LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133162.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.922 | 472 | 482 | 487 | rBV | 99444 | 130799 | 3.06% | 0.418% |
| 2 | 5.340 | 548 | 553 | 556 | rBV | 3936090 | 3621288 | 84.85% | 11.580% |
| 3 | 6.369 | 723 | 728 | 731 | rBV | 3805641 | 3792091 | 88.85% | 12.127% |
| 4 | 6.728 | 785 | 789 | 792 | rBV | 1640524 | 1241447 | 29.09% | 3.970% |
| 5 | 7.293 | 880 | 885 | 888 | rBV | 2930063 | 2487142 | 58.28% | 7.954% |
| 6 | 8.010 | 1003 | 1007 | 1011 | rBV | 2147271 | 1739989 | 40.77% | 5.564% |
| 7 | 9.092 | 1186 | 1191 | 1194 | rBV | 4620579 | 4267757 | 100.00% | 13.648% |
| 8 | 9.763 | 1299 | 1305 | 1308 | rBV | 2439383 | 1968201 | 46.12% | 6.294% |
| 9 | 10.475 | 1423 | 1426 | 1430 | rVB | 326077 | 264948 | 6.21% | 0.847% |
| 10 | 10.551 | 1435 | 1439 | 1442 | rBV | 2811070 | 2428921 | 56.91% | 7.767% |
| 11 | 10.692 | 1458 | 1463 | 1466 | rBV | 43733 | 55117 | 1.29% | 0.176% |
| 12 | 11.245 | 1553 | 1557 | 1560 | rBV | 2401831 | 1953536 | 45.77% | 6.247% |
| 13 | 11.780 | 1645 | 1648 | 1652 | rBV | 331498 | 342332 | 8.02% | 1.095% |
| 14 | 12.569 | 1779 | 1782 | 1785 | rBV2 | 99505 | 99372 | 2.33% | 0.318% |
| 15 | 12.833 | 1823 | 1827 | 1830 | rBV | 4356681 | 4028888 | 94.40% | 12.884% |
| 16 | 13.074 | 1866 | 1868 | 1872 | rBV | 57197 | 45851 | 1.07% | 0.147% |
| 17 | 13.745 | 1980 | 1982 | 1984 | rBV | 76032 | 79472 | 1.86% | 0.254% |
| 18 | 13.880 | 2001 | 2005 | 2011 | rVB | 1355943 | 1194642 | 27.99% | 3.820% |
| 19 | 14.063 | 2033 | 2036 | 2039 | rBV | 73751 | 68457 | 1.60% | 0.219% |
| 20 | 14.369 | 2085 | 2088 | 2092 | rBV | 83182 | 81699 | 1.91% | 0.261% |
| 21 | 14.410 | 2092 | 2095 | 2101 | rBV8 | 60010 | 120693 | 2.83% | 0.386% |
| 22 | 14.986 | 2191 | 2193 | 2197 | rVB2 | 103543 | 103508 | 2.43% | 0.331% |
| 23 | 15.298 | 2242 | 2246 | 2252 | rVB | 966333 | 1049435 | 24.59% | 3.356% |
| 24 | 15.763 | 2321 | 2325 | 2331 | rBV | 80982 | 105257 | 2.47% | 0.337% |

