LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137039.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.158 | 9 | 12 | 24 | rVB2 | 19758 | 36131 | 2.45% | 0.321% |
| 2 | 5.022 | 495 | 499 | 509 | rVB | 71794 | 85678 | 5.80% | 0.761% |
| 3 | 5.434 | 565 | 569 | 587 | rBV | 1205031 | 1221615 | 82.69% | 10.849% |
| 4 | 6.434 | 735 | 739 | 755 | rBV | 1208799 | 1223137 | 82.79% | 10.862% |
| 5 | 6.781 | 795 | 798 | 802 | rBV | 418071 | 339159 | 22.96% | 3.012% |
| 6 | 7.345 | 890 | 894 | 897 | rBV | 895515 | 788026 | 53.34% | 6.998% |
| 7 | 8.057 | 1012 | 1015 | 1019 | rBV | 525934 | 431755 | 29.22% | 3.834% |
| 8 | 9.134 | 1194 | 1198 | 1202 | rBV | 1600566 | 1477388 | 100.00% | 13.120% |
| 9 | 9.816 | 1310 | 1314 | 1318 | rBV | 579258 | 467669 | 31.66% | 4.153% |
| 10 | 10.616 | 1446 | 1450 | 1465 | rBV | 787854 | 806311 | 54.58% | 7.160% |
| 11 | 10.728 | 1465 | 1469 | 1476 | rVB2 | 15468 | 21809 | 1.48% | 0.194% |
| 12 | 11.310 | 1564 | 1568 | 1571 | rBV | 527427 | 447769 | 30.31% | 3.976% |
| 13 | 11.333 | 1571 | 1572 | 1576 | rVV | 92445 | 53874 | 3.65% | 0.478% |
| 14 | 11.386 | 1576 | 1581 | 1584 | rVB | 17089 | 19748 | 1.34% | 0.175% |
| 15 | 11.816 | 1649 | 1654 | 1656 | rBV | 25318 | 27256 | 1.84% | 0.242% |
| 16 | 11.839 | 1656 | 1658 | 1665 | rVV | 195030 | 207938 | 14.07% | 1.847% |
| 17 | 11.928 | 1670 | 1673 | 1675 | rVV | 34782 | 39492 | 2.67% | 0.351% |
| 18 | 11.951 | 1675 | 1677 | 1683 | rVB | 20662 | 18835 | 1.27% | 0.167% |
| 19 | 12.369 | 1744 | 1748 | 1750 | rBV | 21800 | 23593 | 1.60% | 0.210% |
| 20 | 12.457 | 1760 | 1763 | 1767 | rVB3 | 14075 | 17441 | 1.18% | 0.155% |
| 21 | 12.527 | 1772 | 1775 | 1779 | rBV | 125022 | 121329 | 8.21% | 1.077% |
| 22 | 12.633 | 1790 | 1793 | 1798 | rBV | 67337 | 83972 | 5.68% | 0.746% |
| 23 | 12.763 | 1809 | 1815 | 1820 | rVB | 140165 | 135372 | 9.16% | 1.202% |
| 24 | 12.904 | 1835 | 1839 | 1843 | rBV | 1313404 | 1174683 | 79.51% | 10.432% |
| 25 | 12.980 | 1849 | 1852 | 1856 | rBV3 | 15063 | 22465 | 1.52% | 0.200% |
| 26 | 13.069 | 1864 | 1867 | 1869 | rBV4 | 16181 | 21989 | 1.49% | 0.195% |
| 27 | 13.092 | 1869 | 1871 | 1874 | rVB | 19589 | 16704 | 1.13% | 0.148% |
| 28 | 13.198 | 1885 | 1889 | 1893 | rBV2 | 21629 | 20618 | 1.40% | 0.183% |
| 29 | 13.322 | 1907 | 1910 | 1914 | rBV | 17723 | 17739 | 1.20% | 0.158% |
| 30 | 13.474 | 1932 | 1936 | 1939 | rVB4 | 17022 | 17769 | 1.20% | 0.158% |
| 31 | 13.610 | 1956 | 1959 | 1964 | rVB | 17895 | 18167 | 1.23% | 0.161% |
| 32 | 13.716 | 1974 | 1977 | 1979 | rBV | 17878 | 17331 | 1.17% | 0.154% |
| 33 | 13.810 | 1990 | 1993 | 1997 | rVB3 | 24366 | 31216 | 2.11% | 0.277% |
| 34 | 13.857 | 1997 | 2001 | 2004 | rBV2 | 14617 | 17246 | 1.17% | 0.153% |
| 35 | 13.910 | 2004 | 2010 | 2011 | rBV6 | 23684 | 35842 | 2.43% | 0.318% |
| 36 | 13.939 | 2012 | 2015 | 2016 | rVV | 49909 | 56482 | 3.82% | 0.502% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 13.969 | 2016 | 2020 | 2023 | rVV2 | 427238 | 458950 | 31.06% | 4.076% |
| 38 | 13.992 | 2023 | 2024 | 2029 | rVB | 73999 | 61726 | 4.18% | 0.548% |
| 39 | 14.127 | 2044 | 2047 | 2055 | rBV3 | 30975 | 45336 | 3.07% | 0.403% |
| 40 | 14.357 | 2084 | 2086 | 2090 | rVB | 24680 | 24346 | 1.65% | 0.216% |
| 41 | 14.392 | 2090 | 2092 | 2096 | rBV | 17018 | 15977 | 1.08% | 0.142% |
| 42 | 14.433 | 2096 | 2099 | 2105 | rVV4 | 32321 | 40169 | 2.72% | 0.357% |
| 43 | 14.727 | 2145 | 2149 | 2158 | rVB | 225171 | 258780 | 17.52% | 2.298% |
| 44 | 14.816 | 2162 | 2164 | 2169 | rVB2 | 17209 | 19662 | 1.33% | 0.175% |
| 45 | 14.863 | 2169 | 2172 | 2175 | rBV5 | 16870 | 19757 | 1.34% | 0.175% |
| 46 | 15.021 | 2195 | 2199 | 2202 | rBV | 65283 | 89901 | 6.09% | 0.798% |
| 47 | 15.086 | 2207 | 2210 | 2214 | rVB2 | 27097 | 32132 | 2.17% | 0.285% |
| 48 | 15.227 | 2230 | 2234 | 2238 | rVB5 | 10640 | 17807 | 1.21% | 0.158% |
| 49 | 15.327 | 2248 | 2251 | 2257 | rVB | 38701 | 49115 | 3.32% | 0.436% |
| 50 | 15.392 | 2259 | 2262 | 2267 | rVB | 52729 | 68380 | 4.63% | 0.607% |
| 51 | 15.457 | 2268 | 2273 | 2285 | rBV | 314685 | 429035 | 29.04% | 3.810% |
| 52 | 15.915 | 2349 | 2351 | 2356 | rVB4 | 14172 | 18167 | 1.23% | 0.161% |
| 53 | 17.445 | 2607 | 2611 | 2620 | rVB | 20383 | 47829 | 3.24% | 0.425% |

