# LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084296.D
Acq On : 6 Jan 2016 18:20
Operator : SJ/UM
Sample : H1010-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TEMW-2-15

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-BF123115.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 | 3.813 | 149 | 151 | 154 | rVB | 83799 | 118017 | 1.44% | 0.192% |
| 2 | 5.047 | 256 | 259 | 262 | rBV | 707790 | 851246 | 10.36% | 1.383% |
| 3 | 5.218 | 269 | 274 | 279 | rVB | 36182 | 89544 | 1.09% | 0.145% |
| 4 | 5.470 | 294 | 296 | 299 | rVB | 3723574 | 3840357 | 46.72% | 6.239% |
| 5 | 6.499 | 384 | 386 | 389 | rVB | 1949130 | 2702914 | 32.88% | 4.391% |
| 6 | 6.636 | 395 | 398 | 401 | rBV | 6567780 | 6149047 | 74.81% | 9.989% |
| 7 | 6.864 | 416 | 418 | 420 | rBV | 2131092 | 1743548 | 21.21% | 2.832% |
| 8 | 7.024 | 429 | 432 | 434 | rBV | 6713962 | 6016436 | 73.19% | 9.774% |
| 9 | 7.436 | 464 | 468 | 470 | rBV | 5361688 | 5678041 | 69.08% | 9.224% |
| 10 | 7.539 | 473 | 477 | 479 | rBV | 105371 | 175183 | 2.13% | 0.285% |
| 11 | 7.687 | 488 | 490 | 492 | rVB | 98822 | 85525 | 1.04% | 0.139% |
| 12 | 8.156 | 528 | 531 | 533 | rBV | 2329259 | 2313681 | 28.15% | 3.759% |
| 13 | 9.230 | 622 | 625 | 628 | rVB | 8086134 | 8219824 | 100.00% | 13.353% |
| 14 | 9.619 | 657 | 659 | 661 | rBV | 133710 | 141556 | 1.72% | 0.230% |
| 15 | 9.905 | 682 | 684 | 687 | rVB | 2809958 | 2504520 | 30.47% | 4.069% |
| 16 | 10.339 | 719 | 722 | 724 | rBV2 | 115292 | 126809 | 1.54% | 0.206% |
| 17 | 10.556 | 737 | 741 | 745 | rBV2 | 36522 | 82215 | 1.00% | 0.134% |
| 18 | 10.693 | 750 | 753 | 756 | rBV2 | 4504464 | 5610892 | 68.26% | 9.115% |
| 19 | 10.808 | 760 | 763 | 767 | rVV3 | 80336 | 177754 | 2.16% | 0.289% |
| 20 | 11.265 | 801 | 803 | 804 | rBV | 105339 | 109958 | 1.34% | 0.179% |
| 21 | 11.391 | 811 | 814 | 816 | rBV | 2816707 | 2479053 | 30.16% | 4.027% |
| 22 | 12.979 | 950 | 953 | 955 | rBV | 7728794 | 7667833 | 93.28% | 12.457% |
| 23 | 13.471 | 993 | 996 | 998 | rBV3 | 76385 | 87761 | 1.07% | 0.143% |
| 24 | 13.539 | 1000 | 1002 | 1005 | rBV3 | 68227 | 104432 | 1.27% | 0.170% |
| 25 | 13.882 | 1030 | 1032 | 1037 | rVB | 153512 | 255393 | 3.11% | 0.415% |
| 26 | 14.019 | 1042 | 1044 | 1047 | rBV | 1961141 | 2150782 | 26.17% | 3.494% |
| 27 | 14.659 | 1098 | 1100 | 1102 | rBV | 90731 | 99047 | 1.20% | 0.161% |
| 28 | 15.448 | 1166 | 1169 | 1172 | rBV | 1101951 | 1584251 | 19.27% | 2.574% |
| 29 | 16.145 | 1228 | 1230 | 1235 | rVB2 | 133582 | 254318 | 3.09% | 0.413% |
| 30 | 16.671 | 1273 | 1276 | 1281 | rVB5 | 72238 | 136165 | 1.66% | 0.221% |

