LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
Data File : BF106705.D
Acq On : 22 Jun 2018 13:30
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 26KV-TP-11

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 | 5.207 | 483 | 488 | 496 | rBV | 110741 | 151797 | 9.81% | 0.951% |
| 2 | 5.607 | 551 | 556 | 559 | rBV | 1471644 | 1482128 | 95.78% | 9.290% |
| 3 | 6.607 | 720 | 726 | 729 | rBV | 1366589 | 1547496 | 100.00% | 9.699% |
| 4 | 6.736 | 743 | 748 | 751 | rBV | 1490274 | 1540439 | 99.54% | 9.655% |
| 5 | 6.960 | 782 | 786 | 789 | rBV | 496637 | 395108 | 25.53% | 2.476% |
| 6 | 7.119 | 808 | 813 | 816 | rBV | 1182464 | 1135592 | 73.38% | 7.118% |
| 7 | 7.525 | 876 | 882 | 885 | rBV | 1005825 | 1044144 | 67.47% | 6.544% |
| 8 | 8.242 | 1000 | 1004 | 1007 | rBV | 583862 | 522434 | 33.76% | 3.274% |
| 9 | 9.313 | 1180 | 1186 | 1190 | rBV | 1550385 | 1513455 | 97.80% | 9.486% |
| 10 | 9.707 | 1250 | 1253 | 1261 | rVB | 194761 | 155100 | 10.02% | 0.972% |
| 11 | 10.001 | 1299 | 1303 | 1307 | rBV | 714313 | 597190 | 38.59% | 3.743% |
| 12 | 10.201 | 1333 | 1337 | 1340 | rBV2 | 14921 | 15840 | 1.02% | 0.099% |
| 13 | 10.413 | 1370 | 1373 | 1376 | rVB2 | 25645 | 21955 | 1.42% | 0.138% |
| 14 | 10.795 | 1433 | 1438 | 1441 | rBV | 1255665 | 1195254 | 77.24% | 7.492% |
| 15 | 10.883 | 1450 | 1453 | 1463 | rVB | 44205 | 55548 | 3.59% | 0.348% |
| 16 | 11.330 | 1526 | 1529 | 1532 | rBV2 | 30123 | 27151 | 1.75% | 0.170% |
| 17 | 11.495 | 1553 | 1557 | 1559 | rBV | 741327 | 653513 | 42.23% | 4.096% |
| 18 | 11.513 | 1559 | 1560 | 1565 | rVB | 89869 | 74228 | 4.80% | 0.465% |
| 19 | 11.566 | 1565 | 1569 | 1572 | rBV | 21259 | 18483 | 1.19% | 0.116% |
| 20 | 11.995 | 1639 | 1642 | 1644 | rBV | 27753 | 24042 | 1.55% | 0.151% |
| 21 | 12.024 | 1644 | 1647 | 1652 | rVB2 | 29891 | 30923 | 2.00% | 0.194% |
| 22 | 12.107 | 1658 | 1661 | 1663 | rBV2 | 29023 | 35015 | 2.26% | 0.219% |
| 23 | 12.130 | 1663 | 1665 | 1669 | rVB | 22561 | 19413 | 1.25% | 0.122% |
| 24 | 12.289 | 1688 | 1692 | 1694 | rBV | 20468 | 21018 | 1.36% | 0.132% |
| 25 | 12.542 | 1732 | 1735 | 1739 | rBV2 | 33898 | 37767 | 2.44% | 0.237% |
| 26 | 12.707 | 1760 | 1763 | 1767 | rBV | 112445 | 100322 | 6.48% | 0.629% |
| 27 | 12.942 | 1796 | 1803 | 1808 | rBV | 117123 | 169965 | 10.98% | 1.065% |
| 28 | 13.077 | 1822 | 1826 | 1829 | rBV | 1593339 | 1416419 | 91.53% | 8.878% |
| 29 | 13.154 | 1835 | 1839 | 1845 | rVB5 | 17782 | 26772 | 1.73% | 0.168% |
| 30 | 13.265 | 1855 | 1858 | 1860 | rVB3 | 25523 | 17798 | 1.15% | 0.112% |
| 31 | 13.371 | 1872 | 1876 | 1879 | rVB2 | 19304 | 16172 | 1.05% | 0.101% |
| 32 | 13.530 | 1900 | 1903 | 1908 | rVB6 | 17010 | 24431 | 1.58% | 0.153% |
| 33 | 13.630 | 1915 | 1920 | 1922 | rBV2 | 23177 | 31598 | 2.04% | 0.198% |
| 34 | 13.777 | 1943 | 1945 | 1950 | rVB2 | 16751 | 17402 | 1.12% | 0.109% |

