LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

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-BF110817.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 | 3.846 | 291 | 299 | 318 | rBV | 1065712 | 1666299 | 100.00% | 28.322% |
| 2 | 5.046 | 500 | 503 | 508 | rBV | 24677 | 24937 | 1.50% | 0.424% |
| 3 | 5.463 | 570 | 574 | 586 | rBV | 383107 | 372371 | 22.35% | 6.329% |
| 4 | 6.481 | 744 | 747 | 755 | rBV | 450311 | 388001 | 23.29% | 6.595% |
| 5 | 6.622 | 768 | 771 | 775 | rBV | 464409 | 395287 | 23.72% | 6.719% |
| 6 | 6.857 | 808 | 811 | 815 | rBV | 98777 | 79950 | 4.80% | 1.359% |
| 7 | 7.010 | 834 | 837 | 841 | rBV | 384675 | 298092 | 17.89% | 5.067% |
| 8 | 7.416 | 902 | 906 | 909 | rBV | 322221 | 230800 | 13.85% | 3.923% |
| 9 | 8.139 | 1026 | 1029 | 1032 | rBV | 141183 | 102942 | 6.18% | 1.750% |
| 10 | 9.210 | 1208 | 1211 | 1215 | rBV | 556859 | 462786 | 27.77% | 7.866% |
| 11 | 9.604 | 1275 | 1278 | 1281 | rBV | 43747 | 32782 | 1.97% | 0.557% |
| 12 | 9.816 | 1309 | 1314 | 1319 | rVB | 19606 | 21193 | 1.27% | 0.360% |
| 13 | 9.892 | 1324 | 1327 | 1331 | rVB | 153423 | 128316 | 7.70% | 2.181% |
| 14 | 10.310 | 1394 | 1398 | 1403 | rVB2 | 24398 | 32463 | 1.95% | 0.552% |
| 15 | 10.680 | 1458 | 1461 | 1465 | rVB | 398569 | 306495 | 18.39% | 5.209% |
| 16 | 11.380 | 1577 | 1580 | 1583 | rBV | 164607 | 131498 | 7.89% | 2.235% |
| 17 | 11.898 | 1664 | 1668 | 1673 | rBV | 89561 | 82079 | 4.93% | 1.395% |
| 18 | 12.680 | 1798 | 1801 | 1808 | rBV | 46970 | 47932 | 2.88% | 0.815% |
| 19 | 12.963 | 1845 | 1849 | 1852 | rBV | 667455 | 521662 | 31.31% | 8.867% |
| 20 | 13.851 | 1996 | 2000 | 2003 | rBV2 | 51495 | 51970 | 3.12% | 0.883% |
| 21 | 13.886 | 2003 | 2006 | 2010 | rVB | 21690 | 20041 | 1.20% | 0.341% |
| 22 | 13.992 | 2020 | 2024 | 2026 | rBV | 297503 | 236728 | 14.21% | 4.024% |
| 23 | 14.021 | 2026 | 2029 | 2032 | rVB | 145944 | 131761 | 7.91% | 2.240% |
| 24 | 15.486 | 2275 | 2278 | 2285 | rVB | 89251 | 117036 | 7.02% | 1.989% |

