

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052822\  
 Data File : BF128553.D  
 Acq On : 28 May 2022 17:36  
 Operator : CG\JU  
 Sample : N2931-03  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P009-SS003-1218-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128553.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         | 2.951       | 108           | 113         | 121          | rVB2     | 36232          | 56241         | 1.21%           | 0.170%        |
| 2         | 5.063       | 462           | 472         | 481          | rVB      | 138022         | 189808        | 4.09%           | 0.575%        |
| 3         | 5.451       | 533           | 538         | 542          | rBV      | 3448965        | 3770501       | 81.27%          | 11.429%       |
| 4         | 6.292       | 674           | 681         | 691          | rBV3     | 42979          | 81480         | 1.76%           | 0.247%        |
| 5         | 6.463       | 704           | 710         | 713          | rBV      | 3605114        | 3861423       | 83.23%          | 11.705%       |
| 6         | 6.575       | 726           | 729         | 739          | rVB      | 52528          | 59660         | 1.29%           | 0.181%        |
| 7         | 6.839       | 770           | 774         | 777          | rBV      | 1216299        | 1076463       | 23.20%          | 3.263%        |
| 8         | 7.398       | 864           | 869         | 872          | rBV      | 2762632        | 2653320       | 57.19%          | 8.043%        |
| 9         | 7.863       | 945           | 948         | 952          | rVB      | 76447          | 68735         | 1.48%           | 0.208%        |
