 2180         | rVB      | 27124          | 39769         | 5.20%           | 0.845%        |
| 14        | 16.409      | 2186          | 2191        | 2193         | rBV3     | 13707          | 17653         | 2.31%           | 0.375%        |
| 15        | 16.450      | 2193          | 2198        | 2212         | rVB      | 241704         | 371604        | 48.54%          | 7.894%        |
| 16        | 17.707      | 2406          | 2412        | 2419         | rBV      | 212479         | 317236        | 41.44%          | 6.739%        |
| 17        | 18.553      | 2552          | 2556        | 2562         | rBV2     | 7268           | 13863         | 1.81%           | 0.294%        |
| 18        | 20.274      | 2844          | 2849        | 2857         | rBV      | 614029         | 765502        | 100.00%         | 16.261%       |
| 19        | 20.427      | 2869          | 2875        | 2878         | rVB2     | 6504           | 8843          | 1.16%           | 0.188%        |
| 20        | 21.232      | 3008          | 3012        | 3016         | rVB4     | 8968           | 11288         | 1.47%           | 0.240%        |
| 21        | 21.414      | 3036          | 3043        | 3051         | rVB      | 303628         | 438581        | 57.29%          | 9.316%        |
| 22        | 21.578      | 3065          | 3071        | 3079         | rBV8     | 14072          | 38293         | 5.00%           | 0.813%        |
| 23        | 22.013      | 3136          | 3145        | 3154         | rBV      | 202679         | 360261        | 47.06%          | 7.653%        |
| 24        | 22.789      | 3273          | 3277        | 3282         | rBV6     | 4868           | 8227          | 1.07%           | 0.175%        |
| 25        | 23.535      | 3400          | 3404        | 3410         | rVB5     | 7686           | 12337         | 1.61%           | 0.262%        |
| 26        | 24.398      | 3544          | 3551        | 3557         | rBV5     | 13683          | 30847         | 4.03%           | 0.655%        |
| 27        | 25.426      | 3718          | 3726        | 3729         | rBV4     | 9452           | 22483         | 2.94%           | 0.478%        |
| 28        | 25.508      | 3729          | 3740        | 3752         | rVB3     | 113343         | 342709        | 44.77%          | 7.280%        |
| 29        | 26.642      | 3923          | 3933        | 3941         | rBV7     | 12375          | 40518         | 5.29%           | 0.861%        |
| 30        | 29.873      | 4474          | 4483        | 4484         | rBV6     | 5478           | 12111         | 1.58%           | 0.257%        |

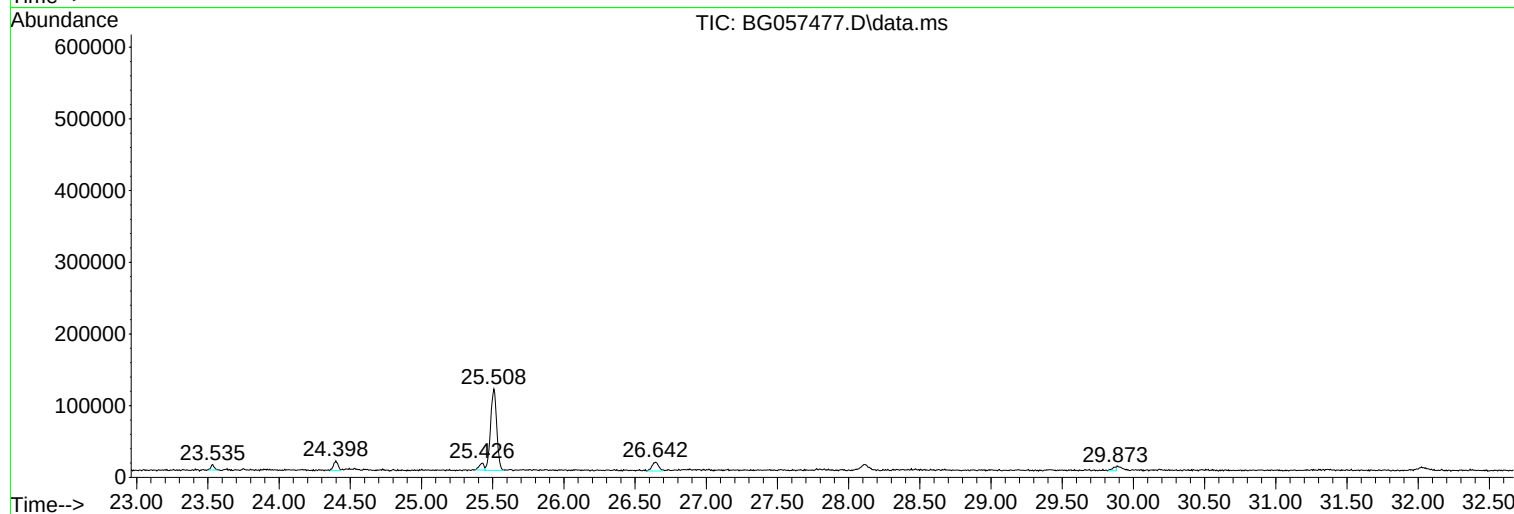
