

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011821\  
 Data File : BF122988.D  
 Acq On : 18 Jan 2021 15:00  
 Operator : JU/CG  
 Sample : M1160-07  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BASIN-3

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-BF011621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122988.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       | 12            | 18          | 23           | rVB      | 611129         | 758617        | 19.46%          | 2.468%        |
| 2         | 5.122       | 507           | 516         | 522          | rBV      | 45121          | 62119         | 1.59%           | 0.202%        |
| 3         | 5.510       | 577           | 582         | 585          | rBV      | 3953413        | 3794249       | 97.35%          | 12.343%       |
| 4         | 6.510       | 747           | 752         | 755          | rBV      | 3421471        | 3670191       | 94.16%          | 11.939%       |
| 5         | 6.716       | 784           | 787         | 795          | rVB      | 58323          | 50277         | 1.29%           | 0.164%        |
| 6         | 6.892       | 814           | 817         | 821          | rBV      | 1227883        | 991577        | 25.44%          | 3.226%        |
| 7         | 7.451       | 907           | 912         | 915          | rBV      | 2539611        | 2397073       | 61.50%          | 7.798%        |
| 8         | 8.175       | 1031          | 1035        | 1039         | rBV      | 1650849        | 1439234       | 36.93%          | 4.682%        |
| 9         | 9.251       | 1213          | 1218        | 1222         | rBV      | 4124829        | 3897680       | 100.00%         | 12.680%       |
| 10        | 9.645       | 1281          | 1285        | 1288         | rBV      | 228789         | 196348        | 5.04%           | 0.639%        |
| 11        | 9.933       | 1327          | 1334        | 1338         | rBV      | 1712028        | 1502719       | 38.55%          | 4.888%        |
| 12        | 10.721      | 1461          | 1468        | 1471         | rBV      | 2656295        | 2343225       | 60.12%          | 7.623%        |
| 13        | 10.763      | 1471          | 1475        | 1480         | rVB      | 32047          | 42231         | 1.08%           | 0.137%        |
| 14        | 11.421      | 1583          | 1587        | 1590         | rBV      | 1487181        | 1193358       | 30.62%          | 3.882%        |
| 15        | 11.945      | 1671          | 1676        | 1689         | rBV      | 544169         | 586136        | 15.04%          | 1.907%        |
| 16        | 12.733      | 1806          | 1810        | 1820         | rBV      | 100754         | 101581        | 2.61%           | 0.330%        |
