# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

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_M\METHODS\8270-BM082120.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 | 7.728 | 794 | 806 | 811 | rBV | 19585111 | 40013971 | 8.01% | 1.719% |
| 2 | 9.369 | 1004 | 1085 | 1086 | rBV | 5107011 | 61860169 | 12.38% | 2.657% |
| 3 | 10.351 | 1214 | 1252 | 1256 | rBV2 | 4662555 | 36346671 | 7.27% | 1.561% |
| 4 | 12.745 | 1625 | 1659 | 1663 | rBV | 4554911 | 26141090 | 5.23% | 1.123% |
| 5 | 14.927 | 1992 | 2030 | 2032 | rBV | 18926558 | 105593551 | 21.13% | 4.536% |
| 6 | 16.221 | 2241 | 2250 | 2254 | rBV | 27833311 | 51862013 | 10.38% | 2.228% |
| 7 | 16.286 | 2254 | 2261 | 2264 | rVV2 | 47714873 | 100489095 | 20.11% | 4.317% |
| 8 | 16.327 | 2264 | 2268 | 2277 | rVB2 | 41189995 | 60627229 | 12.13% | 2.604% |
| 9 | 16.533 | 2289 | 2303 | 2310 | rBV2 | 8696091 | 23415180 | 4.68% | 1.006% |
| 10 | 16.839 | 2344 | 2355 | 2356 | rBV3 | 50450304 | 129124204 | 25.84% | 5.547% |
| 11 | 18.039 | 2537 | 2559 | 2585 | rBV | 37603132 | 144717511 | 28.96% | 6.216% |
| 12 | 18.251 | 2586 | 2595 | 2602 | rVB | 23684932 | 48000442 | 9.60% | 2.062% |
| 13 | 18.862 | 2695 | 2699 | 2708 | rBV2 | 4013352 | 7633471 | 1.53% | 0.328% |
| 14 | 19.133 | 2738 | 2745 | 2752 | rVB2 | 10374940 | 18185953 | 3.64% | 0.781% |
| 15 | 19.268 | 2759 | 2768 | 2774 | rVB | 21014754 | 37447455 | 7.49% | 1.609% |
| 16 | 19.462 | 2796 | 2801 | 2807 | rVB | 29761134 | 35960473 | 7.20% | 1.545% |
| 17 | 19.556 | 2812 | 2817 | 2826 | rVB | 13881083 | 16959920 | 3.39% | 0.729% |
| 18 | 19.645 | 2827 | 2832 | 2834 | rBV | 7675260 | 11026075 | 2.21% | 0.474% |
| 19 | 20.115 | 2906 | 2912 | 2915 | rBV | 16962071 | 20155374 | 4.03% | 0.866% |
| 20 | 20.627 | 2994 | 2999 | 3003 | rBV | 16193336 | 18295523 | 3.66% | 0.786% |
| 21 | 20.950 | 3048 | 3054 | 3058 | rBV | 10079318 | 11838003 | 2.37% | 0.509% |
| 22 | 21.103 | 3076 | 3080 | 3084 | rBV | 16196025 | 17432375 | 3.49% | 0.749% |
| 23 | 21.815 | 3196 | 3201 | 3206 | rVB | 13771254 | 14981436 | 3.00% | 0.644% |
| 24 | 22.239 | 3268 | 3273 | 3281 | rVB | 5099075 | 6315667 | 1.26% | 0.271% |
| 25 | 22.450 | 3303 | 3309 | 3315 | rBV | 7040434 | 11608274 | 2.32% | 0.499% |
| 26 | 22.821 | 3362 | 3372 | 3387 | rVB | 39681653 | 69136125 | 13.83% | 2.970% |
| 27 | 23.256 | 3440 | 3446 | 3451 | rVB | 3694889 | 5999333 | 1.20% | 0.258% |
| 28 | 24.662 | 3662 | 3685 | 3695 | rBV | 56254401 | 455103191 | 91.06% | 19.549% |
| 29 | 26.297 | 3946 | 3963 | 3964 | rBV4 | 3526208 | 14312070 | 2.86% | 0.615% |
| 30 | 26.550 | 3969 | 4006 | 4010 | rVB4 | 55257619 | 499792906 | 100.00% | 21.469% |
| 31 | 27.491 | 4131 | 4166 | 4167 | rBV | 29218732 | 198496633 | 39.72% | 8.527% |
| 32 | 28.556 | 4332 | 4347 | 4360 | rVB | 7418565 | 29098353 | 5.82% | 1.250% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

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_M\METHODS\8270-BM082120.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 2327969736

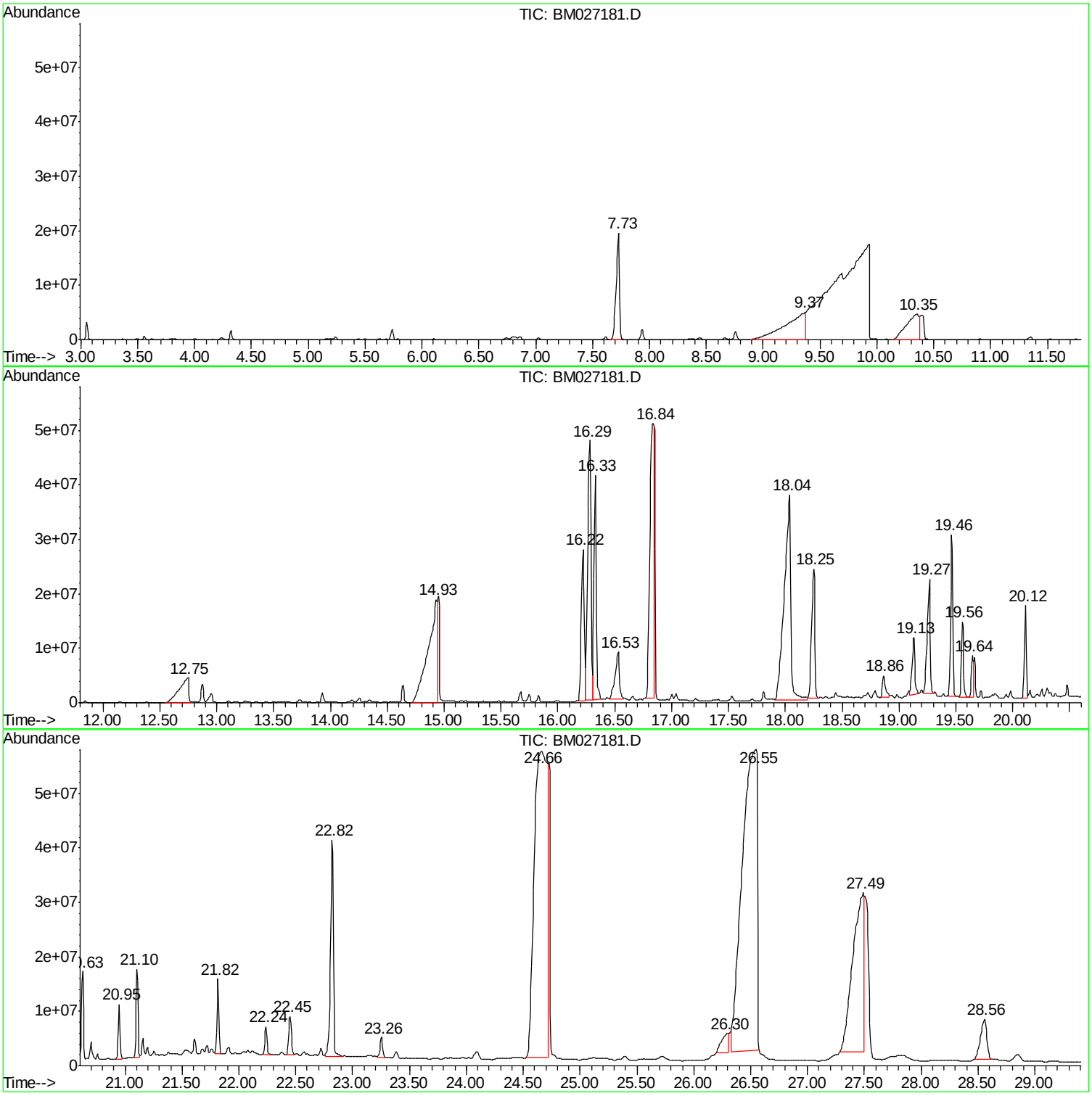
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.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:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

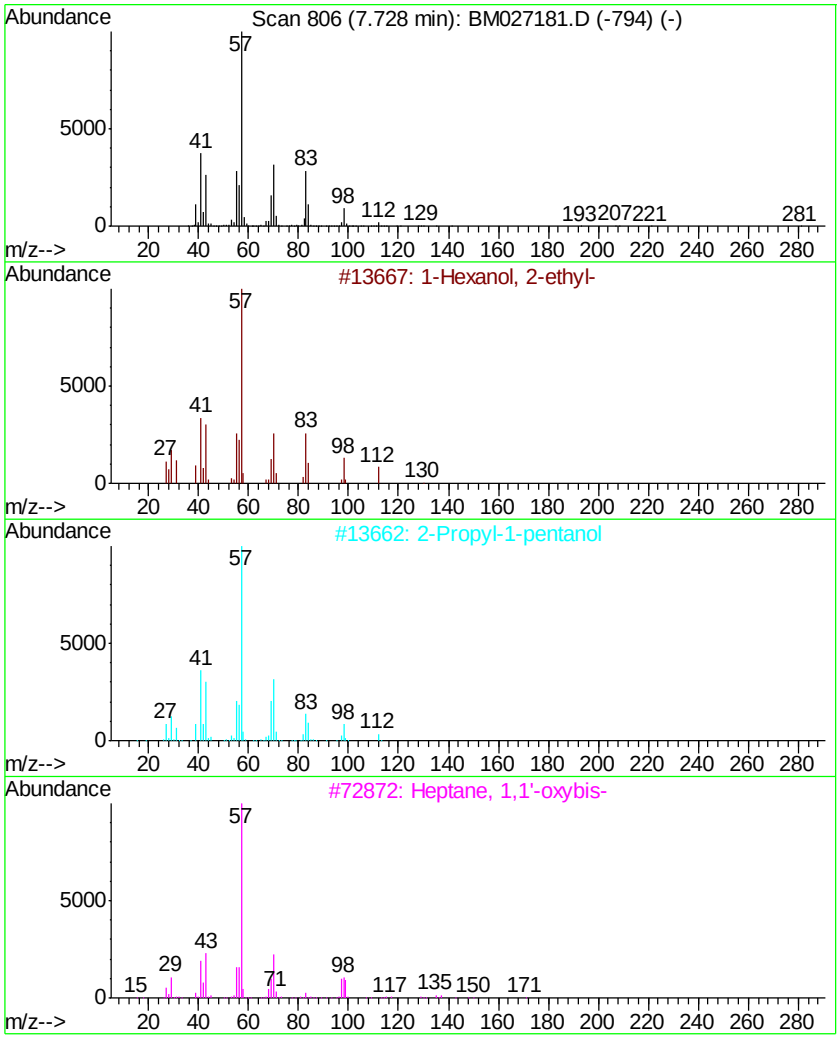
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

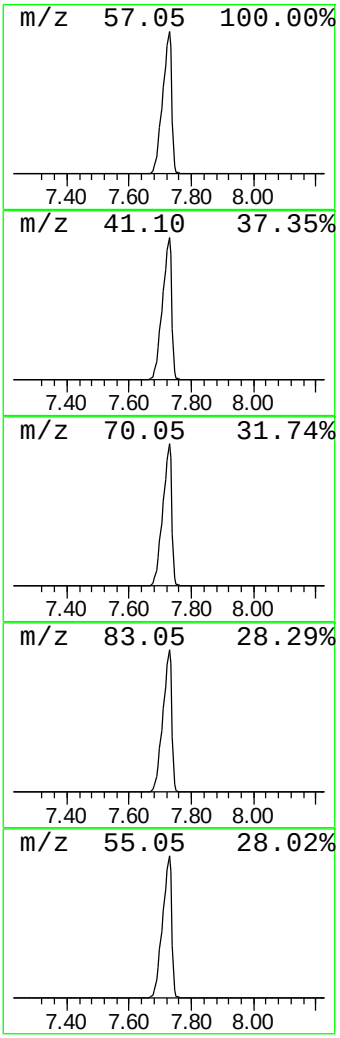
**********

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.73 | 20.00 ng | 40014000 | 1,4-Dichlorobenzene-d4 | 7.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 59 |
| 3 | Heptane, 1,1'-oxybis- | 214 | C14H30O | 000629-64-1 | 53 |
| 4 | Bicyclo[3.1.0]hexan-2-ol | 98 | C6H10O | 1000194-18-6 | 47 |
| 5 | 2-Ethyl-1-hexanol, trifluoroacetate | 226 | C10H17F3O2 | 1000365-19-6 | 47 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