LSC Area Percent Report

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Acq On : 22 Jun 2018 13:30
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 26KV-TP-11

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

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.960 | 1971 | 1976 | 1979 | rBV2 | 98814 | 111964 | 7.24% | 0.702% |
| 36 | 14.148 | 2003 | 2008 | 2011 | rBV | 646099 | 642171 | 41.50% | 4.025% |
| 37 | 14.171 | 2011 | 2012 | 2020 | rVB | 73351 | 66268 | 4.28% | 0.415% |
| 38 | 14.283 | 2028 | 2031 | 2035 | rBV4 | 22246 | 29514 | 1.91% | 0.185% |
| 39 | 14.542 | 2070 | 2075 | 2078 | rBV | 24375 | 29836 | 1.93% | 0.187% |
| 40 | 14.607 | 2083 | 2086 | 2091 | rBV5 | 24311 | 36426 | 2.35% | 0.228% |
| 41 | 14.924 | 2137 | 2140 | 2142 | rVB2 | 19304 | 17010 | 1.10% | 0.107% |
| 42 | 15.230 | 2188 | 2192 | 2196 | rBV | 44017 | 74205 | 4.80% | 0.465% |
| 43 | 15.554 | 2244 | 2247 | 2254 | rVB | 31100 | 40322 | 2.61% | 0.253% |
| 44 | 15.618 | 2254 | 2258 | 2263 | rBV | 44542 | 58577 | 3.79% | 0.367% |
| 45 | 15.695 | 2265 | 2271 | 2283 | rVB | 418688 | 592831 | 38.31% | 3.716% |
| 46 | 16.142 | 2344 | 2347 | 2354 | rVB4 | 15169 | 23102 | 1.49% | 0.145% |
| 47 | 16.683 | 2435 | 2439 | 2443 | rVB3 | 20409 | 30323 | 1.96% | 0.190% |
| 48 | 17.253 | 2531 | 2536 | 2544 | rBV3 | 16959 | 41225 | 2.66% | 0.258% |
| 49 | 17.736 | 2614 | 2618 | 2626 | rVB3 | 12419 | 24960 | 1.61% | 0.156% |

