LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

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-BG102119.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 | 13 | 18 | 30 | rVB | 133959 | 205795 | 10.33% | 1.533% |
| 2 | 5.614 | 423 | 430 | 444 | rBV | 459781 | 844485 | 42.40% | 6.289% |
| 3 | 7.212 | 694 | 702 | 718 | rBV | 534425 | 1057516 | 53.10% | 7.875% |
| 4 | 7.565 | 754 | 762 | 775 | rBV | 564348 | 983040 | 49.36% | 7.321% |
| 5 | 8.023 | 833 | 840 | 847 | rBV | 150781 | 262582 | 13.18% | 1.955% |
| 6 | 8.346 | 887 | 895 | 904 | rBV | 370573 | 665327 | 33.41% | 4.955% |
| 7 | 9.187 | 1028 | 1038 | 1051 | rBV | 300955 | 629172 | 31.59% | 4.685% |
| 8 | 10.832 | 1310 | 1318 | 1329 | rBV | 172462 | 350784 | 17.61% | 2.612% |
| 9 | 13.276 | 1724 | 1734 | 1749 | rBV | 764573 | 1340264 | 67.29% | 9.981% |
| 10 | 14.099 | 1868 | 1874 | 1880 | rBV | 84675 | 142051 | 7.13% | 1.058% |
| 11 | 14.651 | 1960 | 1968 | 1982 | rBV2 | 334071 | 549539 | 27.59% | 4.092% |
| 12 | 16.137 | 2215 | 2221 | 2240 | rBV | 758137 | 1352135 | 67.89% | 10.069% |
| 13 | 17.395 | 2426 | 2435 | 2450 | rBV2 | 377963 | 676244 | 33.95% | 5.036% |
| 14 | 17.512 | 2450 | 2455 | 2460 | rVB4 | 17872 | 28910 | 1.45% | 0.215% |
| 15 | 18.288 | 2582 | 2587 | 2595 | rBV2 | 43330 | 83965 | 4.22% | 0.625% |
| 16 | 20.003 | 2872 | 2879 | 2890 | rBV | 1404233 | 1991654 | 100.00% | 14.832% |
| 17 | 20.802 | 3009 | 3015 | 3019 | rBV4 | 15831 | 23690 | 1.19% | 0.176% |
| 18 | 21.308 | 3097 | 3101 | 3106 | rBV6 | 26206 | 49152 | 2.47% | 0.366% |
| 19 | 21.660 | 3154 | 3161 | 3175 | rBV | 445119 | 821035 | 41.22% | 6.114% |
| 20 | 21.842 | 3188 | 3192 | 3198 | rVB2 | 25569 | 41876 | 2.10% | 0.312% |
| 21 | 22.448 | 3289 | 3295 | 3300 | rBV3 | 37854 | 68339 | 3.43% | 0.509% |
| 22 | 23.129 | 3404 | 3411 | 3421 | rVB5 | 48073 | 112095 | 5.63% | 0.835% |
| 23 | 23.323 | 3439 | 3444 | 3452 | rVB | 58774 | 114381 | 5.74% | 0.852% |
| 24 | 23.922 | 3539 | 3546 | 3554 | rBV3 | 39373 | 98921 | 4.97% | 0.737% |
| 25 | 24.851 | 3695 | 3704 | 3720 | rBV2 | 292278 | 906615 | 45.52% | 6.751% |
| 26 | 25.979 | 3890 | 3896 | 3897 | rBV5 | 19924 | 28797 | 1.45% | 0.214% |

