LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

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-BM060520.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 | 4.116 | 202 | 209 | 225 | rBV | 5093167 | 7337483 | 100.00% | 16.594% |
| 2 | 4.775 | 313 | 321 | 328 | rBV | 105180 | 157896 | 2.15% | 0.357% |
| 3 | 5.040 | 360 | 366 | 384 | rVB | 749435 | 1088738 | 14.84% | 2.462% |
| 4 | 6.610 | 627 | 633 | 647 | rVB | 465675 | 747145 | 10.18% | 1.690% |
| 5 | 7.404 | 759 | 768 | 778 | rBV | 440752 | 679970 | 9.27% | 1.538% |
| 6 | 7.716 | 814 | 821 | 836 | rBV | 1531345 | 2390145 | 32.57% | 5.405% |
| 7 | 8.551 | 956 | 963 | 972 | rVV | 1374853 | 2177971 | 29.68% | 4.925% |
| 8 | 8.634 | 972 | 977 | 983 | rVB | 81940 | 128422 | 1.75% | 0.290% |
| 9 | 10.163 | 1226 | 1237 | 1247 | rBV | 582743 | 956233 | 13.03% | 2.163% |
| 10 | 11.469 | 1451 | 1459 | 1465 | rBV | 73791 | 122981 | 1.68% | 0.278% |
| 11 | 12.616 | 1648 | 1654 | 1658 | rBV | 371953 | 582105 | 7.93% | 1.316% |
| 12 | 12.669 | 1658 | 1663 | 1676 | rVB | 3334844 | 4779677 | 65.14% | 10.809% |
| 13 | 13.527 | 1804 | 1809 | 1815 | rBV | 411709 | 554227 | 7.55% | 1.253% |
| 14 | 13.986 | 1879 | 1887 | 1892 | rBV4 | 46324 | 84871 | 1.16% | 0.192% |
| 15 | 14.057 | 1892 | 1899 | 1906 | rVB | 831050 | 1191888 | 16.24% | 2.695% |
| 16 | 14.833 | 2025 | 2031 | 2036 | rBV | 86830 | 126849 | 1.73% | 0.287% |
| 17 | 15.563 | 2148 | 2155 | 2167 | rBV2 | 2757405 | 4077467 | 55.57% | 9.221% |
| 18 | 16.104 | 2242 | 2247 | 2254 | rBV | 139166 | 193325 | 2.63% | 0.437% |
| 19 | 16.810 | 2361 | 2367 | 2379 | rBV | 1018339 | 1391092 | 18.96% | 3.146% |
| 20 | 17.751 | 2522 | 2527 | 2530 | rBV | 184980 | 256155 | 3.49% | 0.579% |
| 21 | 18.974 | 2731 | 2735 | 2742 | rVB | 670831 | 705615 | 9.62% | 1.596% |
| 22 | 19.045 | 2743 | 2747 | 2754 | rBV2 | 124939 | 194440 | 2.65% | 0.440% |
| 23 | 19.233 | 2775 | 2779 | 2783 | rVB | 89002 | 109400 | 1.49% | 0.247% |
| 24 | 19.286 | 2784 | 2788 | 2797 | rVB | 123097 | 176730 | 2.41% | 0.400% |
| 25 | 19.468 | 2813 | 2819 | 2824 | rBV | 6011080 | 7261539 | 98.96% | 16.422% |
| 26 | 20.298 | 2957 | 2960 | 2966 | rVB2 | 71657 | 96420 | 1.31% | 0.218% |
| 27 | 20.386 | 2972 | 2975 | 2979 | rBV2 | 78691 | 93240 | 1.27% | 0.211% |
| 28 | 20.768 | 3036 | 3040 | 3050 | rBV | 1004287 | 1177619 | 16.05% | 2.663% |
| 29 | 21.021 | 3078 | 3083 | 3091 | rBV | 1183606 | 1543253 | 21.03% | 3.490% |
| 30 | 21.209 | 3112 | 3115 | 3120 | rVB | 118131 | 128533 | 1.75% | 0.291% |
| 31 | 21.627 | 3183 | 3186 | 3193 | rVB | 223592 | 287549 | 3.92% | 0.650% |
| 32 | 22.056 | 3256 | 3259 | 3265 | rVB | 319012 | 384679 | 5.24% | 0.870% |
| 33 | 22.527 | 3335 | 3339 | 3343 | rVB | 401583 | 510240 | 6.95% | 1.154% |
| 34 | 23.044 | 3423 | 3427 | 3432 | rVB | 366930 | 504069 | 6.87% | 1.140% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

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-BM060520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 23.109 | 3433 | 3438 | 3445 | rVB | 940599 | 1551601 | 21.15% | 3.509% |
| 36 | 23.627 | 3522 | 3526 | 3533 | rVB | 275326 | 468765 | 6.39% | 1.060% |

Sum of corrected areas: 44218332

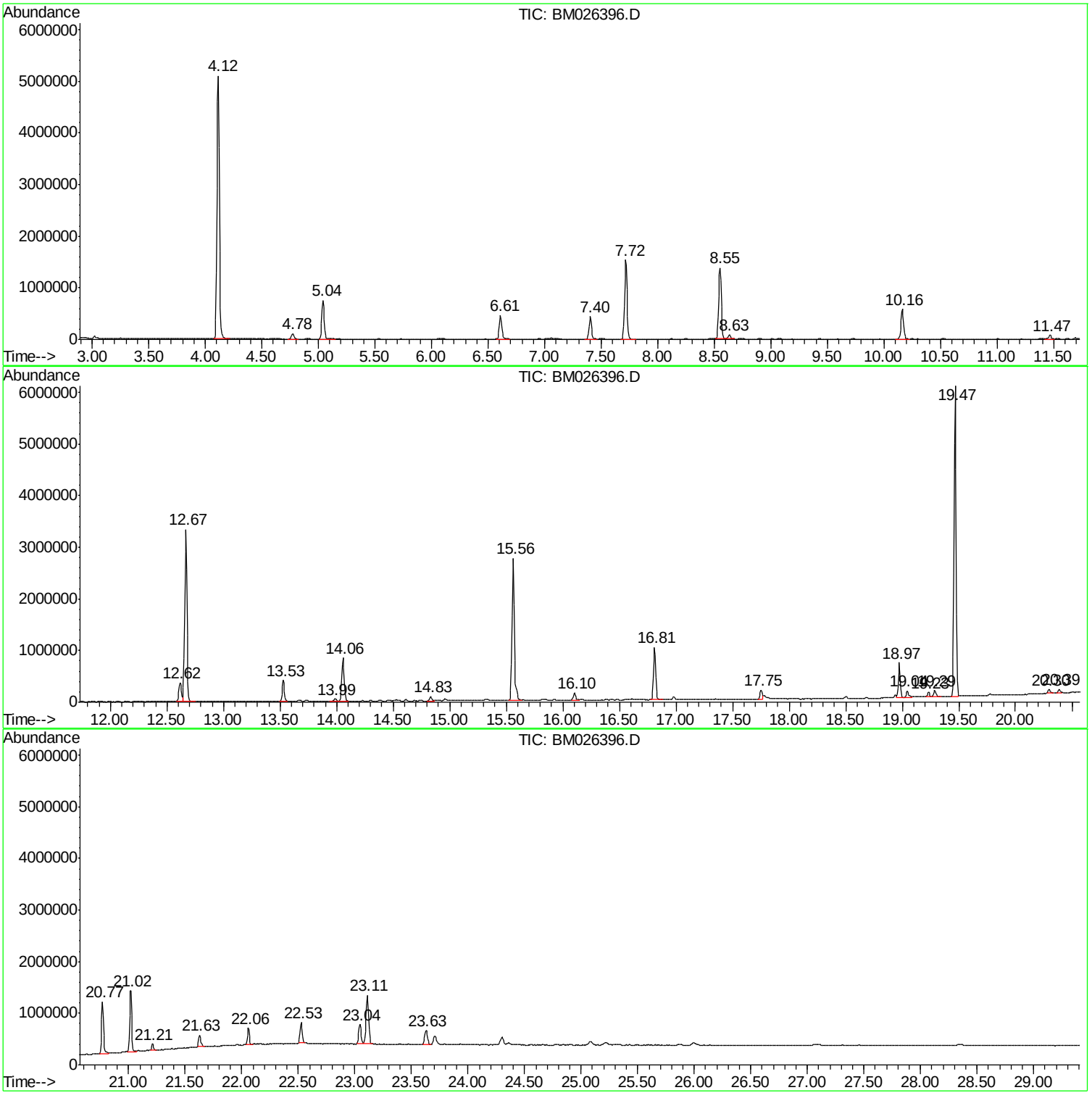
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.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\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

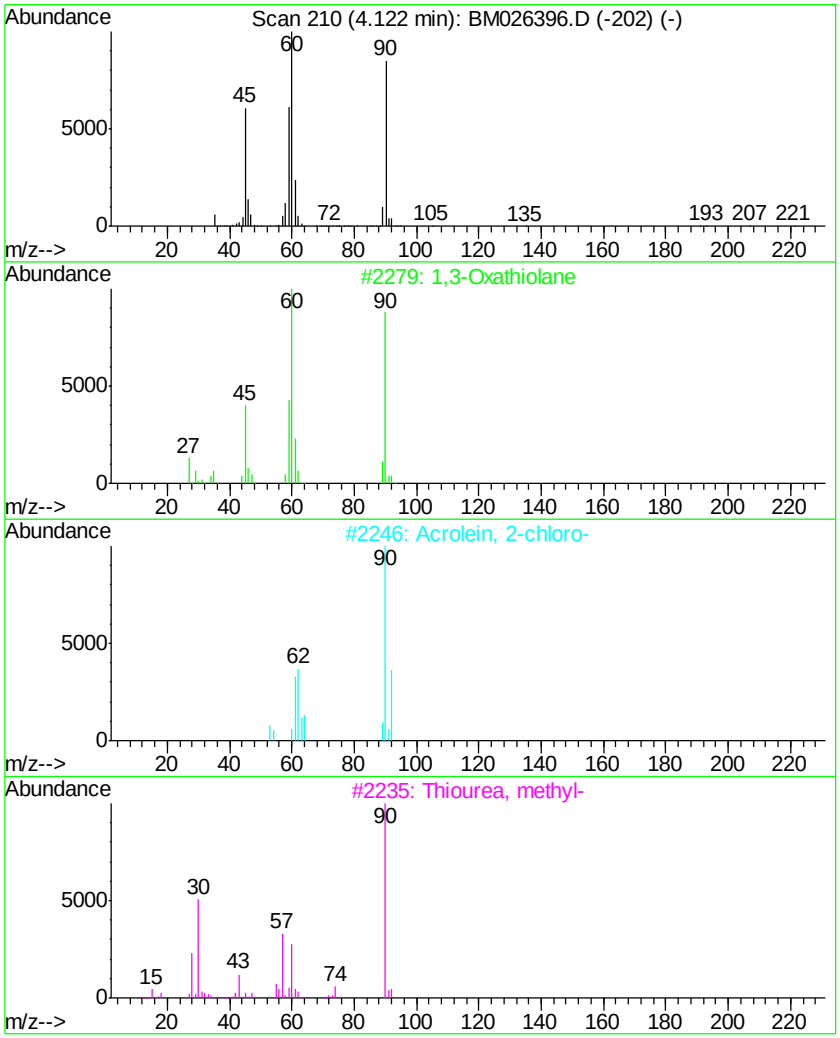
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

