LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110118\
Data File : BG037722.D
Acq On : 1 Nov 2018 17:13
Operator : JU/SJ
Sample : J5741-23
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-6

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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 | 3.763 | 77 | 81 | 90 | rBV | 31789 | 54786 | 1.44% | 0.246% |
| 2 | 5.179 | 316 | 322 | 331 | rBV | 49869 | 80880 | 2.13% | 0.364% |
| 3 | 5.637 | 393 | 400 | 411 | rBV | 1029471 | 1747582 | 45.93% | 7.862% |
| 4 | 7.247 | 665 | 674 | 692 | rBV | 1115872 | 2175869 | 57.18% | 9.789% |
| 5 | 7.623 | 730 | 738 | 751 | rBV | 1043706 | 1866075 | 49.04% | 8.395% |
| 6 | 8.099 | 811 | 819 | 826 | rBV | 175895 | 314414 | 8.26% | 1.414% |
| 7 | 8.422 | 866 | 874 | 883 | rBV | 730629 | 1323341 | 34.78% | 5.953% |
| 8 | 9.274 | 1011 | 1019 | 1028 | rBV | 665584 | 1261572 | 33.16% | 5.675% |
| 9 | 10.919 | 1290 | 1299 | 1306 | rBV | 255659 | 491042 | 12.91% | 2.209% |
| 10 | 13.352 | 1705 | 1713 | 1730 | rBV | 1705360 | 2803782 | 73.69% | 12.613% |
| 11 | 14.174 | 1847 | 1853 | 1860 | rBV | 202494 | 306320 | 8.05% | 1.378% |
| 12 | 14.733 | 1941 | 1948 | 1956 | rBV2 | 445476 | 751108 | 19.74% | 3.379% |
| 13 | 16.219 | 2194 | 2201 | 2217 | rBV | 1382081 | 2230025 | 58.61% | 10.032% |
| 14 | 17.482 | 2408 | 2416 | 2428 | rBV | 580706 | 946385 | 24.87% | 4.258% |
| 15 | 18.334 | 2555 | 2561 | 2571 | rBV2 | 38975 | 73320 | 1.93% | 0.330% |
| 16 | 20.079 | 2852 | 2858 | 2870 | rBV | 2817533 | 3805027 | 100.00% | 17.118% |
| 17 | 21.366 | 3072 | 3077 | 3091 | rBV8 | 30939 | 123627 | 3.25% | 0.556% |
| 18 | 21.765 | 3138 | 3145 | 3156 | rBV | 511325 | 959783 | 25.22% | 4.318% |
| 19 | 23.246 | 3391 | 3397 | 3404 | rBV5 | 25696 | 53573 | 1.41% | 0.241% |
| 20 | 24.080 | 3532 | 3539 | 3546 | rVB5 | 20898 | 45267 | 1.19% | 0.204% |
| 21 | 25.103 | 3699 | 3713 | 3728 | rBV2 | 219979 | 814834 | 21.41% | 3.666% |

