LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041423\
Data File : BG057101.D
Acq On : 14 Apr 2023 15:40
Operator : CG/JU
Sample : 02347-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20230338-COMP-16

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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057101.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.435 | 316 | 323 | 332 | rBV | 80224 | 128877 | 12.13% | 2.189% |
| 2 | 5.917 | 397 | 405 | 416 | rBB | 371346 | 594332 | 55.93% | 10.096% |
| 3 | 7.538 | 672 | 681 | 690 | rBV | 386857 | 656705 | 61.80% | 11.156% |
| 4 | 8.402 | 820 | 828 | 834 | rVB | 66628 | 112618 | 10.60% | 1.913% |
| 5 | 9.583 | 1021 | 1029 | 1037 | rVB | 208125 | 383827 | 36.12% | 6.520% |
| 6 | 11.239 | 1303 | 1311 | 1319 | rBV | 92413 | 160173 | 15.07% | 2.721% |
| 7 | 13.642 | 1713 | 1720 | 1726 | rBV | 519040 | 782997 | 73.68% | 13.301% |
| 8 | 15.017 | 1948 | 1954 | 1960 | rVB2 | 143323 | 214835 | 20.22% | 3.649% |
| 9 | 16.350 | 2174 | 2181 | 2189 | rBV2 | 67007 | 95411 | 8.98% | 1.621% |
| 10 | 16.497 | 2199 | 2206 | 2215 | rBV | 472664 | 706021 | 66.44% | 11.993% |
| 11 | 17.754 | 2412 | 2420 | 2425 | rBV | 167582 | 257460 | 24.23% | 4.374% |
| 12 | 17.795 | 2425 | 2427 | 2432 | rVB2 | 11814 | 13768 | 1.30% | 0.234% |
| 13 | 18.588 | 2558 | 2562 | 2570 | rBV2 | 41359 | 58022 | 5.46% | 0.986% |
| 14 | 19.781 | 2760 | 2765 | 2769 | rBV2 | 10593 | 16359 | 1.54% | 0.278% |
| 15 | 19.839 | 2772 | 2775 | 2779 | rBV6 | 9540 | 14921 | 1.40% | 0.253% |
| 16 | 20.145 | 2824 | 2827 | 2831 | rVB2 | 8973 | 12120 | 1.14% | 0.206% |
| 17 | 20.321 | 2851 | 2857 | 2863 | rVB | 846154 | 1062668 | 100.00% | 18.052% |
| 18 | 21.631 | 3076 | 3080 | 3087 | rBV3 | 26902 | 45837 | 4.31% | 0.779% |
| 19 | 22.072 | 3148 | 3155 | 3160 | rBV | 143798 | 247910 | 23.33% | 4.211% |
| 20 | 22.219 | 3176 | 3180 | 3185 | rVB6 | 8061 | 13405 | 1.26% | 0.228% |
| 21 | 22.871 | 3288 | 3291 | 3297 | rVB6 | 9907 | 18973 | 1.79% | 0.322% |
| 22 | 25.602 | 3741 | 3756 | 3767 | rBV3 | 86765 | 289517 | 27.24% | 4.918% |