Sum of corrected areas: 13428364

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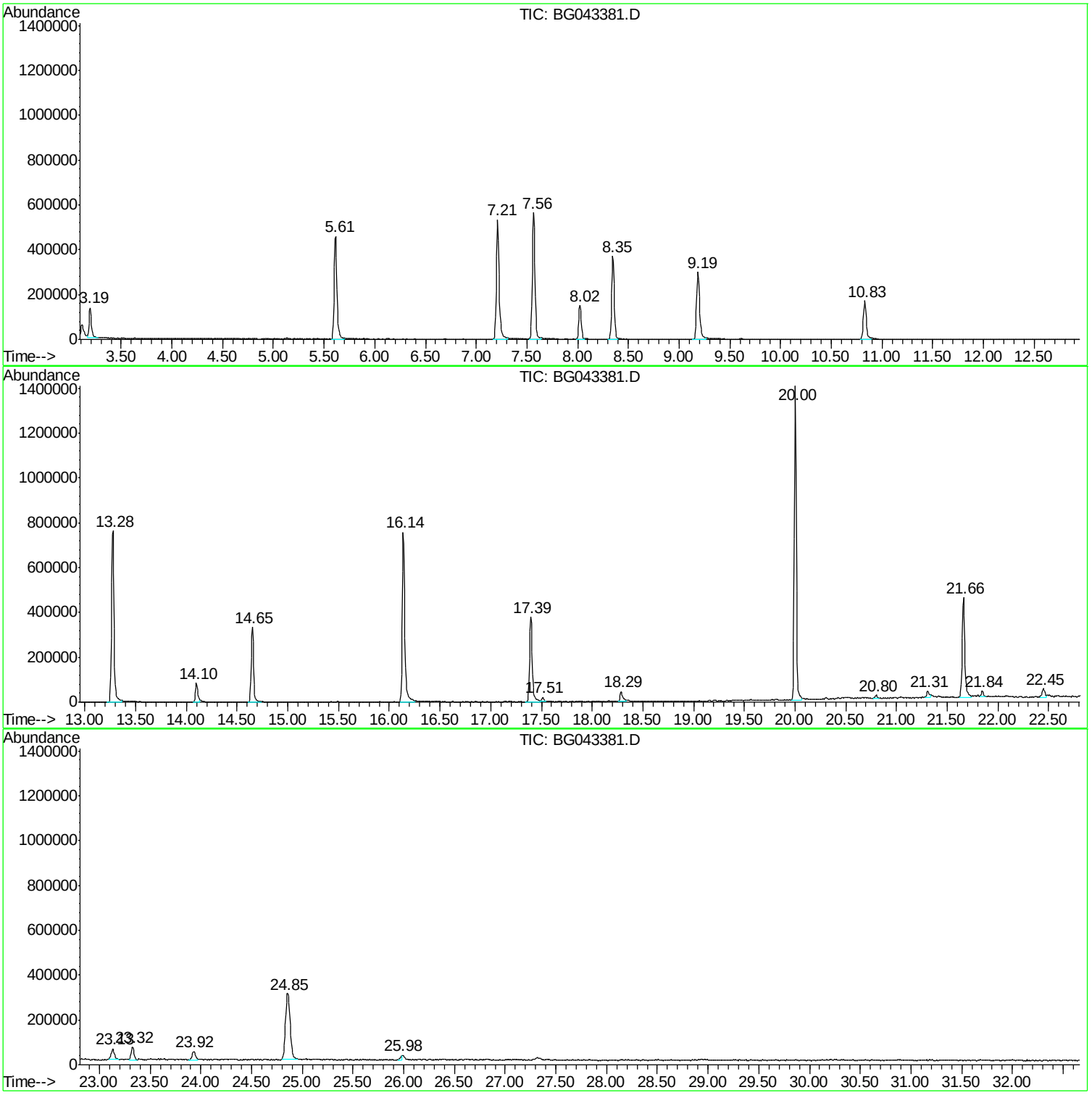
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