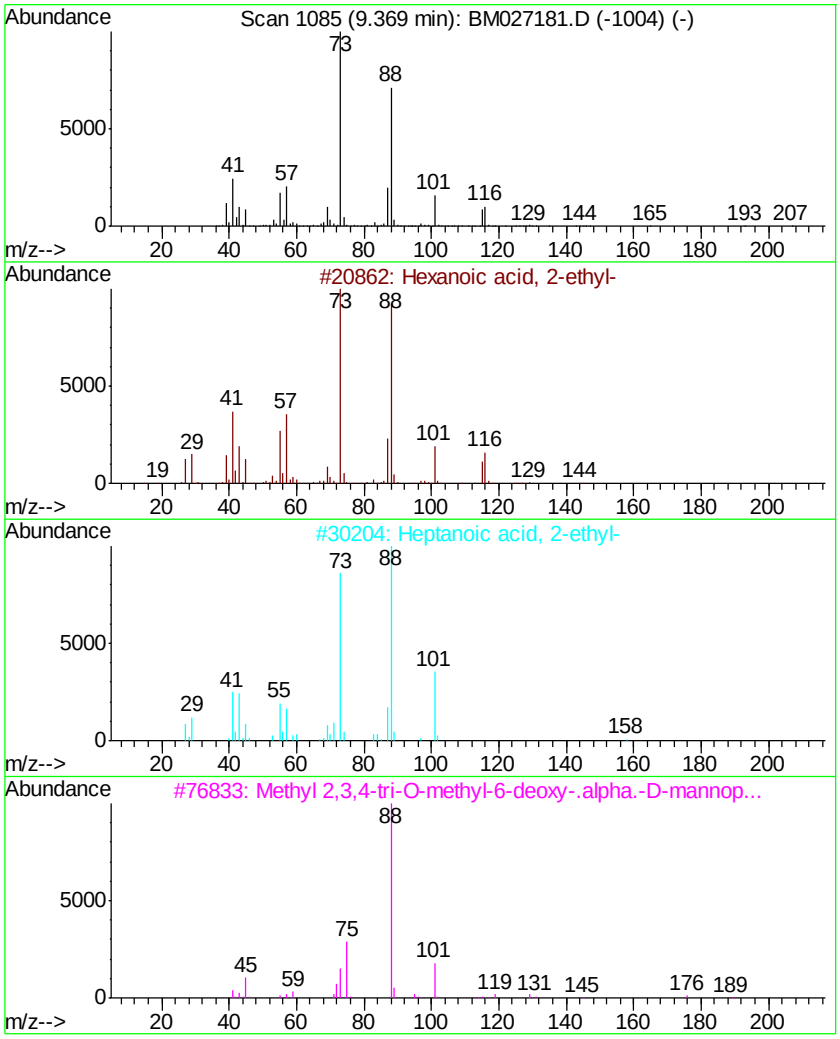
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

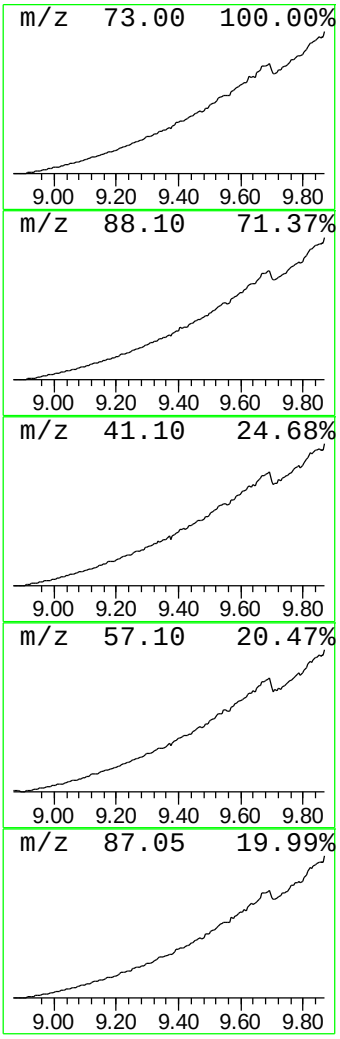
**********

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.37 | 34.04 ng | 61860200 | Naphthalene-d8 | 10.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 72 |
| 2 | Heptanoic acid, 2-ethyl- | 158 | C9H18O2 | 003274-29-1 | 53 |
| 3 | Methyl 2,3,4-tri-O-methyl-6-deox... | 220 | C10H20O5 | 072983-16-5 | 32 |
| 4 | Pentanoic acid, 2,4-dimethyl-, m... | 144 | C8H16O2 | 071672-33-8 | 28 |
| 5 | Propanoic acid, 3-hydroxy-2-meth... | 118 | C5H10O3 | 042998-03-8 | 28 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

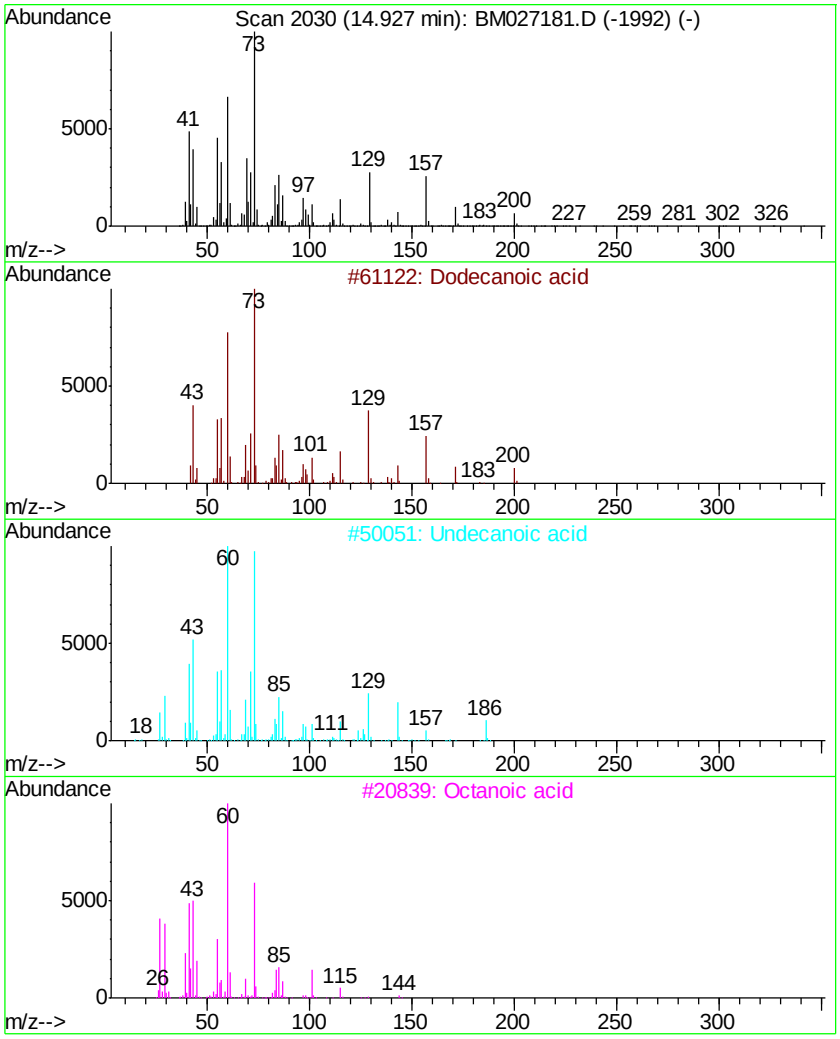
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

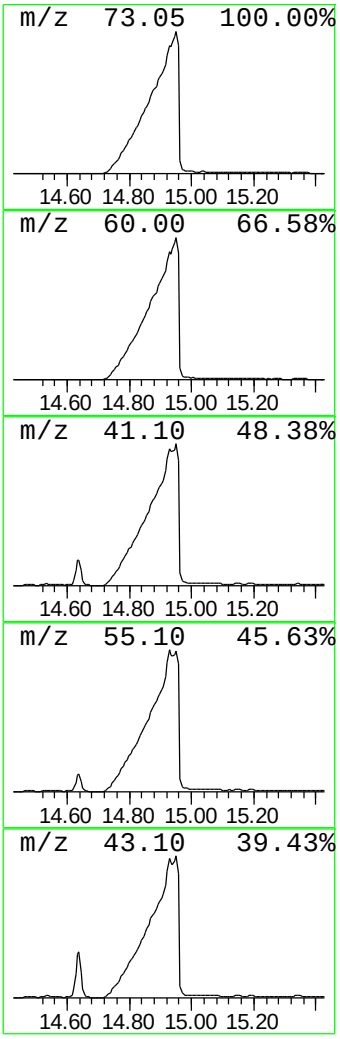
**********

Peak Number 3 Dodecanoic acid Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.93 | 20.00 ng | 105594000 | Acenaphthene-d10 | 14.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 99 |
| 2 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 50 |
| 3 | Octanoic acid | 144 | C8H16O2 | 000124-07-2 | 43 |
| 4 | .alpha.-D-Glucopyranose, 4-O-.be... | 342 | C12H22O11 | 014641-93-1 | 38 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 38 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

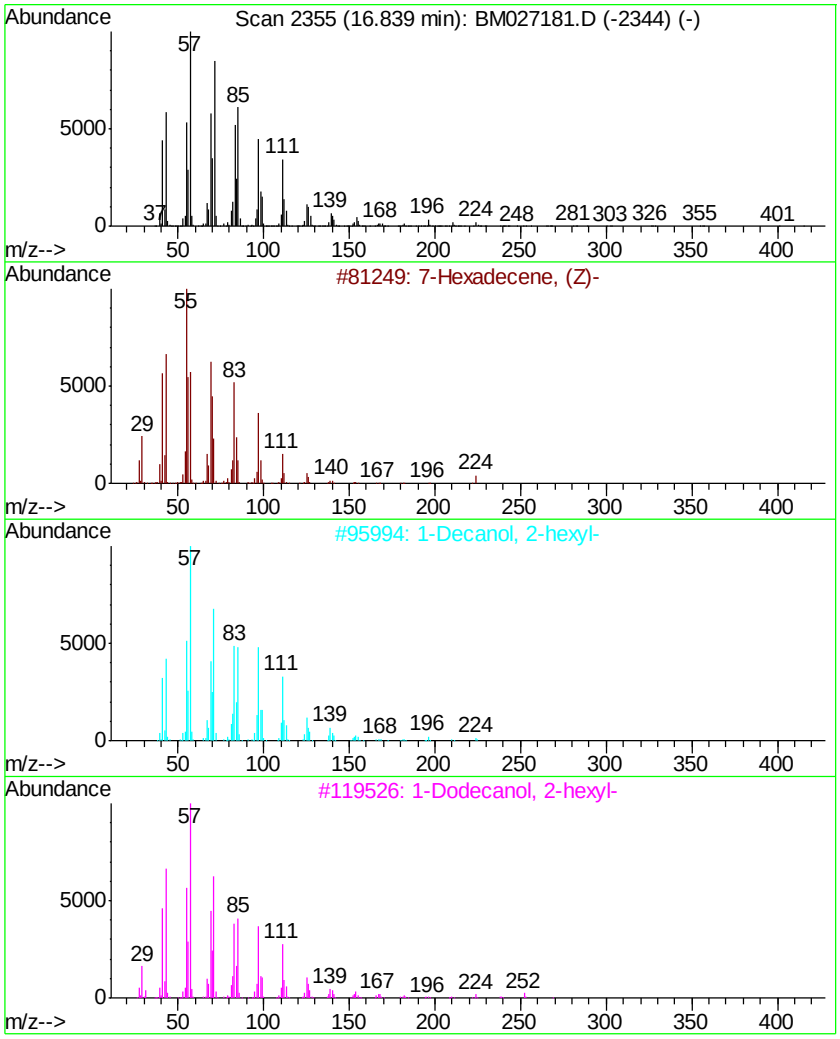
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

