LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102922\
Data File : BG055365.D
Acq On : 29 Oct 2022 14:43
Operator : CG/JU
Sample : N5272-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20221103-COMP-02

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-BG102422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055365.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.324 | 4 | 6 | 14 | rVB | 14532 | 19148 | 1.37% | 0.257% |
| 2 | 5.304 | 337 | 343 | 353 | rBV | 50880 | 78340 | 5.59% | 1.051% |
| 3 | 5.785 | 418 | 425 | 437 | rBV | 390837 | 628995 | 44.85% | 8.438% |
| 4 | 7.407 | 693 | 701 | 716 | rBV | 375553 | 651829 | 46.48% | 8.744% |
| 5 | 8.259 | 839 | 846 | 853 | rBV | 92626 | 153689 | 10.96% | 2.062% |
| 6 | 9.434 | 1039 | 1046 | 1056 | rBV | 214367 | 388285 | 27.69% | 5.209% |
| 7 | 11.091 | 1321 | 1328 | 1339 | rBV | 125738 | 221948 | 15.83% | 2.977% |
| 8 | 13.500 | 1731 | 1738 | 1746 | rBV | 562995 | 867298 | 61.85% | 11.635% |
| 9 | 14.875 | 1965 | 1972 | 1984 | rVB | 212860 | 333651 | 23.79% | 4.476% |
| 10 | 16.355 | 2217 | 2224 | 2251 | rBV | 456731 | 792864 | 56.54% | 10.636% |
| 11 | 17.607 | 2431 | 2437 | 2448 | rBV | 311205 | 447958 | 31.94% | 6.009% |
| 12 | 17.713 | 2452 | 2455 | 2460 | rVB2 | 11561 | 15334 | 1.09% | 0.206% |
| 13 | 20.180 | 2869 | 2875 | 2883 | rBV | 1108449 | 1402304 | 100.00% | 18.812% |
| 14 | 21.485 | 3090 | 3097 | 3115 | rBV4 | 39086 | 164353 | 11.72% | 2.205% |
| 15 | 21.884 | 3158 | 3165 | 3174 | rVB | 308756 | 522168 | 37.24% | 7.005% |
| 16 | 23.382 | 3418 | 3420 | 3429 | rVB6 | 10629 | 18686 | 1.33% | 0.251% |
| 17 | 23.594 | 3450 | 3456 | 3462 | rVB | 38774 | 75773 | 5.40% | 1.016% |
| 18 | 24.234 | 3559 | 3565 | 3570 | rVB3 | 15465 | 31501 | 2.25% | 0.423% |
| 19 | 25.274 | 3728 | 3742 | 3756 | rVB2 | 183402 | 589807 | 42.06% | 7.912% |
| 20 | 26.414 | 3930 | 3936 | 3946 | rVB3 | 17246 | 50419 | 3.60% | 0.676% |

