LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

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-BG092519.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 | 3.179 | 10 | 15 | 24 | rBV | 111230 | 236628 | 6.06% | 1.048% |
| 2 | 3.255 | 24 | 28 | 39 | rVB | 69291 | 108087 | 2.77% | 0.479% |
| 3 | 5.652 | 429 | 436 | 449 | rBV | 843006 | 1379839 | 35.34% | 6.109% |
| 4 | 7.239 | 697 | 706 | 721 | rBV | 913264 | 1634824 | 41.87% | 7.238% |
| 5 | 7.609 | 759 | 769 | 781 | rBV | 865796 | 1534055 | 39.28% | 6.791% |
| 6 | 8.067 | 841 | 847 | 855 | rBV | 253121 | 456094 | 11.68% | 2.019% |
| 7 | 8.396 | 895 | 903 | 913 | rVB | 648909 | 1175027 | 30.09% | 5.202% |
| 8 | 9.230 | 1036 | 1045 | 1054 | rBV | 503694 | 947496 | 24.26% | 4.195% |
| 9 | 10.876 | 1316 | 1325 | 1335 | rBV | 334877 | 632403 | 16.19% | 2.800% |
| 10 | 13.314 | 1732 | 1740 | 1751 | rBV | 1532387 | 2372007 | 60.74% | 10.501% |
| 11 | 13.584 | 1780 | 1786 | 1792 | rVB | 30288 | 46131 | 1.18% | 0.204% |
| 12 | 14.136 | 1874 | 1880 | 1887 | rBV | 246890 | 369571 | 9.46% | 1.636% |
| 13 | 14.689 | 1967 | 1974 | 1982 | rBV2 | 577719 | 939172 | 24.05% | 4.158% |
| 14 | 16.175 | 2219 | 2227 | 2237 | rBV | 1320645 | 2067249 | 52.94% | 9.152% |
| 15 | 17.433 | 2433 | 2441 | 2451 | rBV2 | 759261 | 1196276 | 30.63% | 5.296% |
| 16 | 18.320 | 2586 | 2592 | 2600 | rBV2 | 91436 | 145909 | 3.74% | 0.646% |
| 17 | 19.183 | 2734 | 2739 | 2745 | rBV8 | 25148 | 66231 | 1.70% | 0.293% |
| 18 | 20.041 | 2879 | 2885 | 2894 | rBV | 2886193 | 3904986 | 100.00% | 17.288% |
| 19 | 21.352 | 3103 | 3108 | 3119 | rBV3 | 113782 | 275915 | 7.07% | 1.222% |
| 20 | 21.698 | 3160 | 3167 | 3175 | rBV2 | 810027 | 1441949 | 36.93% | 6.384% |
| 21 | 22.509 | 3302 | 3305 | 3309 | rBV5 | 28614 | 41439 | 1.06% | 0.183% |
| 22 | 24.019 | 3557 | 3562 | 3569 | rBV6 | 37529 | 89641 | 2.30% | 0.397% |
| 23 | 24.924 | 3707 | 3716 | 3731 | rVB3 | 503631 | 1527140 | 39.11% | 6.761% |

