

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022525\  
 Data File : BF141770.D  
 Acq On : 25 Feb 2025 18:04  
 Operator : RC/JU  
 Sample : Q1420-01  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-1-WC

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141770.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         | 3.799       | 284           | 290         | 301          | rVB      | 7657           | 15541         | 1.09%           | 0.127%        |
| 2         | 5.404       | 558           | 563         | 585          | rVB      | 873376         | 1313167       | 92.05%          | 10.746%       |
| 3         | 5.934       | 648           | 653         | 663          | rVB      | 46297          | 64778         | 4.54%           | 0.530%        |
| 4         | 6.422       | 731           | 736         | 764          | rBV      | 869025         | 1324514       | 92.85%          | 10.839%       |
| 5         | 6.781       | 792           | 797         | 806          | rBV      | 314651         | 416042        | 29.16%          | 3.405%        |
| 6         | 7.345       | 887           | 893         | 904          | rBV      | 564669         | 818034        | 57.34%          | 6.694%        |
| 7         | 7.622       | 935           | 940         | 952          | rBV5     | 9283           | 28327         | 1.99%           | 0.232%        |
| 8         | 7.751       | 958           | 962         | 968          | rVB      | 10778          | 14637         | 1.03%           | 0.120%        |
| 9         | 8.063       | 1008          | 1015        | 1029         | rBV      | 324411         | 514662        | 36.08%          | 4.212%        |
| 10        | 8.781       | 1134          | 1137        | 1144         | rBV      | 10574          | 15241         | 1.07%           | 0.125%        |
| 11        | 9.133       | 1192          | 1197        | 1207         | rBV      | 1055452        | 1381577       | 96.85%          | 11.306%       |
| 12        | 9.216       | 1207          | 1211        | 1220         | rVB3     | 15508          | 28529         | 2.00%           | 0.233%        |
| 13        | 9.475       | 1251          | 1255        | 1258         | rVV2     | 10993          | 17568         | 1.23%           | 0.144%        |
| 14        | 9.528       | 1262          | 1264        | 1272         | rVB      | 13597          | 21296         | 1.49%           | 0.174%        |
| 15        | 9.739       | 1297          | 1300        | 1305         | rVB      | 13094          | 16037         | 1.12%           | 0.131%        |
| 16        | 9.810       | 1307          | 1312        | 1317         | rBV      | 357106         | 486847        | 34.13%          | 3.984%        |
| 17        | 10.022      | 1342          | 1348        | 1352         | rBV3     | 10501          | 18201         | 1.28%           | 0.149%        |
| 18        | 10.239      | 1378          | 1385        | 1389         | rBV2     | 25637          | 39085         | 2.74%           | 0.320%        |
| 19        | 10.363      | 1402          | 1406        | 1411         | rBV      | 19623          | 27601         | 1.93%           | 0.226%        |
| 20        | 10.457      | 1418          | 1422        | 1428         | rVB      | 17103          | 26683         | 1.87%           | 0.218%        |
| 21        | 10.527      | 1429          | 1434        | 1440         | rVV      | 127468         | 174598        | 12.24%          | 1.429%        |
| 22        | 10.604      | 1441          | 1447        | 1457         | rVV      | 529061         | 758840        | 53.19%          | 6.210%        |
| 23        | 10.722      | 1461          | 1467        | 1475         | rVB      | 48966          | 86496         | 6.06%           | 0.708%        |
| 24        | 11.157      | 1538          | 1541        | 1544         | rBV      | 22598          | 31492         | 2.21%           | 0.258%        |
| 25        | 11.192      | 1544          | 1547        | 1553         | rVB2     | 27814          | 39254         | 2.75%           | 0.321%        |
| 26        | 11.298      | 1560          | 1565        | 1575         | rBV2     | 355952         | 592999        | 41.57%          | 4.853%        |
| 27        | 11.375      | 1575          | 1578        | 1582         | rVB      | 15715          | 22527         | 1.58%           | 0.184%        |
| 28        | 11.539      | 1603          | 1606        | 1610         | rBV      | 13860          | 20213         | 1.42%           | 0.165%        |
| 29        | 11.586      | 1611          | 1614        | 1618         | rVB      | 21018          | 24888         | 1.74%           | 0.204%        |
| 30        | 11.833      | 1651          | 1656        | 1666         | rBV      | 240982         | 394580        | 27.66%          | 3.229%        |
| 31        | 11.992      | 1680          | 1683        | 1688         | rVB      | 18314          | 23152         | 1.62%           | 0.189%        |
| 32        | 12.380      | 1747          | 1749        | 1755         | rVB3     | 20065          | 25300         | 1.77%           | 0.207%        |
| 33        | 12.510      | 1767          | 1771        | 1775         | rBV      | 77851          | 105377        | 7.39%           | 0.862%        |
| 34        | 12.616      | 1784          | 1789        | 1801         | rBV      | 105109         | 216977        | 15.21%          | 1.776%        |
| 35        | 12.739      | 1806          | 1810        | 1814         | rVV      | 78395          | 137745        | 9.66%           | 1.127%        |
| 36        | 12.774      | 1814          | 1816        | 1826         | rVV      | 52219          | 102107        | 7.16%           | 0.836%        |

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Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

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-BF020625.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |         |         |
|----|--------|------|------|------|------|---------|---------|---------|---------|
| 37 | 12.880 | 1829 | 1834 | 1843 | rVB  | 1120900 | 1426536 | 100.00% | 11.674% |
| 38 | 13.786 | 1984 | 1988 | 2000 | rVB3 | 52625   | 117308  | 8.22%   | 0.960%  |
| 39 | 13.939 | 2008 | 2014 | 2026 | rVB  | 381543  | 592607  | 41.54%  | 4.850%  |
| 40 | 14.686 | 2137 | 2141 | 2152 | rBV3 | 83674   | 157064  | 11.01%  | 1.285%  |
| 41 | 15.386 | 2254 | 2260 | 2276 | rVB  | 325078  | 581339  | 40.75%  | 4.757%  |