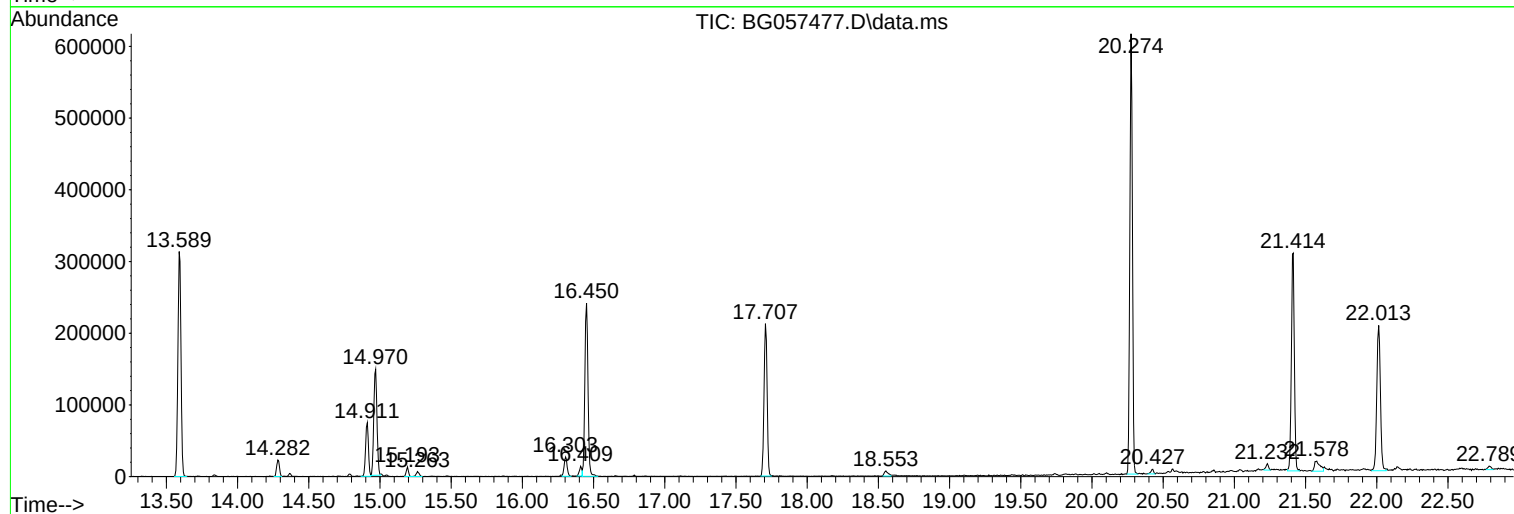
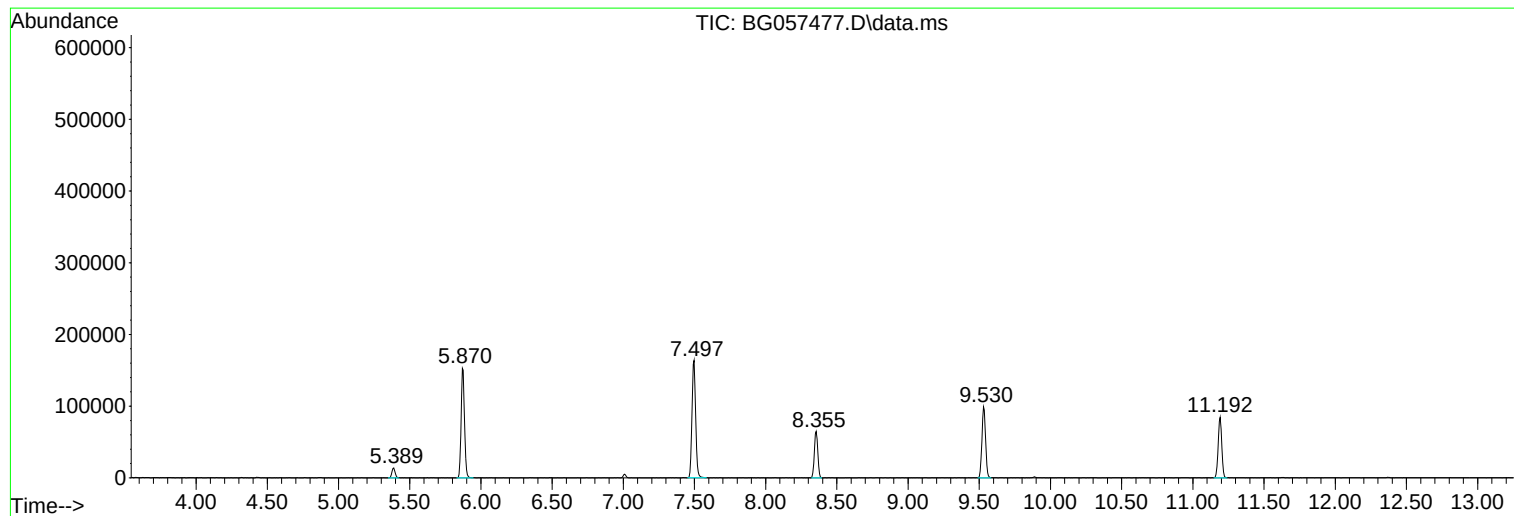
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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.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\BG051923\  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

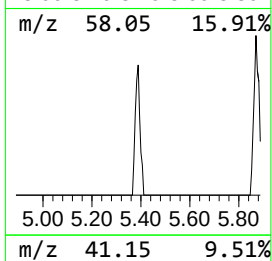
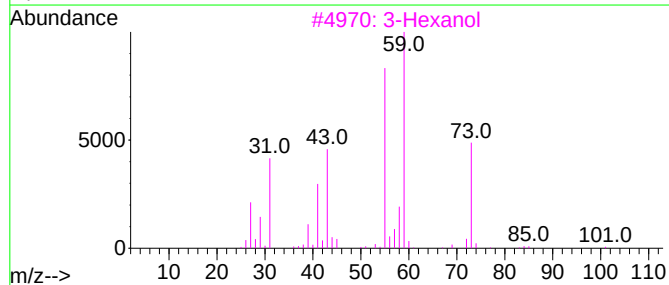
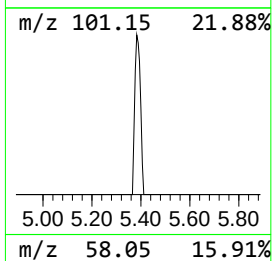
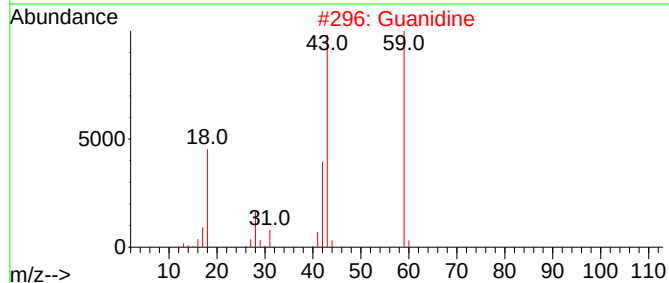
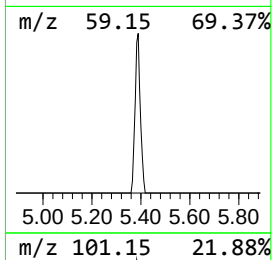
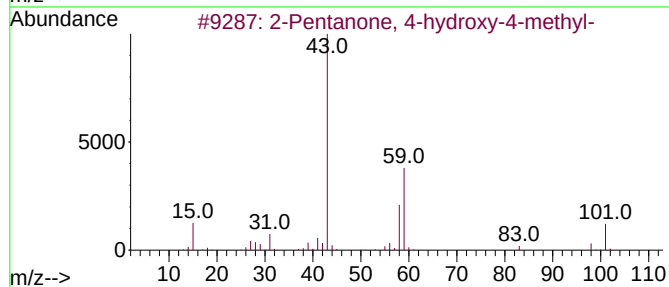
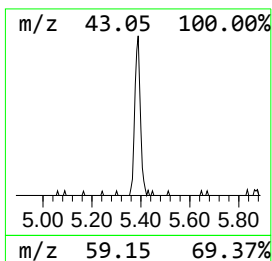
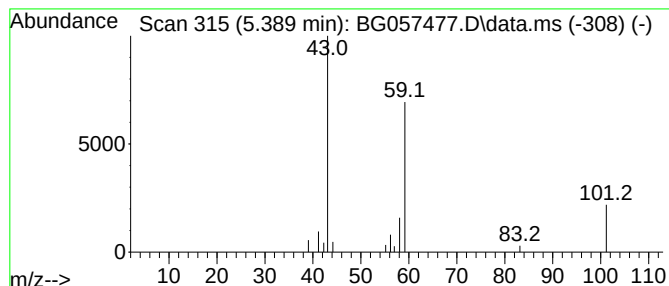
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.389 | 4.00 ng | 21733 | 1,4-Dichlorobenzene-d4 | 8.355 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 72      |      |      |
| 2    | Guanidine                        | 59  | CH5N3        | 000113-00-8 | 9       |      |      |
| 3    | 3-Hexanol                        | 102 | C6H14O       | 000623-37-0 | 9       |      |      |
| 4    | 1,8-Nonanediol, 8-methyl-        | 174 | C10H22O2     | 054725-73-4 | 9       |      |      |
| 5    | 3-Octanol                        | 130 | C8H18O       | 000589-98-0 | 9       |      |      |



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Misc :  
ALS Vial : 9 Sample Multiplier: 1