Sum of corrected areas: 22228612

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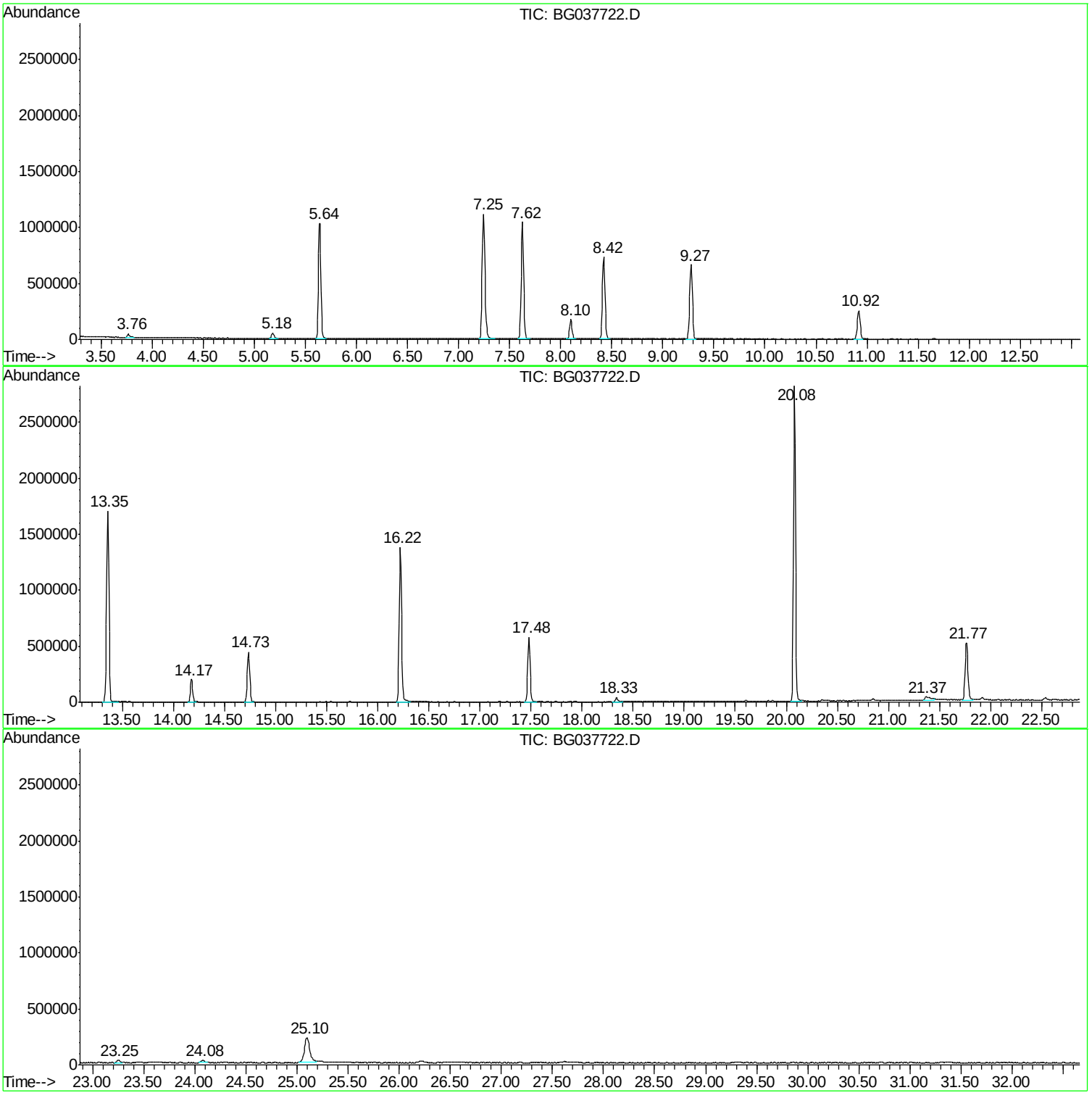
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110118\
Data File : BG037722.D
Acq On : 1 Nov 2018 17:13
Operator : JU/SJ
Sample : J5741-23
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

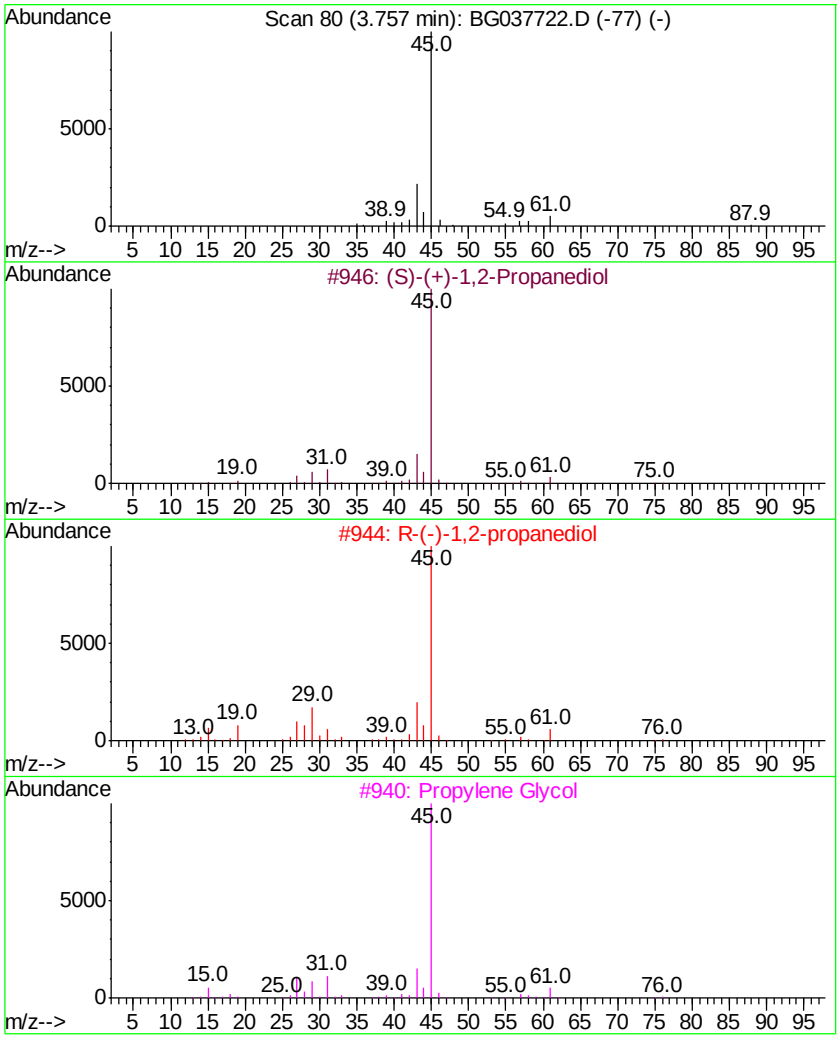
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

