# LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102507.D
Acq On : 27 Jan 2018 13:44
Operator : SJ/JU
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC4

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 | 490 | rVB | 75148 | 104023 | 3.10% | 0.385% |
| 2 | 5.328 | 546 | 551 | 569 | rBV | 3272123 | 3286513 | 97.83% | 12.159% |
| 3 | 6.357 | 721 | 726 | 743 | rBV | 2977221 | 3359565 | 100.00% | 12.430% |
| 4 | 6.487 | 743 | 748 | 751 | rBV | 3325325 | 3291532 | 97.97% | 12.178% |
| 5 | 6.710 | 783 | 786 | 794 | rBV | 1073343 | 920577 | 27.40% | 3.406% |
| 6 | 6.869 | 808 | 813 | 816 | rBV | 2218056 | 2133074 | 63.49% | 7.892% |
| 7 | 7.281 | 878 | 883 | 886 | rBV | 2135624 | 2031773 | 60.48% | 7.517% |
| 8 | 7.375 | 897 | 899 | 908 | rVB3 | 21062 | 35561 | 1.06% | 0.132% |
| 9 | 7.992 | 1000 | 1004 | 1017 | rBV | 1306636 | 1268536 | 37.76% | 4.693% |
| 10 | 9.069 | 1182 | 1187 | 1190 | rBV | 2691841 | 2249011 | 66.94% | 8.321% |
| 11 | 9.463 | 1249 | 1254 | 1262 | rBV | 231403 | 238443 | 7.10% | 0.882% |
| 12 | 9.675 | 1286 | 1290 | 1294 | rBV | 146629 | 129462 | 3.85% | 0.479% |
| 13 | 9.745 | 1298 | 1302 | 1311 | rVB2 | 1498275 | 1327214 | 39.51% | 4.910% |
| 14 | 9.992 | 1341 | 1344 | 1348 | rBV3 | 33816 | 34499 | 1.03% | 0.128% |
| 15 | 10.175 | 1372 | 1375 | 1378 | rVB | 181808 | 136073 | 4.05% | 0.503% |
| 16 | 10.392 | 1408 | 1412 | 1415 | rBV | 45675 | 56281 | 1.68% | 0.208% |
| 17 | 10.539 | 1433 | 1437 | 1448 | rVB | 1501761 | 1519054 | 45.22% | 5.620% |
| 18 | 10.645 | 1452 | 1455 | 1462 | rBV | 156337 | 150424 | 4.48% | 0.557% |
| 19 | 11.092 | 1529 | 1531 | 1534 | rBV | 78640 | 63300 | 1.88% | 0.234% |
| 20 | 11.233 | 1551 | 1555 | 1563 | rBV | 1234172 | 1142573 | 34.01% | 4.227% |
| 21 | 12.816 | 1820 | 1824 | 1833 | rBV | 1747945 | 1546682 | 46.04% | 5.722% |
| 22 | 13.710 | 1973 | 1976 | 1987 | rBV | 117278 | 170454 | 5.07% | 0.631% |
| 23 | 13.869 | 2000 | 2003 | 2011 | rVB | 709089 | 709421 | 21.12% | 2.625% |
| 24 | 15.298 | 2241 | 2246 | 2256 | rBV | 648842 | 864762 | 25.74% | 3.199% |
| 25 | 15.710 | 2312 | 2316 | 2322 | rBV2 | 56857 | 90007 | 2.68% | 0.333% |
| 26 | 16.180 | 2392 | 2396 | 2403 | rVB2 | 64599 | 103127 | 3.07% | 0.382% |
| 27 | 16.733 | 2486 | 2490 | 2495 | rVB3 | 35676 | 66606 | 1.98% | 0.246% |

