LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 7.501 | 925 | 946 | 948 | rBV2 | 183681 | 660796 | 1.17% | 0.564% |
| 2 | 9.719 | 1319 | 1323 | 1334 | rVB | 513303 | 685800 | 1.22% | 0.585% |
| 3 | 12.548 | 1800 | 1804 | 1819 | rBV2 | 483886 | 698908 | 1.24% | 0.597% |
| 4 | 14.959 | 2209 | 2214 | 2229 | rBV | 418428 | 661428 | 1.18% | 0.565% |
| 5 | 16.048 | 2373 | 2399 | 2427 | rBV2 | 4008111 | 26948921 | 47.87% | 23.006% |
| 6 | 17.106 | 2534 | 2579 | 2580 | rBV5 | 6334640 | 56291175 | 100.00% | 48.055% |
| 7 | 17.212 | 2595 | 2597 | 2600 | rVB2 | 3858119 | 3554295 | 6.31% | 3.034% |
| 8 | 17.306 | 2600 | 2613 | 2615 | rVV2 | 4180278 | 11806341 | 20.97% | 10.079% |
| 9 | 17.330 | 2615 | 2617 | 2622 | rVV | 3311081 | 3217024 | 5.71% | 2.746% |
| 10 | 17.377 | 2622 | 2625 | 2629 | rVV | 842077 | 918193 | 1.63% | 0.784% |
| 11 | 17.442 | 2630 | 2636 | 2639 | rVB | 1924930 | 2723881 | 4.84% | 2.325% |
| 12 | 17.959 | 2713 | 2724 | 2730 | rVV | 2514695 | 6151640 | 10.93% | 5.252% |
| 13 | 18.012 | 2730 | 2733 | 2735 | rVV2 | 407925 | 581973 | 1.03% | 0.497% |
| 14 | 18.042 | 2735 | 2738 | 2754 | rVB | 1268535 | 2238738 | 3.98% | 1.911% |

Sum of corrected areas: 117139113

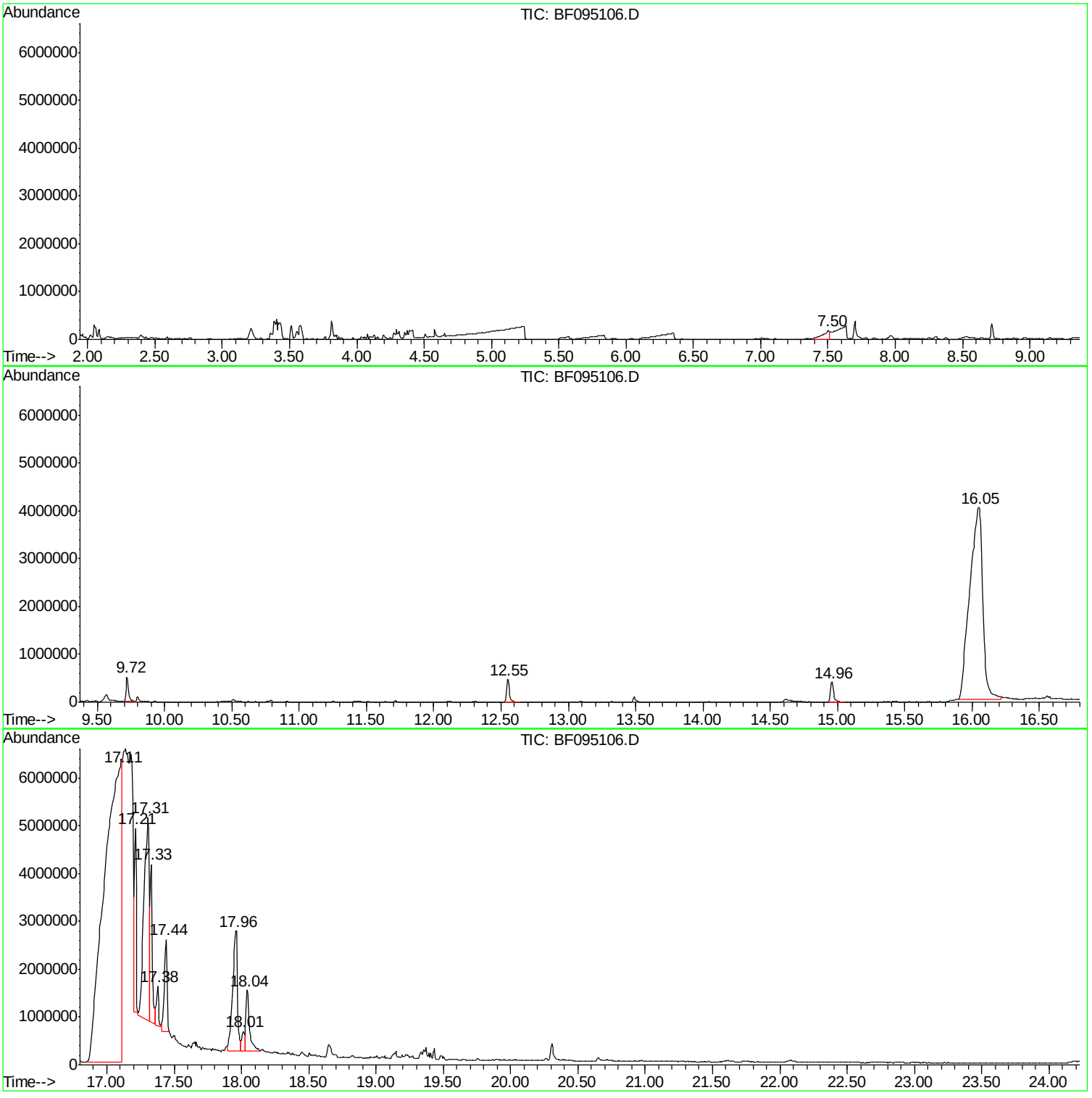
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