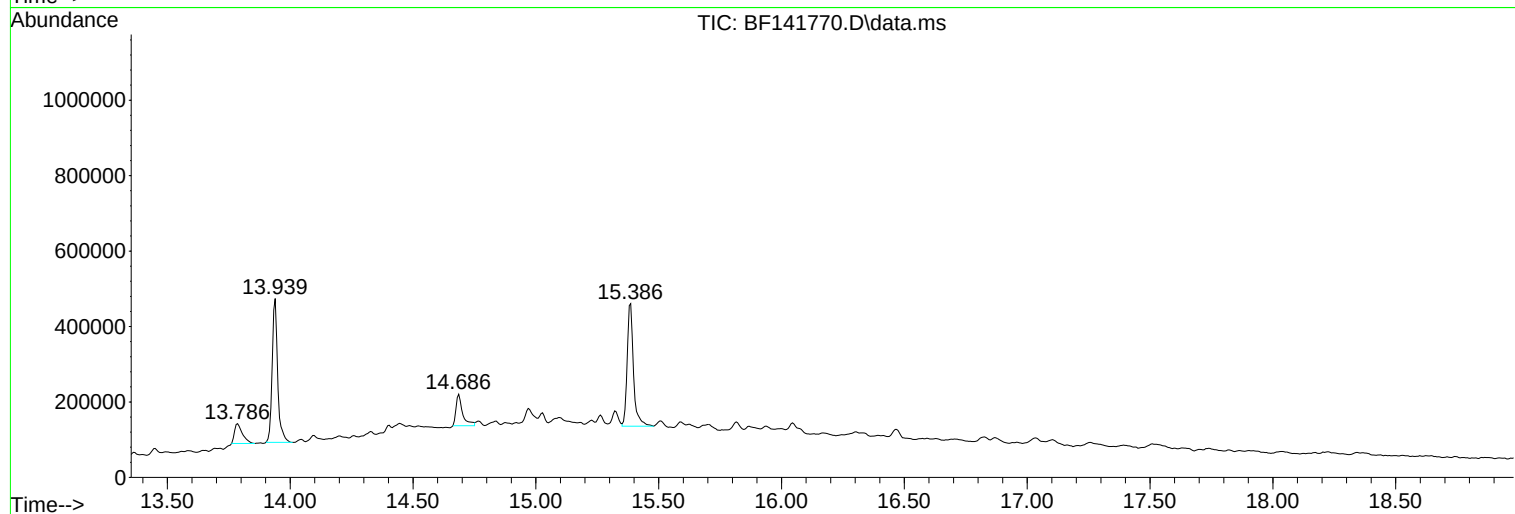
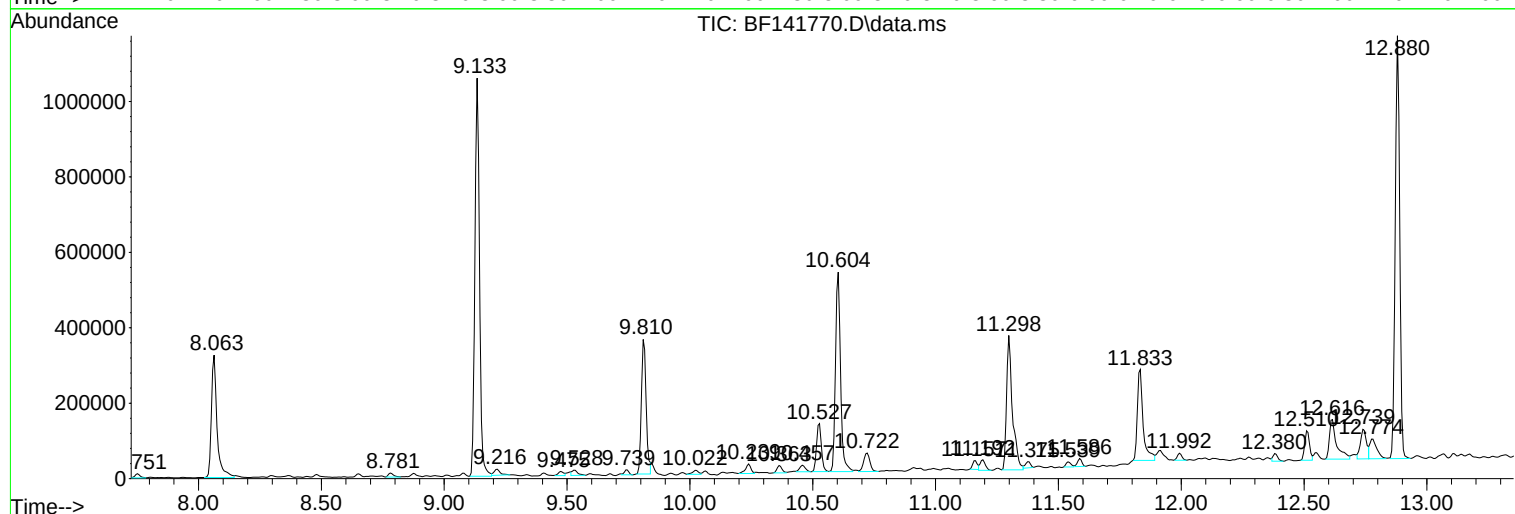
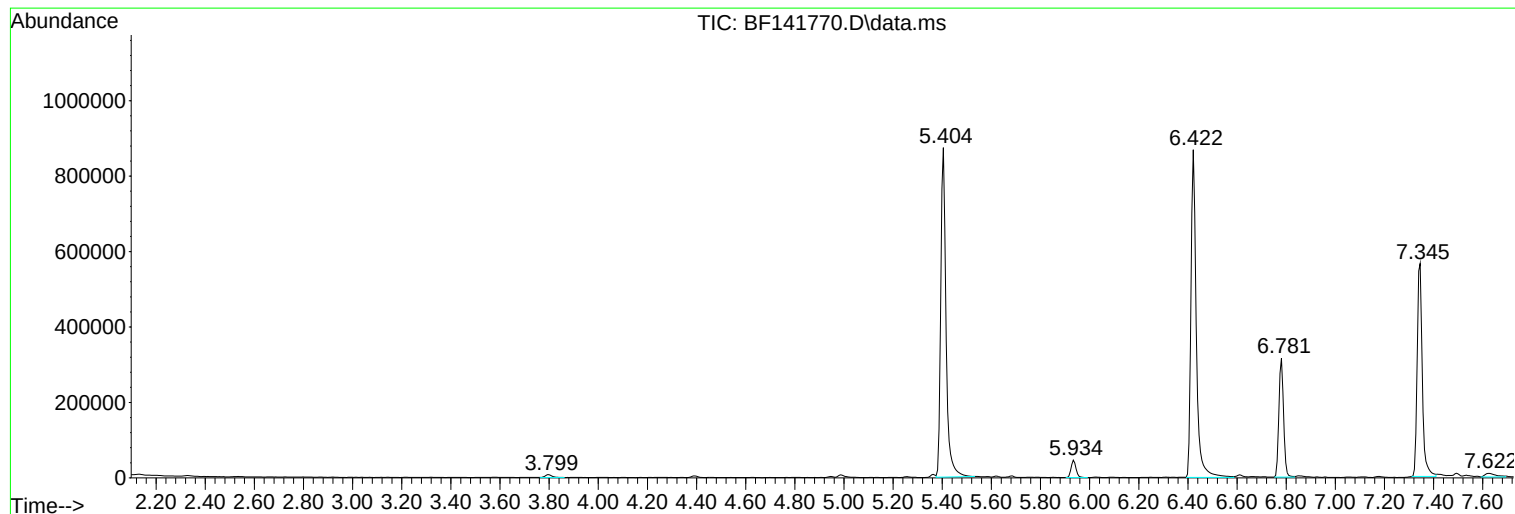
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Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
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TP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.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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Operator : RC/JU  
Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