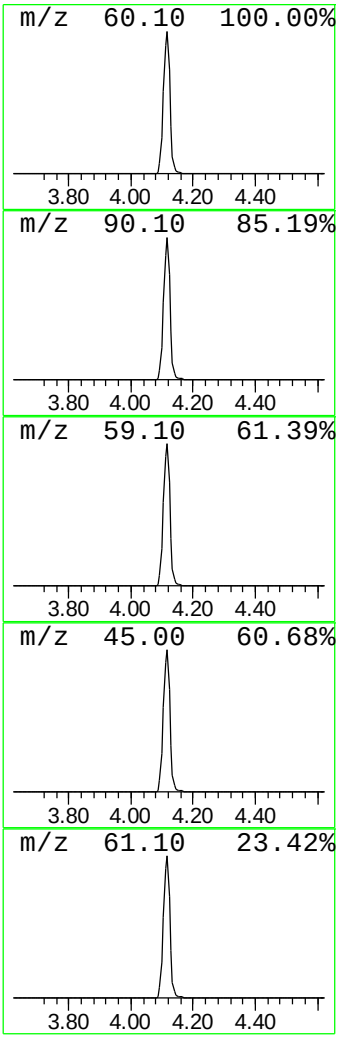
**********

Peak Number 1 1,3-Oxathiolane Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.12 | 215.82 ng | 7337480 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Oxathiolane | 90 | C3H6OS | 002094-97-5 | 90 |
| 2 | Acrolein, 2-chloro- | 90 | C3H3ClO | 000683-51-2 | 59 |
| 3 | Thiourea, methyl- | 90 | C2H6N2S | 000598-52-7 | 50 |
| 4 | Hydrazinecarboxylic acid, methyl... | 90 | C2H6N2O2 | 006294-89-9 | 38 |
| 5 | 3-Thietanol | 90 | C3H6OS | 010304-16-2 | 33 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

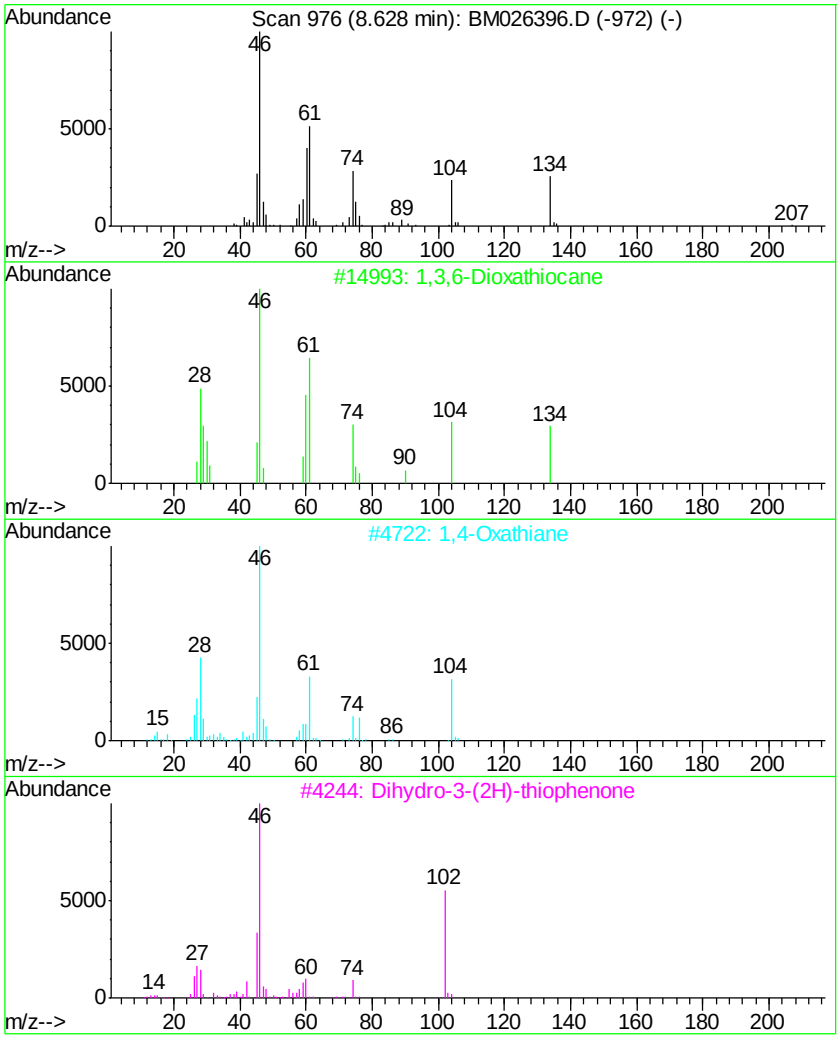
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

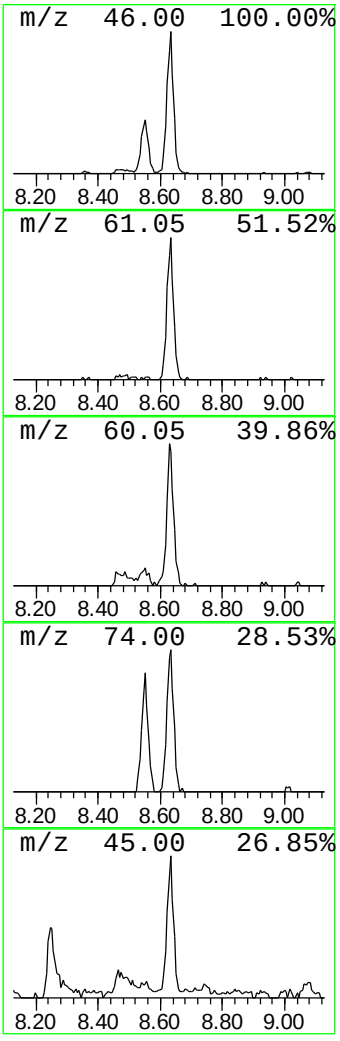
**********

Peak Number 4 1,3,6-Dioxathiocane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.63 | 3.78 ng | 128422 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3,6-Dioxathiocane | 134 | C5H10O2S | 002094-92-0 | 93 |
| 2 | 1,4-Oxathiane | 104 | C4H8OS | 015980-15-1 | 83 |
| 3 | Dihydro-3-(2H)-thiophenone | 102 | C4H6OS | 001003-04-9 | 47 |
| 4 | Thietane | 74 | C3H6S | 000287-27-4 | 43 |
| 5 | Butanoic acid, 4-(methylthio)- | 134 | C5H10O2S | 032391-97-2 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

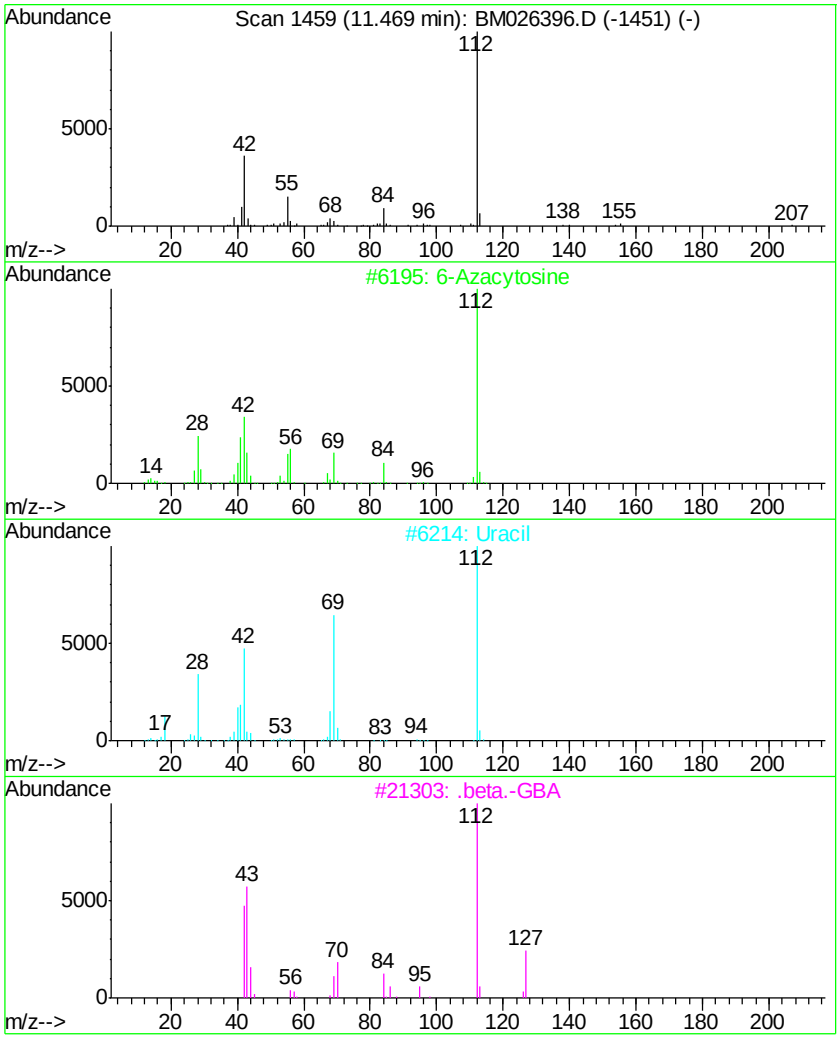
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