| 10        | 8.116       | 987           | 991         | 995          | rBV      | 1535425        | 1419642       | 30.60%          | 4.303%        |
| 11        | 9.198       | 1169          | 1175        | 1178         | rBV      | 5123617        | 4639436       | 100.00%         | 14.063%       |
| 12        | 9.822       | 1275          | 1281        | 1284         | rBV      | 793885         | 615988        | 13.28%          | 1.867%        |
| 13        | 9.875       | 1284          | 1290        | 1294         | rVV      | 1999236        | 1614039       | 34.79%          | 4.892%        |
| 14        | 10.663      | 1419          | 1424        | 1427         | rBV      | 3094004        | 2830286       | 61.00%          | 8.579%        |
| 15        | 10.774      | 1439          | 1443        | 1446         | rVB      | 747894         | 632123        | 13.62%          | 1.916%        |
| 16        | 11.363      | 1539          | 1543        | 1546         | rBV      | 1845730        | 1573594       | 33.92%          | 4.770%        |
| 17        | 11.892      | 1629          | 1633        | 1649         | rBV      | 410668         | 442013        | 9.53%           | 1.340%        |
| 18        | 12.598      | 1748          | 1753        | 1760         | rBV      | 75574          | 97731         | 2.11%           | 0.296%        |
| 19        | 12.674      | 1763          | 1766        | 1774         | rBV      | 89946          | 112189        | 2.42%           | 0.340%        |
| 20        | 12.951      | 1809          | 1813        | 1817         | rBV      | 4030412        | 3918045       | 84.45%          | 11.876%       |
| 21        | 13.910      | 1970          | 1976        | 1987         | rBV2     | 124200         | 333608        | 7.19%           | 1.011%        |
