LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072120\
Data File : BF120958.D
Acq On : 21 Jul 2020 17:17
Operator : JU/CG
Sample : L3351-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SAMPLE-1B

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-BF071620.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 | 2.246 | 25 | 27 | 43 | rVB | 36277 | 83670 | 1.78% | 0.247% |
| 2 | 5.028 | 497 | 500 | 510 | rVB | 111486 | 150860 | 3.20% | 0.446% |
| 3 | 5.434 | 563 | 569 | 572 | rBV | 3350735 | 3463777 | 73.55% | 10.236% |
| 4 | 6.445 | 735 | 741 | 744 | rBV | 3161141 | 3503156 | 74.39% | 10.352% |
| 5 | 6.645 | 772 | 775 | 781 | rBV | 41659 | 48853 | 1.04% | 0.144% |
| 6 | 6.816 | 800 | 804 | 807 | rBV | 1146580 | 1001151 | 21.26% | 2.958% |
| 7 | 7.375 | 894 | 899 | 902 | rBV | 2341699 | 2374487 | 50.42% | 7.017% |
| 8 | 8.098 | 1017 | 1022 | 1025 | rBV | 1484466 | 1319963 | 28.03% | 3.901% |
| 9 | 9.175 | 1199 | 1205 | 1208 | rBV | 4295665 | 4255034 | 90.35% | 12.574% |
| 10 | 9.563 | 1267 | 1271 | 1280 | rBV | 660594 | 585057 | 12.42% | 1.729% |
| 11 | 9.851 | 1315 | 1320 | 1331 | rBV | 1739760 | 1579100 | 33.53% | 4.666% |
| 12 | 10.639 | 1449 | 1454 | 1457 | rBV | 2672568 | 2737167 | 58.12% | 8.089% |
| 13 | 11.333 | 1568 | 1572 | 1575 | rBV | 2002711 | 1747464 | 37.11% | 5.164% |
| 14 | 11.357 | 1575 | 1576 | 1578 | rVB | 165935 | 77965 | 1.66% | 0.230% |
| 15 | 11.945 | 1673 | 1676 | 1678 | rBV | 48633 | 55065 | 1.17% | 0.163% |
| 16 | 12.210 | 1716 | 1721 | 1724 | rBV2 | 52247 | 49770 | 1.06% | 0.147% |
| 17 | 12.310 | 1735 | 1738 | 1741 | rBV | 262257 | 220636 | 4.69% | 0.652% |
| 18 | 12.368 | 1745 | 1748 | 1752 | rVV2 | 36866 | 52666 | 1.12% | 0.156% |
| 19 | 12.421 | 1752 | 1757 | 1762 | rVB5 | 24684 | 49064 | 1.04% | 0.145% |
| 20 | 12.539 | 1774 | 1777 | 1780 | rBV | 184986 | 178954 | 3.80% | 0.529% |
| 21 | 12.768 | 1810 | 1816 | 1819 | rBV | 250433 | 241141 | 5.12% | 0.713% |
| 22 | 12.921 | 1837 | 1842 | 1845 | rBV2 | 4214339 | 4709306 | 100.00% | 13.916% |
| 23 | 13.151 | 1877 | 1881 | 1887 | rBV4 | 40809 | 77822 | 1.65% | 0.230% |
| 24 | 13.445 | 1927 | 1931 | 1935 | rVB | 57788 | 50399 | 1.07% | 0.149% |
| 25 | 13.492 | 1935 | 1939 | 1942 | rBV | 43391 | 48888 | 1.04% | 0.144% |
| 26 | 13.533 | 1942 | 1946 | 1950 | rVB | 151720 | 129514 | 2.75% | 0.383% |
| 27 | 13.768 | 1983 | 1986 | 1990 | rVB2 | 58092 | 50031 | 1.06% | 0.148% |
| 28 | 13.827 | 1992 | 1996 | 2004 | rBV | 588371 | 848699 | 18.02% | 2.508% |
| 29 | 13.968 | 2015 | 2020 | 2023 | rBV | 1856026 | 1709979 | 36.31% | 5.053% |
| 30 | 13.992 | 2023 | 2024 | 2031 | rVB | 121392 | 80992 | 1.72% | 0.239% |
| 31 | 14.139 | 2045 | 2049 | 2052 | rBV | 54827 | 56526 | 1.20% | 0.167% |
| 32 | 14.445 | 2095 | 2101 | 2103 | rBV3 | 70481 | 88601 | 1.88% | 0.262% |
| 33 | 14.474 | 2103 | 2106 | 2114 | rVB5 | 52695 | 91890 | 1.95% | 0.272% |
| 34 | 14.745 | 2150 | 2152 | 2161 | rVB | 61316 | 64239 | 1.36% | 0.190% |

