LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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 | 5.034 | 359 | 365 | 382 | rBV | 2694997 | 3890706 | 43.02% | 8.576% |
| 2 | 6.604 | 625 | 632 | 648 | rBV | 2753603 | 4345317 | 48.05% | 9.578% |
| 3 | 7.398 | 760 | 767 | 775 | rBV | 428903 | 638677 | 7.06% | 1.408% |
| 4 | 7.710 | 812 | 820 | 832 | rBV | 2141991 | 3357174 | 37.12% | 7.400% |
| 5 | 8.545 | 952 | 962 | 976 | rBV | 1850258 | 2961611 | 32.75% | 6.528% |
| 6 | 10.157 | 1229 | 1236 | 1253 | rBV | 527874 | 873151 | 9.66% | 1.925% |
| 7 | 12.663 | 1655 | 1662 | 1677 | rBV | 4133191 | 5965690 | 65.97% | 13.149% |
| 8 | 13.527 | 1803 | 1809 | 1823 | rBV | 484268 | 722734 | 7.99% | 1.593% |
| 9 | 14.051 | 1892 | 1898 | 1908 | rBV | 779756 | 1115221 | 12.33% | 2.458% |
| 10 | 15.557 | 2147 | 2154 | 2177 | rBV | 3555252 | 4931697 | 54.53% | 10.870% |
| 11 | 16.804 | 2357 | 2366 | 2379 | rBV | 948112 | 1314787 | 14.54% | 2.898% |
| 12 | 19.280 | 2782 | 2787 | 2801 | rBV | 221595 | 382232 | 4.23% | 0.843% |
| 13 | 19.462 | 2812 | 2818 | 2823 | rBV | 7514706 | 9043376 | 100.00% | 19.933% |
| 14 | 20.768 | 3035 | 3040 | 3049 | rBV | 221878 | 333273 | 3.69% | 0.735% |
| 15 | 21.009 | 3077 | 3081 | 3087 | rBV | 1223833 | 1526696 | 16.88% | 3.365% |
| 16 | 21.203 | 3111 | 3114 | 3118 | rBV2 | 99464 | 103388 | 1.14% | 0.228% |
| 17 | 21.621 | 3182 | 3185 | 3192 | rVB | 158305 | 178265 | 1.97% | 0.393% |
| 18 | 22.044 | 3252 | 3257 | 3265 | rBV3 | 849760 | 1261513 | 13.95% | 2.781% |
| 19 | 22.515 | 3334 | 3337 | 3342 | rVB | 221353 | 288114 | 3.19% | 0.635% |
| 20 | 23.033 | 3421 | 3425 | 3430 | rBV | 196235 | 295077 | 3.26% | 0.650% |
| 21 | 23.103 | 3431 | 3437 | 3448 | rVB | 919060 | 1593319 | 17.62% | 3.512% |
| 22 | 23.615 | 3521 | 3524 | 3531 | rVB | 152944 | 246367 | 2.72% | 0.543% |

