

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
 Data File : BF139154.D  
 Acq On : 23 Aug 2024 18:44  
 Operator : RC/JU  
 Sample : P3707-04  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S-929-K1-SO-0.5-1-082024

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\_F\Methods\8270-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139154.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         | 2.193       | 9             | 17          | 24           | rVB      | 1025626        | 1596327       | 100.00%         | 12.285%       |
| 2         | 3.399       | 216           | 222         | 252          | rBV      | 43923          | 119658        | 7.50%           | 0.921%        |
| 3         | 5.104       | 503           | 512         | 522          | rVB      | 67134          | 104079        | 6.52%           | 0.801%        |
| 4         | 5.510       | 575           | 581         | 586          | rBV      | 1052799        | 1335538       | 83.66%          | 10.278%       |
| 5         | 6.516       | 746           | 752         | 757          | rBV      | 1078693        | 1398762       | 87.62%          | 10.764%       |
| 6         | 6.716       | 782           | 786         | 792          | rBV      | 30307          | 36729         | 2.30%           | 0.283%        |
| 7         | 6.898       | 812           | 817         | 822          | rBV      | 382799         | 477809        | 29.93%          | 3.677%        |
| 8         | 7.051       | 835           | 843         | 847          | rBV      | 167734         | 202888        | 12.71%          | 1.561%        |
| 9         | 7.322       | 886           | 889         | 893          | rVB      | 16635          | 19028         | 1.19%           | 0.146%        |
| 10        | 7.451       | 905           | 911         | 917          | rBV      | 746238         | 996166        | 62.40%          | 7.666%        |
| 11        | 7.710       | 950           | 955         | 961          | rVB      | 37563          | 44399         | 2.78%           | 0.342%        |
| 12        | 8.175       | 1029          | 1034        | 1039         | rBV      | 484932         | 603771        | 37.82%          | 4.646%        |
| 13        | 8.392       | 1067          | 1071        | 1078         | rVB3     | 17303          | 23453         | 1.47%           | 0.180%        |
| 14        | 8.487       | 1082          | 1087        | 1096         | rBV      | 80202          | 105006        | 6.58%           | 0.808%        |
| 15        | 9.251       | 1212          | 1217        | 1226         | rBV      | 944056         | 1141289       | 71.49%          | 8.783%        |
| 16        | 9.928       | 1327          | 1332        | 1343         | rVB      | 515334         | 669348        | 41.93%          | 5.151%        |
| 17        | 10.028      | 1343          | 1349        | 1356         | rBV2     | 33435          | 60078         | 3.76%           | 0.462%        |
| 18        | 10.716      | 1461          | 1466        | 1471         | rBV      | 601997         | 736044        | 46.11%          | 5.664%        |
| 19        | 10.839      | 1483          | 1487        | 1496         | rVB      | 16259          | 24382         | 1.53%           | 0.188%        |
| 20        | 11.163      | 1539          | 1542        | 1547         | rBV2     | 14891          | 21767         | 1.36%           | 0.168%        |
| 21        | 11.416      | 1575          | 1585        | 1592         | rBV      | 483528         | 626562        | 39.25%          | 4.822%        |
| 22        | 11.528      | 1599          | 1604        | 1609         | rBV4     | 32172          | 49413         | 3.10%           | 0.380%        |
| 23        | 11.851      | 1654          | 1659        | 1668         | rVB      | 49264          | 69751         | 4.37%           | 0.537%        |
| 24        | 11.939      | 1668          | 1674        | 1683         | rBV2     | 138534         | 256479        | 16.07%          | 1.974%        |
| 25        | 12.010      | 1683          | 1686        | 1692         | rVB5     | 14496          | 19861         | 1.24%           | 0.153%        |
| 26        | 12.627      | 1787          | 1791        | 1798         | rBV2     | 9556           | 18293         | 1.15%           | 0.141%        |
| 27        | 12.727      | 1804          | 1808        | 1822         | rBV      | 61788          | 94720         | 5.93%           | 0.729%        |
| 28        | 13.004      | 1849          | 1855        | 1859         | rBV      | 461225         | 584804        | 36.63%          | 4.500%        |
| 29        | 13.904      | 2003          | 2008        | 2020         | rBV      | 83731          | 140093        | 8.78%           | 1.078%        |
| 30        | 14.051      | 2028          | 2033        | 2041         | rVB      | 311819         | 406698        | 25.48%          | 3.130%        |
| 31        | 14.227      | 2058          | 2063        | 2070         | rBV4     | 10808          | 19751         | 1.24%           | 0.152%        |
| 32        | 14.539      | 2110          | 2116        | 2129         | rBV      | 89014          | 156745        | 9.82%           | 1.206%        |
| 33        | 14.845      | 2164          | 2168        | 2177         | rBV4     | 11543          | 24865         | 1.56%           | 0.191%        |
| 34        | 15.192      | 2222          | 2227        | 2230         | rBV      | 42428          | 72417         | 4.54%           | 0.557%        |
| 35        | 15.533      | 2279          | 2285        | 2290         | rBV      | 294149         | 439670        | 27.54%          | 3.384%        |
| 36        | 15.792      | 2324          | 2329        | 2335         | rVB3     | 17651          | 30318         | 1.90%           | 0.233%        |

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Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

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\_F\Methods\8270-BF082024.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |       |       |       |       |        |
|----|--------|------|------|------|-------|-------|-------|-------|--------|
| 37 | 16.033 | 2364 | 2370 | 2374 | rBV   | 36765 | 63412 | 3.97% | 0.488% |
| 38 | 16.080 | 2374 | 2378 | 2386 | rVV2  | 30553 | 69660 | 4.36% | 0.536% |
| 39 | 16.151 | 2387 | 2390 | 2399 | rVB2  | 13875 | 28575 | 1.79% | 0.220% |
| 40 | 16.851 | 2503 | 2509 | 2518 | rVB3  | 25712 | 52482 | 3.29% | 0.404% |
| 41 | 17.257 | 2572 | 2578 | 2588 | rBV10 | 13005 | 37069 | 2.32% | 0.285% |
| 42 | 17.633 | 2638 | 2642 | 2651 | rVB10 | 6899  | 16112 | 1.01% | 0.124% |