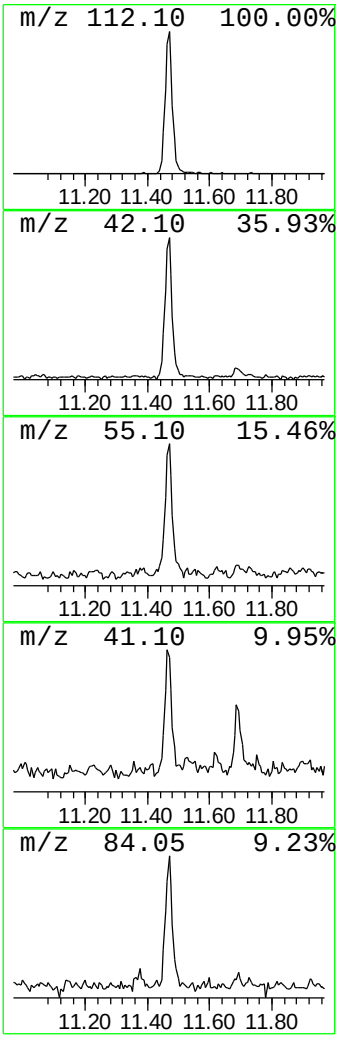
**********

Peak Number 5 6-Azacytosine Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.47 | 2.57 ng | 122981 | Naphthalene-d8 | 10.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Azacytosine | 112 | C3H4N4O | 000931-85-1 | 72 |
| 2 | Uracil | 112 | C4H4N2O2 | 000066-22-8 | 50 |
| 3 | .beta.-GBA | 145 | C5H11N3O2 | 000352-83-0 | 40 |
| 4 | 1,4-Cyclohexanedione | 112 | C6H8O2 | 000637-88-7 | 40 |
| 5 | 4(1H)-Pyridinone, tetrahydro-1-[... | 256 | C15H16N2O2 | 1000350-64-4 | 40 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

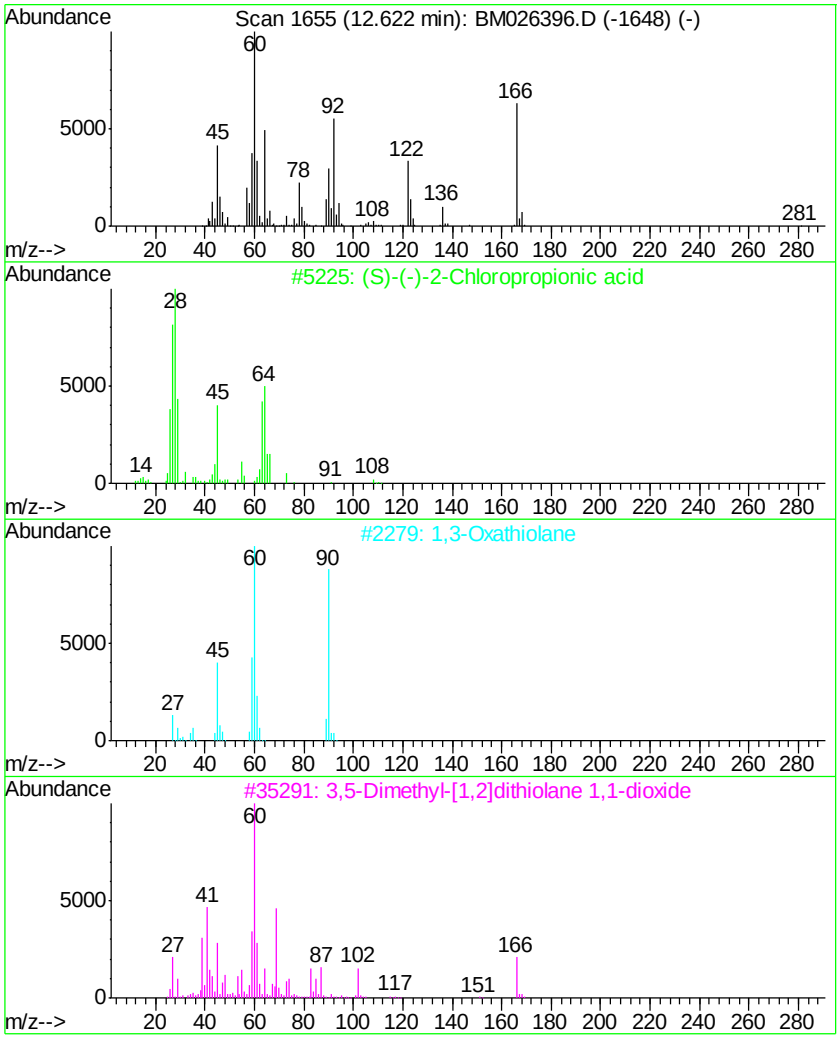
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

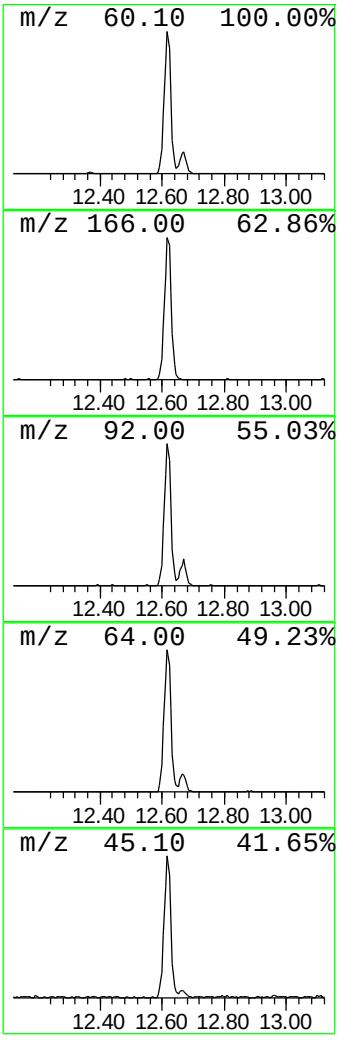
**********

Peak Number 6 unknown12.62 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.62 | 9.77 ng | 582105 | Acenaphthene-d10 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (S)-(-)-2-Chloropropionic acid | 108 | C3H5ClO2 | 029617-66-1 | 27 |
| 2 | 1,3-Oxathiolane | 90 | C3H6OS | 002094-97-5 | 25 |
| 3 | 3,5-Dimethyl-[1,2]dithiolane 1,1... | 166 | C5H10O2S2 | 1000185-07-5 | 16 |
| 4 | 2-Methyl-1,3-oxathiolane | 104 | C4H8OS | 017642-74-9 | 14 |
| 5 | 1,3-Oxathiolane, 2,2-dimethyl- | 118 | C5H10OS | 005684-31-1 | 14 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

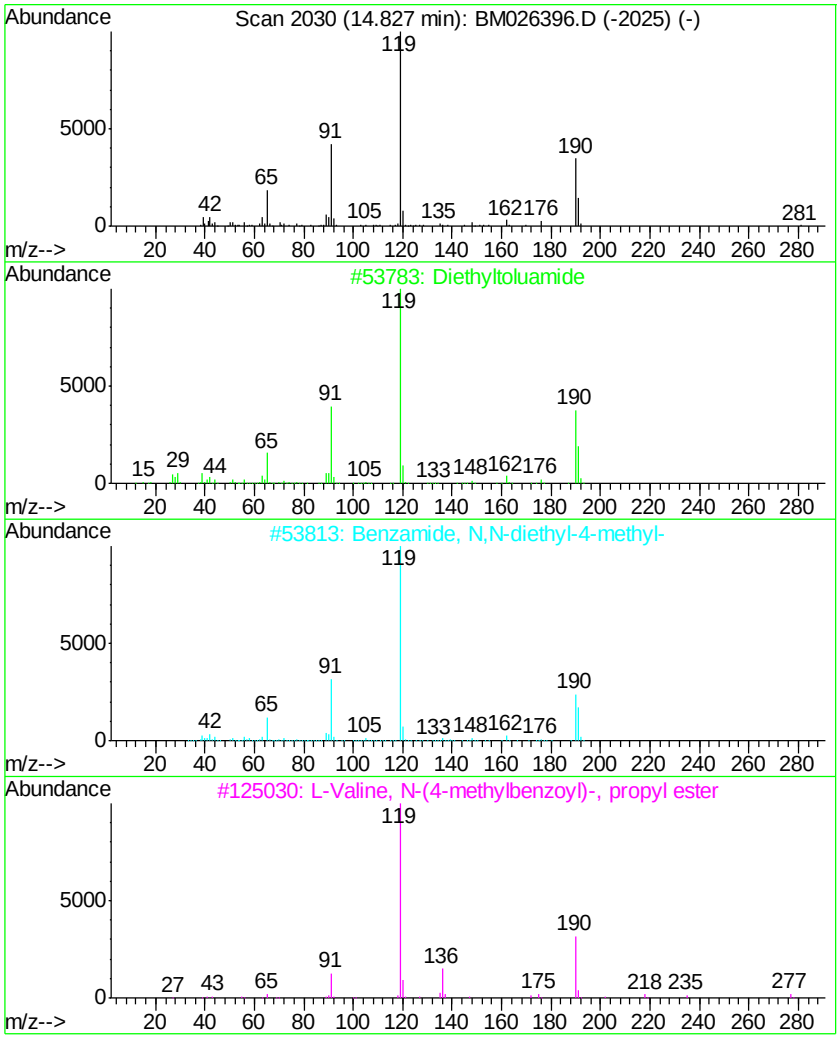
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