Sum of corrected areas: 27028547

LSC Report - Integrated Chromatogram

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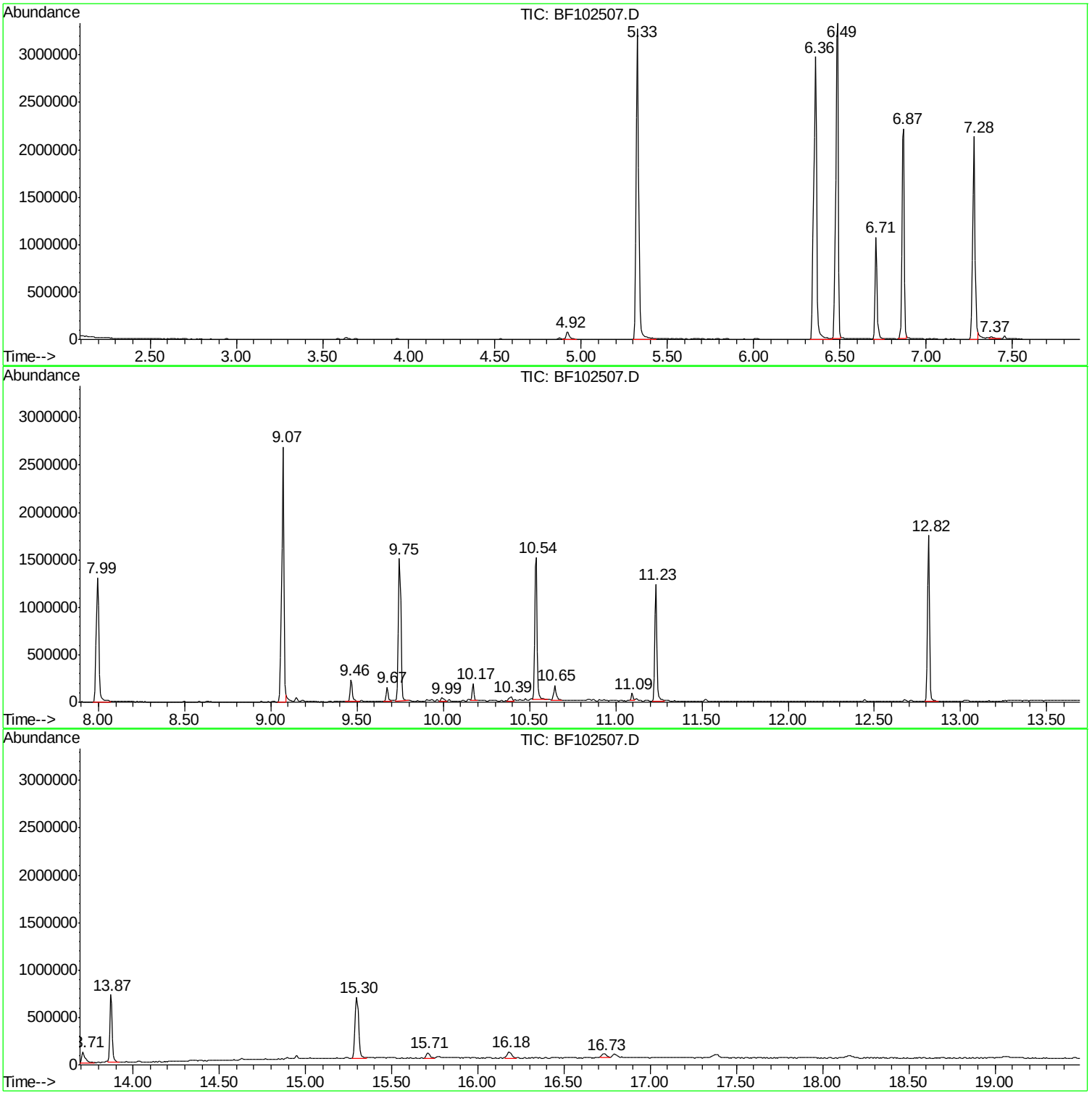
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC4

