LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

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_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134070.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.216 | 18 | 22 | 34 | rVB2 | 22257 | 42260 | 3.45% | 0.439% |
| 2 | 5.075 | 504 | 508 | 520 | rVB | 50388 | 61898 | 5.05% | 0.643% |
| 3 | 5.475 | 572 | 576 | 591 | rBV | 1208938 | 1111106 | 90.69% | 11.536% |
| 4 | 6.475 | 742 | 746 | 761 | rBV | 1180309 | 1090737 | 89.02% | 11.325% |
| 5 | 6.845 | 805 | 809 | 819 | rBV | 738108 | 595543 | 48.61% | 6.183% |
| 6 | 7.404 | 900 | 904 | 916 | rBV | 854716 | 704809 | 57.53% | 7.318% |
| 7 | 8.122 | 1023 | 1026 | 1030 | rBV | 814028 | 701828 | 57.28% | 7.287% |
| 8 | 9.198 | 1206 | 1209 | 1213 | rBV | 1522437 | 1225216 | 100.00% | 12.721% |
| 9 | 9.880 | 1322 | 1325 | 1329 | rBV | 786472 | 649522 | 53.01% | 6.744% |
| 10 | 10.598 | 1443 | 1447 | 1454 | rVB | 216848 | 174641 | 14.25% | 1.813% |
| 11 | 10.674 | 1456 | 1460 | 1466 | rBV | 645832 | 576903 | 47.09% | 5.990% |
| 12 | 10.910 | 1496 | 1500 | 1502 | rBV | 40493 | 33666 | 2.75% | 0.350% |
| 13 | 10.986 | 1507 | 1513 | 1517 | rBV | 15727 | 20063 | 1.64% | 0.208% |
| 14 | 11.286 | 1562 | 1564 | 1569 | rVB | 18875 | 15514 | 1.27% | 0.161% |
| 15 | 11.374 | 1575 | 1579 | 1587 | rBV | 669923 | 597725 | 48.79% | 6.206% |
| 16 | 11.904 | 1666 | 1669 | 1674 | rBV | 85965 | 86377 | 7.05% | 0.897% |
| 17 | 12.698 | 1801 | 1804 | 1808 | rBV6 | 17919 | 26467 | 2.16% | 0.275% |
| 18 | 12.974 | 1847 | 1851 | 1854 | rBV | 1043751 | 1004016 | 81.95% | 10.424% |
| 19 | 13.210 | 1888 | 1891 | 1893 | rBV4 | 14445 | 15057 | 1.23% | 0.156% |
| 20 | 14.039 | 2028 | 2032 | 2038 | rVB | 567819 | 535394 | 43.70% | 5.559% |
| 21 | 15.539 | 2283 | 2287 | 2291 | rBV | 281094 | 362792 | 29.61% | 3.767% |