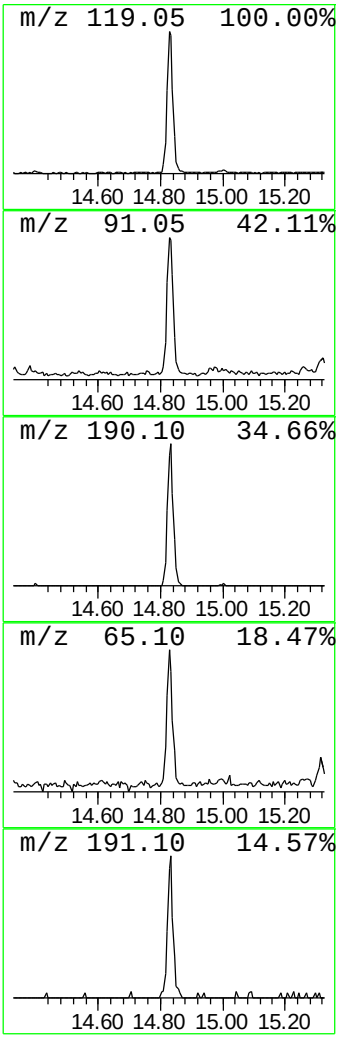
**********

Peak Number 7 Diethyltoluamide Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.83 | 2.13 ng | 126849 | Acenaphthene-d10 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diethyltoluamide | 191 | C12H17NO | 000134-62-3 | 97 |
| 2 | Benzamide, N,N-diethyl-4-methyl- | 191 | C12H17NO | 002728-05-4 | 87 |
| 3 | L-Valine, N-(4-methylbenzoyl)-, ... | 277 | C16H23NO3 | 1000346-63-8 | 78 |
| 4 | Benzamide, 4-methyl-N-2-thiazolyl- | 218 | C11H10N2OS | 150175-93-2 | 53 |
| 5 | 1-Propanone, 2-methyl-1-(4-methy... | 162 | C11H14O | 050390-51-7 | 50 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

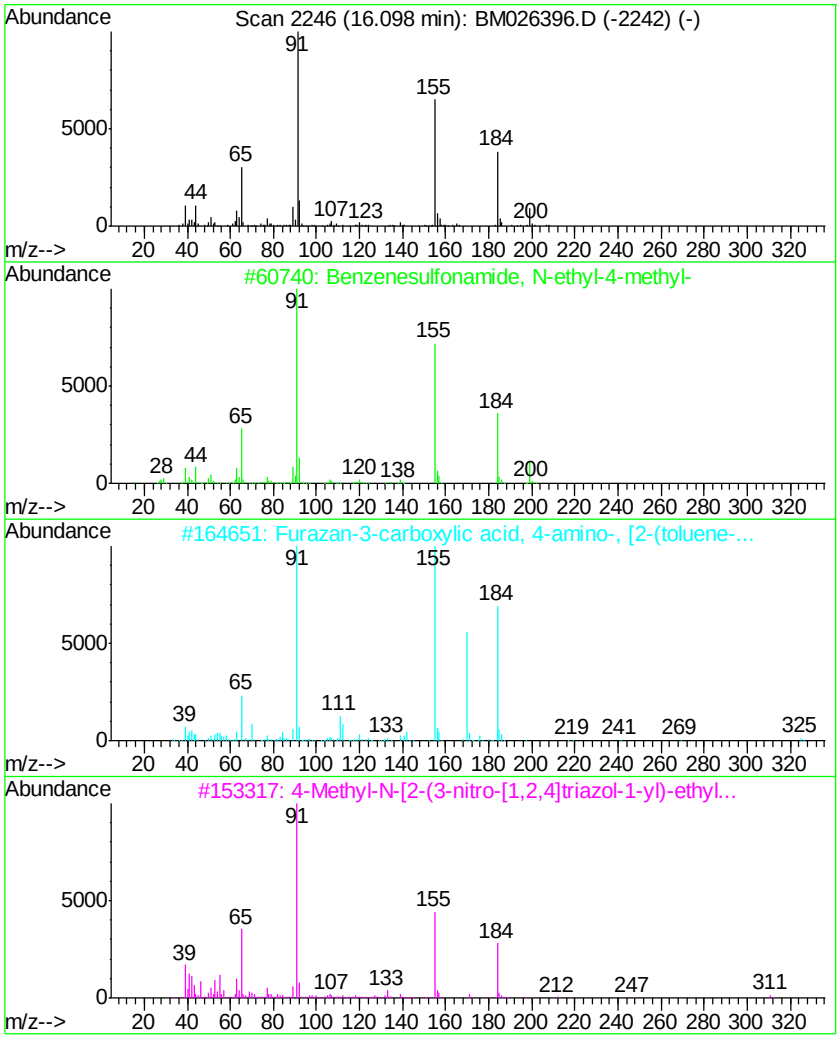
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

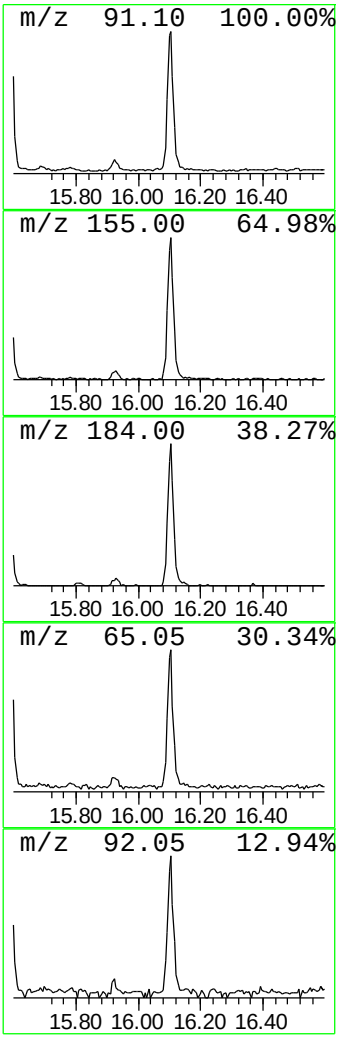
**********

Peak Number 8 Benzenesulfonamide, N-ethyl... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.10 | 2.78 ng | 193325 | Phenanthrene-d10 | 16.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfonamide, N-ethyl-4-me... | 199 | C9H13NO2S | 000080-39-7 | 97 |
| 2 | Furazan-3-carboxylic acid, 4-ami... | 325 | C12H15N5O4S | 1000304-69-4 | 78 |
| 3 | 4-Methyl-N-[2-(3-nitro-[1,2,4]tr... | 311 | C11H13N5O4S | 1000301-03-5 | 78 |
| 4 | Glycine, N-[(4-methylphenyl)sulf... | 229 | C9H11NO4S | 001080-44-0 | 53 |
| 5 | (Toluene-4-sulfonylamino)-acetic... | 283 | C13H17NO4S | 1000190-48-0 | 50 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

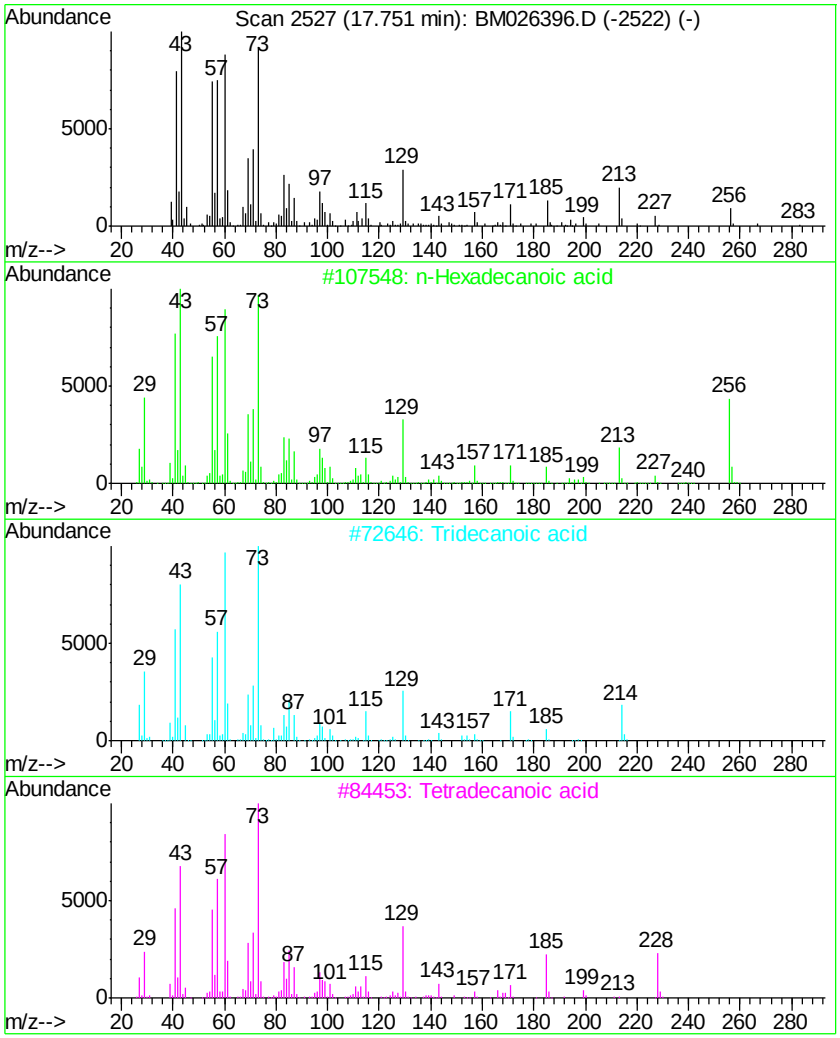
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

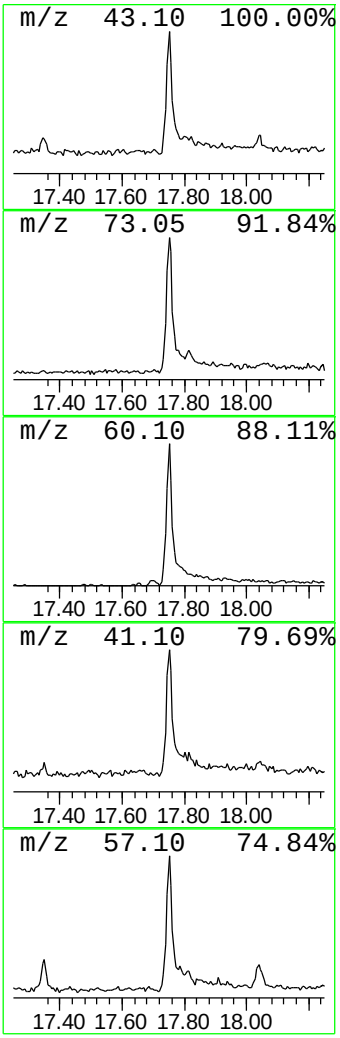
**********

Peak Number 9 n-Hexadecanoic acid Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.75 | 3.68 ng | 256155 | Phenanthrene-d10 | 16.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 62 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

