

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
 Data File : BF136288.D  
 Acq On : 29 Nov 2023 17:39  
 Operator : CG\JU  
 Sample : 05282-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 YORK-20231106

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136288.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         | 4.551       | 415           | 419         | 423          | rVB      | 83706          | 92781         | 2.04%           | 0.483%        |
| 2         | 5.434       | 565           | 569         | 579          | rBV      | 1212093        | 1019955       | 22.43%          | 5.315%        |
| 3         | 6.428       | 734           | 738         | 747          | rBV      | 737507         | 598728        | 13.17%          | 3.120%        |
| 4         | 6.804       | 798           | 802         | 805          | rBV      | 960749         | 746941        | 16.43%          | 3.892%        |
| 5         | 7.363       | 892           | 897         | 900          | rBV      | 2270518        | 2346527       | 51.60%          | 12.228%       |
| 6         | 8.081       | 1014          | 1019        | 1022         | rBV      | 1246076        | 1012633       | 22.27%          | 5.277%        |
| 7         | 9.163       | 1197          | 1203        | 1206         | rBV      | 4996308        | 4547508       | 100.00%         | 23.698%       |
| 8         | 9.833       | 1311          | 1317        | 1321         | rBV      | 1186713        | 1099977       | 24.19%          | 5.732%        |
| 9         | 10.057      | 1348          | 1355        | 1359         | rBV6     | 39057          | 77906         | 1.71%           | 0.406%        |
| 10        | 10.627      | 1448          | 1452        | 1455         | rBV      | 1724123        | 1409194       | 30.99%          | 7.344%        |
| 11        | 11.327      | 1567          | 1571        | 1574         | rBV      | 1142931        | 899175        | 19.77%          | 4.686%        |
| 12        | 11.492      | 1595          | 1599        | 1606         | rVB      | 122262         | 145880        | 3.21%           | 0.760%        |
| 13        | 11.863      | 1656          | 1662        | 1667         | rBV      | 246683         | 274726        | 6.04%           | 1.432%        |
| 14        | 12.004      | 1680          | 1686        | 1691         | rVB3     | 39065          | 58060         | 1.28%           | 0.303%        |
| 15        | 12.198      | 1712          | 1719        | 1731         | rVB6     | 25954          | 97283         | 2.14%           | 0.507%        |
| 16        | 12.574      | 1778          | 1783        | 1789         | rBV      | 85802          | 113671        | 2.50%           | 0.592%        |
| 17        | 12.657      | 1791          | 1797        | 1811         | rVV      | 163105         | 218221        | 4.80%           | 1.137%        |
| 18        | 12.927      | 1838          | 1843        | 1846         | rBV      | 3316696        | 2780860       | 61.15%          | 14.491%       |
| 19        | 13.210      | 1880          | 1891        | 1901         | rBV2     | 39990          | 102068        | 2.24%           | 0.532%        |
| 20        | 13.904      | 2003          | 2009        | 2015         | rBV2     | 55134          | 115799        | 2.55%           | 0.603%        |
| 21        | 13.980      | 2018          | 2022        | 2032         | rVB      | 687405         | 612498        | 13.47%          | 3.192%        |
| 22        | 14.468      | 2100          | 2105        | 2111         | rBV      | 76574          | 108235        | 2.38%           | 0.564%        |
| 23        | 14.998      | 2190          | 2195        | 2202         | rBV2     | 34571          | 65393         | 1.44%           | 0.341%        |
| 24        | 15.462      | 2268          | 2274        | 2279         | rBV      | 534040         | 645592        | 14.20%          | 3.364%        |

