LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125820.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.140 | 3 | 9 | 15 | rBV | 1559341 | 2089014 | 34.75% | 3.674% |
| 2 | 5.069 | 498 | 507 | 517 | rBV | 122925 | 179578 | 2.99% | 0.316% |
| 3 | 5.463 | 569 | 574 | 578 | rBV | 3904562 | 4124657 | 68.60% | 7.254% |
| 4 | 6.469 | 740 | 745 | 748 | rBV | 3866623 | 4336594 | 72.13% | 7.627% |
| 5 | 6.845 | 805 | 809 | 812 | rBV | 1549447 | 1290653 | 21.47% | 2.270% |
| 6 | 7.404 | 898 | 904 | 907 | rBV | 3083740 | 2868107 | 47.70% | 5.044% |
| 7 | 8.028 | 1006 | 1010 | 1019 | rBV | 678991 | 583523 | 9.71% | 1.026% |
| 8 | 8.122 | 1022 | 1026 | 1030 | rBV | 2117824 | 1789589 | 29.77% | 3.148% |
| 9 | 9.198 | 1204 | 1209 | 1212 | rBV | 5950786 | 5472693 | 91.03% | 9.625% |
| 10 | 9.316 | 1226 | 1229 | 1233 | rVB | 194183 | 158419 | 2.63% | 0.279% |
| 11 | 9.874 | 1320 | 1324 | 1328 | rBV | 2514785 | 2082491 | 34.64% | 3.663% |
| 12 | 10.663 | 1454 | 1458 | 1461 | rBV | 3002815 | 2563213 | 42.63% | 4.508% |
| 13 | 11.198 | 1535 | 1549 | 1550 | rBV4 | 308192 | 1002359 | 16.67% | 1.763% |
| 14 | 11.227 | 1552 | 1554 | 1573 | rVV2 | 446047 | 1536647 | 25.56% | 2.703% |
| 15 | 11.357 | 1573 | 1576 | 1579 | rVV | 2200900 | 2070080 | 34.43% | 3.641% |
| 16 | 11.380 | 1579 | 1580 | 1583 | rVV | 241662 | 152178 | 2.53% | 0.268% |
| 17 | 11.427 | 1586 | 1588 | 1592 | rVB2 | 77160 | 76828 | 1.28% | 0.135% |
| 18 | 11.757 | 1641 | 1644 | 1646 | rBV | 85733 | 80282 | 1.34% | 0.141% |
| 19 | 11.880 | 1659 | 1665 | 1677 | rVB2 | 1236078 | 2121713 | 35.29% | 3.732% |
| 20 | 12.021 | 1686 | 1689 | 1694 | rBV3 | 217392 | 329719 | 5.48% | 0.580% |
| 21 | 12.063 | 1694 | 1696 | 1704 | rVB3 | 167540 | 237587 | 3.95% | 0.418% |
| 22 | 12.463 | 1761 | 1764 | 1766 | rBV | 195045 | 173953 | 2.89% | 0.306% |
| 23 | 12.545 | 1773 | 1778 | 1779 | rBV2 | 165633 | 237462 | 3.95% | 0.418% |
| 24 | 12.568 | 1779 | 1782 | 1784 | rVV | 416972 | 352896 | 5.87% | 0.621% |
| 25 | 12.668 | 1793 | 1799 | 1816 | rVB | 3611096 | 6012251 | 100.00% | 10.574% |
| 26 | 12.798 | 1818 | 1821 | 1824 | rVB | 347425 | 306940 | 5.11% | 0.540% |
| 27 | 12.945 | 1842 | 1846 | 1849 | rBV | 5424279 | 4838438 | 80.48% | 8.510% |
| 28 | 13.304 | 1901 | 1907 | 1914 | rVB | 343243 | 727191 | 12.10% | 1.279% |
| 29 | 13.392 | 1919 | 1922 | 1924 | rBV | 60525 | 61222 | 1.02% | 0.108% |
| 30 | 13.851 | 1997 | 2000 | 2009 | rVB2 | 193460 | 304151 | 5.06% | 0.535% |
| 31 | 13.992 | 2019 | 2024 | 2027 | rBV | 1512991 | 1680192 | 27.95% | 2.955% |
| 32 | 14.015 | 2027 | 2028 | 2037 | rVB | 573062 | 718310 | 11.95% | 1.263% |
| 33 | 14.586 | 2120 | 2125 | 2128 | rBV | 564939 | 829749 | 13.80% | 1.459% |
| 34 | 14.621 | 2128 | 2131 | 2144 | rVB | 652644 | 792083 | 13.17% | 1.393% |
| 35 | 14.933 | 2180 | 2184 | 2185 | rBV3 | 72010 | 97810 | 1.63% | 0.172% |
| 36 | 15.021 | 2196 | 2199 | 2202 | rBV | 112646 | 152018 | 2.53% | 0.267% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 15.151 | 2215 | 2221 | 2230 | rVB | 355605 | 663087 | 11.03% | 1.166% |
| 38 | 15.321 | 2247 | 2250 | 2256 | rVB | 90629 | 134677 | 2.24% | 0.237% |
| 39 | 15.380 | 2257 | 2260 | 2264 | rBV | 108551 | 129172 | 2.15% | 0.227% |
| 40 | 15.451 | 2267 | 2272 | 2276 | rBV | 1075074 | 1359828 | 22.62% | 2.392% |
| 41 | 15.792 | 2325 | 2330 | 2340 | rVB | 250275 | 549612 | 9.14% | 0.967% |
| 42 | 16.198 | 2393 | 2399 | 2410 | rBV6 | 199676 | 608380 | 10.12% | 1.070% |
| 43 | 16.533 | 2450 | 2456 | 2470 | rVB2 | 157719 | 445443 | 7.41% | 0.783% |
| 44 | 16.909 | 2513 | 2520 | 2531 | rVB5 | 170217 | 536541 | 8.92% | 0.944% |

Sum of corrected areas: 56857330

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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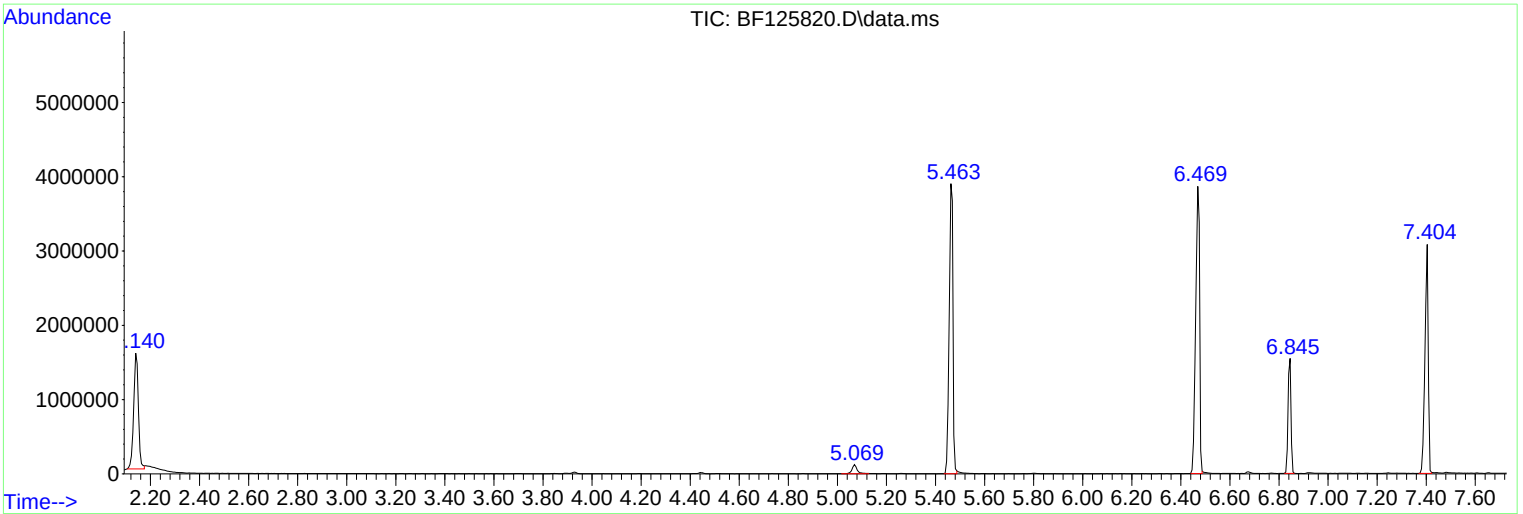
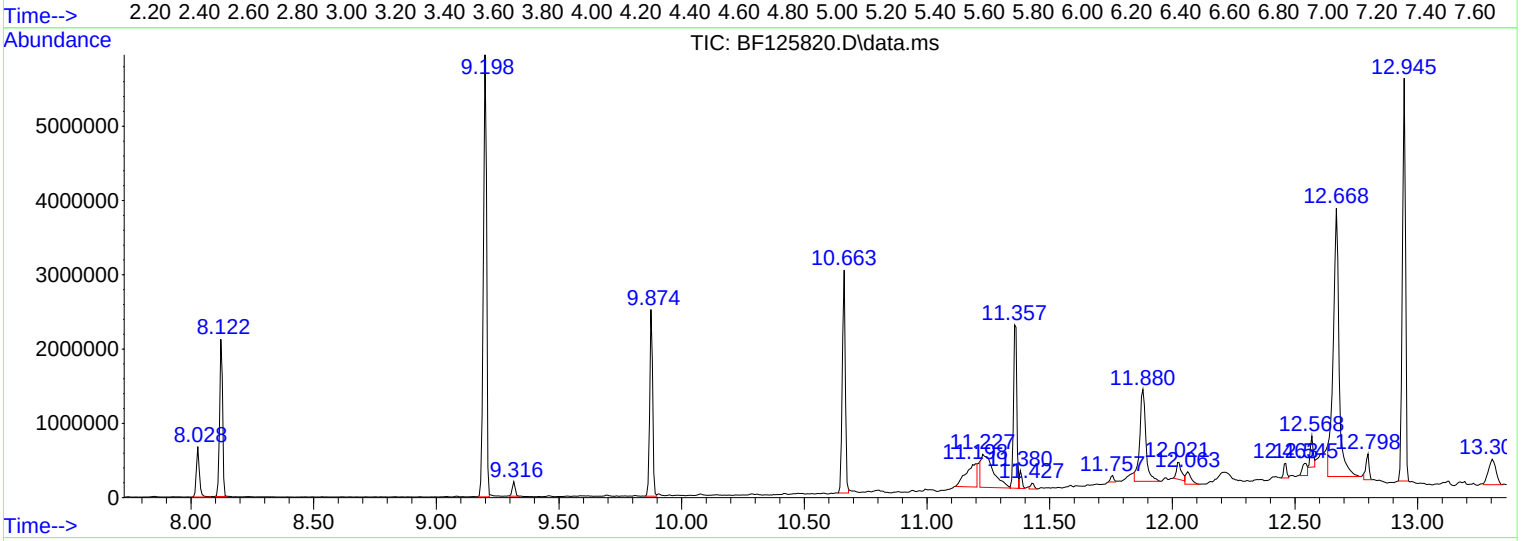
Misc :
ALS Vial : 5 Sample Multiplier: 1

