

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF040822\  
 Data File : BF127711.D  
 Acq On : 08 Apr 2022 14:01  
 Operator : CG\JU  
 Sample : N2317-21  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP2-A

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127711.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         | 2.340       | 3             | 9           | 15           | rVB      | 354423         | 468591        | 12.24%          | 1.603%        |
| 2         | 2.452       | 23            | 28          | 34           | rBV      | 37218          | 47959         | 1.25%           | 0.164%        |
| 3         | 5.210       | 488           | 497         | 507          | rVB      | 172782         | 233965        | 6.11%           | 0.800%        |
| 4         | 5.587       | 555           | 561         | 564          | rBV      | 3167727        | 3153823       | 82.40%          | 10.791%       |
| 5         | 6.245       | 670           | 673         | 677          | rBV      | 83094          | 67780         | 1.77%           | 0.232%        |
| 6         | 6.581       | 723           | 730         | 733          | rBV      | 2833583        | 3317070       | 86.67%          | 11.349%       |
| 7         | 6.963       | 791           | 795         | 798          | rBV      | 1039804        | 826774        | 21.60%          | 2.829%        |
| 8         | 7.528       | 886           | 891         | 894          | rVB      | 2132407        | 2178290       | 56.91%          | 7.453%        |
| 9         | 8.245       | 1008          | 1013        | 1017         | rBV      | 1239292        | 1103105       | 28.82%          | 3.774%        |
| 10        | 9.328       | 1191          | 1197        | 1200         | rBV      | 3792410        | 3749977       | 97.98%          | 12.830%       |
| 11        | 9.392       | 1203          | 1208        | 1212         | rVB3     | 33783          | 45947         | 1.20%           | 0.157%        |
| 12        | 9.439       | 1212          | 1216        | 1218         | rBV      | 49001          | 40766         | 1.07%           | 0.139%        |
| 13        | 9.980       | 1303          | 1308        | 1310         | rBV      | 1518986        | 1263785       | 33.02%          | 4.324%        |
| 14        | 10.010      | 1310          | 1313        | 1316         | rVB      | 1437160        | 1243624       | 32.49%          | 4.255%        |
| 15        | 10.122      | 1329          | 1332        | 1336         | rVB      | 78378          | 62207         | 1.63%           | 0.213%        |
| 16        | 10.739      | 1433          | 1437        | 1440         | rBV      | 72823          | 72628         | 1.90%           | 0.248%        |
