LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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 | 2.869 | 3 | 5 | 22 | rVB | 903215 | 1207917 | 70.37% | 11.579% |
| 2 | 5.102 | 379 | 385 | 393 | rBV | 22895 | 41506 | 2.42% | 0.398% |
| 3 | 5.601 | 463 | 470 | 486 | rBV | 314012 | 605326 | 35.27% | 5.803% |
| 4 | 7.229 | 740 | 747 | 759 | rBV | 333460 | 691189 | 40.27% | 6.626% |
| 5 | 7.581 | 799 | 807 | 819 | rBV | 380474 | 723045 | 42.13% | 6.931% |
| 6 | 8.040 | 879 | 885 | 897 | rVB2 | 67415 | 128630 | 7.49% | 1.233% |
| 7 | 8.363 | 931 | 940 | 954 | rBV | 280693 | 558631 | 32.55% | 5.355% |
| 8 | 9.221 | 1078 | 1086 | 1101 | rBV | 182216 | 410052 | 23.89% | 3.931% |
| 9 | 10.866 | 1357 | 1366 | 1380 | rBV | 103267 | 229043 | 13.34% | 2.196% |
| 10 | 13.304 | 1772 | 1781 | 1795 | rBV | 750410 | 1269767 | 73.98% | 12.172% |