| 17        | 13.015      | 1852          | 1858        | 1861         | rBV      | 3758941        | 3685448       | 94.55%          | 11.989%       |
| 18        | 13.221      | 1889          | 1893        | 1899         | rBV3     | 37144          | 52459         | 1.35%           | 0.171%        |
| 19        | 13.586      | 1945          | 1955        | 1957         | rBV10    | 16449          | 40465         | 1.04%           | 0.132%        |
| 20        | 13.662      | 1960          | 1968        | 1973         | rVV6     | 26778          | 68227         | 1.75%           | 0.222%        |
| 21        | 13.774      | 1984          | 1987        | 1990         | rVB      | 71467          | 63352         | 1.63%           | 0.206%        |
| 22        | 13.909      | 2006          | 2010        | 2021         | rBV      | 1033122        | 1057808       | 27.14%          | 3.441%        |
| 23        | 14.068      | 2032          | 2037        | 2040         | rBV      | 1161726        | 1098170       | 28.17%          | 3.572%        |
| 24        | 14.545      | 2112          | 2118        | 2126         | rBV2     | 99393          | 158004        | 4.05%           | 0.514%        |
| 25        | 15.198      | 2225          | 2229        | 2232         | rBV      | 64135          | 78643         | 2.02%           | 0.256%        |
| 26        | 15.545      | 2282          | 2288        | 2292         | rBV      | 786609         | 921347        | 23.64%          | 2.997%        |
