

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052522\  
 Data File : BF128465.D  
 Acq On : 25 May 2022 17:52  
 Operator : CG\JU  
 Sample : N2894-09  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P004-SS006-0006-01

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-BF052022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128465.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         | 2.357       | 8             | 12          | 21           | rVB3     | 8950           | 18554         | 1.14%           | 0.141%        |
| 2         | 5.034       | 464           | 467         | 471          | rBV      | 20818          | 28854         | 1.77%           | 0.219%        |
| 3         | 5.440       | 532           | 536         | 556          | rBV      | 1479687        | 1625537       | 99.54%          | 12.316%       |
| 4         | 6.245       | 665           | 673         | 676          | rBV2     | 32208          | 41450         | 2.54%           | 0.314%        |
| 5         | 6.463       | 707           | 710         | 724          | rBV      | 1366110        | 1632984       | 100.00%         | 12.372%       |
| 6         | 6.810       | 765           | 769         | 773          | rBV      | 555939         | 484397        | 29.66%          | 3.670%        |
| 7         | 6.916       | 782           | 787         | 790          | rVB2     | 45399          | 40857         | 2.50%           | 0.310%        |
| 8         | 7.228       | 832           | 840         | 845          | rBV8     | 9393           | 25135         | 1.54%           | 0.190%        |
| 9         | 7.304       | 848           | 853         | 857          | rVV3     | 15322          | 27651         | 1.69%           | 0.209%        |
| 10        | 7.375       | 861           | 865         | 879          | rVB      | 1065753        | 1008156       | 61.74%          | 7.638%        |