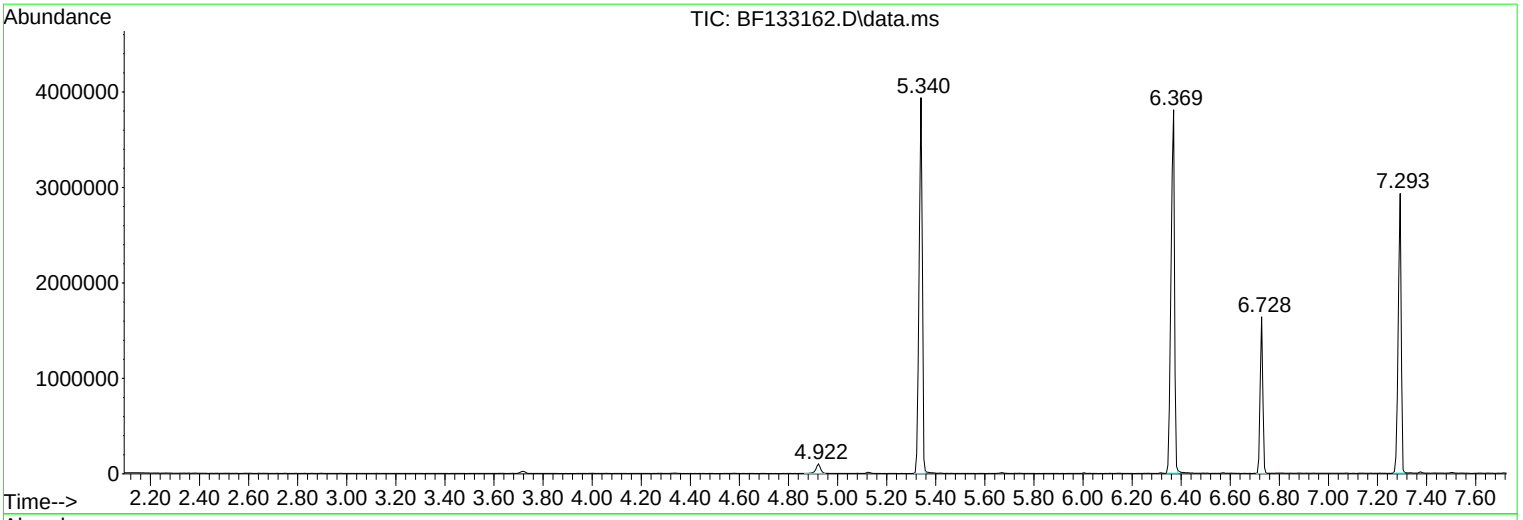
Sum of corrected areas: 31270842

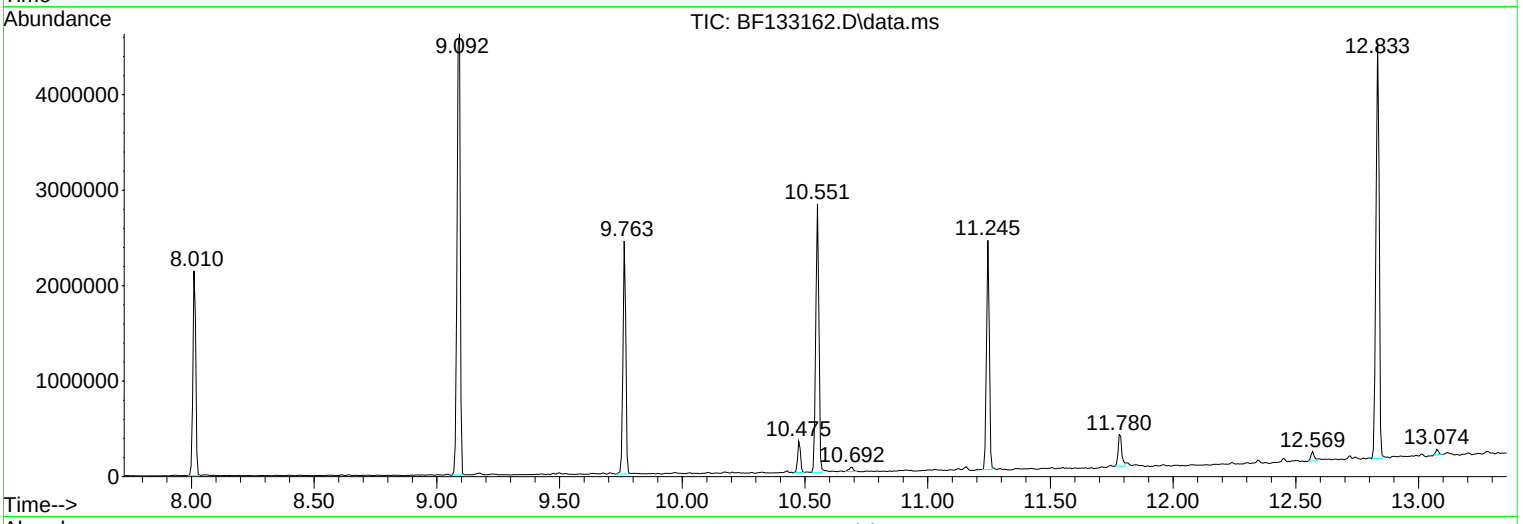
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