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



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

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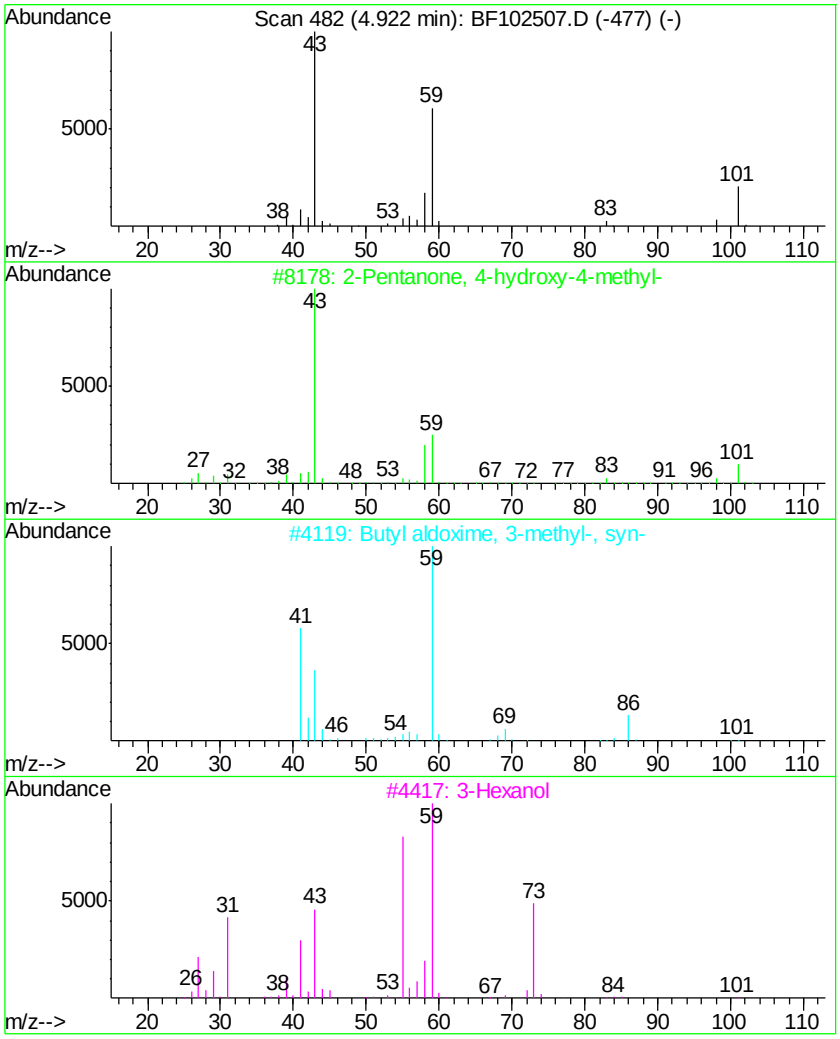
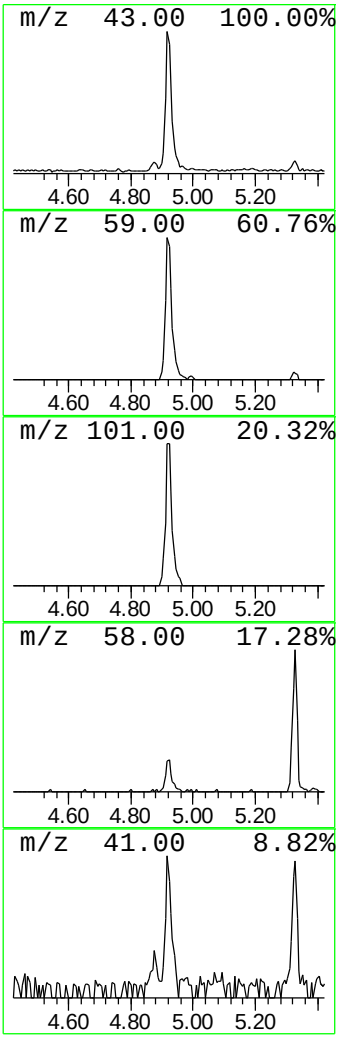
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 2.26 ng | 104023 | 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 | 59 |
| 2 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 37 |
| 3 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 36 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102507.D
Acq On : 27 Jan 2018 13:44
Operator : SJ/JU
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC4

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

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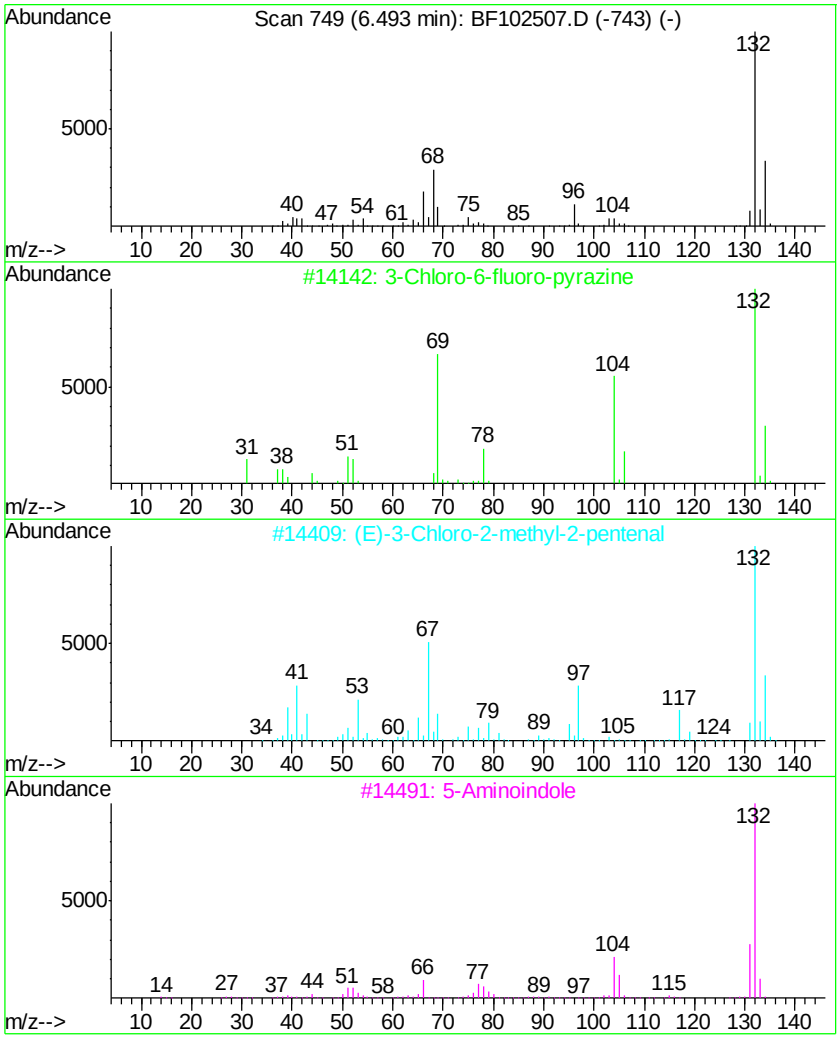
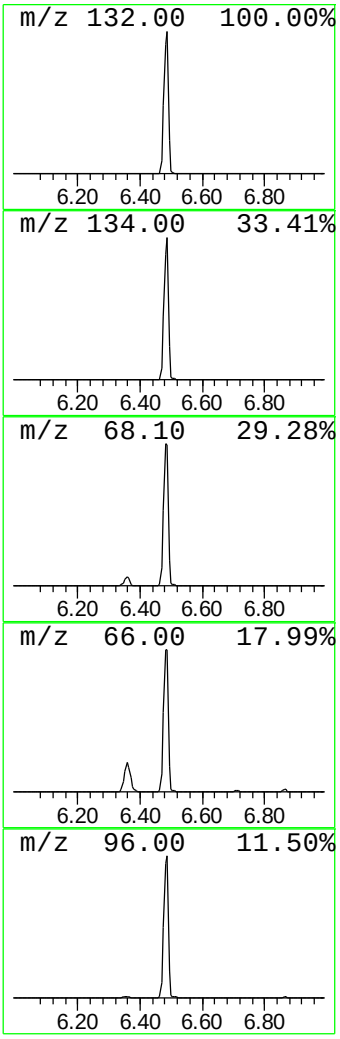
Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.49 | 71.51 ng | 3291530 | 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 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 9 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