| 27        | 15.586      | 2292          | 2295        | 2299         | rVB      | 38062          | 45954         | 1.18%           | 0.149%        |
| 28        | 16.033      | 2366          | 2371        | 2375         | rBV2     | 59812          | 91115         | 2.34%           | 0.296%        |
| 29        | 16.080      | 2375          | 2379        | 2388         | rVV2     | 104562         | 198593        | 5.10%           | 0.646%        |
| 30        | 16.550      | 2454          | 2459        | 2464         | rBV2     | 25782          | 41603         | 1.07%           | 0.135%        |
| 31        | 17.256      | 2574          | 2579        | 2591         | rVB9     | 21952          | 61616         | 1.58%           | 0.200%        |
| 32        | 17.656      | 2640          | 2647        | 2654         | rBV10    | 19906          | 50561         | 1.30%           | 0.164%        |

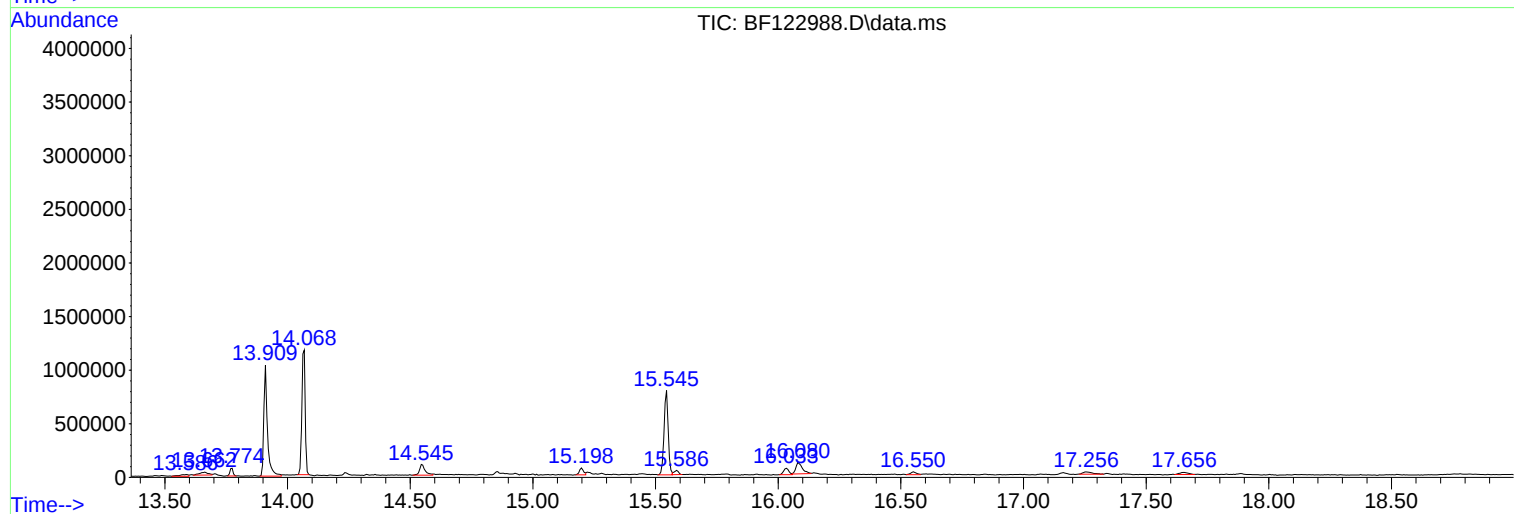
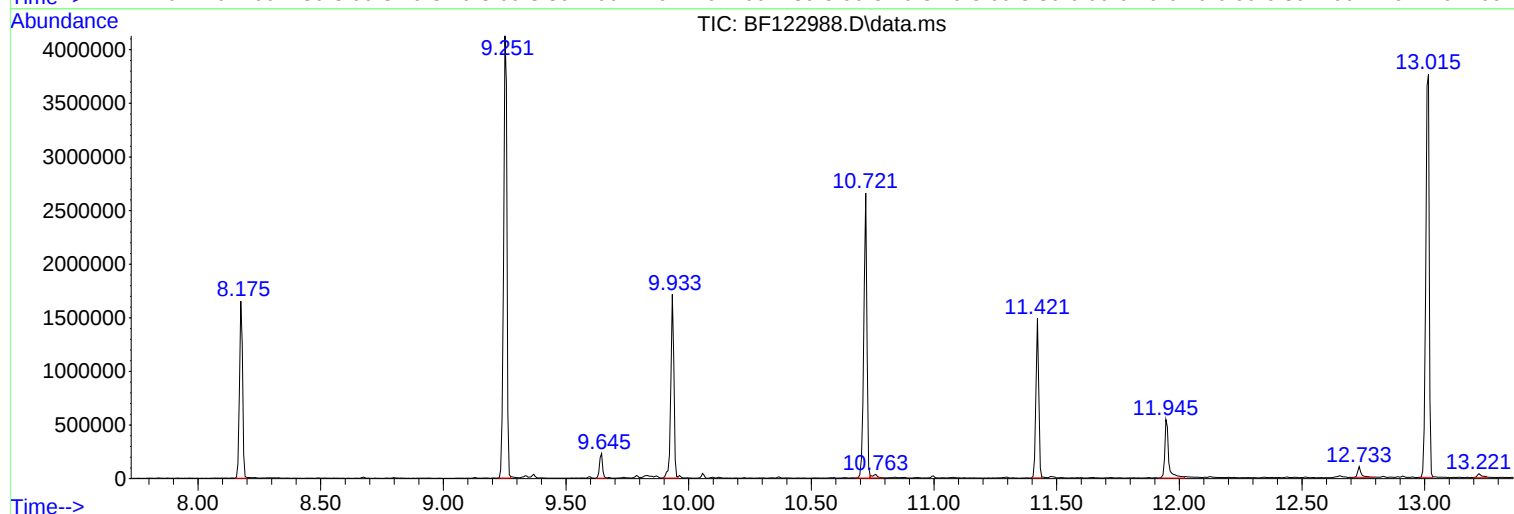
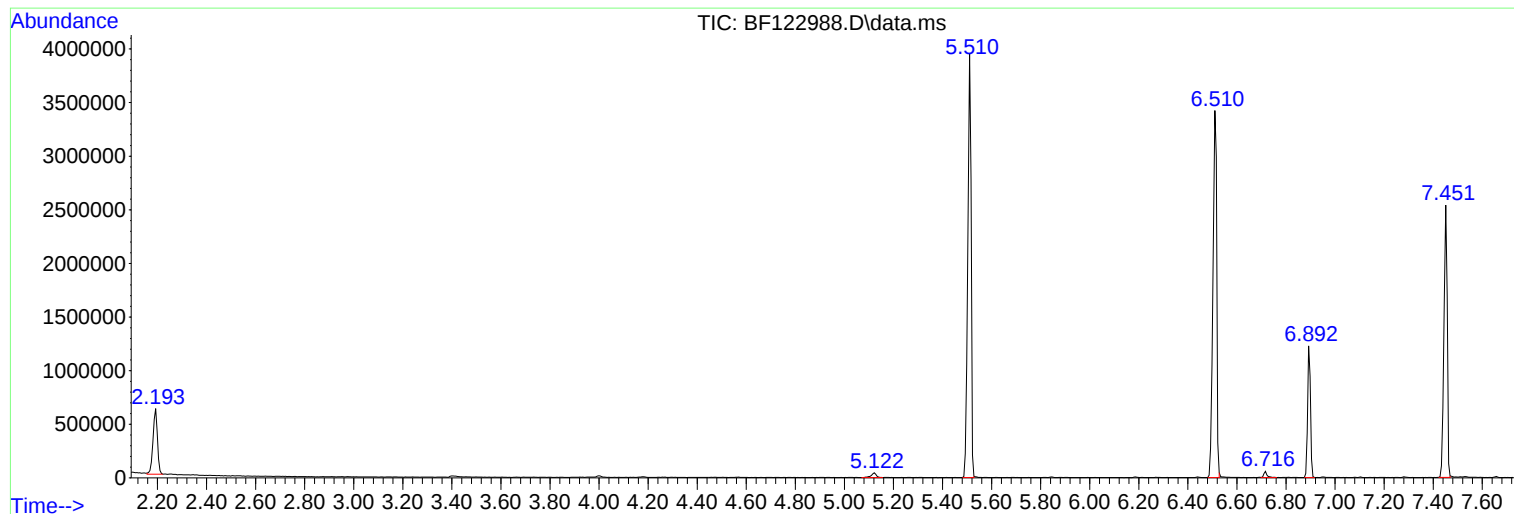
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Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BASIN-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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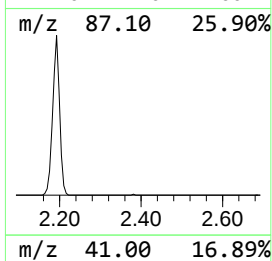
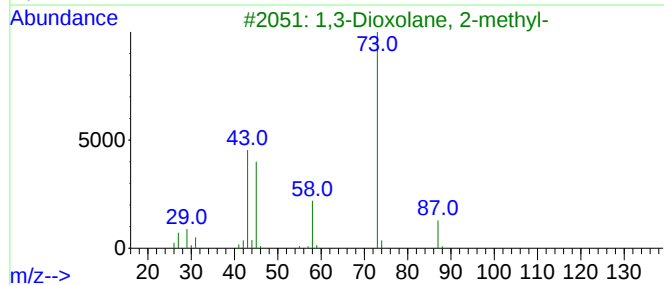
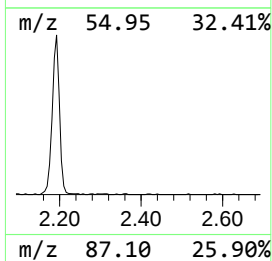
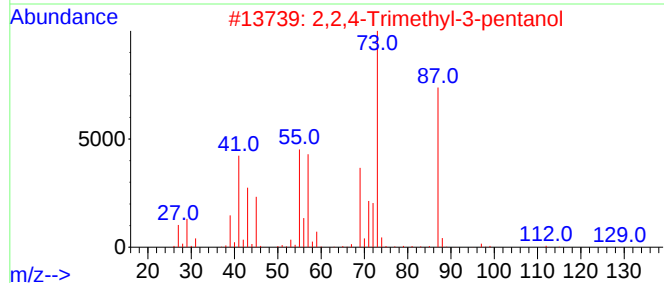
