# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106658.D
Acq On : 21 Jun 2018 13:39
Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

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-BF061918.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 | 5.201 | 482 | 487 | 496 | rVB | 144468 | 184824 | 7.90% | 0.895% |
| 2 | 5.601 | 551 | 555 | 559 | rBV | 1871990 | 1900660 | 81.22% | 9.206% |
| 3 | 6.607 | 721 | 726 | 735 | rBV | 1914563 | 2030201 | 86.76% | 9.834% |
| 4 | 6.736 | 744 | 748 | 751 | rBV | 2042746 | 1999630 | 85.45% | 9.686% |
| 5 | 6.960 | 782 | 786 | 789 | rVB | 703352 | 550344 | 23.52% | 2.666% |
| 6 | 7.119 | 808 | 813 | 816 | rBV | 1690597 | 1579965 | 67.52% | 7.653% |
| 7 | 7.525 | 877 | 882 | 885 | rBV | 1389930 | 1363149 | 58.25% | 6.603% |
| 8 | 8.242 | 1000 | 1004 | 1020 | rBB | 875134 | 719334 | 30.74% | 3.484% |
| 9 | 9.319 | 1182 | 1187 | 1190 | rBV | 2569319 | 2340060 | 100.00% | 11.335% |
| 10 | 9.707 | 1249 | 1253 | 1261 | rVB | 355470 | 275299 | 11.76% | 1.333% |
| 11 | 9.913 | 1284 | 1288 | 1292 | rBV | 49250 | 40042 | 1.71% | 0.194% |
| 12 | 10.001 | 1299 | 1303 | 1307 | rBV2 | 929474 | 803744 | 34.35% | 3.893% |
| 13 | 10.413 | 1371 | 1373 | 1376 | rVB | 67362 | 46833 | 2.00% | 0.227% |
| 14 | 10.713 | 1421 | 1424 | 1429 | rVB | 36242 | 27494 | 1.17% | 0.133% |
| 15 | 10.795 | 1434 | 1438 | 1442 | rBV | 1610395 | 1521318 | 65.01% | 7.369% |
| 16 | 10.883 | 1450 | 1453 | 1463 | rVB | 57056 | 60930 | 2.60% | 0.295% |
| 17 | 11.336 | 1526 | 1530 | 1532 | rBV | 30237 | 25275 | 1.08% | 0.122% |
| 18 | 11.495 | 1553 | 1557 | 1560 | rBV | 923273 | 779874 | 33.33% | 3.778% |
| 19 | 12.936 | 1796 | 1802 | 1804 | rBV3 | 26575 | 35680 | 1.52% | 0.173% |
| 20 | 13.077 | 1822 | 1826 | 1830 | rBV | 2247196 | 2264135 | 96.76% | 10.967% |
| 21 | 13.289 | 1859 | 1862 | 1866 | rVB | 29578 | 24965 | 1.07% | 0.121% |
| 22 | 13.630 | 1916 | 1920 | 1923 | rBV2 | 48677 | 46022 | 1.97% | 0.223% |
| 23 | 13.959 | 1972 | 1976 | 1983 | rBV | 103195 | 110246 | 4.71% | 0.534% |
| 24 | 14.148 | 2003 | 2008 | 2011 | rBV | 736869 | 729782 | 31.19% | 3.535% |
| 25 | 14.283 | 2028 | 2031 | 2035 | rBV | 73903 | 68718 | 2.94% | 0.333% |
| 26 | 14.601 | 2082 | 2085 | 2090 | rBV | 89412 | 88535 | 3.78% | 0.429% |
| 27 | 14.918 | 2136 | 2139 | 2143 | rBV | 68925 | 78370 | 3.35% | 0.380% |
| 28 | 15.001 | 2150 | 2153 | 2157 | rVB | 87841 | 87560 | 3.74% | 0.424% |
| 29 | 15.230 | 2188 | 2192 | 2196 | rBV2 | 23178 | 44425 | 1.90% | 0.215% |
| 30 | 15.277 | 2197 | 2200 | 2204 | rVB | 62235 | 71275 | 3.05% | 0.345% |
| 31 | 15.612 | 2255 | 2257 | 2263 | rVB | 21982 | 29849 | 1.28% | 0.145% |
| 32 | 15.683 | 2264 | 2269 | 2278 | rVB | 444053 | 623526 | 26.65% | 3.020% |
| 33 | 16.142 | 2343 | 2347 | 2353 | rVB | 35260 | 55843 | 2.39% | 0.270% |
| 34 | 16.683 | 2435 | 2439 | 2444 | rVB4 | 20008 | 37281 | 1.59% | 0.181% |

LSC Area Percent Report

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Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 20645188