| 22        | 13.998      | 1987          | 1991        | 1995         | rVV      | 1092096        | 1058915       | 22.82%          | 3.210%        |
| 23        | 14.098      | 2003          | 2008        | 2013         | rBV      | 444276         | 485419        | 10.46%          | 1.471%        |
| 24        | 14.527      | 2077          | 2081        | 2086         | rBV2     | 134979         | 154193        | 3.32%           | 0.467%        |
| 25        | 14.868      | 2135          | 2139        | 2143         | rBV      | 230661         | 236033        | 5.09%           | 0.715%        |
| 26        | 15.468      | 2235          | 2241        | 2246         | rBV      | 710337         | 946475        | 20.40%          | 2.869%        |
| 27        | 15.951      | 2319          | 2323        | 2331         | rVB3     | 35913          | 62758         | 1.35%           | 0.190%        |

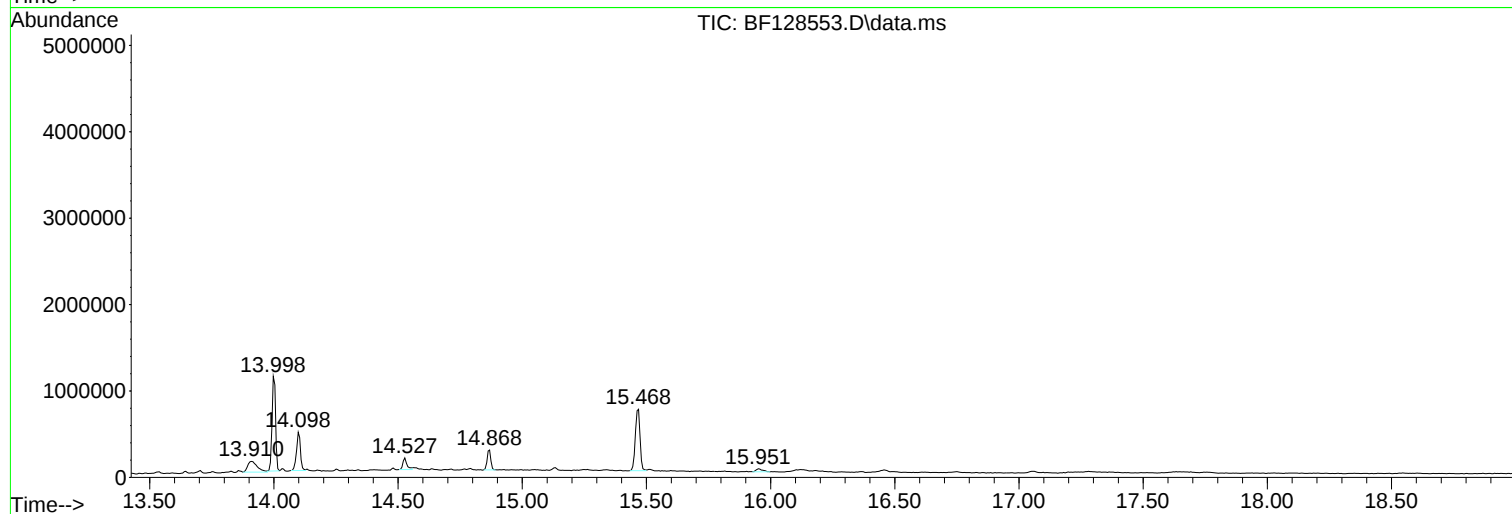
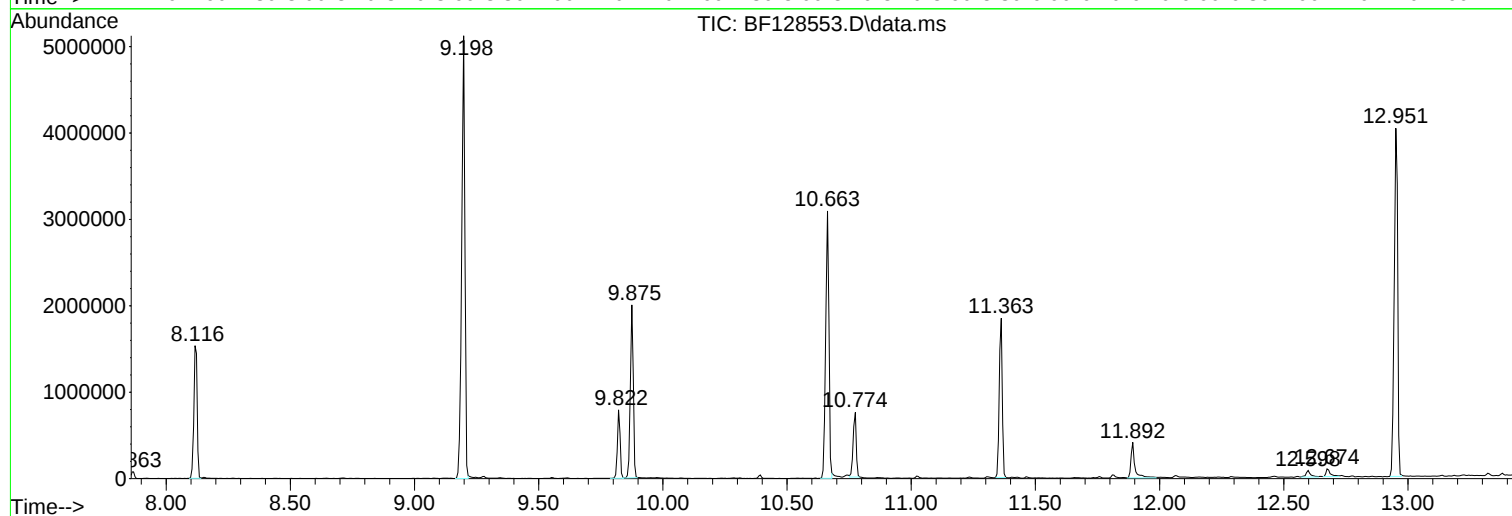
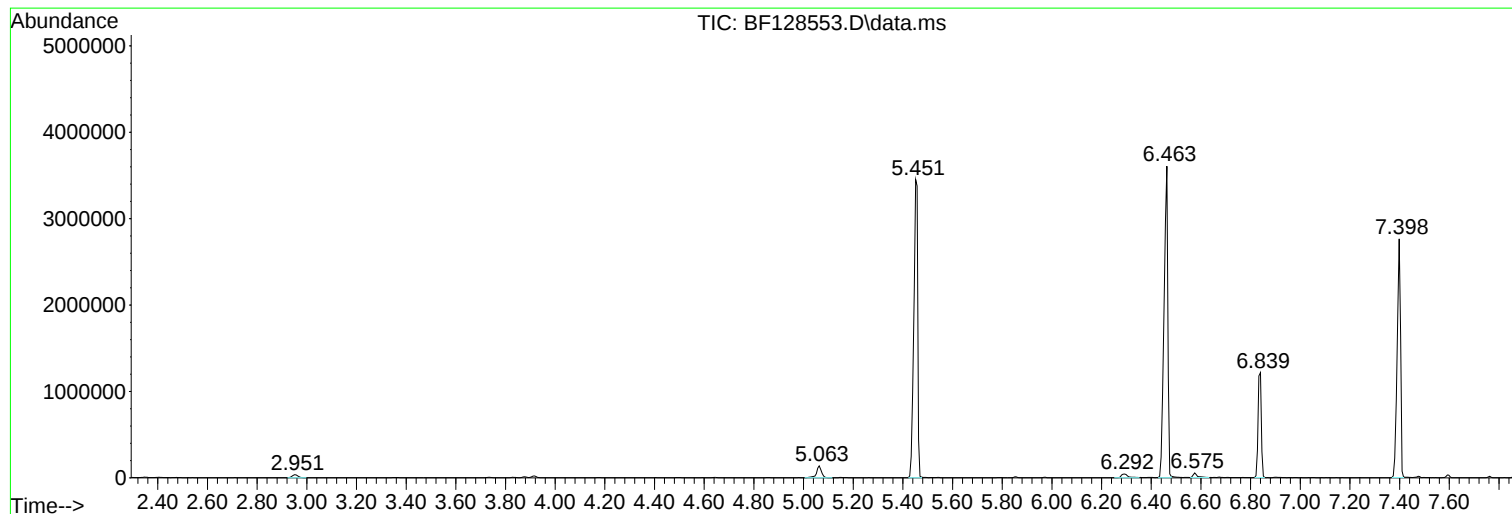
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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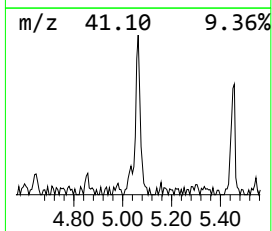
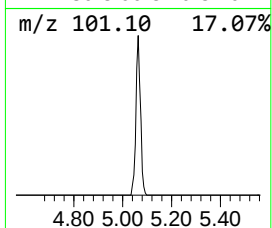
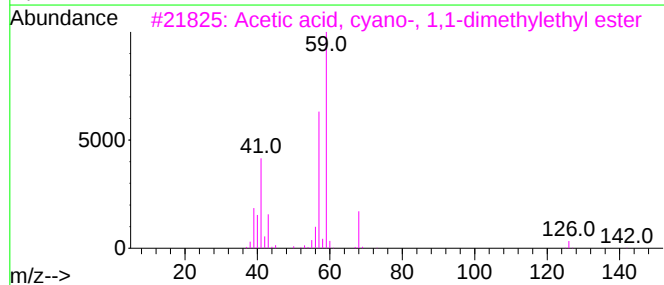
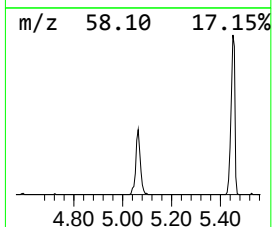
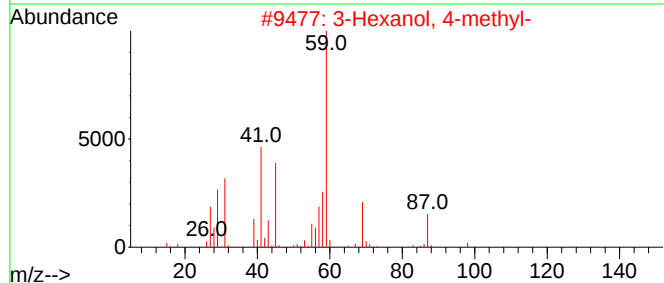
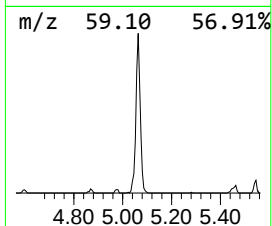
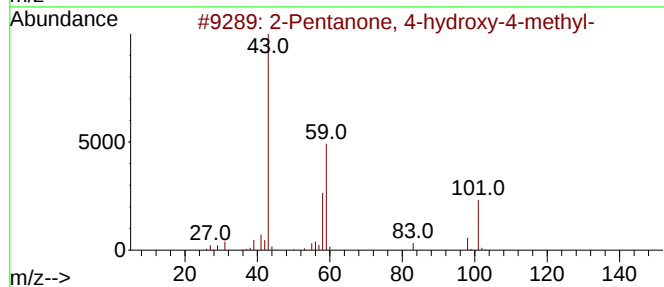
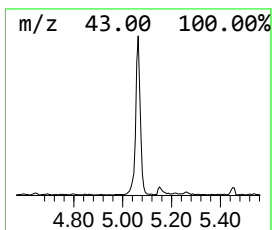
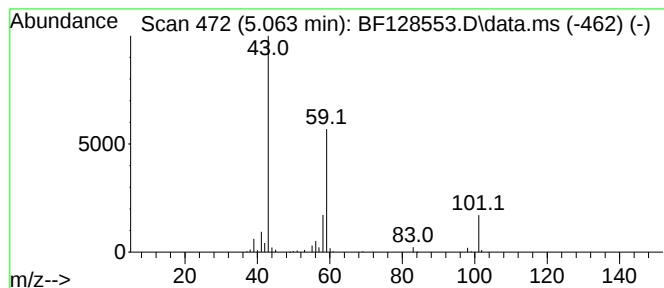
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.063 | 3.53 ng | 189808 | 1,4-Dichlorobenzene-d4 | 6.839 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 72      |      |      |
| 2    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 33      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 25      |      |      |