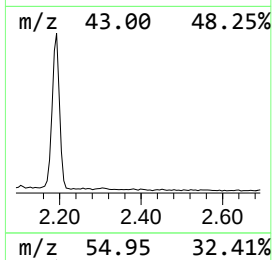
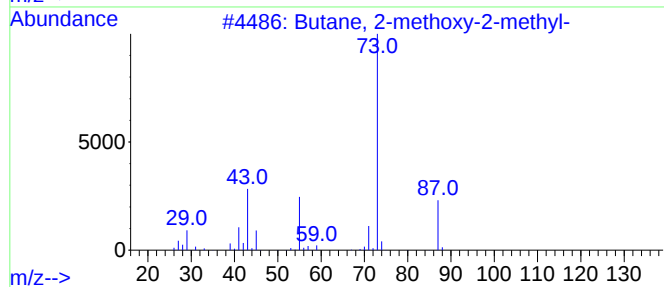
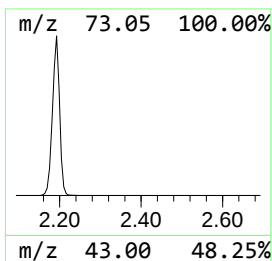
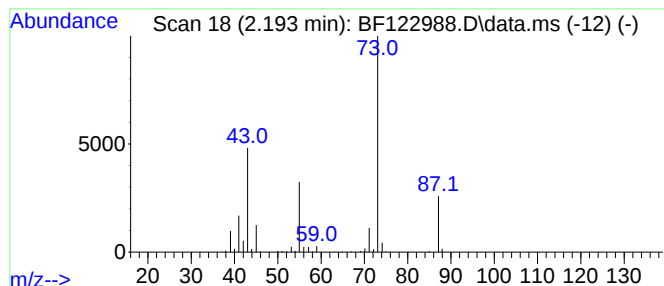
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 2.193 | 15.30 ng | 758617 | 1,4-Dichlorobenzene-d4 | 6.892 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |
| 5    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |



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BASIN-3

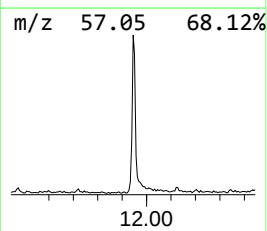
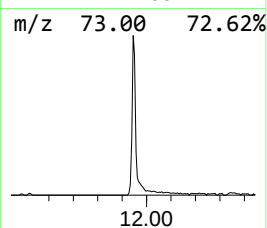
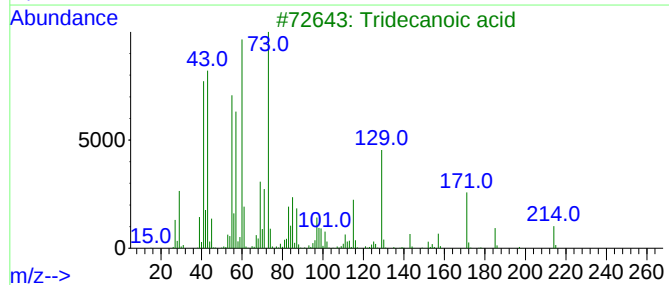
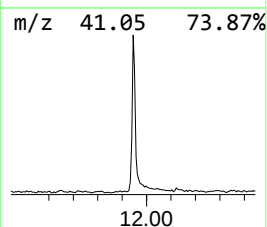
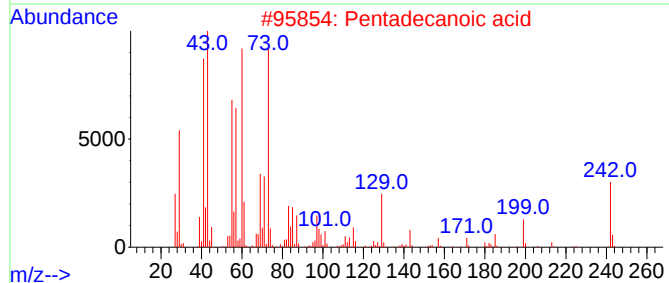
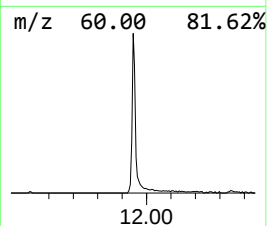
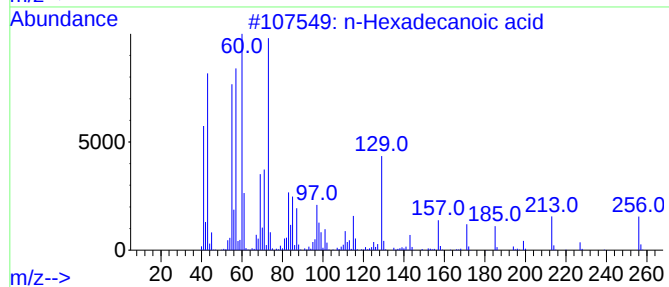
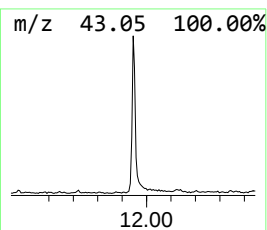
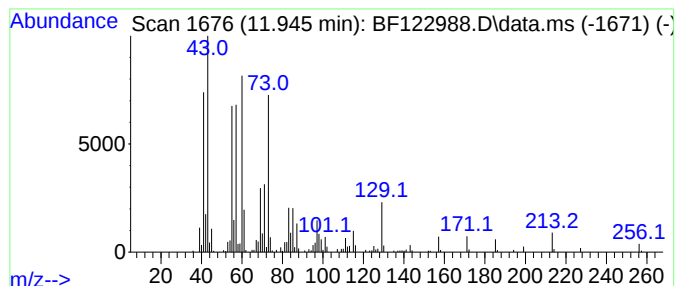
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.945 | 9.82 ng | 586136 | Phenanthrene-d10 | 11.421 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 76   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 35   |



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Sample : M1160-07  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BASIN-3

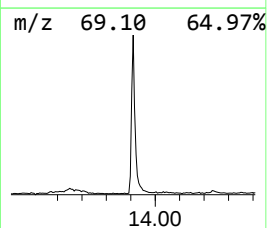
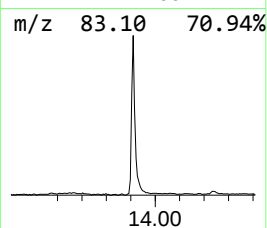
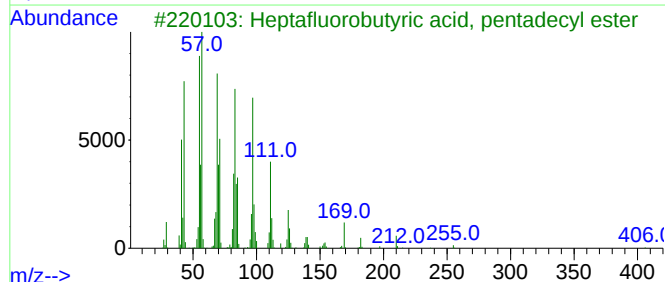
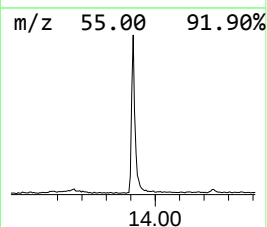
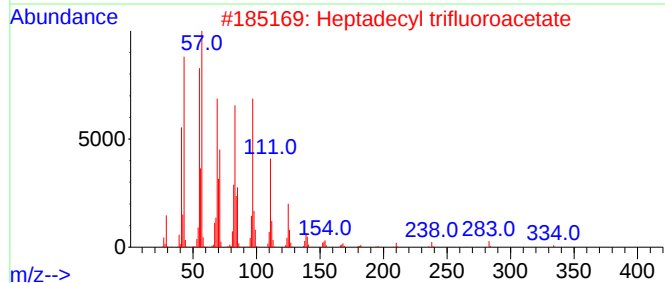