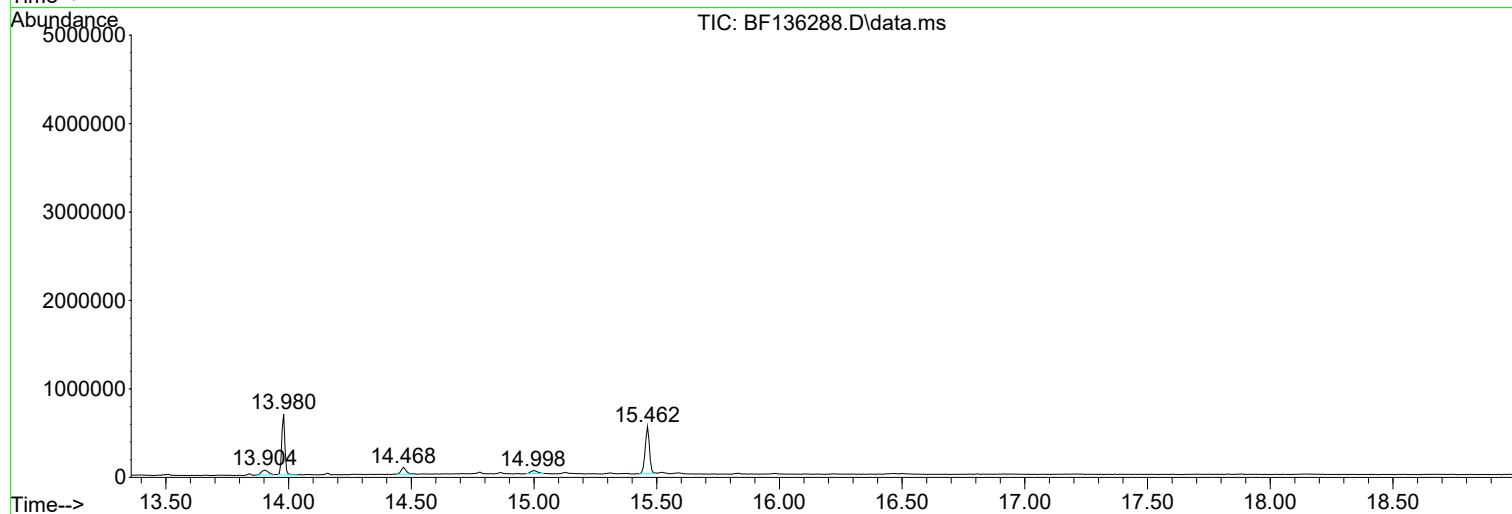
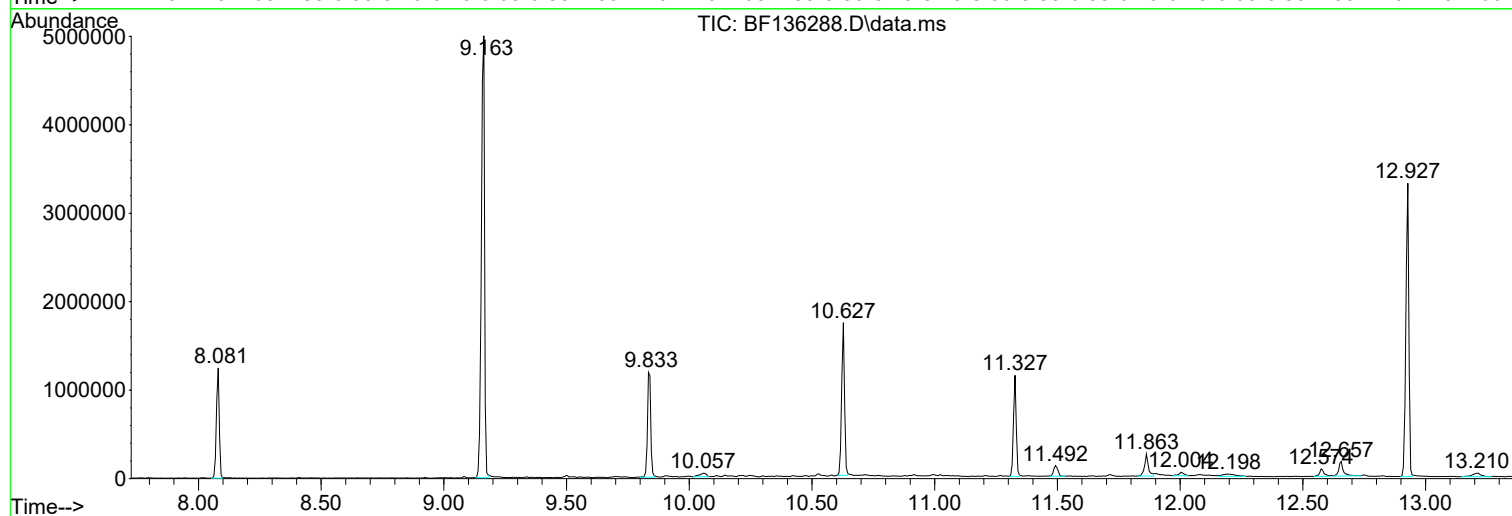
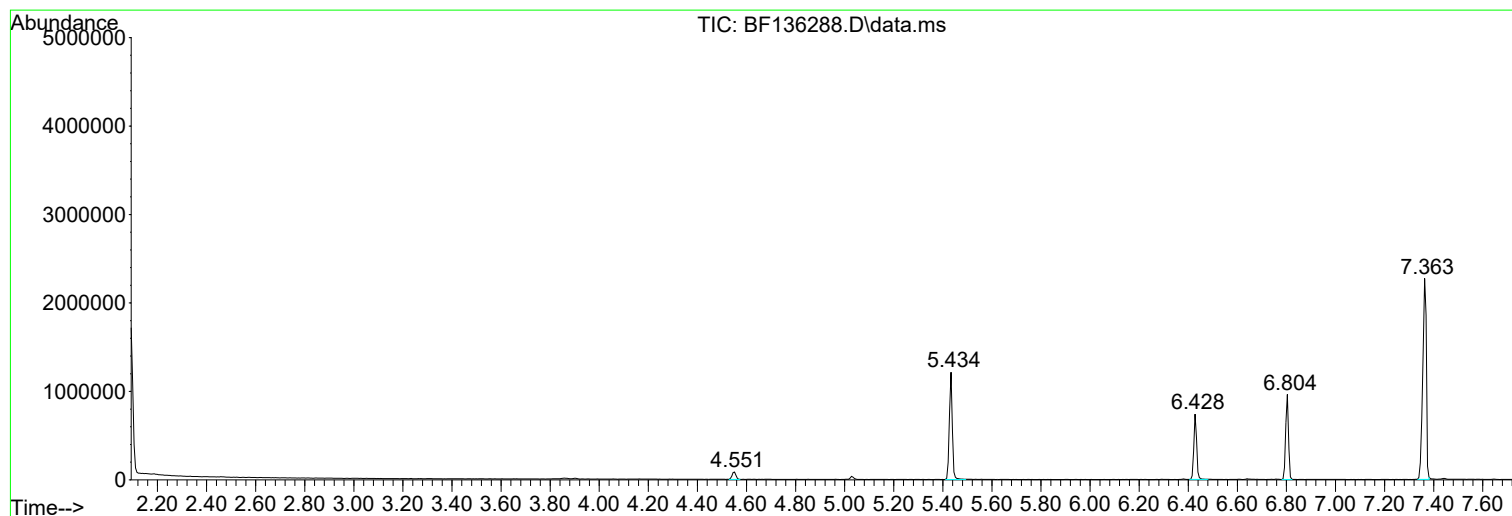
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

