

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
 Data File : BF140079.D  
 Acq On : 28 Oct 2024 11:31  
 Operator : RC/JU  
 Sample : PB164444BL  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB164444BL

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140079.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         | 2.246       | 20            | 26          | 40           | rVB      | 60072          | 108884        | 2.67%           | 0.408%        |
| 2         | 4.022       | 321           | 328         | 334          | rBV      | 93912          | 147840        | 3.62%           | 0.554%        |
| 3         | 5.516       | 575           | 582         | 587          | rBV      | 2379442        | 3421011       | 83.78%          | 12.815%       |
| 4         | 6.510       | 744           | 751         | 756          | rBV      | 2331665        | 3426748       | 83.92%          | 12.837%       |
| 5         | 6.887       | 810           | 815         | 820          | rVB      | 625889         | 757614        | 18.55%          | 2.838%        |
| 6         | 7.445       | 903           | 910         | 915          | rBV      | 1658563        | 2322515       | 56.88%          | 8.700%        |
| 7         | 8.169       | 1027          | 1033        | 1038         | rBV      | 769758         | 999772        | 24.48%          | 3.745%        |
| 8         | 9.245       | 1209          | 1216        | 1221         | rBV      | 2955121        | 4083263       | 100.00%         | 15.296%       |
| 9         | 9.922       | 1325          | 1331        | 1350         | rBV      | 888634         | 1150328       | 28.17%          | 4.309%        |
| 10        | 10.710      | 1459          | 1465        | 1479         | rBV      | 1742785        | 2374056       | 58.14%          | 8.893%        |
| 11        | 11.410      | 1578          | 1584        | 1589         | rBV      | 925255         | 1151100       | 28.19%          | 4.312%        |
| 12        | 11.916      | 1654          | 1670        | 1693         | rBV4     | 134194         | 476747        | 11.68%          | 1.786%        |
| 13        | 12.710      | 1798          | 1805        | 1819         | rBV      | 77196          | 174157        | 4.27%           | 0.652%        |
| 14        | 12.904      | 1830          | 1838        | 1848         | rVB      | 123444         | 267755        | 6.56%           | 1.003%        |
| 15        | 12.998      | 1848          | 1854        | 1859         | rBV      | 2651055        | 3536154       | 86.60%          | 13.247%       |
| 16        | 13.610      | 1951          | 1958        | 1969         | rBV      | 119466         | 225935        | 5.53%           | 0.846%        |
| 17        | 14.045      | 2027          | 2032        | 2044         | rVB      | 478740         | 638690        | 15.64%          | 2.393%        |
| 18        | 14.174      | 2047          | 2054        | 2062         | rBV      | 120925         | 206612        | 5.06%           | 0.774%        |
| 19        | 14.651      | 2129          | 2135        | 2144         | rBV      | 83690          | 147643        | 3.62%           | 0.553%        |
| 20        | 15.157      | 2214          | 2221        | 2227         | rBV      | 58409          | 119213        | 2.92%           | 0.447%        |
| 21        | 15.527      | 2277          | 2284        | 2300         | rBV      | 441980         | 752741        | 18.43%          | 2.820%        |
| 22        | 15.727      | 2312          | 2318        | 2328         | rVB      | 31989          | 66705         | 1.63%           | 0.250%        |
| 23        | 16.380      | 2425          | 2429        | 2439         | rVB      | 19521          | 43026         | 1.05%           | 0.161%        |
| 24        | 17.539      | 2619          | 2626        | 2638         | rVB2     | 34805          | 95983         | 2.35%           | 0.360%        |