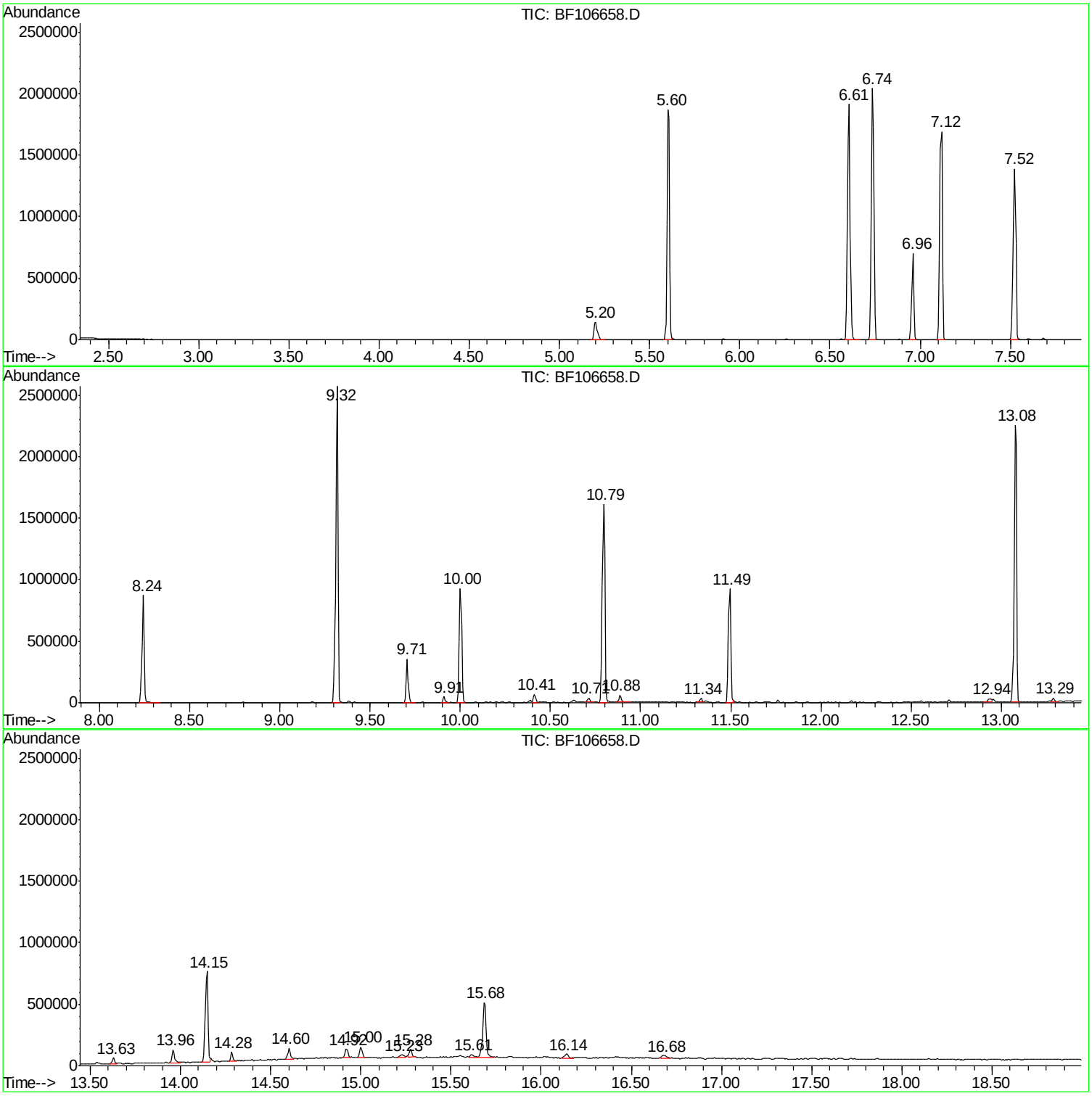
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106658.D
Acq On : 21 Jun 2018 13:39
Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106658.D
Acq On : 21 Jun 2018 13:39
Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

