LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

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-BG041520.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 | 3.194 | 15 | 18 | 26 | rVB | 114179 | 141197 | 2.08% | 0.460% |
| 2 | 3.482 | 62 | 67 | 76 | rVB | 107417 | 152306 | 2.24% | 0.496% |
| 3 | 4.633 | 257 | 263 | 271 | rBV2 | 56236 | 112036 | 1.65% | 0.365% |
| 4 | 5.086 | 335 | 340 | 350 | rVB3 | 51340 | 79932 | 1.18% | 0.260% |
| 5 | 5.579 | 417 | 424 | 435 | rBV | 1238223 | 2080927 | 30.67% | 6.780% |
| 6 | 7.171 | 687 | 695 | 707 | rBV | 1255959 | 2224283 | 32.78% | 7.247% |
| 7 | 8.005 | 831 | 837 | 845 | rVB | 258923 | 435781 | 6.42% | 1.420% |
| 8 | 8.334 | 885 | 893 | 902 | rBV | 1228958 | 2225513 | 32.80% | 7.251% |
| 9 | 9.163 | 1025 | 1034 | 1045 | rBV | 996017 | 1851430 | 27.29% | 6.032% |
| 10 | 10.813 | 1307 | 1315 | 1325 | rBV | 352702 | 641955 | 9.46% | 2.092% |
| 11 | 13.269 | 1725 | 1733 | 1741 | rBV | 2987523 | 4692628 | 69.16% | 15.290% |
| 12 | 14.643 | 1959 | 1967 | 1975 | rBV2 | 609343 | 980211 | 14.45% | 3.194% |
| 13 | 16.130 | 2213 | 2220 | 2231 | rBV | 2612232 | 4076210 | 60.08% | 13.281% |
| 14 | 17.387 | 2428 | 2434 | 2441 | rBV | 758111 | 1182478 | 17.43% | 3.853% |
| 15 | 18.597 | 2634 | 2640 | 2648 | rBV2 | 75198 | 155795 | 2.30% | 0.508% |
| 16 | 19.466 | 2784 | 2788 | 2794 | rVB2 | 81036 | 100900 | 1.49% | 0.329% |
| 17 | 19.707 | 2824 | 2829 | 2833 | rBV2 | 51178 | 72933 | 1.07% | 0.238% |
| 18 | 20.001 | 2873 | 2879 | 2886 | rVB | 4954030 | 6784859 | 100.00% | 22.107% |
| 19 | 20.535 | 2966 | 2970 | 2975 | rBV3 | 53869 | 78583 | 1.16% | 0.256% |
| 20 | 20.670 | 2989 | 2993 | 2997 | rVB | 260316 | 291158 | 4.29% | 0.949% |
| 21 | 21.651 | 3153 | 3160 | 3166 | rBV2 | 720343 | 1190892 | 17.55% | 3.880% |
| 22 | 24.830 | 3692 | 3701 | 3710 | rBV2 | 408242 | 1139036 | 16.79% | 3.711% |