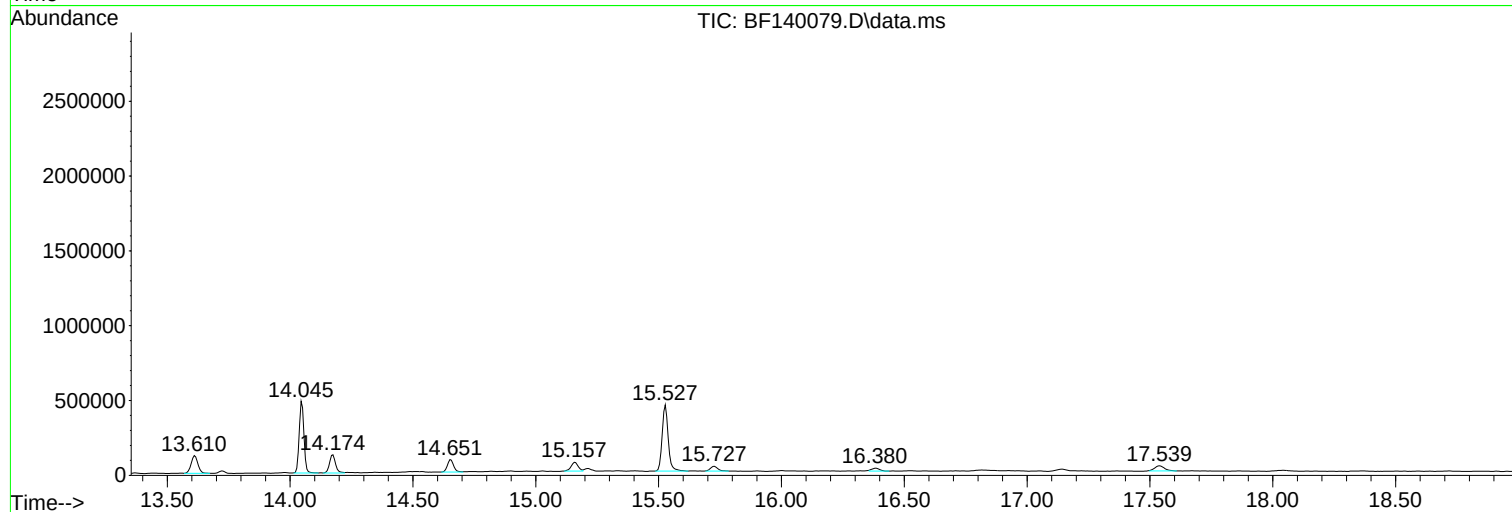
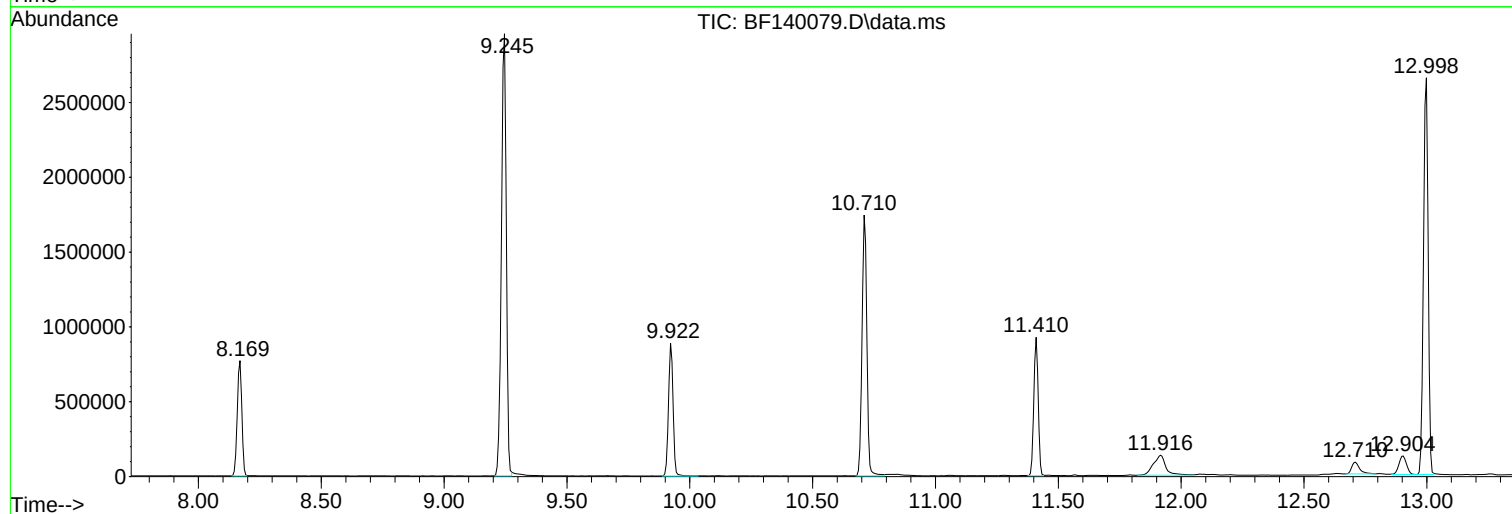
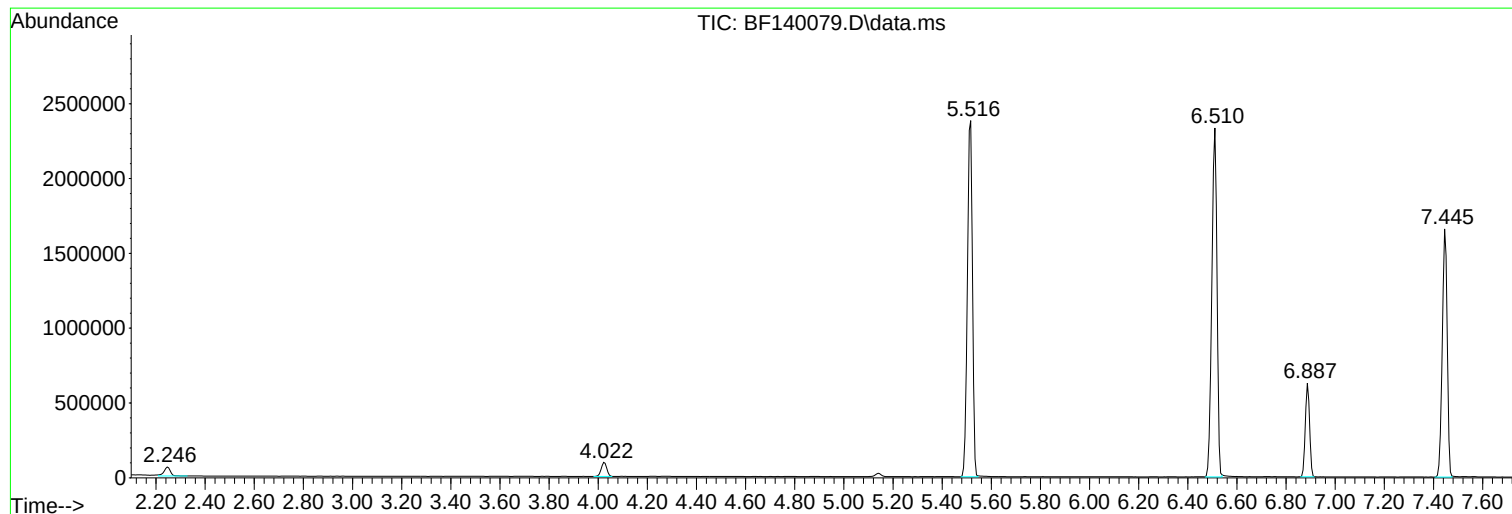
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BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.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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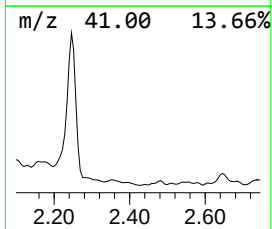
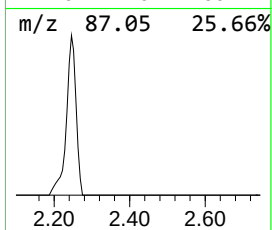
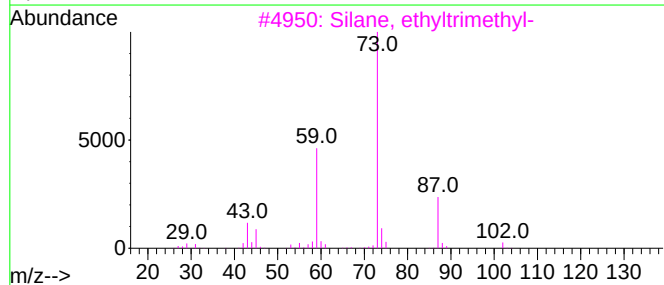
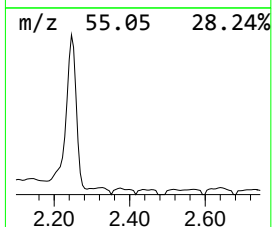
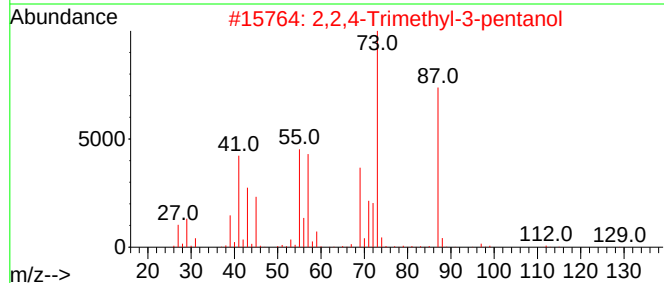
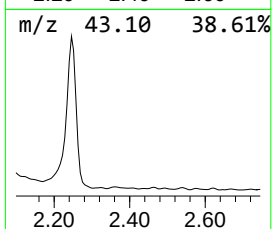
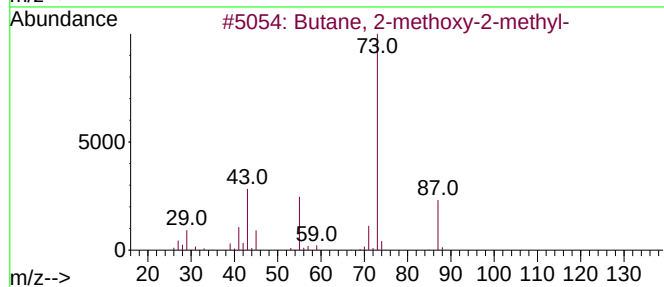
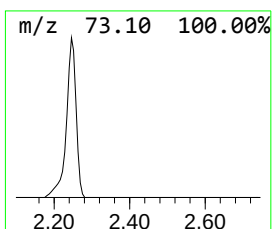
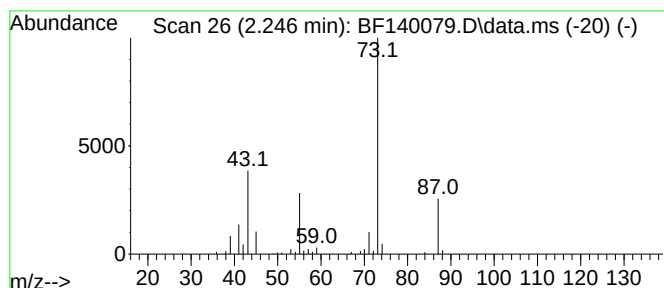
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 2.246 | 2.87 ng | 108884 | 1,4-Dichlorobenzene-d4 | 6.886 |

