LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082718\
Data File : BG036441.D
Acq On : 27 Aug 2018 21:16
Operator : JU/SJ
Sample : J4583-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

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-BG082318.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 | 5.168 | 315 | 320 | 328 | rBV | 65207 | 95984 | 1.93% | 0.368% |
| 2 | 5.633 | 391 | 399 | 409 | rBV | 1195015 | 1887538 | 37.99% | 7.241% |
| 3 | 7.219 | 661 | 669 | 682 | rBV | 1228457 | 2139800 | 43.06% | 8.208% |
| 4 | 7.595 | 724 | 733 | 741 | rBV | 1148585 | 1964522 | 39.54% | 7.536% |
| 5 | 8.065 | 806 | 813 | 821 | rBV | 222699 | 378947 | 7.63% | 1.454% |
| 6 | 8.388 | 860 | 868 | 879 | rVB | 854956 | 1473234 | 29.65% | 5.651% |
| 7 | 9.223 | 1001 | 1010 | 1019 | rBV | 698666 | 1264370 | 25.45% | 4.850% |
| 8 | 10.874 | 1282 | 1291 | 1298 | rBV | 305528 | 549013 | 11.05% | 2.106% |
| 9 | 13.318 | 1696 | 1707 | 1716 | rBV | 1922796 | 3057966 | 61.54% | 11.730% |
| 10 | 14.134 | 1840 | 1846 | 1853 | rBV | 247717 | 358734 | 7.22% | 1.376% |
| 11 | 14.687 | 1933 | 1940 | 1950 | rVB2 | 492338 | 796318 | 16.03% | 3.055% |
| 12 | 16.173 | 2185 | 2193 | 2206 | rBV | 1684847 | 2519511 | 50.71% | 9.665% |
| 13 | 17.431 | 2399 | 2407 | 2413 | rBV | 690072 | 1038691 | 20.90% | 3.984% |
| 14 | 18.318 | 2553 | 2558 | 2568 | rBV | 107491 | 174211 | 3.51% | 0.668% |
| 15 | 19.734 | 2795 | 2799 | 2804 | rVB3 | 42242 | 57416 | 1.16% | 0.220% |
| 16 | 20.039 | 2845 | 2851 | 2857 | rBV | 3731570 | 4968954 | 100.00% | 19.061% |
| 17 | 21.355 | 3069 | 3075 | 3083 | rBV | 102903 | 201437 | 4.05% | 0.773% |
| 18 | 21.696 | 3126 | 3133 | 3143 | rVB | 784557 | 1240331 | 24.96% | 4.758% |
| 19 | 21.908 | 3164 | 3169 | 3177 | rBV2 | 43324 | 61434 | 1.24% | 0.236% |
| 20 | 22.525 | 3269 | 3274 | 3284 | rBV3 | 37903 | 75536 | 1.52% | 0.290% |
| 21 | 23.224 | 3388 | 3393 | 3401 | rVB5 | 35526 | 68582 | 1.38% | 0.263% |
| 22 | 23.412 | 3418 | 3425 | 3433 | rVB | 200662 | 366155 | 7.37% | 1.405% |
| 23 | 24.029 | 3526 | 3530 | 3538 | rVB3 | 28380 | 60504 | 1.22% | 0.232% |
| 24 | 24.916 | 3669 | 3681 | 3690 | rBV | 425299 | 1206682 | 24.28% | 4.629% |
| 25 | 26.132 | 3882 | 3888 | 3898 | rVB6 | 24381 | 62778 | 1.26% | 0.241% |