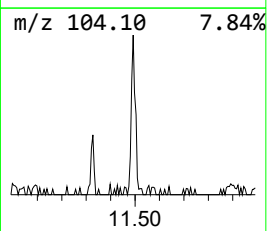
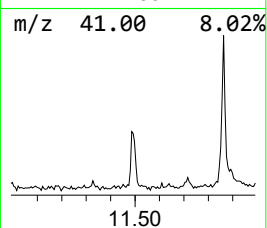
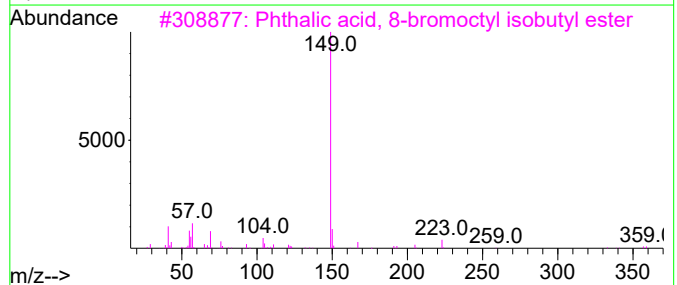
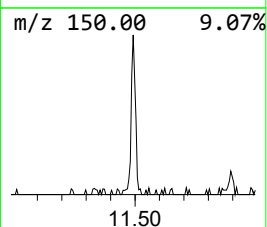
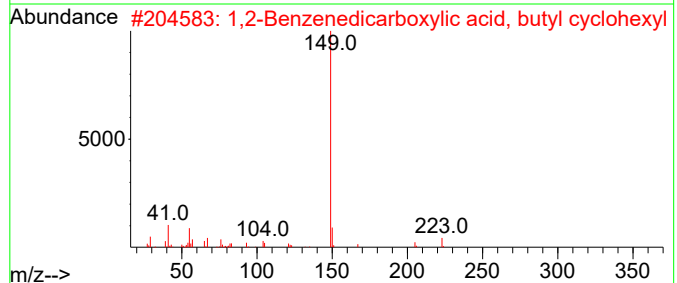
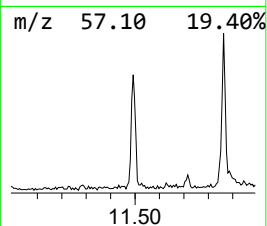
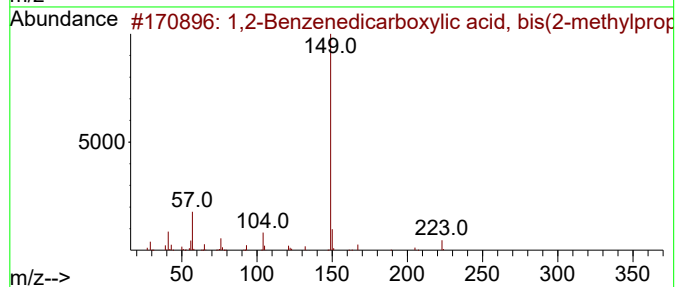
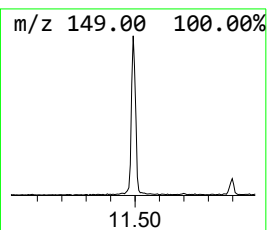
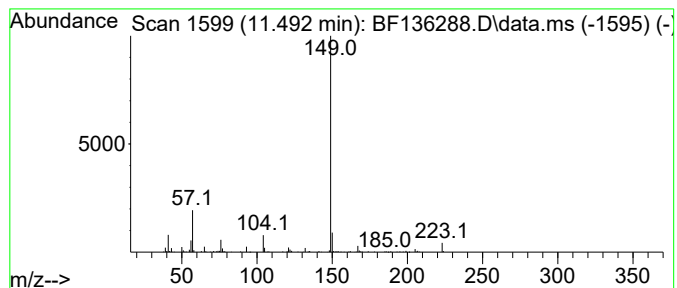
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.492 | 3.24 ng | 145880 | Phenanthrene-d10 | 11.327 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 1,2-Benzenedicarboxylic acid, bi...  | 278 | C16H22O4   | 000084-69-5  | 87   |
| 2    |    |   | 1,2-Benzenedicarboxylic acid, bu...  | 304 | C18H24O4   | 000084-64-0  | 78   |
| 3    |    |   | Phthalic acid, 8-bromooctyl isobu... | 412 | C20H29BrO4 | 1000382-55-3 | 78   |
| 4    |    |   | Phthalic acid, isobutyl 6-methyl...  | 334 | C20H30O4   | 1000377-95-7 | 78   |
| 5    |    |   | Phthalic acid, isobutyl non-5-yn...  | 344 | C21H28O4   | 1000315-18-8 | 78   |



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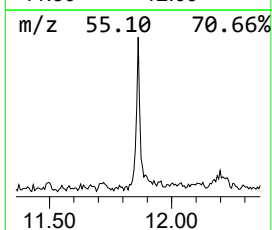
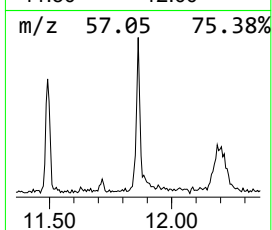
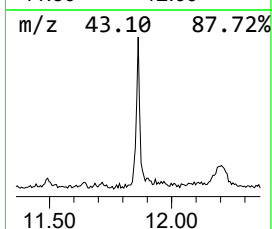
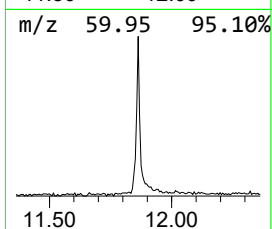
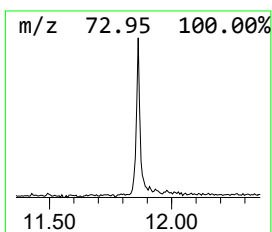
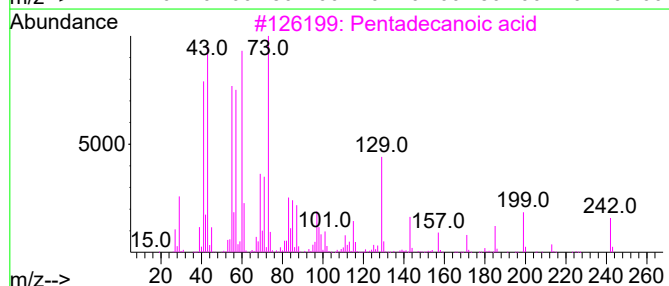
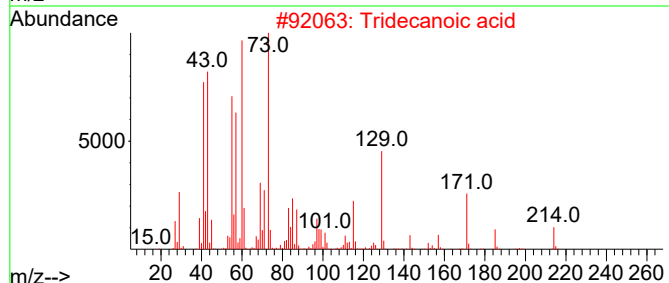
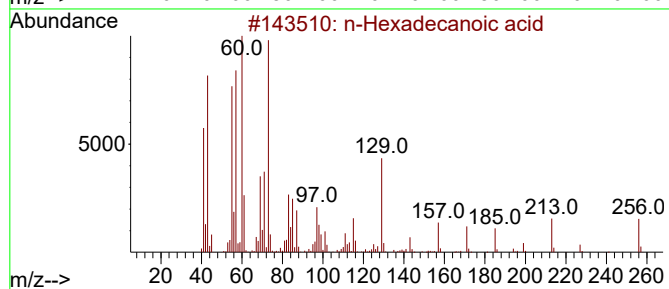
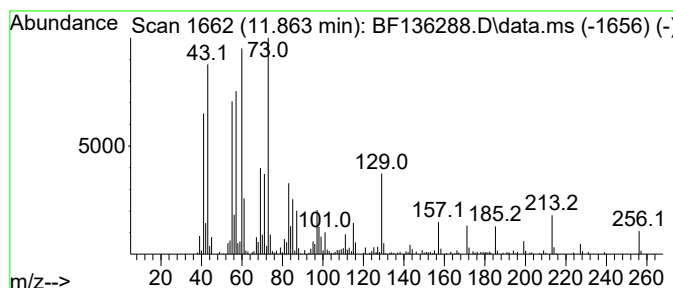
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 11.863    | 6.11 ng             | 274726 | Phenanthrene-d10 | 11.327      |      |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 99   |
| 2         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 91   |
| 3         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 90   |
| 4         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 72   |
| 5         | Undecanoic acid     | 186    | C11H22O2         | 000112-37-8 | 68   |