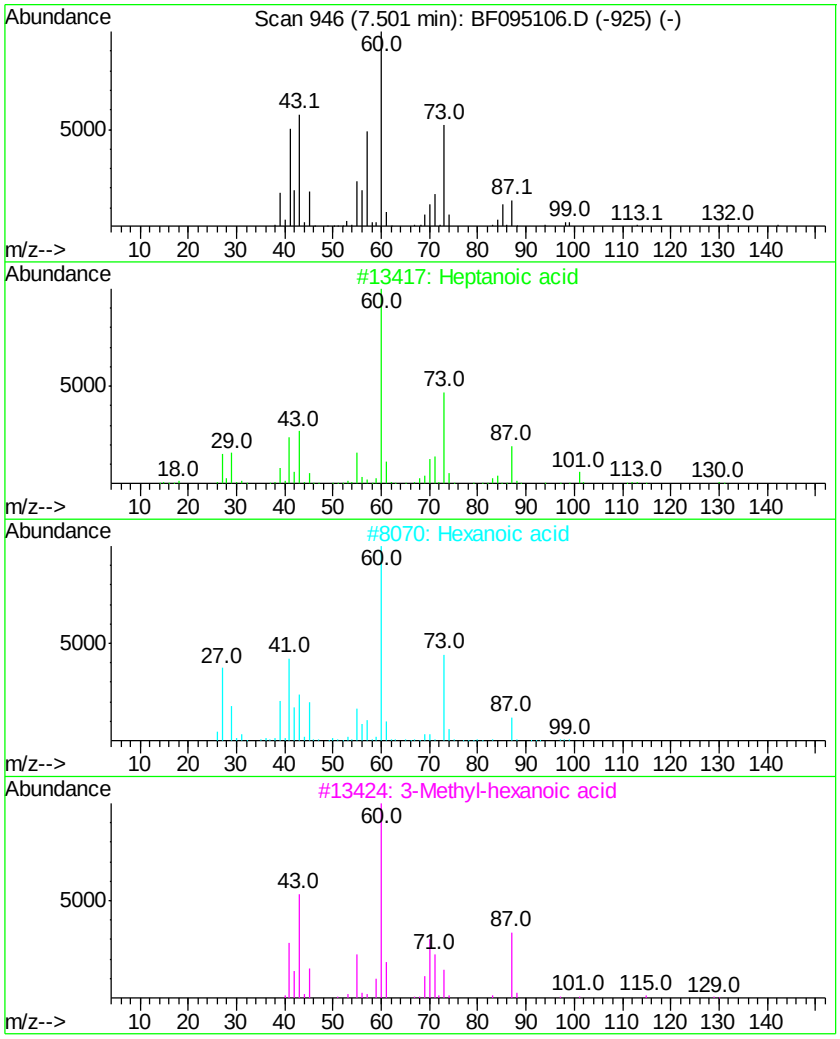
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

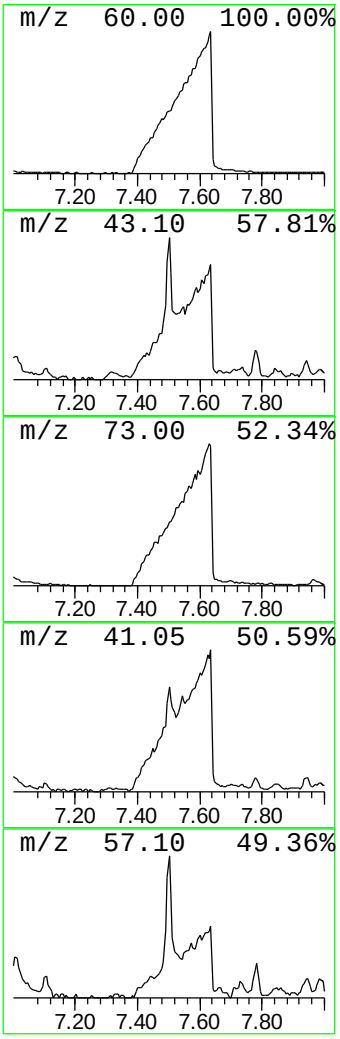
**********

Peak Number 1 Heptanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.50 | 20.00 ng | 660796 | 1,4-Dichlorobenzene-d4 | 7.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptanoic acid | 130 | C7H14O2 | 000111-14-8 | 64 |
| 2 | Hexanoic acid | 116 | C6H12O2 | 000142-62-1 | 53 |
| 3 | 3-Methyl-hexanoic acid | 130 | C7H14O2 | 1000365-65-4 | 53 |
| 4 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 47 |
| 5 | Propanedioic acid, propyl- | 146 | C6H10O4 | 000616-62-6 | 42 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

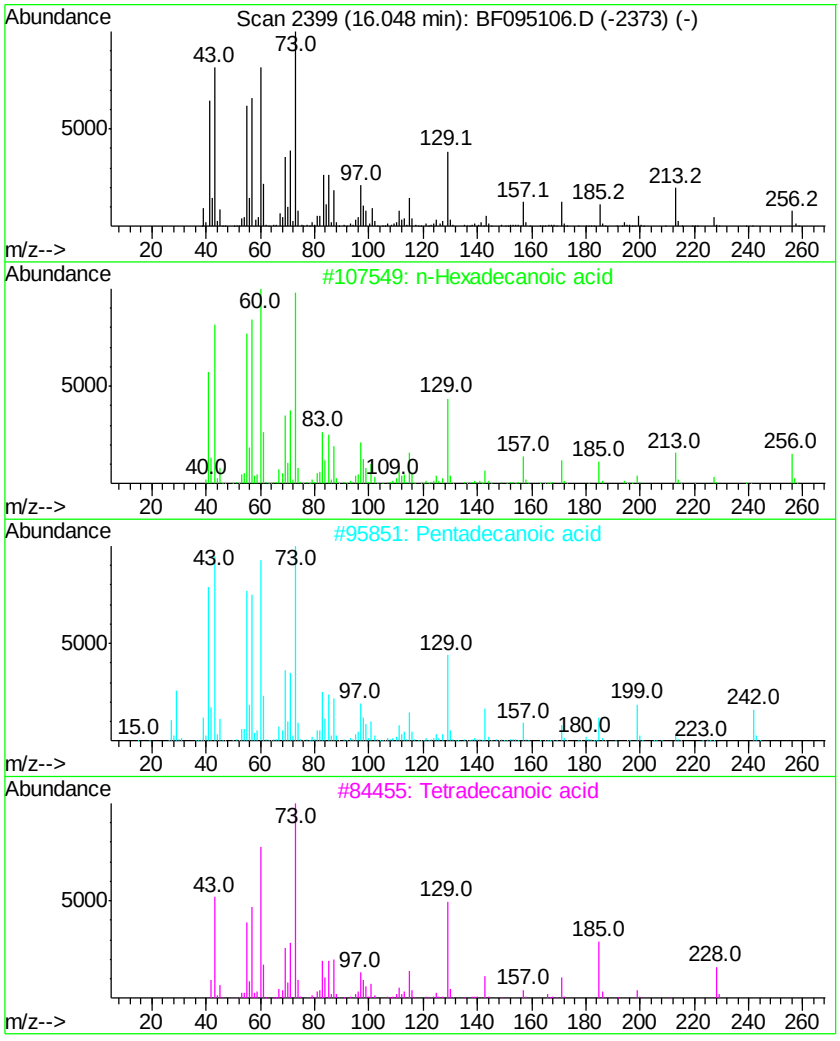
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