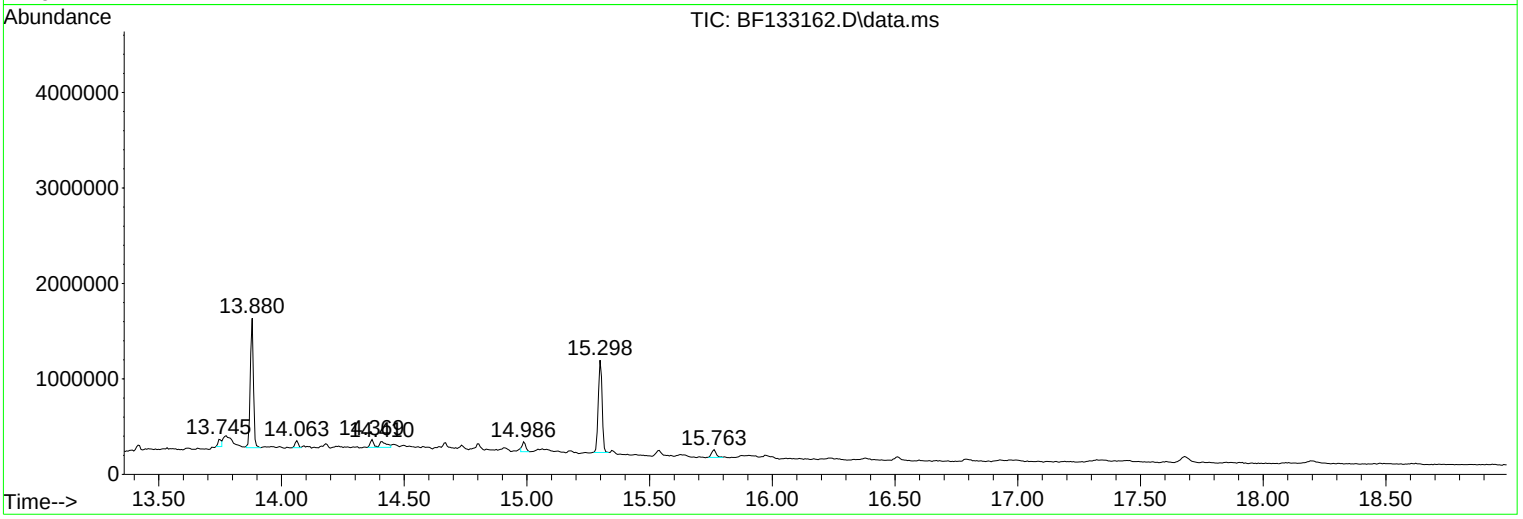
**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