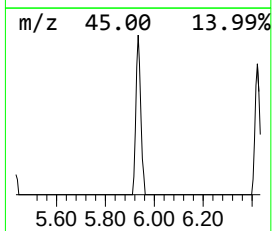
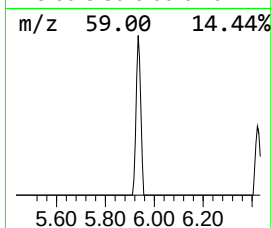
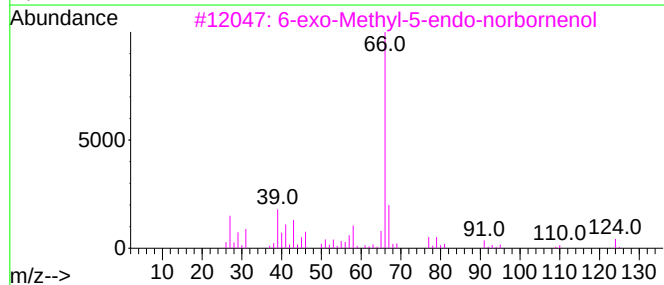
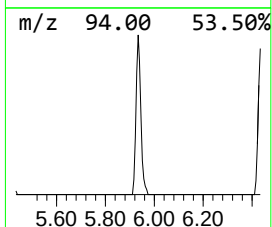
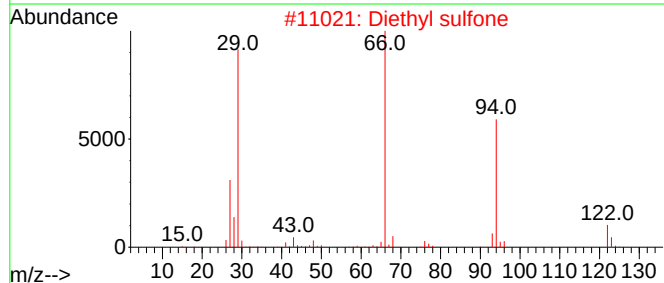
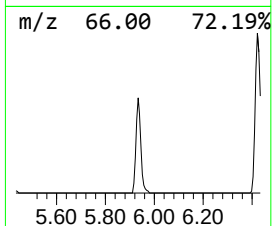
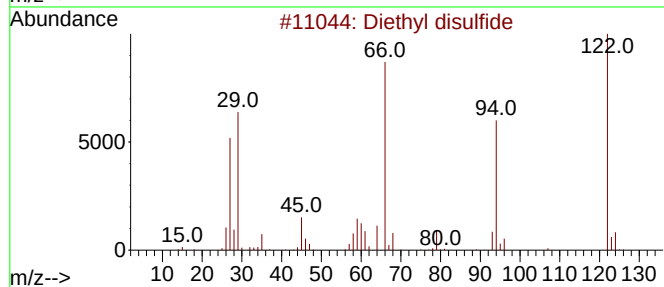
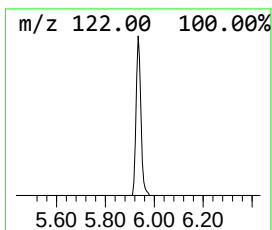
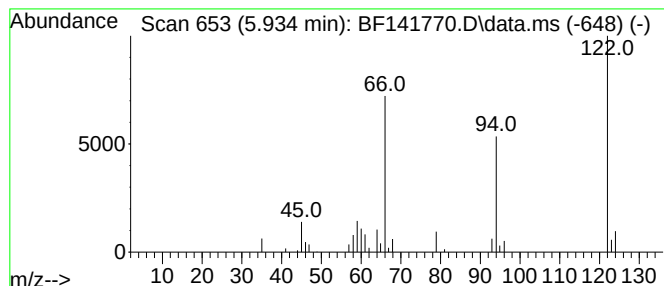
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Diethyl disulfide Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.934 | 3.11 ng | 64778 | 1,4-Dichlorobenzene-d4 | 6.781 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Diethyl disulfide                   | 122 | C4H10S2   | 000110-81-6 | 96   |
| 2    |    |   | Diethyl sulfone                     | 122 | C4H10O2S  | 000597-35-3 | 38   |
| 3    |    |   | 6-exo-Methyl-5-endo-norbornenol     | 124 | C8H12O    | 041414-52-2 | 38   |
| 4    |    |   | Dixanthogen                         | 242 | C6H10O2S4 | 000502-55-6 | 17   |
| 5    |    |   | 3-Pyridinecarboxaldehyde, oxime,... | 122 | C6H6N2O   | 051892-16-1 | 9    |



