LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129757.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.475 | 539 | 542 | 554 | rBV | 272825 | 292871 | 2.76% | 0.989% |
| 2 | 6.493 | 712 | 715 | 724 | rBV | 263911 | 268744 | 2.53% | 0.907% |
| 3 | 6.834 | 769 | 773 | 776 | rBV | 677350 | 618080 | 5.83% | 2.086% |
| 4 | 7.393 | 865 | 868 | 876 | rBV | 184324 | 161040 | 1.52% | 0.544% |
| 5 | 8.116 | 987 | 991 | 994 | rBV | 827661 | 722011 | 6.81% | 2.437% |
| 6 | 9.187 | 1169 | 1173 | 1176 | rBV | 410984 | 326617 | 3.08% | 1.103% |
| 7 | 9.869 | 1283 | 1289 | 1292 | rBV | 1039316 | 811719 | 7.65% | 2.740% |
| 8 | 10.663 | 1421 | 1424 | 1427 | rBV | 225839 | 195305 | 1.84% | 0.659% |
| 9 | 11.363 | 1539 | 1543 | 1545 | rBV | 980451 | 901436 | 8.50% | 3.043% |
| 10 | 11.381 | 1545 | 1546 | 1550 | rVB | 167761 | 141718 | 1.34% | 0.478% |
| 11 | 11.739 | 1603 | 1607 | 1610 | rBV | 2771541 | 2126504 | 20.04% | 7.179% |
| 12 | 11.880 | 1629 | 1631 | 1638 | rVB3 | 253259 | 277243 | 2.61% | 0.936% |
| 13 | 11.975 | 1644 | 1647 | 1650 | rBV3 | 113976 | 122486 | 1.15% | 0.413% |
| 14 | 12.439 | 1719 | 1726 | 1727 | rBV | 9125811 | 10608780 | 100.00% | 35.812% |
| 15 | 12.457 | 1727 | 1729 | 1734 | rVB2 | 8009381 | 6947577 | 65.49% | 23.453% |
| 16 | 12.533 | 1739 | 1742 | 1746 | rVB | 1932734 | 1545465 | 14.57% | 5.217% |
| 17 | 12.580 | 1746 | 1750 | 1752 | rBV | 833223 | 952994 | 8.98% | 3.217% |
| 18 | 12.810 | 1786 | 1789 | 1795 | rVB | 365723 | 403767 | 3.81% | 1.363% |
| 19 | 12.945 | 1809 | 1812 | 1815 | rVB | 497453 | 385324 | 3.63% | 1.301% |
| 20 | 13.257 | 1863 | 1865 | 1871 | rVB | 186573 | 162026 | 1.53% | 0.547% |
| 21 | 13.927 | 1976 | 1979 | 1985 | rBV | 224996 | 245880 | 2.32% | 0.830% |
| 22 | 14.010 | 1989 | 1993 | 1996 | rBV2 | 813716 | 912291 | 8.60% | 3.080% |
| 23 | 15.486 | 2242 | 2244 | 2249 | rVB | 418205 | 493296 | 4.65% | 1.665% |

