LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.916 | 477 | 481 | 489 | rVB | 77388 | 106486 | 2.85% | 0.323% |
| 2 | 5.328 | 546 | 551 | 568 | rBV | 3318355 | 3576315 | 95.80% | 10.842% |
| 3 | 6.363 | 721 | 727 | 743 | rBV | 3079887 | 3733293 | 100.00% | 11.318% |
| 4 | 6.486 | 743 | 748 | 751 | rBV | 3728844 | 3559764 | 95.35% | 10.792% |
| 5 | 6.710 | 783 | 786 | 795 | rBV | 1129759 | 934362 | 25.03% | 2.833% |
| 6 | 6.869 | 808 | 813 | 816 | rBV | 3025162 | 2802229 | 75.06% | 8.495% |
| 7 | 7.281 | 878 | 883 | 886 | rBV | 2403686 | 2258517 | 60.50% | 6.847% |
| 8 | 7.457 | 910 | 913 | 916 | rVB | 47181 | 41572 | 1.11% | 0.126% |
| 9 | 7.992 | 1000 | 1004 | 1023 | rVB | 1388663 | 1281689 | 34.33% | 3.886% |
| 10 | 9.069 | 1183 | 1187 | 1190 | rBV | 3940309 | 3666848 | 98.22% | 11.117% |
| 11 | 9.145 | 1197 | 1200 | 1203 | rVB | 59497 | 43927 | 1.18% | 0.133% |
| 12 | 9.463 | 1249 | 1254 | 1261 | rBV | 447548 | 426669 | 11.43% | 1.294% |
| 13 | 9.674 | 1287 | 1290 | 1294 | rBV | 176355 | 144398 | 3.87% | 0.438% |
| 14 | 9.745 | 1298 | 1302 | 1311 | rVB2 | 1498155 | 1350423 | 36.17% | 4.094% |
| 15 | 9.992 | 1341 | 1344 | 1348 | rVB2 | 42709 | 39810 | 1.07% | 0.121% |
| 16 | 10.174 | 1372 | 1375 | 1378 | rVB | 187885 | 153617 | 4.11% | 0.466% |
| 17 | 10.392 | 1407 | 1412 | 1414 | rBV | 47738 | 58806 | 1.58% | 0.178% |
| 18 | 10.539 | 1433 | 1437 | 1447 | rBV | 2090002 | 2010021 | 53.84% | 6.094% |
| 19 | 10.645 | 1452 | 1455 | 1461 | rBV | 161882 | 164026 | 4.39% | 0.497% |
| 20 | 11.092 | 1528 | 1531 | 1533 | rBV | 69709 | 51698 | 1.38% | 0.157% |
| 21 | 11.233 | 1551 | 1555 | 1558 | rBV | 1253859 | 1166108 | 31.24% | 3.535% |
| 22 | 11.368 | 1574 | 1578 | 1581 | rBV | 296459 | 275818 | 7.39% | 0.836% |
| 23 | 11.410 | 1582 | 1585 | 1588 | rVB | 106439 | 92504 | 2.48% | 0.280% |
| 24 | 12.445 | 1759 | 1761 | 1764 | rVB | 104365 | 87805 | 2.35% | 0.266% |
| 25 | 12.674 | 1795 | 1800 | 1804 | rBV | 84025 | 100849 | 2.70% | 0.306% |
| 26 | 12.815 | 1820 | 1824 | 1827 | rBV | 2742334 | 2558205 | 68.52% | 7.756% |
| 27 | 13.710 | 1972 | 1976 | 1986 | rVB | 188365 | 237815 | 6.37% | 0.721% |
| 28 | 13.845 | 1996 | 1999 | 2000 | rBV | 53441 | 51948 | 1.39% | 0.157% |
| 29 | 13.868 | 2000 | 2003 | 2007 | rVV | 844905 | 838178 | 22.45% | 2.541% |
| 30 | 14.892 | 2174 | 2177 | 2180 | rBV | 49792 | 63027 | 1.69% | 0.191% |
| 31 | 15.180 | 2223 | 2226 | 2230 | rVB | 43753 | 51078 | 1.37% | 0.155% |
| 32 | 15.239 | 2233 | 2236 | 2241 | rVV | 52169 | 56107 | 1.50% | 0.170% |
| 33 | 15.298 | 2241 | 2246 | 2257 | rVV | 740148 | 946915 | 25.36% | 2.871% |
| 34 | 15.709 | 2313 | 2316 | 2321 | rVB3 | 36873 | 54226 | 1.45% | 0.164% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-49-9.5-10.0

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:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 32985053

