

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\  
 Data File : BG021090.D  
 Acq On : 26 Feb 2016 22:46  
 Operator : UM/SJ  
 Sample : H1558-03  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 S5

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG022616.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 3.094       | 37            | 43          | 59           | rVV      | 322570         | 475501        | 100.00%         | 19.999%       |
| 2         | 3.235       | 62            | 67          | 75           | rVV2     | 7180           | 14443         | 3.04%           | 0.607%        |
| 3         | 5.262       | 407           | 412         | 419          | rBB      | 14471          | 21194         | 4.46%           | 0.891%        |
| 4         | 5.726       | 485           | 491         | 497          | rBB      | 70706          | 111116        | 23.37%          | 4.673%        |
| 5         | 7.312       | 754           | 761         | 768          | rBB      | 77975          | 125827        | 26.46%          | 5.292%        |
| 6         | 7.700       | 820           | 827         | 833          | rBB      | 73724          | 121770        | 25.61%          | 5.121%        |
| 7         | 8.170       | 902           | 907         | 913          | rBB      | 19097          | 29112         | 6.12%           | 1.224%        |
| 8         | 8.493       | 956           | 962         | 969          | rBB      | 52288          | 88558         | 18.62%          | 3.725%        |
| 9         | 9.334       | 1098          | 1105        | 1111         | rBB      | 46031          | 78412         | 16.49%          | 3.298%        |
| 10        | 10.985      | 1379          | 1386        | 1392         | rBB      | 25588          | 43310         | 9.11%           | 1.822%        |
| 11        | 13.405      | 1792          | 1798        | 1805         | rBB      | 136116         | 199335        | 41.92%          | 8.384%        |
| 12        | 14.222      | 1932          | 1937        | 1942         | rBB      | 13501          | 16880         | 3.55%           | 0.710%        |
| 13        | 14.780      | 2026          | 2032        | 2038         | rBB2     | 41674          | 66424         | 13.97%          | 2.794%        |
| 14        | 15.609      | 2169          | 2173        | 2176         | rBB      | 4072           | 5044          | 1.06%           | 0.212%        |
| 15        | 16.255      | 2277          | 2283        | 2289         | rBB2     | 123405         | 170246        | 35.80%          | 7.160%        |
| 16        | 16.466      | 2315          | 2319        | 2326         | rBB2     | 4239           | 6851          | 1.44%           | 0.288%        |
| 17        | 17.512      | 2490          | 2497        | 2503         | rBV      | 65516          | 92422         | 19.44%          | 3.887%        |
| 18        | 18.382      | 2641          | 2645        | 2652         | rBV2     | 14914          | 18139         | 3.81%           | 0.763%        |