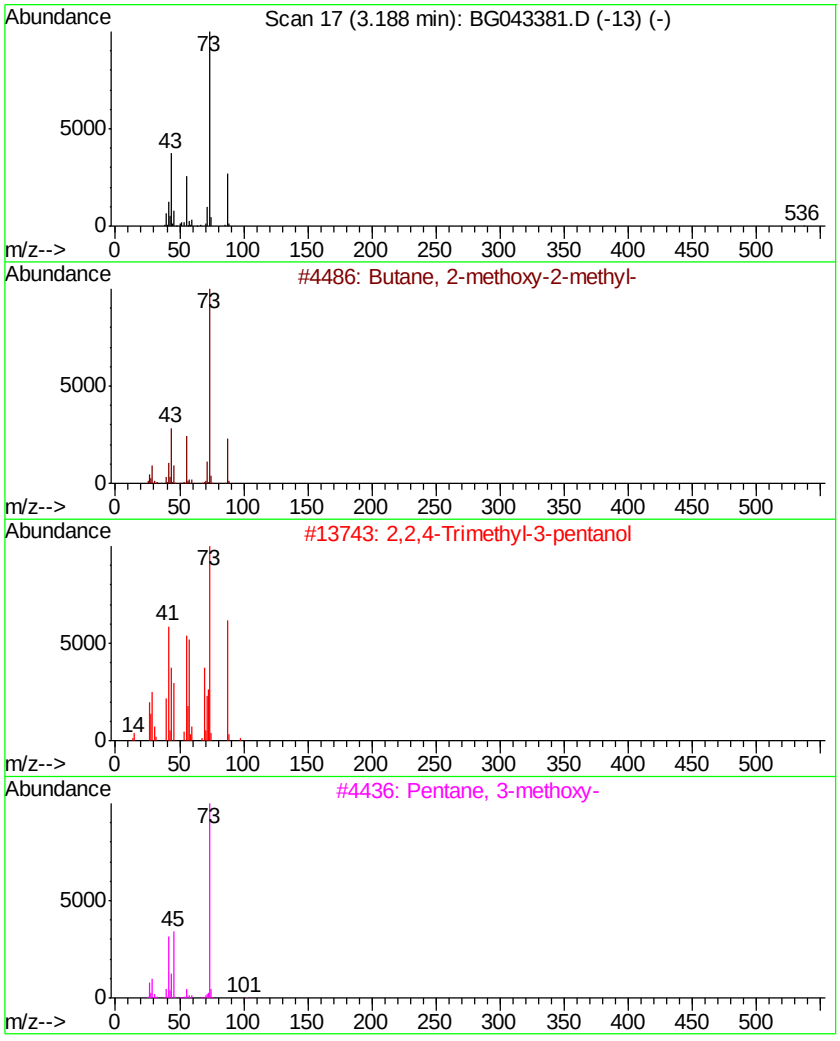
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

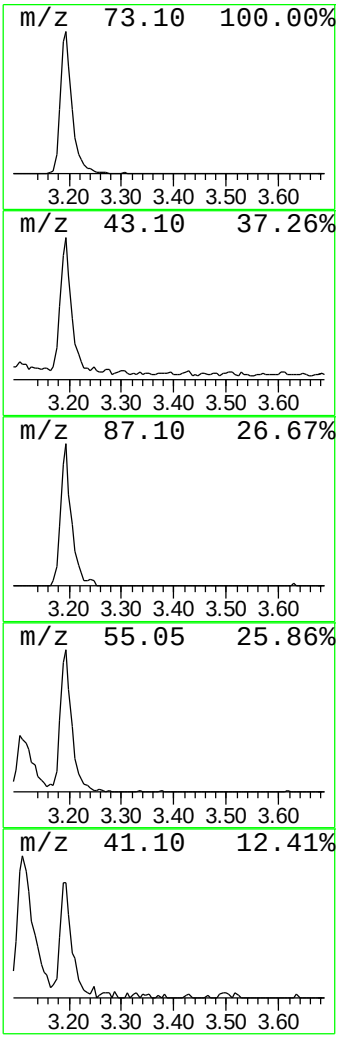
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.19 | 15.67 ng | 205795 | 1,4-Dichlorobenzene-d4 | 8.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 56 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 50 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

