LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128923.D
Acq On : 22 Jun 2022 03:42
Operator : CG\JU
Sample : N3412-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128923.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.387 | 524 | 527 | 540 | rBV | 1678412 | 1642415 | 3.93% | 2.144% |
| 2 | 6.416 | 698 | 702 | 713 | rBV | 1653986 | 1647552 | 3.94% | 2.151% |
| 3 | 6.757 | 756 | 760 | 763 | rBV | 688463 | 574694 | 1.38% | 0.750% |
| 4 | 7.322 | 852 | 856 | 859 | rBV | 1280366 | 1038994 | 2.49% | 1.356% |
| 5 | 8.039 | 972 | 978 | 981 | rBV | 811157 | 672109 | 1.61% | 0.877% |
| 6 | 9.116 | 1157 | 1161 | 1164 | rVB | 2159227 | 1710530 | 4.09% | 2.233% |
| 7 | 9.792 | 1268 | 1276 | 1279 | rBV | 795309 | 670218 | 1.60% | 0.875% |
| 8 | 10.586 | 1408 | 1411 | 1414 | rBV | 965013 | 814126 | 1.95% | 1.063% |
| 9 | 11.280 | 1526 | 1529 | 1531 | rBV | 784824 | 630046 | 1.51% | 0.823% |
| 10 | 11.686 | 1592 | 1598 | 1601 | rBV | 9815116 | 11856459 | 28.38% | 15.479% |
| 11 | 11.839 | 1617 | 1624 | 1630 | rBV2 | 798207 | 1170128 | 2.80% | 1.528% |
| 12 | 12.410 | 1709 | 1721 | 1723 | rBV3 | 12071084 | 41781056 | 100.00% | 54.547% |
| 13 | 12.486 | 1730 | 1734 | 1736 | rBV | 6638808 | 5747153 | 13.76% | 7.503% |
| 14 | 12.527 | 1738 | 1741 | 1743 | rBV | 1130827 | 1383344 | 3.31% | 1.806% |
| 15 | 12.710 | 1769 | 1772 | 1774 | rBV3 | 509186 | 485788 | 1.16% | 0.634% |
| 16 | 12.733 | 1774 | 1776 | 1785 | rVB2 | 441558 | 716447 | 1.71% | 0.935% |
| 17 | 12.880 | 1797 | 1801 | 1803 | rBV | 1727248 | 1385223 | 3.32% | 1.808% |
| 18 | 13.057 | 1828 | 1831 | 1836 | rVB2 | 348579 | 566373 | 1.36% | 0.739% |
| 19 | 13.192 | 1852 | 1854 | 1857 | rVB | 605009 | 525954 | 1.26% | 0.687% |
| 20 | 13.627 | 1922 | 1928 | 1931 | rBV3 | 241517 | 454696 | 1.09% | 0.594% |
| 21 | 13.863 | 1965 | 1968 | 1971 | rVB | 615912 | 523698 | 1.25% | 0.684% |
| 22 | 13.927 | 1975 | 1979 | 1982 | rVV2 | 500624 | 598730 | 1.43% | 0.782% |

