

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP110620\  
 Data File : BP003842.D  
 Acq On : 06 Nov 2020 16:16  
 Operator : CG/JU  
 Sample : L4653-01  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 TP-7-COMP

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\_P\METHODS\8270-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003842.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         | 2.952       | 5             | 11          | 29           | rVB      | 6281500        | 9542731       | 100.00%         | 20.379%       |
| 2         | 3.105       | 30            | 37          | 48           | rVV      | 155799         | 390838        | 4.10%           | 0.835%        |
| 3         | 3.199       | 48            | 53          | 65           | rVB      | 297150         | 461893        | 4.84%           | 0.986%        |
| 4         | 5.822       | 491           | 499         | 513          | rBV      | 2321493        | 3497233       | 36.65%          | 7.468%        |
| 5         | 7.469       | 770           | 779         | 792          | rBV      | 2211333        | 3627093       | 38.01%          | 7.746%        |
| 6         | 8.305       | 913           | 921         | 928          | rBV      | 536857         | 862725        | 9.04%           | 1.842%        |
| 7         | 9.463       | 1102          | 1118        | 1127         | rBV      | 1402959        | 2319707       | 24.31%          | 4.954%        |
| 8         | 11.134      | 1393          | 1402        | 1409         | rBV      | 699493         | 1166225       | 12.22%          | 2.490%        |
| 9         | 13.540      | 1804          | 1811        | 1822         | rBV      | 3310457        | 4821245       | 50.52%          | 10.296%       |
| 10        | 14.340      | 1941          | 1947        | 1954         | rBV      | 427564         | 566101        | 5.93%           | 1.209%        |
| 11        | 14.916      | 2038          | 2045        | 2052         | rVB      | 1049583        | 1500671       | 15.73%          | 3.205%        |
| 12        | 16.392      | 2289          | 2296        | 2311         | rBV      | 2557022        | 3703080       | 38.81%          | 7.908%        |
| 13        | 17.639      | 2502          | 2508        | 2513         | rBV      | 1201786        | 1740518       | 18.24%          | 3.717%        |
| 14        | 17.681      | 2513          | 2515        | 2521         | rVB      | 79179          | 99056         | 1.04%           | 0.212%        |
| 15        | 18.475      | 2645          | 2650        | 2656         | rBV2     | 217323         | 312833        | 3.28%           | 0.668%        |