Sum of corrected areas: 5883421

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
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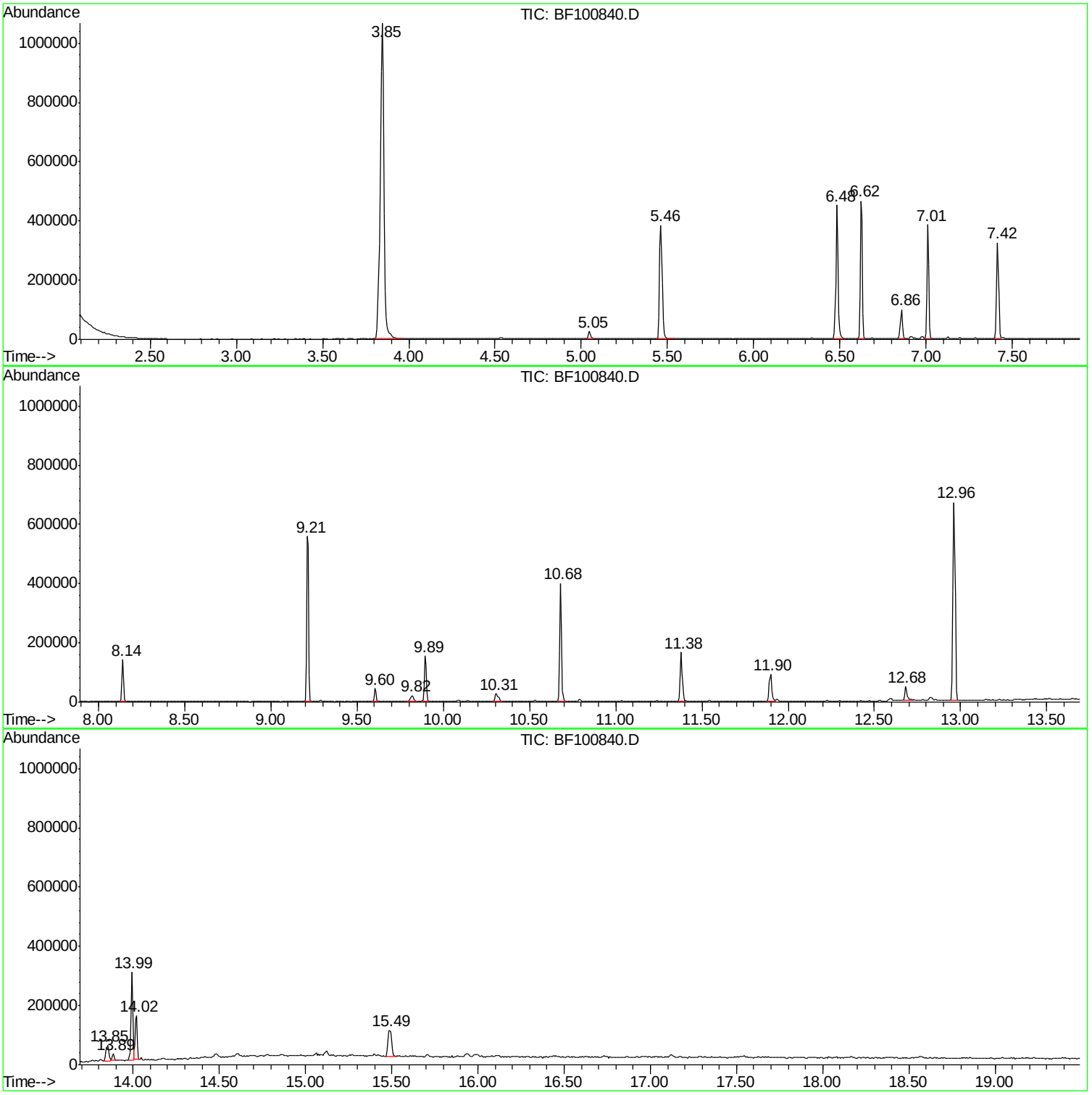
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

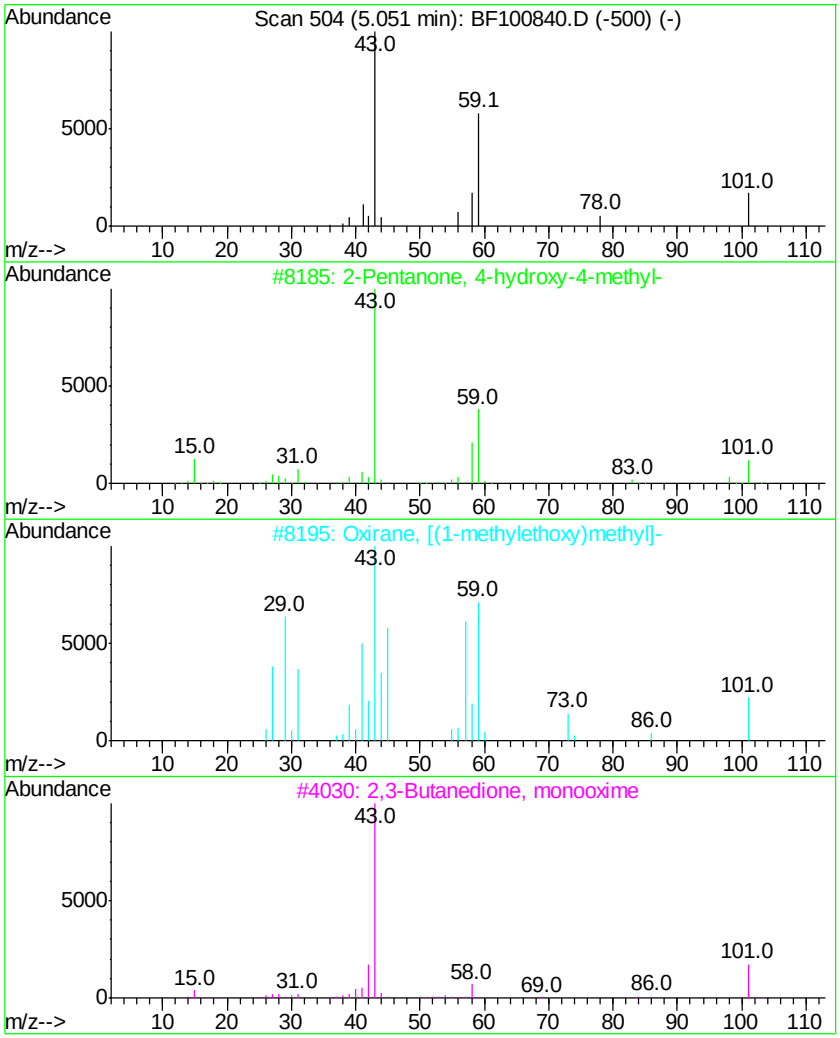
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