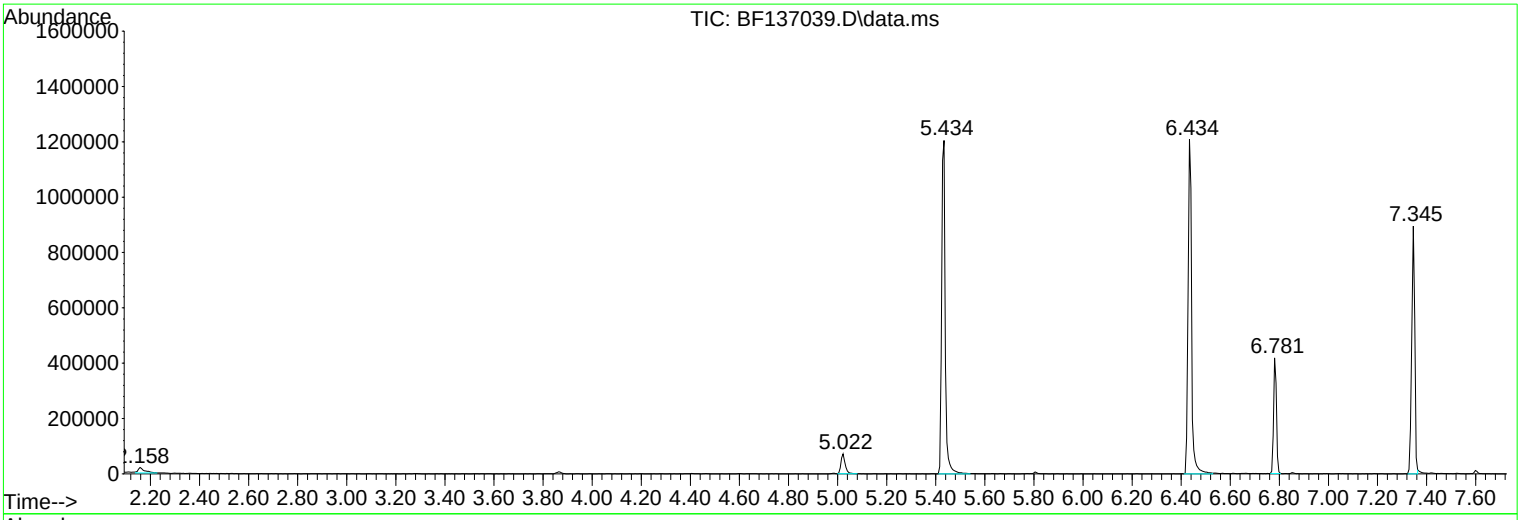
Sum of corrected areas: 11260617

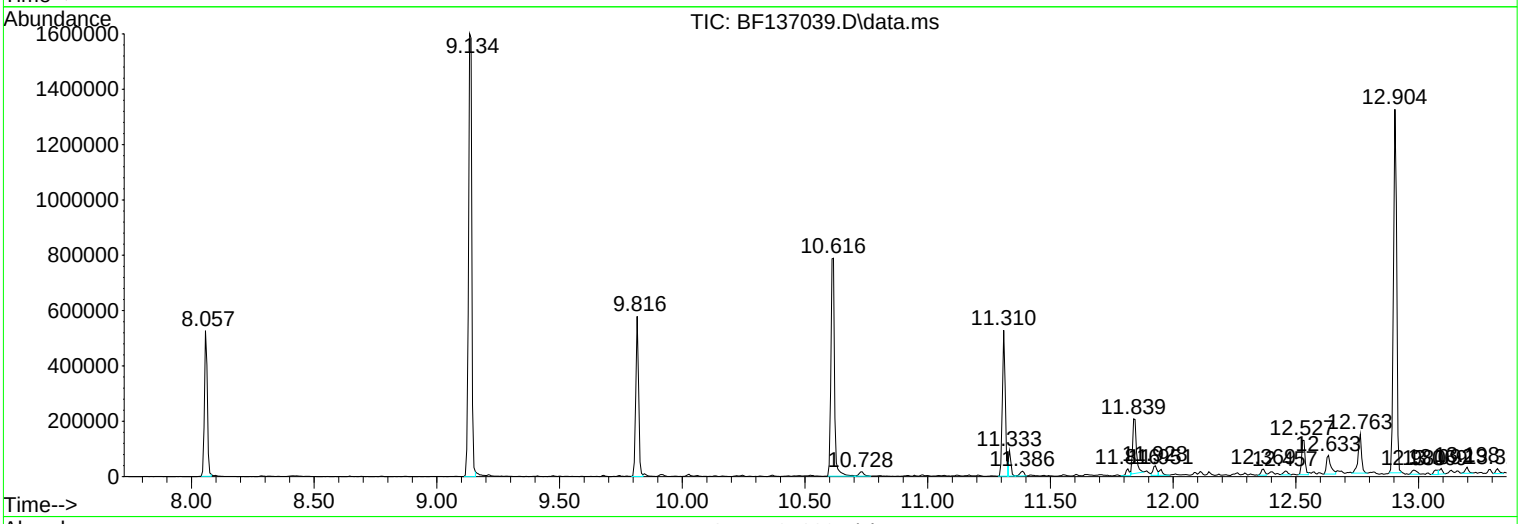