| 11 | 14.127 | 1915 | 1921 | 1928 | rBV | 90728 | 148443 | 8.65% | 1.423% |
| 12 | 14.679 | 2008 | 2015 | 2025 | rBV2 | 203093 | 371213 | 21.63% | 3.559% |
| 13 | 16.177 | 2263 | 2270 | 2288 | rBV | 479293 | 866214 | 50.47% | 8.304% |
| 14 | 16.359 | 2296 | 2301 | 2311 | rVB3 | 11436 | 26433 | 1.54% | 0.253% |
| 15 | 17.147 | 2430 | 2435 | 2439 | rBV4 | 13523 | 20682 | 1.20% | 0.198% |
| 16 | 17.429 | 2476 | 2483 | 2497 | rBV2 | 233291 | 435522 | 25.37% | 4.175% |
| 17 | 17.781 | 2532 | 2543 | 2551 | rBV4 | 23142 | 62125 | 3.62% | 0.596% |
| 18 | 17.881 | 2556 | 2560 | 2570 | rVB2 | 17580 | 31814 | 1.85% | 0.305% |
| 19 | 19.144 | 2770 | 2775 | 2781 | rBV7 | 13174 | 24797 | 1.44% | 0.238% |
| 20 | 19.937 | 2908 | 2910 | 2918 | rBV7 | 10163 | 18545 | 1.08% | 0.178% |
| 21 | 20.020 | 2918 | 2924 | 2942 | rBV | 1119682 | 1716426 | 100.00% | 16.454% |