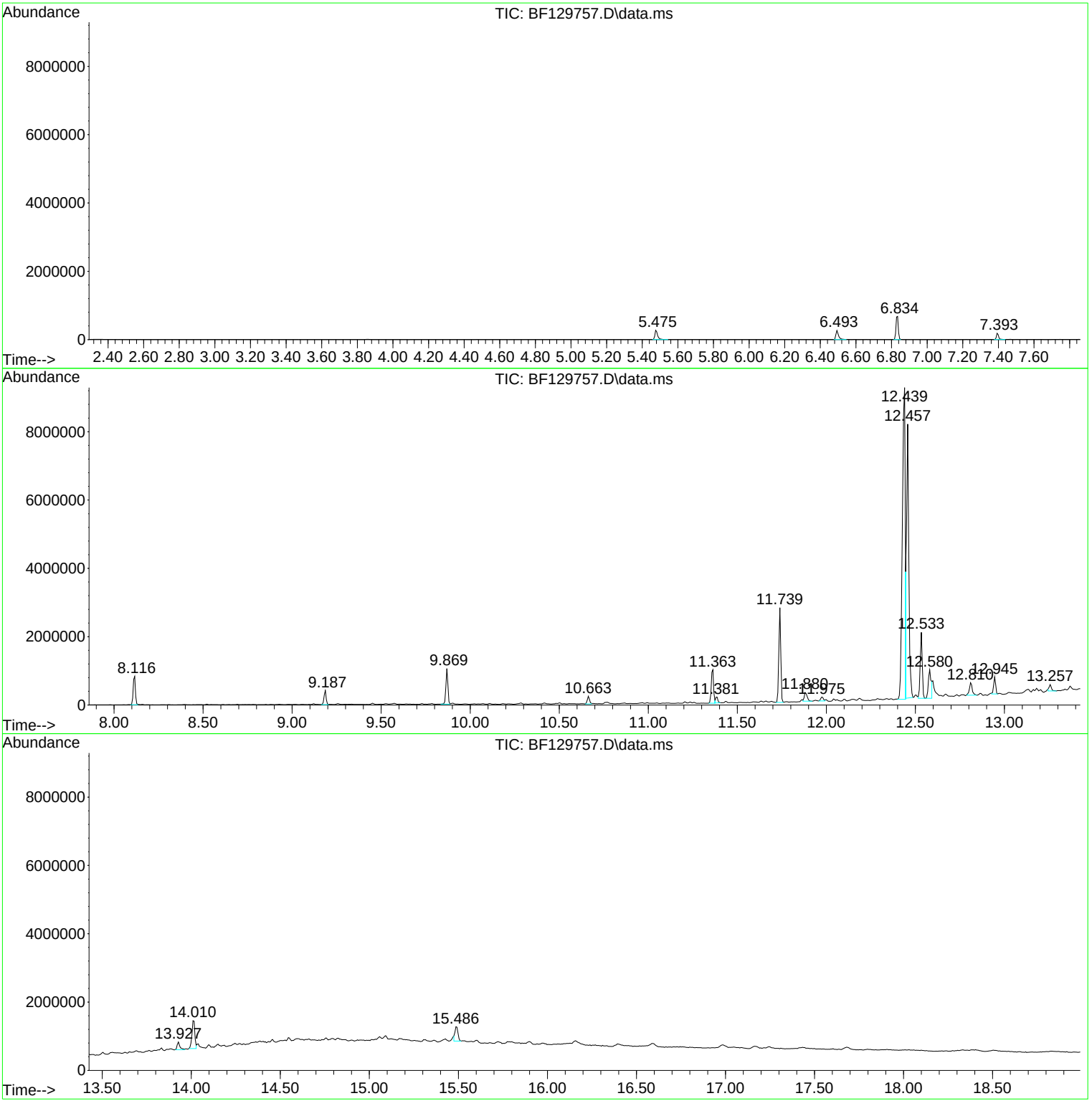
Sum of corrected areas: 29623174

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

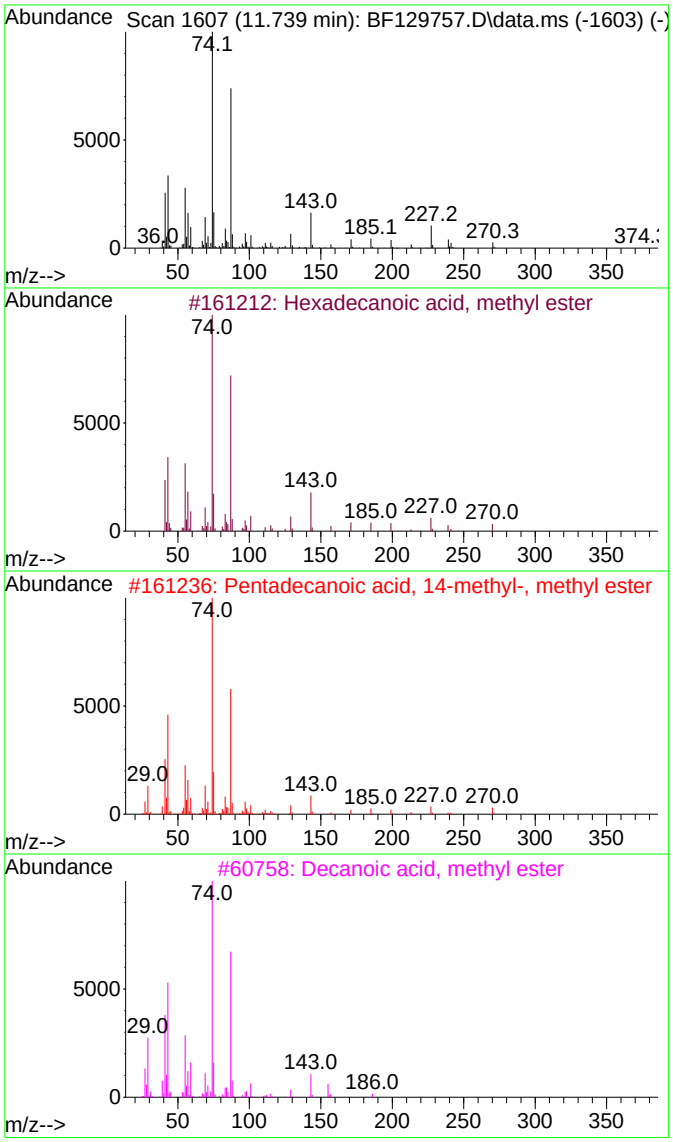
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