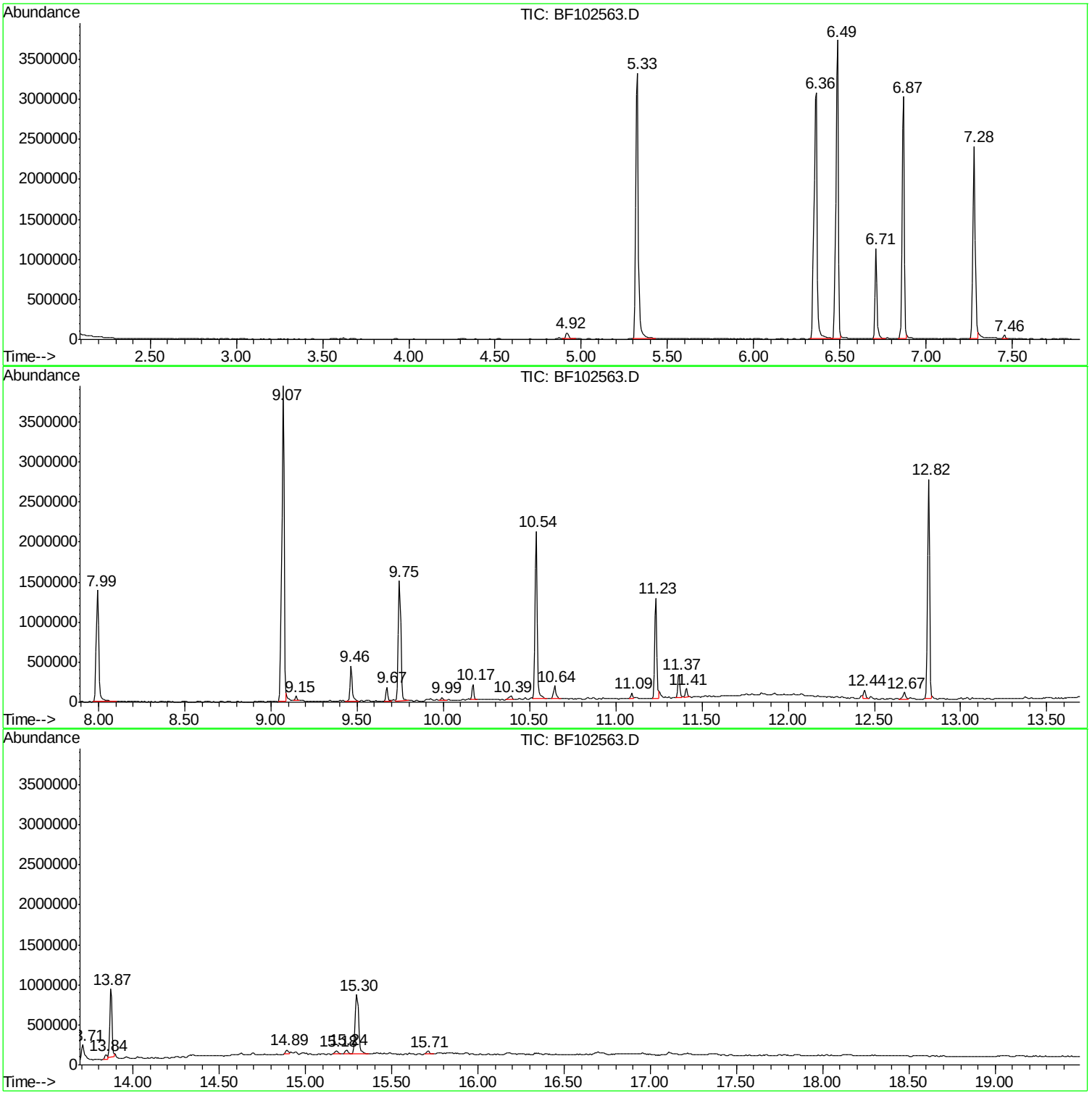
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

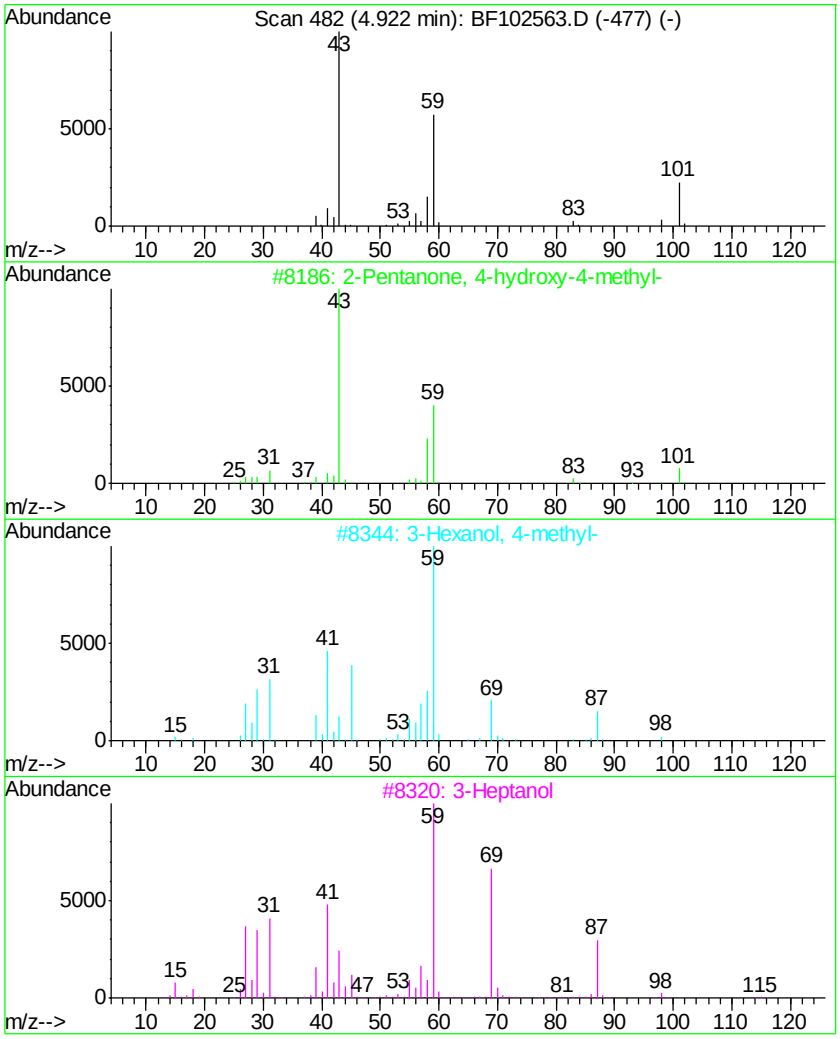
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