| 22 | 21.541 | 3180 | 3183 | 3192 | rVB | 30747 | 53186 | 3.10% | 0.510% |
| 23 | 21.694 | 3202 | 3209 | 3225 | rVB | 188561 | 391526 | 22.81% | 3.753% |
| 24 | 23.322 | 3482 | 3486 | 3497 | rVB3 | 18617 | 42673 | 2.49% | 0.409% |
| 25 | 24.926 | 3750 | 3759 | 3775 | rVB3 | 110667 | 356949 | 20.80% | 3.422% |

Sum of corrected areas: 10431654

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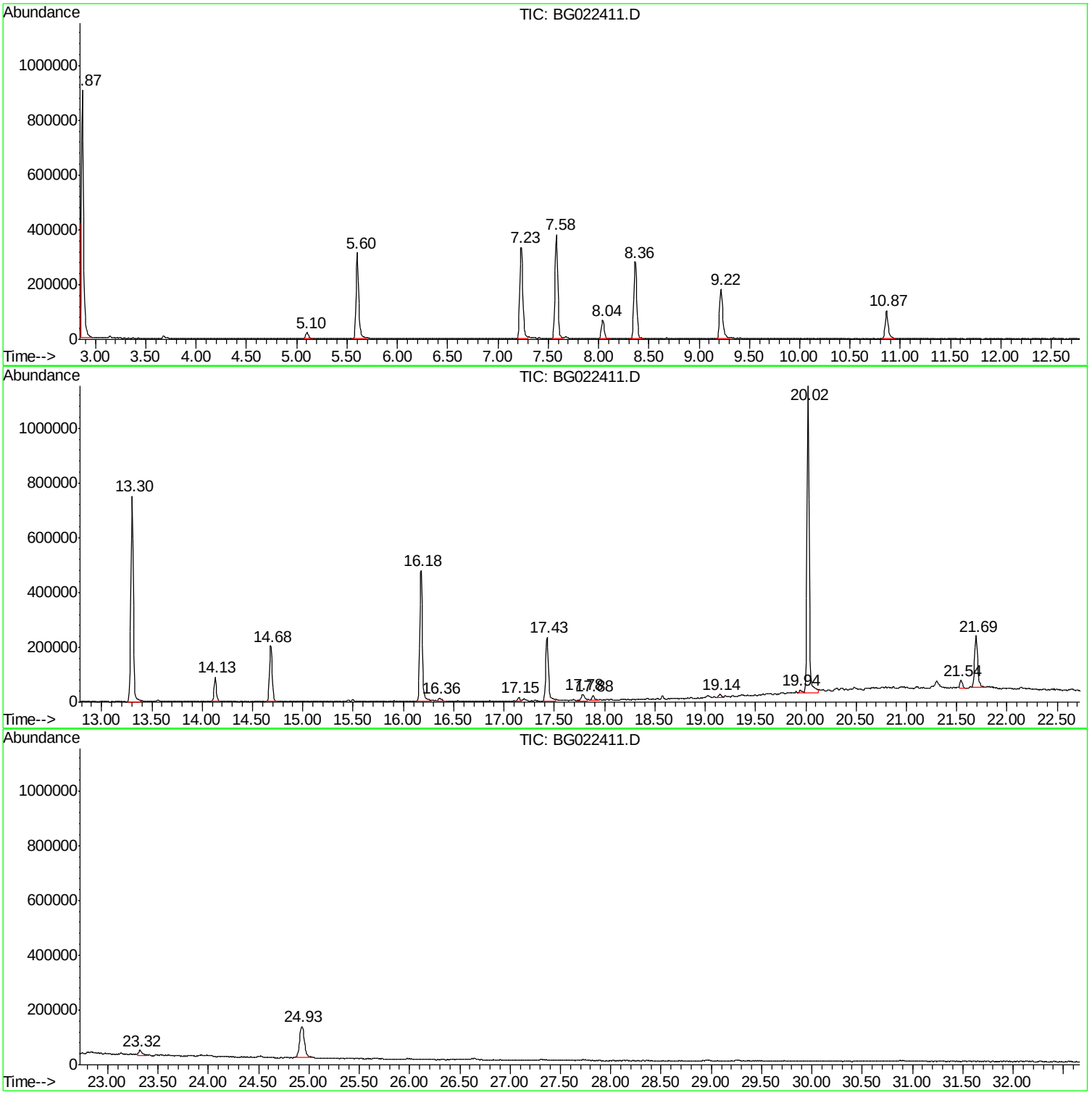
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SB4-1-3

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\BG061716\
Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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

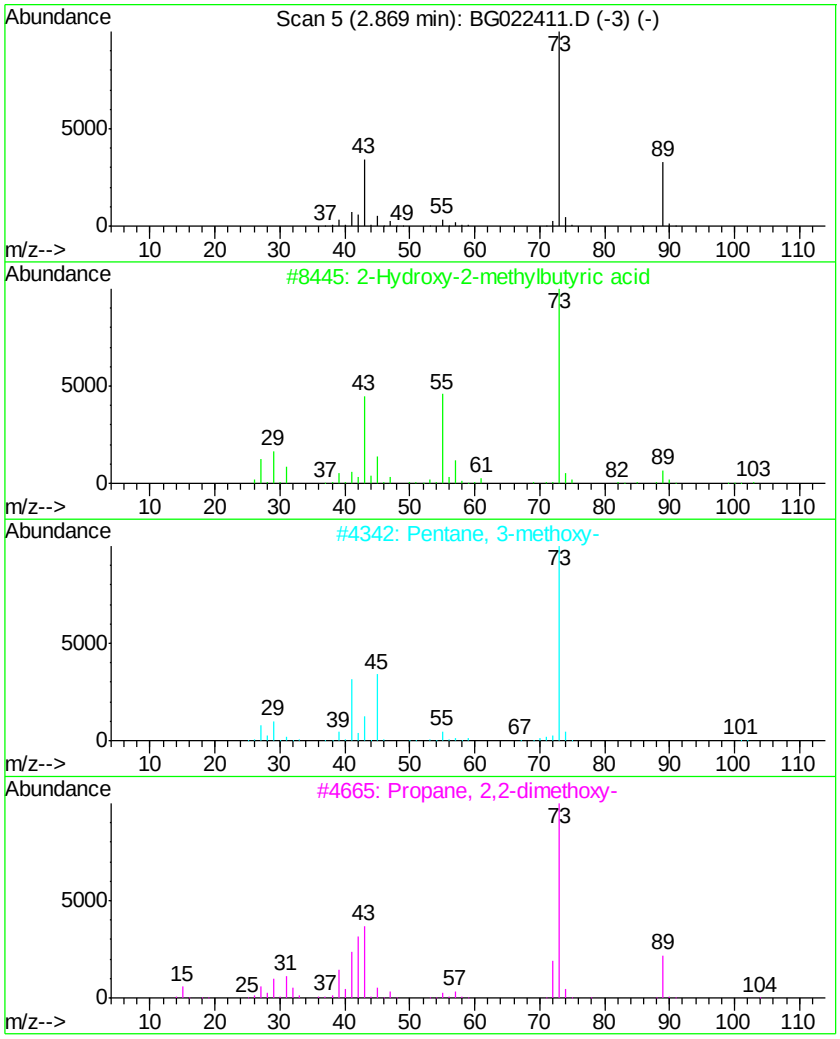
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

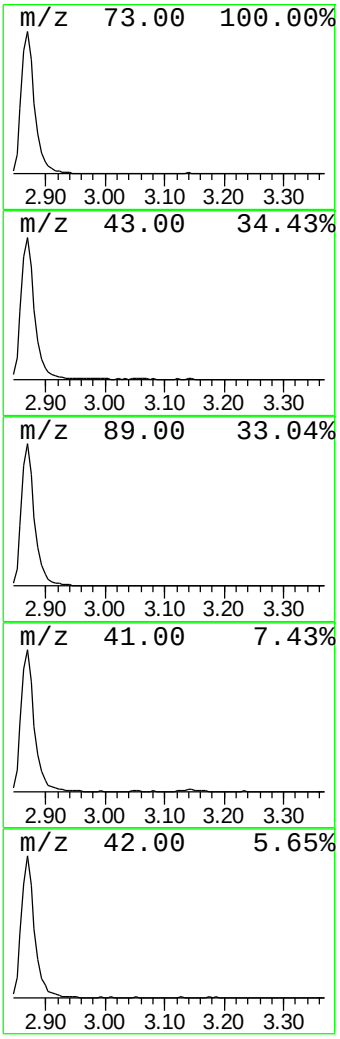