| 17        | 10.798      | 1441          | 1447        | 1450         | rBV      | 2935846        | 2765379       | 72.25%          | 9.462%        |
| 18        | 11.504      | 1562          | 1567        | 1570         | rBV      | 1469214        | 1375630       | 35.94%          | 4.707%        |
| 19        | 12.016      | 1648          | 1654        | 1660         | rBV      | 106661         | 119542        | 3.12%           | 0.409%        |
| 20        | 12.733      | 1767          | 1776        | 1786         | rBV2     | 65290          | 112228        | 2.93%           | 0.384%        |
| 21        | 13.092      | 1832          | 1837        | 1840         | rBV      | 4046497        | 3827427       | 100.00%         | 13.095%       |
| 22        | 13.857      | 1963          | 1967        | 1970         | rBV      | 879017         | 761217        | 19.89%          | 2.604%        |
| 23        | 13.998      | 1986          | 1991        | 2003         | rBV2     | 104422         | 268864        | 7.02%           | 0.920%        |
| 24        | 14.151      | 2013          | 2017        | 2020         | rVB      | 1221932        | 1056956       | 27.62%          | 3.616%        |
| 25        | 14.245      | 2026          | 2033        | 2050         | rBV      | 144078         | 236206        | 6.17%           | 0.808%        |