| 4    | 4-Penten-2-one, 4-methyl-           | 98  | C6H10O       | 003744-02-3 | 14      |      |      |
| 5    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 12      |      |      |



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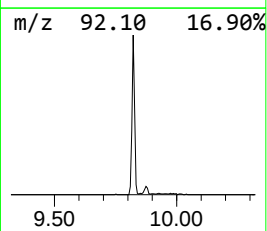
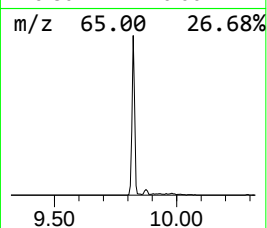
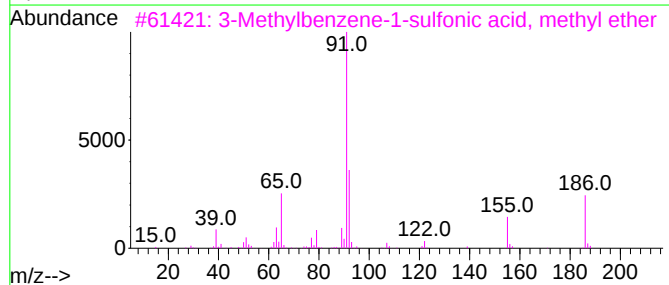
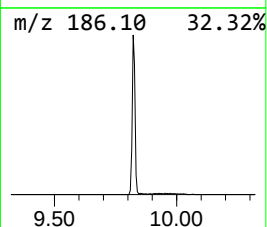
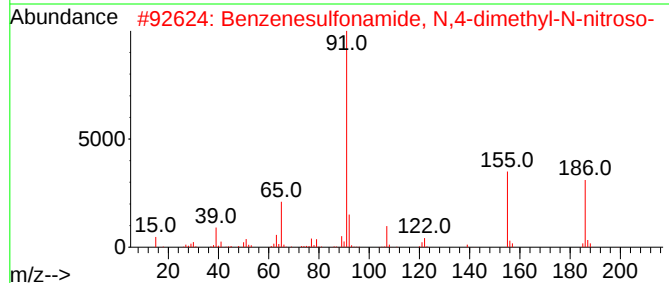
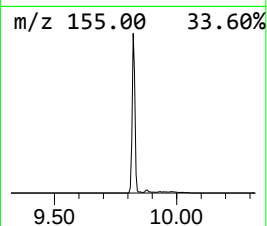
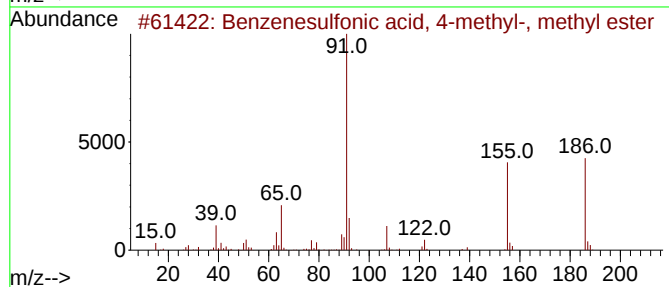
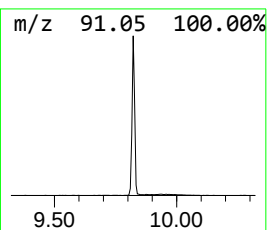
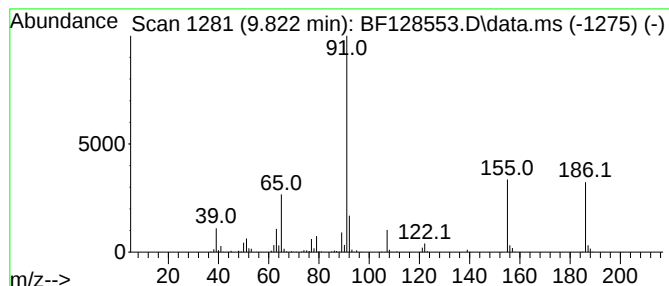
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzenesulfonic acid, 4-met... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 9.822 | 7.63 ng | 615988 | Acenaphthene-d10 | 9.874 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Benzenesulfonic acid, 4-methyl-,... | 186 | C8H10O3S   | 000080-48-8 | 93   |
| 2    |    |   | Benzenesulfonamide, N,4-dimethyl... | 214 | C8H10N2O3S | 000080-11-5 | 91   |
| 3    |    |   | 3-Methylbenzene-1-sulfonic acid,... | 186 | C8H10O3S   | 126865-07-4 | 76   |
| 4    |    |   | 4-Toluenesulfonylmethyl isocyanide  | 195 | C9H9N02S   | 036635-61-7 | 43   |
| 5    |    |   | Thiocyanic acid, phenylmethyl ester | 149 | C8H7NS     | 003012-37-1 | 38   |



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Sample : N2931-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

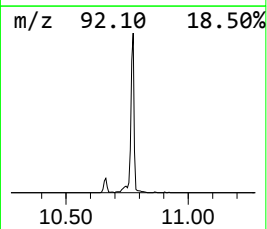
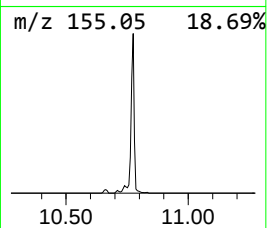
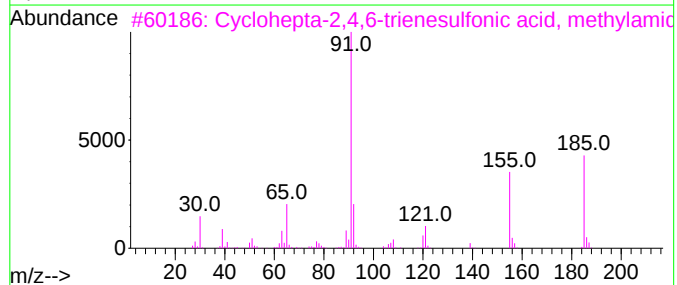
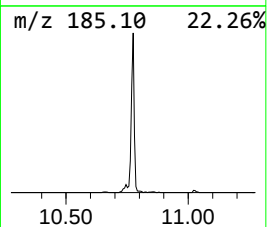
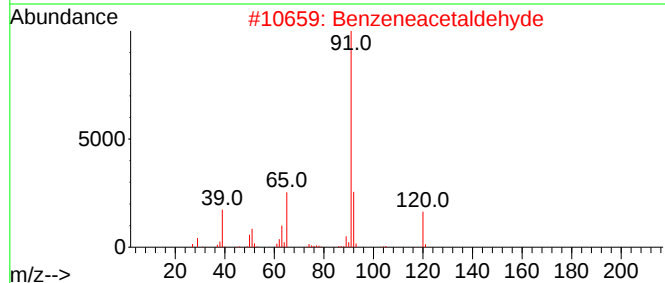
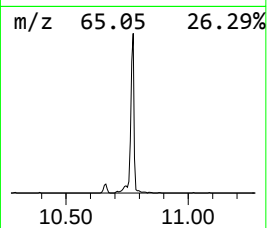
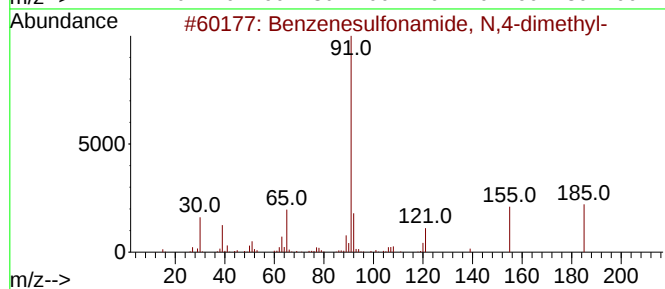
