LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106979.D
Acq On : 29 Jun 2018 18:00
Operator : JU/SJ
Sample : J3677-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 93-95-B3(0-2.5)

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 | 5.196 | 482 | 486 | 495 | rBV | 148986 | 184497 | 10.26% | 1.136% |
| 2 | 5.595 | 550 | 554 | 557 | rBV | 1582639 | 1455472 | 80.94% | 8.963% |
| 3 | 6.595 | 719 | 724 | 738 | rVB | 1408227 | 1554556 | 86.45% | 9.573% |
| 4 | 6.731 | 742 | 747 | 750 | rBV | 1690474 | 1537903 | 85.53% | 9.471% |
| 5 | 6.954 | 781 | 785 | 788 | rBV | 499702 | 445026 | 24.75% | 2.741% |
| 6 | 7.107 | 807 | 811 | 815 | rBV | 1410343 | 1267293 | 70.48% | 7.804% |
| 7 | 7.519 | 876 | 881 | 884 | rBV | 1045403 | 979666 | 54.48% | 6.033% |
| 8 | 7.601 | 890 | 895 | 903 | rVB | 16673 | 22429 | 1.25% | 0.138% |
| 9 | 8.236 | 999 | 1003 | 1006 | rBV | 608670 | 552283 | 30.71% | 3.401% |
| 10 | 9.307 | 1181 | 1185 | 1188 | rBV | 1993731 | 1798190 | 100.00% | 11.074% |
| 11 | 9.701 | 1248 | 1252 | 1258 | rVB | 246027 | 214645 | 11.94% | 1.322% |
| 12 | 9.901 | 1282 | 1286 | 1289 | rBV | 44336 | 35777 | 1.99% | 0.220% |
| 13 | 9.995 | 1298 | 1302 | 1306 | rBV | 687378 | 599295 | 33.33% | 3.691% |
| 14 | 10.401 | 1369 | 1371 | 1374 | rVB | 64234 | 46112 | 2.56% | 0.284% |
| 15 | 10.619 | 1403 | 1408 | 1411 | rBV2 | 17403 | 23534 | 1.31% | 0.145% |
| 16 | 10.789 | 1433 | 1437 | 1440 | rBV | 1185219 | 1060808 | 58.99% | 6.533% |
| 17 | 10.872 | 1448 | 1451 | 1458 | rBV | 47018 | 58248 | 3.24% | 0.359% |
| 18 | 11.325 | 1525 | 1528 | 1531 | rBV2 | 28105 | 24095 | 1.34% | 0.148% |
| 19 | 11.489 | 1552 | 1556 | 1558 | rBV | 592218 | 566683 | 31.51% | 3.490% |
| 20 | 11.507 | 1558 | 1559 | 1563 | rVV | 118228 | 92797 | 5.16% | 0.571% |
| 21 | 11.566 | 1566 | 1569 | 1572 | rVB | 21803 | 21232 | 1.18% | 0.131% |
| 22 | 12.019 | 1643 | 1646 | 1650 | rVB2 | 24340 | 23041 | 1.28% | 0.142% |
| 23 | 12.101 | 1657 | 1660 | 1663 | rBV2 | 22968 | 27630 | 1.54% | 0.170% |
| 24 | 12.536 | 1731 | 1734 | 1738 | rBV2 | 17628 | 22531 | 1.25% | 0.139% |
| 25 | 12.701 | 1759 | 1762 | 1767 | rVB | 163610 | 153248 | 8.52% | 0.944% |
| 26 | 12.919 | 1795 | 1799 | 1800 | rBV2 | 28050 | 33124 | 1.84% | 0.204% |
| 27 | 12.936 | 1800 | 1802 | 1807 | rVB | 167152 | 134539 | 7.48% | 0.829% |
| 28 | 13.071 | 1820 | 1825 | 1828 | rBV | 1875551 | 1666346 | 92.67% | 10.262% |
| 29 | 13.154 | 1835 | 1839 | 1843 | rBV3 | 13165 | 19245 | 1.07% | 0.119% |
| 30 | 13.260 | 1855 | 1857 | 1863 | rVB2 | 26238 | 30707 | 1.71% | 0.189% |
| 31 | 13.536 | 1900 | 1904 | 1914 | rVB | 41482 | 52441 | 2.92% | 0.323% |
| 32 | 13.889 | 1958 | 1964 | 1966 | rBV2 | 14539 | 19096 | 1.06% | 0.118% |
| 33 | 13.948 | 1971 | 1974 | 1979 | rBV4 | 53736 | 64026 | 3.56% | 0.394% |
| 34 | 14.089 | 1996 | 1998 | 2002 | rBV | 49629 | 46694 | 2.60% | 0.288% |