Sum of corrected areas: 22588069

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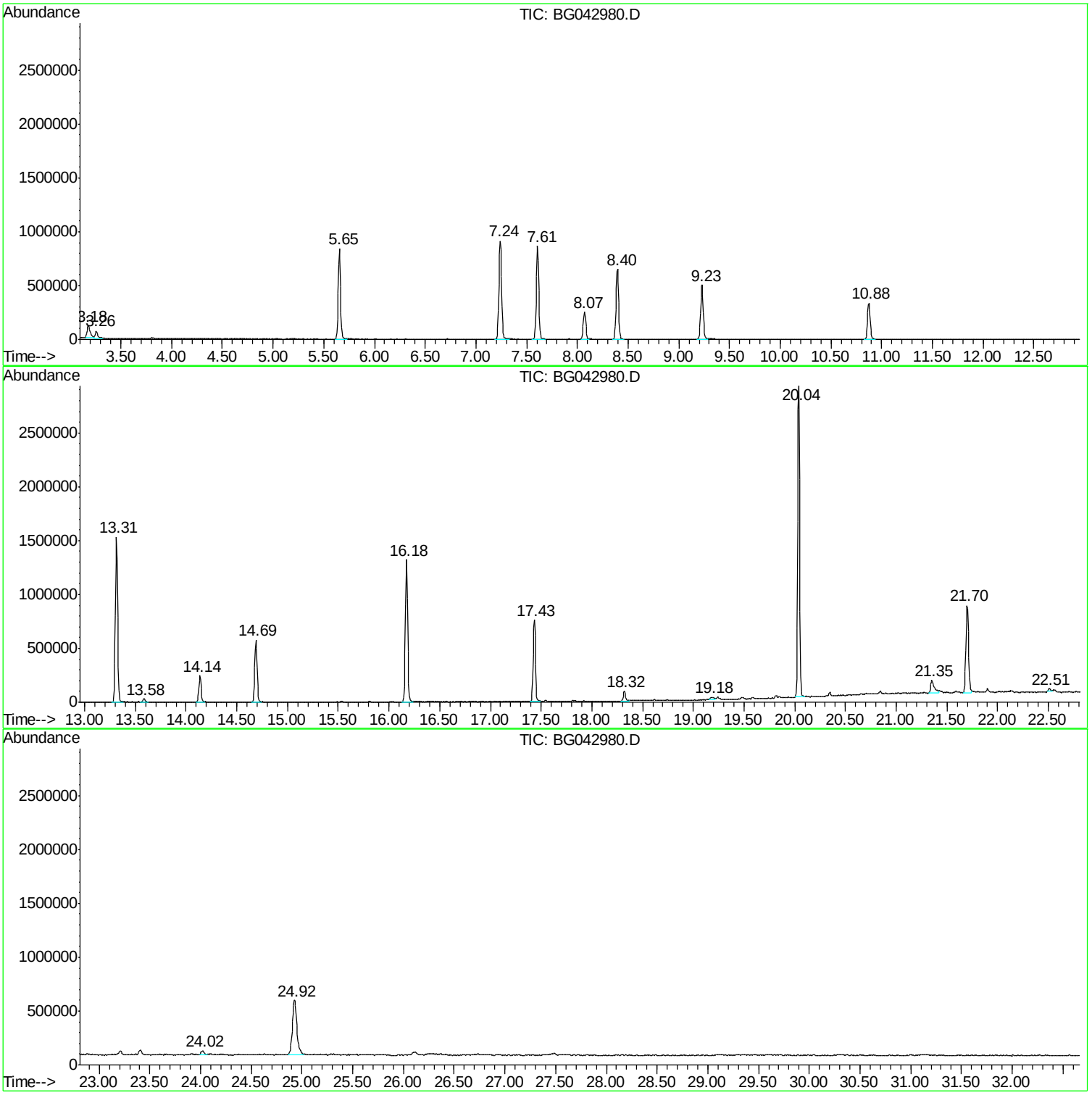
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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\BG100119\
Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

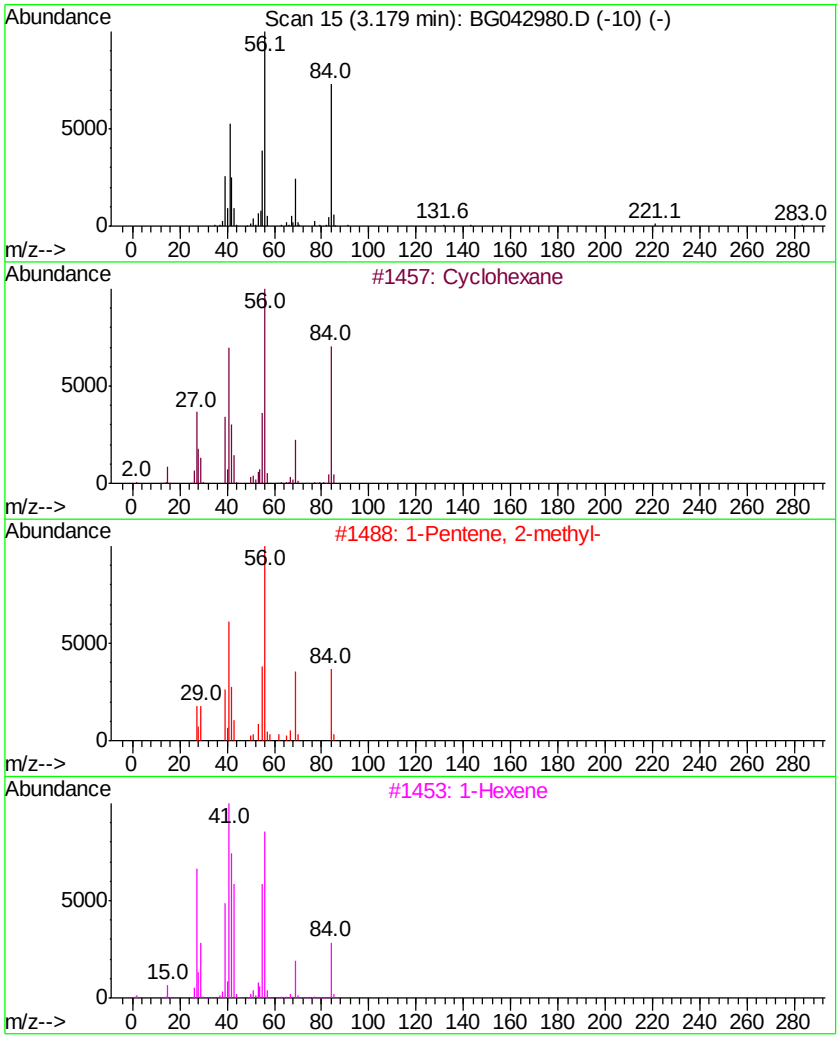
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