Sum of corrected areas: 61556102

LSC Report - Integrated Chromatogram

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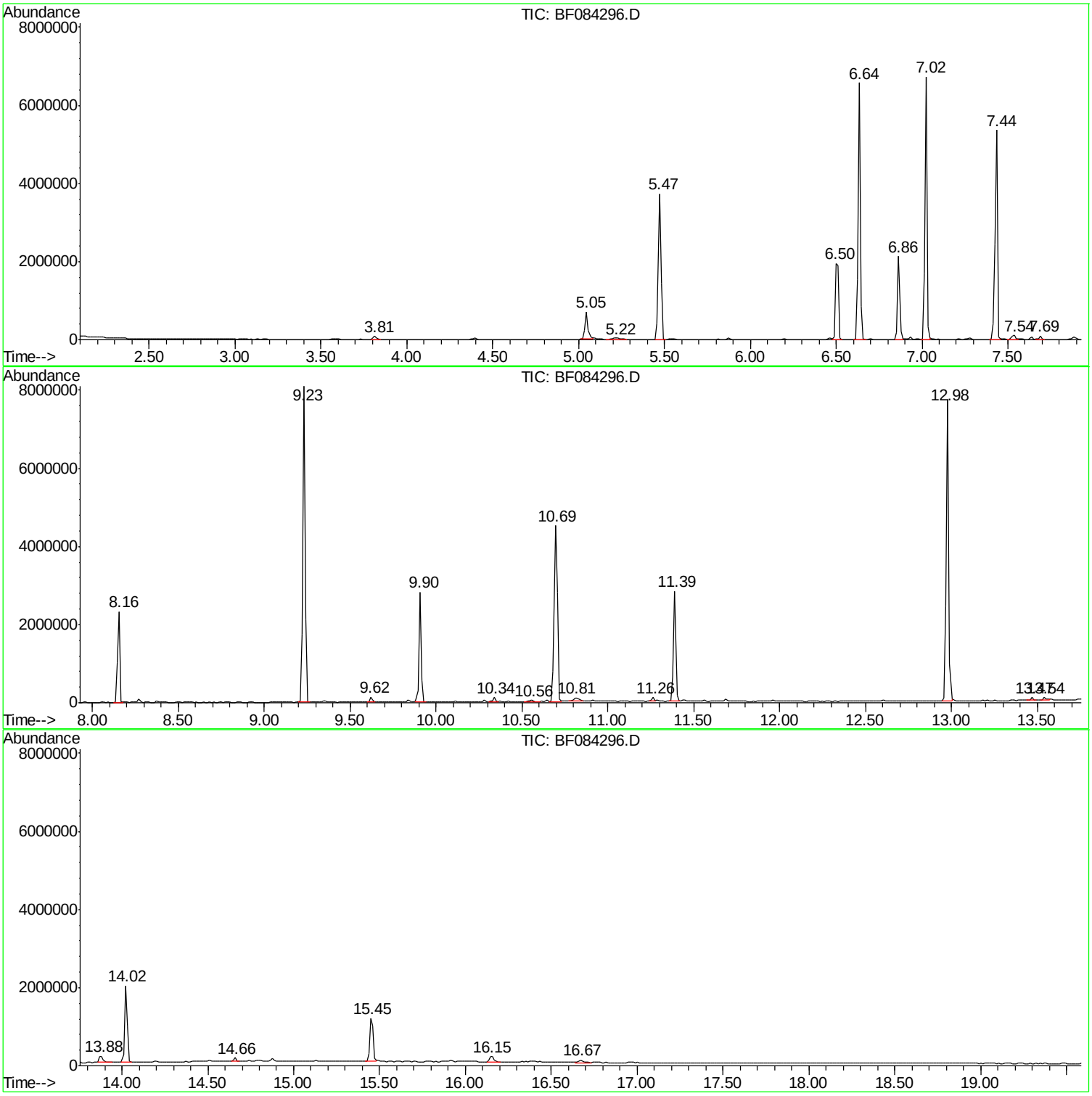
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TEMW-2-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