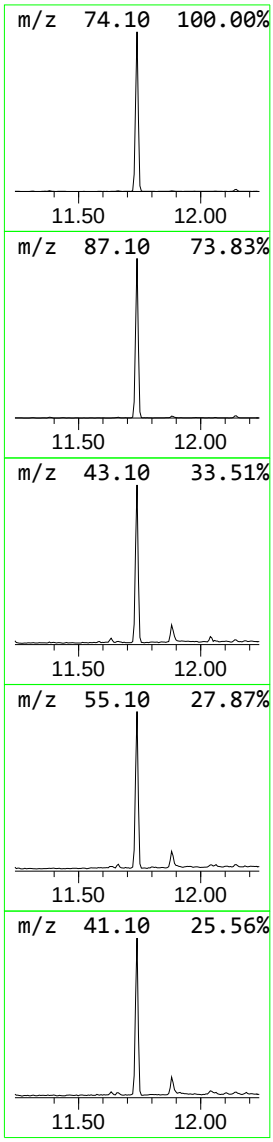
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.739 | 47.18 ng | 2126500 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 98 |
| 2 | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 93 |
| 3 | Decanoic acid, methyl ester | 186 | C11H22O2 | 000110-42-9 | 87 |
| 4 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 86 |
| 5 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

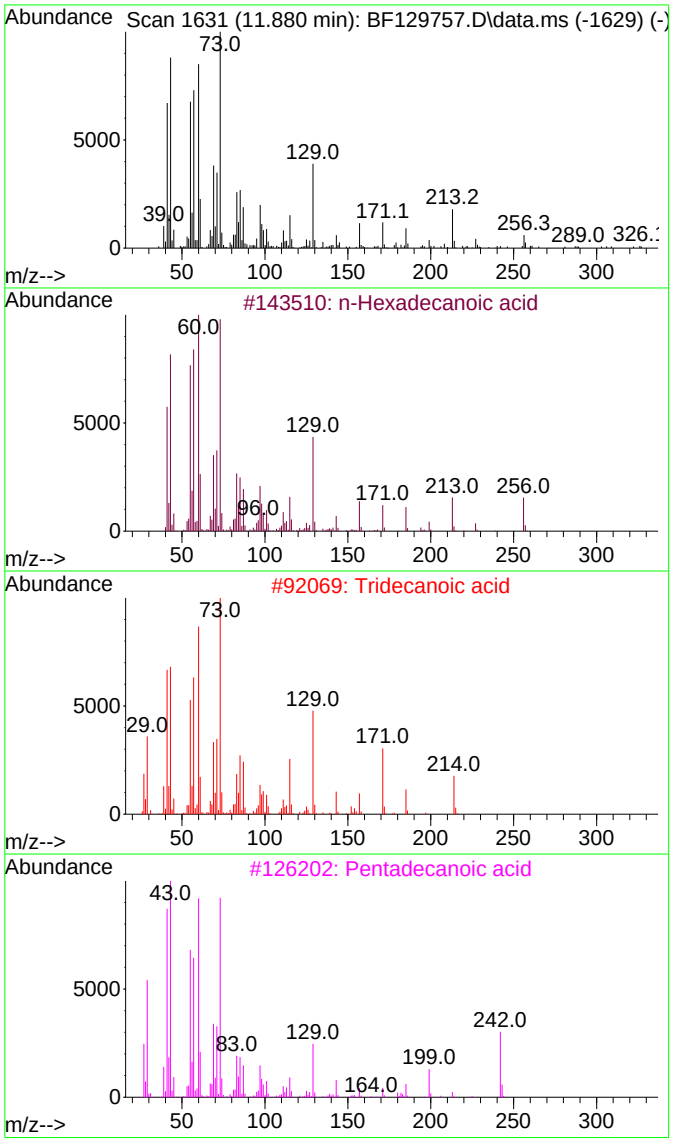
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