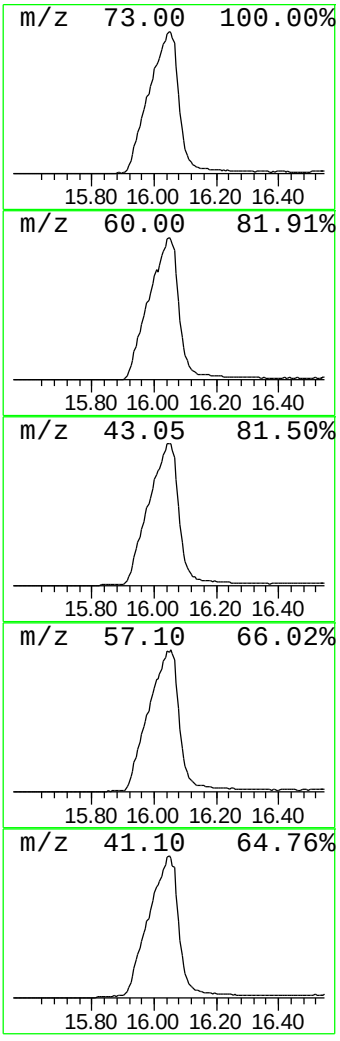
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.05 | 814.87 ng | 26948900 | Phenanthrene-d10 | 14.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 90 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

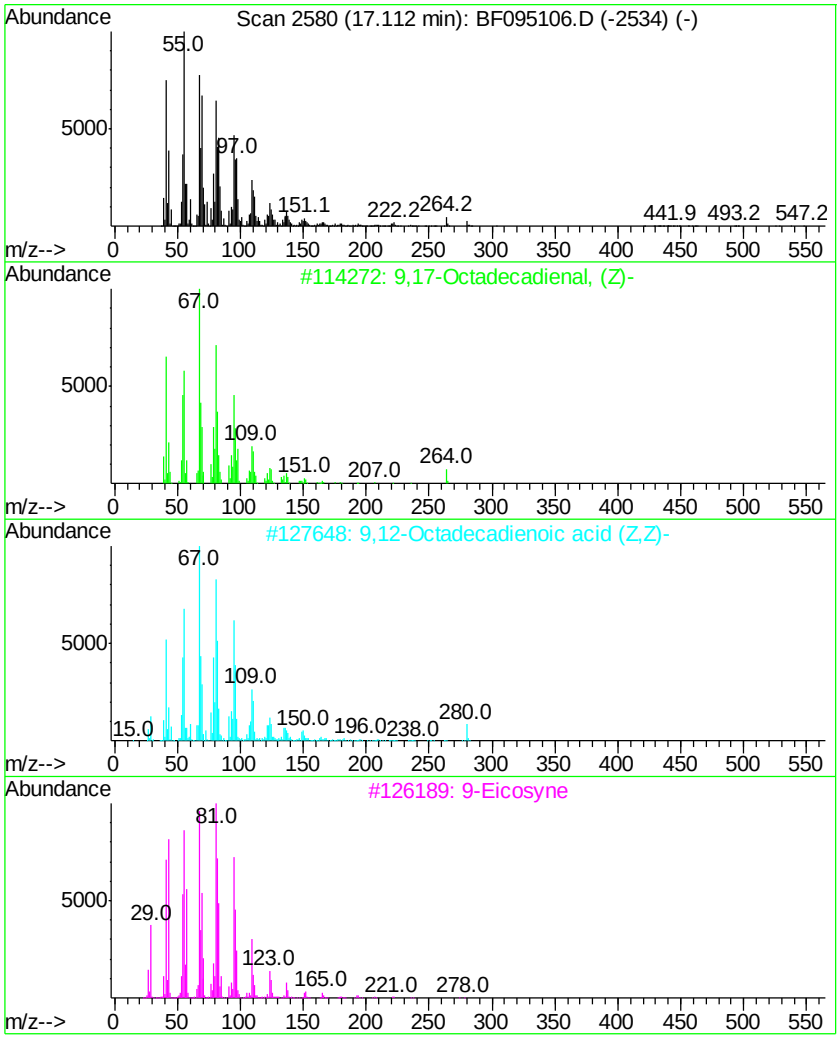
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

