LSC Area Percent Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

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-BG062619.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 | 5.568 | 416 | 422 | 436 | rBV | 380513 | 622759 | 32.19% | 6.409% |
| 2 | 7.189 | 691 | 698 | 715 | rVB | 395040 | 702269 | 36.30% | 7.228% |
| 3 | 7.559 | 754 | 761 | 772 | rBV | 386789 | 683340 | 35.33% | 7.033% |
| 4 | 8.029 | 835 | 841 | 848 | rBV | 92171 | 158516 | 8.19% | 1.631% |
| 5 | 8.352 | 889 | 896 | 905 | rBV | 308275 | 536431 | 27.73% | 5.521% |
| 6 | 9.210 | 1035 | 1042 | 1052 | rBV | 234060 | 440629 | 22.78% | 4.535% |
| 7 | 10.855 | 1315 | 1322 | 1331 | rBV | 99187 | 195304 | 10.10% | 2.010% |
| 8 | 13.294 | 1730 | 1737 | 1748 | rBV | 639082 | 955428 | 49.39% | 9.833% |
| 9 | 14.122 | 1872 | 1878 | 1886 | rBV | 58089 | 93111 | 4.81% | 0.958% |
| 10 | 14.675 | 1966 | 1972 | 1983 | rBV2 | 180075 | 285728 | 14.77% | 2.941% |
| 11 | 16.167 | 2220 | 2226 | 2239 | rBV | 572704 | 923156 | 47.72% | 9.501% |
| 12 | 17.424 | 2433 | 2440 | 2454 | rBV | 270681 | 428440 | 22.15% | 4.409% |
| 13 | 18.282 | 2580 | 2586 | 2597 | rBV2 | 40191 | 75375 | 3.90% | 0.776% |
| 14 | 19.551 | 2798 | 2802 | 2809 | rBV9 | 11644 | 21358 | 1.10% | 0.220% |
| 15 | 20.021 | 2876 | 2882 | 2894 | rBV | 1493812 | 1934414 | 100.00% | 19.909% |
| 16 | 21.296 | 3092 | 3099 | 3114 | rBV7 | 25169 | 90982 | 4.70% | 0.936% |
| 17 | 21.696 | 3160 | 3167 | 3182 | rBV2 | 341211 | 588452 | 30.42% | 6.056% |
| 18 | 21.837 | 3186 | 3191 | 3198 | rVB3 | 16608 | 26798 | 1.39% | 0.276% |
| 19 | 22.442 | 3289 | 3294 | 3300 | rBV3 | 28152 | 48275 | 2.50% | 0.497% |
| 20 | 23.135 | 3407 | 3412 | 3418 | rVB3 | 42828 | 73204 | 3.78% | 0.753% |
| 21 | 23.329 | 3438 | 3445 | 3453 | rBV2 | 36520 | 69774 | 3.61% | 0.718% |
| 22 | 23.946 | 3542 | 3550 | 3561 | rVB4 | 36298 | 91880 | 4.75% | 0.946% |
| 23 | 24.904 | 3705 | 3713 | 3717 | rBV2 | 27278 | 62746 | 3.24% | 0.646% |
| 24 | 24.980 | 3717 | 3726 | 3736 | rVB2 | 188530 | 536223 | 27.72% | 5.519% |
| 25 | 26.038 | 3899 | 3906 | 3916 | rVB6 | 17705 | 50448 | 2.61% | 0.519% |
| 26 | 27.413 | 4132 | 4140 | 4145 | rVB8 | 7315 | 21413 | 1.11% | 0.220% |