| 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    |    |   | Silane, ethyltrimethyl-          | 102 | C5H14Si  | 003439-38-1 | 33   |
| 4    |    |   | 3-Hexanol, 2-methyl-             | 116 | C7H16O   | 000617-29-8 | 25   |
| 5    |    |   | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17   |



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ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

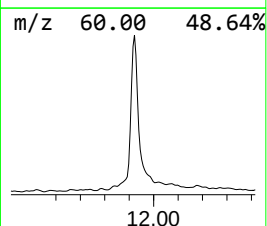
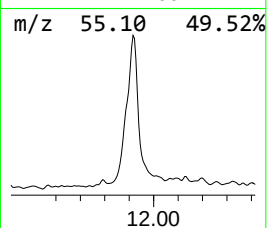
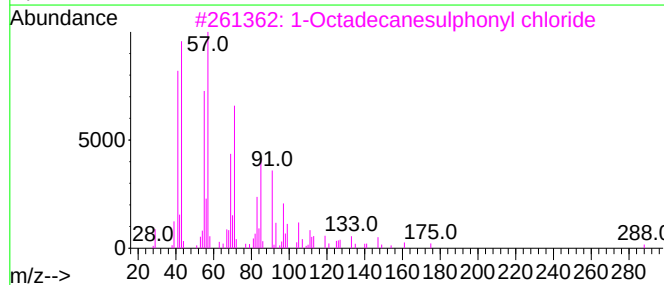
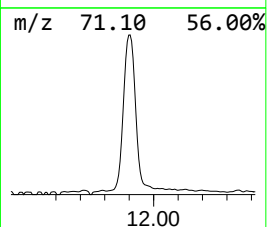
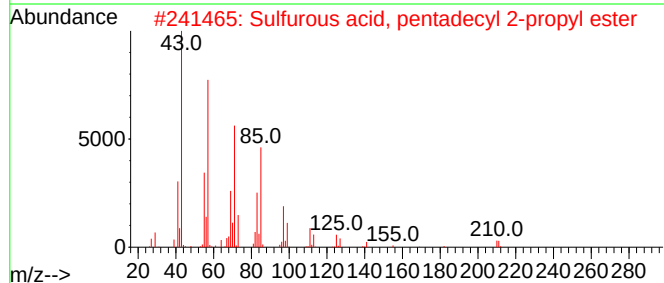
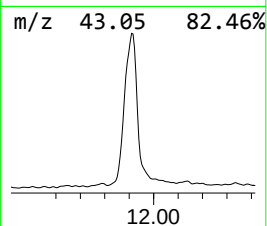
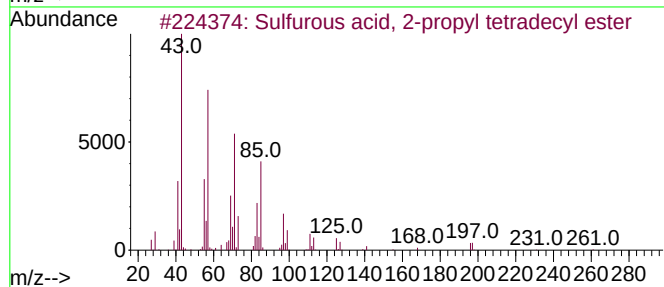
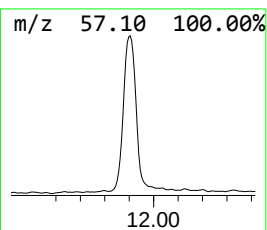
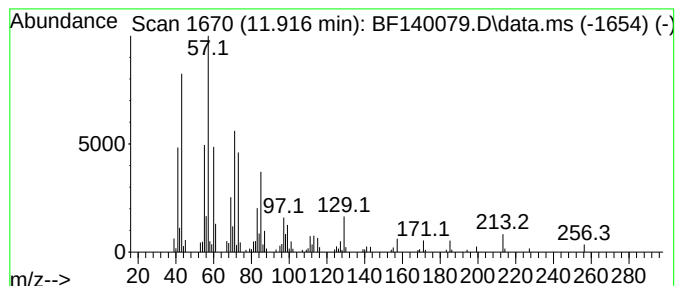
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Sulfurous acid, 2-propyl te... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.916 | 8.28 ng | 476747 | Phenanthrene-d10 | 11.410 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Sulfurous acid, 2-propyl tetradec... | 320 | C17H36O3S   | 1010309-12-5 | 53   |
| 2    |    |   | Sulfurous acid, pentadecyl 2-pro...  | 334 | C18H38O3S   | 1000309-12-6 | 53   |
| 3    |    |   | 1-Octadecanesulphonyl chloride       | 352 | C18H37ClO2S | 1000342-70-4 | 49   |
| 4    |    |   | Heptacosane, 1-chloro-               | 414 | C27H55Cl    | 062016-79-9  | 49   |
| 5    |    |   | Octadecane, 1-chloro-                | 288 | C18H37Cl    | 003386-33-2  | 49   |