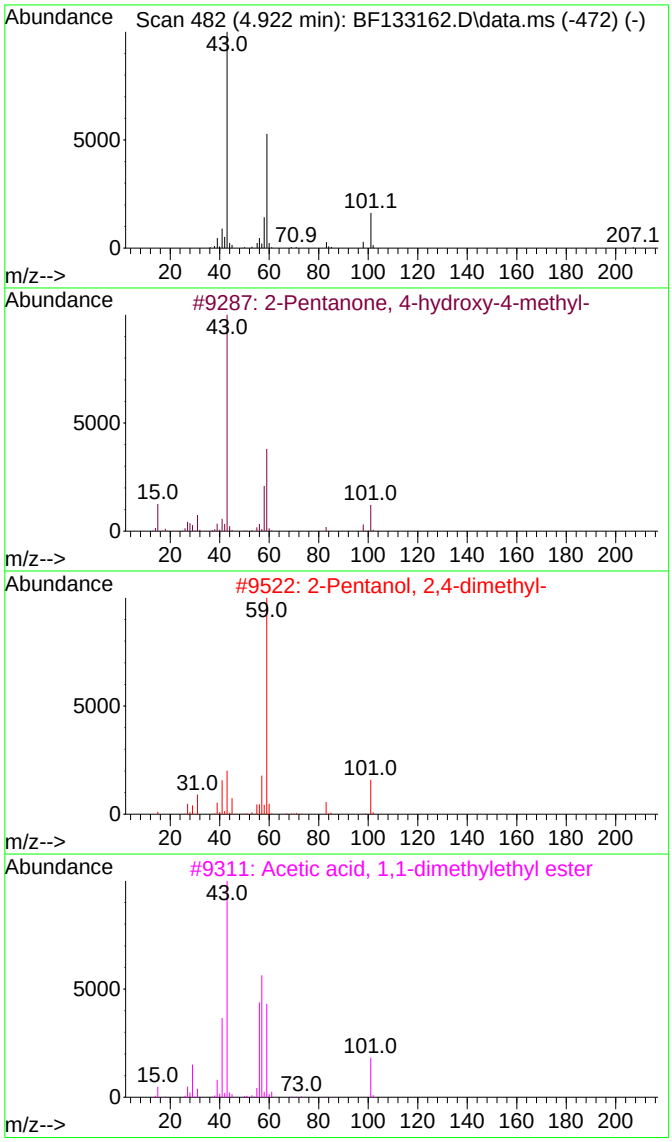
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

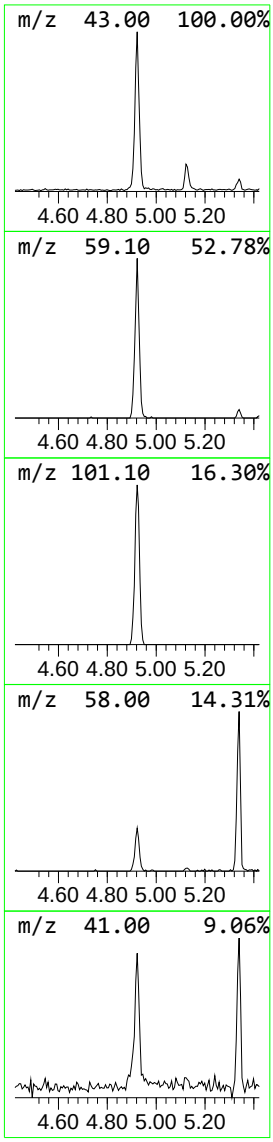
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.922 | 2.11 ng | 130799 | 1,4-Dichlorobenzene-d4 | 6.728 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 42 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 25 |
| 5 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 23 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