Sum of corrected areas: 5886756

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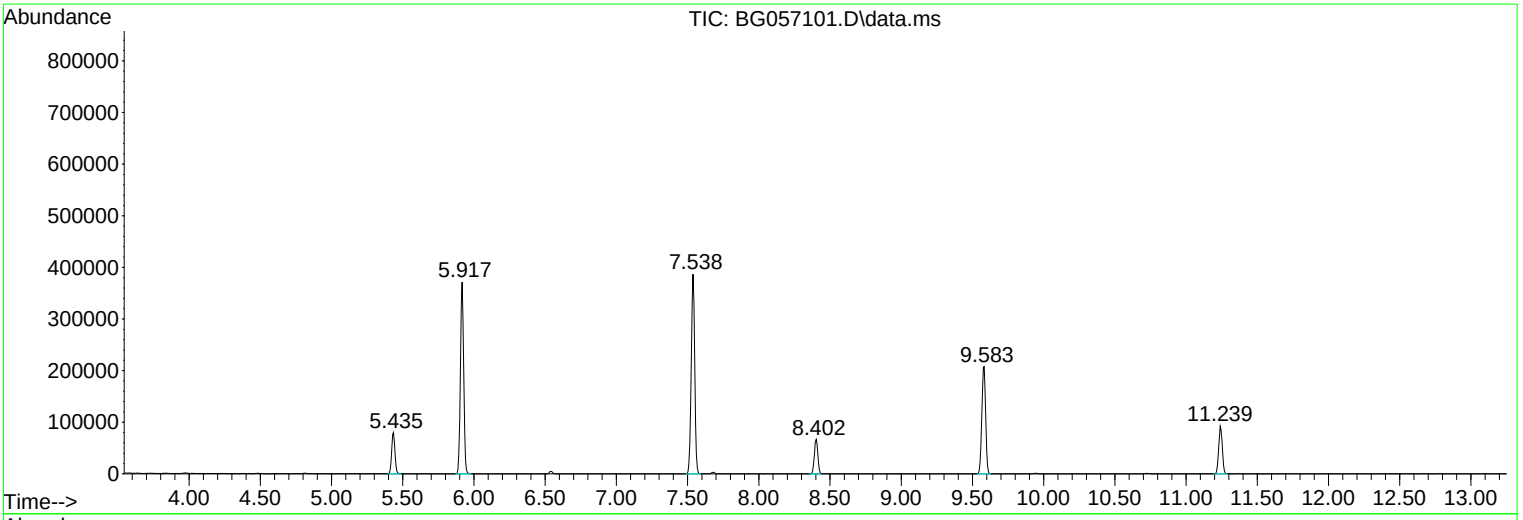
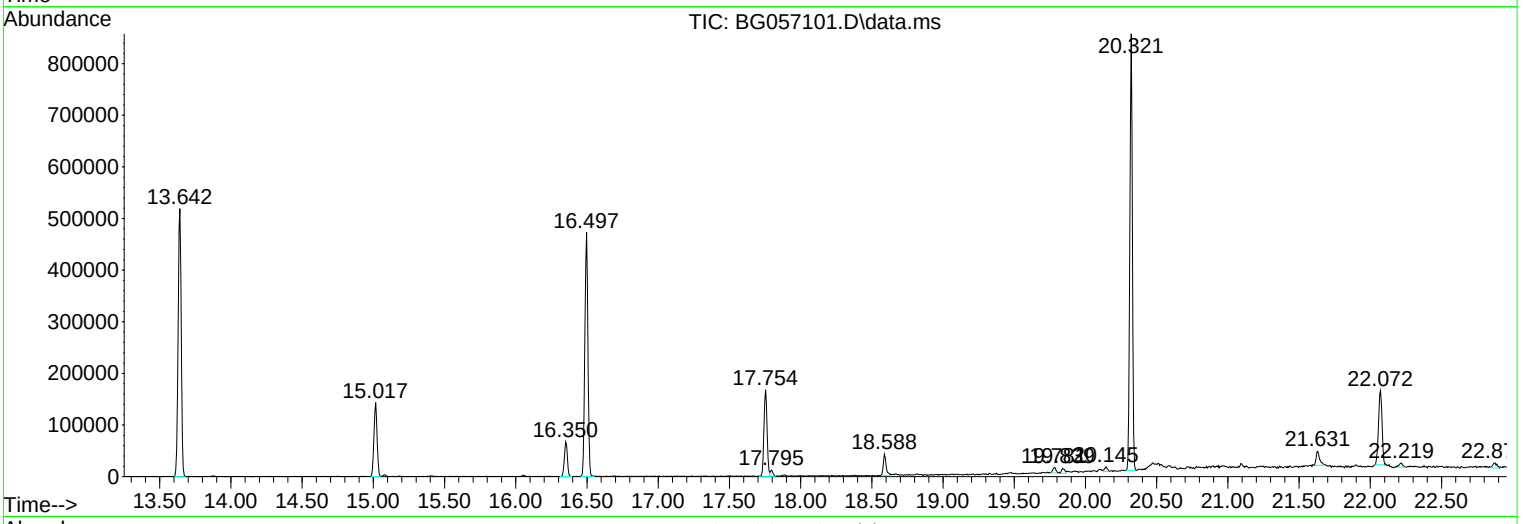
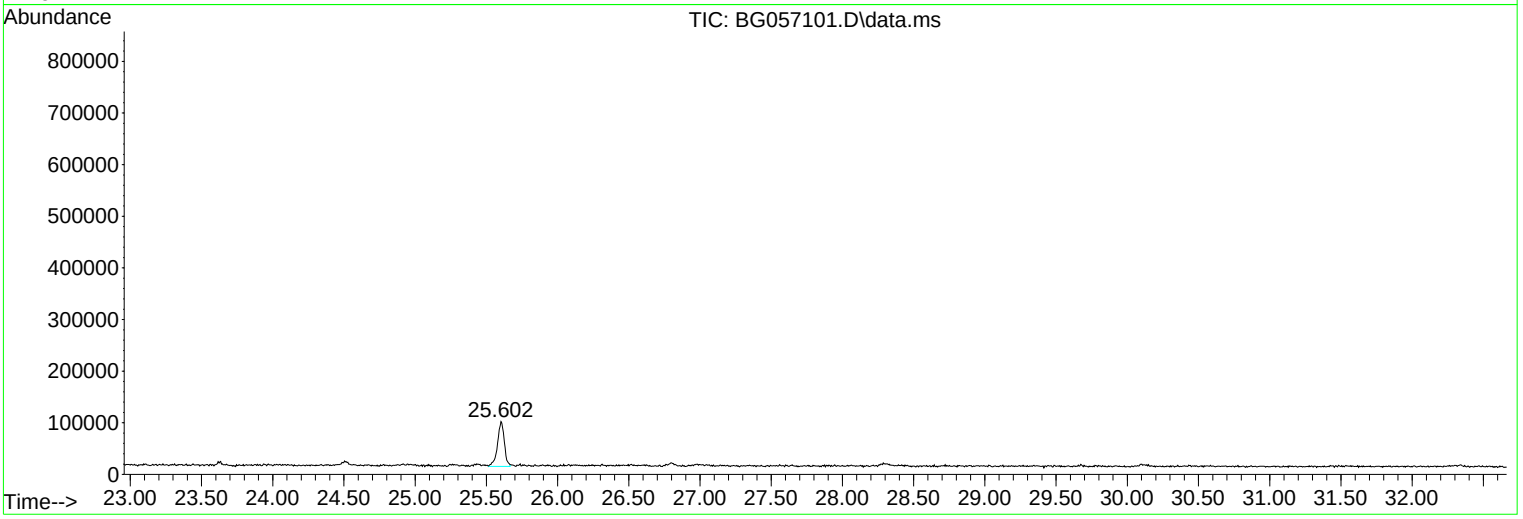
BNA_G
**ClientSampleId :**