Sum of corrected areas: 30691043

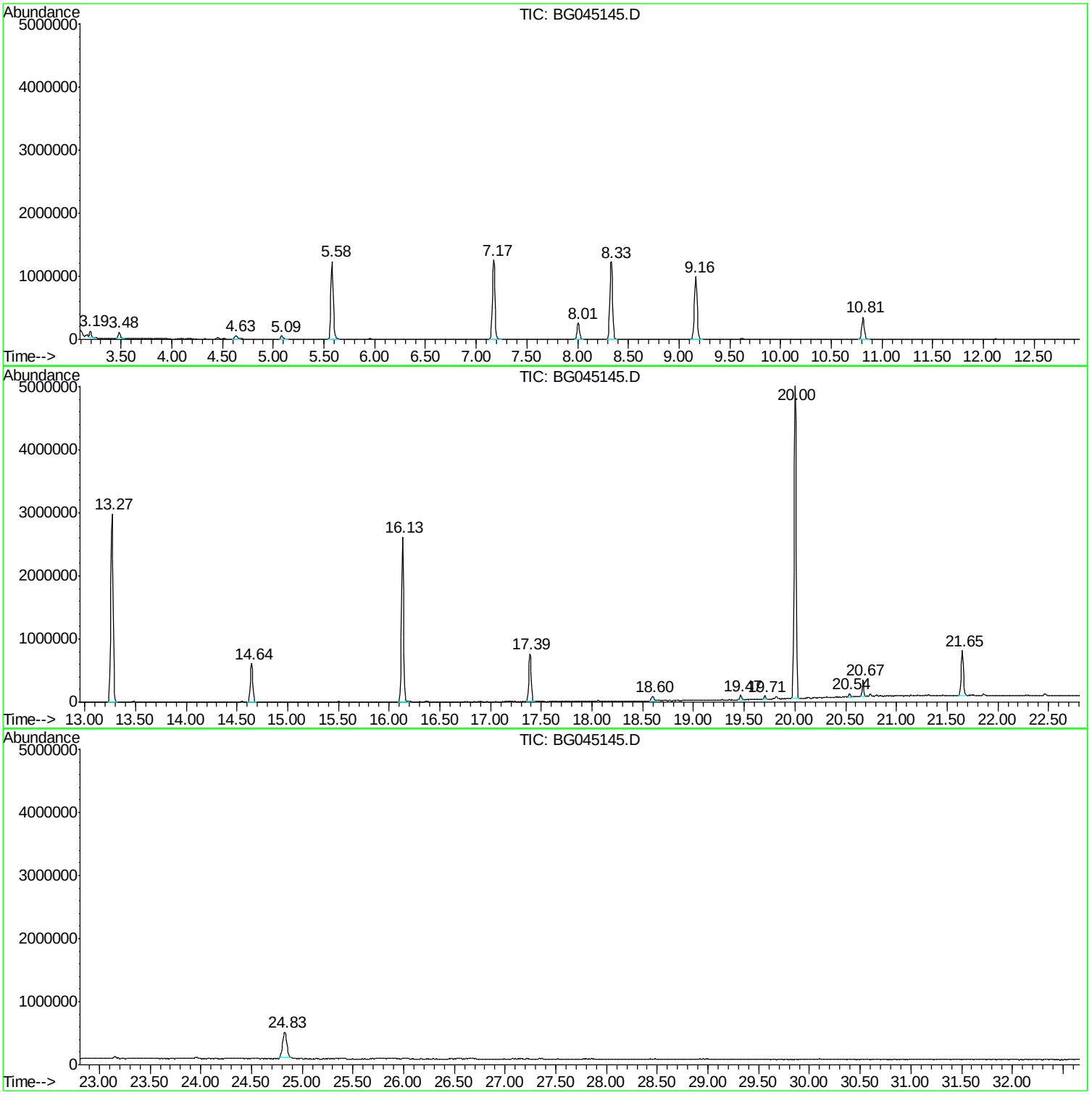
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.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\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

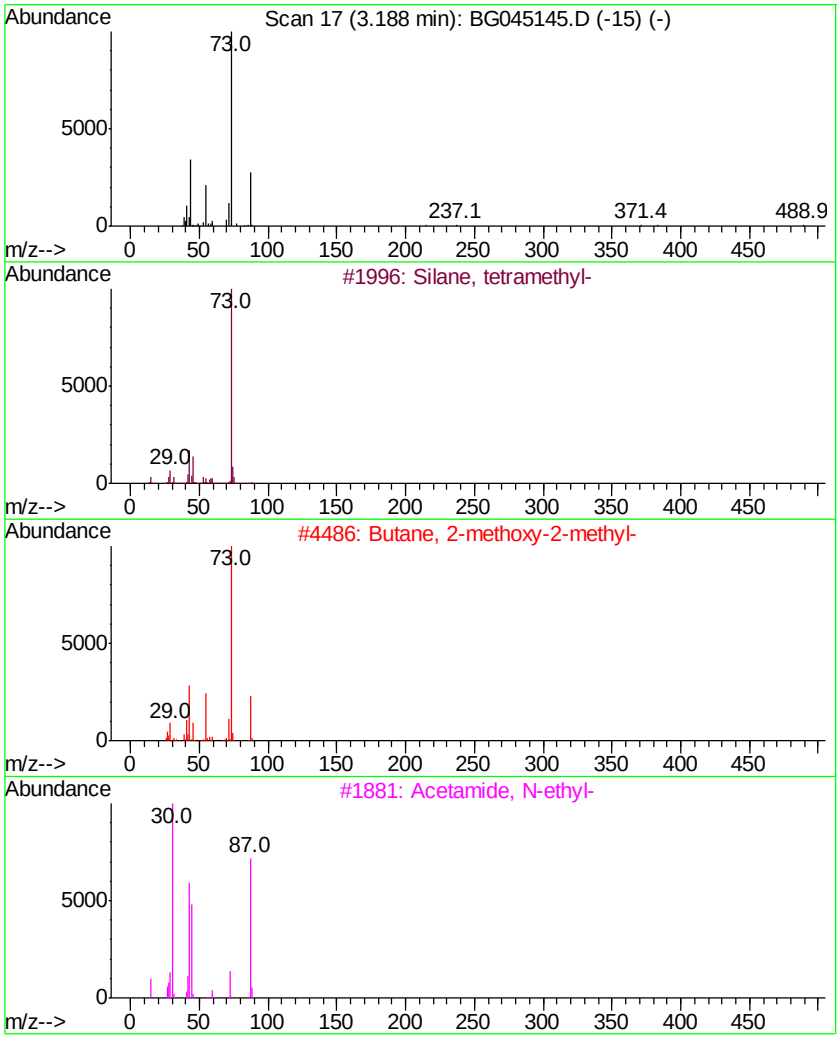
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