| 11        | 7.610       | 902           | 905         | 912          | rBV      | 18454          | 22228         | 1.36%           | 0.168%        |
| 12        | 8.022       | 970           | 975         | 977          | rBV5     | 14495          | 19158         | 1.17%           | 0.145%        |
| 13        | 8.092       | 983           | 987         | 990          | rBV      | 669465         | 557021        | 34.11%          | 4.220%        |
| 14        | 8.122       | 990           | 992         | 999          | rVB5     | 16076          | 23384         | 1.43%           | 0.177%        |
| 15        | 8.810       | 1106          | 1109        | 1115         | rBV3     | 11673          | 18788         | 1.15%           | 0.142%        |
| 16        | 9.163       | 1165          | 1169        | 1173         | rBV      | 1746947        | 1612829       | 98.77%          | 12.219%       |
| 17        | 9.222       | 1176          | 1179        | 1180         | rVV3     | 19297          | 20456         | 1.25%           | 0.155%        |
| 18        | 9.263       | 1184          | 1186        | 1191         | rVB4     | 15601          | 19568         | 1.20%           | 0.148%        |
| 19        | 9.686       | 1254          | 1258        | 1260         | rBV3     | 27795          | 32256         | 1.98%           | 0.244%        |
| 20        | 9.751       | 1267          | 1269        | 1276         | rVB6     | 13012          | 23129         | 1.42%           | 0.175%        |
| 21        | 9.816       | 1276          | 1280        | 1281         | rBV3     | 16125          | 19740         | 1.21%           | 0.150%        |
| 22        | 9.845       | 1282          | 1285        | 1291         | rVB      | 638264         | 565447        | 34.63%          | 4.284%        |