20230338-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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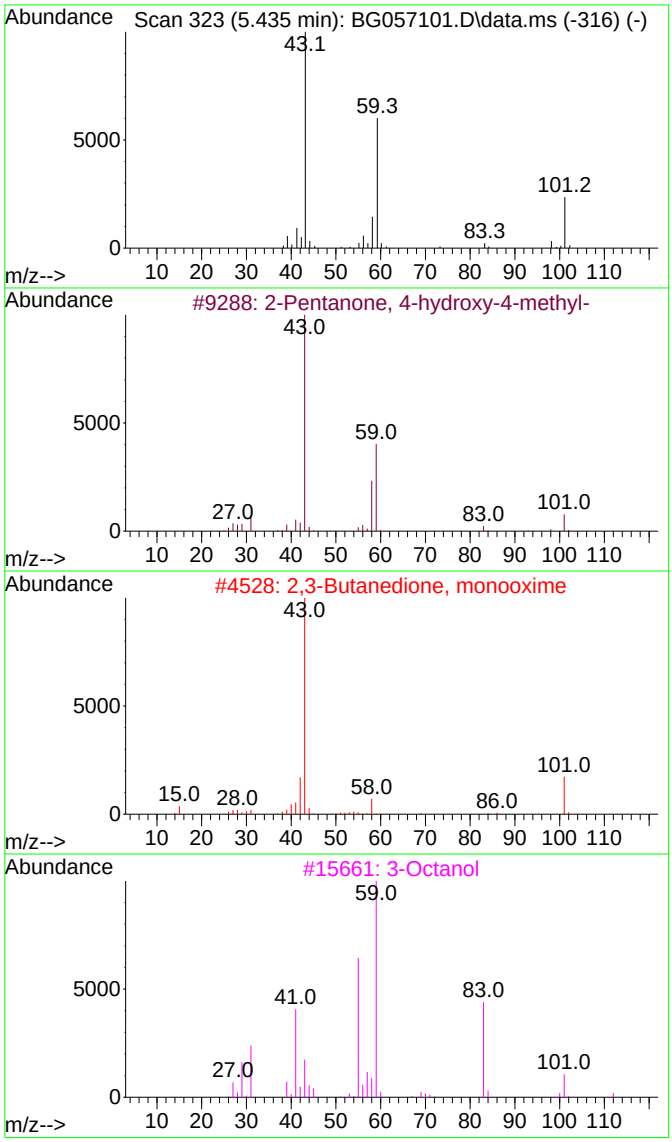
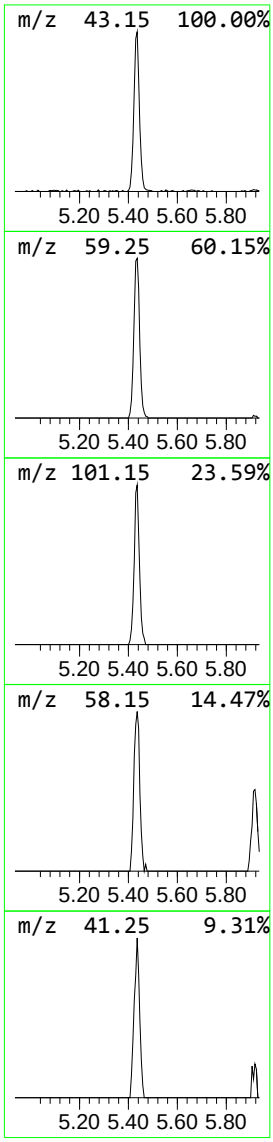
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.435 | 22.89 ng | 128877 | 1,4-Dichlorobenzene-d4 | 8.402 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 3 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 28 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 25 |
| 5 | Butanamide, 2-hydroxy-2,N-dimethyl- | 117 | C5H11NO2 | 039961-72-3 | 25 |