Sum of corrected areas: 26068648

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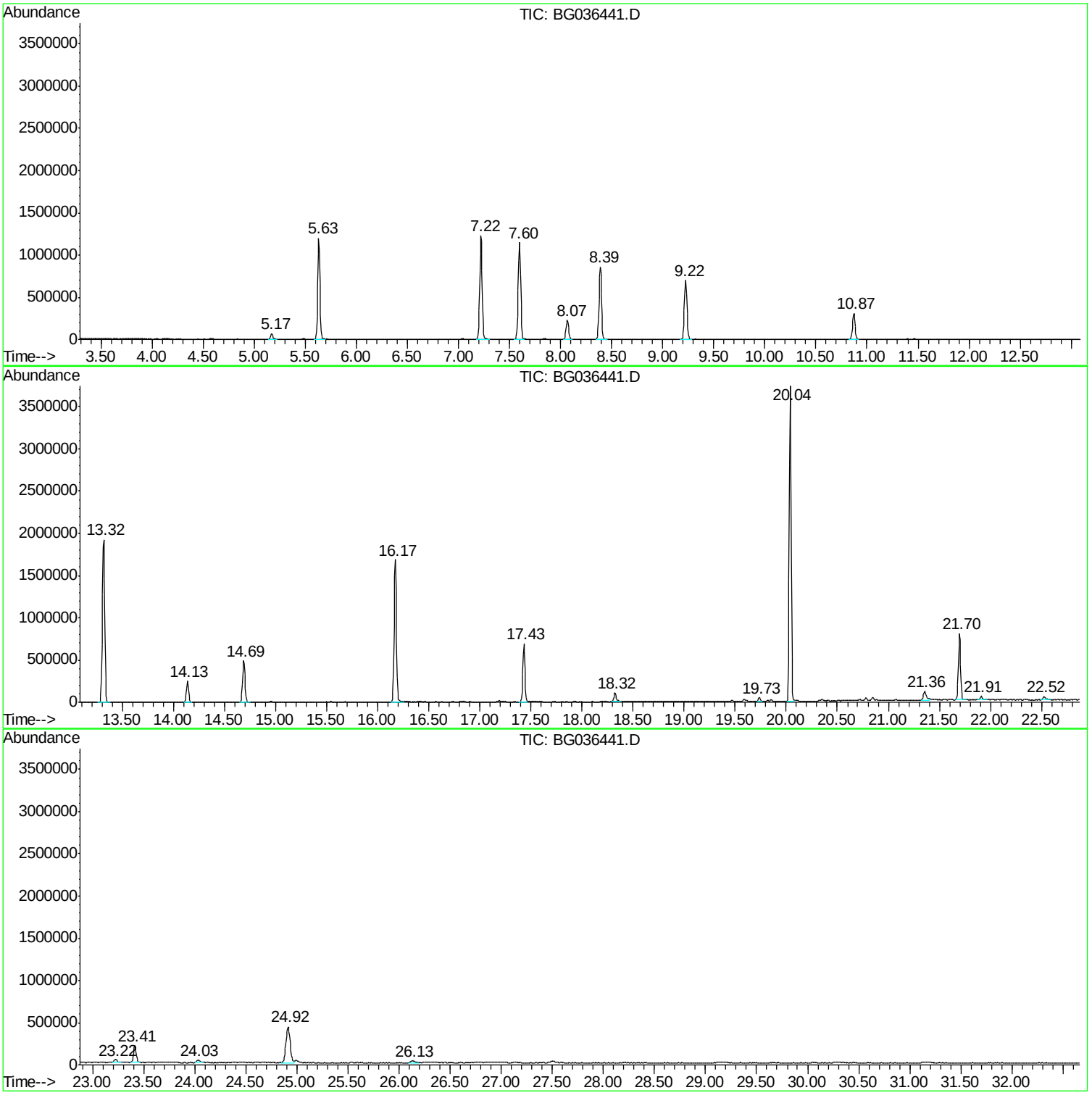
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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\BG082718\
Data File : BG036441.D
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**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