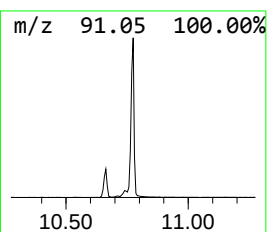
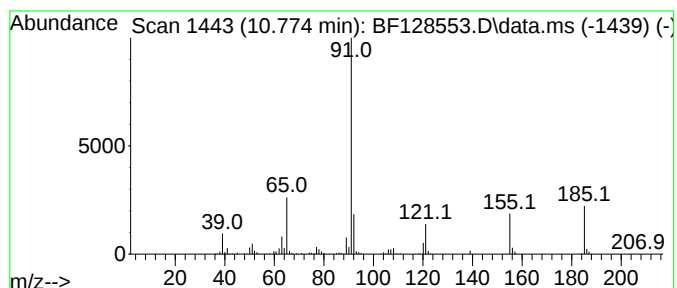
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.775 | 8.03 ng | 632123 | Phenanthrene-d10 | 11.363 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzenesulfonamide, N,4-dimethyl-   | 185 | C8H11NO2S  | 000640-61-9  | 95   |
| 2    |    |   | Benzeneacetaldehyde                 | 120 | C8H8O      | 000122-78-1  | 55   |
| 3    |    |   | Cyclohepta-2,4,6-trienesulfonic ... | 185 | C8H11NO2S  | 1000187-28-7 | 52   |
| 4    |    |   | Benzenesulfonamide, N,4-dimethyl... | 214 | C8H10N2O3S | 000080-11-5  | 50   |
| 5    |    |   | (O-p-Tosylisonitroso)malononitrile  | 249 | C10H7N3O3S | 020893-01-0  | 47   |



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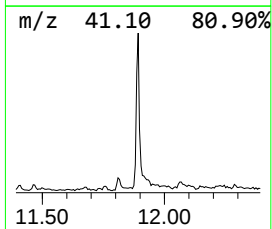
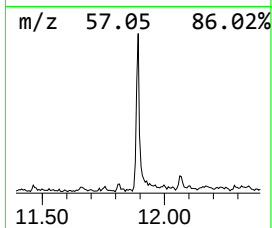
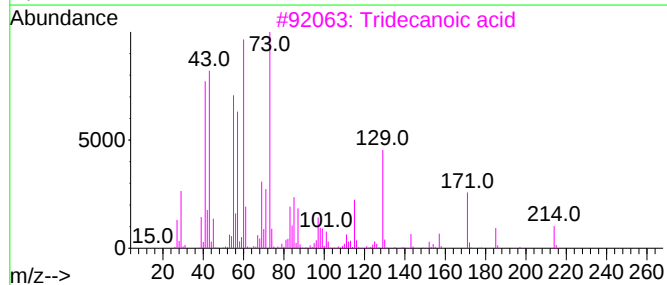
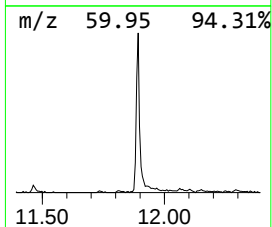
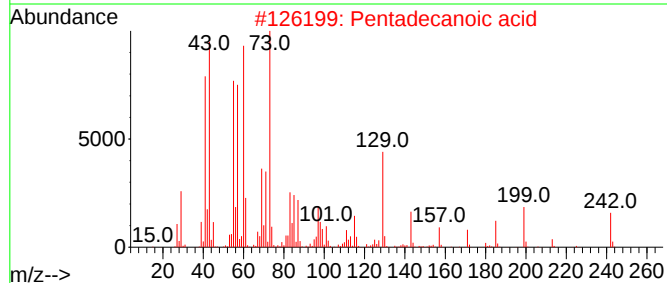
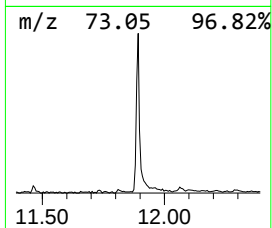
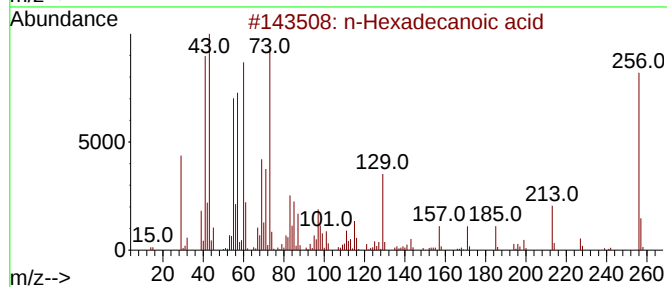
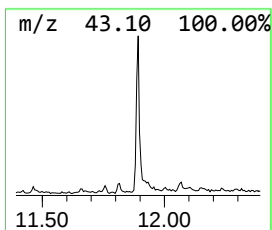
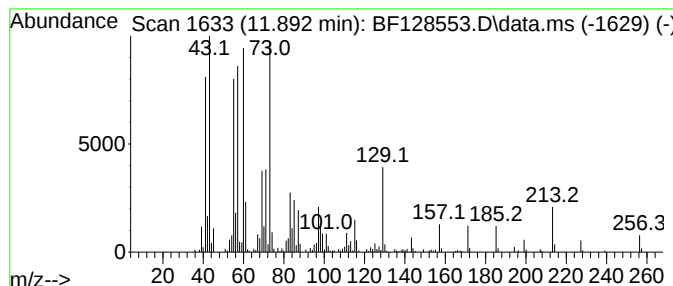
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.892 | 5.62 ng | 442013 | Phenanthrene-d10 | 11.363 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 93   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 76   |



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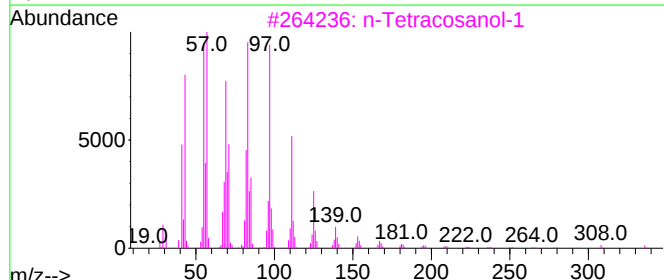
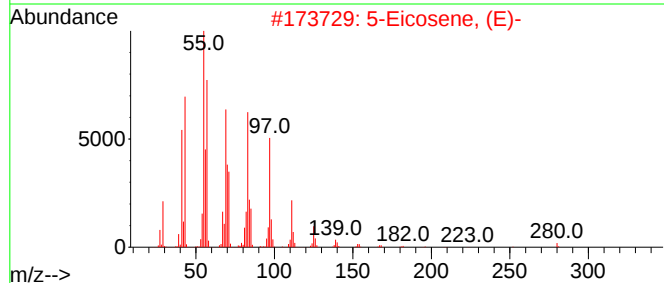
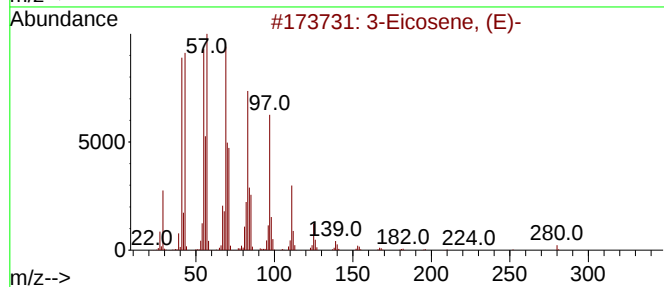
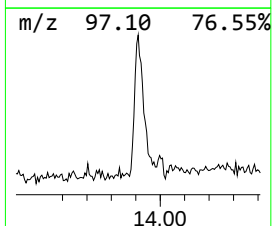
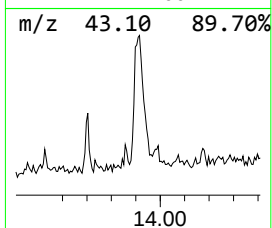
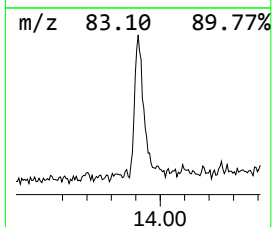
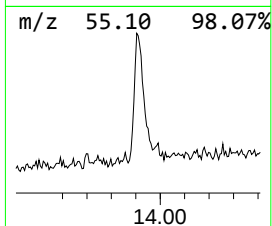
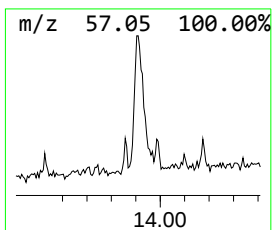
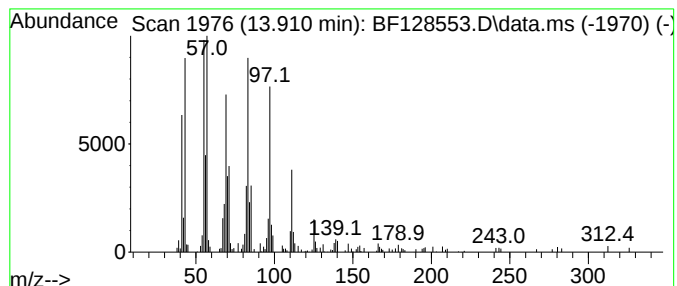