LSC Area Percent Report

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Operator : JU/CG
Sample : L3351-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SAMPLE-1B

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.992 | 2190 | 2194 | 2203 | rVB | 66154 | 133591 | 2.84% | 0.395% |
| 36 | 15.080 | 2205 | 2209 | 2215 | rBV2 | 66529 | 89856 | 1.91% | 0.266% |
| 37 | 15.292 | 2241 | 2245 | 2251 | rVB | 39379 | 50804 | 1.08% | 0.150% |
| 38 | 15.351 | 2251 | 2255 | 2260 | rBV2 | 53683 | 68819 | 1.46% | 0.203% |
| 39 | 15.415 | 2260 | 2266 | 2270 | rVV | 1075995 | 1334618 | 28.34% | 3.944% |
| 40 | 15.451 | 2270 | 2272 | 2279 | rVB2 | 72217 | 91850 | 1.95% | 0.271% |
| 41 | 15.880 | 2341 | 2345 | 2351 | rVB | 49138 | 69574 | 1.48% | 0.206% |
| 42 | 15.956 | 2352 | 2358 | 2369 | rBV5 | 62447 | 167876 | 3.56% | 0.496% |
| 43 | 16.368 | 2424 | 2428 | 2434 | rBV2 | 30382 | 50973 | 1.08% | 0.151% |

Sum of corrected areas: 33839847

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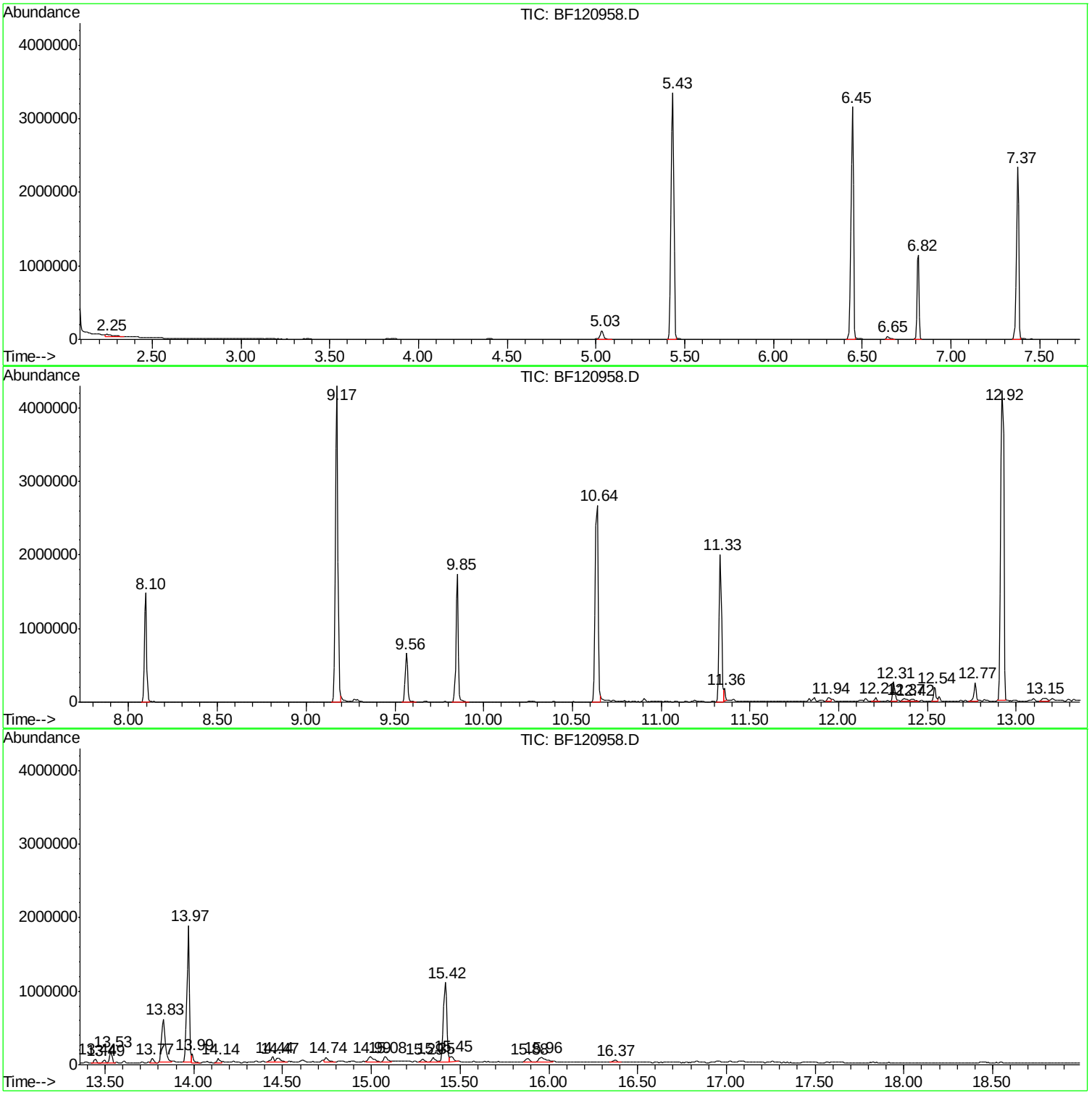
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SAMPLE-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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\BF072120\
Data File : BF120958.D
Acq On : 21 Jul 2020 17:17
Operator : JU/CG
Sample : L3351-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SAMPLE-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

