LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

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_G\METHODS\8270-BG060616.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 | 2.909 | 6 | 12 | 24 | rBV | 317514 | 494125 | 26.28% | 4.767% |
| 2 | 5.130 | 383 | 390 | 401 | rBV | 20771 | 39073 | 2.08% | 0.377% |
| 3 | 5.617 | 464 | 473 | 489 | rBV | 339780 | 650670 | 34.61% | 6.277% |
| 4 | 7.233 | 740 | 748 | 765 | rBV | 387146 | 767528 | 40.82% | 7.405% |
| 5 | 7.603 | 803 | 811 | 826 | rBV | 405643 | 790667 | 42.05% | 7.628% |
| 6 | 8.067 | 883 | 890 | 898 | rBV | 66074 | 126697 | 6.74% | 1.222% |
| 7 | 8.396 | 936 | 946 | 963 | rBV | 289054 | 567085 | 30.16% | 5.471% |
| 8 | 9.243 | 1082 | 1090 | 1101 | rBV | 214550 | 441281 | 23.47% | 4.257% |
| 9 | 10.894 | 1363 | 1371 | 1384 | rBV | 105044 | 220481 | 11.73% | 2.127% |
| 10 | 13.326 | 1778 | 1785 | 1799 | rBV | 696843 | 1229822 | 65.41% | 11.865% |
| 11 | 14.154 | 1918 | 1926 | 1935 | rBV | 95783 | 159692 | 8.49% | 1.541% |
| 12 | 14.707 | 2013 | 2020 | 2032 | rBV2 | 214797 | 374191 | 19.90% | 3.610% |
| 13 | 16.199 | 2267 | 2274 | 2290 | rBV | 563602 | 934286 | 49.69% | 9.013% |
| 14 | 17.451 | 2481 | 2487 | 2499 | rBV2 | 260156 | 447731 | 23.81% | 4.319% |
| 15 | 19.724 | 2870 | 2874 | 2883 | rVB4 | 13174 | 23471 | 1.25% | 0.226% |
| 16 | 20.048 | 2923 | 2929 | 2949 | rBV | 1312674 | 1880129 | 100.00% | 18.138% |
| 17 | 20.717 | 3037 | 3043 | 3048 | rBV3 | 32946 | 72514 | 3.86% | 0.700% |
| 18 | 20.758 | 3048 | 3050 | 3059 | rVB5 | 26146 | 41527 | 2.21% | 0.401% |
| 19 | 21.334 | 3141 | 3148 | 3156 | rBV4 | 22797 | 55042 | 2.93% | 0.531% |
| 20 | 21.575 | 3186 | 3189 | 3196 | rVB2 | 13393 | 21733 | 1.16% | 0.210% |
| 21 | 21.722 | 3207 | 3214 | 3227 | rBV | 241124 | 463240 | 24.64% | 4.469% |
| 22 | 22.874 | 3402 | 3410 | 3419 | rBV | 64896 | 133862 | 7.12% | 1.291% |
| 23 | 24.989 | 3759 | 3770 | 3784 | rBV2 | 135219 | 430584 | 22.90% | 4.154% |