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Data File : BF102507.D
Acq On : 27 Jan 2018 13:44
Operator : SJ/JU
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC4

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

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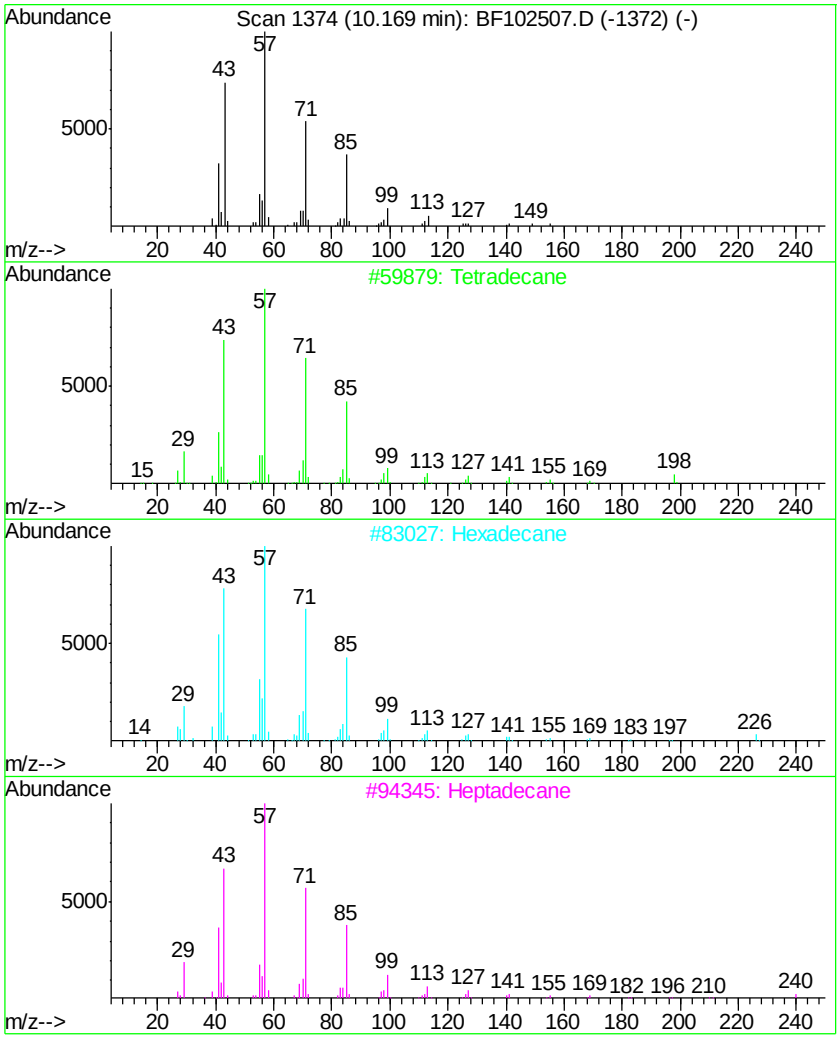
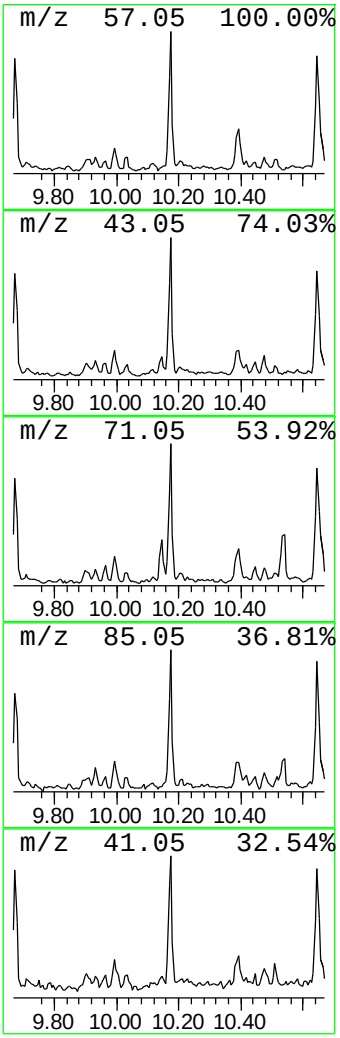
Peak Number 4 Tetradecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.17 | 2.05 ng | 136073 | Acenaphthene-d10 | 9.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 83 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |
| 5 | Nonadecane | 268 | C19H40 | 000629-92-5 | 80 |