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

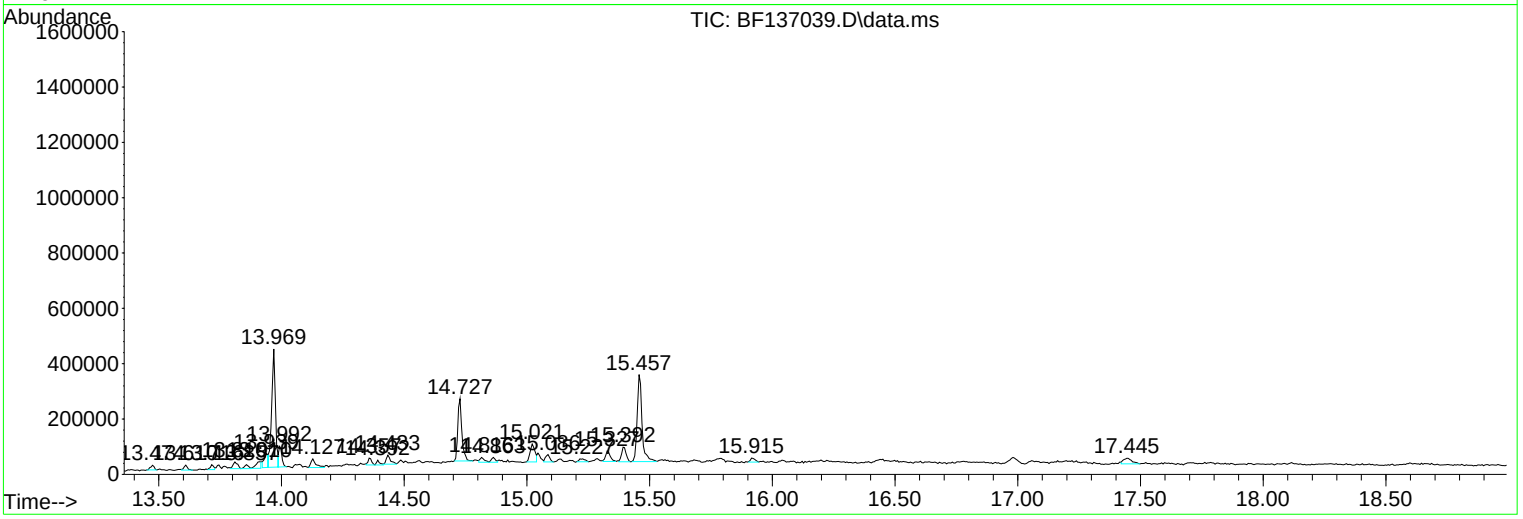
**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

