

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071924\  
 Data File : BF138589.D  
 Acq On : 19 Jul 2024 14:58  
 Operator : RC/JU  
 Sample : P3246-06  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 WC-CTW2-BL-02

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138589.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         | 2.152       | 3             | 10          | 20           | rVB      | 1421369        | 2257202       | 100.00%         | 12.383%       |
| 2         | 3.381       | 213           | 219         | 244          | rBV      | 43843          | 114381        | 5.07%           | 0.627%        |
| 3         | 5.081       | 504           | 508         | 517          | rVB      | 104800         | 157636        | 6.98%           | 0.865%        |
| 4         | 5.487       | 571           | 577         | 582          | rBV      | 1576331        | 2037492       | 90.27%          | 11.178%       |
| 5         | 6.492       | 742           | 748         | 753          | rBV      | 1609914        | 2169138       | 96.10%          | 11.900%       |
| 6         | 6.687       | 773           | 781         | 792          | rBV      | 17190          | 24909         | 1.10%           | 0.137%        |
| 7         | 6.857       | 805           | 810         | 815          | rVB      | 355855         | 427547        | 18.94%          | 2.346%        |
| 8         | 7.422       | 899           | 906         | 911          | rBV      | 997213         | 1343677       | 59.53%          | 7.371%        |
| 9         | 8.139       | 1022          | 1028        | 1033         | rBV      | 454425         | 560642        | 24.84%          | 3.076%        |
| 10        | 8.451       | 1076          | 1081        | 1094         | rBV      | 29749          | 49719         | 2.20%           | 0.273%        |