| 23        | 9.957       | 1301          | 1304        | 1307         | rBV2     | 53767          | 45339         | 2.78%           | 0.344%        |
| 24        | 10.080      | 1322          | 1325        | 1328         | rVB2     | 80411          | 74436         | 4.56%           | 0.564%        |
| 25        | 10.122      | 1328          | 1332        | 1340         | rVB4     | 33002          | 49596         | 3.04%           | 0.376%        |
| 26        | 10.263      | 1349          | 1356        | 1359         | rBV4     | 30103          | 35406         | 2.17%           | 0.268%        |
| 27        | 10.474      | 1389          | 1392        | 1397         | rVB5     | 29709          | 35190         | 2.15%           | 0.267%        |
| 28        | 10.598      | 1410          | 1413        | 1417         | rBV      | 84427          | 73920         | 4.53%           | 0.560%        |
| 29        | 10.639      | 1417          | 1420        | 1424         | rBV      | 877520         | 833314        | 51.03%          | 6.313%        |
| 30        | 10.886      | 1460          | 1462        | 1467         | rVB3     | 20983          | 22975         | 1.41%           | 0.174%        |
| 31        | 11.339      | 1536          | 1539        | 1543         | rBV      | 612638         | 553760        | 33.91%          | 4.195%        |
| 32        | 11.380      | 1543          | 1546        | 1551         | rVB      | 57464          | 54269         | 3.32%           | 0.411%        |
| 33        | 11.451      | 1556          | 1558        | 1564         | rVB5     | 25453          | 26765         | 1.64%           | 0.203%        |
| 34        | 11.539      | 1570          | 1573        | 1575         | rBV3     | 23146          | 22623         | 1.39%           | 0.171%        |
| 35        | 11.721      | 1601          | 1604        | 1606         | rVB      | 78997          | 61392         | 3.76%           | 0.465%        |