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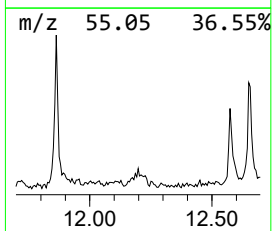
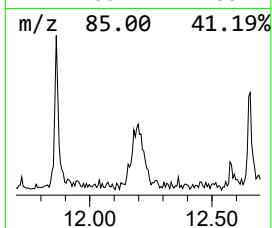
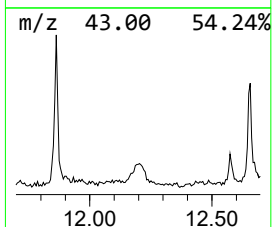
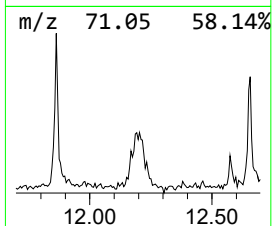
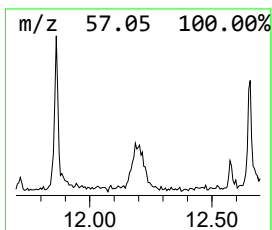
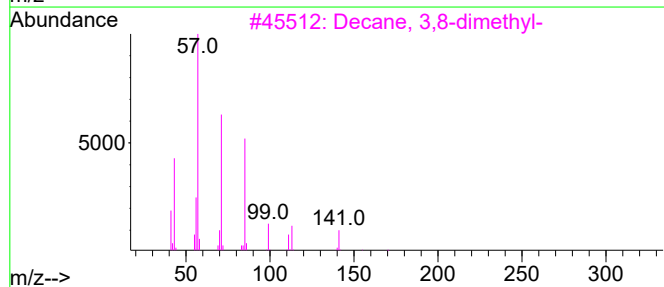
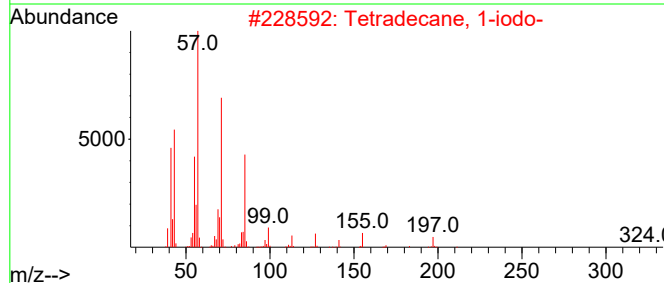
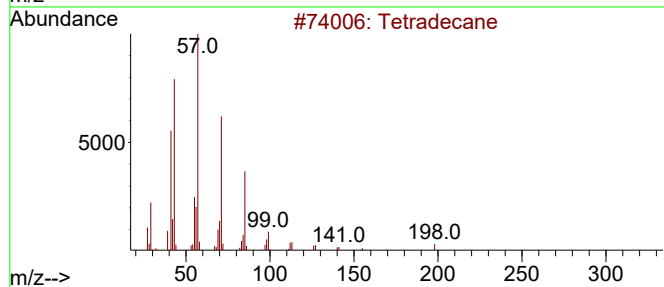
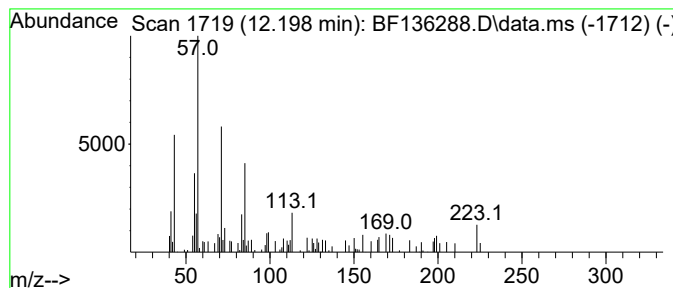
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tetradecane Concentration Rank 9

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.198 | 2.16 ng | 97283 | Phenanthrene-d10 | 11.327 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Tetradecane                         | 198 | C14H30    | 000629-59-4  | 64   |
| 2    |    |   | Tetradecane, 1-iodo-                | 324 | C14H29I   | 019218-94-1  | 59   |
| 3    |    |   | Decane, 3,8-dimethyl-               | 170 | C12H26    | 017312-55-9  | 59   |
| 4    |    |   | Octane, 2-methyl-                   | 128 | C9H20     | 003221-61-2  | 58   |
| 5    |    |   | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 53   |



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ClientSampleId :  
YORK-20231106