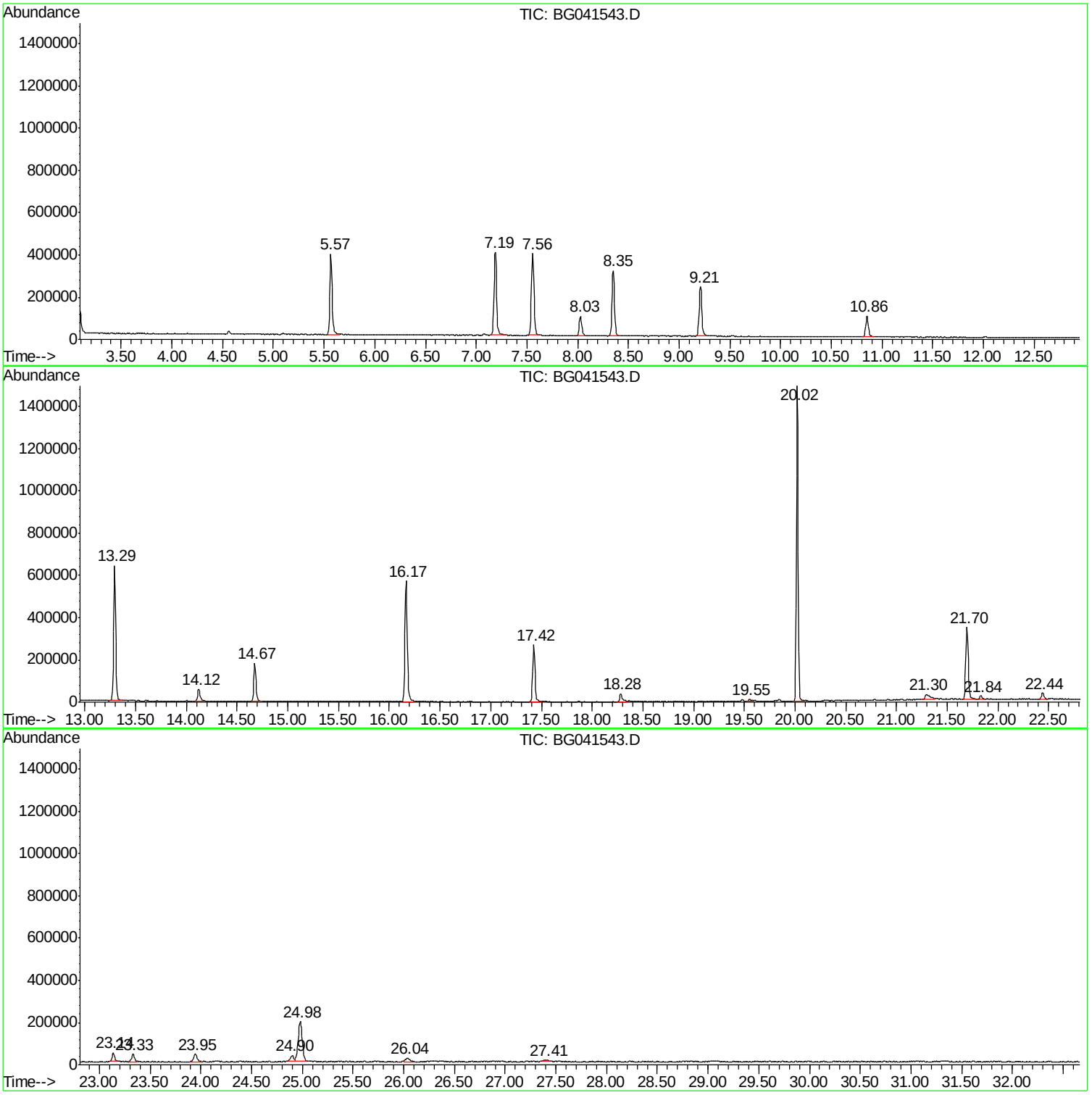
Sum of corrected areas: 9716453

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

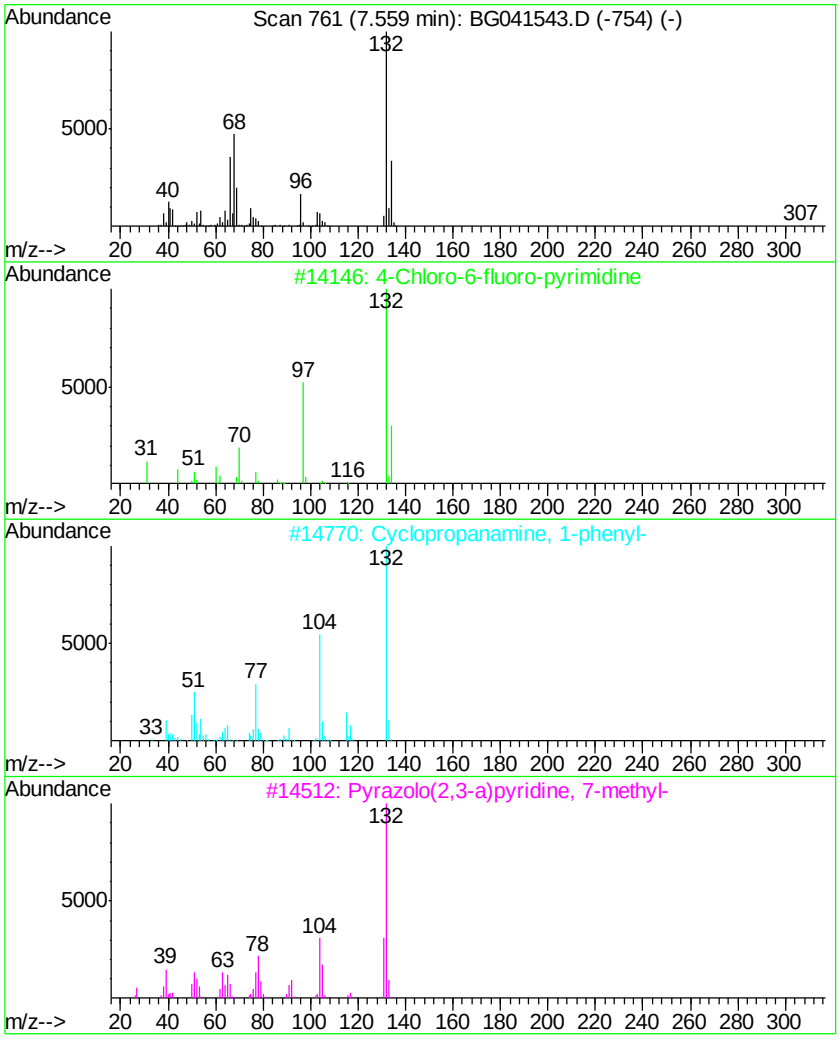
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