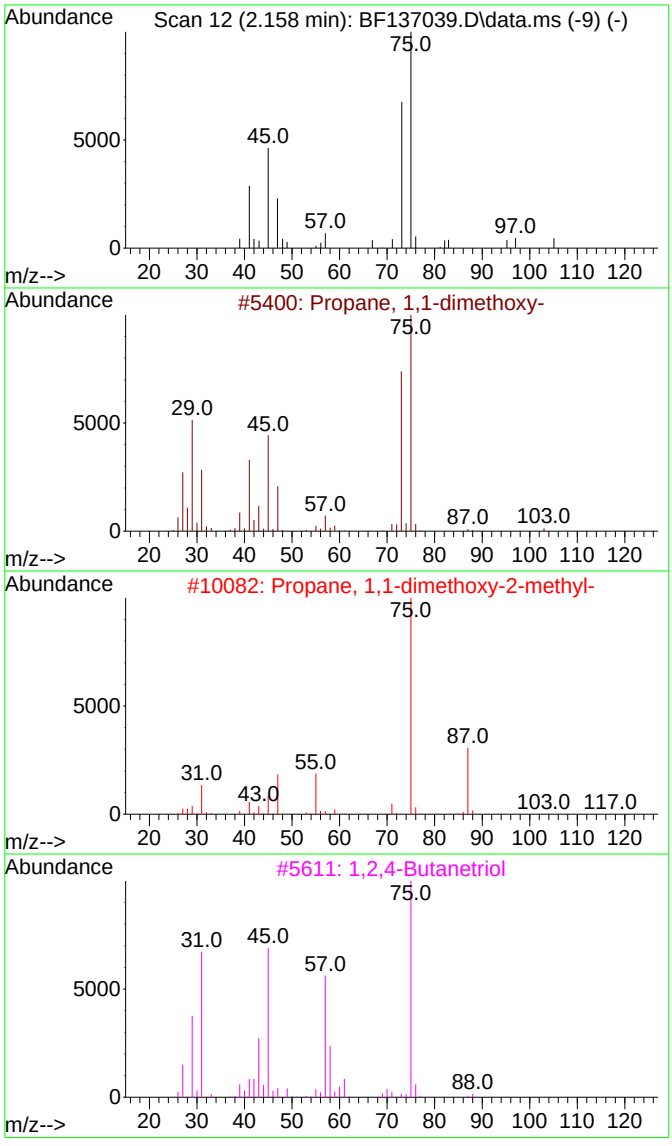
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

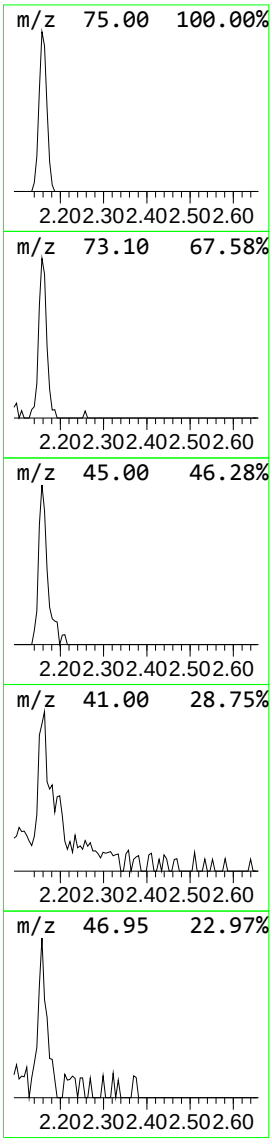
**********

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.158 | 2.13 ng | 36131 | 1,4-Dichlorobenzene-d4 | 6.781 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 72 |
| 2 | Propane, 1,1-dimethoxy-2-methyl- | 118 | C6H14O2 | 041632-89-7 | 28 |
| 3 | 1,2,4-Butanetriol | 106 | C4H10O3 | 003068-00-6 | 9 |
| 4 | Ethane, 2-chloro-1,1-dimethoxy- | 124 | C4H9ClO2 | 000097-97-2 | 9 |
| 5 | 1-Cyclohexyl-3-ethoxy-butan-2-one | 198 | C12H22O2 | 074897-69-1 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