| 16        | 19.610      | 2838          | 2843        | 2848         | rVB      | 177502         | 226993        | 2.38%           | 0.485%        |
| 17        | 19.957      | 2899          | 2902        | 2909         | rVB      | 142822         | 190754        | 2.00%           | 0.407%        |
| 18        | 20.133      | 2927          | 2932        | 2937         | rBV      | 5447689        | 6525184       | 68.38%          | 13.935%       |
| 19        | 21.316      | 3129          | 3133        | 3142         | rVB      | 662028         | 785906        | 8.24%           | 1.678%        |
| 20        | 21.392      | 3142          | 3146        | 3149         | rBV      | 116331         | 130519        | 1.37%           | 0.279%        |
| 21        | 21.663      | 3186          | 3192        | 3197         | rBV      | 1409141        | 1938103       | 20.31%          | 4.139%        |
| 22        | 22.733      | 3369          | 3374        | 3380         | rBV      | 448199         | 666701        | 6.99%           | 1.424%        |
| 23        | 24.139      | 3606          | 3613        | 3620         | rBV      | 870650         | 1751140       | 18.35%          | 3.740%        |

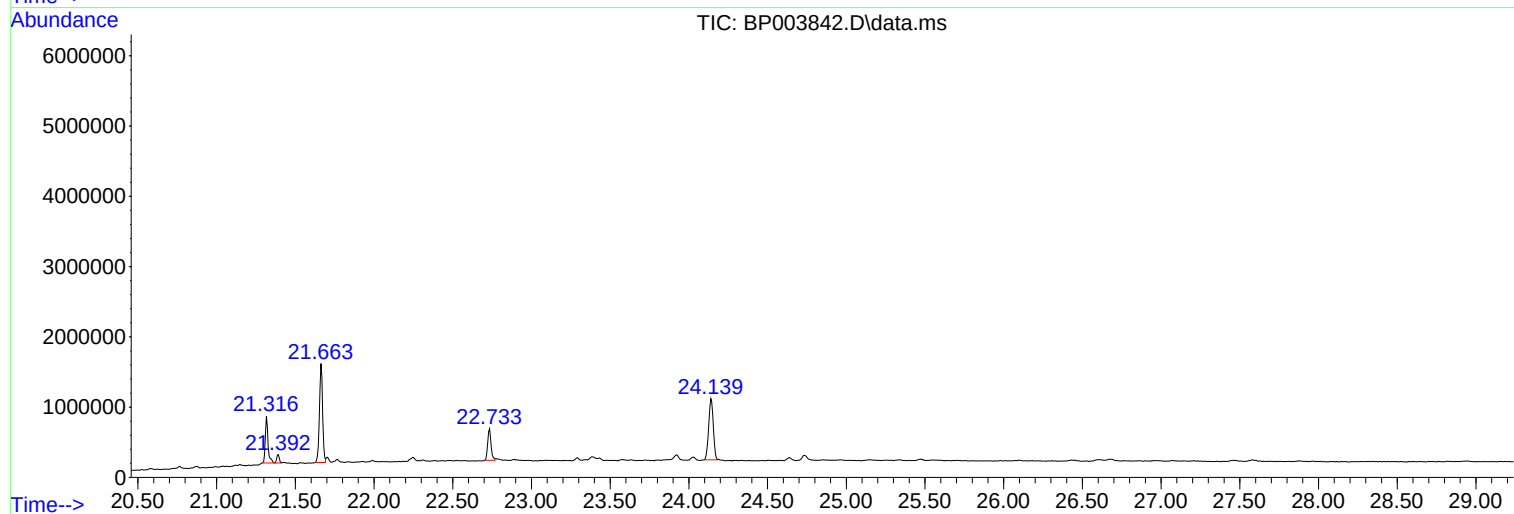
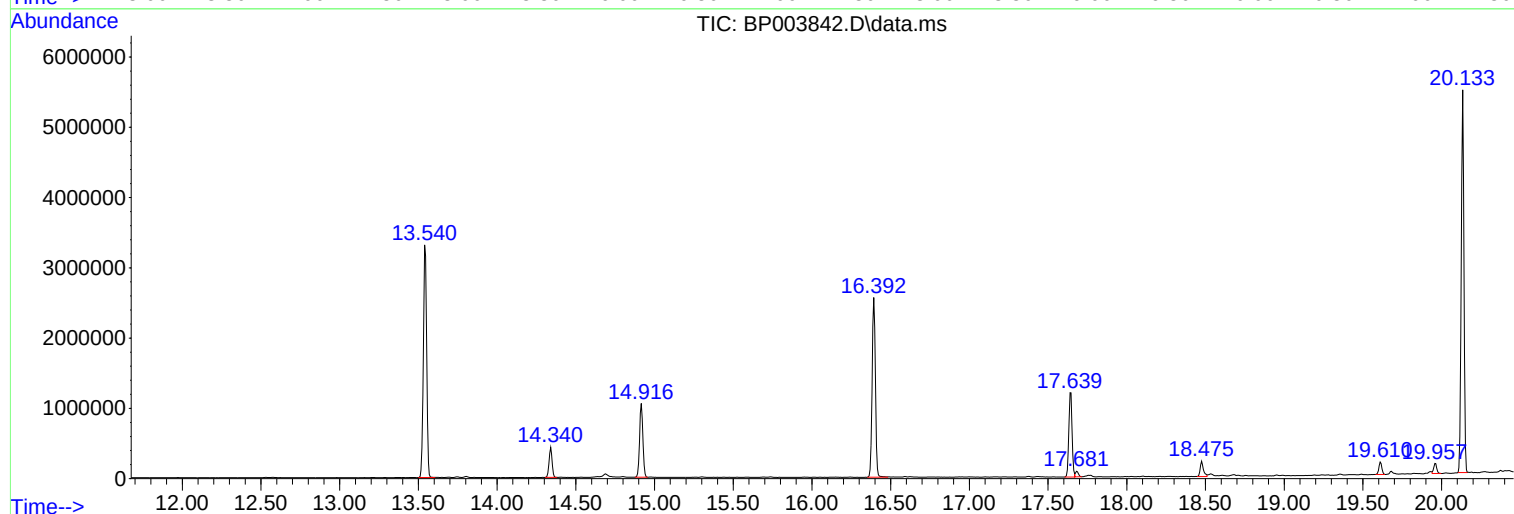
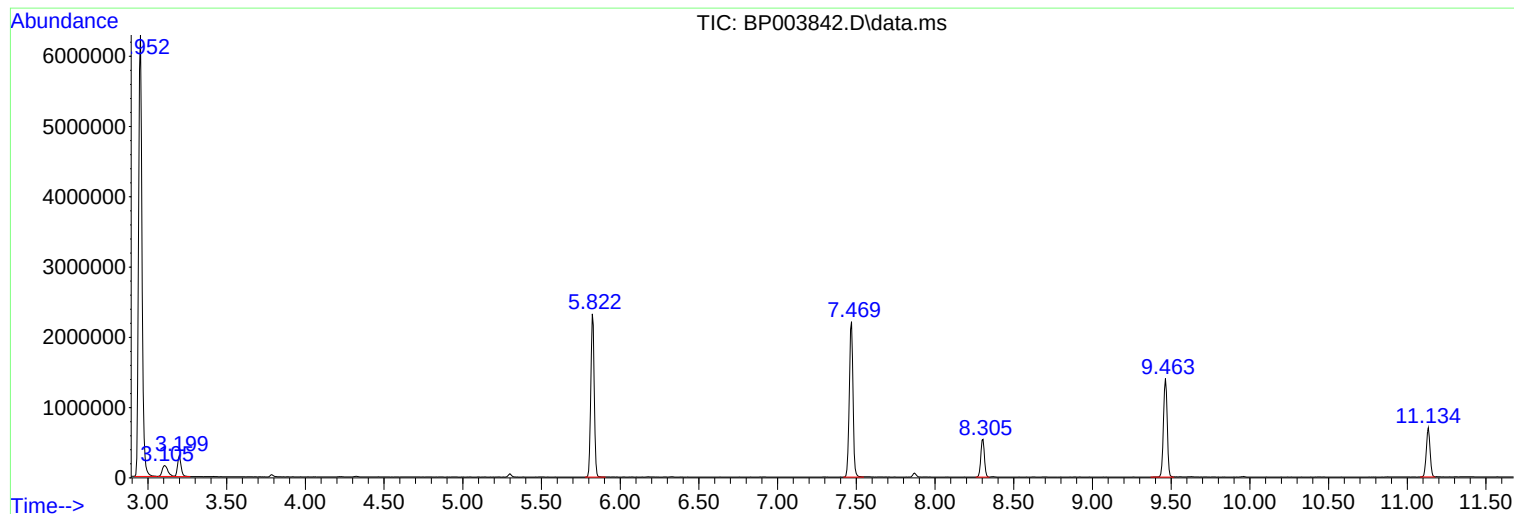
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BNA\_P  
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TP-7-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP110320.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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TP-7-COMP

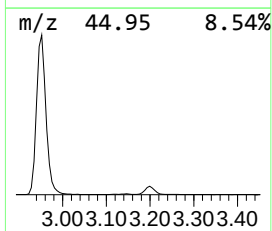
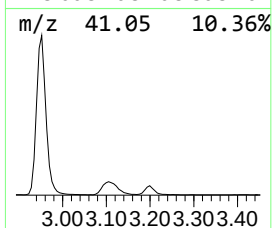
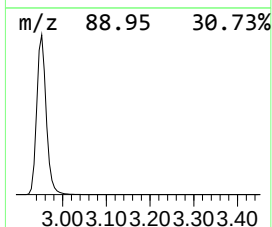
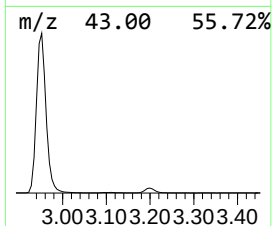
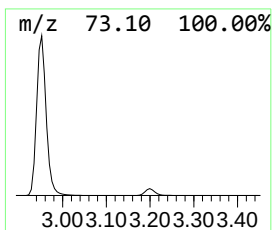
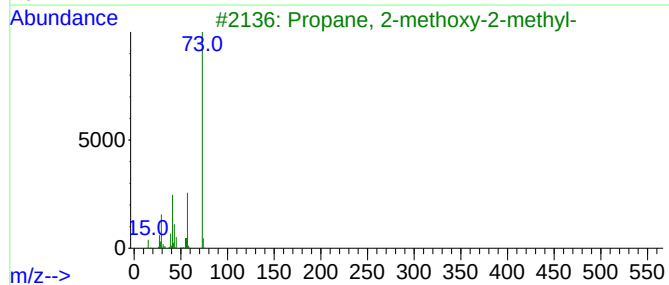
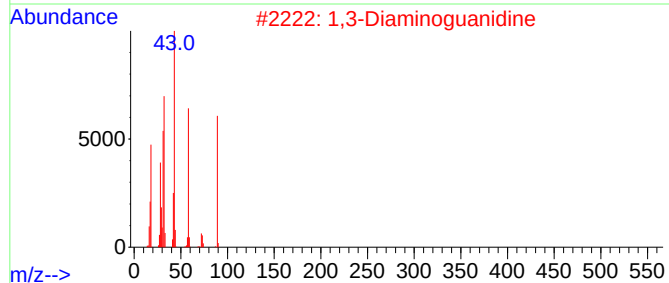
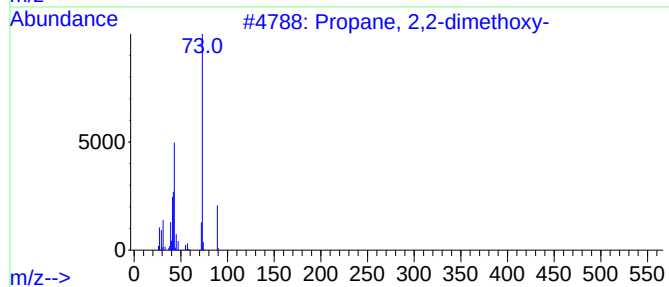
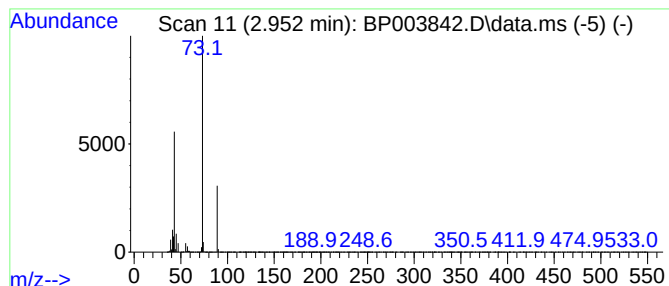
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown2.95 Concentration Rank 1

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 2.952 | 221.22 ng | 9542730 | 1,4-Dichlorobenzene-d4 | 8.305 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propane, 2,2-dimethoxy-             | 104 | C5H12O2 | 000077-76-9 | 38   |
| 2    |    |   | 1,3-Diaminoguanidine                | 89  | CH7N5   | 004364-78-7 | 9    |
| 3    |    |   | Propane, 2-methoxy-2-methyl-        | 88  | C5H12O  | 001634-04-4 | 9    |