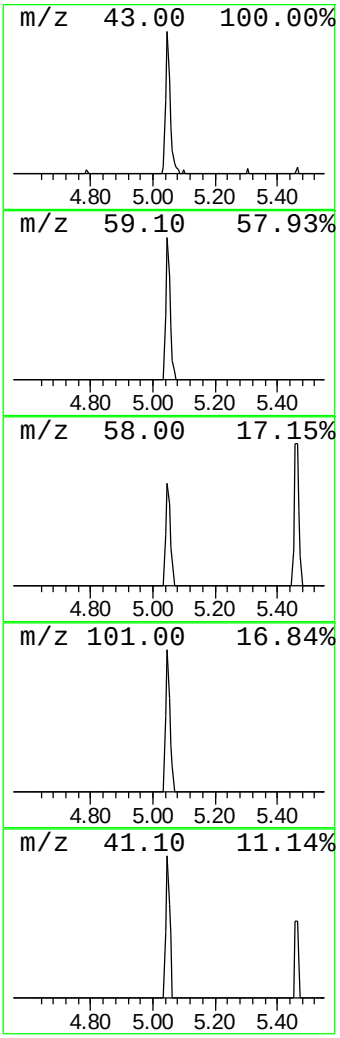
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.05 | 6.24 ng | 24937 | 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 | 56 |
| 2 | Oxirane, [(1-methylethoxy)methyl]- | 116 | C6H12O2 | 004016-14-2 | 40 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | 2-Heptanone, 7,7-dichloro- | 182 | C7H12Cl2O | 066241-43-8 | 9 |
| 5 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

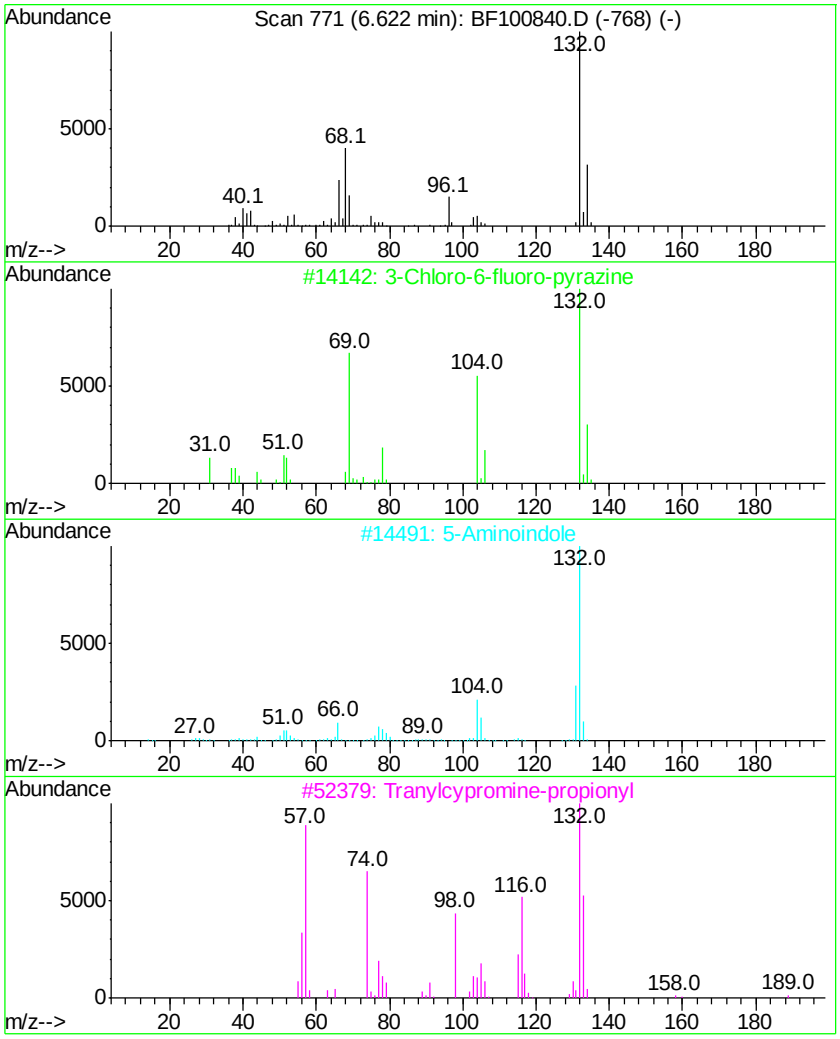
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