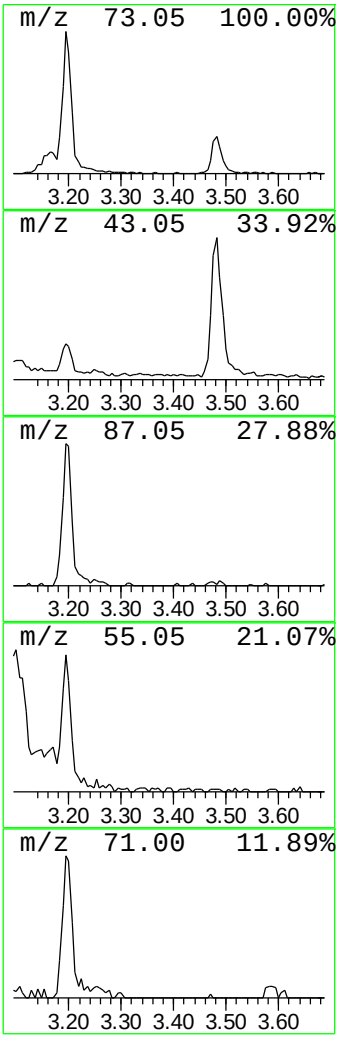
**********

Peak Number 1 unknown3.19 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.19 | 6.48 ng | 141197 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 10 |
| 2 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 9 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 4 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 4 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 4 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

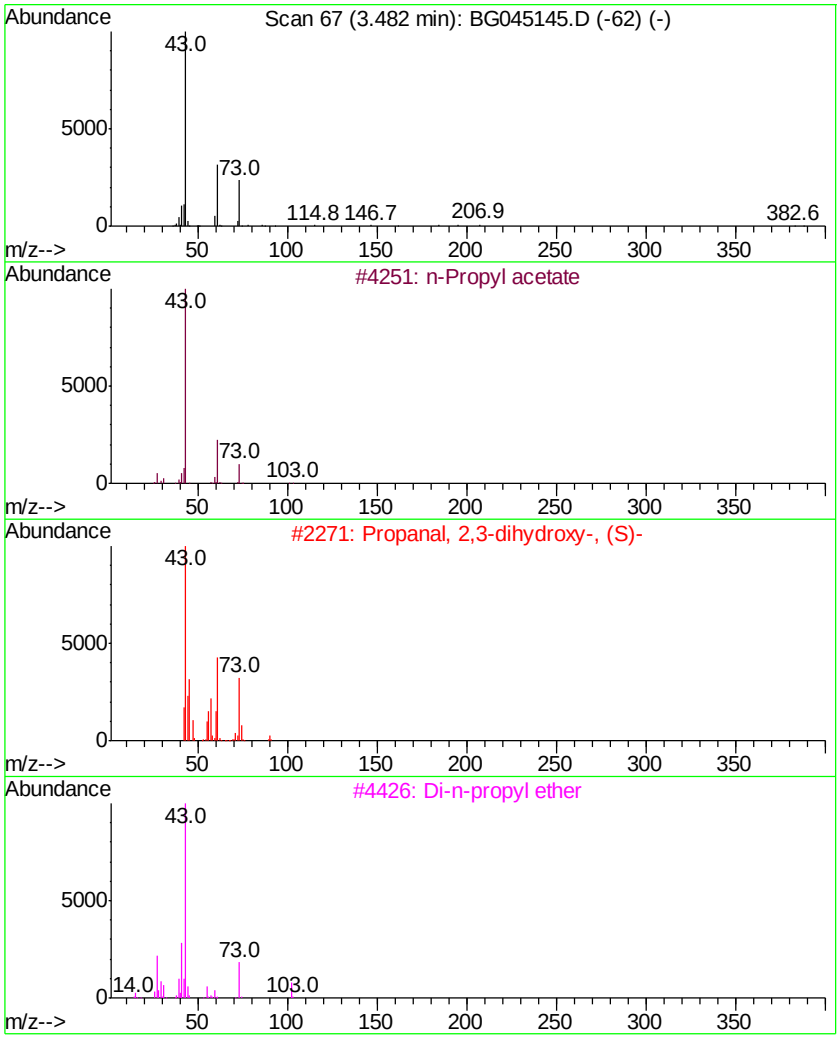
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

