LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
Data File : BF092959.D
Acq On : 15 Feb 2017 19:03
Operator : SJ/MA
Sample : I1822-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 38-SB-01-65-70

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-BF013017.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 | 3.790 | 146 | 149 | 153 | rBV | 123757 | 212168 | 5.65% | 0.619% |
| 2 | 5.036 | 255 | 258 | 268 | rBV | 898291 | 1315539 | 35.06% | 3.836% |
| 3 | 5.470 | 293 | 296 | 298 | rBV | 3132951 | 3283268 | 87.50% | 9.573% |
| 4 | 6.510 | 384 | 387 | 389 | rBV | 2466058 | 3467729 | 92.42% | 10.111% |
| 5 | 6.636 | 395 | 398 | 400 | rBV | 3368253 | 3263609 | 86.98% | 9.516% |
| 6 | 6.864 | 416 | 418 | 421 | rBV | 1065842 | 888203 | 23.67% | 2.590% |
| 7 | 7.024 | 429 | 432 | 434 | rBV | 2724404 | 2585451 | 68.90% | 7.538% |
| 8 | 7.436 | 465 | 468 | 470 | rBV | 1881345 | 2183151 | 58.18% | 6.365% |
| 9 | 7.539 | 473 | 477 | 483 | rBV | 38142 | 68875 | 1.84% | 0.201% |
| 10 | 8.156 | 528 | 531 | 533 | rBV | 836459 | 1133444 | 30.21% | 3.305% |
| 11 | 9.230 | 622 | 625 | 627 | rBV | 3642298 | 3752325 | 100.00% | 10.941% |
| 12 | 9.619 | 657 | 659 | 662 | rBV | 529162 | 510102 | 13.59% | 1.487% |
| 13 | 9.825 | 674 | 677 | 680 | rVV2 | 113113 | 197829 | 5.27% | 0.577% |
| 14 | 9.905 | 682 | 684 | 686 | rVB | 1642492 | 1394740 | 37.17% | 4.067% |
| 15 | 10.305 | 713 | 719 | 720 | rBV3 | 26742 | 52275 | 1.39% | 0.152% |
| 16 | 10.339 | 720 | 722 | 723 | rVB | 77398 | 98576 | 2.63% | 0.287% |
| 17 | 10.556 | 737 | 741 | 744 | rBV | 38883 | 68374 | 1.82% | 0.199% |
| 18 | 10.693 | 750 | 753 | 755 | rBV | 2051173 | 1982567 | 52.84% | 5.781% |
| 19 | 10.808 | 761 | 763 | 767 | rBV | 136773 | 163431 | 4.36% | 0.477% |
| 20 | 11.253 | 800 | 802 | 803 | rBV | 96276 | 83163 | 2.22% | 0.242% |
| 21 | 11.391 | 811 | 814 | 816 | rBV | 1378493 | 1376545 | 36.69% | 4.014% |
| 22 | 11.608 | 831 | 833 | 837 | rBV | 79754 | 111995 | 2.98% | 0.327% |
| 23 | 11.676 | 837 | 839 | 843 | rVB | 33551 | 38384 | 1.02% | 0.112% |
| 24 | 12.431 | 903 | 905 | 907 | rBV | 35992 | 45039 | 1.20% | 0.131% |
| 25 | 12.968 | 950 | 952 | 955 | rBV | 2684239 | 3348614 | 89.24% | 9.763% |
| 26 | 13.859 | 1028 | 1030 | 1038 | rBV | 88919 | 133365 | 3.55% | 0.389% |
| 27 | 14.019 | 1042 | 1044 | 1047 | rVB | 1397775 | 1280582 | 34.13% | 3.734% |
| 28 | 14.854 | 1115 | 1117 | 1119 | rVB | 73974 | 85160 | 2.27% | 0.248% |
| 29 | 15.460 | 1167 | 1170 | 1174 | rBV | 794208 | 1131119 | 30.14% | 3.298% |
| 30 | 16.374 | 1247 | 1250 | 1258 | rVB2 | 17555 | 41718 | 1.11% | 0.122% |