Sum of corrected areas: 10365431

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
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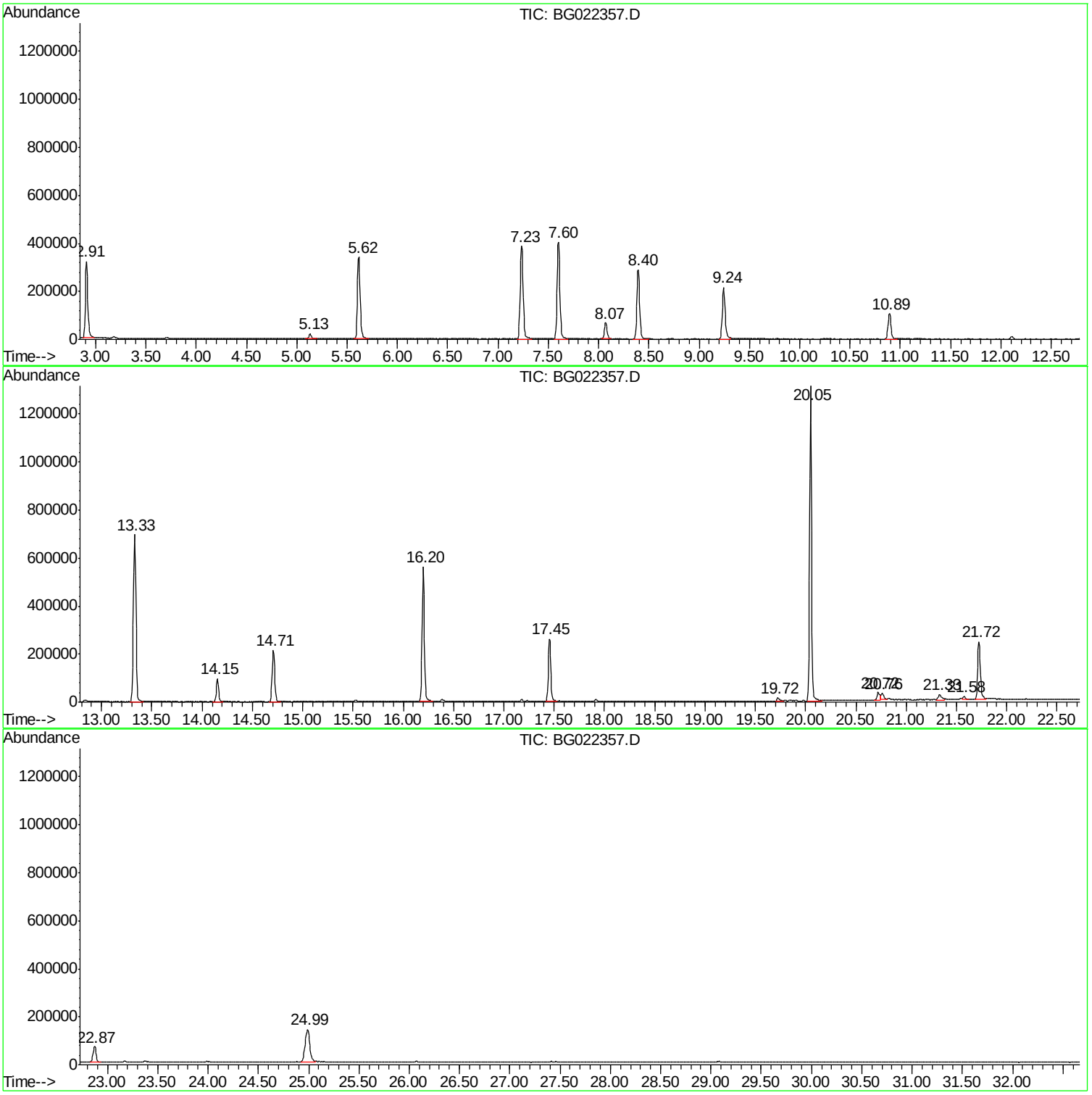
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

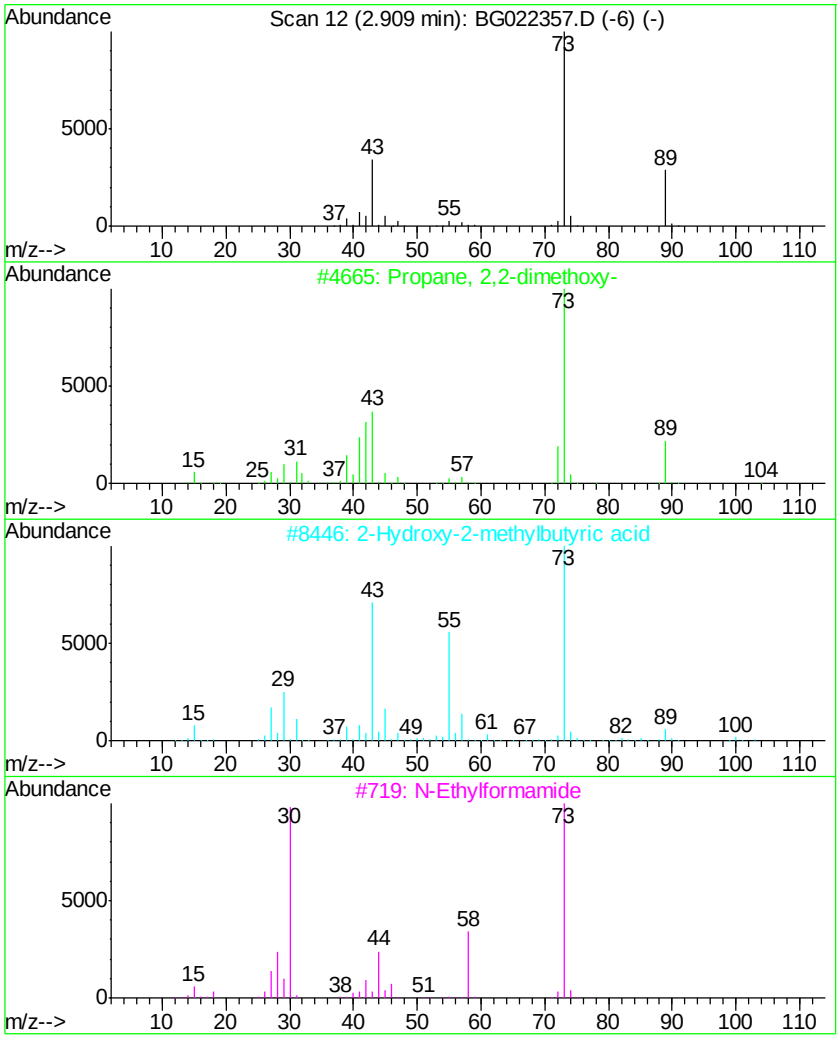
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