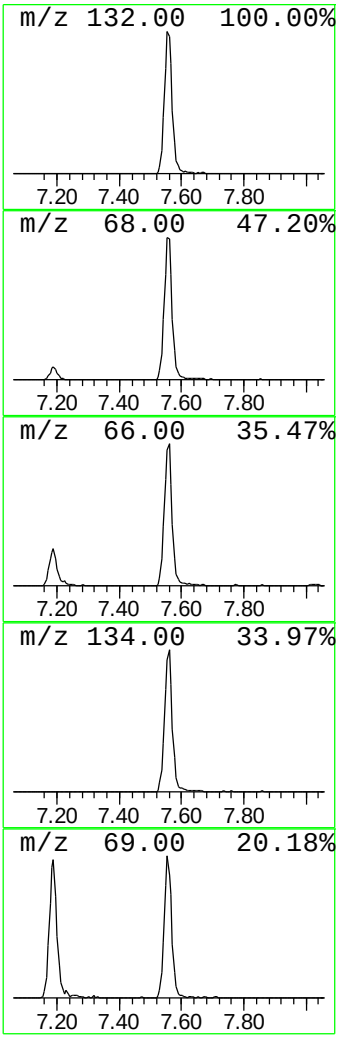
**********

Peak Number 1 unknown7.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.56 | 86.22 ng | 683340 | 1,4-Dichlorobenzene-d4 | 8.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 22 |
| 3 | Pyrazolo(2,3-a)pyridine, 7-methyl- | 132 | C8H8N2 | 034760-58-2 | 22 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

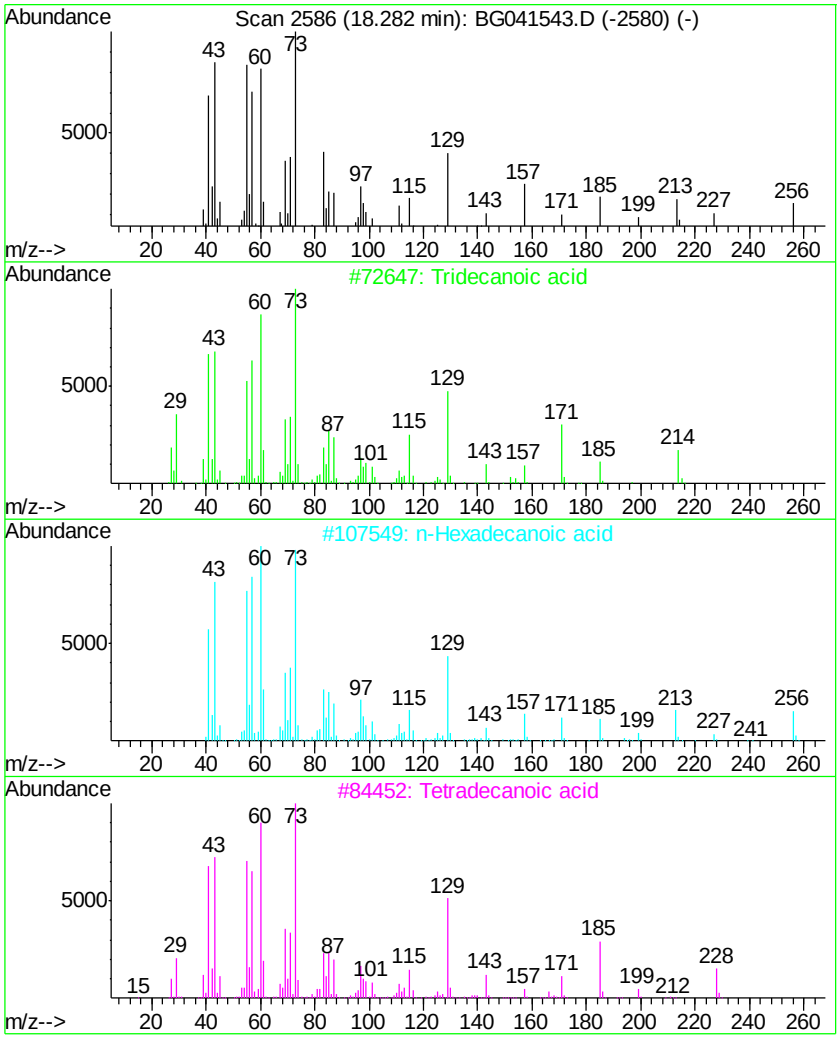
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