LSC Area Percent Report

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Sample : J3677-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 93-95-B3(0-2.5)

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

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Peak separation: 5

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

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.142 | 2002 | 2007 | 2010 | rVV | 619449 | 640793 | 35.64% | 3.946% |
| 36 | 14.166 | 2010 | 2011 | 2017 | rVB | 76915 | 58119 | 3.23% | 0.358% |
| 37 | 14.542 | 2070 | 2075 | 2077 | rBV | 18252 | 20683 | 1.15% | 0.127% |
| 38 | 15.065 | 2161 | 2164 | 2167 | rVB4 | 19246 | 22584 | 1.26% | 0.139% |
| 39 | 15.230 | 2188 | 2192 | 2195 | rBV | 49817 | 76767 | 4.27% | 0.473% |
| 40 | 15.260 | 2195 | 2197 | 2201 | rVB2 | 35624 | 37079 | 2.06% | 0.228% |
| 41 | 15.554 | 2243 | 2247 | 2253 | rVB | 30463 | 40839 | 2.27% | 0.252% |
| 42 | 15.618 | 2254 | 2258 | 2262 | rVV | 41767 | 53990 | 3.00% | 0.332% |
| 43 | 15.689 | 2264 | 2270 | 2281 | rVB | 314611 | 435055 | 24.19% | 2.679% |
| 44 | 16.124 | 2340 | 2344 | 2348 | rVB4 | 12889 | 19052 | 1.06% | 0.117% |