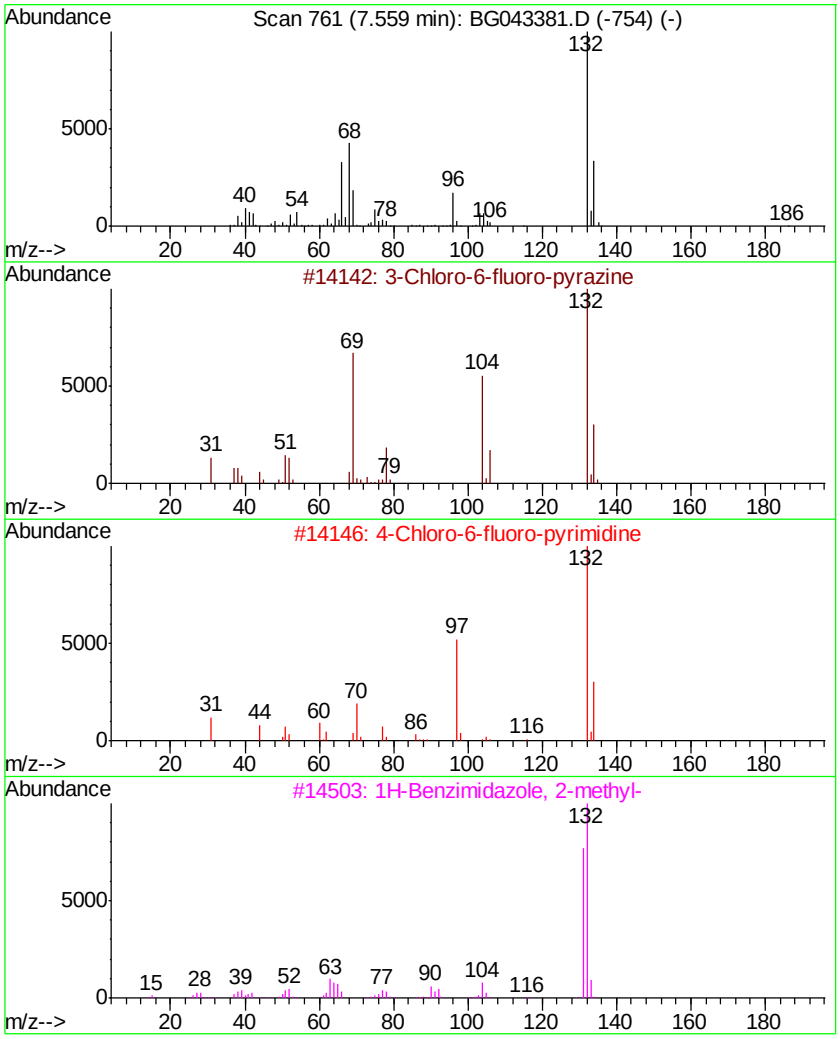
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

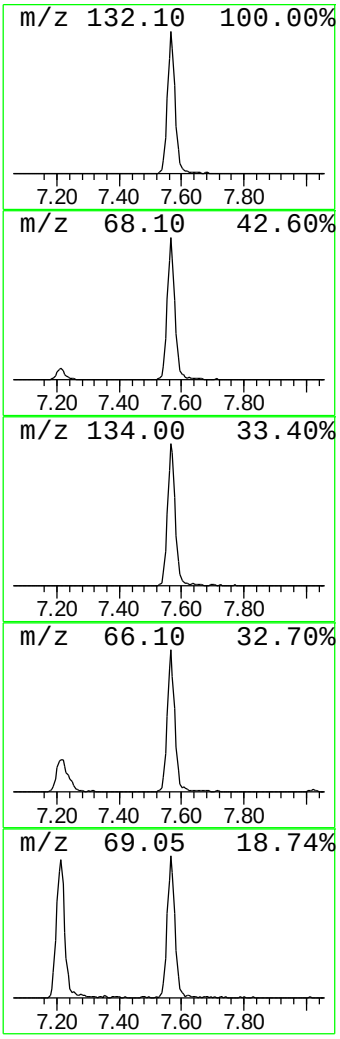
**********

Peak Number 2 unknown7.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.56 | 74.87 ng | 983040 | 1,4-Dichlorobenzene-d4 | 8.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 12 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