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Data File : BF102507.D
Acq On : 27 Jan 2018 13:44
Operator : SJ/JU
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC4

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

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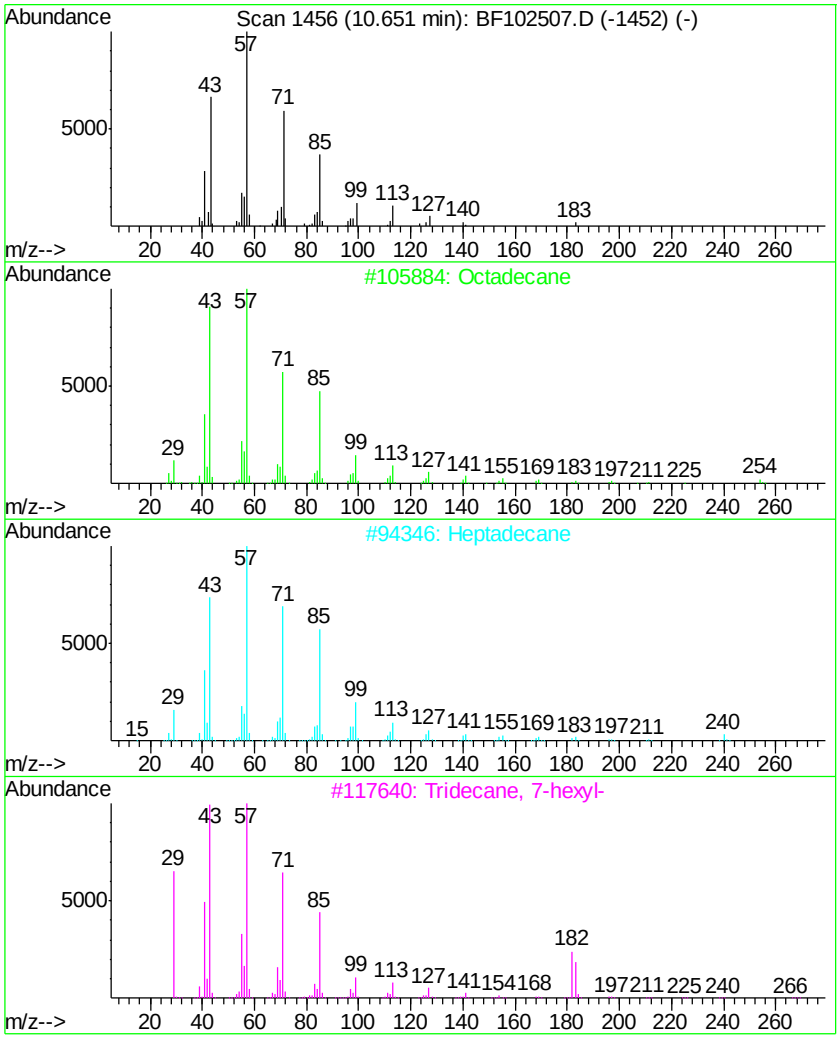
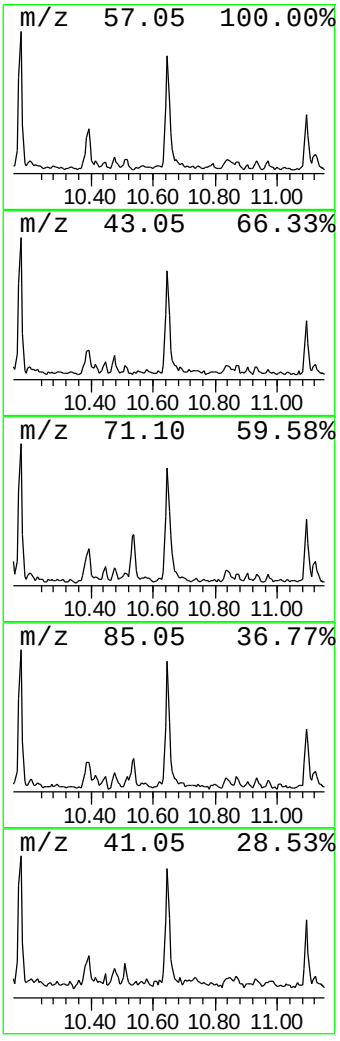
Peak Number 5 Octadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.65 | 2.63 ng | 150424 | Phenanthrene-d10 | 11.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 90 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 86 |
| 3 | Tridecane, 7-hexyl- | 268 | C19H40 | 007225-66-3 | 86 |
| 4 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 78 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 78 |