Sum of corrected areas: 7454350

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BNA_G
**ClientSampleId :**
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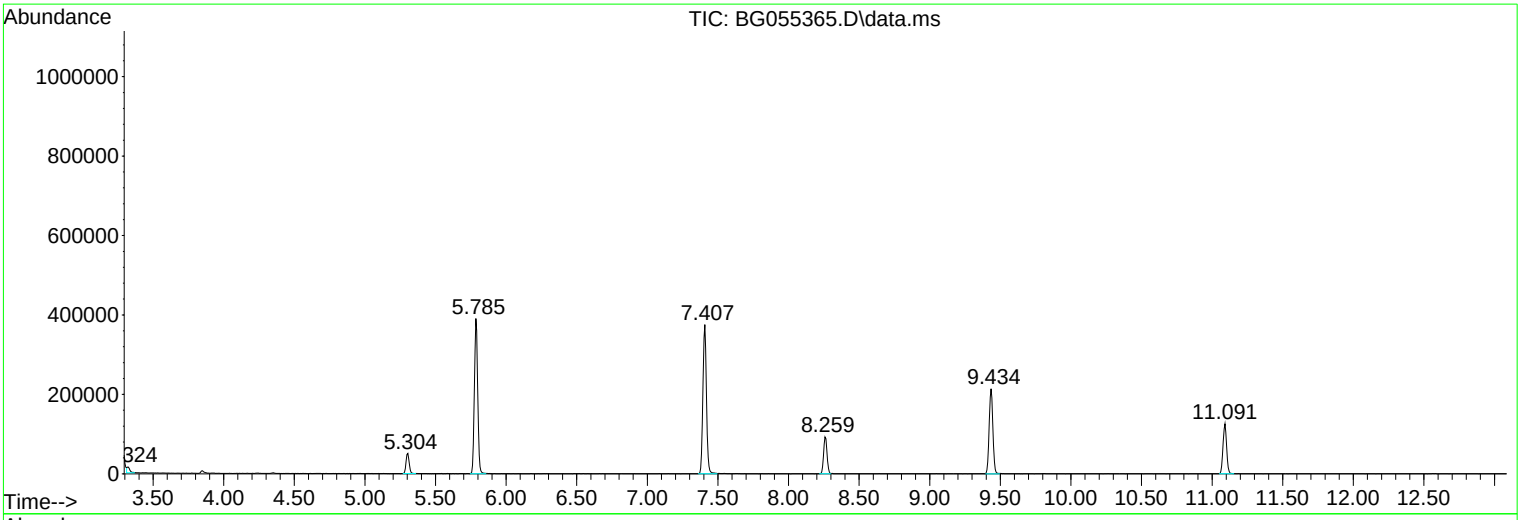
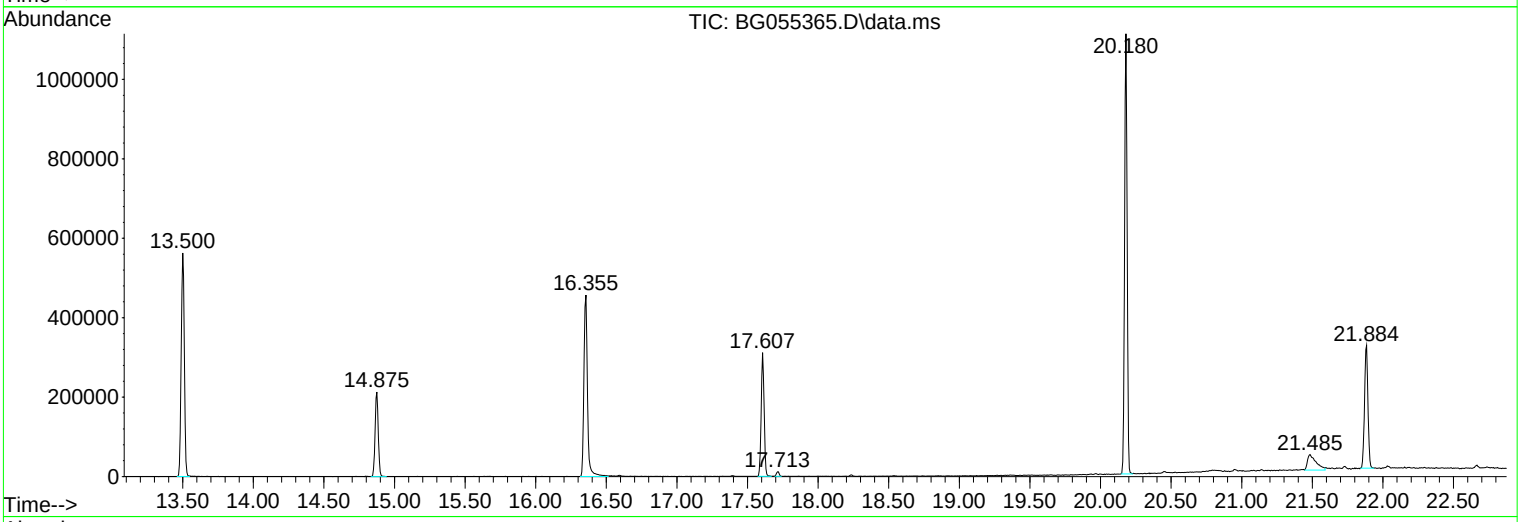