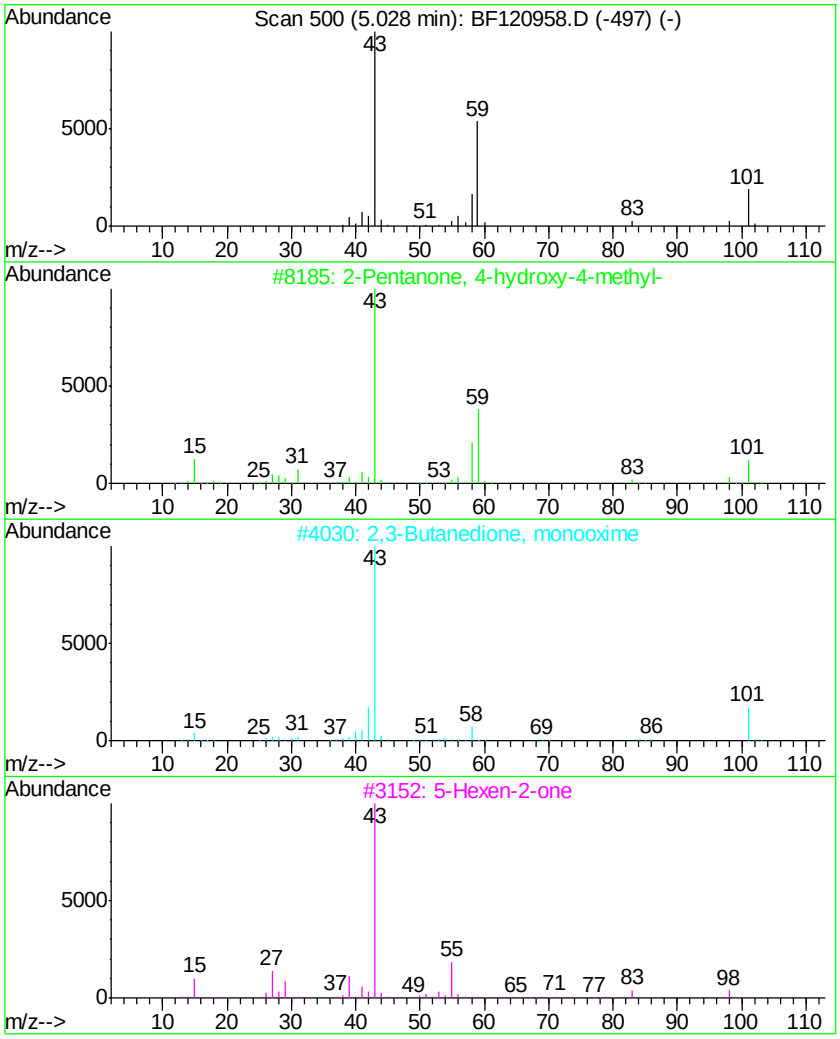
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