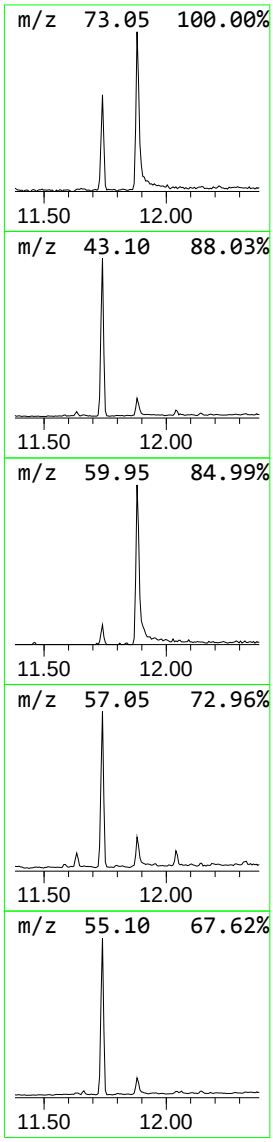
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.881 | 6.15 ng | 277243 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 96 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

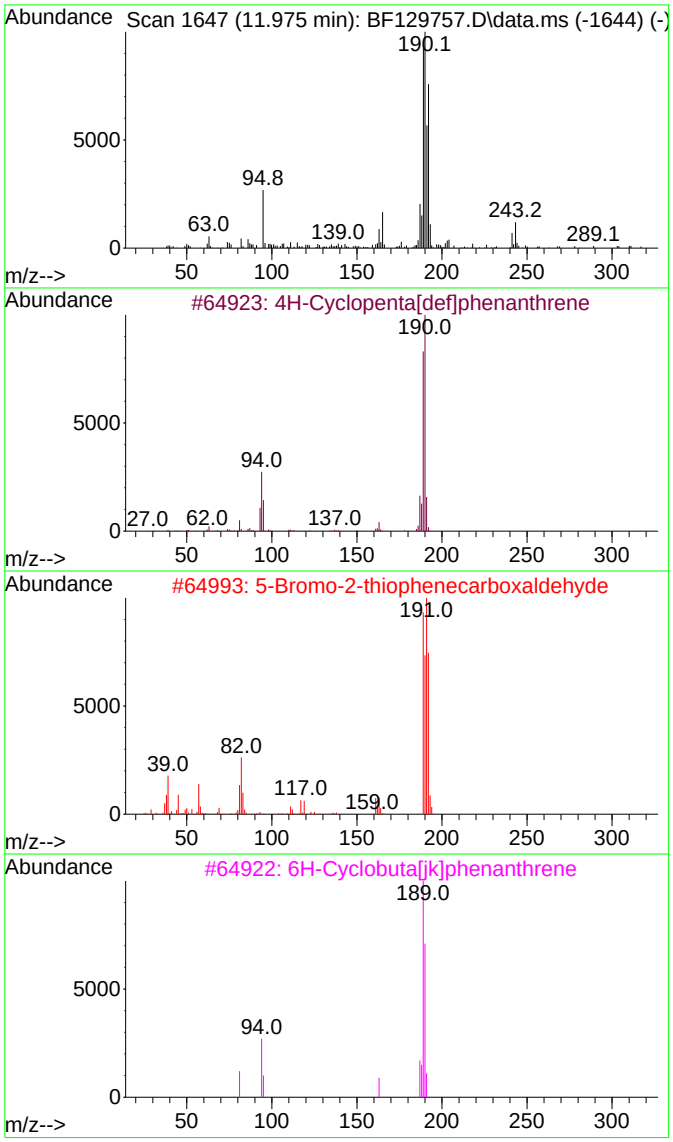
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