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Operator : SJ/JU
Sample : J1306-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC4

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

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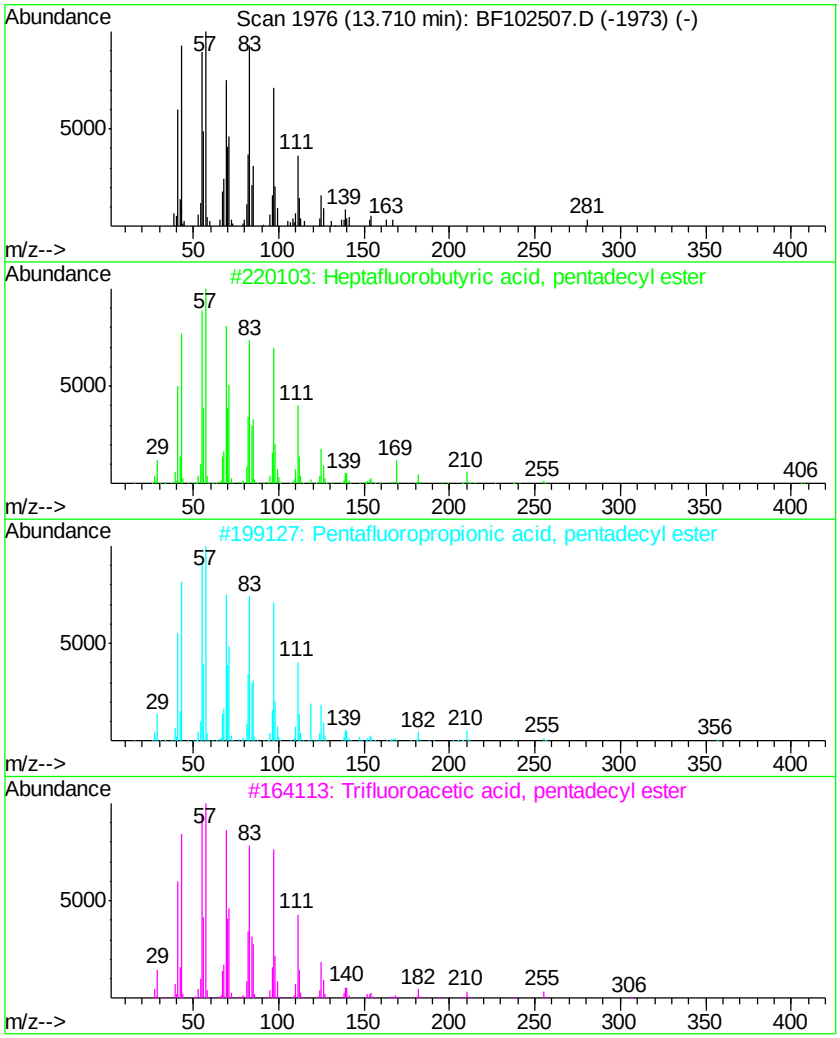
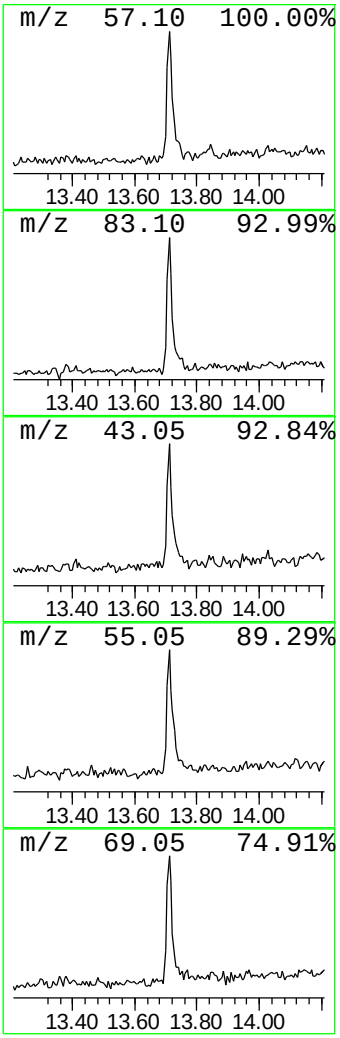
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.71 | 4.81 ng | 170454 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 2 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 3 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 4 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |



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Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
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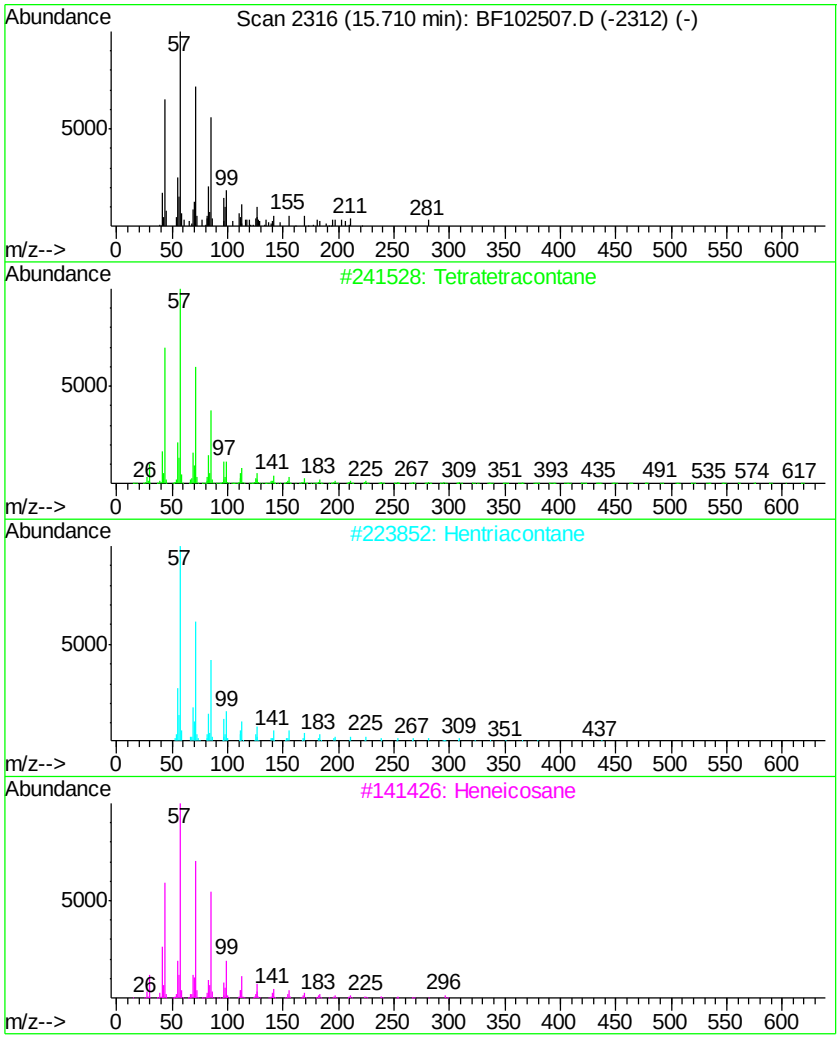
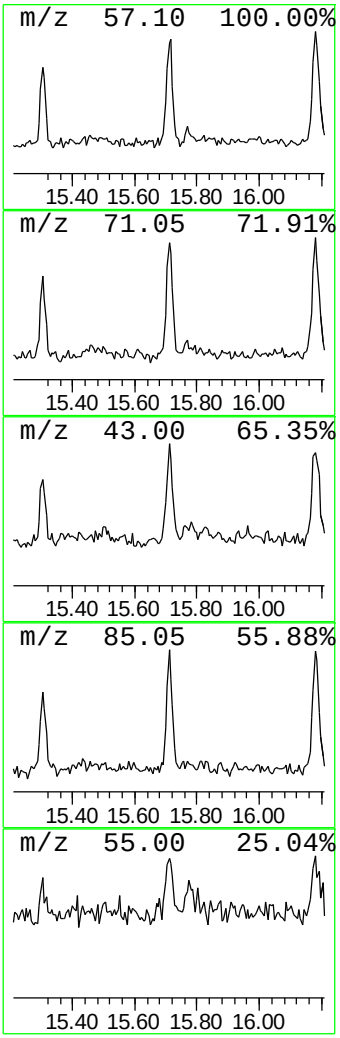
Peak Number 7 Tetratetracontane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.71 | 2.08 ng | 90007 | Perylene-d12 | 15.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 90 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 4 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 86 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 83 |