| 11        | 9.216       | 1204          | 1211        | 1216         | rBV      | 1709598        | 2220299       | 98.37%          | 12.181%       |
| 12        | 9.892       | 1319          | 1326        | 1331         | rBV      | 518971         | 635546        | 28.16%          | 3.487%        |
| 13        | 9.986       | 1336          | 1342        | 1348         | rBV      | 58714          | 95085         | 4.21%           | 0.522%        |
| 14        | 10.298      | 1391          | 1395        | 1401         | rVB2     | 18149          | 33755         | 1.50%           | 0.185%        |
| 15        | 10.680      | 1454          | 1460        | 1471         | rBV      | 1130803        | 1489827       | 66.00%          | 8.173%        |
| 16        | 11.380      | 1573          | 1579        | 1586         | rBV      | 534133         | 692370        | 30.67%          | 3.798%        |
| 17        | 11.904      | 1663          | 1668        | 1681         | rBV2     | 124242         | 206149        | 9.13%           | 1.131%        |
| 18        | 12.592      | 1781          | 1785        | 1789         | rBV      | 23898          | 32315         | 1.43%           | 0.177%        |
| 19        | 12.686      | 1797          | 1801        | 1807         | rBV2     | 23168          | 40016         | 1.77%           | 0.220%        |
| 20        | 12.816      | 1820          | 1823        | 1828         | rBV      | 16131          | 22692         | 1.01%           | 0.124%        |
| 21        | 12.963      | 1842          | 1848        | 1853         | rBV      | 1717225        | 2205578       | 97.71%          | 12.100%       |
| 22        | 13.857      | 1995          | 2000        | 2015         | rBV      | 112450         | 216881        | 9.61%           | 1.190%        |