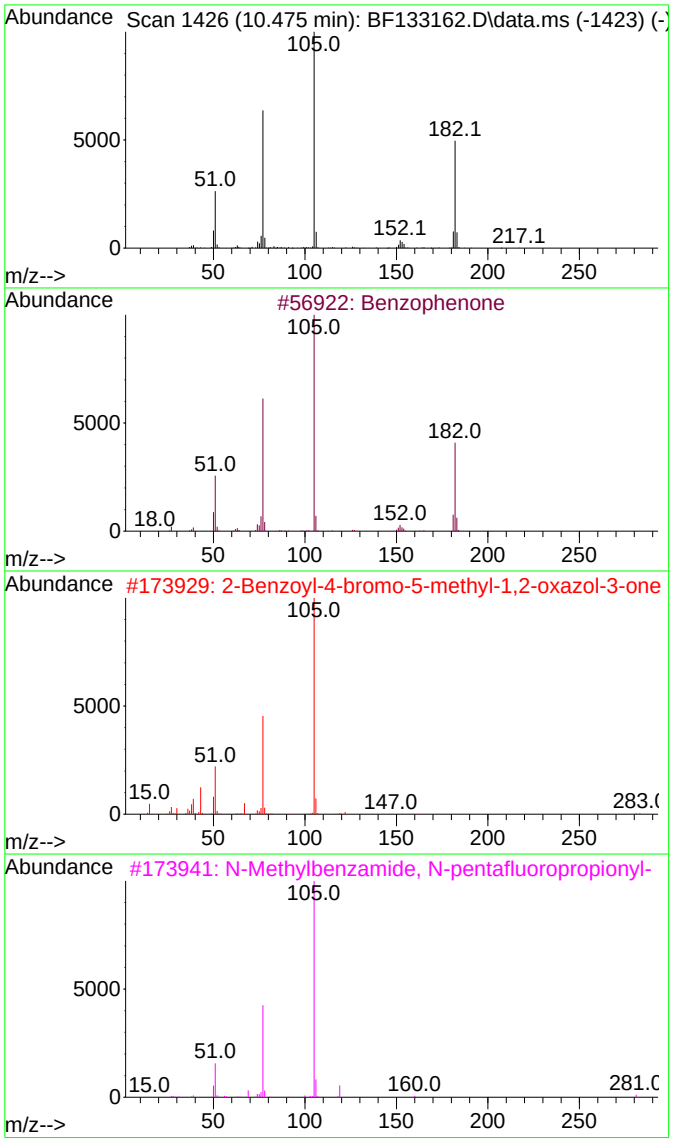
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

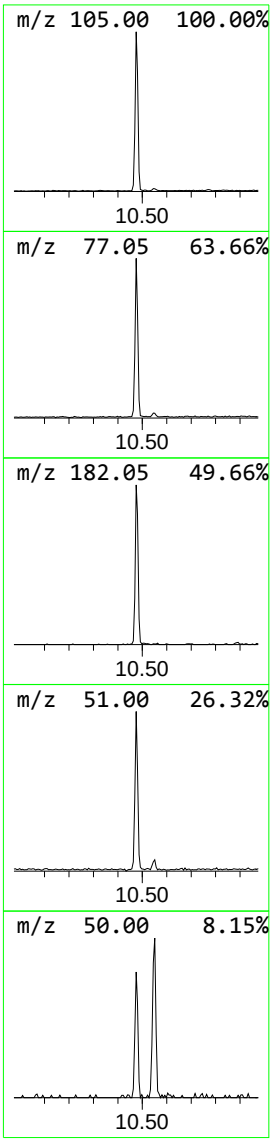
**********

Peak Number 2 Benzophenone Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.475 | 2.69 ng | 264948 | Acenaphthene-d10 | 9.763 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | 2-Benzoyl-4-bromo-5-methyl-1,2-o... | 281 | C11H8BrNO3 | 1000444-92-3 | 47 |
| 3 | N-Methylbenzamide, N-pentafluoro... | 281 | C11H8F5NO2 | 1000446-98-1 | 47 |
| 4 | Vinyl benzoate | 148 | C9H8O2 | 000769-78-8 | 47 |
| 5 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