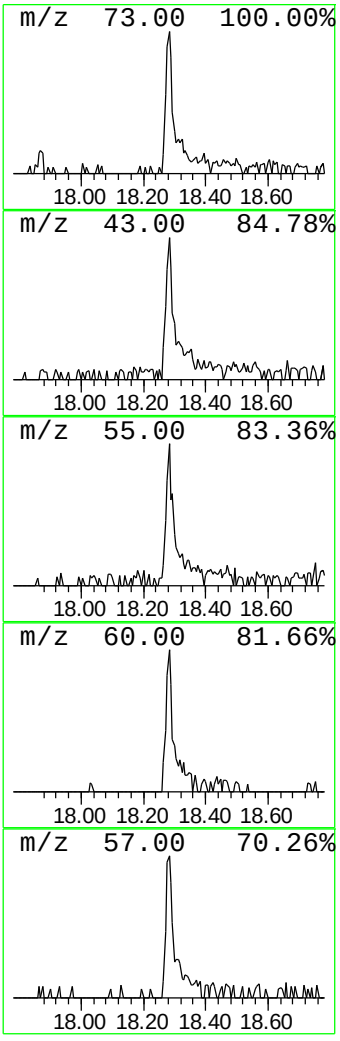
**********

Peak Number 3 Tridecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.28 | 3.52 ng | 75375 | Phenanthrene-d10 | 17.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 89 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 86 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 64 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 47 |



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

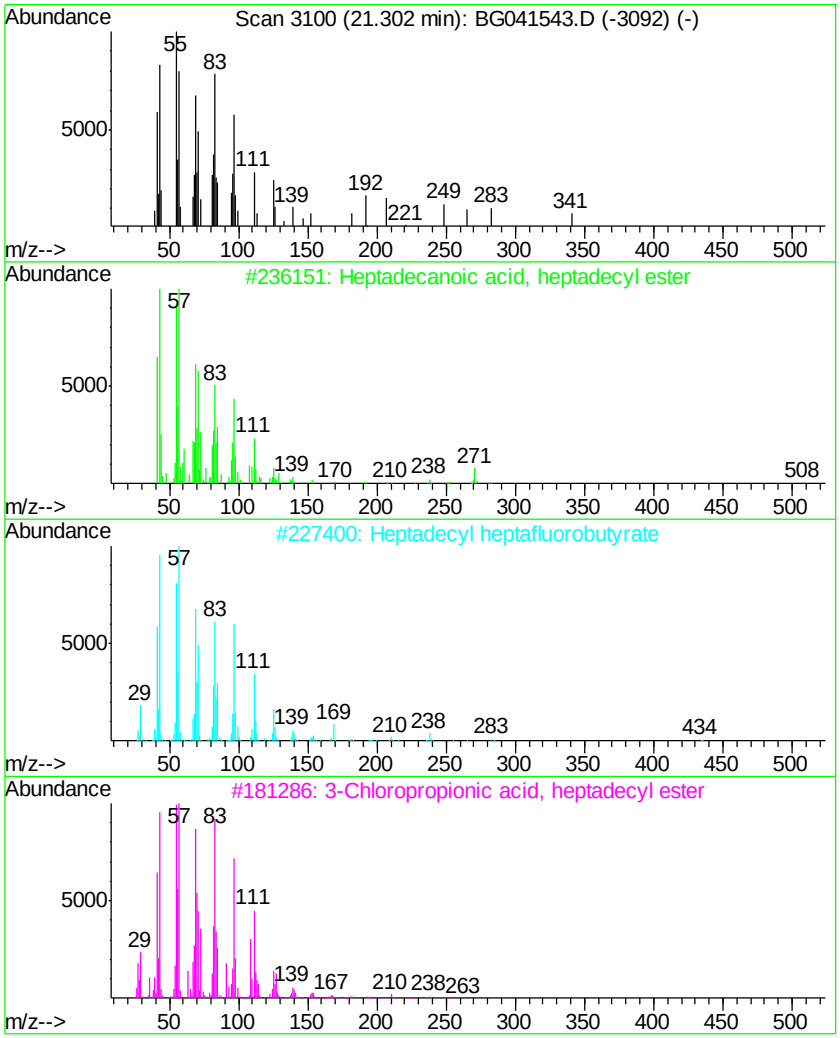
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