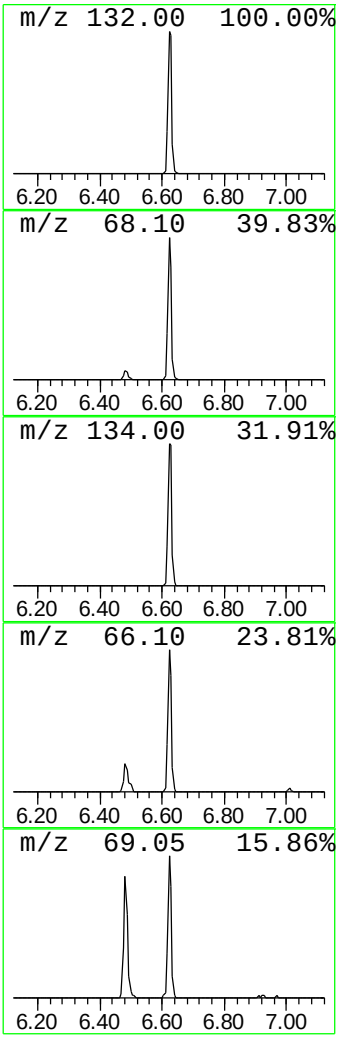
**********

Peak Number 3 unknown6.62 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 98.88 ng | 395287 | 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-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

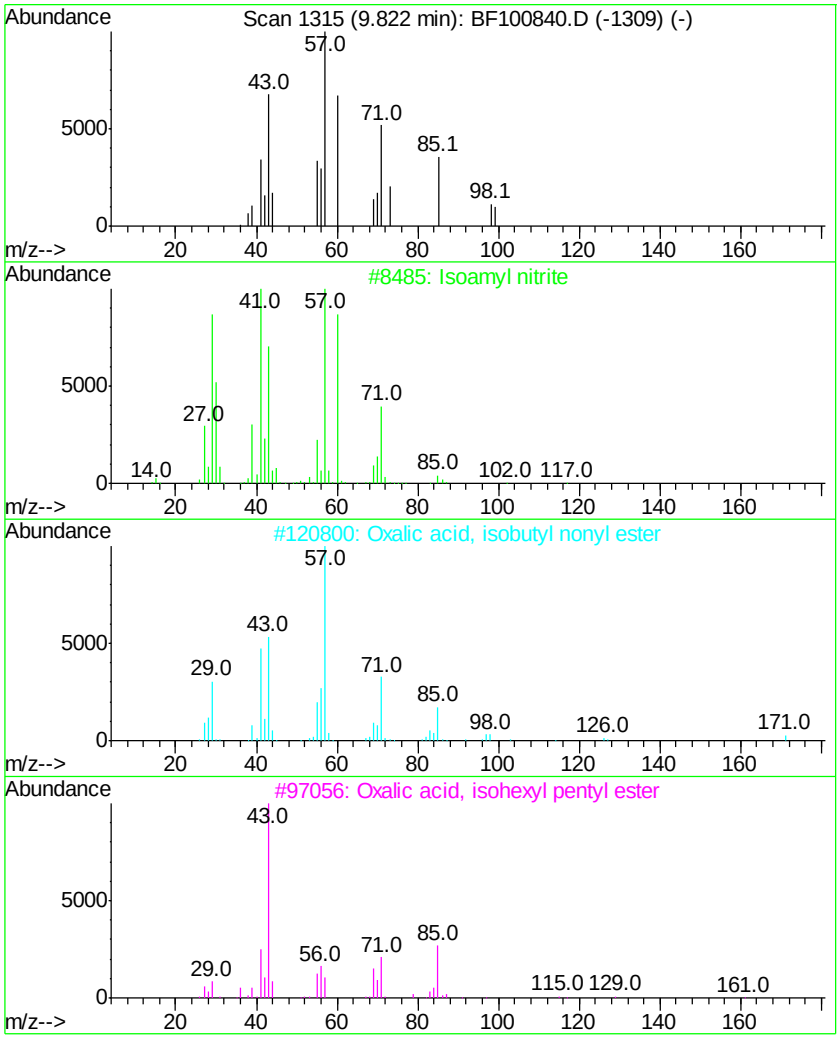
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