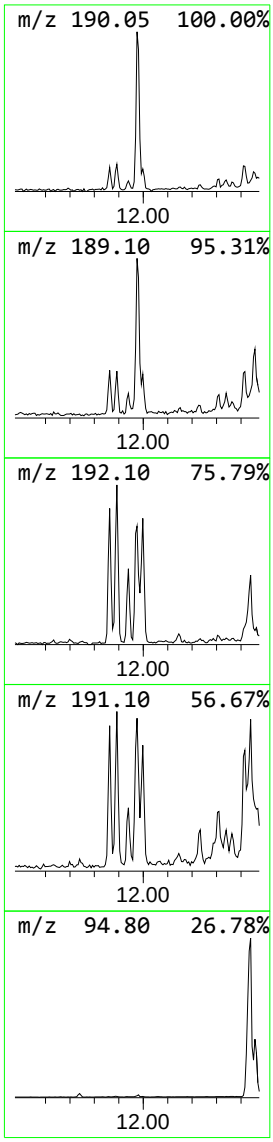
**********

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.975 | 2.72 ng | 122486 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 60 |
| 2 | 5-Bromo-2-thiophenecarboxaldehyde | 190 | C5H3BrOS | 004701-17-1 | 53 |
| 3 | 6H-Cyclobuta[jk]phenanthrene | 190 | C15H10 | 083469-43-6 | 46 |
| 4 | Pyrazole-4-carboxaldehyde, 3-(4-... | 190 | C10H7FN2O | 306936-57-2 | 43 |
| 5 | 2,2'-Bis(4,5-dimethylimidazole) | 190 | C10H14N4 | 069286-06-2 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

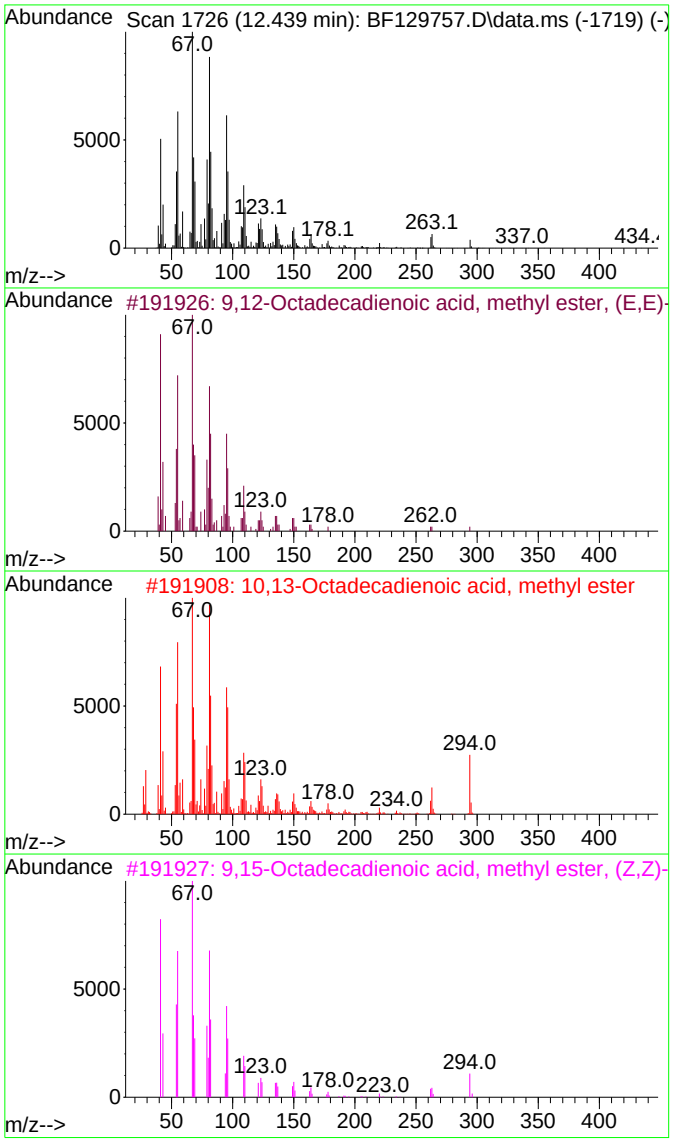
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

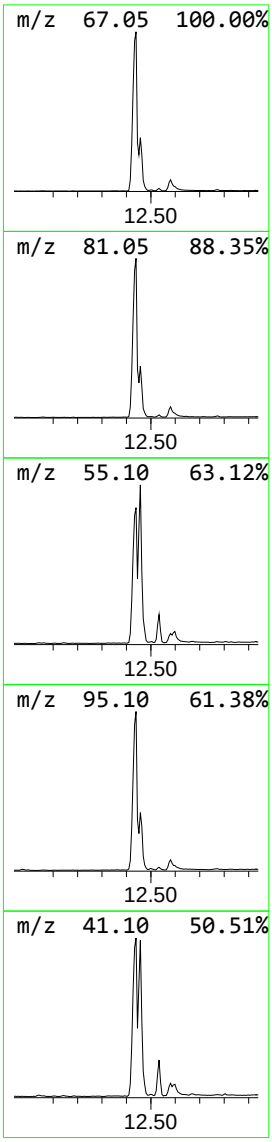
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.439 | 235.38 ng | 10608800 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |
| 2 | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 99 |
| 3 | 9,15-Octadecadienoic acid, methy... | 294 | C19H34O2 | 017309-05-6 | 99 |
| 4 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 99 |
| 5 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