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Sample : 02347-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20230338-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

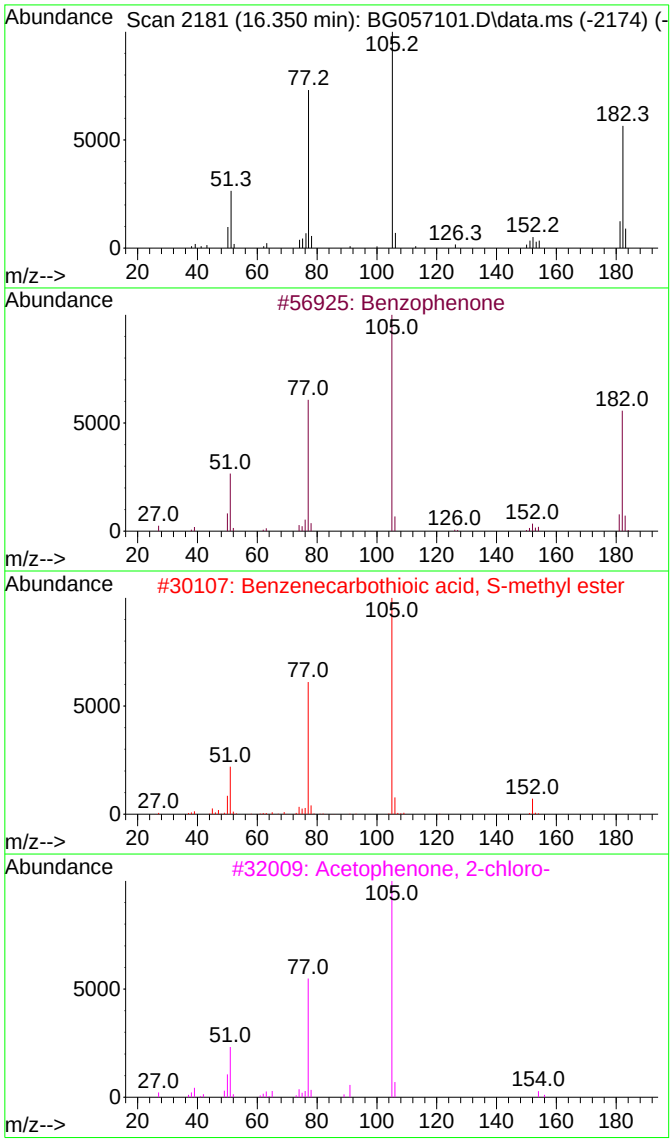
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

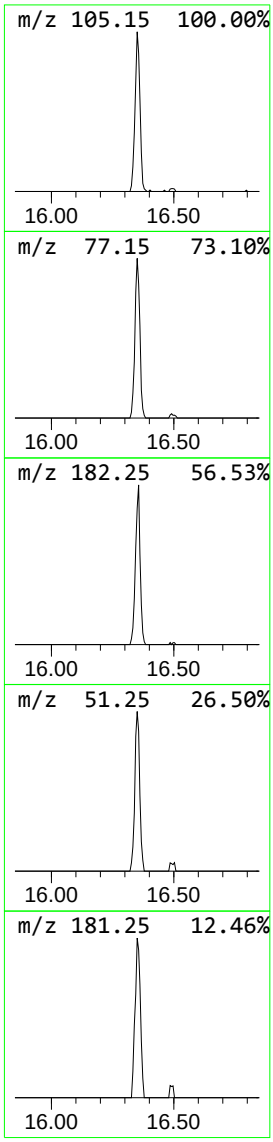
**********

Peak Number 2 Benzophenone Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.350 | 8.88 ng | 95411 | Acenaphthene-d10 | 15.017 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 97 |
| 2 | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS | 005925-68-8 | 46 |
| 3 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 46 |
| 4 | Benzoylformic acid | 150 | C8H6O3 | 000611-73-4 | 43 |
| 5 | Benzoyl isothiocyanate | 163 | C8H5NOS | 000532-55-8 | 38 |



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Operator : CG/JU
Sample : 02347-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
20230338-COMP-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