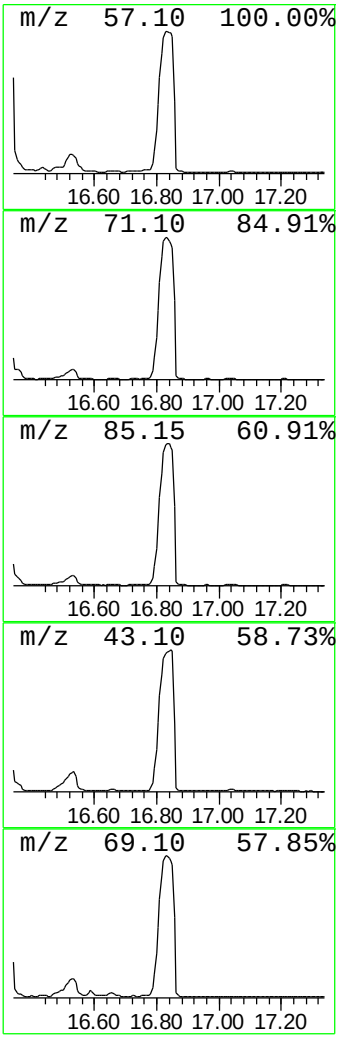
**********

Peak Number 4 7-Hexadecene, (Z)- Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.84 | 20.00 ng | 129124000 | Phenanthrene-d10 | 17.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7-Hexadecene, (Z)- | 224 | C16H32 | 035507-09-6 | 95 |
| 2 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 94 |
| 3 | 1-Dodecanol, 2-hexyl- | 270 | C18H38O | 110225-00-8 | 91 |
| 4 | 1-Decanol, 2-octyl- | 270 | C18H38O | 045235-48-1 | 91 |
| 5 | 2-Hexyl-1-octanol | 214 | C14H30O | 019780-79-1 | 91 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

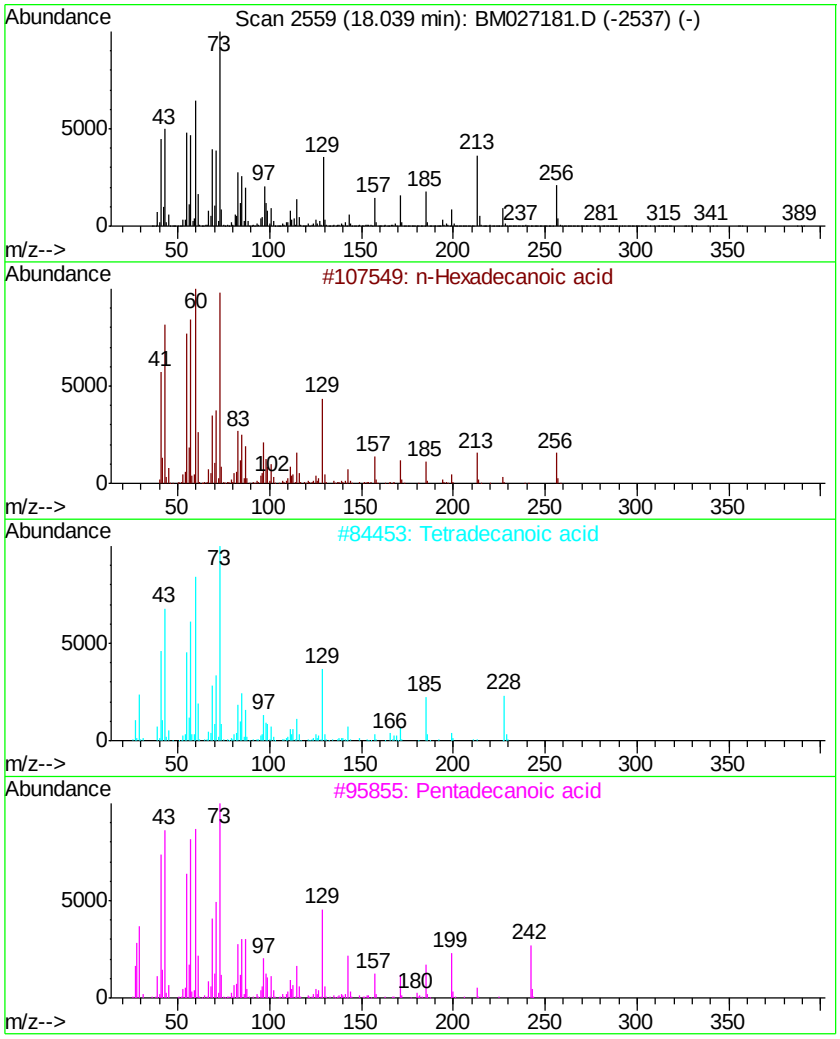
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

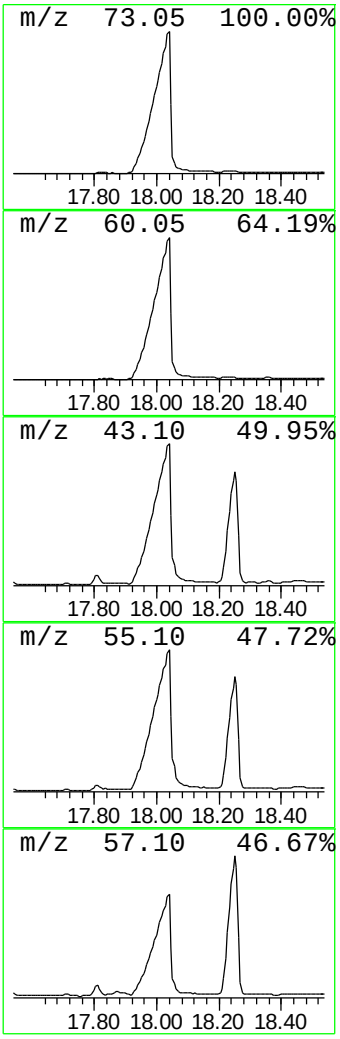
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 n-Hexadecanoic acid Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.04 | 22.42 ng | 144718000 | Phenanthrene-d10 | 17.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 92 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 60 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 58 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 50 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 43 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

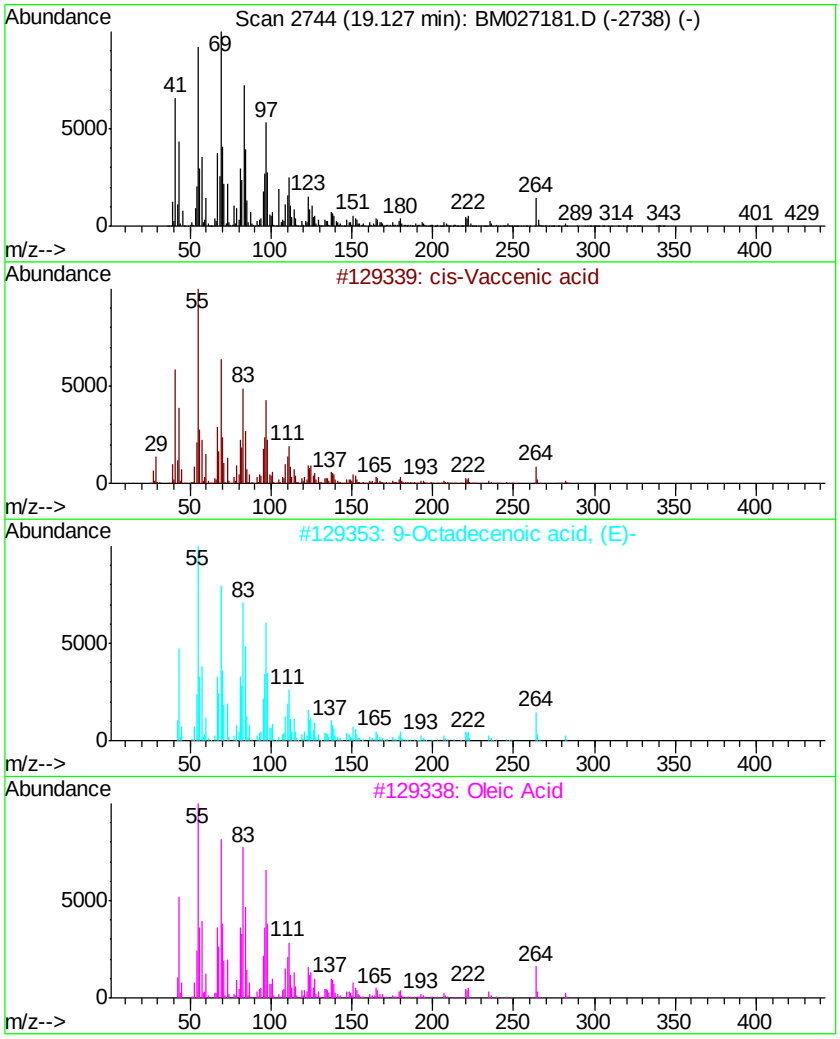
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

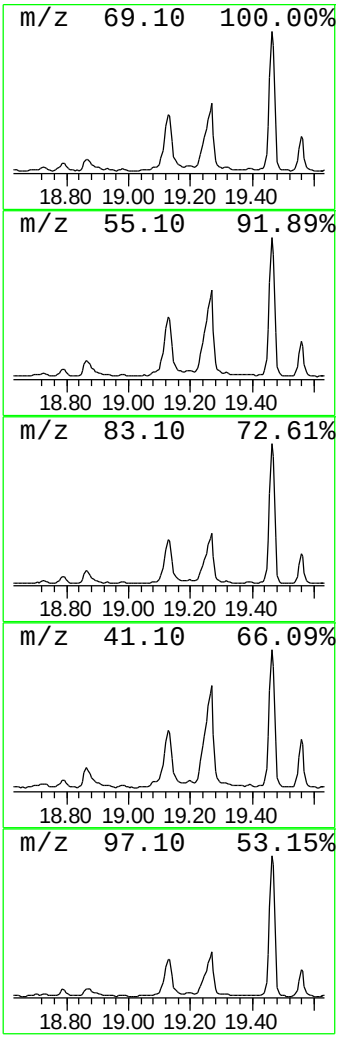
**********

Peak Number 6 cis-Vaccenic acid Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.13 | 20.86 ng | 18186000 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-Vaccenic acid | 282 | C18H34O2 | 000506-17-2 | 97 |
| 2 | 9-Octadecenoic acid, (E)- | 282 | C18H34O2 | 000112-79-8 | 97 |
| 3 | Oleic Acid | 282 | C18H34O2 | 000112-80-1 | 94 |
| 4 | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 80 |
| 5 | trans-13-Octadecenoic acid | 282 | C18H34O2 | 000693-71-0 | 70 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

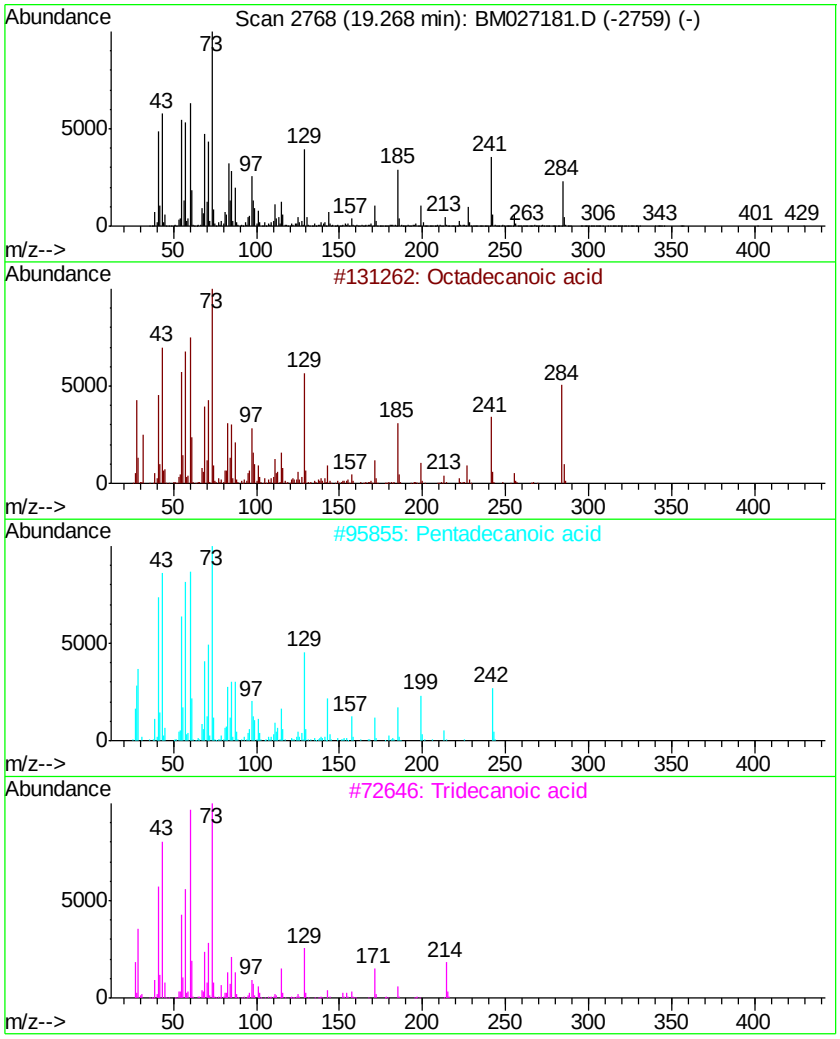
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