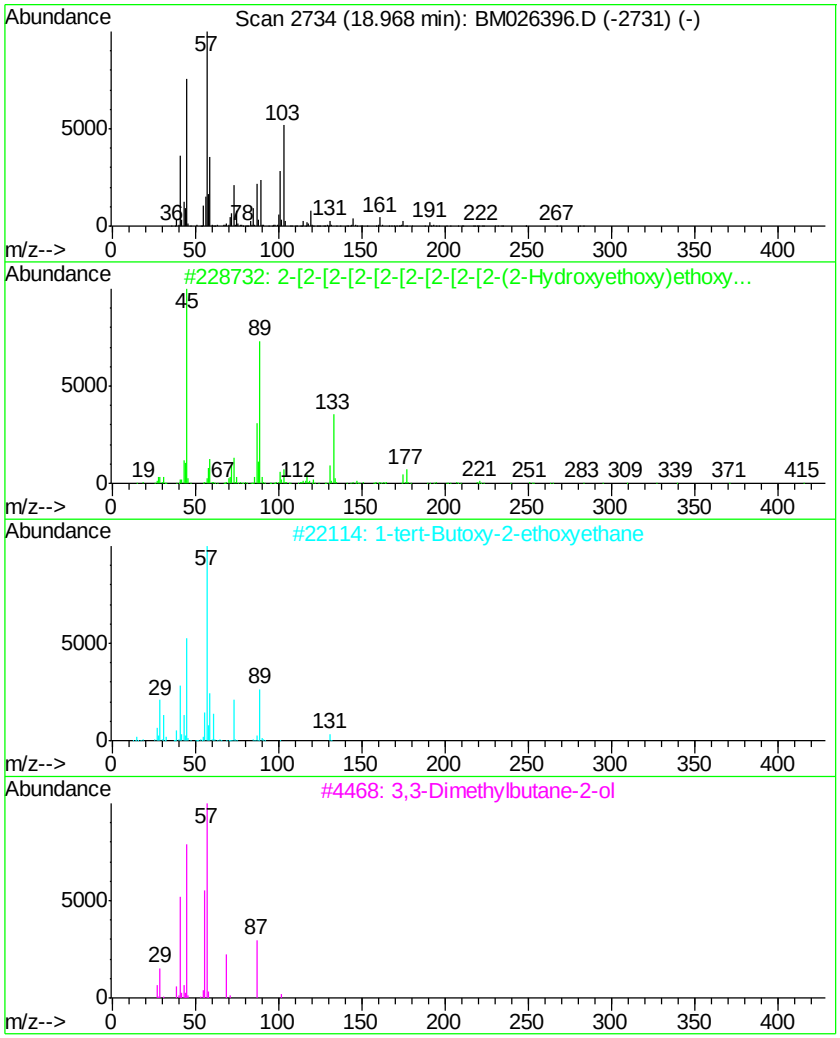
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

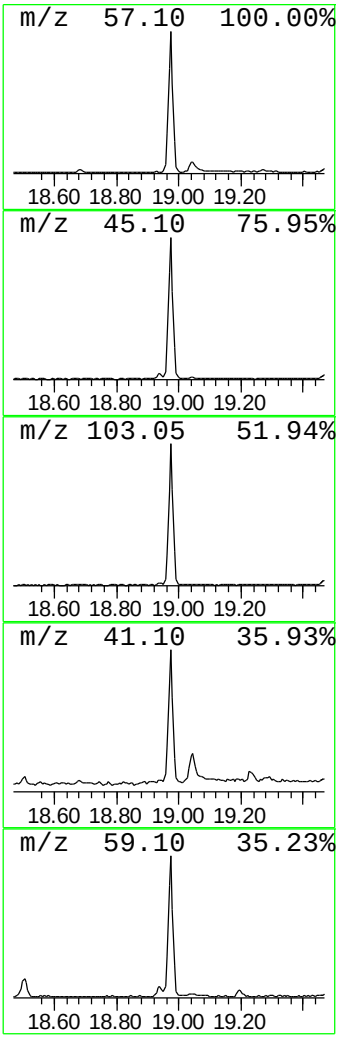
**********

Peak Number 10 unknown18.97 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.97 | 9.14 ng | 705615 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd... | 458 | C20H42O11 | 1000352-12-6 | 38 |
| 2 | 1-tert-Butoxy-2-ethoxyethane | 146 | C8H18O2 | 051422-54-9 | 38 |
| 3 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 38 |
| 4 | Di-sec-butyl ether | 130 | C8H18O | 006863-58-7 | 38 |
| 5 | 2-[2-[2-[2-[2-[2-[2-[2-[2-(2-... | 502 | C22H46O12 | 1000352-13-2 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

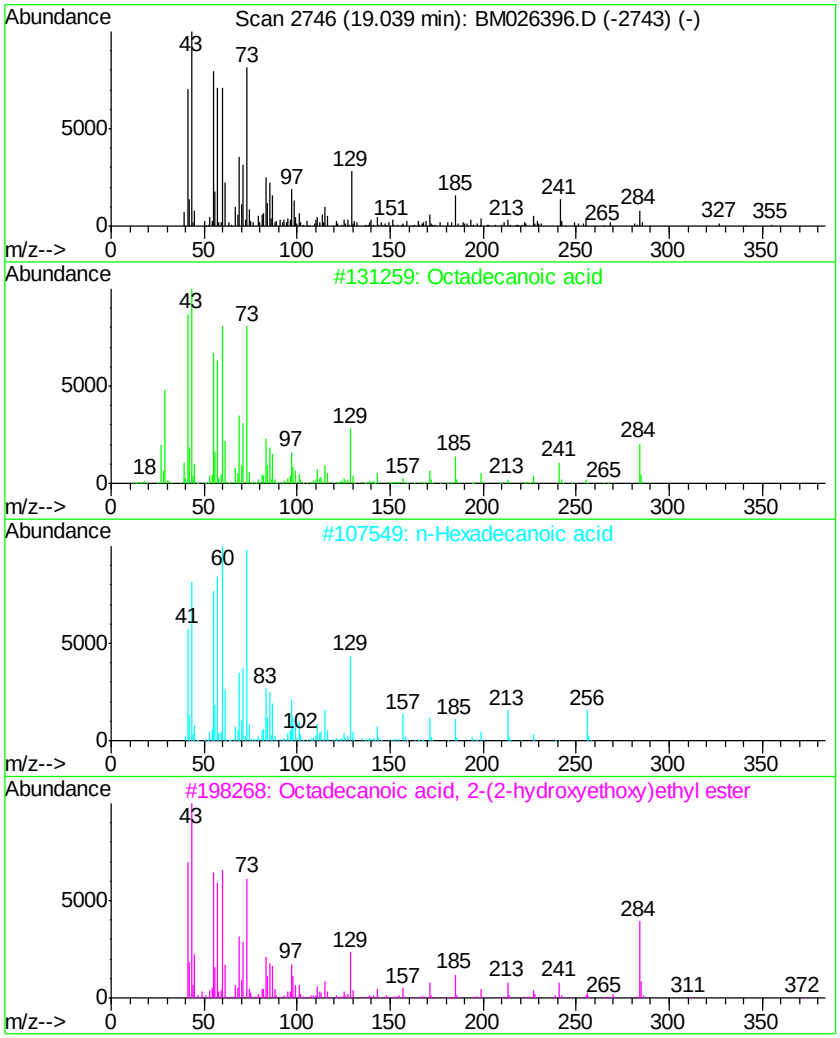
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

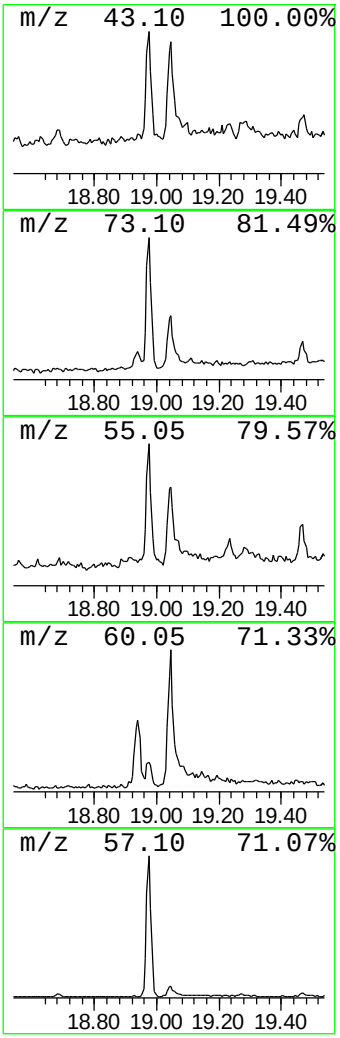
**********

Peak Number 11 Octadecanoic acid Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.04 | 2.52 ng | 194440 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 96 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 87 |
| 3 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

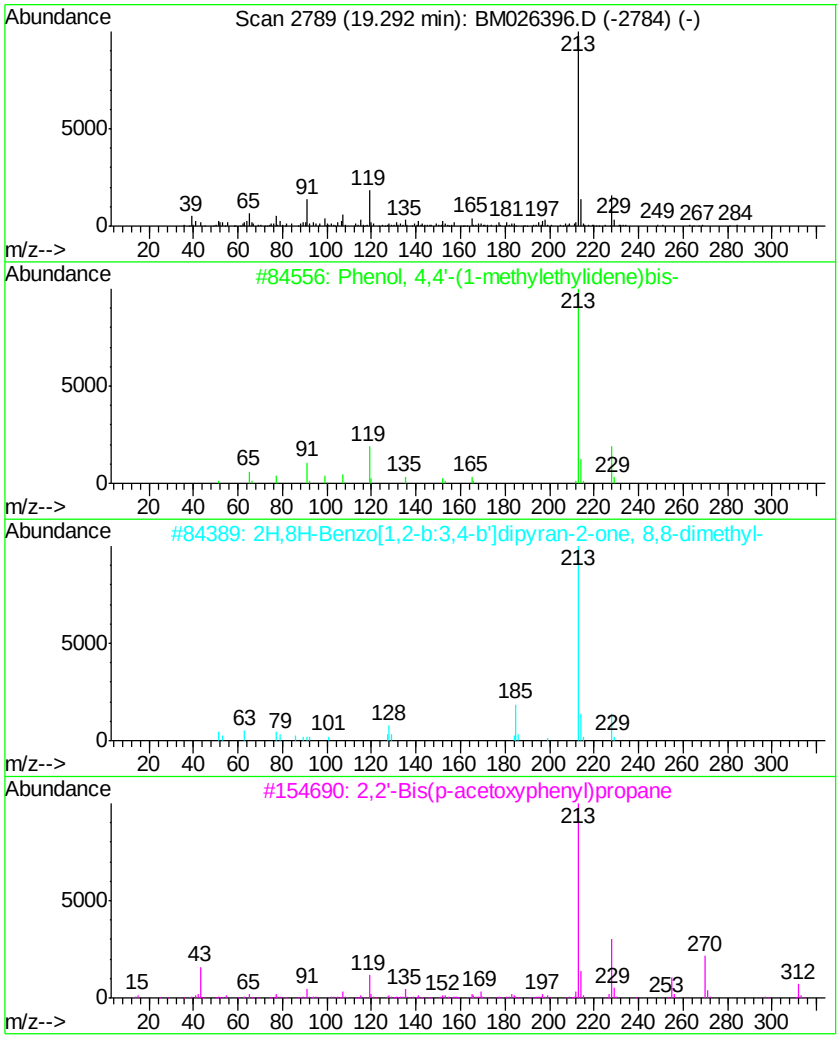
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