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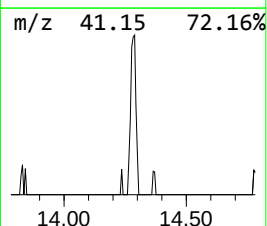
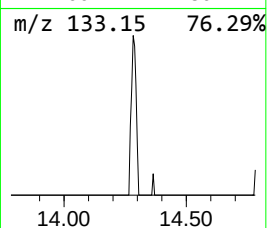
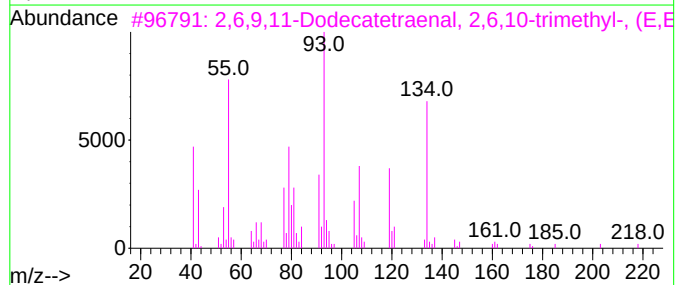
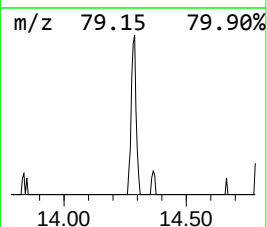
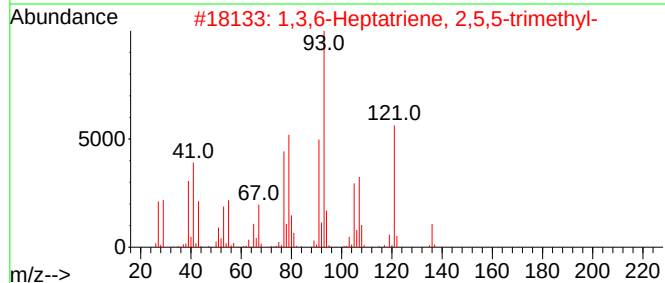
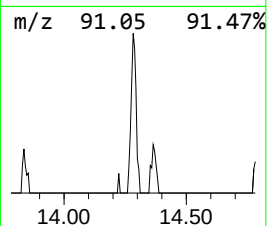
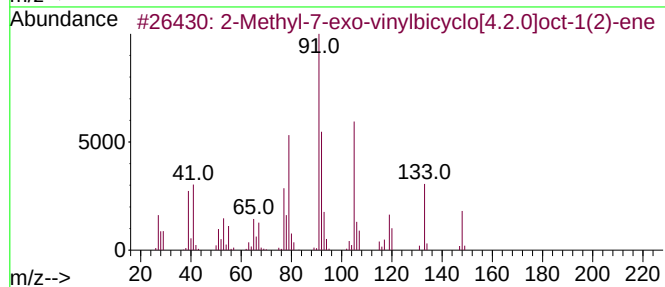
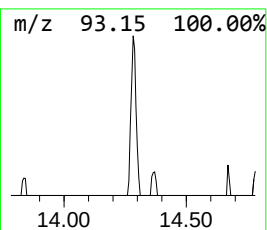
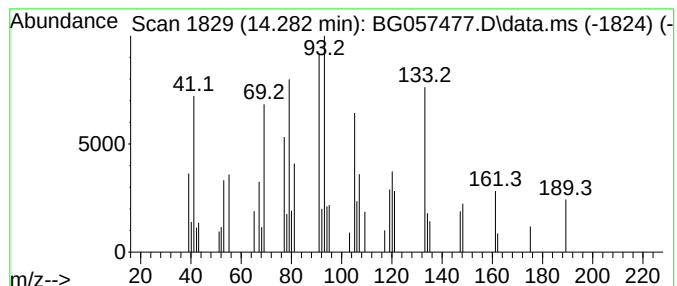
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown14.282 Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.282 | 2.79 ng | 31921 | Acenaphthene-d10 | 14.970 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | 2-Methyl-7-exo-vinylbicyclo[4.2.... | 148 | C11H16  | 107914-89-6  | 43   |
| 2    |    |   | 1,3,6-Heptatriene, 2,5,5-trimethyl- | 136 | C10H16  | 029548-02-5  | 35   |
| 3    |    |   | 2,6,9,11-Dodecatetraenal, 2,6,10... | 218 | C15H22O | 017909-77-2  | 27   |
| 4    |    |   | Spiro[4.4]nona-1,3-diene, 1,2-di... | 148 | C11H16  | 1000163-57-6 | 27   |
| 5    |    |   | 1-Methylene-2-vinylcyclopentane     | 108 | C8H12   | 006196-78-7  | 27   |





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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP3

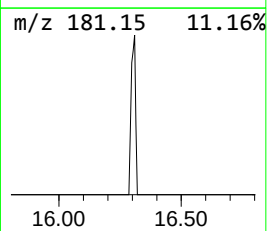
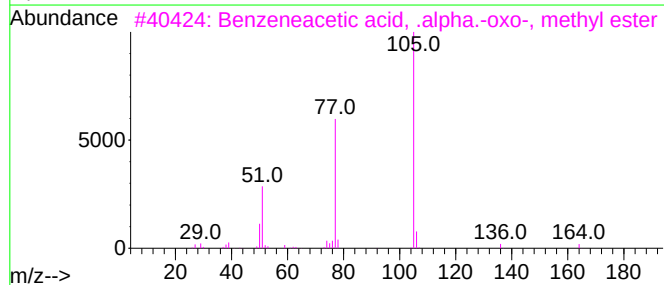
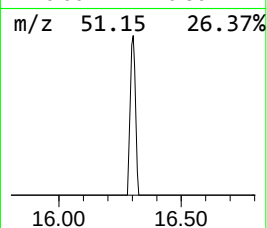
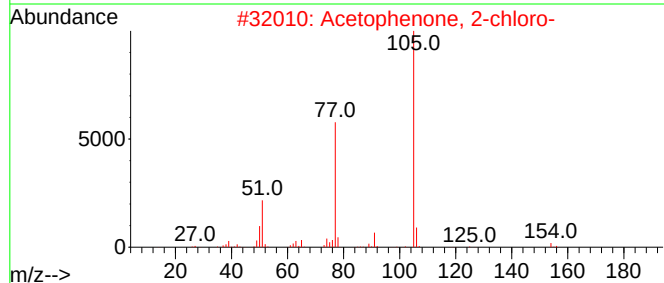