Sum of corrected areas: 45368385

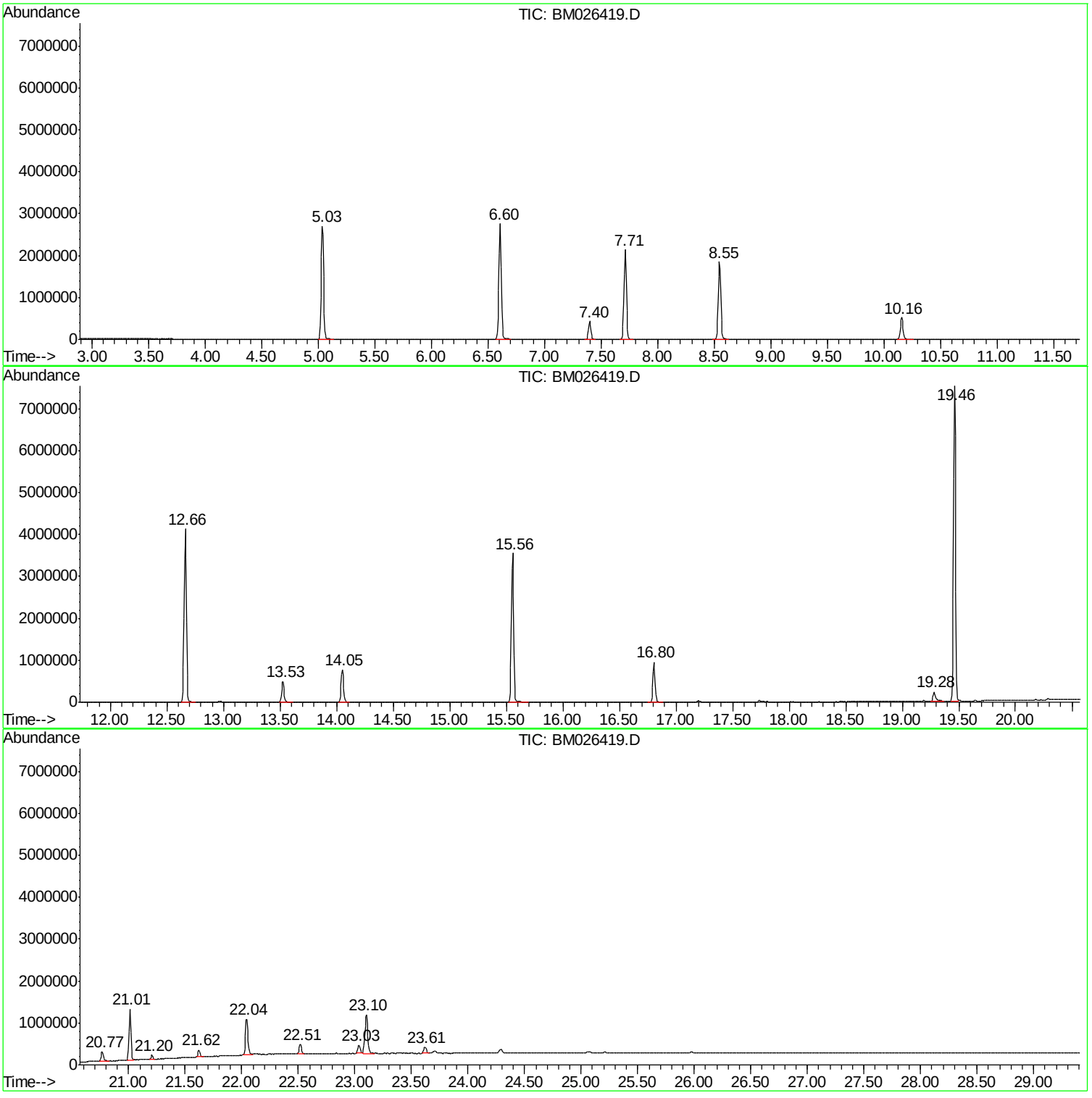
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MW-24(19-21)

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\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