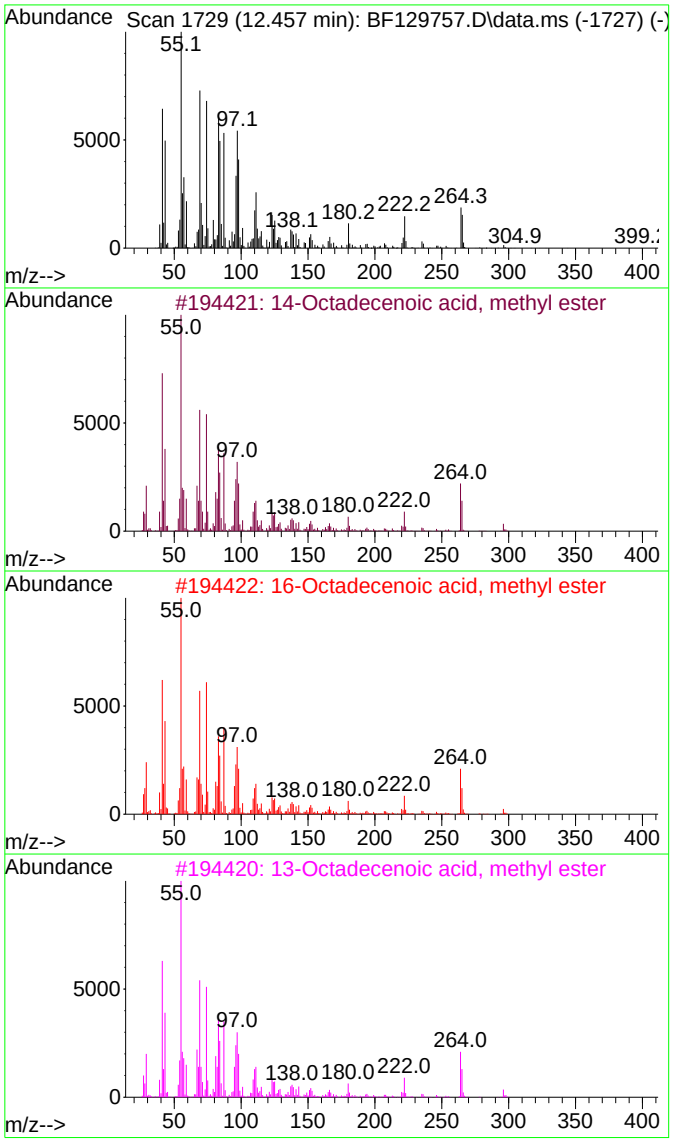
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

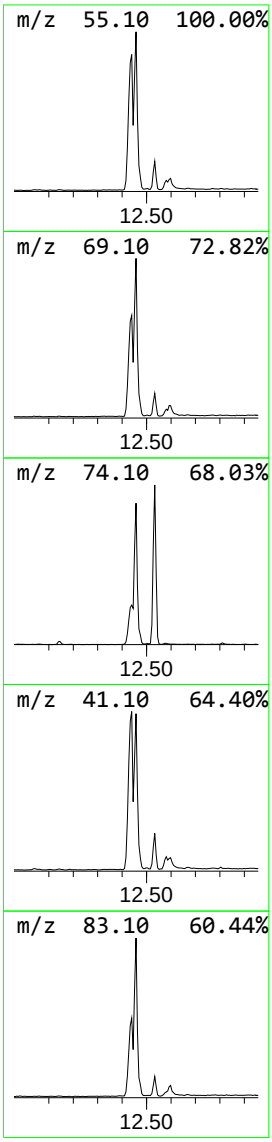
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 14-Octadecenoic acid, methy... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.457 | 154.15 ng | 6947580 | Phenanthrene-d10 | 11.363 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 14-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-48-4 | 94 |
| 2 | 16-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-49-5 | 93 |
| 3 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 93 |
| 4 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 91 |
| 5 | 11-Octadecenoic acid, methyl est... | 296 | C19H36O2 | 001937-63-9 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