| 36        | 11.863      | 1625          | 1628        | 1632         | rBV      | 191315         | 193436        | 11.85%          | 1.466%        |

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Sample : N2894-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

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-BF052022.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 37 | 12.427 | 1722 | 1724 | 1727 | rBV  | 46884   | 36249   | 2.22%  | 0.275%  |
| 38 | 12.651 | 1760 | 1762 | 1767 | rVB2 | 45851   | 48457   | 2.97%  | 0.367%  |
| 39 | 12.927 | 1805 | 1809 | 1812 | rBV  | 1636175 | 1351074 | 82.74% | 10.236% |
| 40 | 13.033 | 1824 | 1827 | 1830 | rBV  | 253687  | 205276  | 12.57% | 1.555%  |
| 41 | 13.310 | 1871 | 1874 | 1877 | rBV  | 396513  | 365755  | 22.40% | 2.771%  |
| 42 | 13.398 | 1886 | 1889 | 1892 | rBV  | 301602  | 261697  | 16.03% | 1.983%  |
| 43 | 13.839 | 1962 | 1964 | 1969 | rBV  | 134344  | 185024  | 11.33% | 1.402%  |
| 44 | 13.957 | 1981 | 1984 | 1987 | rBV  | 481199  | 425637  | 26.06% | 3.225%  |
| 45 | 13.992 | 1987 | 1990 | 1994 | rVV  | 406462  | 369786  | 22.64% | 2.802%  |

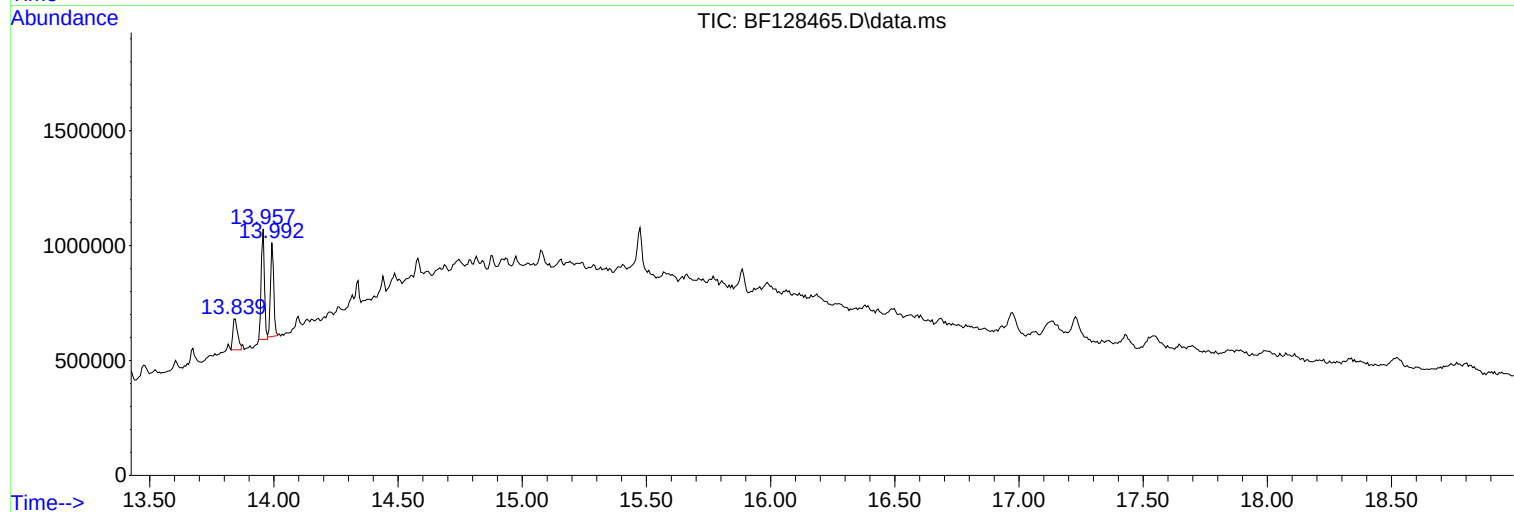
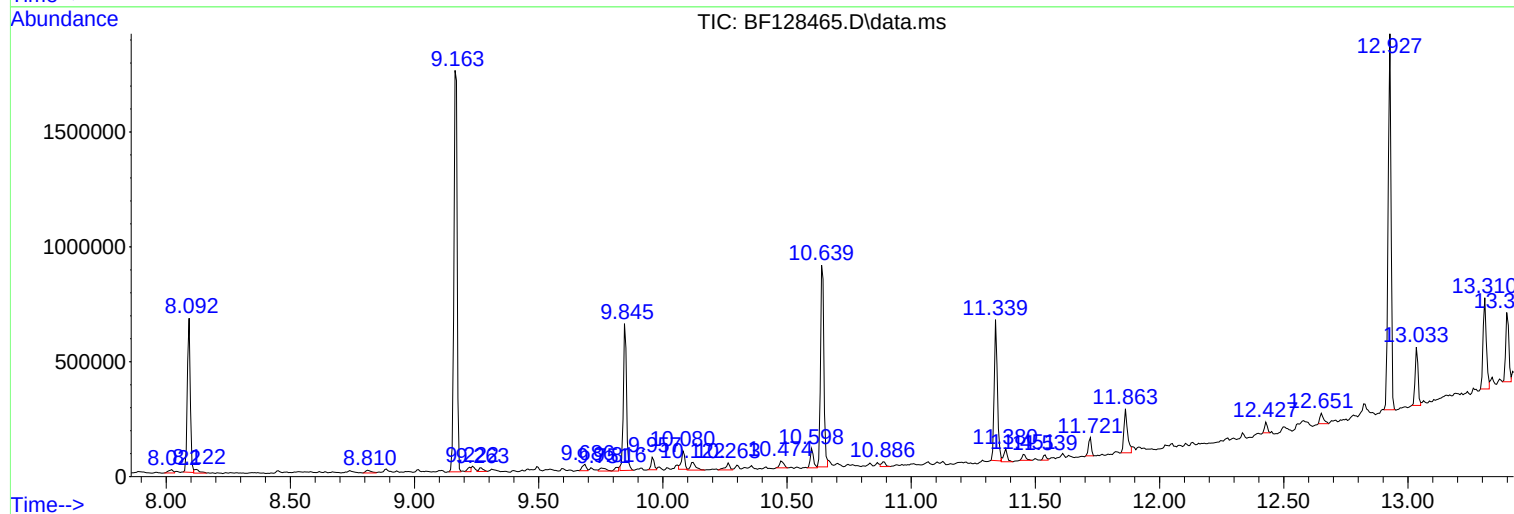
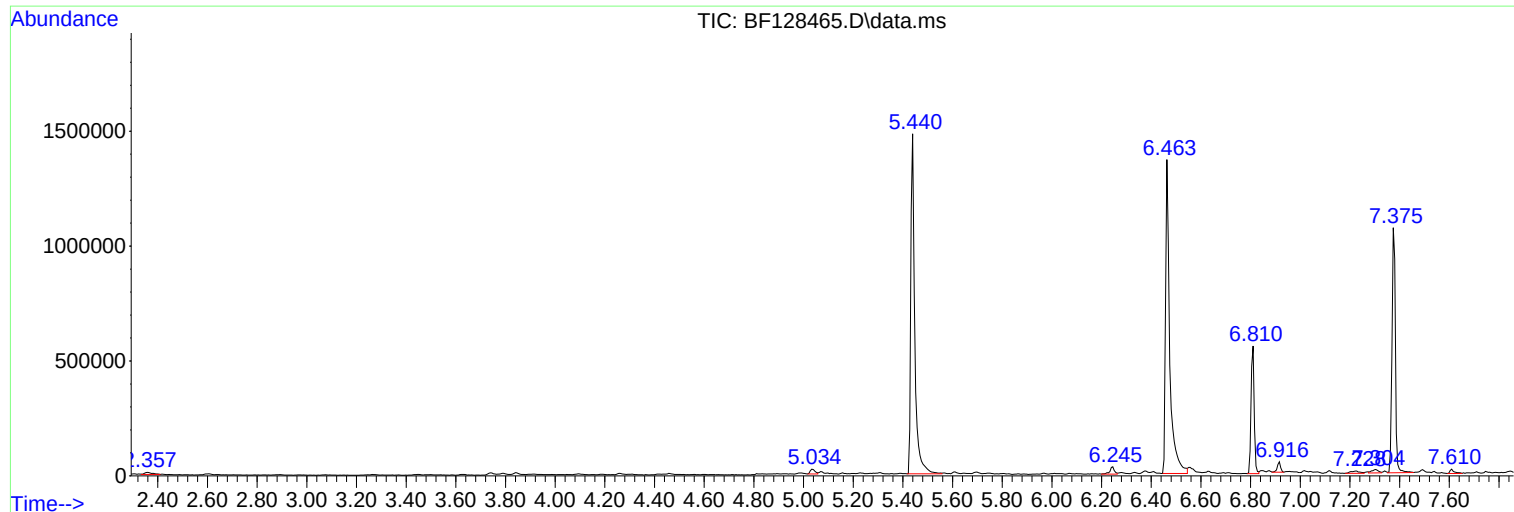
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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.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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Misc :  
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Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

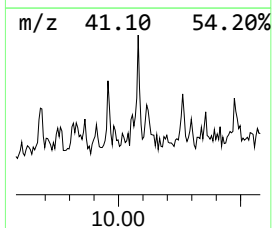
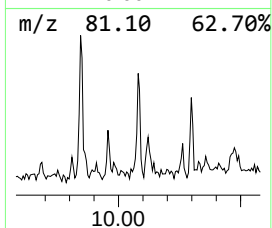
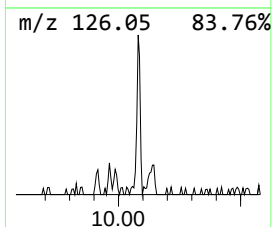
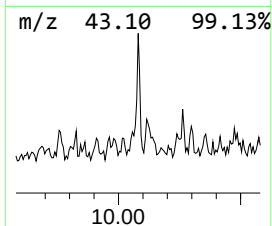
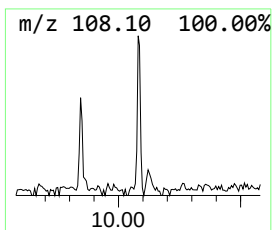