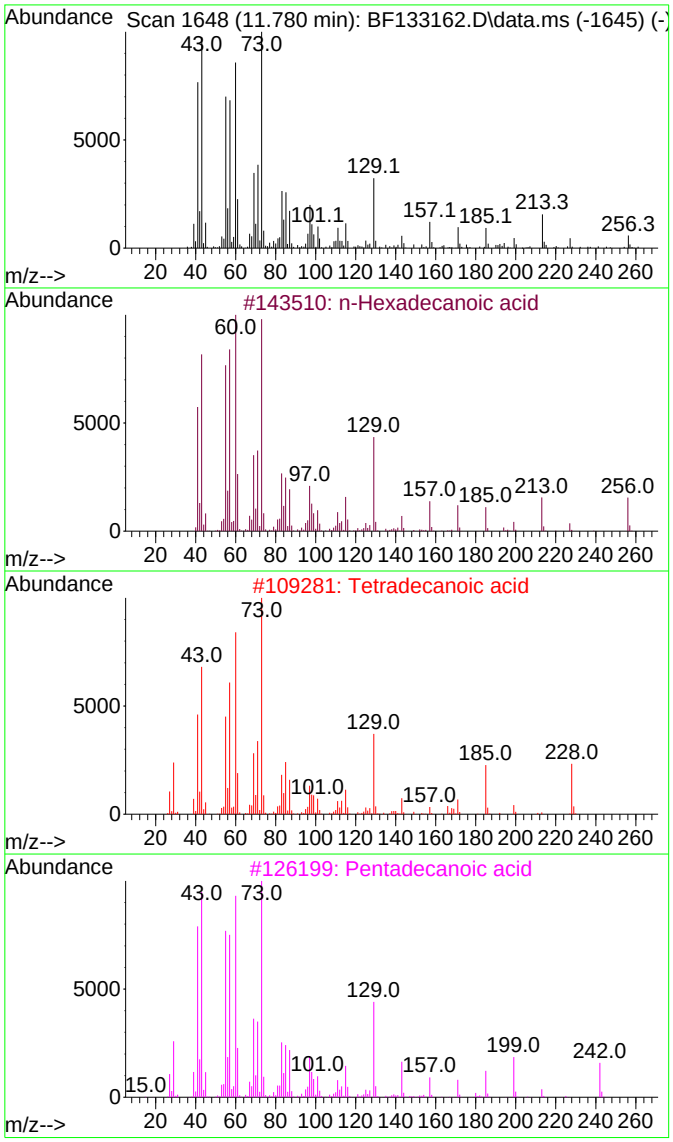
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

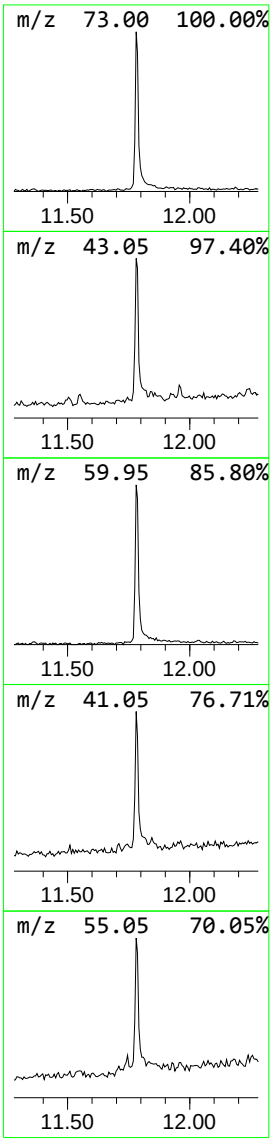
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.781 | 3.50 ng | 342332 | Phenanthrene-d10 | 11.245 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 94 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 87 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

