LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098363.D
Acq On : 8 Sep 2017 21:07
Operator : SJ/JU
Sample : I5137-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1-COMP

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-BF081517.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 | 4.881 | 471 | 475 | 487 | rVB | 134000 | 203116 | 8.03% | 1.029% |
| 2 | 5.298 | 541 | 546 | 549 | rBV | 2301702 | 2376464 | 93.99% | 12.044% |
| 3 | 6.334 | 717 | 722 | 733 | rBV | 2189297 | 2528450 | 100.00% | 12.814% |
| 4 | 6.457 | 738 | 743 | 746 | rBV | 2494870 | 2323488 | 91.89% | 11.775% |
| 5 | 6.681 | 778 | 781 | 785 | rBV | 640829 | 550797 | 21.78% | 2.791% |
| 6 | 6.839 | 804 | 808 | 811 | rBV | 2006632 | 1849600 | 73.15% | 9.373% |
| 7 | 7.251 | 873 | 878 | 881 | rBV | 1443711 | 1397855 | 55.29% | 7.084% |
| 8 | 7.969 | 995 | 1000 | 1003 | rBV | 715872 | 661688 | 26.17% | 3.353% |
| 9 | 9.045 | 1177 | 1183 | 1186 | rBV | 2642272 | 2316069 | 91.60% | 11.737% |
| 10 | 9.439 | 1246 | 1250 | 1253 | rBV | 337050 | 257868 | 10.20% | 1.307% |
| 11 | 9.716 | 1293 | 1297 | 1301 | rBV | 682468 | 598337 | 23.66% | 3.032% |
| 12 | 10.510 | 1427 | 1432 | 1435 | rBV | 1110614 | 1033974 | 40.89% | 5.240% |
| 13 | 10.622 | 1448 | 1451 | 1458 | rBV | 28762 | 33840 | 1.34% | 0.171% |
| 14 | 11.198 | 1546 | 1549 | 1553 | rBV | 609828 | 532527 | 21.06% | 2.699% |
| 15 | 12.410 | 1752 | 1755 | 1759 | rVB | 38952 | 32176 | 1.27% | 0.163% |
| 16 | 12.639 | 1791 | 1794 | 1797 | rVB | 34218 | 30439 | 1.20% | 0.154% |
| 17 | 12.786 | 1815 | 1819 | 1822 | rBV | 1945133 | 1733553 | 68.56% | 8.785% |
| 18 | 13.345 | 1911 | 1914 | 1919 | rBV7 | 21193 | 32579 | 1.29% | 0.165% |
| 19 | 13.686 | 1968 | 1972 | 1978 | rBV3 | 105895 | 140630 | 5.56% | 0.713% |
| 20 | 13.833 | 1993 | 1997 | 2000 | rBV | 667443 | 638513 | 25.25% | 3.236% |
| 21 | 15.245 | 2232 | 2237 | 2244 | rBV | 362552 | 460261 | 18.20% | 2.333% |