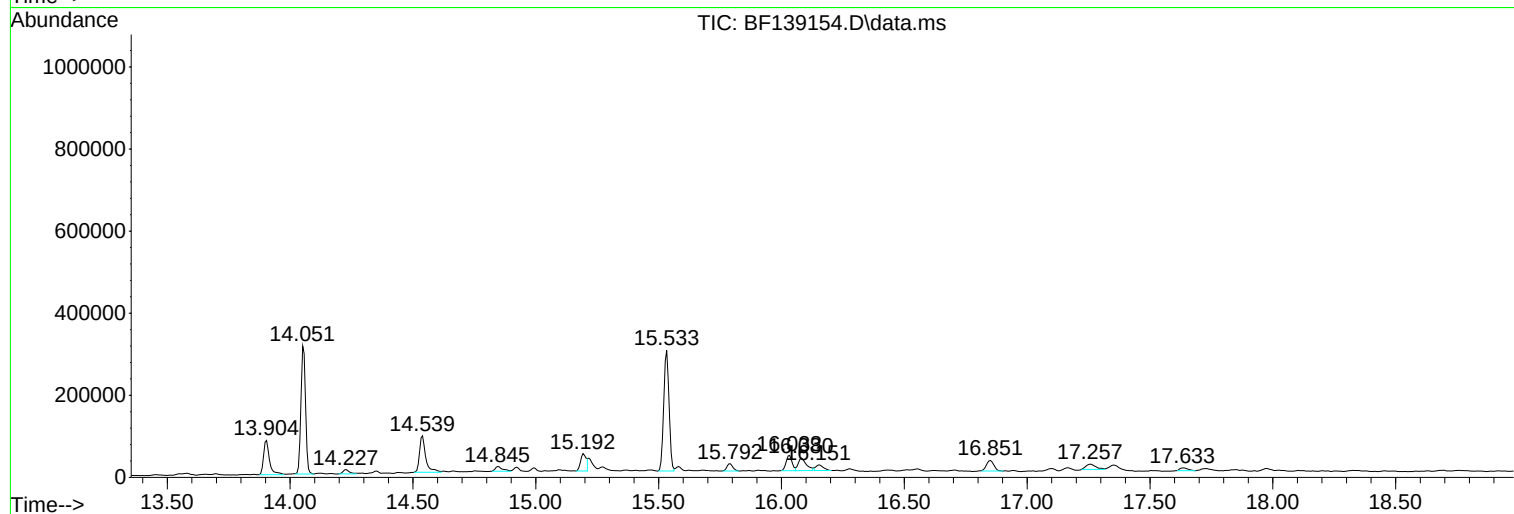
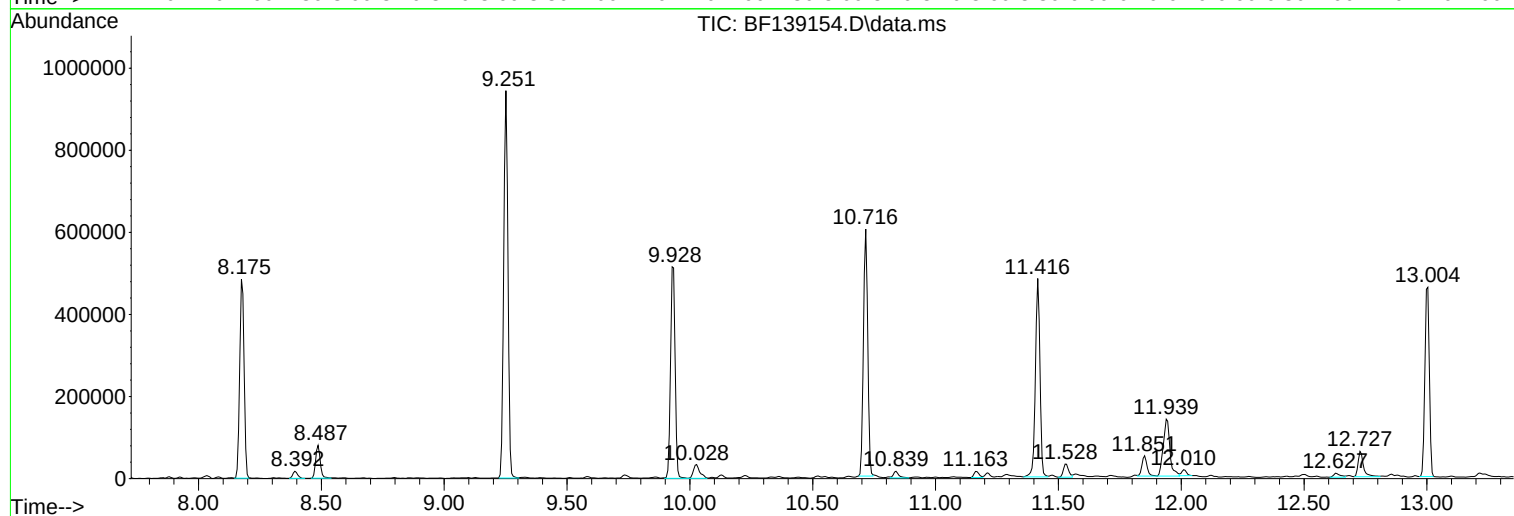
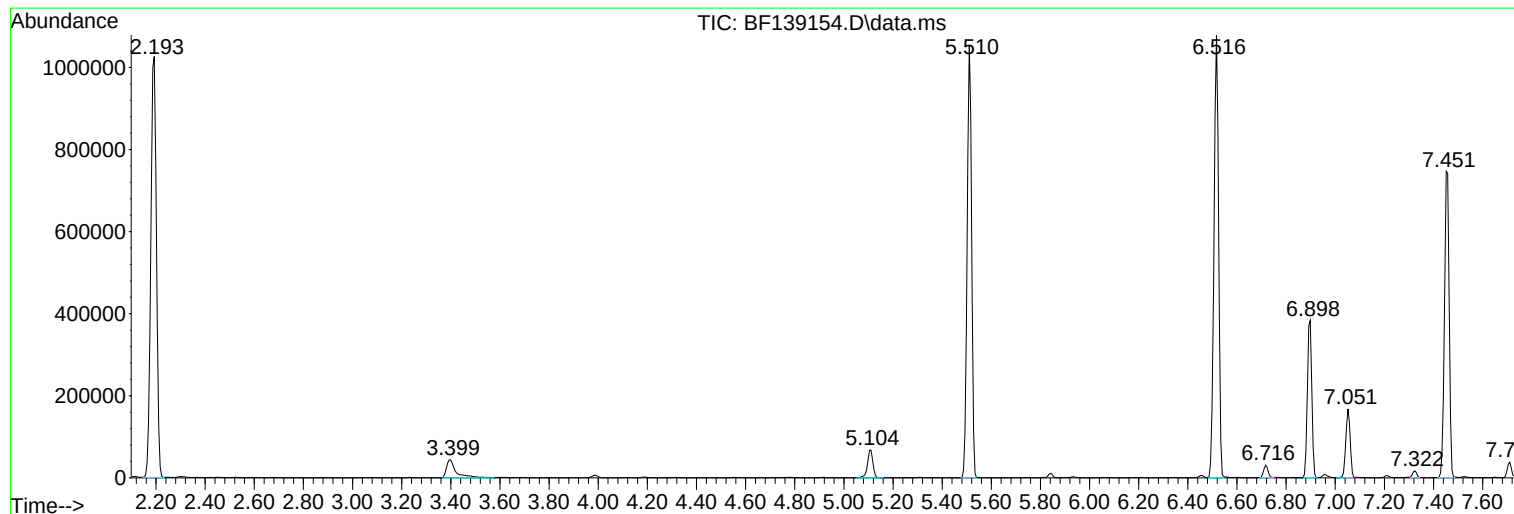
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BNA\_F  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
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Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

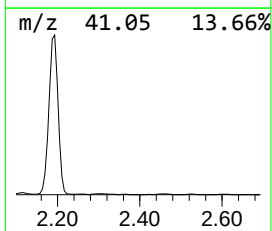
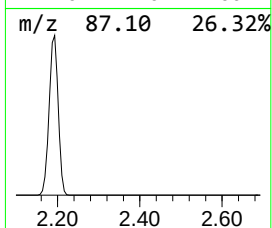
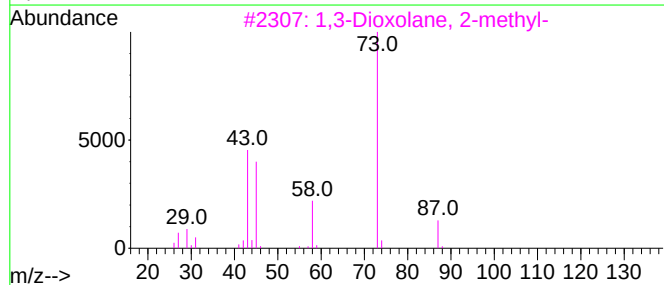
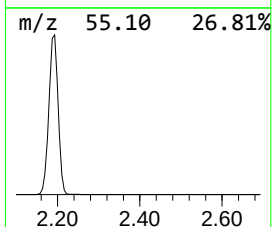
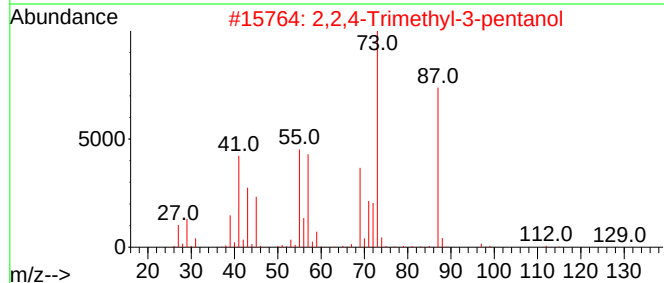
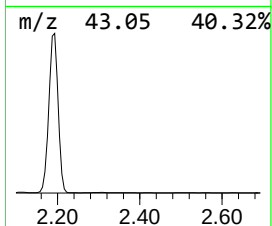
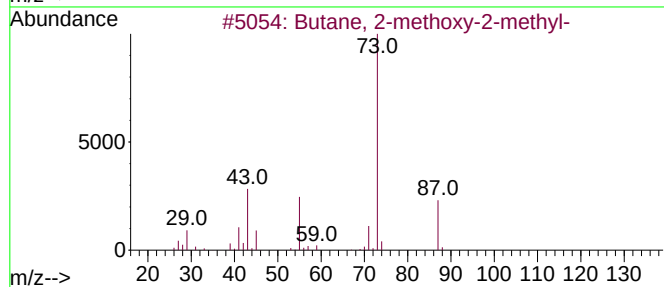
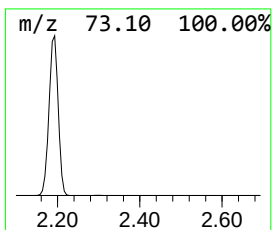
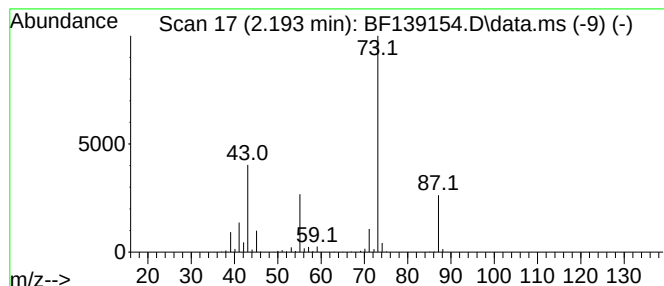
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.193 | 66.82 ng | 1596330 | 1,4-Dichlorobenzene-d4 | 6.898 |

| 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 | 39   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |
| 5    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 9    |



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BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