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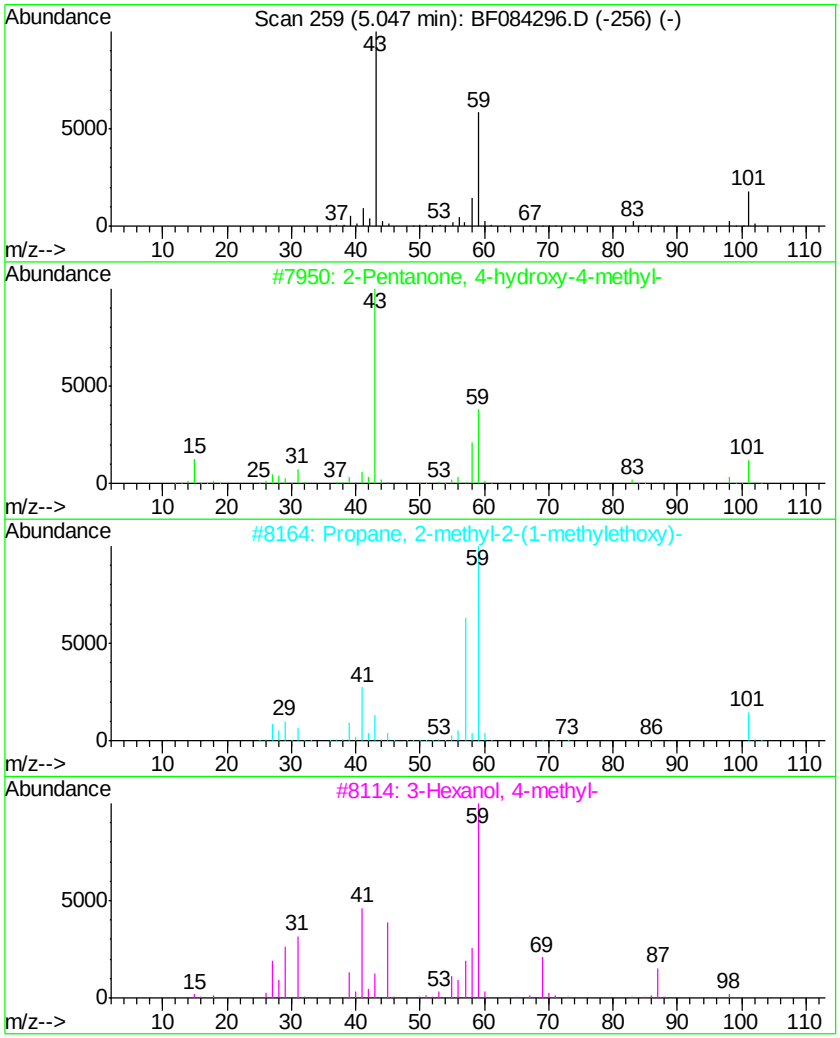
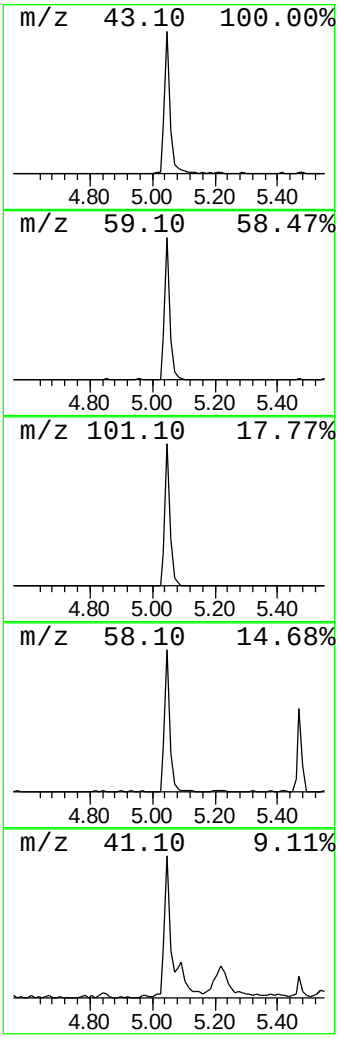
**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.05 | 9.76 ng | 851246 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 5 | 1,2-Butanediol, (.+/-.)- | 90 | C4H10O2 | 026171-83-5 | 28 |