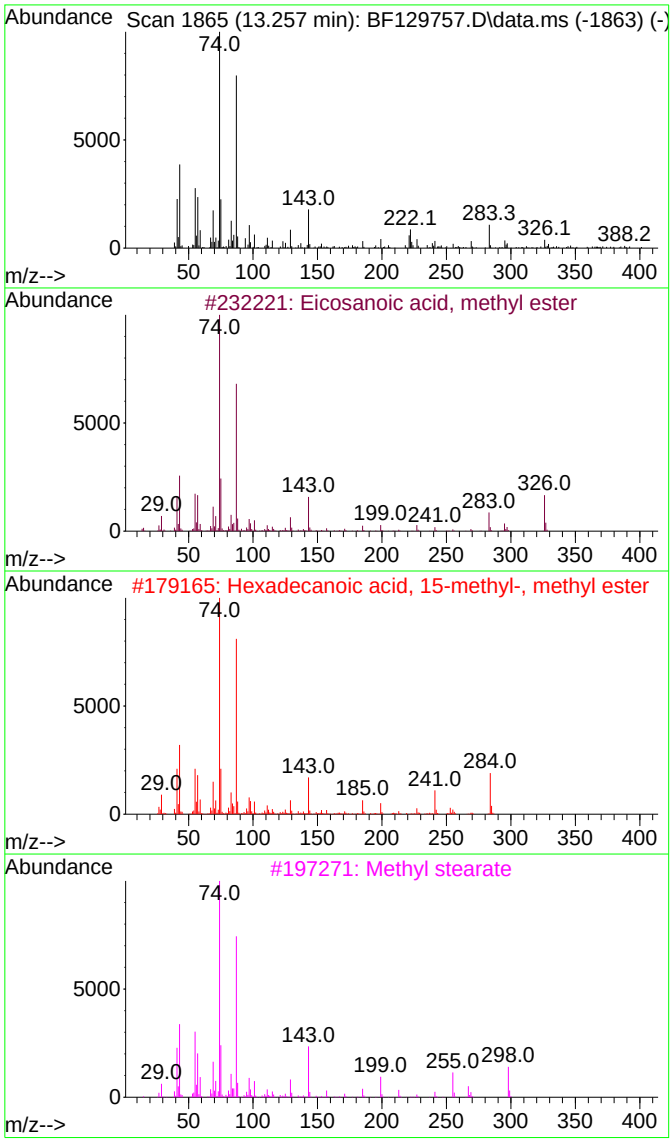
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

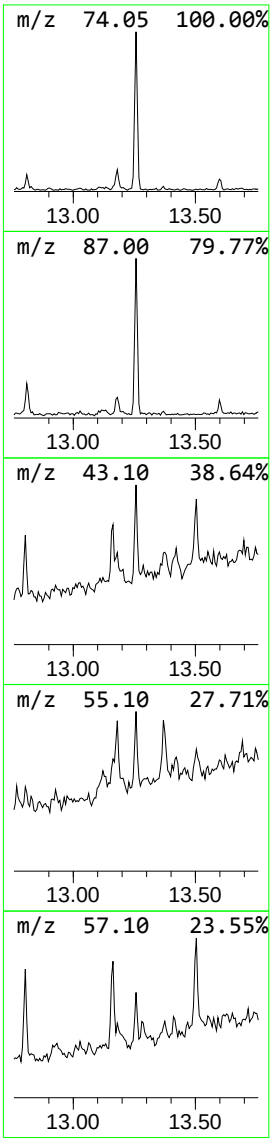
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Eicosanoic acid, methyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.257 | 3.55 ng | 162026 | Chrysene-d12 | 14.016 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosanoic acid, methyl ester | 326 | C21H42O2 | 001120-28-1 | 91 |
| 2 | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0 | 87 |
| 3 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 87 |
| 4 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 83 |
| 5 | Nonadecanoic acid, methyl ester | 312 | C20H40O2 | 001731-94-8 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