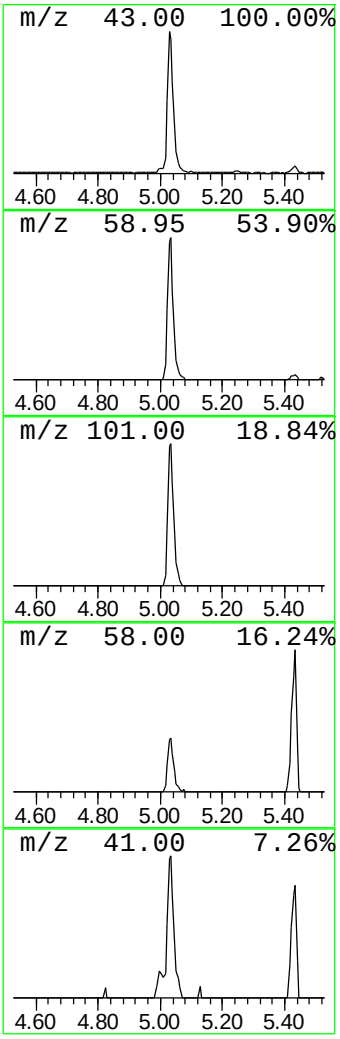
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.03 | 3.01 ng | 150860 | 1,4-Dichlorobenzene-d4 | 6.82 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 9 |



# Library Search Compound Report

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Sample : L3351-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SAMPLE-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

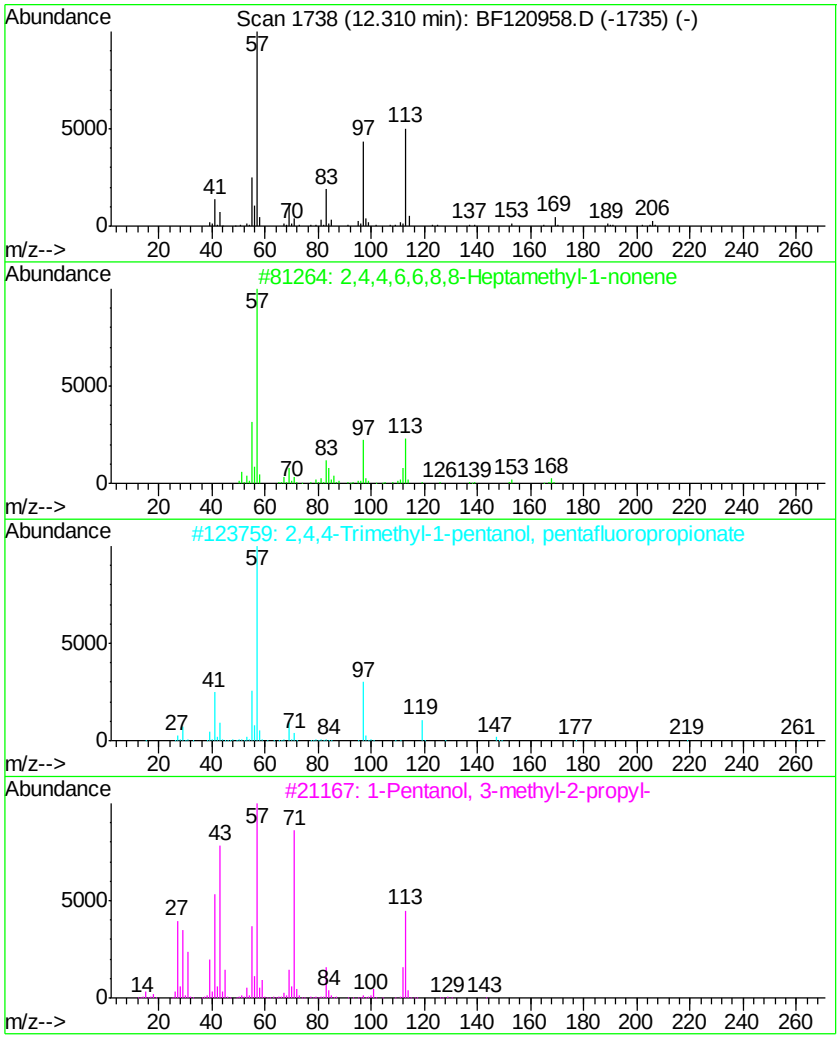
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