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Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

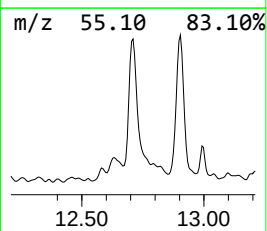
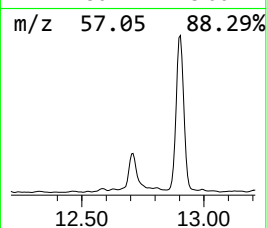
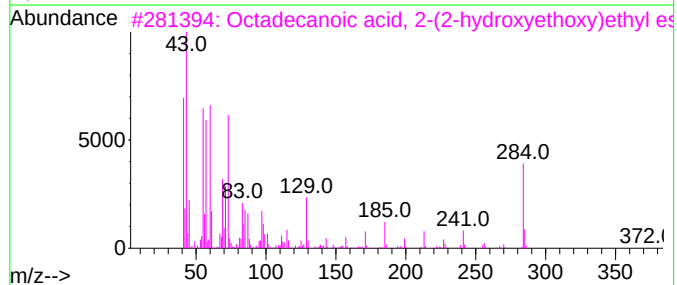
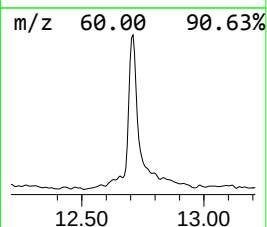
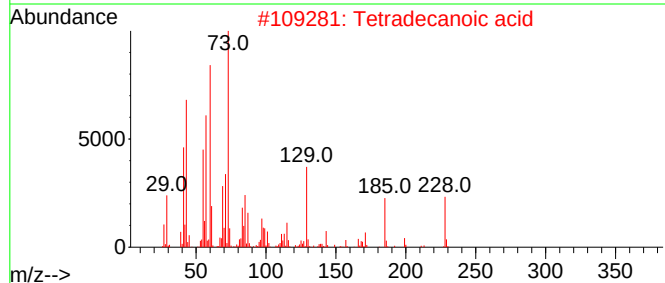
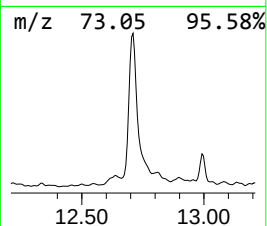
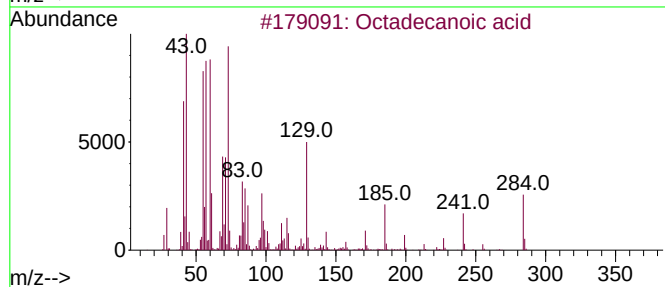
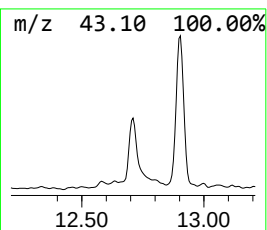
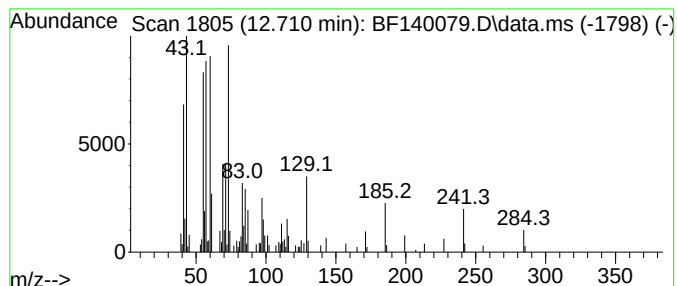
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Octadecanoic acid Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.710 | 3.03 ng | 174157 | Phenanthrene-d10 | 11.410 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 3    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 80   |
| 4    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 74   |
| 5    |    |   | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9 | 58   |



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Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

