

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\  
 Data File : BF099561.D  
 Acq On : 16 Oct 2017 23:12  
 Operator : SJ/JU  
 Sample : I5782-09  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S5(1-3)

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\_F\METHODS\8270-BF092317.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         | 5.069       | 504           | 507         | 521          | rBV      | 331850         | 459170        | 17.69%          | 2.130%        |
| 2         | 5.469       | 571           | 575         | 598          | rBV      | 2064401        | 2144001       | 82.58%          | 9.946%        |
| 3         | 6.481       | 742           | 747         | 766          | rBV      | 2088968        | 2317765       | 89.27%          | 10.752%       |
| 4         | 6.616       | 766           | 770         | 773          | rBV      | 2480272        | 2251944       | 86.74%          | 10.447%       |
| 5         | 6.845       | 805           | 809         | 817          | rBV      | 639623         | 581370        | 22.39%          | 2.697%        |
| 6         | 6.998       | 831           | 835         | 839          | rBV      | 2103280        | 1849215       | 71.23%          | 8.579%        |
| 7         | 7.410       | 900           | 905         | 908          | rBV      | 1523485        | 1401714       | 53.99%          | 6.503%        |
| 8         | 8.122       | 1023          | 1026        | 1041         | rBV      | 870765         | 796328        | 30.67%          | 3.694%        |
| 9         | 9.198       | 1204          | 1209        | 1212         | rBV      | 2832157        | 2596264       | 100.00%         | 12.045%       |
| 10        | 9.592       | 1273          | 1276        | 1284         | rVB      | 611426         | 462810        | 17.83%          | 2.147%        |
| 11        | 9.881       | 1321          | 1325        | 1334         | rVB      | 1030020        | 863151        | 33.25%          | 4.004%        |
| 12        | 10.592      | 1443          | 1446        | 1451         | rBB      | 95442          | 74673         | 2.88%           | 0.346%        |
| 13        | 10.675      | 1455          | 1460        | 1474         | rBV      | 1211098        | 1190890       | 45.87%          | 5.525%        |
| 14        | 11.369      | 1574          | 1578        | 1582         | rBV      | 903133         | 754375        | 29.06%          | 3.500%        |
| 15        | 12.951      | 1843          | 1847        | 1850         | rBV      | 2074398        | 1847439       | 71.16%          | 8.571%        |
| 16        | 13.833      | 1994          | 1997        | 2007         | rBV3     | 37479          | 58012         | 2.23%           | 0.269%        |
| 17        | 14.010      | 2024          | 2027        | 2035         | rBV      | 545211         | 535071        | 20.61%          | 2.482%        |