Sum of corrected areas: 16238170

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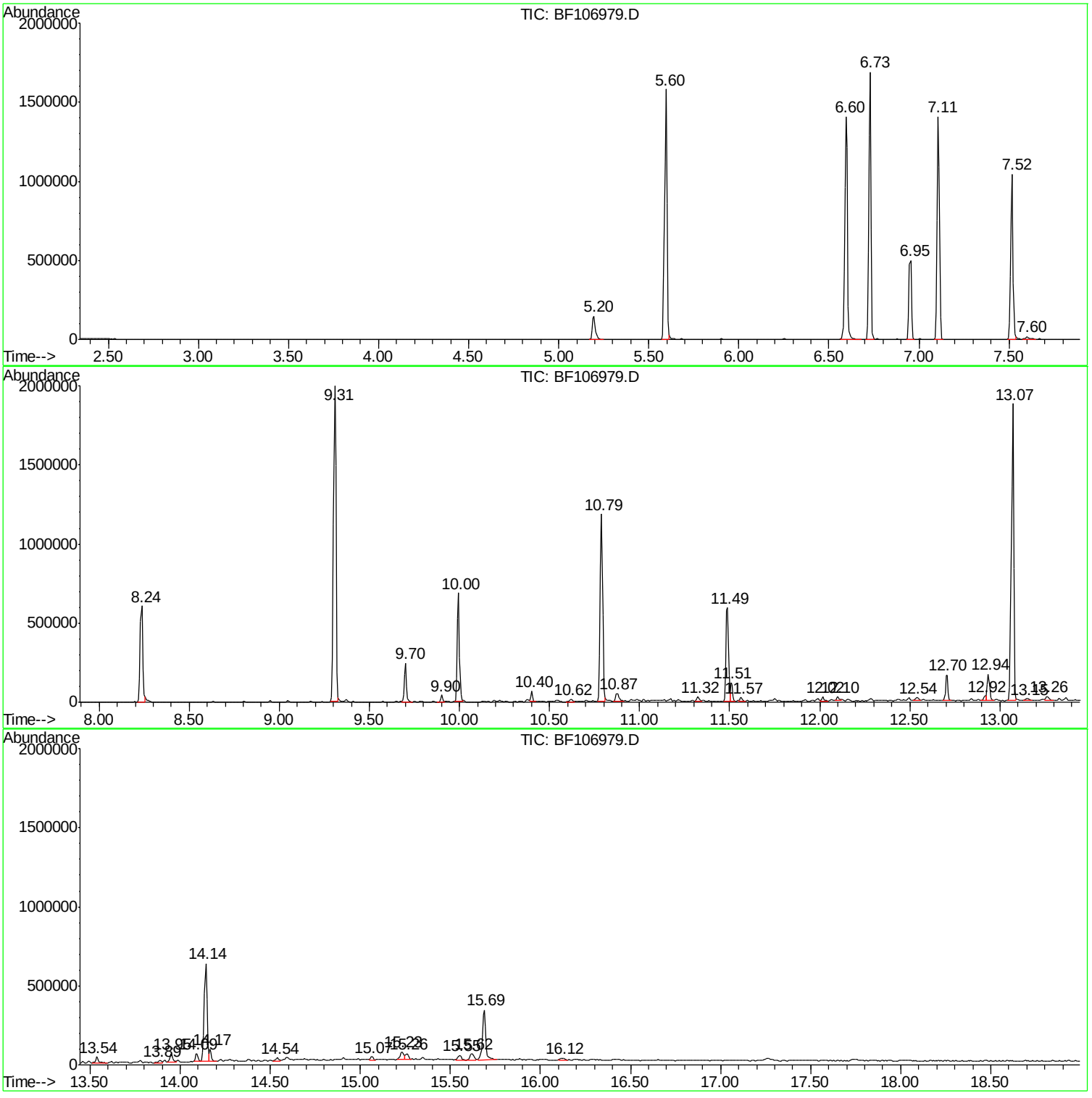
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
93-95-B3(0-2.5)

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\BF062918\
Data File : BF106979.D
Acq On : 29 Jun 2018 18:00
Operator : JU/SJ
Sample : J3677-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 93-95-B3(0-2.5)