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 3-Eicosene, (E)- Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.910 | 6.30 ng | 333608 | Chrysene-d12     | 13.998 |

| Hit# | of | 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Eicosene, (E)- | 280 | C20H40  | 074685-33-9 | 98   |
| 2    |    |   | 5-Eicosene, (E)- | 280 | C20H40  | 074685-30-6 | 96   |
| 3    |    |   | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94   |
| 4    |    |   | 1-Docosene       | 308 | C22H44  | 001599-67-3 | 94   |
| 5    |    |   | 1-Heneicosanol   | 312 | C21H44O | 015594-90-8 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052822\  
Data File : BF128553.D  
Acq On : 28 May 2022 17:36  
Operator : CG\JU  
Sample : N2931-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P009-SS003-1218-01

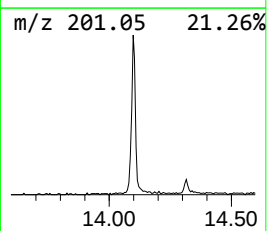
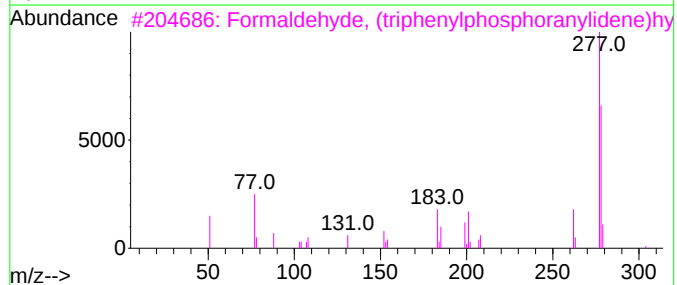
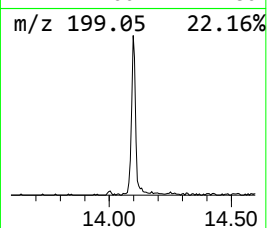
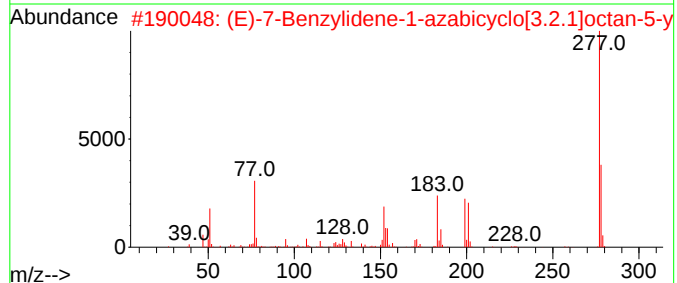
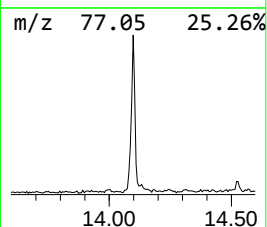
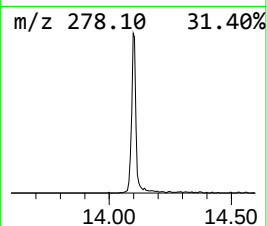
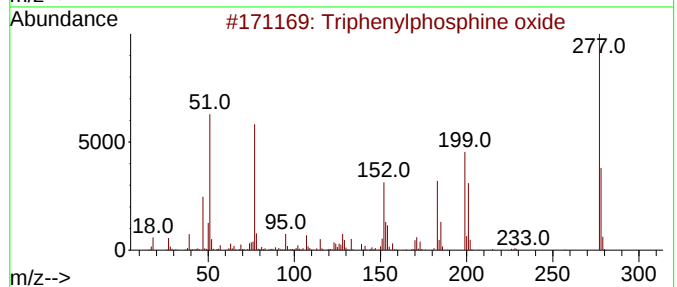
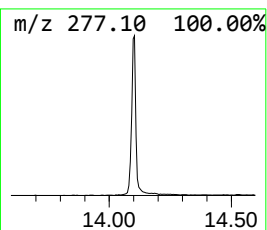
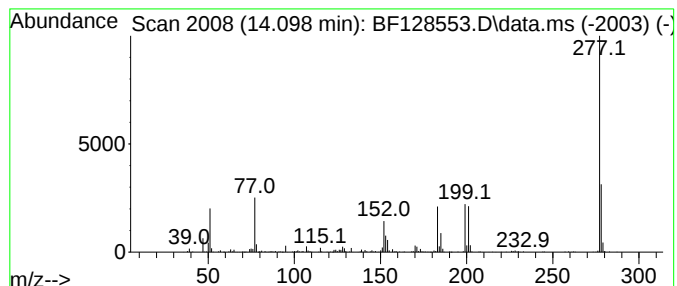
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.098 | 9.17 ng | 485419 | Chrysene-d12     | 13.998 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 96   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S | 1000483-83-4 | 60   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 50   |
| 4    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd...  | 277 | C18H15NO2  | 299962-12-2  | 37   |
| 5    |    |   | Cobalt,(.eta.<5>-2,4-cyclopentad...  | 277 | C16H15BCo  | 036682-12-9  | 27   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052822\  
Data File : BF128553.D  