Sum of corrected areas: 19732224

LSC Report - Integrated Chromatogram

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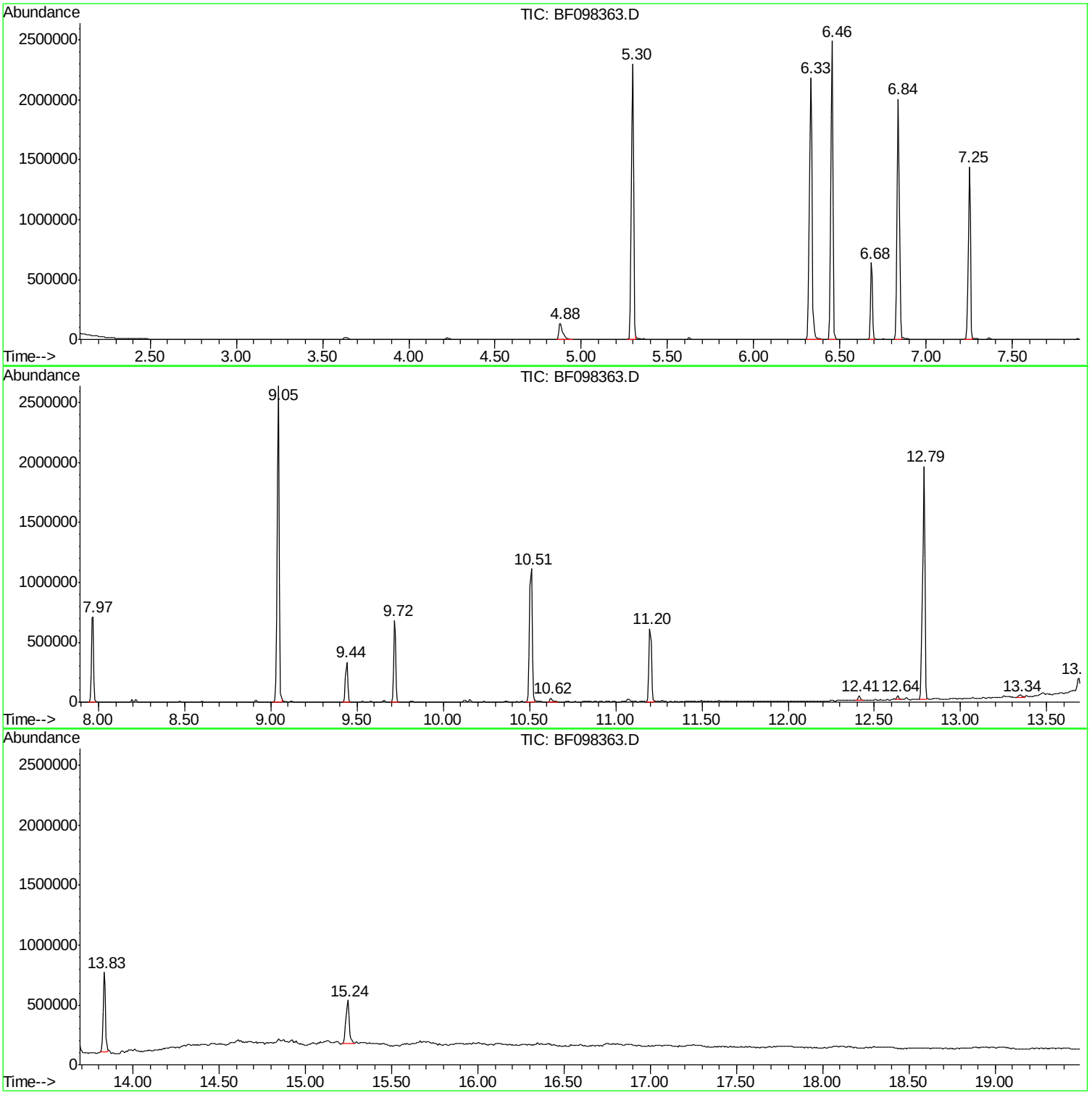
Sample : I5137-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098363.D
Acq On : 8 Sep 2017 21:07
Operator : SJ/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