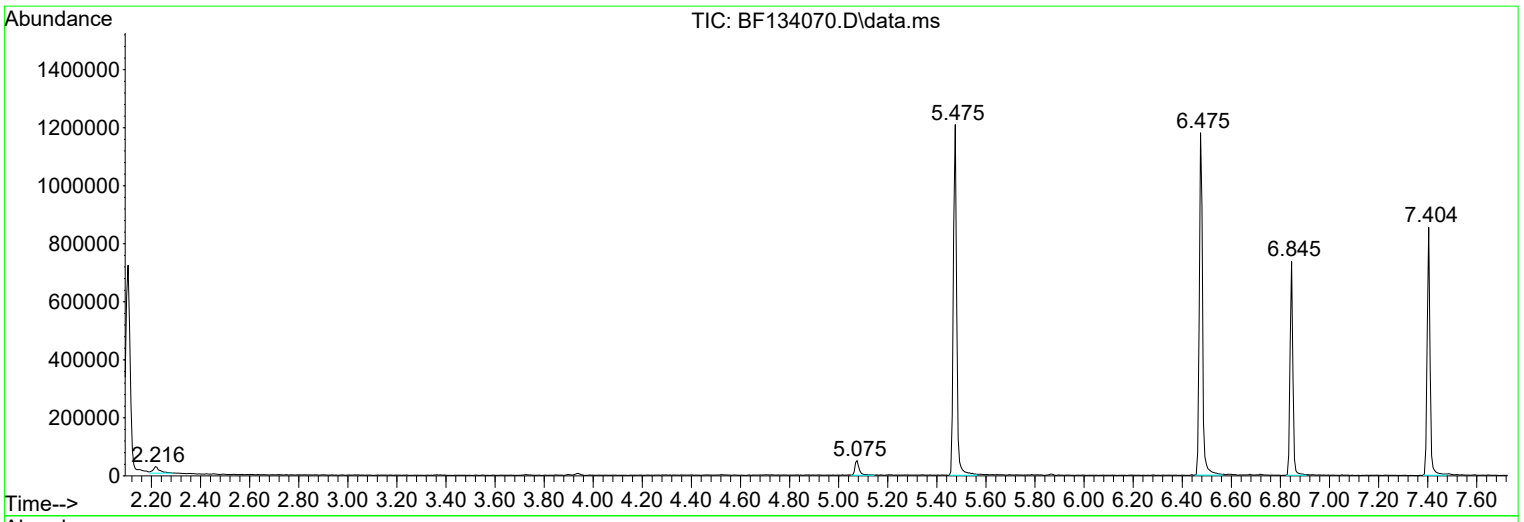
Sum of corrected areas: 9631534

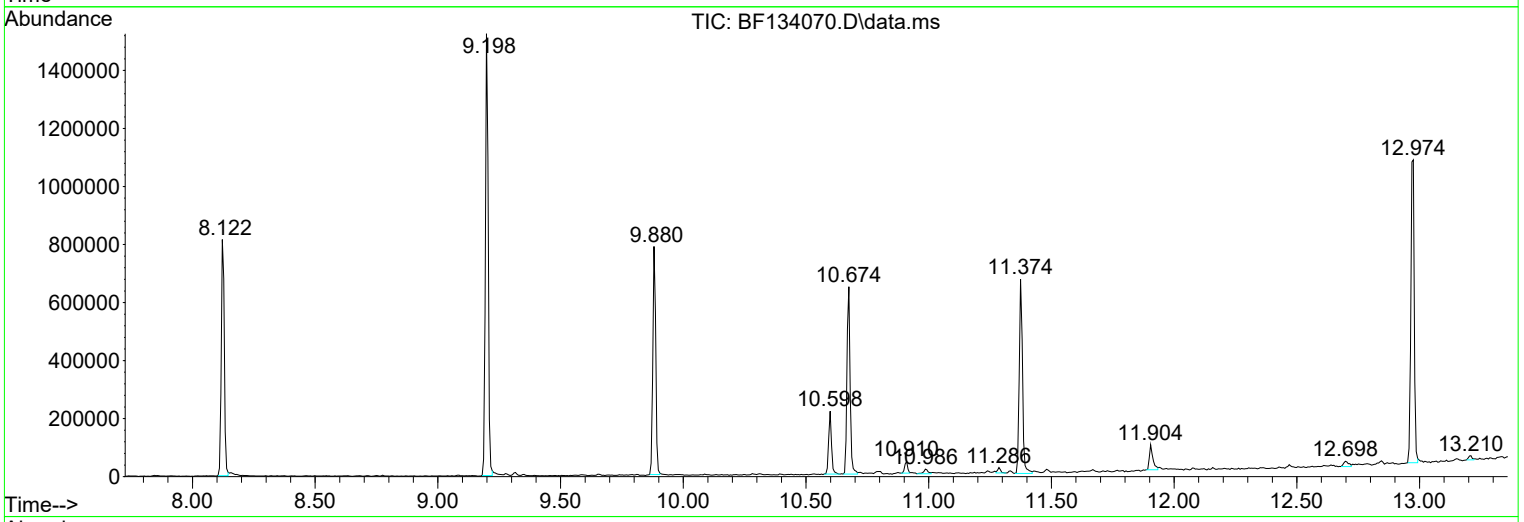
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