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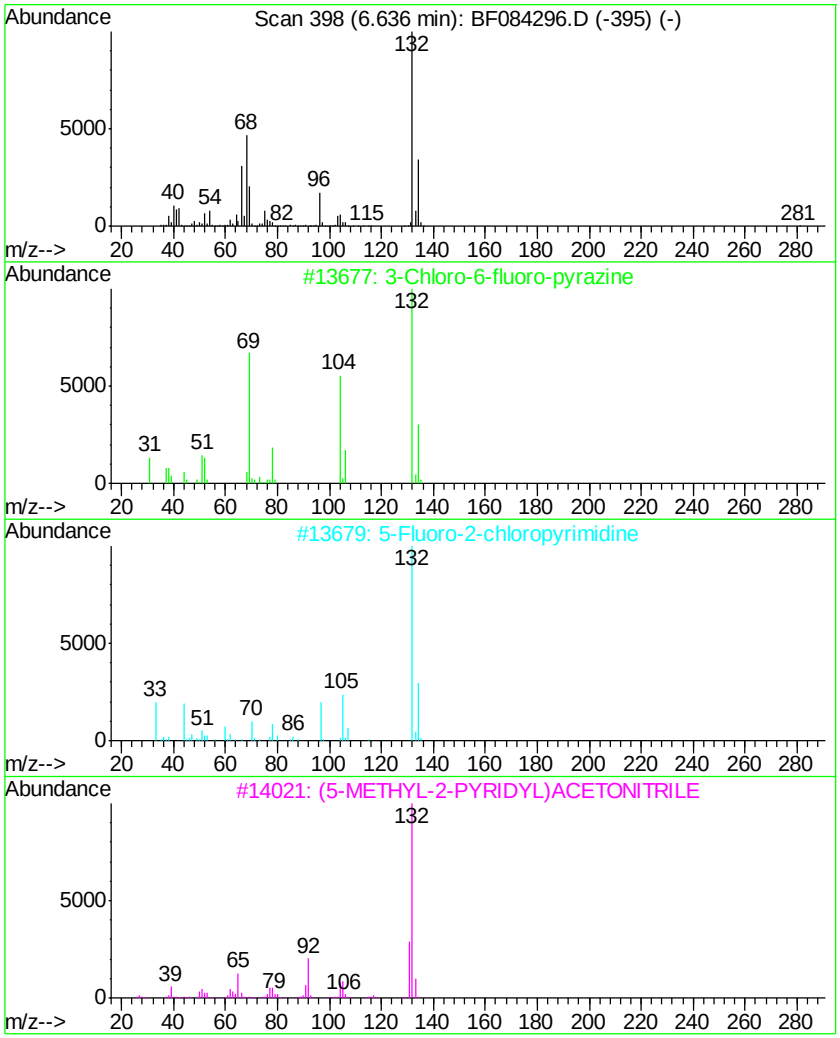
TIC Integration Parameters: LSCINT.P

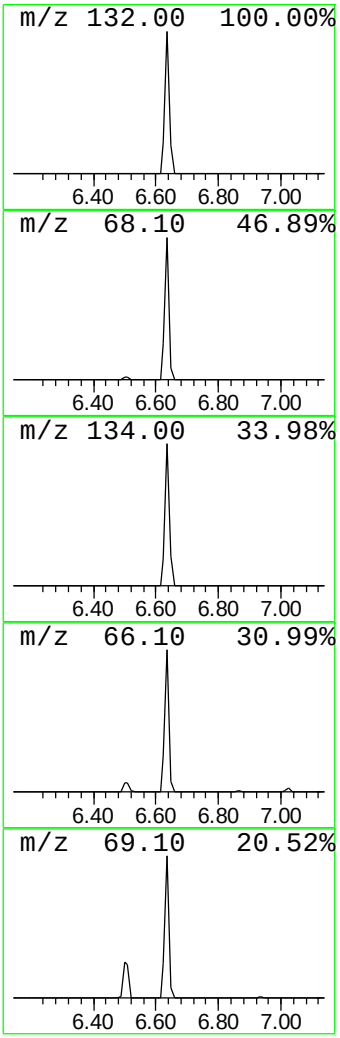
**********

Peak Number 2 unknown6.64 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.64 | 70.53 ng | 6149050 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | 1,2,3-Trifluorobenzene | 132 | C6H3F3 | 001489-53-8 | 9 |



