LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120116\
Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

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-BF112916.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 | 5.041 | 238 | 241 | 243 | rBV | 499771 | 737289 | 11.53% | 1.682% |
| 2 | 5.453 | 274 | 277 | 280 | rBV | 2707246 | 2570839 | 40.21% | 5.865% |
| 3 | 6.482 | 364 | 367 | 369 | rBV | 2094527 | 1928247 | 30.16% | 4.399% |
| 4 | 6.630 | 377 | 380 | 382 | rBV | 3460734 | 4676098 | 73.14% | 10.668% |
| 5 | 6.859 | 397 | 400 | 402 | rBV | 1421677 | 1196191 | 18.71% | 2.729% |
| 6 | 7.019 | 411 | 414 | 416 | rVB | 4353727 | 4302644 | 67.30% | 9.816% |
| 7 | 7.419 | 446 | 449 | 452 | rBV | 2796422 | 3364114 | 52.62% | 7.675% |
| 8 | 8.139 | 510 | 512 | 515 | rBV | 1299028 | 1442266 | 22.56% | 3.291% |
| 9 | 9.225 | 604 | 607 | 609 | rBV | 6178450 | 6042399 | 94.52% | 13.786% |
| 10 | 9.613 | 639 | 641 | 643 | rBV | 169256 | 136852 | 2.14% | 0.312% |
| 11 | 9.899 | 663 | 666 | 668 | rBV | 2033510 | 1787660 | 27.96% | 4.079% |
| 12 | 10.333 | 700 | 704 | 706 | rBV2 | 51672 | 74932 | 1.17% | 0.171% |
| 13 | 10.688 | 732 | 735 | 737 | rBV | 3880127 | 4201563 | 65.72% | 9.586% |
| 14 | 10.813 | 743 | 746 | 749 | rBV | 64988 | 82844 | 1.30% | 0.189% |
| 15 | 11.385 | 793 | 796 | 798 | rVB | 1214430 | 1666163 | 26.06% | 3.801% |
| 16 | 11.911 | 840 | 842 | 850 | rBV2 | 261969 | 316516 | 4.95% | 0.722% |
