

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062822\  
 Data File : BG054123.D  
 Acq On : 28 Jun 2022 18:51  
 Operator : CG/JU  
 Sample : N3488-03  
 Misc :  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-9-22.5-24.5-20220623

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-BG061322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054123.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         | 4.563       | 194           | 200         | 210          | rVB      | 26733          | 46749         | 3.53%           | 0.638%        |
| 2         | 5.162       | 296           | 302         | 313          | rBV      | 108086         | 184927        | 13.98%          | 2.525%        |
| 3         | 5.638       | 374           | 383         | 394          | rBV      | 192423         | 326898        | 24.72%          | 4.463%        |
| 4         | 7.230       | 646           | 654         | 665          | rBV      | 275041         | 490589        | 37.09%          | 6.699%        |
| 5         | 8.070       | 790           | 797         | 804          | rBV      | 81435          | 145178        | 10.98%          | 1.982%        |
| 6         | 9.228       | 986           | 994         | 1003         | rBV      | 174302         | 327589        | 24.77%          | 4.473%        |
| 7         | 10.879      | 1266          | 1275        | 1286         | rBV      | 121829         | 231449        | 17.50%          | 3.160%        |
| 8         | 13.323      | 1683          | 1691        | 1700         | rVB      | 551324         | 892208        | 67.46%          | 12.182%       |
| 9         | 14.698      | 1918          | 1925        | 1932         | rVB      | 225355         | 362121        | 27.38%          | 4.944%        |
| 10        | 15.538      | 2063          | 2068        | 2073         | rVB      | 13339          | 18577         | 1.40%           | 0.254%        |
| 11        | 16.179      | 2168          | 2177        | 2184         | rBV      | 63528          | 104445        | 7.90%           | 1.426%        |
| 12        | 16.396      | 2210          | 2214        | 2216         | rBV2     | 18564          | 23849         | 1.80%           | 0.326%        |
| 13        | 16.420      | 2216          | 2218        | 2223         | rVB3     | 16342          | 21694         | 1.64%           | 0.296%        |
| 14        | 17.189      | 2344          | 2349        | 2353         | rBV4     | 17451          | 22682         | 1.71%           | 0.310%        |
| 15        | 17.248      | 2353          | 2359        | 2366         | rVB4     | 10445          | 20515         | 1.55%           | 0.280%        |
| 16        | 17.442      | 2385          | 2392        | 2396         | rBV      | 288571         | 458061        | 34.63%          | 6.254%        |
| 17        | 17.483      | 2396          | 2399        | 2406         | rVV      | 50855          | 78417         | 5.93%           | 1.071%        |
| 18        | 17.571      | 2410          | 2414        | 2420         | rVB      | 10609          | 17814         | 1.35%           | 0.243%        |
| 19        | 17.930      | 2471          | 2475        | 2483         | rVB2     | 16522          | 22510         | 1.70%           | 0.307%        |
| 20        | 18.364      | 2544          | 2549        | 2556         | rVB3     | 16447          | 30900         | 2.34%           | 0.422%        |
| 21        | 18.441      | 2556          | 2562        | 2564         | rBV4     | 9092           | 14648         | 1.11%           | 0.200%        |
| 22        | 18.617      | 2588          | 2592        | 2598         | rBV      | 17428          | 26918         | 2.04%           | 0.368%        |
| 23        | 18.805      | 2620          | 2624        | 2628         | rBV3     | 10607          | 17328         | 1.31%           | 0.237%        |
| 24        | 19.022      | 2657          | 2661        | 2664         | rVB4     | 19562          | 24656         | 1.86%           | 0.337%        |
| 25        | 19.228      | 2691          | 2696        | 2697         | rBV2     | 19534          | 27966         | 2.11%           | 0.382%        |
| 26        | 19.422      | 2726          | 2729        | 2735         | rVB5     | 14441          | 19794         | 1.50%           | 0.270%        |
| 27        | 19.492      | 2735          | 2741        | 2746         | rBV      | 106819         | 162247        | 12.27%          | 2.215%        |
| 28        | 19.821      | 2793          | 2797        | 2799         | rBV2     | 37906          | 56176         | 4.25%           | 0.767%        |
| 29        | 19.857      | 2799          | 2803        | 2811         | rVB      | 157241         | 263102        | 19.89%          | 3.592%        |
| 30        | 19.927      | 2811          | 2815        | 2816         | rBV4     | 15243          | 19510         | 1.48%           | 0.266%        |
| 31        | 19.957      | 2817          | 2820        | 2824         | rVB      | 39410          | 49161         | 3.72%           | 0.671%        |
| 32        | 20.045      | 2830          | 2835        | 2841         | rVB      | 960743         | 1322613       | 100.00%         | 18.059%       |
| 33        | 20.350      | 2884          | 2887        | 2893         | rVB2     | 32268          | 43441         | 3.28%           | 0.593%        |
| 34        | 20.850      | 2969          | 2972        | 2976         | rVB2     | 34675          | 43706         | 3.30%           | 0.597%        |
| 35        | 21.349      | 3053          | 3057        | 3062         | rBV3     | 88224          | 136691        | 10.33%          | 1.866%        |
| 36        | 21.713      | 3112          | 3119        | 3125         | rBV2     | 284683         | 578732        | 43.76%          | 7.902%        |