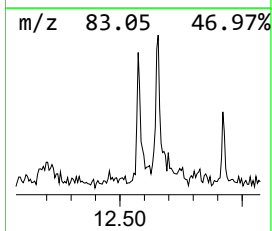
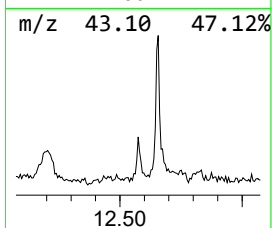
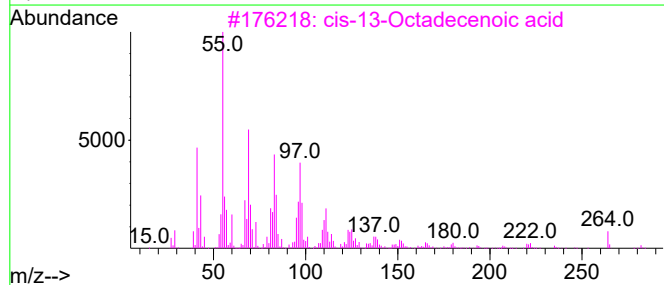
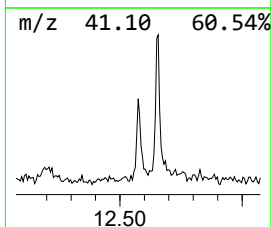
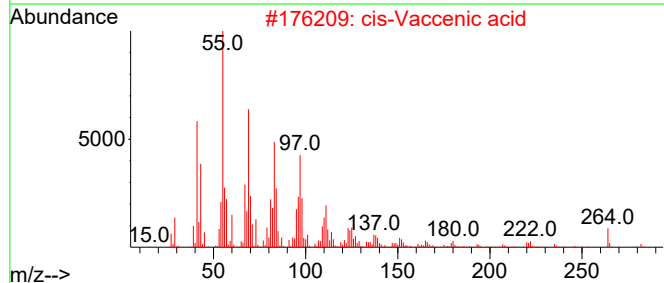
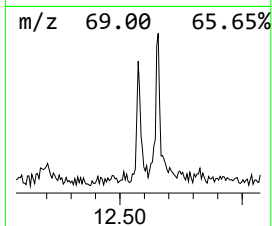
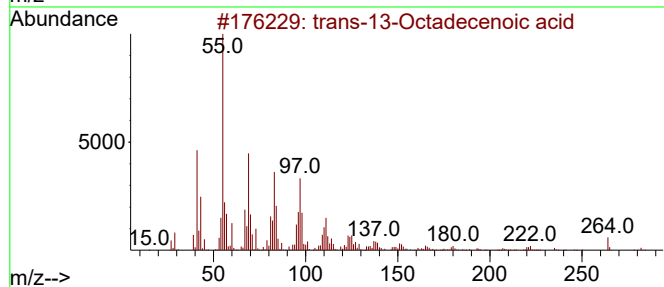
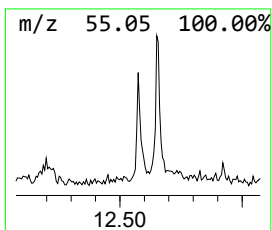
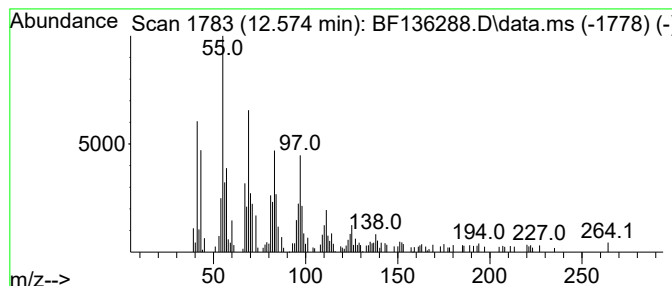
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Peak Number 5 trans-13-Octadecenoic acid Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.574 | 2.53 ng | 113671 | Phenanthrene-d10 | 11.327 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------------|-----|----------|-------------|------|
| 1    |    |   | trans-13-Octadecenoic acid | 282 | C18H34O2 | 000693-71-0 | 90   |
| 2    |    |   | cis-Vaccenic acid          | 282 | C18H34O2 | 000506-17-2 | 90   |
| 3    |    |   | cis-13-Octadecenoic acid   | 282 | C18H34O2 | 013126-39-1 | 90   |
| 4    |    |   | 9-Octadecenoic acid, (E)-  | 282 | C18H34O2 | 000112-79-8 | 90   |
| 5    |    |   | Oleic Acid                 | 282 | C18H34O2 | 000112-80-1 | 87   |



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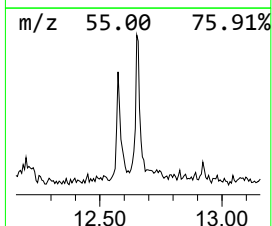
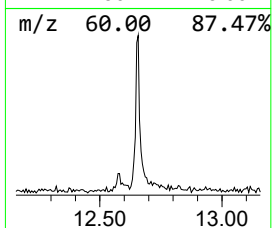
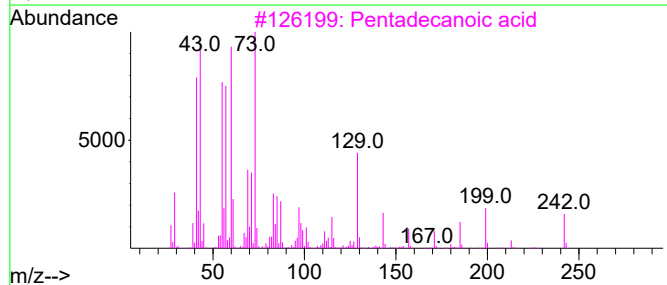
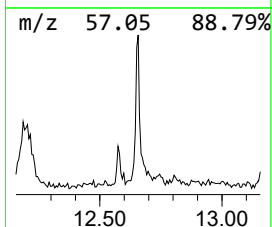
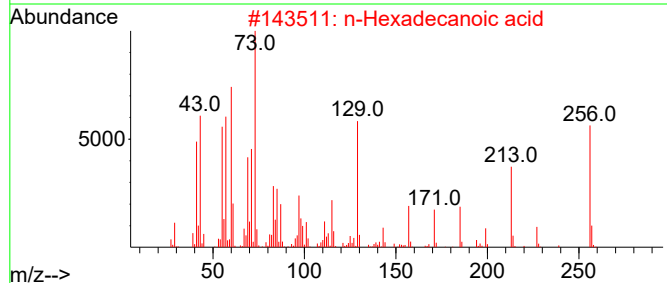
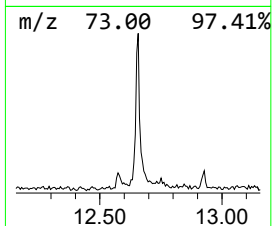
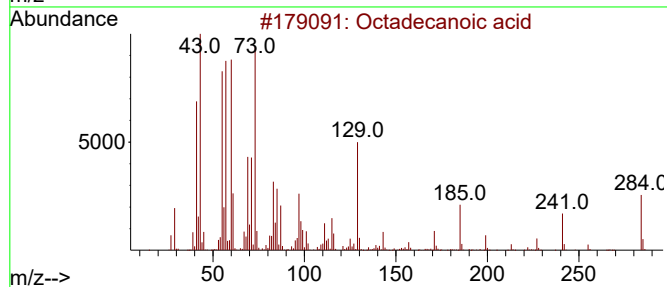
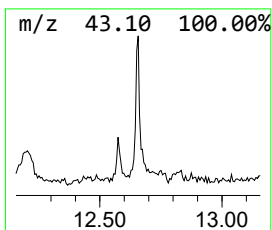
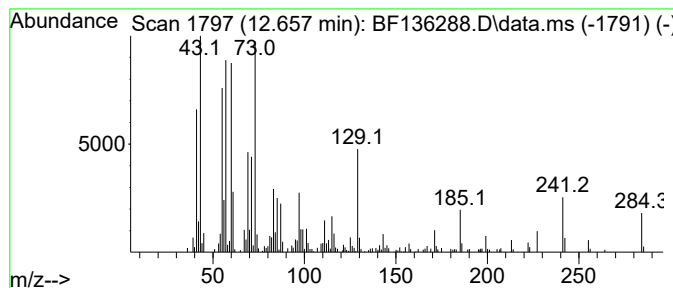
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Octadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.657 | 7.13 ng | 218221 | Chrysene-d12     | 13.980 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 89   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 78   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 70   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
Data File : BF136288.D  
Acq On : 29 Nov 2023 17:39  
Operator : CG\JU  
Sample : 05282-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