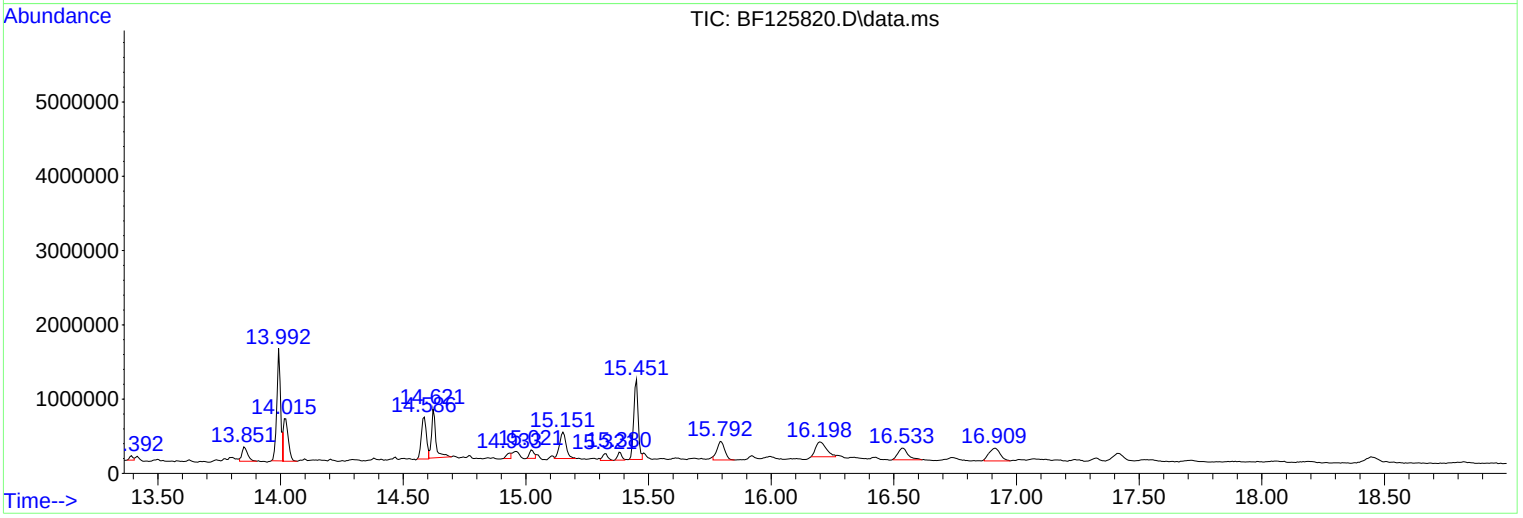
**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

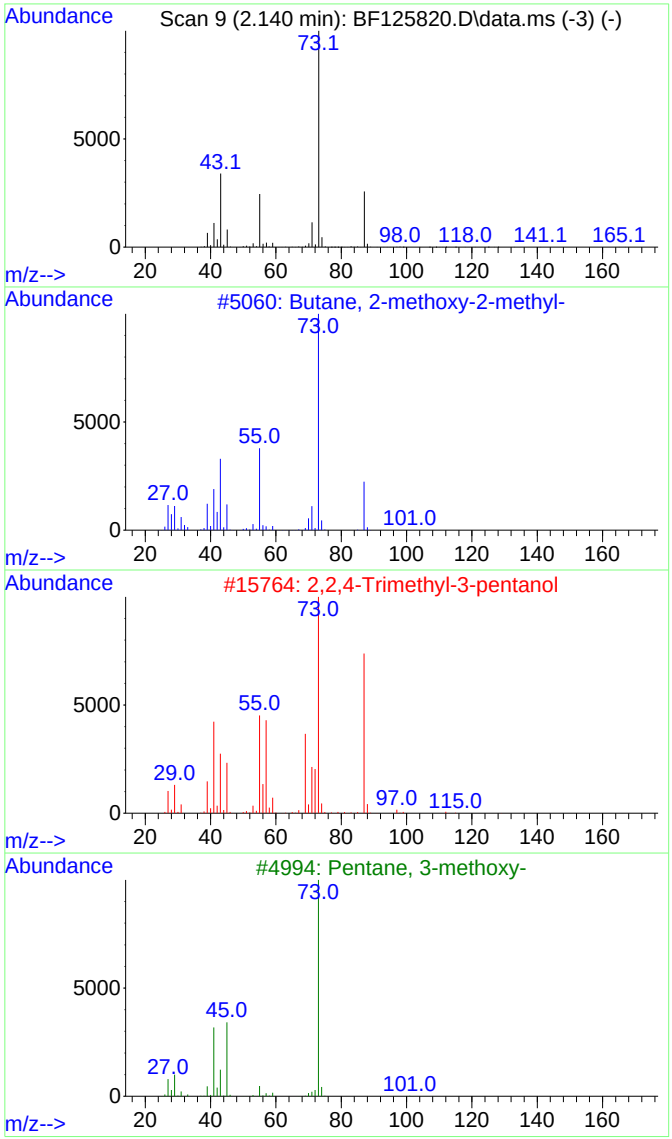
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

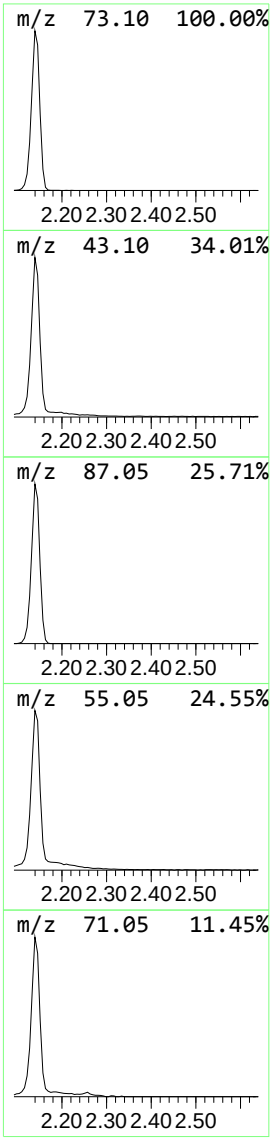
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.140 | 32.37 ng | 2089010 | 1,4-Dichlorobenzene-d4 | 6.845 |

| 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 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

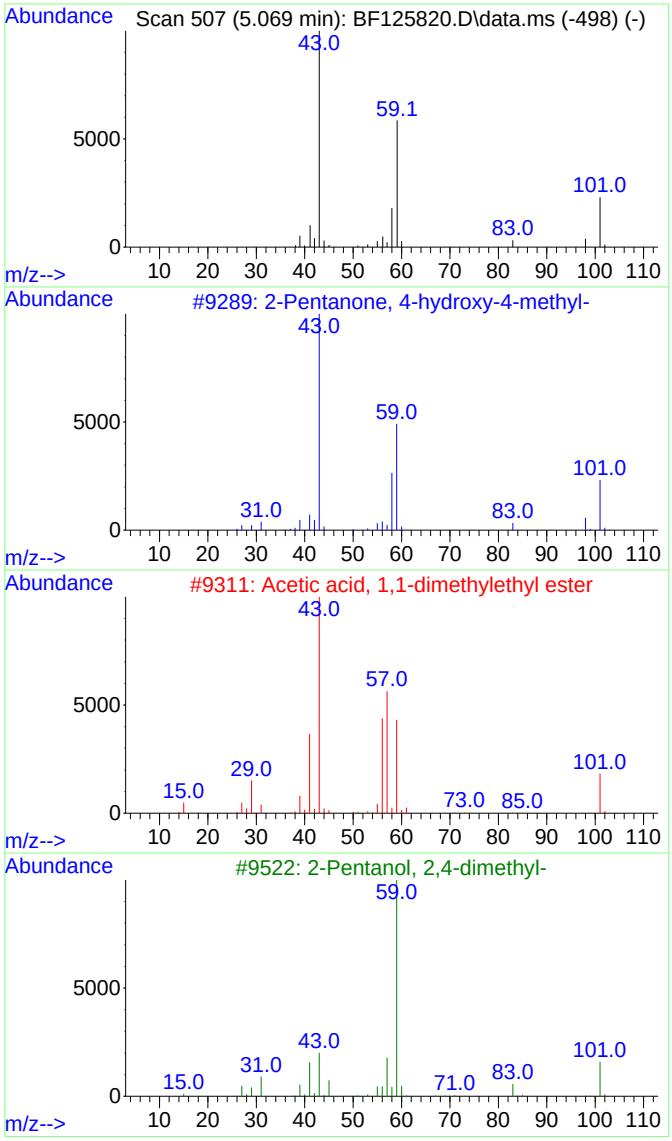
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

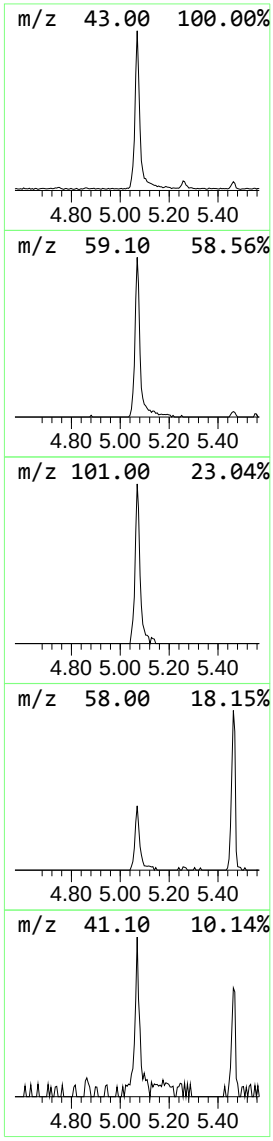
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.069 | 2.78 ng | 179578 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 25 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 23 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