| 18        | 14.763      | 2151          | 2155        | 2158         | rBV      | 25737          | 27269         | 1.05%           | 0.127%        |
| 19        | 14.833      | 2164          | 2167        | 2172         | rVB      | 91801          | 86495         | 3.33%           | 0.401%        |
| 20        | 15.092      | 2207          | 2211        | 2215         | rVB      | 55740          | 56423         | 2.17%           | 0.262%        |
| 21        | 15.486      | 2270          | 2278        | 2286         | rBV      | 462068         | 650529        | 25.06%          | 3.018%        |
| 22        | 15.898      | 2342          | 2348        | 2355         | rVB      | 89225          | 134230        | 5.17%           | 0.623%        |
| 23        | 16.392      | 2427          | 2432        | 2439         | rBV      | 86636          | 149790        | 5.77%           | 0.695%        |
| 24        | 16.980      | 2526          | 2532        | 2540         | rVB2     | 57321          | 120057        | 4.62%           | 0.557%        |
| 25        | 17.674      | 2643          | 2650        | 2661         | rVB3     | 41547          | 105842        | 4.08%           | 0.491%        |
| 26        | 18.486      | 2780          | 2788        | 2789         | rBV4     | 24078          | 40768         | 1.57%           | 0.189%        |

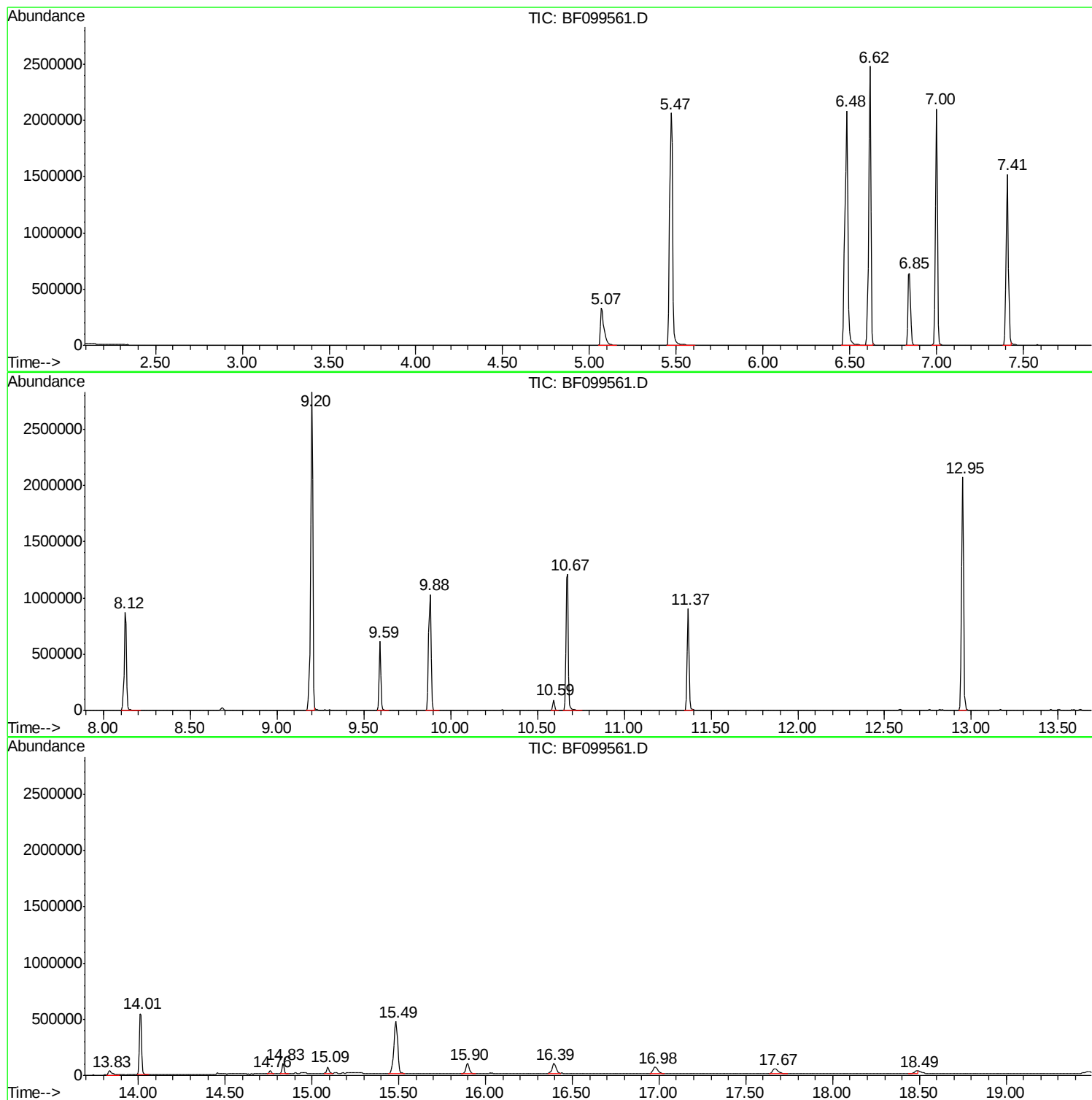
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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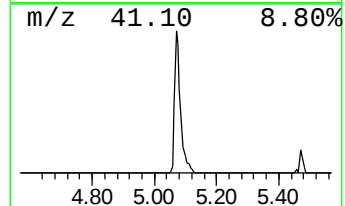
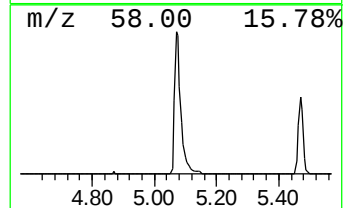
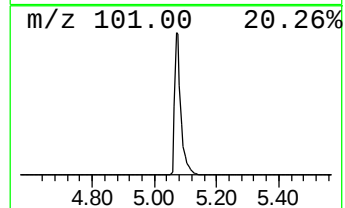
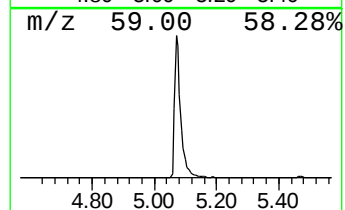
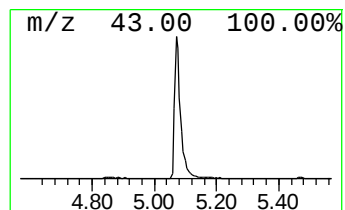
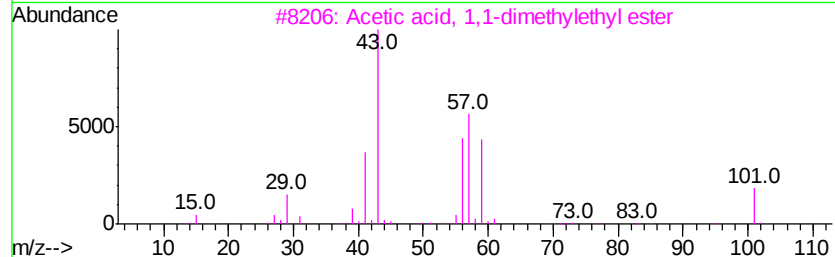
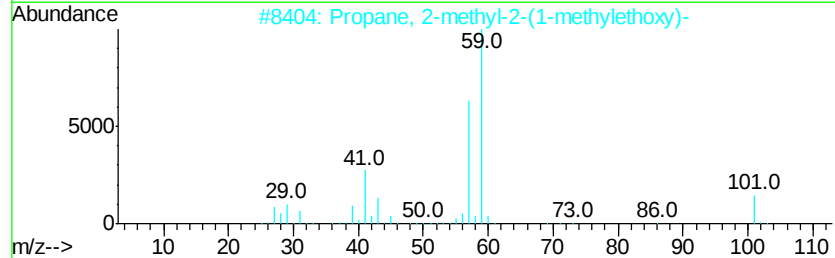
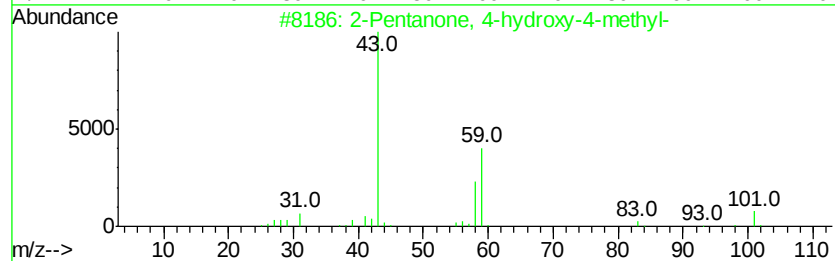
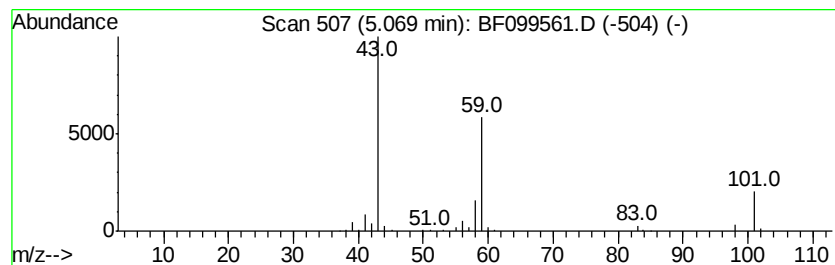
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 5.07 | 15.80 ng | 459170 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 42   |
| 2    |    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 4    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 5    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



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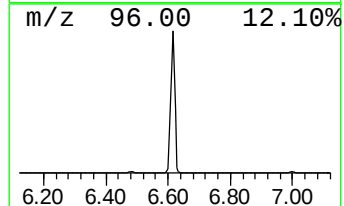
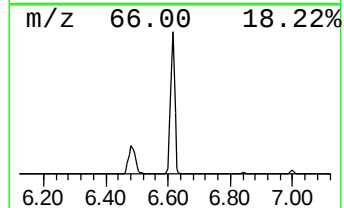
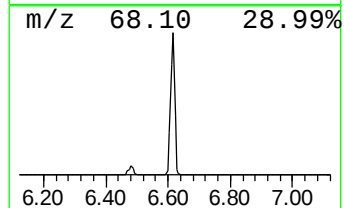
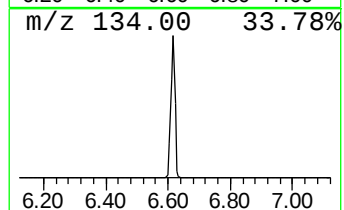
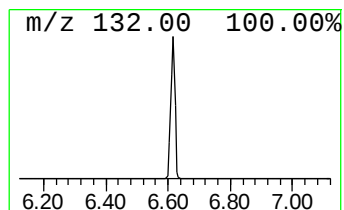
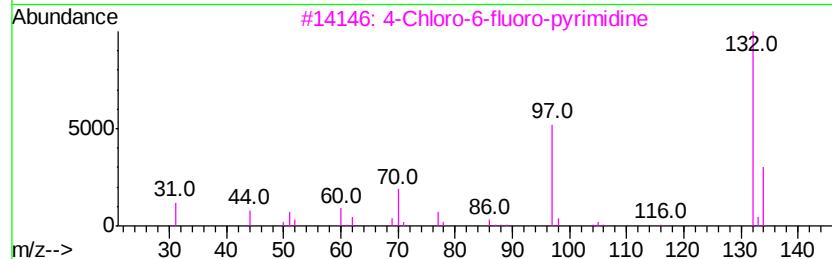
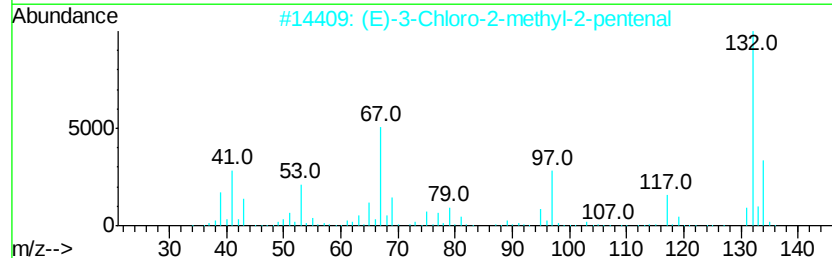
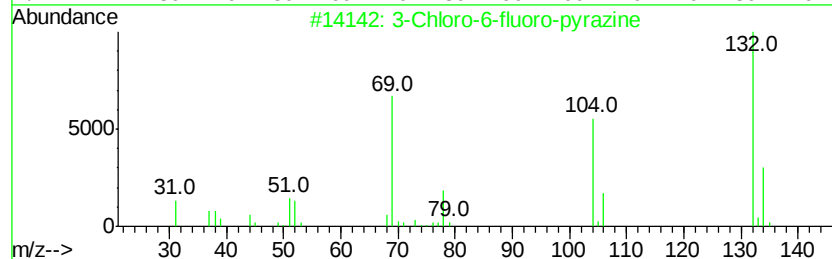
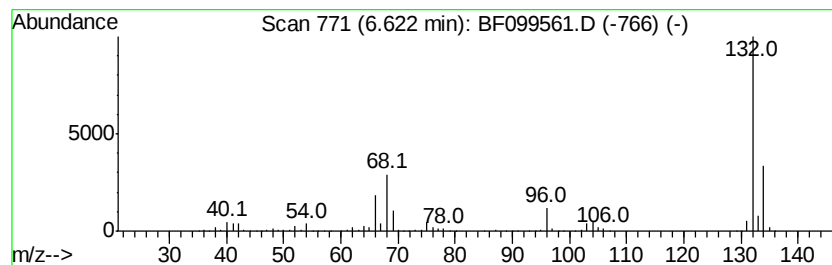