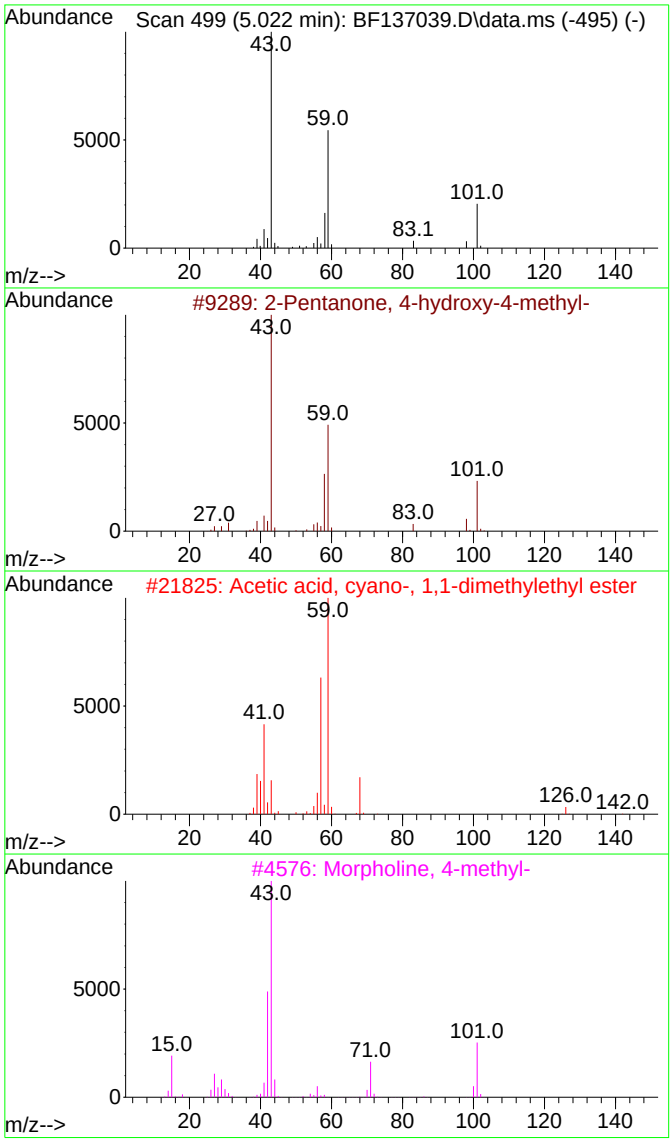
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

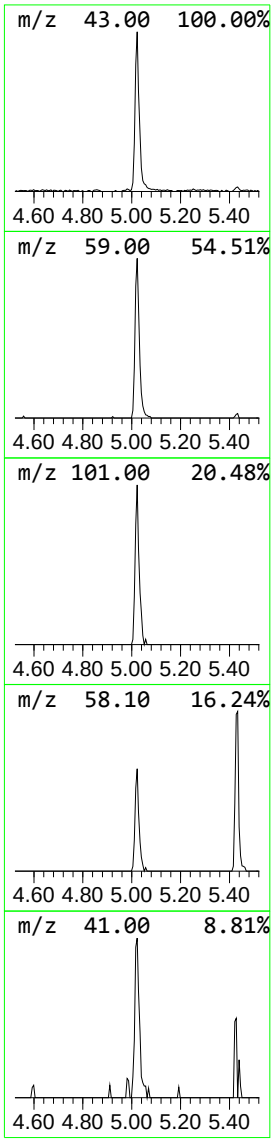
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.022 | 5.05 ng | 85678 | 1,4-Dichlorobenzene-d4 | 6.781 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 47 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

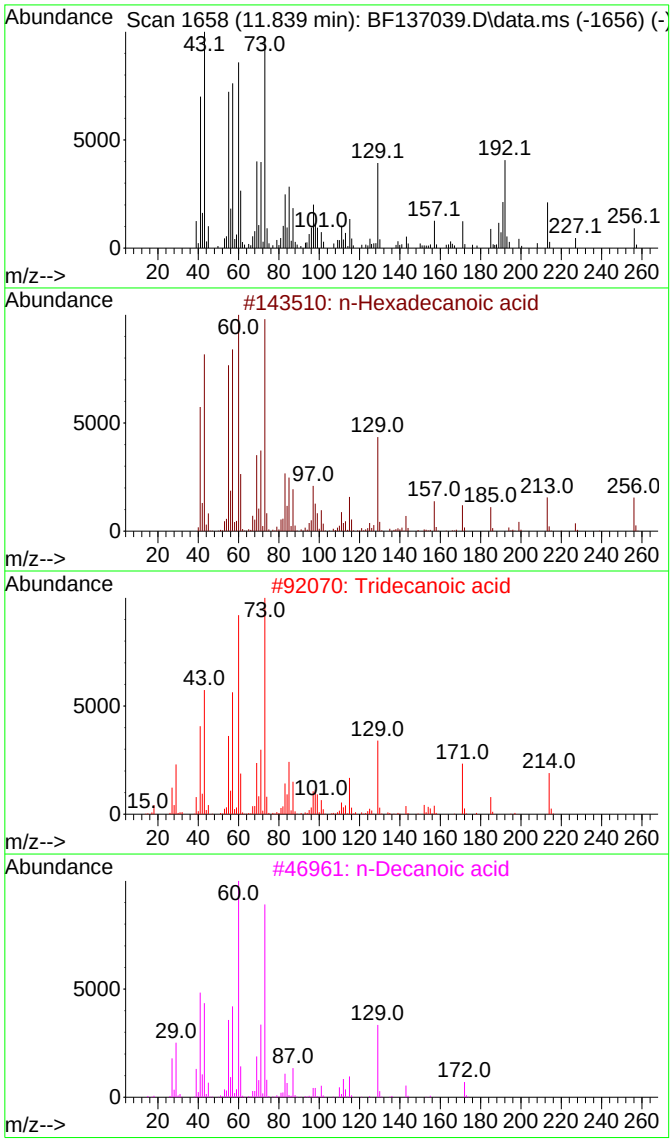
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