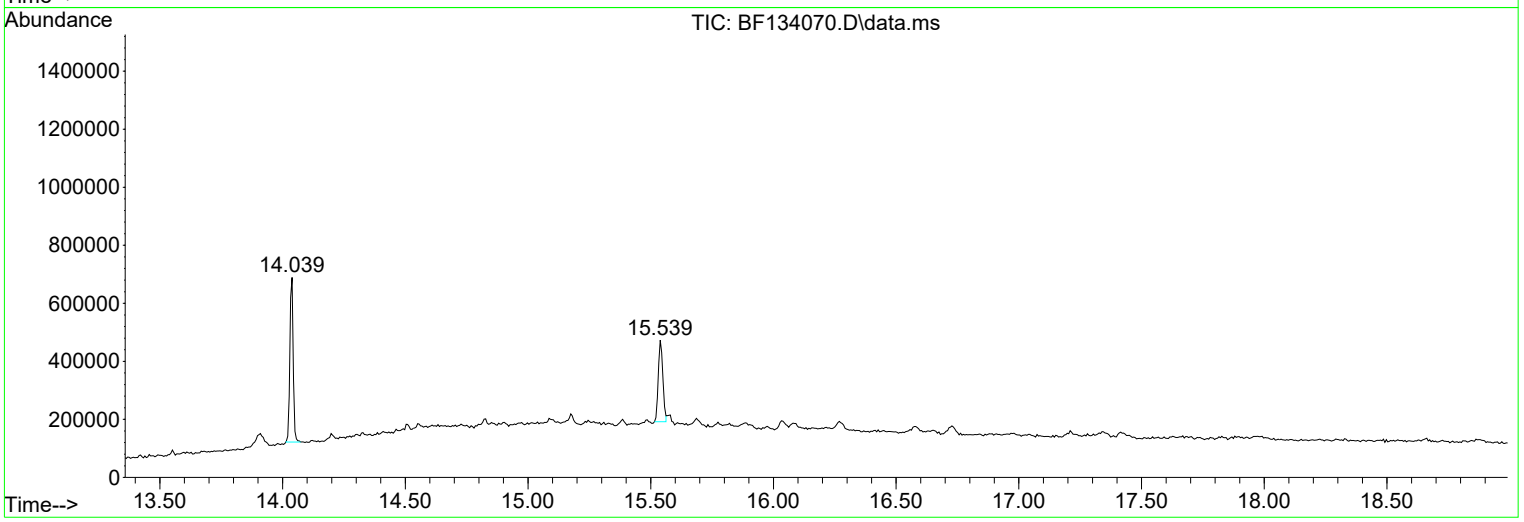
**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

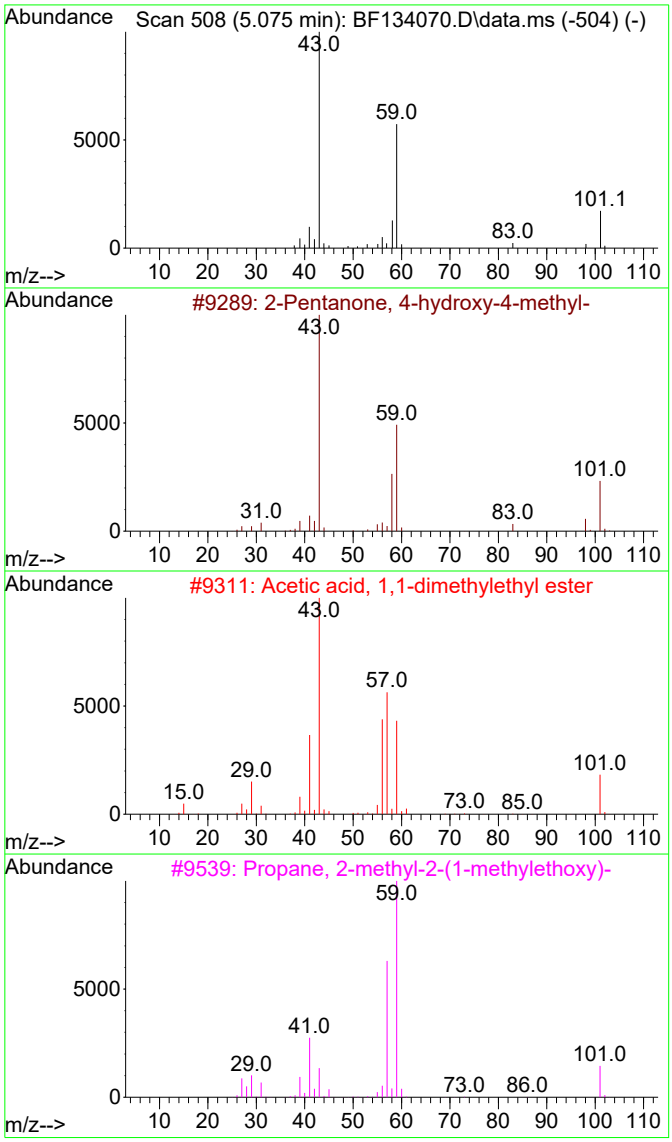
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