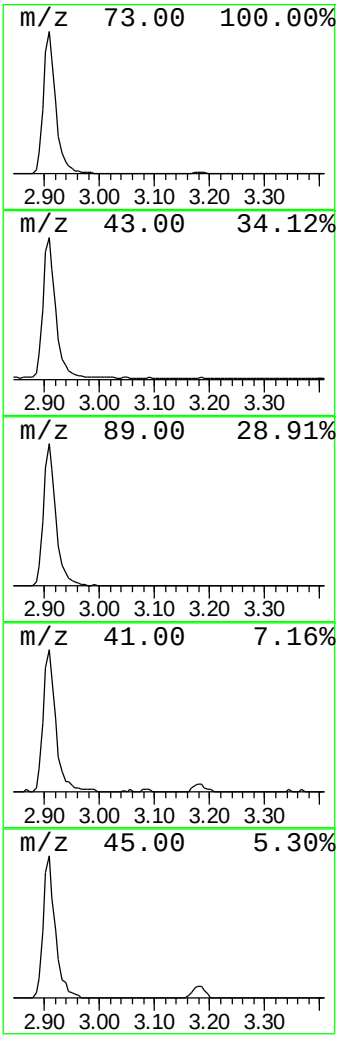
**********

Peak Number 1 unknown2.91 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.91 | 78.00 ng | 494125 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 38 |
| 2 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 7 |
| 4 | Methane, isothiocyanato- | 73 | C2H3NS | 000556-61-6 | 7 |
| 5 | 1,3,5-Trioxane | 90 | C3H6O3 | 000110-88-3 | 4 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

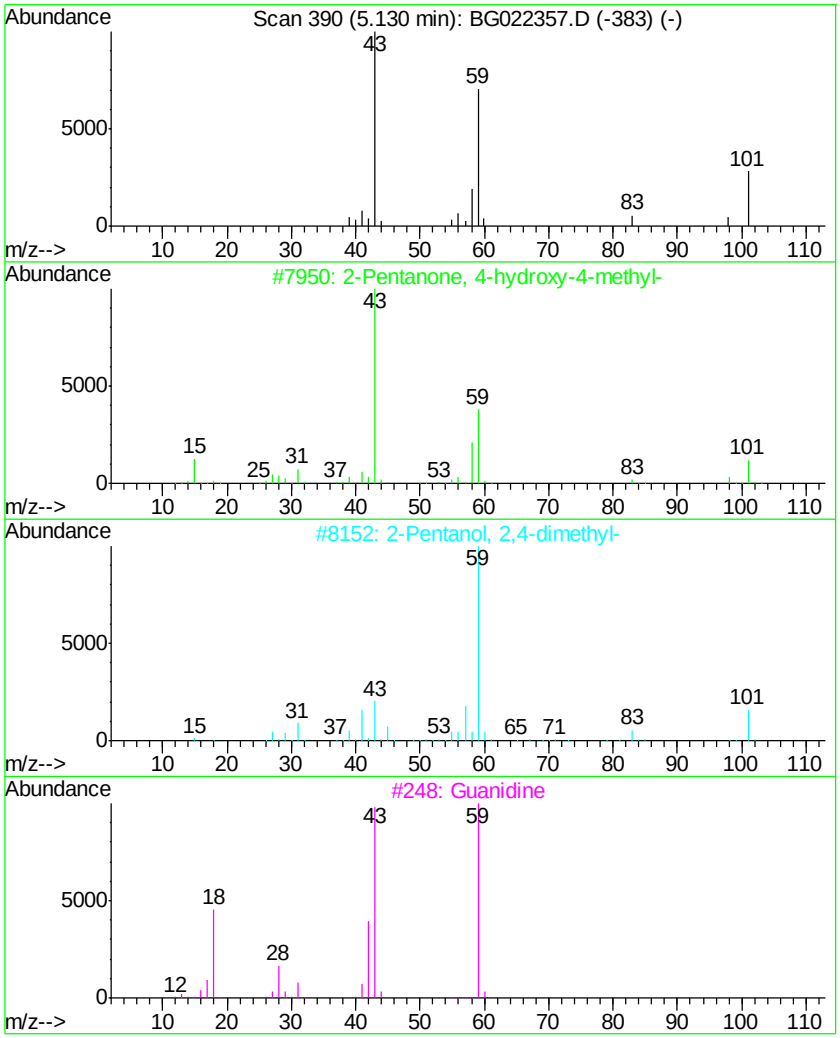
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