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Sample : N3488-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

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-BG061322.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 21.913 | 3149 | 3153 | 3158 | rVB2 | 49520  | 73029  | 5.52%  | 0.997% |
| 38 | 22.524 | 3253 | 3257 | 3262 | rBV2 | 56322  | 90005  | 6.81%  | 1.229% |
| 39 | 24.974 | 3666 | 3674 | 3688 | rVB2 | 166023 | 526932 | 39.84% | 7.195% |

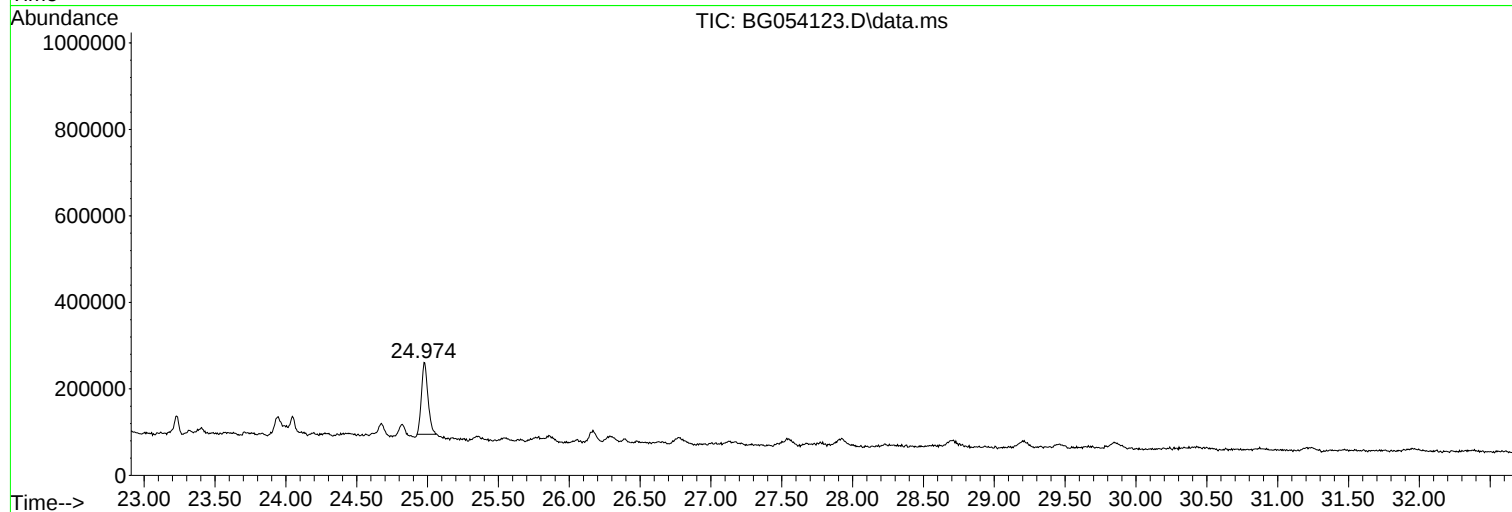