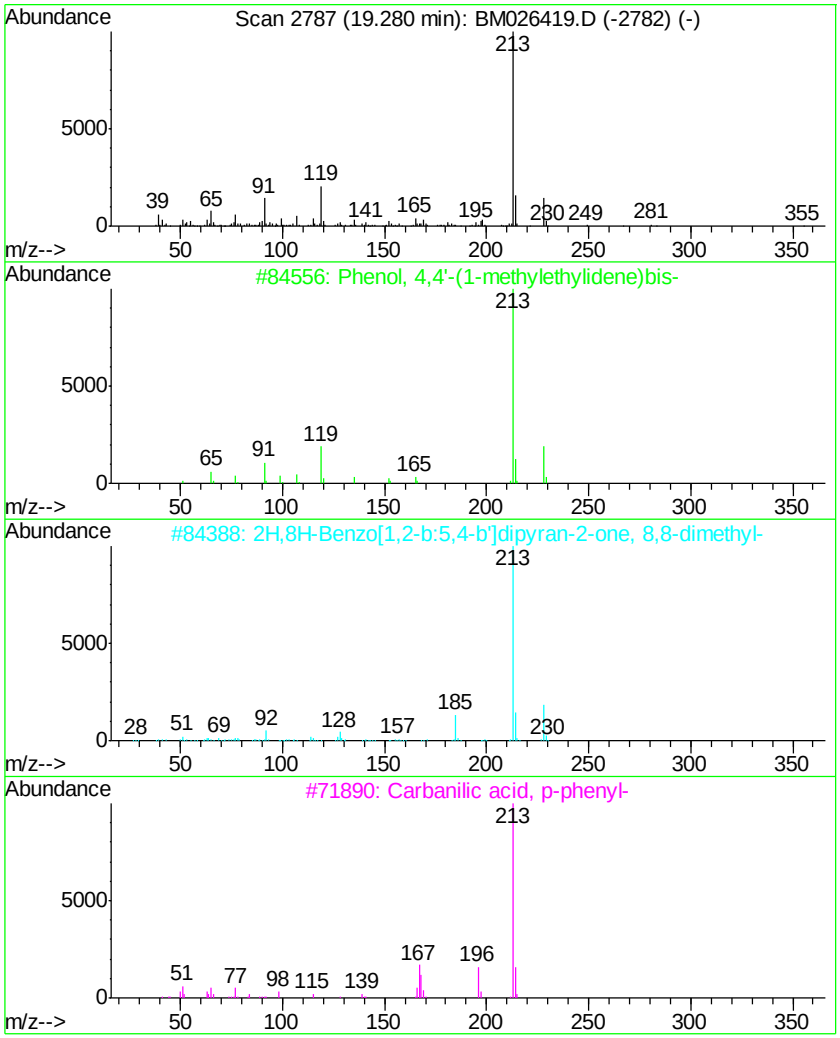
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

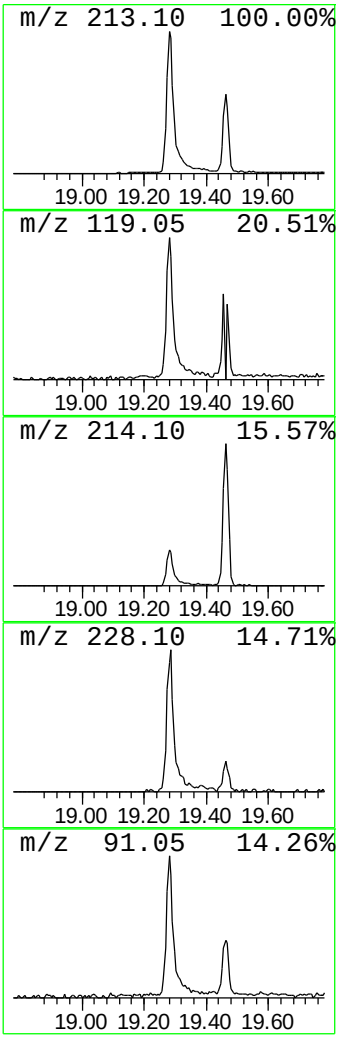
**********

Peak Number 2 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.28 | 5.01 ng | 382232 | Chrysene-d12 | 21.01 |

| 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:5,4-b']dipyran... | 228 | C14H12O3 | 000553-19-5 | 58 |
| 3 | Carbanilic acid, p-phenyl- | 213 | C13H11NO2 | 004474-53-7 | 52 |
| 4 | 9-Propanoyl-1,2,3,4,5,6,7,8-octa... | 242 | C17H22O | 1000255-01-4 | 50 |
| 5 | Naphthalene-2,6-dicarboxylic aci... | 376 | C24H24O4 | 1000189-60-8 | 47 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