| 19        | 19.645      | 2857          | 2860        | 2864         | rBV2     | 4830           | 4900          | 1.03%           | 0.206%        |
| 20        | 20.103      | 2933          | 2938        | 2944         | rVB      | 326055         | 410665        | 86.36%          | 17.272%       |
| 21        | 21.408      | 3156          | 3160        | 3164         | rBV2     | 15419          | 18911         | 3.98%           | 0.795%        |
| 22        | 21.778      | 3217          | 3223        | 3230         | rBV2     | 75621          | 123755        | 26.03%          | 5.205%        |
| 23        | 23.505      | 3512          | 3517        | 3525         | rVB      | 15029          | 27923         | 5.87%           | 1.174%        |
| 24        | 25.068      | 3775          | 3783        | 3794         | rVB      | 39187          | 106918        | 22.49%          | 4.497%        |

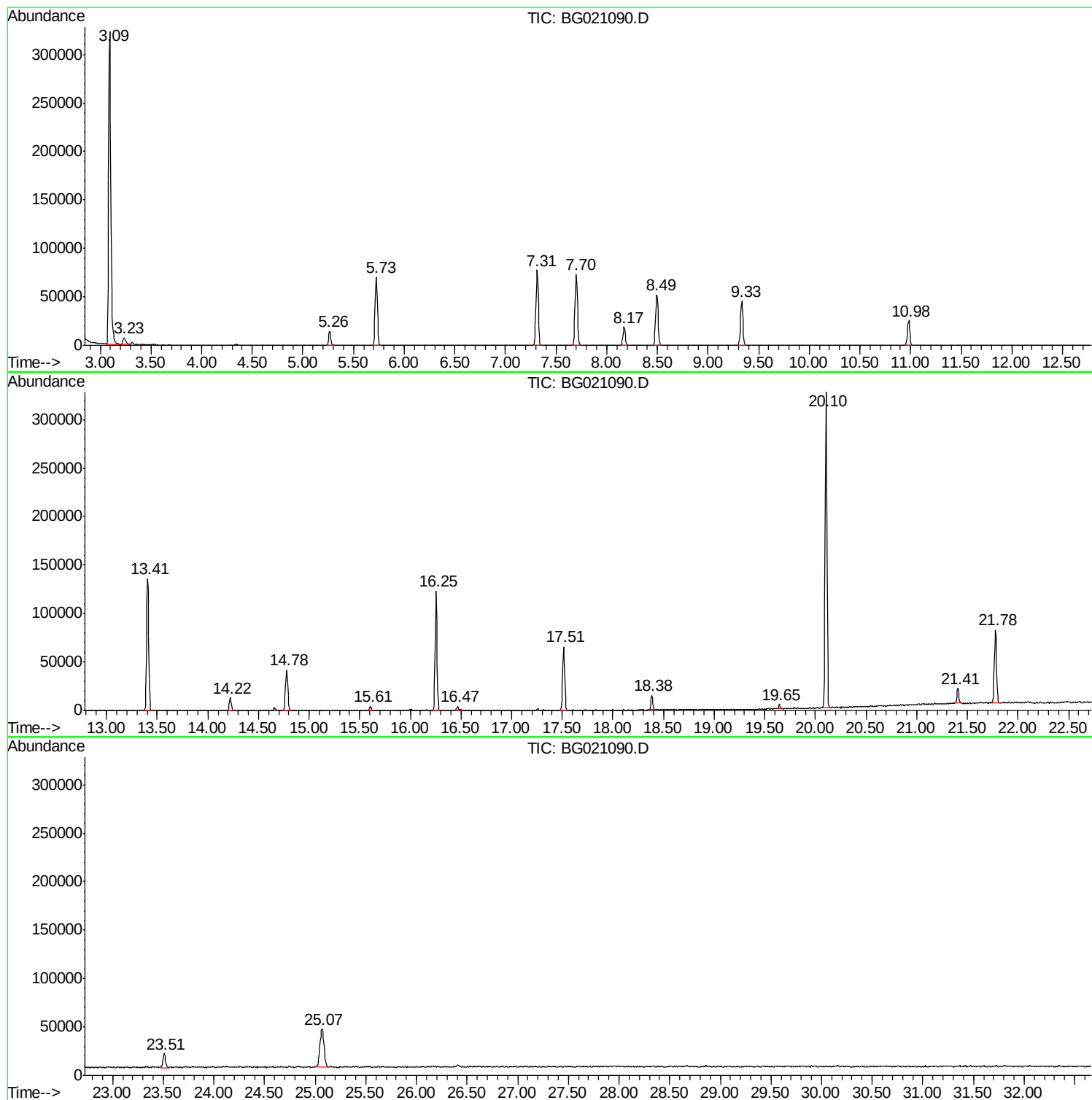
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Instrument :  
BNA\_G  
ClientSampleId :  
S5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022616.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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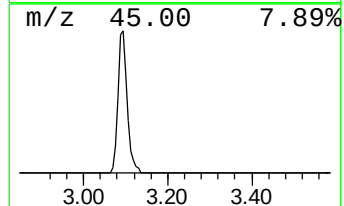
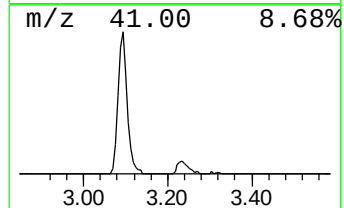
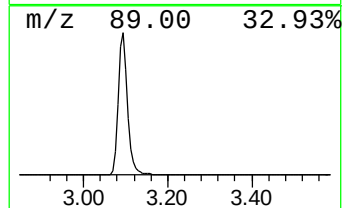
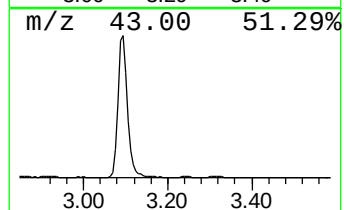
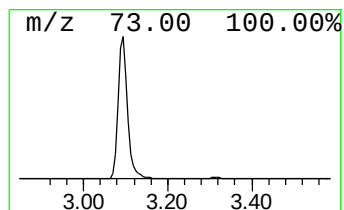