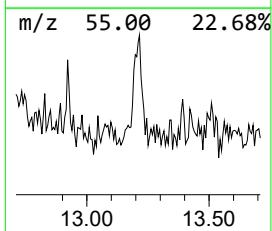
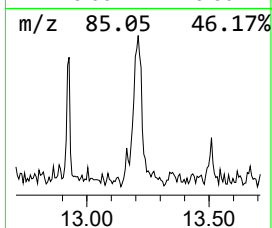
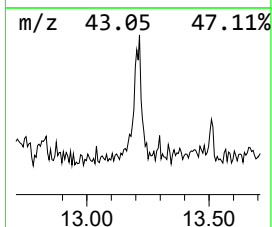
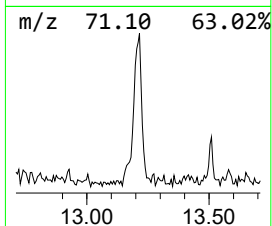
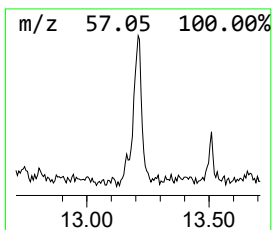
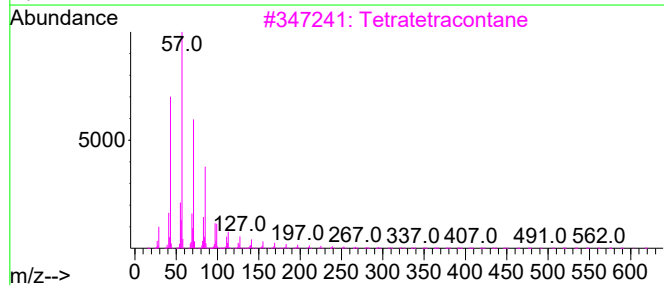
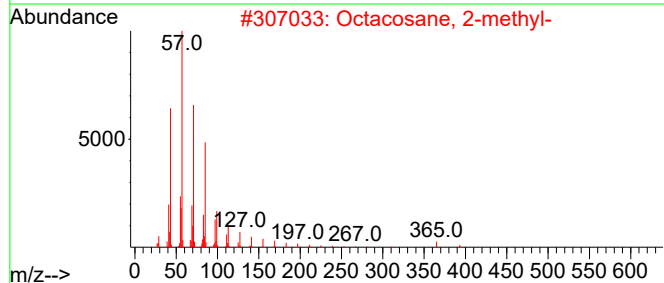
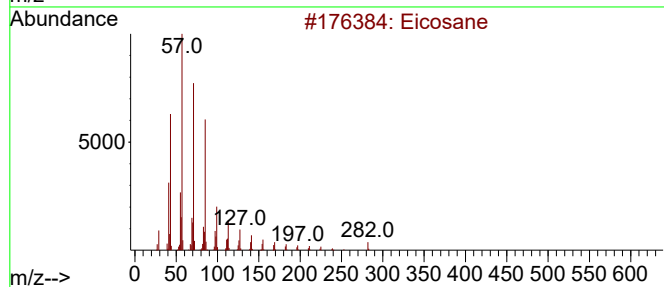
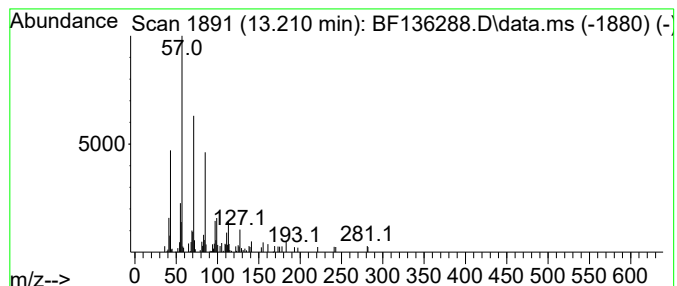
Instrument :  
BNA\_F  
ClientSampleId :  
YORK-20231106

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 7 Eicosane Concentration Rank 5

| R.T.      | EstConc               | Area   | Relative to ISTD |         | R.T.        |      |
|-----------|-----------------------|--------|------------------|---------|-------------|------|
| 13.210    | 3.33 ng               | 102068 | Chrysene-d12     |         | 13.980      |      |
| Hit# of 5 | Tentative ID          |        | MW               | MolForm | CAS#        | Qual |
| 1         | Eicosane              |        | 282              | C20H42  | 000112-95-8 | 96   |
| 2         | Octacosane, 2-methyl- |        | 408              | C29H60  | 001560-98-1 | 91   |
| 3         | Tetratetracontane     |        | 619              | C44H90  | 007098-22-8 | 91   |
| 4         | 2-Methyltetracosane   |        | 352              | C25H52  | 001560-78-7 | 90   |
| 5         | Hentriacontane        |        | 437              | C31H64  | 000630-04-6 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
Data File : BF136288.D  
Acq On : 29 Nov 2023 17:39  
Operator : CG\JU  
Sample : 05282-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
YORK-20231106

