

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG081721\  
 Data File : BG049879.D  
 Acq On : 17 Aug 2021 15:47  
 Operator : CG/JU  
 Sample : M3424-11  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 19S

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049879.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         | 3.138       | 11            | 17          | 29           | rVB      | 118134         | 239380        | 18.49%          | 2.484%        |
| 2         | 5.106       | 347           | 352         | 359          | rVB3     | 15633          | 25419         | 1.96%           | 0.264%        |
| 3         | 5.588       | 424           | 434         | 442          | rBV      | 500608         | 854977        | 66.04%          | 8.871%        |
| 4         | 7.197       | 699           | 708         | 722          | rBV      | 546438         | 960041        | 74.16%          | 9.962%        |
| 5         | 8.026       | 843           | 849         | 856          | rVB      | 128865         | 216727        | 16.74%          | 2.249%        |
| 6         | 9.195       | 1041          | 1048        | 1065         | rVB      | 336942         | 628334        | 48.54%          | 6.520%        |
| 7         | 10.610      | 1281          | 1289        | 1300         | rBV4     | 33176          | 78860         | 6.09%           | 0.818%        |
| 8         | 10.845      | 1317          | 1329        | 1336         | rBV      | 174500         | 323424        | 24.98%          | 3.356%        |
| 9         | 12.249      | 1564          | 1568        | 1573         | rVB4     | 10675          | 15104         | 1.17%           | 0.157%        |
| 10        | 13.201      | 1725          | 1730        | 1734         | rVB4     | 9815           | 14914         | 1.15%           | 0.155%        |
| 11        | 13.295      | 1738          | 1746        | 1756         | rBV      | 780696         | 1233984       | 95.32%          | 12.804%       |
| 12        | 13.489      | 1772          | 1779        | 1782         | rBV7     | 10080          | 17619         | 1.36%           | 0.183%        |
| 13        | 13.994      | 1858          | 1865        | 1871         | rBV10    | 8228           | 16011         | 1.24%           | 0.166%        |
| 14        | 14.141      | 1884          | 1890        | 1895         | rBV4     | 8517           | 13851         | 1.07%           | 0.144%        |
| 15        | 14.681      | 1973          | 1982        | 1988         | rVB      | 255446         | 409832        | 31.66%          | 4.252%        |
| 16        | 14.740      | 1988          | 1992        | 1998         | rBV4     | 9413           | 18543         | 1.43%           | 0.192%        |
| 17        | 15.081      | 2045          | 2050        | 2055         | rBV4     | 11079          | 20135         | 1.56%           | 0.209%        |
| 18        | 15.727      | 2155          | 2160        | 2164         | rBV6     | 10822          | 18779         | 1.45%           | 0.195%        |
| 19        | 16.021      | 2206          | 2210        | 2214         | rVB5     | 9095           | 13415         | 1.04%           | 0.139%        |
| 20        | 16.173      | 2230          | 2236        | 2243         | rBV      | 702256         | 1109625       | 85.72%          | 11.514%       |
| 21        | 17.084      | 2388          | 2391        | 2397         | rVB7     | 8116           | 13539         | 1.05%           | 0.140%        |
| 22        | 17.166      | 2400          | 2405        | 2409         | rBV7     | 14209          | 27591         | 2.13%           | 0.286%        |
| 23        | 17.225      | 2411          | 2415        | 2417         | rBV4     | 9708           | 14291         | 1.10%           | 0.148%        |
| 24        | 17.307      | 2425          | 2429        | 2437         | rVB7     | 18375          | 38359         | 2.96%           | 0.398%        |
| 25        | 17.431      | 2445          | 2450        | 2454         | rBV      | 273529         | 425665        | 32.88%          | 4.417%        |
| 26        | 17.478      | 2454          | 2458        | 2466         | rVB      | 144840         | 216894        | 16.75%          | 2.251%        |
| 27        | 17.566      | 2468          | 2473        | 2478         | rVB      | 27531          | 46151         | 3.57%           | 0.479%        |
| 28        | 17.736      | 2498          | 2502        | 2507         | rBV5     | 27646          | 43219         | 3.34%           | 0.448%        |
| 29        | 17.830      | 2514          | 2518        | 2519         | rBV4     | 15590          | 20697         | 1.60%           | 0.215%        |
| 30        | 17.906      | 2527          | 2531        | 2536         | rBV5     | 29261          | 40173         | 3.10%           | 0.417%        |
| 31        | 18.312      | 2596          | 2600        | 2604         | rBV2     | 46028          | 67491         | 5.21%           | 0.700%        |
| 32        | 18.365      | 2606          | 2609        | 2613         | rVB2     | 29580          | 38354         | 2.96%           | 0.398%        |
| 33        | 18.511      | 2629          | 2634        | 2637         | rBV6     | 28595          | 52898         | 4.09%           | 0.549%        |
| 34        | 18.600      | 2647          | 2649        | 2652         | rBV3     | 16756          | 18608         | 1.44%           | 0.193%        |
| 35        | 19.487      | 2796          | 2800        | 2806         | rBV      | 205722         | 285598        | 22.06%          | 2.963%        |
| 36        | 19.816      | 2852          | 2856        | 2858         | rBV3     | 40597          | 64754         | 5.00%           | 0.672%        |

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Sample : M3424-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
19S