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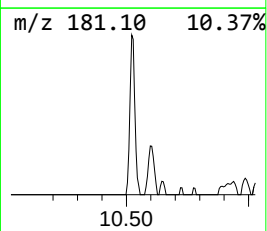
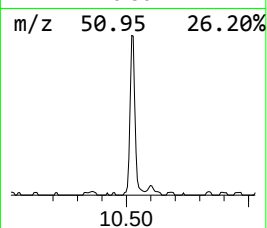
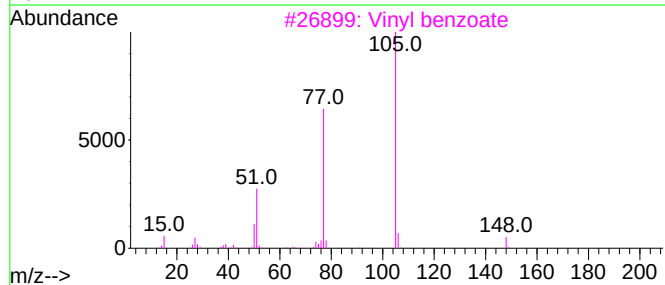
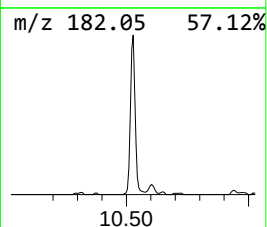
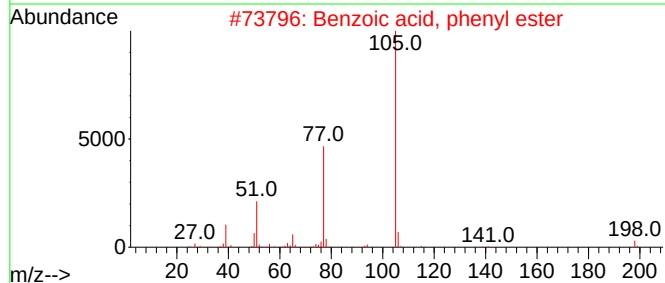
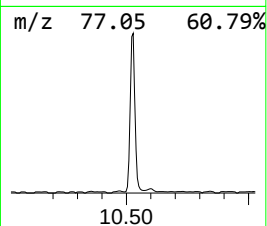
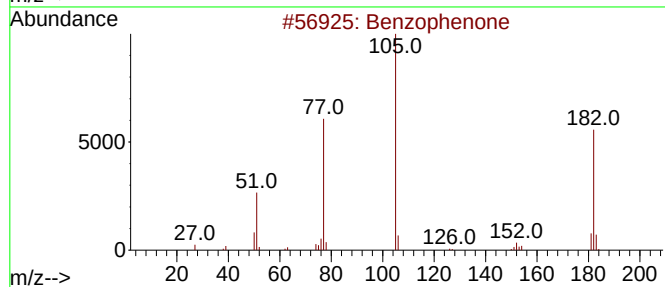
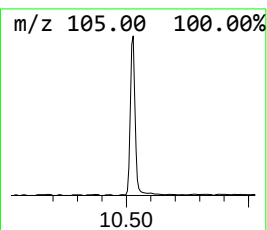
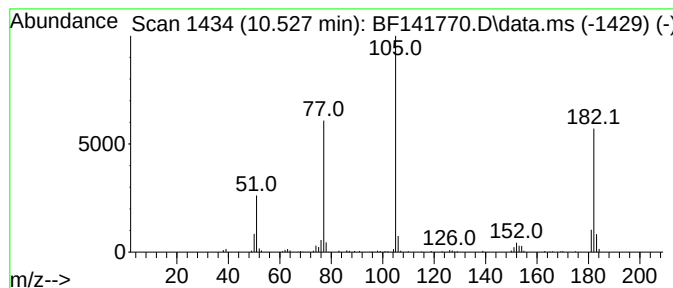
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.528 | 7.17 ng | 174598 | Acenaphthene-d10 | 9.810 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-----------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Benzoic acid, phenyl ester  | 198 | C13H10O2 | 000093-99-2 | 47   |
| 3    |    |   | Vinyl benzoate              | 148 | C9H8O2   | 000769-78-8 | 47   |
| 4    |    |   | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 47   |
| 5    |    |   | Phenyl 4-pyridyl ketone     | 183 | C12H9NO  | 014548-46-0 | 47   |



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Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