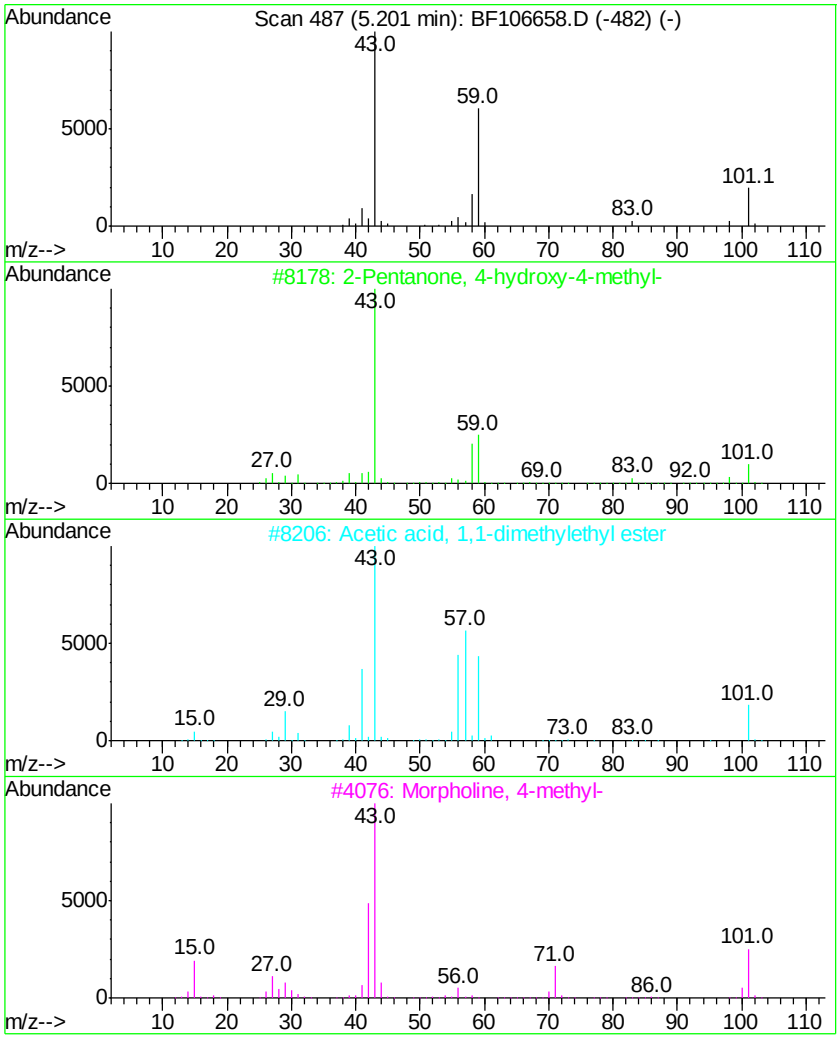
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

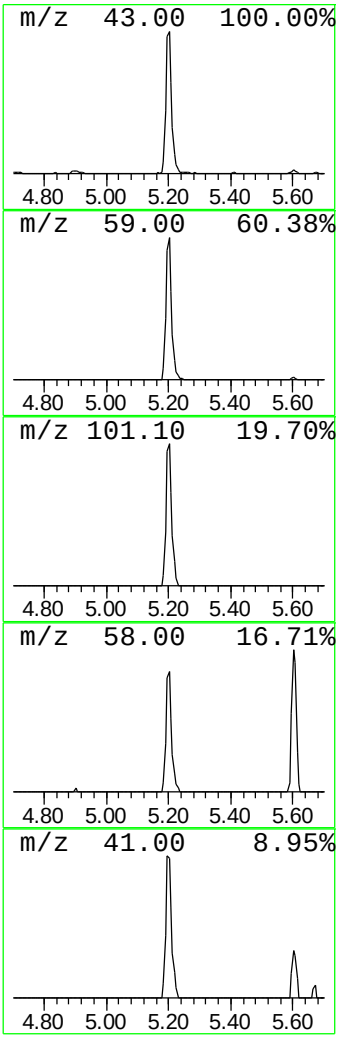
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.20 | 6.72 ng | 184824 | 1,4-Dichlorobenzene-d4 | 6.96 |

| 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 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106658.D
Acq On : 21 Jun 2018 13:39
Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

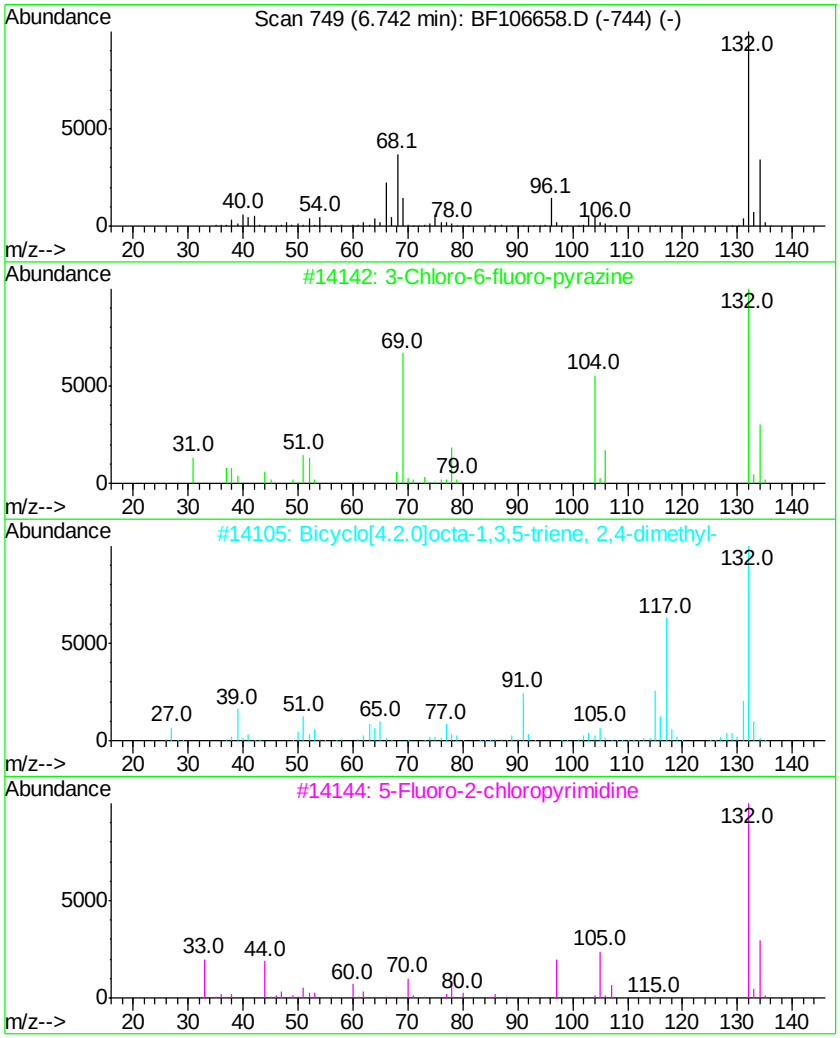
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