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-BG080321.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 19.851 | 2858 | 2862 | 2870 | rVB  | 182389  | 271870  | 21.00%  | 2.821%  |
| 38 | 20.045 | 2890 | 2895 | 2901 | rVB  | 1004893 | 1294551 | 100.00% | 13.433% |
| 39 | 21.719 | 3175 | 3180 | 3185 | rVB3 | 236611  | 427774  | 33.04%  | 4.439%  |

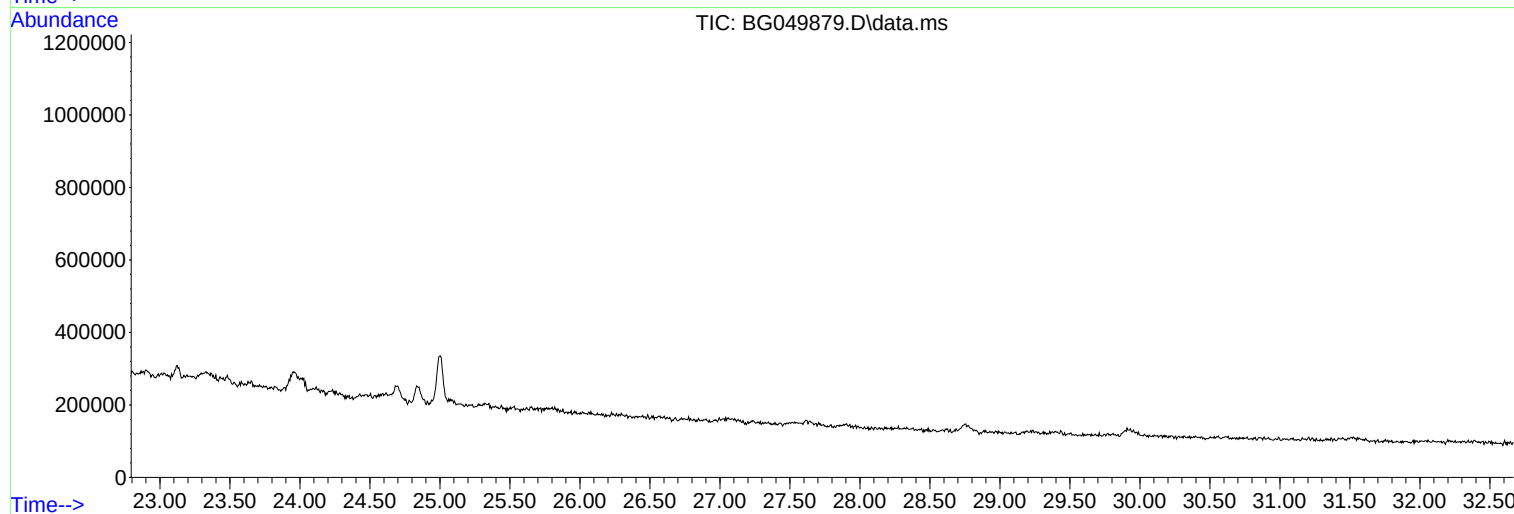
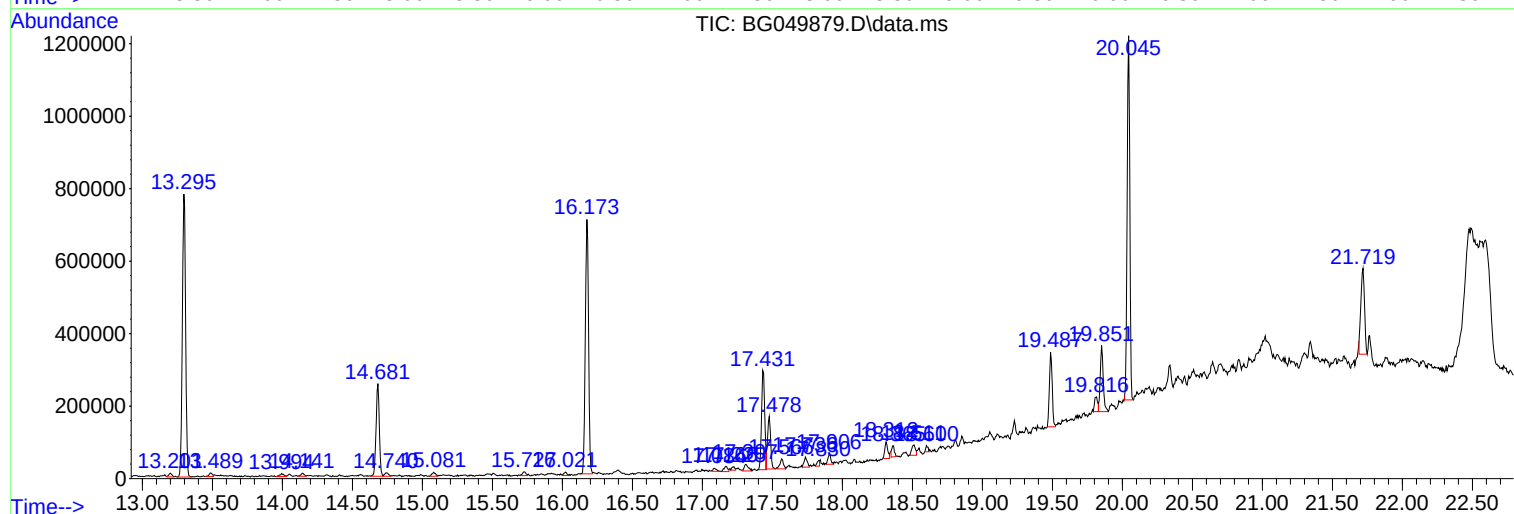
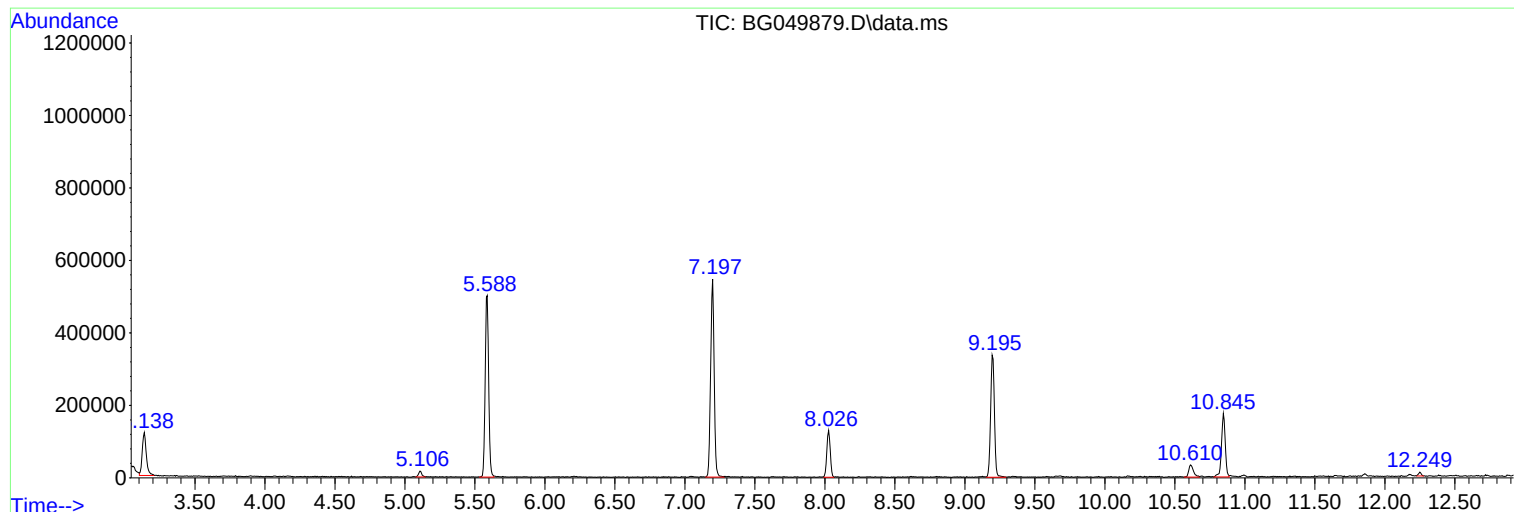
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BNA\_G  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG081721\  
Data File : BG049879.D  
Acq On : 17 Aug 2021 15:47  
Operator : CG/JU  
Sample : M3424-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
19S