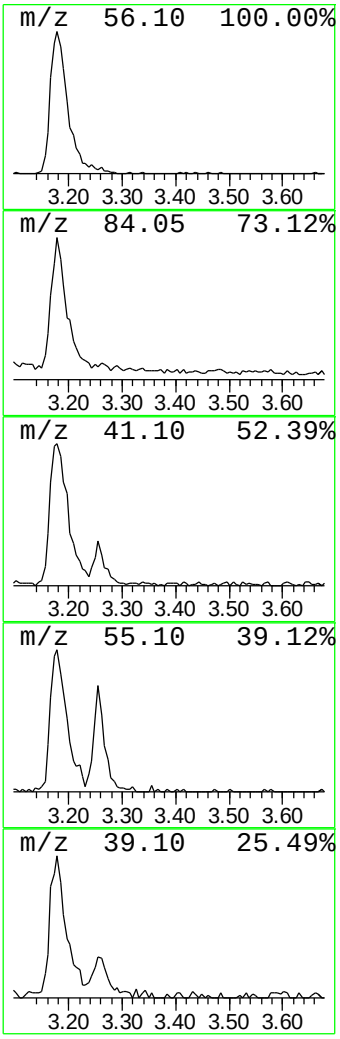
**********

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.18 | 10.38 ng | 236628 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane | 84 | C6H12 | 000110-82-7 | 91 |
| 2 | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 86 |
| 3 | 1-Hexene | 84 | C6H12 | 000592-41-6 | 59 |
| 4 | Cyclopentanone, 2-ethyl- | 112 | C7H12O | 004971-18-0 | 50 |
| 5 | 2-Pentene, 2-methyl- | 84 | C6H12 | 000625-27-4 | 47 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