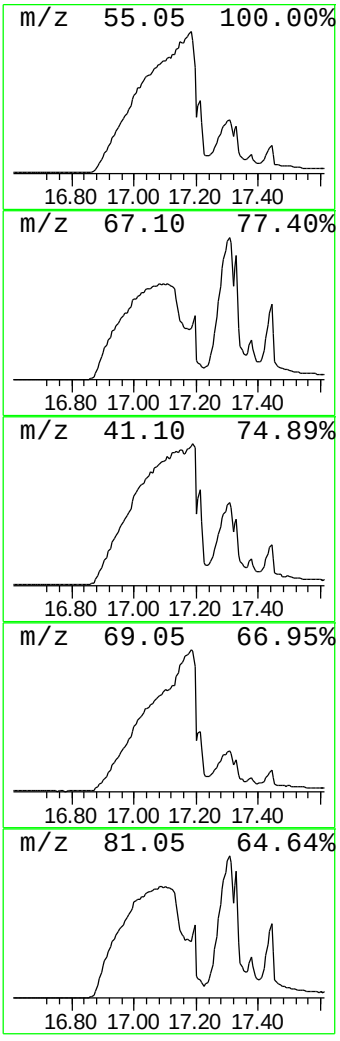
**********

Peak Number 3 9,17-Octadecadienal, (Z)- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.11 | 502.88 ng | 56291200 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,17-Octadecadienal, (Z)- | 264 | C18H32O | 056554-35-9 | 98 |
| 2 | 9,12-Octadecadienoic acid (Z,Z)- | 280 | C18H32O2 | 000060-33-3 | 96 |
| 3 | 9-Eicosyne | 278 | C20H38 | 071899-38-2 | 95 |
| 4 | 2-Methyl-Z,Z-3,13-octadecadienol | 280 | C19H36O | 1000130-90-5 | 93 |
| 5 | trans-13-Octadecenoic acid | 282 | C18H34O2 | 000693-71-0 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

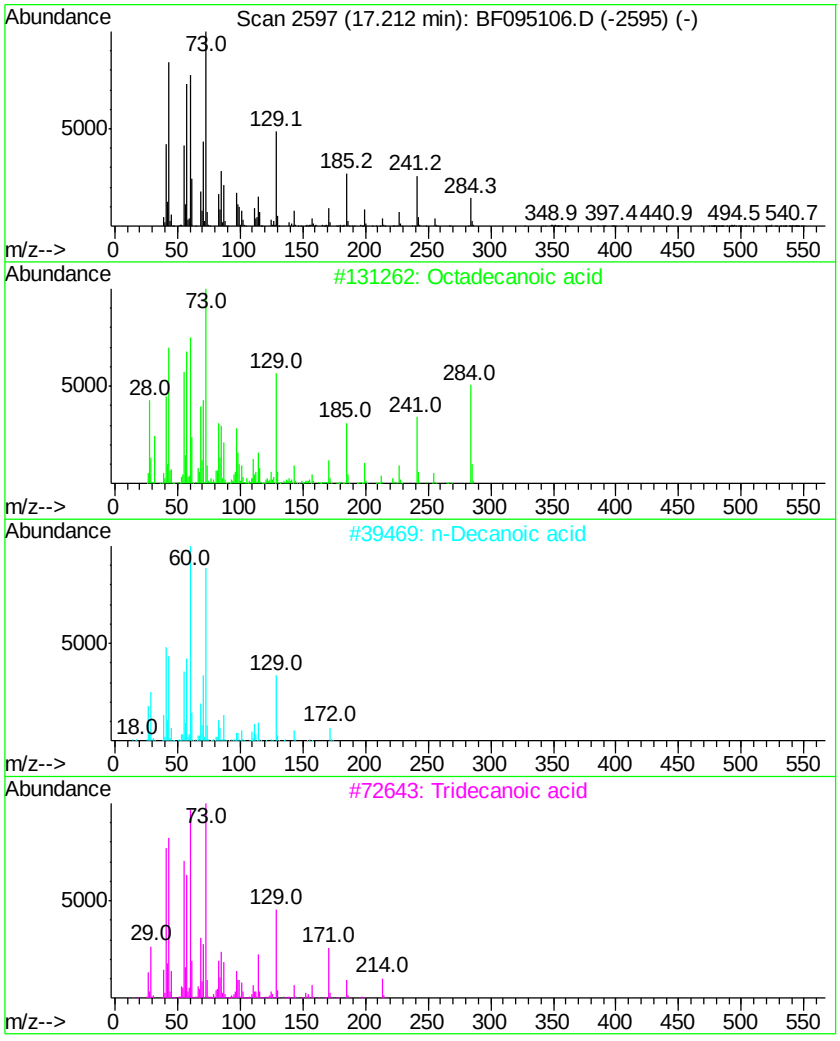
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

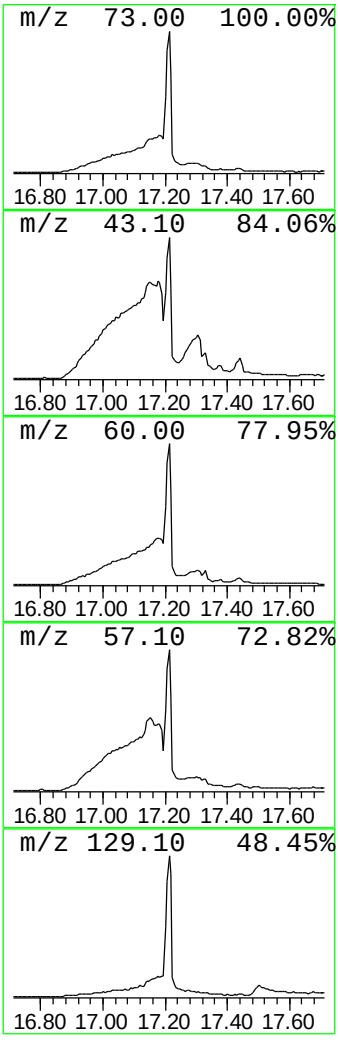
**********

Peak Number 4 Octadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.21 | 31.75 ng | 3554300 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 90 |
| 2 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 68 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