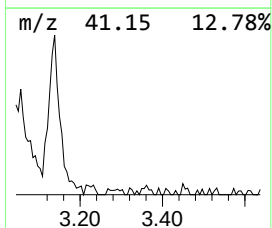
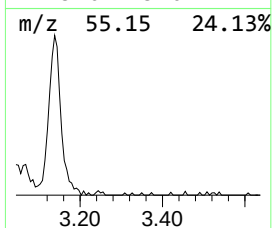
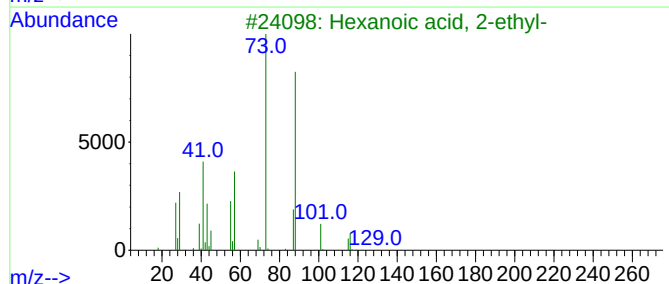
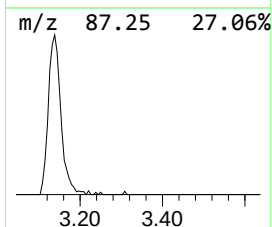
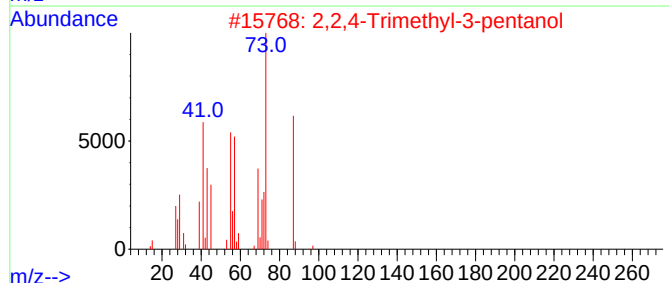
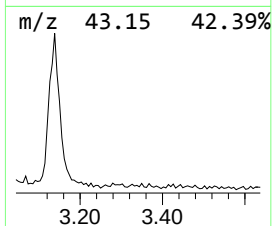
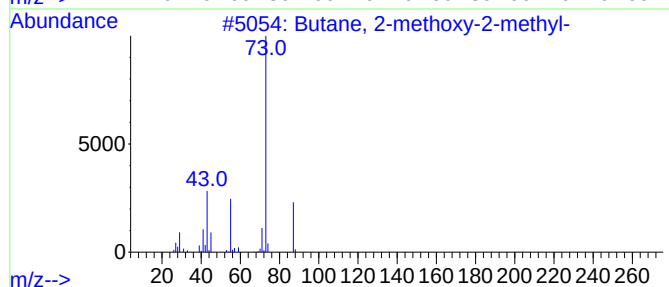
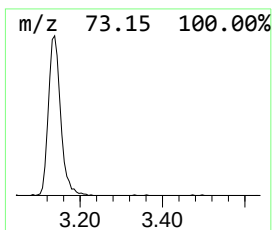
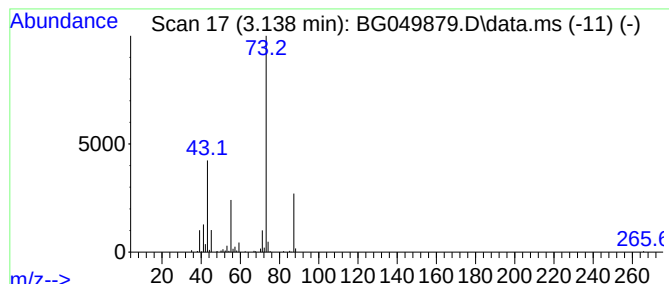
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.138 | 22.09 ng | 239380 | 1,4-Dichlorobenzene-d4 | 8.026 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl-         | 102 | C6H14O   | 000994-05-8  | 72   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol          | 130 | C8H18O   | 005162-48-1  | 56   |
| 3    |    |   | Hexanoic acid, 2-ethyl-             | 144 | C8H16O2  | 000149-57-5  | 28   |
| 4    |    |   | 1-(2-Methoxyethoxy)-2-methyl-2-p... | 162 | C8H18O3  | 1000364-24-4 | 17   |
| 5    |    |   | Octanal, 7-methoxy-3,7-dimethyl-    | 186 | C11H22O2 | 003613-30-7  | 12   |