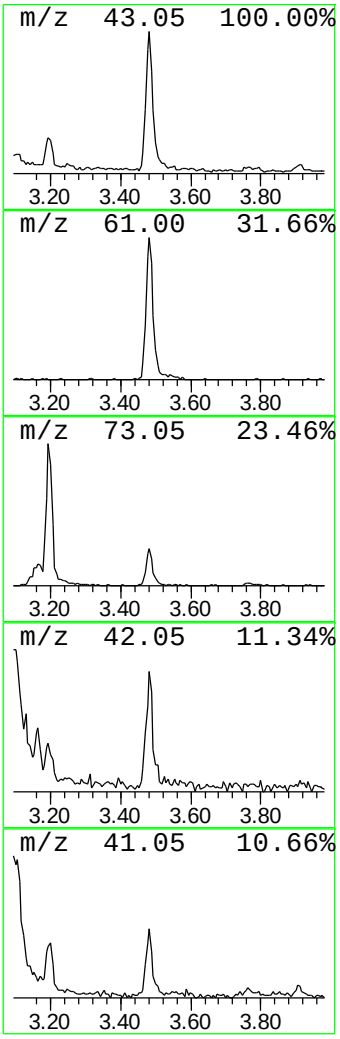
**********

Peak Number 2 n-Propyl acetate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.48 | 6.99 ng | 152306 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Propyl acetate | 102 | C5H10O2 | 000109-60-4 | 72 |
| 2 | Propanal, 2,3-dihydroxy-, (S)- | 90 | C3H6O3 | 000497-09-6 | 39 |
| 3 | Di-n-propyl ether | 102 | C6H14O | 000111-43-3 | 9 |
| 4 | Propanoic acid, 2-methyl- | 88 | C4H8O2 | 000079-31-2 | 9 |
| 5 | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

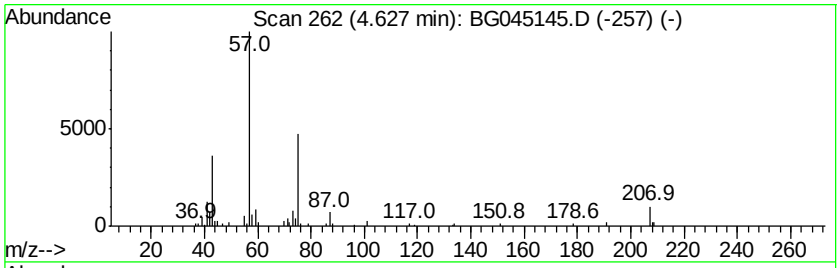
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

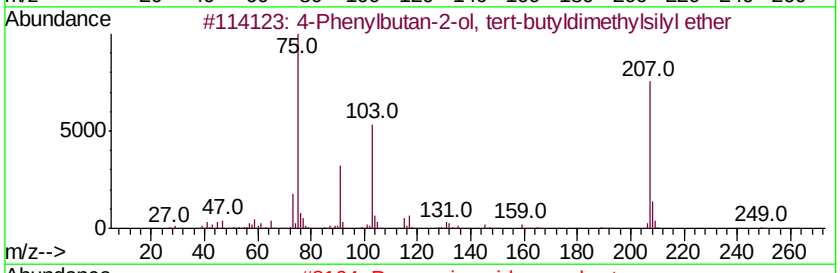
**********

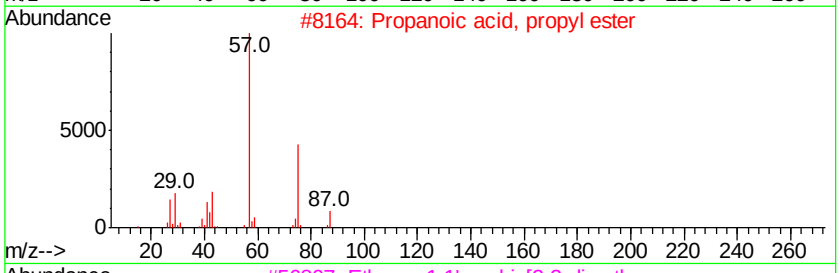
Peak Number 3 4-Phenylbutan-2-ol, tert-bu... Concentration Rank 4