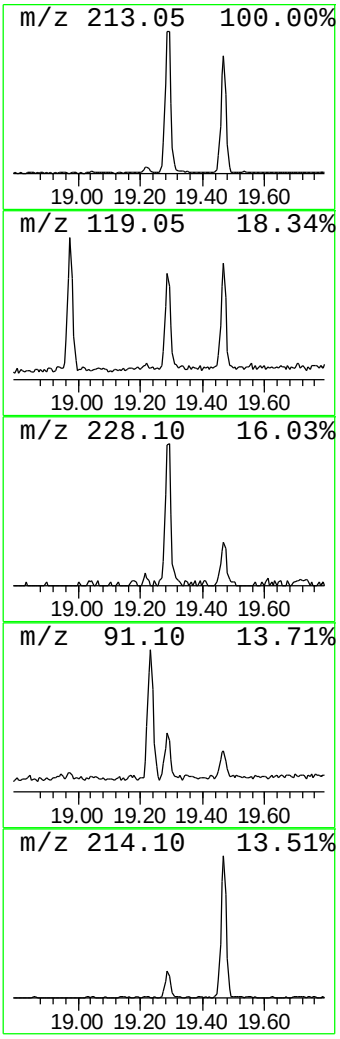
**********

Peak Number 12 Phenol, 4,4'-(1-methylethyl... Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.29 | 2.29 ng | 176730 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4,4'-(1-methylethylidene... | 228 | C15H16O2 | 000080-05-7 | 96 |
| 2 | 2H,8H-Benzo[1,2-b:3,4-b']dipyran... | 228 | C14H12O3 | 000523-59-1 | 53 |
| 3 | 2,2'-Bis(p-acetoxyphenyl)propane | 312 | C19H20O4 | 010192-62-8 | 50 |
| 4 | 9-Propanoyl-1,2,3,4,5,6,7,8-octa... | 242 | C17H22O | 1000255-01-4 | 50 |
| 5 | Carbanilic acid, p-phenyl- | 213 | C13H11NO2 | 004474-53-7 | 49 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

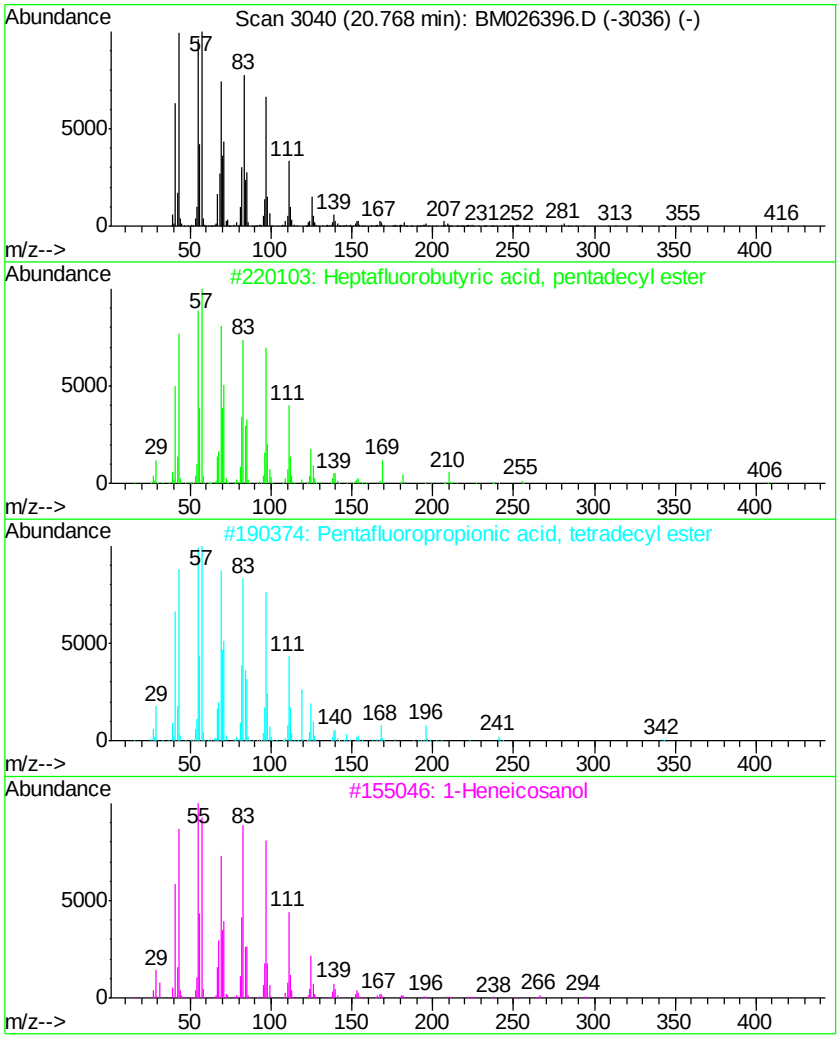
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

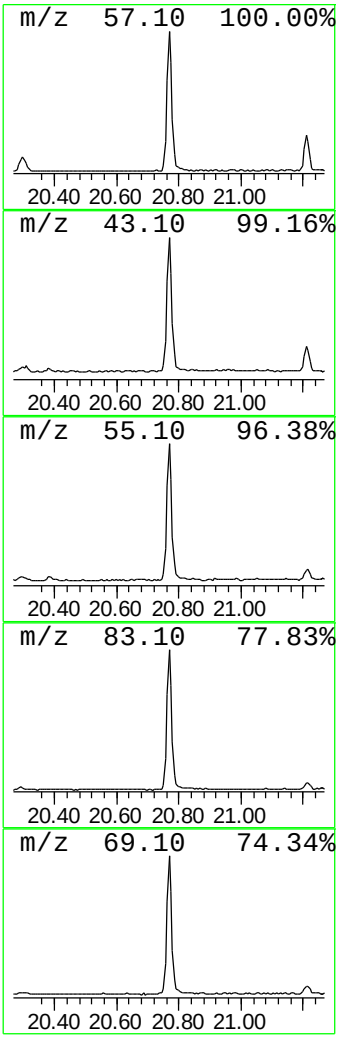
**********

Peak Number 13 Heptafluorobutyric acid, pe... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.77 | 15.26 ng | 1177620 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 2 | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 94 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 4 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 5 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

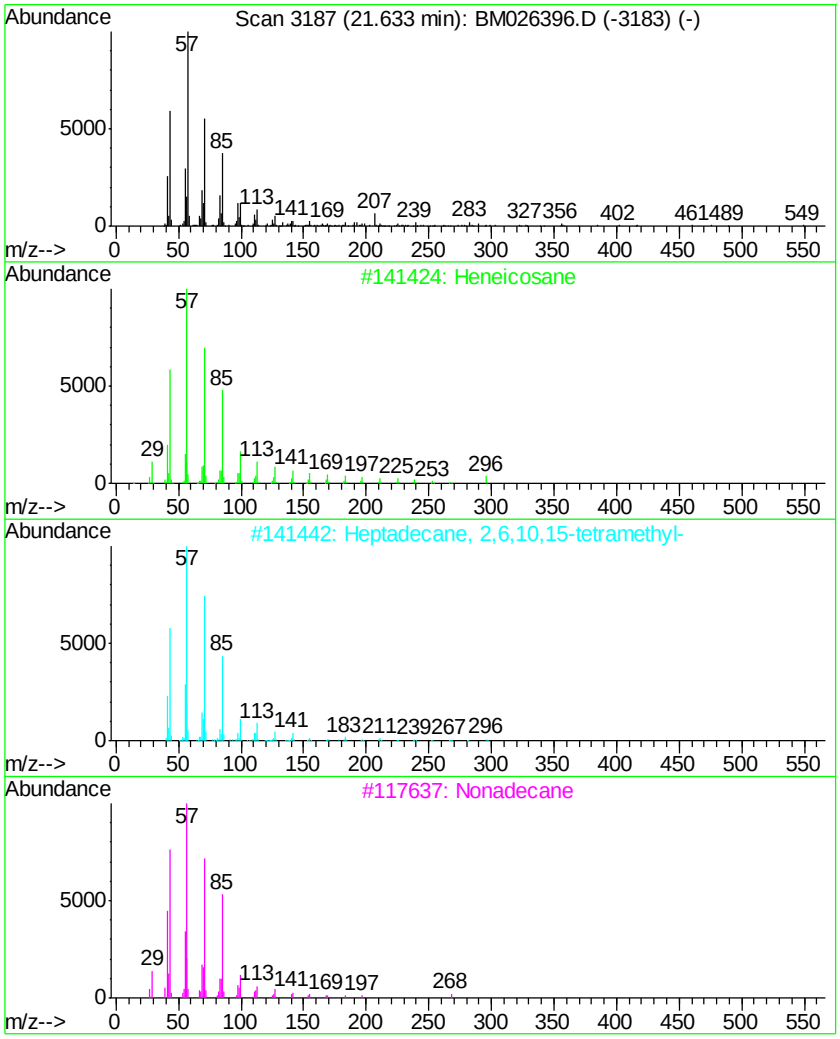
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