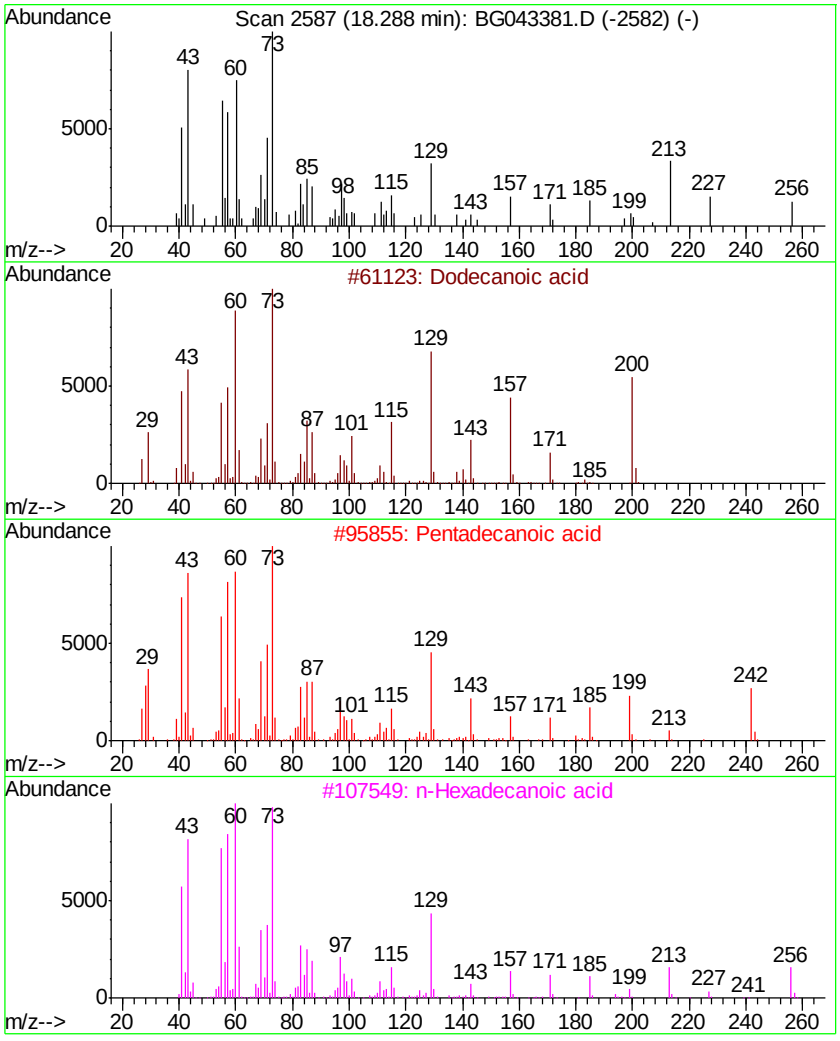
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

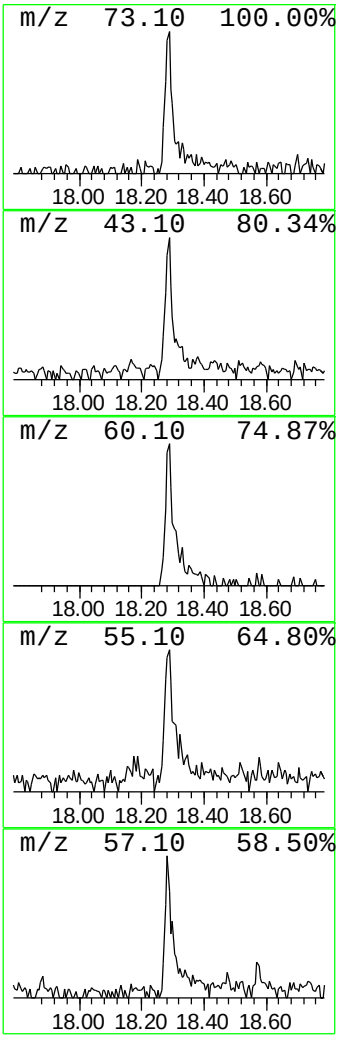
**********

Peak Number 4 Dodecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.29 | 2.48 ng | 83965 | Phenanthrene-d10 | 17.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 86 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 64 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 64 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 58 |
| 5 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 50 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