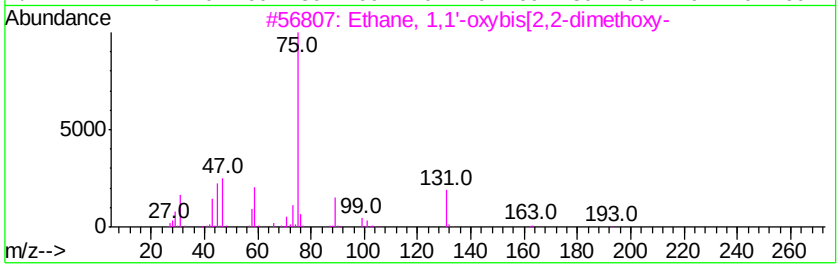
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.63 | 5.14 ng | 112036 | 1,4-Dichlorobenzene-d4 | 8.01 |

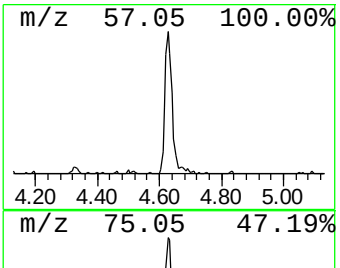
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Phenylbutan-2-ol, tert-butyldi... | 264 | C16H28OSi | 1000373-40-0 | 50 |
| 2 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 43 |
| 3 | Ethane, 1,1'-oxybis[2,2-dimethoxy- | 194 | C8H18O5 | 078082-46-9 | 12 |
| 4 | 2,2-Dimethyl-1-dimethyl(isopropy... | 188 | C10H24OSi | 1000278-74-3 | 12 |
| 5 | exo-Norbornanol, allyldimethylsi... | 210 | C12H22OSi | 1000245-87-6 | 12 |

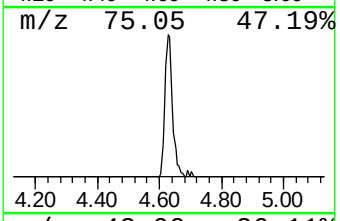


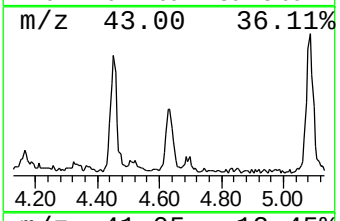



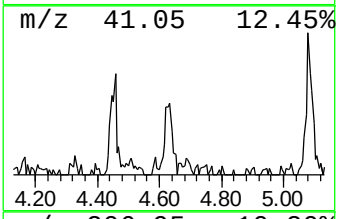



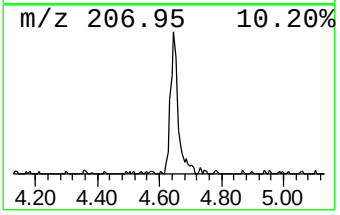



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

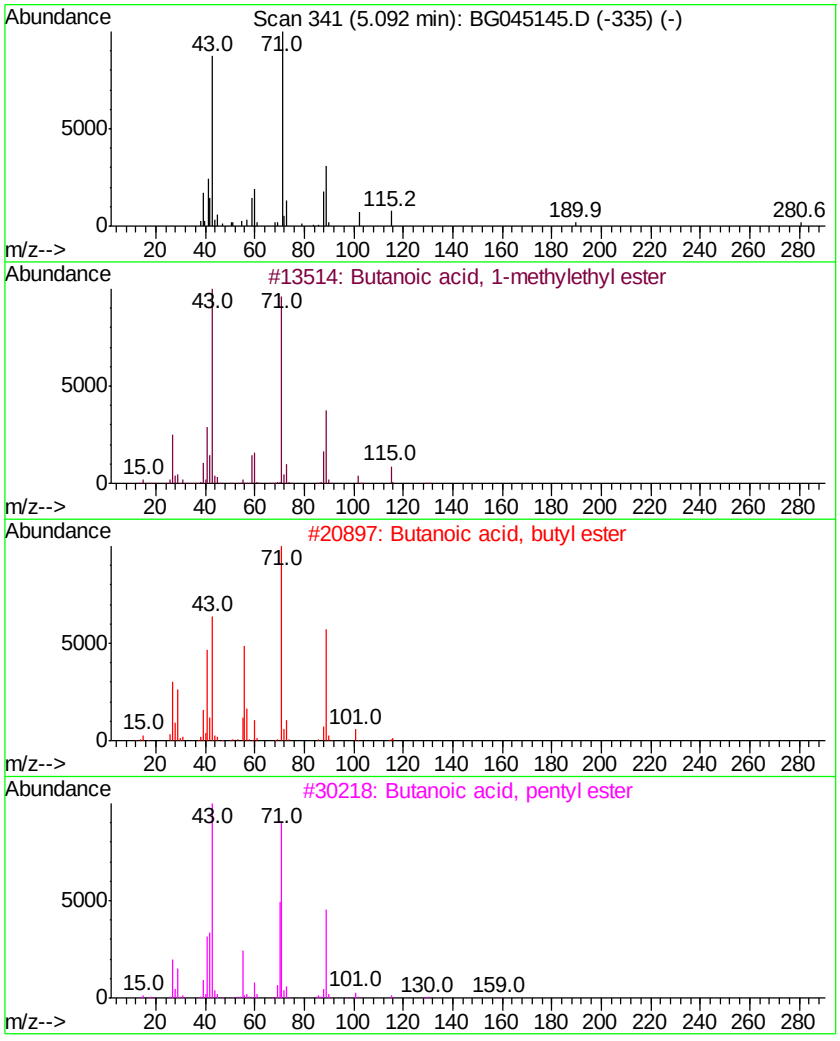
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