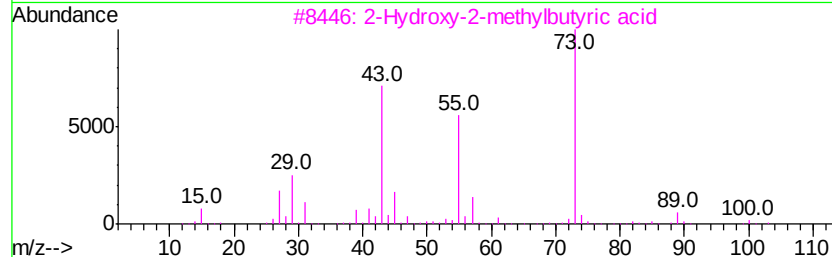
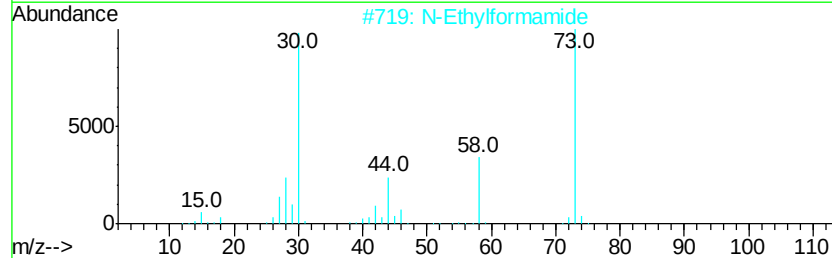
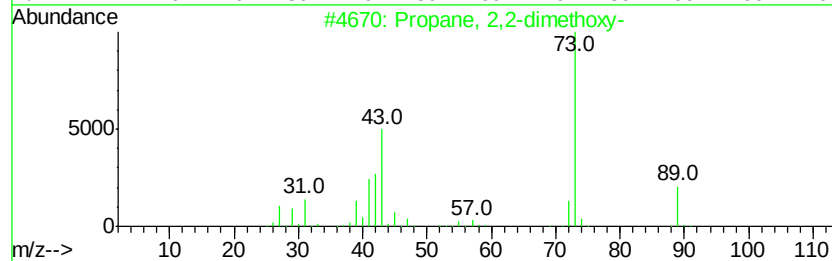
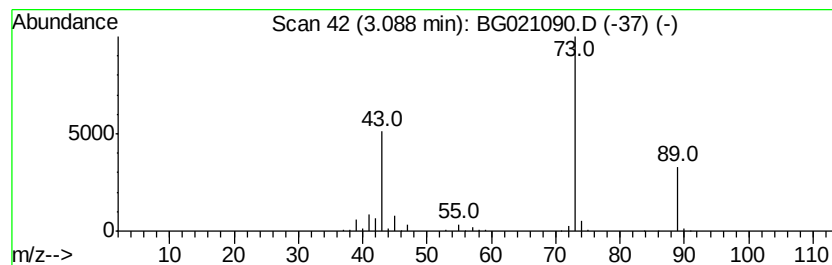
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD       | R.T. |
|------|-----------|--------|------------------------|------|
| 3.09 | 326.67 ng | 475501 | 1,4-Dichlorobenzene-d4 | 8.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-             | 104 | C5H12O2  | 000077-76-9 | 50   |
| 2    |    | N-Ethylformamide                    | 73  | C3H7NO   | 000627-45-2 | 9    |
| 3    |    | 2-Hydroxy-2-methylbutyric acid      | 118 | C5H10O3  | 003739-30-8 | 9    |
| 4    |    | 1-Hexen-4-ol, 1-chloro-3,5-dimet... | 162 | C8H15ClO | 100244-09-5 | 9    |
| 5    |    | Propane, 2-methoxy-2-methyl-        | 88  | C5H12O   | 001634-04-4 | 9    |



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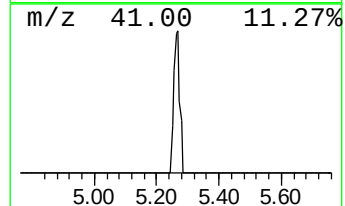
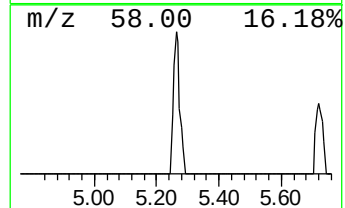
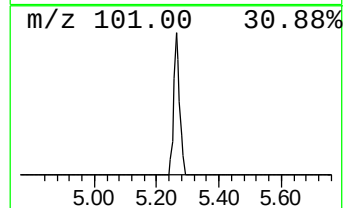
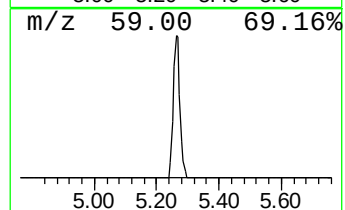
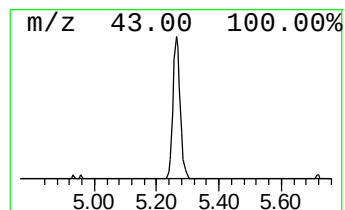
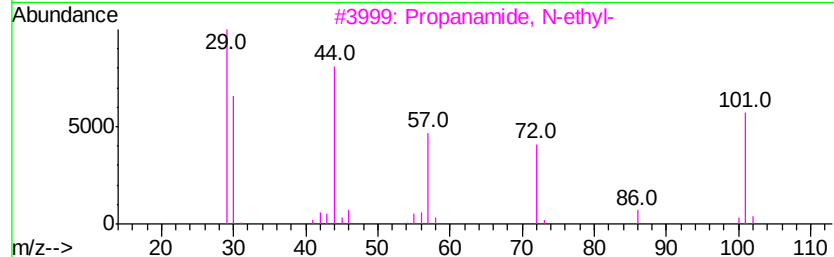
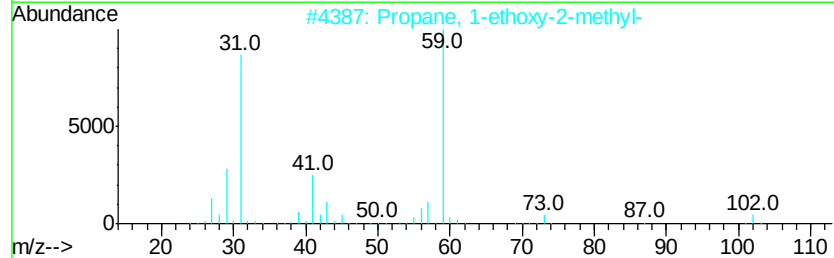
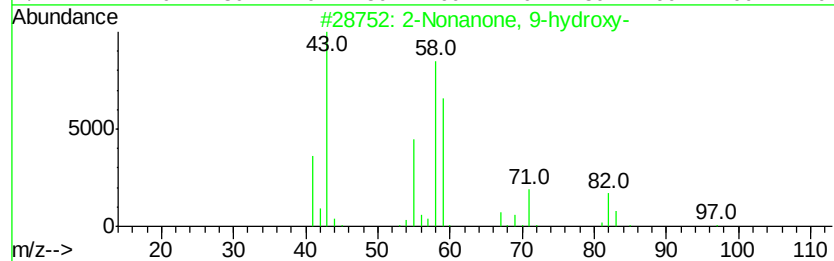
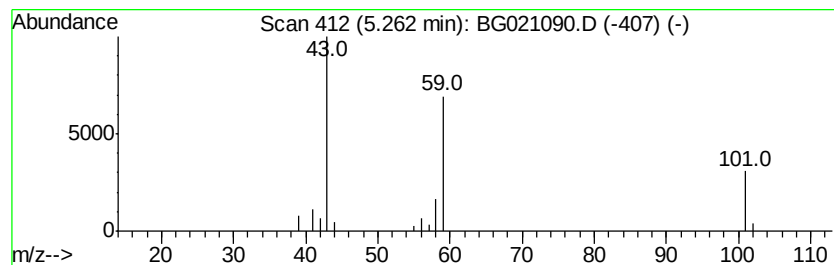
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown5.26 Concentration Rank 4

| R.T. | EstConc  | Area  | Relative to ISTD       | R.T. |
|------|----------|-------|------------------------|------|
| 5.26 | 14.56 ng | 21194 | 1,4-Dichlorobenzene-d4 | 8.17 |