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Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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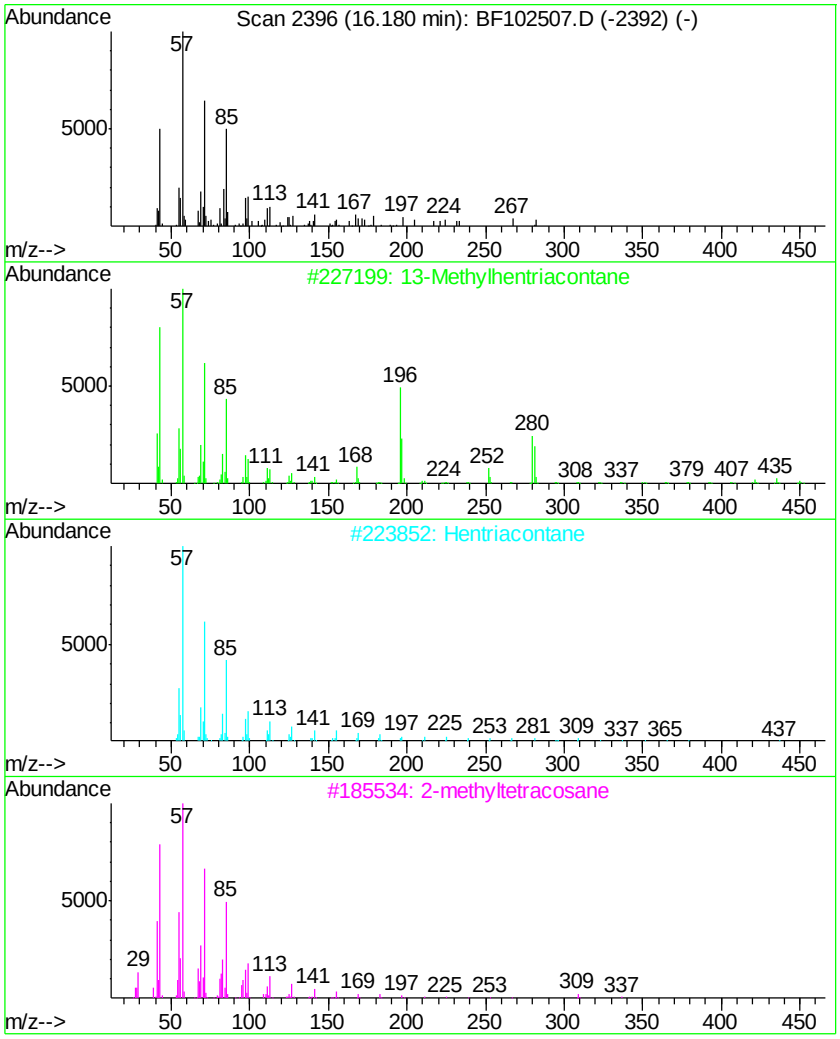
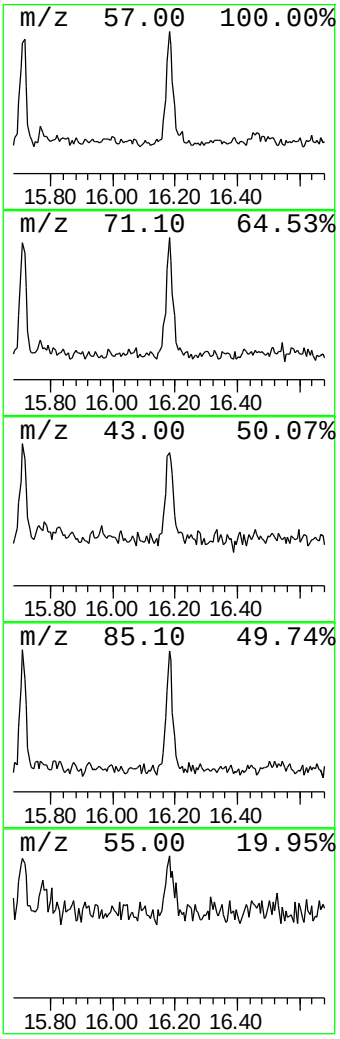
**********

Peak Number 8 13-Methylhentriacontane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.18 | 2.39 ng | 103127 | Perylene-d12 | 15.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 13-Methylhentriacontane | 451 | C32H66 | 1000131-19-4 | 90 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |
| 3 | 2-methyltetracosane | 352 | C25H52 | 1000376-72-6 | 87 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |
| 5 | Sulfurous acid, dodecyl 2-propyl... | 292 | C15H32O3S | 1000309-12-3 | 86 |



Tentatively Identified Compound (LSC) summary

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**ClientSampleId :** WC4

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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 | 104023 | 1 | 6.71 | 920577 | 20.0 |
| unknown6.49 | 6.49 | 71.5 | ng | 3291530 | 1 | 6.71 | 920577 | 20.0 |
| Tetradecane | 10.17 | 2.0 | ng | 136073 | 3 | 9.75 | 1327210 | 20.0 |
| Octadecane | 10.65 | 2.6 | ng | 150424 | 4 | 11.23 | 1142570 | 20.0 |
| Heptafluorobutyri... | 13.71 | 4.8 | ng | 170454 | 5 | 13.87 | 709421 | 20.0 |
| Tetratetracontane | 15.71 | 2.1 | ng | 90007 | 6 | 15.30 | 864762 | 20.0 |
| 13-Methylhentriac... | 16.18 | 2.4 | ng | 103127 | 6 | 15.30 | 864762 | 20.0 |