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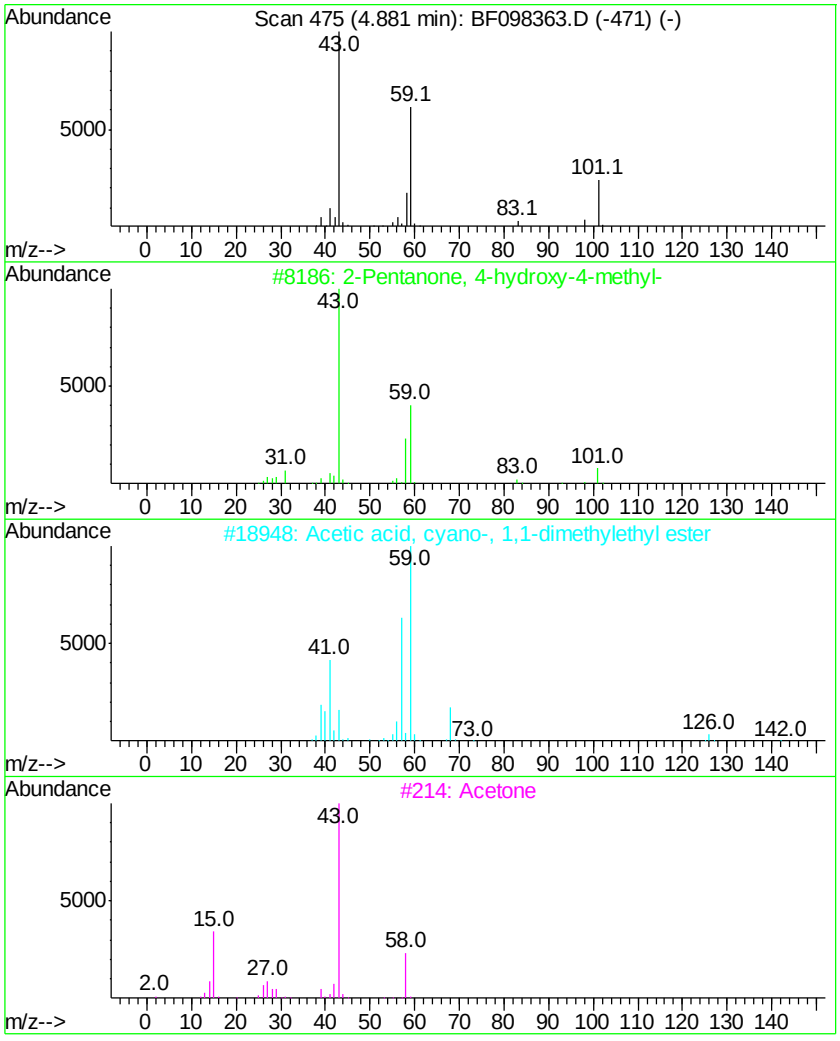
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

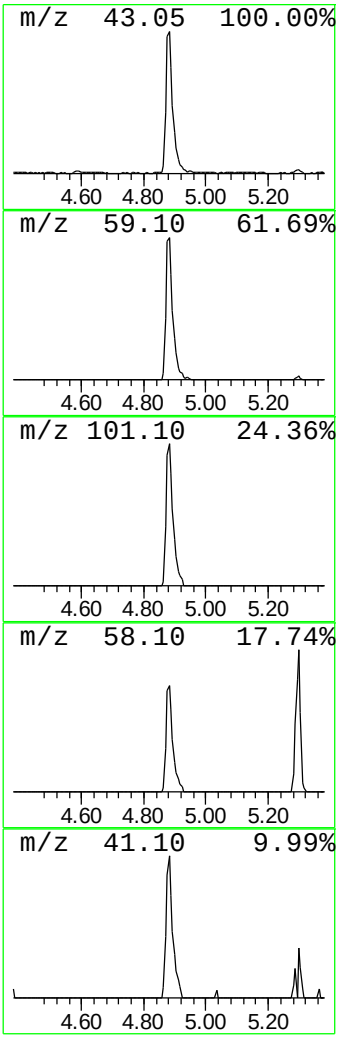
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.88 | 7.38 ng | 203116 | 1,4-Dichlorobenzene-d4 | 6.68 |

| 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, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 10 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



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Sample : I5137-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

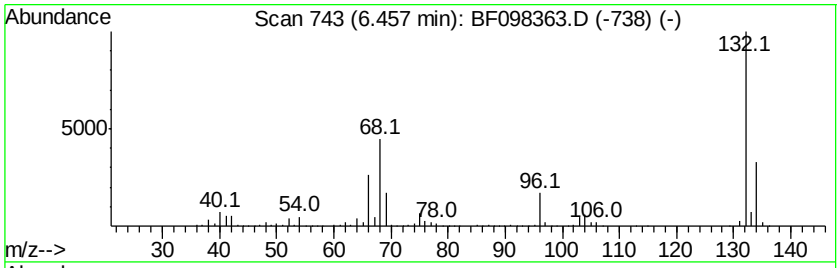
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