| Hit# | of 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|------|------------------------------------|-----|---------|-------------|------|
| 1    |      | 2-Nonanone, 9-hydroxy-             | 158 | C9H18O2 | 025368-56-3 | 33   |
| 2    |      | Propane, 1-ethoxy-2-methyl-        | 102 | C6H14O  | 000627-02-1 | 17   |
| 3    |      | Propanamide, N-ethyl-              | 101 | C5H11NO | 005129-72-6 | 10   |
| 4    |      | Morpholine, 4-methyl-              | 101 | C5H11NO | 000109-02-4 | 9    |
| 5    |      | (+)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9    |



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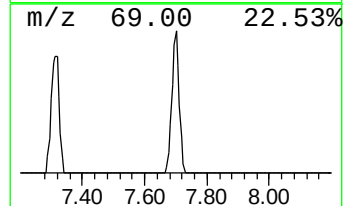
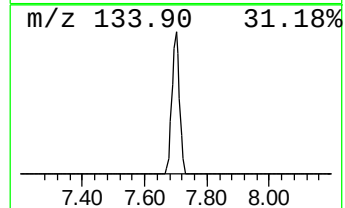
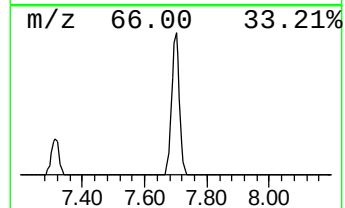
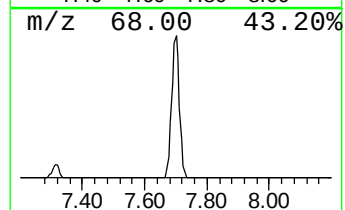
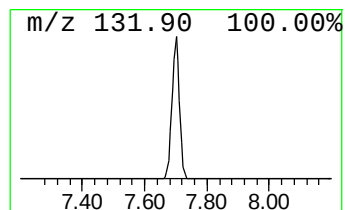
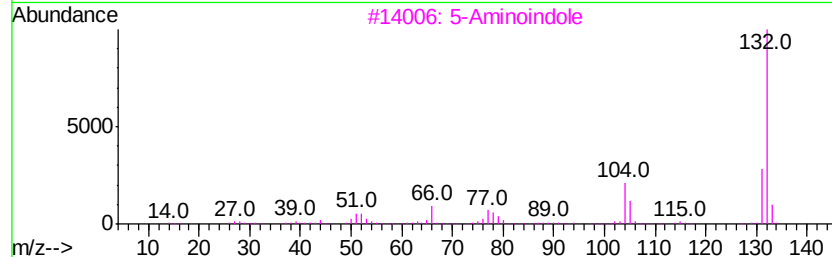
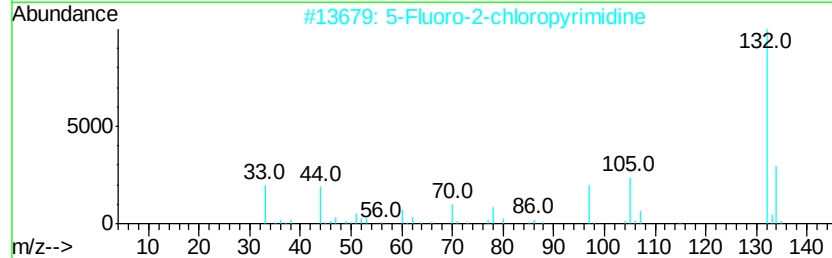
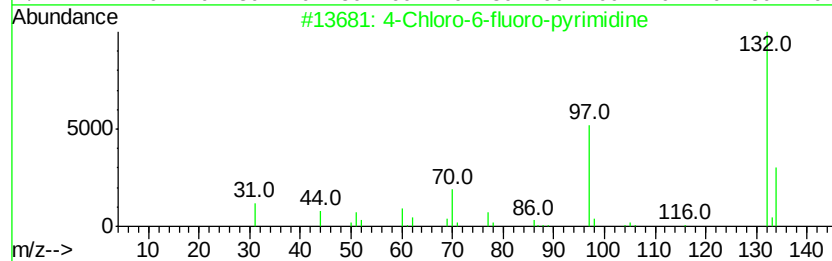
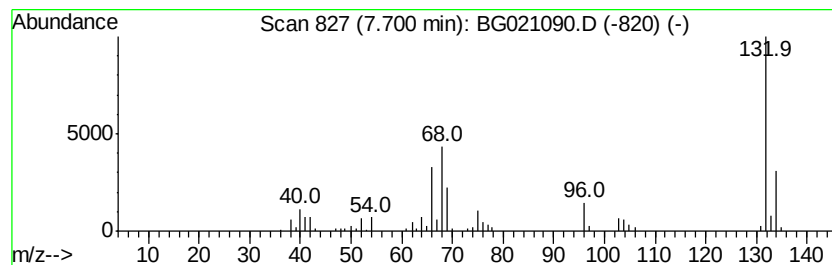
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown7.70 Concentration Rank 2

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 7.70 | 83.66 ng | 121770 | 1,4-Dichlorobenzene-d4 | 8.17 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|----------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0 | 27   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0 | 27   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6 | 22   |