| 26        | 15.298      | 2208          | 2212        | 2216         | rBV      | 36716          | 39521         | 1.03%           | 0.135%        |
| 27        | 15.674      | 2271          | 2276        | 2287         | rVB2     | 628534         | 788438        | 20.60%          | 2.698%        |

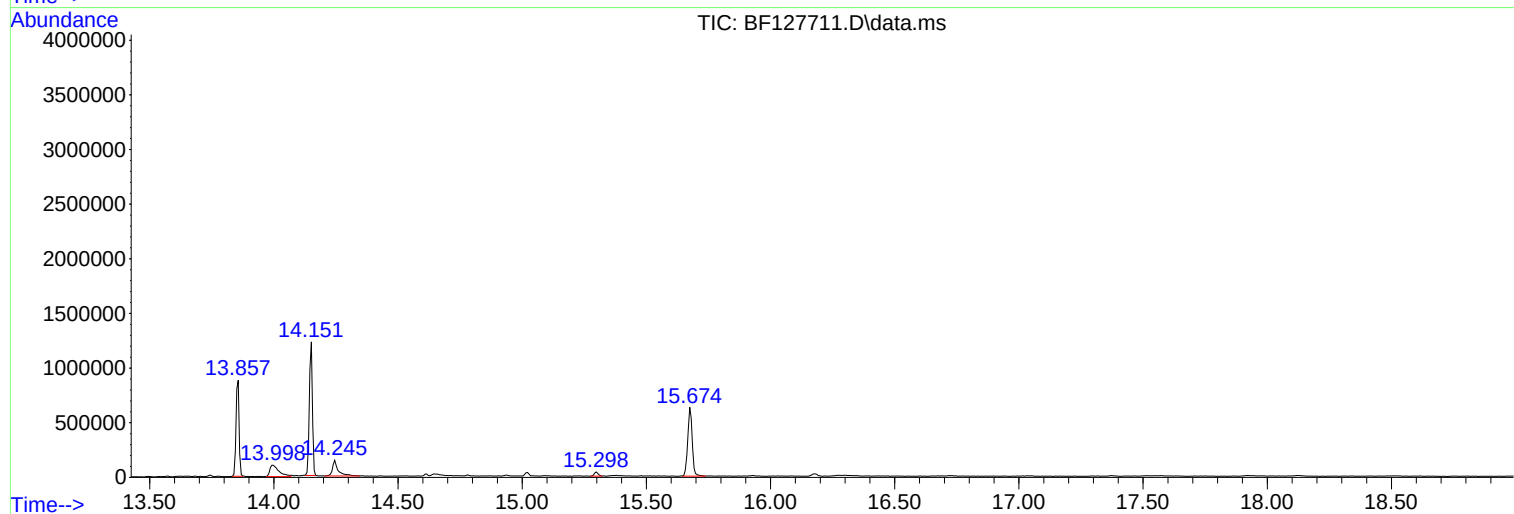
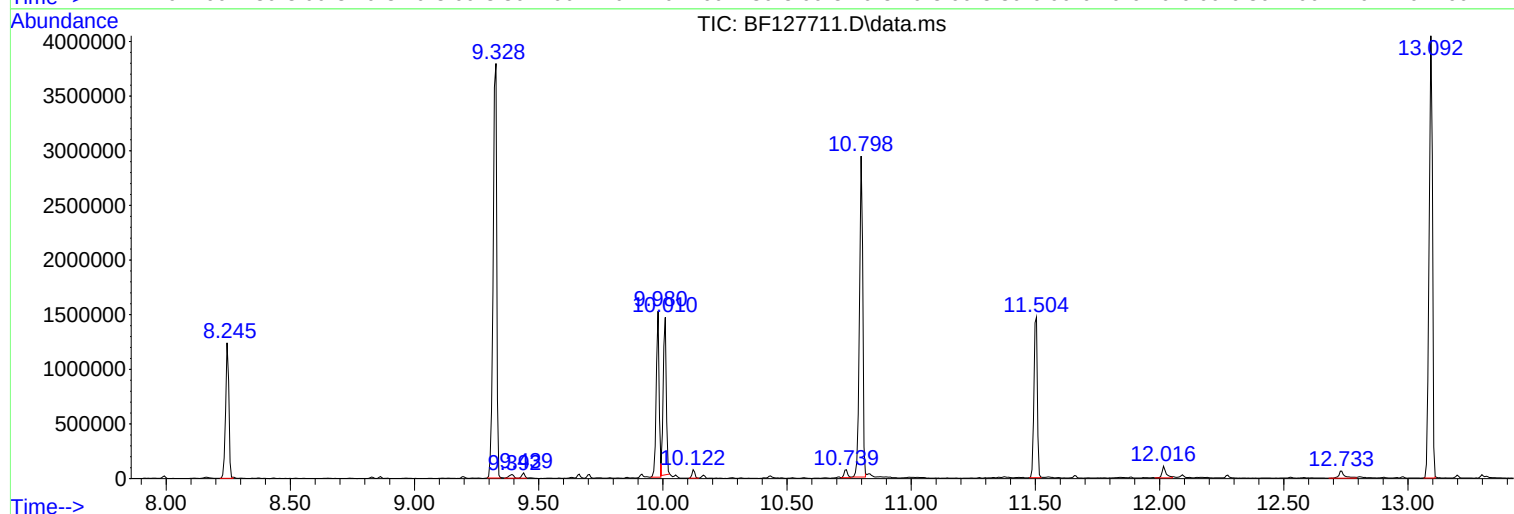
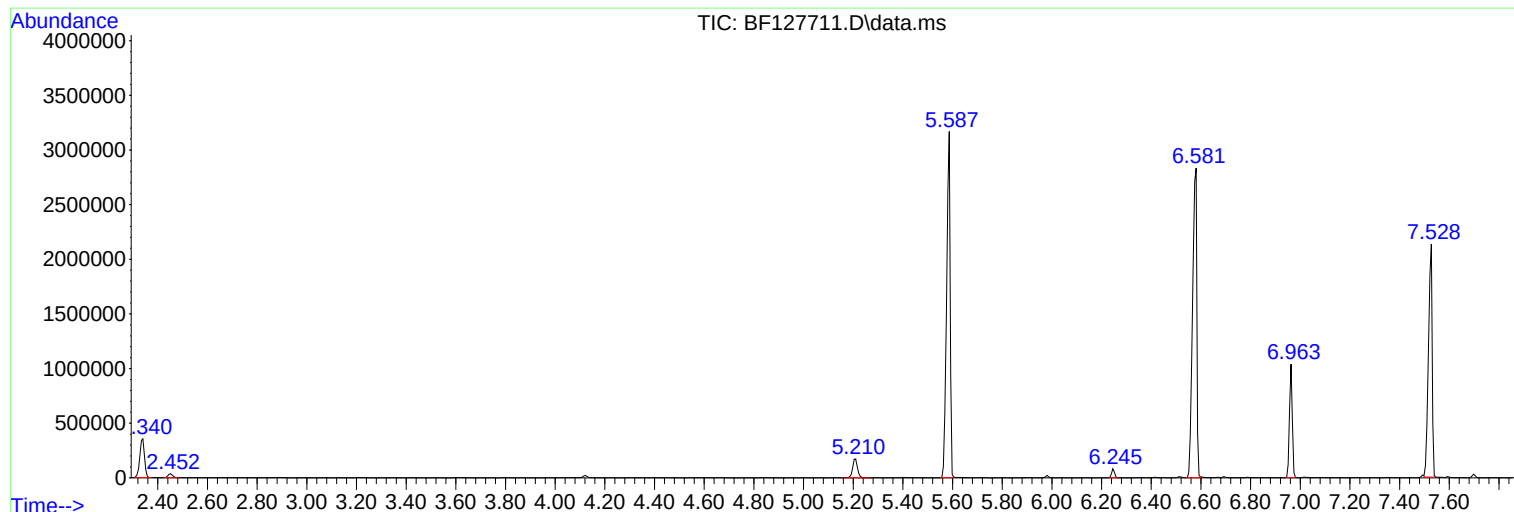
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Instrument :  
BNA\_F  
ClientSampleId :  
TP2-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF040622.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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Instrument :  
BNA\_F  
ClientSampleId :  
TP2-A

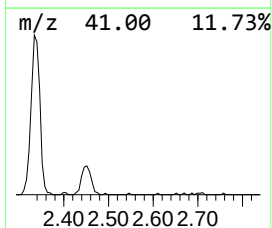
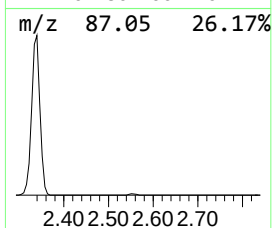
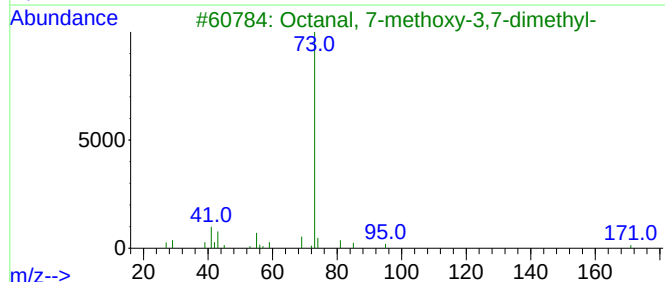
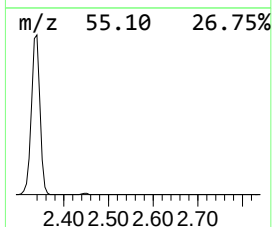
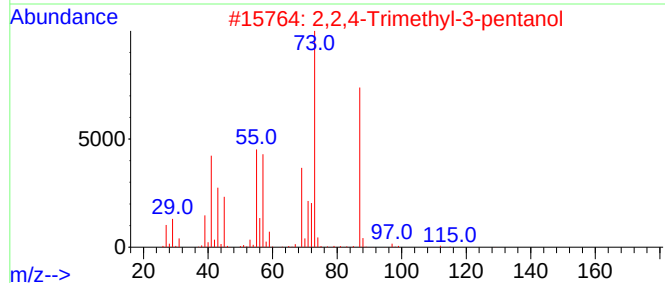
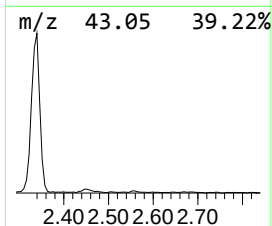
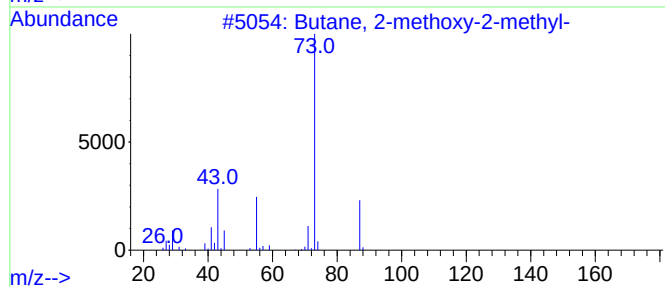
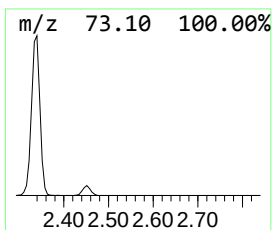
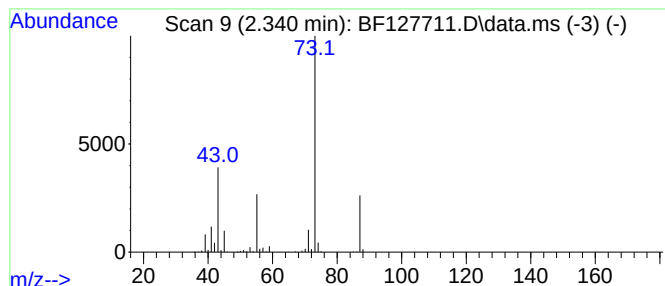
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF040622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 2

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 2.340 | 11.34 ng | 468591 | 1,4-Dichlorobenzene-d4 | 6.963 |