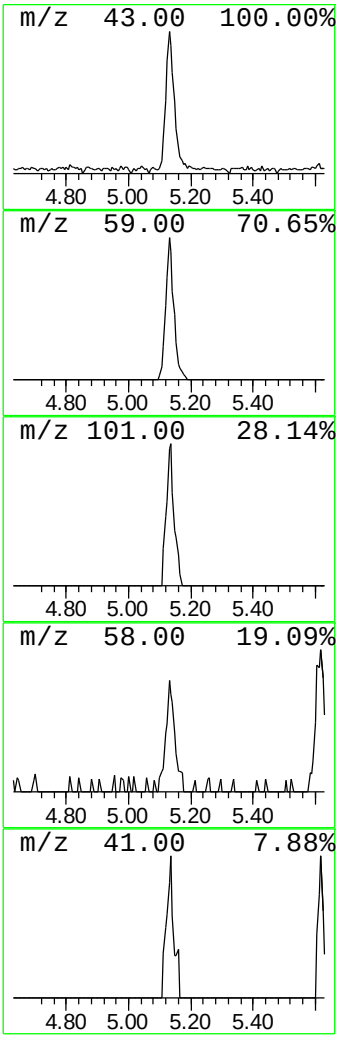
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.13 | 6.17 ng | 39073 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 38 |
| 3 | Guanidine | 59 | CH5N3 | 000113-00-8 | 38 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 37 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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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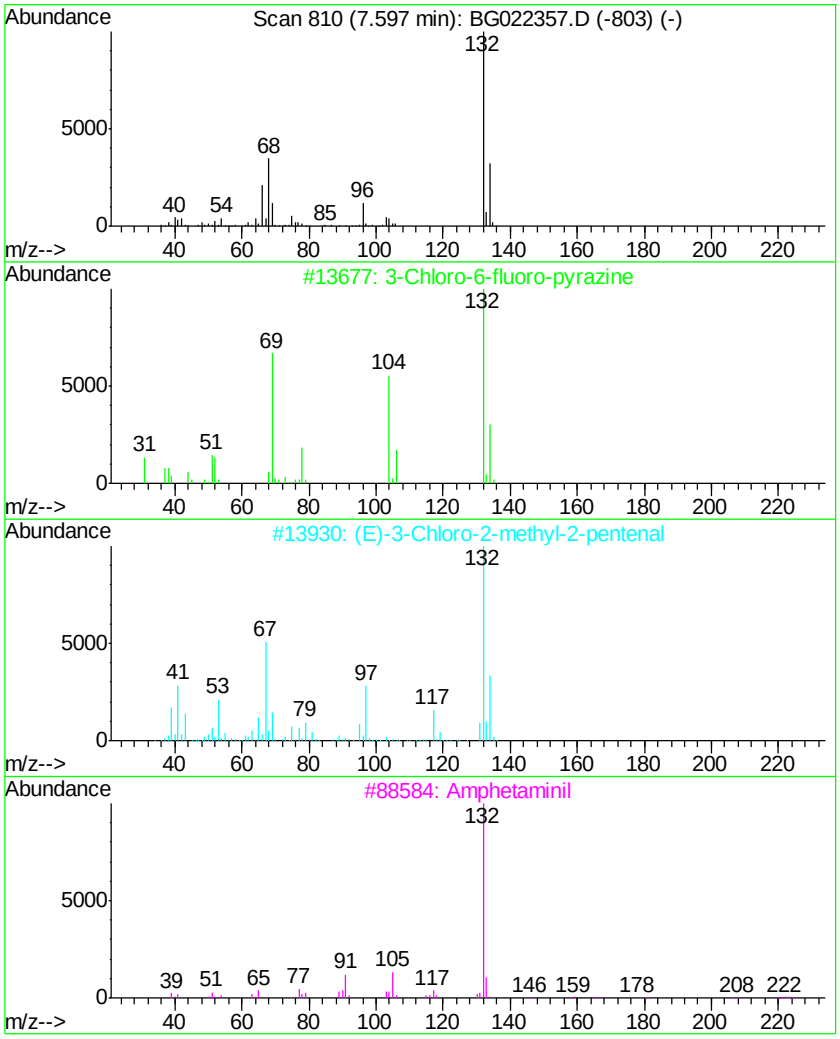
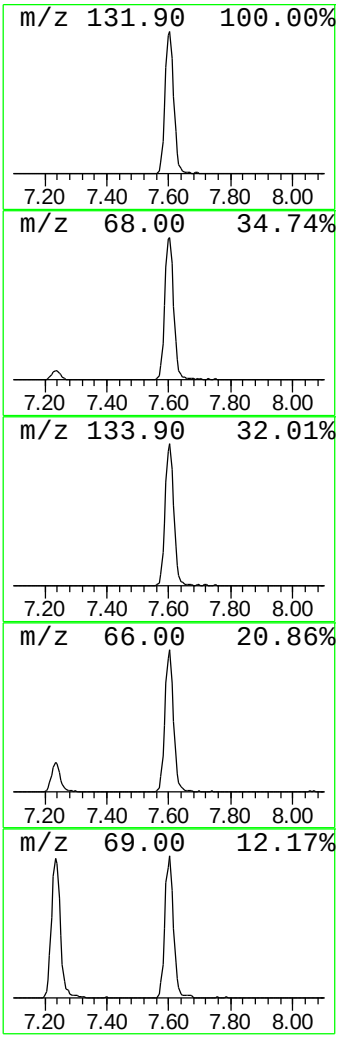
Peak Number 3 unknown7.60 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.60 | 124.81 ng | 790667 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