| 5    |    | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2  | 014203-19-1 | 17   |



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S5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022616.M  
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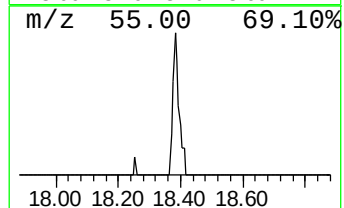
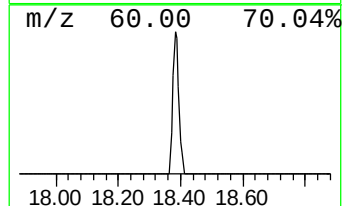
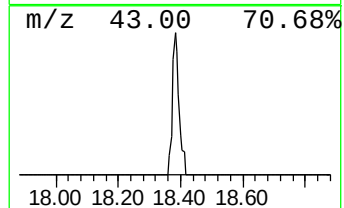
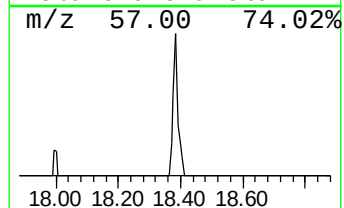
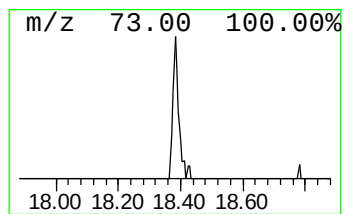
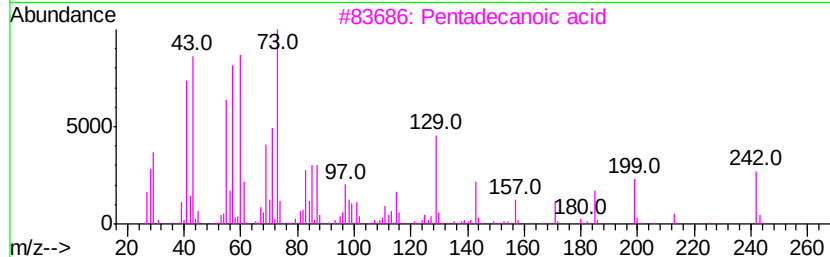
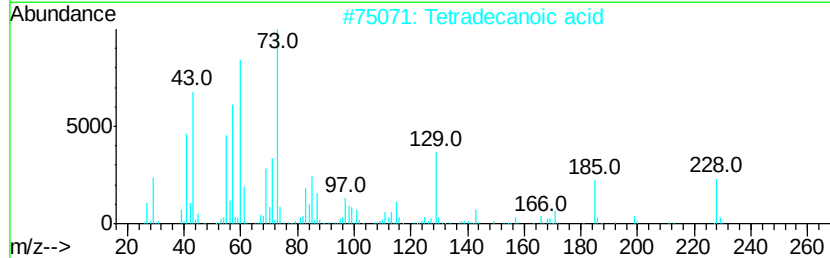
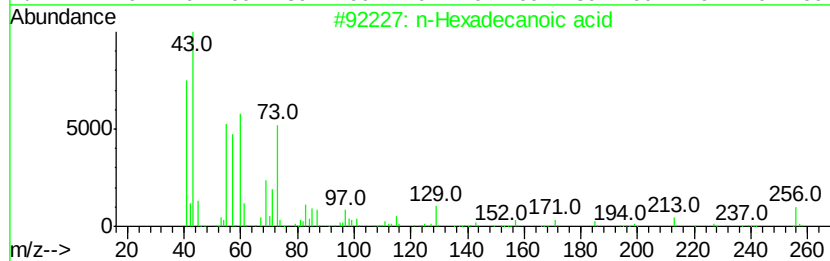
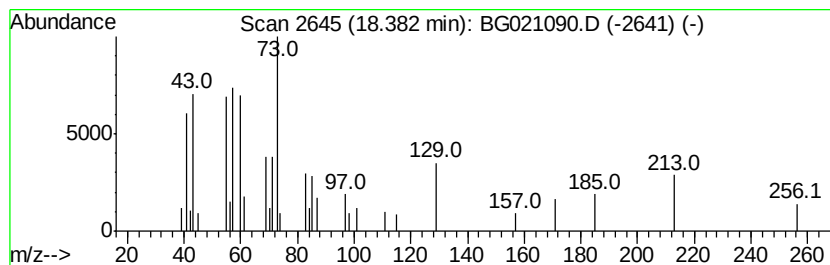
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 18.38 | 3.93 ng | 18139 | Phenanthrene-d10 | 17.51 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97   |
| 2    |    | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 3    |    | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 58   |
| 4    |    | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 47   |
| 5    |    | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 43   |



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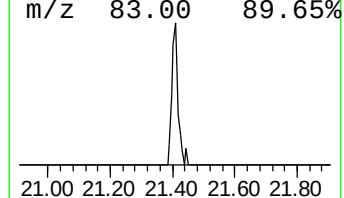
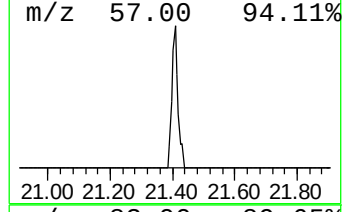
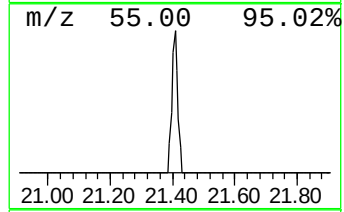
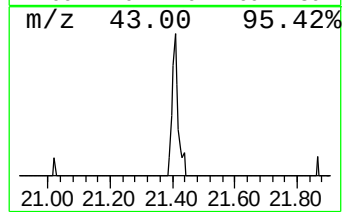
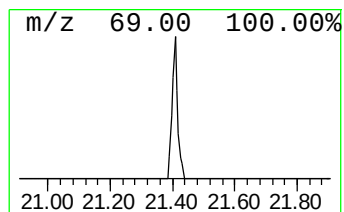
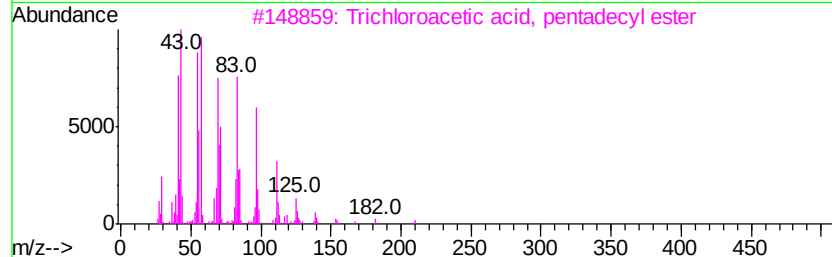
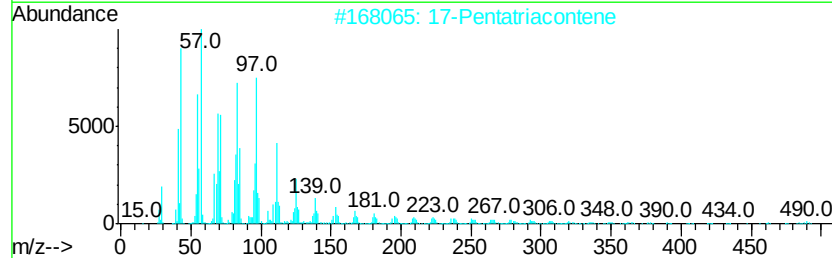
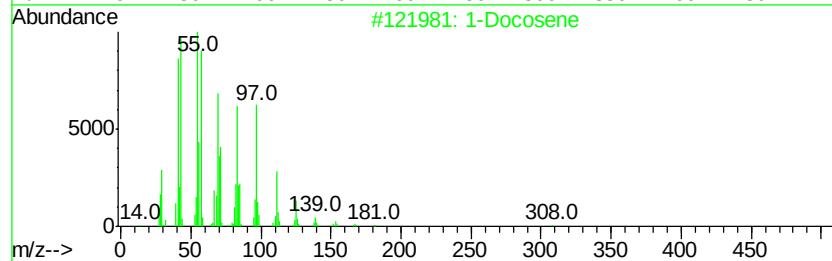