Acq On : 28 May 2022 17:36  
Operator : CG\JU  
Sample : N2931-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P009-SS003-1218-01

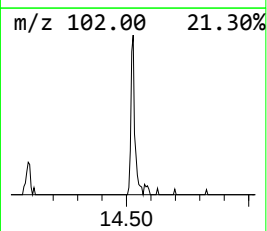
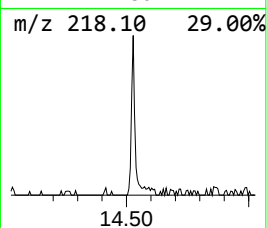
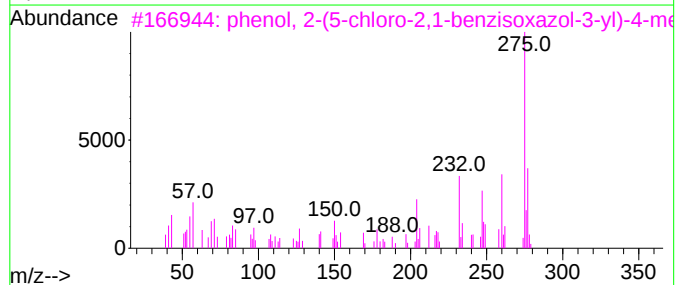
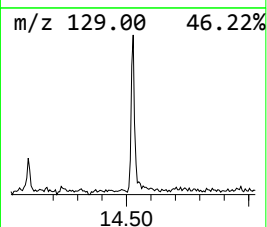
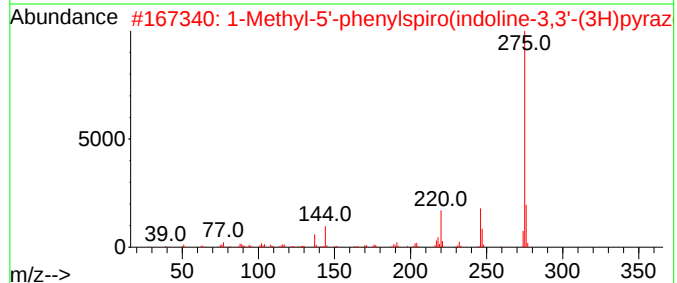
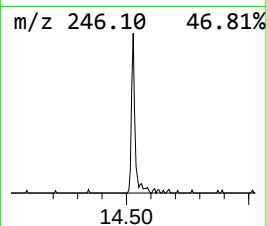
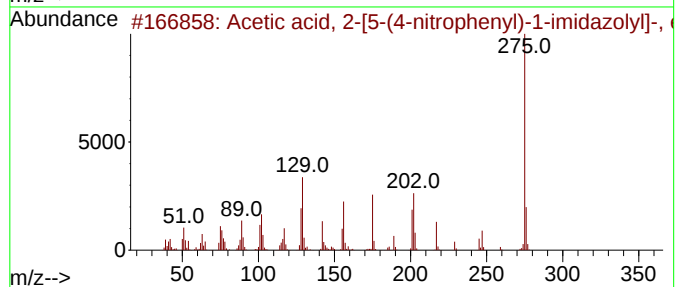
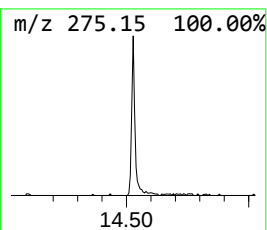
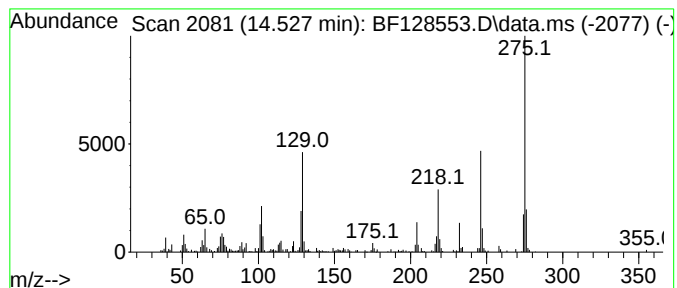
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.527 | 2.91 ng | 154193 | Chrysene-d12     | 13.998 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Acetic acid, 2-[5-(4-nitrophenyl)... | 275 | C13H13N3O4  | 351064-45-4  | 64   |
| 2    |    |   | 1-Methyl-5'-phenylspiro(indoline...  | 275 | C17H13N3O   | 015970-21-5  | 43   |
| 3    |    |   | phenol, 2-(5-chloro-2,1-benzisox...  | 275 | C14H10ClNO3 | 1000397-06-6 | 43   |
| 4    |    |   | 5H-[1]Benzopyrano[4,3-d]pyrimidi...  | 275 | C16H9N3O2   | 1000337-49-1 | 38   |
| 5    |    |   | 8H-Benzo[g]-1,3-benzodioxolo[6,5...  | 275 | C17H9NO3    | 000475-75-2  | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052822\  
Data File : BF128553.D  
Acq On : 28 May 2022 17:36  
Operator : CG\JU  
Sample : N2931-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P009-SS003-1218-01

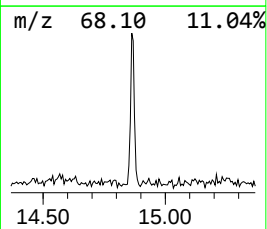
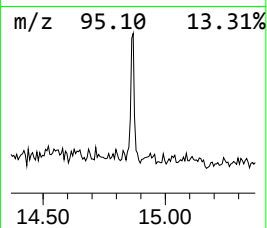
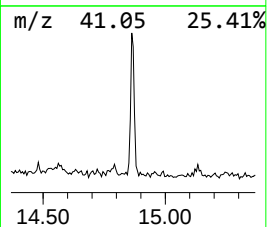
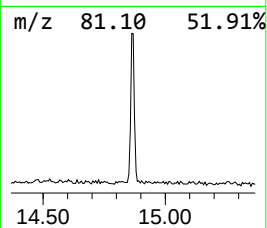
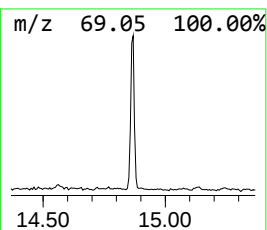
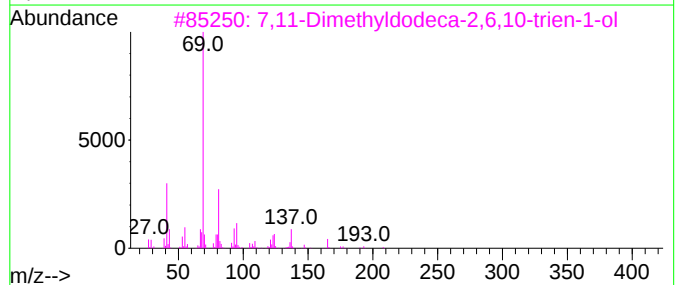
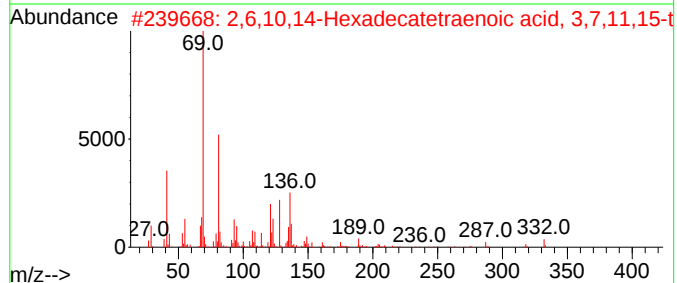
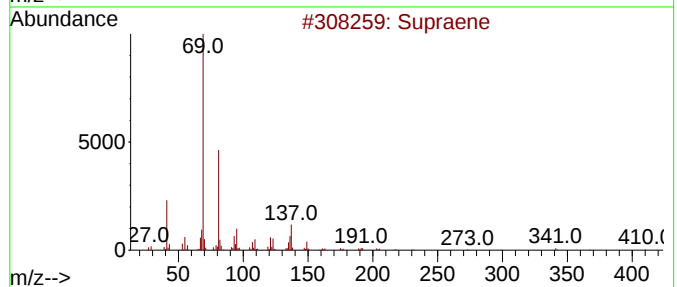
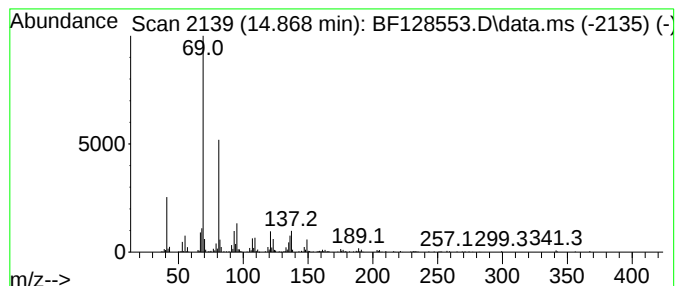