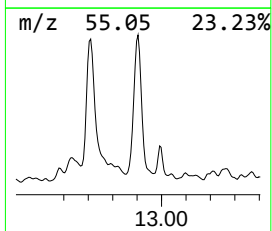
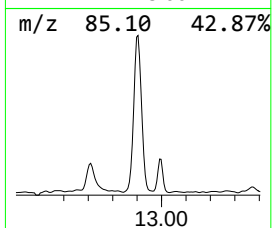
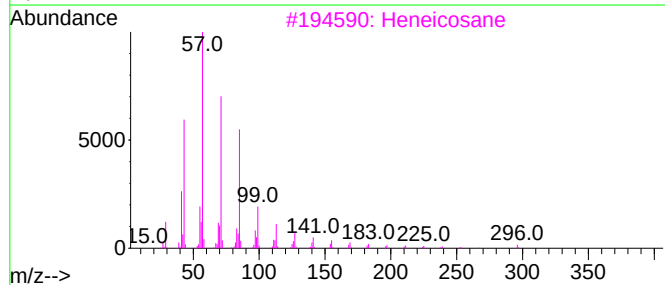
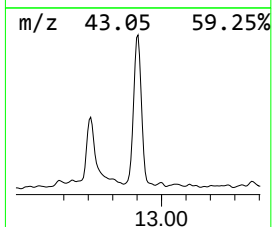
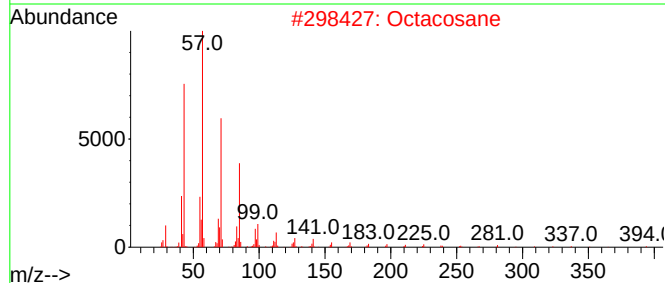
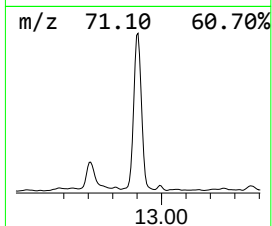
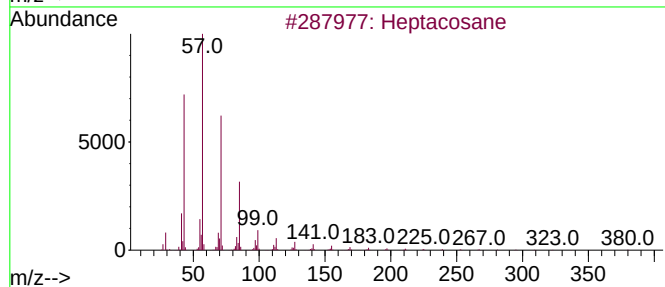
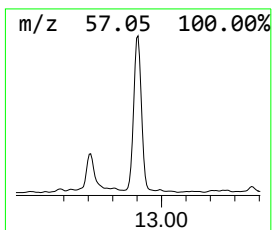
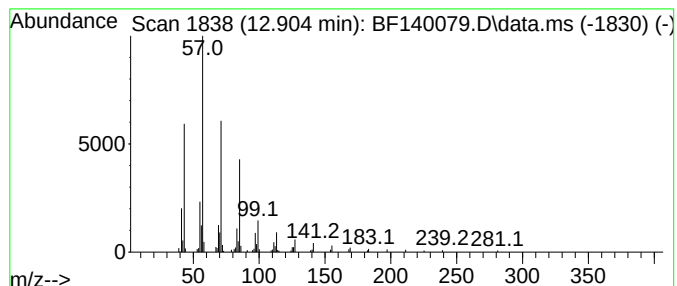
TIC Library : C:\Database\NIST20.L  
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Peak Number 5 Heptacosane Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.904 | 8.38 ng | 267755 | Chrysene-d12     | 14.045 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Heptacosane           | 380 | C27H56  | 000593-49-7 | 91   |
| 2    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 3    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 4    |    |   | Pentacosane           | 352 | C25H52  | 000629-99-2 | 91   |
| 5    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 90   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

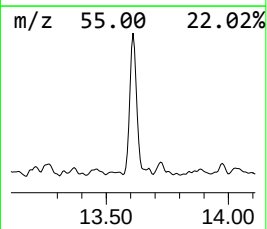
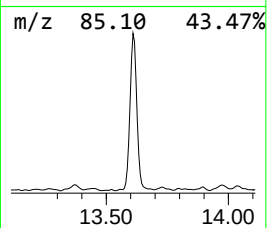
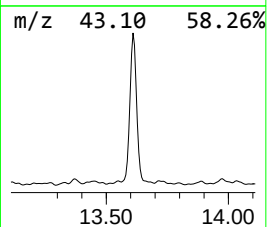
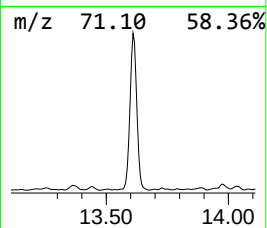
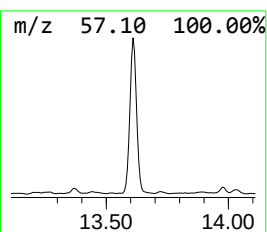
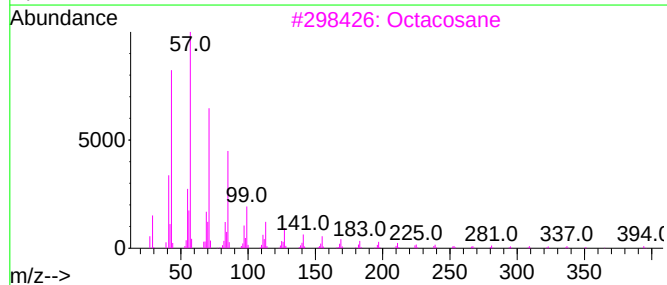
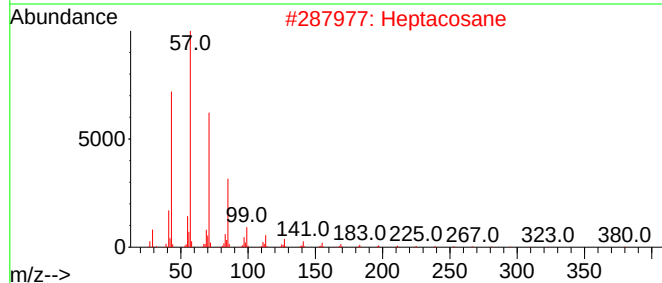
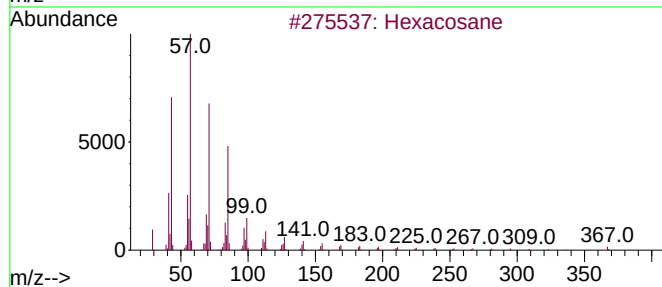
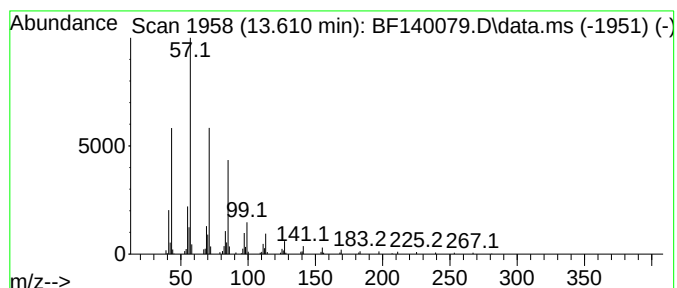
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Hexacosane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.610 | 7.07 ng | 225935 | Chrysene-d12     | 14.045 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 91   |
| 2    |    |   | Heptacosane           | 380 | C27H56  | 000593-49-7 | 91   |
| 3    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 90   |
| 5    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
Data File : BF140079.D  
Acq On : 28 Oct 2024 11:31  
Operator : RC/JU  
Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