| 23        | 14.015      | 2022          | 2027        | 2037         | rVB      | 352701         | 472153        | 20.92%          | 2.590%        |
| 24        | 14.174      | 2051          | 2054        | 2063         | rVB2     | 13586          | 22808         | 1.01%           | 0.125%        |
| 25        | 14.486      | 2102          | 2107        | 2114         | rBV5     | 26853          | 79779         | 3.53%           | 0.438%        |
| 26        | 14.545      | 2114          | 2117        | 2122         | rVB      | 22137          | 29221         | 1.29%           | 0.160%        |
| 27        | 14.780      | 2155          | 2157        | 2173         | rVB      | 18708          | 30954         | 1.37%           | 0.170%        |
| 28        | 15.121      | 2211          | 2215        | 2219         | rBV      | 34625          | 47553         | 2.11%           | 0.261%        |
| 29        | 15.480      | 2270          | 2276        | 2288         | rBV      | 287852         | 470707        | 20.85%          | 2.582%        |
| 30        | 15.933      | 2349          | 2353        | 2359         | rVB      | 26902          | 42238         | 1.87%           | 0.232%        |

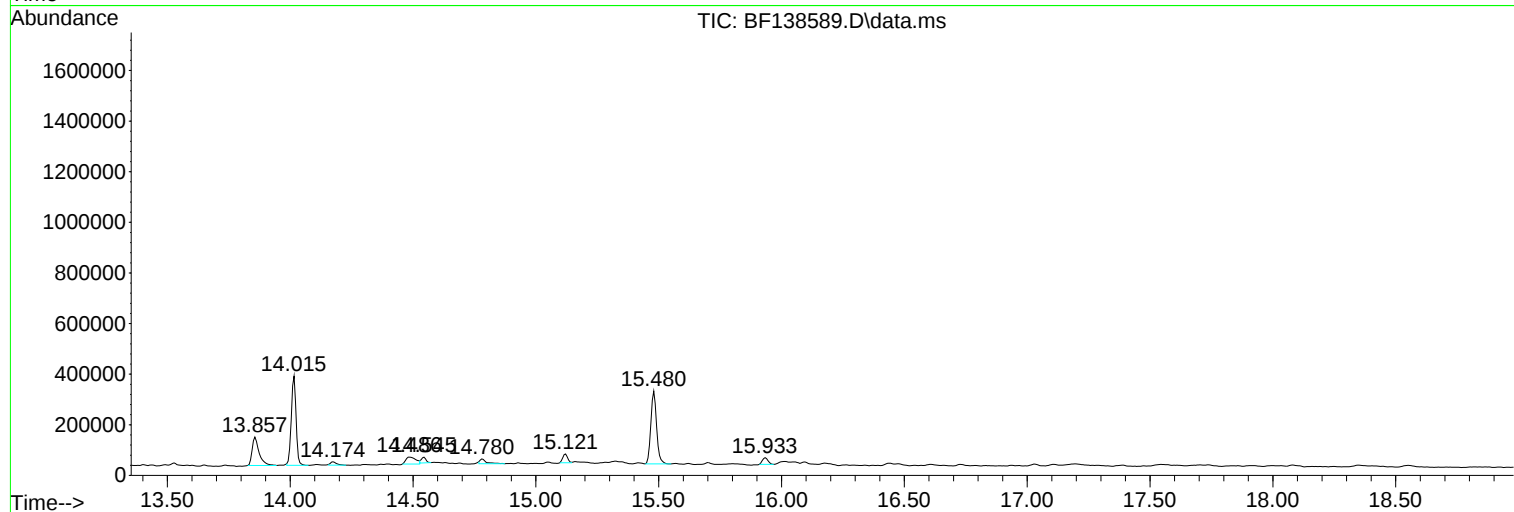
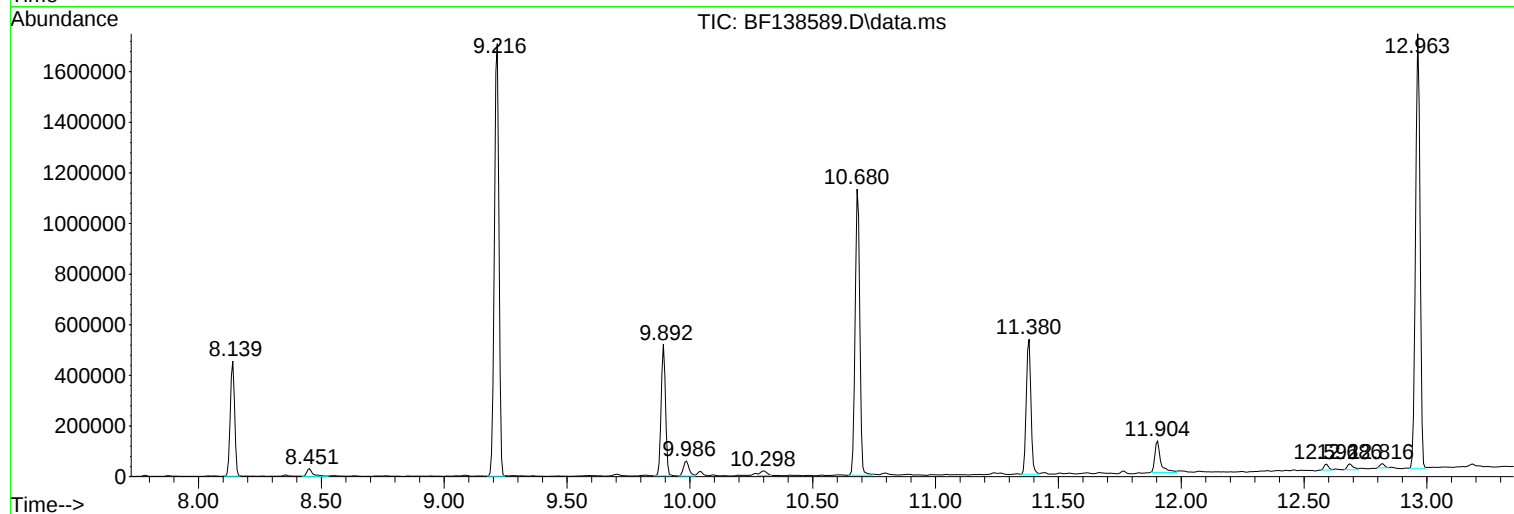
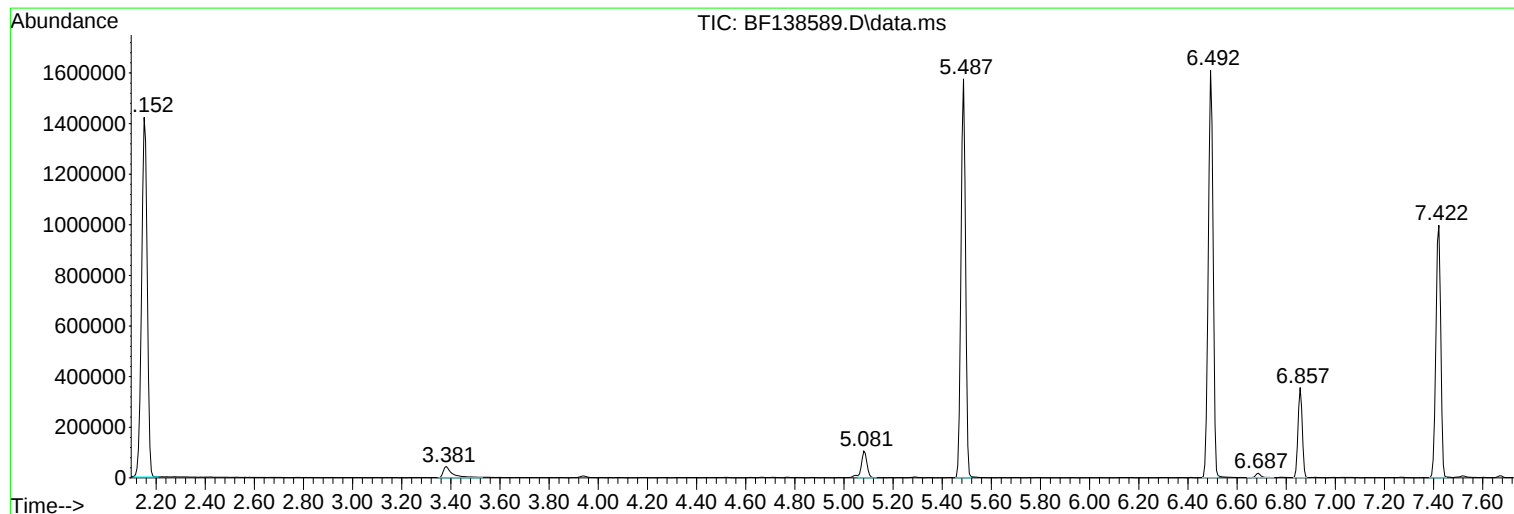
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ALS Vial : 13 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
WC-CTW2-BL-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.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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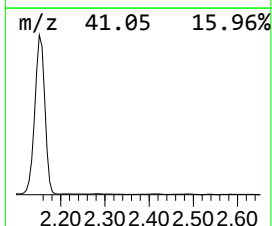
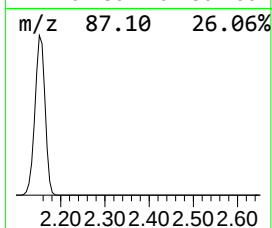
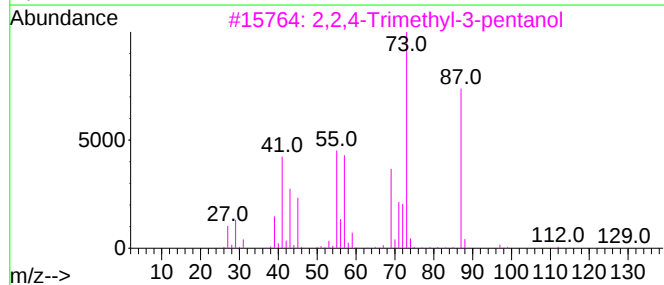
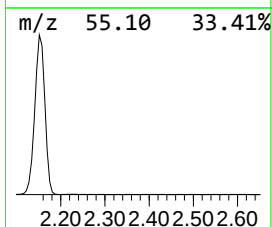
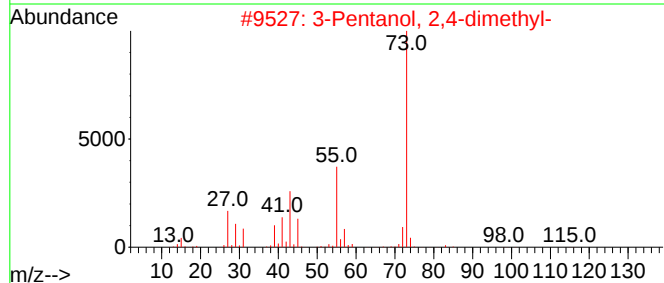