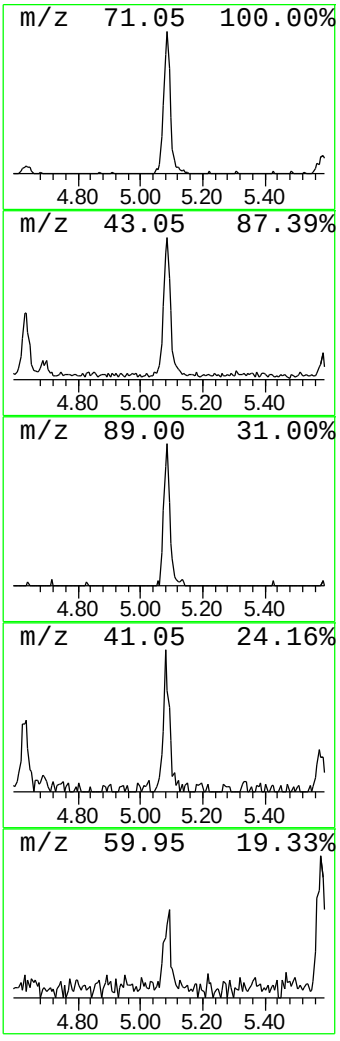
**********

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 3.67 ng | 79932 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, 1-methylethyl ester | 130 | C7H14O2 | 000638-11-9 | 78 |
| 2 | Butanoic acid, butyl ester | 144 | C8H16O2 | 000109-21-7 | 72 |
| 3 | Butanoic acid, pentyl ester | 158 | C9H18O2 | 000540-18-1 | 72 |
| 4 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 64 |
| 5 | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

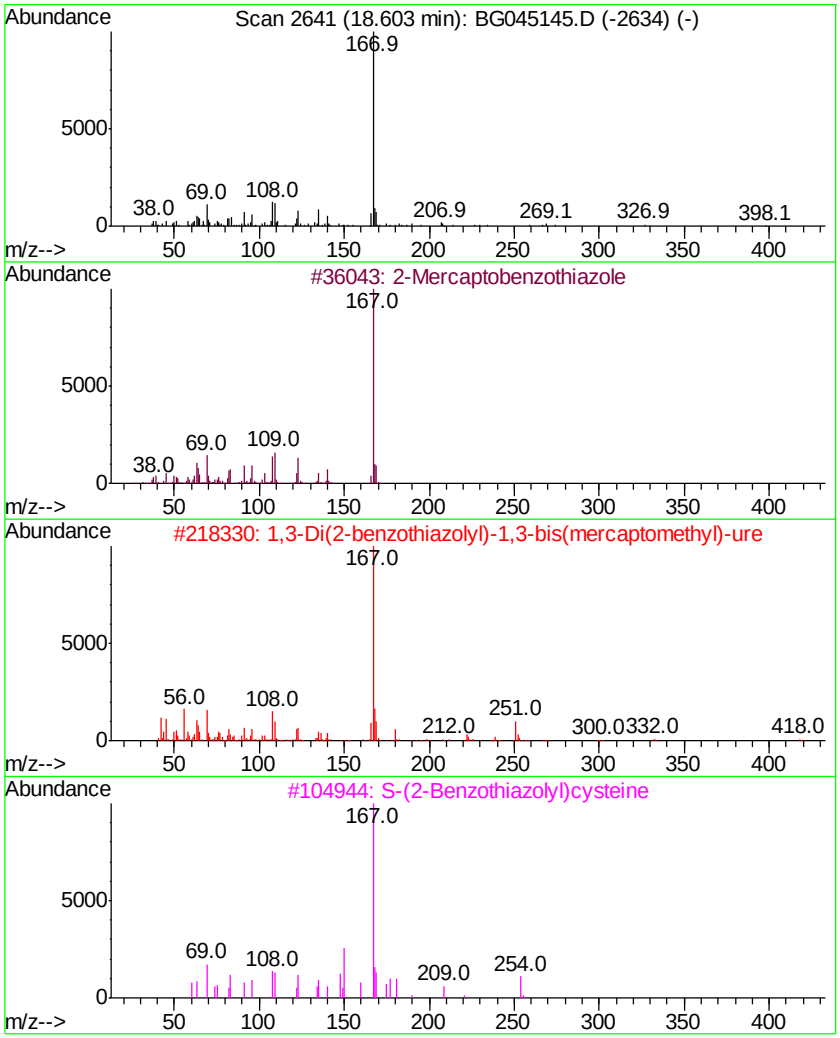
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