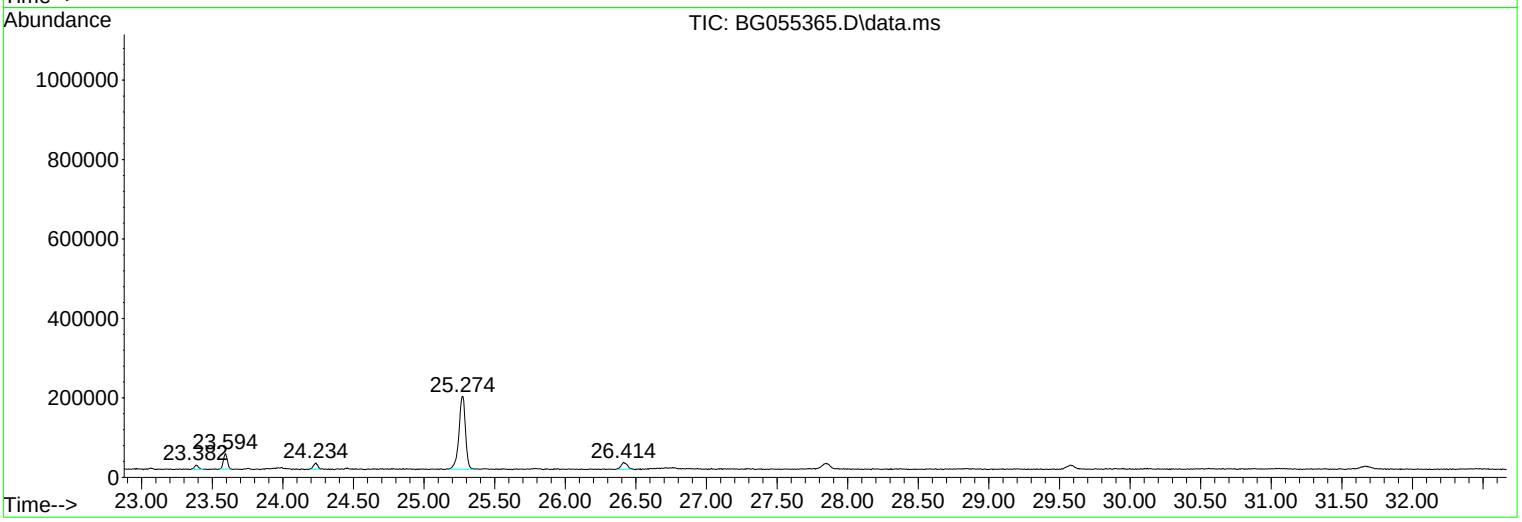
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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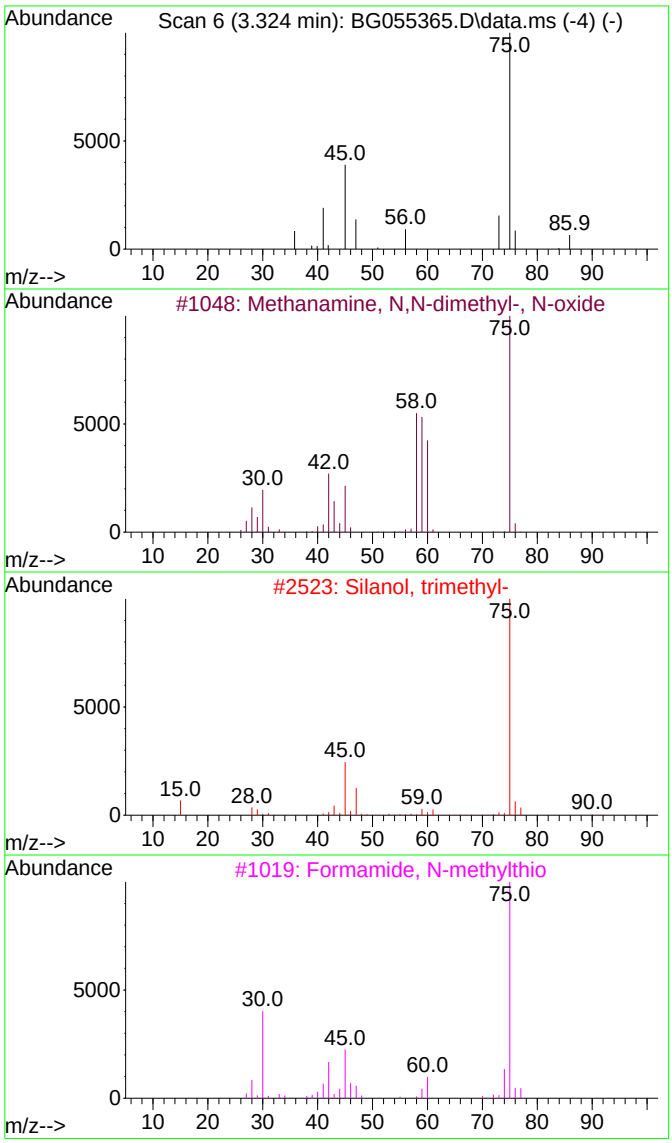
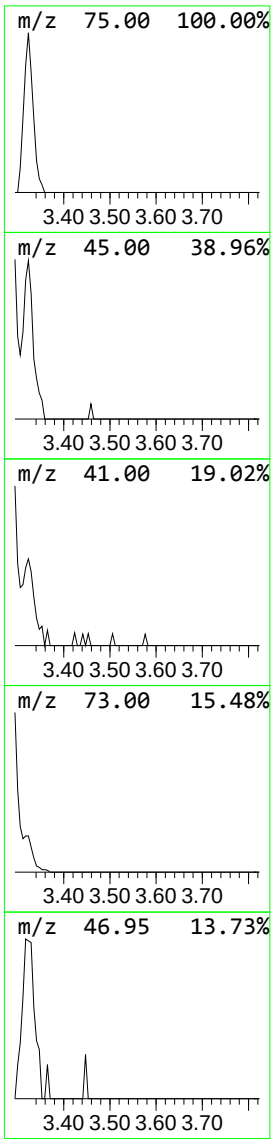
**********