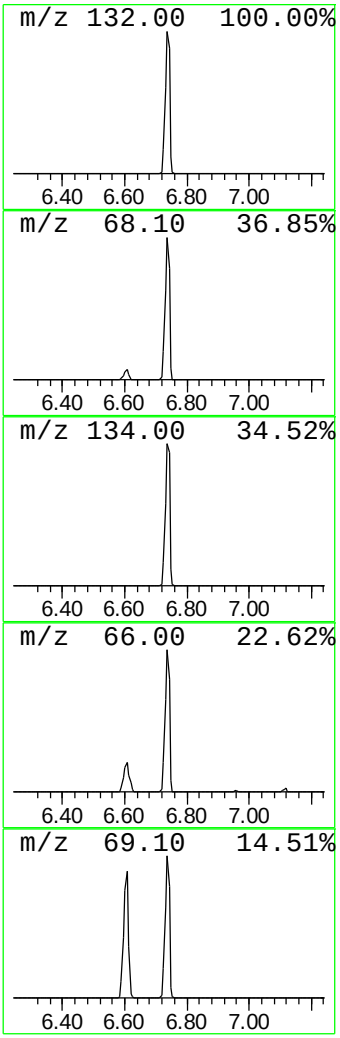
**********

Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.74 | 72.67 ng | 1999630 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Library Search Compound Report

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Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

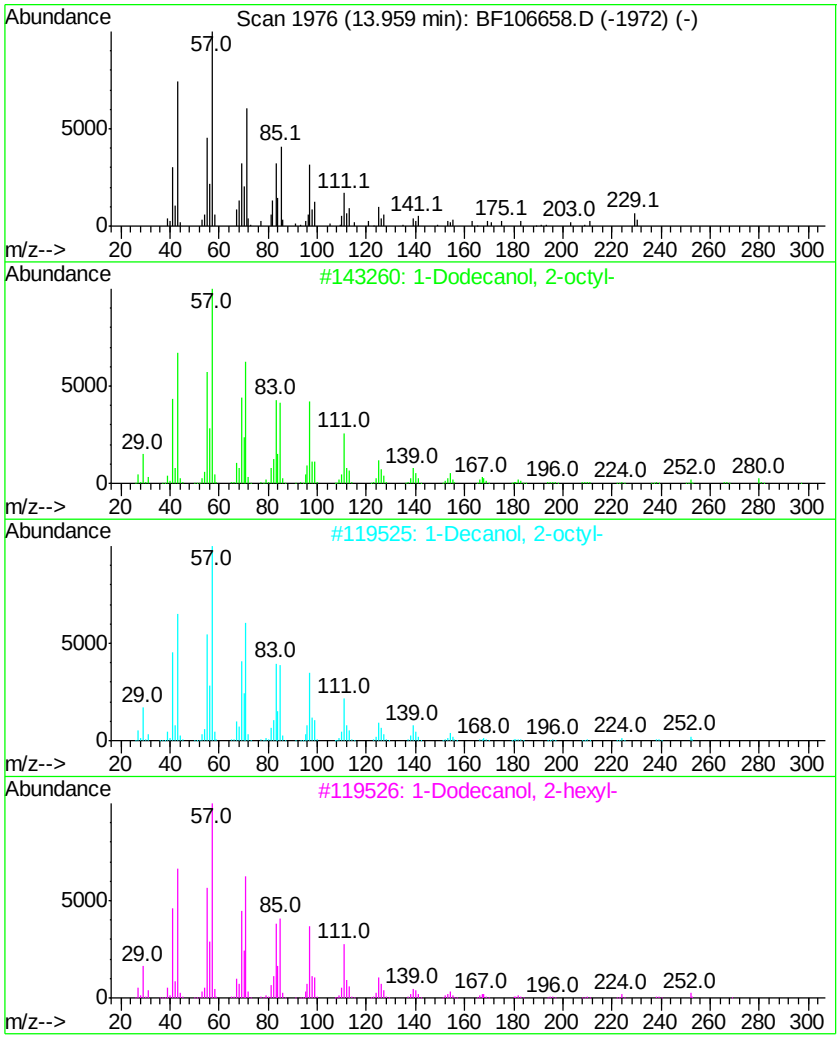
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