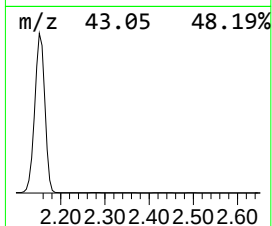
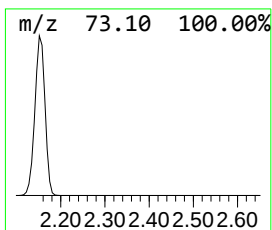
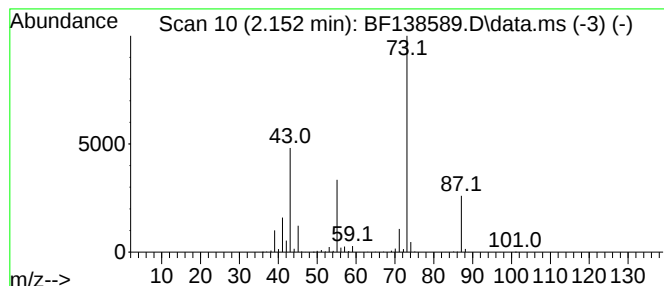
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 2.152 | 105.59 ng | 2257200 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 43   |
| 3    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 38   |
| 5    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |



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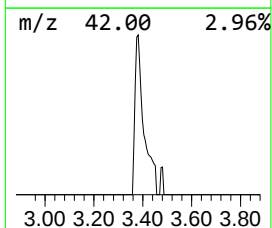
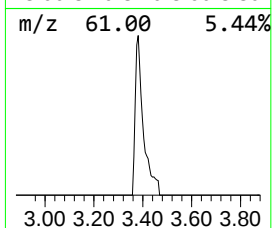
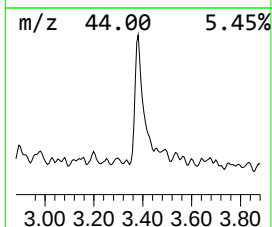
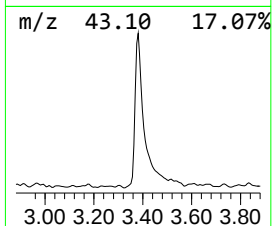
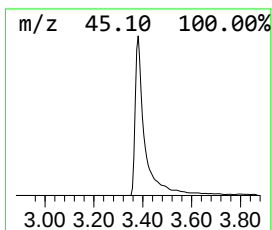
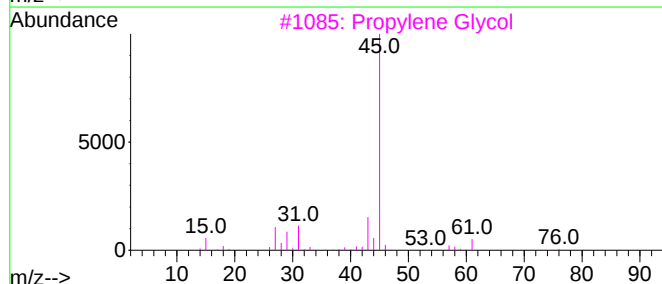
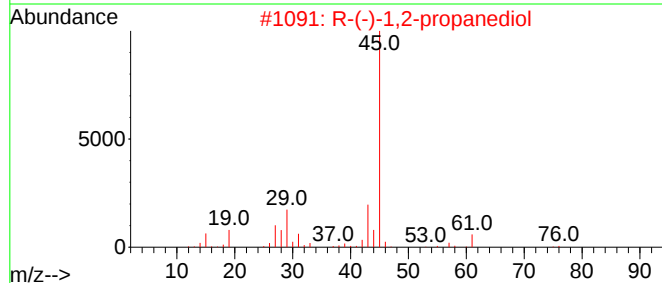
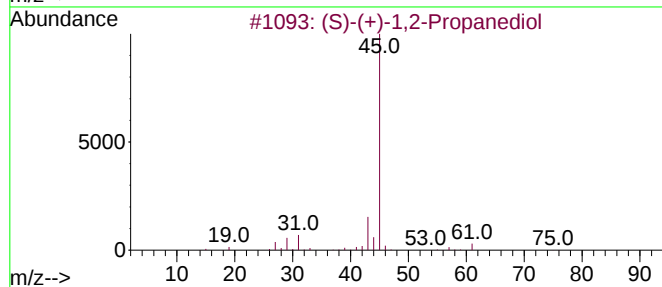
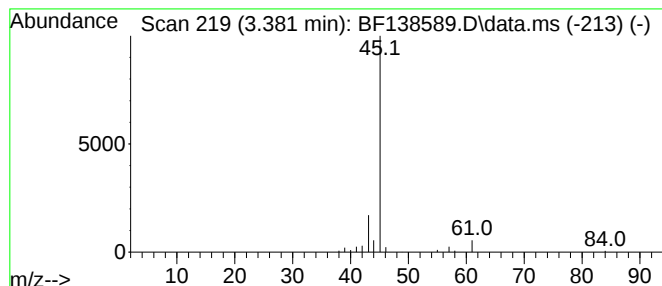
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.381 | 5.35 ng | 114381 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------------------------|-----|---------|-------------|------|
| 1    |      | (S)-(+)-1,2-Propanediol             | 76  | C3H8O2  | 004254-15-3 | 64   |
| 2    |      | R-(-)-1,2-propanediol               | 76  | C3H8O2  | 004254-14-2 | 43   |
| 3    |      | Propylene Glycol                    | 76  | C3H8O2  | 000057-55-6 | 9    |
| 4    |      | Isopropyl Alcohol                   | 60  | C3H8O   | 000067-63-0 | 9    |
| 5    |      | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3  | 000547-64-8 | 9    |



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Instrument :  
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ClientSampleId :  
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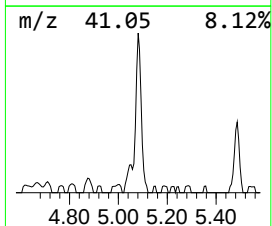
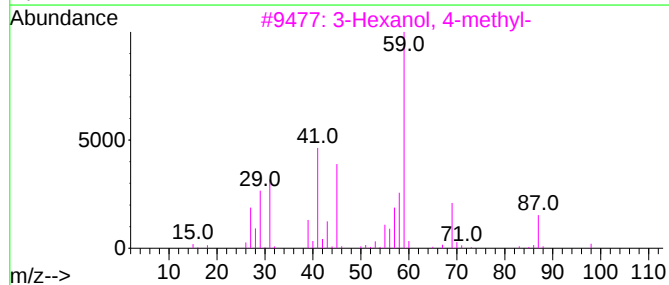
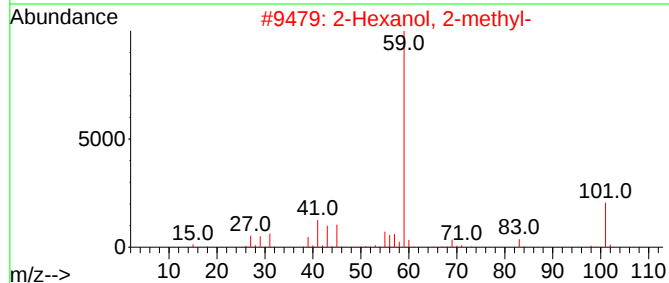