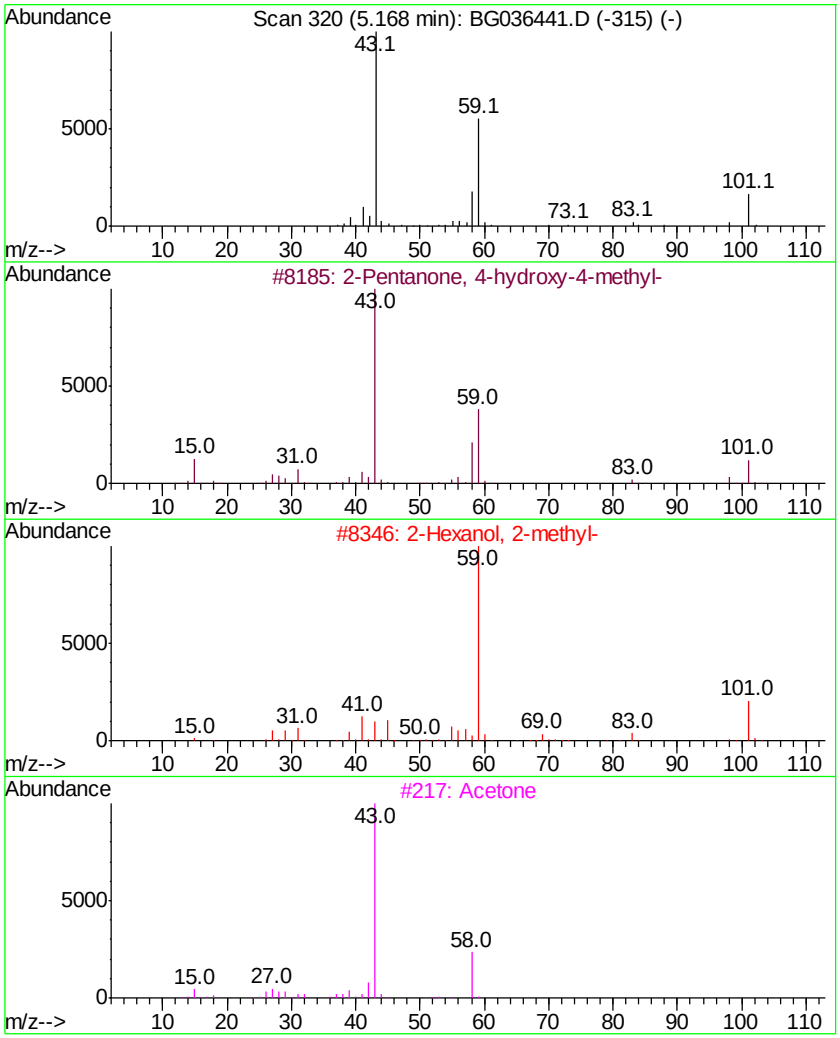
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

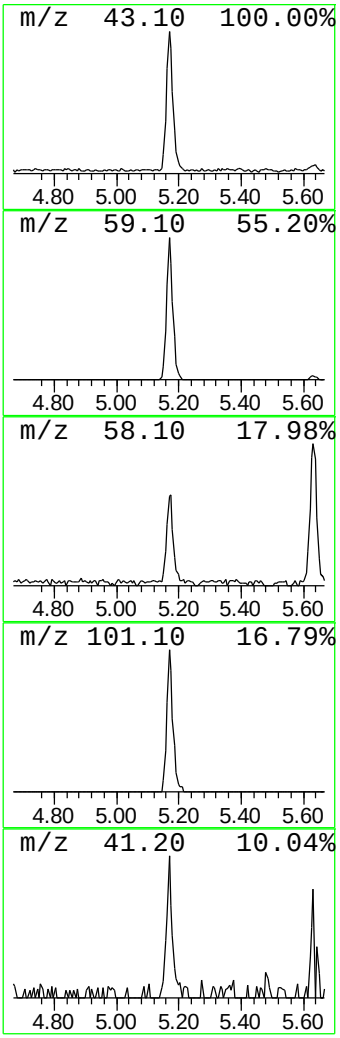
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 5.07 ng | 95984 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 25 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 22 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 17 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 12 |



# Library Search Compound Report

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Operator : JU/SJ
Sample : J4583-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