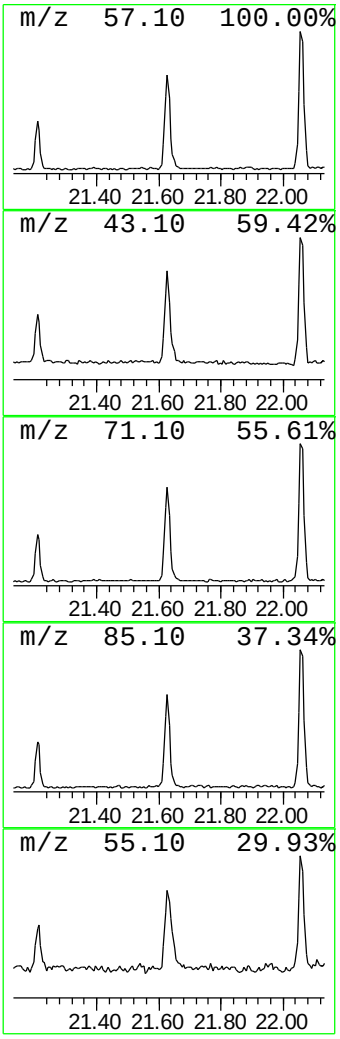
**********

Peak Number 14 Heneicosane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.63 | 3.73 ng | 287549 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 94 |
| 2 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 91 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 90 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

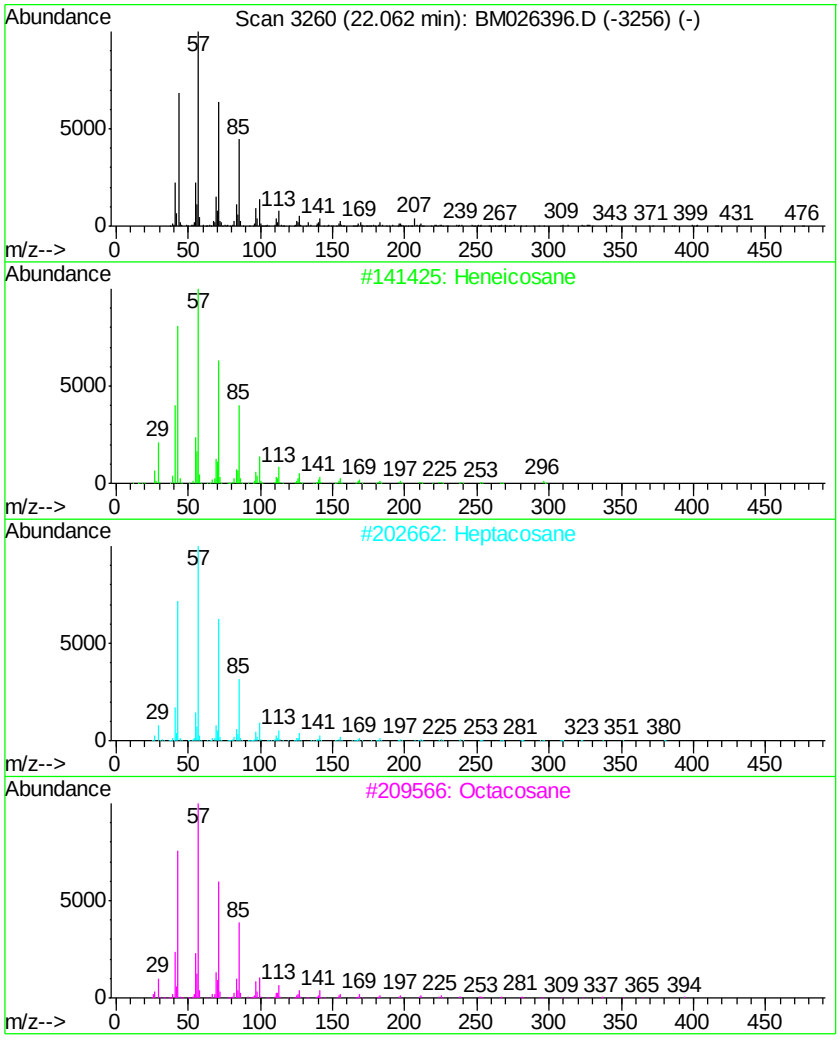
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

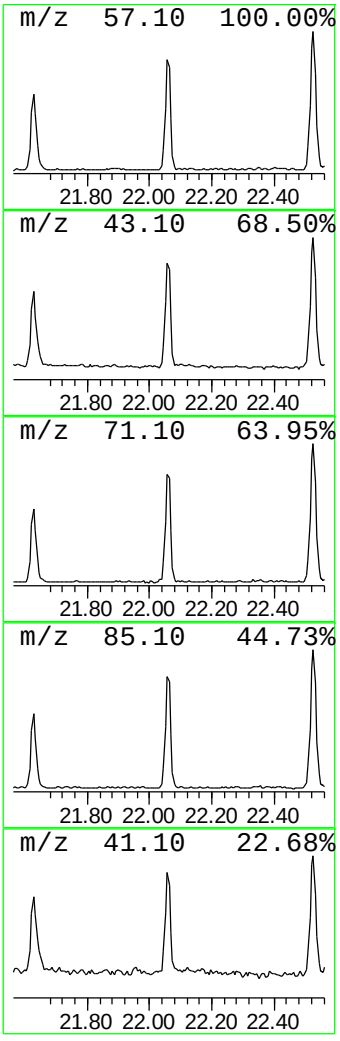
**********

Peak Number 15 Heptacosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.06 | 4.99 ng | 384679 | Chrysene-d12 | 21.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

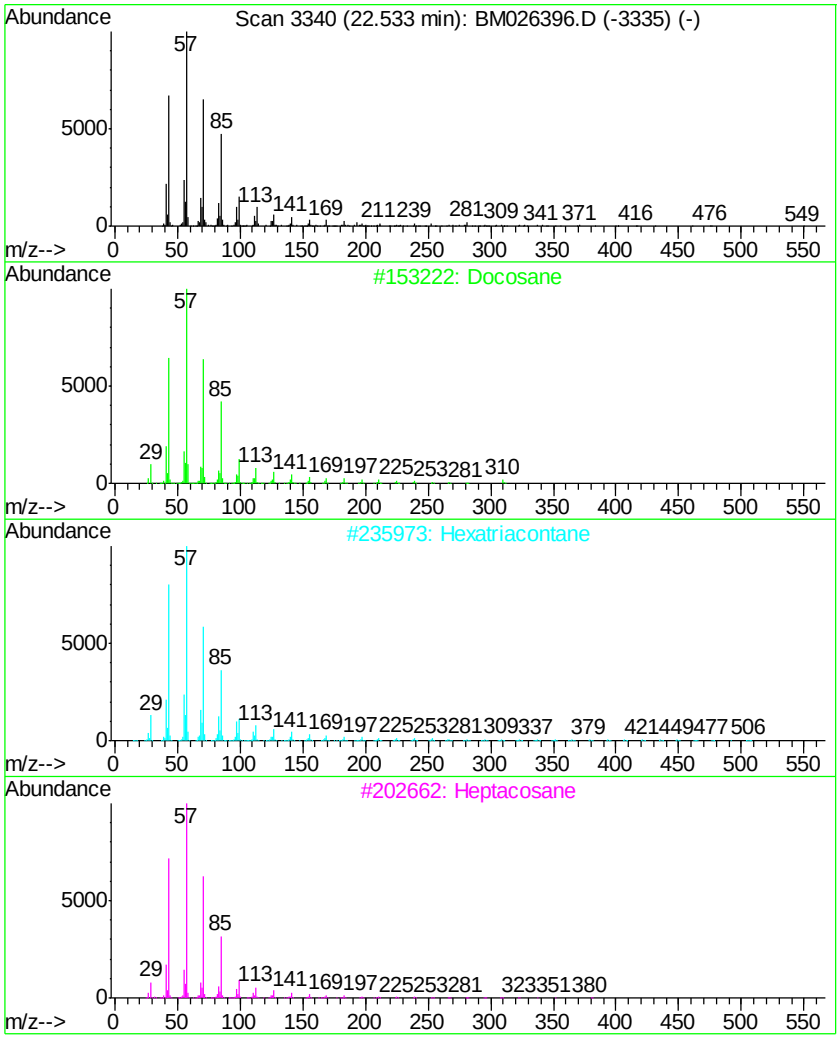
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

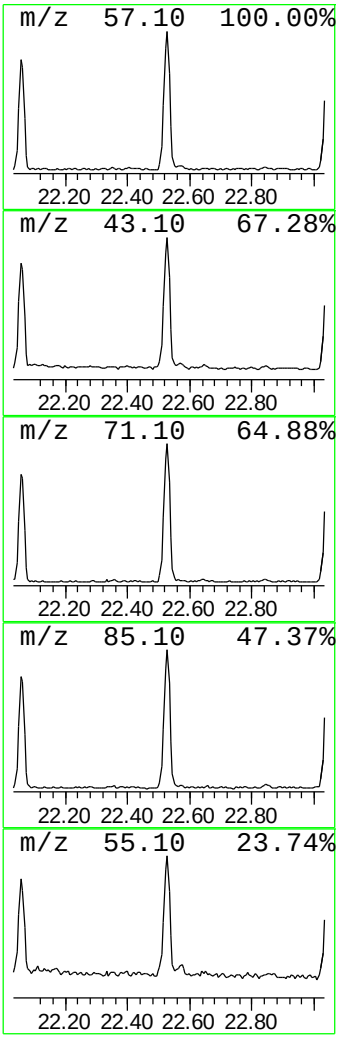
**********

Peak Number 16 Docosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.53 | 6.58 ng | 510240 | Perylene-d12 | 23.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane | 310 | C22H46 | 000629-97-0 | 94 |
| 2 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 91 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 5 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