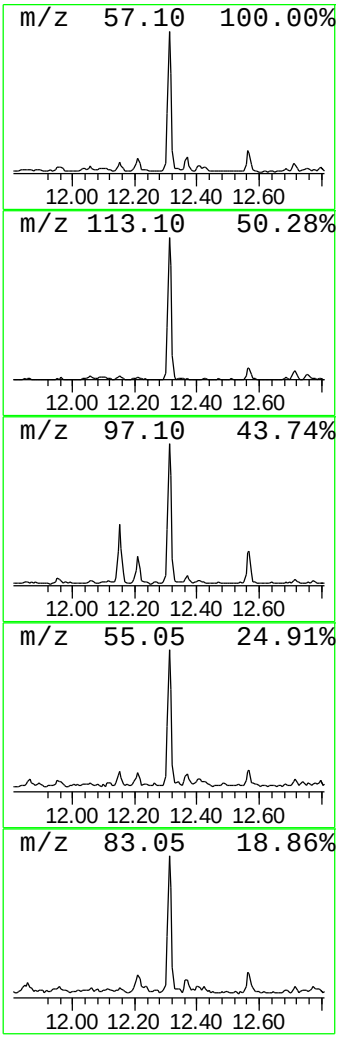
**********

Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.31 | 2.53 ng | 220636 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,4,6,6,8,8-Heptamethyl-1-nonene | 224 | C16H32 | 015796-04-0 | 56 |
| 2 | 2,4,4-Trimethyl-1-pentanol, pent... | 276 | C11H17F5O2 | 1000365-51-0 | 37 |
| 3 | 1-Pentanol, 3-methyl-2-propyl- | 144 | C9H20O | 054004-40-9 | 33 |
| 4 | 2,4,4-Trimethyl-1-pentanol, trif... | 226 | C10H17F3O2 | 1000365-19-5 | 32 |
| 5 | (1-Propoxy-pentyl)-cyclopropane | 170 | C11H22O | 094883-97-3 | 22 |



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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SAMPLE-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