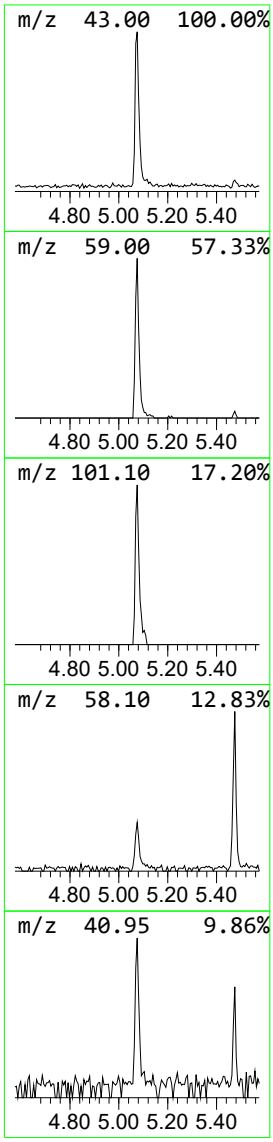
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.075 | 2.08 ng | 61898 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 36 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

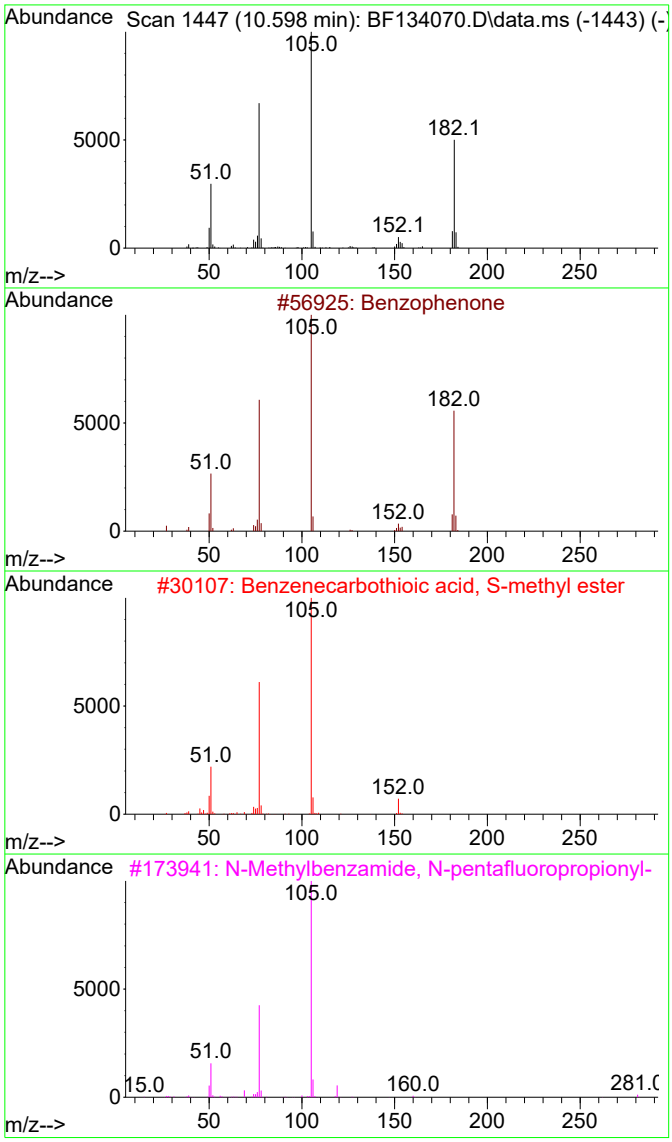
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

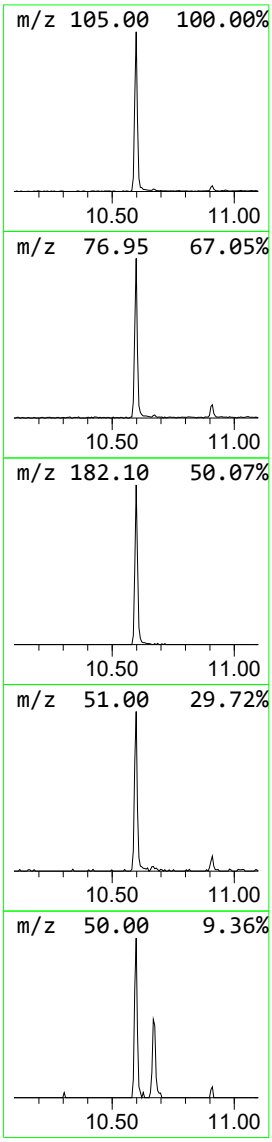
**********

Peak Number 2 Benzophenone Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.598 | 5.38 ng | 174641 | Acenaphthene-d10 | 9.880 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS | 005925-68-8 | 52 |
| 3 | N-Methylbenzamide, N-pentafluoro... | 281 | C11H8F5NO2 | 1000446-98-1 | 50 |
| 4 | Methyl hippurate, N-trifluoroace... | 289 | C12H10F3NO4 | 073749-76-5 | 50 |
| 5 | 1-Propanone, 3-chloro-1-phenyl- | 168 | C9H9ClO | 000936-59-4 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