| 17 | 12.699 | 909 | 911 | 918 | rBV | 281415 | 332905 | 5.21% | 0.760% |
| 18 | 12.974 | 932 | 935 | 937 | rBV | 5896831 | 6392921 | 100.00% | 14.585% |
| 19 | 13.877 | 1012 | 1014 | 1018 | rBV | 107250 | 127584 | 2.00% | 0.291% |
| 20 | 14.014 | 1023 | 1026 | 1028 | rBV | 1483023 | 1426171 | 22.31% | 3.254% |
| 21 | 15.442 | 1148 | 1151 | 1154 | rBV | 847988 | 1024823 | 16.03% | 2.338% |

Sum of corrected areas: 43831021

LSC Report - Integrated Chromatogram

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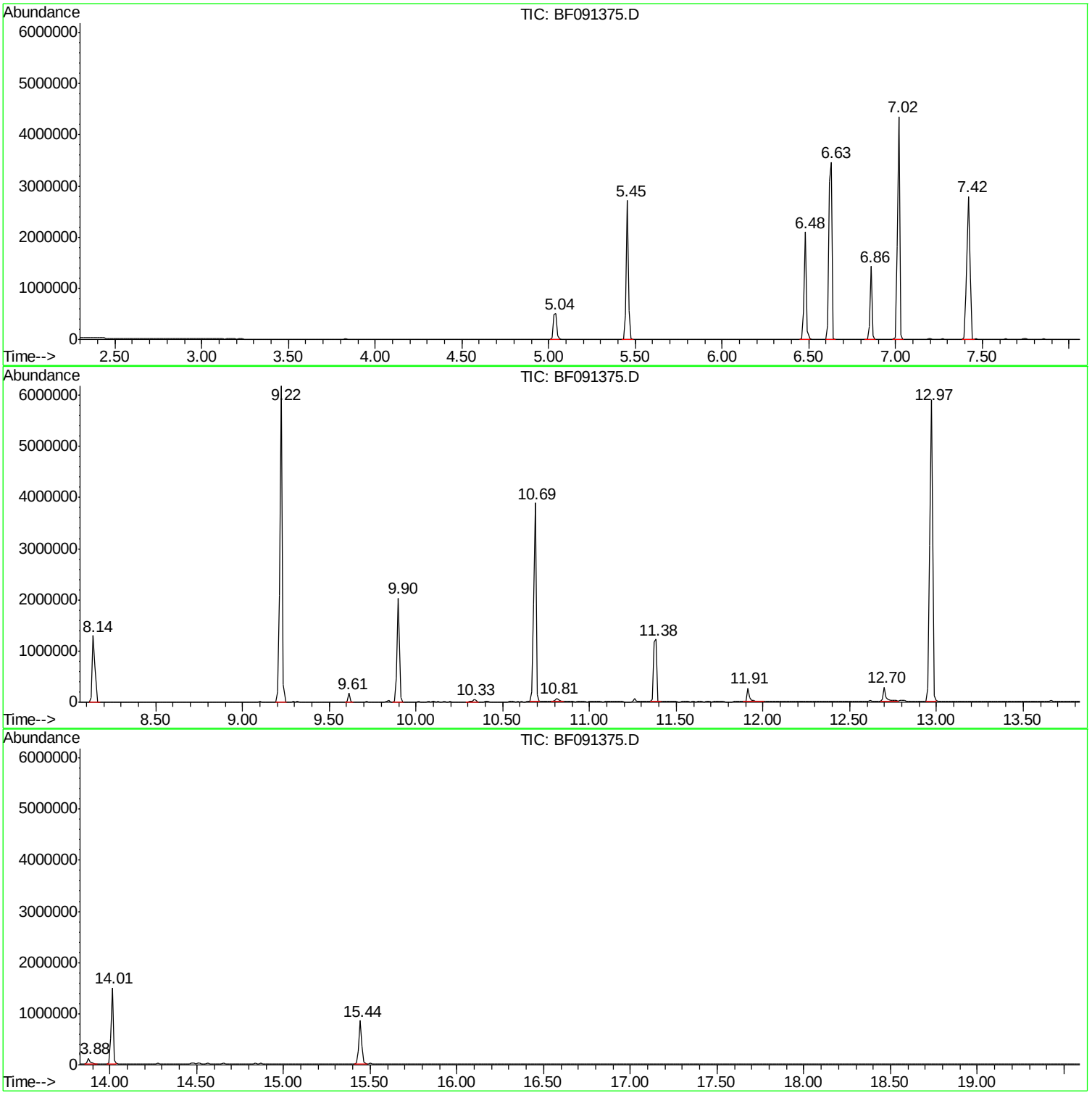
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120116\
Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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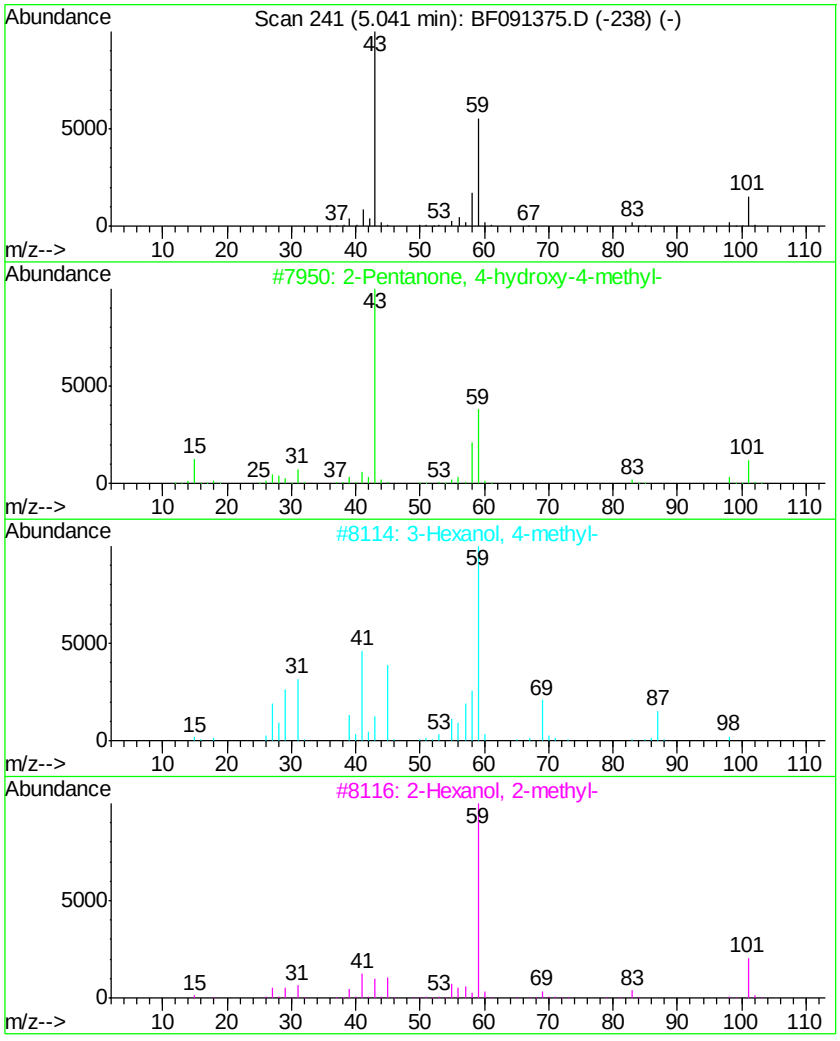