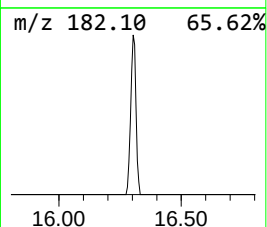
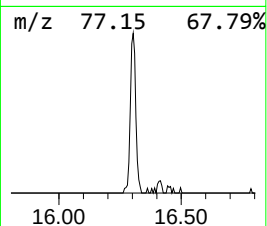
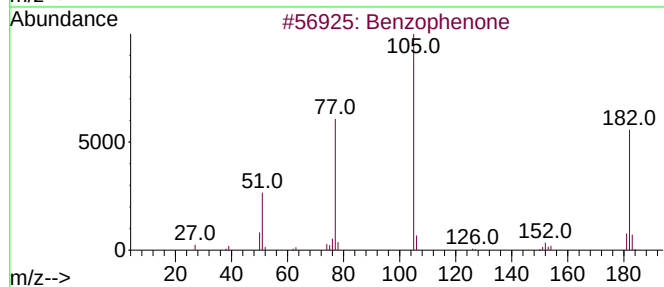
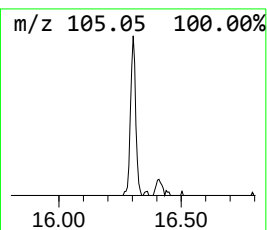
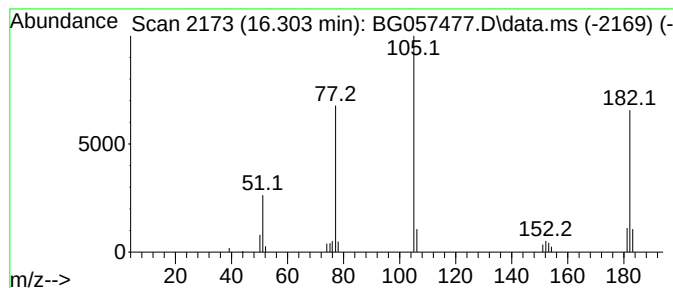
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Benzophenone Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.303 | 3.47 ng | 39769 | Acenaphthene-d10 | 14.970 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9  | 95   |
| 2    |    |   | Acetophenone, 2-chloro-             | 154 | C8H7ClO  | 000532-27-4  | 46   |
| 3    |    |   | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3   | 015206-55-0  | 43   |
| 4    |    |   | 1,2(4H)-Oxazine-3-ol, 5,6-dihydr... | 219 | C11H9N04 | 1000253-25-6 | 43   |
| 5    |    |   | 1-Propanone, 3-chloro-1-phenyl-     | 168 | C9H9ClO  | 000936-59-4  | 43   |



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Instrument :  
BNA\_G  
ClientSampleId :  
TP3

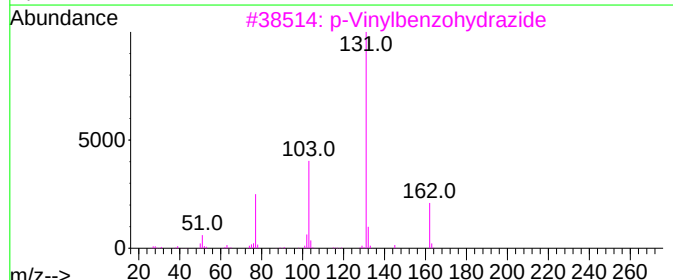
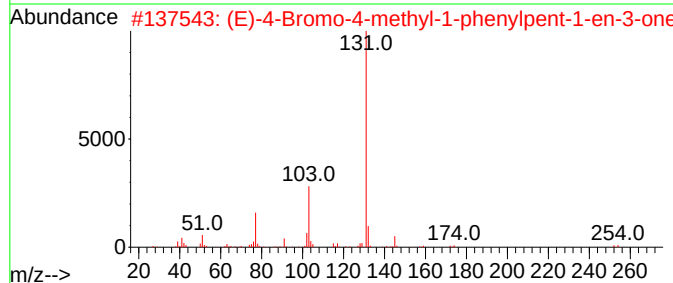
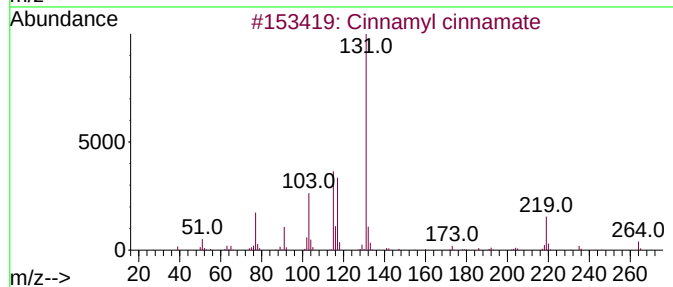
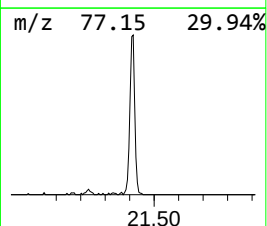
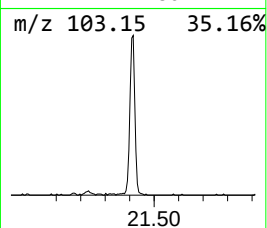
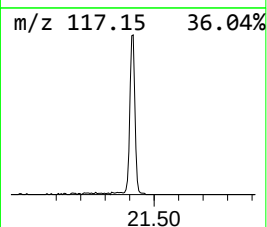
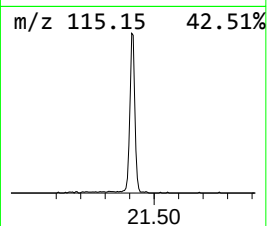
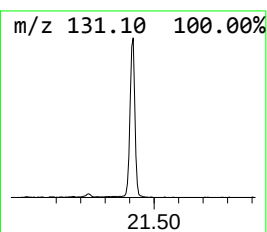
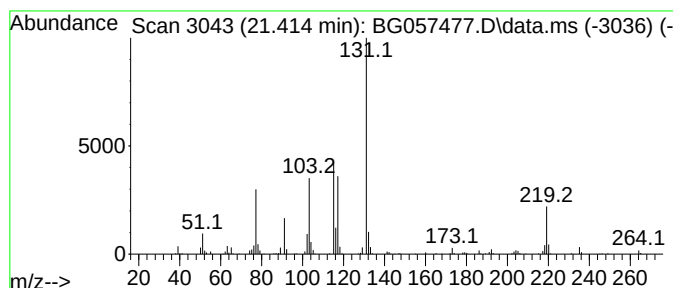