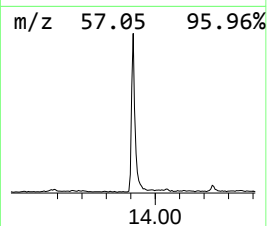
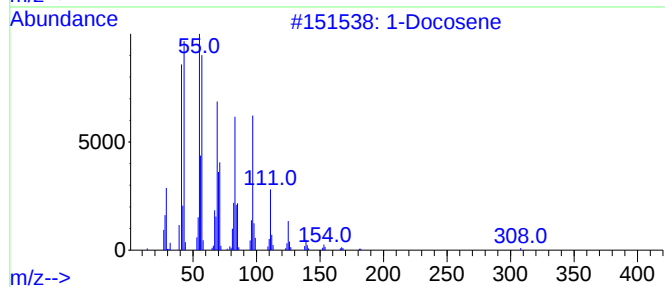
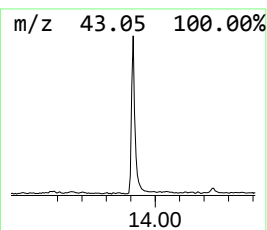
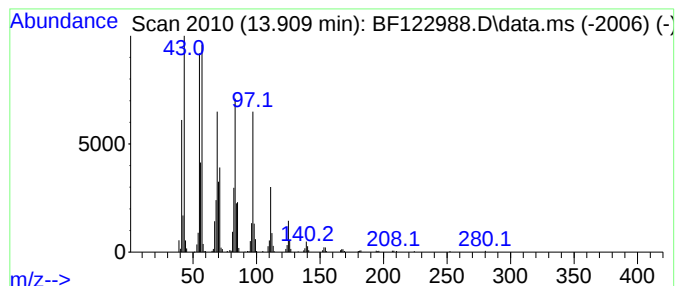
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 1-Docosene Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 13.910 | 19.26 ng | 1057810 | Chrysene-d12     | 14.068 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm    | CAS#         | Qual |
|------|-------------------------------------|---|--------------|-----|------------|--------------|------|
| 1    | 1-Docosene                          |   |              | 308 | C22H44     | 001599-67-3  | 95   |
| 2    | Heptadecyl trifluoroacetate         |   |              | 352 | C19H35F3O2 | 1000351-87-0 | 94   |
| 3    | Heptafluorobutyric acid, pentade... |   |              | 424 | C19H31F7O2 | 959261-23-5  | 94   |
| 4    | Pentafluoropropionic acid, penta... |   |              | 374 | C18H31F5O2 | 959092-08-1  | 94   |
| 5    | Trifluoroacetic acid, pentadecyl... |   |              | 324 | C17H31F3O2 | 959010-23-2  | 94   |



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ClientSampleId :  
BASIN-3

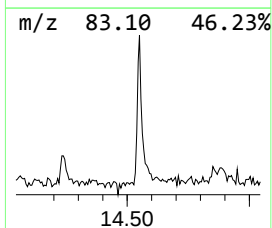
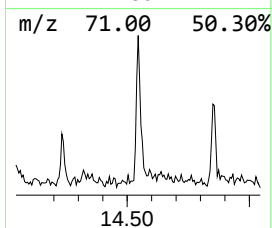
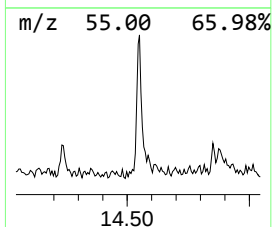
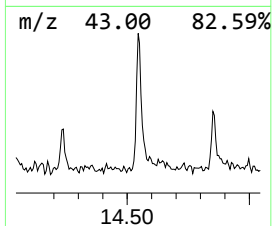
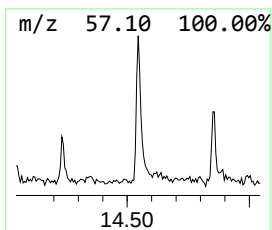
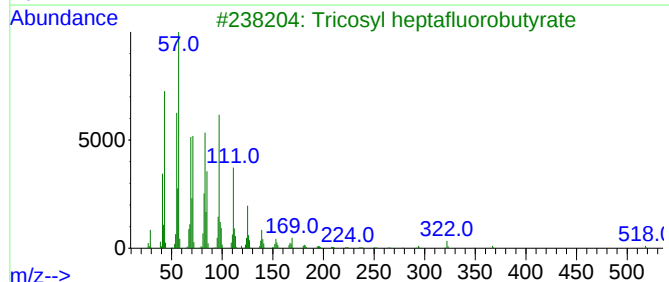
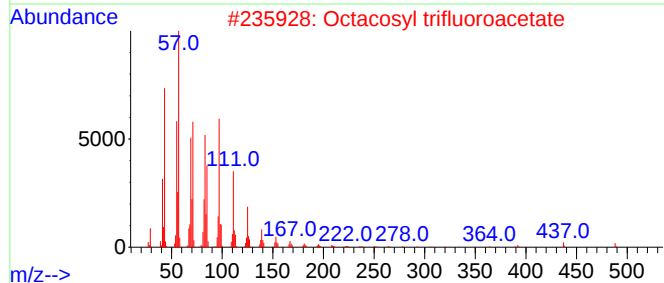