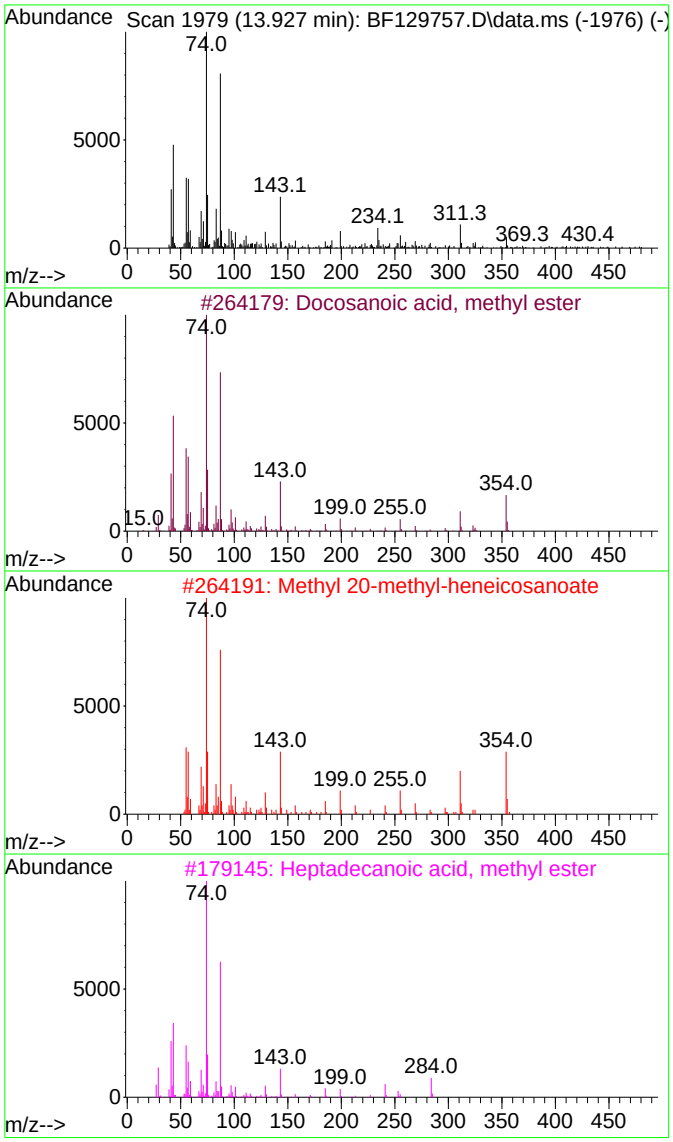
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

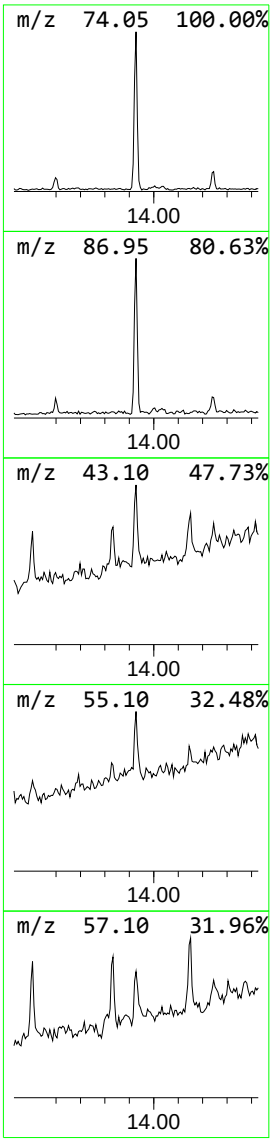
**********

Peak Number 7 Docosanoic acid, methyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.927 | 5.39 ng | 245880 | Chrysene-d12 | 14.016 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosanoic acid, methyl ester | 354 | C23H46O2 | 000929-77-1 | 98 |
| 2 | Methyl 20-methyl-heneicosanoate | 354 | C23H46O2 | 1000336-47-4 | 93 |
| 3 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 91 |
| 4 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 87 |
| 5 | Nonadecanoic acid, methyl ester | 312 | C20H40O2 | 001731-94-8 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129757.D
Acq On : 12 Aug 2022 22:07
Operator : CG\JU
Sample : N4153-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TR-04-081022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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 |
| Hexadecanoic ac... | 11.739 | 47.2 | ng | 2126500 | 4 | 11.363 | 901436 | 20.0 |
| n-Hexadecanoic ... | 11.881 | 6.2 | ng | 277243 | 4 | 11.363 | 901436 | 20.0 |
| 4H-Cyclopenta[d... | 11.975 | 2.7 | ng | 122486 | 4 | 11.363 | 901436 | 20.0 |
| 9,12-Octadecadi... | 12.439 | 235.4 | ng | 10608800 | 4 | 11.363 | 901436 | 20.0 |
| 14-Octadecenoic... | 12.457 | 154.2 | ng | 6947580 | 4 | 11.363 | 901436 | 20.0 |
| Eicosanoic acid... | 13.257 | 3.5 | ng | 162026 | 5 | 14.016 | 912291 | 20.0 |
| Docosanoic acid... | 13.927 | 5.4 | ng | 245880 | 5 | 14.016 | 912291 | 20.0 |