Sum of corrected areas: 34297340

LSC Report - Integrated Chromatogram

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Data File : BF092959.D
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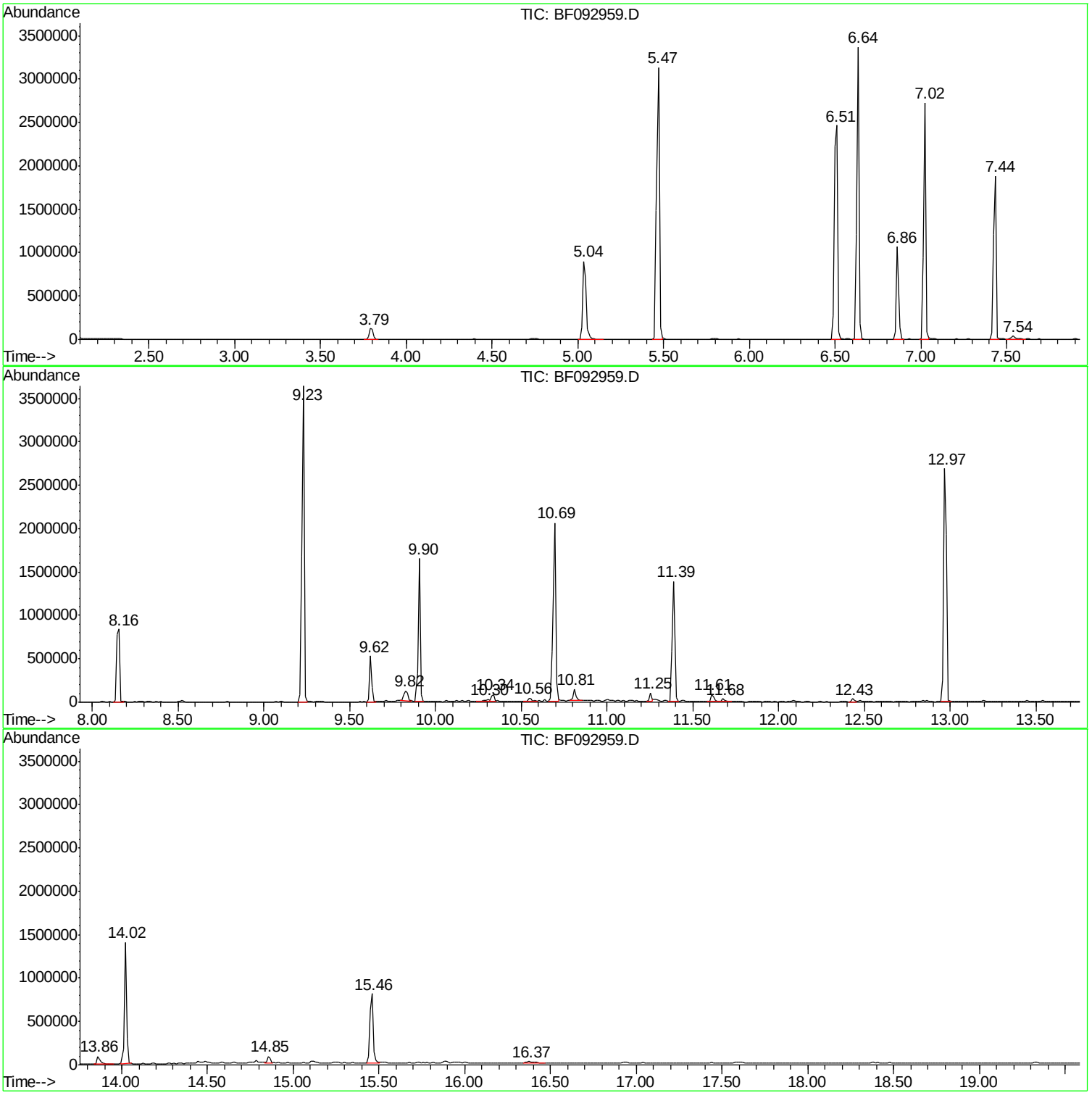
Operator : SJ/MA
Sample : I1822-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 38-SB-01-65-70