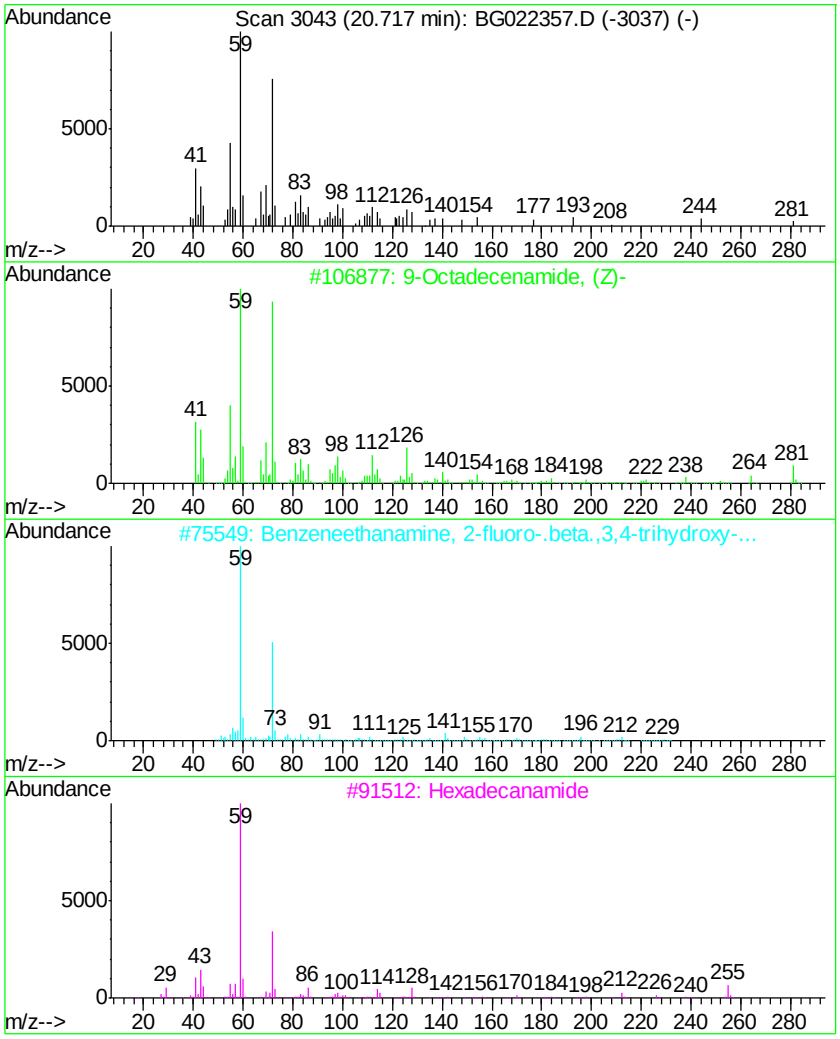
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