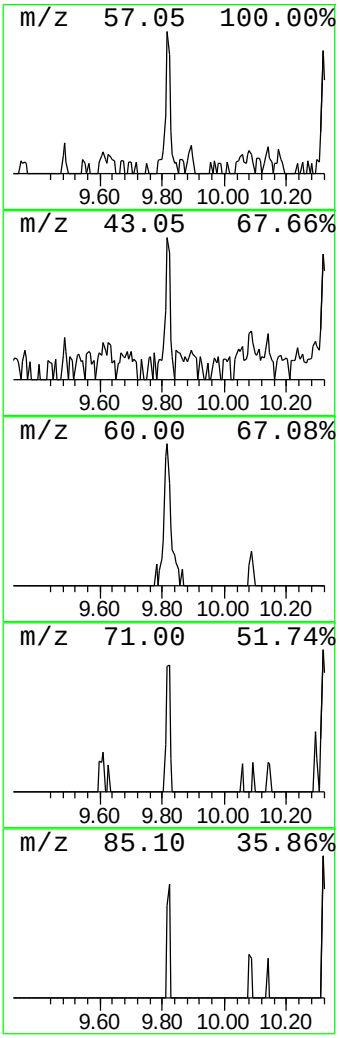
**********

Peak Number 5 unknown9.82 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.82 | 3.30 ng | 21193 | Acenaphthene-d10 | 9.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isoamyl nitrite | 117 | C5H11NO2 | 000110-46-3 | 36 |
| 2 | Oxalic acid, isobutyl nonyl ester | 272 | C15H28O4 | 1000309-37-4 | 32 |
| 3 | Oxalic acid, isohexyl pentyl ester | 244 | C13H24O4 | 1000309-32-8 | 27 |
| 4 | Acetamide, N-(2-hydroxyethyl)- | 103 | C4H9NO2 | 000142-26-7 | 23 |
| 5 | .alpha.-L-Galactopyranoside, met... | 178 | C7H14O5 | 014687-15-1 | 17 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

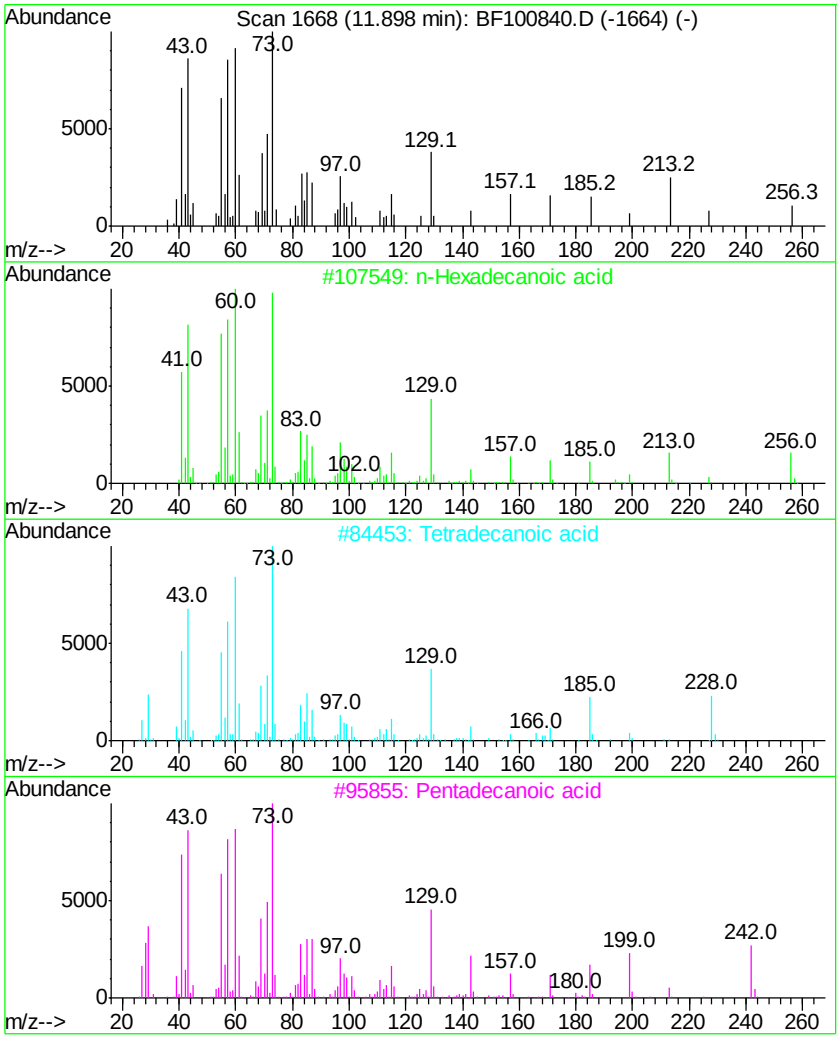
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

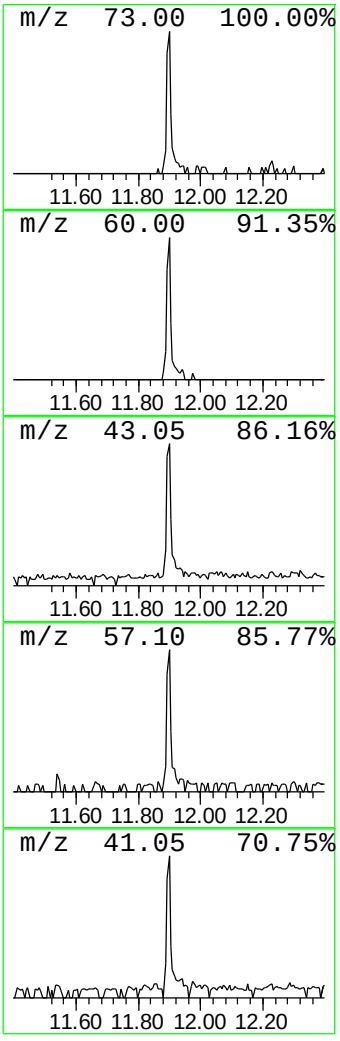
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.90 | 12.48 ng | 82079 | Phenanthrene-d10 | 11.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 58 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