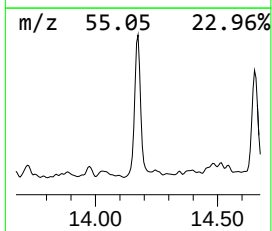
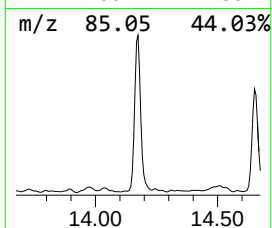
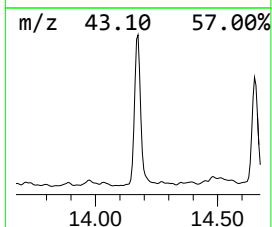
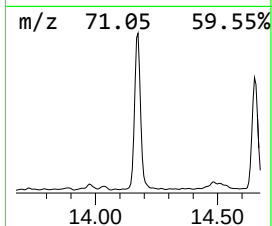
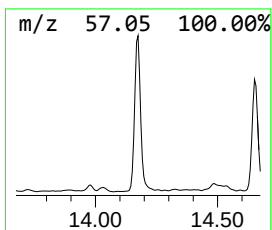
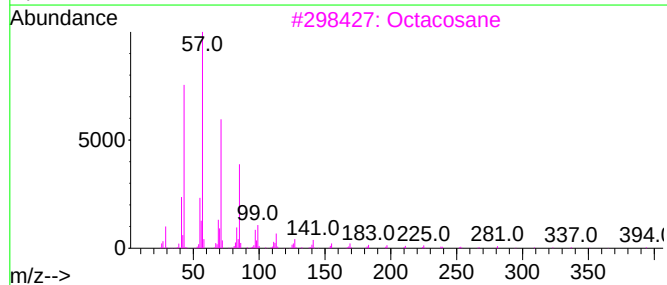
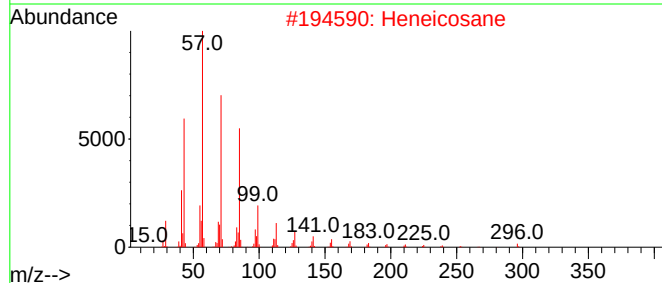
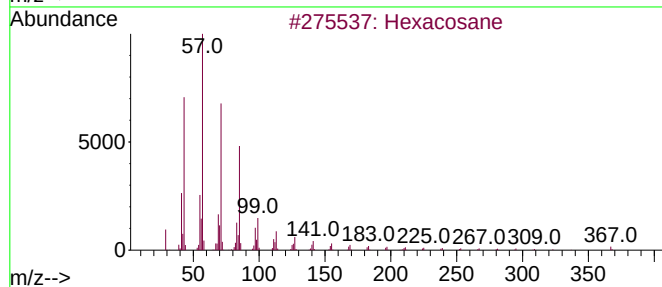
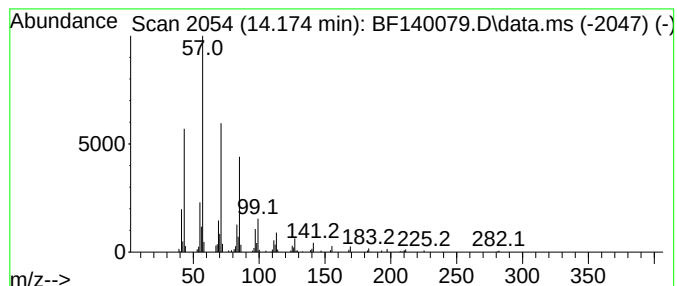
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Peak Number 7 Heneicosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.174 | 6.47 ng | 206612 | Chrysene-d12     | 14.045 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | Hexacosane                       | 366 | C26H54  | 000630-01-3 | 91   |
| 2    |    |   | Heneicosane                      | 296 | C21H44  | 000629-94-7 | 91   |
| 3    |    |   | Octacosane                       | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    |   | Hentriacontane                   | 437 | C31H64  | 000630-04-6 | 91   |
| 5    |    |   | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54  | 055282-11-6 | 91   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
Data File : BF140079.D  
Acq On : 28 Oct 2024 11:31  
Operator : RC/JU  
Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

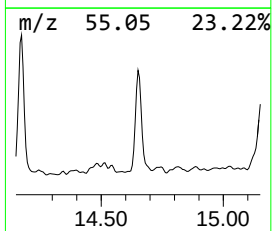
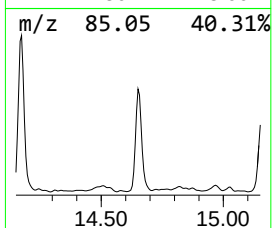
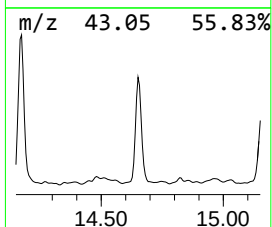
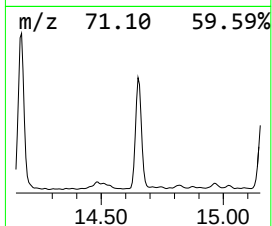
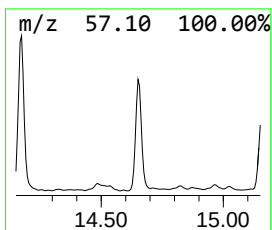
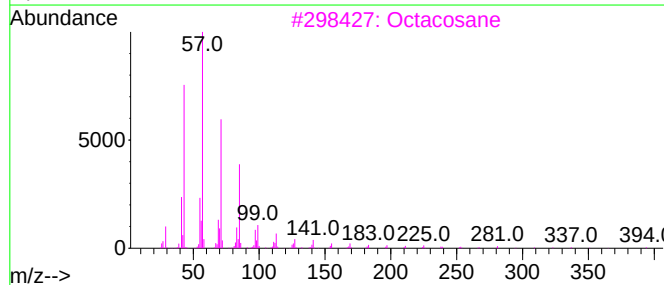
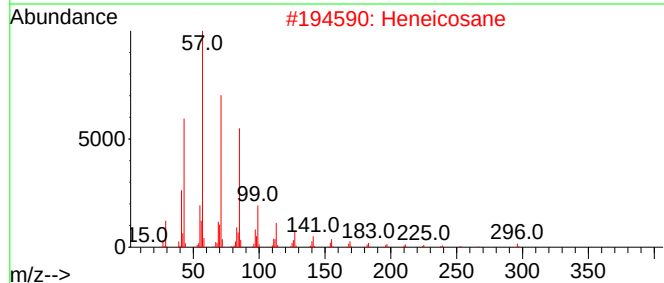
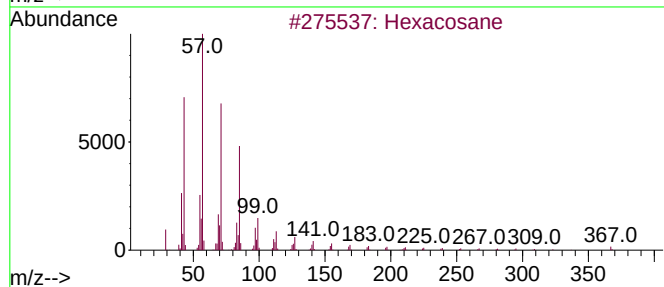
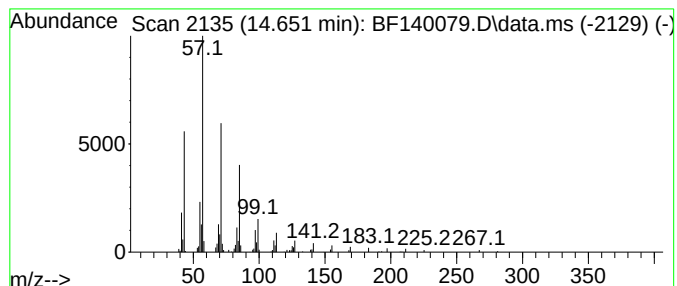
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Peak Number 8 Octacosane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.651 | 4.62 ng | 147643 | Chrysene-d12     | 14.045 |