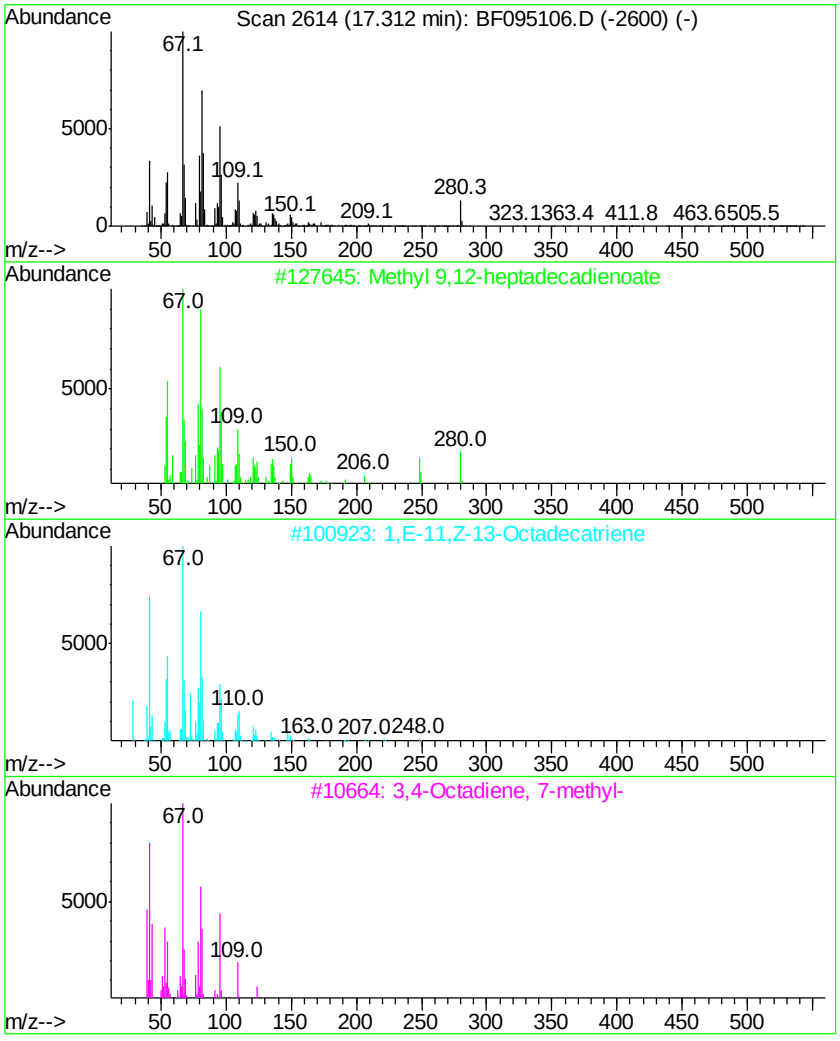
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

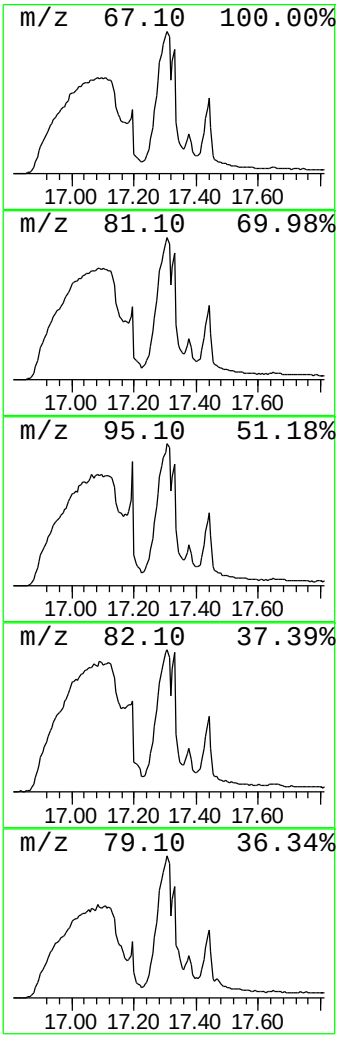
**********

Peak Number 5 Methyl 9,12-heptadecadienoate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.31 | 105.47 ng | 11806300 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 9,12-heptadecadienoate | 280 | C18H32O2 | 1000336-36-2 | 87 |
| 2 | 1,E-11,Z-13-Octadecatriene | 248 | C18H32 | 080625-36-1 | 80 |
| 3 | 3,4-Octadiene, 7-methyl- | 124 | C9H16 | 037050-05-8 | 74 |
| 4 | 11-Hexadecyn-1-ol | 238 | C16H30O | 065686-49-9 | 72 |
| 5 | 7-Hexadecyne | 222 | C16H30 | 074685-28-2 | 72 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

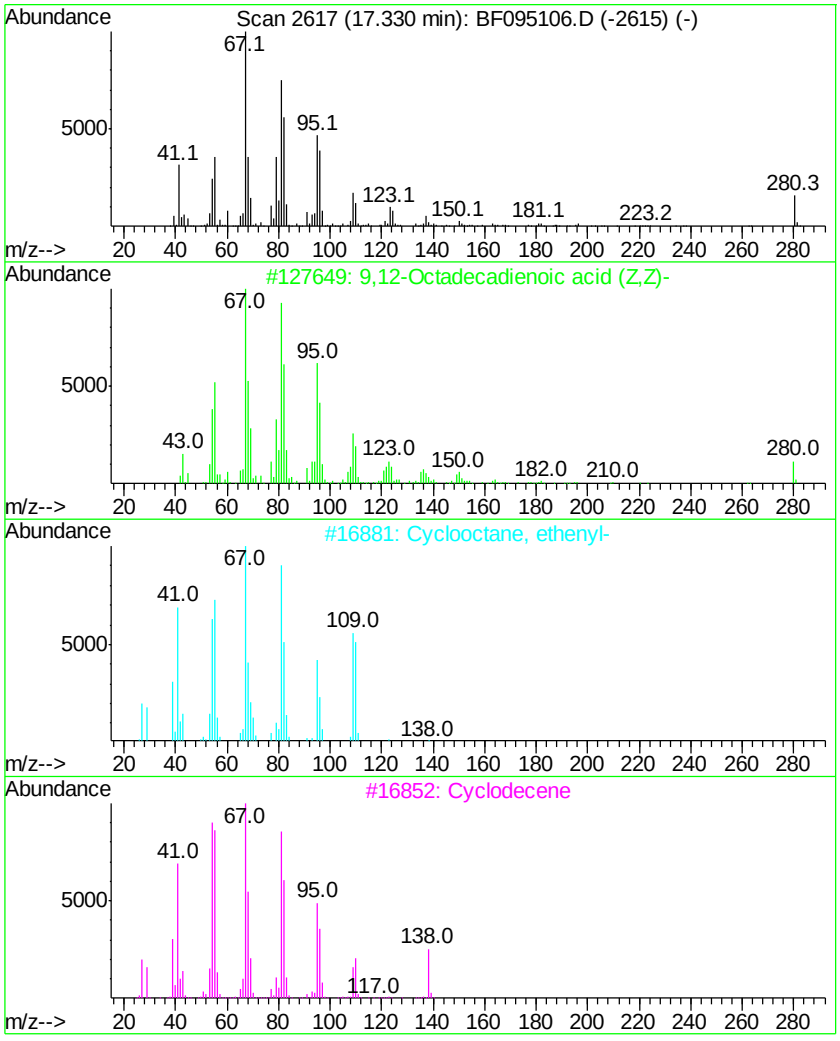
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