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Instrument :  
BNA\_G  
ClientSampled :  
19S

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

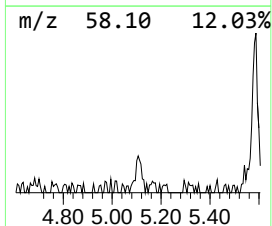
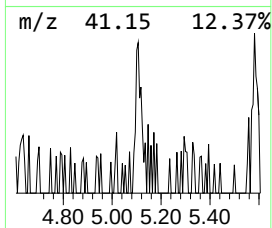
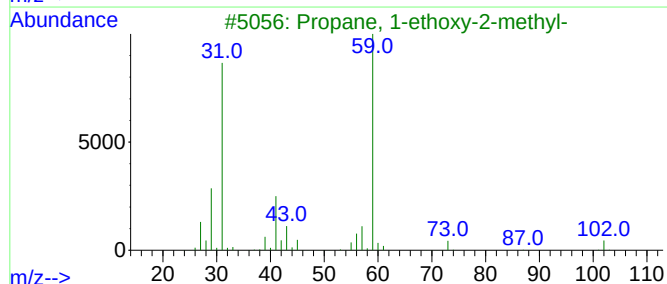
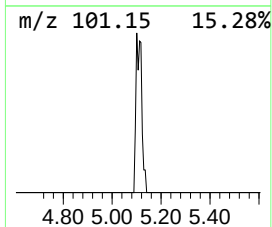
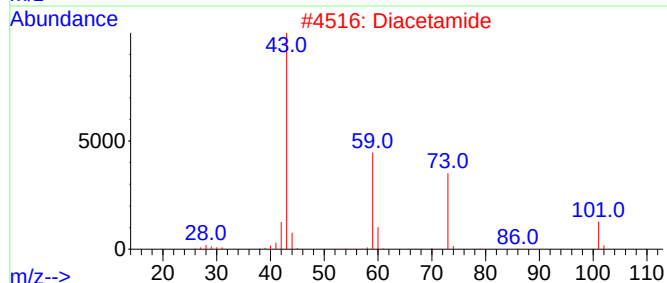
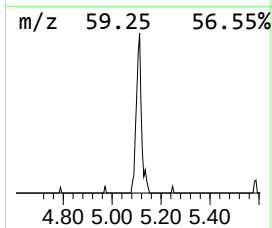
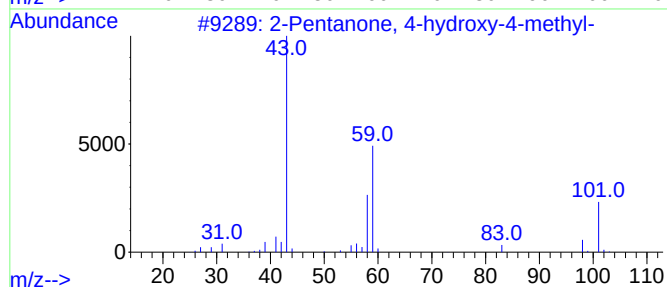
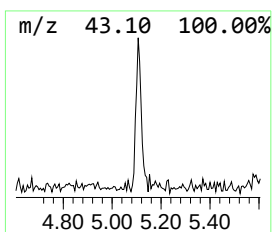
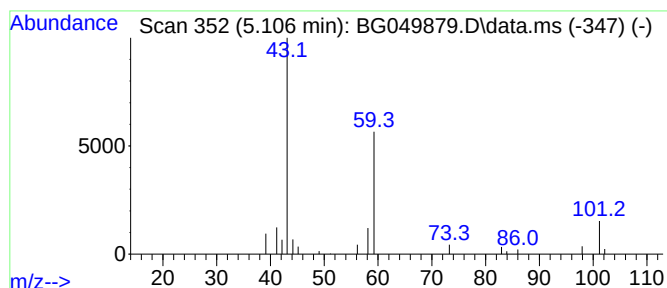
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.106 | 2.35 ng | 25419 | 1,4-Dichlorobenzene-d4 | 8.026 |