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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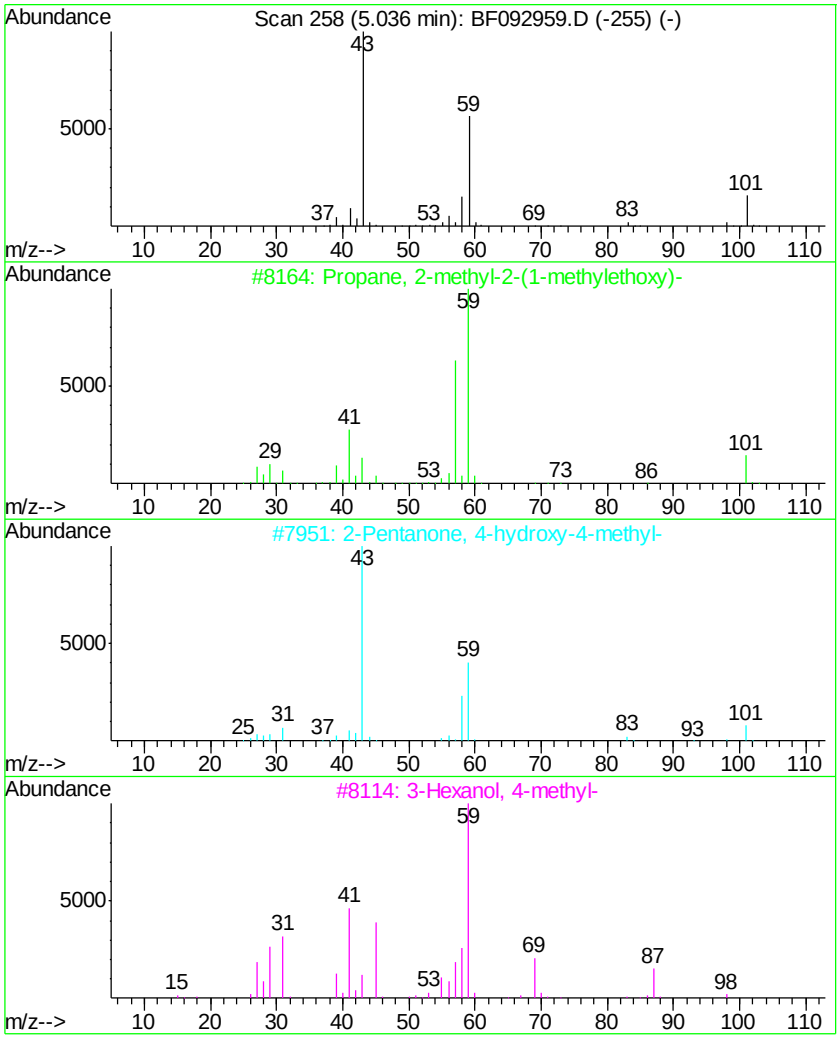
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