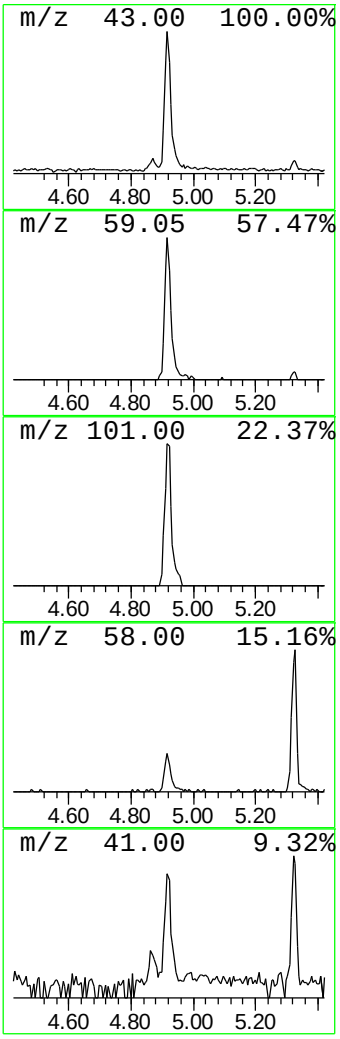
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 2.28 ng | 106486 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 3-Heptanol | 116 | C7H16O | 000589-82-2 | 25 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 5 | 2-Propyn-1-ol, acetate | 98 | C5H6O2 | 000627-09-8 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

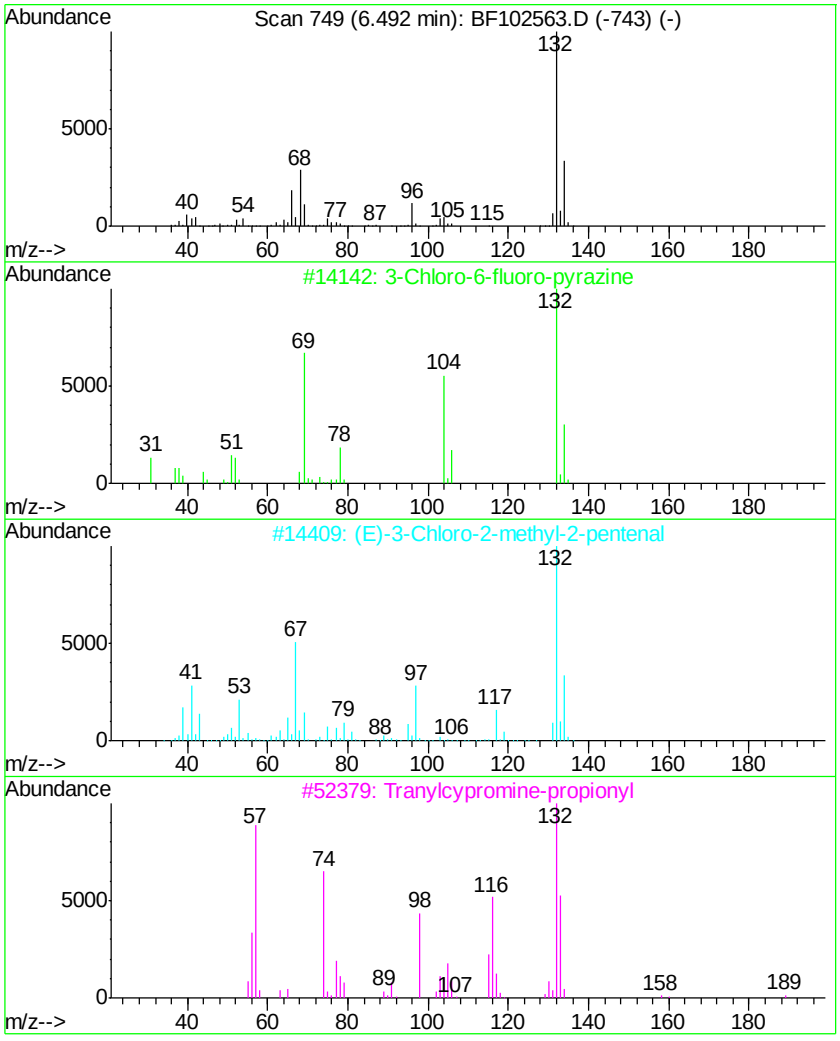
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