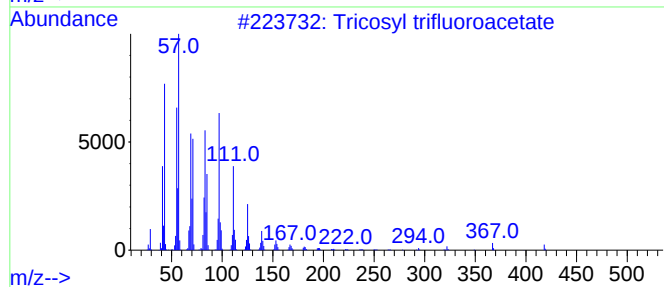
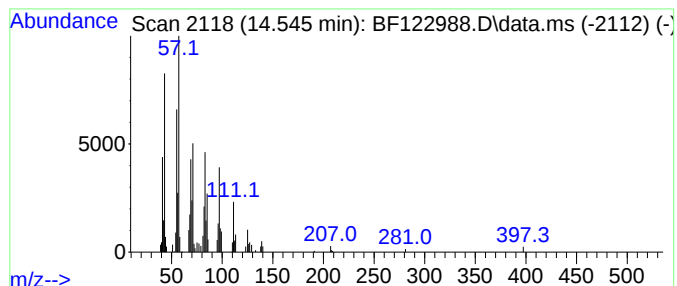
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Tricosyl trifluoroacetate Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.545 | 2.88 ng | 158004 | Chrysene-d12     | 14.068 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------|-----|------------|--------------|------|
| 1    |    |   | Tricosyl trifluoroacetate      | 436 | C25H47F3O2 | 1000351-75-1 | 91   |
| 2    |    |   | Octacosyl trifluoroacetate     | 506 | C30H57F3O2 | 1000351-74-9 | 91   |
| 3    |    |   | Tricosyl heptafluorobutyrate   | 536 | C27H47F7O2 | 1000351-83-4 | 91   |
| 4    |    |   | Tetracosyl trifluoroacetate    | 450 | C26H49F3O2 | 1000351-76-4 | 91   |
| 5    |    |   | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6  | 91   |



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BASIN-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
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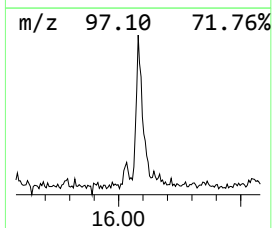
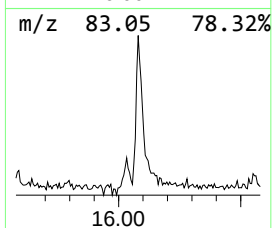
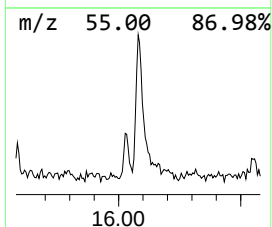
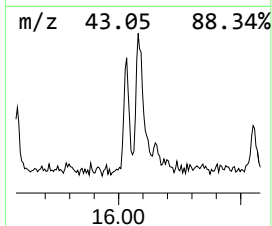
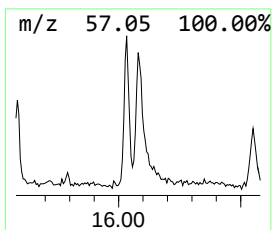
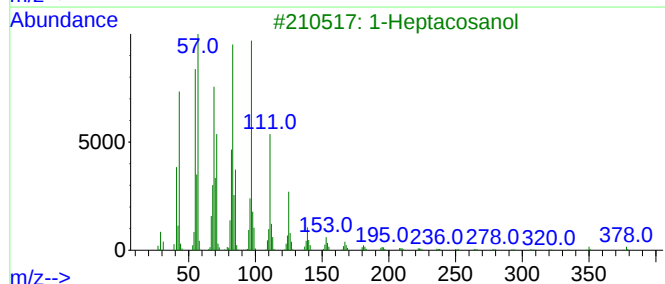
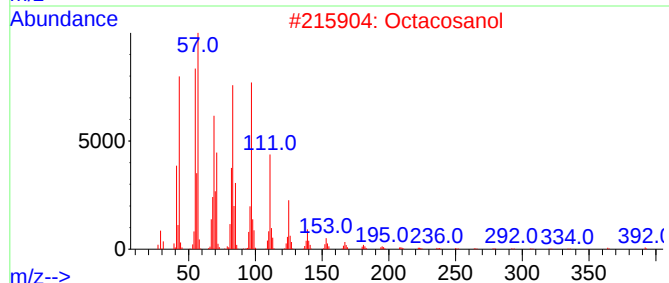
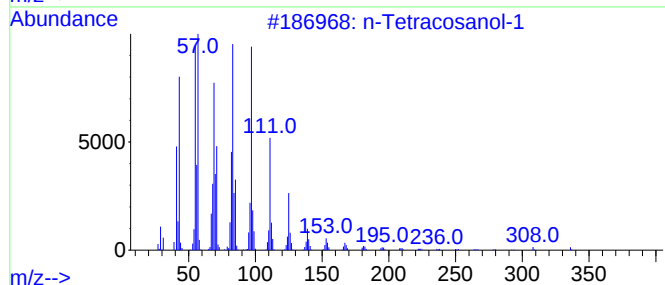
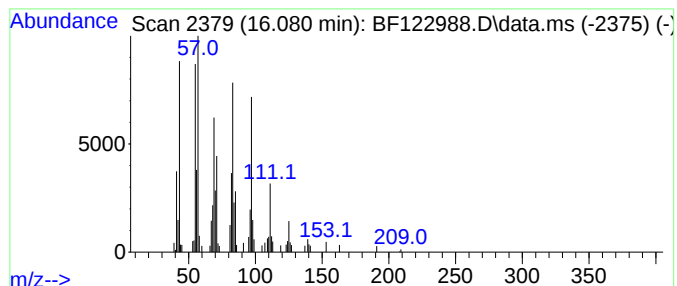