Sum of corrected areas: 15954646

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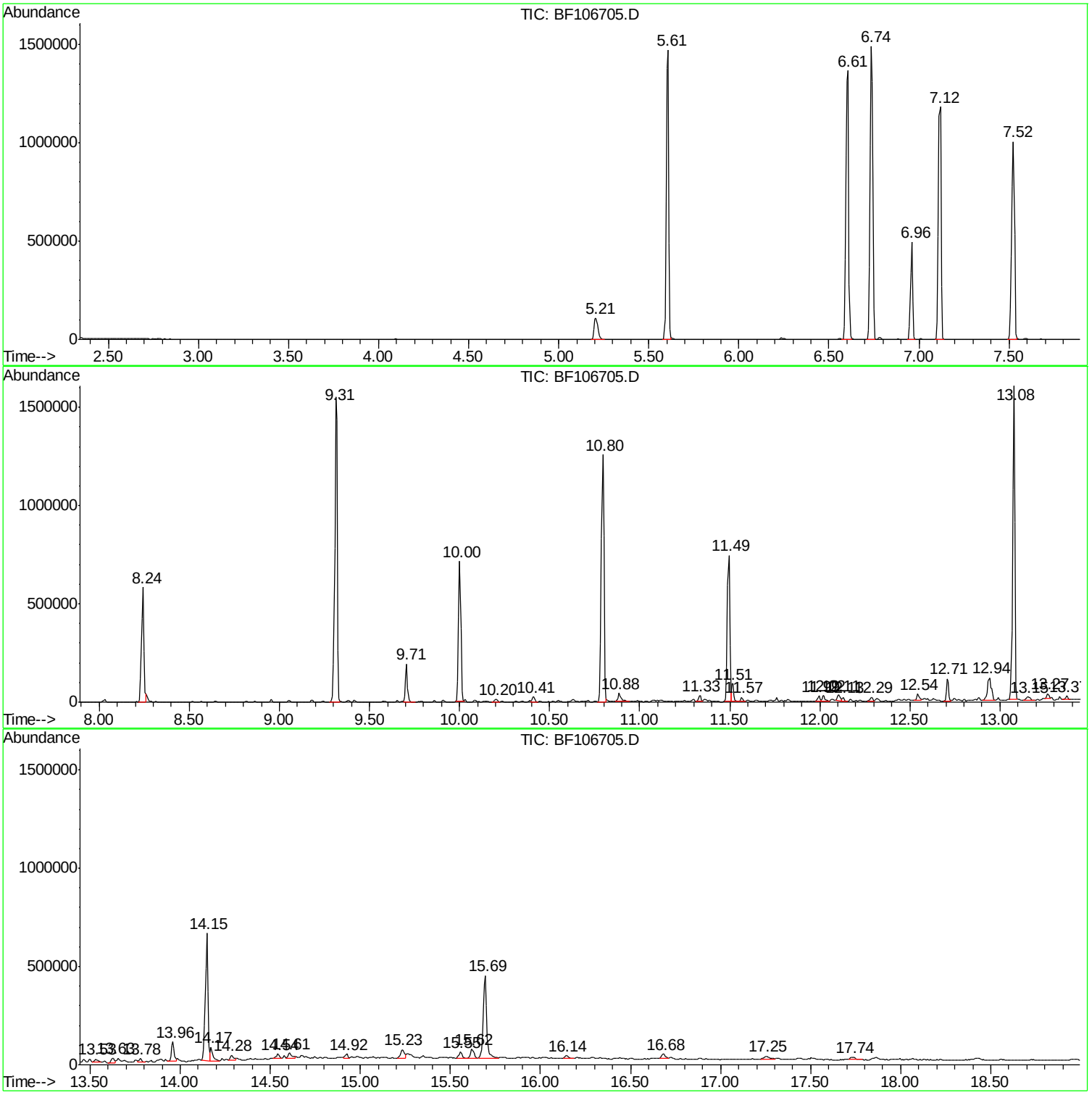
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
26KV-TP-11

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\BF062218\
Data File : BF106705.D
Acq On : 22 Jun 2018 13:30
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 26KV-TP-11