| Hit# | of 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|------|----------------------------------|-----|---------|-------------|------|
| 1    |      | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59   |
| 2    |      | Diacetamide                      | 101 | C4H7NO2 | 000625-77-4 | 36   |
| 3    |      | Propane, 1-ethoxy-2-methyl-      | 102 | C6H14O  | 000627-02-1 | 25   |
| 4    |      | 3-Hexanol                        | 102 | C6H14O  | 000623-37-0 | 23   |
| 5    |      | Butane, 1-ethoxy-                | 102 | C6H14O  | 000628-81-9 | 9    |



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Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
19S

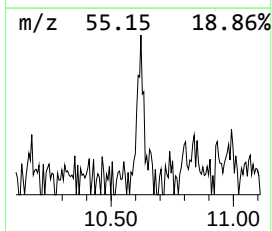
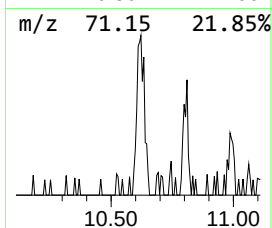
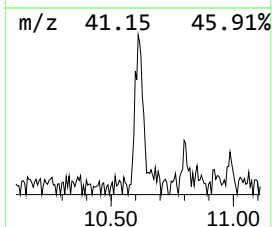
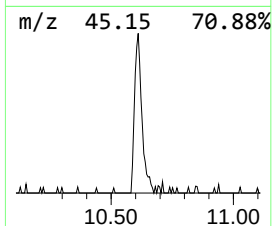
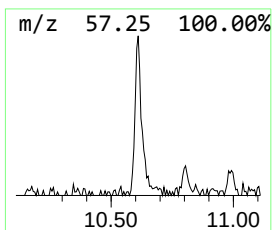
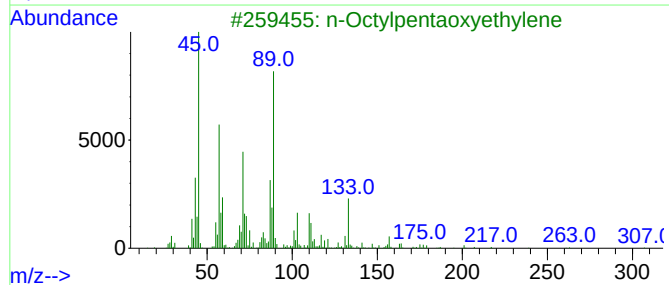
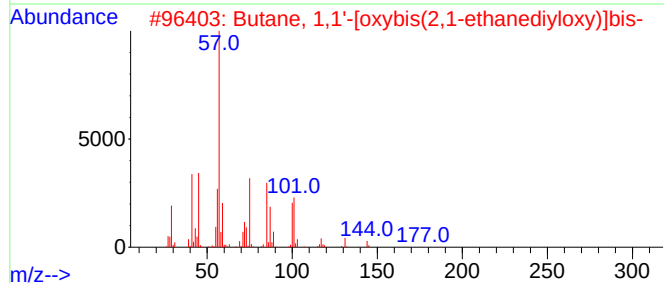
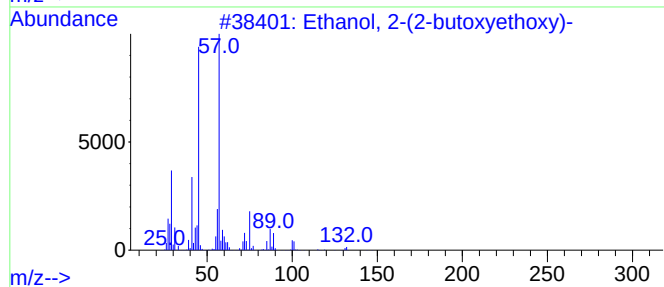
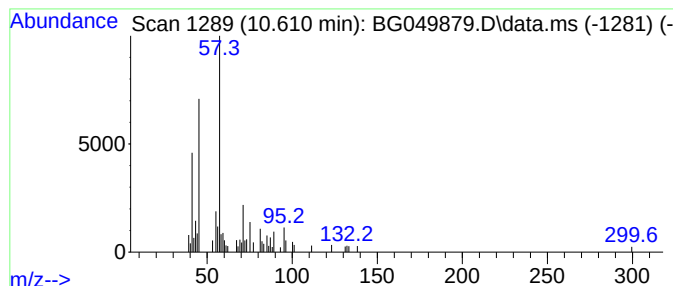
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown10.610 Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 10.610 | 4.88 ng | 78860 | Naphthalene-d8   | 10.845 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-butoxyethoxy)-         | 162 | C8H18O3  | 000112-34-5 | 49   |
| 2    |    |   | Butane, 1,1'-[oxybis(2,1-ethaned...  | 218 | C12H26O3 | 000112-73-2 | 43   |
| 3    |    |   | n-Octylpentaoxyethylene              | 350 | C18H38O6 | 019327-40-3 | 38   |
| 4    |    |   | Butane, 1,1'-[ethylidenebis(oxy)...] | 174 | C10H22O2 | 000871-22-7 | 38   |
| 5    |    |   | 3,6,9,12,15-Pentaoxanonadecan-1-ol   | 294 | C14H30O6 | 001786-94-3 | 35   |