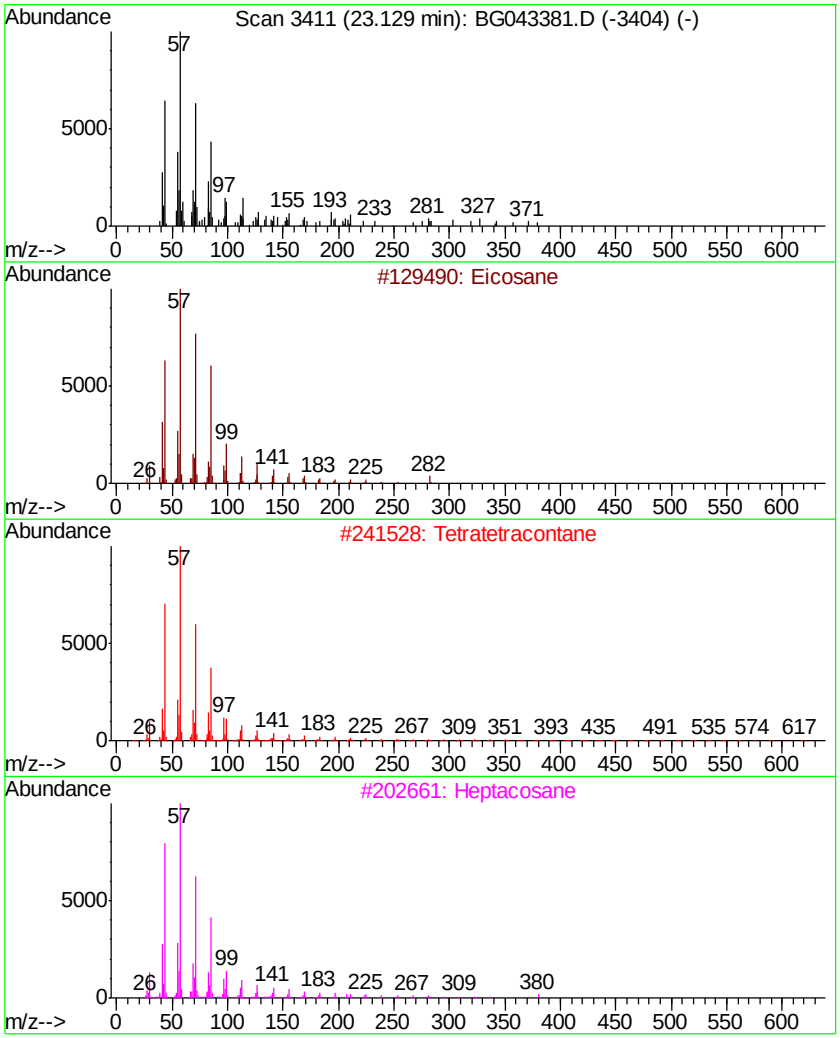
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

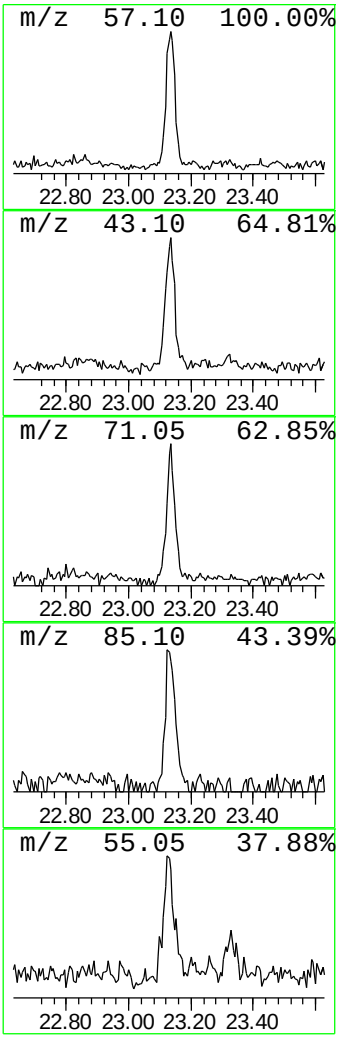
**********

Peak Number 5 Eicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.13 | 2.73 ng | 112095 | Chrysene-d12 | 21.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 76 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 74 |
| 4 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 68 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 68 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

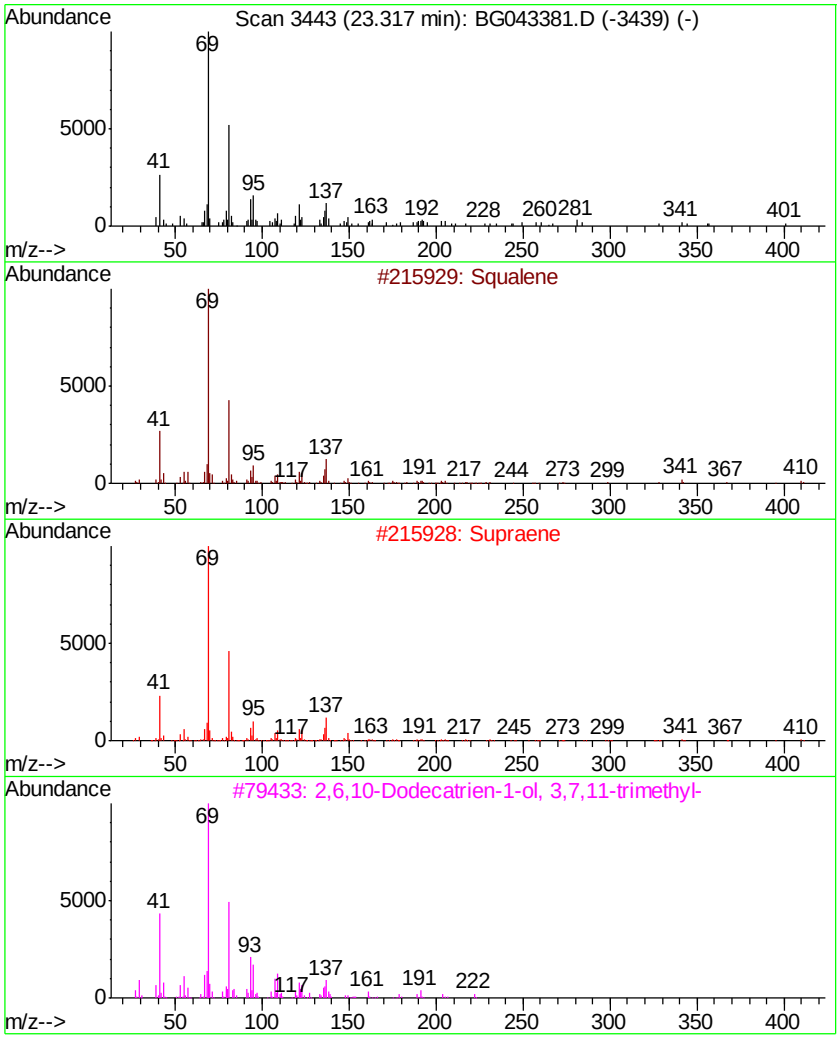
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