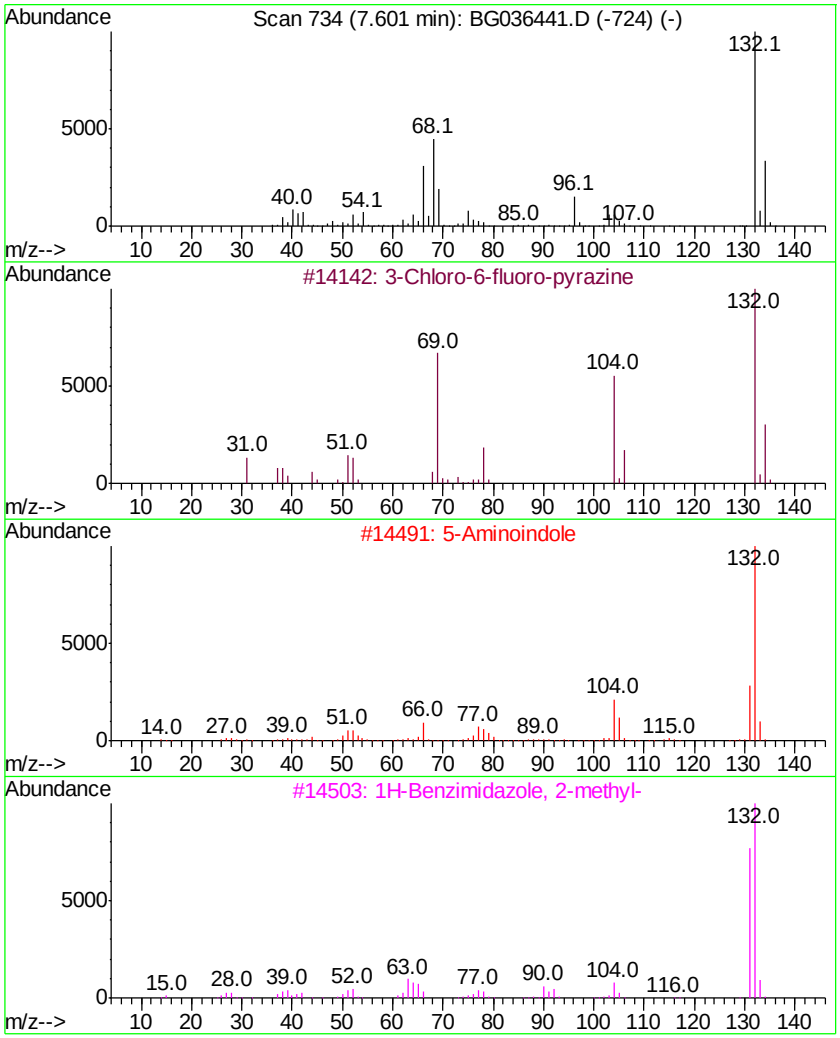
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

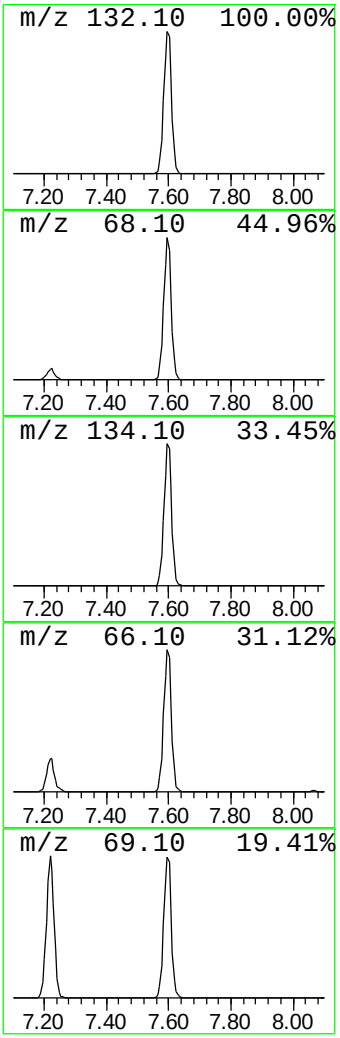
**********

Peak Number 2 unknown7.60 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.60 | 103.68 ng | 1964520 | 1,4-Dichlorobenzene-d4 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 10 |



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Data File : BG036441.D
Acq On : 27 Aug 2018 21:16
Operator : JU/SJ
Sample : J4583-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

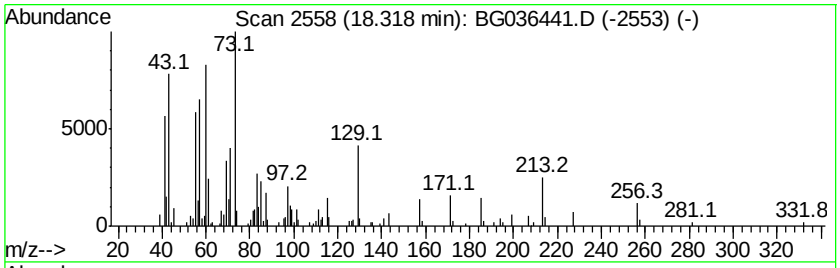
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