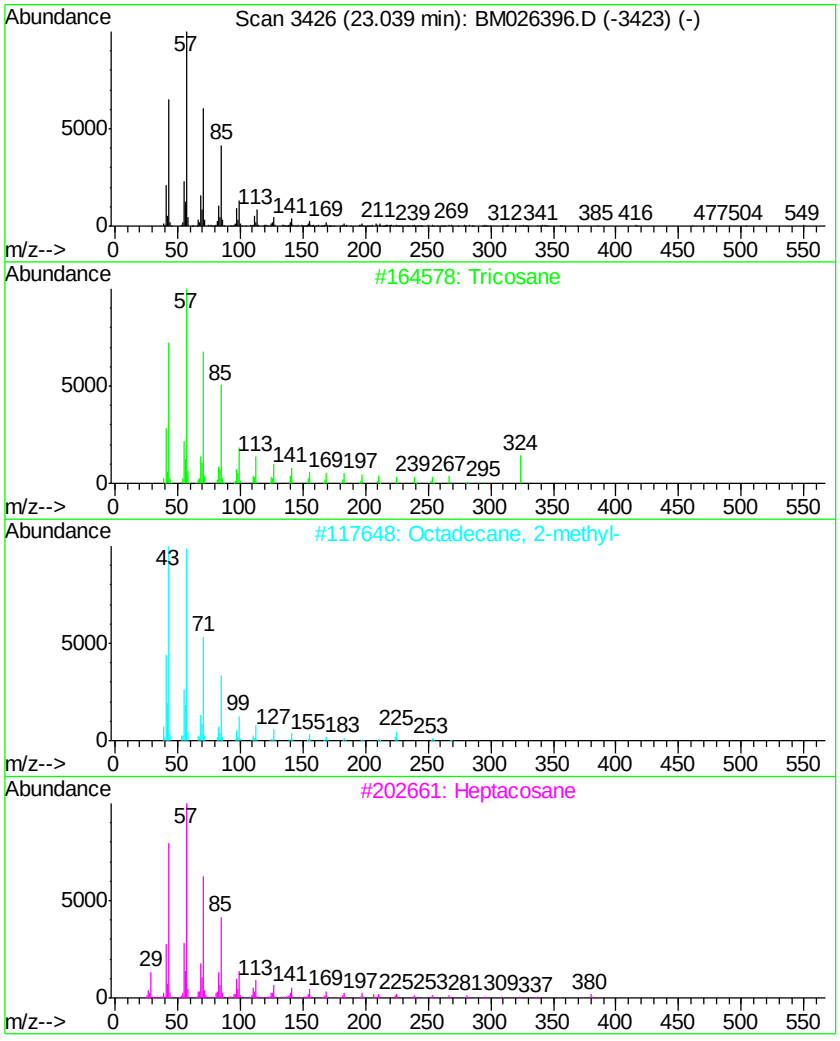
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

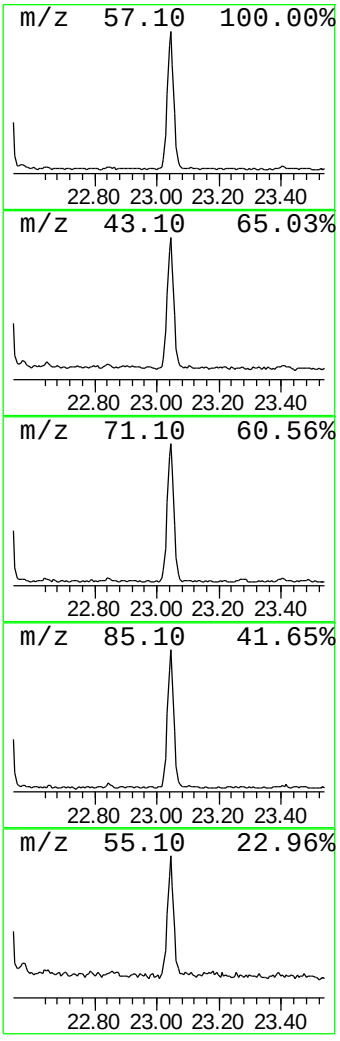
**********

Peak Number 17 Tricosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.04 | 6.50 ng | 504069 | Perylene-d12 | 23.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricosane | 324 | C23H48 | 000638-67-5 | 95 |
| 2 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 91 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

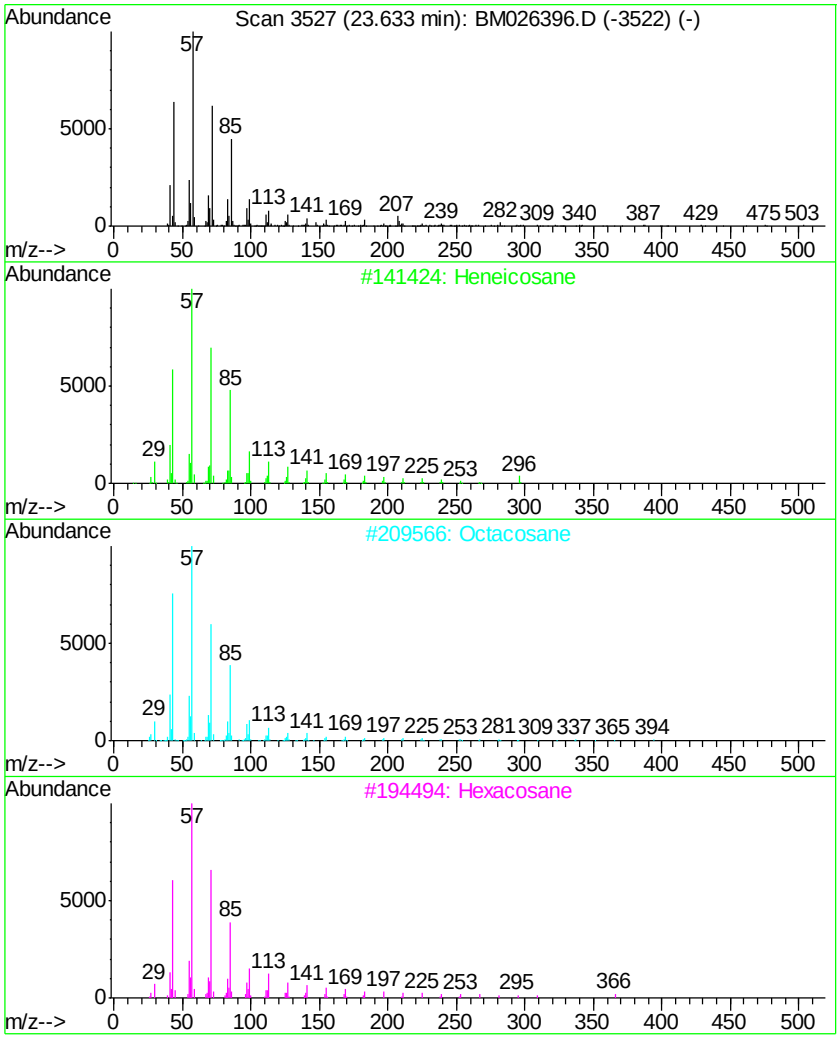
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

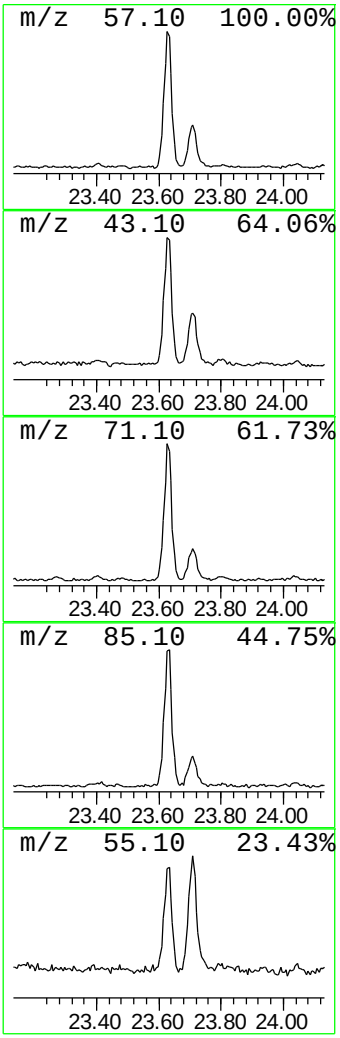
**********

Peak Number 18 Octacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.63 | 6.04 ng | 468765 | Perylene-d12 | 23.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 95 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 4 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 87 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM061520\
Data File : BM026396.D
Acq On : 15 Jun 2020 17:56
Operator : JU/CG
Sample : L3005-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF017MW001-200611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.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 |
| 1,3-Oxathiolane | 4.12 | 215.8 | ng | 7337480 | 1 | 7.40 | 679970 | 20.0 |
| 1,3,6-Dioxathiocane | 8.63 | 3.8 | ng | 128422 | 1 | 7.40 | 679970 | 20.0 |
| 6-Azacytosine | 11.47 | 2.6 | ng | 122981 | 2 | 10.16 | 956233 | 20.0 |
| unknown12.62 | 12.62 | 9.8 | ng | 582105 | 3 | 14.06 | 1191890 | 20.0 |
| Diethyltoluamide | 14.83 | 2.1 | ng | 126849 | 3 | 14.06 | 1191890 | 20.0 |
| Benzenesulfonamid... | 16.10 | 2.8 | ng | 193325 | 4 | 16.81 | 1391090 | 20.0 |
| n-Hexadecanoic acid | 17.75 | 3.7 | ng | 256155 | 4 | 16.81 | 1391090 | 20.0 |
| unknown18.97 | 18.97 | 9.1 | ng | 705615 | 5 | 21.02 | 1543250 | 20.0 |
| Octadecanoic acid | 19.04 | 2.5 | ng | 194440 | 5 | 21.02 | 1543250 | 20.0 |
| Phenol, 4,4'-(1-m... | 19.29 | 2.3 | ng | 176730 | 5 | 21.02 | 1543250 | 20.0 |
| Heptafluorobutyri... | 20.77 | 15.3 | ng | 1177620 | 5 | 21.02 | 1543250 | 20.0 |
| Heneicosane | 21.63 | 3.7 | ng | 287549 | 5 | 21.02 | 1543250 | 20.0 |
| Heptacosane | 22.06 | 5.0 | ng | 384679 | 5 | 21.02 | 1543250 | 20.0 |
| Docosane | 22.53 | 6.6 | ng | 510240 | 6 | 23.11 | 1551600 | 20.0 |
| Tricosane | 23.04 | 6.5 | ng | 504069 | 6 | 23.11 | 1551600 | 20.0 |
| Octacosane | 23.63 | 6.0 | ng | 468765 | 6 | 23.11 | 1551600 | 20.0 |