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

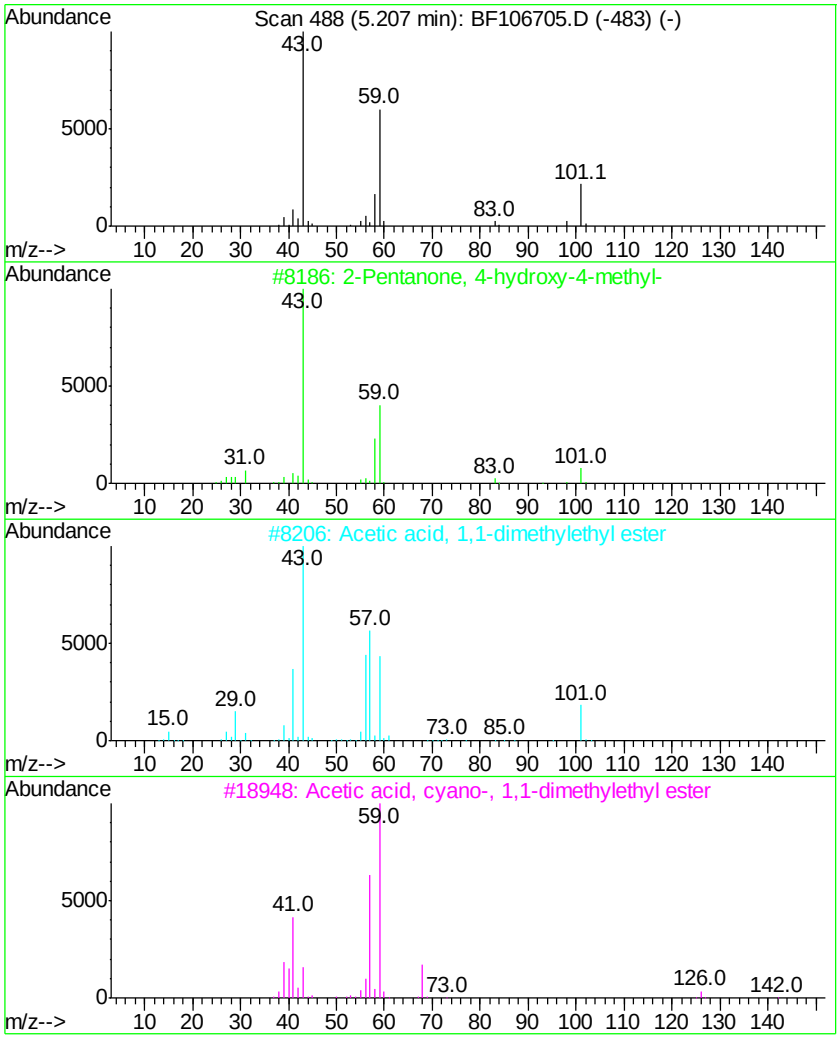
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

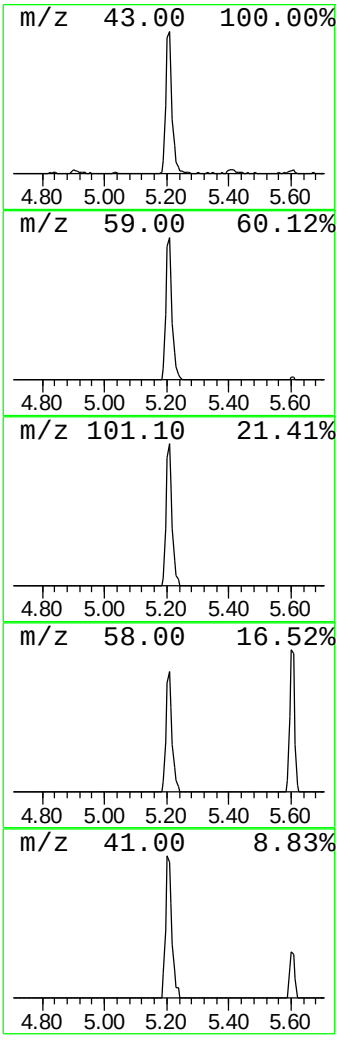
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.21 | 7.68 ng | 151797 | 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 | 56 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



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Data File : BF106705.D
Acq On : 22 Jun 2018 13:30
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 26KV-TP-11