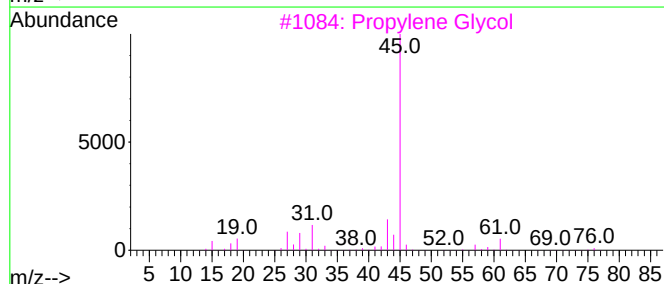
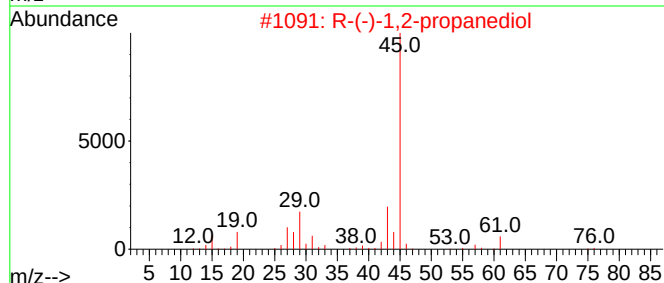
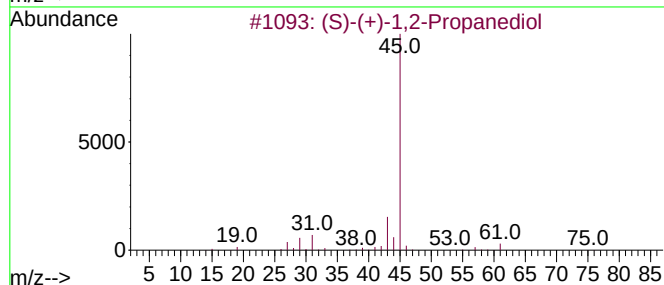
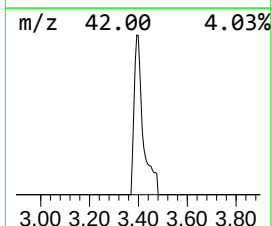
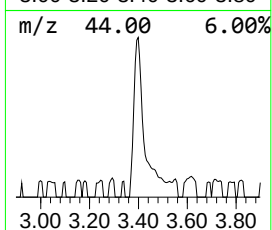
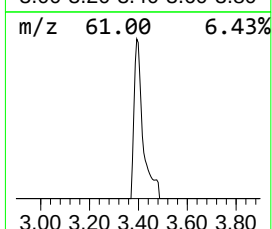
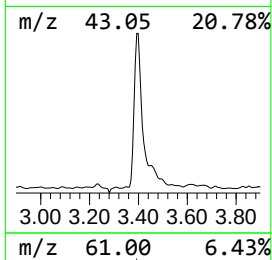
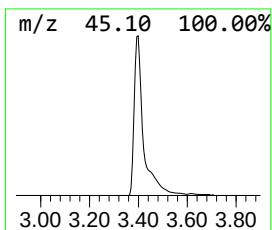
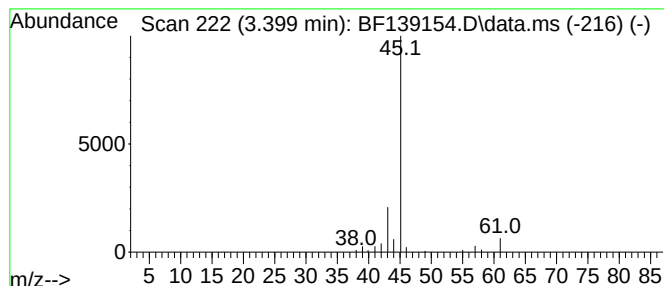
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.399 | 5.01 ng | 119658 | 1,4-Dichlorobenzene-d4 | 6.898 |

| Hit# | of 5 | Tentative ID            | MW | MolForm | CAS#        | Qual |
|------|------|-------------------------|----|---------|-------------|------|
| 1    |      | (S)-(+)-1,2-Propanediol | 76 | C3H8O2  | 004254-15-3 | 74   |
| 2    |      | R-(-)-1,2-propanediol   | 76 | C3H8O2  | 004254-14-2 | 64   |
| 3    |      | Propylene Glycol        | 76 | C3H8O2  | 000057-55-6 | 9    |
| 4    |      | Isopropyl Alcohol       | 60 | C3H8O   | 000067-63-0 | 9    |
| 5    |      | Formamide               | 45 | CH3NO   | 000075-12-7 | 5    |



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Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

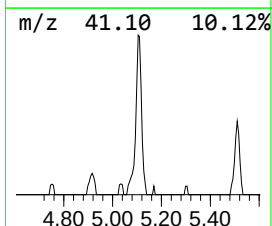
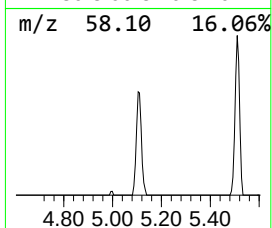
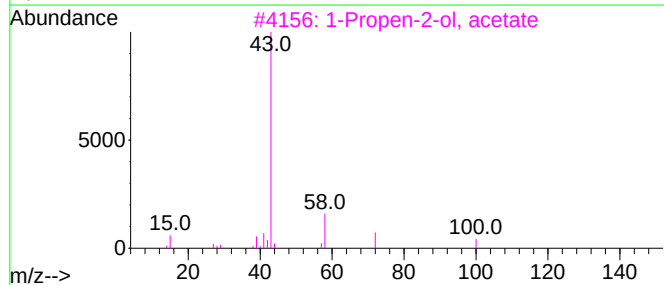
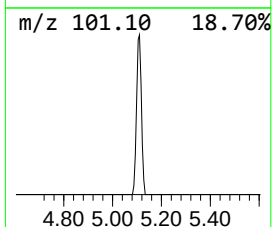
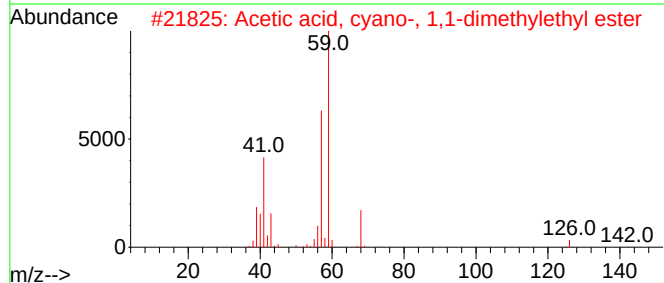
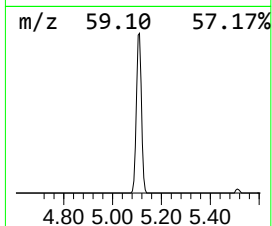
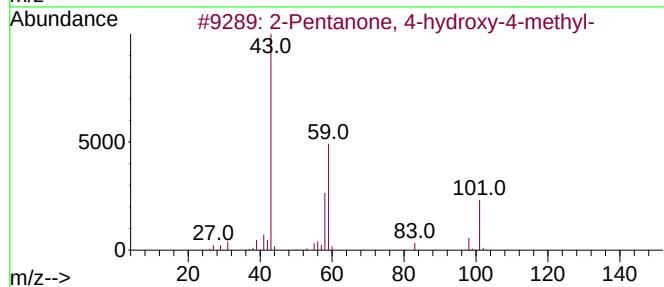
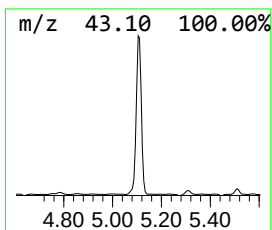
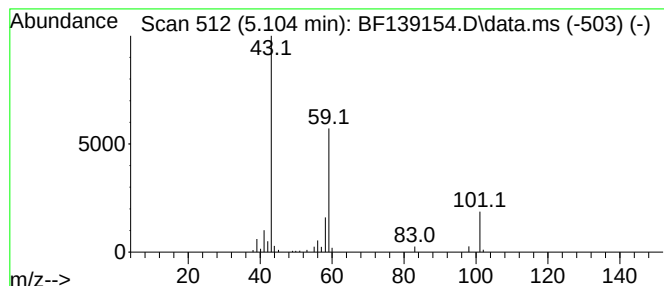
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.104 | 4.36 ng | 104079 | 1,4-Dichlorobenzene-d4 | 6.898 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32   |
| 3    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 12   |
| 4    |    |   | Acetone                             | 58  | C3H6O    | 000067-64-1 | 9    |
| 5    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



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ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