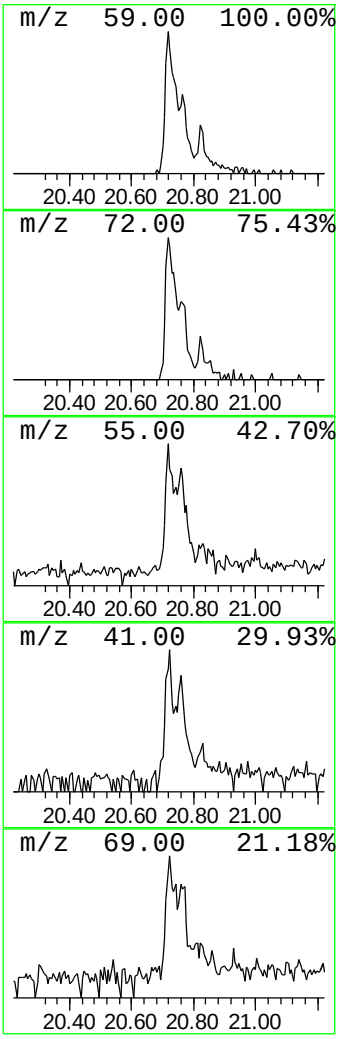
**********

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.72 | 3.13 ng | 72514 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 90 |
| 2 | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 59 |
| 3 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 56 |
| 4 | Mannosamine hydrochloride | 179 | C6H13NO5 | 1000127-68-8 | 50 |
| 5 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 47 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

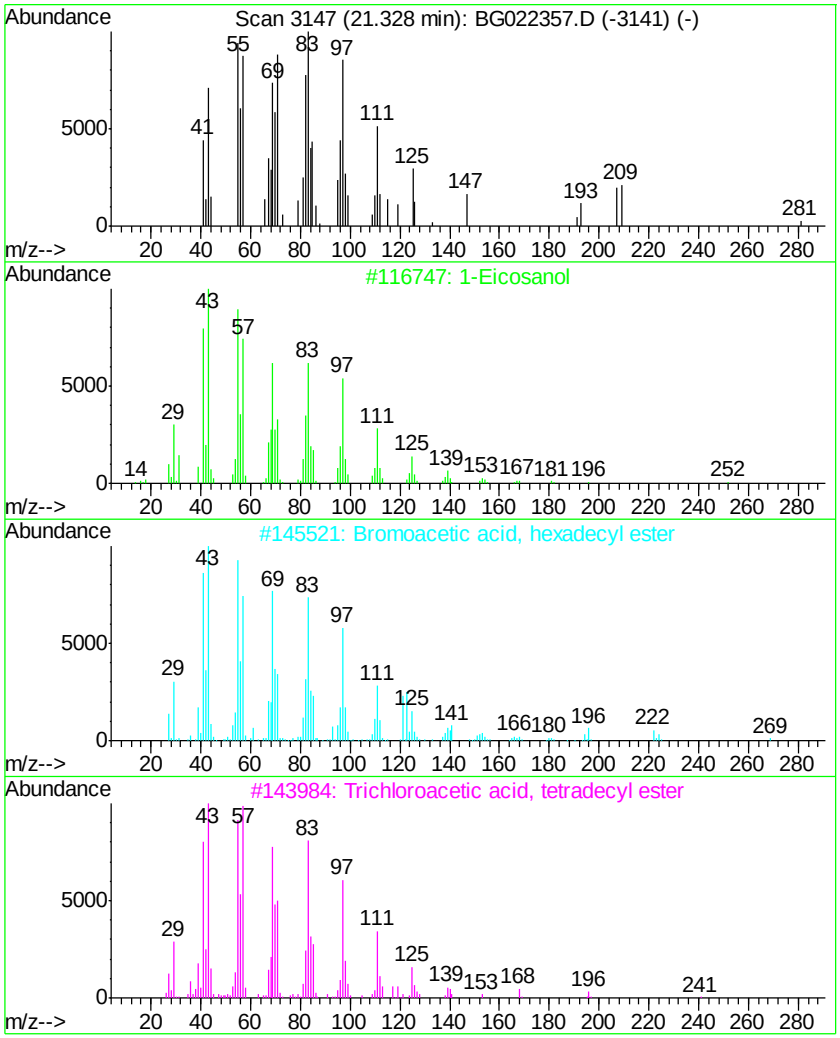
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