| 4    |    |   | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 9    |
| 5    |    |   | 2-Hydroxy-2-methylbutyric acid      | 118 | C5H10O3 | 003739-30-8 | 9    |



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TP-7-COMP

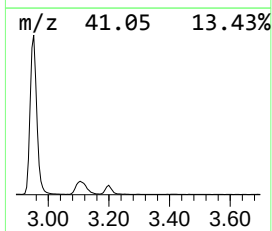
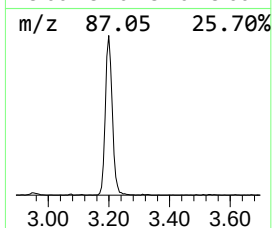
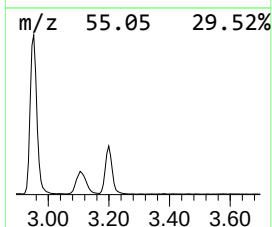
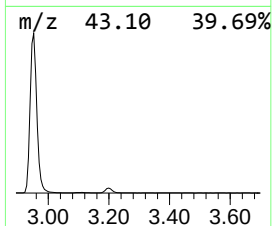
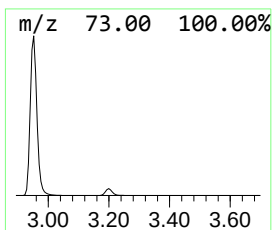
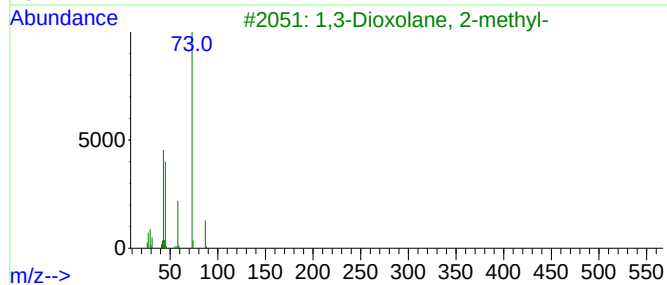
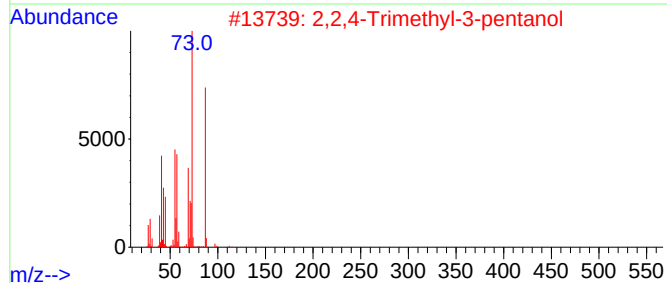
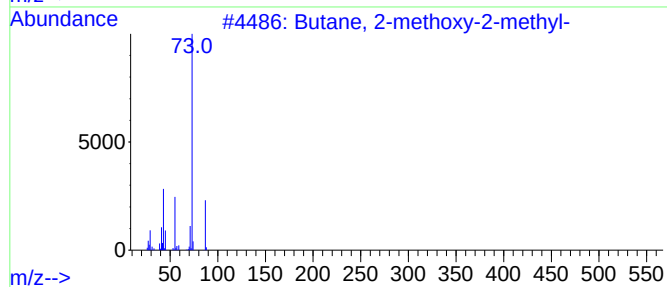
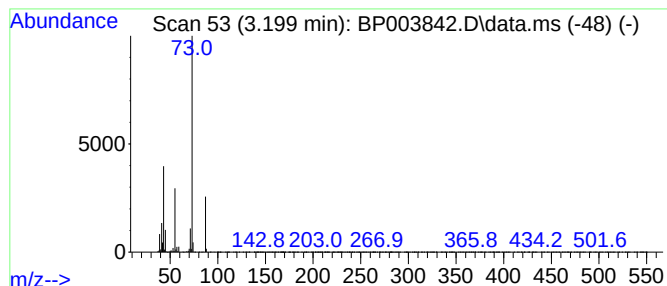
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP110320.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.199 | 10.71 ng | 461893 | 1,4-Dichlorobenzene-d4 | 8.305 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |
| 4    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 22   |
| 5    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |



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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
TP-7-COMP

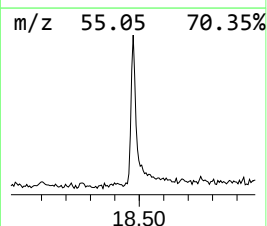
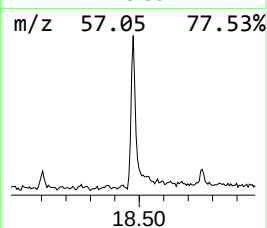
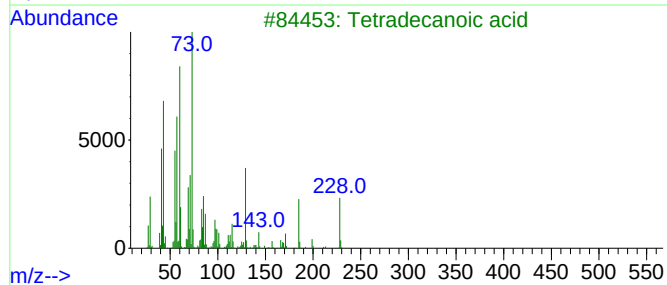
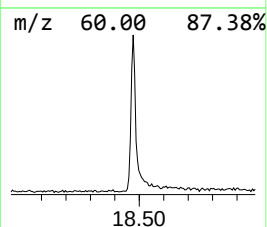
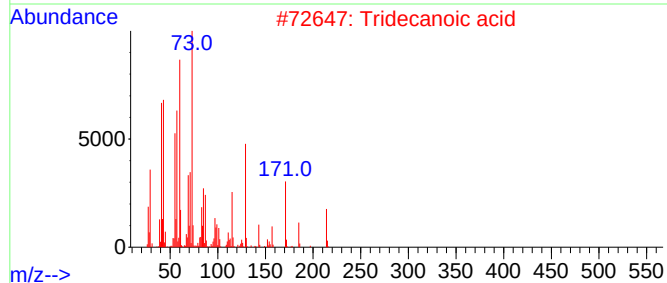
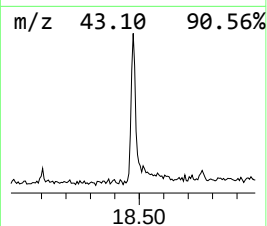