Sum of corrected areas: 76595733

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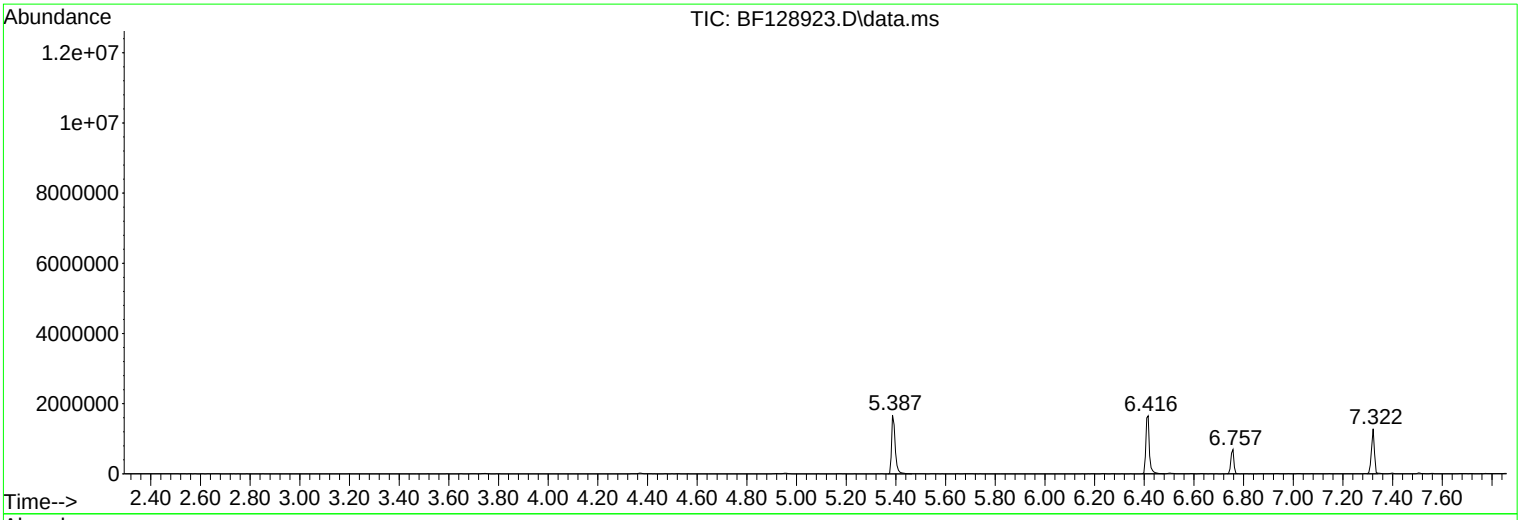
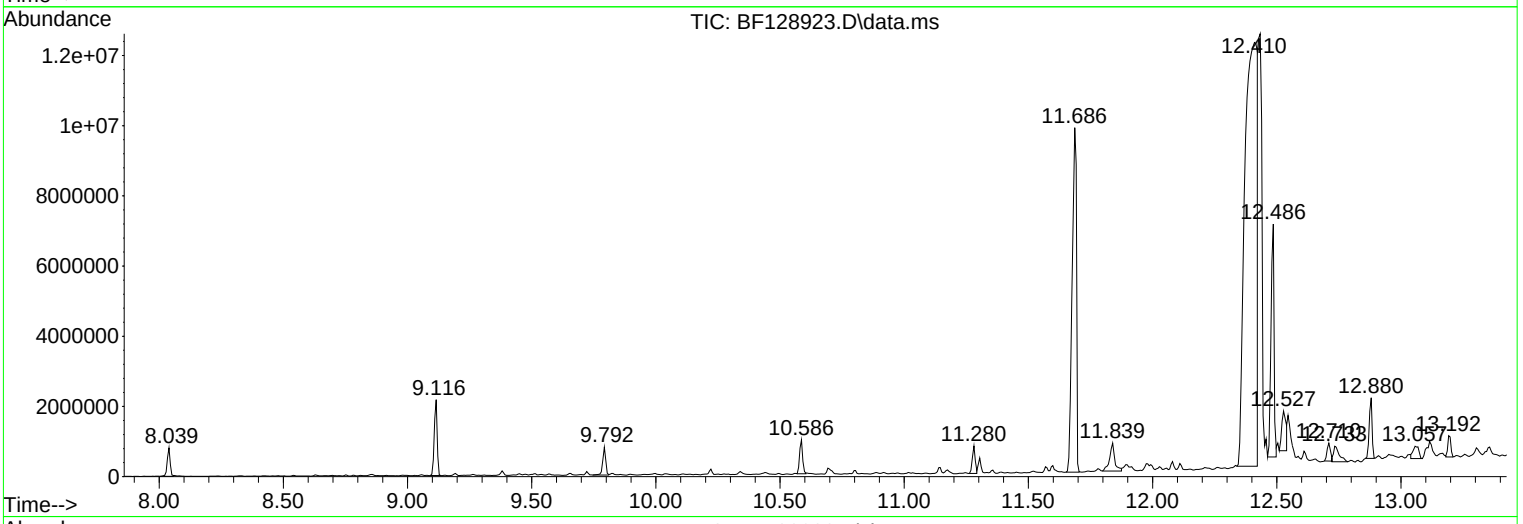
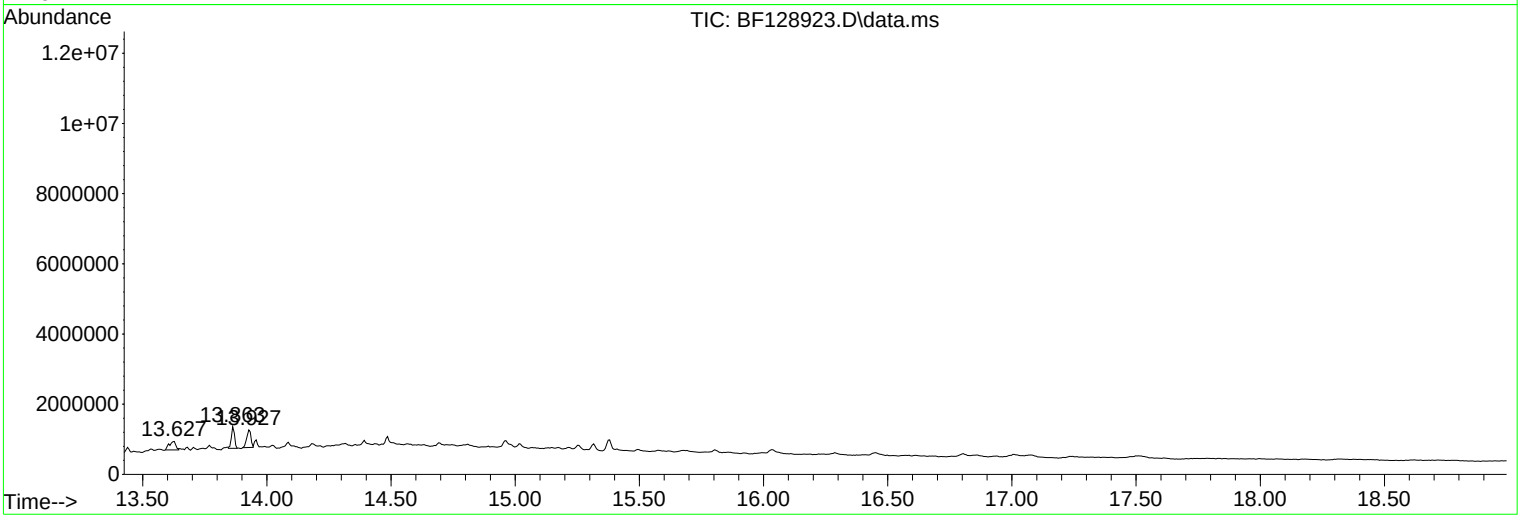
**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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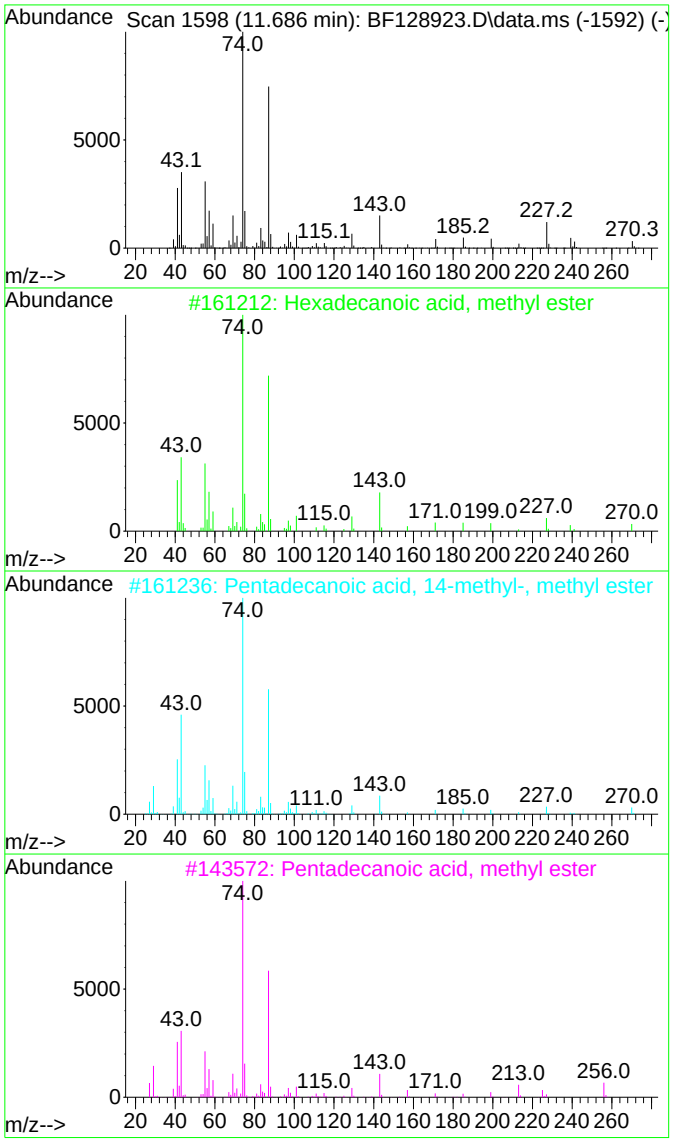
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