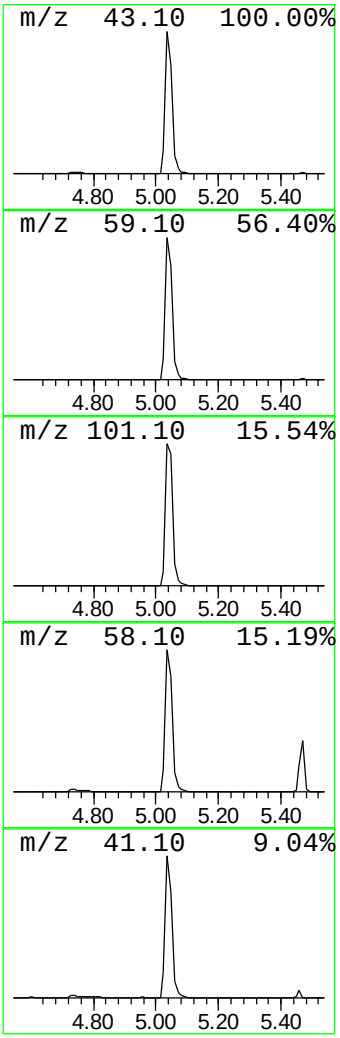
**********

Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.04 | 29.62 ng | 1315540 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 53 |
| 2 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |



# Library Search Compound Report

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Data File : BF092959.D
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Operator : SJ/MA
Sample : I1822-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 38-SB-01-65-70

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

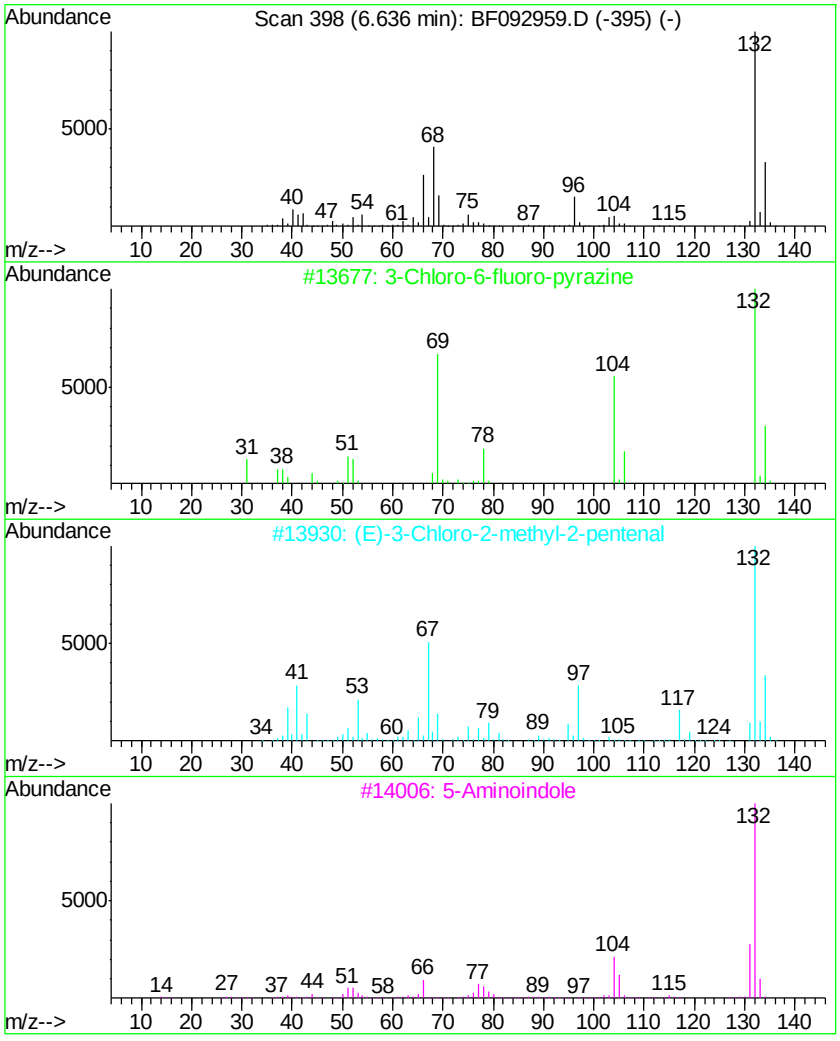
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