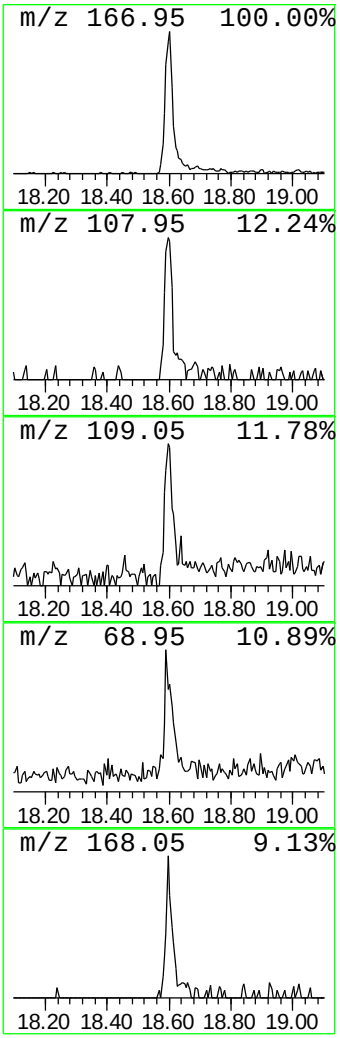
**********

Peak Number 6 2-Mercaptobenzothiazole Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.60 | 2.64 ng | 155795 | Phenanthrene-d10 | 17.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Mercaptobenzothiazole | 167 | C7H5NS2 | 000149-30-4 | 95 |
| 2 | 1,3-Di(2-benzothiazolyl)-1,3-bis... | 418 | C17H14N4OS4 | 064216-20-2 | 87 |
| 3 | S-(2-Benzothiazolyl)cysteine | 254 | C10H10N2O2S2 | 000399-82-6 | 74 |
| 4 | Benzothiazole, 2-(2-hydroxyethyl... | 211 | C9H9NOS2 | 004665-63-8 | 72 |
| 5 | Mandelic acid, 3,4-dimethoxy-, m... | 226 | C11H14O5 | 002911-73-1 | 56 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