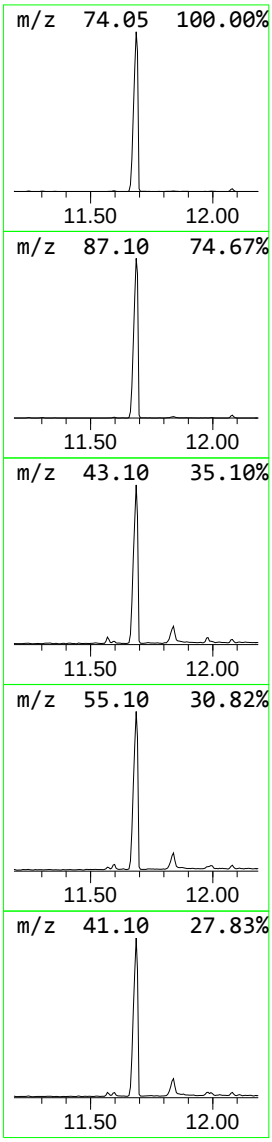
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.686 | 376.37 ng | 11856500 | Phenanthrene-d10 | 11.280 |

| 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 | 96 |
| 3 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 90 |
| 4 | Tridecanoic acid, methyl ester | 228 | C14H28O2 | 001731-88-0 | 90 |
| 5 | Methyl 9-methyltetradecanoate | 256 | C16H32O2 | 213617-69-7 | 86 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128923.D
Acq On : 22 Jun 2022 03:42
Operator : CG\JU
Sample : N3412-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