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Supraene Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.868 | 4.99 ng | 236033 | Perylene-d12     | 15.468 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50   | 007683-64-9 | 91   |
| 2    |    |   | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 72   |
| 3    |    |   | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O  | 125529-10-4 | 72   |
| 4    |    |   | Squalene                            | 410 | C30H50   | 000111-02-4 | 50   |
| 5    |    |   | 2,3,5-Trimethyl-2,3,5-hexanetric... | 203 | C12H17N3 | 003974-79-6 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052822\  
Data File : BF128553.D  
Acq On : 28 May 2022 17:36  
Operator : CG\JU  
Sample : N2931-03  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P009-SS003-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.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 |
| 2-Pentanone, 4-... | 5.063  | 3.5     | ng    | 189808   | 1                     | 6.839  | 1076460 | 20.0 |
| Benzenesulfonic... | 9.822  | 7.6     | ng    | 615988   | 3                     | 9.874  | 1614040 | 20.0 |
| Benzenesulfonam... | 10.775 | 8.0     | ng    | 632123   | 4                     | 11.363 | 1573590 | 20.0 |
| n-Hexadecanoic ... | 11.892 | 5.6     | ng    | 442013   | 4                     | 11.363 | 1573590 | 20.0 |
| 3-Eicosene, (E)-   | 13.910 | 6.3     | ng    | 333608   | 5                     | 13.998 | 1058920 | 20.0 |
| Triphenylphosph... | 14.098 | 9.2     | ng    | 485419   | 5                     | 13.998 | 1058920 | 20.0 |
| Acetic acid, 2-... | 14.527 | 2.9     | ng    | 154193   | 5                     | 13.998 | 1058920 | 20.0 |
| Supraene           | 14.868 | 5.0     | ng    | 236033   | 6                     | 15.468 | 946475  | 20.0 |