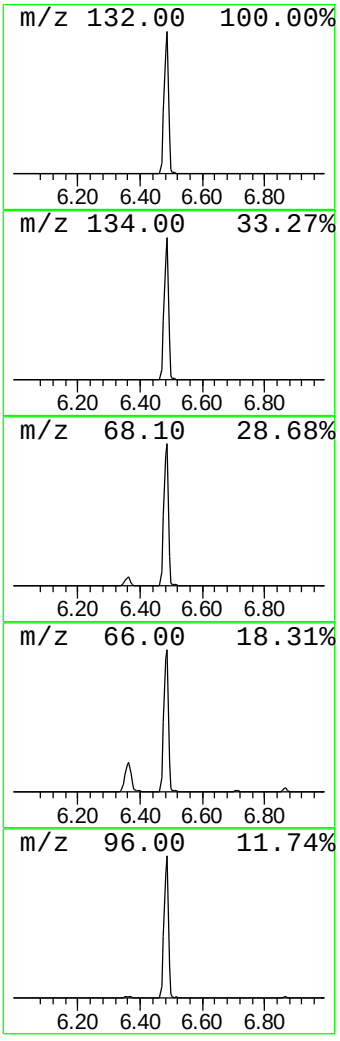
**********

Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.49 | 76.20 ng | 3559760 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

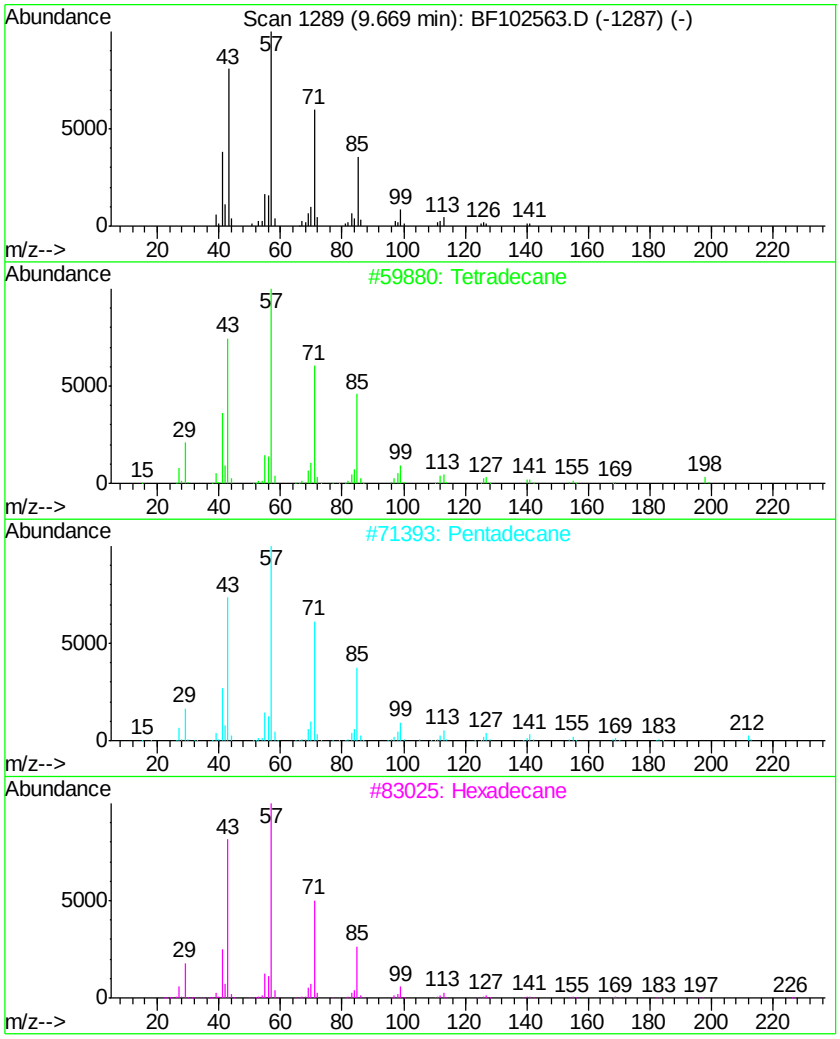
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