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

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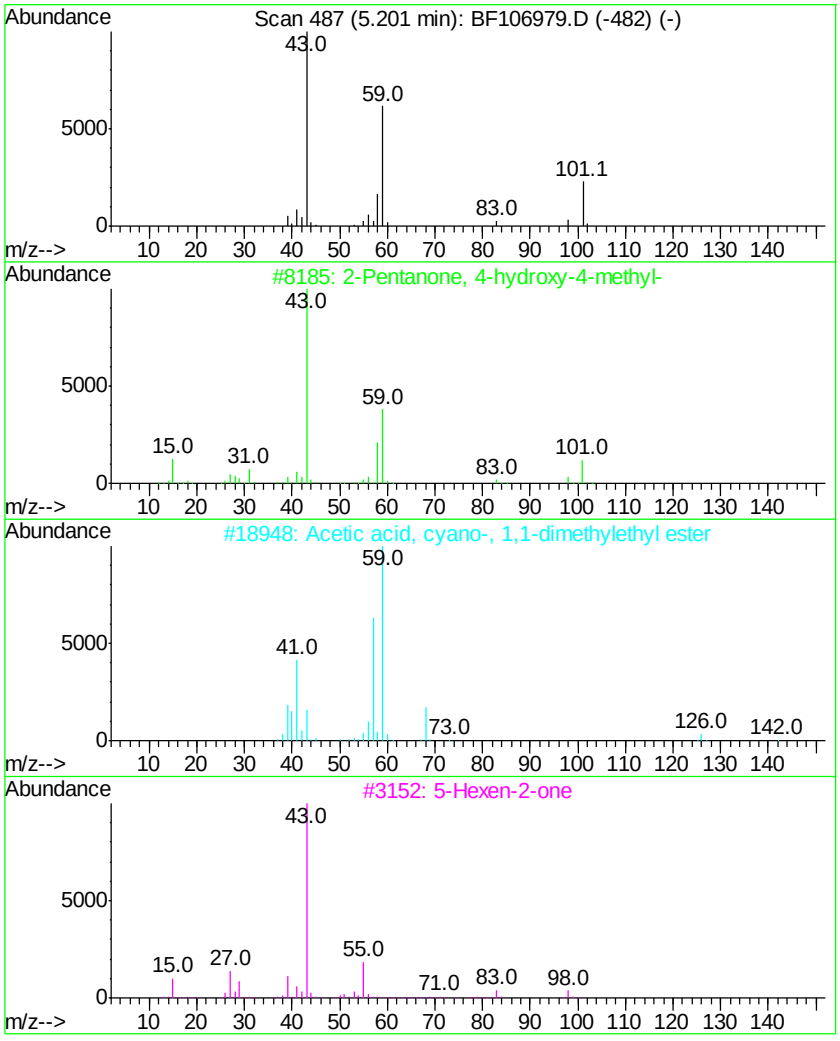
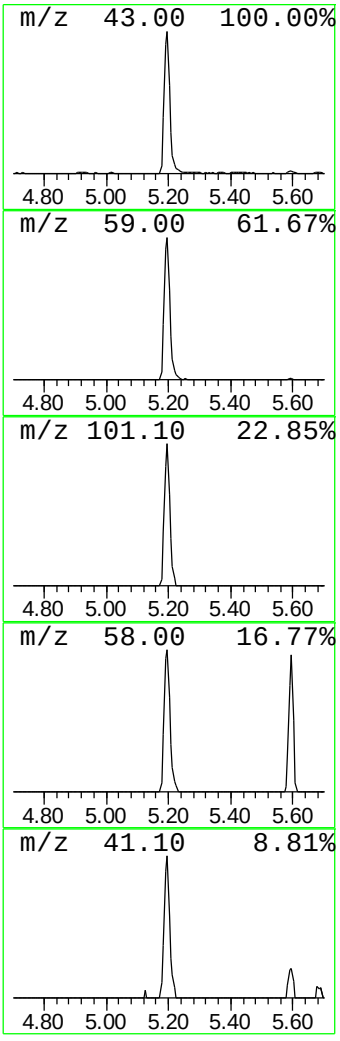
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.20 | 8.29 ng | 184497 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |



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Misc :
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**Instrument :** BNA_F
**ClientSampleId :** 93-95-B3(0-2.5)