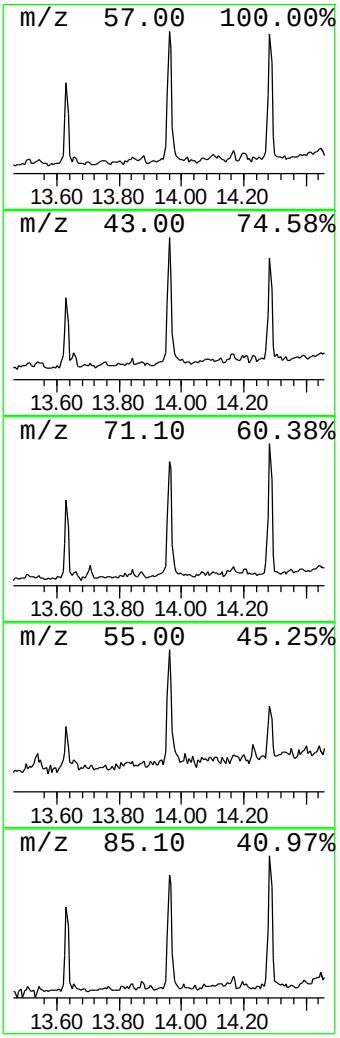
**********

Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.96 | 3.02 ng | 110246 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 91 |
| 2 | 1-Decanol, 2-octyl- | 270 | C18H38O | 045235-48-1 | 91 |
| 3 | 1-Dodecanol, 2-hexyl- | 270 | C18H38O | 110225-00-8 | 91 |
| 4 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 62 |
| 5 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 60 |



Library Search Compound Report

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Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

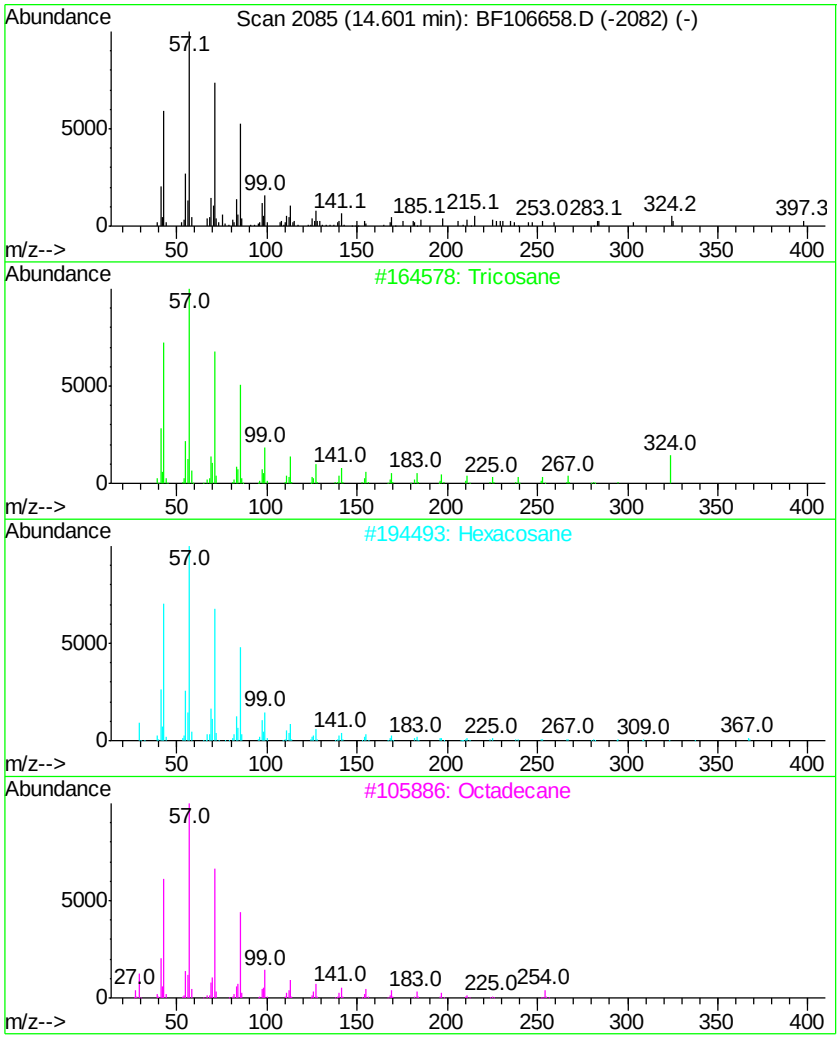
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