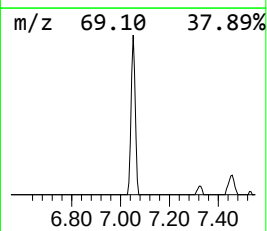
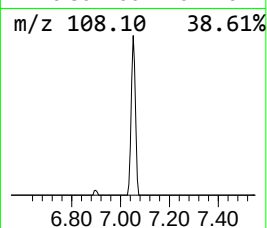
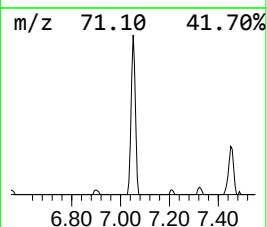
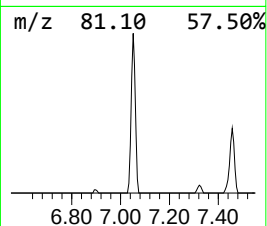
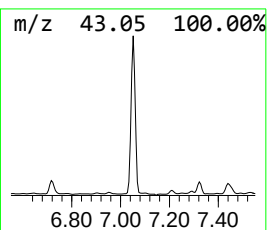
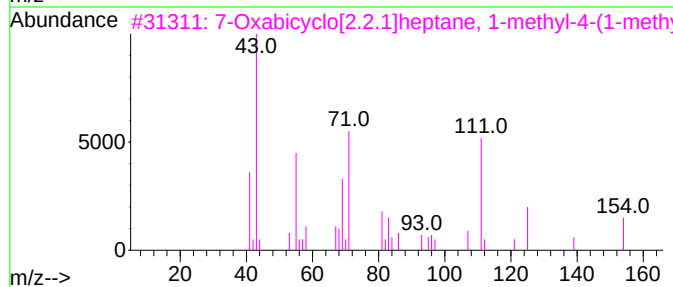
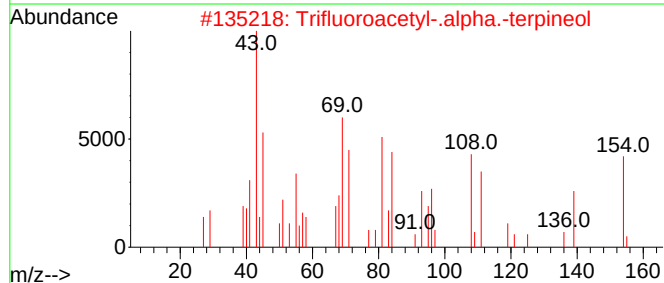
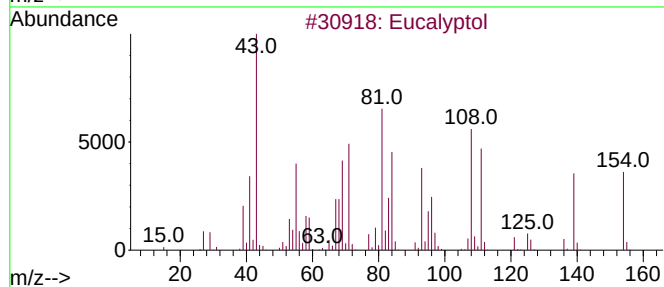
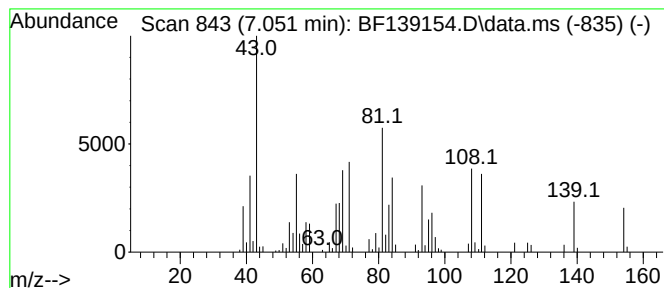
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Eucalyptol Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 7.051 | 8.49 ng | 202888 | 1,4-Dichlorobenzene-d4 | 6.898 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Eucalyptol                          | 154 | C10H18O    | 000470-82-6  | 97   |
| 2    |    |   | Trifluoroacetyl-.alpha.-terpineol   | 250 | C12H17F3O2 | 1000058-17-6 | 38   |
| 3    |    |   | 7-Oxabicyclo[2.2.1]heptane, 1-me... | 154 | C10H18O    | 000470-67-7  | 32   |
| 4    |    |   | 2-Isopropyl-5-methylhex-2-enal      | 154 | C10H18O    | 035158-25-9  | 27   |
| 5    |    |   | 4-Isopropyl-1-methylcyclohex-2-enol | 154 | C10H18O    | 000619-62-5  | 25   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

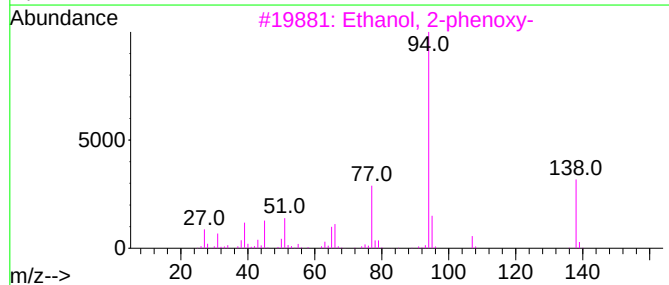
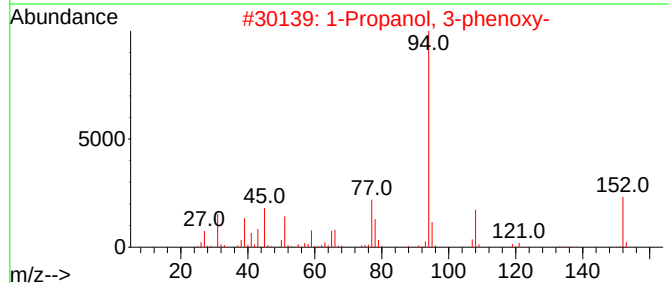
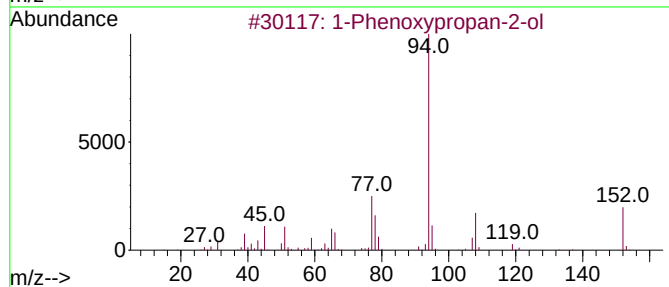
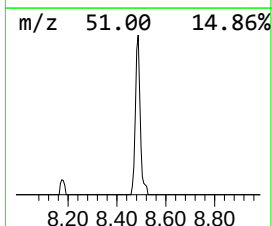
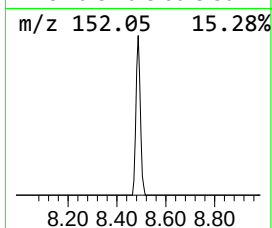
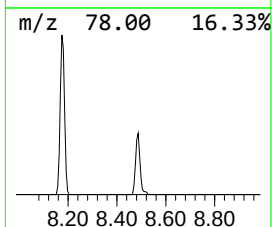
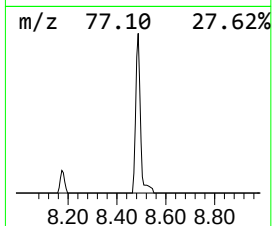
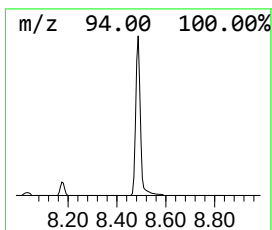
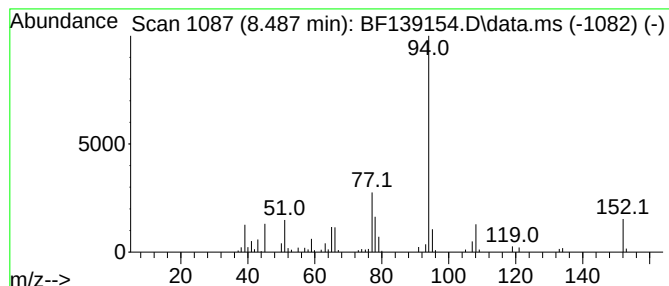
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.487 | 3.48 ng | 105006 | Naphthalene-d8   | 8.175 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1-Phenoxypropan-2-ol                | 152 | C9H12O2  | 000770-35-4 | 96   |
| 2    |    |   | 1-Propanol, 3-phenoxy-              | 152 | C9H12O2  | 006180-61-6 | 87   |
| 3    |    |   | Ethanol, 2-phenoxy-                 | 138 | C8H10O2  | 000122-99-6 | 64   |
| 4    |    |   | Carbonic acid, neopentyl phenyl ... | 208 | C12H16O3 | 013183-19-2 | 59   |
| 5    |    |   | 1-Propanol, 2-phenoxy-              | 152 | C9H12O2  | 004169-04-4 | 59   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

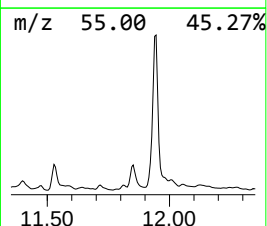
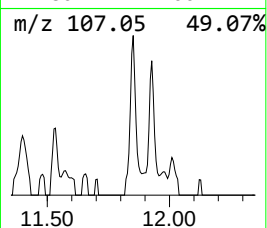
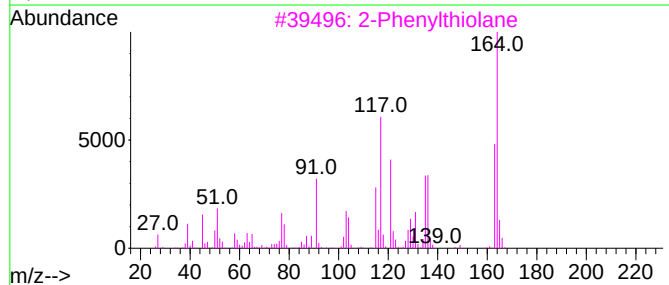
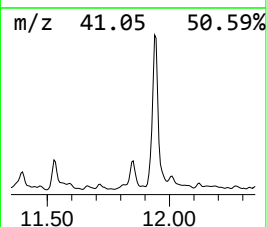
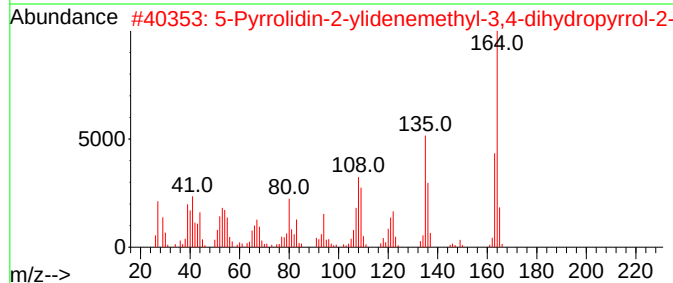
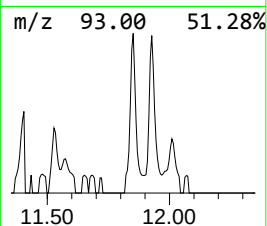
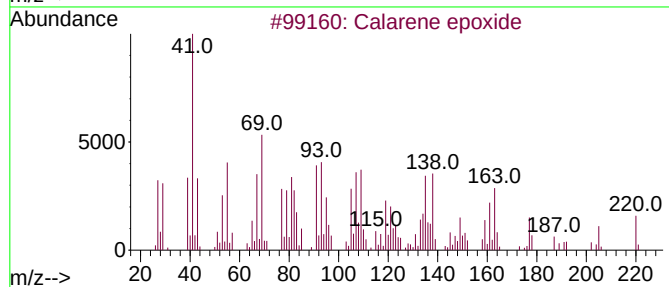
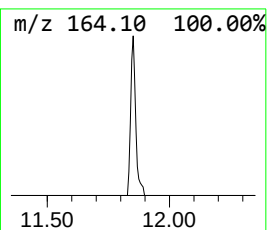
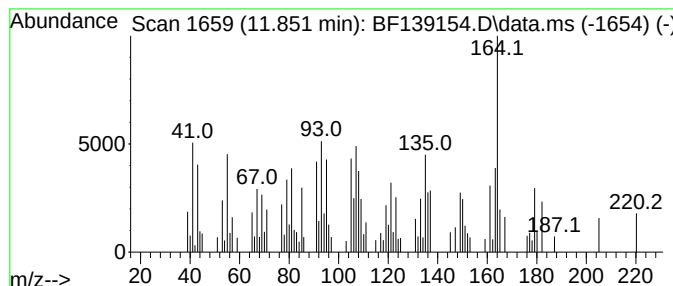
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Calarene epoxide Concentration Rank 14