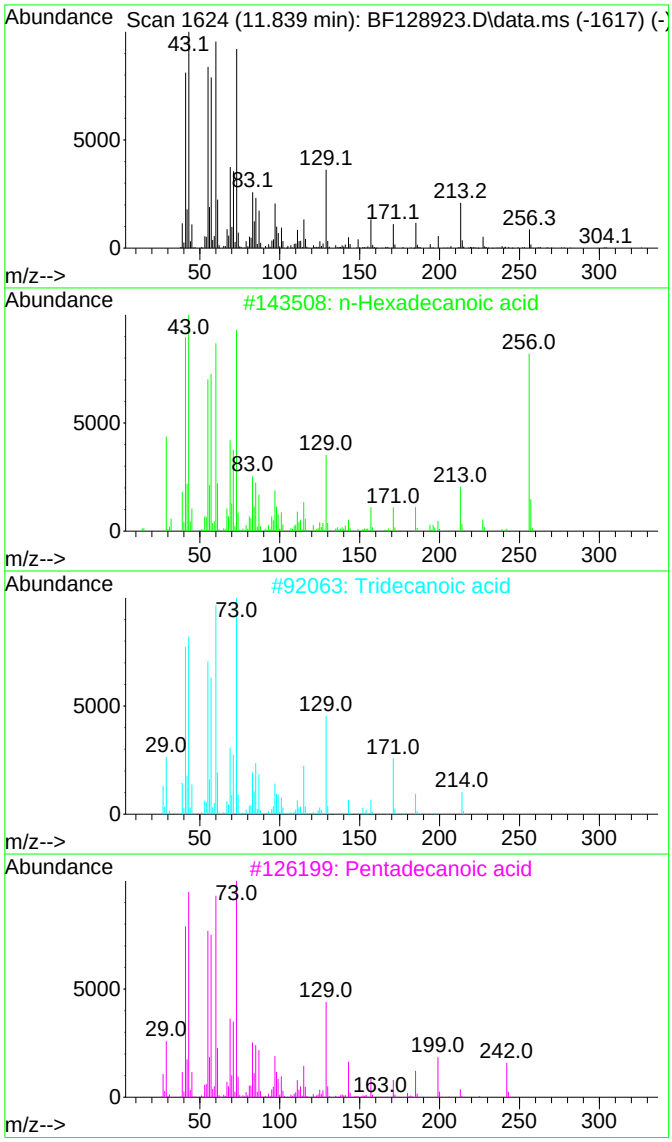
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

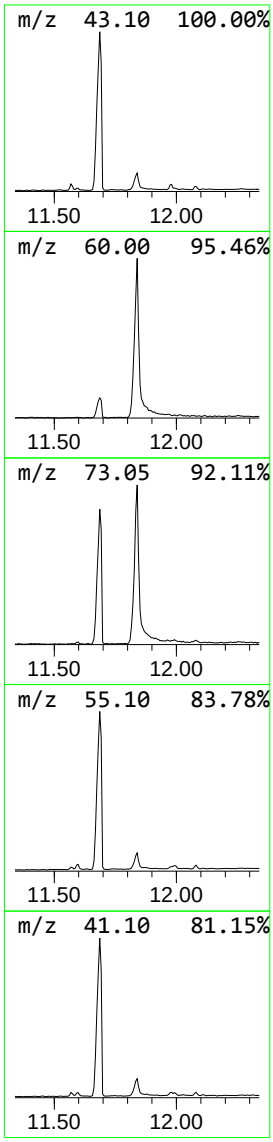
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.839 | 37.14 ng | 1170130 | Phenanthrene-d10 | 11.280 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 94 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 68 |
| 5 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128923.D
Acq On : 22 Jun 2022 03:42
Operator : CG\JU
Sample : N3412-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

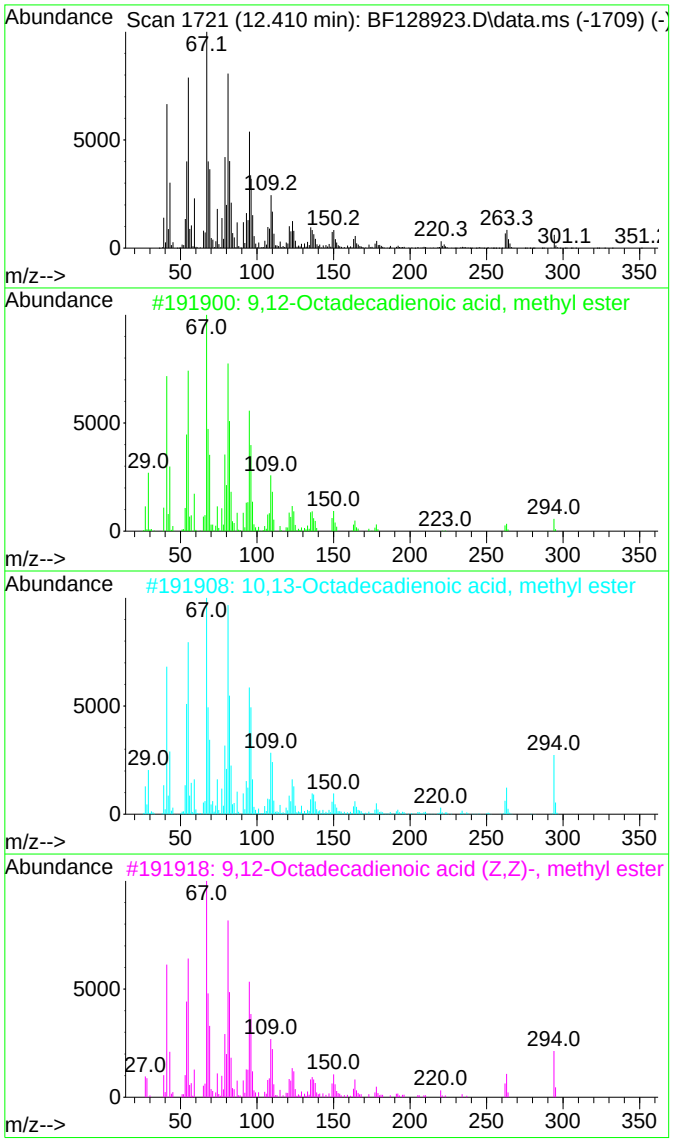
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