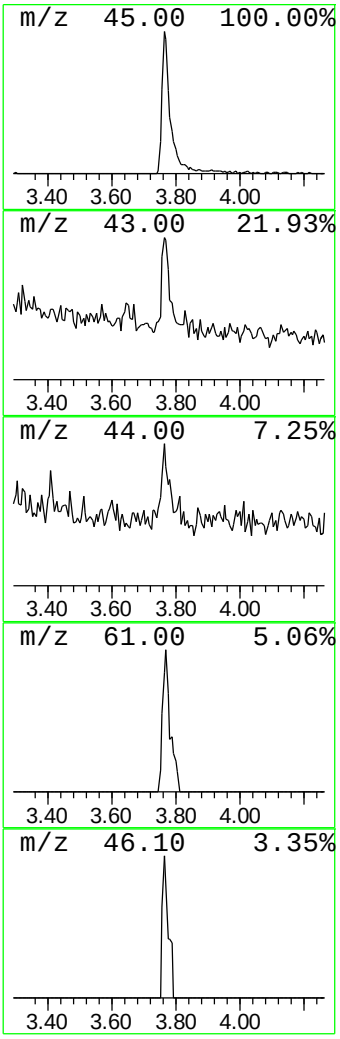
**********

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.76 | 3.48 ng | 54786 | 1,4-Dichlorobenzene-d4 | 8.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (S)-(+)-1,2-Propanediol | 76 | C3H8O2 | 004254-15-3 | 56 |
| 2 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 40 |
| 3 | Propylene Glycol | 76 | C3H8O2 | 000057-55-6 | 40 |
| 4 | 1-Butene, 4-methoxy | 86 | C5H10O | 004696-30-4 | 9 |
| 5 | 2-Butanol, (R)- | 74 | C4H10O | 014898-79-4 | 9 |



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Data File : BG037722.D
Acq On : 1 Nov 2018 17:13
Operator : JU/SJ
Sample : J5741-23
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-6