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

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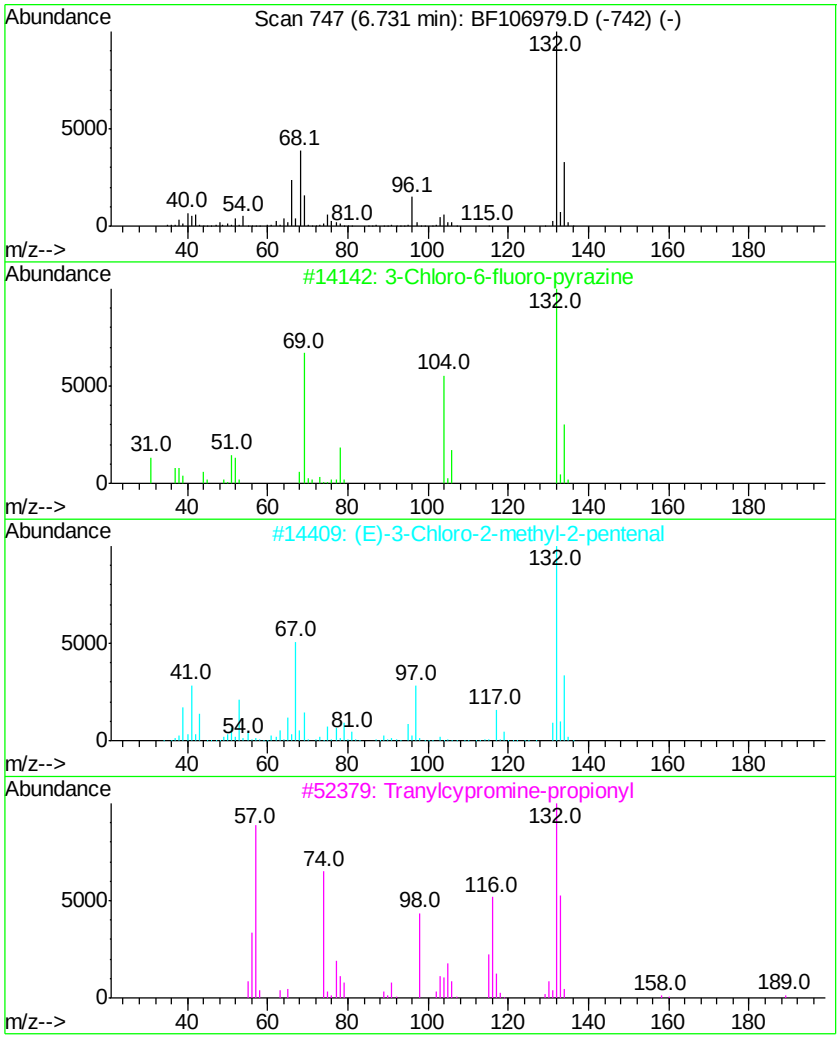
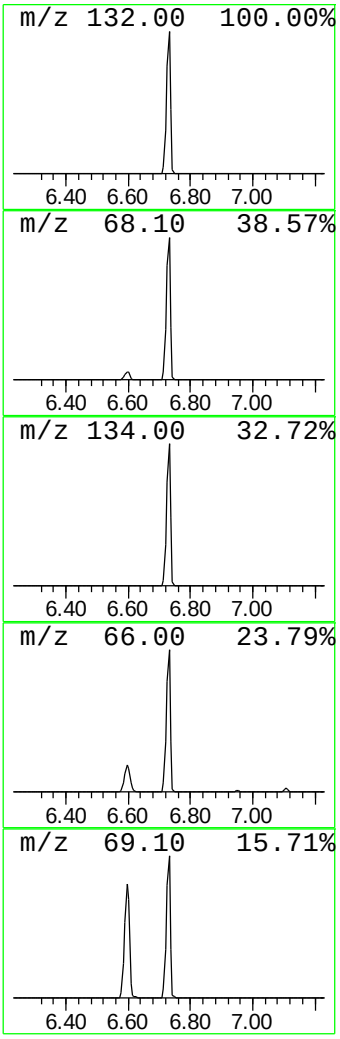
Peak Number 2 unknown6.73 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.73 | 69.12 ng | 1537900 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



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Operator : JU/SJ
Sample : J3677-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 93-95-B3(0-2.5)