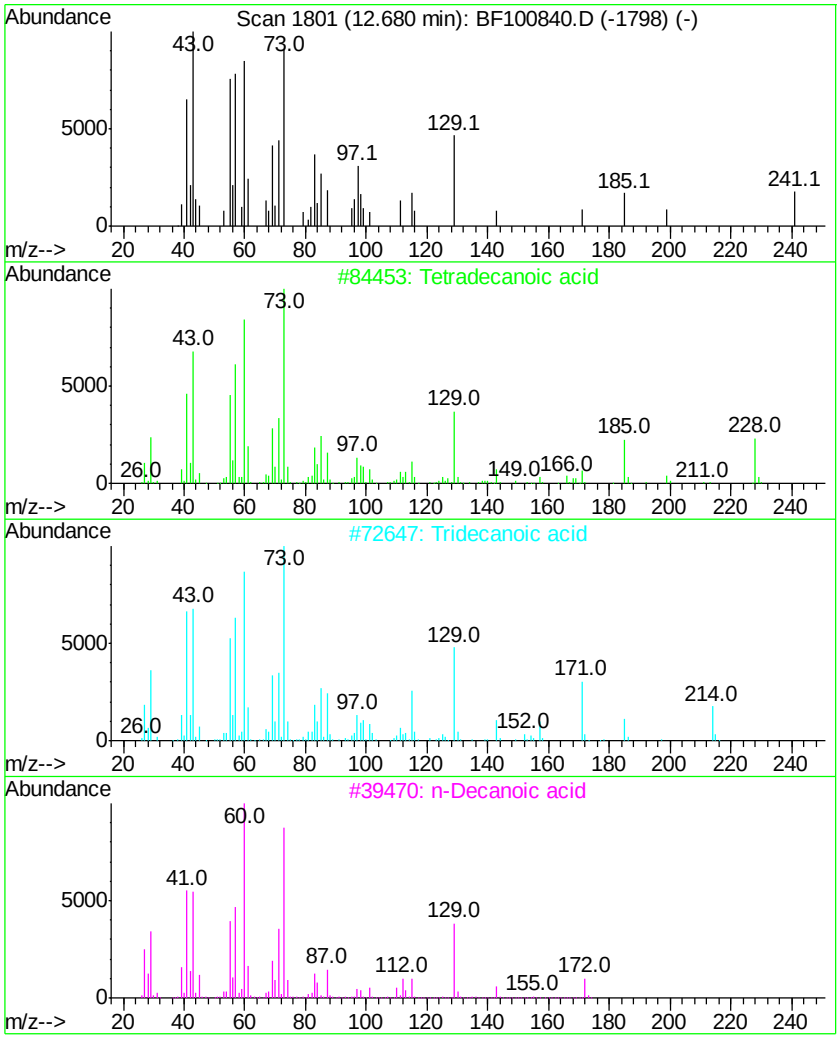
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

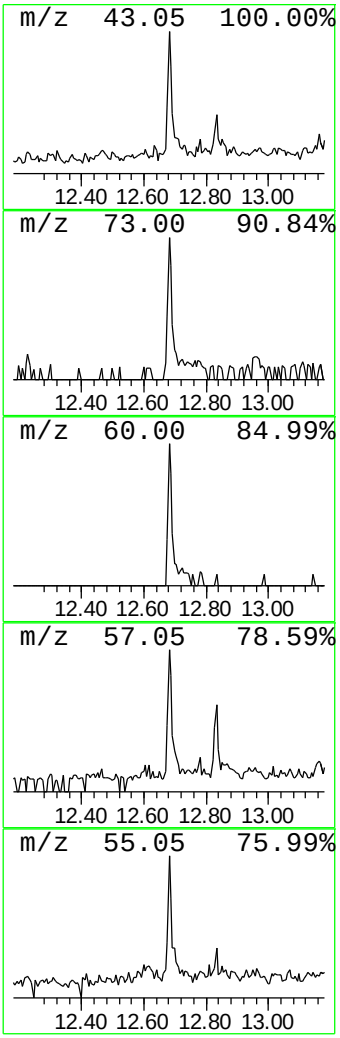
**********

Peak Number 7 Tetradecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.68 | 7.29 ng | 47932 | Phenanthrene-d10 | 11.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | .alpha.-D-Glucopyranoside, O-.al... | 504 | C18H32O16 | 000597-12-6 | 35 |
| 5 | Xylose | 150 | C5H10O5 | 000058-86-6 | 27 |



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Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