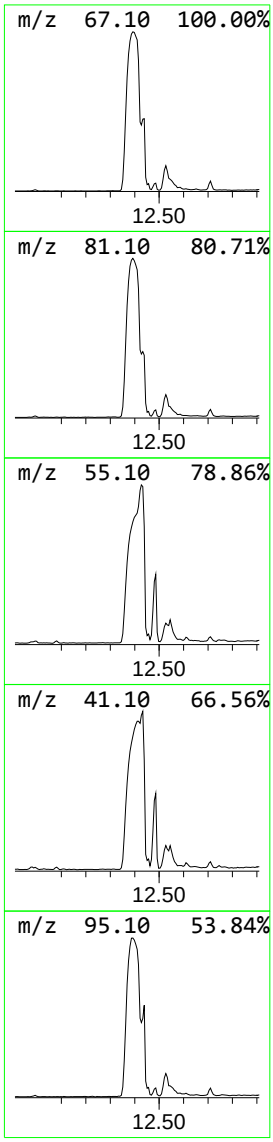
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.410 | 1326.29 ng | 41781100 | Phenanthrene-d10 | 11.280 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |
| 2 | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 99 |
| 3 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 99 |
| 4 | Methyl 9-cis,11-trans-octadecadi... | 294 | C19H34O2 | 013058-52-1 | 99 |
| 5 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |



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Operator : CG\JU
Sample : N3412-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

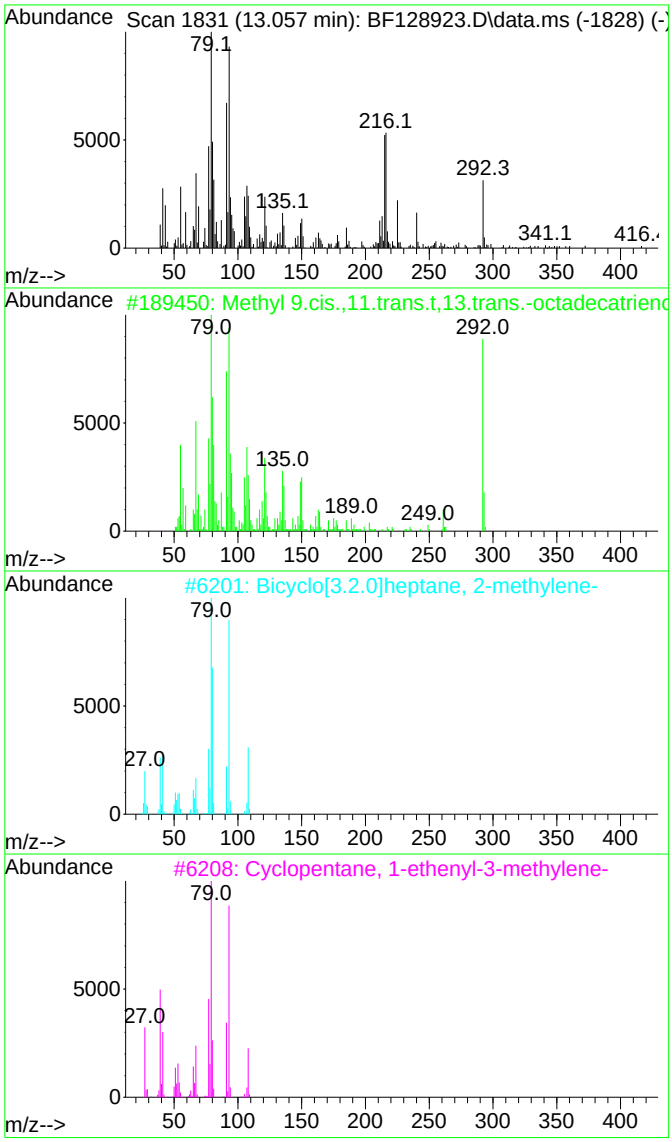
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