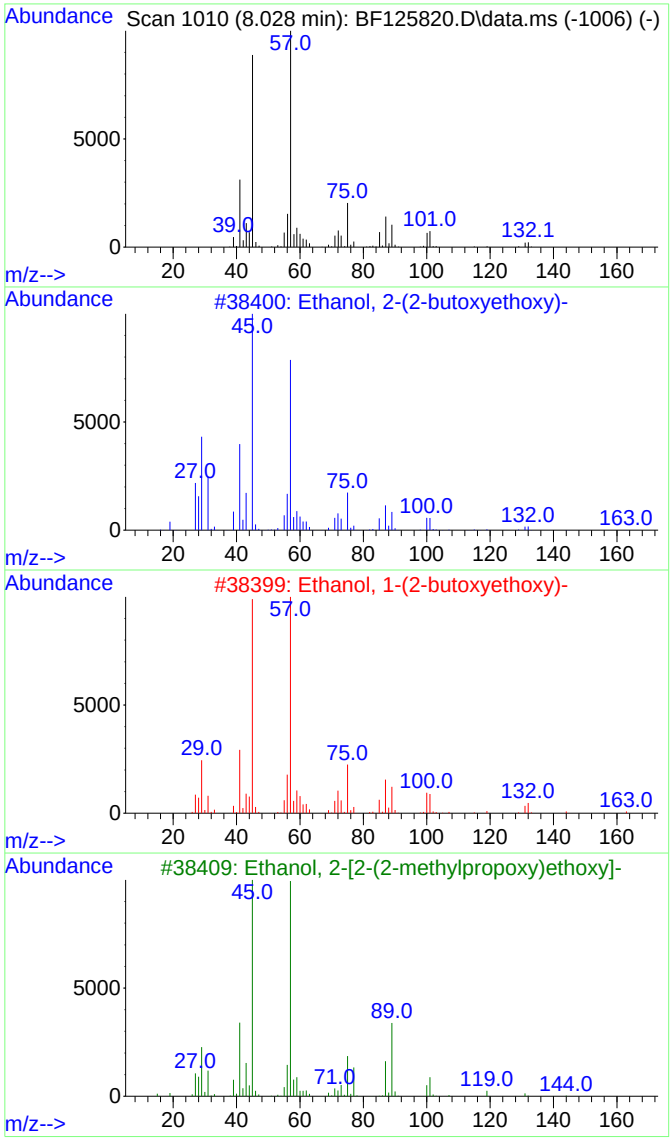
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

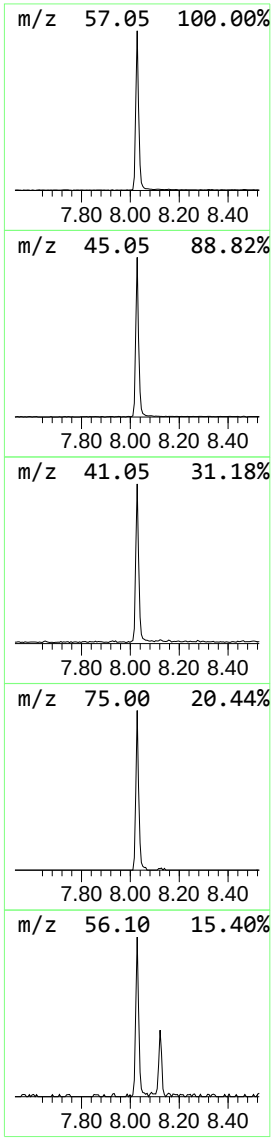
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.028 | 6.52 ng | 583523 | Naphthalene-d8 | 8.122 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 83 |
| 3 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 64 |
| 4 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64 |
| 5 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

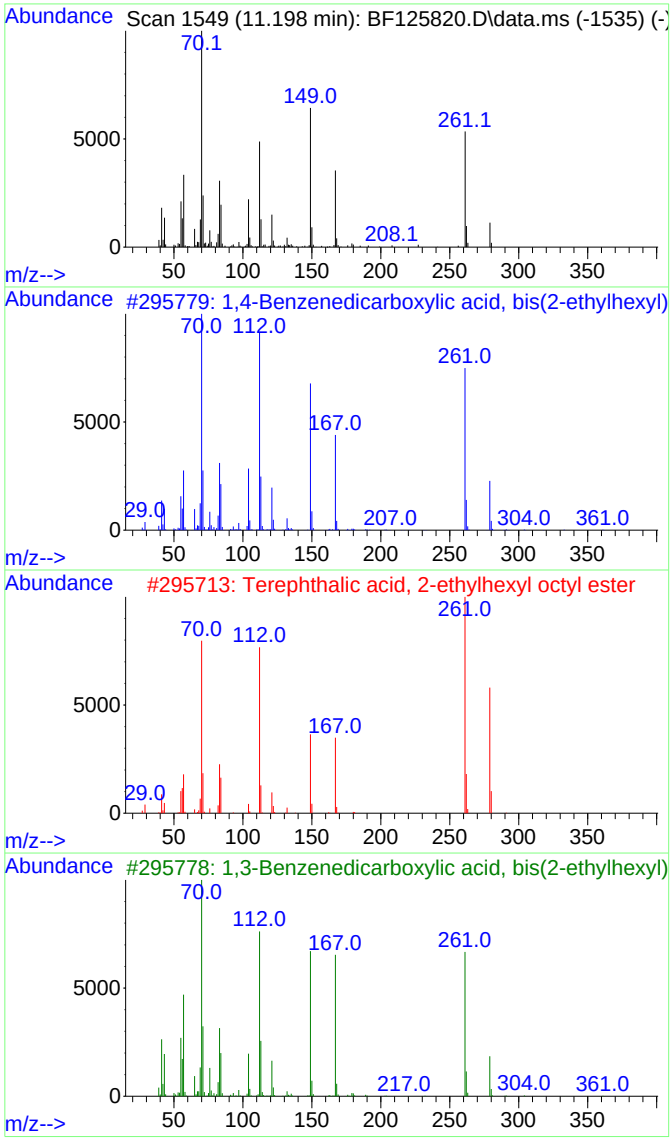
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

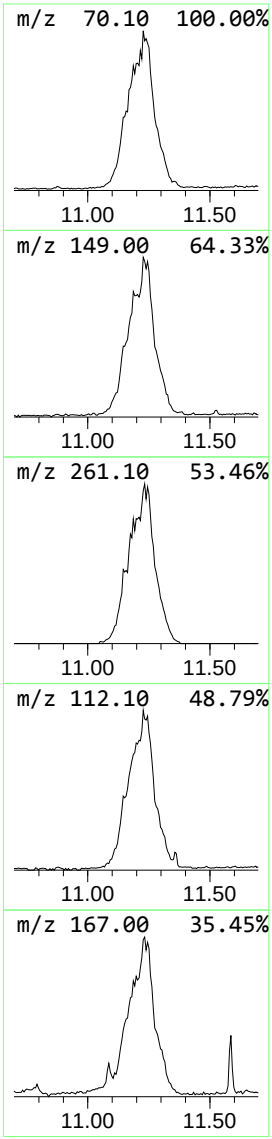
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.198 | 9.68 ng | 1002360 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 006422-86-2 | 64 |
| 2 | Terephthalic acid, 2-ethylhexyl ... | 390 | C24H38O4 | 1000324-00-5 | 52 |
| 3 | 1,3-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 000137-89-3 | 49 |
| 4 | Terephthalic acid, 3-methylbut-2... | 348 | C21H32O4 | 1000356-27-6 | 49 |
| 5 | Terephthalic acid, di(4-octyl) e... | 390 | C24H38O4 | 1000323-74-2 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

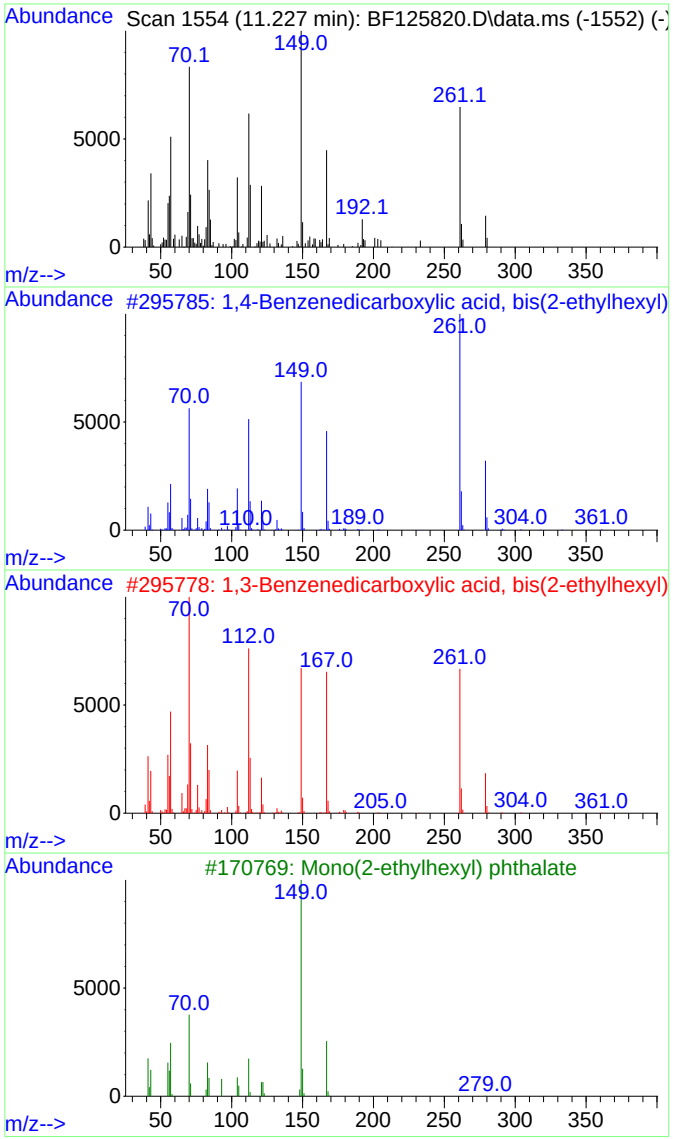
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

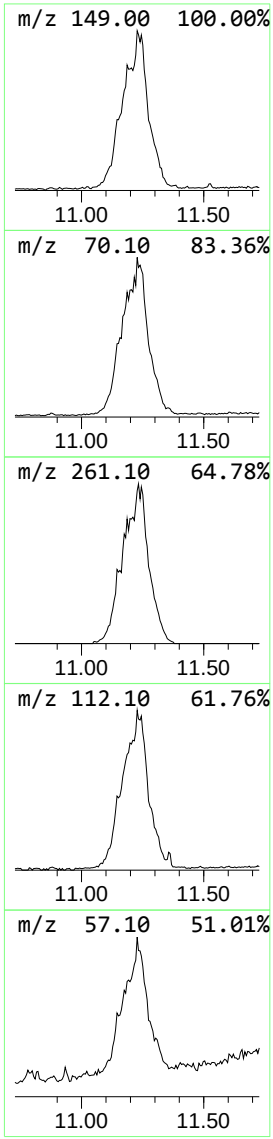
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 1,3-Benzenedicarboxylic aci... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.227 | 14.85 ng | 1536650 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 006422-86-2 | 91 |
| 2 | 1,3-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 000137-89-3 | 72 |
| 3 | Mono(2-ethylhexyl) phthalate | 278 | C16H22O4 | 004376-20-9 | 43 |
| 4 | 1,3-oxazole-4-carboxylic acid, 4... | 185 | C9H15NO3 | 1000197-69-0 | 22 |
| 5 | Phthalic acid, hexyl oct-3-yl ester | 362 | C22H34O4 | 1000377-71-5 | 14 |