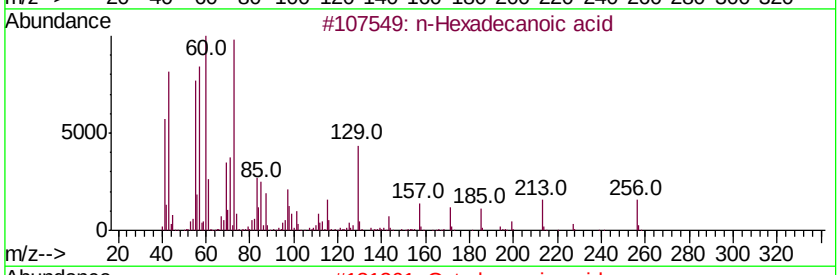
**********

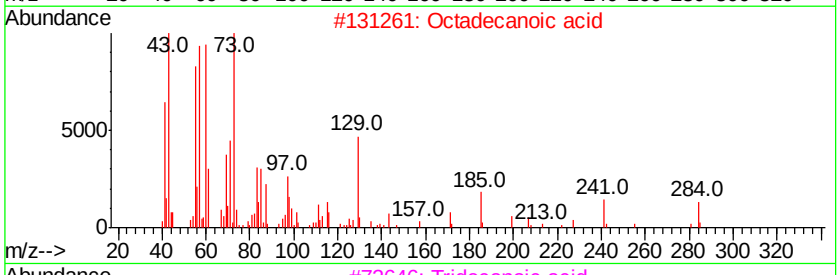
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

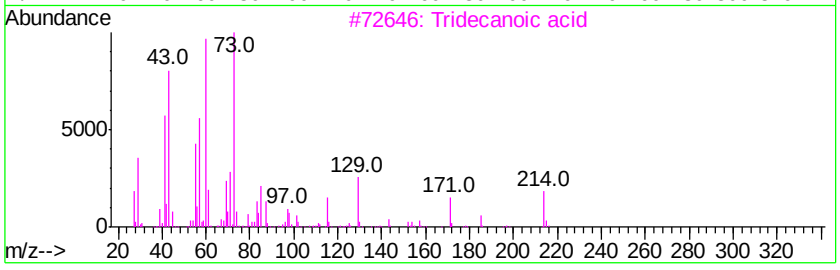
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.32 | 3.35 ng | 174211 | Phenanthrene-d10 | 17.43 |

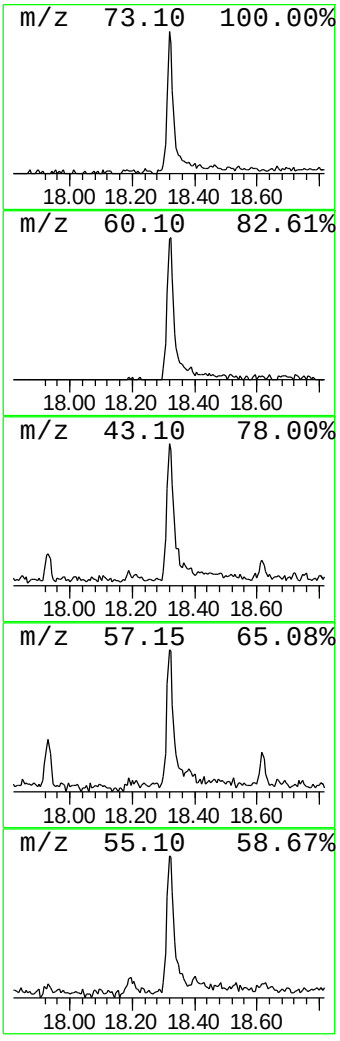
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 93 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 89 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