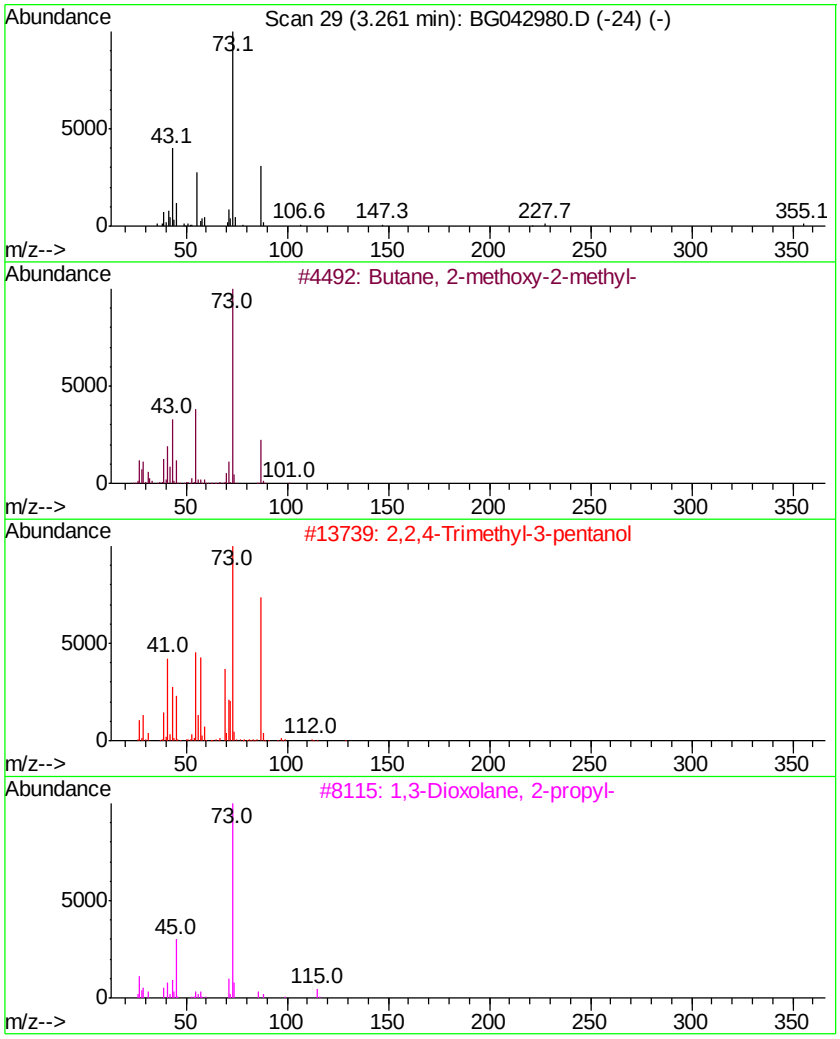
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

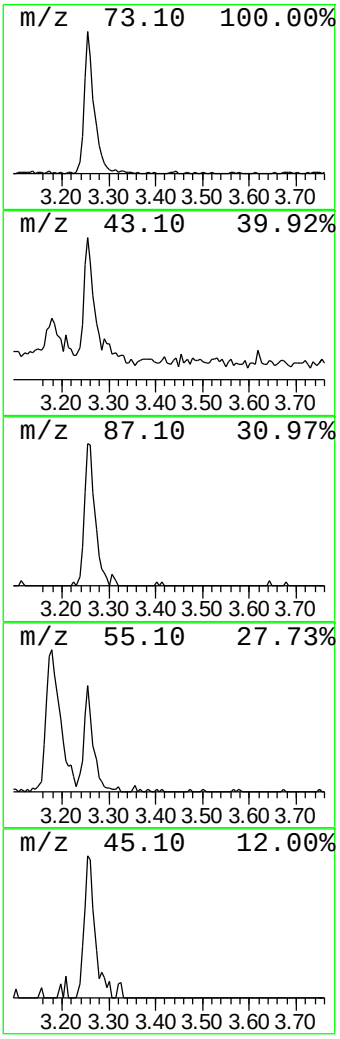
**********

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.26 | 4.74 ng | 108087 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | 1,3-Dioxolane, 2-propyl- | 116 | C6H12O2 | 003390-13-4 | 33 |
| 4 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 25 |
| 5 | 2,5-Dimethyl-4-hydroxy-3-hexanone | 144 | C8H16O2 | 000815-77-0 | 23 |



# Library Search Compound Report

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Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

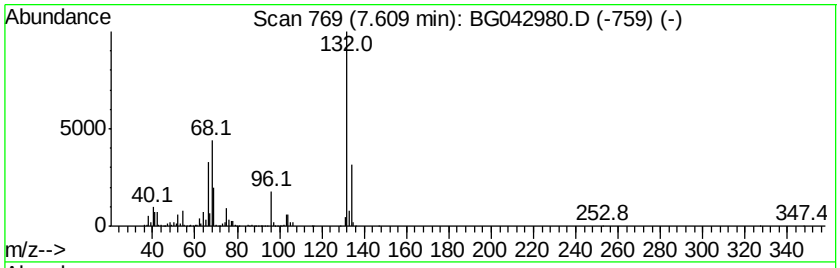
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