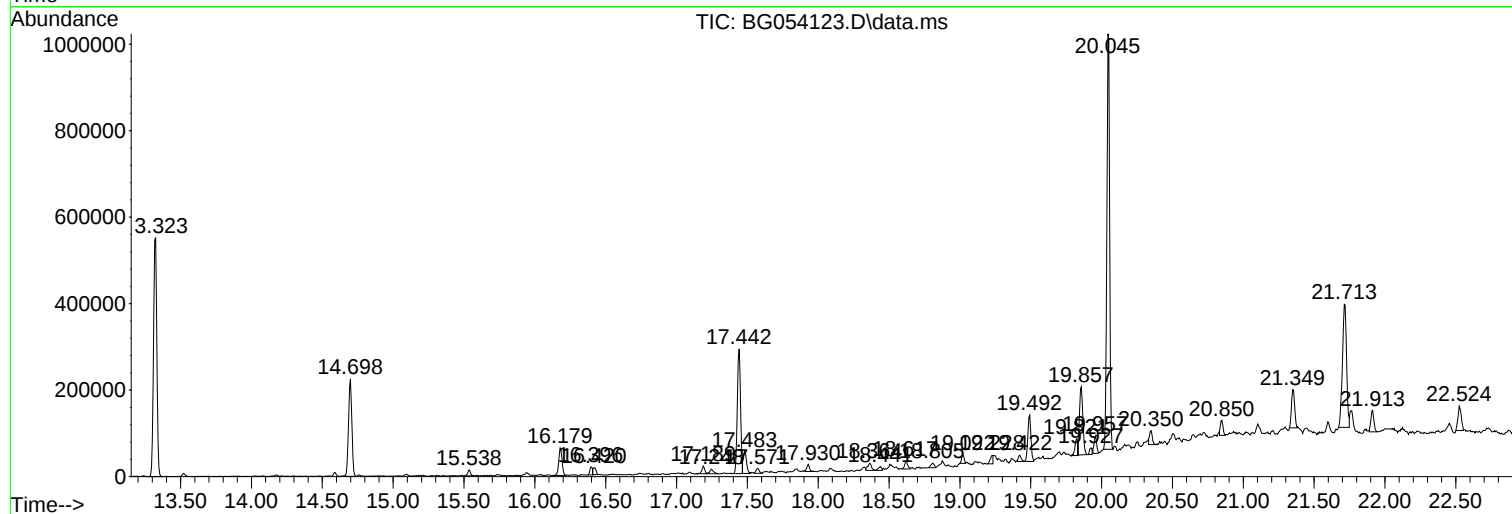
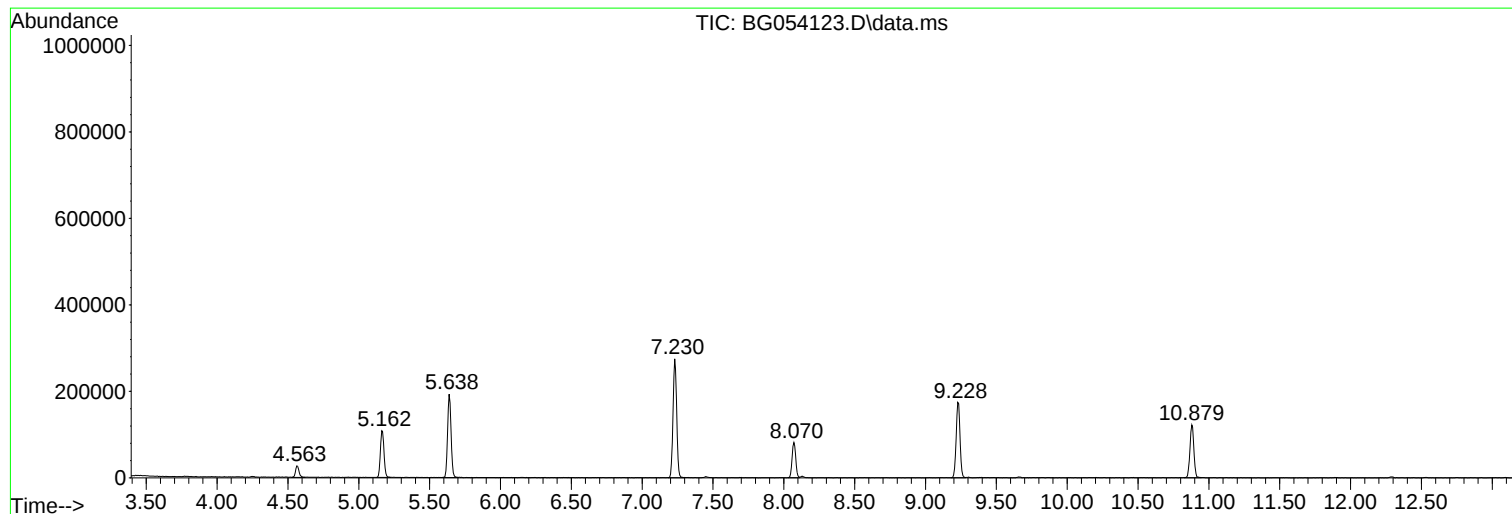
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062822\  
Data File : BG054123.D  
Acq On : 28 Jun 2022 18:51  
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Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.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\BG062822\  
Data File : BG054123.D  
Acq On : 28 Jun 2022 18:51  
Operator : CG/JU  
Sample : N3488-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