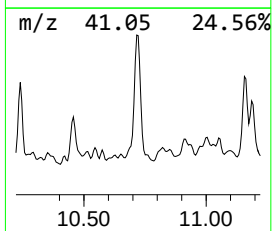
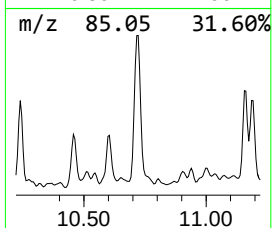
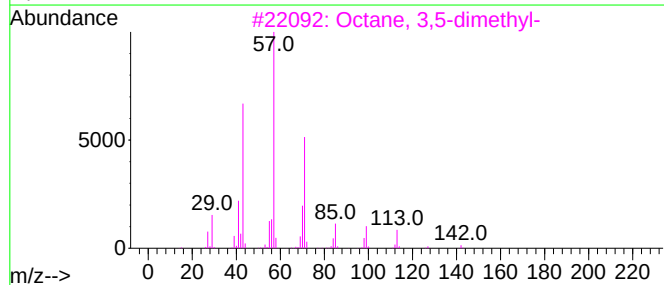
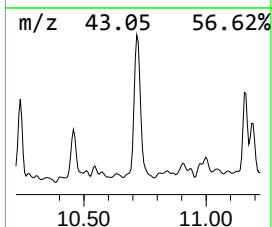
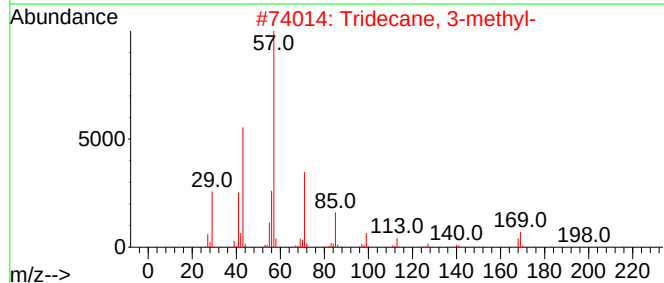
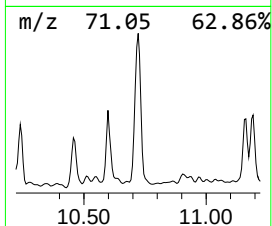
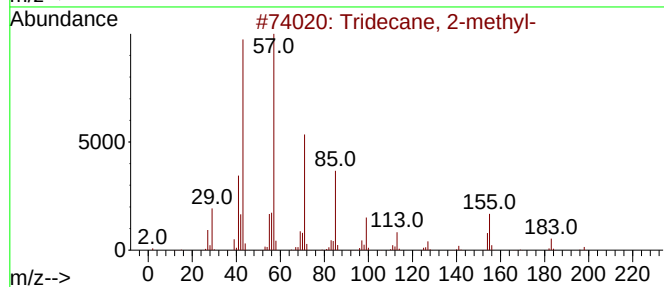
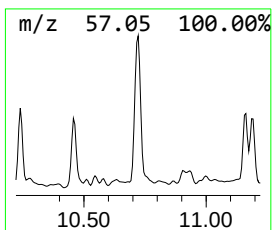
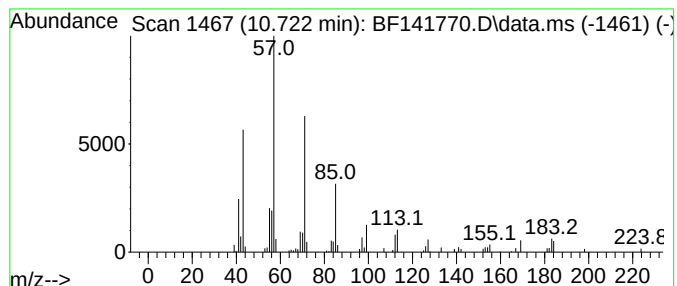
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Tridecane, 2-methyl- Concentration Rank 7

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 10.722 | 2.92 ng | 86496 | Phenanthrene-d10 | 11.298 |

| Hit# | of 5 | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|------|------------------------|-----|---------|-------------|------|
| 1    |      | Tridecane, 2-methyl-   | 198 | C14H30  | 001560-96-9 | 94   |
| 2    |      | Tridecane, 3-methyl-   | 198 | C14H30  | 006418-41-3 | 80   |
| 3    |      | Octane, 3,5-dimethyl-  | 142 | C10H22  | 015869-93-9 | 74   |
| 4    |      | Heptadecane, 2-methyl- | 254 | C18H38  | 001560-89-0 | 72   |
| 5    |      | Tetradecane, 1-iodo-   | 324 | C14H29I | 019218-94-1 | 64   |



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ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