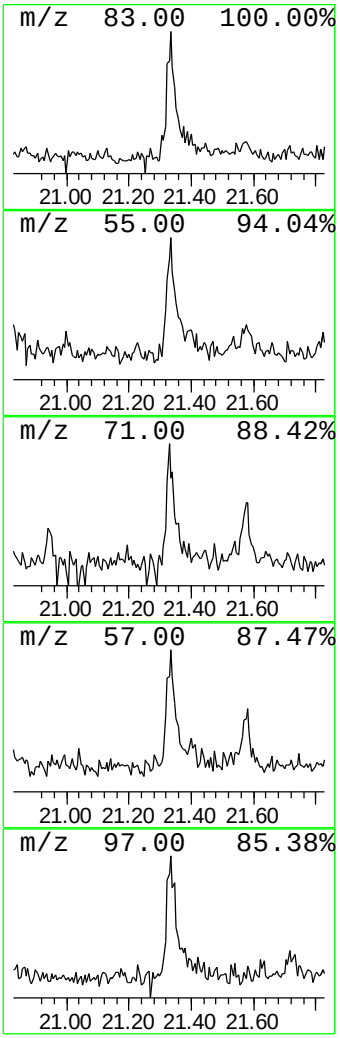
**********

Peak Number 6 1-Eicosanol Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.33 | 2.38 ng | 55042 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Eicosanol | 298 | C20H42O | 000629-96-9 | 91 |
| 2 | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 83 |
| 3 | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 81 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 81 |
| 5 | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1 | 81 |



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Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

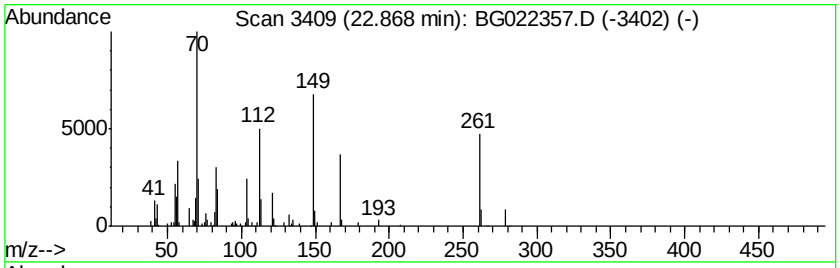
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

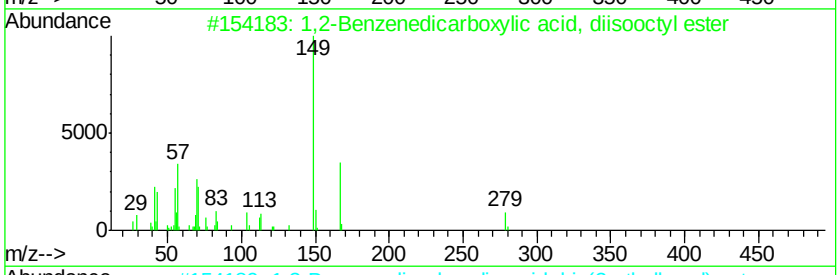
**********

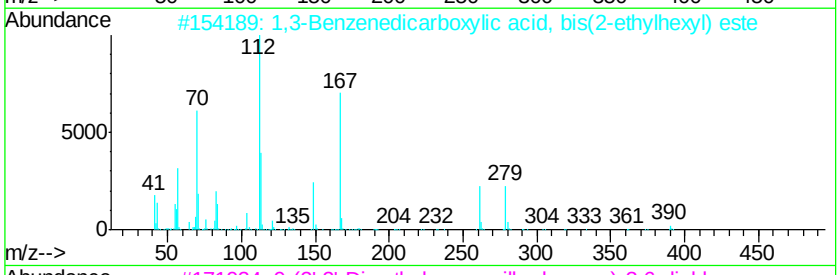
Peak Number 7 unknown22.87 Concentration Rank 5