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Instrument :  
BNA\_G  
ClientSampleId :  
19S

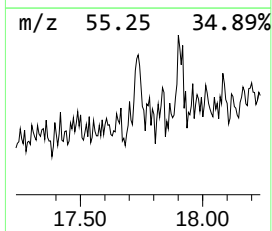
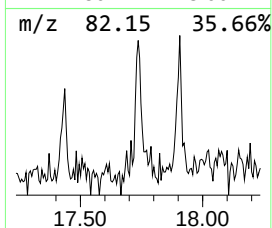
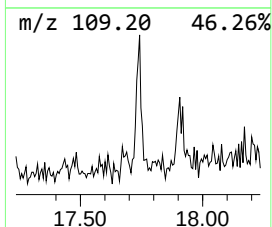
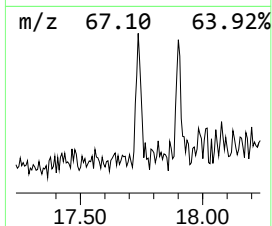
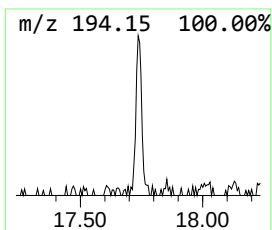
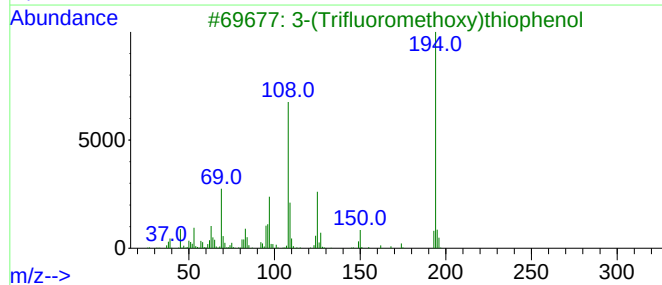
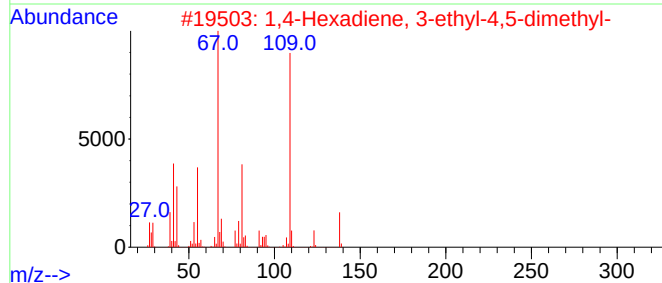
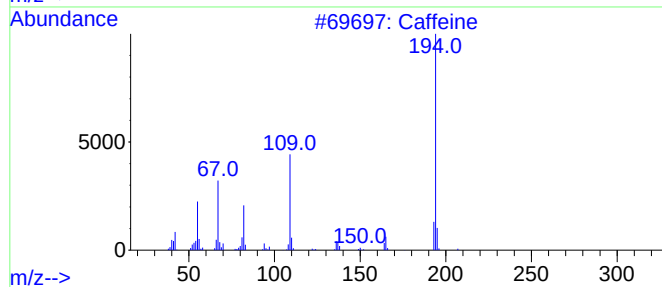
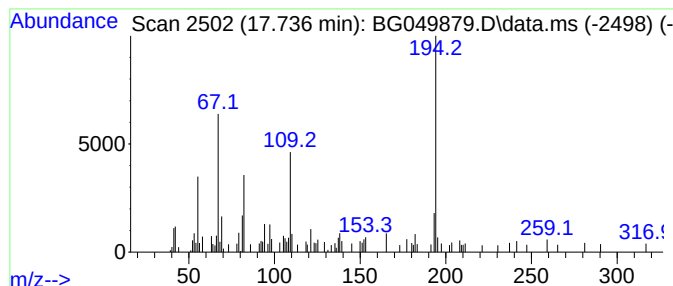
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Caffeine Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 17.736 | 2.03 ng | 43219 | Phenanthrene-d10 | 17.431 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Caffeine                            | 194 | C8H10N4O2 | 000058-08-2  | 58   |
| 2    |    |   | 1,4-Hexadiene, 3-ethyl-4,5-dimet... | 138 | C10H18    | 1000154-09-2 | 30   |
| 3    |    |   | 3-(Trifluoromethoxy)thiophenol      | 194 | C7H5F3OS  | 220239-66-7  | 27   |
| 4    |    |   | 4-Amino-6,8-difluoro-2-methylqui... | 194 | C10H8F2N2 | 288151-32-6  | 27   |
| 5    |    |   | 9-Acridinamine                      | 194 | C13H10N2  | 000090-45-9  | 27   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG081721\  
Data File : BG049879.D  
Acq On : 17 Aug 2021 15:47  
Operator : CG/JU  
Sample : M3424-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampled :  
19S