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.62 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.62 | 77.47 ng | 2251940 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 38   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6  | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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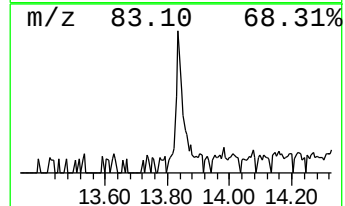
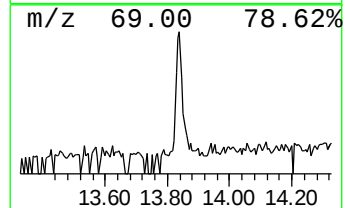
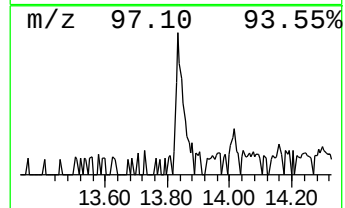
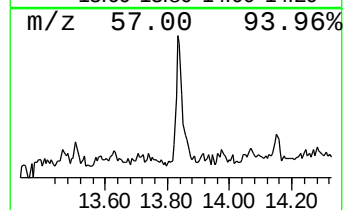
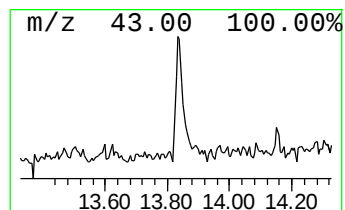
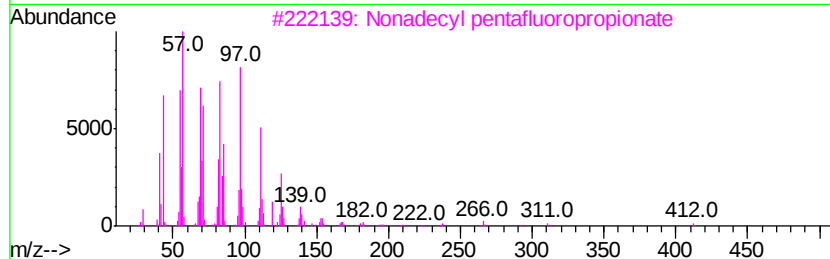
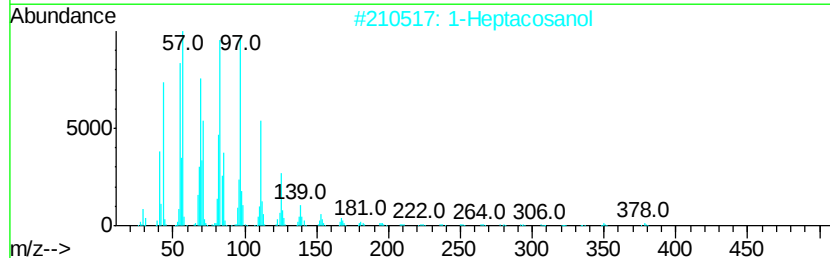
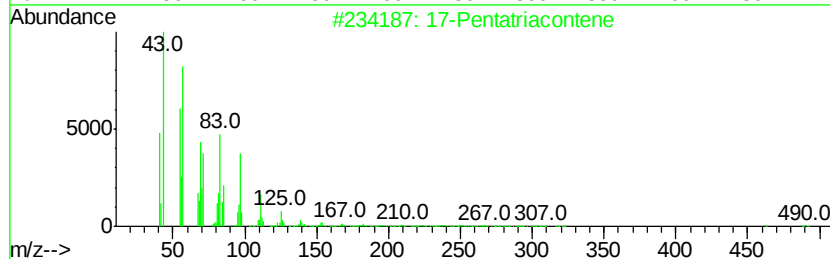
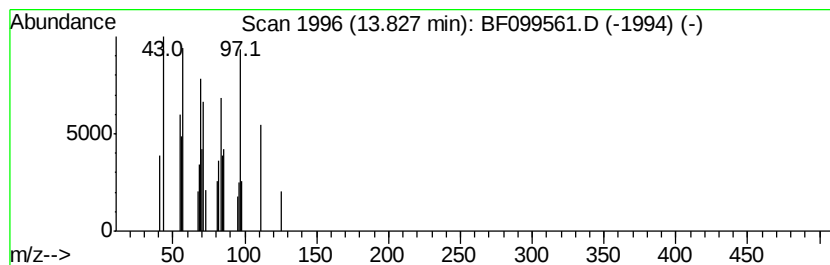
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 17-Pentatriacontene Concentration Rank 9

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 13.83 | 2.17 ng | 58012 | Chrysene-d12     | 14.02 |

| Hit# of | 5 | Tentative ID                    | MW  | MolForm    | CAS#         | Qual |
|---------|---|---------------------------------|-----|------------|--------------|------|
| 1       |   | 17-Pentatriacontene             | 491 | C35H70     | 006971-40-0  | 91   |
| 2       |   | 1-Heptacosanol                  | 396 | C27H56O    | 002004-39-9  | 91   |
| 3       |   | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91   |
| 4       |   | Octadecyl trifluoroacetate      | 366 | C20H37F3O2 | 079392-43-1  | 91   |
| 5       |   | Heneicosyl heptafluorobutyrate  | 508 | C25H43F7O2 | 1000351-83-8 | 91   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