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Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

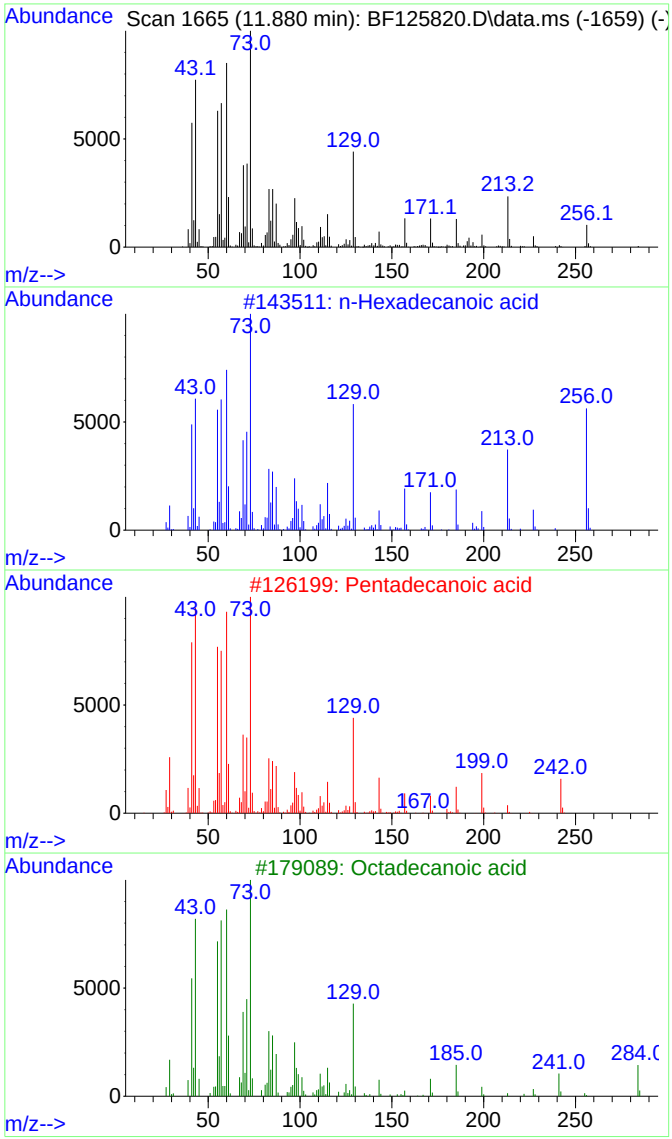
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

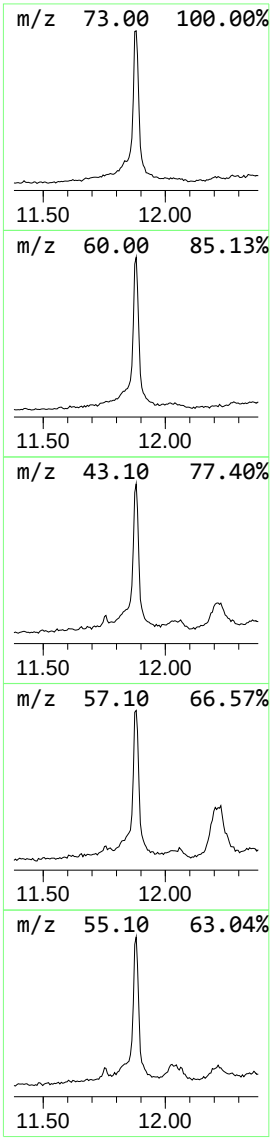
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.880 | 20.50 ng | 2121710 | Phenanthrene-d10 | 11.363 |

| 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 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 93 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

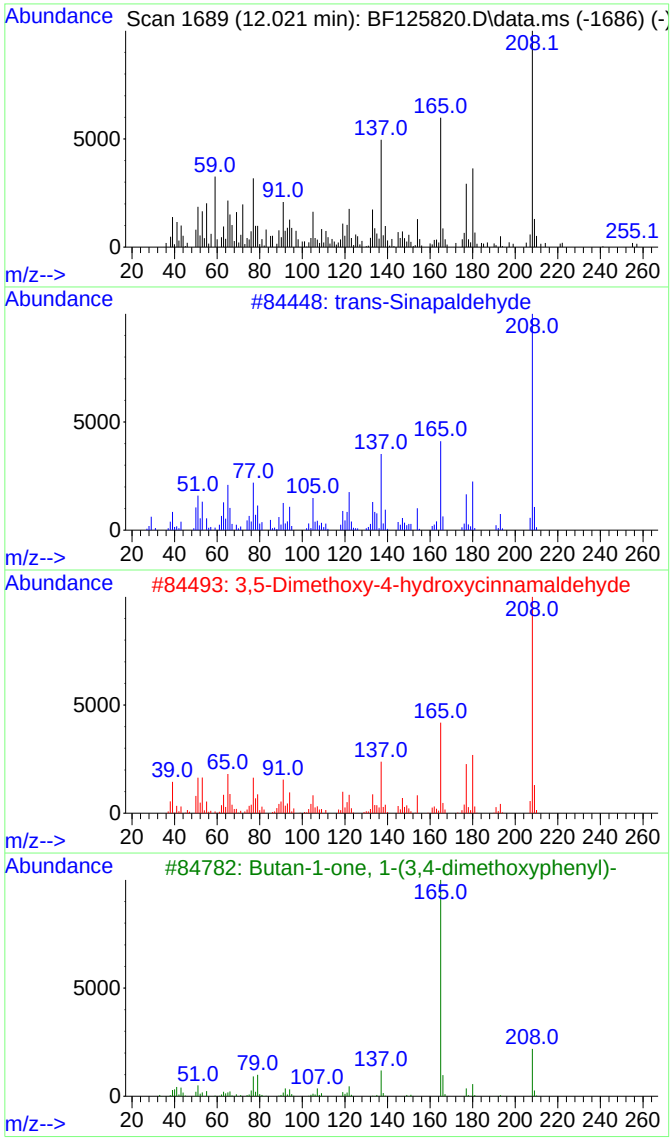
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

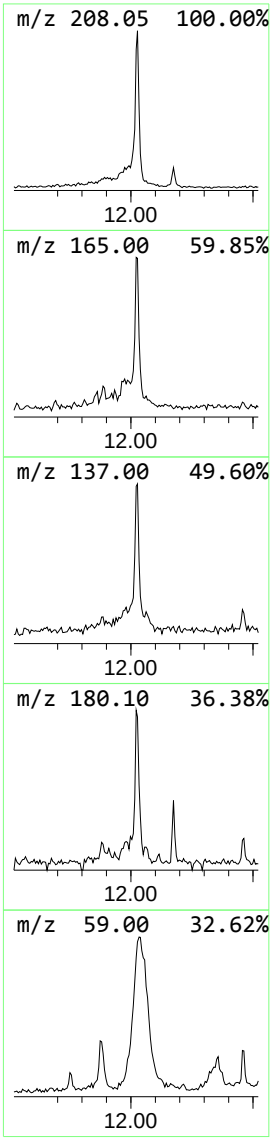
**********

Peak Number 7 trans-Sinapaldehyde Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.021 | 3.19 ng | 329719 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-Sinapaldehyde | 208 | C11H12O4 | 004206-58-0 | 94 |
| 2 | 3,5-Dimethoxy-4-hydroxycinnamald... | 208 | C11H12O4 | 087345-53-7 | 93 |
| 3 | Butan-1-one, 1-(3,4-dimethoxyphe... | 208 | C12H16O3 | 054419-21-5 | 53 |
| 4 | 3-tert-Butyl-4-hydroxyanisole | 180 | C11H16O2 | 000121-00-6 | 47 |
| 5 | 4-(2-Amino-1,3-thiazol-4-yl)-1,3... | 208 | C9H8N2O2S | 090850-44-5 | 41 |



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Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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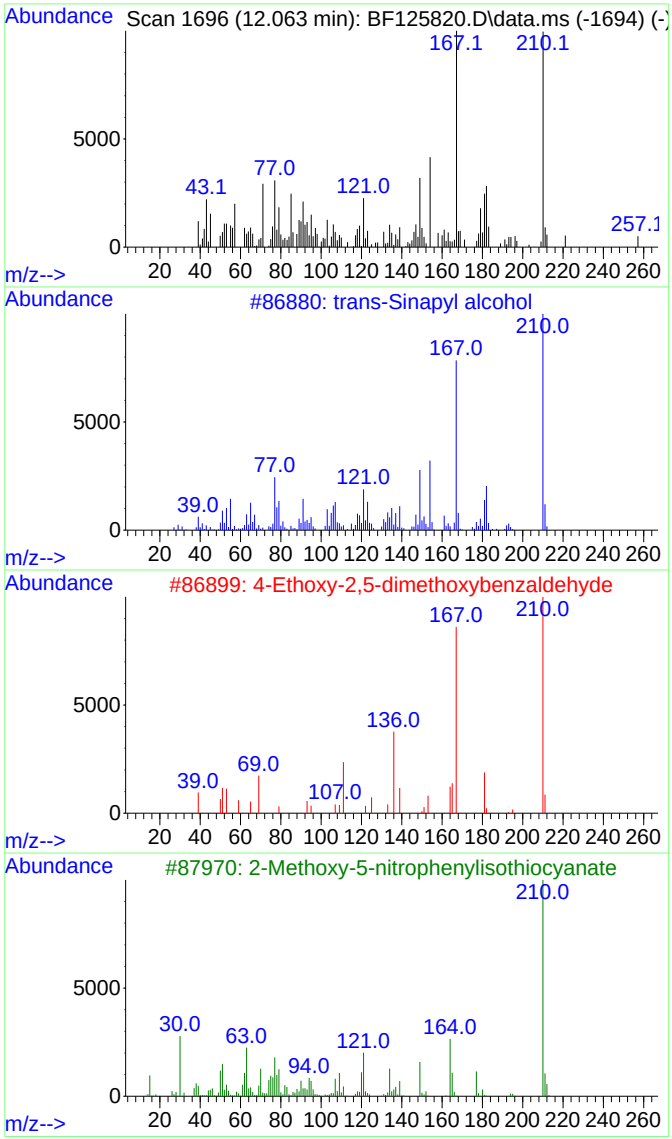
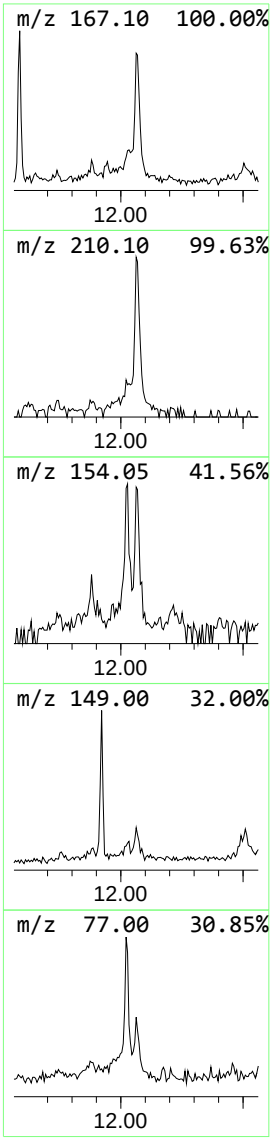
Peak Number 8 trans-Sinapyl alcohol Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.063 | 2.30 ng | 237587 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-Sinapyl alcohol | 210 | C11H14O4 | 020675-96-1 | 87 |
| 2 | 4-Ethoxy-2,5-dimethoxybenzaldehyde | 210 | C11H14O4 | 1000121-30-2 | 47 |
| 3 | 2-Methoxy-5-nitrophenylisothiocy... | 210 | C8H6N2O3S | 071793-51-6 | 30 |
| 4 | 5-Methyl-2-(methylthio)[1,2,4]tr... | 210 | C8H10N4OS | 113362-33-7 | 30 |
| 5 | 3H-Indazol-3-one, 1,2-dihydro-2-... | 210 | C13H10N2O | 017049-65-9 | 22 |