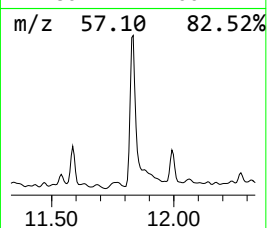
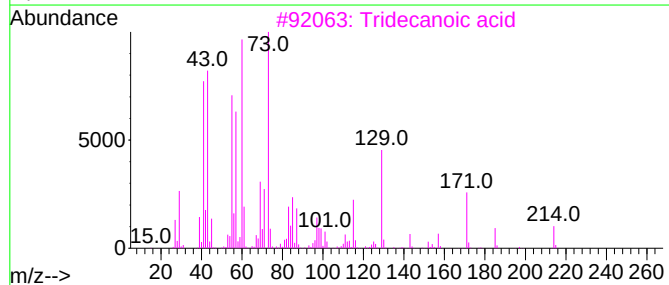
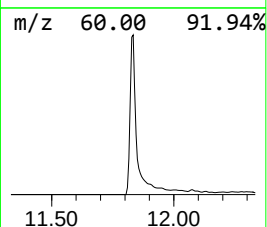
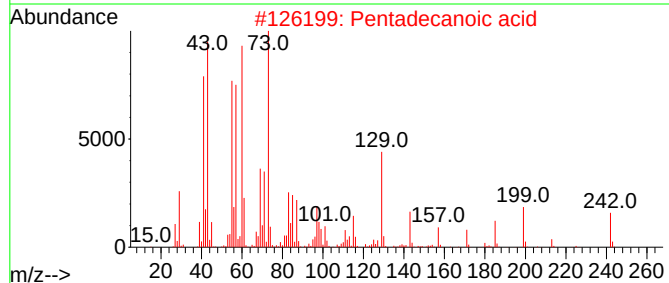
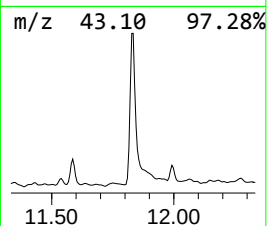
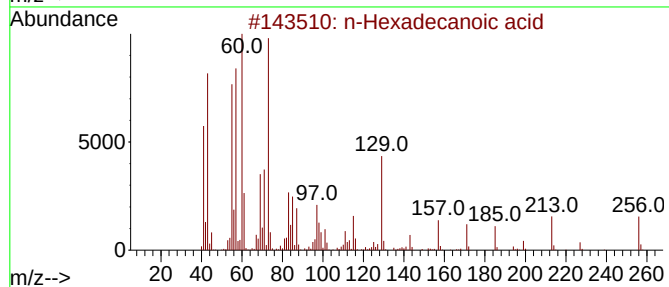
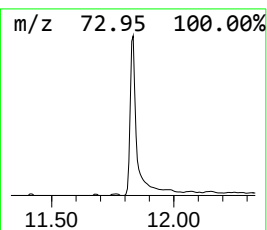
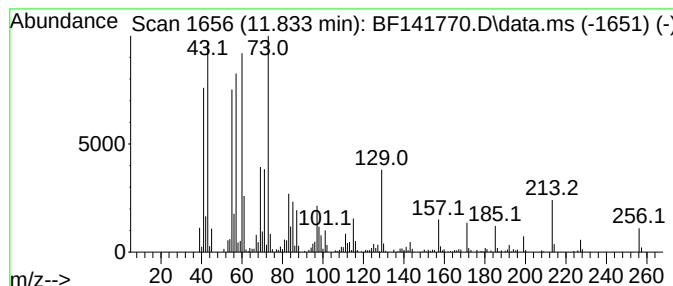
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 11.833 | 13.31 ng | 394580 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 91   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 68   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 68   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022525\  
Data File : BF141770.D  
Acq On : 25 Feb 2025 18:04  
Operator : RC/JU  
Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

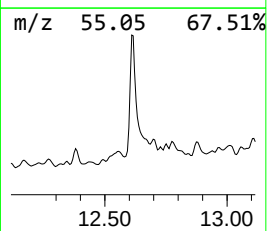
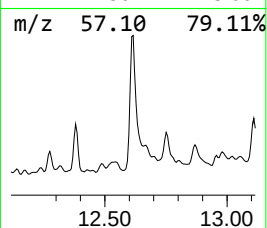
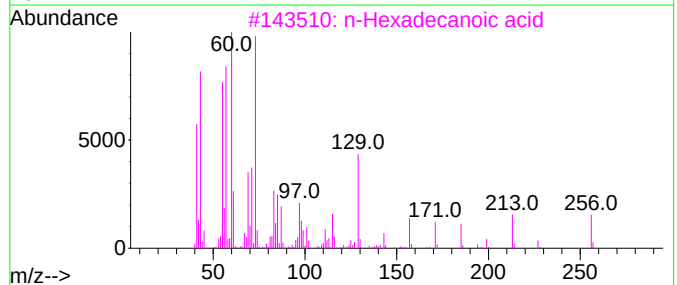
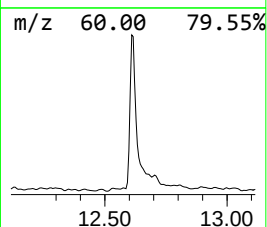
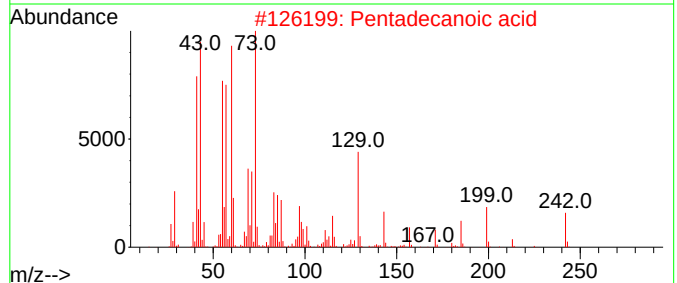
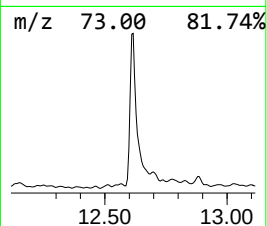
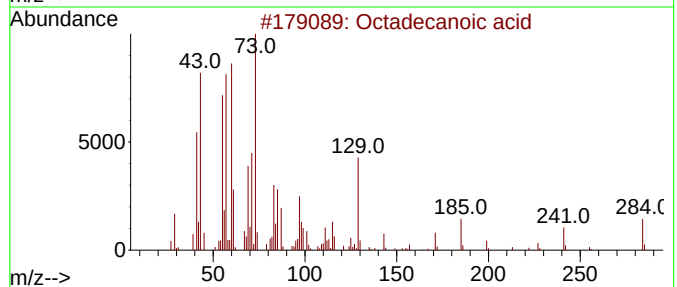
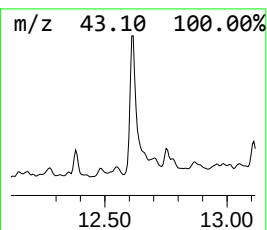
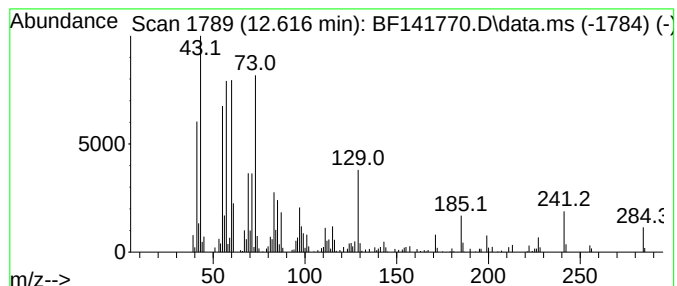
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.616 | 7.32 ng | 216977 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 94   |
| 3    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 93   |
| 4    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 86   |
| 5    |    |   | Isopropyl palmitate                 | 298 | C19H38O2 | 000142-91-6 | 72   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022525\  
Data File : BF141770.D  
Acq On : 25 Feb 2025 18:04  
Operator : RC/JU  
Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