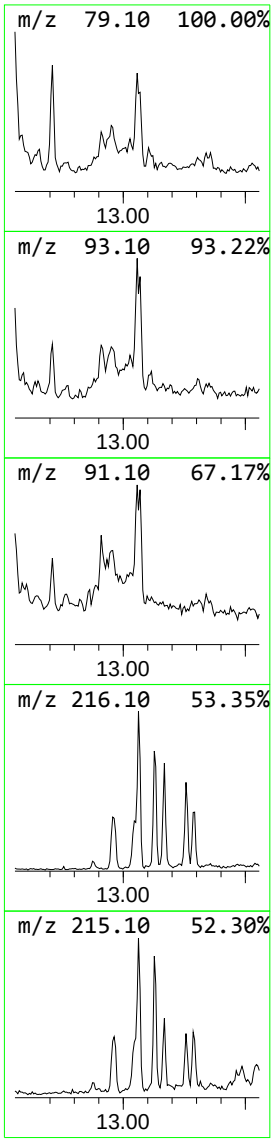
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Methyl 9.cis.,11.trans.t,13... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.057 | 18.92 ng | 566373 | Chrysene-d12 | 13.927 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 9.cis.,11.trans.t,13.tran... | 292 | C19H32O2 | 1000336-42-6 | 84 |
| 2 | Bicyclo[3.2.0]heptane, 2-methylene- | 108 | C8H12 | 089243-94-7 | 49 |
| 3 | Cyclopentane, 1-ethenyl-3-methyl... | 108 | C8H12 | 029668-63-1 | 46 |
| 4 | Bicyclo[2.2.1]heptane, 2,2-dimet... | 136 | C10H16 | 005794-03-6 | 46 |
| 5 | Bicyclo[3.1.1]heptane, 6,6-dimet... | 136 | C10H16 | 016022-04-1 | 46 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062122\
Data File : BF128923.D
Acq On : 22 Jun 2022 03:42
Operator : CG\JU
Sample : N3412-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
NB-7-062022

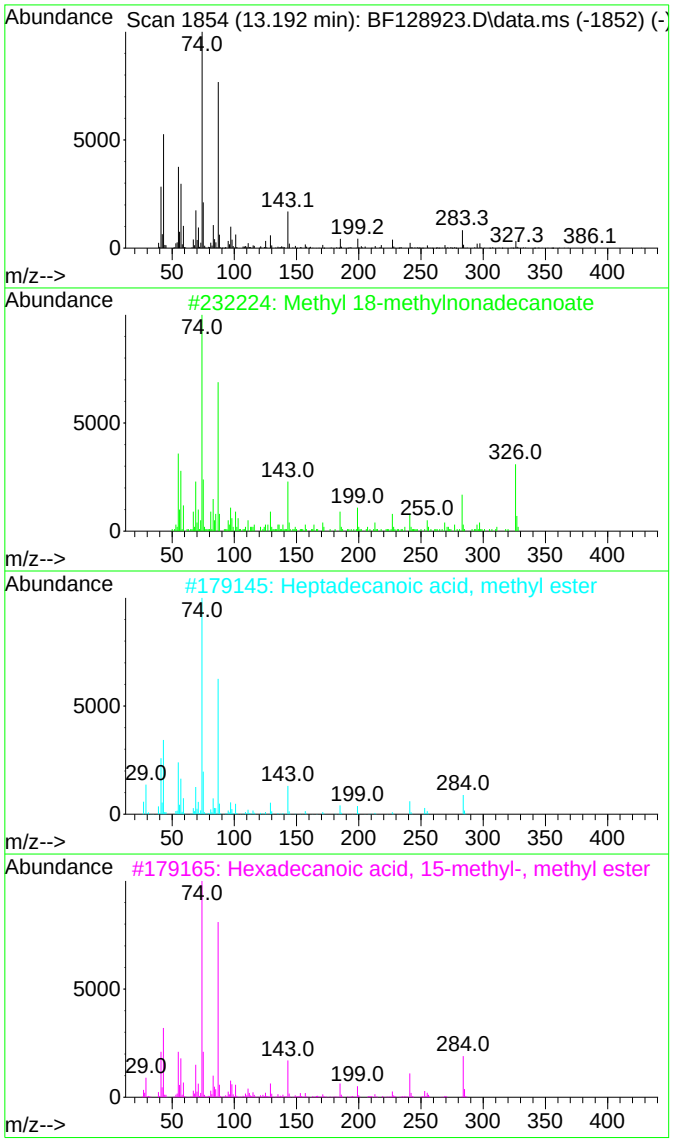
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