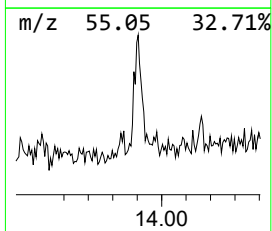
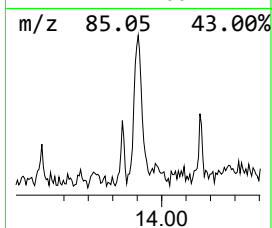
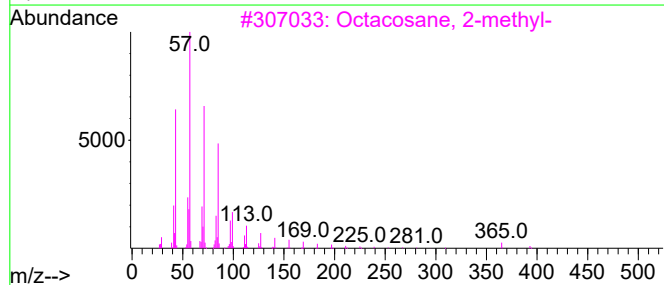
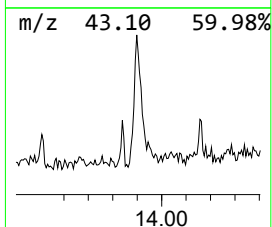
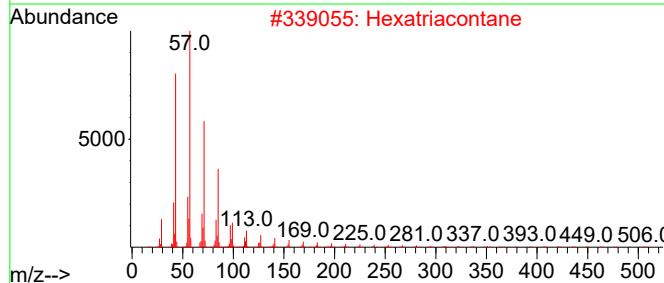
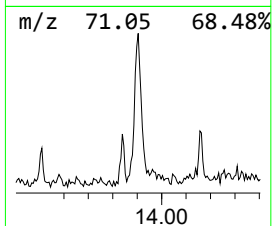
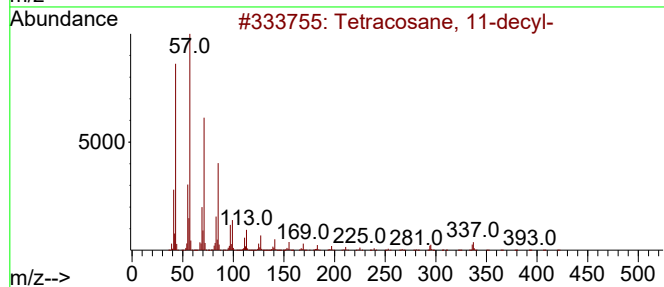
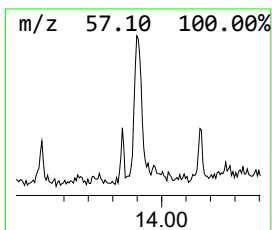
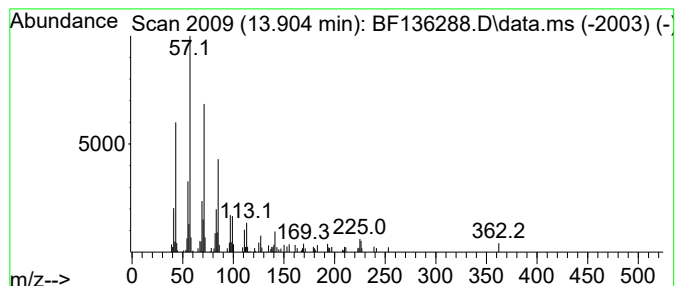
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Tetracosane, 11-decyl- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.904 | 3.78 ng | 115799 | Chrysene-d12     | 13.980 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------|-----|---------|-------------|------|
| 1    |    |   | Tetracosane, 11-decyl- | 479 | C34H70  | 055429-84-0 | 91   |
| 2    |    |   | Hexatriacontane        | 507 | C36H74  | 000630-06-8 | 91   |
| 3    |    |   | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1 | 90   |
| 4    |    |   | Tetratetracontane      | 619 | C44H90  | 007098-22-8 | 90   |
| 5    |    |   | Docosane, 11-decyl-    | 451 | C32H66  | 055401-55-3 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
Data File : BF136288.D  
Acq On : 29 Nov 2023 17:39  
Operator : CG\JU  
Sample : 05282-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
YORK-20231106

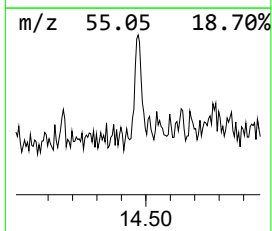
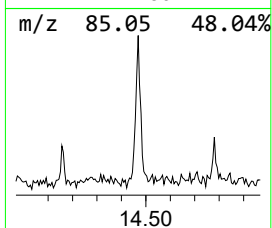
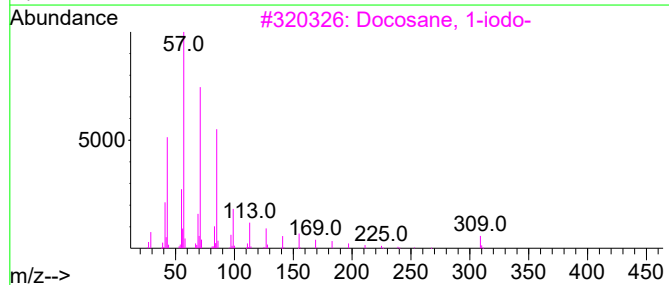
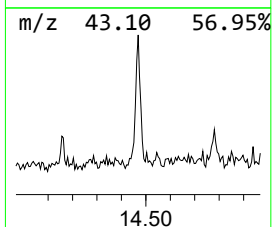
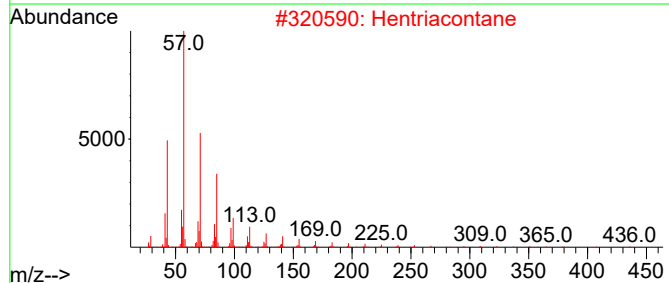
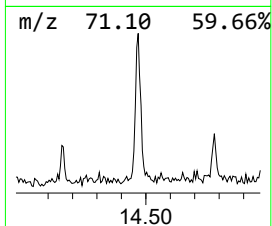
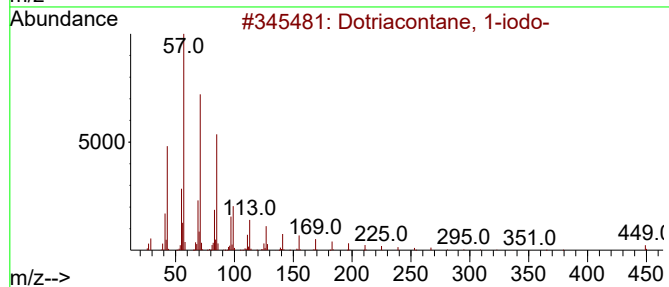
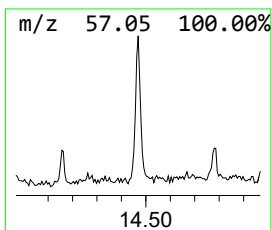
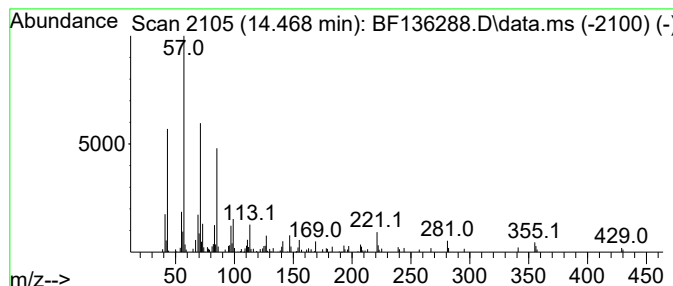
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 9 Dotriacontane, 1-iodo- Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.468 | 3.53 ng | 108235 | Chrysene-d12     | 13.980 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#         | Qual |
|------|----|---|------------------------|-----|---------|--------------|------|
| 1    |    |   | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 81   |
| 2    |    |   | Hentriacontane         | 437 | C31H64  | 000630-04-6  | 81   |
| 3    |    |   | Docosane, 1-iodo-      | 436 | C22H45I | 1000406-31-9 | 76   |
| 4    |    |   | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1  | 74   |
| 5    |    |   | Octacosane, 1-iodo-    | 520 | C28H57I | 1000406-32-2 | 74   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
Data File : BF136288.D  
Acq On : 29 Nov 2023 17:39  
Operator : CG\JU  
Sample : 05282-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
YORK-20231106