| Hit# | of 5 | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------|-----|---------|-------------|------|
| 1    |      | Hexacosane        | 366 | C26H54  | 000630-01-3 | 91   |
| 2    |      | Heneicosane       | 296 | C21H44  | 000629-94-7 | 91   |
| 3    |      | Octacosane        | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |      | Hentriacontane    | 437 | C31H64  | 000630-04-6 | 91   |
| 5    |      | Tetratetracontane | 619 | C44H90  | 007098-22-8 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
Data File : BF140079.D  
Acq On : 28 Oct 2024 11:31  
Operator : RC/JU  
Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

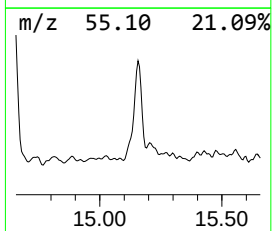
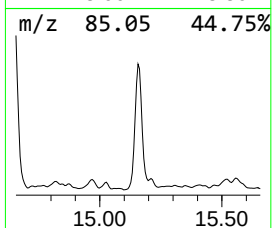
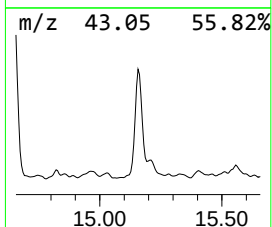
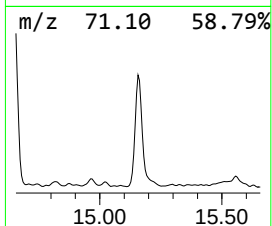
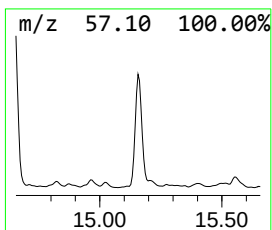
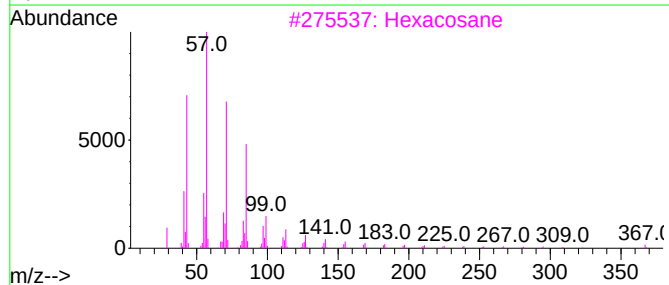
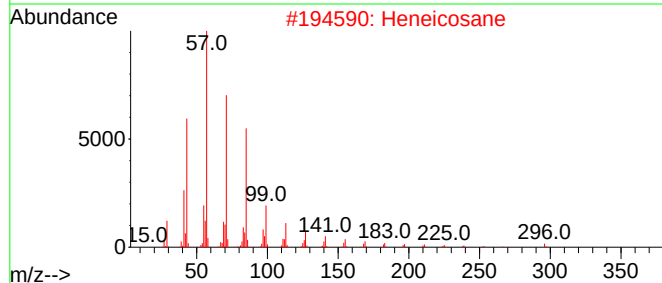
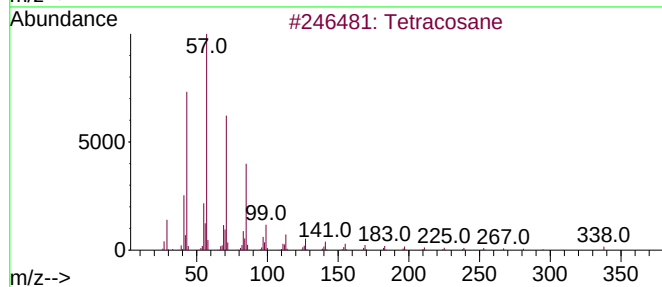
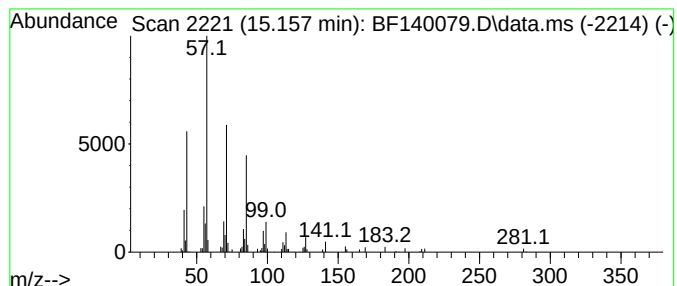
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 Tetracosane Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.157 | 3.17 ng | 119213 | Perylene-d12     | 15.527 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Tetracosane           | 338 | C24H50  | 000646-31-1 | 91   |
| 2    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 3    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 91   |
| 4    |    |   | Hentriacontane        | 437 | C31H64  | 000630-04-6 | 91   |
| 5    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
Data File : BF140079.D  
Acq On : 28 Oct 2024 11:31  
Operator : RC/JU  
Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