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Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

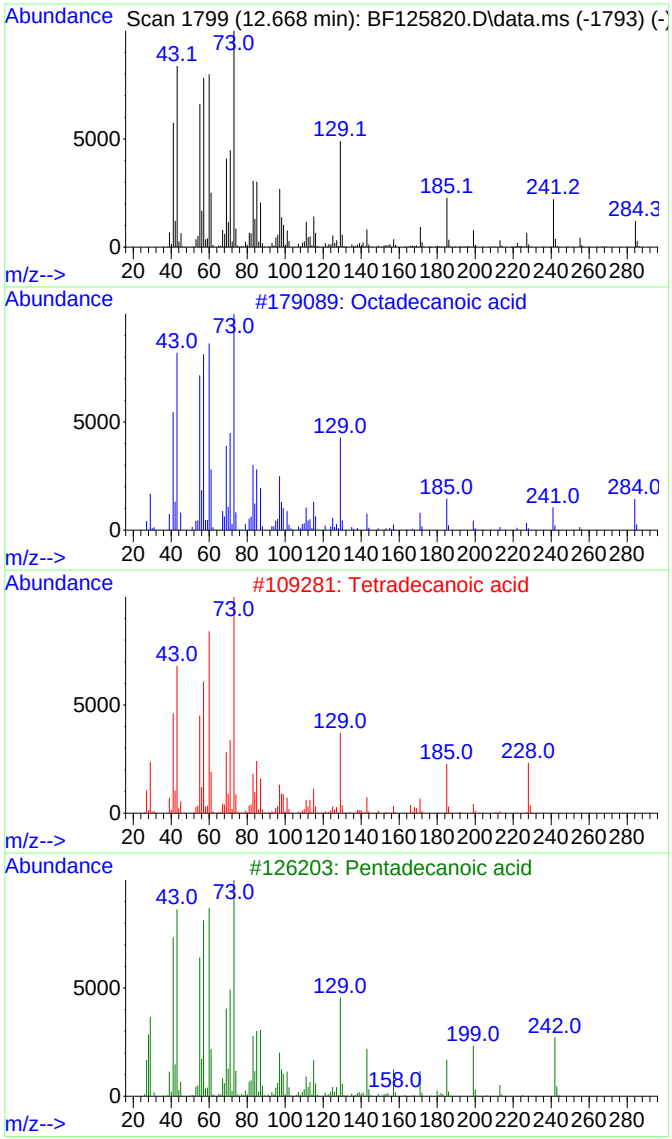
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

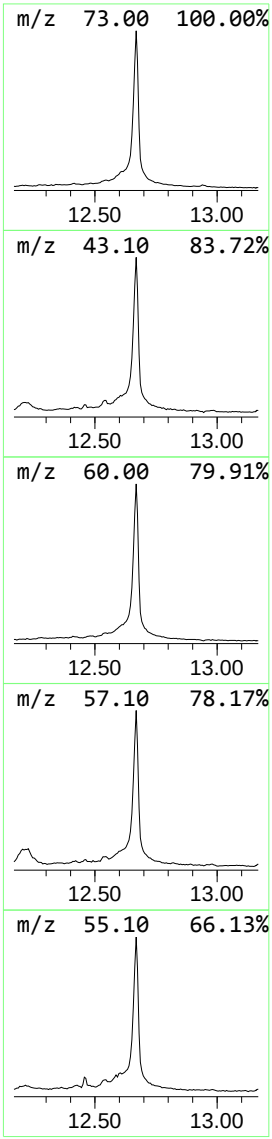
**********

Peak Number 9 Octadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.668 | 58.09 ng | 6012250 | Phenanthrene-d10 | 11.363 |

| 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 | 87 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 5 | Oxalic acid, propyl tetradecyl e... | 328 | C19H36O4 | 1000309-26-7 | 25 |



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Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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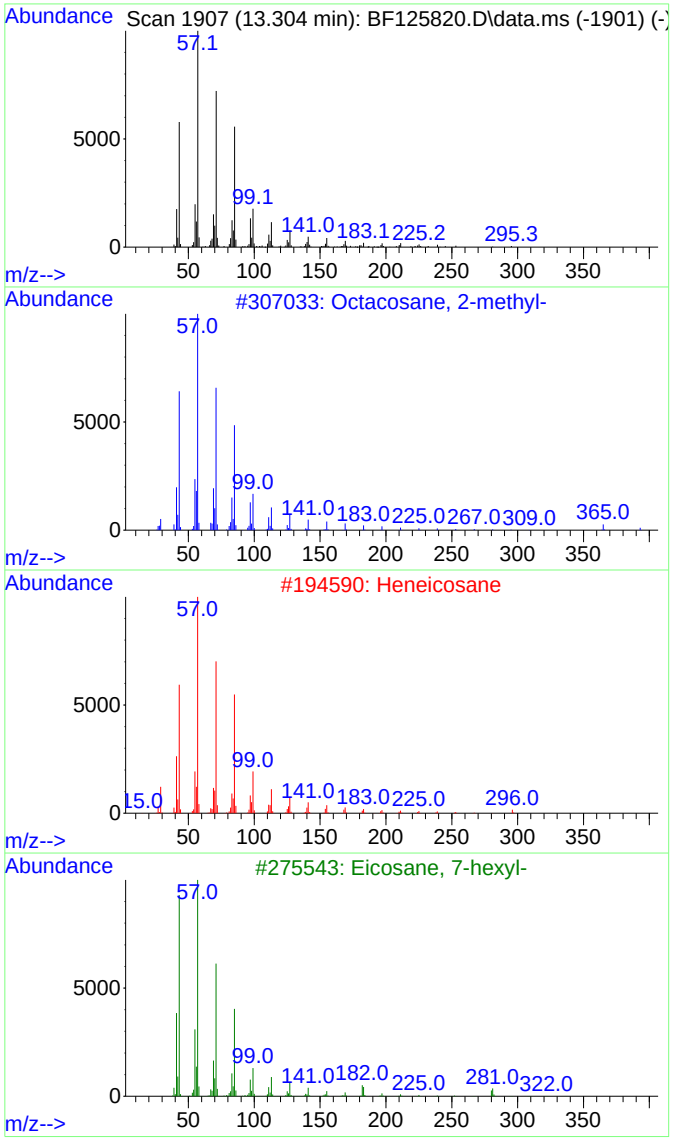
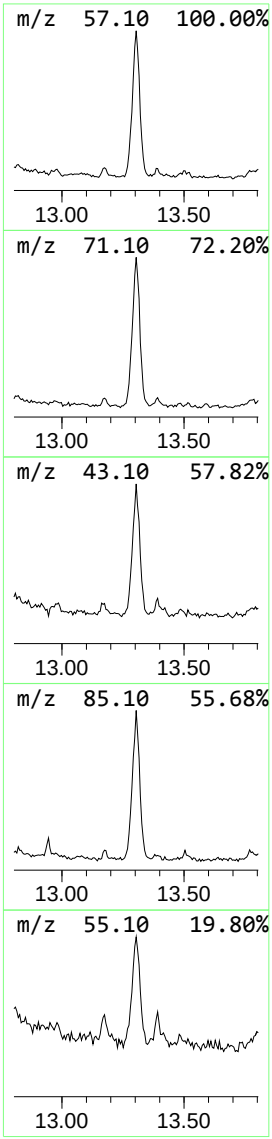
Peak Number 10 Octacosane, 2-methyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.304 | 8.66 ng | 727191 | Chrysene-d12 | 13.992 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 90 |
| 4 | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 87 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |



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Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

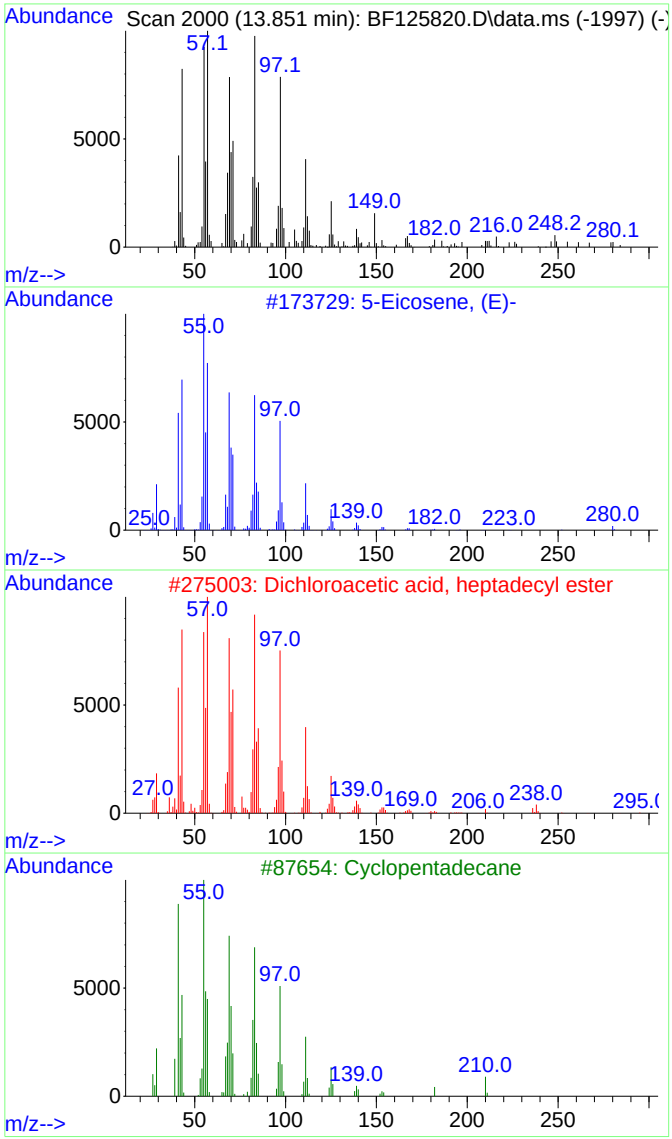
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