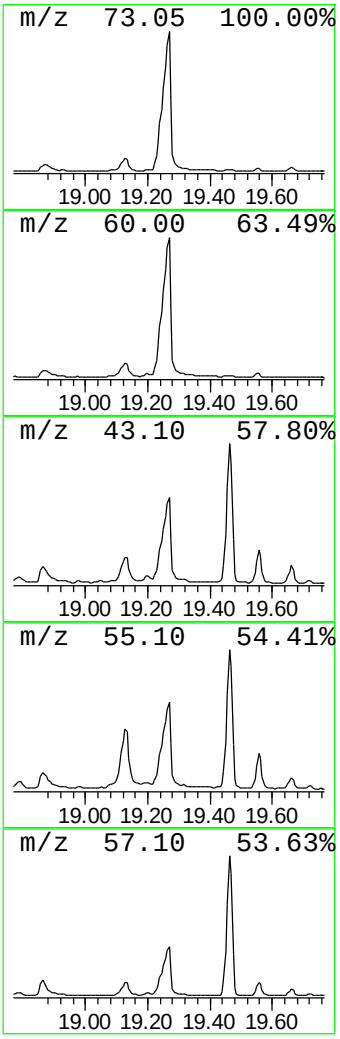
**********

Peak Number 7 Octadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.27 | 42.96 ng | 37447500 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 86 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 60 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 52 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

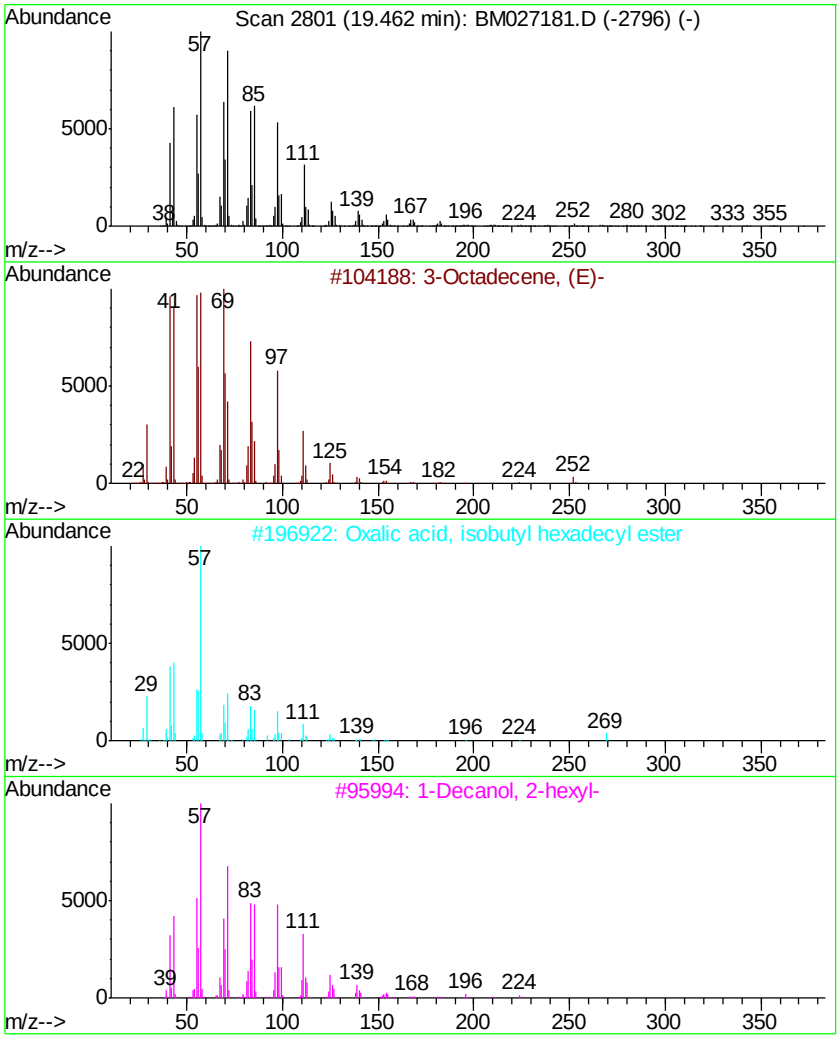
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

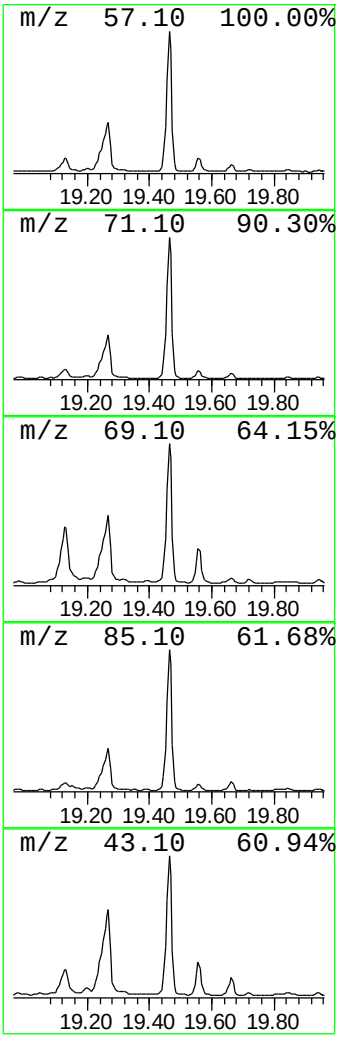
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 3-Octadecene, (E)- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.46 | 41.26 ng | 35960500 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 92 |
| 2 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 91 |
| 3 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 91 |
| 4 | Oxalic acid, isobutyl pentadecyl... | 356 | C21H40O4 | 1000309-38-0 | 83 |
| 5 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 74 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

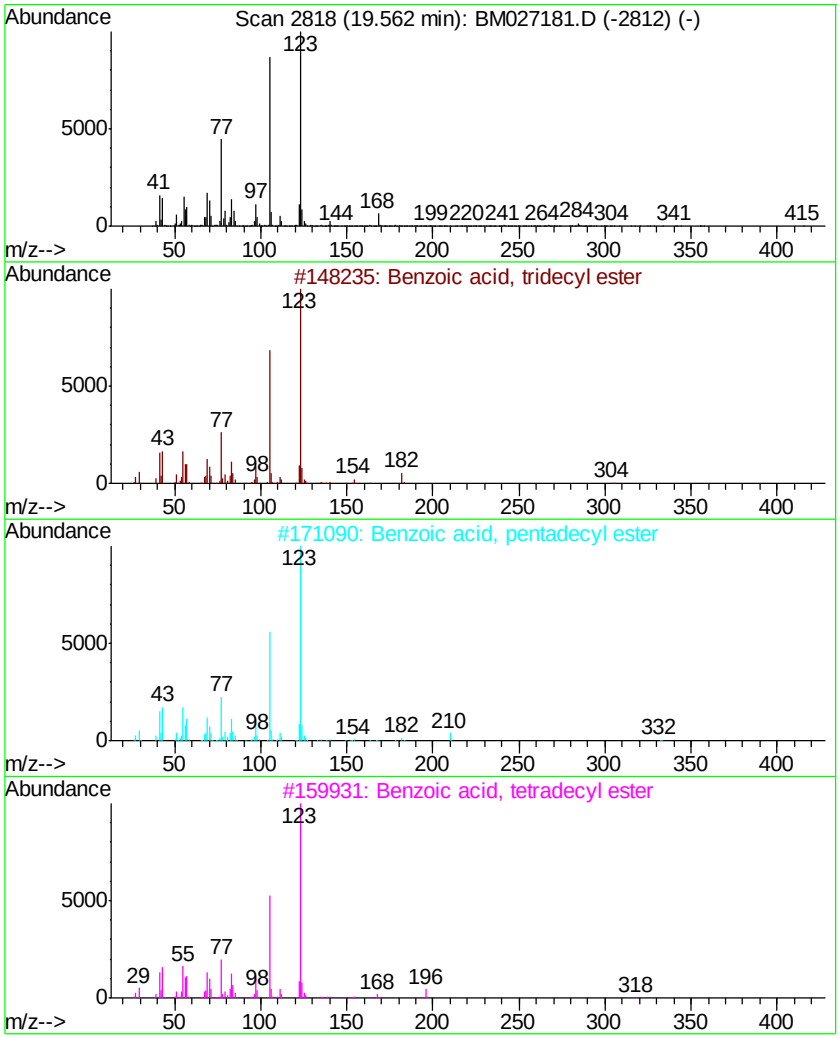
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

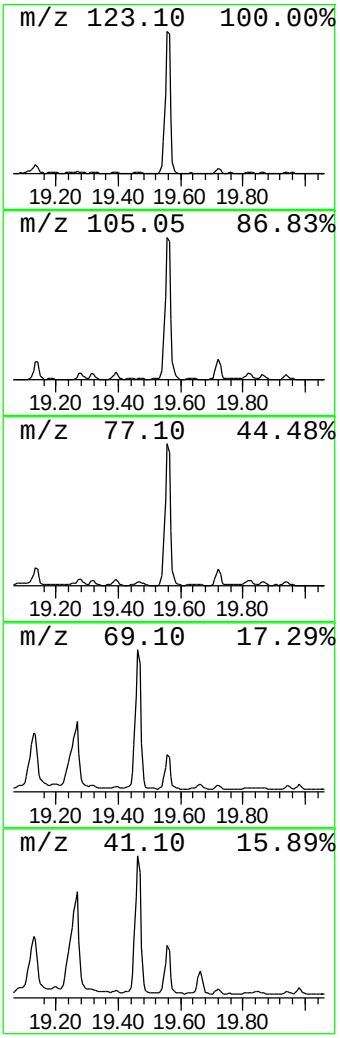
**********

Peak Number 9 Benzoic acid, tridecyl ester Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.56 | 19.46 ng | 16959900 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, tridecyl ester | 304 | C20H32O2 | 1000340-22-6 | 95 |
| 2 | Benzoic acid, pentadecyl ester | 332 | C22H36O2 | 1000340-22-8 | 94 |
| 3 | Benzoic acid, tetradecyl ester | 318 | C21H34O2 | 1000340-22-7 | 74 |
| 4 | Benzoic acid, octadecyl ester | 374 | C25H42O2 | 1000340-23-1 | 68 |
| 5 | Benzoic acid, octyl ester | 234 | C15H22O2 | 000094-50-8 | 64 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

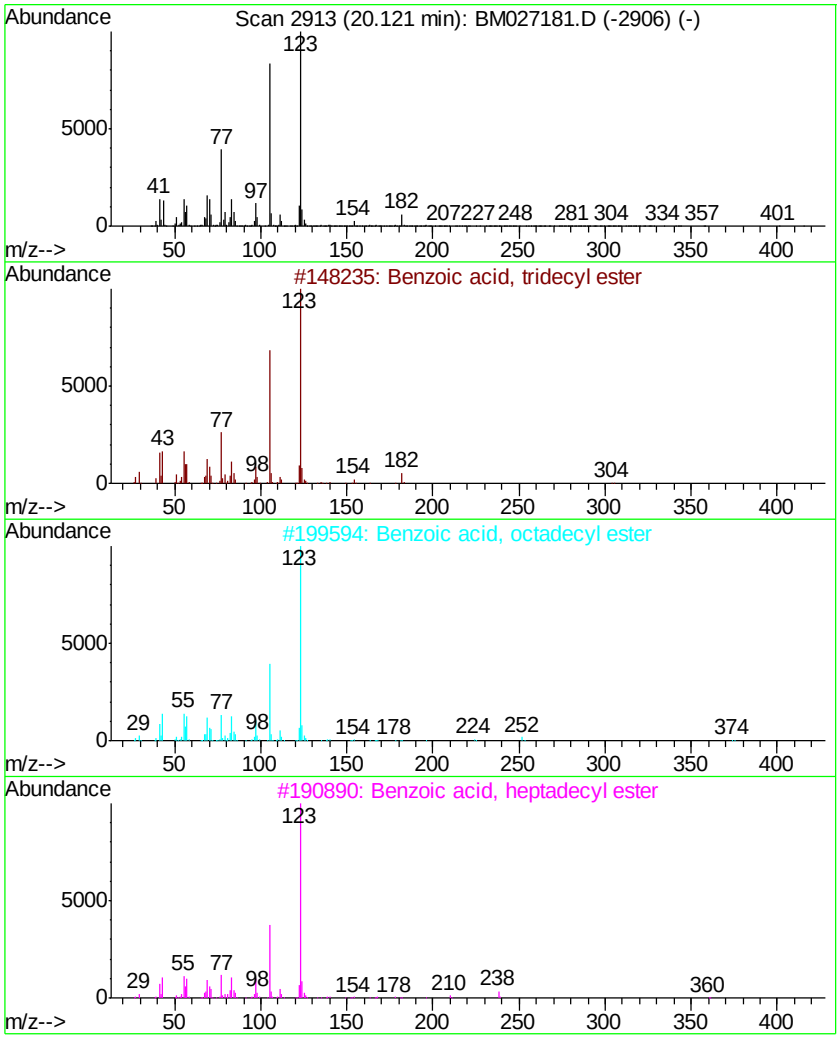
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