| 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    |    |   | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17   |
| 4    |    |   | Silane, tetramethyl-             | 88  | C4H12Si  | 000075-76-3 | 17   |
| 5    |    |   | Pentane, 3-methoxy-              | 102 | C6H14O   | 036839-67-5 | 12   |



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BNA\_F  
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TP2-A

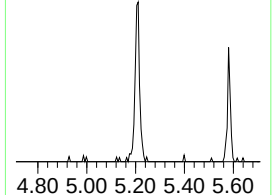
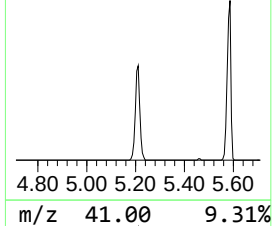
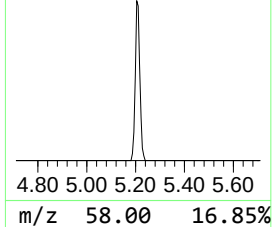
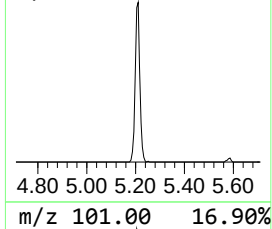
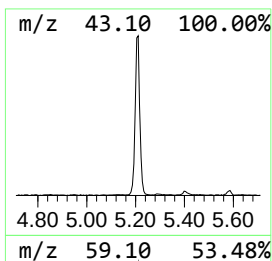
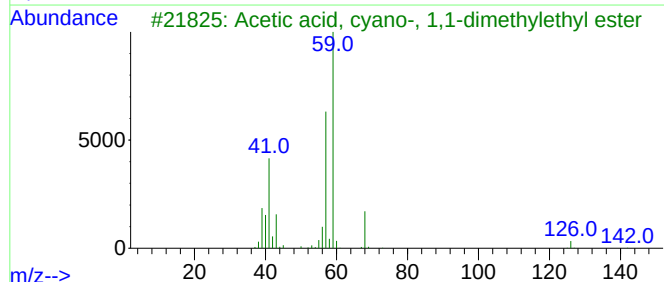
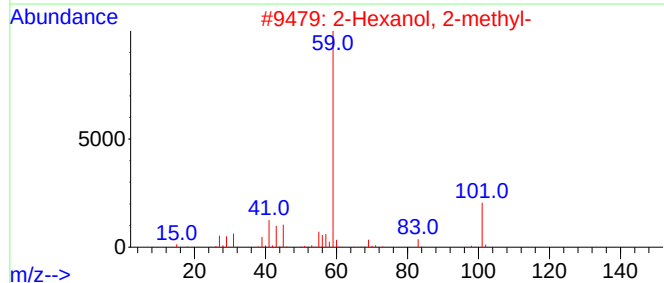
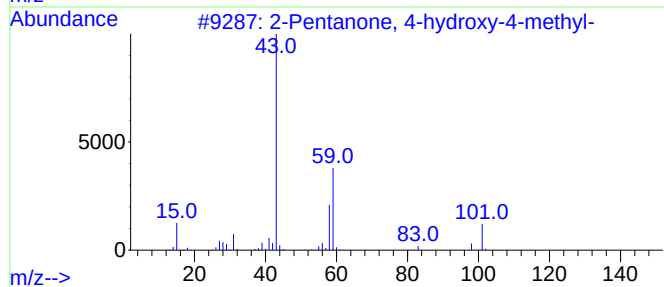
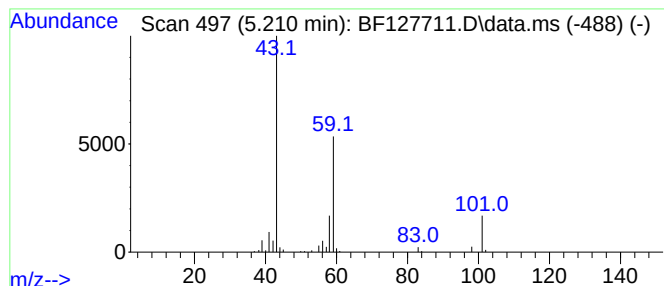
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|--------|------------------------|-------------|------|
| 5.210     | 5.66 ng                             | 233965 | 1,4-Dichlorobenzene-d4 | 6.963       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    | 116    | C6H12O2                | 000123-42-2 | 59   |
| 2         | 2-Hexanol, 2-methyl-                | 116    | C7H16O                 | 000625-23-0 | 28   |
| 3         | Acetic acid, cyano-, 1,1-dimethy... | 141    | C7H11NO2               | 001116-98-9 | 25   |
| 4         | Acetone                             | 58     | C3H6O                  | 000067-64-1 | 12   |