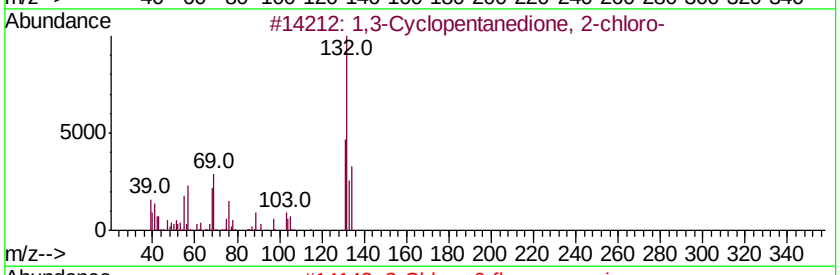
**********

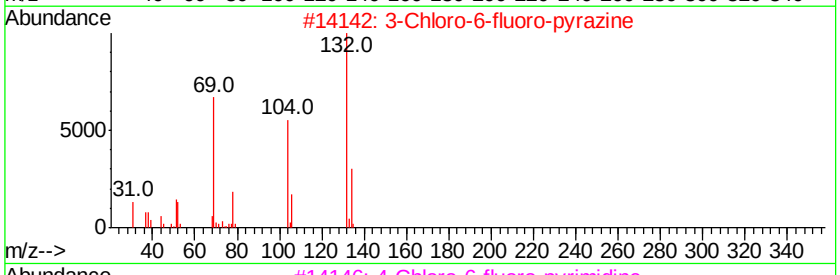
Peak Number 3 unknown7.61 Concentration Rank 1

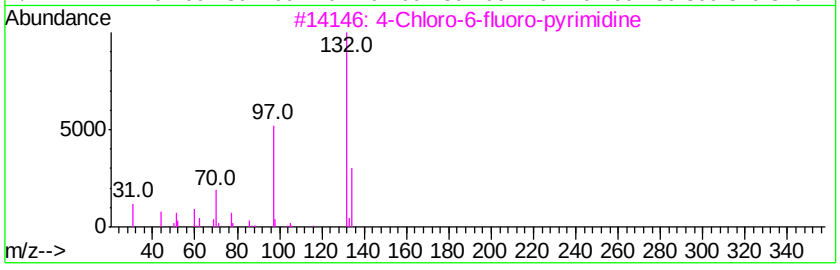
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.61 | 67.27 ng | 1534060 | 1,4-Dichlorobenzene-d4 | 8.07 |

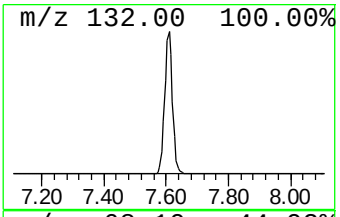
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 35 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 12 |

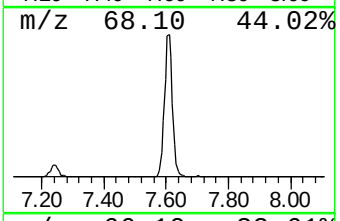


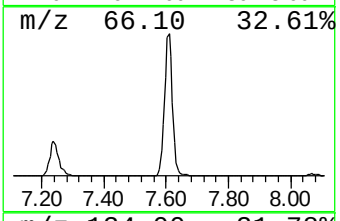



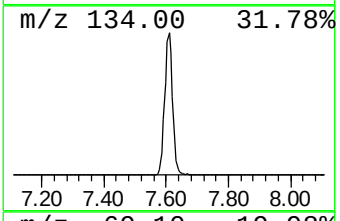



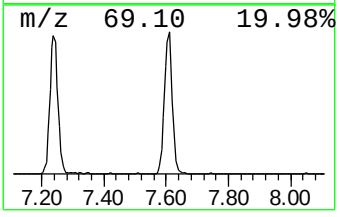



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ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