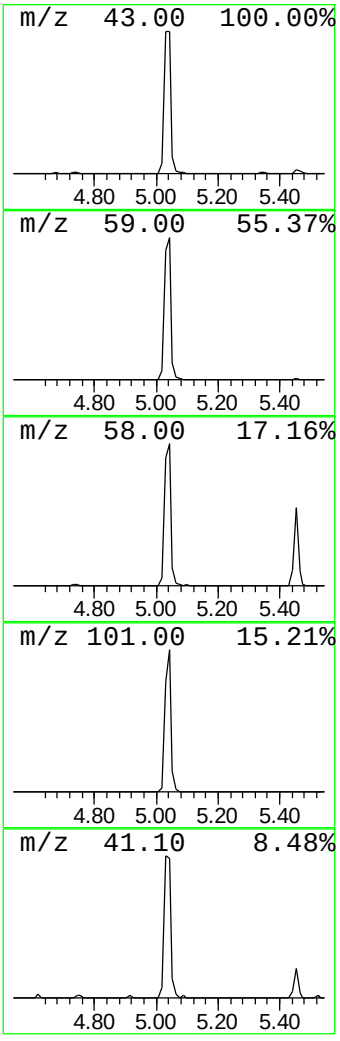
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.04 | 12.33 ng | 737289 | 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 | 59 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 32 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



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Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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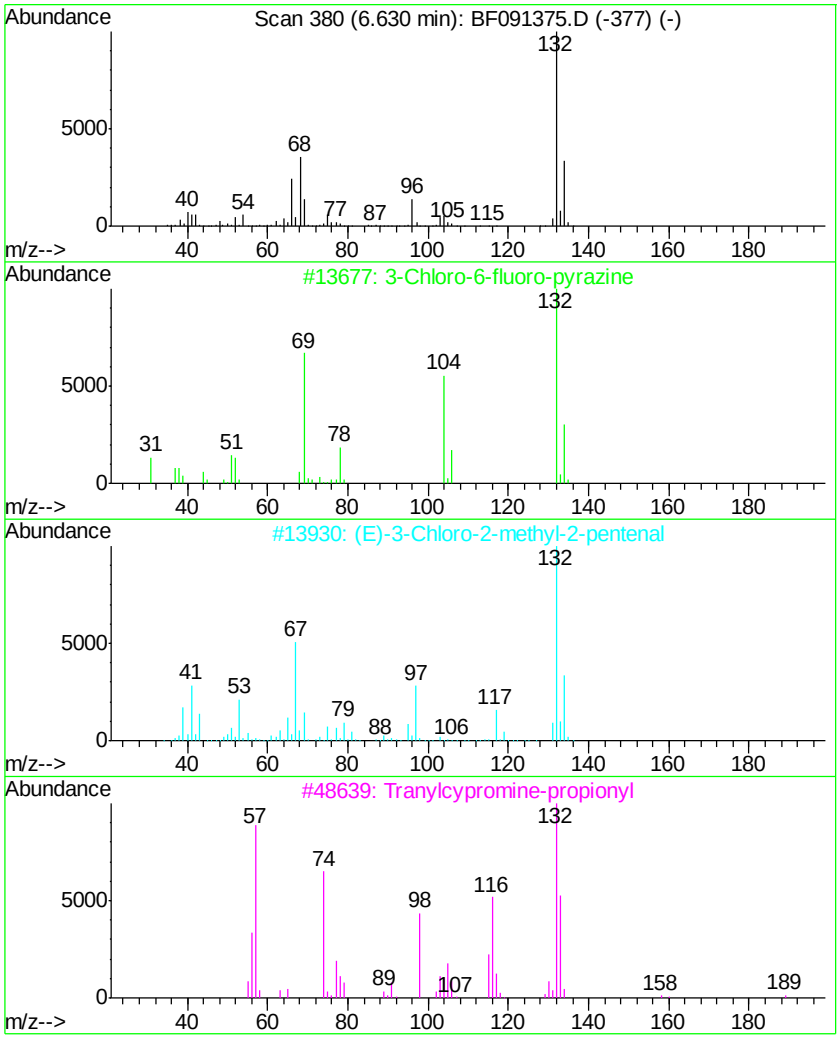
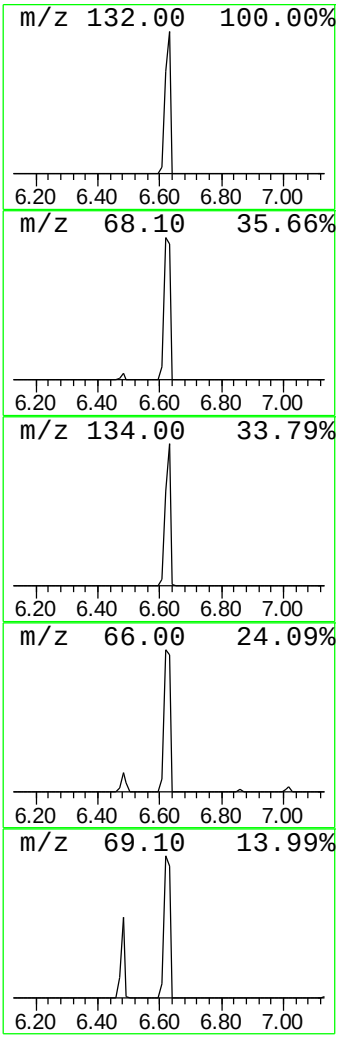
Peak Number 2 unknown6.63 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 78.18 ng | 4676100 | 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 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 25 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120116\
Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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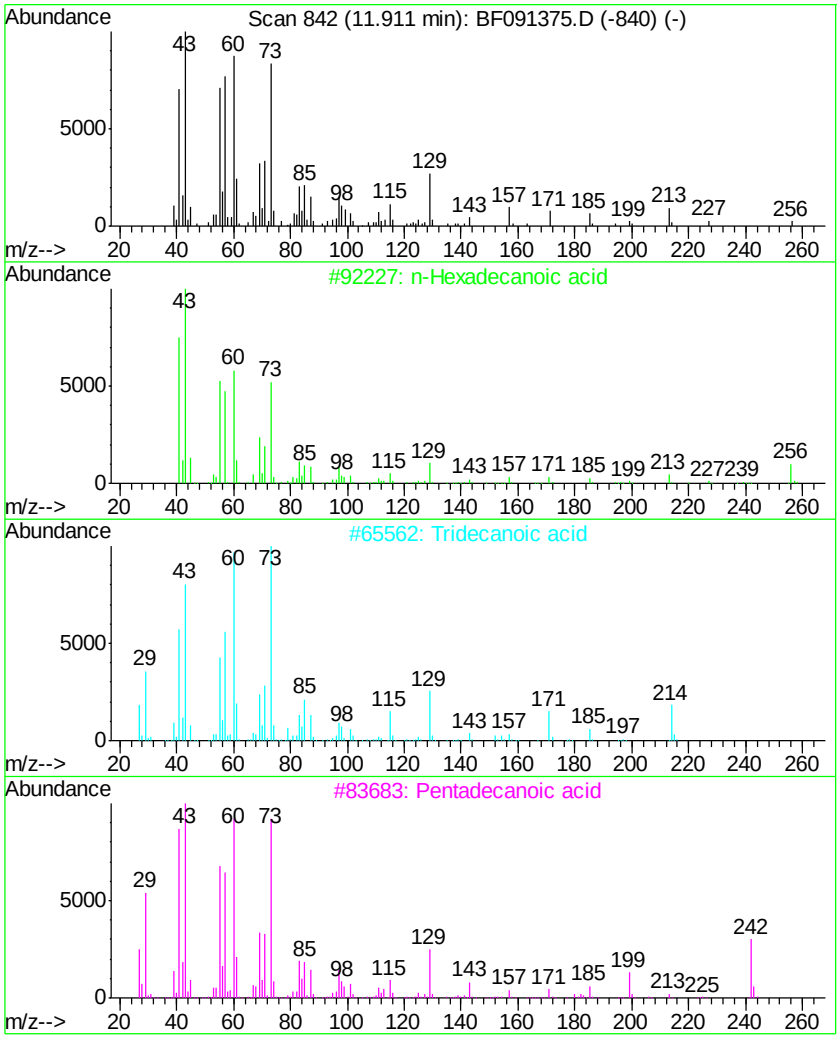
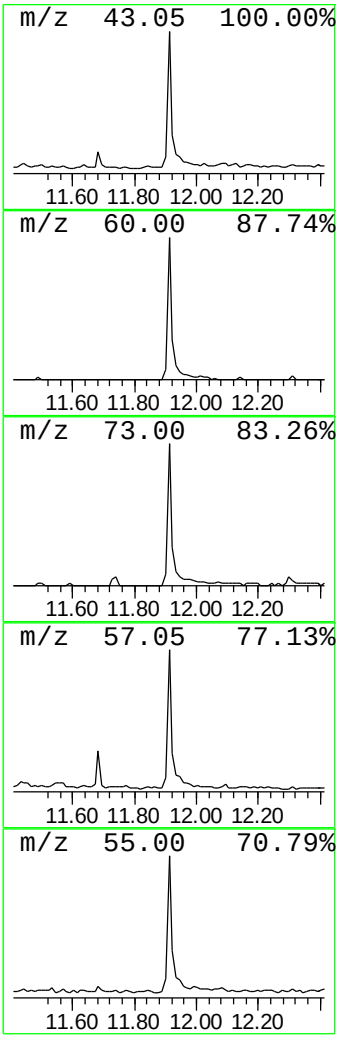
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.91 | 3.80 ng | 316516 | Phenanthrene-d10 | 11.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 86 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120116\
Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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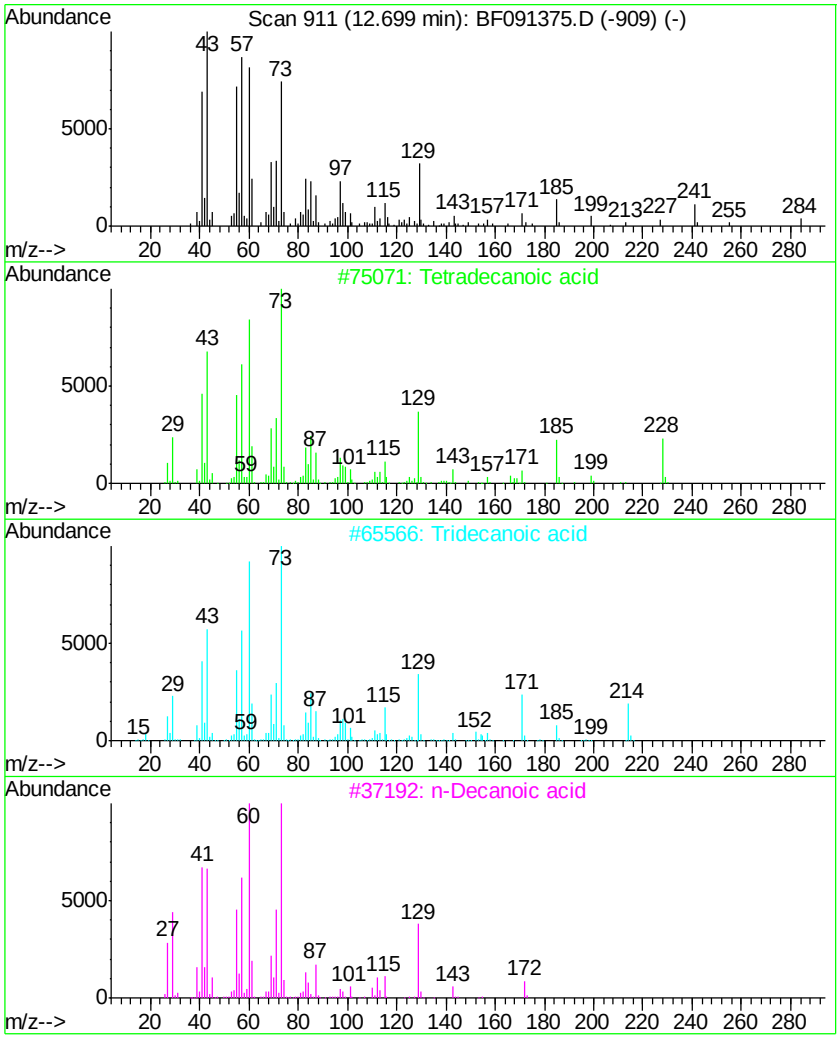
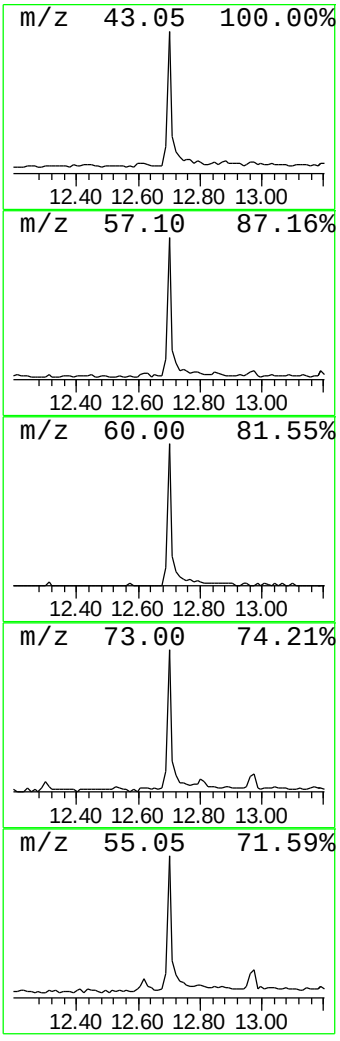
Peak Number 5 Tetradecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.70 | 4.00 ng | 332905 | Phenanthrene-d10 | 11.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 50 |
| 5 | .alpha.-D-Glucopyranoside, .alph... | 342 | C12H22O11 | 000099-20-7 | 47 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120116\
Data File : BF091375.D
Acq On : 1 Dec 2016 16:21
Operator : UM/SJ
Sample : H5801-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6-112916

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.04 | 12.3 | ng | 737289 | 1 | 6.86 | 1196190 | 20.0 |
| unknown6.63 | 6.63 | 78.2 | ng | 4676100 | 1 | 6.86 | 1196190 | 20.0 |
| n-Hexadecanoic acid | 11.91 | 3.8 | ng | 316516 | 4 | 11.38 | 1666160 | 20.0 |
| Tetradecanoic acid | 12.70 | 4.0 | ng | 332905 | 4 | 11.38 | 1666160 | 20.0 |