| 5         | 1-Propen-2-ol, acetate              | 100    | C5H8O2                 | 000108-22-5 | 12   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP2-A

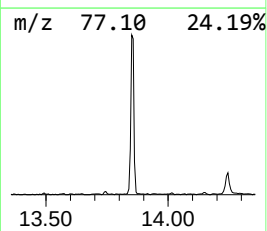
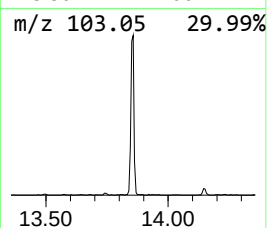
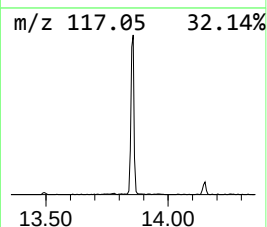
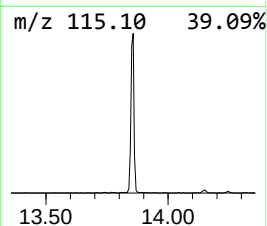
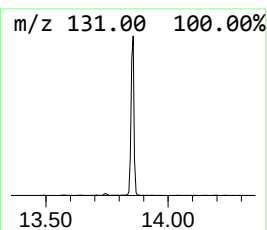
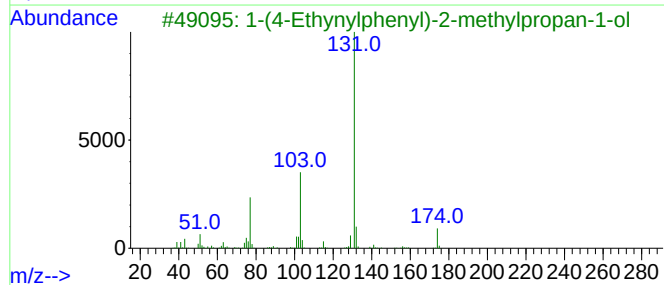
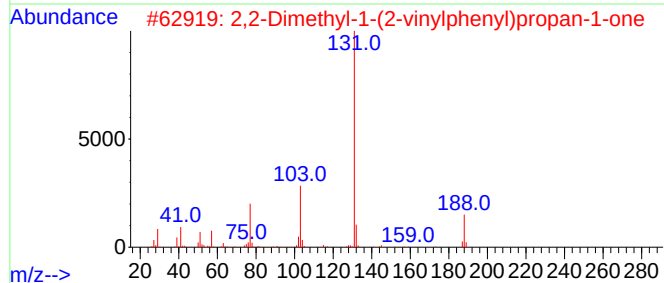
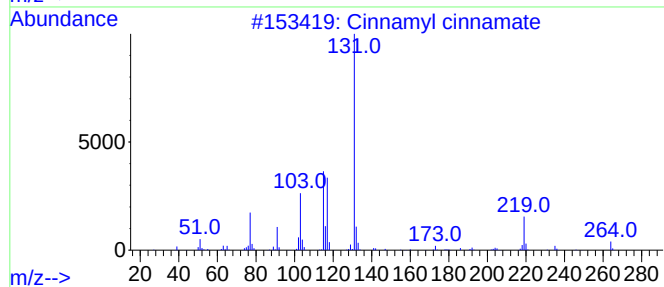
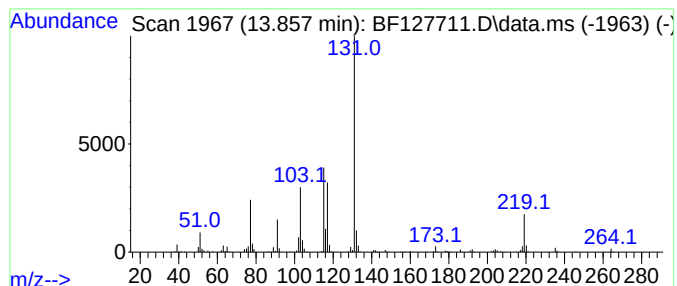
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Cinnamyl cinnamate Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.857 | 14.40 ng | 761217 | Chrysene-d12     | 14.151 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Cinnamyl cinnamate                  | 264 | C18H16O2    | 000122-69-0  | 91   |
| 2    |    |   | 2,2-Dimethyl-1-(2-vinylphenyl)pr... | 188 | C13H16O     | 1000210-99-9 | 49   |
| 3    |    |   | 1-(4-Ethynylphenyl)-2-methylprop... | 174 | C12H14O     | 1000466-39-4 | 47   |
| 4    |    |   | 1-Penten-3-one, 4,4-dimethyl-1-p... | 188 | C13H16O     | 000538-44-3  | 47   |
| 5    |    |   | N-(4-Fluorophenyl)-3-phenyl-2-pr... | 337 | C17H11F4NO2 | 1000492-37-5 | 47   |



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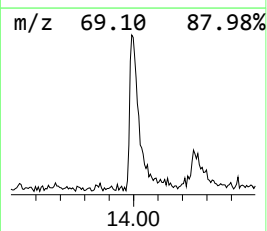
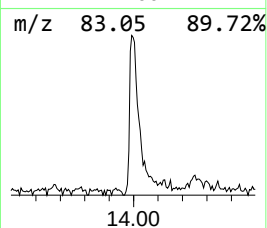