Peak Number 1 unknown3.324 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.324 | 2.49 ng | 19148 | 1,4-Dichlorobenzene-d4 | 8.259 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methanamine, N,N-dimethyl-, N-oxide | 75 | C3H9NO | 001184-78-7 | 4 |
| 2 | Silanol, trimethyl- | 90 | C3H10OSi | 001066-40-6 | 4 |
| 3 | Formamide, N-methylthio | 75 | C2H5NS | 018952-41-5 | 4 |
| 4 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 4 |
| 5 | Glycine | 75 | C2H5NO2 | 000056-40-6 | 3 |



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**Instrument :**
BNA_G
**ClientSampleId :**
20221103-COMP-02

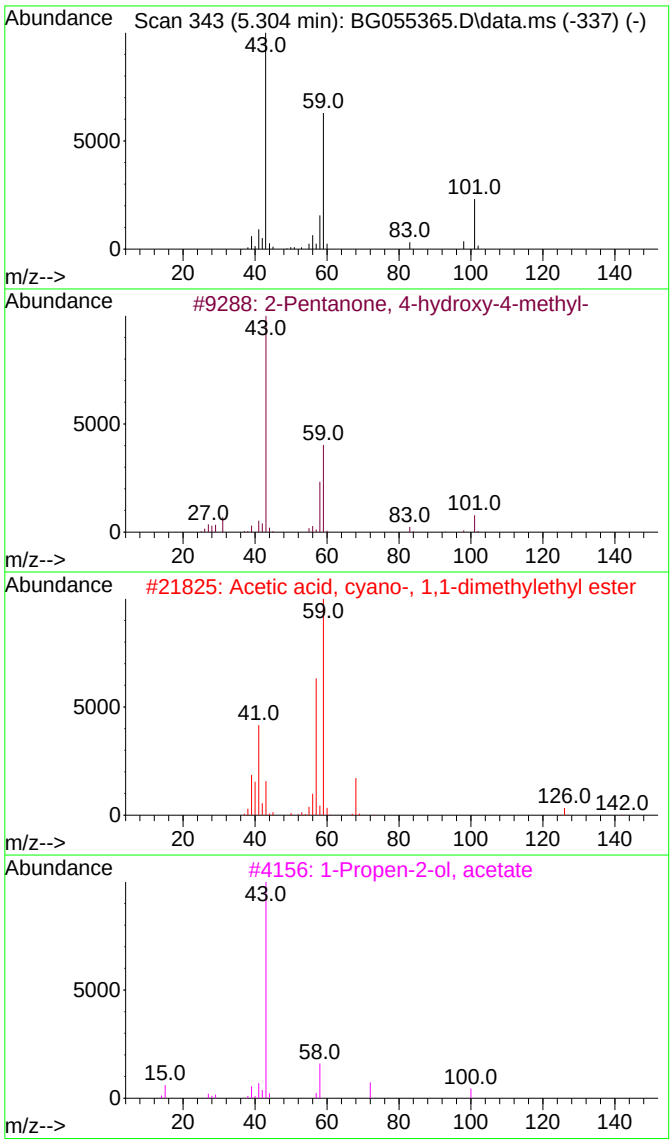
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