**********

Peak Number 1 unknown2.87 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.87 | 187.81 ng | 1207920 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 25 |
| 2 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 3 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 9 |
| 4 | 1,3,5-Trioxane | 90 | C3H6O3 | 000110-88-3 | 7 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 7 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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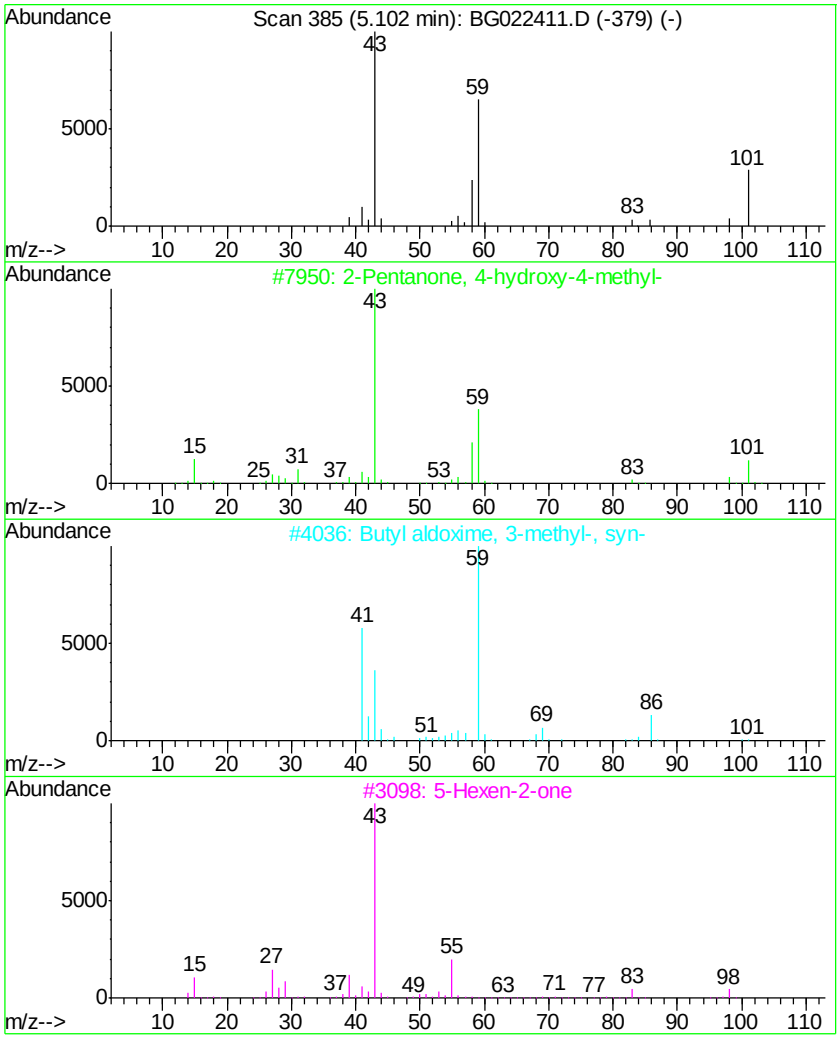
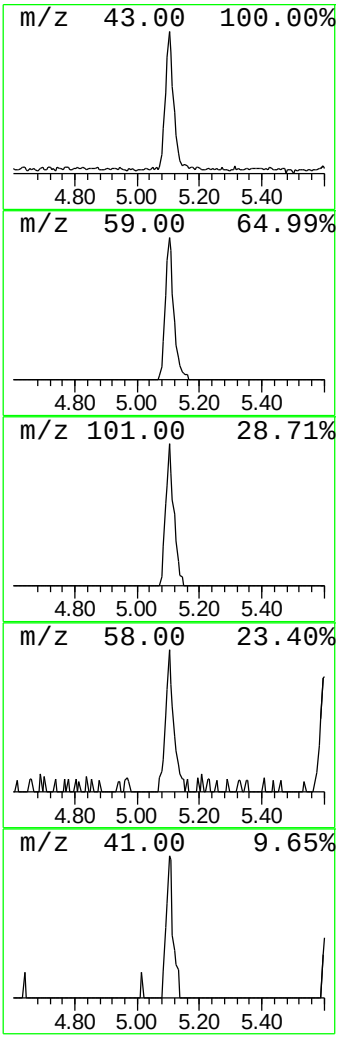
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 6.45 ng | 41506 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 12 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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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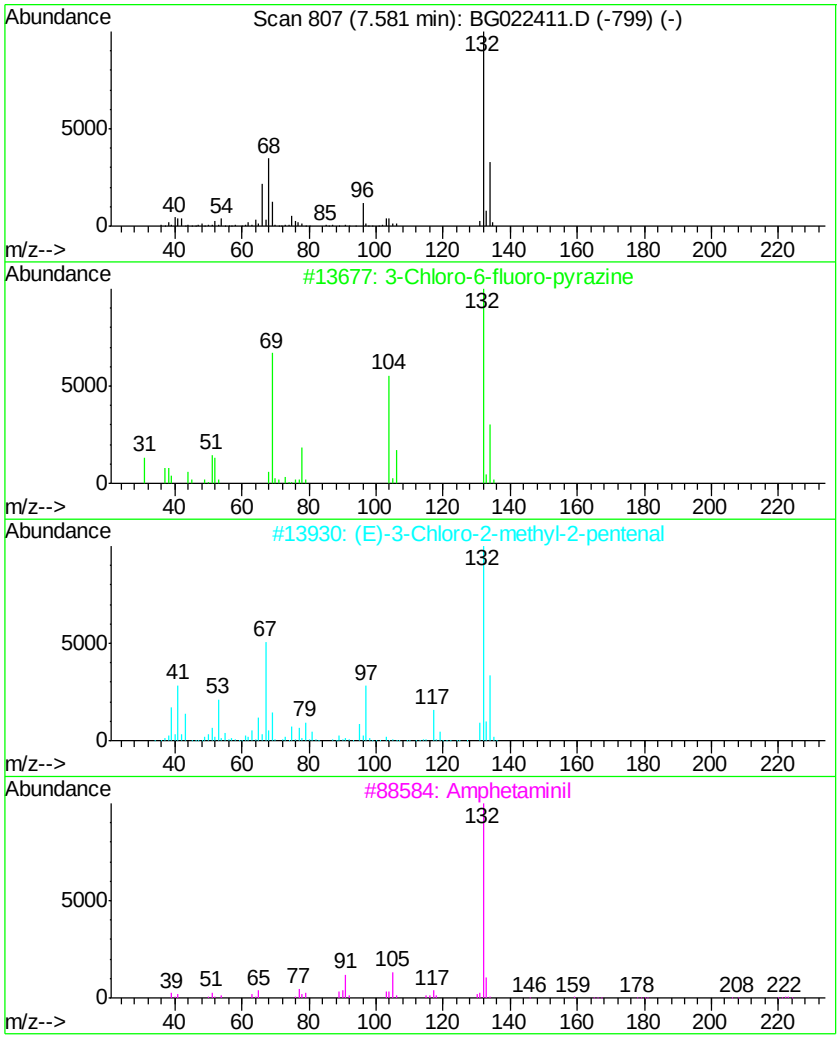