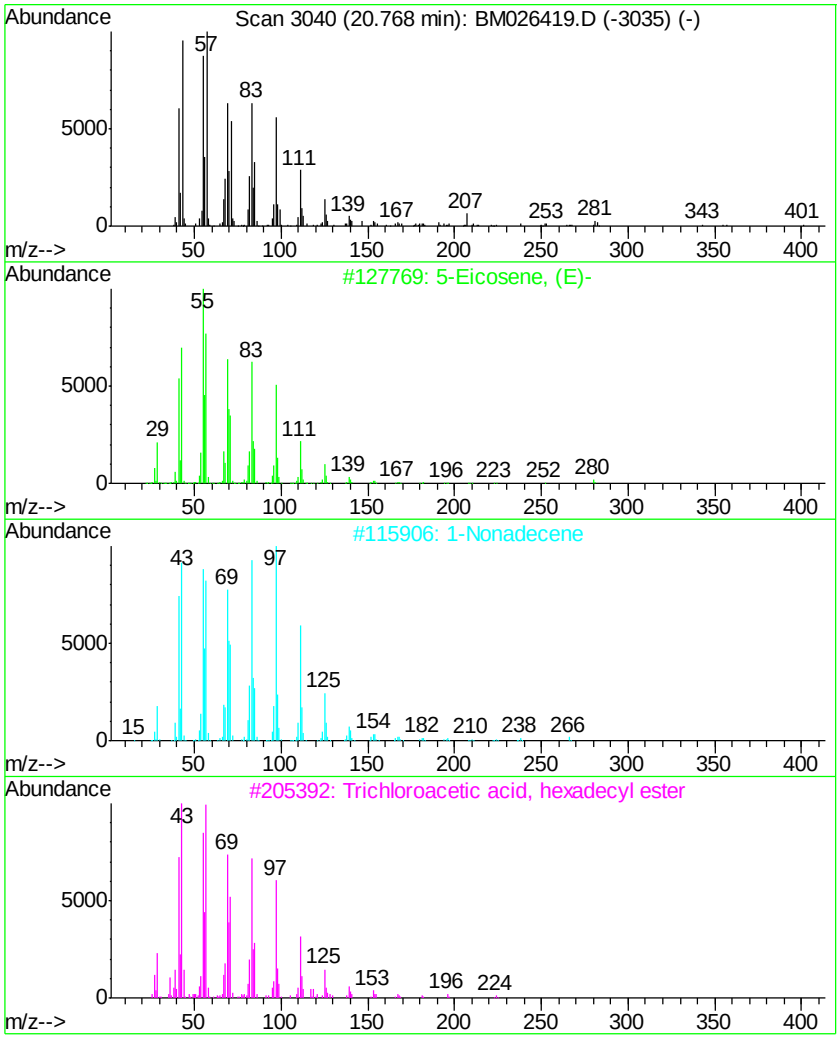
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

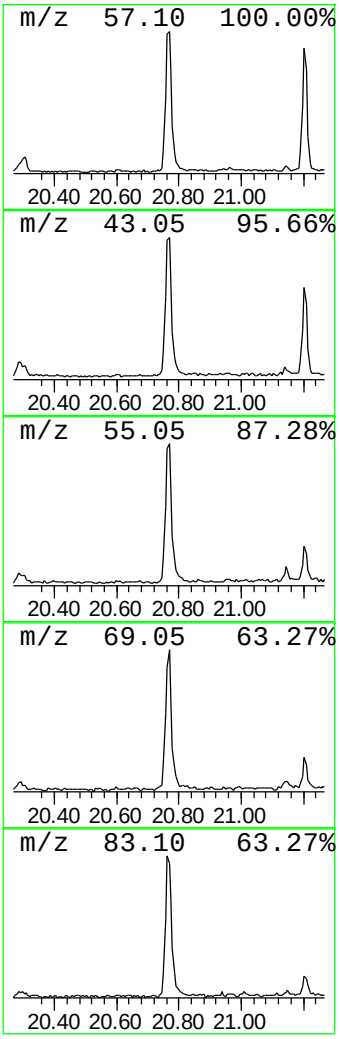
**********

Peak Number 3 5-Eicosene, (E)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.77 | 4.37 ng | 333273 | Chrysene-d12 | 21.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 95 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 95 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 4 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 5 | Cyclohexadecane, 1,2-diethyl- | 280 | C20H40 | 1000155-85-3 | 93 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