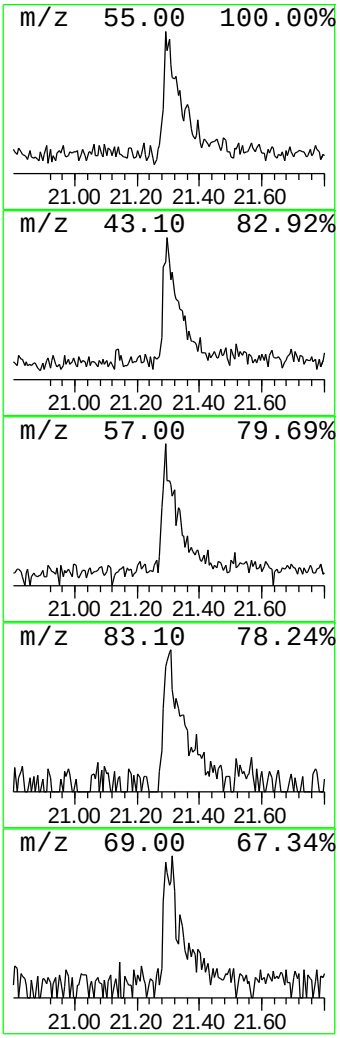
**********

Peak Number 4 Heptadecanoic acid, heptade... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.30 | 3.09 ng | 90982 | Chrysene-d12 | 21.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecanoic acid, heptadecyl e... | 509 | C34H68O2 | 036617-50-2 | 72 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 58 |
| 3 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 58 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 52 |
| 5 | Octacosanol | 410 | C28H58O | 000557-61-9 | 52 |



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

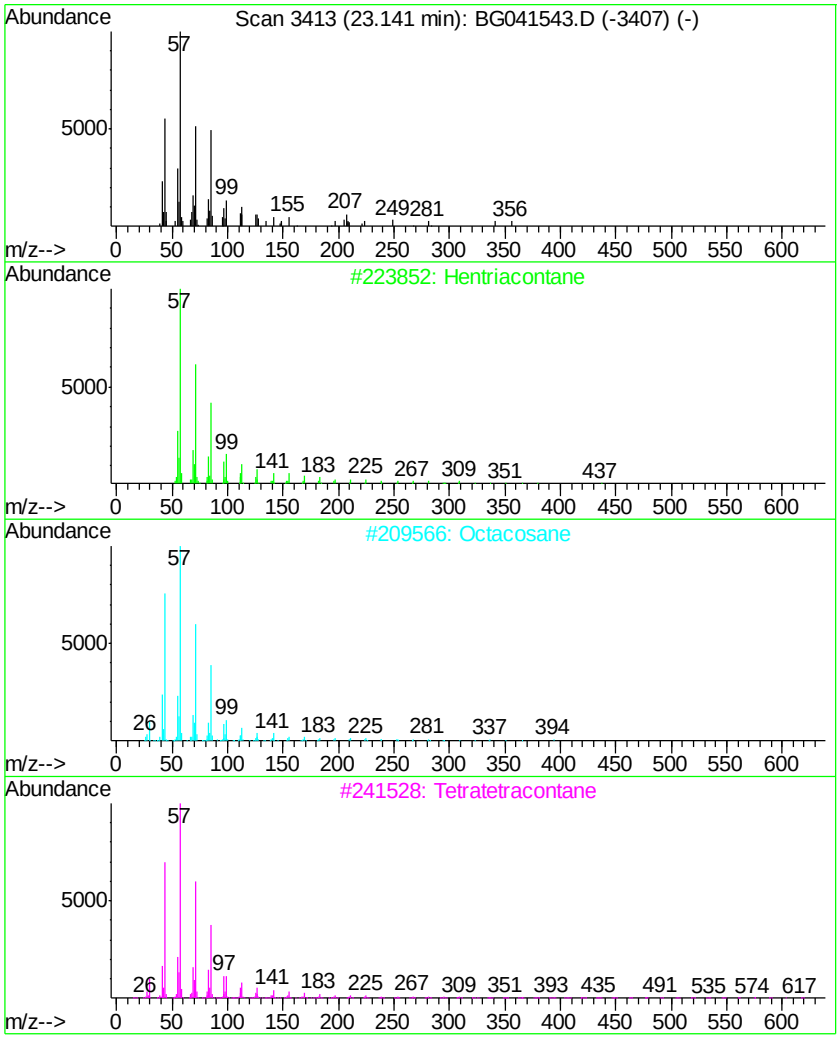
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

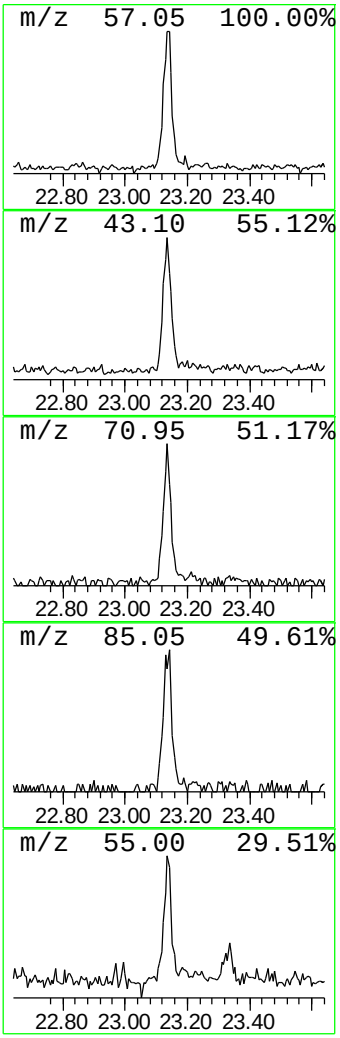
**********

Peak Number 5 Hentriacontane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.14 | 2.49 ng | 73204 | Chrysene-d12 | 21.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 86 |