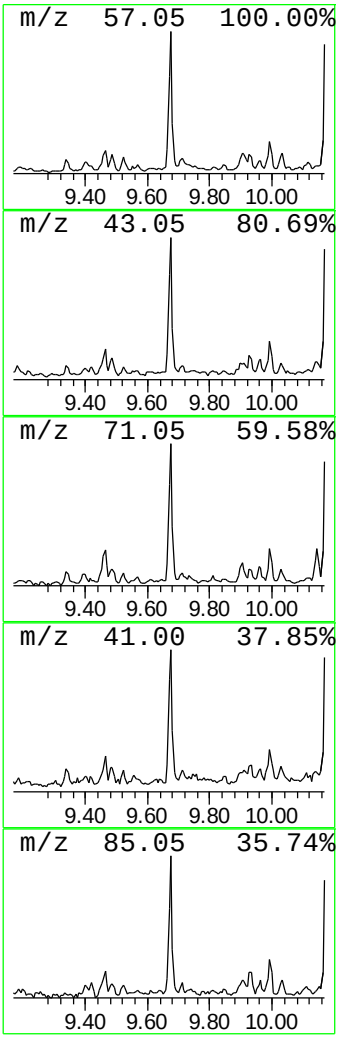
**********

Peak Number 4 Tetradecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.67 | 2.14 ng | 144398 | Acenaphthene-d10 | 9.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 80 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 59 |
| 5 | Sulfurous acid, hexyl heptyl ester | 264 | C13H28O3S | 1000309-12-9 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

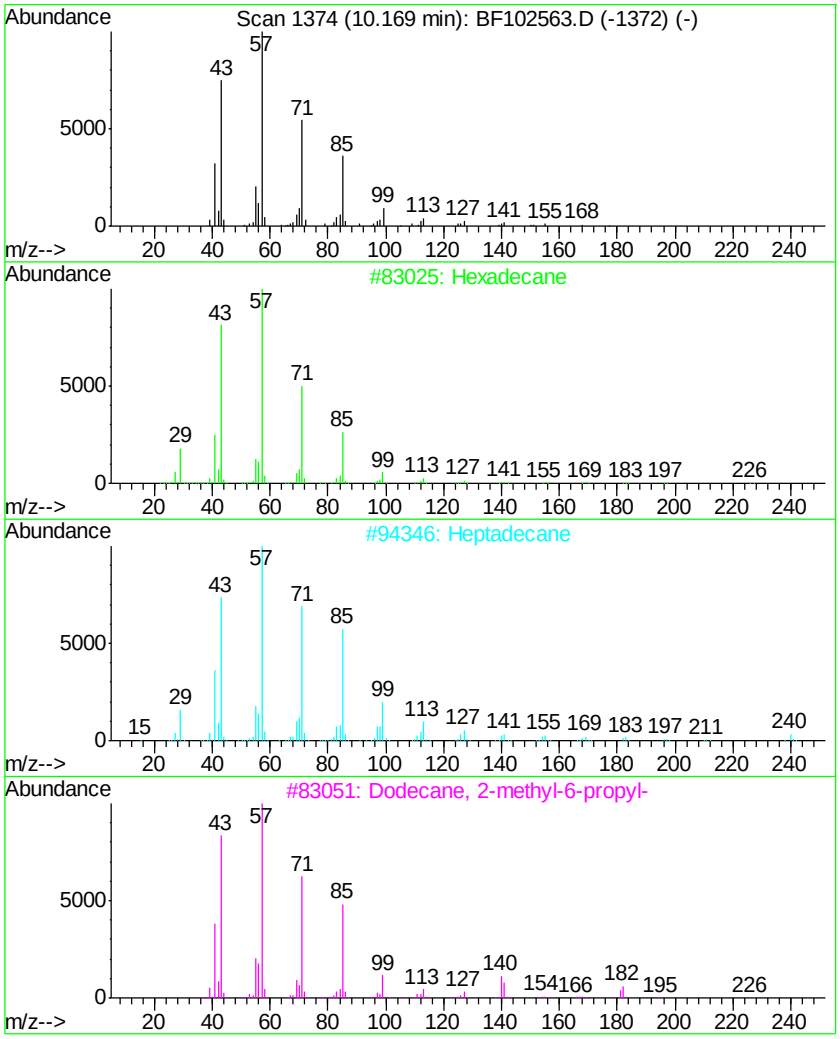
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

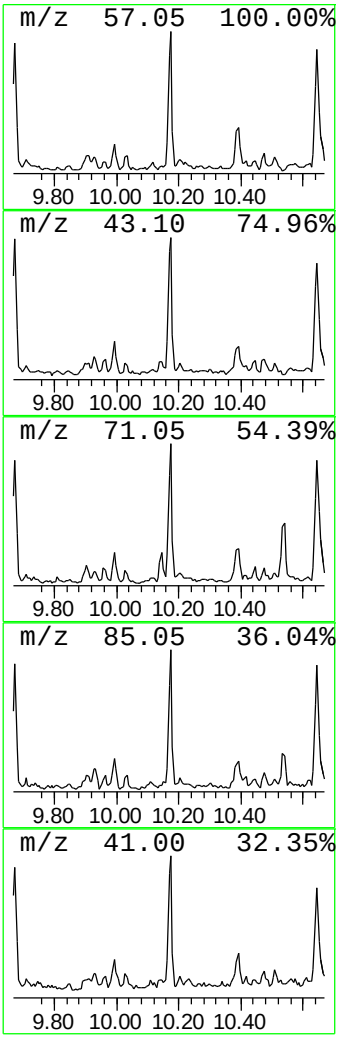
**********

Peak Number 5 Hexadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.17 | 2.28 ng | 153617 | Acenaphthene-d10 | 9.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 97 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 83 |
| 3 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 80 |
| 4 | Sulfurous acid, pentadecyl 2-pro... | 334 | C18H38O3S | 1000309-12-6 | 72 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 72 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