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.851 | 2.23 ng | 69751 | Phenanthrene-d10 | 11.416 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Calarene epoxide                    | 220 | C15H24O  | 1000151-46-0 | 50   |
| 2    |    |   | 5-Pyrrolidin-2-ylidenemethyl-3,4... | 164 | C9H12N2O | 1010192-09-5 | 46   |
| 3    |    |   | 2-Phenylthiolane                    | 164 | C10H12S  | 002060-65-3  | 38   |
| 4    |    |   | Bicyclo[2.2.2]oct-2-ene, 1,2,3,6... | 164 | C12H20   | 062376-14-1  | 38   |
| 5    |    |   | 8-Amino-2H-1,4-benzoxazin-3(4H)-one | 164 | C8H8N2O2 | 321126-82-3  | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

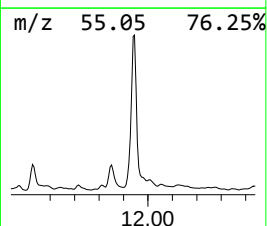
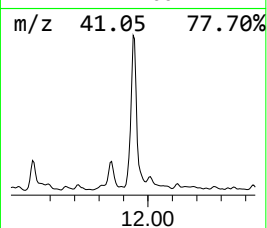
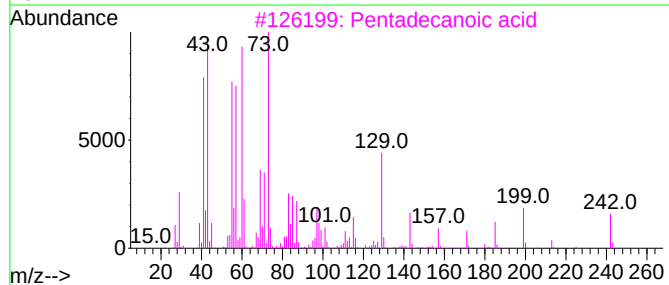
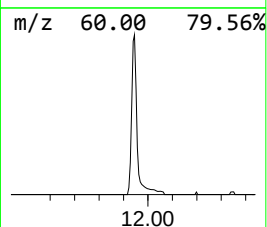
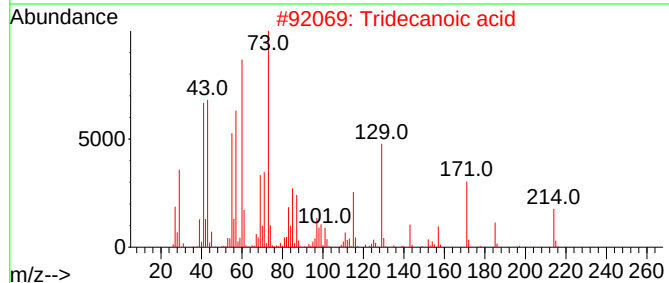
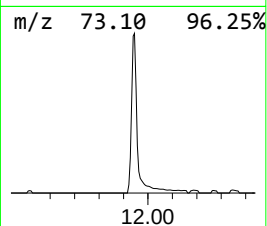
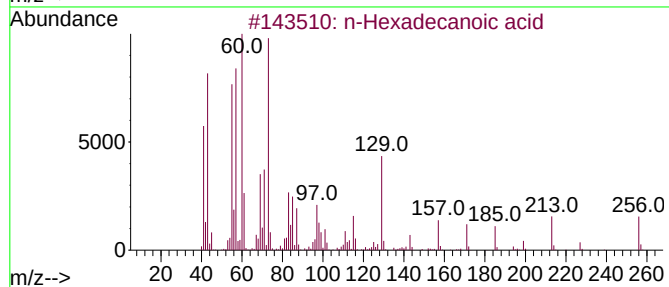
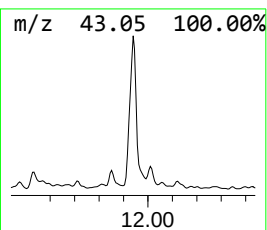
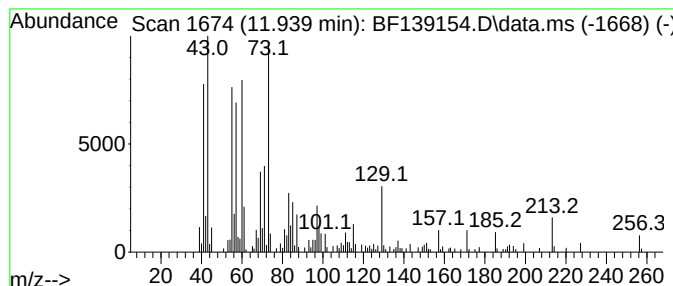
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.939 | 8.19 ng | 256479 | Phenanthrene-d10 | 11.416 |

| 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  | 83   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 74   |
| 4    |    |   | Oxalic acid, cyclobutyl heptadec... | 382 | C23H42O4 | 1000309-70-7 | 18   |
| 5    |    |   | Oxalic acid, allyl hexadecyl ester  | 354 | C21H38O4 | 1000309-24-4 | 18   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

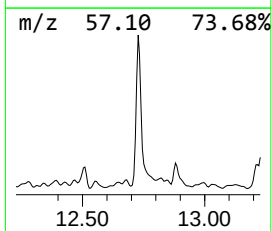
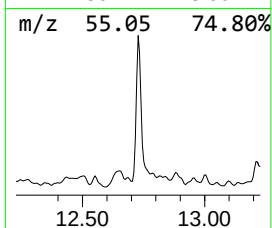
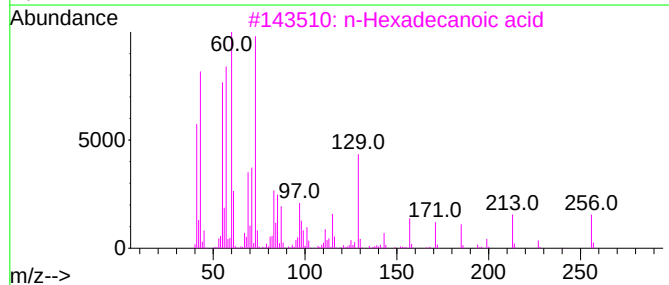
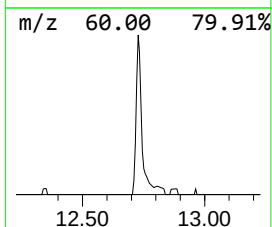
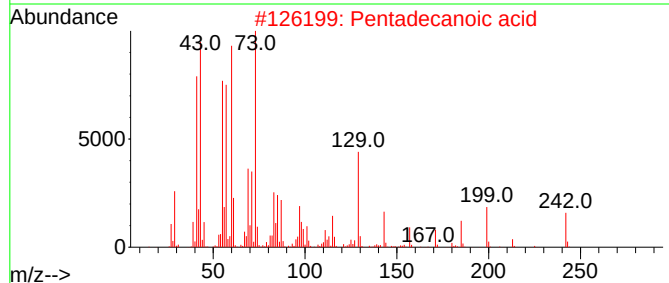
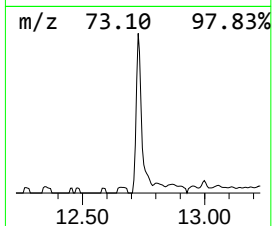
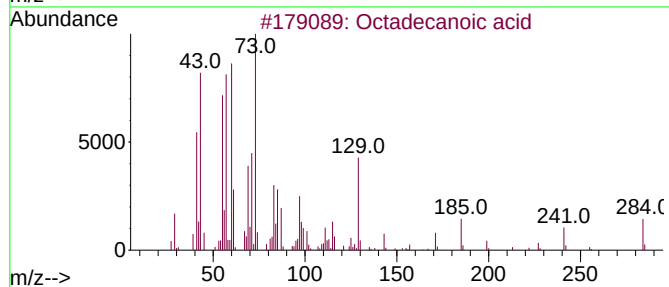
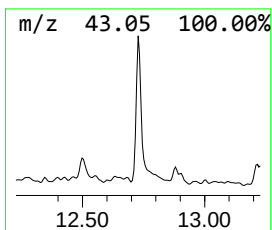
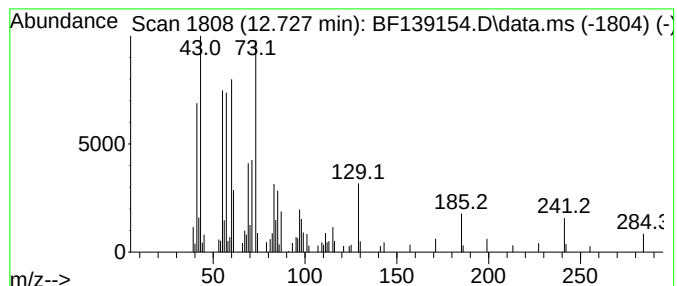
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Octadecanoic acid Concentration Rank 11