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

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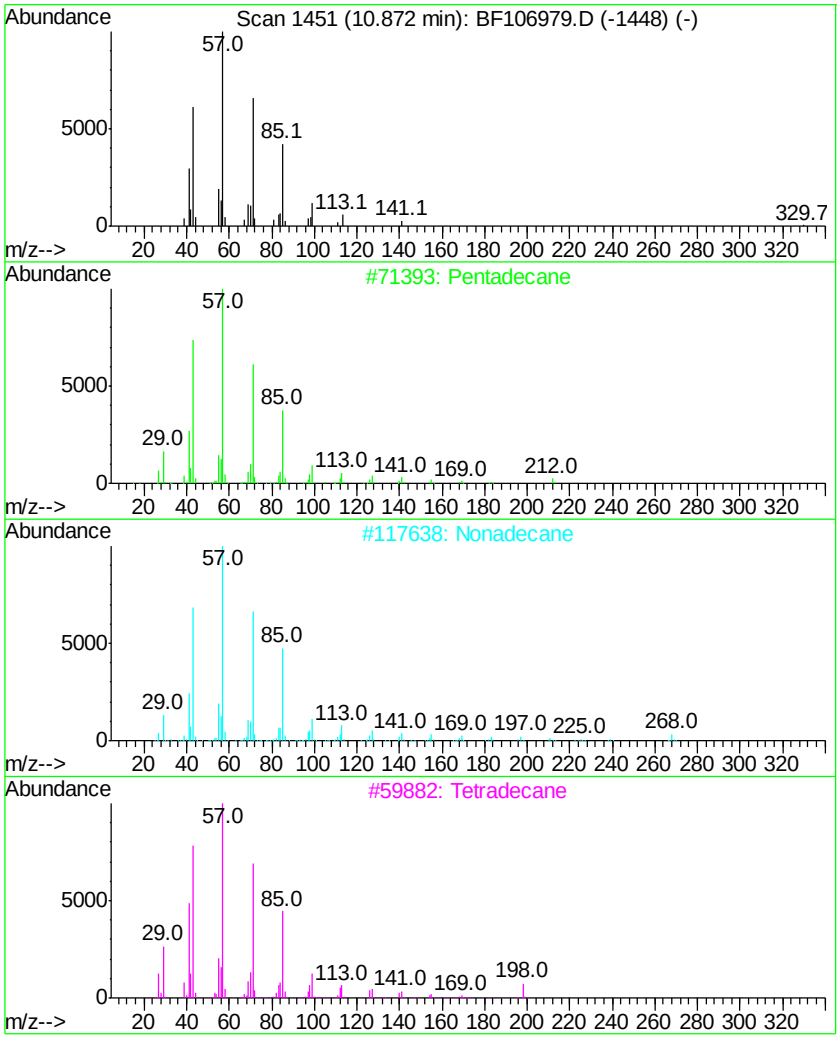
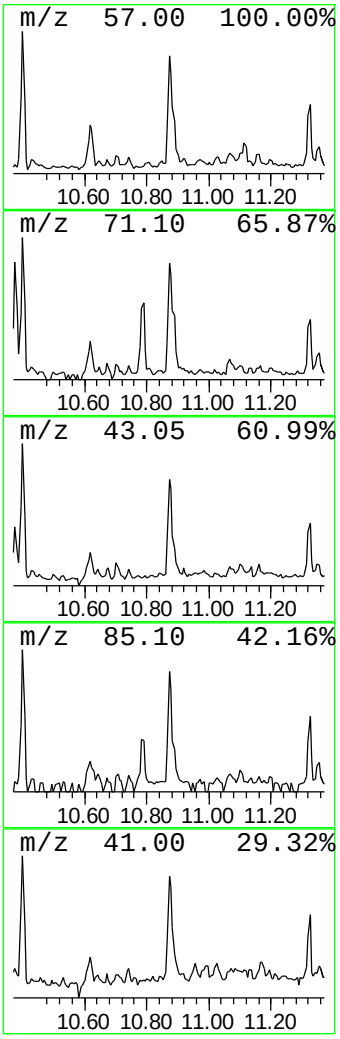
Peak Number 4 Pentadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.87 | 2.06 ng | 58248 | Phenanthrene-d10 | 11.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 90 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 5 | Hexadecane, 7,9-dimethyl- | 254 | C18H38 | 021164-95-4 | 86 |



Tentatively Identified Compound (LSC) summary

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Data File : BF106979.D
Acq On : 29 Jun 2018 18:00
Operator : JU/SJ
Sample : J3677-05
Misc :
ALS Vial : 19 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
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.20 | 8.3 | ng | 184497 | 1 | 6.95 | 445026 | 20.0 |
| unknown6.73 | 6.73 | 69.1 | ng | 1537900 | 1 | 6.95 | 445026 | 20.0 |
| Pentadecane | 10.87 | 2.1 | ng | 58248 | 4 | 11.49 | 566683 | 20.0 |