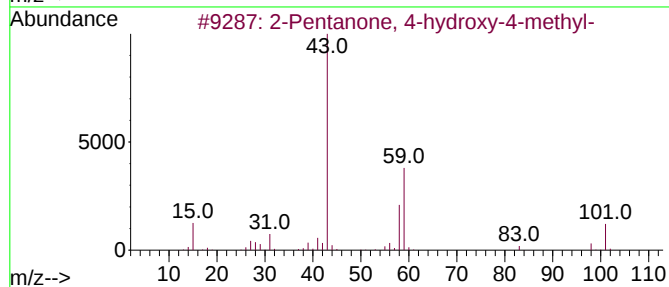
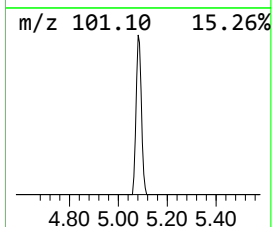
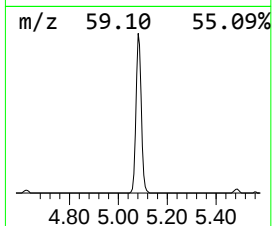
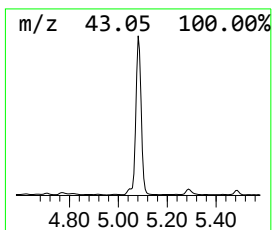
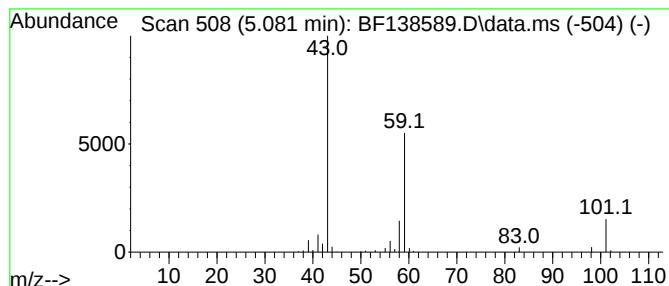
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.081 | 7.37 ng | 157636 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 3    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 5    |    |   | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O   | 000627-02-1 | 9    |



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Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

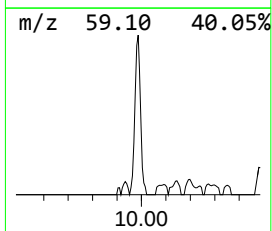
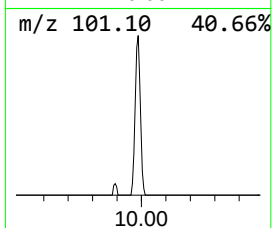
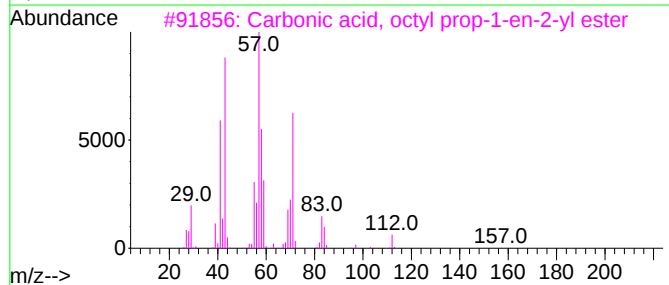
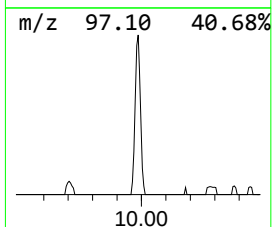
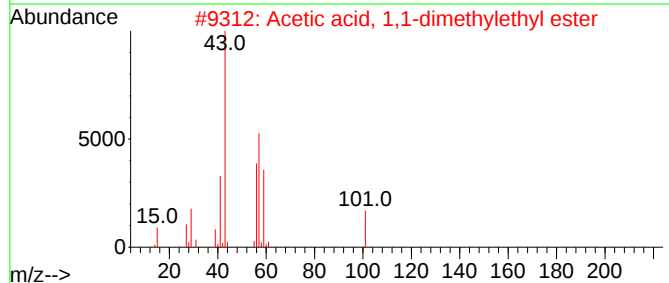
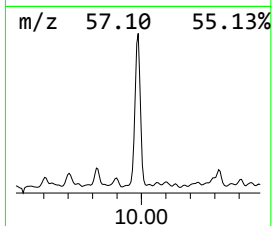
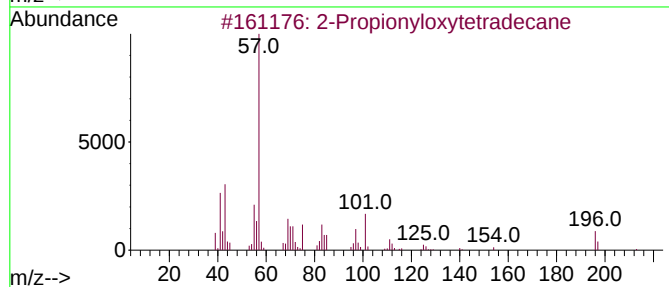
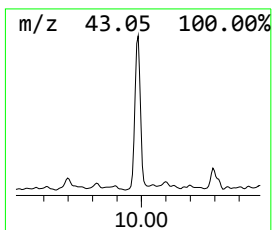
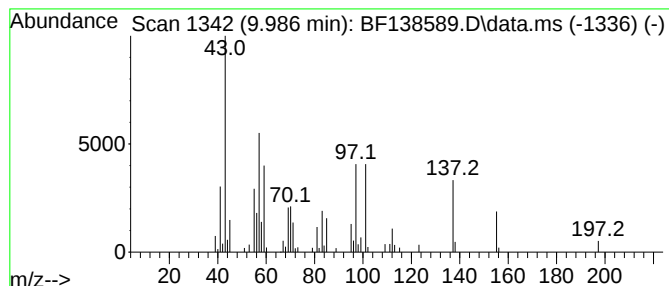
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown9.986 Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 9.986 | 2.99 ng | 95085 | Acenaphthene-d10 | 9.892 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Propionyloxytetradecane           | 270 | C17H34O2 | 1000245-62-7 | 27   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5  | 22   |
| 3    |    |   | Carbonic acid, octyl prop-1-en-2... | 214 | C12H22O3 | 1000382-54-0 | 16   |
| 4    |    |   | 5-Ethyl-3-nonanol                   | 172 | C11H24O  | 019780-71-3  | 16   |
| 5    |    |   | 3-Hexene-2,5-dione                  | 112 | C6H8O2   | 004436-75-3  | 11   |



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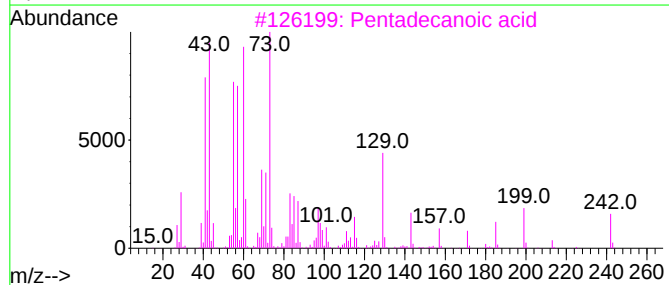
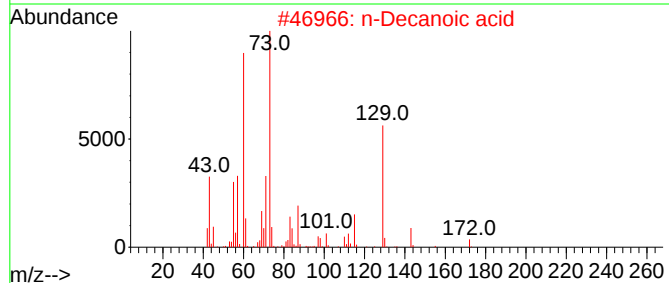
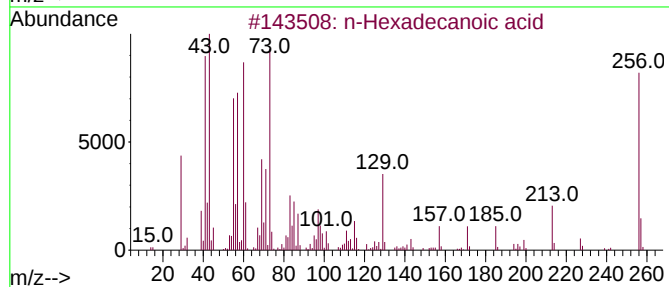
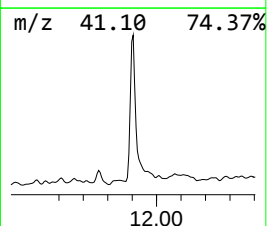