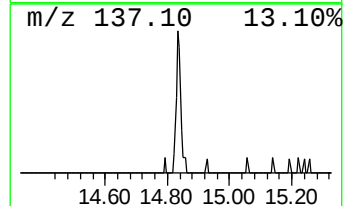
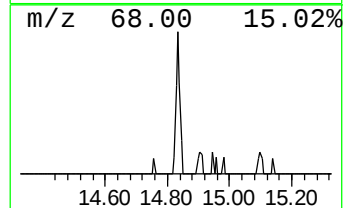
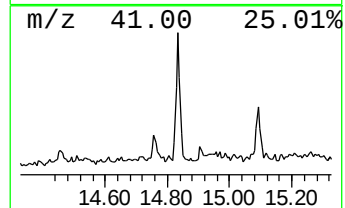
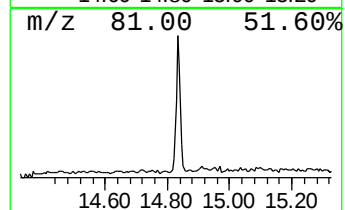
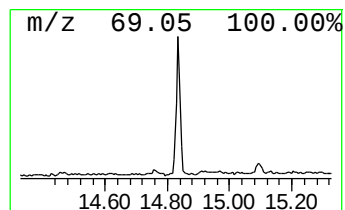
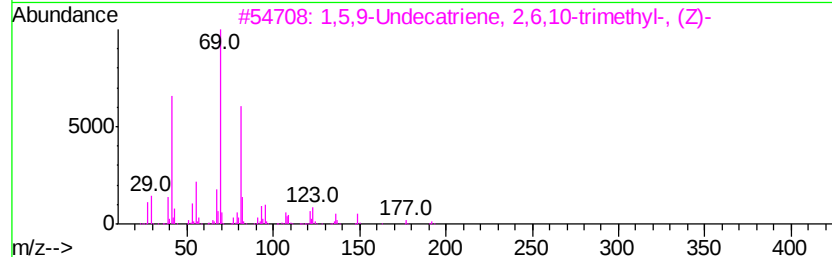
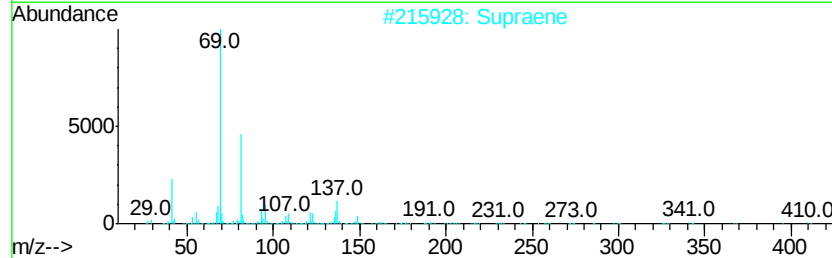
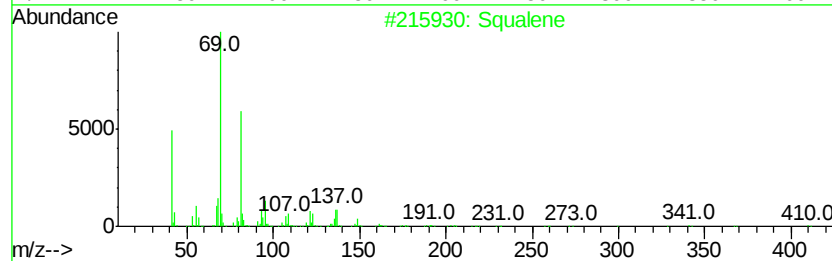
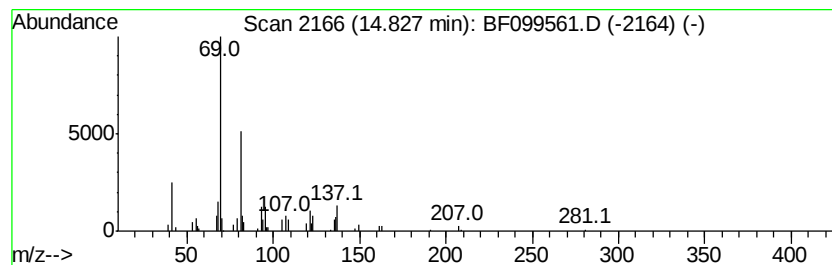
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 Squalene Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.83 | 2.66 ng | 86495 | Perylene-d12     | 15.49 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50   | 000111-02-4  | 91   |
| 2    |    | Supraene                            | 410 | C30H50   | 007683-64-9  | 91   |
| 3    |    | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24   | 062951-96-6  | 80   |
| 4    |    | 4,9,13,17-Tetramethyl-4,8,12,16-... | 316 | C22H36O  | 056882-09-8  | 78   |
| 5    |    | Farnesol, acetate                   | 264 | C17H28O2 | 1000352-67-2 | 64   |



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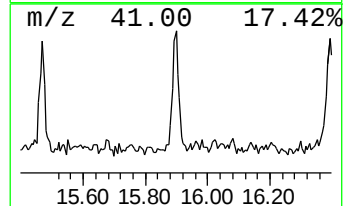
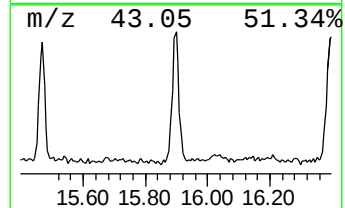
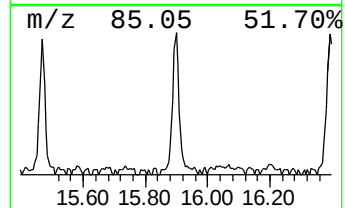
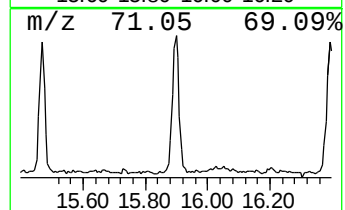
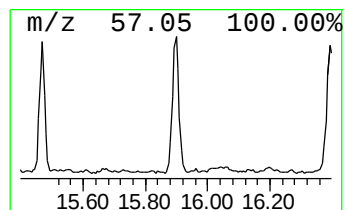
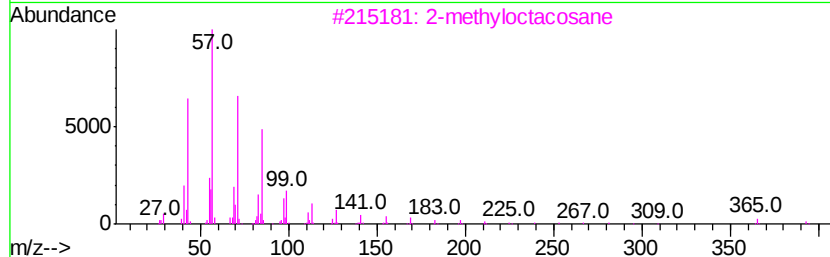
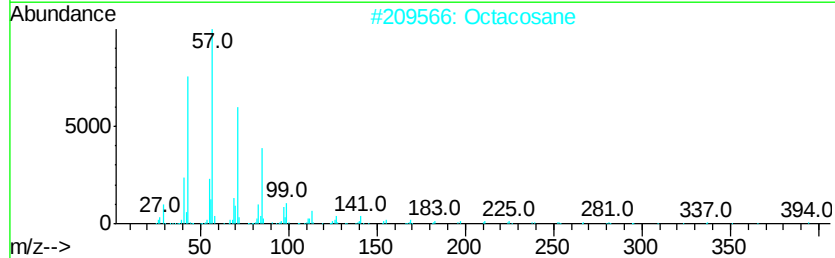
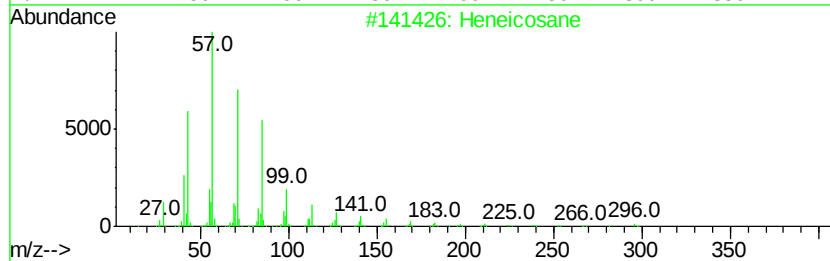
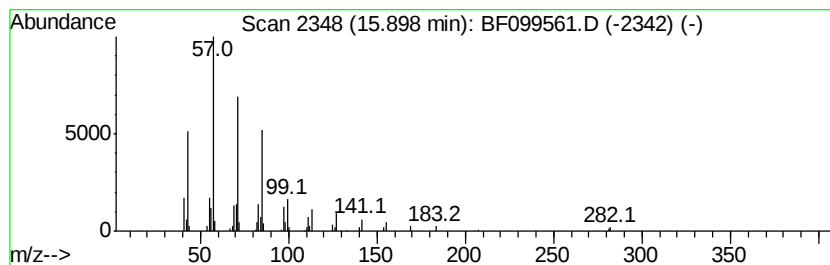