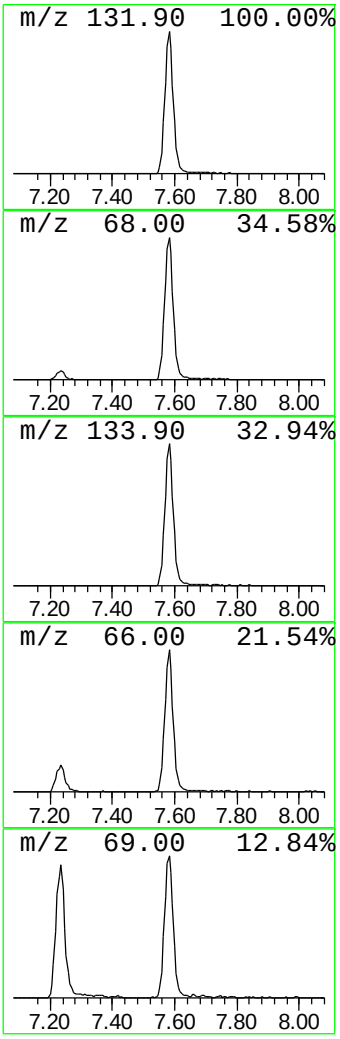
Peak Number 3 unknown7.58 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.58 | 112.42 ng | 723045 | 1,4-Dichlorobenzene-d4 | 8.04 |

| 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 | 38 |
| 3 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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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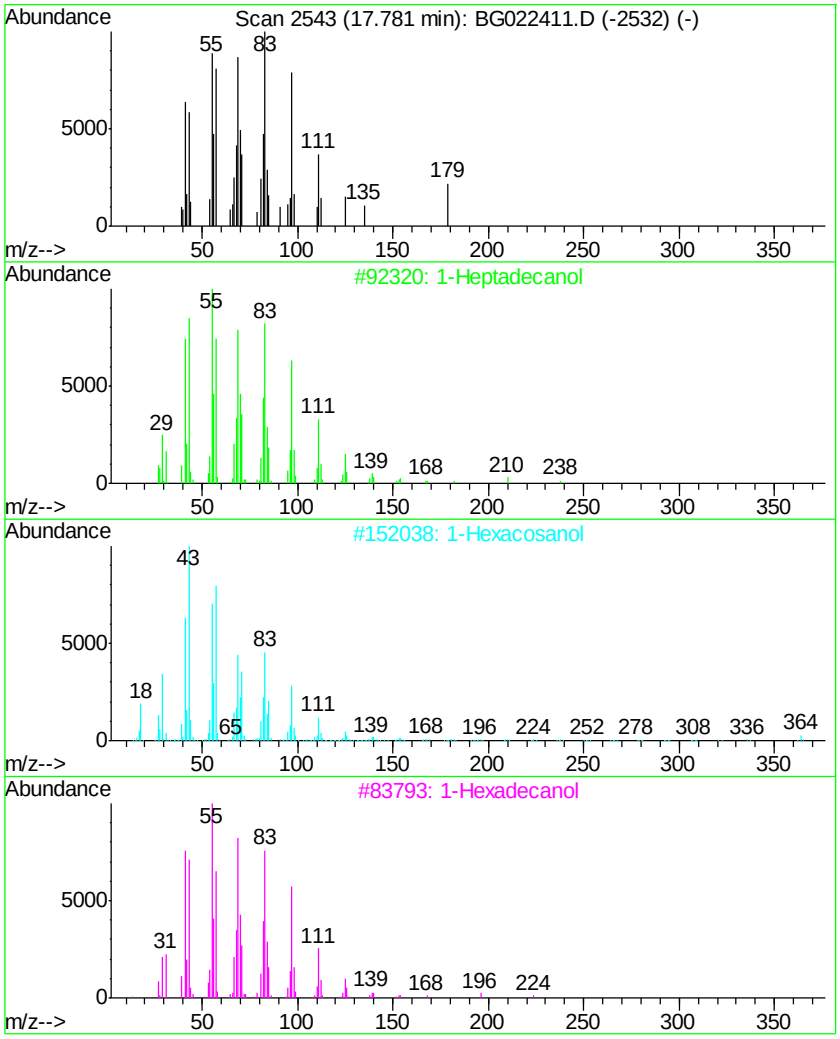
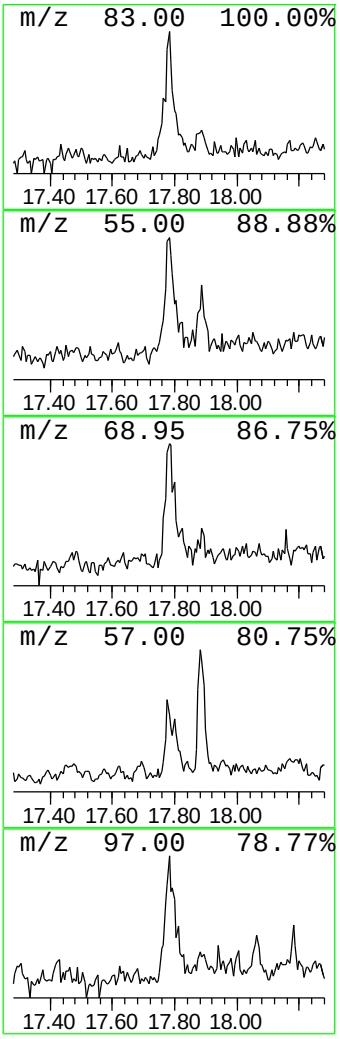
Peak Number 5 1-Heptadecanol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.78 | 2.85 ng | 62125 | Phenanthrene-d10 | 17.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heptadecanol | 256 | C17H36O | 001454-85-9 | 95 |
| 2 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 86 |