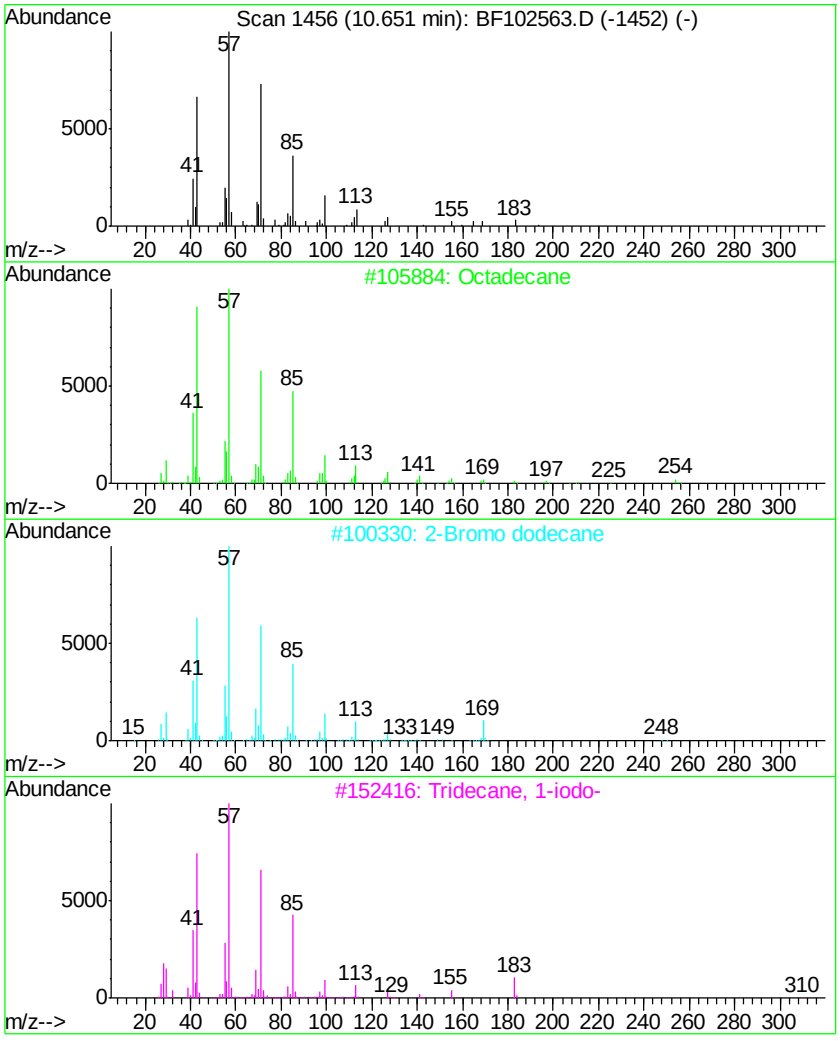
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

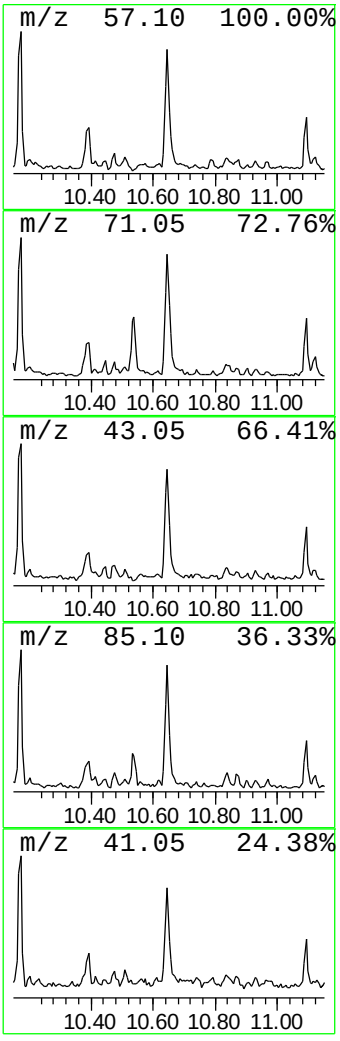
**********

Peak Number 6 Octadecane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.65 | 2.81 ng | 164026 | Phenanthrene-d10 | 11.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 91 |
| 2 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 91 |
| 3 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 83 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 83 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