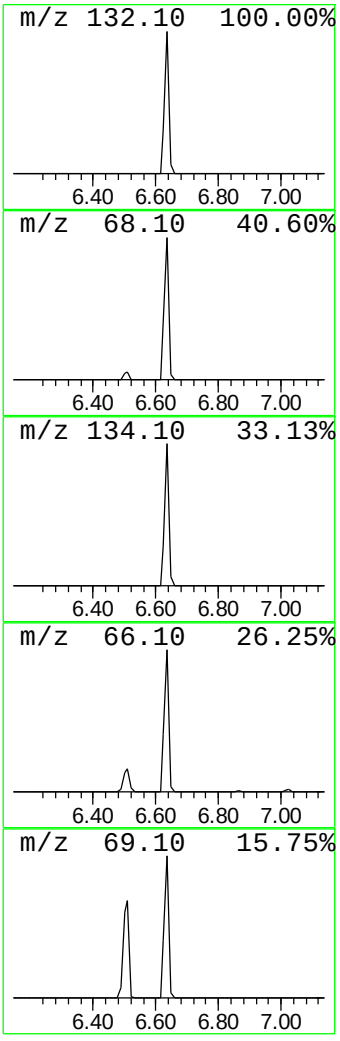
**********

Peak Number 3 unknown6.64 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.64 | 73.49 ng | 3263610 | 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 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 9 |