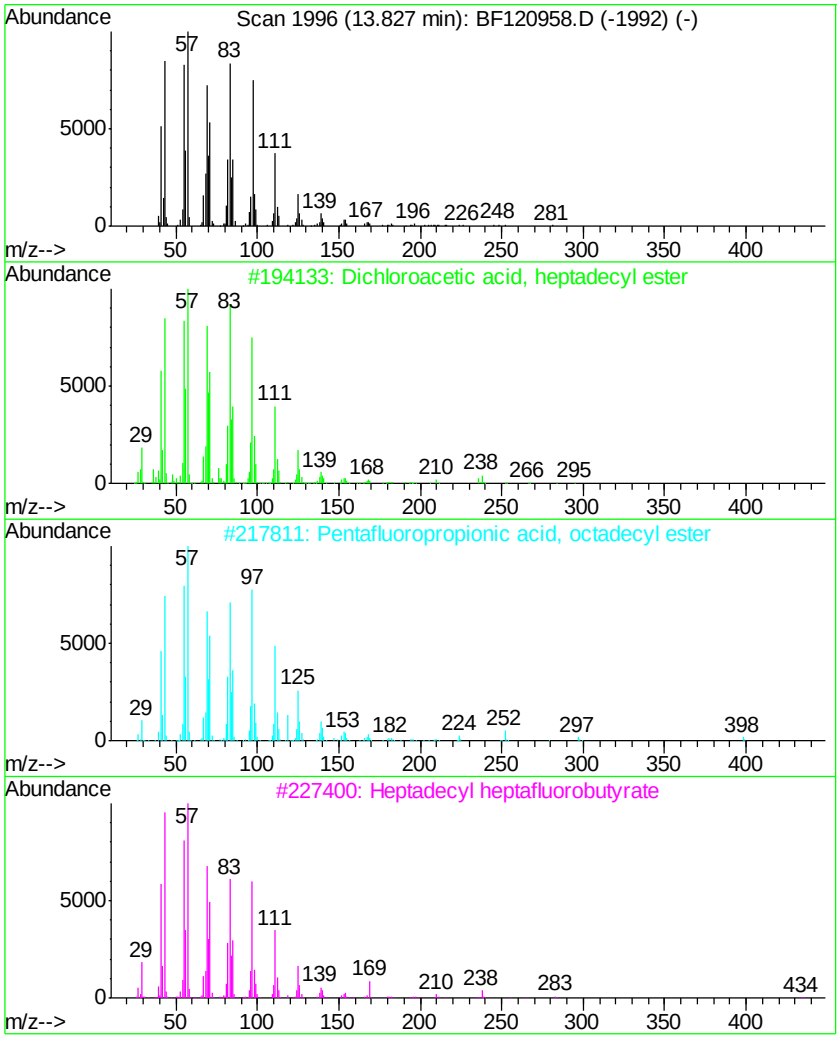
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

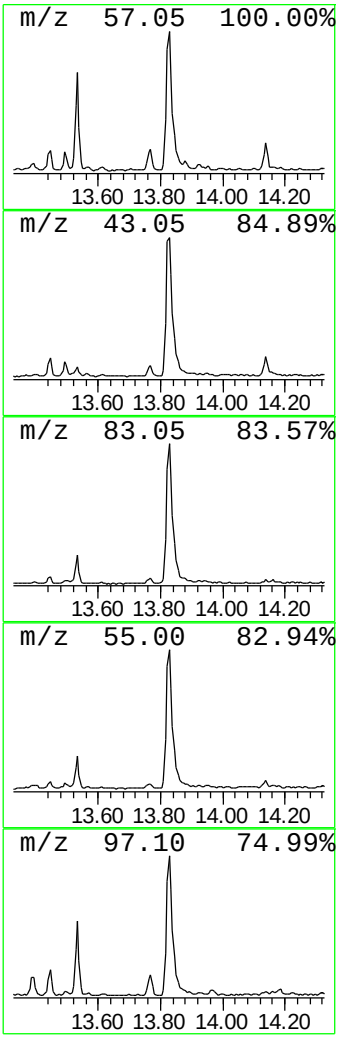
**********

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.83 | 9.93 ng | 848699 | Chrysene-d12 | 13.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 94 |
| 2 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 959261-25-7 | 94 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 4 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |



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ALS Vial : 14 Sample Multiplier: 1

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**ClientSampleId :** SAMPLE-1B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