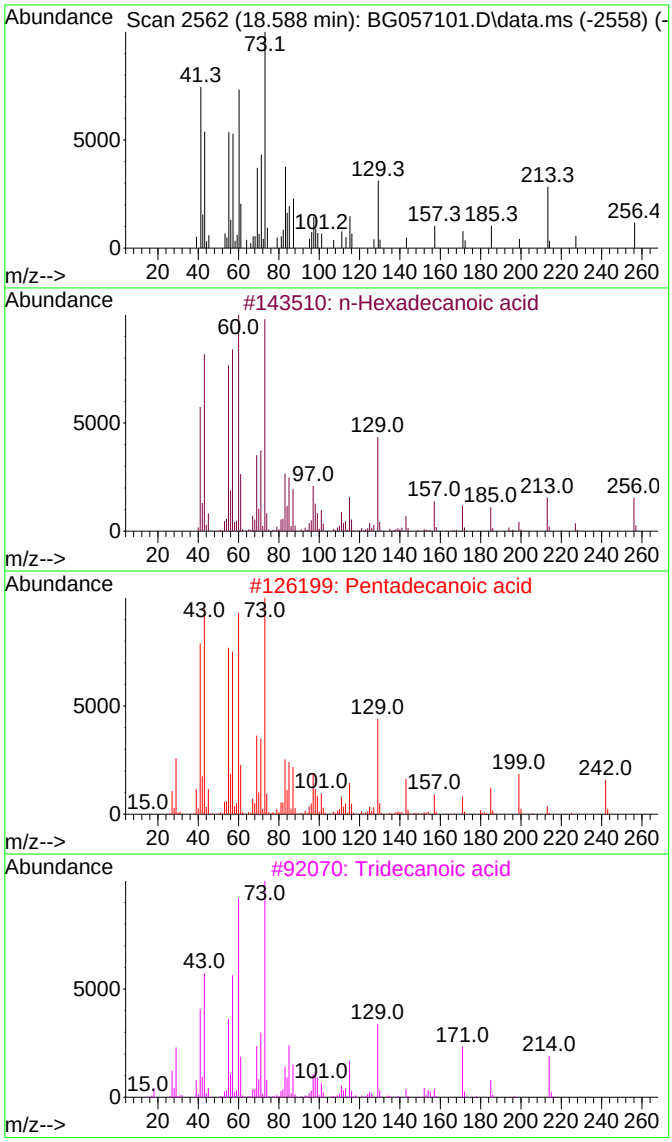
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

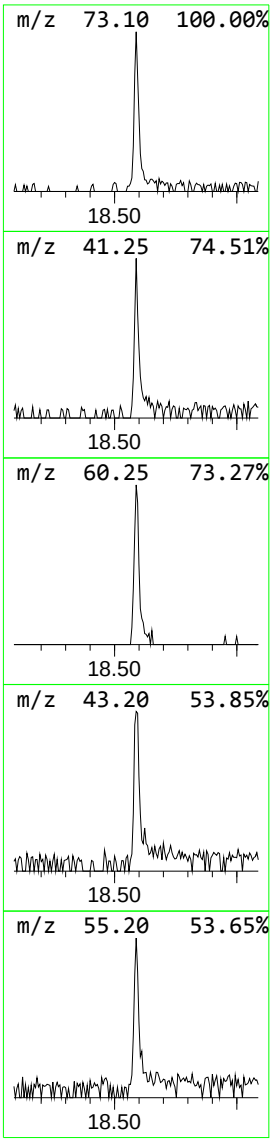
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.588 | 4.51 ng | 58022 | Phenanthrene-d10 | 17.754 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 59 |
| 5 | Trehalose | 342 | C12H22O11 | 000099-20-7 | 47 |