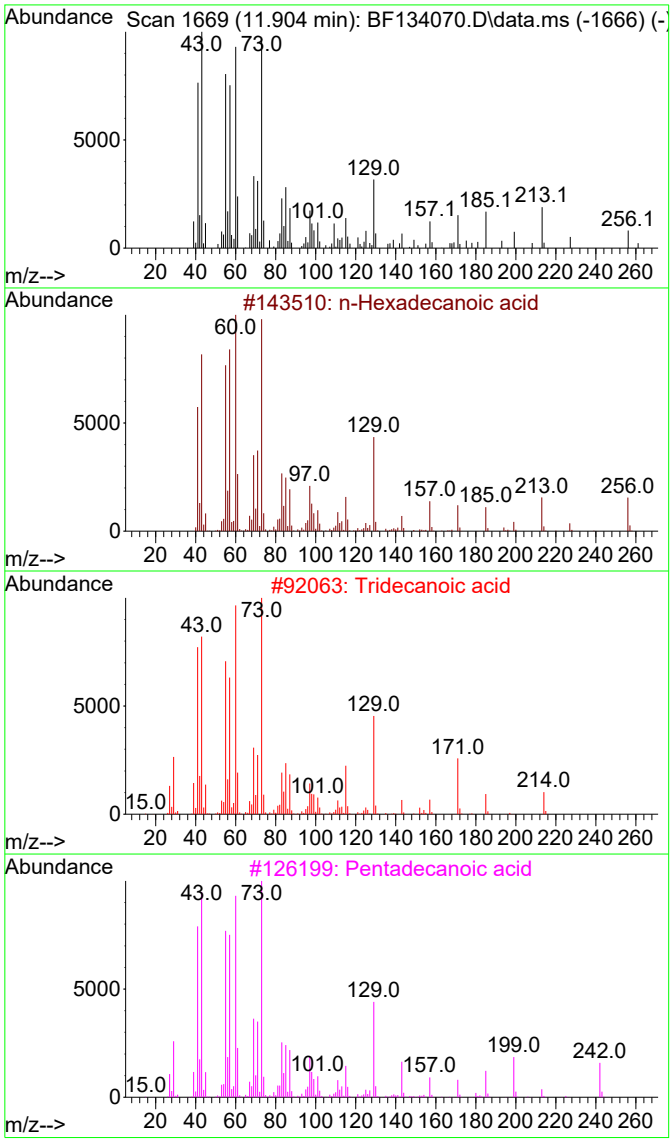
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

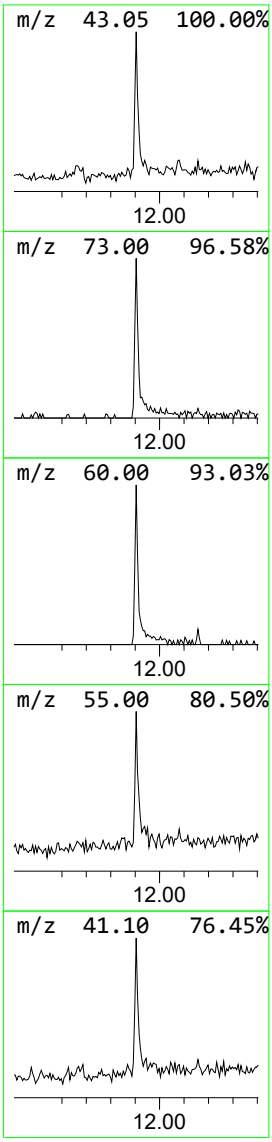
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.904 | 2.89 ng | 86377 | Phenanthrene-d10 | 11.374 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 53 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134070.D
Acq On : 01 Jul 2023 01:28
Operator : CG\JU
Sample : 03428-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PNNL-APM-0621-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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-... | 5.075 | 2.1 | ng | 61898 | 1 | 6.845 | 595543 | 20.0 |
| Benzophenone | 10.598 | 5.4 | ng | 174641 | 3 | 9.880 | 649522 | 20.0 |
| n-Hexadecanoic ... | 11.904 | 2.9 | ng | 86377 | 4 | 11.374 | 597725 | 20.0 |