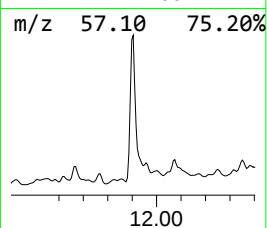
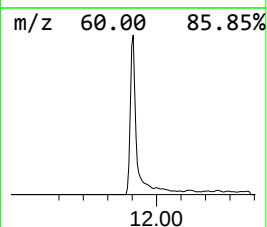
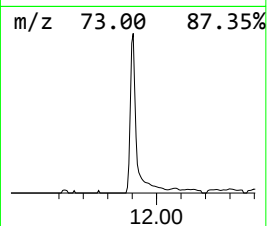
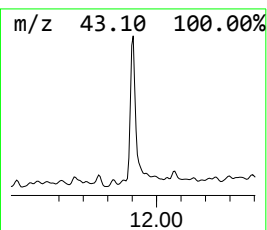
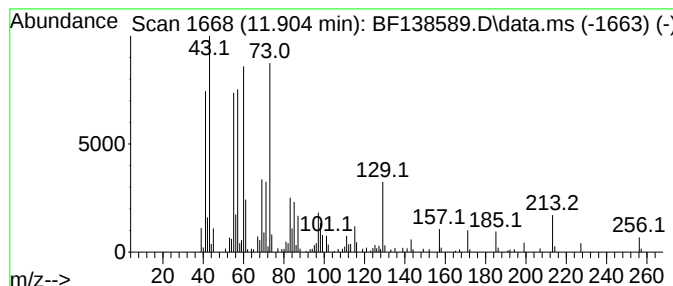
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.904 | 5.95 ng | 206149 | Phenanthrene-d10 | 11.380 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 91   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071924\  
Data File : BF138589.D  
Acq On : 19 Jul 2024 14:58  
Operator : RC/JU  
Sample : P3246-06  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-CTW2-BL-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

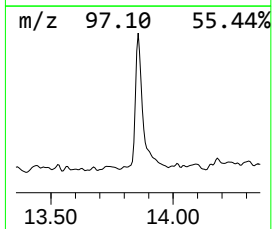
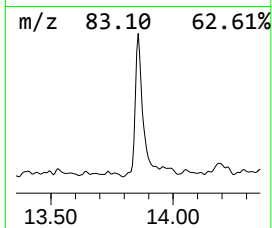
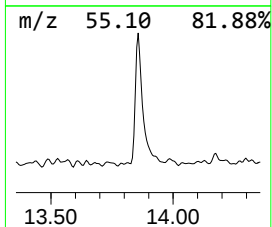
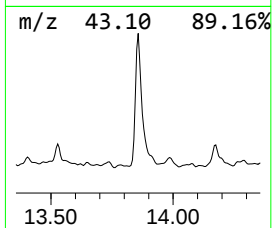
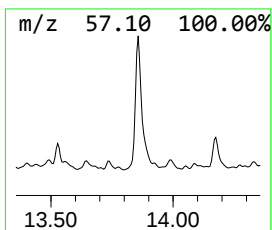
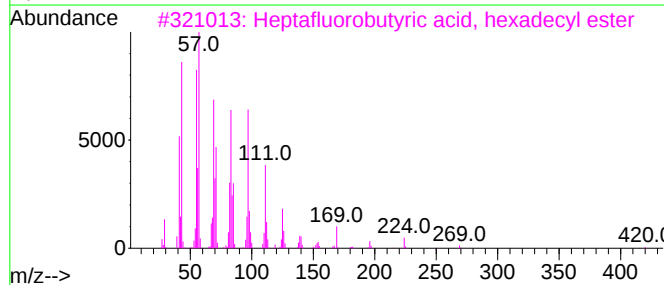
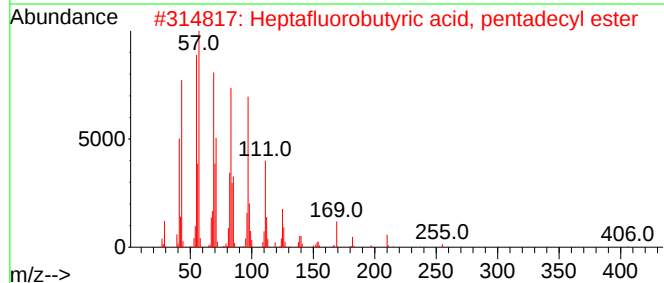
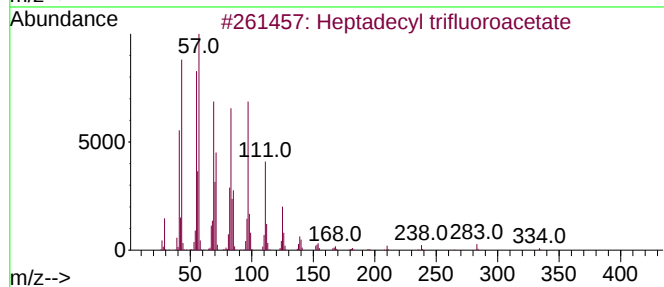
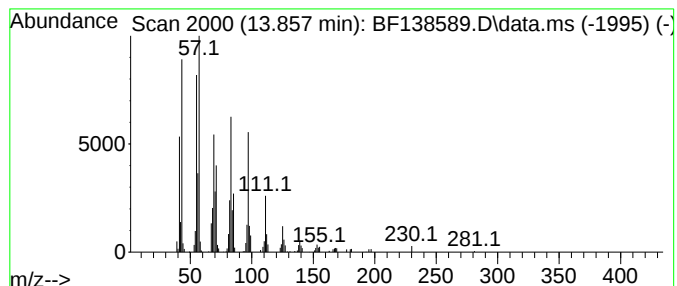
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Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.857 | 9.19 ng | 216881 | Chrysene-d12     | 14.015 |

| Hit# | of | 5 | Tentative ID                              | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Heptadecyl trifluoroacetate               | 352 | C19H35F3O2 | 1010351-87-0 | 94   |
| 2    |    |   | Heptafluorobutyric acid, pentadecyl ester | 424 | C19H31F7O2 | 959261-23-5  | 94   |
| 3    |    |   | Heptafluorobutyric acid, hexadecyl ester  | 438 | C20H33F7O2 | 006385-15-5  | 94   |
| 4    |    |   | Heptadecyl heptafluorobutyrate            | 452 | C21H35F7O2 | 959085-66-6  | 94   |
| 5    |    |   | Trifluoroacetoxy hexadecane               | 338 | C18H33F3O2 | 006222-03-3  | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071924\  