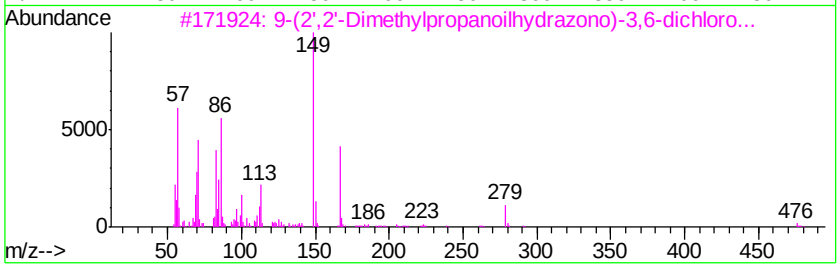
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.87 | 5.78 ng | 133862 | Chrysene-d12 | 21.72 |

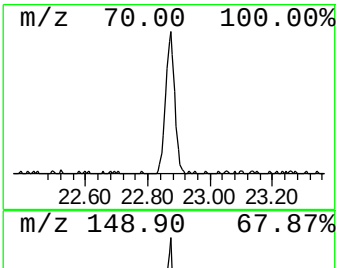
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzenedicarboxylic acid, di... | 390 | C24H38O4 | 027554-26-3 | 25 |
| 2 | 1,3-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 000137-89-3 | 23 |
| 3 | 9-(2',2'-Dimethylpropanoilhydraz... | 576 | C30H42Cl2N4O3 | 1000111-04-6 | 22 |
| 4 | Di-n-octyl phthalate | 390 | C24H38O4 | 000117-84-0 | 22 |
| 5 | Aziridine, 1-(1,1-dimethylethyl)... | 127 | C8H17N | 056082-94-1 | 16 |

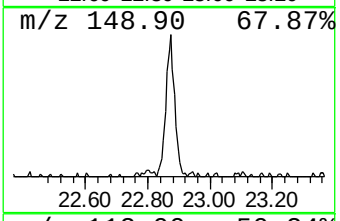


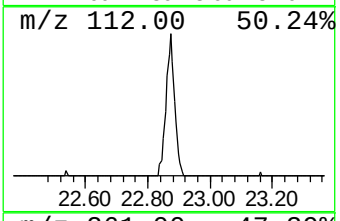



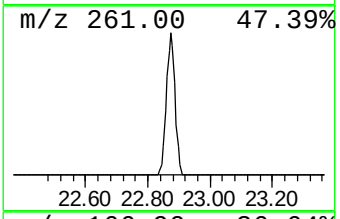



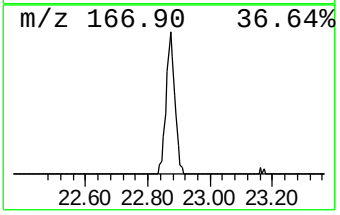



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061416\
Data File : BG022357.D
Acq On : 15 Jun 2016 6:42
Operator : UM/SJ
Sample : H3492-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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 |
| unknown2.91 | 2.91 | 78.0 | ng | 494125 | 1 | 8.07 | 126697 | 20.0 |
| 2-Pentanone, 4-hy... | 5.13 | 6.2 | ng | 39073 | 1 | 8.07 | 126697 | 20.0 |
| unknown7.60 | 7.60 | 124.8 | ng | 790667 | 1 | 8.07 | 126697 | 20.0 |
| 9-Octadecenamide,... | 20.72 | 3.1 | ng | 72514 | 5 | 21.72 | 463240 | 20.0 |
| 1-Eicosanol | 21.33 | 2.4 | ng | 55042 | 5 | 21.72 | 463240 | 20.0 |
| unknown22.87 | 22.87 | 5.8 | ng | 133862 | 5 | 21.72 | 463240 | 20.0 |