Library Search Compound Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

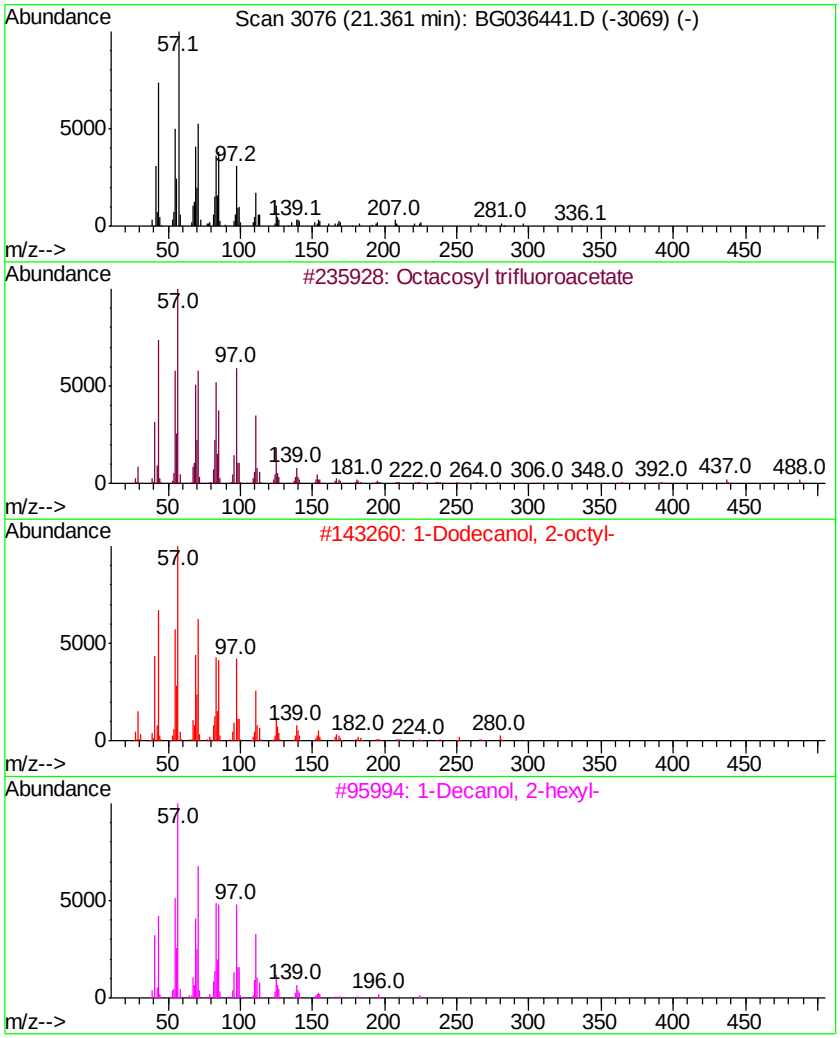
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

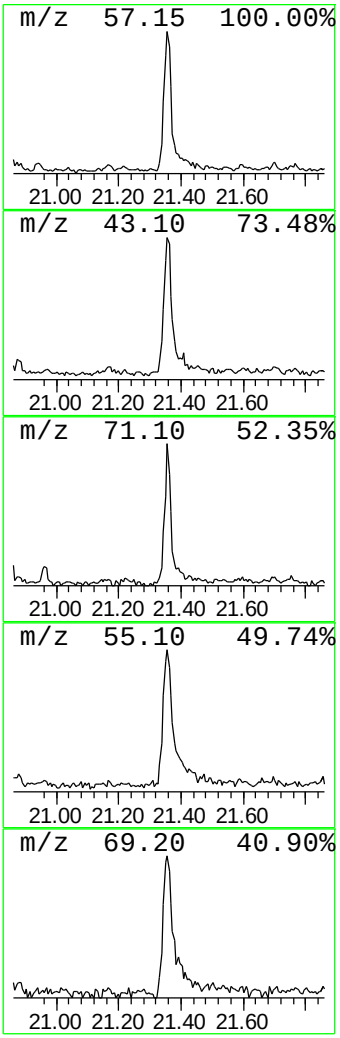
**********

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.36 | 3.25 ng | 201437 | Chrysene-d12 | 21.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 91 |
| 2 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 91 |
| 3 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 91 |
| 4 | Oxalic acid, isobutyl pentadecyl... | 356 | C21H40O4 | 1000309-38-0 | 87 |
| 5 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 87 |



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ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOD1-SB-101-02-03-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