Data File : BF138589.D  
Acq On : 19 Jul 2024 14:58  
Operator : RC/JU  
Sample : P3246-06  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-CTW2-BL-02

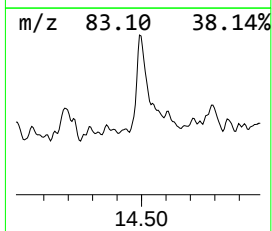
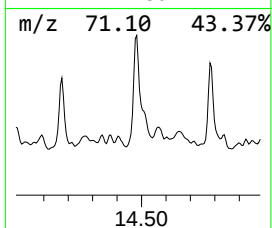
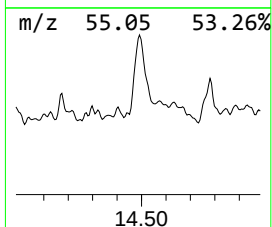
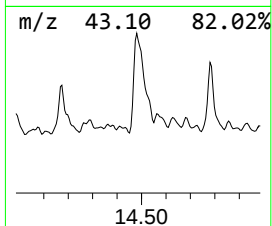
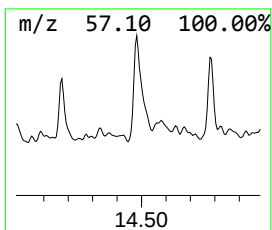
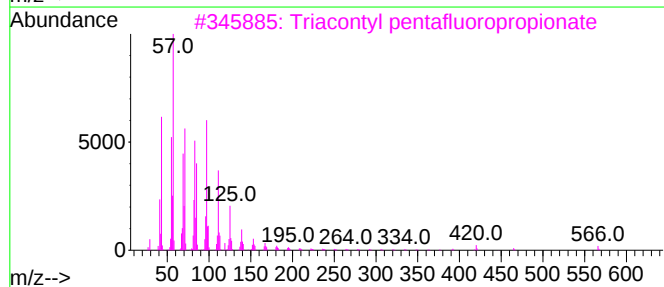
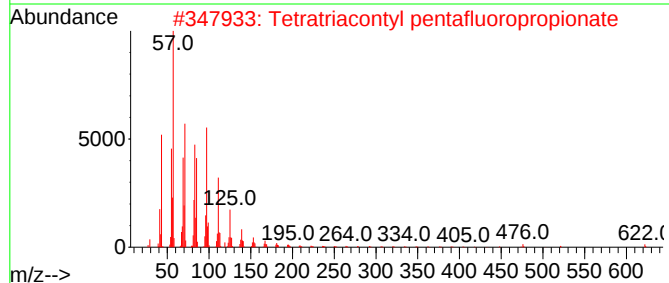
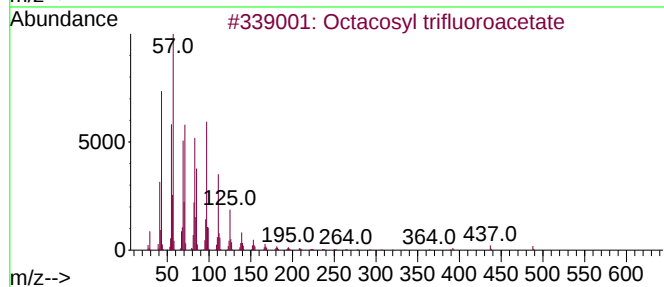
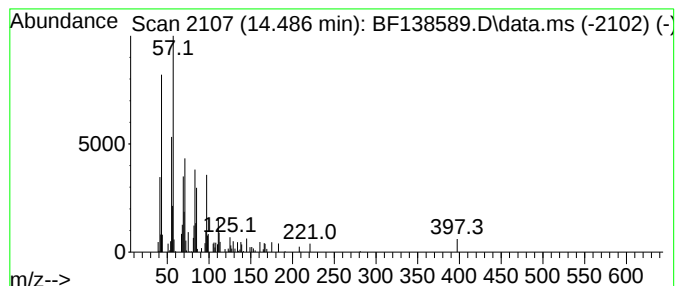
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 6

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 14.486    | 3.38 ng                             | 79779 | Chrysene-d12     | 14.015       |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | Octacosyl trifluoroacetate          | 506   | C30H57F3O2       | 1000351-74-9 | 91   |
| 2         | Tetratriacontyl pentafluoropropi... | 641   | C37H69F5O2       | 1000351-81-5 | 91   |
| 3         | Triacontyl pentafluoropropionate    | 584   | C33H61F5O2       | 1000351-80-0 | 91   |
| 4         | Triacontyl trifluoroacetate         | 534   | C32H61F3O2       | 1000351-75-7 | 91   |
| 5         | Tetratriacontyl trifluoroacetate    | 591   | C36H69F3O2       | 1000351-75-3 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071924\  
Data File : BF138589.D  
Acq On : 19 Jul 2024 14:58  
Operator : RC/JU  
Sample : P3246-06  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-CTW2-BL-02

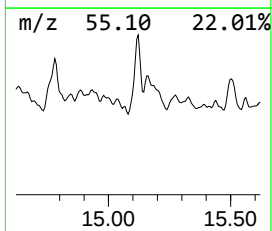
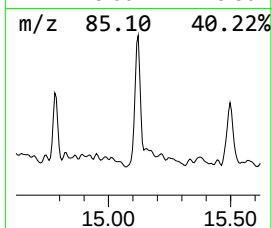
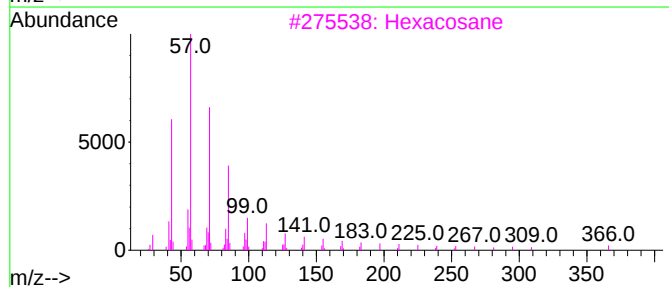
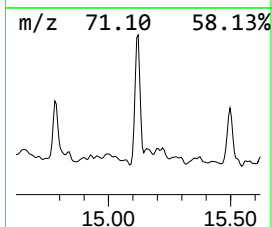
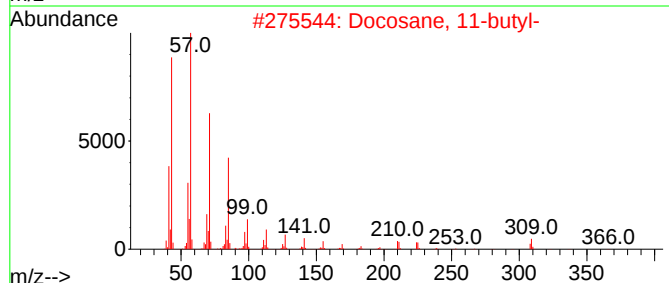
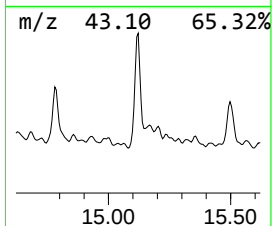
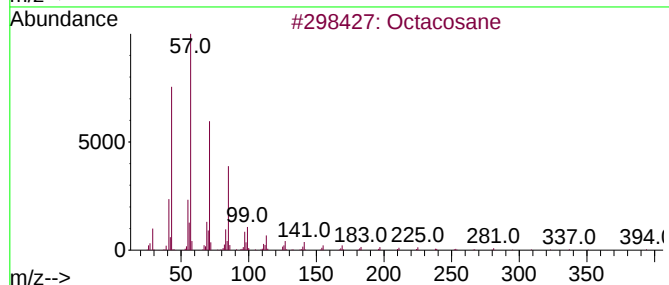
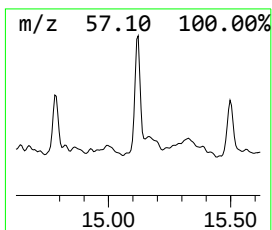