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

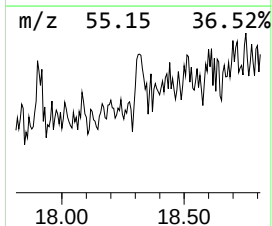
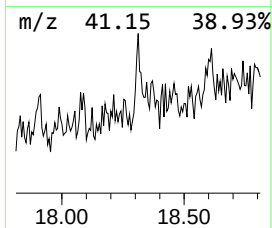
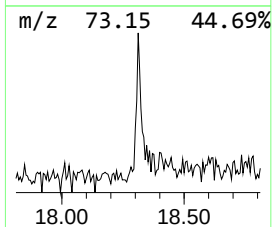
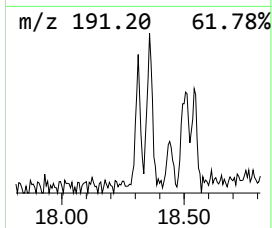
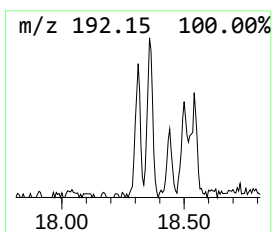
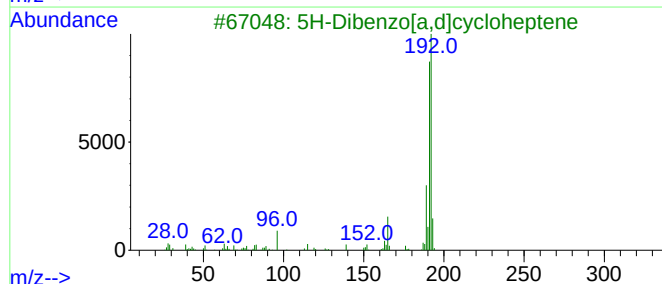
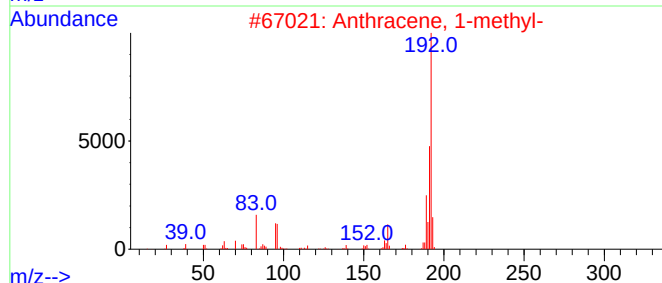
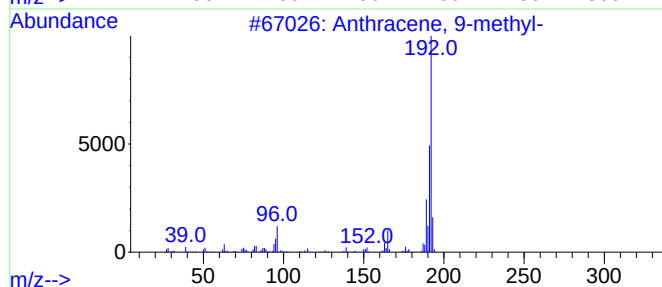
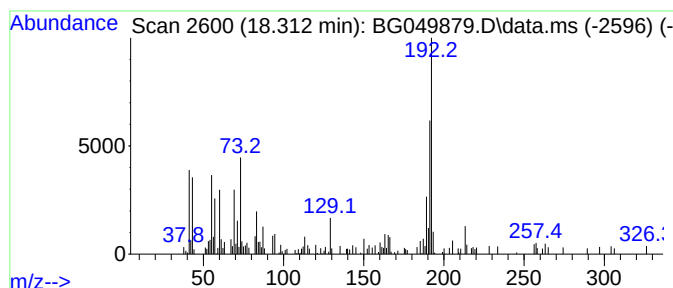
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Anthracene, 9-methyl- Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.312 | 3.17 ng | 67491 | Phenanthrene-d10 | 17.431 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Anthracene, 9-methyl-       | 192 | C15H12  | 000779-02-2 | 53   |
| 2    |    |   | Anthracene, 1-methyl-       | 192 | C15H12  | 000610-48-0 | 49   |
| 3    |    |   | 5H-Dibenzo[a,d]cycloheptene | 192 | C15H12  | 000256-81-5 | 49   |
| 4    |    |   | 1H-Indene, 2-phenyl-        | 192 | C15H12  | 004505-48-0 | 49   |
| 5    |    |   | Phenanthrene, 3-methyl-     | 192 | C15H12  | 000832-71-3 | 43   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG081721\  
Data File : BG049879.D  
Acq On : 17 Aug 2021 15:47  
Operator : CG/JU  
Sample : M3424-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
19S