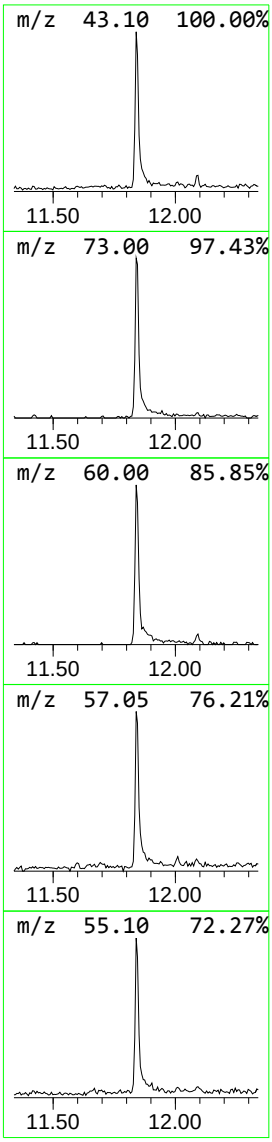
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.839 | 9.29 ng | 207938 | Phenanthrene-d10 | 11.310 |

| 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 | 83 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 60 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 53 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

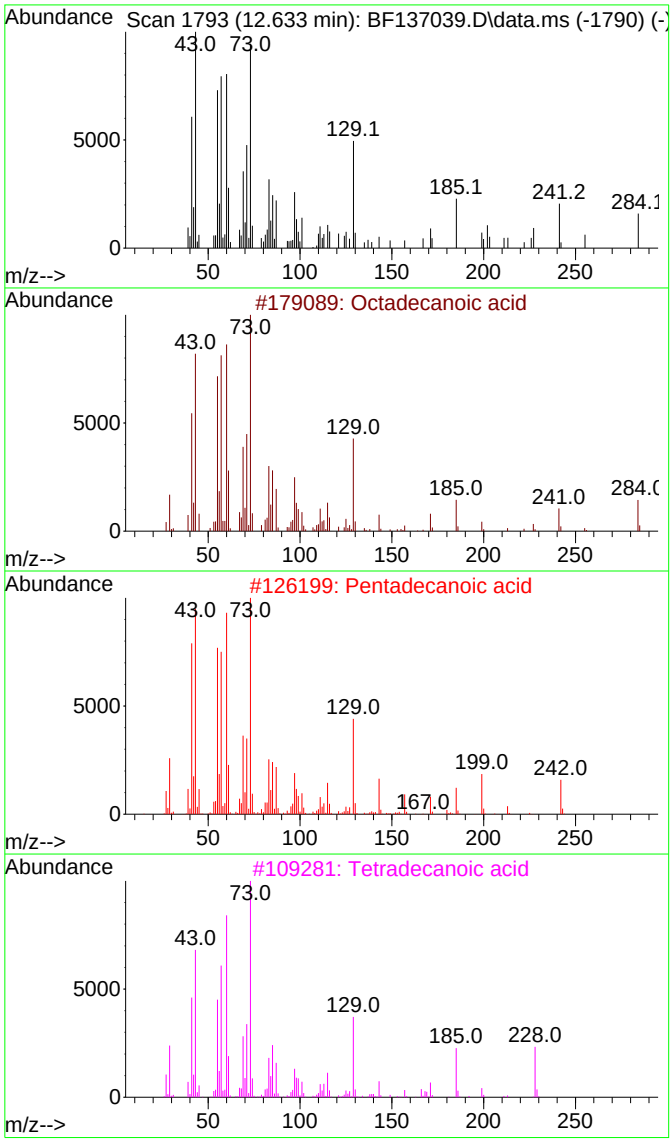
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