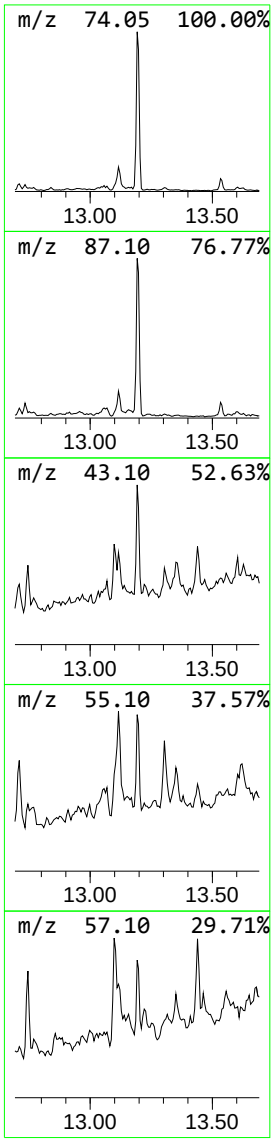
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Methyl 18-methylnonadecanoate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.192 | 17.57 ng | 525954 | Chrysene-d12 | 13.927 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 18-methylnonadecanoate | 326 | C21H42O2 | 1000424-52-4 | 94 |
| 2 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 94 |
| 3 | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0 | 93 |
| 4 | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 91 |
| 5 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 90 |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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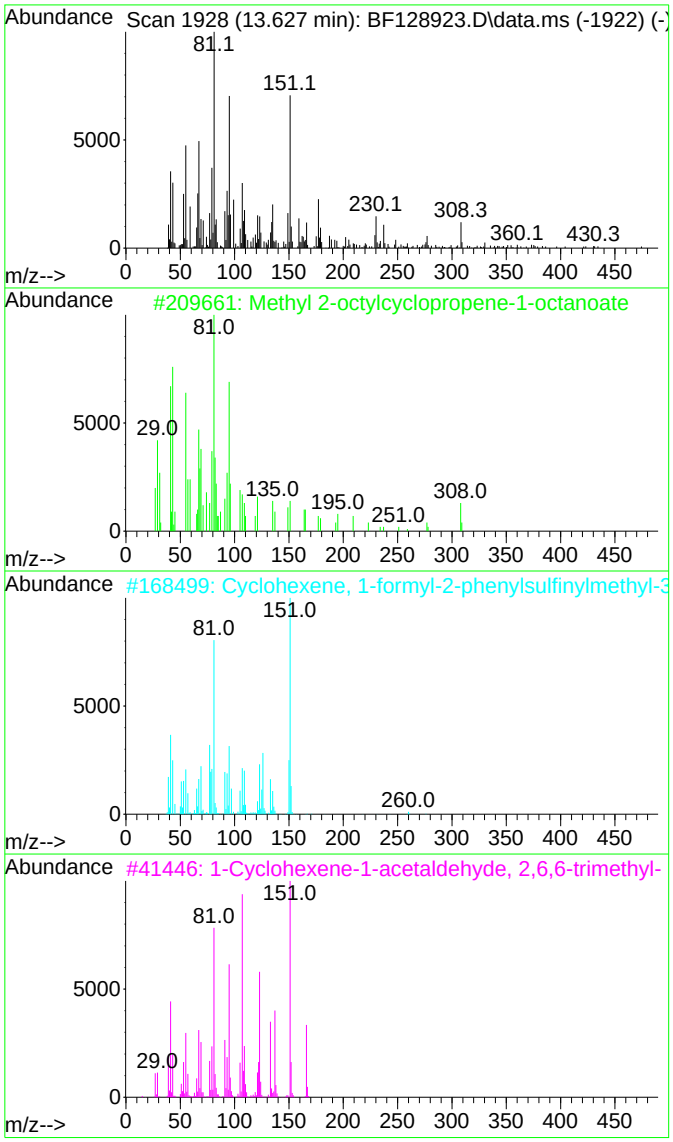
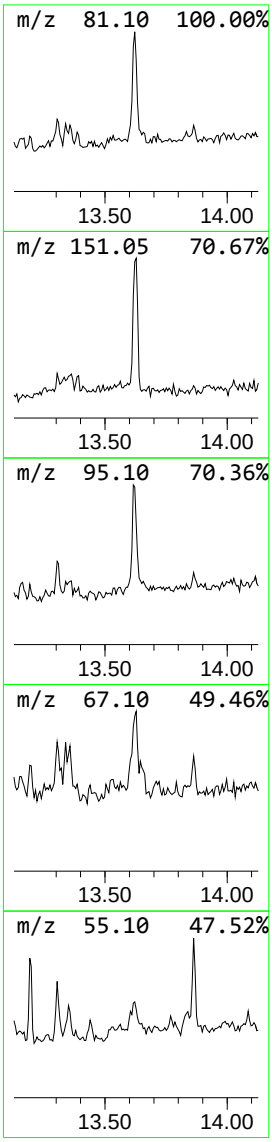
**********

Peak Number 6 unknown13.267 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.627 | 15.19 ng | 454696 | Chrysene-d12 | 13.927 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 2-octylcyclopropene-1-oct... | 308 | C20H36O2 | 003220-60-8 | 46 |
| 2 | Cyclohexene, 1-formyl-2-phenylsu... | 276 | C16H20O2S | 081054-00-4 | 35 |
| 3 | 1-Cyclohexene-1-acetaldehyde, 2,... | 166 | C11H18O | 000472-66-2 | 27 |
| 4 | 6,10,14,18,22-Tetracosapentaen-2... | 506 | C30H51BrO | 065746-05-6 | 25 |
| 5 | 2,2'-Bi(bicyclo[2.2.1]heptane) | 190 | C14H22 | 018947-78-9 | 22 |