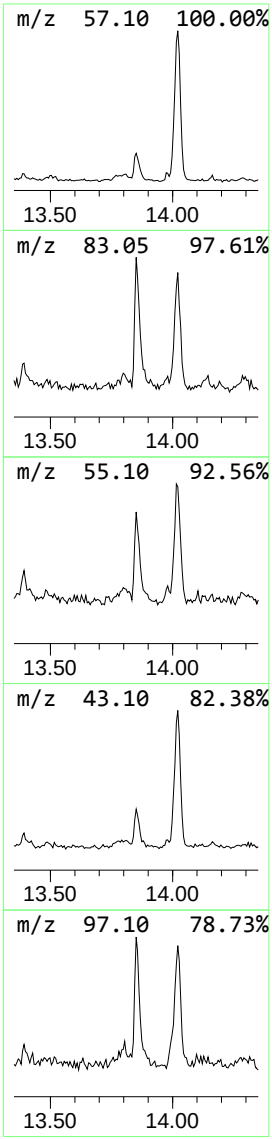
**********

Peak Number 11 5-Eicosene, (E)- Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.851 | 3.62 ng | 304151 | Chrysene-d12 | 13.992 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 96 |
| 2 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 95 |
| 3 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 94 |
| 4 | 1-Tetracosene | 336 | C24H48 | 010192-32-2 | 94 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |



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Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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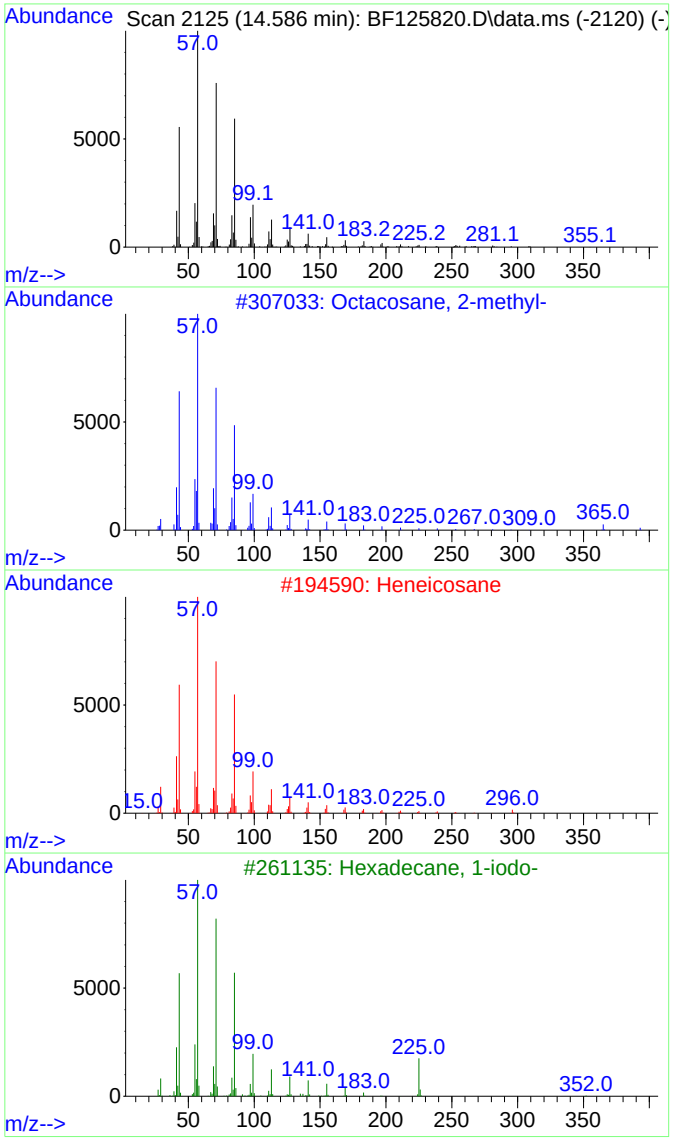
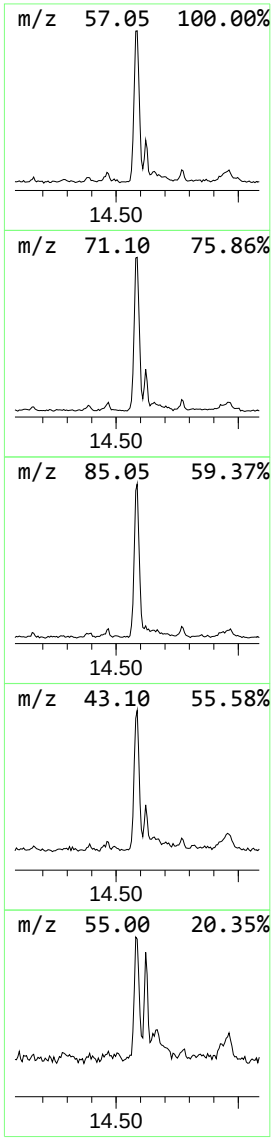
Peak Number 12 Heneicosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.586 | 9.88 ng | 829749 | Chrysene-d12 | 13.992 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 91 |
| 4 | Pentacosane | 352 | C25H52 | 000629-99-2 | 91 |
| 5 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |



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Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

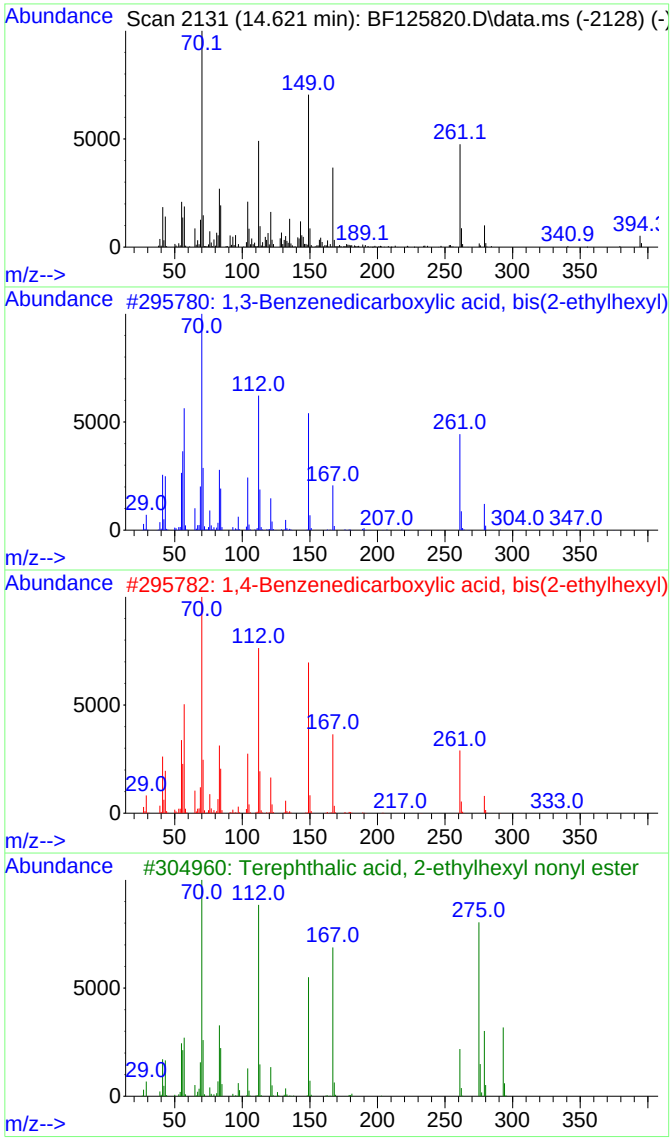
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

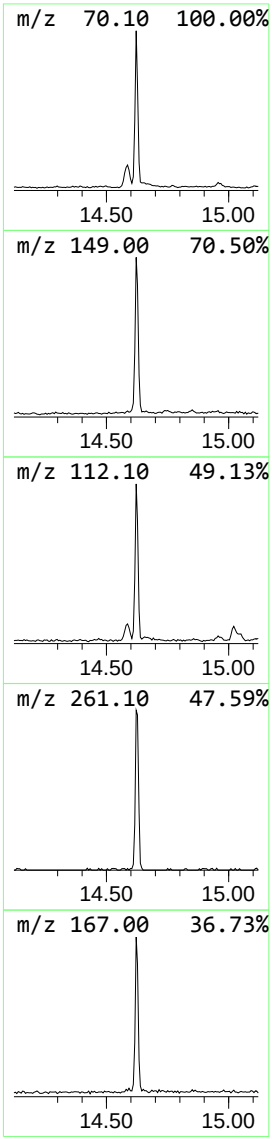
**********

Peak Number 13 unknown14.621 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.621 | 9.43 ng | 792083 | Chrysene-d12 | 13.992 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 000137-89-3 | 90 |
| 2 | 1,4-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 006422-86-2 | 52 |
| 3 | Terephthalic acid, 2-ethylhexyl ... | 404 | C25H40O4 | 1000324-00-6 | 38 |
| 4 | Benzeneethanamine, N-(1-methylet... | 161 | C11H15N | 010433-34-8 | 14 |
| 5 | l-Proline, N-(3-cyclopentylpropi... | 253 | C14H23NO3 | 1000299-65-4 | 14 |