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Sample : I1822-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
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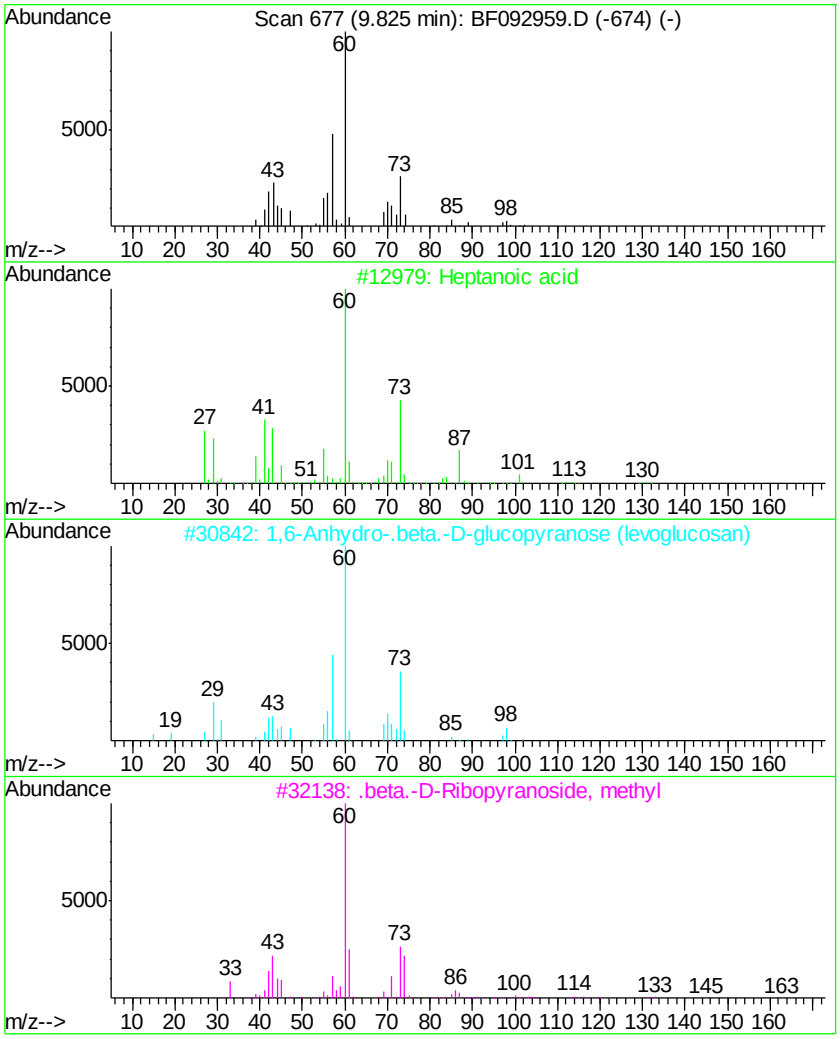
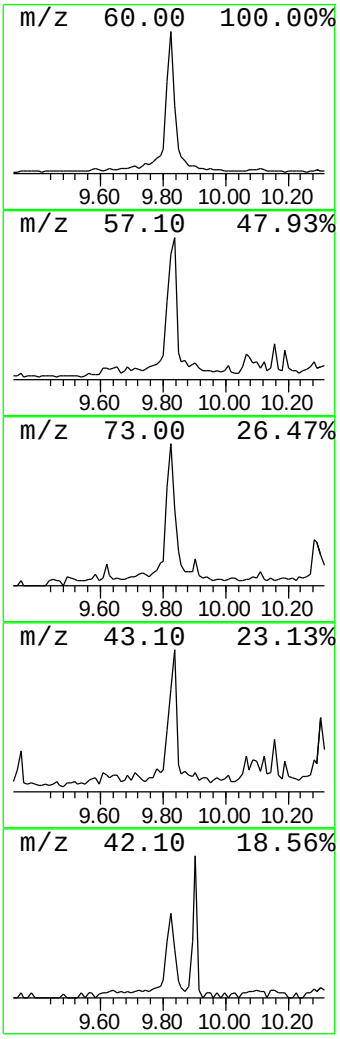
**********