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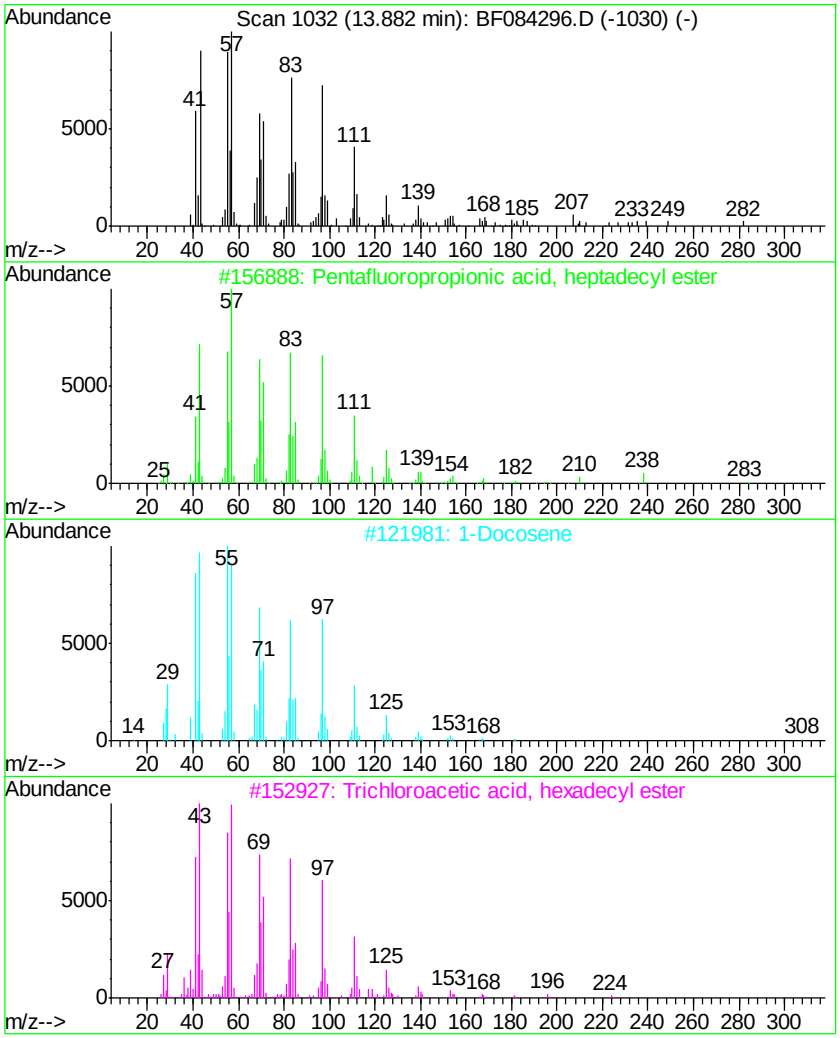
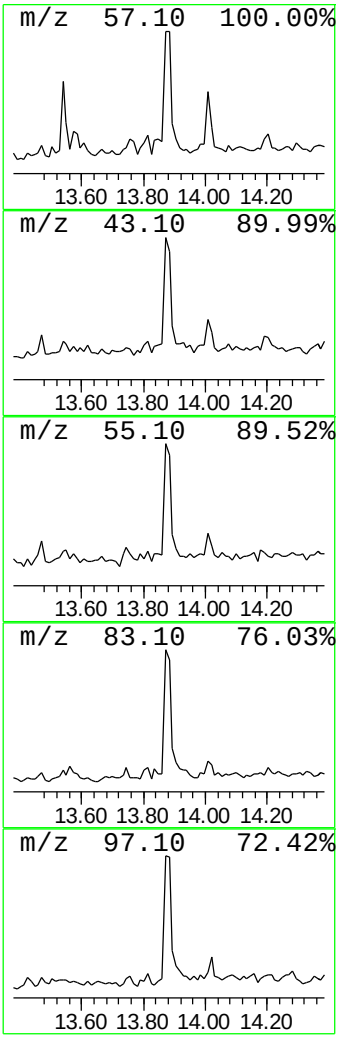
**********
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.88 | 2.37 ng | 255393 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 1000283-04-2 | 94 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 4 | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1 | 91 |
| 5 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 91 |