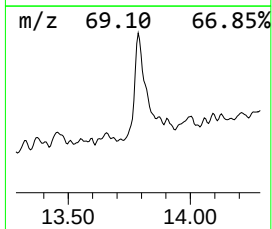
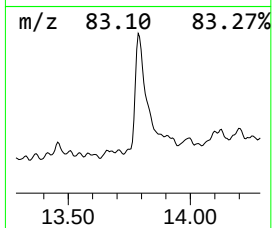
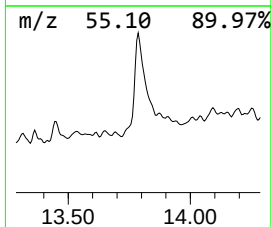
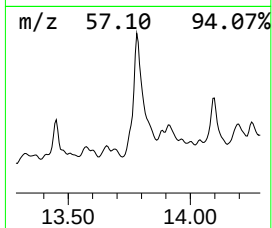
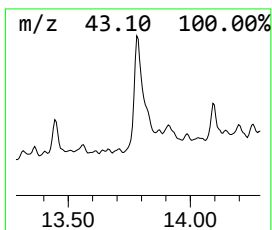
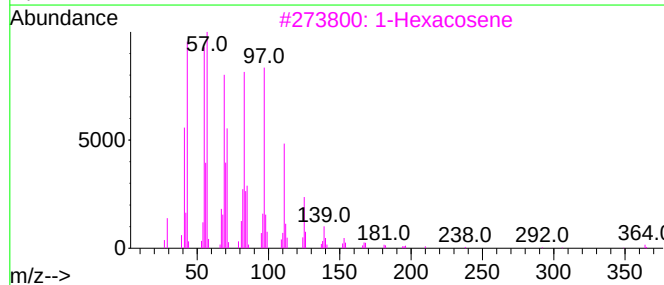
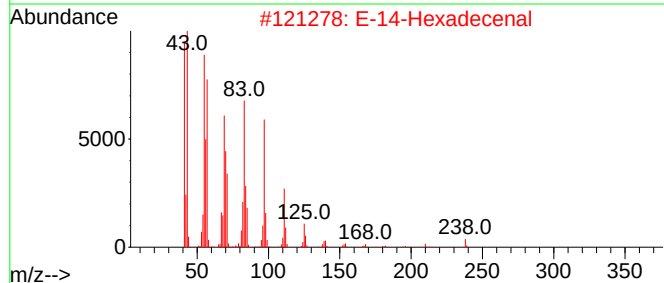
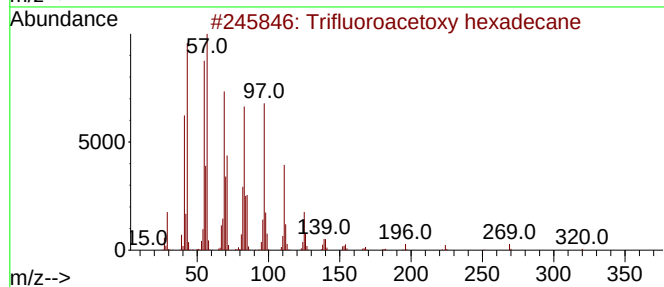
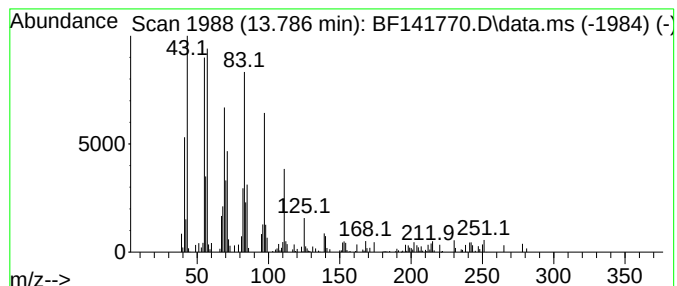
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.786 | 3.96 ng | 117308 | Chrysene-d12     | 13.939 |

| Hit# | of 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|------|-----------------------------|-----|------------|--------------|------|
| 1    |      | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3  | 93   |
| 2    |      | E-14-Hexadecenal            | 238 | C16H30O    | 330207-53-9  | 90   |
| 3    |      | 1-Hexacosene                | 364 | C26H52     | 018835-33-1  | 90   |
| 4    |      | Cyclooctadecane, ethyl-     | 280 | C20H40     | 1000151-22-5 | 87   |
| 5    |      | 16-Hentriacontanol          | 452 | C31H64O    | 001070-54-8  | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022525\  
Data File : BF141770.D  
Acq On : 25 Feb 2025 18:04  
Operator : RC/JU  
Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