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

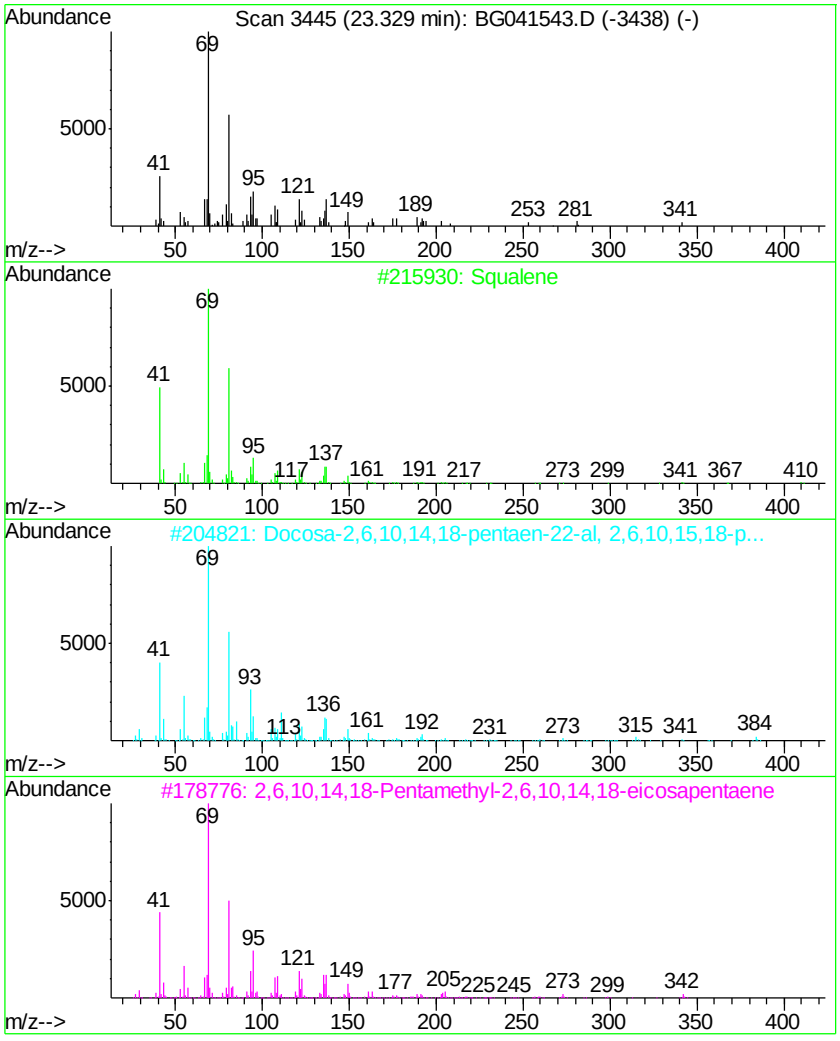
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

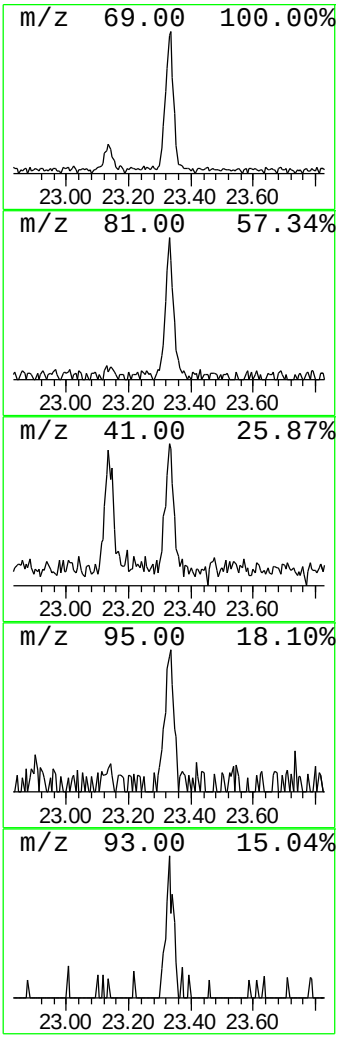
**********

Peak Number 6 Squalene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.33 | 2.37 ng | 69774 | Chrysene-d12 | 21.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 87 |
| 2 | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O | 1000163-04-7 | 86 |
| 3 | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42 | 075581-03-2 | 80 |
| 4 | Supraene | 410 | C30H50 | 007683-64-9 | 72 |
| 5 | 3-Cyclohexene-1-carboxaldehyde, ... | 192 | C13H20O | 052475-89-5 | 58 |



Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

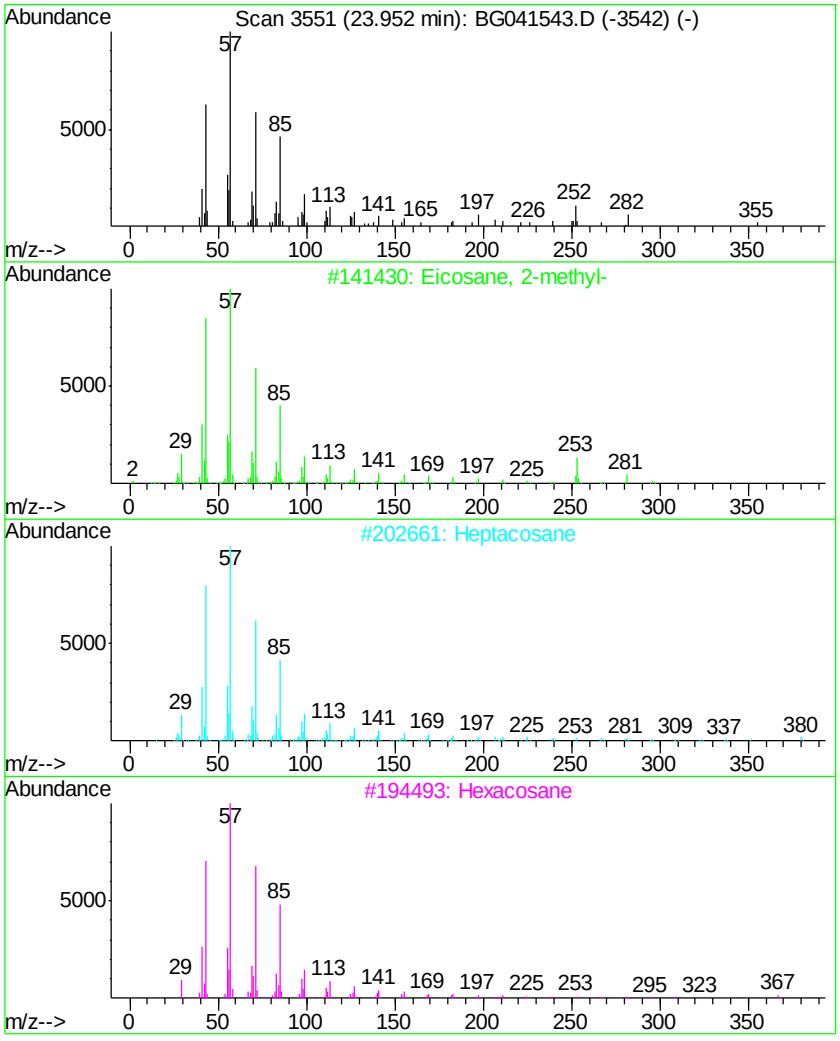
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

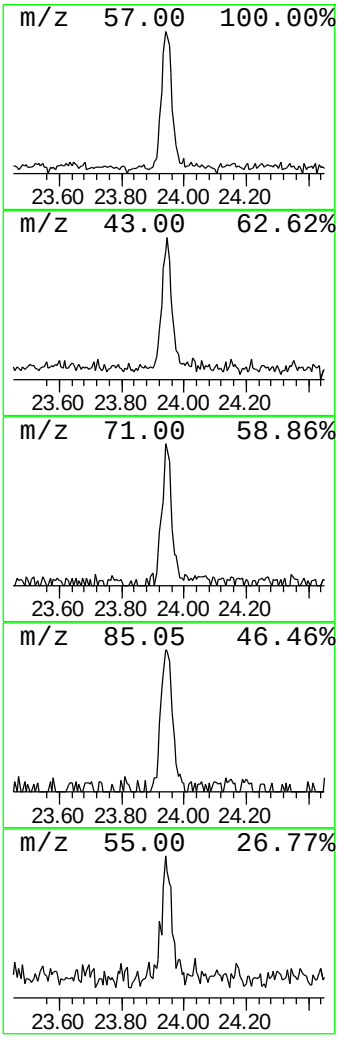
**********

Peak Number 7 Eicosane, 2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.95 | 3.43 ng | 91880 | Perylene-d12 | 24.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane, 2-methyl- | 296 | C21H44 | 001560-84-5 | 91 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 86 |