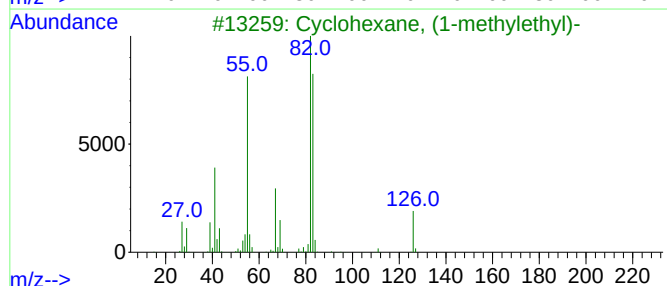
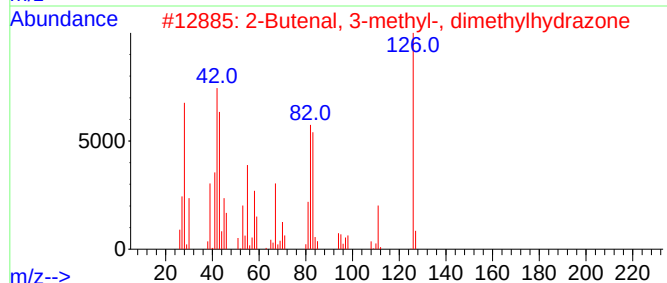
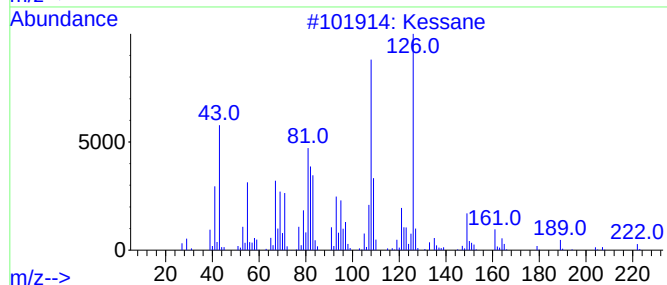
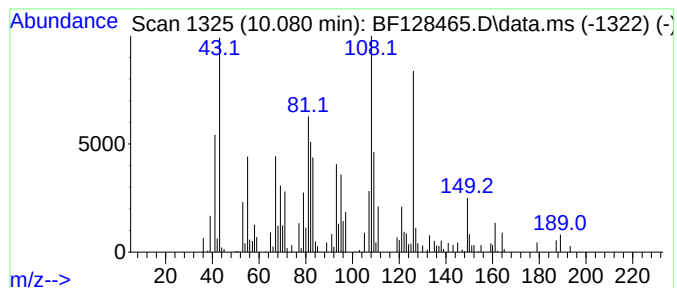
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Kessane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.  |
|--------|---------|-------|------------------|-------|
| 10.080 | 2.63 ng | 74436 | Acenaphthene-d10 | 9.845 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Kessane                             | 222 | C15H26O | 003321-66-2 | 58   |
| 2    |    |   | 2-Butenal, 3-methyl-, dimethylhy... | 126 | C7H14N2 | 016713-48-7 | 38   |
| 3    |    |   | Cyclohexane, (1-methylethyl)-       | 126 | C9H18   | 000696-29-7 | 30   |
| 4    |    |   | 2-Cyclopenten-1-one, 3-ethyl-2-h... | 126 | C7H10O2 | 021835-01-8 | 25   |
| 5    |    |   | 2-Fluorophenylhydrazine             | 126 | C6H7FN2 | 002368-80-1 | 25   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

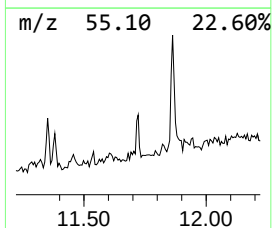
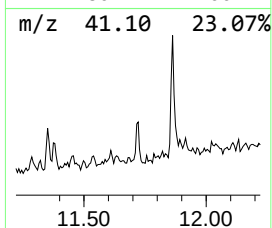
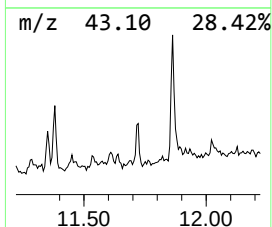
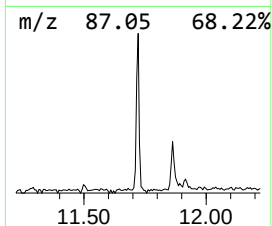
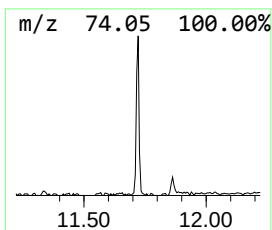
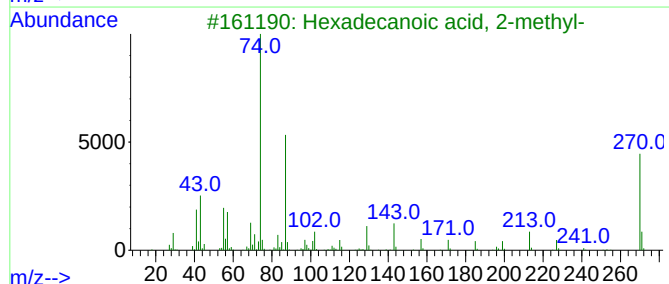
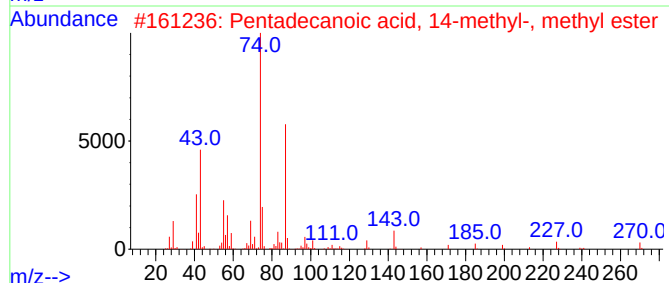
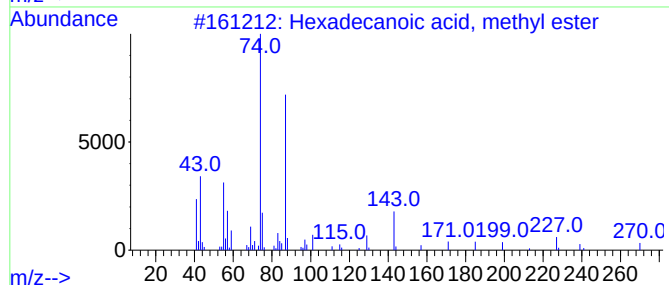
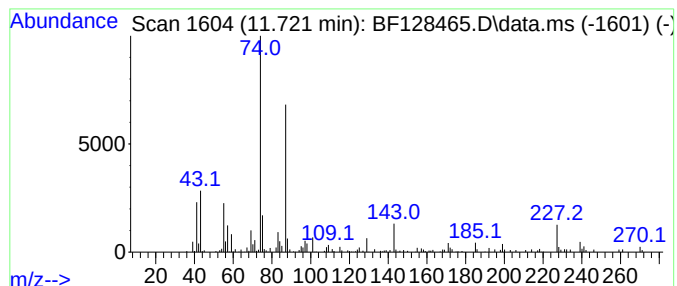
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.722 | 2.22 ng | 61392 | Phenanthrene-d10 | 11.339 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Hexadecanoic acid, methyl ester     | 270 | C17H34O2 | 000112-39-0 | 98   |
| 2    |    |   | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 87   |
| 3    |    |   | Hexadecanoic acid, 2-methyl-        | 270 | C17H34O2 | 027147-71-3 | 83   |
| 4    |    |   | Tridecanoic acid, methyl ester      | 228 | C14H28O2 | 001731-88-0 | 81   |
| 5    |    |   | Decanoic acid, methyl ester         | 186 | C11H22O2 | 000110-42-9 | 81   |