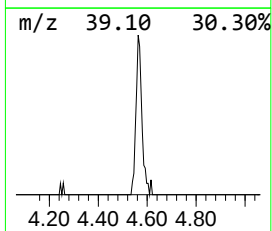
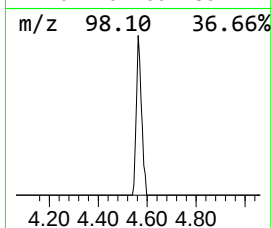
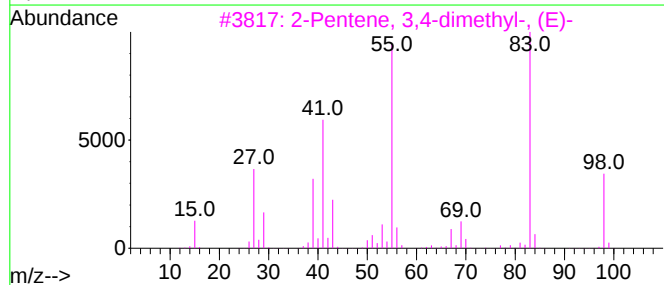
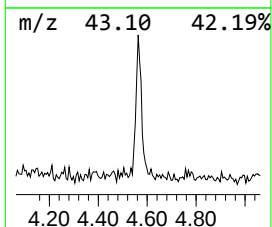
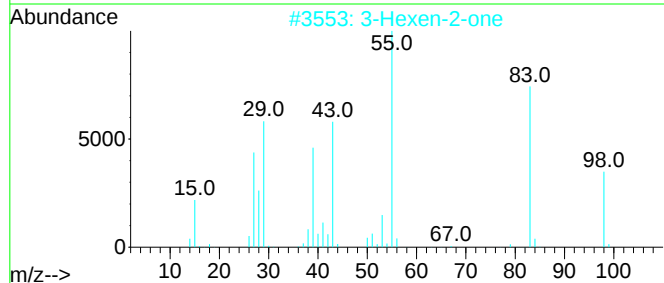
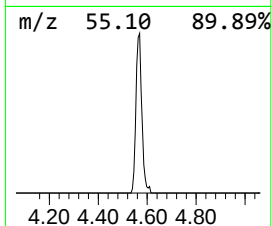
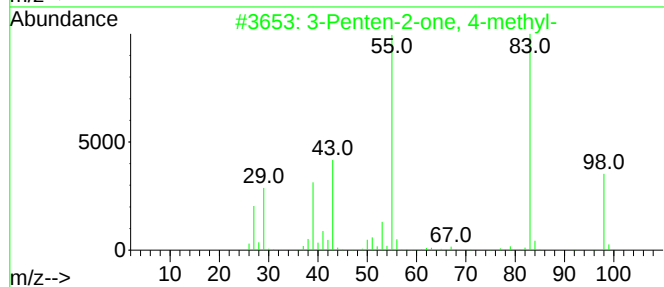
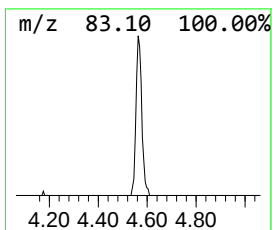
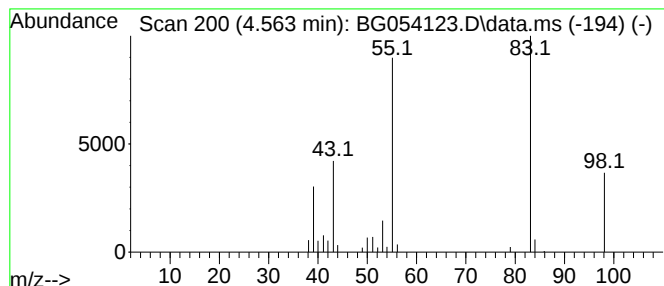
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.563 | 6.44 ng | 46749 | 1,4-Dichlorobenzene-d4 | 8.070 |

| Hit# | of 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|------|--------------------------------|----|---------|-------------|------|
| 1    |      | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |      | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |      | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 86   |
| 4    |      | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 72   |
| 5    |      | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14   | 000762-63-0 | 72   |



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Sample : N3488-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