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.080 | 4.31 ng | 198593 | Perylene-d12     | 15.545 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-----------------------------|-----|------------|--------------|------|
| 1    |    |   | n-Tetracosanol-1            | 354 | C24H50O    | 000506-51-4  | 94   |
| 2    |    |   | Octacosanol                 | 410 | C28H58O    | 000557-61-9  | 94   |
| 3    |    |   | 1-Heptacosanol              | 396 | C27H56O    | 002004-39-9  | 94   |
| 4    |    |   | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 5    |    |   | 1-Docosene                  | 308 | C22H44     | 001599-67-3  | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011821\  
Data File : BF122988.D  
Acq On : 18 Jan 2021 15:00  
Operator : JU/CG  
Sample : M1160-07  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BASIN-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF011621.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 2.193  | 15.3    | ng    | 758617   | 1                     | 6.892  | 991577  | 20.0 |
| n-Hexadecanoic ... | 11.945 | 9.8     | ng    | 586136   | 4                     | 11.421 | 1193360 | 20.0 |
| 1-Docosene         | 13.910 | 19.3    | ng    | 1057810  | 5                     | 14.068 | 1098170 | 20.0 |
| Tricosyl triflu... | 14.545 | 2.9     | ng    | 158004   | 5                     | 14.068 | 1098170 | 20.0 |
| n-Tetracosanol-1   | 16.080 | 4.3     | ng    | 198593   | 6                     | 15.545 | 921347  | 20.0 |