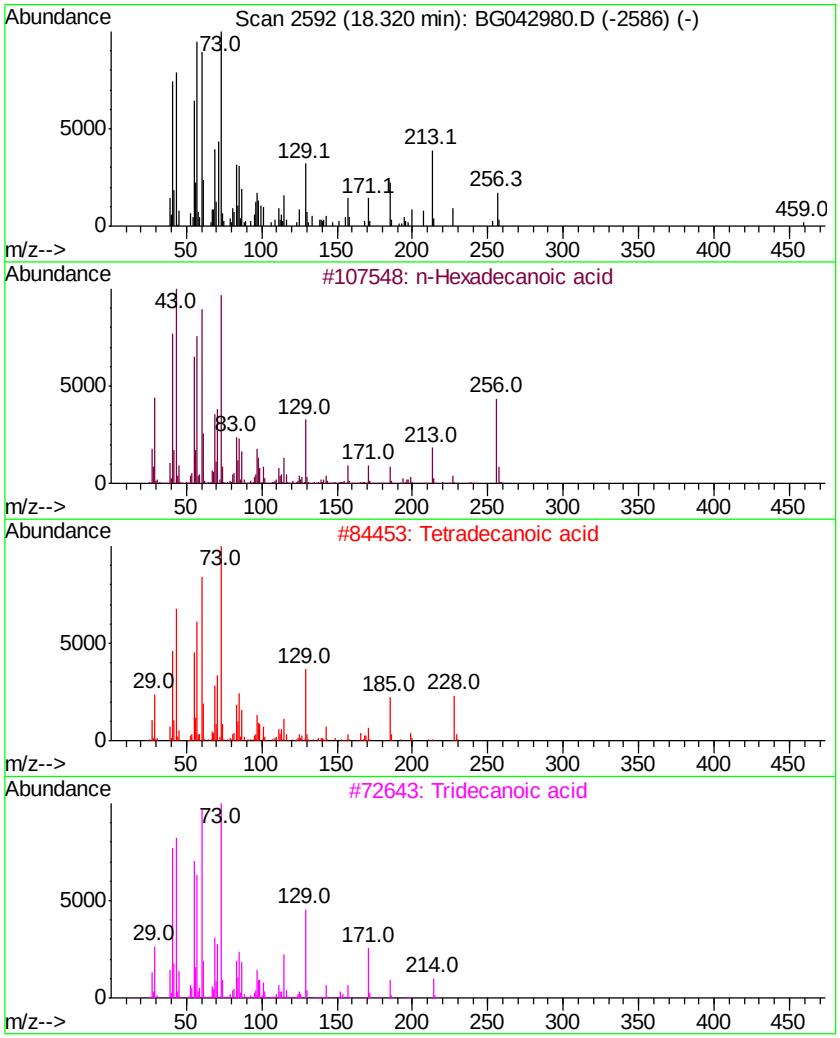
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

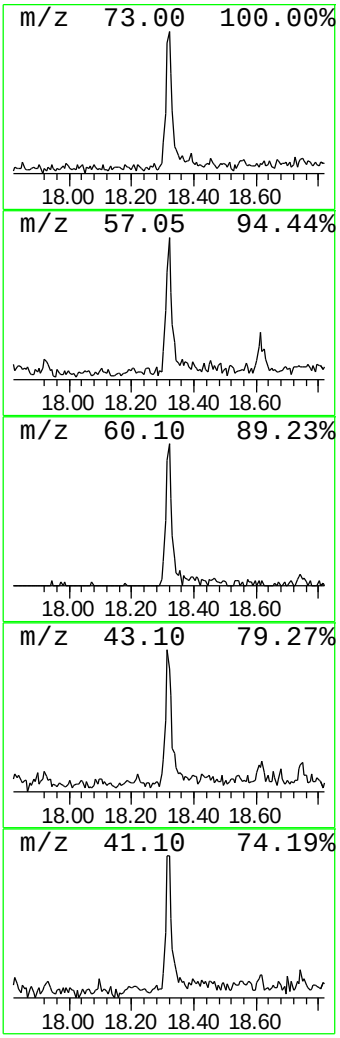
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.32 | 2.44 ng | 145909 | Phenanthrene-d10 | 17.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 64 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 62 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

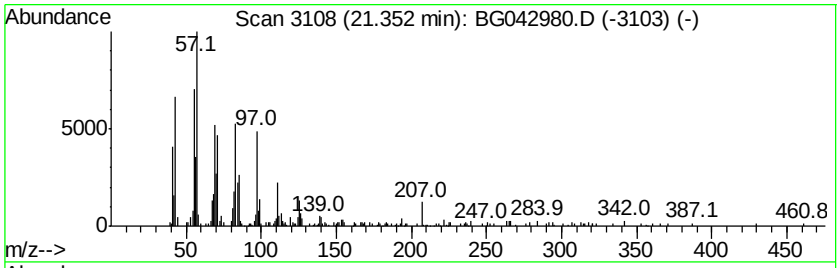
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