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

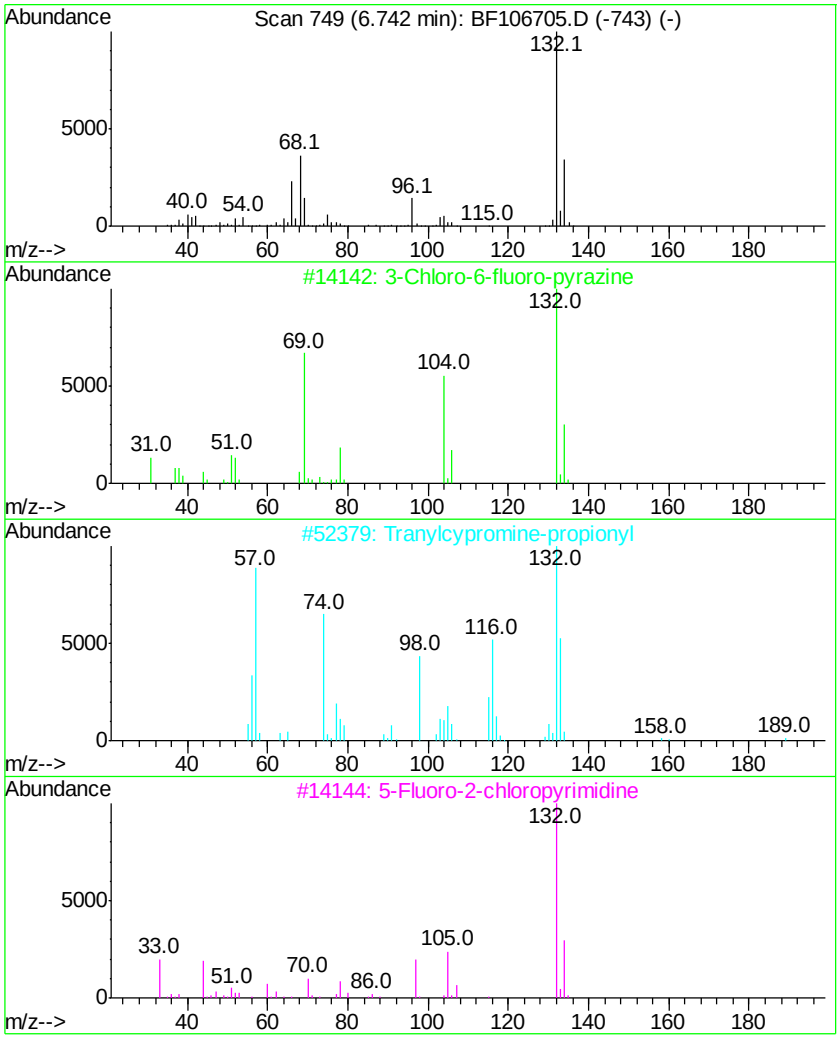
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

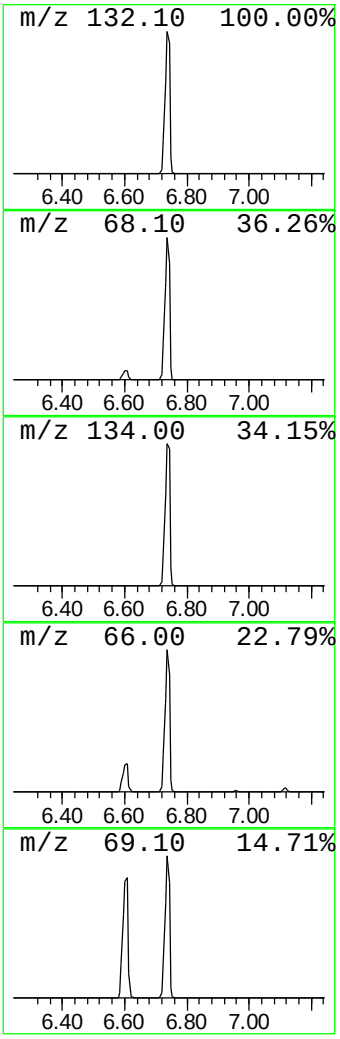
**********

Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.74 | 77.98 ng | 1540440 | 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 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