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.727 | 3.02 ng | 94720 | Phenanthrene-d10 | 11.416 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2  | 000057-11-4  | 98   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2  | 001002-84-2  | 91   |
| 3    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2  | 000057-10-3  | 80   |
| 4    |    |   | Oxalic acid, propyl tetradecyl e... | 328 | C19H36O4  | 1000309-26-7 | 25   |
| 5    |    |   | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 25   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

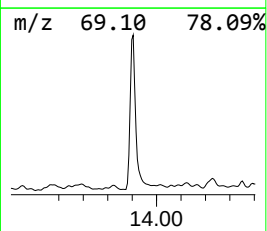
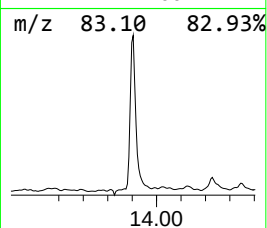
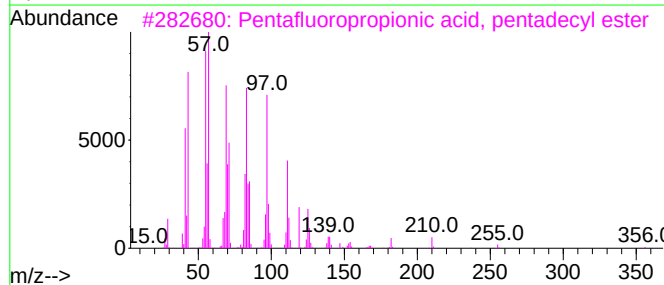
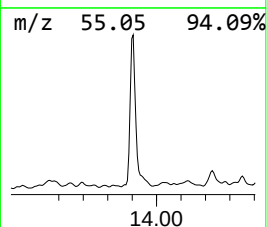
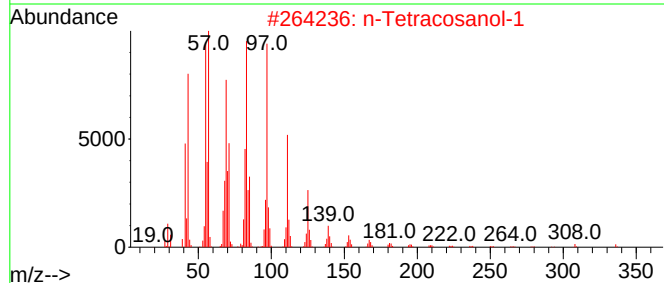
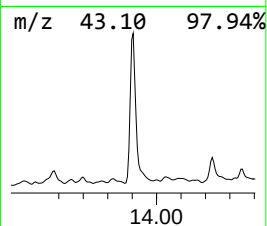
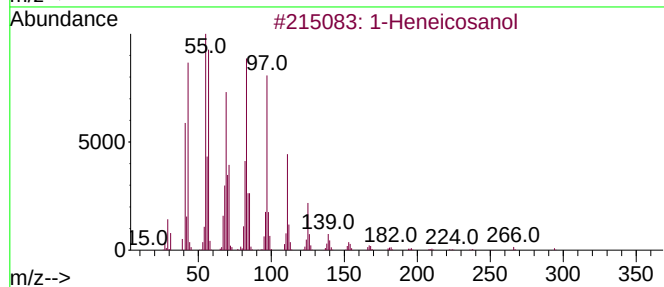
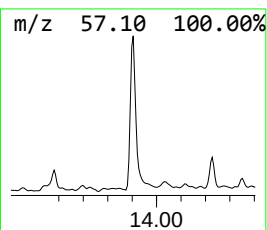
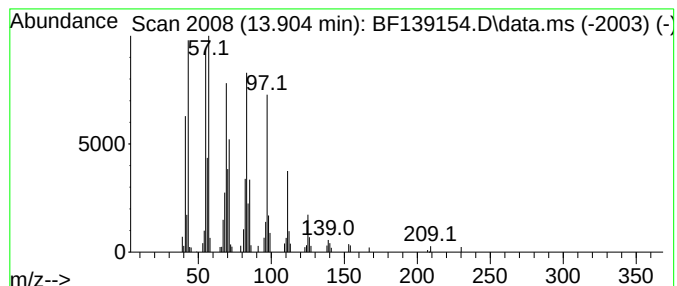
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 9 1-Heneicosanol Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.904 | 6.89 ng | 140093 | Chrysene-d12     | 14.051 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 95   |
| 2    |    |   | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4 | 94   |
| 3    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 91   |
| 4    |    |   | 3-Eicosene, (E)-                    | 280 | C20H40     | 074685-33-9 | 91   |
| 5    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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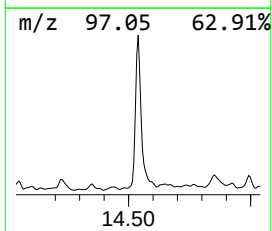
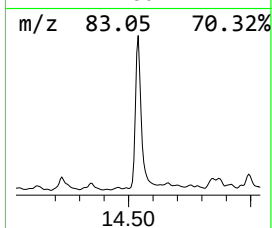
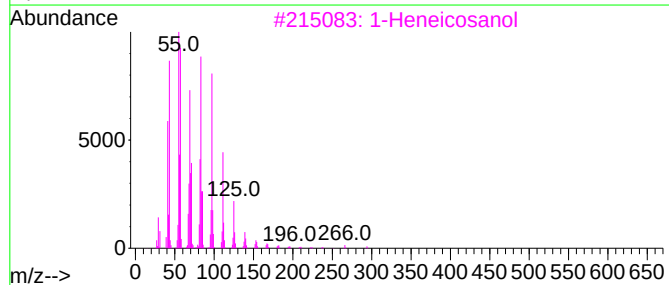
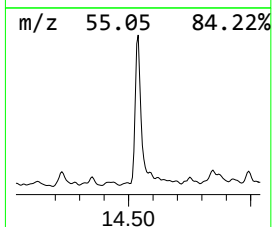
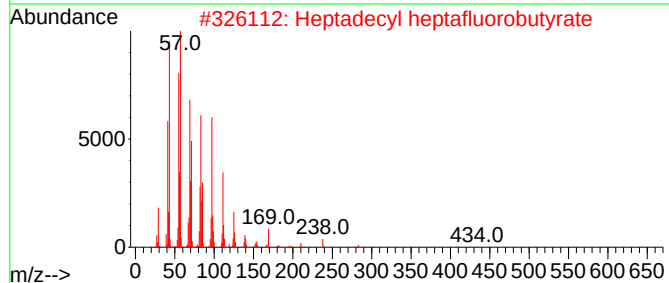
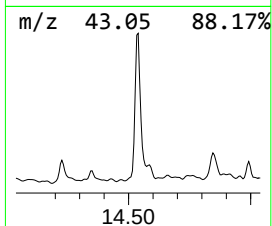
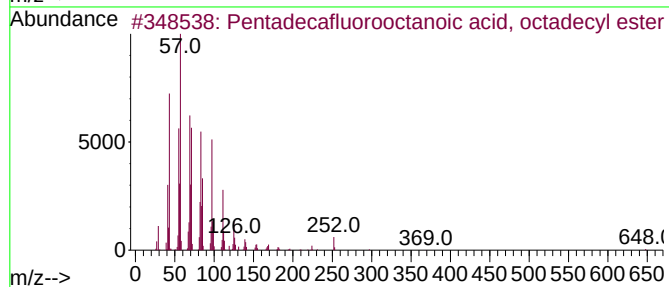
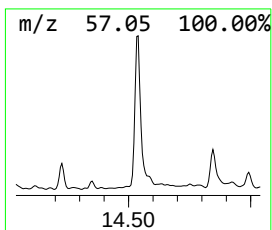
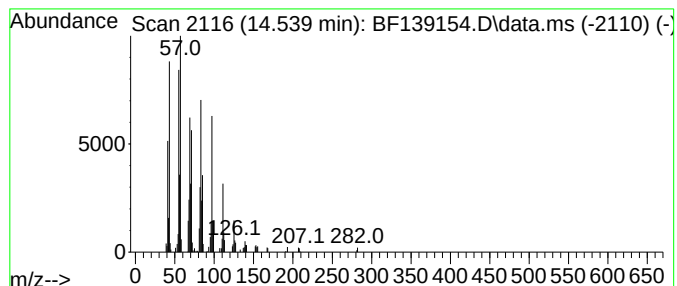
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 4

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 14.539    | 7.71 ng                             | 156745 | Chrysene-d12     | 14.051       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Pentadecafluorooctanoic acid, oc... | 666    | C26H37F15O2      | 1000406-04-8 | 95   |
| 2         | Heptadecyl heptafluorobutyrate      | 452    | C21H35F7O2       | 959085-66-6  | 95   |
| 3         | 1-Heneicosanol                      | 312    | C21H44O          | 015594-90-8  | 93   |
| 4         | 1-Heptacosanol                      | 396    | C27H56O          | 002004-39-9  | 91   |
| 5         | Heptadecyl trifluoroacetate         | 352    | C19H35F3O2       | 1010351-87-0 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