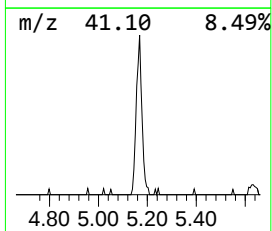
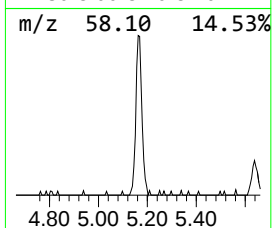
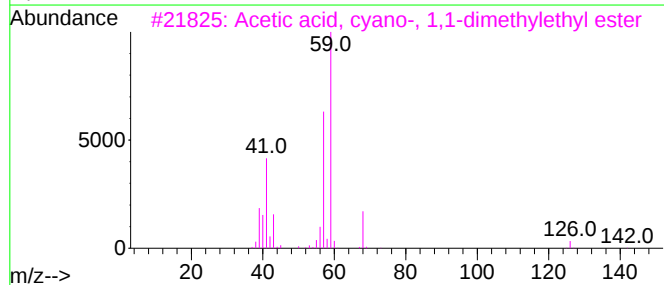
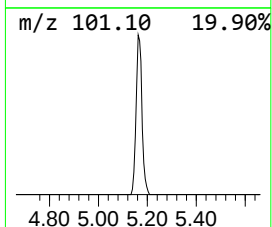
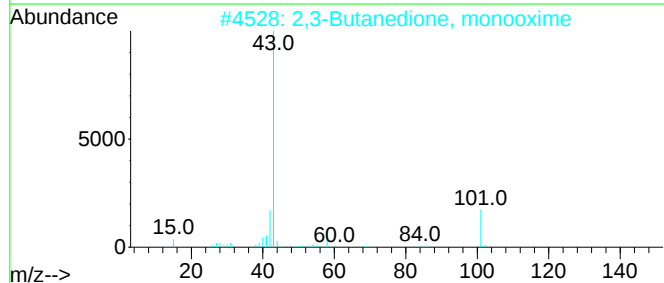
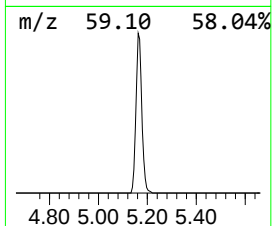
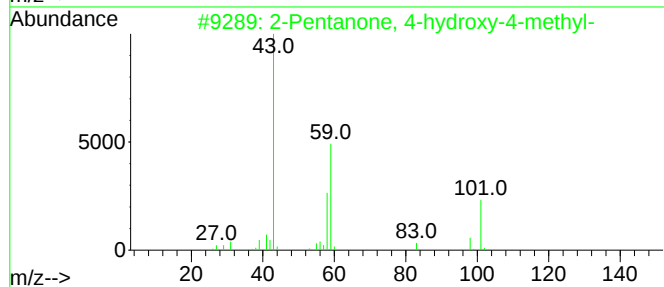
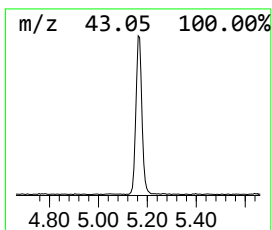
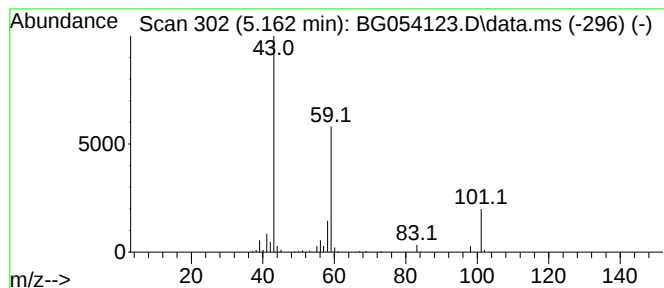
Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.      | EstConc                             | Area   | Relative to ISTD       |          |             | R.T.  |
|-----------|-------------------------------------|--------|------------------------|----------|-------------|-------|
| 5.162     | 25.48 ng                            | 184927 | 1,4-Dichlorobenzene-d4 |          |             | 8.070 |
| Hit# of 5 | Tentative ID                        |        | MW                     | MolForm  | CAS#        | Qual  |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    |        | 116                    | C6H12O2  | 000123-42-2 | 56    |
| 2         | 2,3-Butanedione, monooxime          |        | 101                    | C4H7NO2  | 000057-71-6 | 35    |
| 3         | Acetic acid, cyano-, 1,1-dimethy... |        | 141                    | C7H11NO2 | 001116-98-9 | 32    |
| 4         | 1,8-Nonanediol, 8-methyl-           |        | 174                    | C10H22O2 | 054725-73-4 | 25    |
| 5         | 1-Propen-2-ol, acetate              |        | 100                    | C5H8O2   | 000108-22-5 | 10    |



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Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