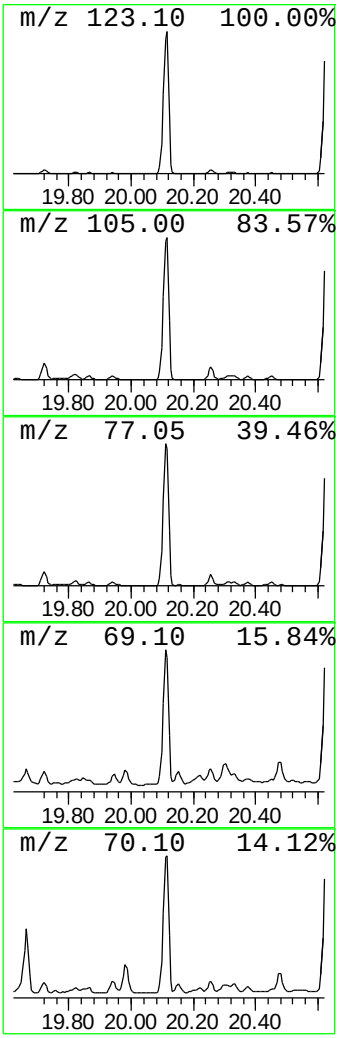
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 Benzoic acid, octadecyl ester Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.12 | 23.12 ng | 20155400 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, tridecyl ester | 304 | C20H32O2 | 1000340-22-6 | 95 |
| 2 | Benzoic acid, octadecyl ester | 374 | C25H42O2 | 1000340-23-1 | 74 |
| 3 | Benzoic acid, heptadecyl ester | 360 | C24H40O2 | 1000340-23-0 | 74 |
| 4 | 2,6-Pyridinedicarboxylic acid | 167 | C7H5NO4 | 000499-83-2 | 72 |
| 5 | Benzoic acid, nonadecyl ester | 388 | C26H44O2 | 1000340-23-2 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

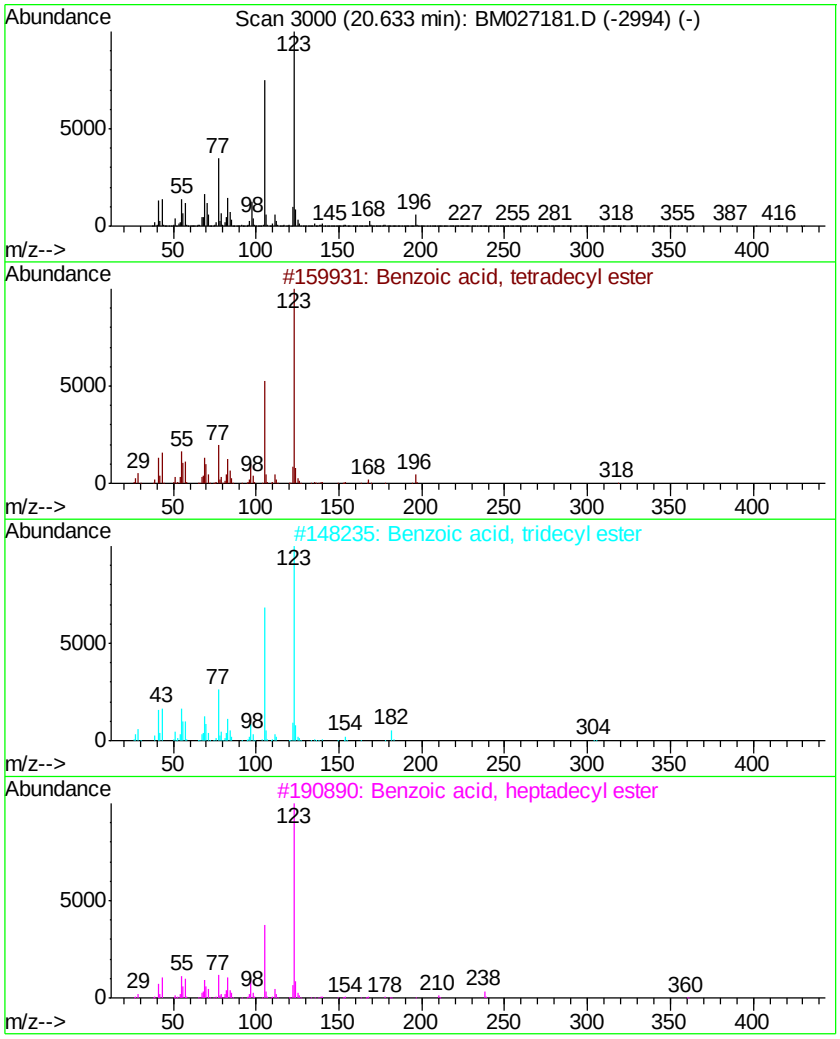
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

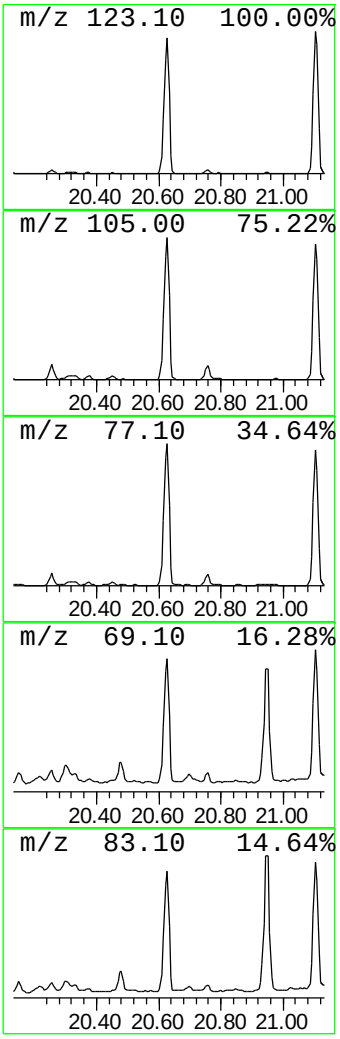
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 Benzoic acid, tetradecyl ester Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.63 | 20.99 ng | 18295500 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, tetradecyl ester | 318 | C21H34O2 | 1000340-22-7 | 97 |
| 2 | Benzoic acid, tridecyl ester | 304 | C20H32O2 | 1000340-22-6 | 91 |
| 3 | Benzoic acid, heptadecyl ester | 360 | C24H40O2 | 1000340-23-0 | 86 |
| 4 | Benzoic acid, nonadecyl ester | 388 | C26H44O2 | 1000340-23-2 | 86 |
| 5 | Benzoic acid, octadecyl ester | 374 | C25H42O2 | 1000340-23-1 | 83 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

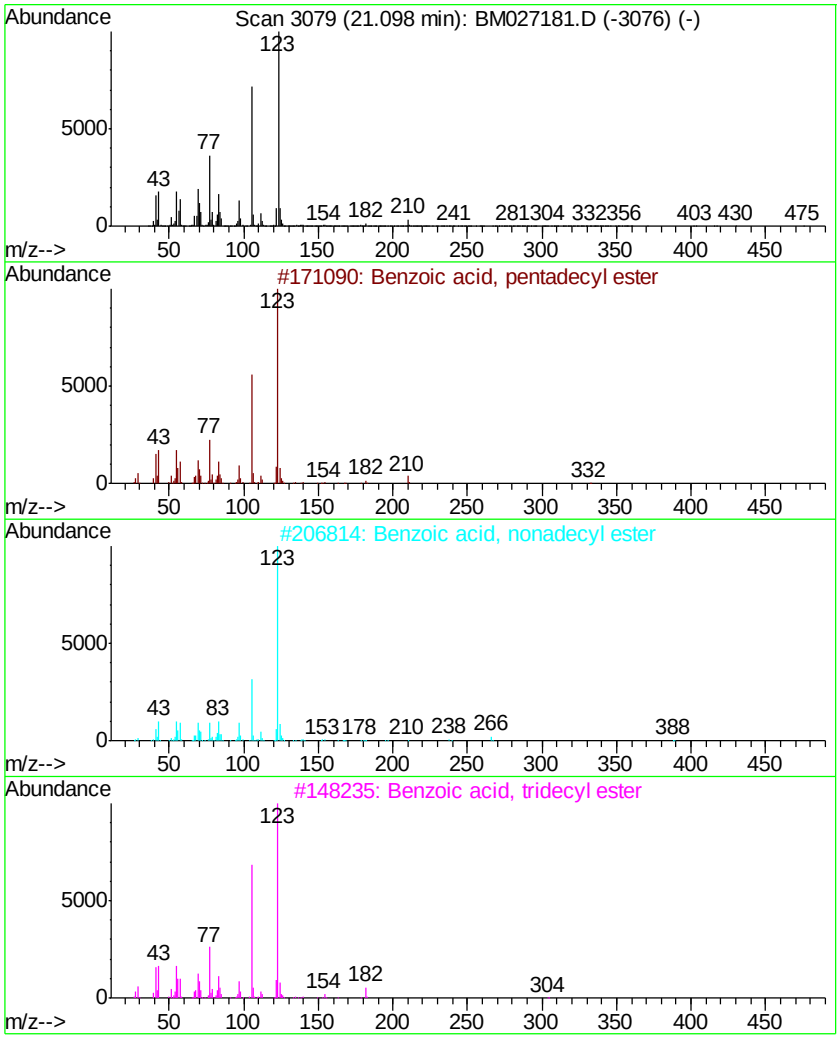
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

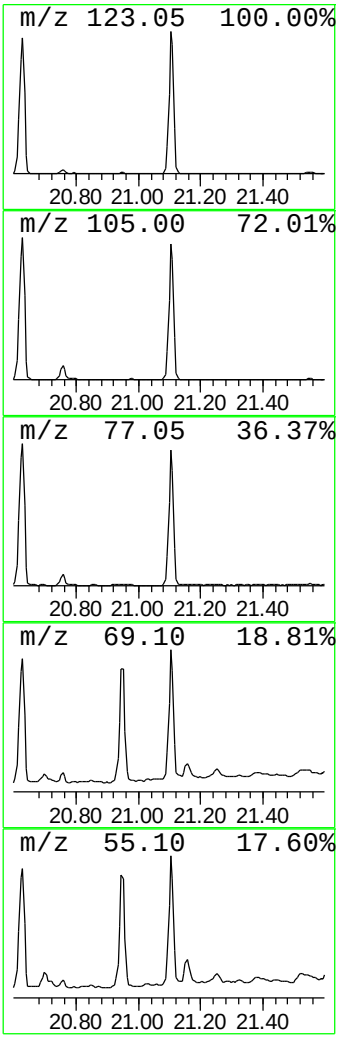
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 12 Benzoic acid, pentadecyl ester Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.10 | 20.00 ng | 17432400 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, pentadecyl ester | 332 | C22H36O2 | 1000340-22-8 | 99 |
| 2 | Benzoic acid, nonadecyl ester | 388 | C26H44O2 | 1000340-23-2 | 91 |
| 3 | Benzoic acid, tridecyl ester | 304 | C20H32O2 | 1000340-22-6 | 91 |
| 4 | Benzoic acid, undecyl ester | 276 | C18H28O2 | 006316-30-9 | 90 |
| 5 | Benzoic acid, heptadecyl ester | 360 | C24H40O2 | 1000340-23-0 | 90 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

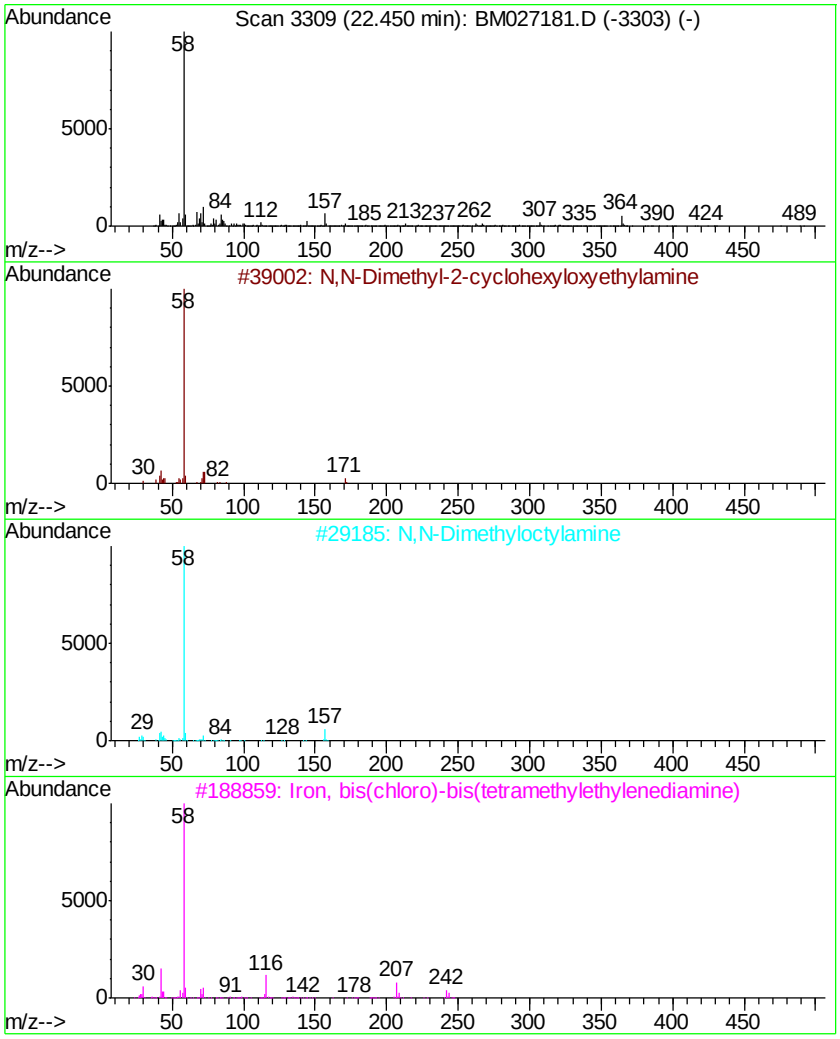
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