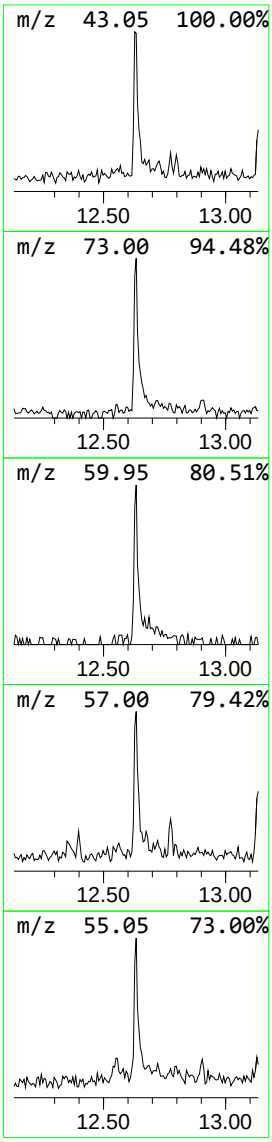
**********

Peak Number 4 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.633 | 3.75 ng | 83972 | Phenanthrene-d10 | 11.310 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 98 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 89 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 4 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 68 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

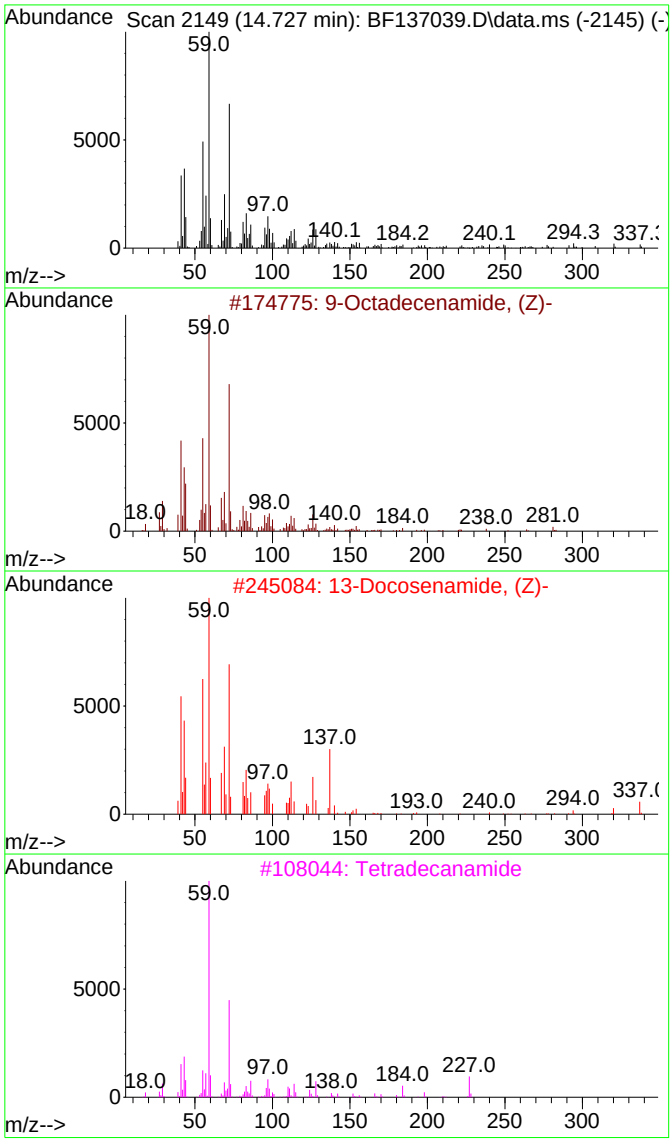
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

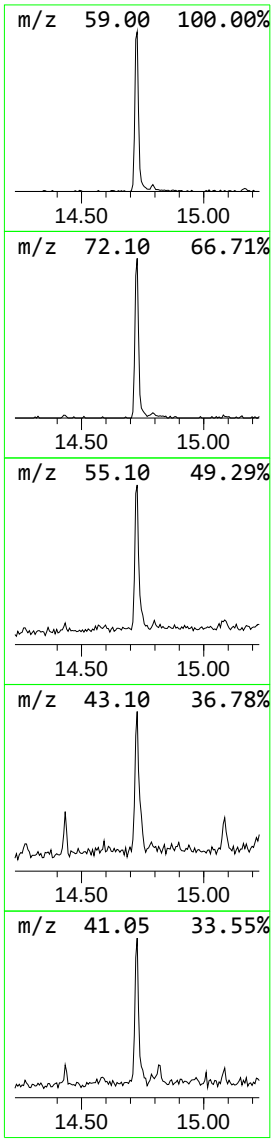
**********

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.727 | 12.06 ng | 258780 | Perylene-d12 | 15.457 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 97 |
| 2 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 83 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 78 |
| 4 | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 68 |
| 5 | Octadecanamide | 283 | C18H37NO | 000124-26-5 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