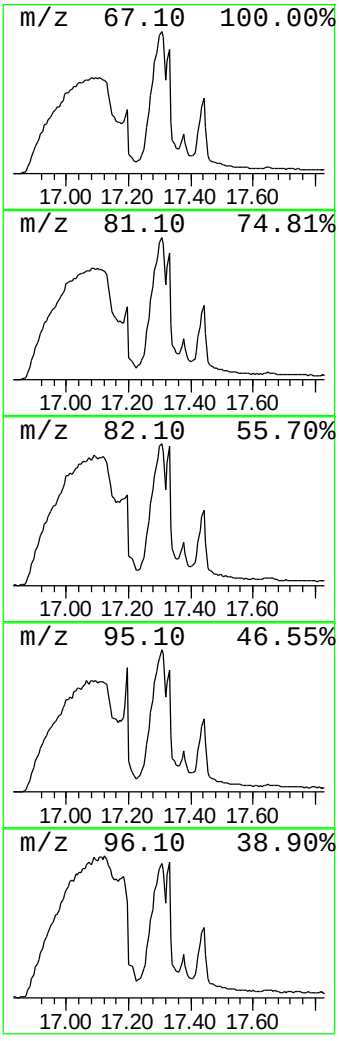
**********

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.33 | 28.74 ng | 3217020 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid (Z,Z)- | 280 | C18H32O2 | 000060-33-3 | 91 |
| 2 | Cyclooctane, ethenyl- | 138 | C10H18 | 061142-41-4 | 76 |
| 3 | Cyclodecene | 138 | C10H18 | 003618-12-0 | 60 |
| 4 | Methyl 9,12-heptadecadienoate | 280 | C18H32O2 | 1000336-36-2 | 58 |
| 5 | Bicyclo[2.2.2]octane | 110 | C8H14 | 000280-33-1 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

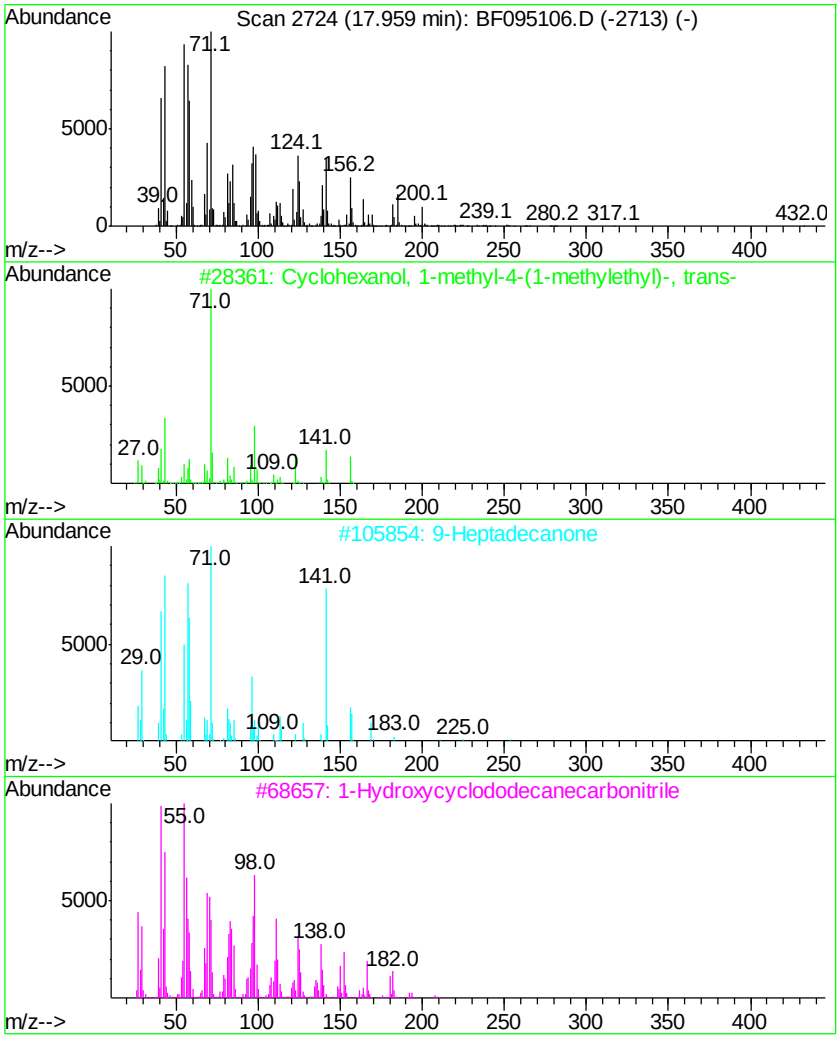
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