# Library Search Compound Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

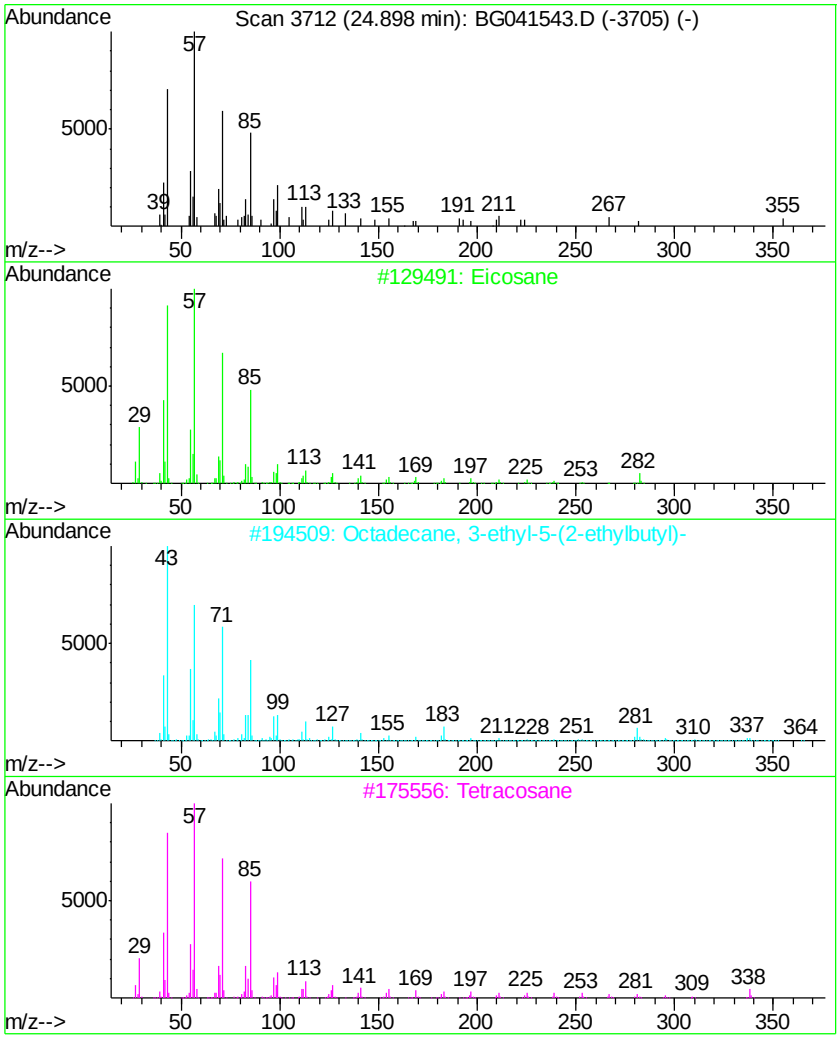
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

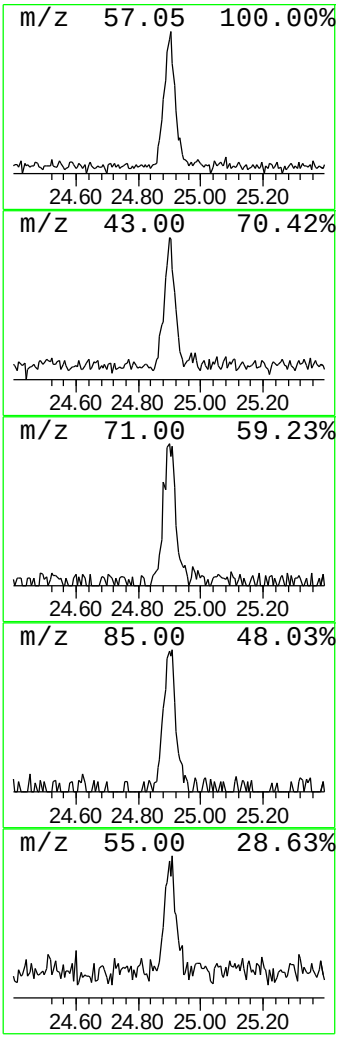
**********

Peak Number 8 Eicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.90 | 2.34 ng | 62746 | Perylene-d12 | 24.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 95 |
| 2 | Octadecane, 3-ethyl-5-(2-ethylbu... | 366 | C26H54 | 055282-12-7 | 80 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 80 |
| 4 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 72 |
| 5 | Docosane, 11-decyl- | 451 | C32H66 | 055401-55-3 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_G\DATA\BG062919\
Data File : BG041543.D
Acq On : 29 Jun 2019 12:59
Operator : HP/JU
Sample : K3555-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SAMPLE-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG062619.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 |
| unknown7.56 | 7.56 | 86.2 | ng | 683340 | 1 | 8.03 | 158516 | 20.0 |
| Tridecanoic acid | 18.28 | 3.5 | ng | 75375 | 4 | 17.42 | 428440 | 20.0 |
| Heptadecanoic aci... | 21.30 | 3.1 | ng | 90982 | 5 | 21.70 | 588452 | 20.0 |
| Hentriacontane | 23.14 | 2.5 | ng | 73204 | 5 | 21.70 | 588452 | 20.0 |
| Squalene | 23.33 | 2.4 | ng | 69774 | 5 | 21.70 | 588452 | 20.0 |
| Eicosane, 2-methyl- | 23.95 | 3.4 | ng | 91880 | 6 | 24.98 | 536223 | 20.0 |
| Eicosane | 24.90 | 2.3 | ng | 62746 | 6 | 24.98 | 536223 | 20.0 |