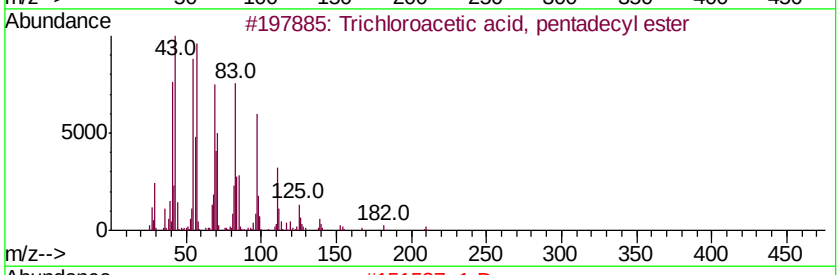
**********

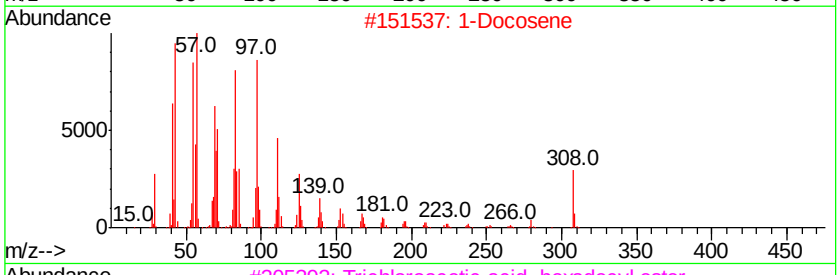
Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

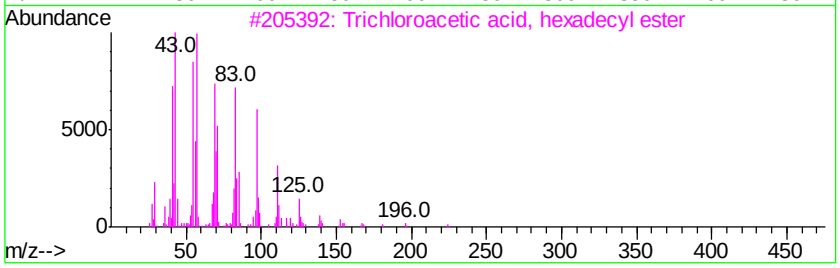
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.35 | 3.83 ng | 275915 | Chrysene-d12 | 21.70 |

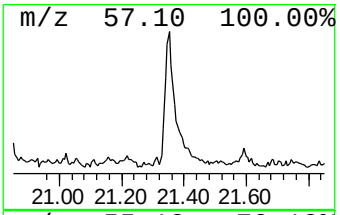
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 93 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 4 | 10-Heneicosene (c,t) | 294 | C21H42 | 095008-11-0 | 89 |
| 5 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 87 |

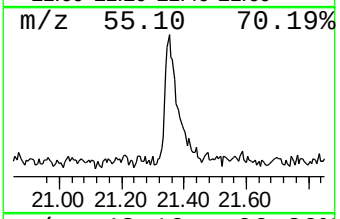


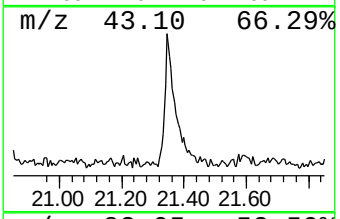



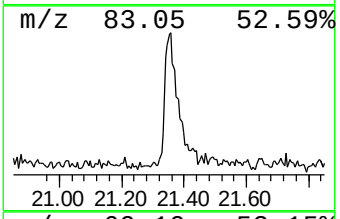



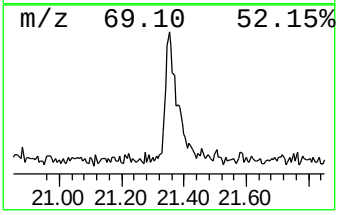



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100119\
Data File : BG042980.D
Acq On : 1 Oct 2019 23:29
Operator : JU
Sample : K4946-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GP-1_(10-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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 |
| 1-Pentene, 2-methyl- | 3.18 | 10.4 | ng | 236628 | 1 | 8.07 | 456094 | 20.0 |
| Butane, 2-methoxy... | 3.26 | 4.7 | ng | 108087 | 1 | 8.07 | 456094 | 20.0 |
| unknown7.61 | 7.61 | 67.3 | ng | 1534060 | 1 | 8.07 | 456094 | 20.0 |
| n-Hexadecanoic acid | 18.32 | 2.4 | ng | 145909 | 4 | 17.43 | 1196280 | 20.0 |
| Trichloroacetic a... | 21.35 | 3.8 | ng | 275915 | 5 | 21.70 | 1441950 | 20.0 |