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Cinnamyl cinnamate Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 21.414 | 24.35 ng | 438581 | Chrysene-d12     | 22.013 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Cinnamyl cinnamate                  | 264 | C18H16O2  | 000122-69-0  | 87   |
| 2    |    |   | (E)-4-Bromo-4-methyl-1-phenylpen... | 252 | C12H13BrO | 1000443-02-8 | 49   |
| 3    |    |   | p-Vinylbenzohydrazide               | 162 | C9H10N2O  | 1000244-74-9 | 47   |
| 4    |    |   | N-(4-Fluorophenyl)-3-phenyl-2-pr... | 241 | C15H12FNO | 019358-27-1  | 47   |
| 5    |    |   | 2,2-Dimethyl-1-(2-vinylphenyl)pr... | 188 | C13H16O   | 1000210-99-9 | 47   |



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TP3

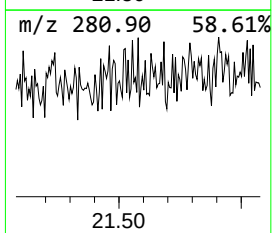
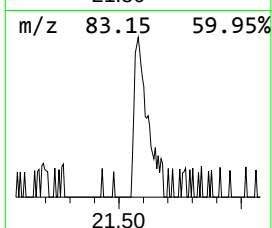
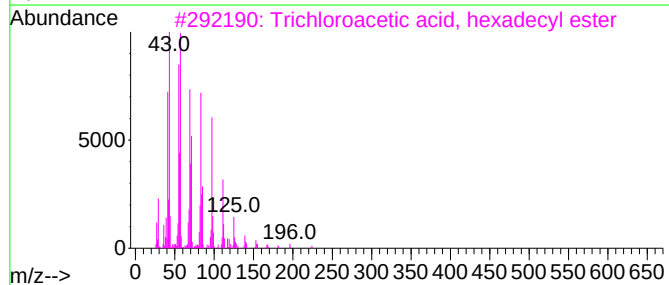
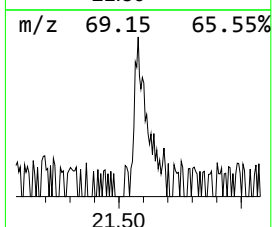
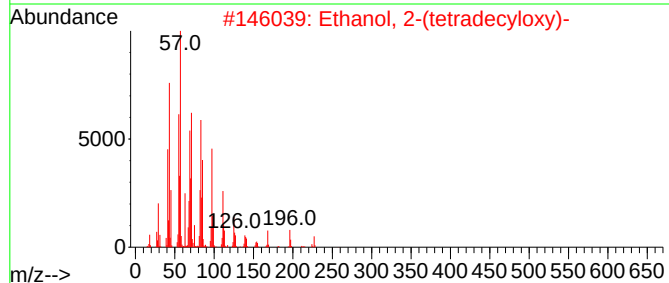
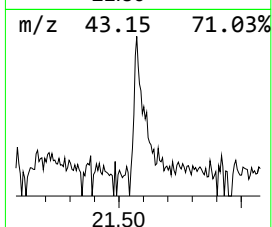
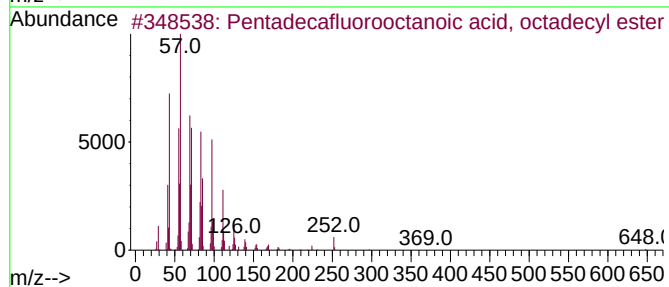
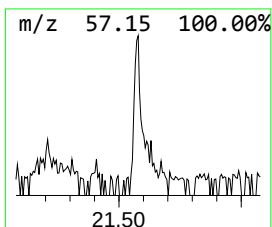
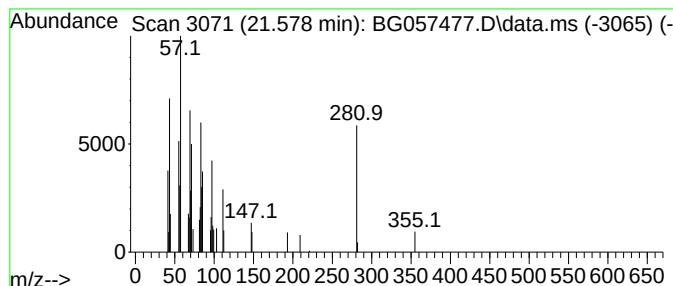
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 7

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 21.578    | 2.13 ng                             | 38293 | Chrysene-d12     | 22.013       |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | Pentadecafluorooctanoic acid, oc... | 666   | C26H37F15O2      | 1000406-04-8 | 70   |