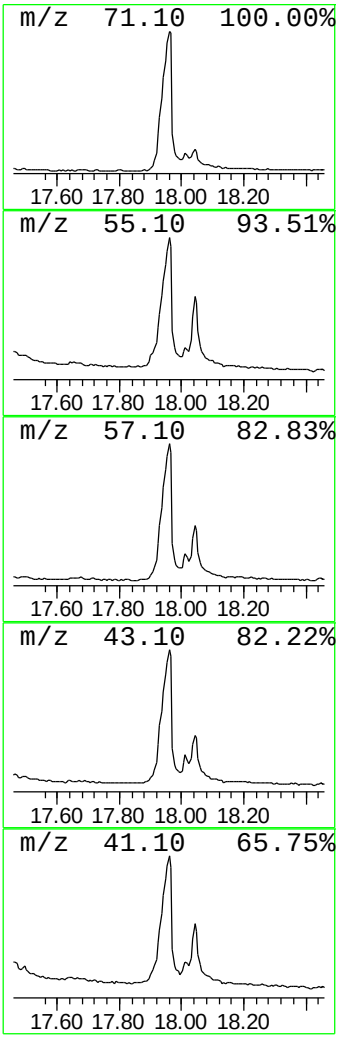
**********

Peak Number 9 unknown17.96 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.96 | 54.96 ng | 6151640 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexanol, 1-methyl-4-(1-meth... | 156 | C10H20O | 003901-93-7 | 43 |
| 2 | 9-Heptadecanone | 254 | C17H34O | 000540-08-9 | 41 |
| 3 | 1-Hydroxycyclododecanecarbonitrile | 209 | C13H23NO | 000882-83-7 | 38 |
| 4 | 2-Nonen-1-ol, 2-methyl- | 156 | C10H20O | 091008-40-1 | 38 |
| 5 | Bicyclo[2.2.1]heptan-2-ol, 2,3,3... | 154 | C10H18O | 000465-31-6 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

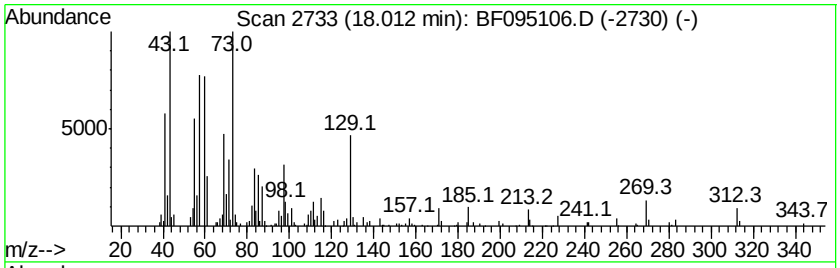
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

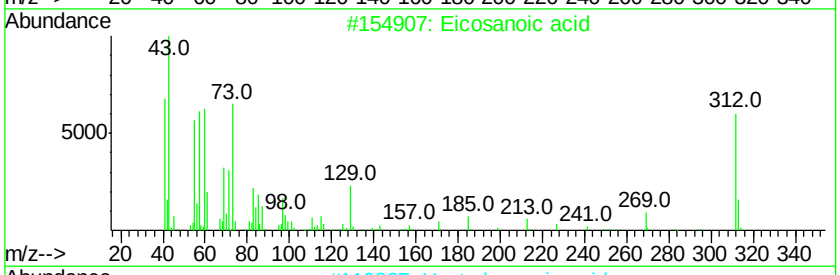
**********

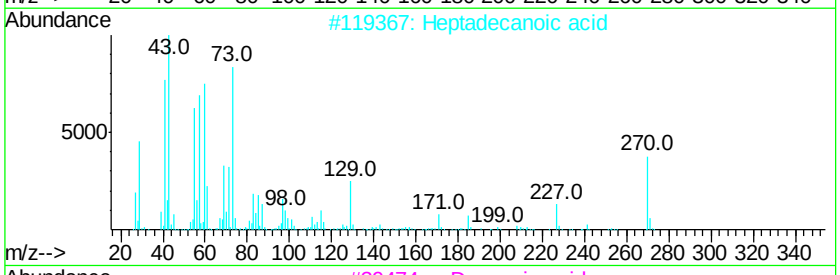
Peak Number 10 Eicosanoic acid Concentration Rank 11

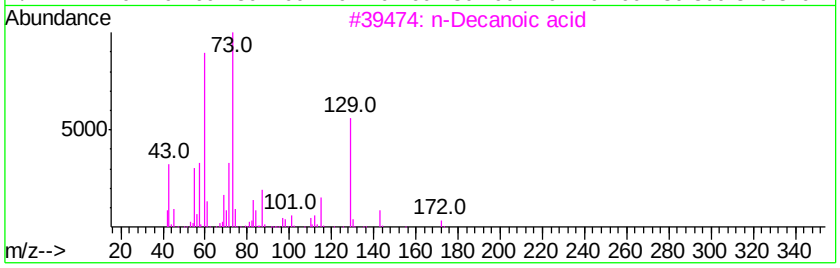
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.01 | 5.20 ng | 581973 | Chrysene-d12 | 18.65 |

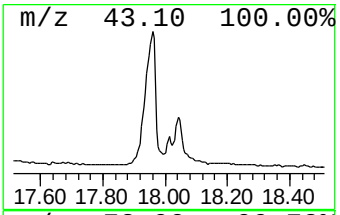
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosanoic acid | 312 | C20H40O2 | 000506-30-9 | 93 |
| 2 | Heptadecanoic acid | 270 | C17H34O2 | 000506-12-7 | 91 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 86 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |

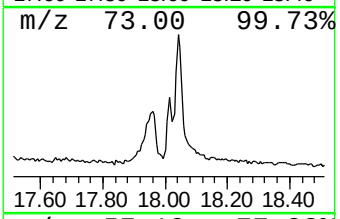


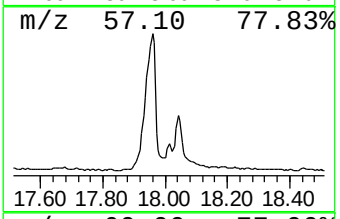



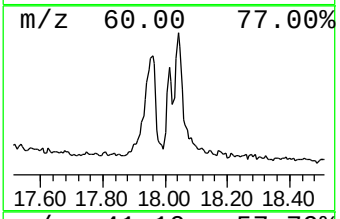



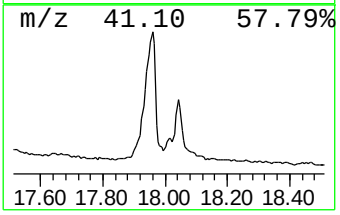



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

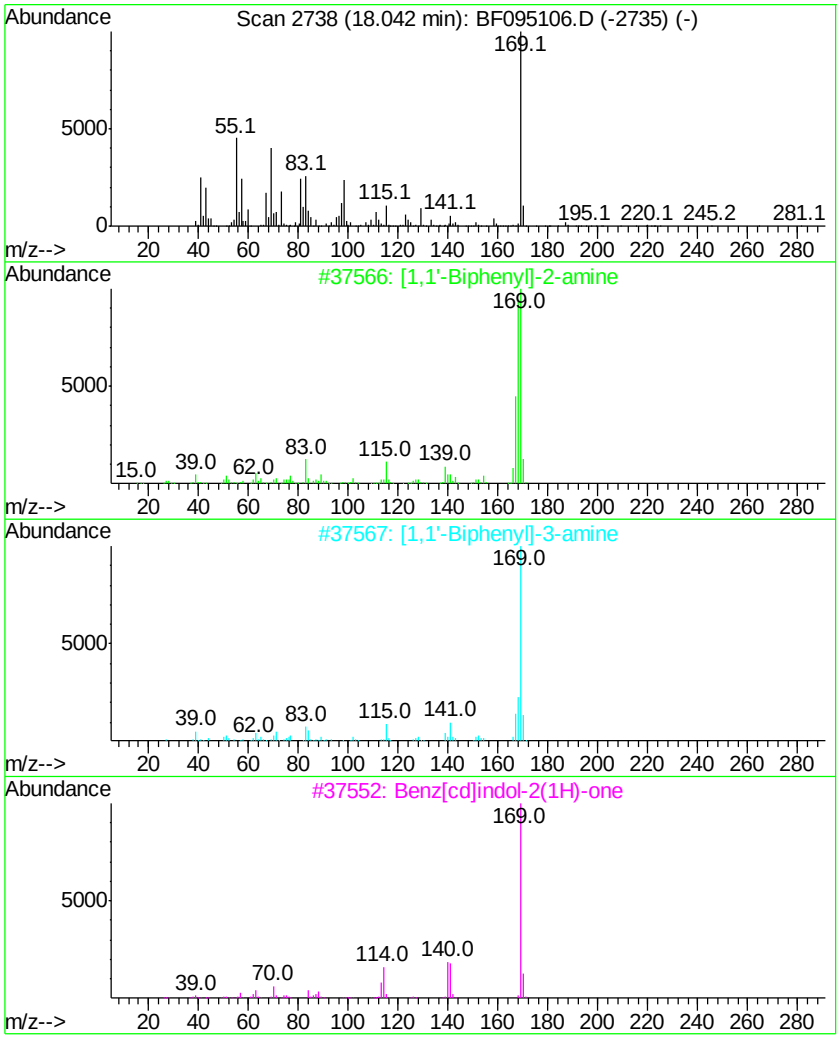
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

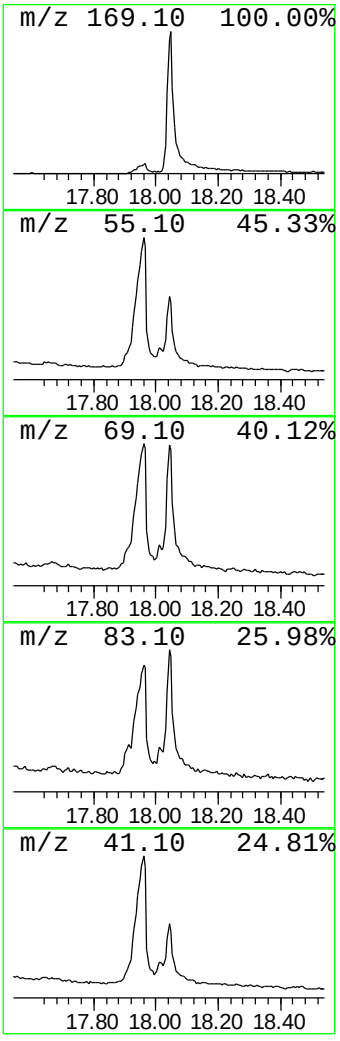
**********

Peak Number 11 unknown18.04 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.04 | 20.00 ng | 2238740 | Chrysene-d12 | 18.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | [1,1'-Biphenyl]-2-amine | 169 | C12H11N | 000090-41-5 | 47 |
| 2 | [1,1'-Biphenyl]-3-amine | 169 | C12H11N | 002243-47-2 | 43 |
| 3 | Benz[cd]indol-2(1H)-one | 169 | C11H7NO | 000130-00-7 | 43 |
| 4 | [1,1'-Biphenyl]-4-amine | 169 | C12H11N | 000092-67-1 | 43 |
| 5 | 3-Chlorophenyl isothiocyanate | 169 | C7H4ClNS | 002392-68-9 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
Data File : BF095106.D
Acq On : 12 May 2017 8:35
Operator : SJ/MA
Sample : I3058-04 20X
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** KY032MW006-170508

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Heptanoic acid | 7.50 | 20.0 | ng | 660796 | 1 | 7.70 | 660796 | 20.0 |
| n-Hexadecanoic acid | 16.05 | 814.9 | ng | 26948900 | 4 | 14.96 | 661428 | 20.0 |
| 9,17-Octadecadien... | 17.11 | 502.9 | ng | 56291200 | 5 | 18.65 | 2238740 | 20.0 |
| Octadecanoic acid | 17.21 | 31.8 | ng | 3554300 | 5 | 18.65 | 2238740 | 20.0 |
| Methyl 9,12-hepta... | 17.31 | 105.5 | ng | 11806300 | 5 | 18.65 | 2238740 | 20.0 |
| 9,12-Octadecadien... | 17.33 | 28.7 | ng | 3217020 | 5 | 18.65 | 2238740 | 20.0 |
| unknown17.96 | 17.96 | 55.0 | ng | 6151640 | 5 | 18.65 | 2238740 | 20.0 |
| Eicosanoic acid | 18.01 | 5.2 | ng | 581973 | 5 | 18.65 | 2238740 | 20.0 |
| unknown18.04 | 18.04 | 20.0 | ng | 2238740 | 5 | 18.65 | 2238740 | 20.0 |