Peak Number 5 Heptanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.82 | 2.84 ng | 197829 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptanoic acid | 130 | C7H14O2 | 000111-14-8 | 59 |
| 2 | 1,6-Anhydro-.beta.-D-glucopyrano... | 162 | C6H10O5 | 000498-07-7 | 56 |
| 3 | .beta.-D-Ribopyranoside, methyl | 164 | C6H12O5 | 017289-61-1 | 45 |
| 4 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 42 |
| 5 | 3,4-Altrosan | 162 | C6H10O5 | 1000129-76-4 | 25 |



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Operator : SJ/MA
Sample : I1822-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 38-SB-01-65-70

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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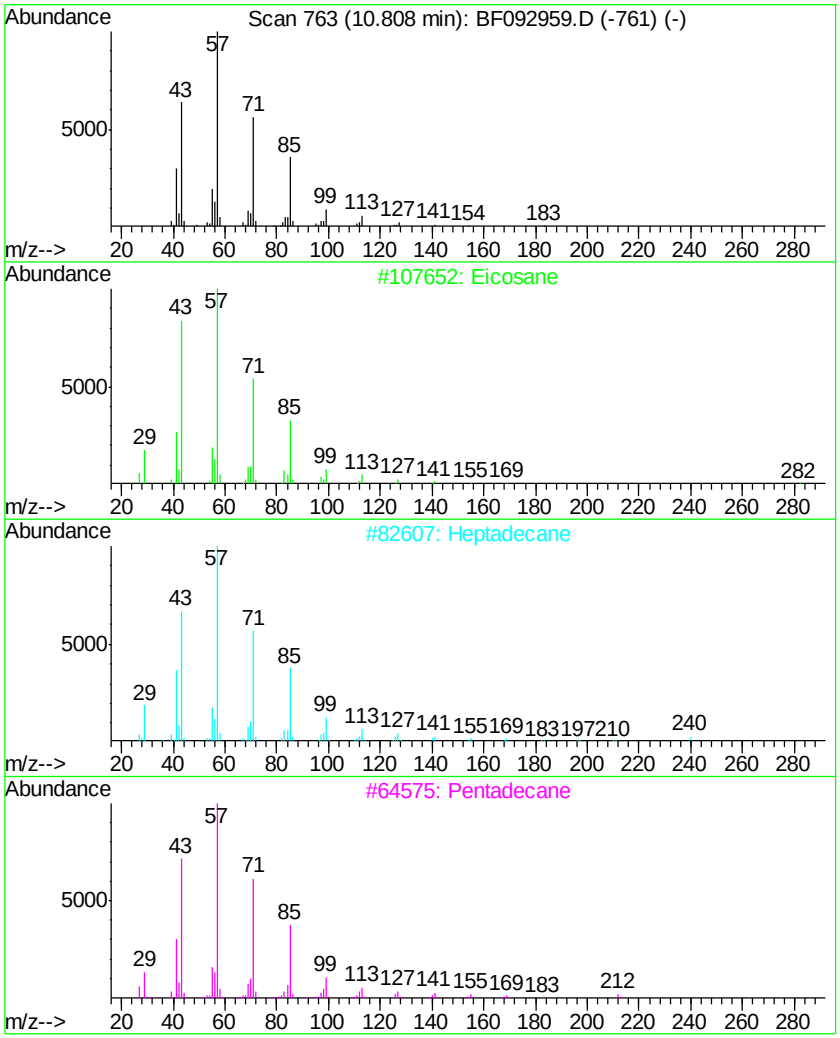
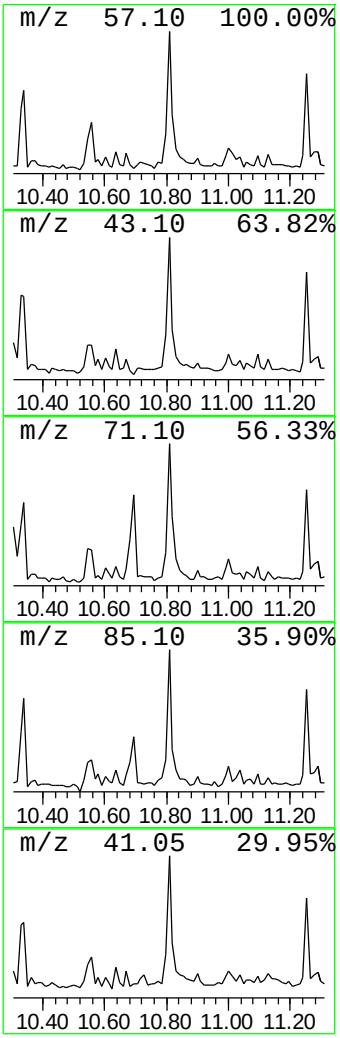
**********

Peak Number 6 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.81 | 2.37 ng | 163431 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 5 | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 86 |



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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**ClientSampleId :** 38-SB-01-65-70