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Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
P004-SS006-0006-01

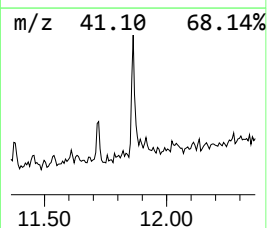
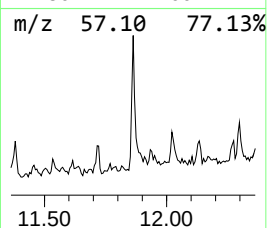
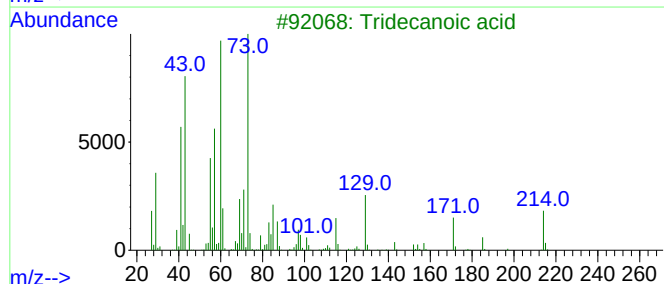
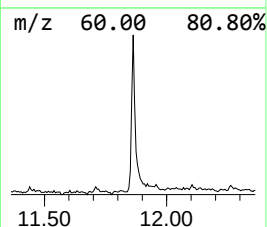
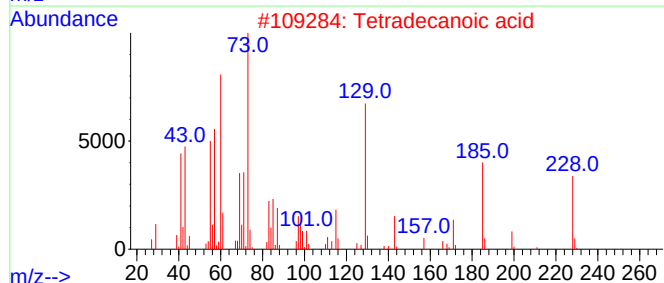
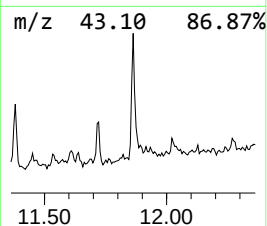
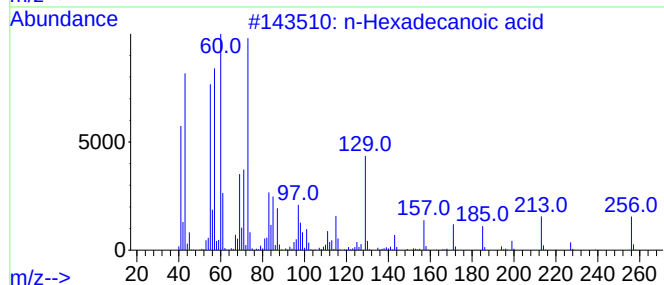
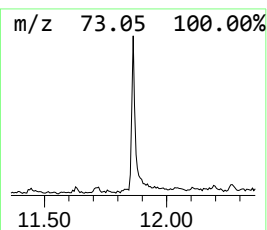
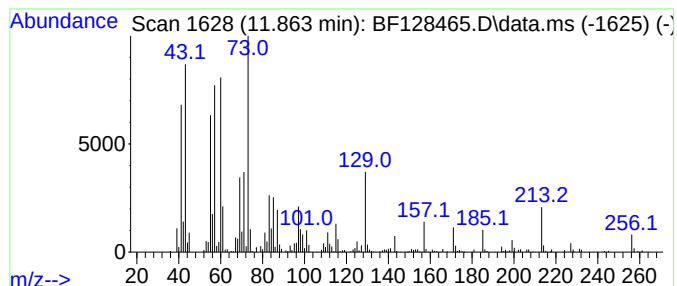
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.863 | 6.99 ng | 193436 | Phenanthrene-d10 | 11.339 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 95   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 68   |



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Misc :  
ALS Vial : 14 Sample Multiplier: 1

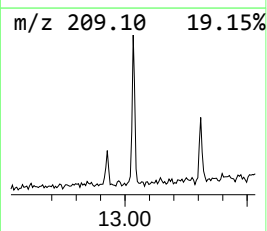
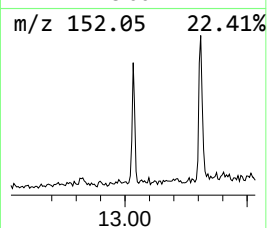
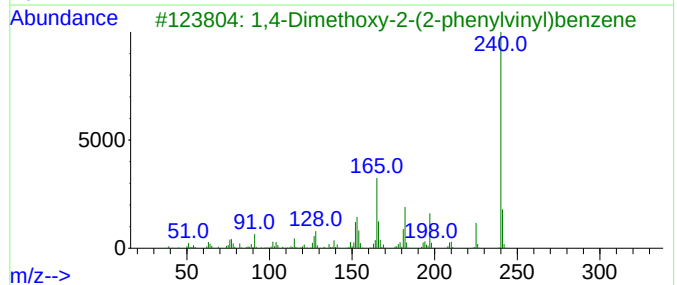
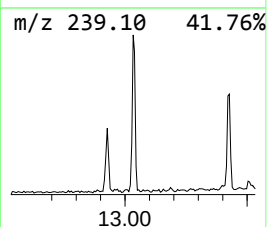
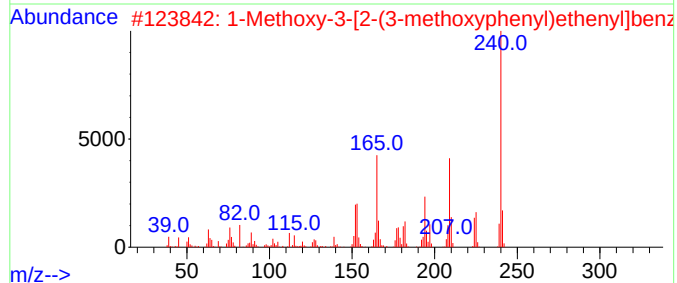
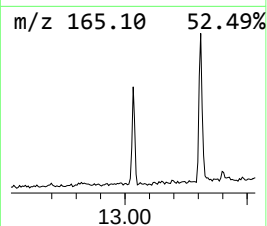
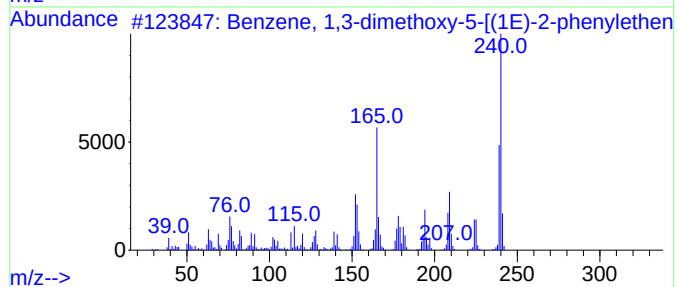
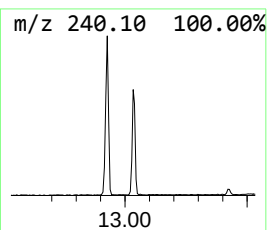
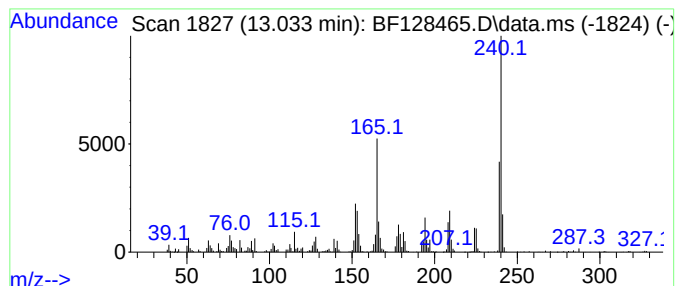
Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.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 Benzene, 1,3-dimethoxy-5-[(... Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|----------|-------------|------|
| 13.033    | 11.10 ng                            | 205276 | Chrysene-d12     |          | 13.992      |      |
| Hit# of 5 | Tentative ID                        |        | MW               | MolForm  | CAS#        | Qual |
| 1         | Benzene, 1,3-dimethoxy-5-[(1E)-2... |        | 240              | C16H16O2 | 021956-56-9 | 99   |
| 2         | 1-Methoxy-3-[2-(3-methoxyphenyl)... |        | 240              | C16H16O2 | 006325-63-9 | 89   |