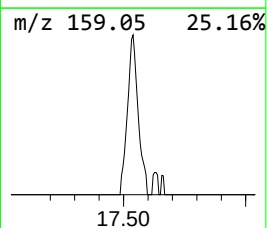
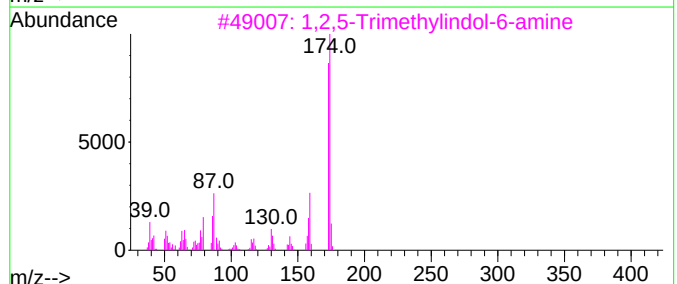
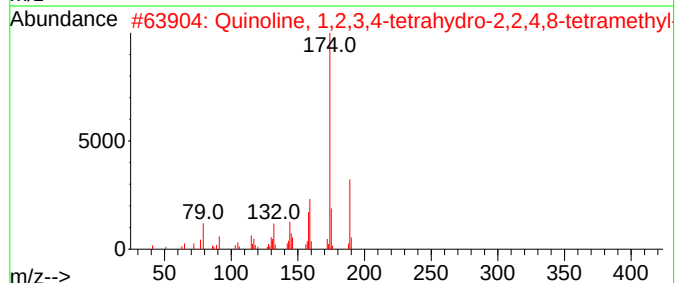
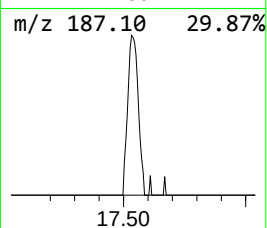
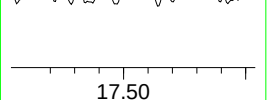
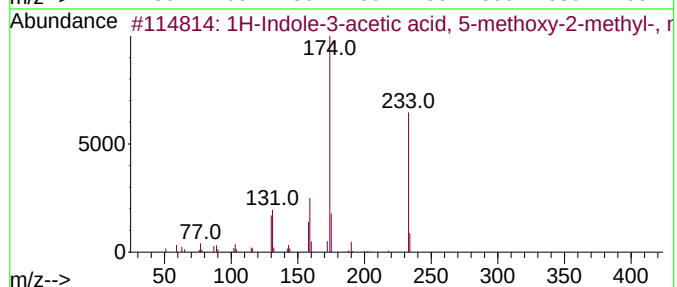
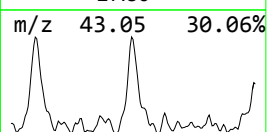
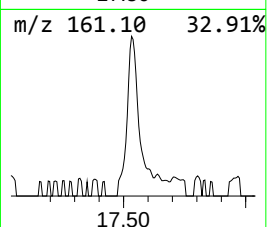
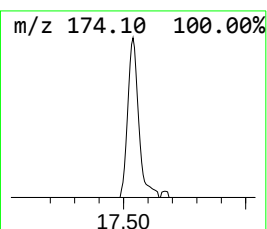
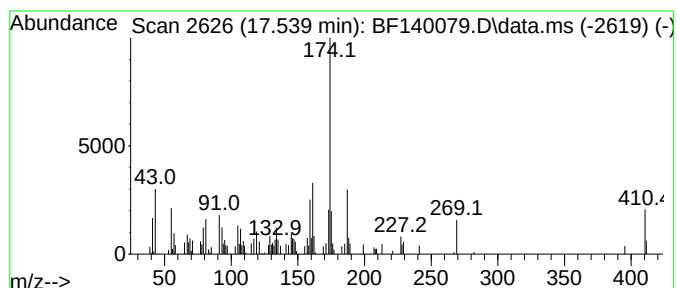
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 10 unknown17.539 Concentration Rank 10

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 17.539 | 2.55 ng | 95983 | Perylene-d12     | 15.527 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|------|-------------------------------------|-----|-------------|--------------|------|
| 1    |      | 1H-Indole-3-acetic acid, 5-metho... | 233 | C13H15NO3   | 007588-36-5  | 43   |
| 2    |      | Quinoline, 1,2,3,4-tetrahydro-2,... | 189 | C13H19N     | 1000308-78-8 | 43   |
| 3    |      | 1,2,5-Trimethylindol-6-amine        | 174 | C11H14N2    | 1000389-10-0 | 38   |
| 4    |      | [+]-2,4-Dihydroxy-3,3-dimethyl-N... | 411 | C18H25N3O6S | 028124-68-7  | 38   |
| 5    |      | N-(Isopropyl)-1-phenylcyclohexyl... | 217 | C15H23N     | 002201-48-1  | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102824\  
Data File : BF140079.D  
Acq On : 28 Oct 2024 11:31  
Operator : RC/JU  
Sample : PB164444BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB164444BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.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 |
| Butane, 2-metho... | 2.246  | 2.9     | ng    | 108884   | 1                     | 6.886  | 757614  | 20.0 |
| Sulfurous acid,... | 11.916 | 8.3     | ng    | 476747   | 4                     | 11.410 | 1151100 | 20.0 |
| Octadecanoic acid  | 12.710 | 3.0     | ng    | 174157   | 4                     | 11.410 | 1151100 | 20.0 |
| Heptacosane        | 12.904 | 8.4     | ng    | 267755   | 5                     | 14.045 | 638690  | 20.0 |
| Hexacosane         | 13.610 | 7.1     | ng    | 225935   | 5                     | 14.045 | 638690  | 20.0 |
| Heneicosane        | 14.174 | 6.5     | ng    | 206612   | 5                     | 14.045 | 638690  | 20.0 |
| Octacosane         | 14.651 | 4.6     | ng    | 147643   | 5                     | 14.045 | 638690  | 20.0 |
| Tetracosane        | 15.157 | 3.2     | ng    | 119213   | 6                     | 15.527 | 752741  | 20.0 |
| unknown17.539      | 17.539 | 2.5     | ng    | 95983    | 6                     | 15.527 | 752741  | 20.0 |