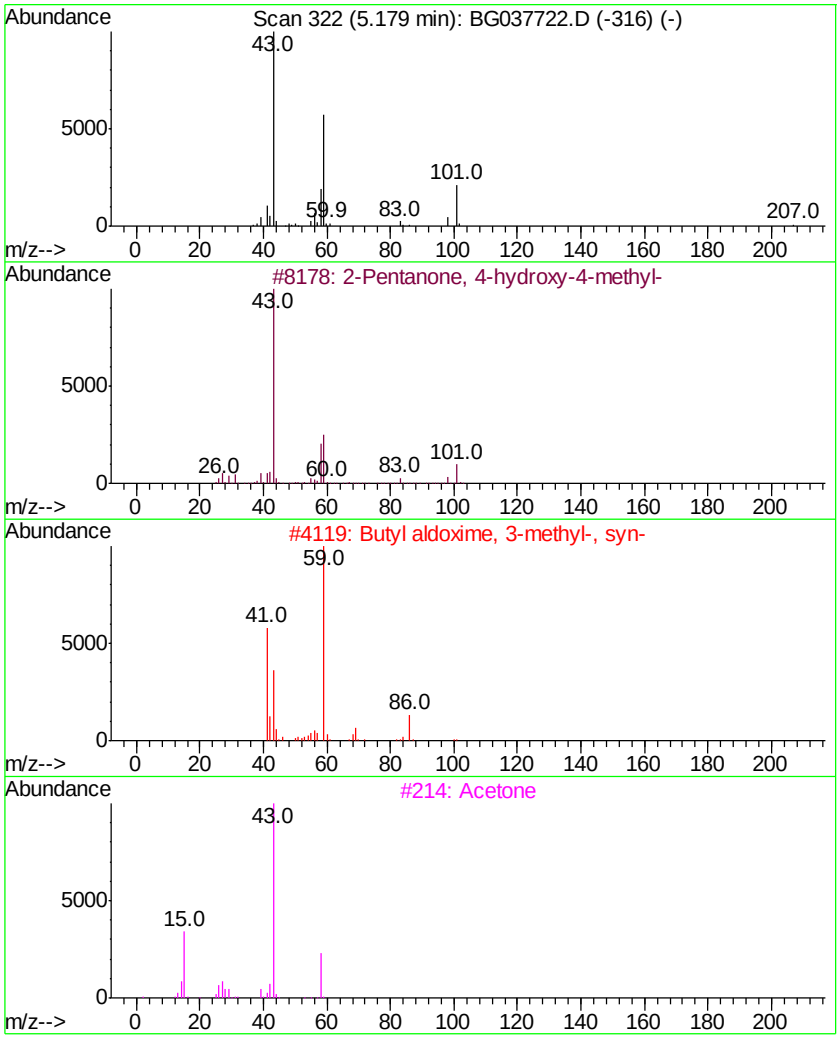
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

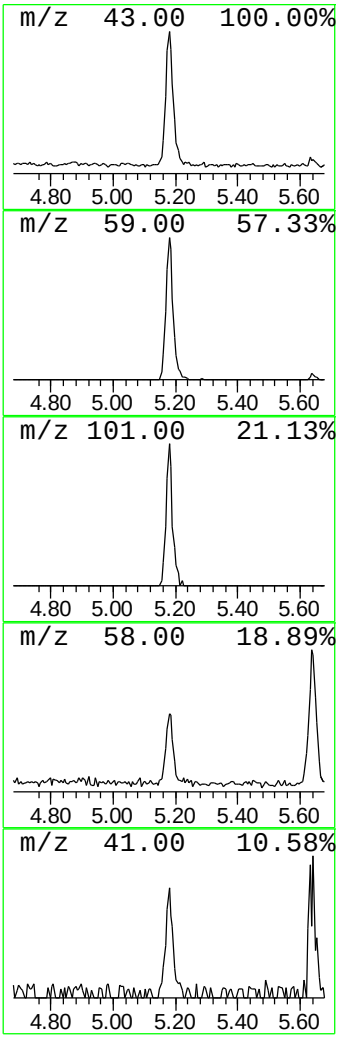
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 5.14 ng | 80880 | 1,4-Dichlorobenzene-d4 | 8.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 12 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