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Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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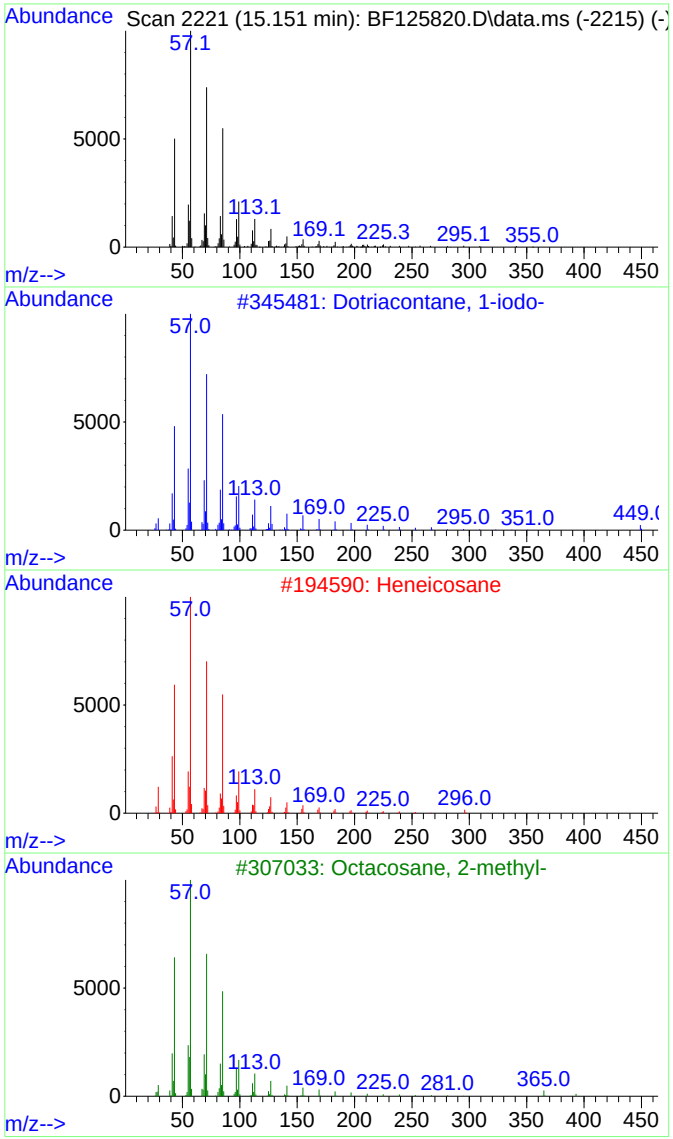
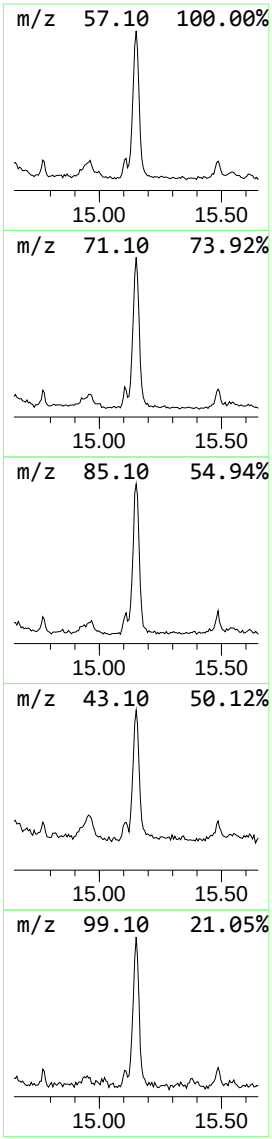
Peak Number 14 Dotriacontane, 1-iodo- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.151 | 9.75 ng | 663087 | Perylene-d12 | 15.451 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



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Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

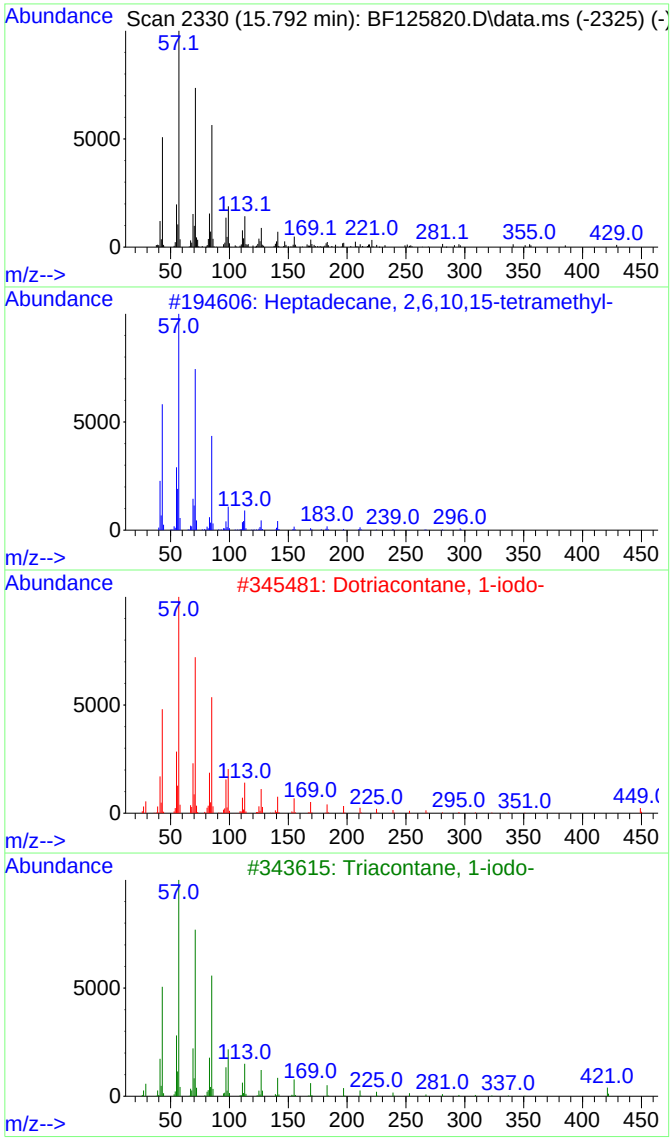
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