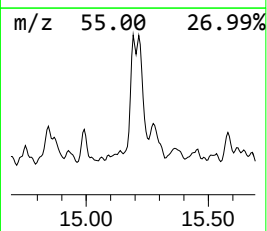
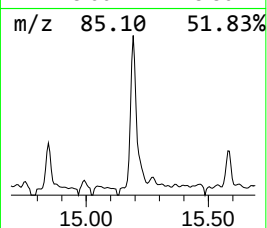
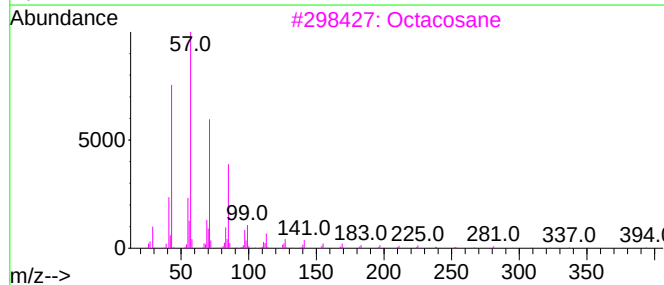
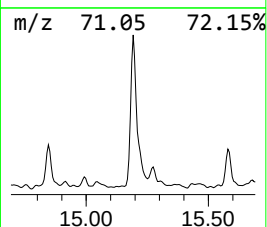
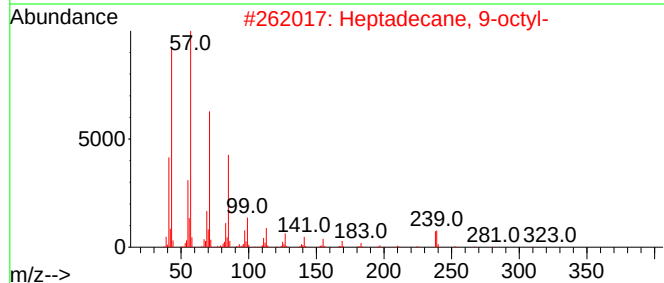
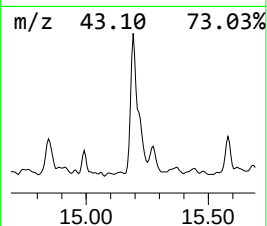
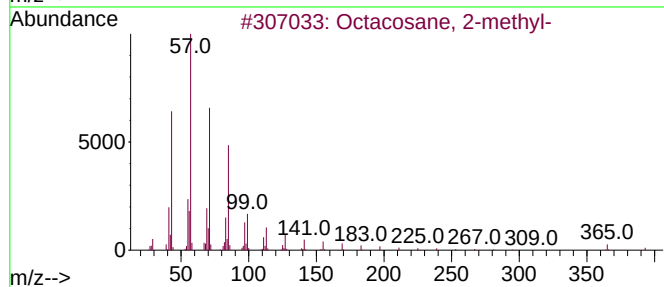
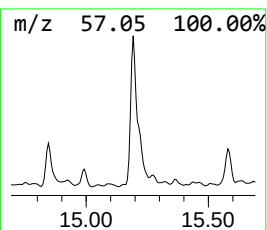
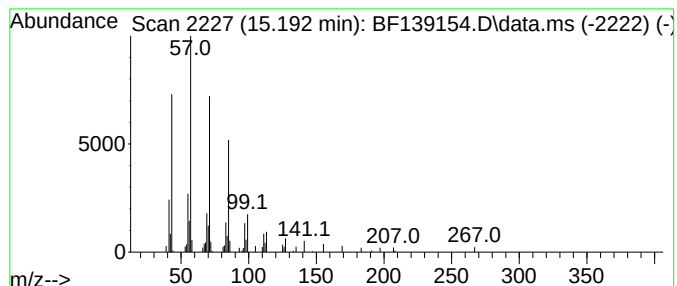
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 11 Octacosane, 2-methyl- Concentration Rank 9

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.192 | 3.29 ng | 72417 | Perylene-d12     | 15.533 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 91   |
| 2    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 91   |
| 3    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 5    |    |   | Heptacosane           | 380 | C27H56  | 000593-49-7 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

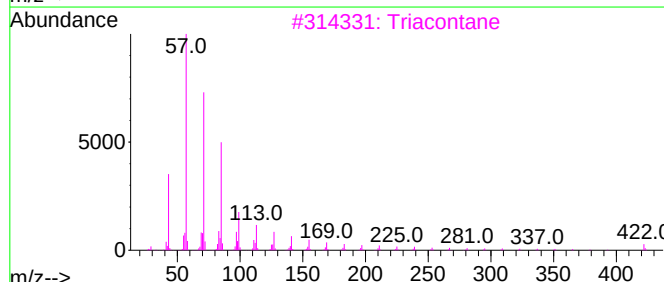
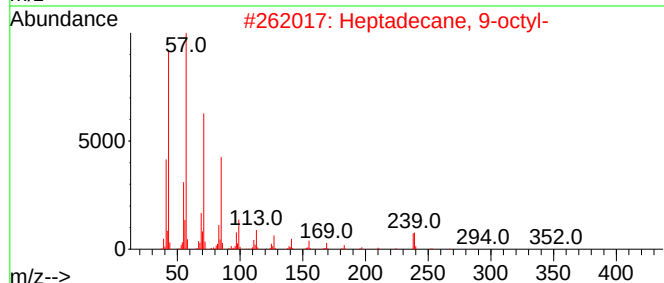
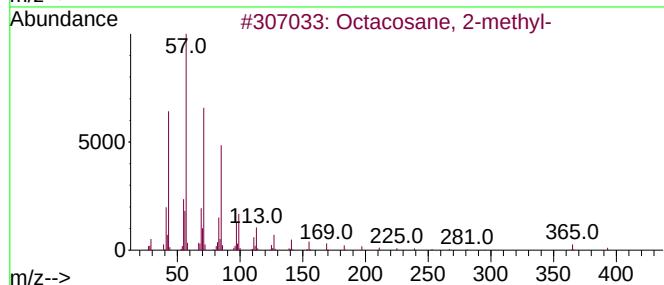
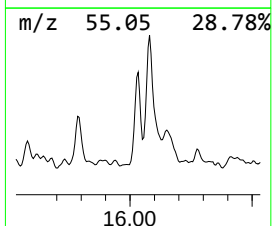
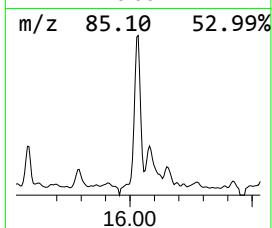
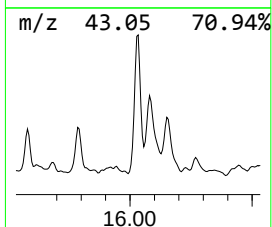
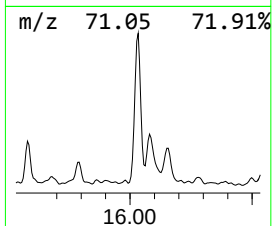
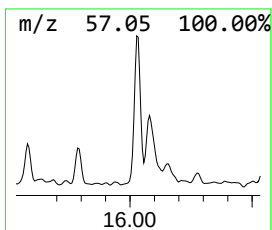
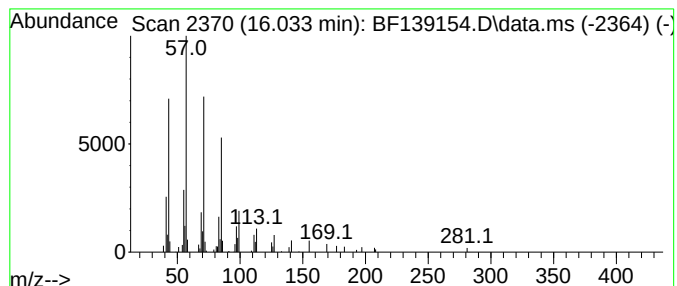
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 12

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.033 | 2.88 ng | 63412 | Perylene-d12     | 15.533 |

| Hit# | of 5 | Tentative ID           | MW  | MolForm | CAS#         | Qual |
|------|------|------------------------|-----|---------|--------------|------|
| 1    |      | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1  | 91   |
| 2    |      | Heptadecane, 9-octyl-  | 352 | C25H52  | 007225-64-1  | 91   |
| 3    |      | Triacontane            | 422 | C30H62  | 000638-68-6  | 91   |
| 4    |      | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 91   |
| 5    |      | Heneicosane            | 296 | C21H44  | 000629-94-7  | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