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Sample : N3412-01
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ALS Vial : 24 Sample Multiplier: 1

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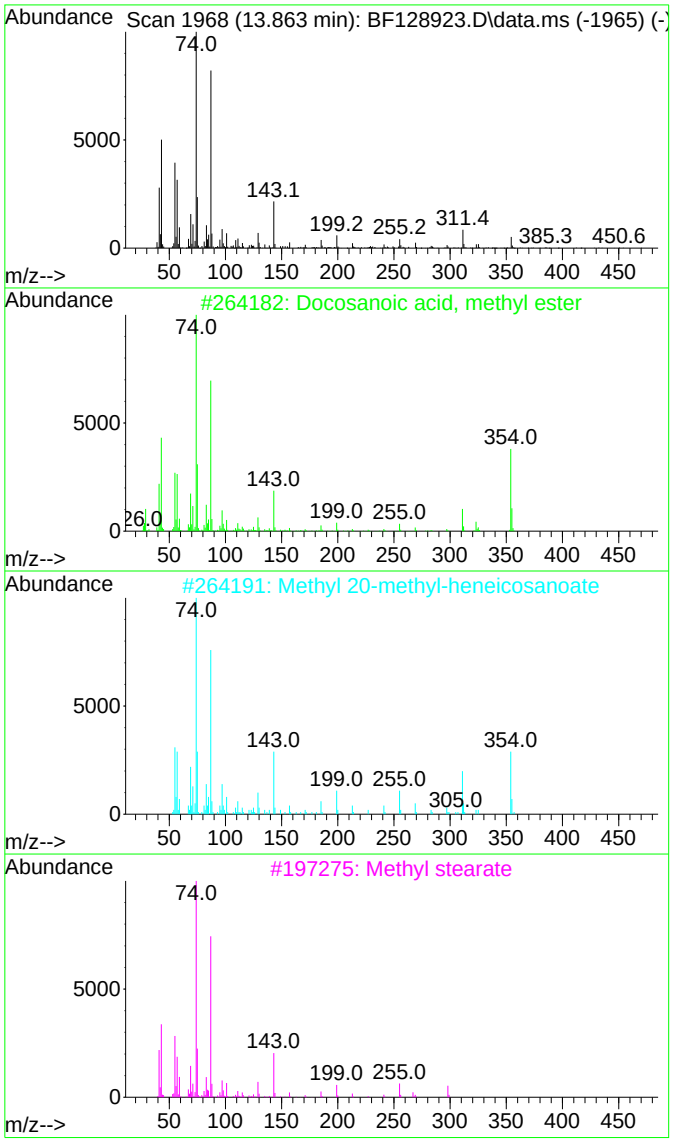
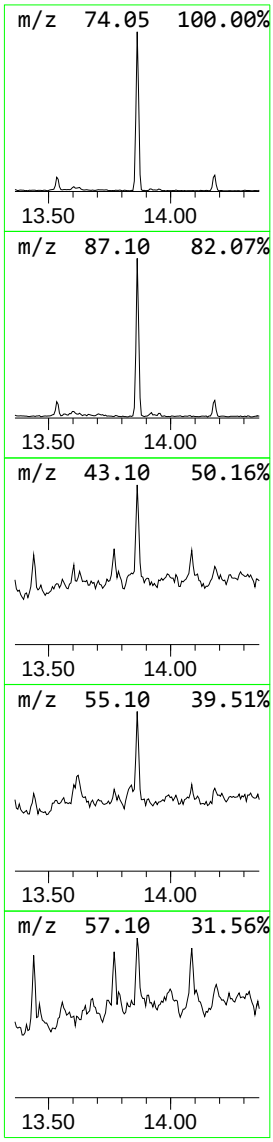
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 Docosanoic acid, methyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.863 | 17.49 ng | 523698 | Chrysene-d12 | 13.927 |

| 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 | 95 |
| 3 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 87 |
| 4 | Nonadecanoic acid, methyl ester | 312 | C20H40O2 | 001731-94-8 | 86 |
| 5 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 86 |



Tentatively Identified Compound (LSC) summary

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Operator : CG\JU
Sample : N3412-01
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**Instrument :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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... | 11.686 | 376.4 | ng | 11856500 | 4 | 11.280 | 630046 | 20.0 |
| n-Hexadecanoic ... | 11.839 | 37.1 | ng | 1170130 | 4 | 11.280 | 630046 | 20.0 |
| 9,12-Octadecadi... | 12.410 | 1326.3 | ng | 41781100 | 4 | 11.280 | 630046 | 20.0 |
| Methyl 9.cis.,1... | 13.057 | 18.9 | ng | 566373 | 5 | 13.927 | 598730 | 20.0 |
| Methyl 18-methy... | 13.192 | 17.6 | ng | 525954 | 5 | 13.927 | 598730 | 20.0 |
| unknown13.267 | 13.627 | 15.2 | ng | 454696 | 5 | 13.927 | 598730 | 20.0 |
| Docosanoic acid... | 13.863 | 17.5 | ng | 523698 | 5 | 13.927 | 598730 | 20.0 |