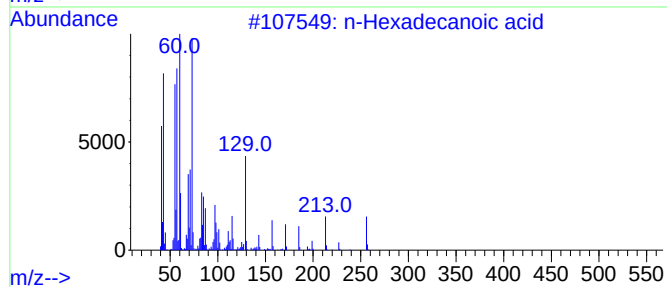
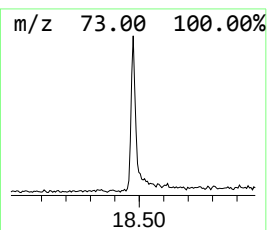
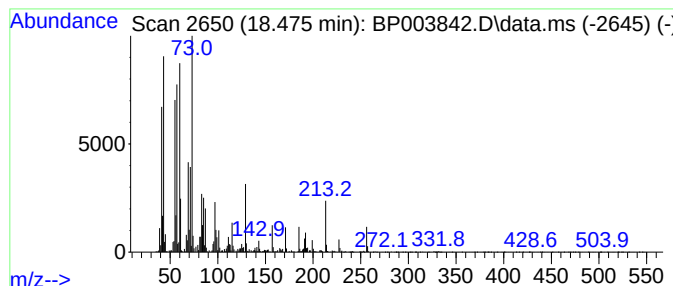
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP110320.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.475 | 3.59 ng | 312833 | Phenanthrene-d10 | 17.640 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 95   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 93   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 5    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 64   |



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Instrument :  
BNA\_P  
ClientSampleId :  
TP-7-COMP

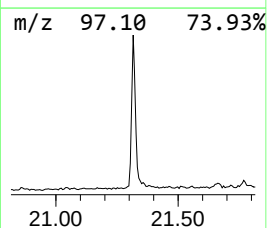
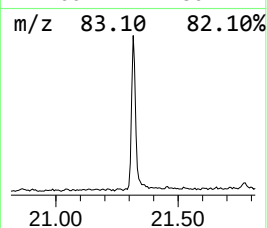
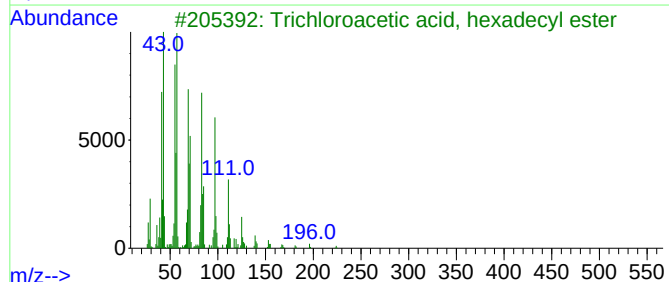
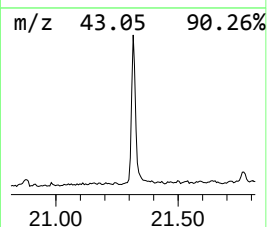
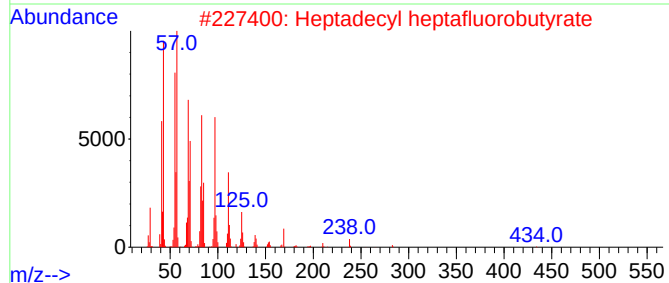
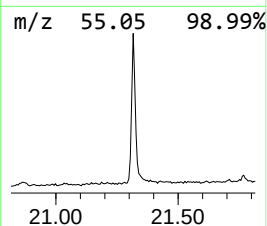
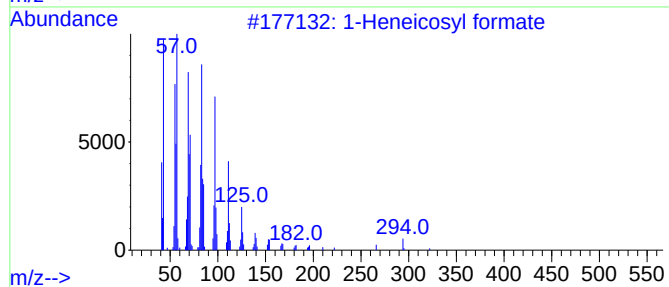
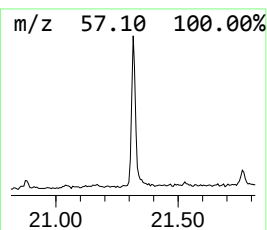
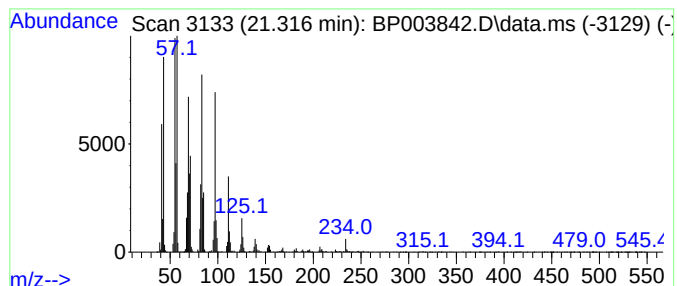
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP110320.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 1-Heneicosyl formate Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.316 | 8.11 ng | 785906 | Chrysene-d12     | 21.663 |