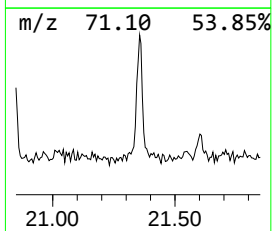
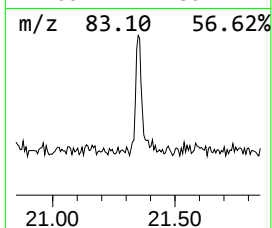
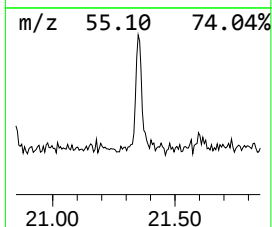
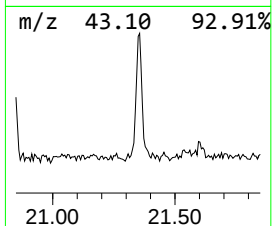
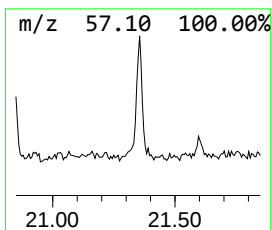
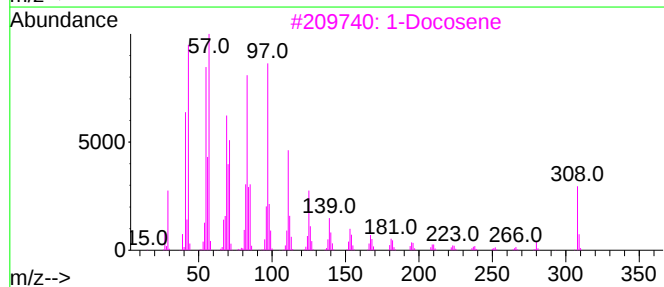
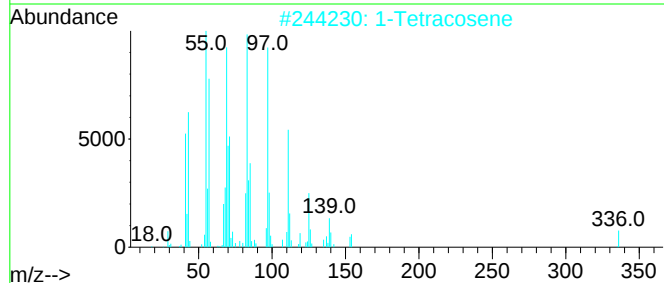
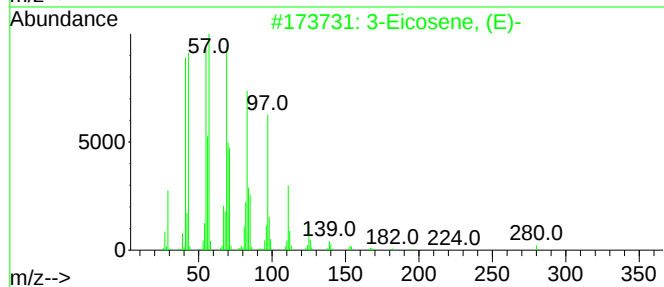
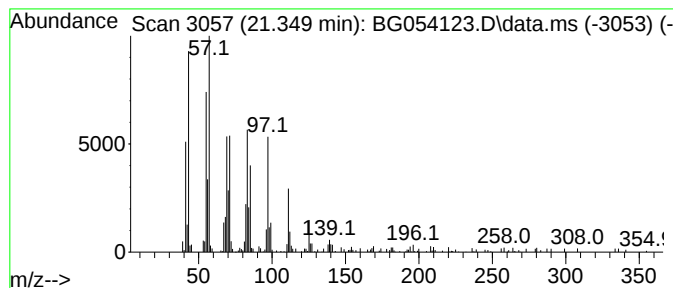
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 3-Eicosene, (E)- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.349 | 4.72 ng | 136691 | Chrysene-d12     | 21.719 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | 3-Eicosene, (E)-                    | 280 | C20H40      | 074685-33-9  | 98   |
| 2    |    |   | 1-Tetracosene                       | 336 | C24H48      | 010192-32-2  | 97   |
| 3    |    |   | 1-Docosene                          | 308 | C22H44      | 001599-67-3  | 95   |
| 4    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94   |
| 5    |    |   | 5-Eicosene, (E)-                    | 280 | C20H40      | 074685-30-6  | 92   |