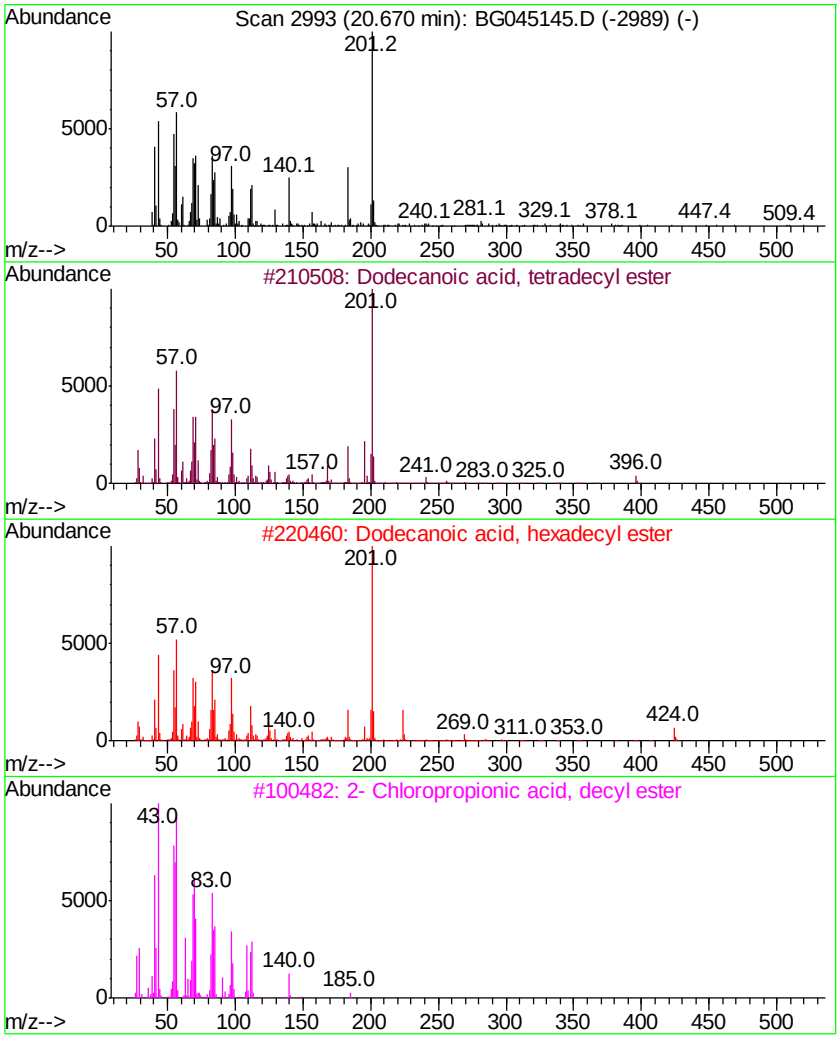
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

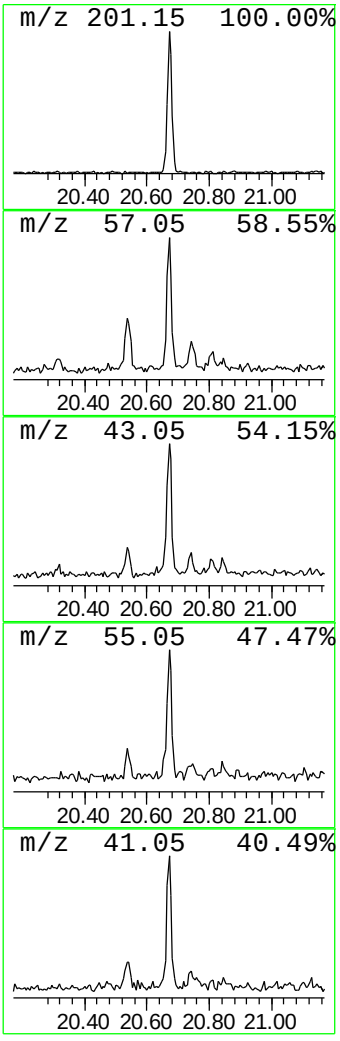
**********

Peak Number 7 Dodecanoic acid, tetradecyl... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.67 | 4.89 ng | 291158 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid, tetradecyl ester | 396 | C26H52O2 | 022412-97-1 | 64 |
| 2 | Dodecanoic acid, hexadecyl ester | 424 | C28H56O2 | 020834-06-4 | 40 |
| 3 | 2- Chloropropionic acid, decyl e... | 248 | C13H25ClO2 | 086711-78-6 | 35 |
| 4 | Dodecanoic acid, undecyl ester | 354 | C23H46O2 | 003658-44-4 | 32 |
| 5 | Dodecane, 1,1'-thiobis- | 370 | C24H50S | 002469-45-6 | 25 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042320\
Data File : BG045145.D
Acq On : 23 Apr 2020 17:10
Operator : CG/JU
Sample : L2350-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.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 |
| unknown3.19 | 3.19 | 6.5 | ng | 141197 | 1 | 8.01 | 435781 | 20.0 |
| n-Propyl acetate | 3.48 | 7.0 | ng | 152306 | 1 | 8.01 | 435781 | 20.0 |
| 4-Phenylbutan-2-o... | 4.63 | 5.1 | ng | 112036 | 1 | 8.01 | 435781 | 20.0 |
| Butanoic acid, 1-... | 5.09 | 3.7 | ng | 79932 | 1 | 8.01 | 435781 | 20.0 |
| 2-Mercaptobenzoth... | 18.60 | 2.6 | ng | 155795 | 4 | 17.39 | 1182480 | 20.0 |
| Dodecanoic acid, ... | 20.67 | 4.9 | ng | 291158 | 5 | 21.65 | 1190890 | 20.0 |