| 3         | 1,4-Dimethoxy-2-(2-phenylvinyl)b... |        | 240              | C16H16O2 | 021889-09-8 | 70   |
| 4         | Benzene, 1,1'-(1,2-ethenediyl)bi... |        | 240              | C16H16O2 | 004705-34-4 | 55   |
| 5         | Cyclohexane, hexaethylidene-        |        | 240              | C18H24   | 001482-93-5 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052522\  
Data File : BF128465.D  
Acq On : 25 May 2022 17:52  
Operator : CG\JU  
Sample : N2894-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

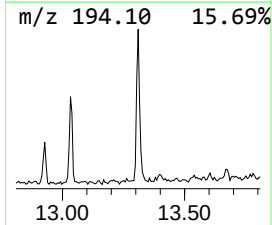
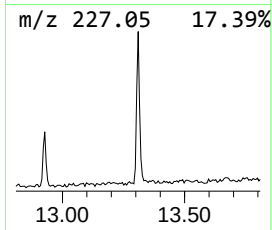
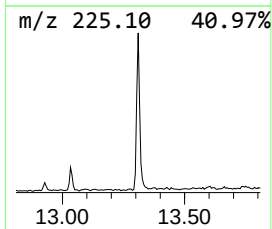
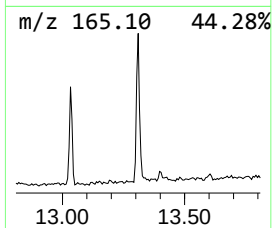
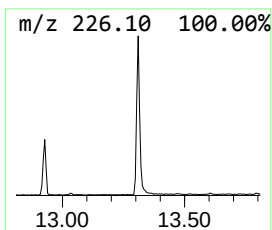
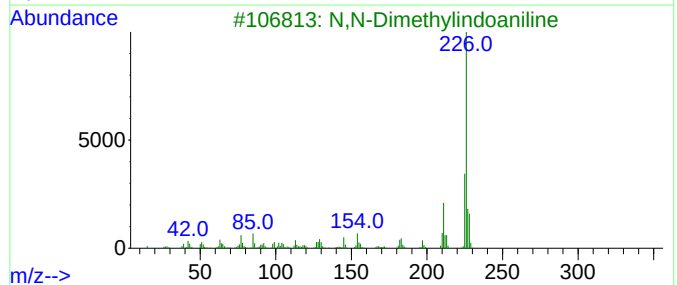
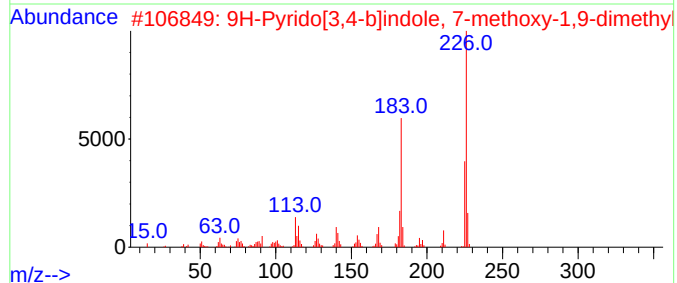
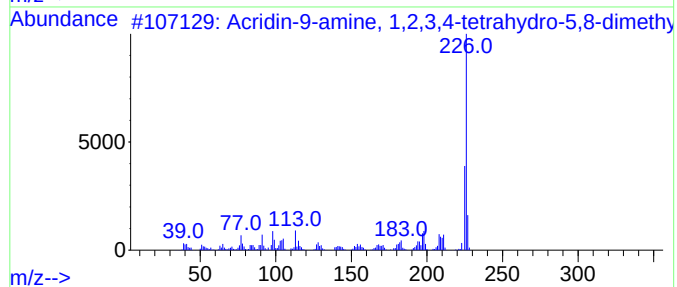
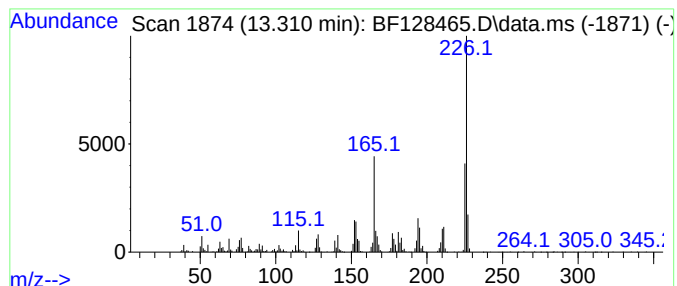
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.310 | 19.78 ng | 365755 | Chrysene-d12     | 13.992 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2   | 297758-19-1  | 70   |
| 2    |    |   | 9H-Pyrido[3,4-b]indole, 7-methox... | 226 | C14H14N2O  | 143502-37-8  | 52   |
| 3    |    |   | N,N-Dimethylindooaniline            | 226 | C14H14N2O  | 002150-58-5  | 47   |
| 4    |    |   | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2   | 1000300-57-6 | 46   |
| 5    |    |   | Benzenamine, N-[(4-nitrophenyl)m... | 226 | C13H10N2O2 | 000785-80-8  | 46   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052522\  
Data File : BF128465.D  
Acq On : 25 May 2022 17:52  
Operator : CG\JU  
Sample : N2894-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

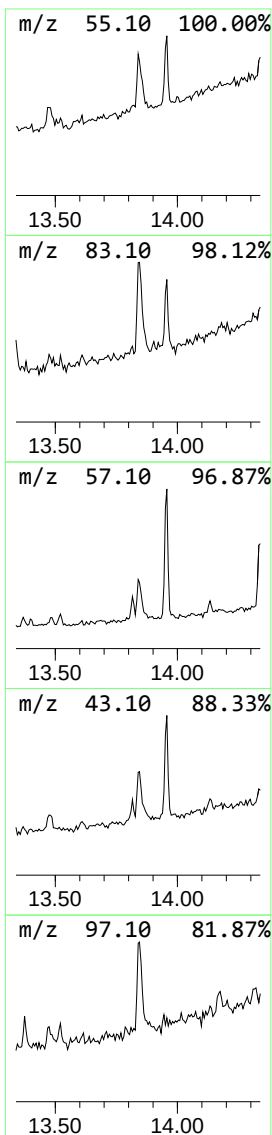
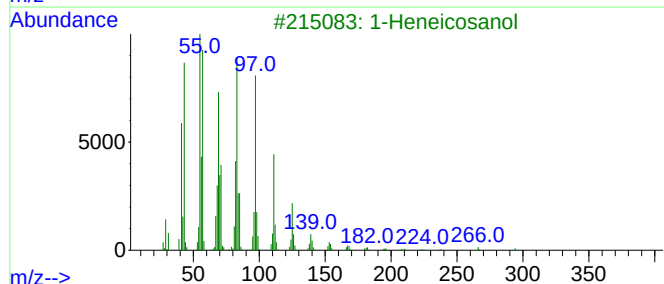
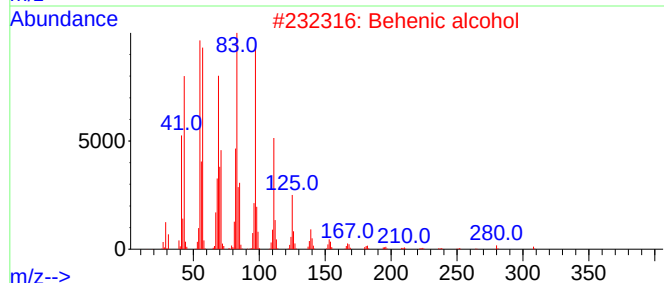
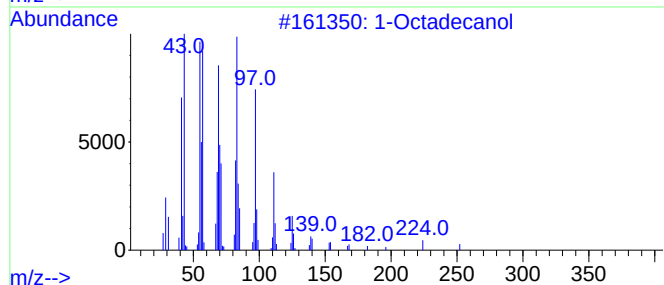