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SB-9-22.5-24.5-20220623

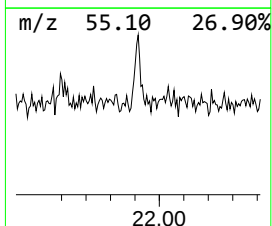
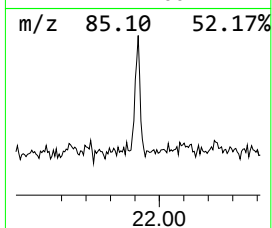
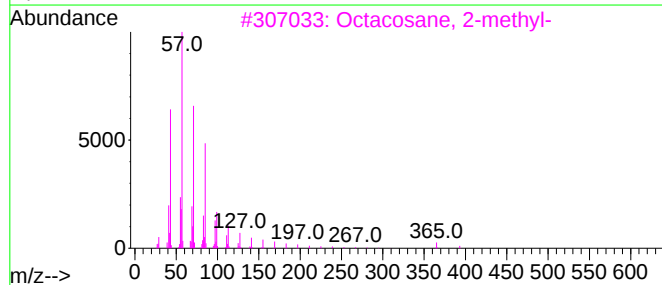
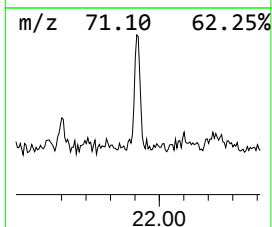
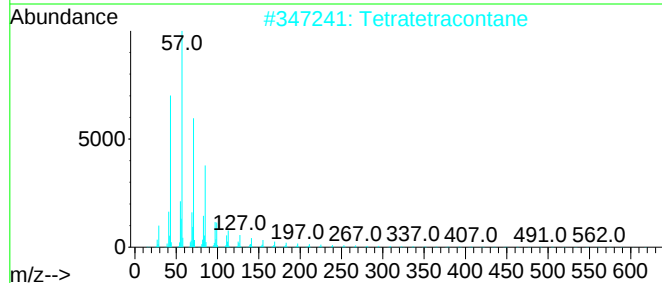
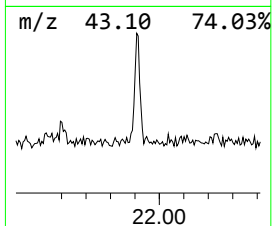
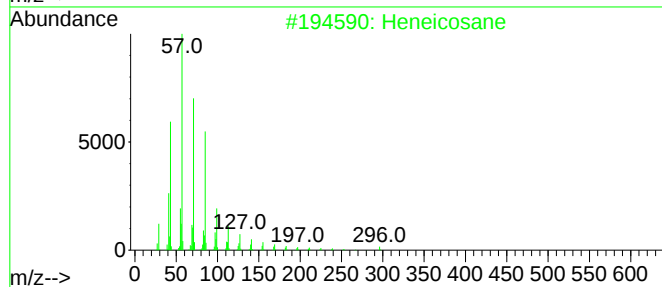
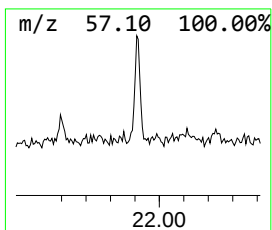
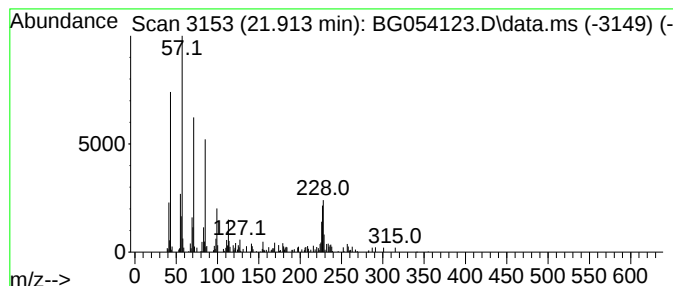
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Heneicosane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.913 | 2.52 ng | 73029 | Chrysene-d12     | 21.719 |

| Hit# | of 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|------|-----------------------|-----|---------|-------------|------|
| 1    |      | Heneicosane           | 296 | C21H44  | 000629-94-7 | 55   |
| 2    |      | Tetratetracontane     | 619 | C44H90  | 007098-22-8 | 45   |
| 3    |      | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 45   |
| 4    |      | Hexacosane            | 366 | C26H54  | 000630-01-3 | 45   |
| 5    |      | Octacosane            | 394 | C28H58  | 000630-02-4 | 45   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062822\  
Data File : BG054123.D  
Acq On : 28 Jun 2022 18:51  
Operator : CG/JU  
Sample : N3488-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