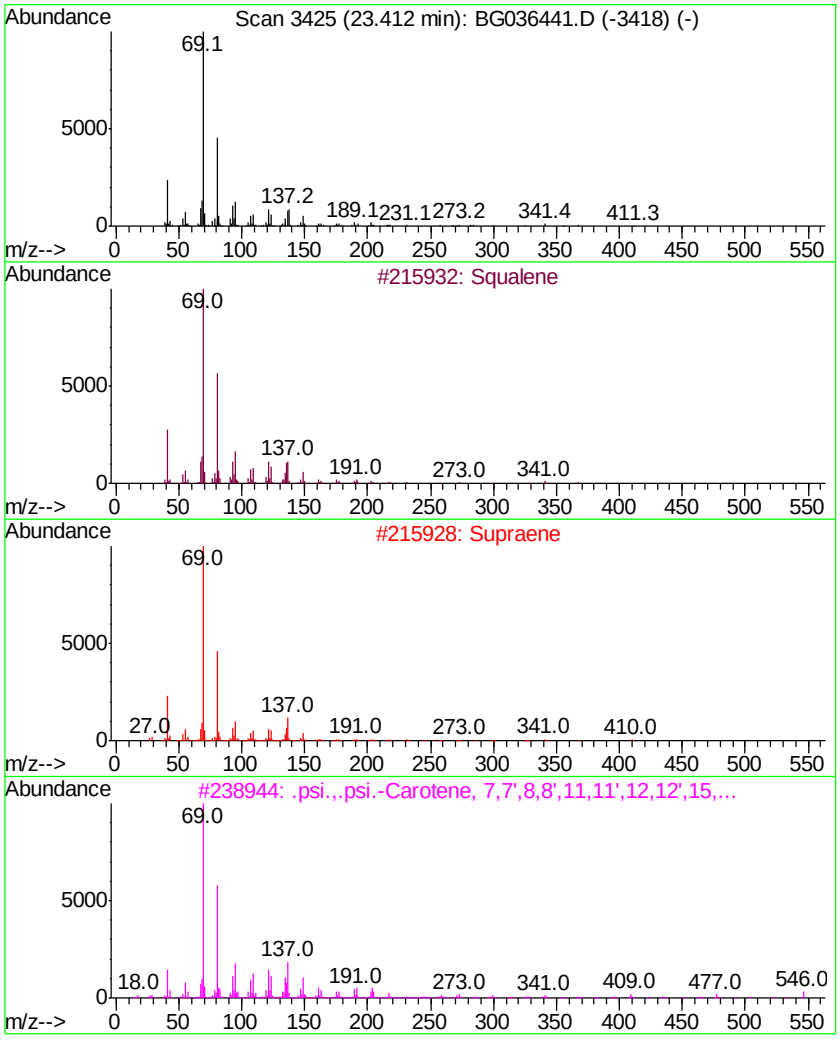
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

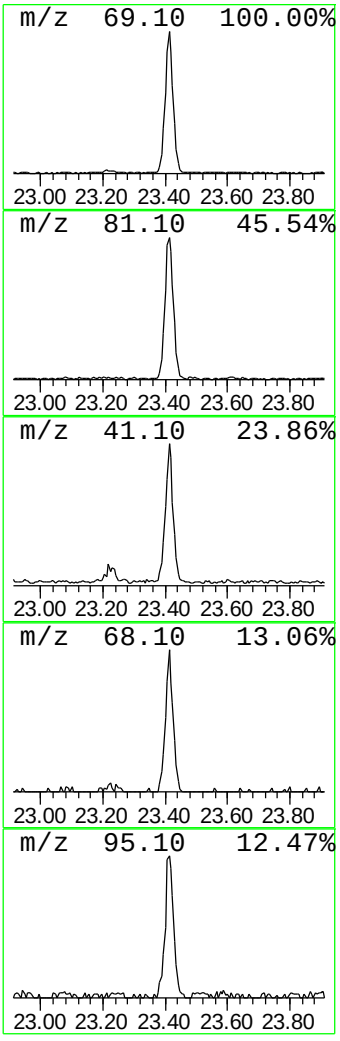
**********

Peak Number 6 Squalene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.41 | 6.07 ng | 366155 | Perylene-d12 | 24.91 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 3 | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66 | 000502-62-5 | 78 |
| 4 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 72 |
| 5 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 72 |



Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.17 | 5.1 | ng | 95984 | 1 | 8.07 | 378947 | 20.0 |
| unknown7.60 | 7.60 | 103.7 | ng | 1964520 | 1 | 8.07 | 378947 | 20.0 |
| n-Hexadecanoic acid | 18.32 | 3.4 | ng | 174211 | 4 | 17.43 | 1038690 | 20.0 |
| Octacosyl trifluo... | 21.36 | 3.3 | ng | 201437 | 5 | 21.70 | 1240330 | 20.0 |
| Squalene | 23.41 | 6.1 | ng | 366155 | 6 | 24.91 | 1206680 | 20.0 |