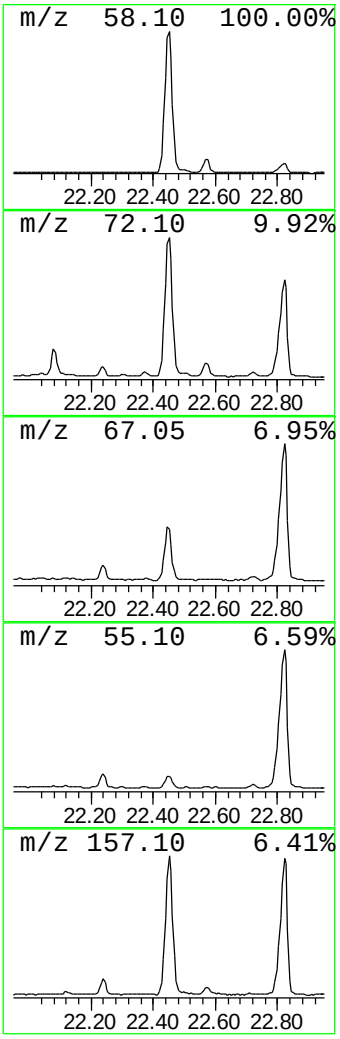
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 13 N,N-Dimethyl-2-cyclohexylox... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.45 | 38.70 ng | 11608300 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | N,N-Dimethyl-2-cyclohexyloxyethy... | 171 | C10H21NO | 071126-60-8 | 64 |
| 2 | N,N-Dimethyloctylamine | 157 | C10H23N | 007378-99-6 | 64 |
| 3 | Iron, bis(chloro)-bis(tetramethy... | 358 | C12H32Cl2FeN4 | 1000163-25-7 | 64 |
| 4 | Acetoxyacetic acid, 2-dimethylam... | 189 | C8H15NO4 | 1000331-22-6 | 64 |
| 5 | N,N-Dimethyl-2-tert-butoxyethyla... | 145 | C8H19NO | 071126-61-9 | 64 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

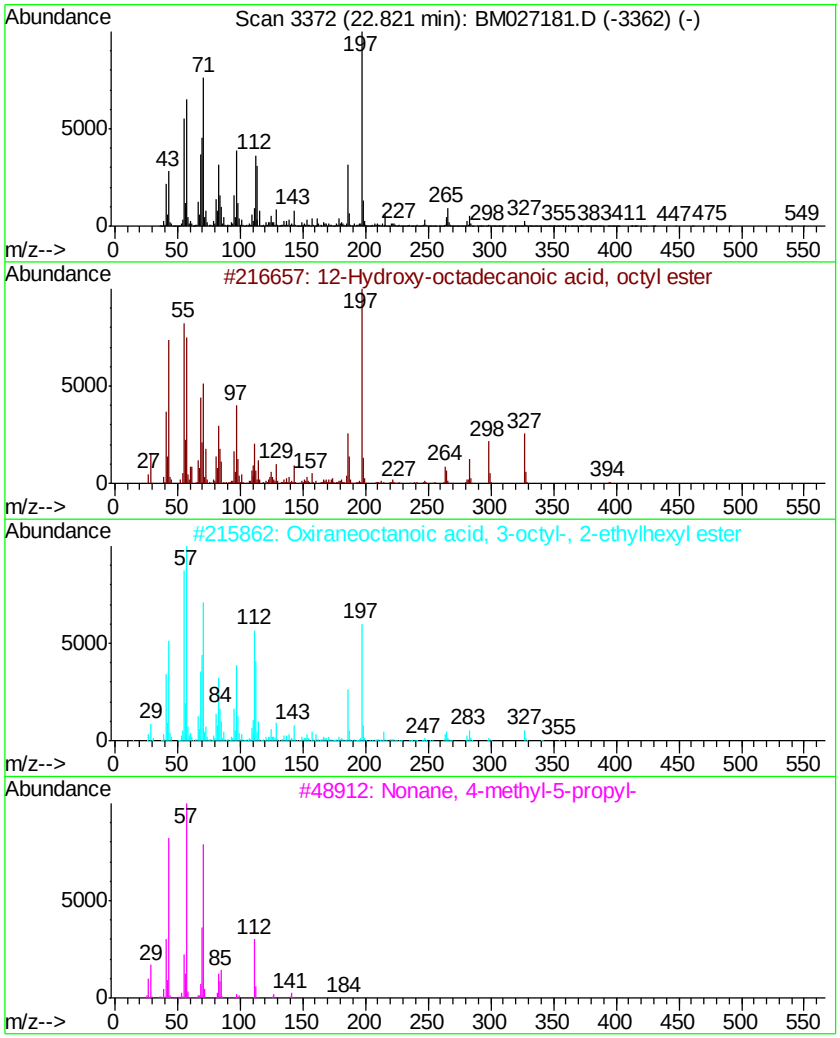
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

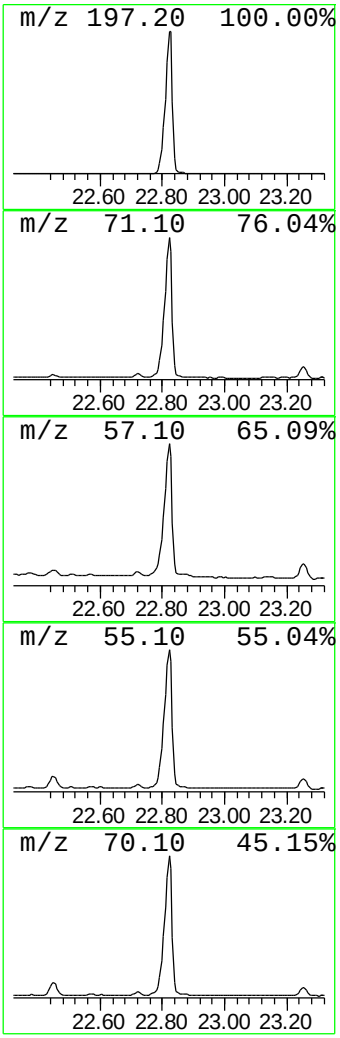
**********

Peak Number 14 12-Hydroxy-octadecanoic aci... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.82 | 230.48 ng | 69136100 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 12-Hydroxy-octadecanoic acid, oc... | 412 | C26H52O3 | 074819-90-2 | 50 |
| 2 | Oxiraneoctanoic acid, 3-octyl-, ... | 410 | C26H50O3 | 000141-38-8 | 45 |
| 3 | Nonane, 4-methyl-5-propyl- | 184 | C13H28 | 062185-55-1 | 35 |
| 4 | Methoxyacetic acid, 2-ethylhexyl... | 202 | C11H22O3 | 1000282-41-4 | 35 |
| 5 | Decane, 5,6-dipropyl- | 226 | C16H34 | 119209-20-0 | 30 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

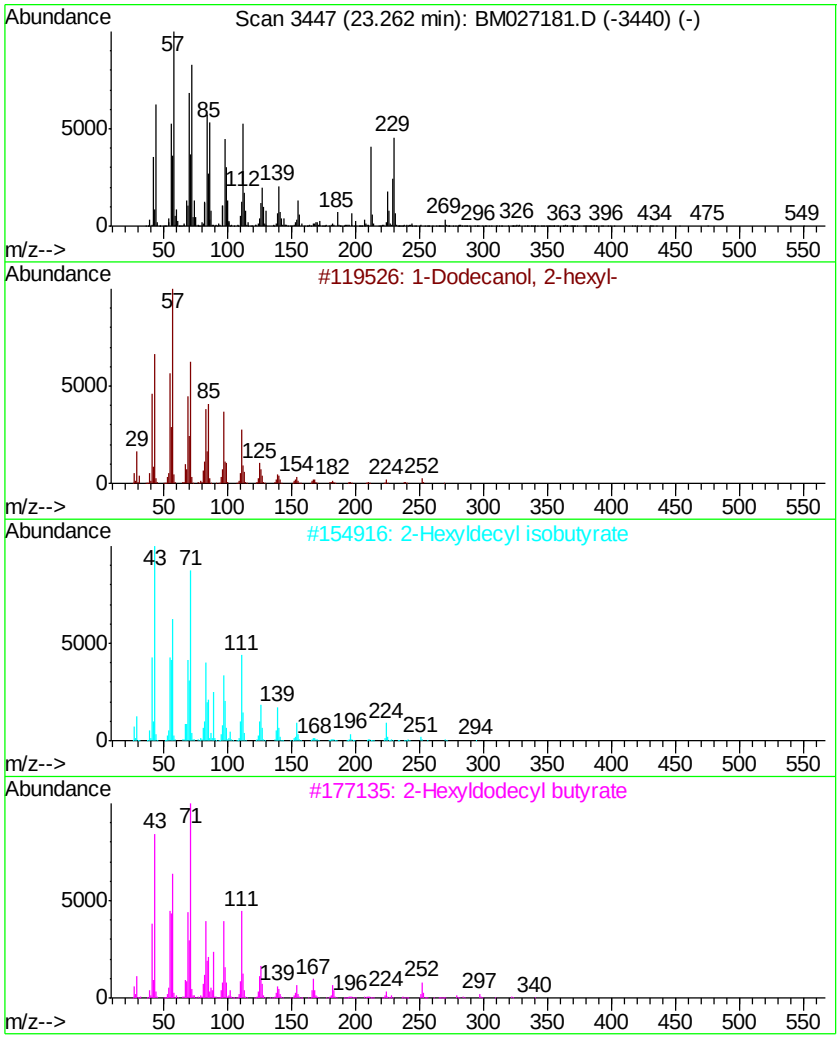
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

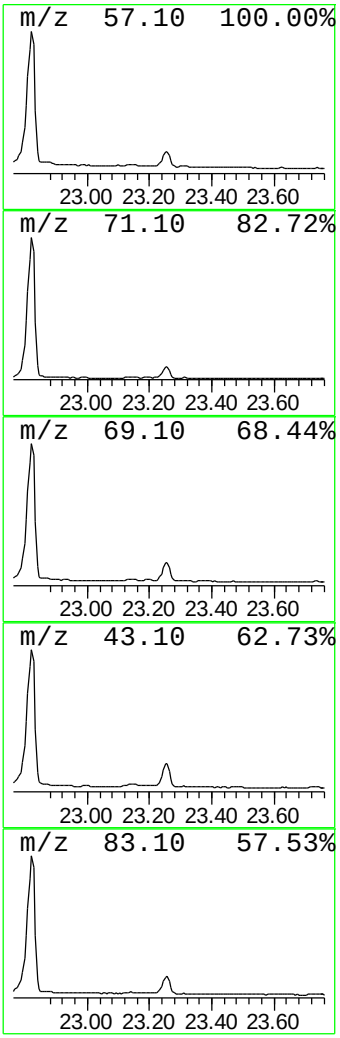
**********

Peak Number 15 1-Dodecanol, 2-hexyl- Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.26 | 20.00 ng | 5999330 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Dodecanol, 2-hexyl- | 270 | C18H38O | 110225-00-8 | 58 |
| 2 | 2-Hexyldecyl isobutyrate | 312 | C20H40O2 | 1000368-55-3 | 58 |
| 3 | 2-Hexyldodecyl butyrate | 340 | C22H44O2 | 1000368-56-1 | 55 |
| 4 | 2-Hexyldecyl acetate | 284 | C18H36O2 | 082409-75-4 | 50 |
| 5 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 49 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