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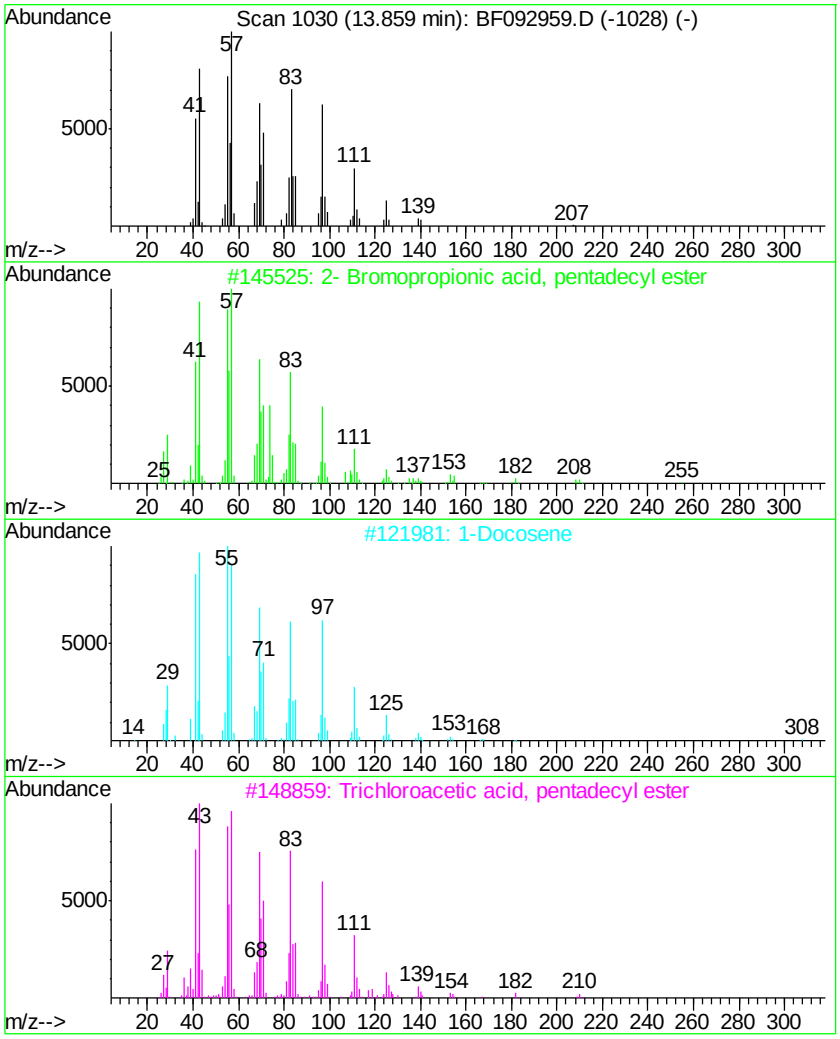
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

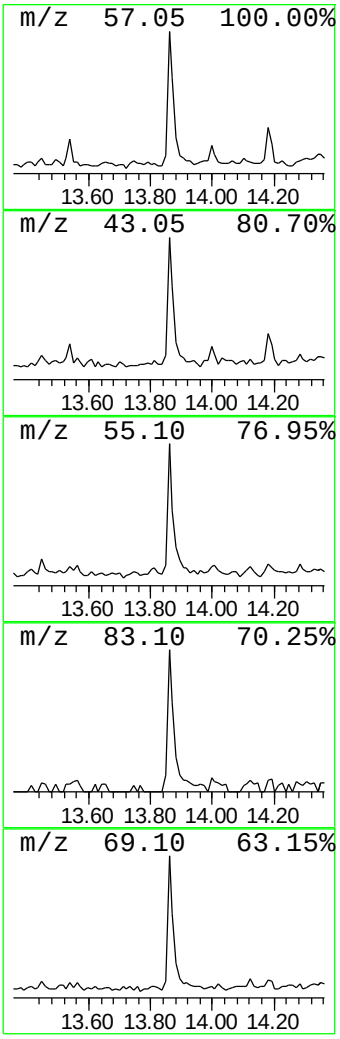
**********

Peak Number 7 2- Bromopropionic acid, pen... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.86 | 2.08 ng | 133365 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2- Bromopropionic acid, pentadec... | 362 | C18H35BrO2 | 1000292-44-2 | 91 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 4 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 90 |
| 5 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Propane, 2-methyl... | 5.04 | 29.6 | ng | 1315540 | 1 | 6.86 | 888203 | 20.0 |
| unknown6.64 | 6.64 | 73.5 | ng | 3263610 | 1 | 6.86 | 888203 | 20.0 |
| Heptanoic acid | 9.82 | 2.8 | ng | 197829 | 3 | 9.90 | 1394740 | 20.0 |
| Eicosane | 10.81 | 2.4 | ng | 163431 | 4 | 11.39 | 1376550 | 20.0 |
| 2- Bromopropionic... | 13.86 | 2.1 | ng | 133365 | 5 | 14.02 | 1280580 | 20.0 |