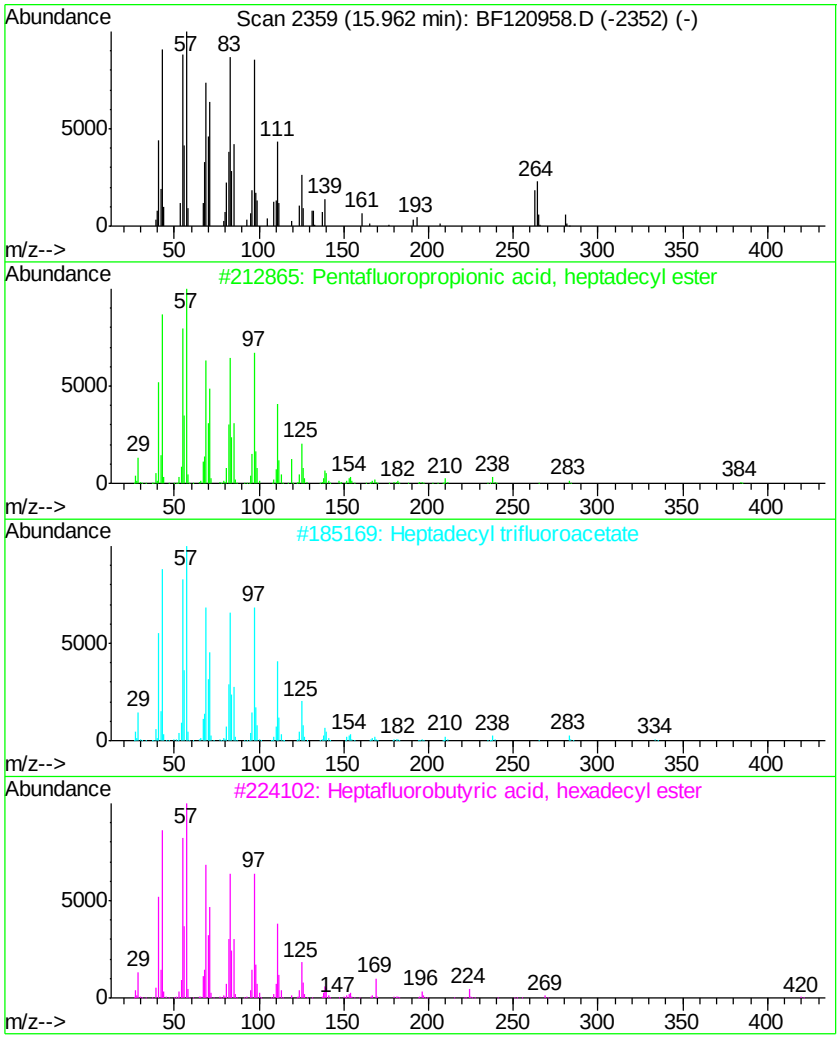
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

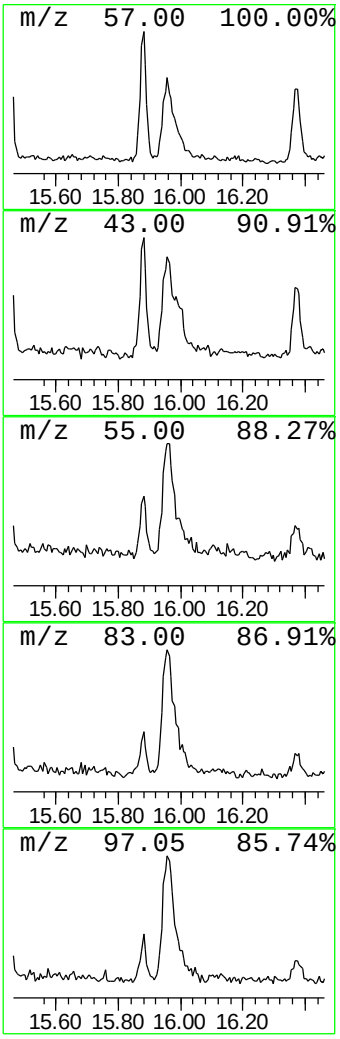
**********

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.96 | 2.52 ng | 167876 | Perylene-d12 | 15.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 93 |
| 2 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 93 |
| 3 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 93 |
| 4 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 90 |



Tentatively Identified Compound (LSC) summary

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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... | 5.03 | 3.0 | ng | 150860 | 1 | 6.82 | 1001150 | 20.0 |
| 2,4,4,6,6,8,8-Hep... | 12.31 | 2.5 | ng | 220636 | 4 | 11.33 | 1747460 | 20.0 |
| Dichloroacetic ac... | 13.83 | 9.9 | ng | 848699 | 5 | 13.97 | 1709980 | 20.0 |
| Pentafluoropropio... | 15.96 | 2.5 | ng | 167876 | 6 | 15.42 | 1334620 | 20.0 |