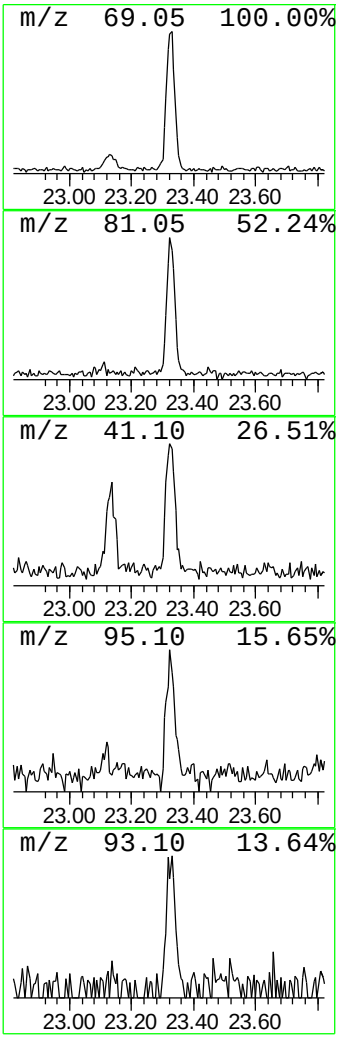
**********

Peak Number 6 Squalene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.32 | 2.52 ng | 114381 | Perylene-d12 | 24.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 64 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 64 |
| 3 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0 | 50 |
| 4 | 1,5-Heptadiene, 3,3,5-trimethyl- | 138 | C10H18 | 074630-29-8 | 49 |
| 5 | Cyclopropanecarboxylic acid, 4-i... | 204 | C13H16O2 | 1000331-01-9 | 47 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

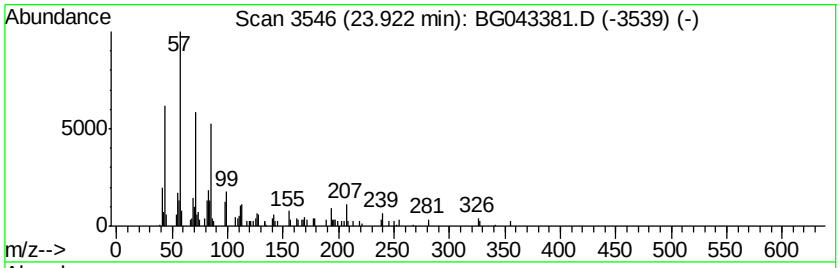
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