| 2         | Ethanol, 2-(tetradecyloxy)-         | 258   | C16H34O2         | 002136-70-1  | 62   |
| 3         | Trichloroacetic acid, hexadecyl ... | 386   | C18H33Cl3O2      | 074339-54-1  | 62   |
| 4         | Heptadecyl heptafluorobutyrate      | 452   | C21H35F7O2       | 959085-66-6  | 62   |
| 5         | Pentafluoropropionic acid, tetra... | 360   | C17H29F5O2       | 006222-06-6  | 49   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG051923\  
Data File : BG057477.D  
Acq On : 19 May 2023 21:36  
Operator : CG/JU  
Sample : 02845-21  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP3

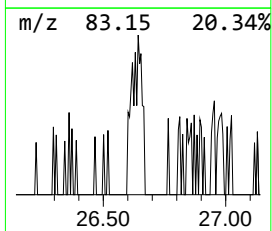
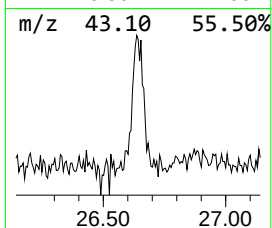
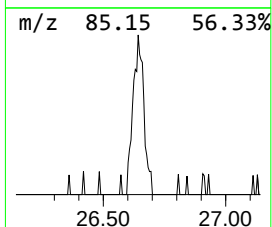
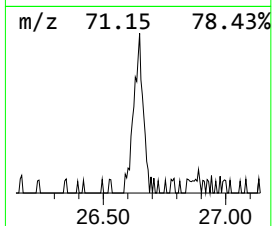
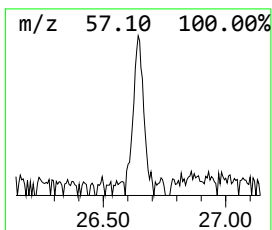
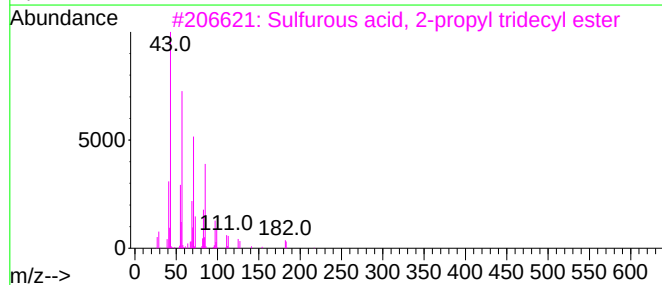
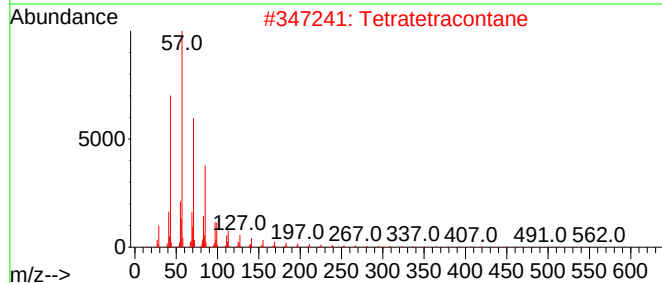
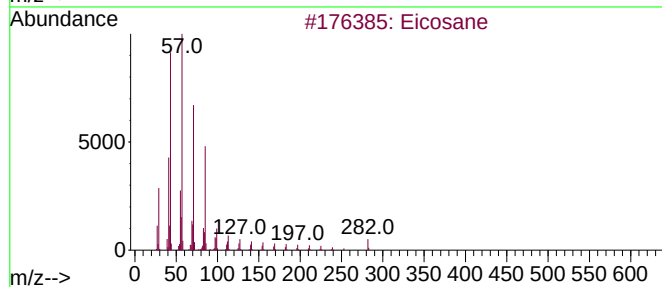
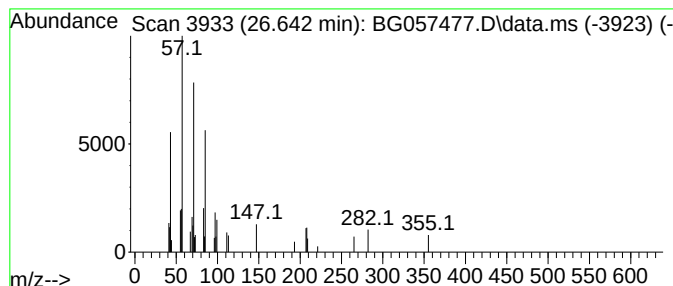
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Eicosane Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 26.642 | 2.36 ng | 40518 | Perylene-d12     | 25.508 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Eicosane                            | 282 | C20H42    | 000112-95-8  | 86   |