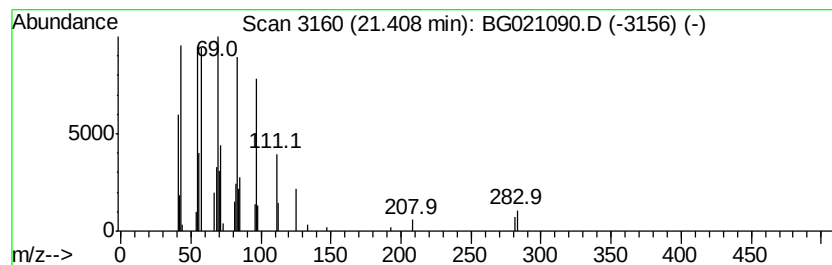
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 1-Docosene Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 21.41 | 3.06 ng | 18911 | Chrysene-d12     | 21.78 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | 1-Docosene                          | 308 | C22H44      | 001599-67-3  | 53   |
| 2    |    | 17-Pentatriacontene                 | 491 | C35H70      | 006971-40-0  | 49   |
| 3    |    | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0  | 49   |
| 4    |    | Heptafluorobutyric acid, n-penta... | 424 | C19H31F7O2  | 1000216-79-3 | 49   |
| 5    |    | 2-Chloropropionic acid, octadec...  | 360 | C21H41ClO2  | 088104-31-8  | 49   |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\  
Data File : BG021090.D  
Acq On : 26 Feb 2016 22:46  
Operator : UM/SJ  
Sample : H1558-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
S5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022616.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

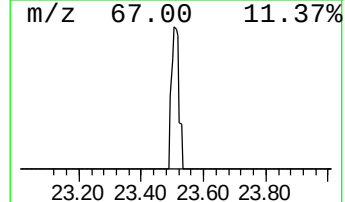
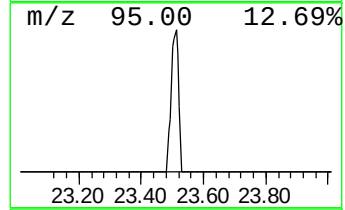
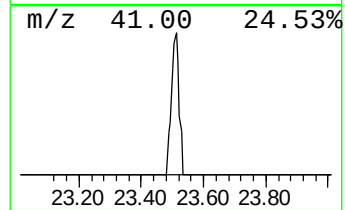
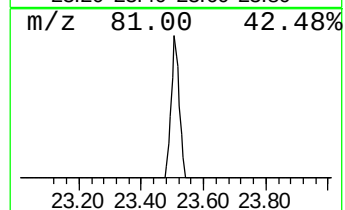
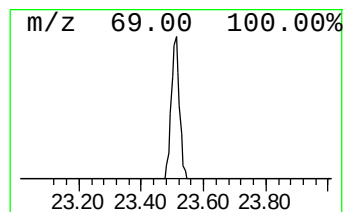
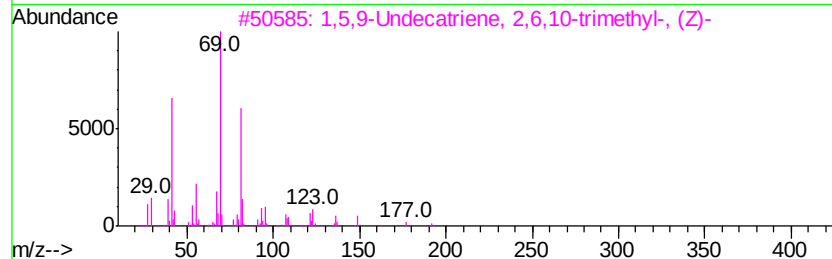
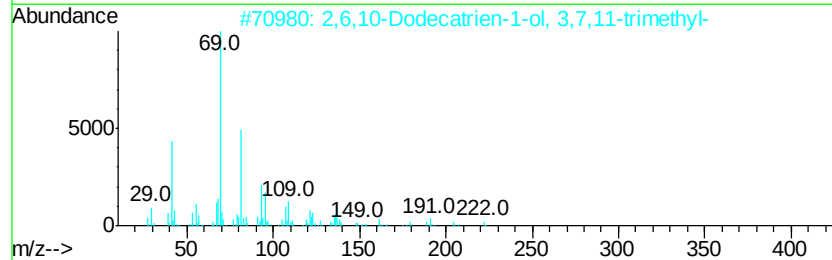
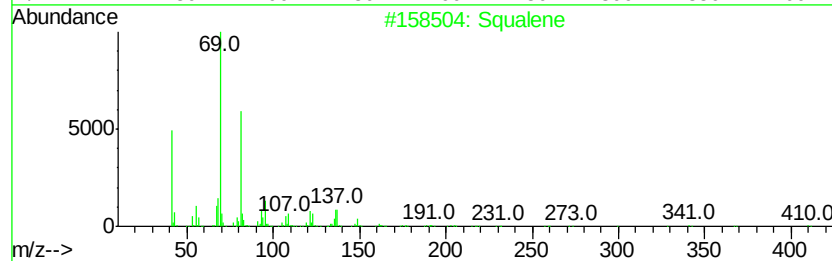
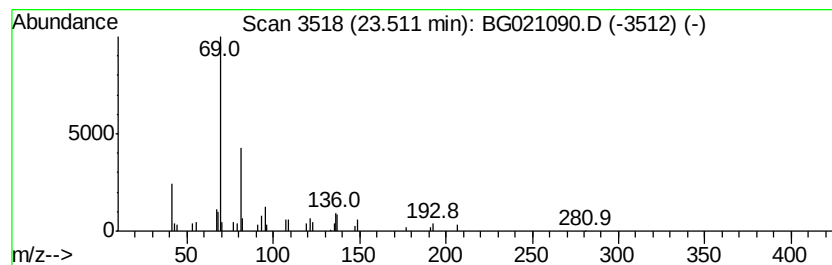