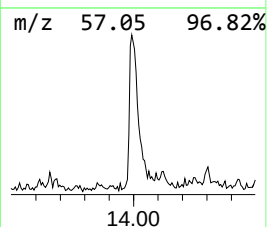
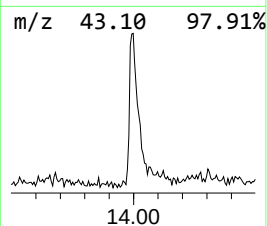
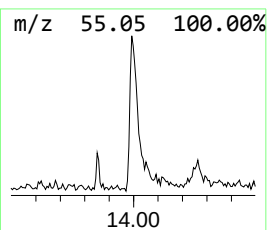
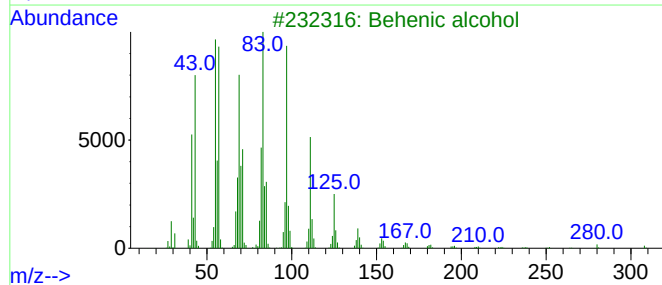
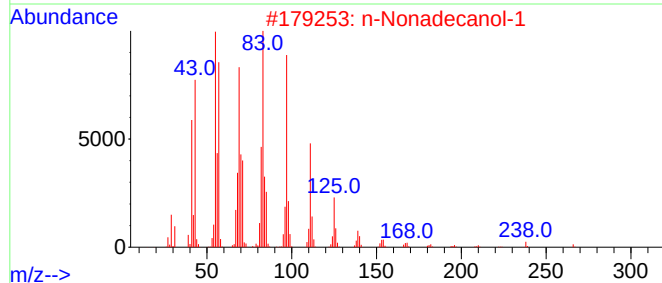
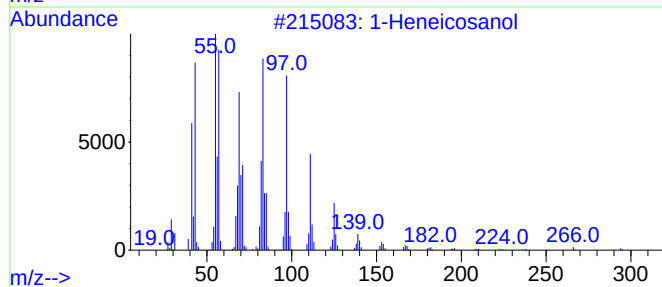
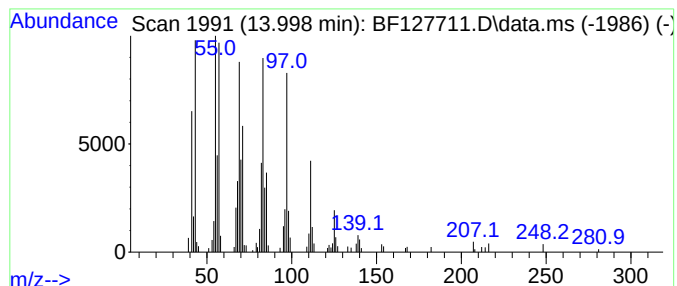
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 1-Heneicosanol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.998 | 5.09 ng | 268864 | Chrysene-d12     | 14.151 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 95   |
| 2    |    |   | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 95   |
| 3    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 95   |
| 4    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94   |
| 5    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94   |



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BNA\_F  
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TP2-A

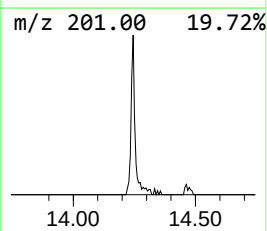
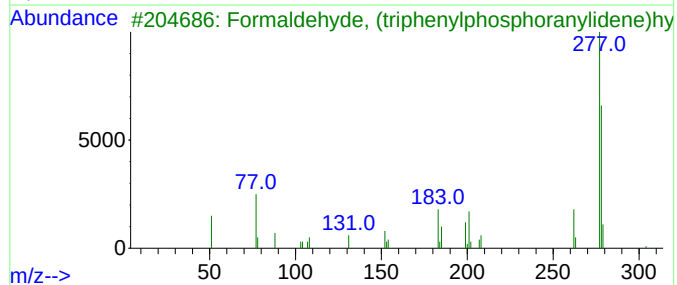
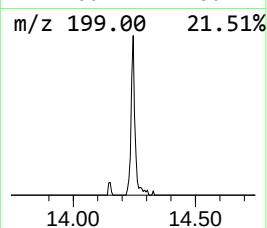
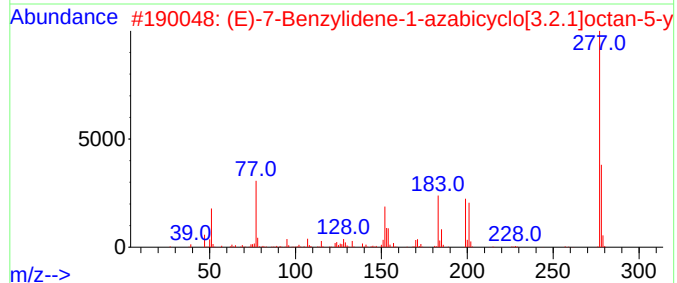
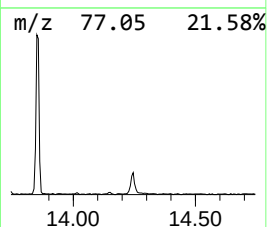
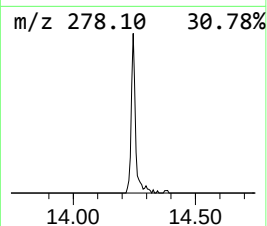
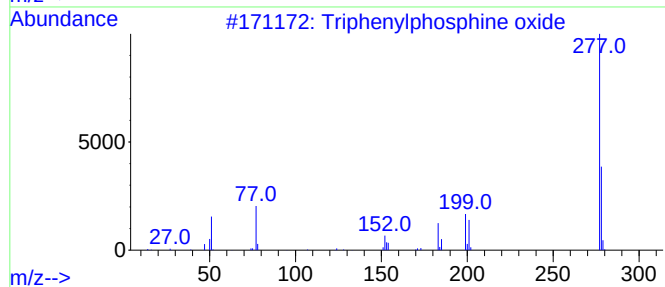
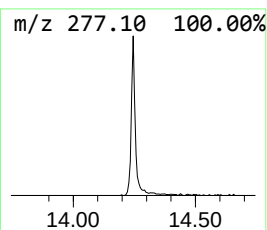
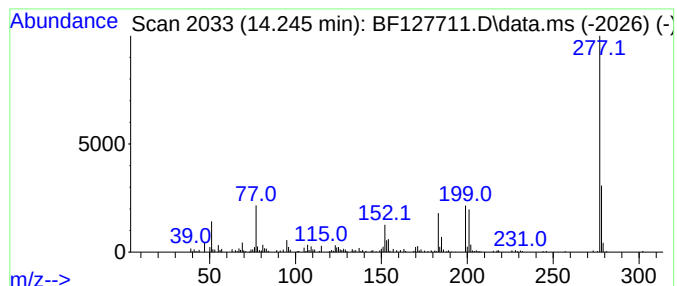