| 3 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 76 |
| 4 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 72 |
| 5 | 9-Octadecene, (E)- | 252 | C18H36 | 007206-25-9 | 68 |



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Data File : BG022411.D
Acq On : 18 Jun 2016 6:35
Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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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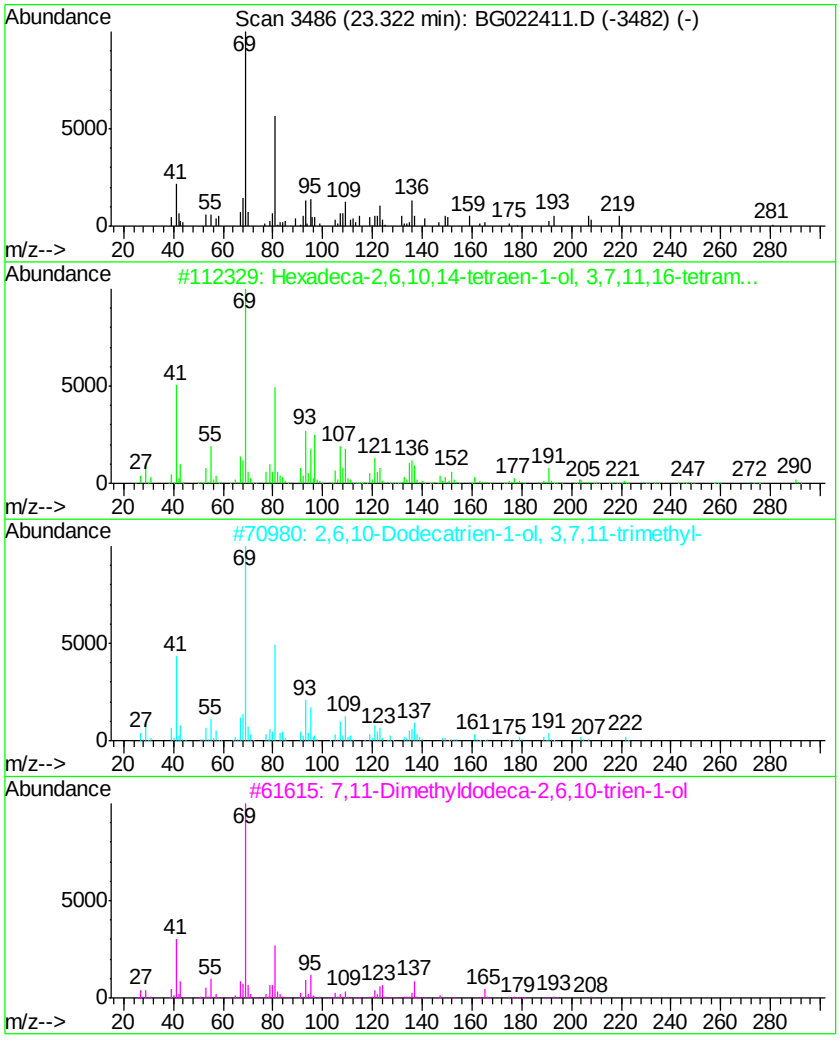
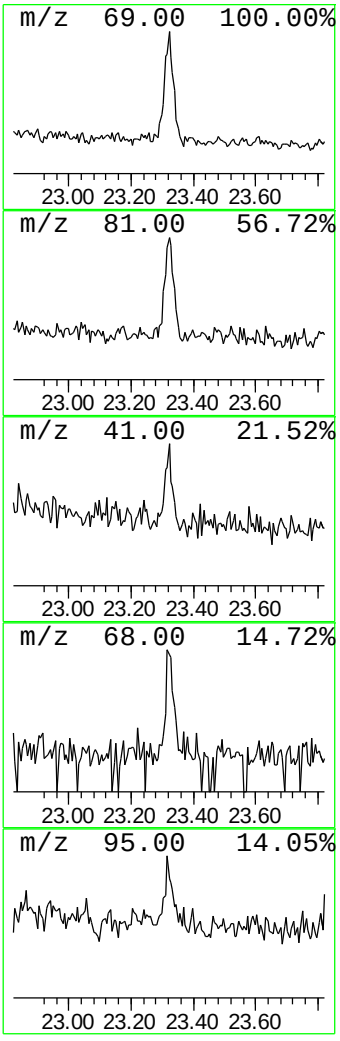
Peak Number 6 Hexadeca-2,6,10,14-tetraen-... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.32 | 2.39 ng | 42673 | Perylene-d12 | 24.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadeca-2,6,10,14-tetraen-1-ol,... | 290 | C20H34O | 007614-21-3 | 59 |
| 2 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0 | 53 |
| 3 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 53 |
| 4 | 5,9,13-Pentadecatrien-2-one, 6,1... | 262 | C18H30O | 001117-52-8 | 53 |
| 5 | 2,6,10,14,18,22-Tetracosahexaene... | 410 | C30H50 | 000111-02-4 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061716\
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Operator : UM/SJ
Sample : H3501-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB4-1-3

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 |
| unknown2.87 | 2.87 | 187.8 | ng | 1207920 | 1 | 8.04 | 128630 | 20.0 |
| 2-Pentanone, 4-hy... | 5.10 | 6.5 | ng | 41506 | 1 | 8.04 | 128630 | 20.0 |
| unknown7.58 | 7.58 | 112.4 | ng | 723045 | 1 | 8.04 | 128630 | 20.0 |
| 1-Heptadecanol | 17.78 | 2.9 | ng | 62125 | 4 | 17.43 | 435522 | 20.0 |
| Hexadeca-2,6,10,1... | 23.32 | 2.4 | ng | 42673 | 6 | 24.93 | 356949 | 20.0 |