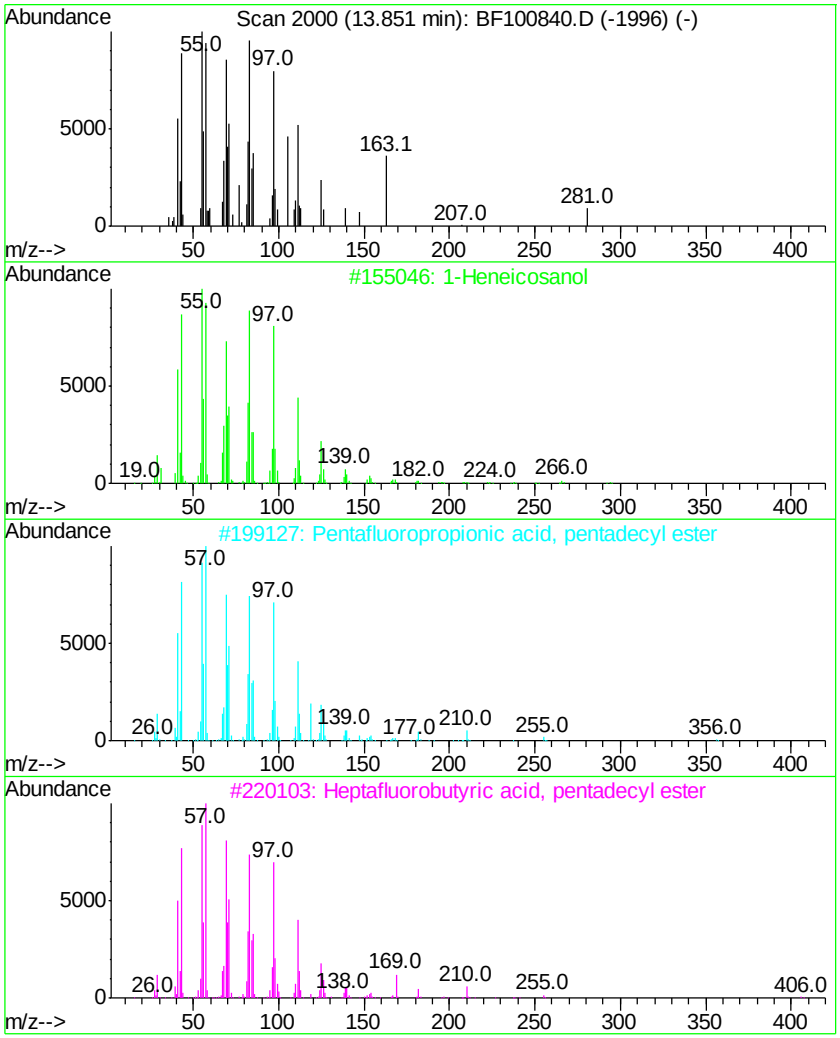
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

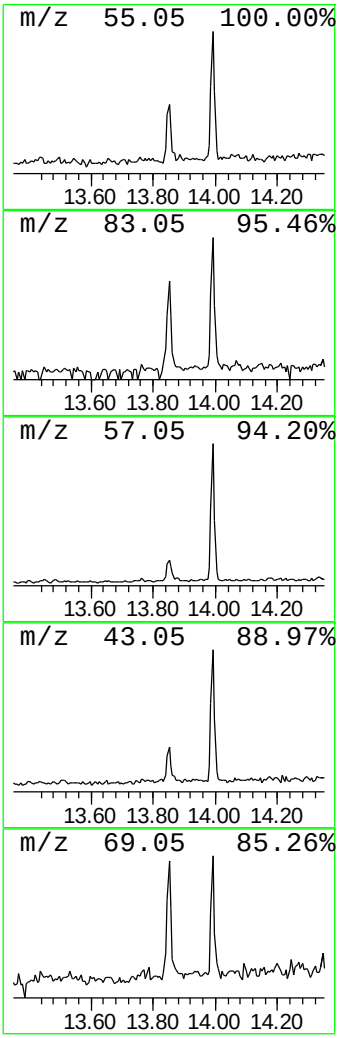
**********

Peak Number 8 1-Heneicosanol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.85 | 7.89 ng | 51970 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 2 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 93 |
| 3 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 93 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 90 |



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Data File : BF100840.D
Acq On : 22 Nov 2017 23:01
Operator : SJ/JU
Sample : I6513-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