| 2    |    |   | Tetratetracontane                   | 619 | C44H90    | 007098-22-8  | 58   |
| 3    |    |   | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 58   |
| 4    |    |   | Sulfurous acid, 2-propyl tetrad...  | 320 | C17H36O3S | 1010309-12-5 | 58   |
| 5    |    |   | Hexacosane                          | 366 | C26H54    | 000630-01-3  | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG051923\  
Data File : BG057477.D  
Acq On : 19 May 2023 21:36  
Operator : CG/JU  
Sample : 02845-21  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.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-... | 5.389  | 4.0     | ng    | 21733    | 1                     | 8.355  | 108753 | 20.0 |
| unknown14.282      | 14.282 | 2.8     | ng    | 31921    | 3                     | 14.970 | 228923 | 20.0 |
| (1R,2S,6S,7S,8S... | 14.911 | 9.0     | ng    | 103221   | 3                     | 14.970 | 228923 | 20.0 |
| Benzophenone       | 16.303 | 3.5     | ng    | 39769    | 3                     | 14.970 | 228923 | 20.0 |
| Cinnamyl cinnamate | 21.414 | 24.4    | ng    | 438581   | 5                     | 22.013 | 360261 | 20.0 |
| Pentadecafluoro... | 21.578 | 2.1     | ng    | 38293    | 5                     | 22.013 | 360261 | 20.0 |
| Eicosane           | 26.642 | 2.4     | ng    | 40518    | 6                     | 25.508 | 342709 | 20.0 |