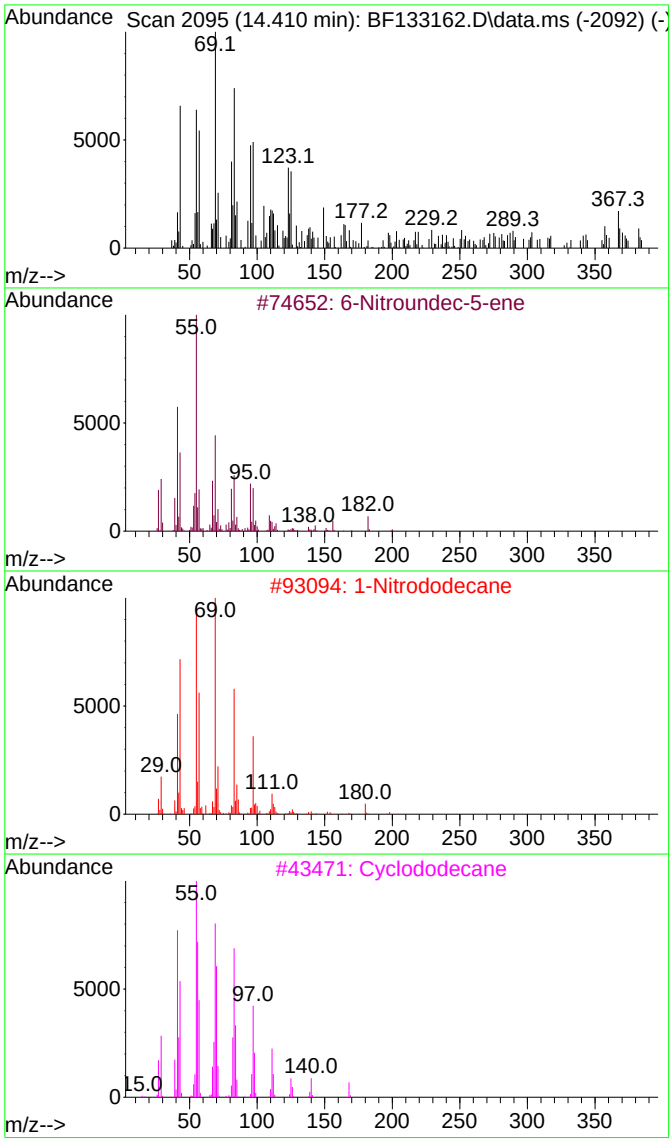
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

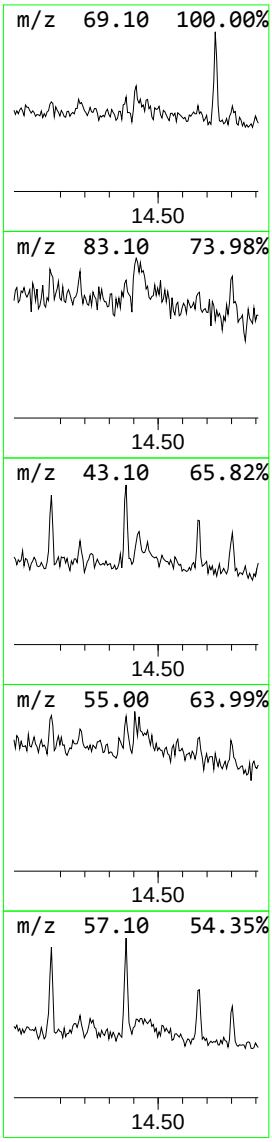
**********

Peak Number 4 6-Nitroundec-5-ene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.410 | 2.02 ng | 120693 | Chrysene-d12 | 13.880 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Nitroundec-5-ene | 199 | C11H21NO2 | 1000192-40-3 | 59 |
| 2 | 1-Nitrododecane | 215 | C12H25NO2 | 016891-99-9 | 47 |
| 3 | Cyclododecane | 168 | C12H24 | 000294-62-2 | 47 |
| 4 | Cyclohexane, 3-ethyl-5-methyl-1-... | 168 | C12H24 | 1000151-39-5 | 43 |
| 5 | 1-Tridecene | 182 | C13H26 | 002437-56-1 | 30 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