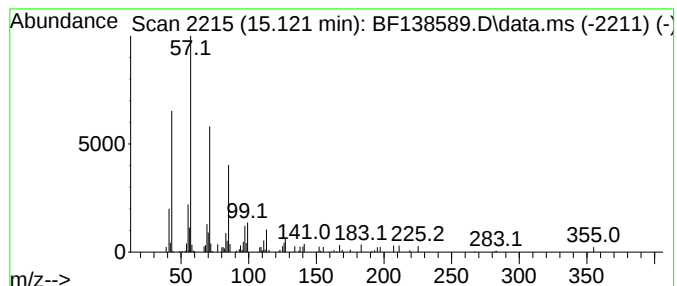
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Octacosane Concentration Rank 8

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.121 | 2.02 ng | 47553 | Perylene-d12     | 15.480 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane          | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    |   | Docosane, 11-butyl- | 366 | C26H54  | 013475-76-8 | 91   |
| 3    |    |   | Hexacosane          | 366 | C26H54  | 000630-01-3 | 91   |
| 4    |    |   | Tetracosane         | 338 | C24H50  | 000646-31-1 | 91   |
| 5    |    |   | Pentacosane         | 352 | C25H52  | 000629-99-2 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071924\  
Data File : BF138589.D  
Acq On : 19 Jul 2024 14:58  
Operator : RC/JU  
Sample : P3246-06  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-CTW2-BL-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.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... | 2.152  | 105.6   | ng    | 2257200  | 1                     | 6.857  | 427547 | 20.0 |
| (S)-(+)-1,2-Pro... | 3.381  | 5.3     | ng    | 114381   | 1                     | 6.857  | 427547 | 20.0 |
| 2-Pentanone, 4-... | 5.081  | 7.4     | ng    | 157636   | 1                     | 6.857  | 427547 | 20.0 |
| unknown9.986       | 9.986  | 3.0     | ng    | 95085    | 3                     | 9.892  | 635546 | 20.0 |
| n-Hexadecanoic ... | 11.904 | 6.0     | ng    | 206149   | 4                     | 11.380 | 692370 | 20.0 |
| Heptadecyl trif... | 13.857 | 9.2     | ng    | 216881   | 5                     | 14.015 | 472153 | 20.0 |
| Octacosyl trifl... | 14.486 | 3.4     | ng    | 79779    | 5                     | 14.015 | 472153 | 20.0 |
| Octacosane         | 15.121 | 2.0     | ng    | 47553    | 6                     | 15.480 | 470707 | 20.0 |