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Data File : BG037722.D
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Operator : JU/SJ
Sample : J5741-23
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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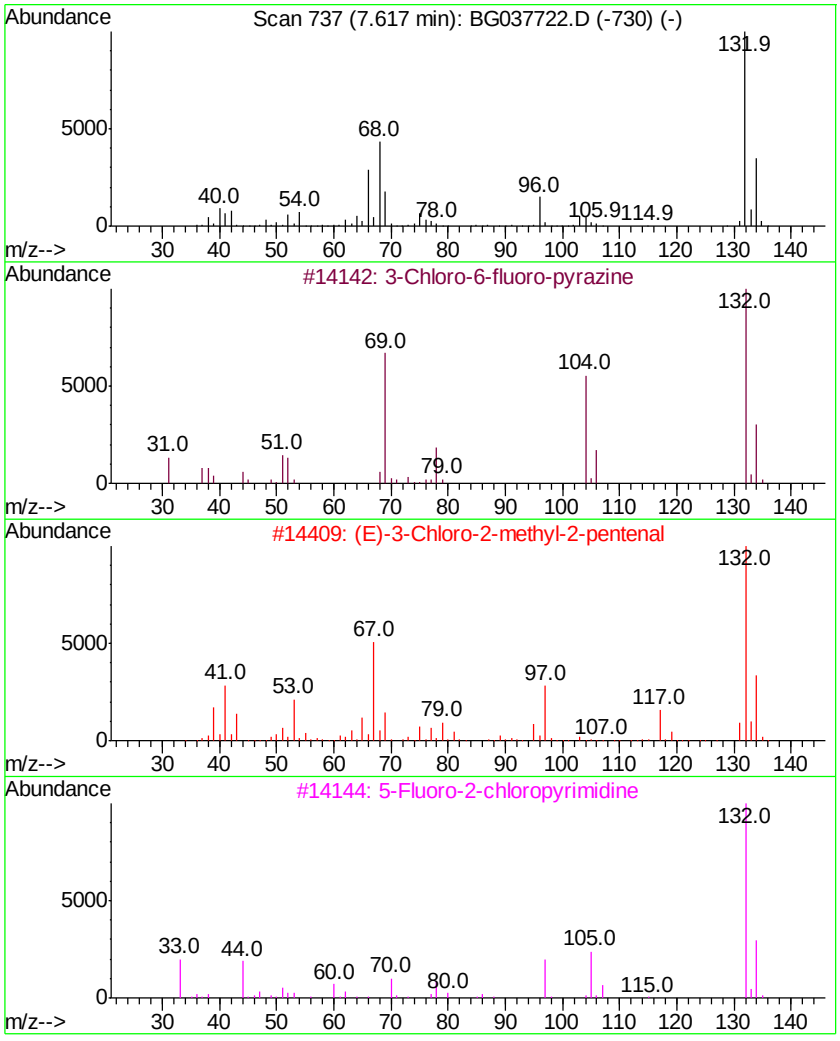
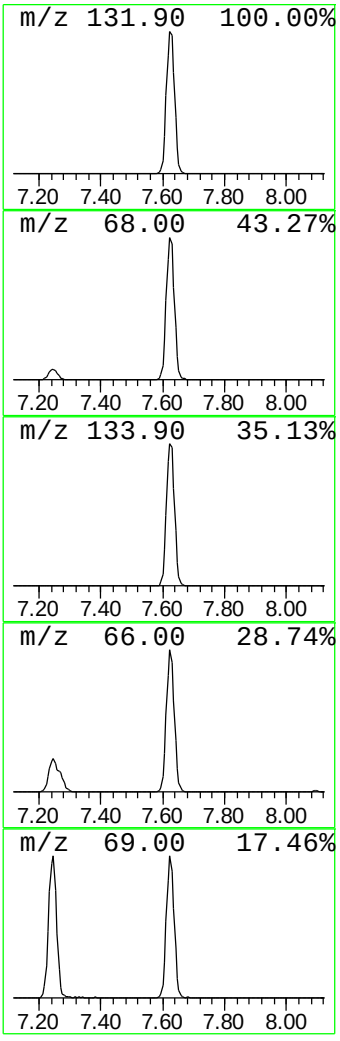
**********

Peak Number 3 unknown7.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.62 | 118.70 ng | 1866080 | 1,4-Dichlorobenzene-d4 | 8.10 |

| 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-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