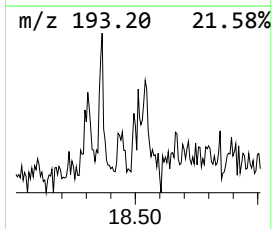
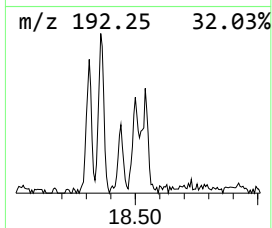
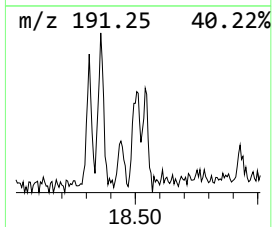
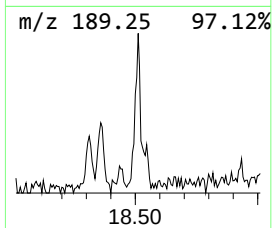
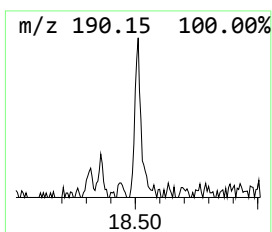
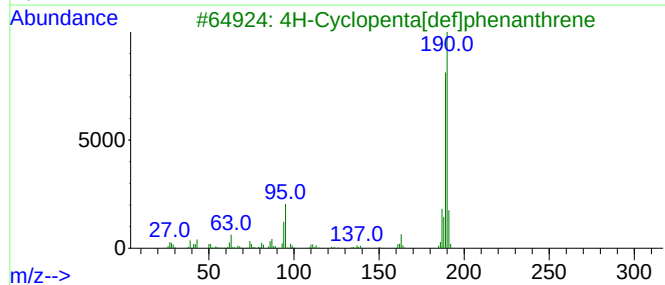
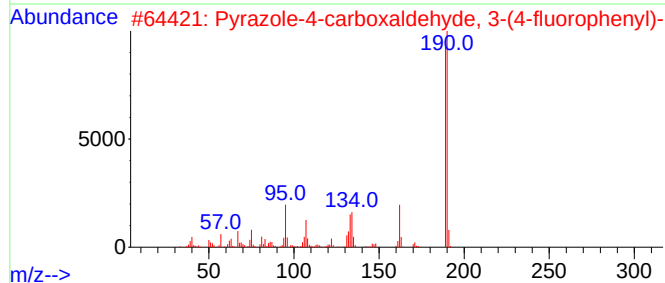
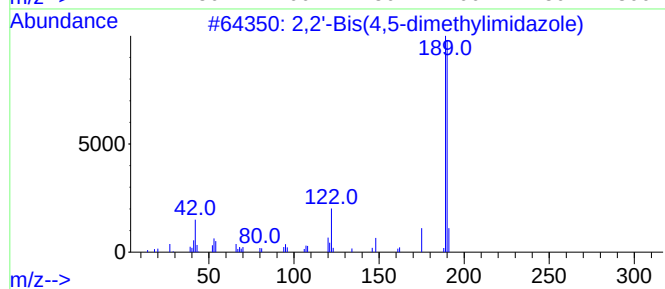
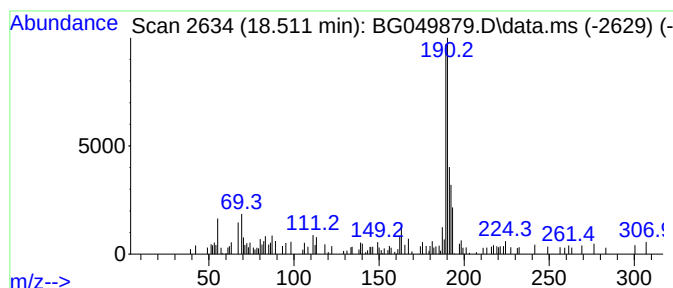
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 2,2'-Bis(4,5-dimethylimidaz... Concentration Rank 4

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 18.512    | 2.49 ng                             | 52898 | Phenanthrene-d10 | 17.431       |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | 2,2'-Bis(4,5-dimethylimidazole)     | 190   | C10H14N4         | 069286-06-2  | 50   |
| 2         | Pyrazole-4-carboxaldehyde, 3-(4-... | 190   | C10H7FN2O        | 306936-57-2  | 47   |
| 3         | 4H-Cyclopenta[def]phenanthrene      | 190   | C15H10           | 000203-64-5  | 40   |
| 4         | Glaucyl alcohol                     | 220   | C15H24O          | 087745-32-2  | 35   |
| 5         | l-Alanine, n-pentafluoropropiony... | 403   | C18H30F5NO3      | 1000323-37-9 | 35   |



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Data File : BG049879.D  
Acq On : 17 Aug 2021 15:47  
Operator : CG/JU  
Sample : M3424-11  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
19S

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG080321.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 |
| Butane, 2-metho... | 3.138  | 22.1    | ng    | 239380   | 1                     | 8.026  | 216727 | 20.0 |
| 2-Pentanone, 4-... | 5.106  | 2.4     | ng    | 25419    | 1                     | 8.026  | 216727 | 20.0 |
| unknown10.610      | 10.610 | 4.9     | ng    | 78860    | 2                     | 10.845 | 323424 | 20.0 |
| Caffeine           | 17.736 | 2.0     | ng    | 43219    | 4                     | 17.431 | 425665 | 20.0 |
| Anthracene, 9-m... | 18.312 | 3.2     | ng    | 67491    | 4                     | 17.431 | 425665 | 20.0 |
| 2,2'-Bis(4,5-di... | 18.512 | 2.5     | ng    | 52898    | 4                     | 17.431 | 425665 | 20.0 |