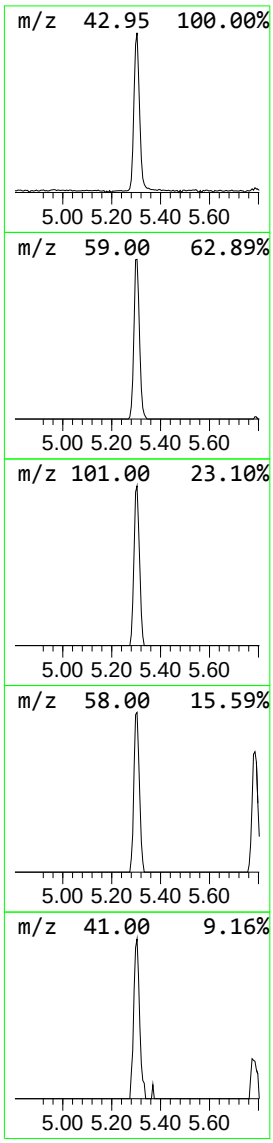
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.304 | 10.19 ng | 78340 | 1,4-Dichlorobenzene-d4 | 8.259 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 5 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |



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Sample : N5272-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20221103-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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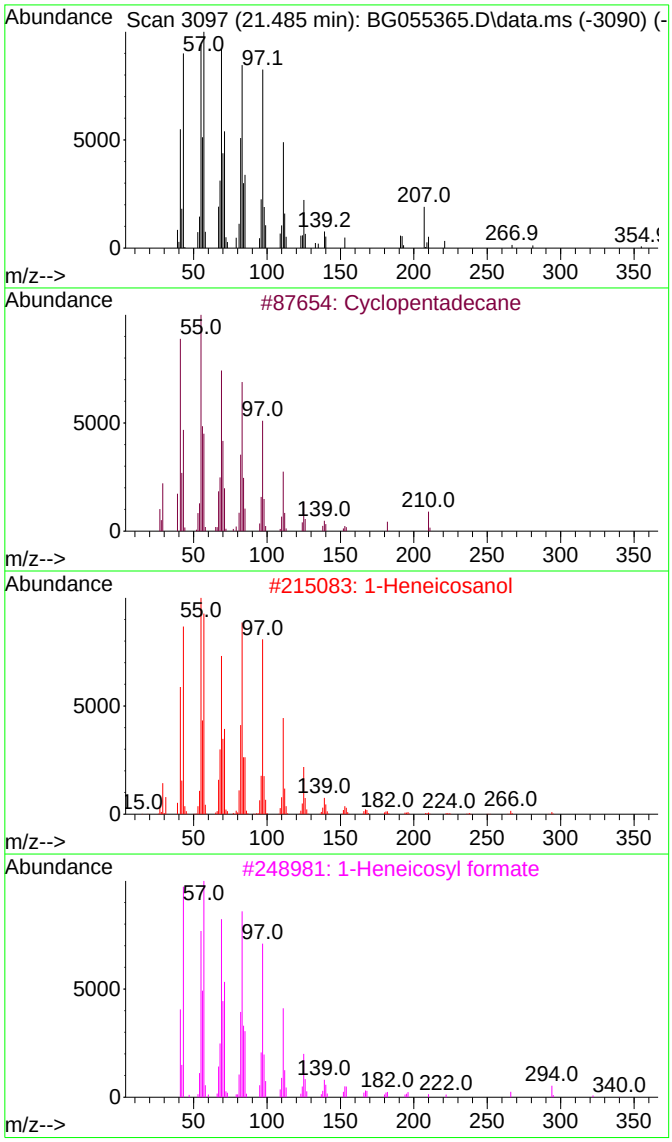
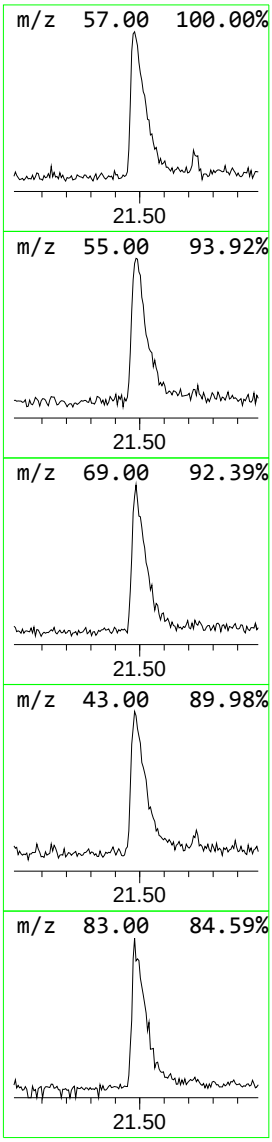
Peak Number 3 Cyclopentadecane Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.485 | 6.30 ng | 164353 | Chrysene-d12 | 21.884 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 97 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 95 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 94 |