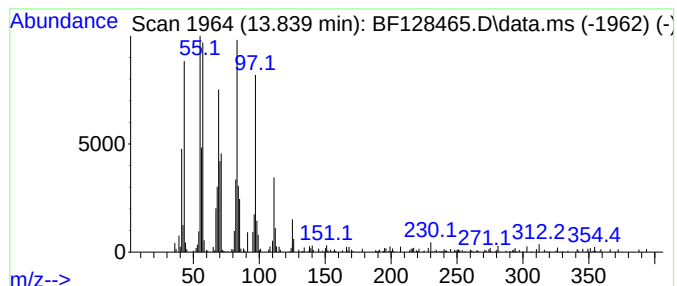
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 1-Octadecanol Concentration Rank 3

| R.T.      | EstConc              | Area   | Relative to ISTD | R.T.        |      |
|-----------|----------------------|--------|------------------|-------------|------|
| 13.839    | 10.01 ng             | 185024 | Chrysene-d12     | 13.992      |      |
| Hit# of 5 | Tentative ID         | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Octadecanol        | 270    | C18H38O          | 000112-92-5 | 91   |
| 2         | Behenic alcohol      | 326    | C22H46O          | 000661-19-8 | 91   |
| 3         | 1-Heneicosanol       | 312    | C21H44O          | 015594-90-8 | 91   |
| 4         | 1-Heneicosyl formate | 340    | C22H44O2         | 077899-03-7 | 91   |
| 5         | n-Heptadecanol-1     | 256    | C17H36O          | 001454-85-9 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052522\  
Data File : BF128465.D  
Acq On : 25 May 2022 17:52  
Operator : CG\JU  
Sample : N2894-09  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P004-SS006-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052022.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 |
| Kessane            | 10.080 | 2.6     | ng    | 74436    | 3                     | 9.845  | 565447 | 20.0 |
| Hexadecanoic ac... | 11.722 | 2.2     | ng    | 61392    | 4                     | 11.339 | 553760 | 20.0 |
| n-Hexadecanoic ... | 11.863 | 7.0     | ng    | 193436   | 4                     | 11.339 | 553760 | 20.0 |
| Benzene, 1,3-di... | 13.033 | 11.1    | ng    | 205276   | 5                     | 13.992 | 369786 | 20.0 |
| Acridin-9-amine... | 13.310 | 19.8    | ng    | 365755   | 5                     | 13.992 | 369786 | 20.0 |
| 1-Octadecanol      | 13.839 | 10.0    | ng    | 185024   | 5                     | 13.992 | 369786 | 20.0 |