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Heneicosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.90 | 4.13 ng | 134230 | Perylene-d12     | 15.49 |

| Hit# of | 5                     | Tentative ID | MW  | MolForm | CAS#         | Qual |
|---------|-----------------------|--------------|-----|---------|--------------|------|
| 1       | Heneicosane           |              | 296 | C21H44  | 000629-94-7  | 91   |
| 2       | Octacosane            |              | 394 | C28H58  | 000630-02-4  | 91   |
| 3       | 2-methyloctacosane    |              | 408 | C29H60  | 1000376-72-8 | 91   |
| 4       | Heptadecane, 9-octyl- |              | 352 | C25H52  | 007225-64-1  | 91   |
| 5       | triacontane           |              | 422 | C30H62  | 000638-68-6  | 91   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101617\  
Data File : BF099561.D  
Acq On : 16 Oct 2017 23:12  
Operator : SJ/JU  
Sample : I5782-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S5(1-3)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

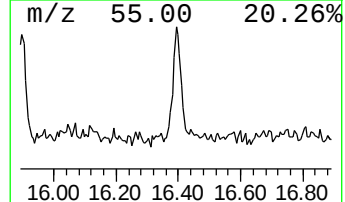
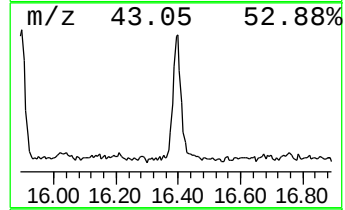
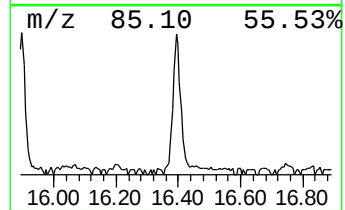
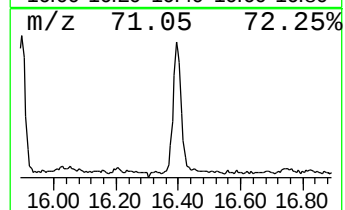
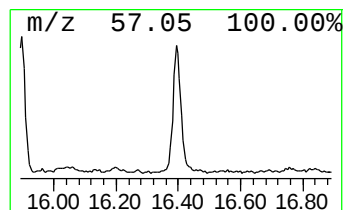
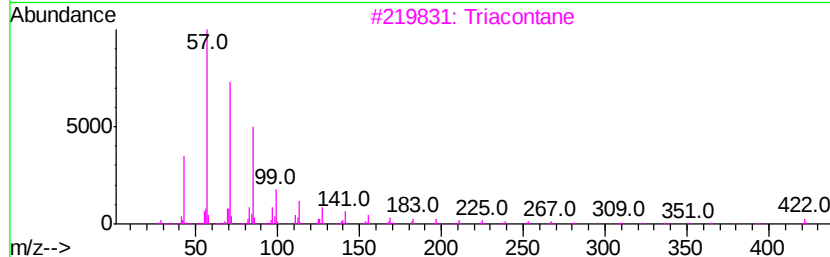
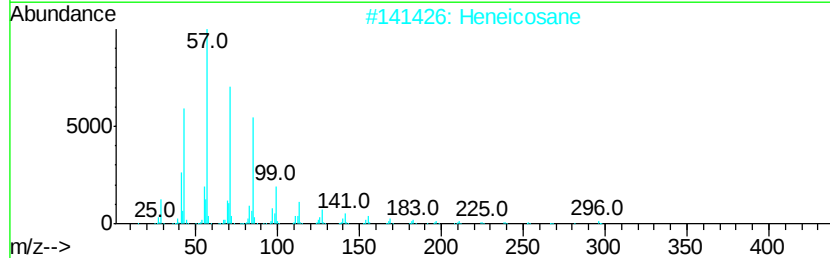
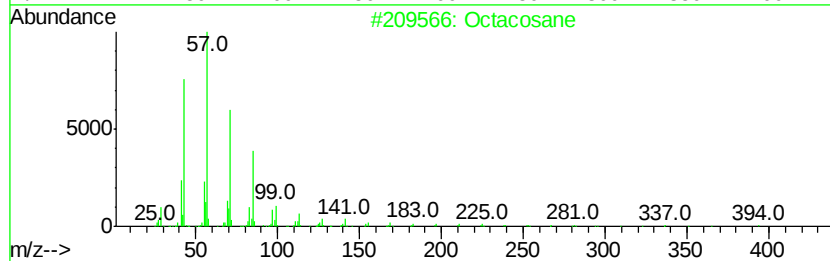
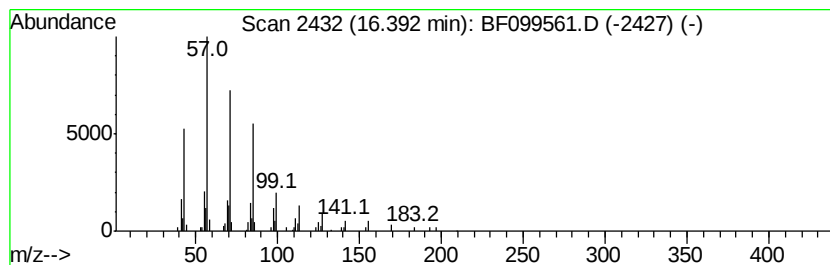