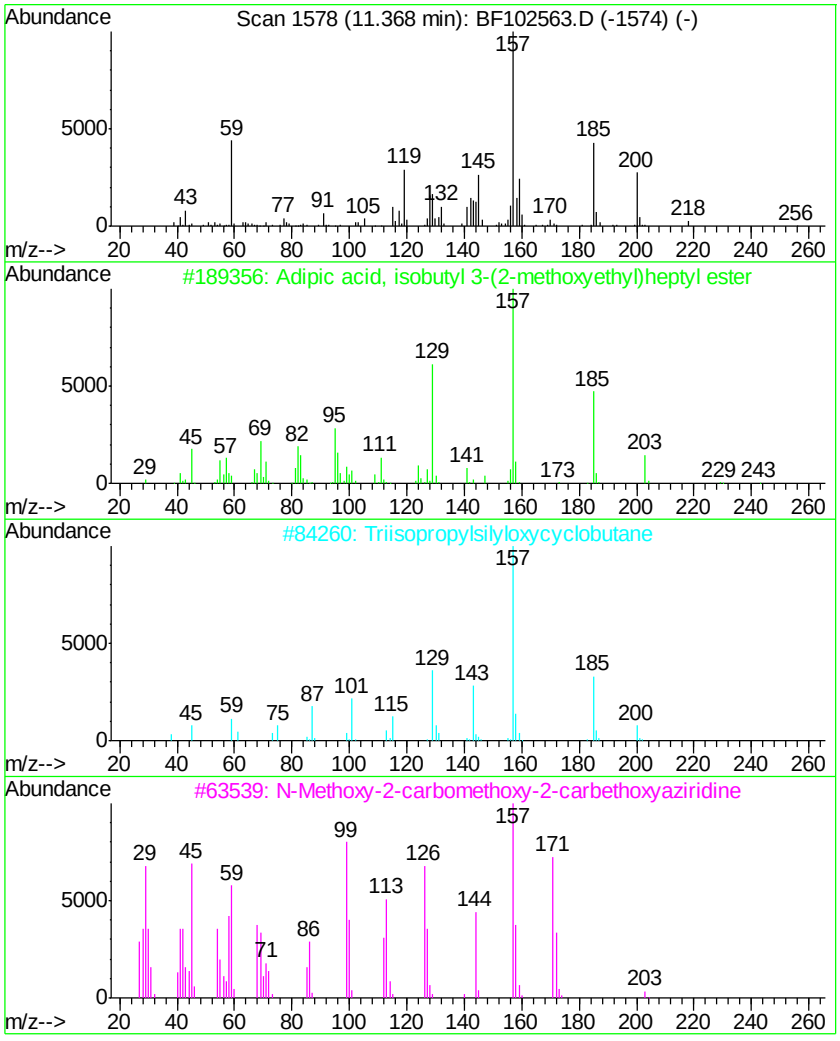
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

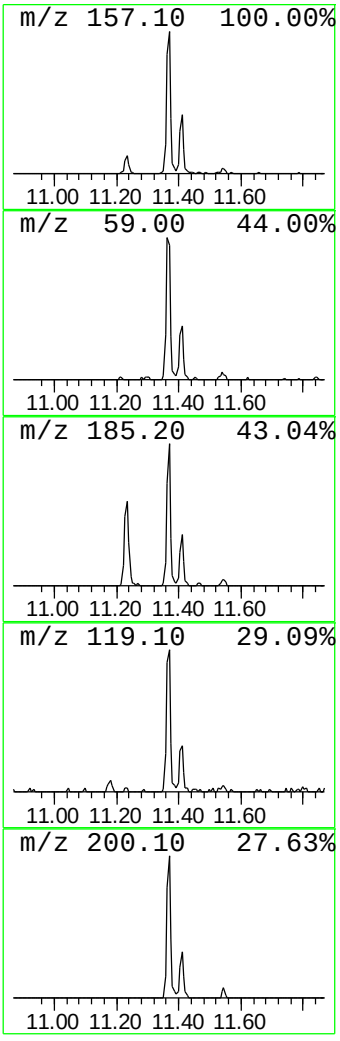
**********

Peak Number 7 unknown11.37 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.37 | 4.73 ng | 275818 | Phenanthrene-d10 | 11.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Adipic acid, isobutyl 3-(2-metho... | 358 | C20H38O5 | 1000324-28-7 | 37 |
| 2 | Triisopropylsilyloxycyclobutane | 228 | C13H28OSi | 1000283-09-4 | 35 |
| 3 | N-Methoxy-2-carbomethoxy-2-carbe... | 203 | C8H13NO5 | 063859-01-8 | 35 |
| 4 | 2-Pyrimidinamine, 5-chloro-4,6-d... | 157 | C6H8ClN3 | 007749-61-3 | 27 |
| 5 | Quinoline, 4,8-dimethyl- | 157 | C11H11N | 013362-80-6 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