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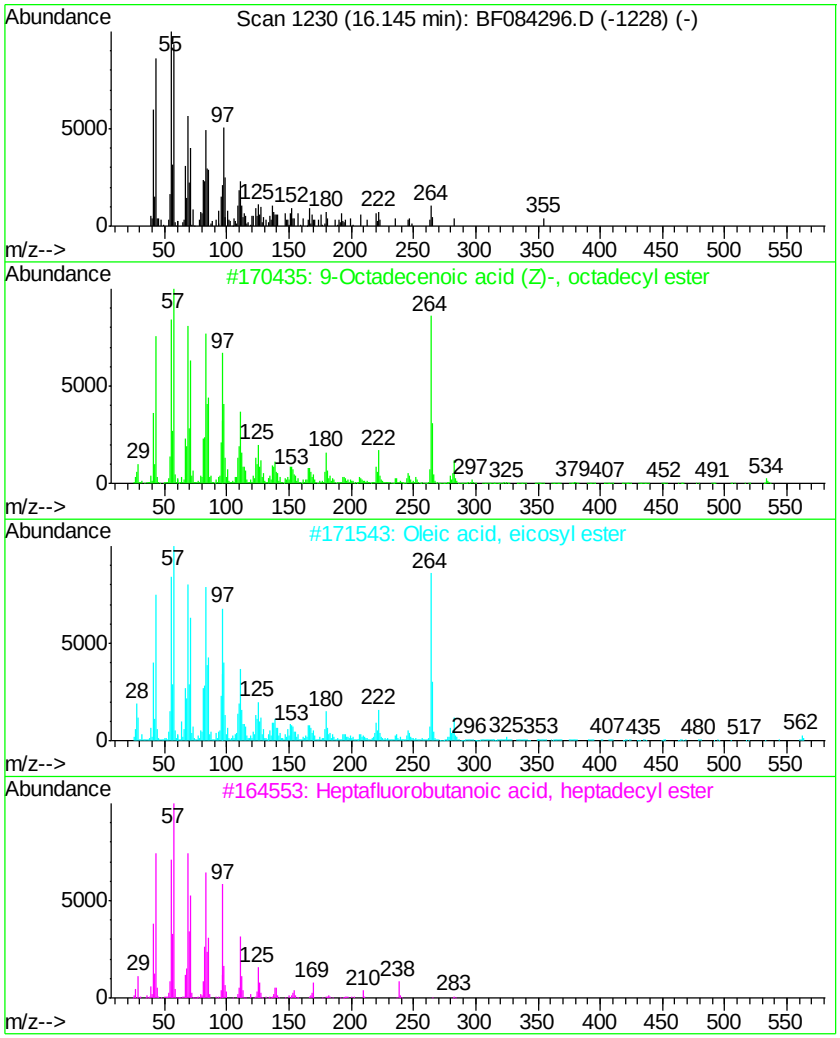
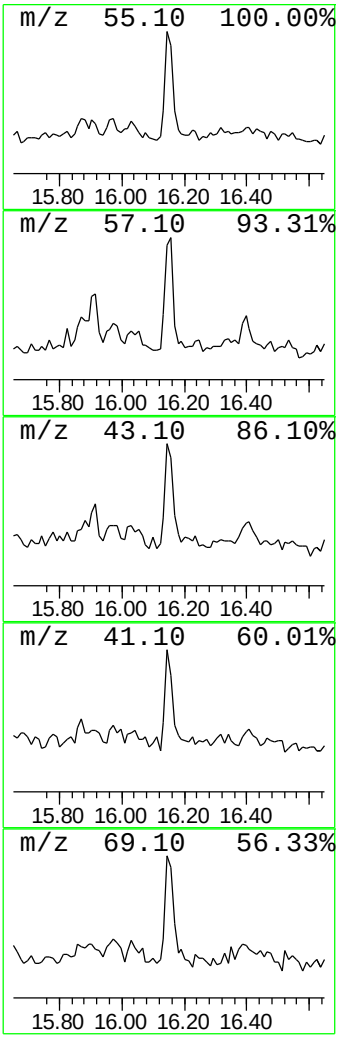
**********
Peak Number 5 9-Octadecenoic acid (Z)-, o... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.15 | 3.21 ng | 254318 | Perylene-d12 | 15.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenoic acid (Z)-, octade... | 535 | C36H70O2 | 017673-49-3 | 91 |
| 2 | Oleic acid, eicosyl ester | 563 | C38H74O2 | 022393-88-0 | 91 |
| 3 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 76 |
| 4 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 1000283-04-2 | 76 |
| 5 | Trifluoroacetic acid, n-octadecy... | 366 | C20H37F3O2 | 079392-43-1 | 72 |



Tentatively Identified Compound (LSC) summary

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| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| 2-Pentanone, 4-hy... | 5.05 | 9.8 | ng | 851246 | 1 | 6.86 | 1743550 | 20.0 |
| unknown6.64 | 6.64 | 70.5 | ng | 6149050 | 1 | 6.86 | 1743550 | 20.0 |
| Pentafluoropropio... | 13.88 | 2.4 | ng | 255393 | 5 | 14.02 | 2150780 | 20.0 |
| 9-Octadecenoic ac... | 16.15 | 3.2 | ng | 254318 | 6 | 15.45 | 1584250 | 20.0 |