| Hit# | of | 5 | Tentative ID                             | MW  | MolForm     | CAS#        | Qual |
|------|----|---|------------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | 1-Heneicosyl formate                     | 340 | C22H44O2    | 077899-03-7 | 95   |
| 2    |    |   | Heptadecyl heptafluorobutyrate           | 452 | C21H35F7O2  | 959085-66-6 | 94   |
| 3    |    |   | Trichloroacetic acid, hexadecyl ...      | 386 | C18H33Cl3O2 | 074339-54-1 | 94   |
| 4    |    |   | Pentafluoropropionic acid, hexadecyl ... | 388 | C19H33F5O2  | 006222-07-7 | 94   |
| 5    |    |   | Heptafluorobutyric acid, hexadecyl ...   | 438 | C20H33F7O2  | 006385-15-5 | 94   |



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BNA\_P  
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TP-7-COMP

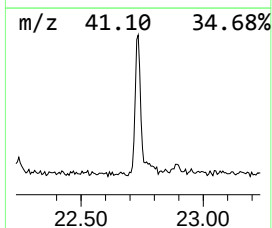
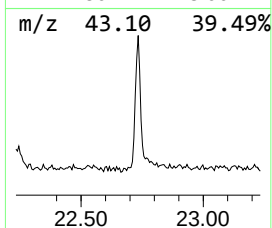
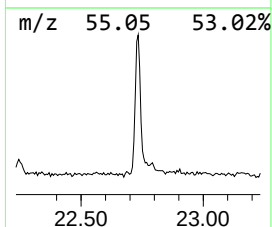
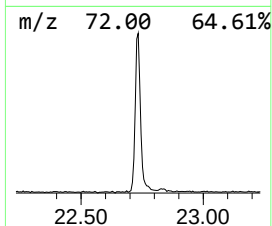
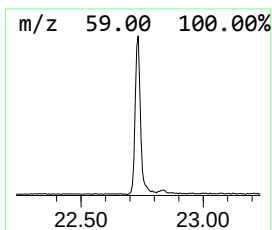
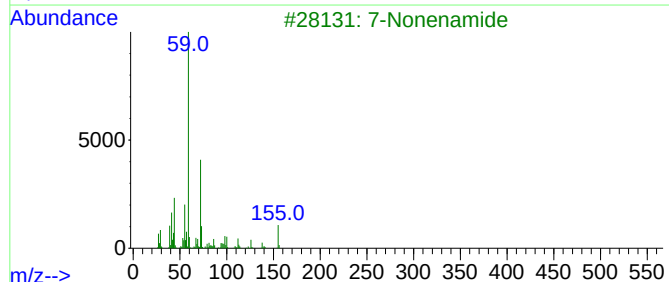
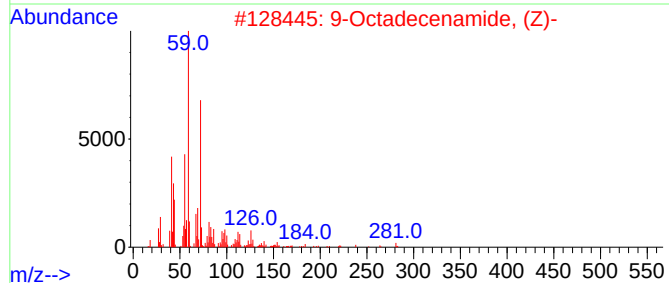
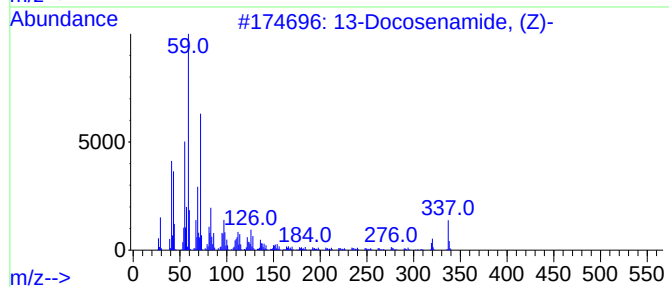
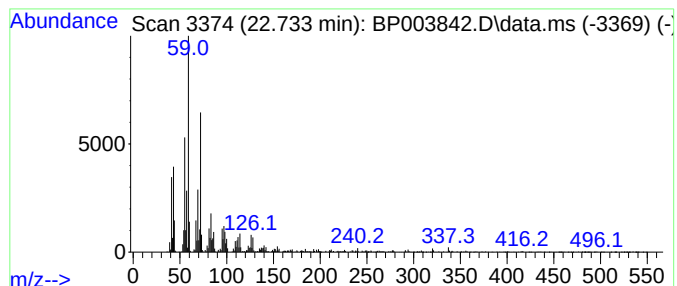
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.733 | 6.88 ng | 666701 | Chrysene-d12     | 21.663 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 13-Docosenamide, (Z)-               | 337 | C22H43NO   | 000112-84-5 | 93   |
| 2    |    |   | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 91   |
| 3    |    |   | 7-Nonenamide                        | 155 | C9H17NO    | 090949-53-4 | 64   |
| 4    |    |   | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 53   |
| 5    |    |   | Decanamide-                         | 171 | C10H21NO   | 002319-29-1 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP110620\  
Data File : BP003842.D  
Acq On : 06 Nov 2020 16:16  
Operator : CG/JU  
Sample : L4653-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
TP-7-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP110320.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 |
| unknown2.95        | 2.952  | 221.2   | ng    | 9542730  | 1                     | 8.305  | 862725  | 20.0 |
| Butane, 2-metho... | 3.199  | 10.7    | ng    | 461893   | 1                     | 8.305  | 862725  | 20.0 |
| n-Hexadecanoic ... | 18.475 | 3.6     | ng    | 312833   | 4                     | 17.640 | 1740520 | 20.0 |
| 1-Heneicosyl fo... | 21.316 | 8.1     | ng    | 785906   | 5                     | 21.663 | 1938100 | 20.0 |
| 13-Docosenamide... | 22.733 | 6.9     | ng    | 666701   | 5                     | 21.663 | 1938100 | 20.0 |