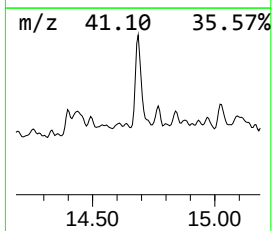
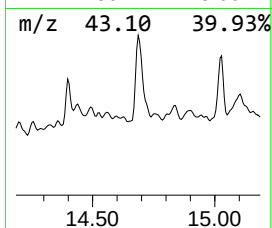
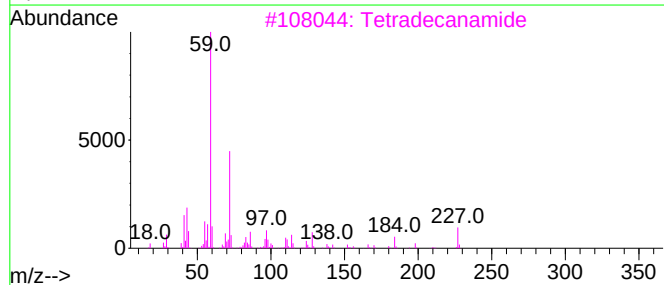
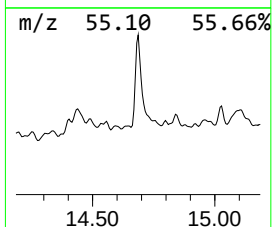
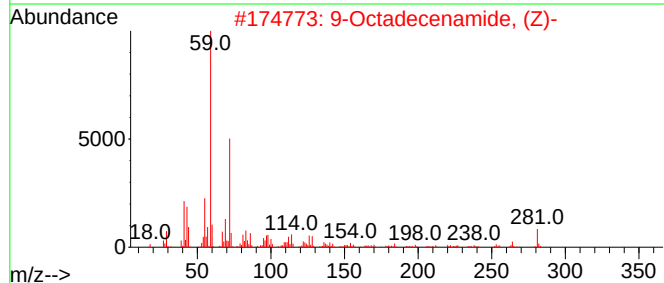
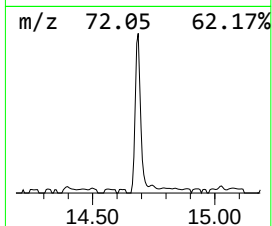
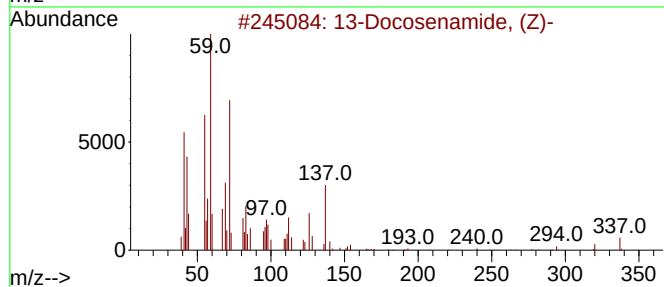
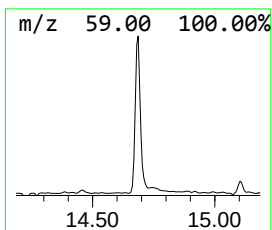
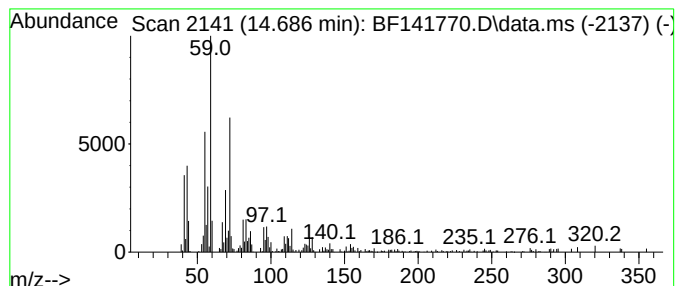
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.686 | 5.40 ng | 157064 | Perylene-d12     | 15.386 |

| Hit# | of 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|------|------|------------------------|-----|----------|-------------|------|
| 1    |      | 13-Docosenamide, (Z)-  | 337 | C22H43NO | 000112-84-5 | 87   |
| 2    |      | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 86   |
| 3    |      | Tetradecanamide        | 227 | C14H29NO | 000638-58-4 | 78   |
| 4    |      | Octadecanamide         | 283 | C18H37NO | 000124-26-5 | 72   |
| 5    |      | Decanamide-            | 171 | C10H21NO | 002319-29-1 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022525\  
Data File : BF141770.D  
Acq On : 25 Feb 2025 18:04  
Operator : RC/JU  
Sample : Q1420-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020625.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 |
| Diethyl disulfide  | 5.934  | 3.1     | ng    | 64778    | 1                     | 6.781  | 416042 | 20.0 |
| Benzophenone       | 10.528 | 7.2     | ng    | 174598   | 3                     | 9.810  | 486847 | 20.0 |
| Tridecane, 2-me... | 10.722 | 2.9     | ng    | 86496    | 4                     | 11.298 | 592999 | 20.0 |
| n-Hexadecanoic ... | 11.833 | 13.3    | ng    | 394580   | 4                     | 11.298 | 592999 | 20.0 |
| Octadecanoic acid  | 12.616 | 7.3     | ng    | 216977   | 4                     | 11.298 | 592999 | 20.0 |
| Trifluoroacetox... | 13.786 | 4.0     | ng    | 117308   | 5                     | 13.939 | 592607 | 20.0 |
| 13-Docosenamide... | 14.686 | 5.4     | ng    | 157064   | 6                     | 15.386 | 581339 | 20.0 |