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Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
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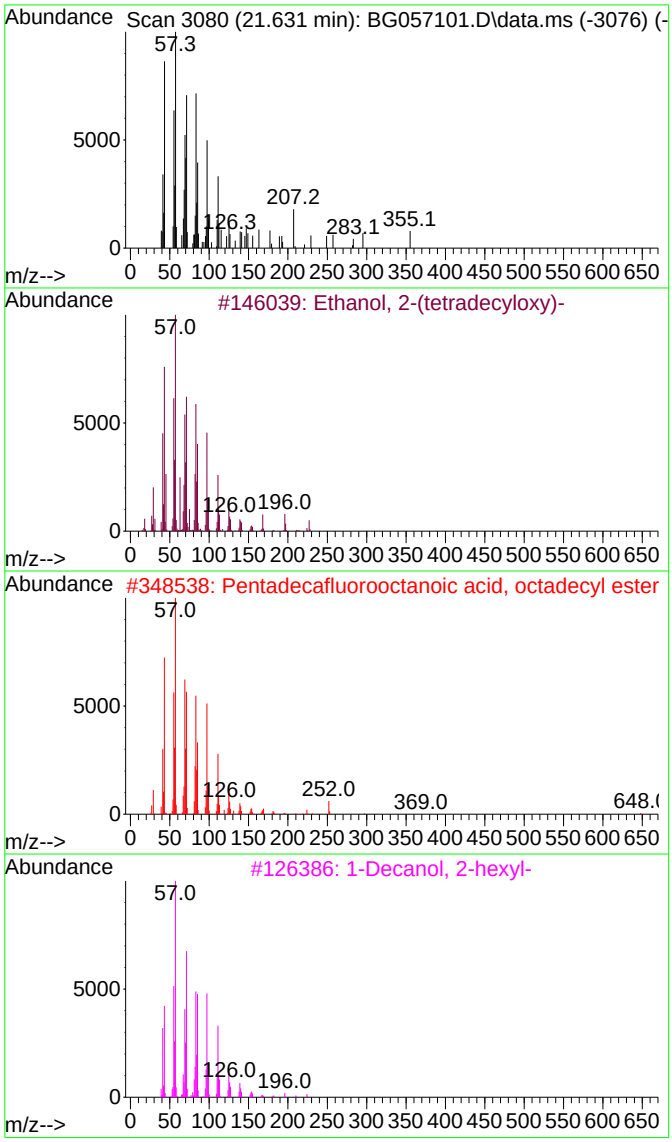
TIC Integration Parameters: LSCINT.P

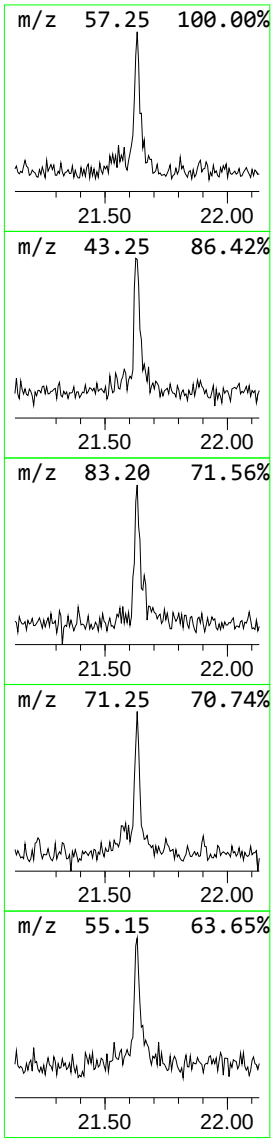
**********

Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.631 | 3.70 ng | 45837 | Chrysene-d12 | 22.072 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 91 |
| 2 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 87 |
| 3 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 87 |
| 4 | Hexadecyl propyl ether | 284 | C19H40O | 1000406-27-9 | 83 |
| 5 | Octadecyl propyl ether | 312 | C21H44O | 1000406-28-0 | 83 |



Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 5.435 | 22.9 | ng | 128877 | 1 | 8.402 | 112618 | 20.0 |
| Benzophenone | 16.350 | 8.9 | ng | 95411 | 3 | 15.017 | 214835 | 20.0 |
| n-Hexadecanoic ... | 18.588 | 4.5 | ng | 58022 | 4 | 17.754 | 257460 | 20.0 |
| Ethanol, 2-(tet... | 21.631 | 3.7 | ng | 45837 | 5 | 22.072 | 247910 | 20.0 |