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Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20221103-COMP-02

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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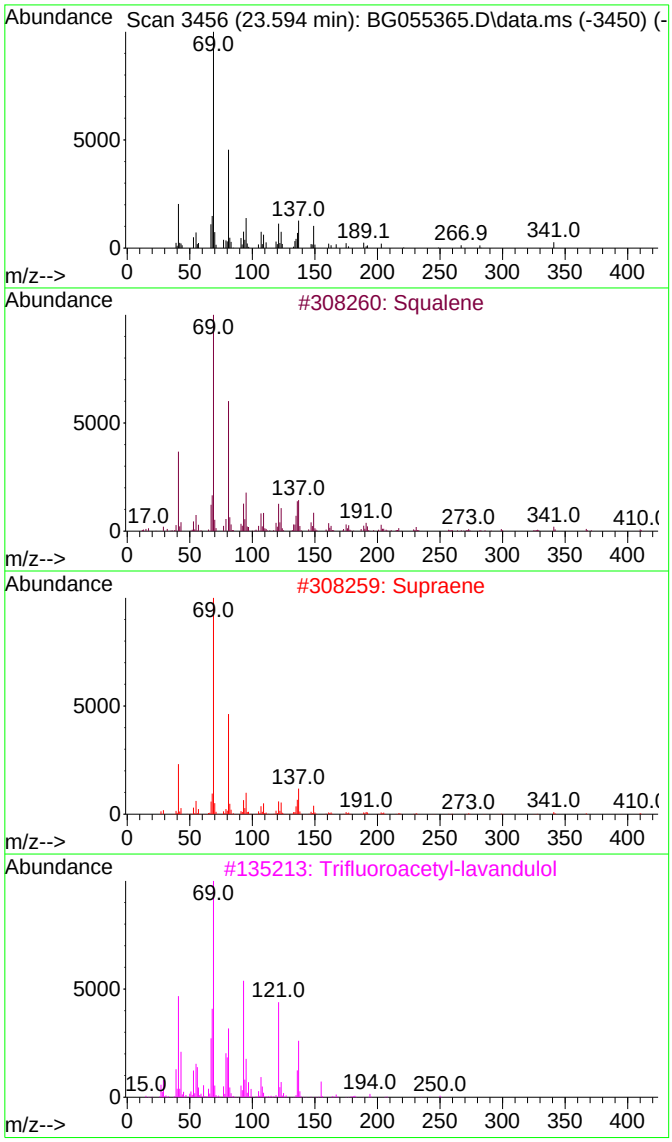
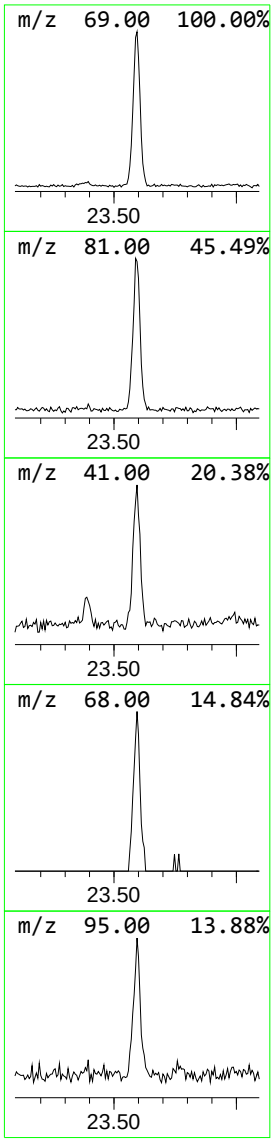
Peak Number 4 Squalene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.594 | 2.57 ng | 75773 | Perylene-d12 | 25.269 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 3 | Trifluoroacetyl-lavandulol | 250 | C12H17F3O2 | 028673-24-7 | 64 |
| 4 | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 64 |
| 5 | Farnesol (E), methyl ether | 236 | C16H28O | 1000352-67-3 | 64 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 7 Sample Multiplier: 1

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown3.324 | 3.324 | 2.5 | ng | 19148 | 1 | 8.259 | 153689 | 20.0 |
| 2-Pentanone, 4-... | 5.304 | 10.2 | ng | 78340 | 1 | 8.259 | 153689 | 20.0 |
| Cyclopentadecane | 21.485 | 6.3 | ng | 164353 | 5 | 21.884 | 522168 | 20.0 |
| Squalene | 23.594 | 2.6 | ng | 75773 | 6 | 25.269 | 589807 | 20.0 |