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 8 Squalene Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 23.51 | 5.22 ng | 27923 | Perylene-d12     | 25.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50  | 007683-64-9  | 72   |
| 2    |    | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0  | 64   |
| 3    |    | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24  | 062951-96-6  | 59   |
| 4    |    | 4,9,13,17-Tetramethyl-4,8,12,16-... | 316 | C22H36O | 056882-09-8  | 50   |
| 5    |    | Farnesol isomer a                   | 222 | C15H26O | 1000108-92-4 | 50   |





Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG022616\  
Data File : BG021090.D  
Acq On : 26 Feb 2016 22:46  
Operator : UM/SJ  
Sample : H1558-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
S5

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG022616.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| Propane, 2,2-dime... | 3.09  | 326.7   | ng    | 475501   | 1                     | 8.17  | 29112  | 20.0 |
| unknown5.26          | 5.26  | 14.6    | ng    | 21194    | 1                     | 8.17  | 29112  | 20.0 |
| unknown7.70          | 7.70  | 83.7    | ng    | 121770   | 1                     | 8.17  | 29112  | 20.0 |
| n-Hexadecanoic acid  | 18.38 | 3.9     | ng    | 18139    | 4                     | 17.51 | 92422  | 20.0 |
| 1-Docosene           | 21.41 | 3.1     | ng    | 18911    | 5                     | 21.78 | 123755 | 20.0 |
| Squalene             | 23.51 | 5.2     | ng    | 27923    | 6                     | 25.07 | 106918 | 20.0 |