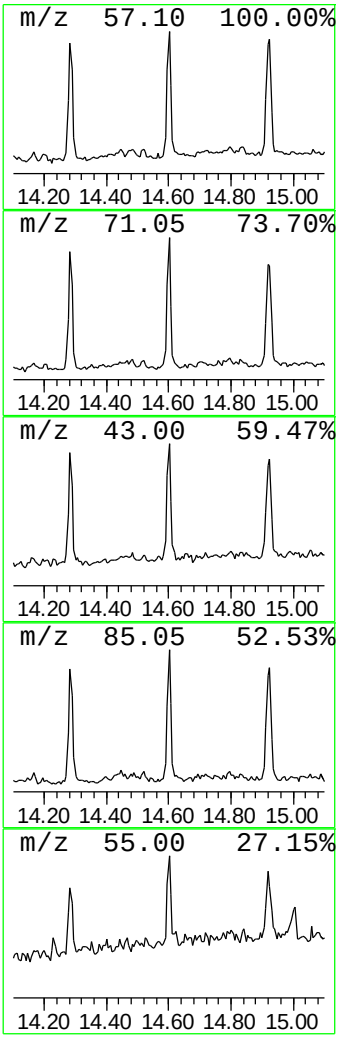
**********

Peak Number 5 Tricosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.60 | 2.43 ng | 88535 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricosane | 324 | C23H48 | 000638-67-5 | 93 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 3 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |
| 4 | Triacontane | 422 | C30H62 | 000638-68-6 | 87 |
| 5 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 87 |



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ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
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TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

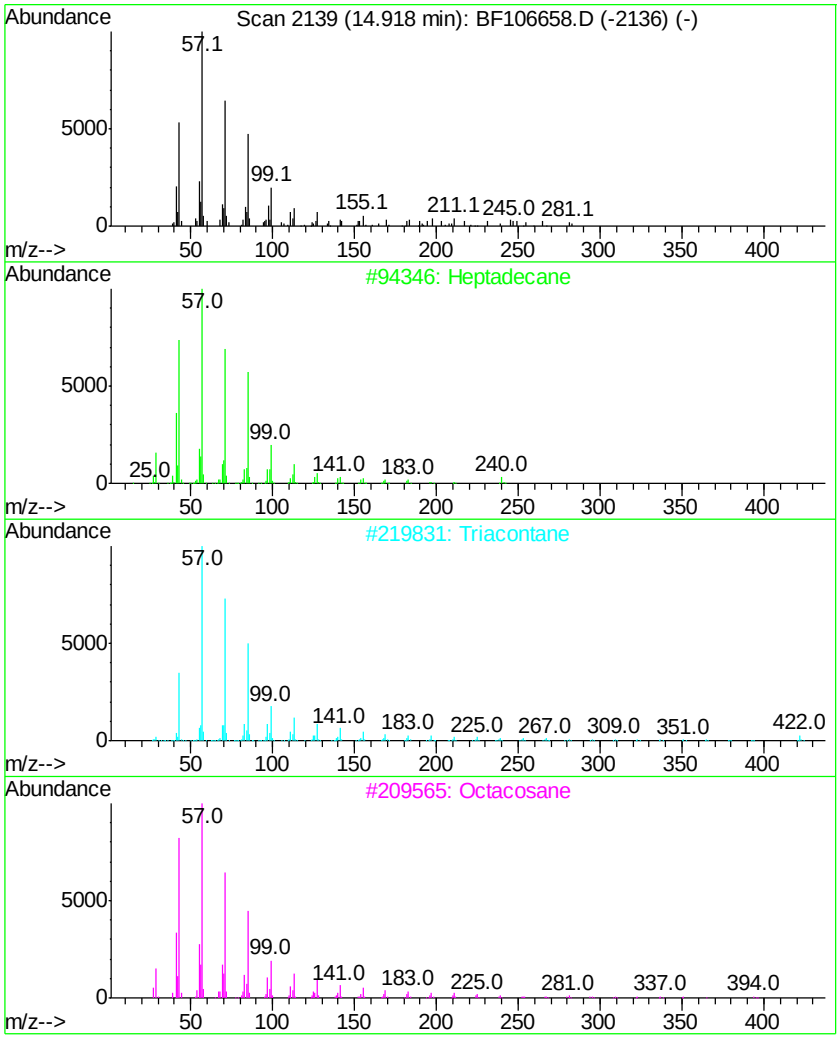
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

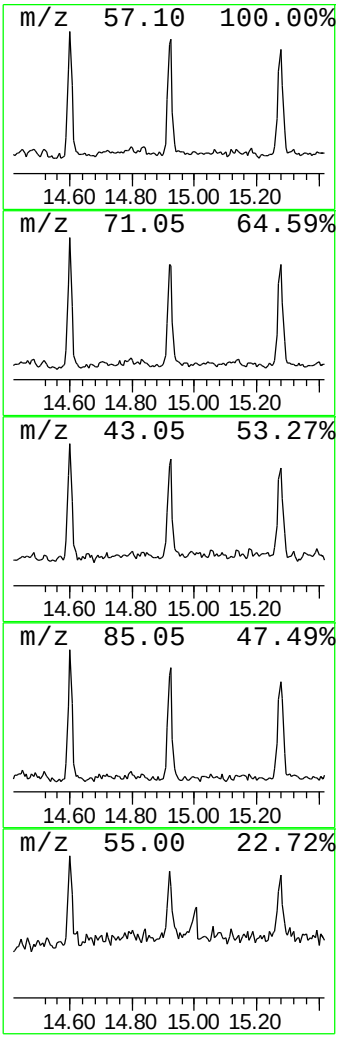
**********

Peak Number 6 Heptadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.92 | 2.51 ng | 78370 | Perylene-d12 | 15.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Triacontane | 422 | C30H62 | 000638-68-6 | 87 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 4 | 6,6-Diethylhoctadecane | 310 | C22H46 | 1000360-41-8 | 86 |
| 5 | Eicosane, 2-methyl- | 296 | C21H44 | 001560-84-5 | 86 |