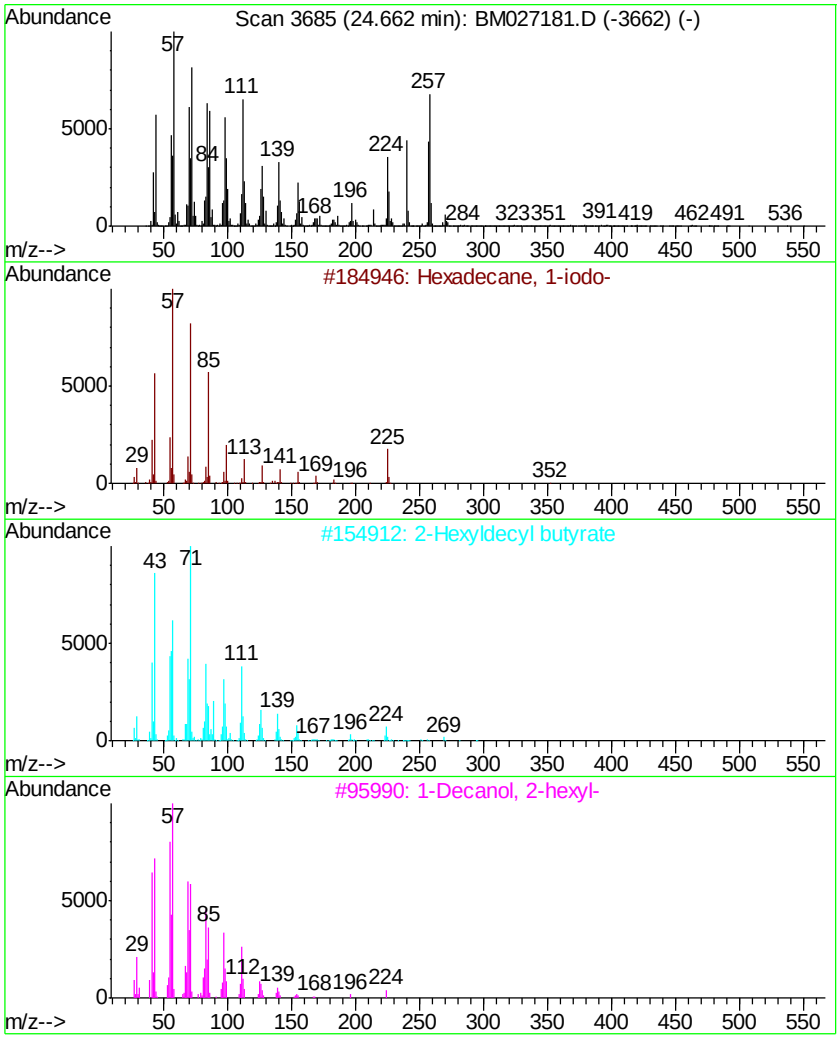
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

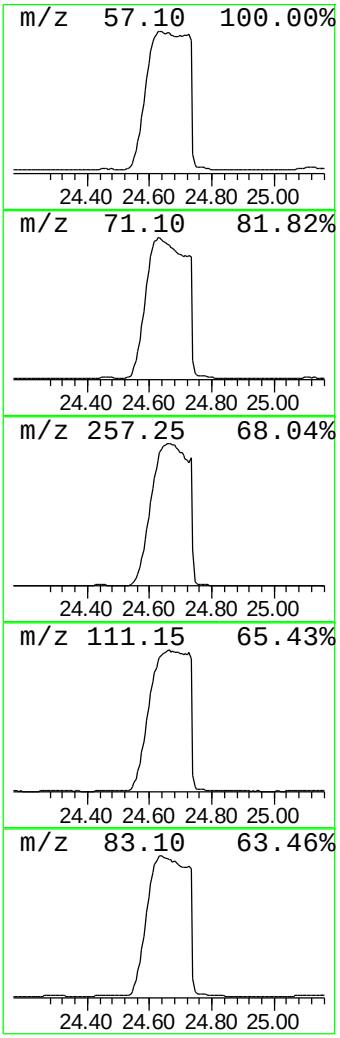
**********

Peak Number 16 Hexadecane, 1-iodo- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.66 | 1517.18 ng | 455103000 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 92 |
| 2 | 2-Hexyldecyl butyrate | 312 | C20H40O2 | 1072782-00-3 | 55 |
| 3 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 50 |
| 4 | 2-Hexyldecyl isobutyrate | 312 | C20H40O2 | 1000368-55-3 | 49 |
| 5 | Isobutyl nonyl carbonate | 244 | C14H28O3 | 959311-27-4 | 41 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

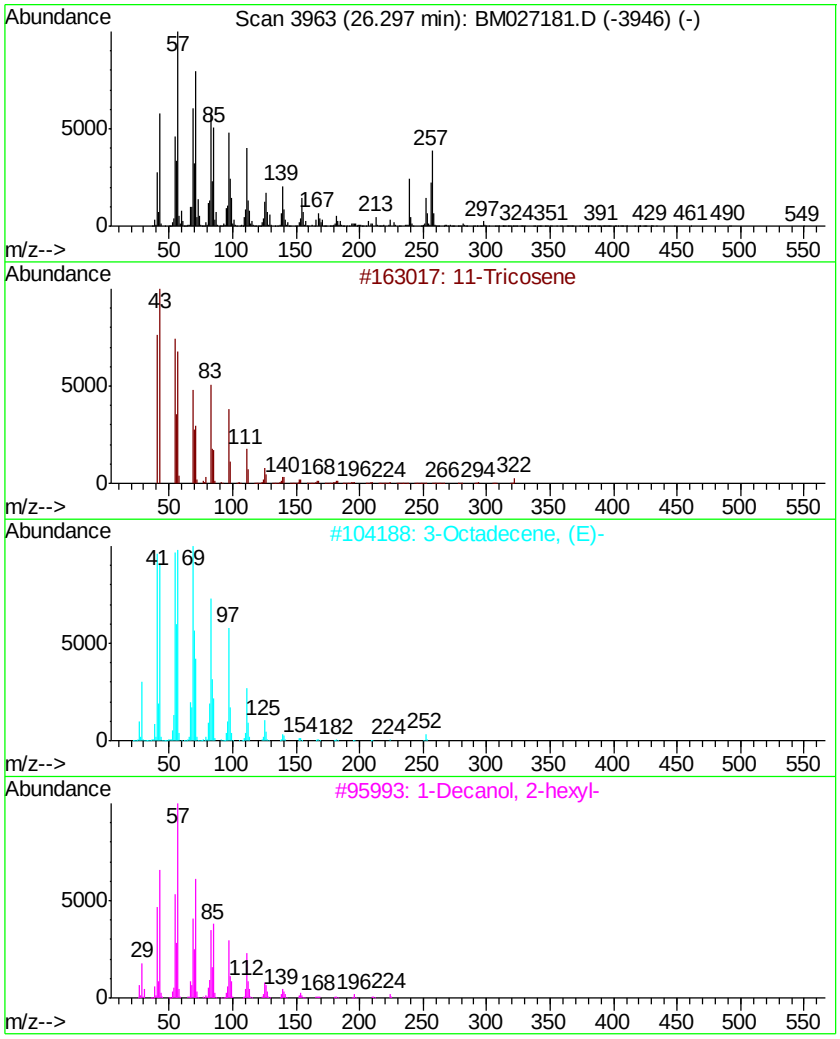
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

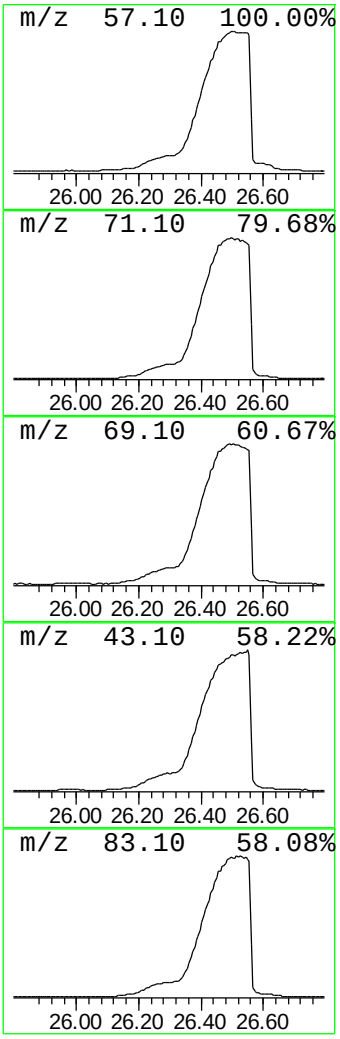
**********

Peak Number 17 11-Tricosene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.30 | 47.71 ng | 14312100 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 11-Tricosene | 322 | C23H46 | 052078-56-5 | 68 |
| 2 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 64 |
| 3 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 64 |
| 4 | 1-Dodecanol, 2-hexyl- | 270 | C18H38O | 110225-00-8 | 64 |
| 5 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 53 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

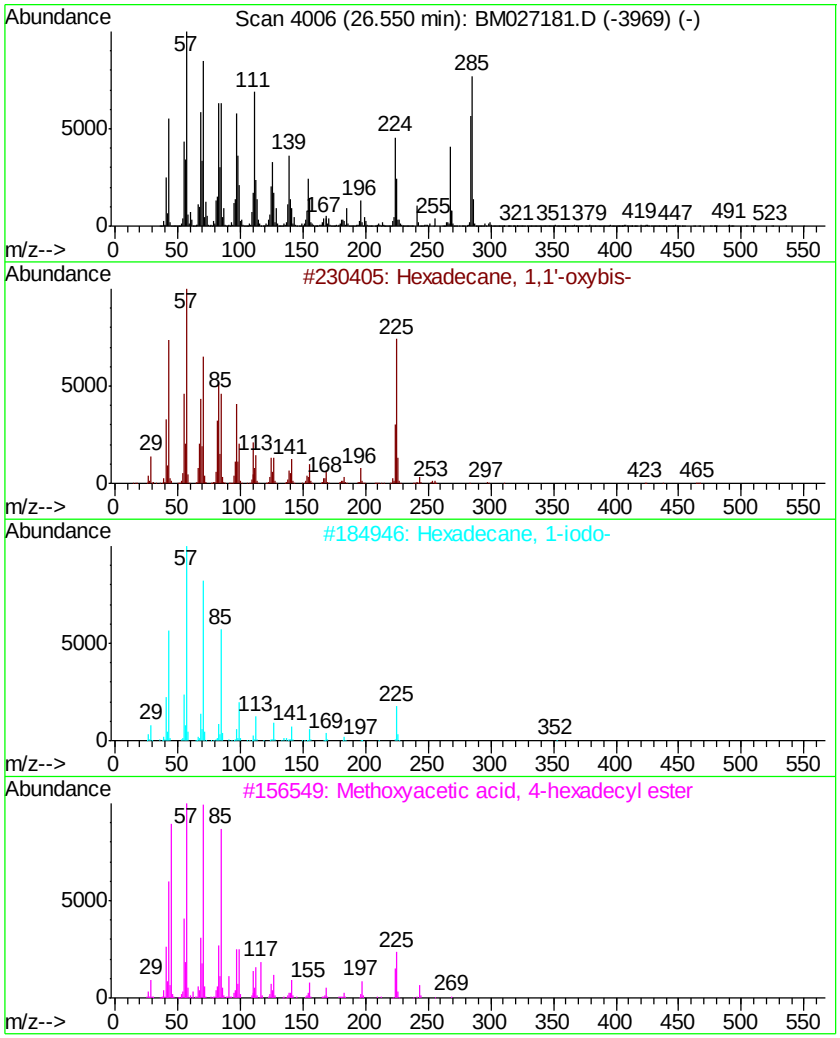
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

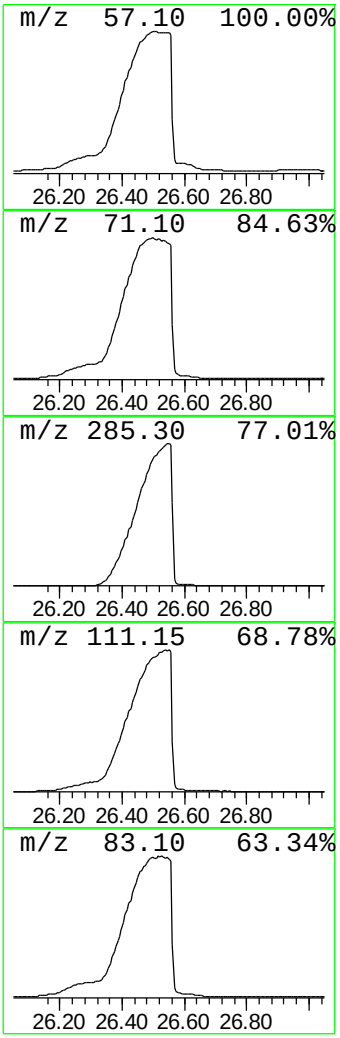
**********

Peak Number 18 unknown26.55 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.55 | 1666.16 ng | 499793000 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane, 1,1'-oxybis- | 467 | C32H66O | 004113-12-6 | 38 |
| 2 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 30 |
| 3 | Methoxyacetic acid, 4-hexadecyl ... | 314 | C19H38O3 | 1000282-99-0 | 27 |
| 4 | Trihexadecyl borate | 735 | C48H99BO3 | 002665-11-4 | 25 |
| 5 | Hexadecane, 5-butyl- | 282 | C20H42 | 006912-07-8 | 22 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