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 Octacosane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.39 | 4.61 ng | 149790 | Perylene-d12     | 15.49 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane   | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    |   | Heneicosane  | 296 | C21H44  | 000629-94-7 | 91   |
| 3    |    |   | Triacontane  | 422 | C30H62  | 000638-68-6 | 91   |
| 4    |    |   | Octadecane   | 254 | C18H38  | 000593-45-3 | 87   |
| 5    |    |   | Hexacosane   | 366 | C26H54  | 000630-01-3 | 87   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101617\  
Data File : BF099561.D  
Acq On : 16 Oct 2017 23:12  
Operator : SJ/JU  
Sample : I5782-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S5(1-3)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.07  | 15.8    | ng    | 459170   | 1                     | 6.85  | 581370 | 20.0 |
| unknown6.62          | 6.62  | 77.5    | ng    | 2251940  | 1                     | 6.85  | 581370 | 20.0 |
| 17-Pentatriacontene  | 13.83 | 2.2     | ng    | 58012    | 5                     | 14.02 | 535071 | 20.0 |
| Squalene             | 14.83 | 2.7     | ng    | 86495    | 6                     | 15.49 | 650529 | 20.0 |
| Heneicosane          | 15.90 | 4.1     | ng    | 134230   | 6                     | 15.49 | 650529 | 20.0 |
| Octacosane           | 16.39 | 4.6     | ng    | 149790   | 6                     | 15.49 | 650529 | 20.0 |