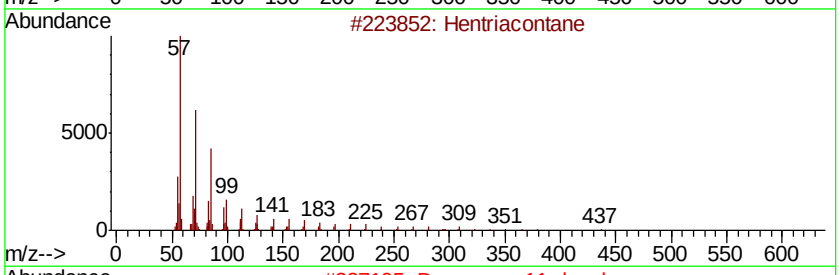
**********

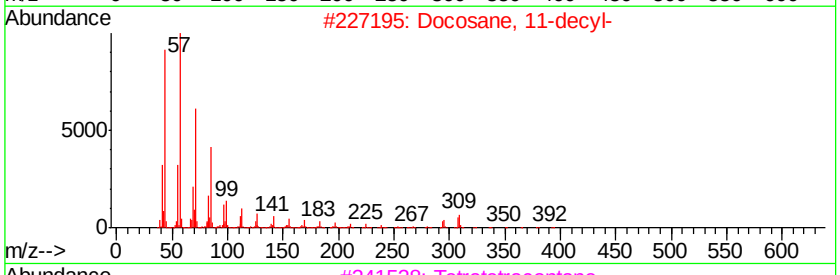
Peak Number 7 Hentriacontane Concentration Rank 7

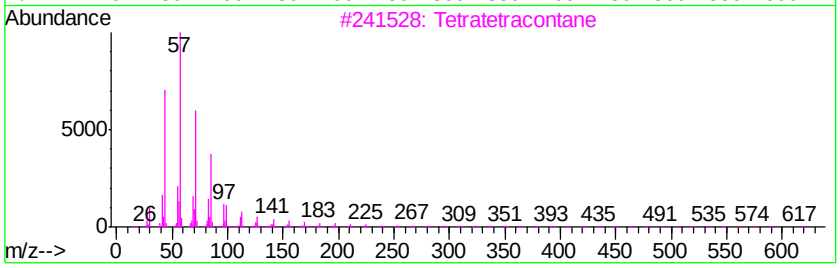
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.92 | 2.18 ng | 98921 | Perylene-d12 | 24.85 |

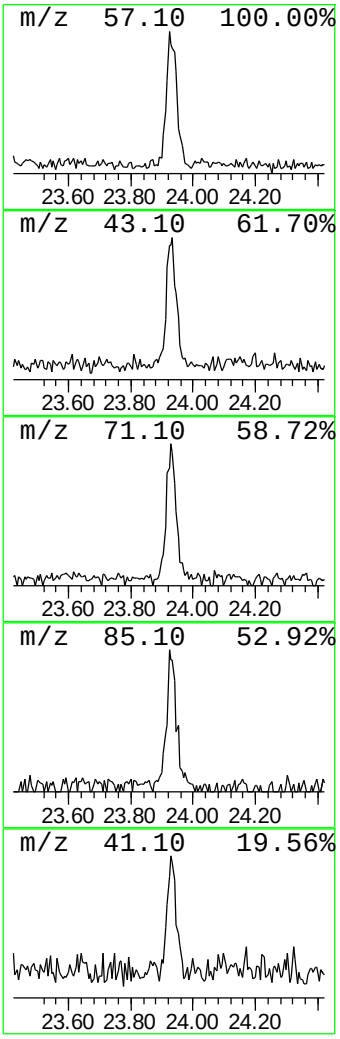
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 74 |
| 2 | Docosane, 11-decyl- | 451 | C32H66 | 055401-55-3 | 72 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 72 |
| 4 | Tetracosane, 11-decyl- | 479 | C34H70 | 055429-84-0 | 72 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102919\
Data File : BG043381.D
Acq On : 29 Oct 2019 19:36
Operator : JU
Sample : K5540-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 154-82-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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 |
| Butane, 2-methoxy... | 3.19 | 15.7 | ng | 205795 | 1 | 8.02 | 262582 | 20.0 |
| unknown7.56 | 7.56 | 74.9 | ng | 983040 | 1 | 8.02 | 262582 | 20.0 |
| Dodecanoic acid | 18.29 | 2.5 | ng | 83965 | 4 | 17.39 | 676244 | 20.0 |
| Eicosane | 23.13 | 2.7 | ng | 112095 | 5 | 21.66 | 821035 | 20.0 |
| Squalene | 23.32 | 2.5 | ng | 114381 | 6 | 24.85 | 906615 | 20.0 |
| Hentriacontane | 23.92 | 2.2 | ng | 98921 | 6 | 24.85 | 906615 | 20.0 |