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

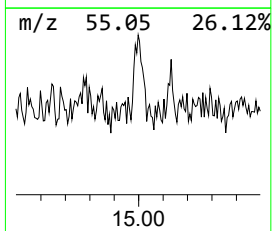
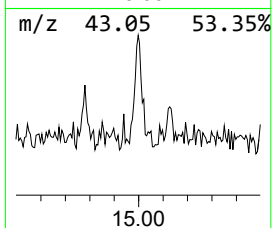
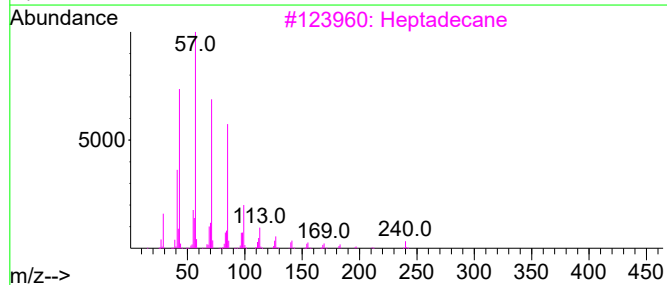
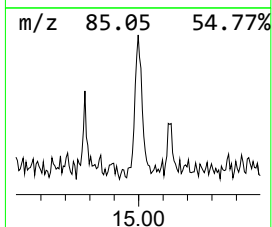
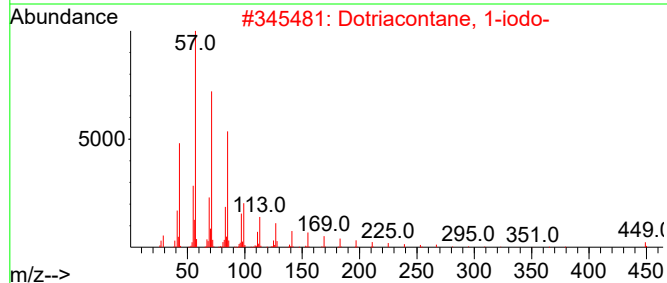
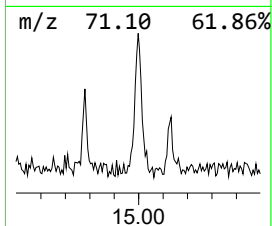
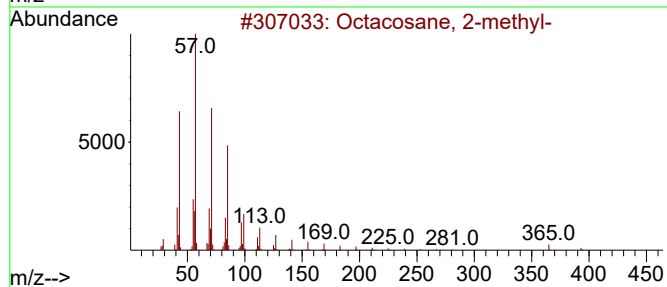
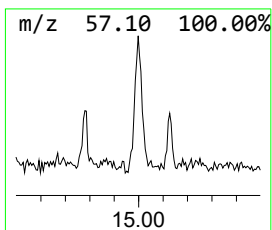
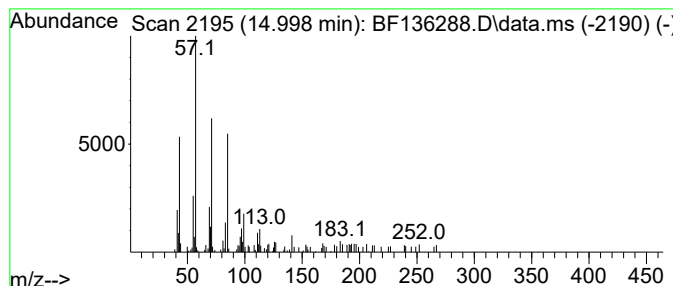
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 10 Octacosane, 2-methyl- Concentration Rank 10

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.998 | 2.03 ng | 65393 | Perylene-d12     | 15.462 |

| Hit# | of 5 | Tentative ID           | MW  | MolForm | CAS#         | Qual |
|------|------|------------------------|-----|---------|--------------|------|
| 1    |      | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1  | 86   |
| 2    |      | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 86   |
| 3    |      | Heptadecane            | 240 | C17H36  | 000629-78-7  | 80   |
| 4    |      | Nonadecane, 2-methyl-  | 282 | C20H42  | 001560-86-7  | 80   |
| 5    |      | 10-Methylnonadecane    | 282 | C20H42  | 056862-62-5  | 78   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112923\  
Data File : BF136288.D  
Acq On : 29 Nov 2023 17:39  
Operator : CG\JU  
Sample : 05282-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
YORK-20231106

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.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 |
| 1,2-Benzenedica... | 11.492 | 3.2     | ng    | 145880   | 4                     | 11.327 | 899175 | 20.0 |
| n-Hexadecanoic ... | 11.863 | 6.1     | ng    | 274726   | 4                     | 11.327 | 899175 | 20.0 |
| Tetradecane        | 12.198 | 2.2     | ng    | 97283    | 4                     | 11.327 | 899175 | 20.0 |
| trans-13-Octade... | 12.574 | 2.5     | ng    | 113671   | 4                     | 11.327 | 899175 | 20.0 |
| Octadecanoic acid  | 12.657 | 7.1     | ng    | 218221   | 5                     | 13.980 | 612498 | 20.0 |
| Eicosane           | 13.210 | 3.3     | ng    | 102068   | 5                     | 13.980 | 612498 | 20.0 |
| Tetracosane, 11... | 13.904 | 3.8     | ng    | 115799   | 5                     | 13.980 | 612498 | 20.0 |
| Dotriacontane, ... | 14.468 | 3.5     | ng    | 108235   | 5                     | 13.980 | 612498 | 20.0 |
| Octacosane, 2-m... | 14.998 | 2.0     | ng    | 65393    | 6                     | 15.462 | 645592 | 20.0 |