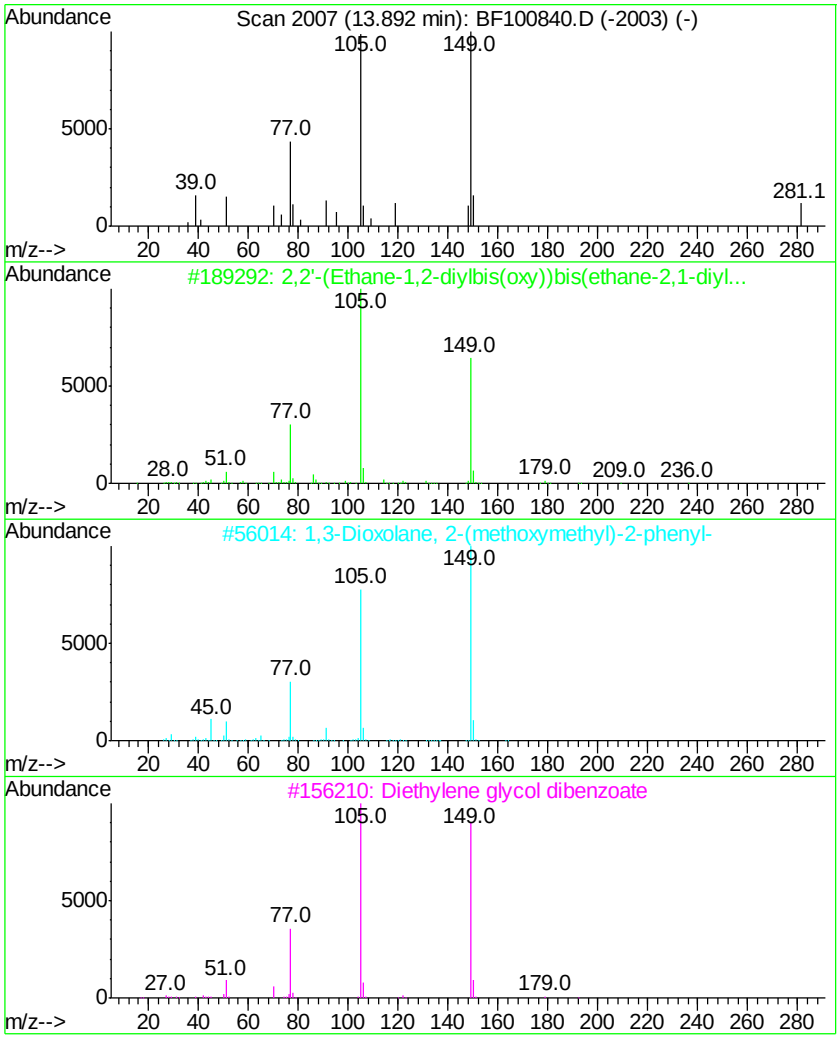
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

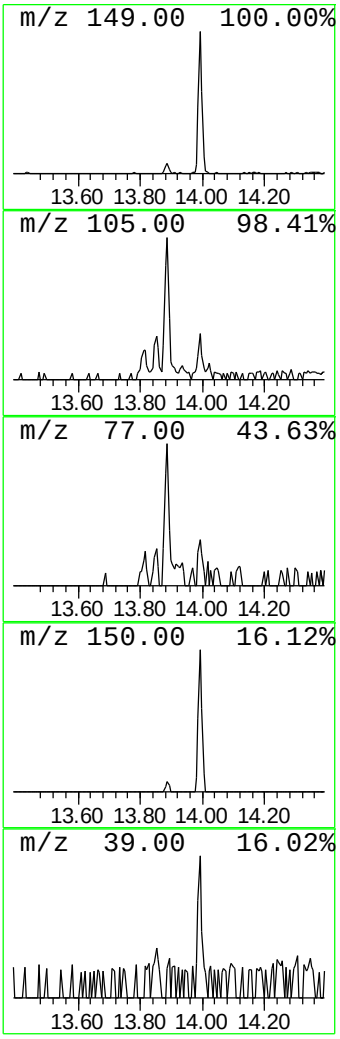
**********

Peak Number 9 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.89 | 3.04 ng | 20041 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,2'-(Ethane-1,2-divlbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 78 |
| 2 | 1,3-Dioxolane, 2-(methoxymethyl)... | 194 | C11H14O3 | 1000156-71-2 | 78 |
| 3 | Diethylene glycol dibenzoate | 314 | C18H18O5 | 000120-55-8 | 78 |
| 4 | Benzoic acid, 2-(4-nitrophenoxy)... | 287 | C15H13NO5 | 1000368-92-7 | 64 |
| 5 | 2-(2-(2-Methoxyethoxy)ethoxy)eth... | 268 | C14H20O5 | 1000366-99-1 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
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ALS Vial : 13 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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... | 5.05 | 6.2 | ng | 24937 | 1 | 6.86 | 79950 | 20.0 |
| unknown6.62 | 6.62 | 98.9 | ng | 395287 | 1 | 6.86 | 79950 | 20.0 |
| unknown9.82 | 9.82 | 3.3 | ng | 21193 | 3 | 9.89 | 128316 | 20.0 |
| n-Hexadecanoic acid | 11.90 | 12.5 | ng | 82079 | 4 | 11.38 | 131498 | 20.0 |
| Tetradecanoic acid | 12.68 | 7.3 | ng | 47932 | 4 | 11.38 | 131498 | 20.0 |
| 1-Heneicosanol | 13.85 | 7.9 | ng | 51970 | 5 | 14.02 | 131761 | 20.0 |
| 2,2'-(Ethane-1,2-... | 13.89 | 3.0 | ng | 20041 | 5 | 14.02 | 131761 | 20.0 |