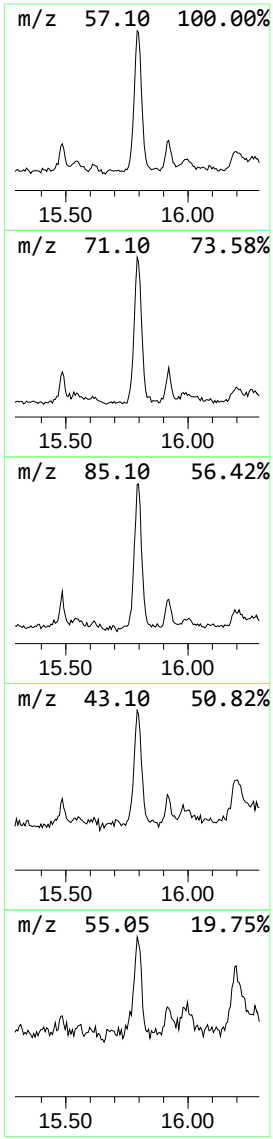
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 15 Heptadecane, 2,6,10,15-tetr... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.792 | 8.08 ng | 549612 | Perylene-d12 | 15.451 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 93 |
| 2 | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 91 |
| 3 | Triacontane, 1-iodo- | 548 | C30H61I | 1000406-32-3 | 91 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 5 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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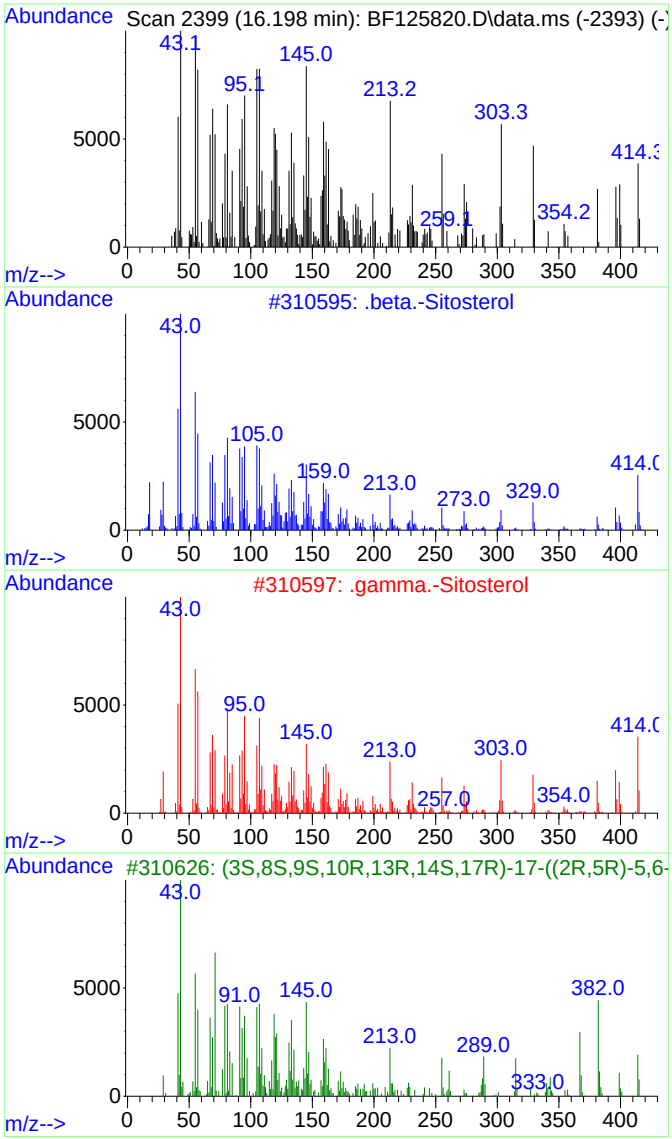
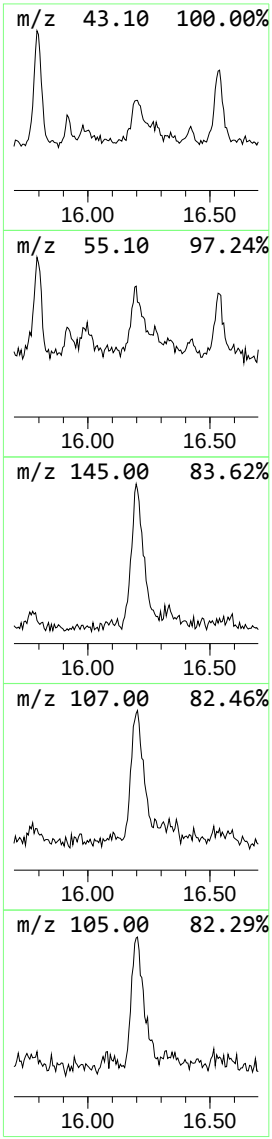
Peak Number 16 .beta.-Sitosterol Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.198 | 8.95 ng | 608380 | Perylene-d12 | 15.451 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .beta.-Sitosterol | 414 | C29H50O | 000083-46-5 | 98 |
| 2 | .gamma.-Sitosterol | 414 | C29H50O | 000083-47-6 | 95 |
| 3 | (3S,8S,9S,10R,13R,14S,17R)-17-((... | 414 | C29H50O | 029365-29-5 | 78 |
| 4 | .beta.-Sitosterol acetate | 456 | C31H52O2 | 000915-05-9 | 46 |
| 5 | Pregn-5-en-3-ol, 21-bromo-20-met... | 394 | C22H35BrO | 055103-80-5 | 35 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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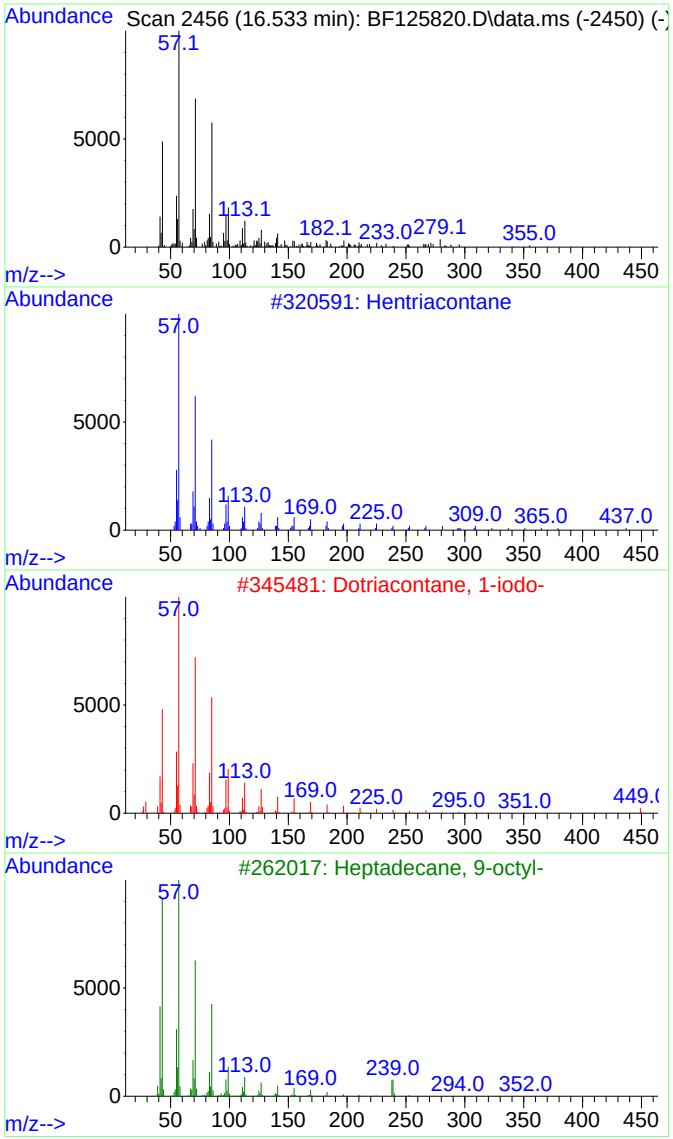
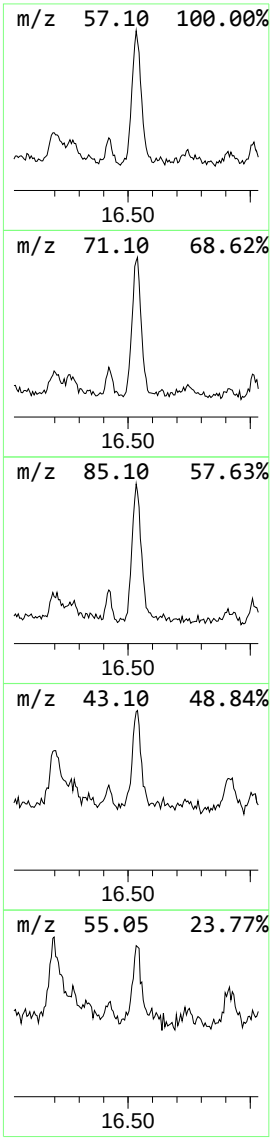
Peak Number 17 Hentriacontane Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.533 | 6.55 ng | 445443 | Perylene-d12 | 15.451 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |
| 2 | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 87 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 4 | Pentacosane | 352 | C25H52 | 000629-99-2 | 87 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 86 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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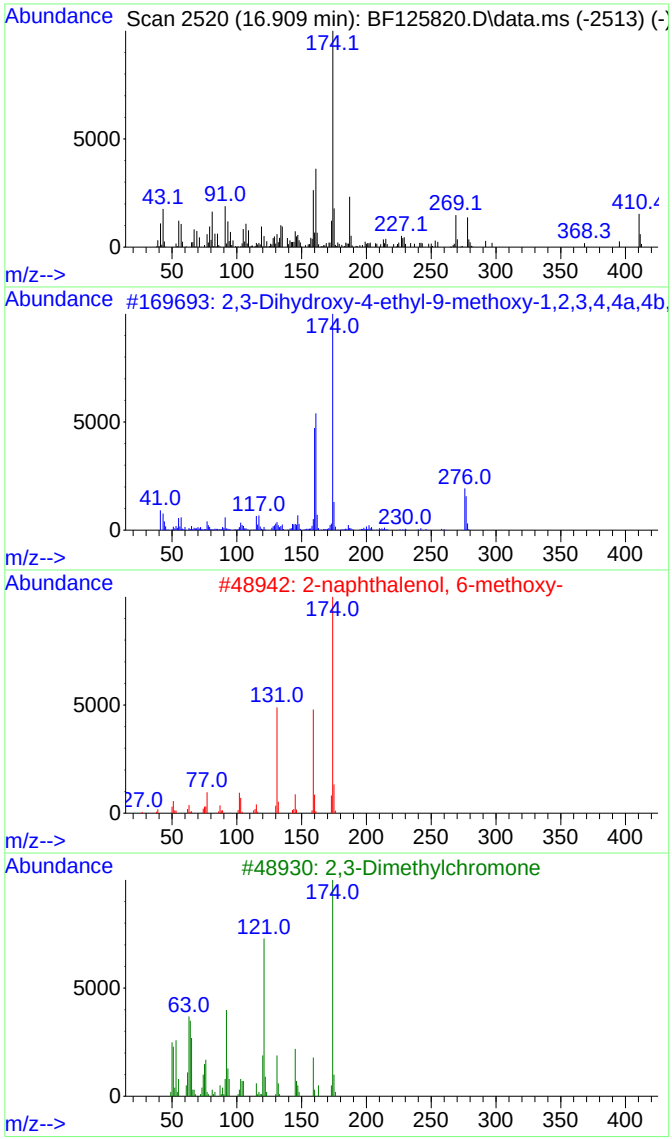
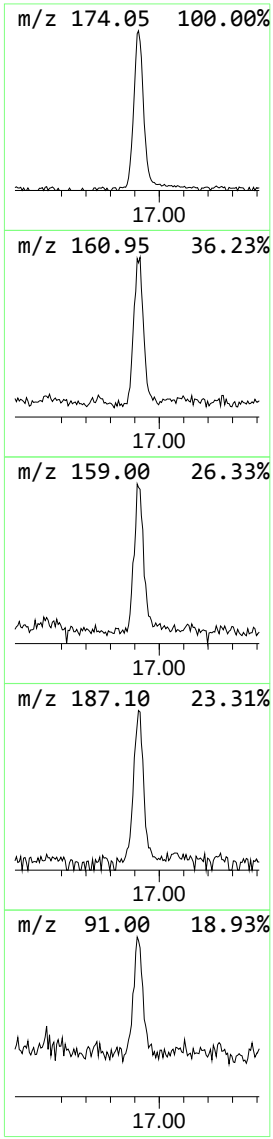
Peak Number 18 unknown16.909 Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.909 | 7.89 ng | 536541 | Perylene-d12 | 15.451 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,3-Dihydroxy-4-ethyl-9-methoxy-... | 277 | C16H23NO3 | 1000111-32-1 | 43 |
| 2 | 2-naphthalenol, 6-methoxy- | 174 | C11H10O2 | 1000404-68-0 | 43 |
| 3 | 2,3-Dimethylchromone | 174 | C11H10O2 | 017584-90-6 | 38 |
| 4 | Quinazoline, 4-ethyl-, 3-oxide | 174 | C10H10N2O | 037920-74-4 | 38 |
| 5 | Butanamide, 4,4,4-trifluoro-3-ox... | 312 | C15H15F3N2O2 | 1000351-42-8 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125820.D
Acq On : 13 Oct 2021 11:36
Operator : JU/CG
Sample : M4158-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.140 | 32.4 | ng | 2089010 | 1 | 6.845 | 1290650 | 20.0 |
| 2-Pentanone, 4-... | 5.069 | 2.8 | ng | 179578 | 1 | 6.845 | 1290650 | 20.0 |
| Ethanol, 2-(2-b... | 8.028 | 6.5 | ng | 583523 | 2 | 8.122 | 1789590 | 20.0 |
| 1,4-Benzenedica... | 11.198 | 9.7 | ng | 1002360 | 4 | 11.363 | 2070080 | 20.0 |
| 1,3-Benzenedica... | 11.227 | 14.9 | ng | 1536650 | 4 | 11.363 | 2070080 | 20.0 |
| n-Hexadecanoic ... | 11.880 | 20.5 | ng | 2121710 | 4 | 11.363 | 2070080 | 20.0 |
| trans-Sinapalde... | 12.021 | 3.2 | ng | 329719 | 4 | 11.363 | 2070080 | 20.0 |
| trans-Sinapyl a... | 12.063 | 2.3 | ng | 237587 | 4 | 11.363 | 2070080 | 20.0 |
| Octadecanoic acid | 12.668 | 58.1 | ng | 6012250 | 4 | 11.363 | 2070080 | 20.0 |
| Octacosane, 2-m... | 13.304 | 8.7 | ng | 727191 | 5 | 13.992 | 1680190 | 20.0 |
| 5-Eicosene, (E)- | 13.851 | 3.6 | ng | 304151 | 5 | 13.992 | 1680190 | 20.0 |
| Heneicosane | 14.586 | 9.9 | ng | 829749 | 5 | 13.992 | 1680190 | 20.0 |
| unknown14.621 | 14.621 | 9.4 | ng | 792083 | 5 | 13.992 | 1680190 | 20.0 |
| Dotriacontane, ... | 15.151 | 9.8 | ng | 663087 | 6 | 15.451 | 1359830 | 20.0 |
| Heptadecane, 2,... | 15.792 | 8.1 | ng | 549612 | 6 | 15.451 | 1359830 | 20.0 |
| .beta.-Sitosterol | 16.198 | 8.9 | ng | 608380 | 6 | 15.451 | 1359830 | 20.0 |
| Hentriacontane | 16.533 | 6.5 | ng | 445443 | 6 | 15.451 | 1359830 | 20.0 |
| unknown16.909 | 16.909 | 7.9 | ng | 536541 | 6 | 15.451 | 1359830 | 20.0 |