Library Search Compound Report

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ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

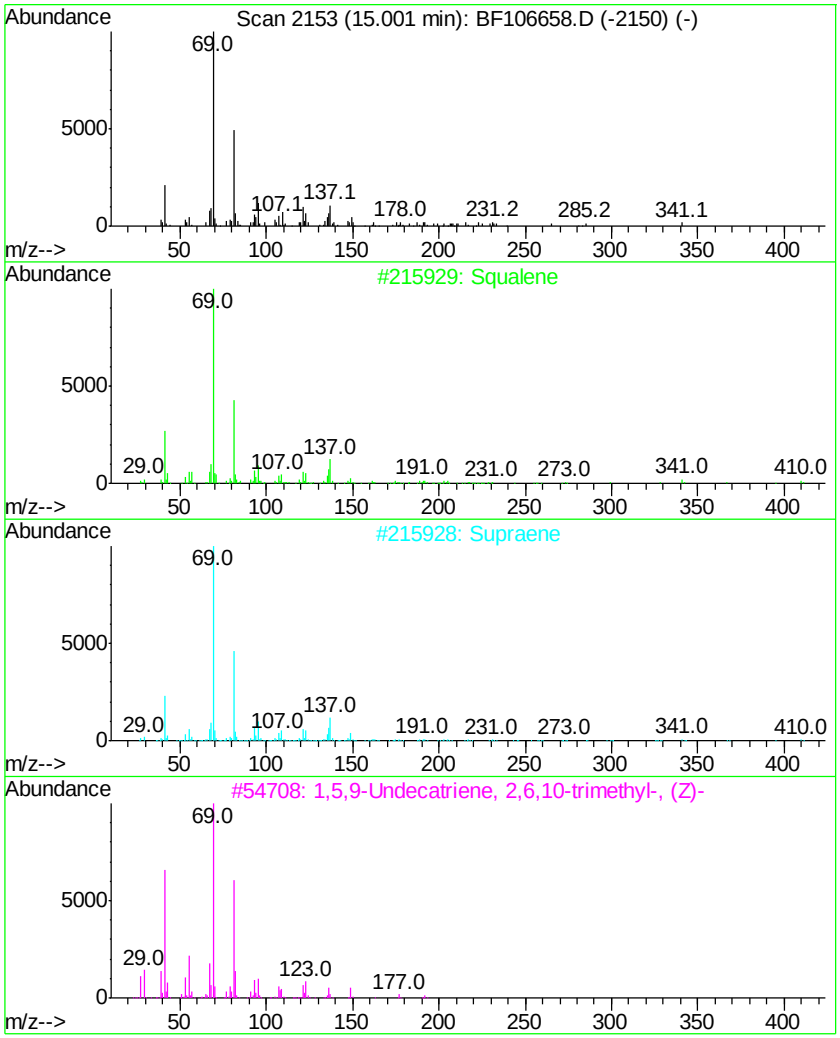
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

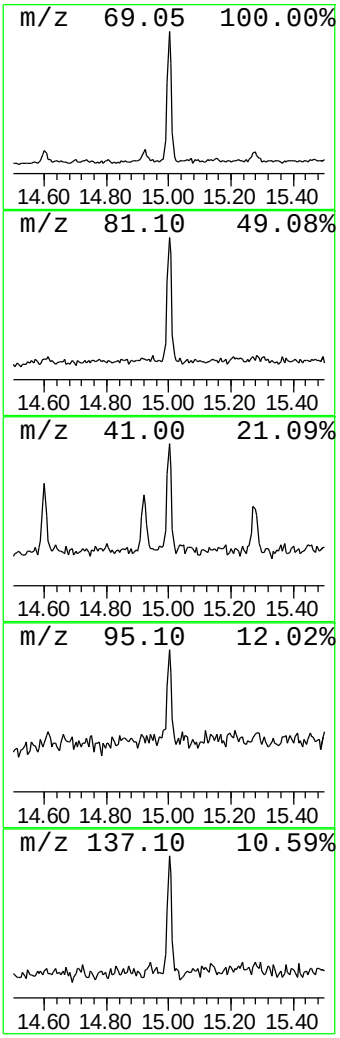
**********

Peak Number 7 Squalene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.00 | 2.81 ng | 87560 | Perylene-d12 | 15.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 86 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 83 |
| 3 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 72 |
| 4 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72 |
| 5 | 5,9,13-Pentadecatrien-2-one, 6,1... | 262 | C18H30O | 001117-52-8 | 59 |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