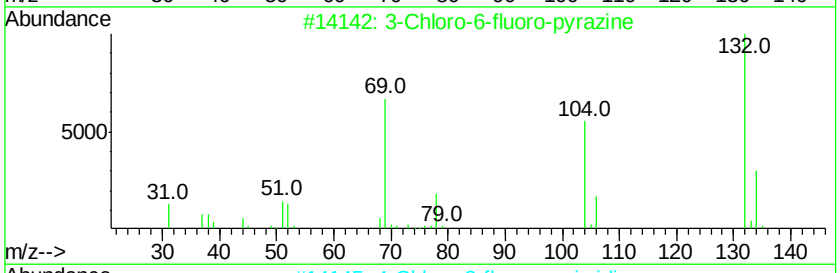
**********

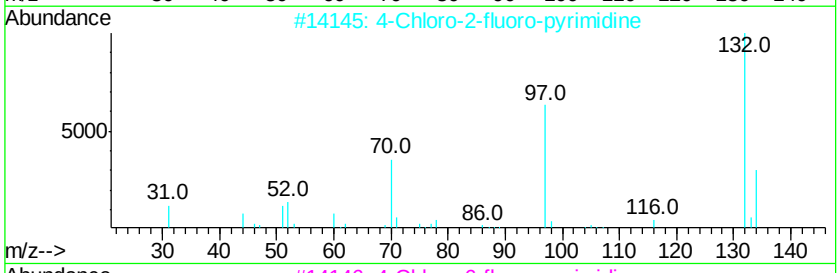
Peak Number 2 unknown6.46 Concentration Rank 1

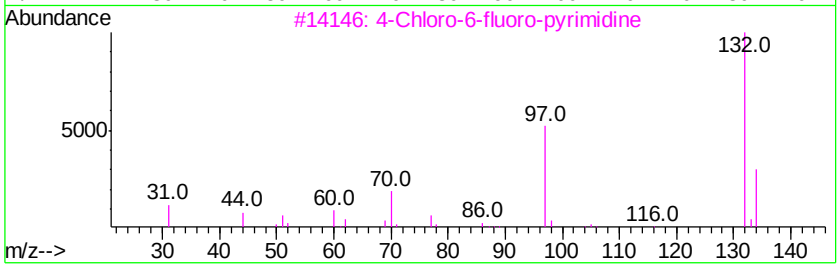
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.46 | 84.37 ng | 2323490 | 1,4-Dichlorobenzene-d4 | 6.68 |

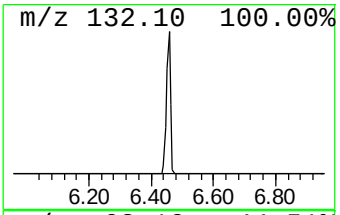
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |

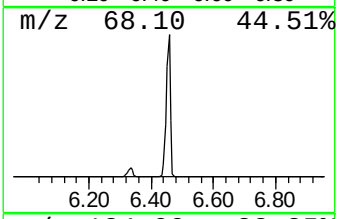


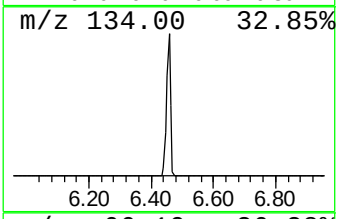



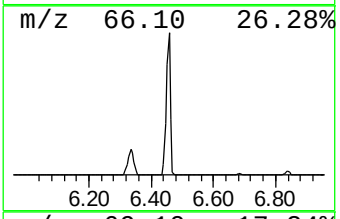



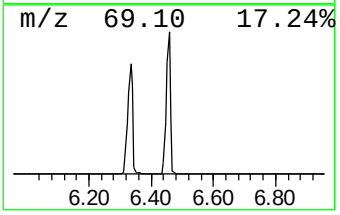



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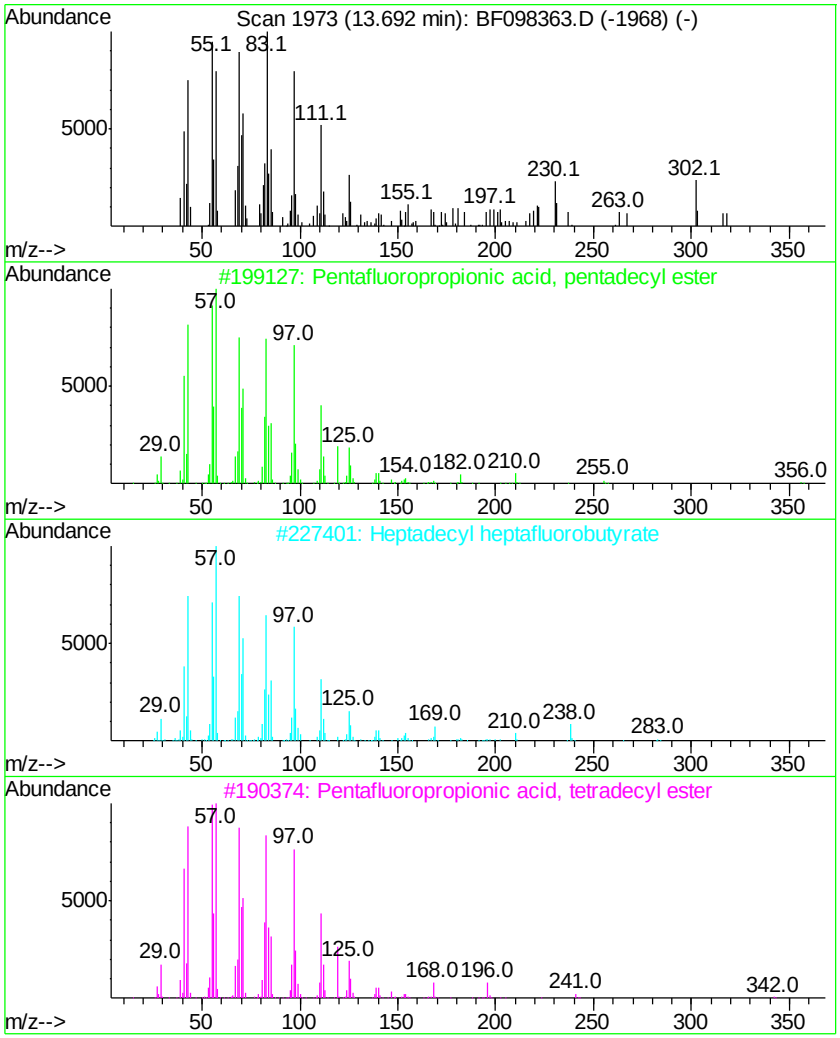
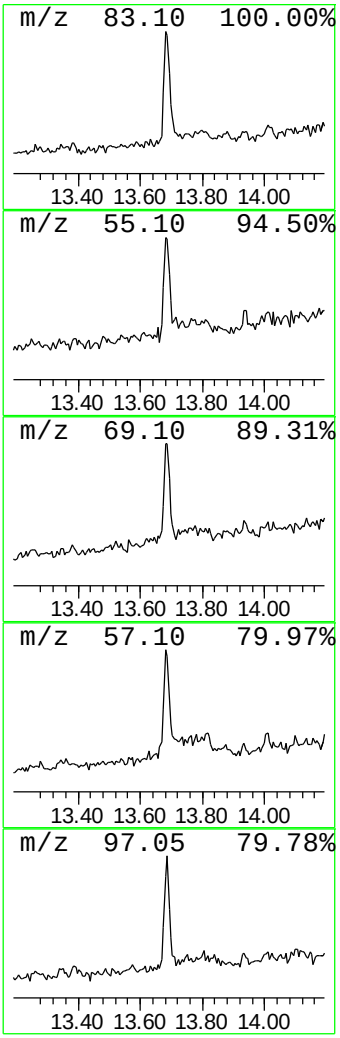
**********

Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.69 | 4.40 ng | 140630 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 3 | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 94 |
| 4 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 5 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.88 | 7.4 | ng | 203116 | 1 | 6.68 | 550797 | 20.0 |
| unknown6.46 | 6.46 | 84.4 | ng | 2323490 | 1 | 6.68 | 550797 | 20.0 |
| Pentafluoropropio... | 13.69 | 4.4 | ng | 140630 | 5 | 13.83 | 638513 | 20.0 |