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**Instrument :** BNA_G
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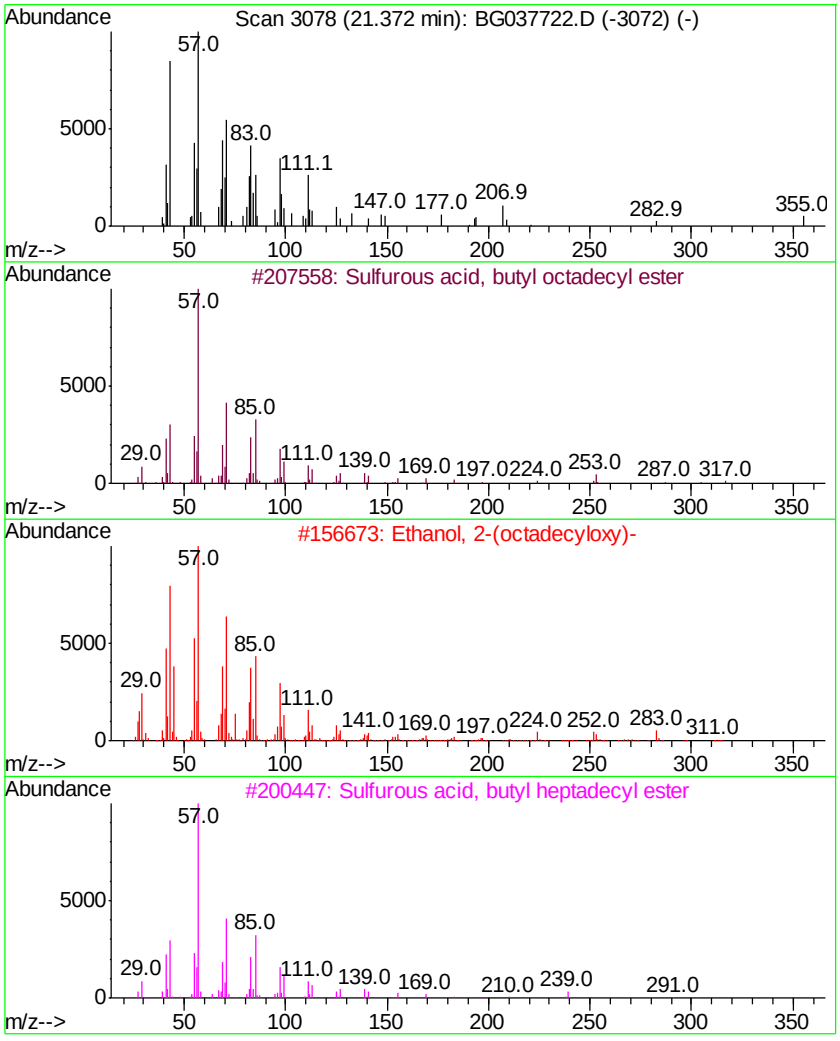
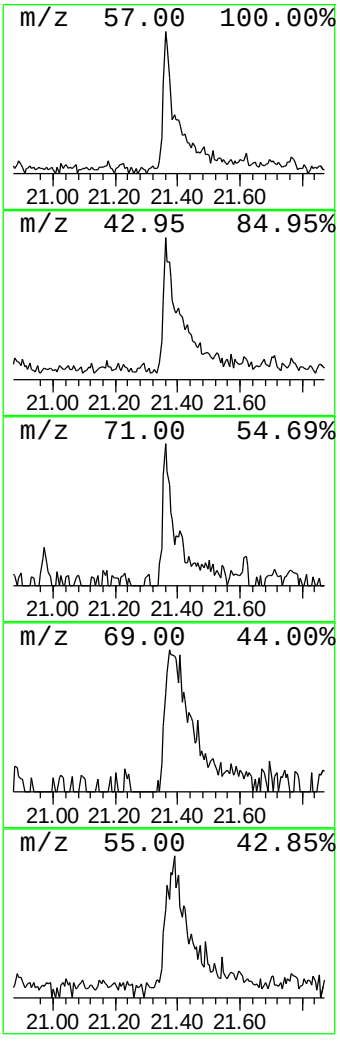
**********

Peak Number 5 Sulfurous acid, butyl octad... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.37 | 2.58 ng | 123627 | Chrysene-d12 | 21.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, butyl octadecyl ... | 390 | C22H46O3S | 1000309-18-5 | 86 |
| 2 | Ethanol, 2-(octadecyloxy)- | 314 | C20H42O2 | 002136-72-3 | 80 |
| 3 | Sulfurous acid, butyl heptadecyl... | 376 | C21H44O3S | 1000309-18-4 | 80 |
| 4 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 74 |
| 5 | 1-Decanol, 2-octyl- | 270 | C18H38O | 045235-48-1 | 74 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110118\
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Acq On : 1 Nov 2018 17:13
Operator : JU/SJ
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
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 |
| (S)-(+)-1,2-Propa... | 3.76 | 3.5 | ng | 54786 | 1 | 8.10 | 314414 | 20.0 |
| 2-Pentanone, 4-hy... | 5.18 | 5.1 | ng | 80880 | 1 | 8.10 | 314414 | 20.0 |
| unknown7.62 | 7.62 | 118.7 | ng | 1866080 | 1 | 8.10 | 314414 | 20.0 |
| Sulfurous acid, b... | 21.37 | 2.6 | ng | 123627 | 5 | 21.77 | 959783 | 20.0 |