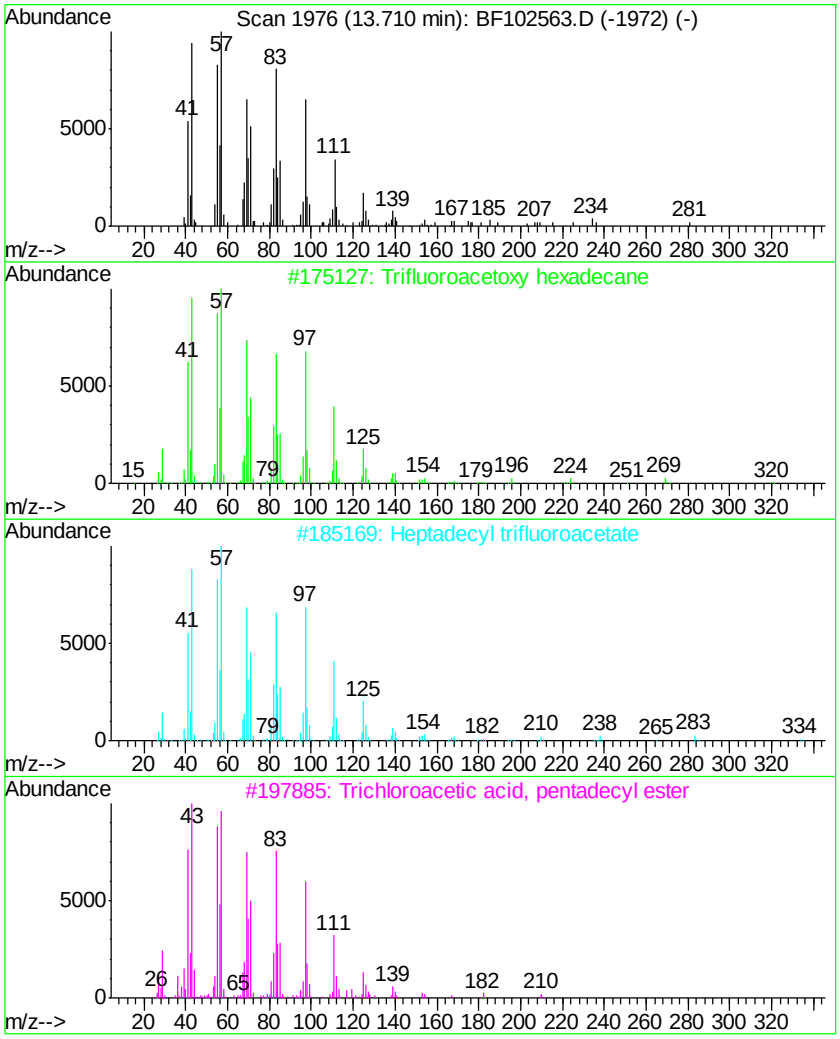
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

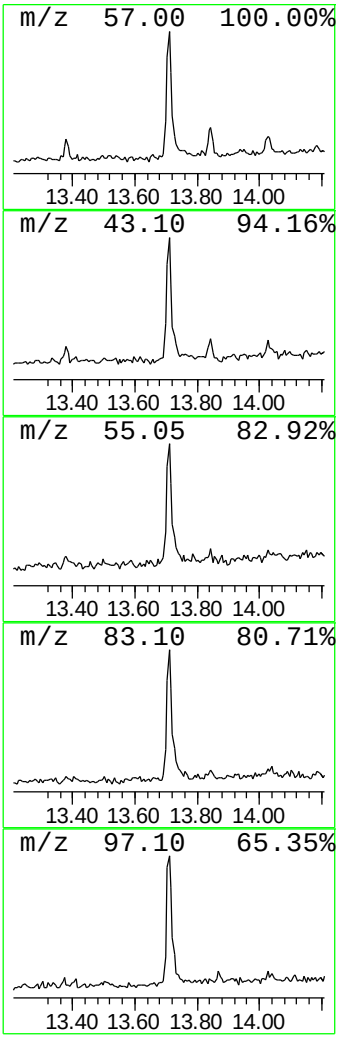
**********

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.71 | 5.67 ng | 237815 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 95 |
| 2 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 94 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 94 |
| 4 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012818\
Data File : BF102563.D
Acq On : 28 Jan 2018 17:54
Operator : SJ/JU
Sample : J1290-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-49-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.92 | 2.3 | ng | 106486 | 1 | 6.71 | 934362 | 20.0 |
| unknown6.49 | 6.49 | 76.2 | ng | 3559760 | 1 | 6.71 | 934362 | 20.0 |
| Tetradecane | 9.67 | 2.1 | ng | 144398 | 3 | 9.75 | 1350420 | 20.0 |
| Hexadecane | 10.17 | 2.3 | ng | 153617 | 3 | 9.75 | 1350420 | 20.0 |
| Octadecane | 10.65 | 2.8 | ng | 164026 | 4 | 11.23 | 1166110 | 20.0 |
| unknown11.37 | 11.37 | 4.7 | ng | 275818 | 4 | 11.23 | 1166110 | 20.0 |
| Trifluoroacetoxy ... | 13.71 | 5.7 | ng | 237815 | 5 | 13.87 | 838178 | 20.0 |