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF040622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.245 | 4.47 ng | 236206 | Chrysene-d12     | 14.151 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 94   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S  | 1000483-83-4 | 58   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...] | 304 | C19H17N2P   | 015990-54-2  | 50   |
| 4    |    |   | (Carbethoxymethyl)-triphenylphos...  | 428 | C22H22BrO2P | 001530-45-6  | 38   |
| 5    |    |   | Vanadium, cycloheptatrienyl-(pen...  | 277 | C17H22V     | 1000155-20-5 | 25   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF040822\  
Data File : BF127711.D  
Acq On : 08 Apr 2022 14:01  
Operator : CG\JU  
Sample : N2317-21  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP2-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF040622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 2.340  | 11.3    | ng    | 468591   | 1                     | 6.963  | 826774  | 20.0 |
| 2-Pentanone, 4-... | 5.210  | 5.7     | ng    | 233965   | 1                     | 6.963  | 826774  | 20.0 |
| Cinnamyl cinnamate | 13.857 | 14.4    | ng    | 761217   | 5                     | 14.151 | 1056960 | 20.0 |
| 1-Heneicosanol     | 13.998 | 5.1     | ng    | 268864   | 5                     | 14.151 | 1056960 | 20.0 |
| Triphenylphosph... | 14.245 | 4.5     | ng    | 236206   | 5                     | 14.151 | 1056960 | 20.0 |