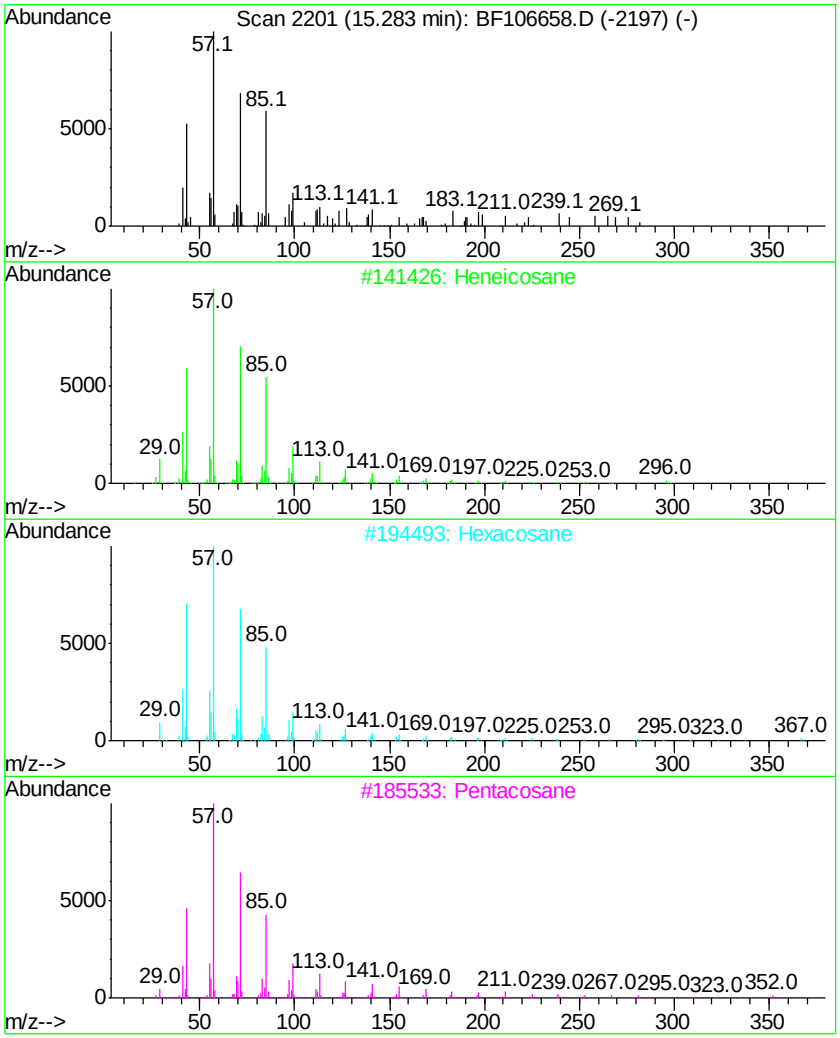
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

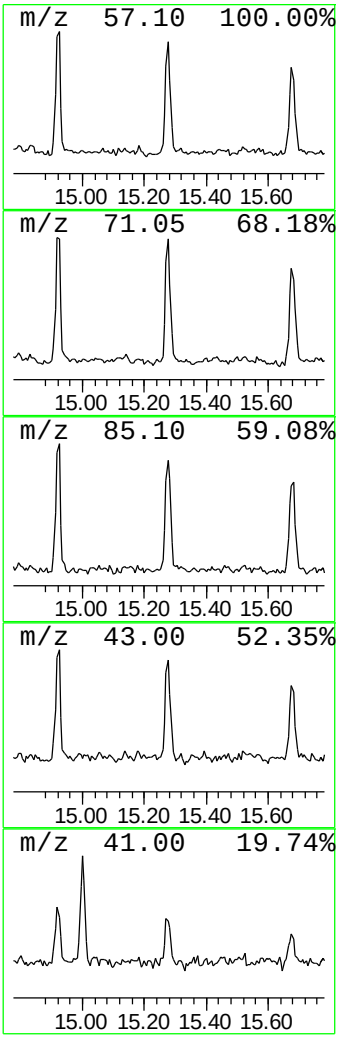
**********

Peak Number 8 Heneicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.28 | 2.29 ng | 71275 | Perylene-d12 | 15.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 3 | Pentacosane | 352 | C25H52 | 000629-99-2 | 83 |
| 4 | Triacontane | 422 | C30H62 | 000638-68-6 | 80 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062118\
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Operator : JU/SJ
Sample : J3584-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-12-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| 2-Pentanone, 4-hy... | 5.20 | 6.7 | ng | 184824 | 1 | 6.96 | 550344 | 20.0 |
| unknown6.74 | 6.74 | 72.7 | ng | 1999630 | 1 | 6.96 | 550344 | 20.0 |
| 1-Dodecanol, 2-oc... | 13.96 | 3.0 | ng | 110246 | 5 | 14.15 | 729782 | 20.0 |
| Tricosane | 14.60 | 2.4 | ng | 88535 | 5 | 14.15 | 729782 | 20.0 |
| Heptadecane | 14.92 | 2.5 | ng | 78370 | 6 | 15.69 | 623526 | 20.0 |
| Squalene | 15.00 | 2.8 | ng | 87560 | 6 | 15.69 | 623526 | 20.0 |
| Heneicosane | 15.28 | 2.3 | ng | 71275 | 6 | 15.69 | 623526 | 20.0 |