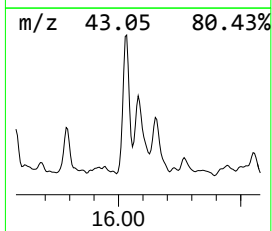
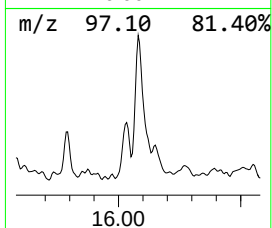
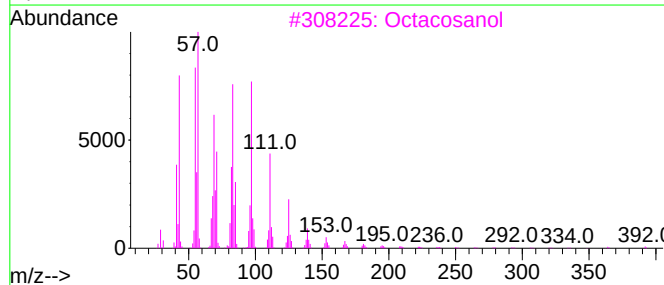
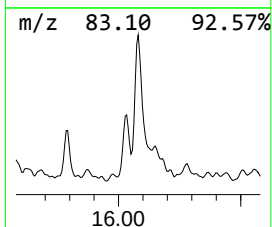
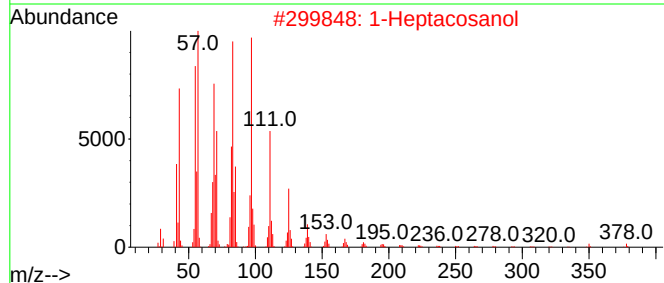
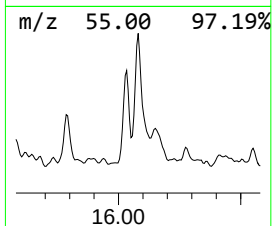
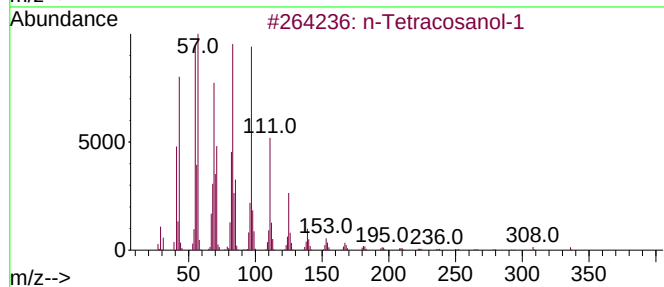
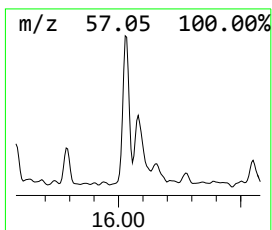
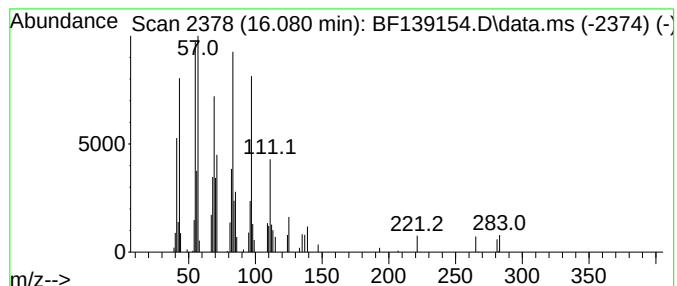
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 13 n-Tetracosanol-1 Concentration Rank 10

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.080 | 3.17 ng | 69660 | Perylene-d12     | 15.533 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-----------------------------|-----|------------|--------------|------|
| 1    |    |   | n-Tetracosanol-1            | 354 | C24H50O    | 000506-51-4  | 94   |
| 2    |    |   | 1-Heptacosanol              | 396 | C27H56O    | 002004-39-9  | 91   |
| 3    |    |   | Octacosanol                 | 410 | C28H58O    | 000557-61-9  | 91   |
| 4    |    |   | Behenic alcohol             | 326 | C22H46O    | 000661-19-8  | 91   |
| 5    |    |   | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1010351-87-0 | 91   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

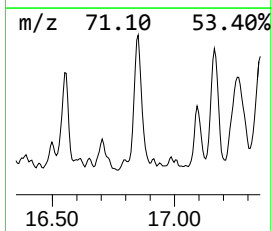
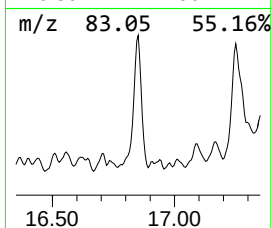
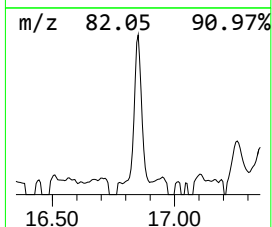
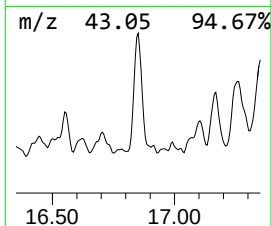
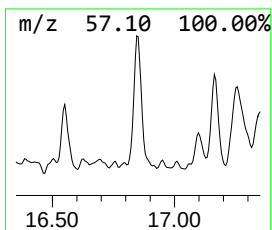
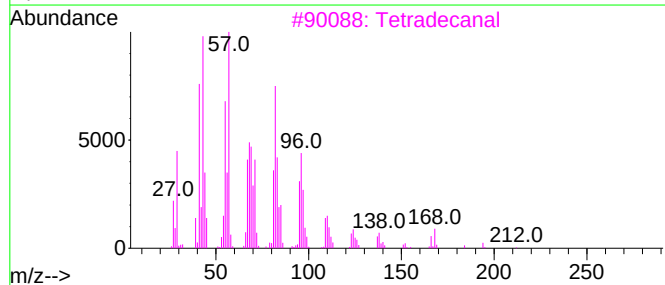
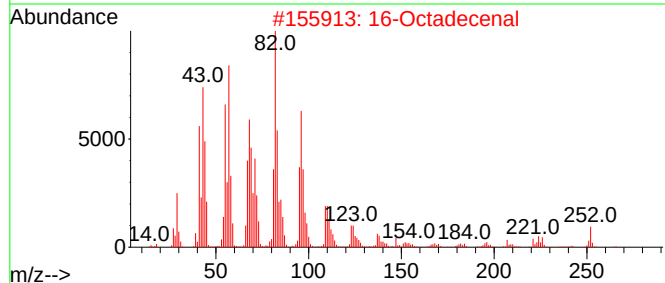
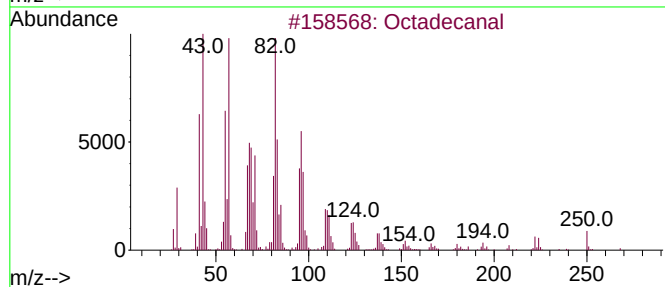
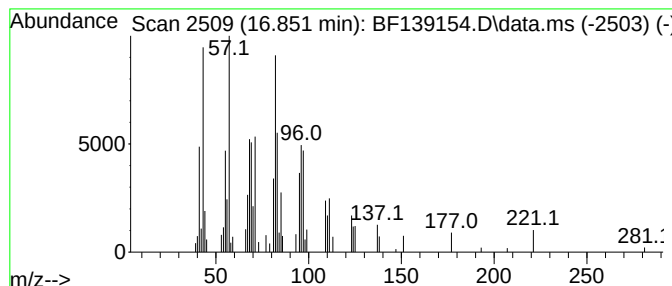
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Peak Number 14 Octadecanal Concentration Rank 13

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.851 | 2.39 ng | 52482 | Perylene-d12     | 15.533 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------|-----|---------|-------------|------|
| 1    |      | Octadecanal         | 268 | C18H36O | 000638-66-4 | 91   |
| 2    |      | 16-Octadecenal      | 266 | C18H34O | 056554-87-1 | 80   |
| 3    |      | Tetradecanal        | 212 | C14H28O | 000124-25-4 | 80   |
| 4    |      | Oxirane, dodecyl-   | 212 | C14H28O | 003234-28-4 | 72   |
| 5    |      | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 68   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082324\  
Data File : BF139154.D  
Acq On : 23 Aug 2024 18:44  
Operator : RC/JU  
Sample : P3707-04  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-929-K1-SO-0.5-1-082024

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF082024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.193  | 66.8    | ng    | 1596330  | 1                     | 6.898  | 477809 | 20.0 |
| (S)-(+)-1,2-Pro... | 3.399  | 5.0     | ng    | 119658   | 1                     | 6.898  | 477809 | 20.0 |
| 2-Pentanone, 4-... | 5.104  | 4.4     | ng    | 104079   | 1                     | 6.898  | 477809 | 20.0 |
| Eucalyptol         | 7.051  | 8.5     | ng    | 202888   | 1                     | 6.898  | 477809 | 20.0 |
| 1-Phenoxypropan... | 8.487  | 3.5     | ng    | 105006   | 2                     | 8.175  | 603771 | 20.0 |
| Calarene epoxide   | 11.851 | 2.2     | ng    | 69751    | 4                     | 11.416 | 626562 | 20.0 |
| n-Hexadecanoic ... | 11.939 | 8.2     | ng    | 256479   | 4                     | 11.416 | 626562 | 20.0 |
| Octadecanoic acid  | 12.727 | 3.0     | ng    | 94720    | 4                     | 11.416 | 626562 | 20.0 |
| 1-Heneicosanol     | 13.904 | 6.9     | ng    | 140093   | 5                     | 14.051 | 406698 | 20.0 |
| Pentadecafluoro... | 14.539 | 7.7     | ng    | 156745   | 5                     | 14.051 | 406698 | 20.0 |
| Octacosane, 2-m... | 15.192 | 3.3     | ng    | 72417    | 6                     | 15.533 | 439670 | 20.0 |
| Heptadecane, 9-... | 16.033 | 2.9     | ng    | 63412    | 6                     | 15.533 | 439670 | 20.0 |
| n-Tetracosanol-1   | 16.080 | 3.2     | ng    | 69660    | 6                     | 15.533 | 439670 | 20.0 |
| Octadecanal        | 16.851 | 2.4     | ng    | 52482    | 6                     | 15.533 | 439670 | 20.0 |