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Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062218\
Data File : BF106705.D
Acq On : 22 Jun 2018 13:30
Operator : JU/SJ
Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 26KV-TP-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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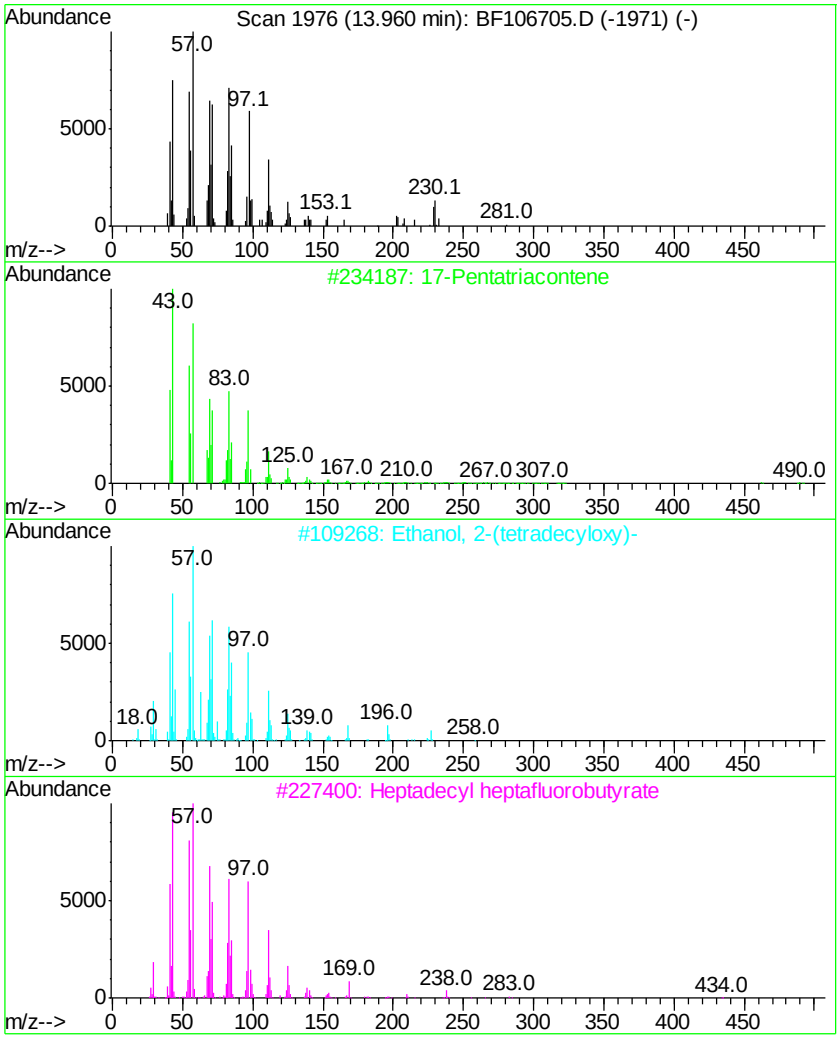
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

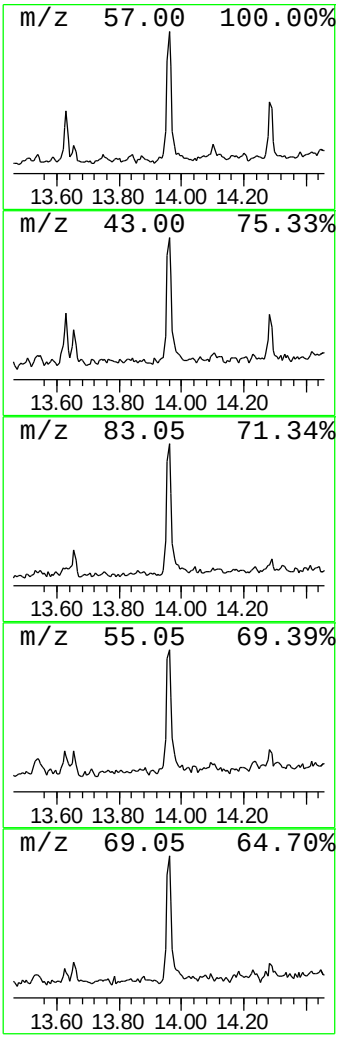
**********

Peak Number 4 17-Pentatriacontene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.96 | 3.49 ng | 111964 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |
| 2 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 90 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 81 |
| 4 | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 81 |
| 5 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 76 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
Data File : BF106705.D
Acq On : 22 Jun 2018 13:30
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Sample : J3603-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
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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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.21 | 7.7 | ng | 151797 | 1 | 6.96 | 395108 | 20.0 |
| unknown6.74 | 6.74 | 78.0 | ng | 1540440 | 1 | 6.96 | 395108 | 20.0 |
| 17-Pentatriacontene | 13.96 | 3.5 | ng | 111964 | 5 | 14.15 | 642171 | 20.0 |