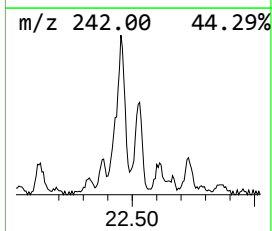
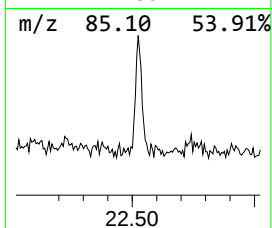
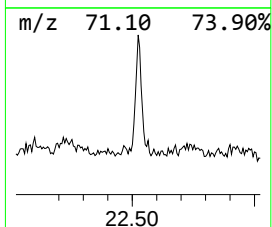
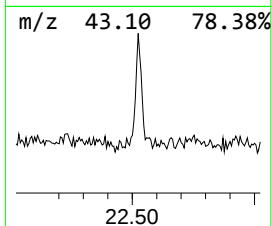
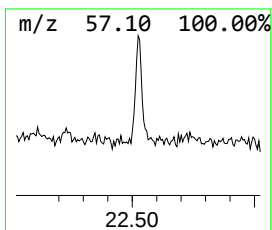
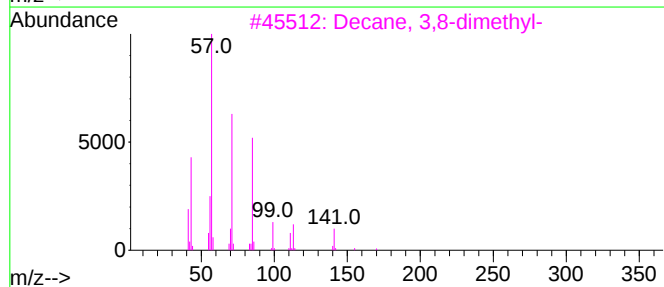
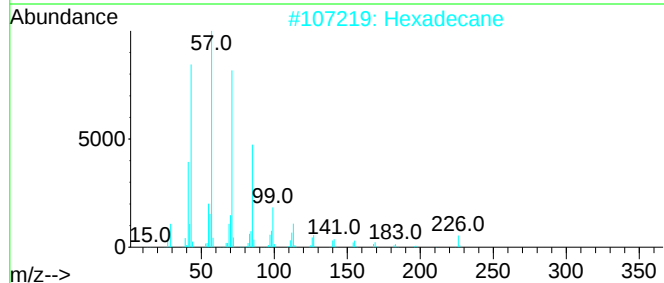
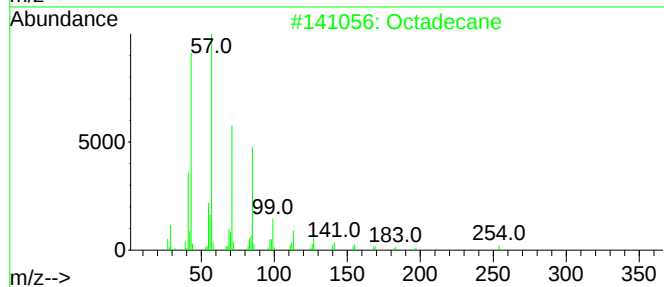
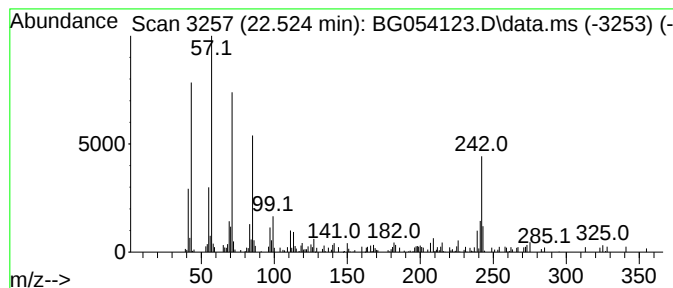
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Octadecane Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 22.524 | 3.11 ng | 90005 | Chrysene-d12     | 21.719 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Octadecane            | 254 | C18H38  | 000593-45-3 | 90   |
| 2    |    |   | Hexadecane            | 226 | C16H34  | 000544-76-3 | 78   |
| 3    |    |   | Decane, 3,8-dimethyl- | 170 | C12H26  | 017312-55-9 | 60   |
| 4    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 58   |
| 5    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062822\  
Data File : BG054123.D  
Acq On : 28 Jun 2022 18:51  
Operator : CG/JU  
Sample : N3488-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-9-22.5-24.5-20220623

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061322.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 |
| 3-Penten-2-one,... | 4.563  | 6.4     | ng    | 46749    | 1                     | 8.070  | 145178 | 20.0 |
| 2-Pentanone, 4-... | 5.162  | 25.5    | ng    | 184927   | 1                     | 8.070  | 145178 | 20.0 |
| 3-Eicosene, (E)-   | 21.349 | 4.7     | ng    | 136691   | 5                     | 21.719 | 578732 | 20.0 |
| Heneicosane        | 21.913 | 2.5     | ng    | 73029    | 5                     | 21.719 | 578732 | 20.0 |
| Octadecane         | 22.524 | 3.1     | ng    | 90005    | 5                     | 21.719 | 578732 | 20.0 |