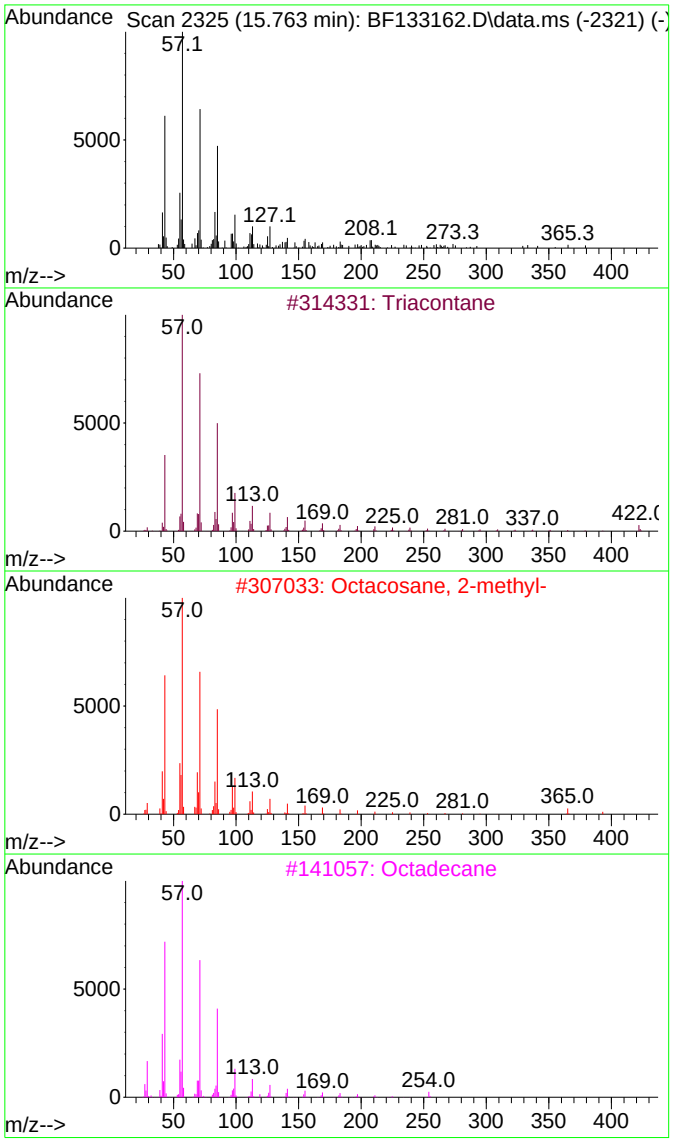
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

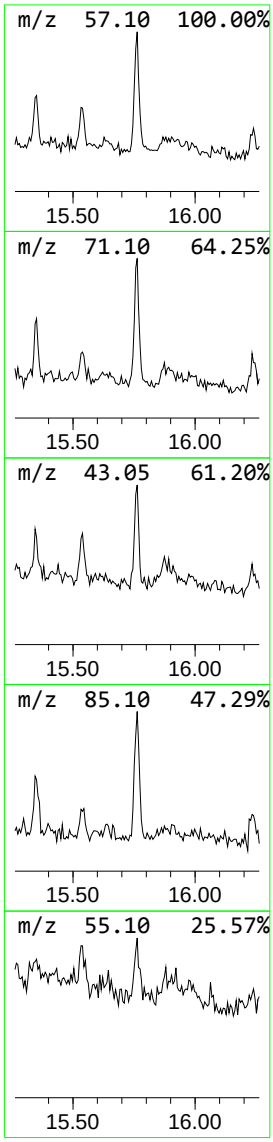
**********

Peak Number 5 Triacontane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.762 | 2.01 ng | 105257 | Perylene-d12 | 15.298 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triacontane | 422 | C30H62 | 000638-68-6 | 90 |
| 2 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 87 |
| 3 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |
| 4 | 4-Methylheneicosane | 310 | C22H46 | 025117-29-7 | 87 |
| 5 | Pentadecane | 212 | C15H32 | 000629-62-9 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133162.D
Acq On : 01 May 2023 18:37
Operator : CG\JU
Sample : 02558-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P001-SS013-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-... | 4.922 | 2.1 | ng | 130799 | 1 | 6.728 | 1241450 | 20.0 |
| Benzophenone | 10.475 | 2.7 | ng | 264948 | 3 | 9.763 | 1968200 | 20.0 |
| n-Hexadecanoic ... | 11.781 | 3.5 | ng | 342332 | 4 | 11.245 | 1953540 | 20.0 |
| 6-Nitroundec-5-ene | 14.410 | 2.0 | ng | 120693 | 5 | 13.880 | 1194640 | 20.0 |
| Triacontane | 15.762 | 2.0 | ng | 105257 | 6 | 15.298 | 1049440 | 20.0 |