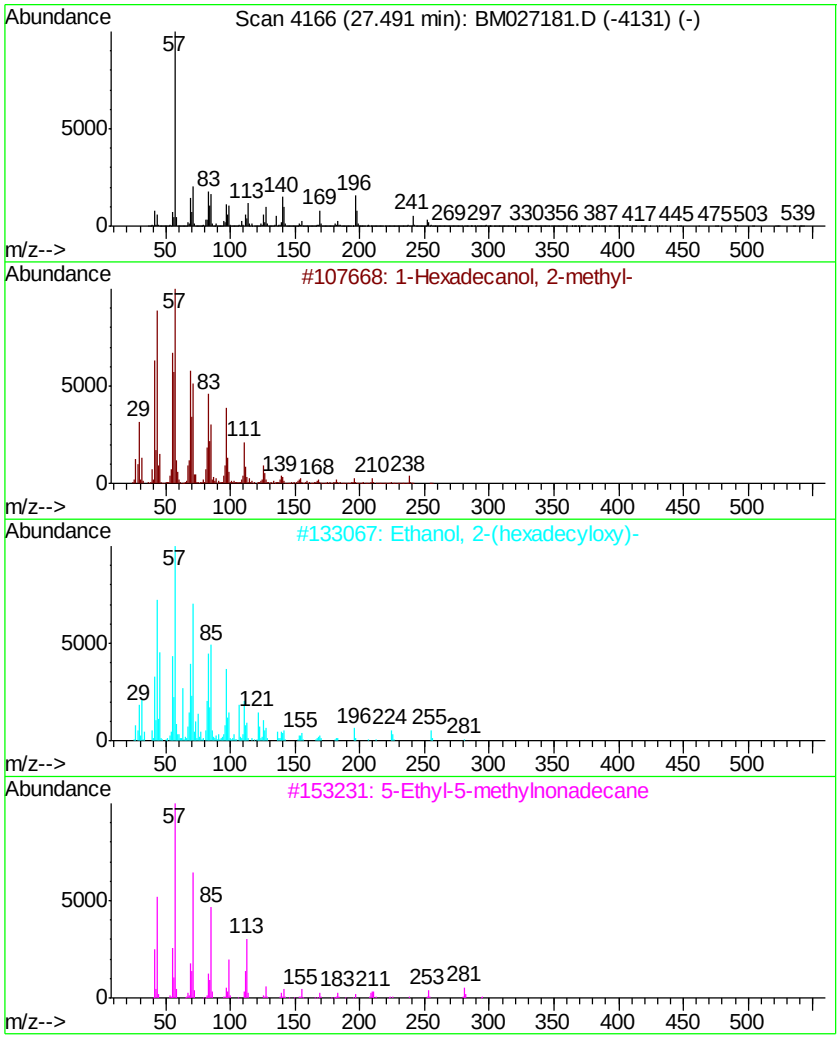
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

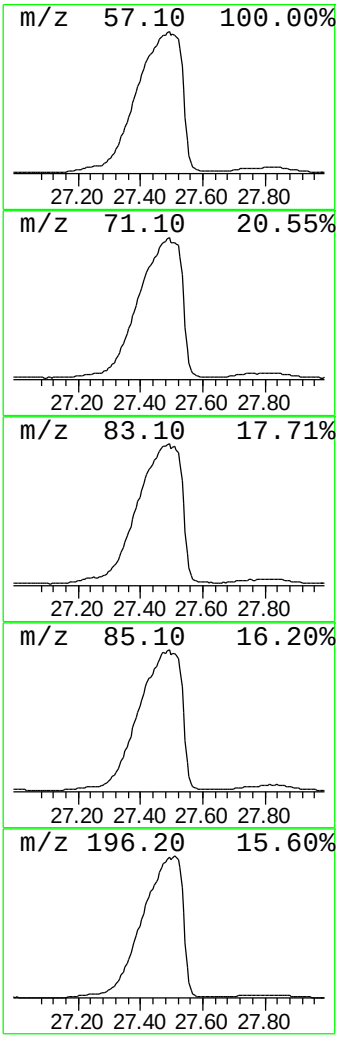
**********

Peak Number 19 unknown27.49 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 27.49 | 661.73 ng | 198497000 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexadecanol, 2-methyl- | 256 | C17H36O | 002490-48-4 | 30 |
| 2 | Ethanol, 2-(hexadecyloxy)- | 286 | C18H38O2 | 002136-71-2 | 27 |
| 3 | 5-Ethyl-5-methylnonadecane | 310 | C22H46 | 1000360-42-7 | 27 |
| 4 | Disulfide, di-tert-dodecyl | 402 | C24H50S2 | 027458-90-8 | 27 |
| 5 | Pentanoic acid, 2,4-dimethyl-, t... | 186 | C11H22O2 | 1000163-75-4 | 22 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

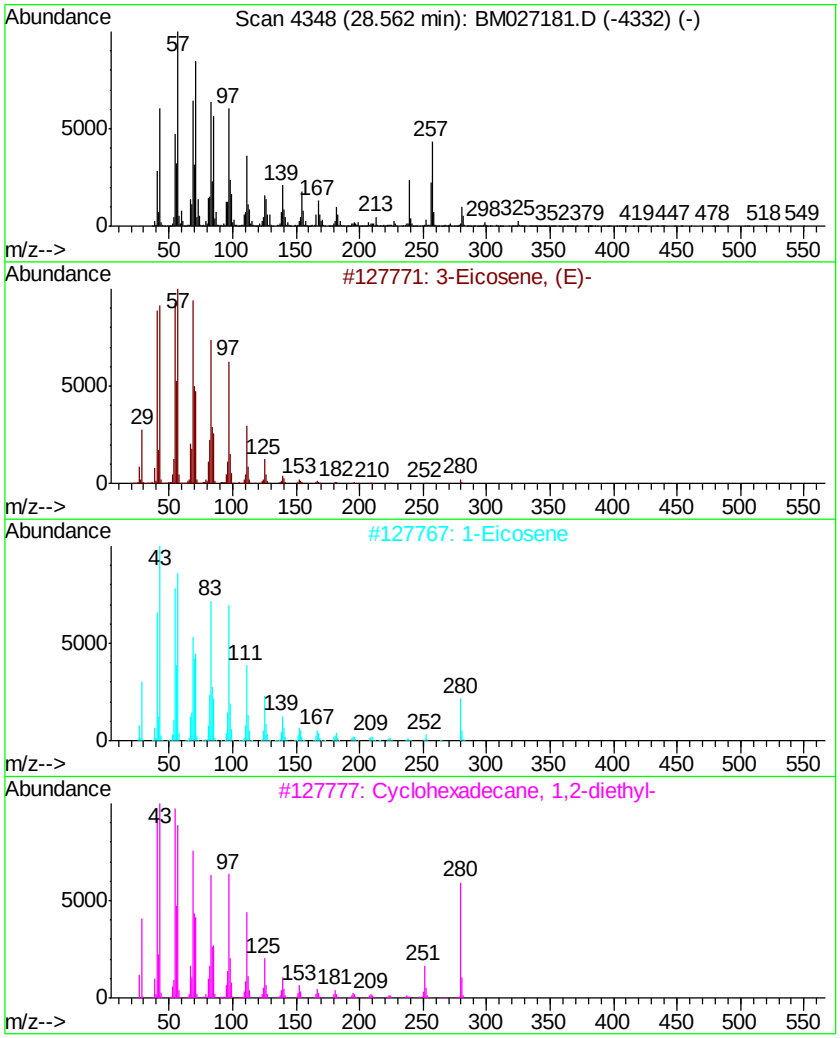
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

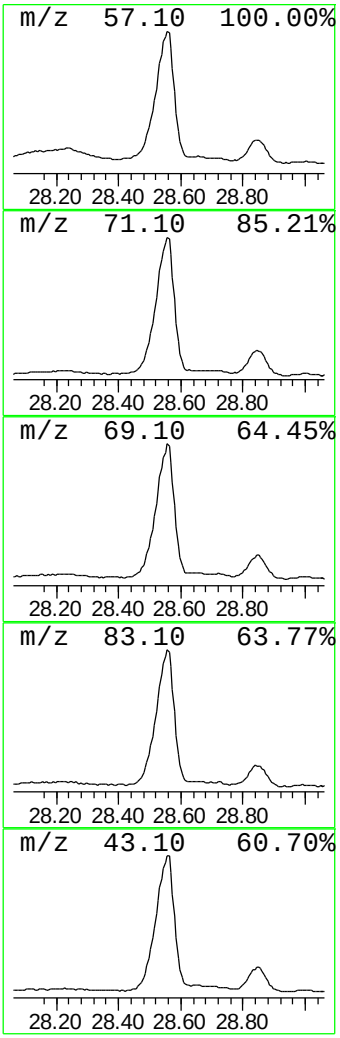
**********

Peak Number 20 3-Eicosene, (E)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 28.56 | 97.01 ng | 29098400 | Perylene-d12 | 23.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 93 |
| 2 | 1-Eicosene | 280 | C20H40 | 003452-07-1 | 72 |
| 3 | Cyclohexadecane, 1,2-diethyl- | 280 | C20H40 | 1000155-85-3 | 72 |
| 4 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 70 |
| 5 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 68 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082120\
Data File : BM027181.D
Acq On : 21 Aug 2020 22:05
Operator : JU/CG
Sample : L3706-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
EFF-WW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| 1-Hexanol, 2-ethyl- | 7.73 | 20.0 | ng | 40014000 | 1 | 7.62 | 40014000 | 20.0 |
| Hexanoic acid, 2-... | 9.37 | 34.0 | ng | 61860200 | 2 | 10.39 | 36346700 | 20.0 |
| Dodecanoic acid | 14.93 | 20.0 | ng | 105594000 | 3 | 14.26 | 105594000 | 20.0 |
| 7-Hexadecene, (Z)- | 16.84 | 20.0 | ng | 129124000 | 4 | 17.00 | 129124000 | 20.0 |
| n-Hexadecanoic acid | 18.04 | 22.4 | ng | 144718000 | 4 | 17.00 | 129124000 | 20.0 |
| cis-Vaccenic acid | 19.13 | 20.9 | ng | 18186000 | 5 | 21.20 | 17432400 | 20.0 |
| Octadecanoic acid | 19.27 | 43.0 | ng | 37447500 | 5 | 21.20 | 17432400 | 20.0 |
| 3-Octadecene, (E)- | 19.46 | 41.3 | ng | 35960500 | 5 | 21.20 | 17432400 | 20.0 |
| Benzoic acid, tri... | 19.56 | 19.5 | ng | 16959900 | 5 | 21.20 | 17432400 | 20.0 |
| Benzoic acid, oct... | 20.12 | 23.1 | ng | 20155400 | 5 | 21.20 | 17432400 | 20.0 |
| Benzoic acid, tet... | 20.63 | 21.0 | ng | 18295500 | 5 | 21.20 | 17432400 | 20.0 |
| Benzoic acid, pen... | 21.10 | 20.0 | ng | 17432400 | 5 | 21.20 | 17432400 | 20.0 |
| N,N-Dimethyl-2-cy... | 22.45 | 38.7 | ng | 11608300 | 6 | 23.39 | 5999330 | 20.0 |
| 12-Hydroxy-octade... | 22.82 | 230.5 | ng | 69136100 | 6 | 23.39 | 5999330 | 20.0 |
| 1-Dodecanol, 2-he... | 23.26 | 20.0 | ng | 5999330 | 6 | 23.39 | 5999330 | 20.0 |
| Hexadecane, 1-iodo- | 24.66 | 1517.2 | ng | 455103000 | 6 | 23.39 | 5999330 | 20.0 |
| 11-Tricosene | 26.30 | 47.7 | ng | 14312100 | 6 | 23.39 | 5999330 | 20.0 |
| unknown26.55 | 26.55 | 1666.2 | ng | 499793000 | 6 | 23.39 | 5999330 | 20.0 |
| unknown27.49 | 27.49 | 661.7 | ng | 198497000 | 6 | 23.39 | 5999330 | 20.0 |
| 3-Eicosene, (E)- | 28.56 | 97.0 | ng | 29098400 | 6 | 23.39 | 5999330 | 20.0 |