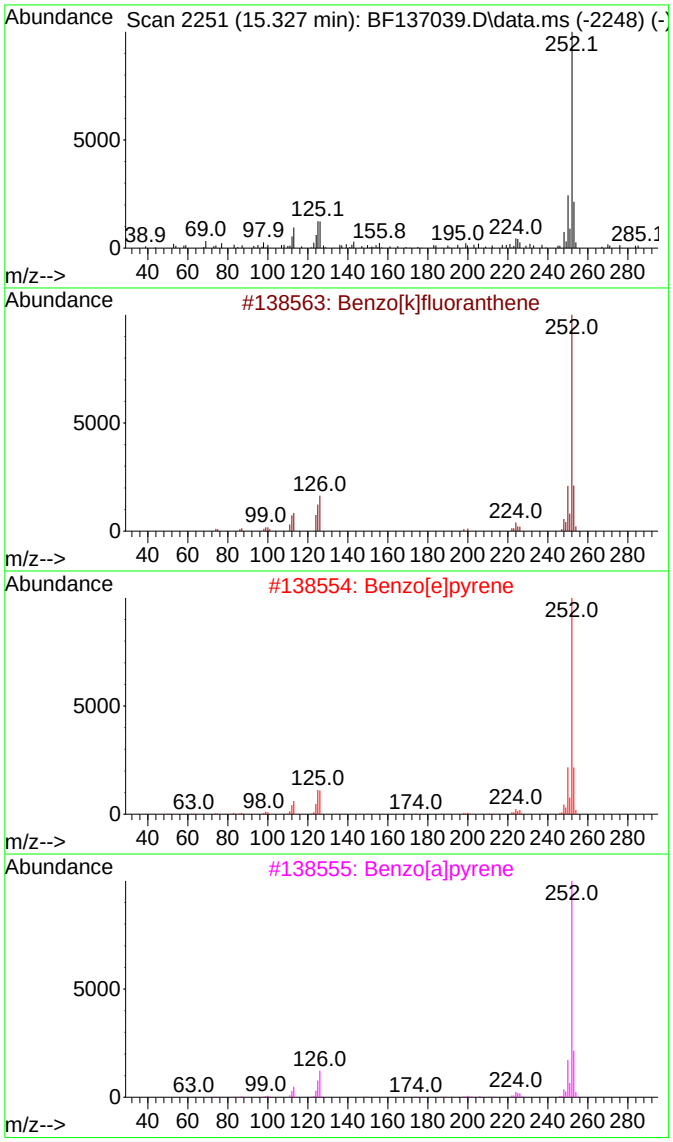
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

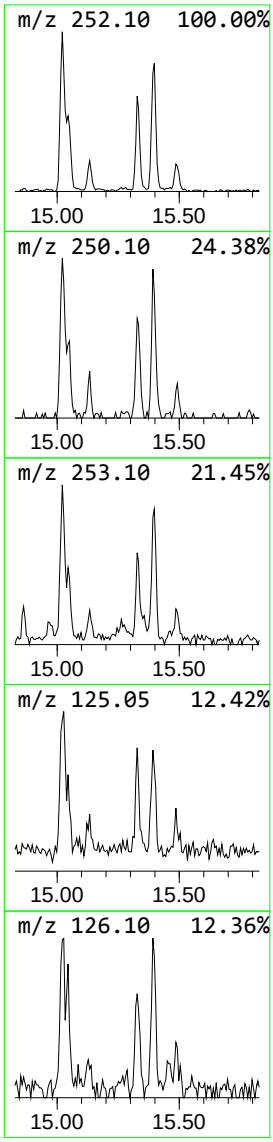
**********

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.327 | 2.29 ng | 49115 | Perylene-d12 | 15.457 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 96 |
| 2 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 96 |
| 3 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 94 |
| 4 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 93 |
| 5 | Perylene | 252 | C20H12 | 000198-55-0 | 81 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137039.D
Acq On : 11 Jan 2024 15:19
Operator : CG\JU
Sample : P1100-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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 |
| Propane, 1,1-di... | 2.158 | 2.1 | ng | 36131 | 1 | 6.781 | 339159 | 20.0 |
| 2-Pentanone, 4-... | 5.022 | 5.0 | ng | 85678 | 1 | 6.781 | 339159 | 20.0 |
| n-Hexadecanoic ... | 11.839 | 9.3 | ng | 207938 | 4 | 11.310 | 447769 | 20.0 |
| Octadecanoic acid | 12.633 | 3.8 | ng | 83972 | 4 | 11.310 | 447769 | 20.0 |
| 9-Octadecenamid... | 14.727 | 12.1 | ng | 258780 | 6 | 15.457 | 429035 | 20.0 |
| Benzo[e]pyrene | 15.327 | 2.3 | ng | 49115 | 6 | 15.457 | 429035 | 20.0 |