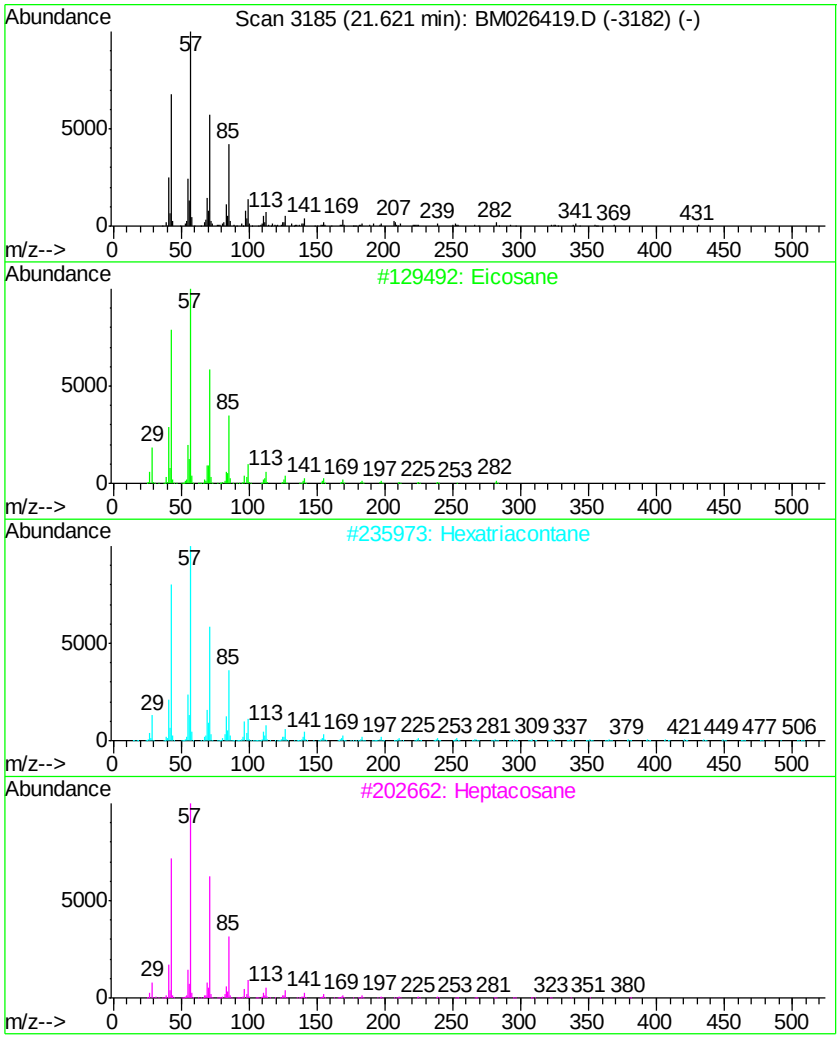
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

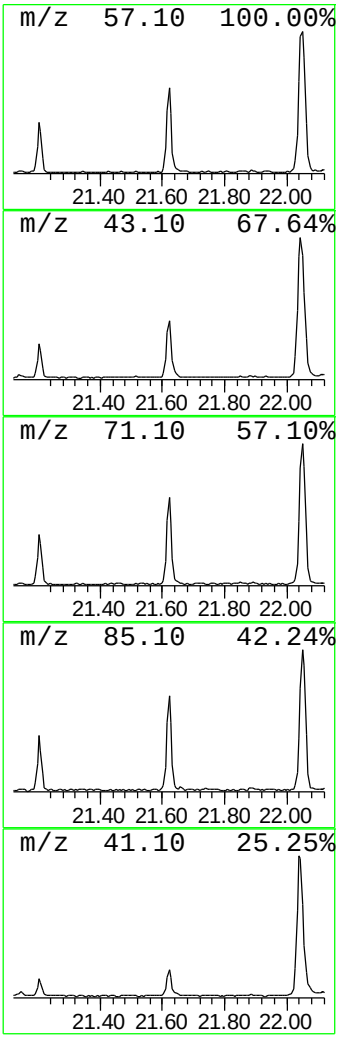
**********

Peak Number 4 Eicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.62 | 2.34 ng | 178265 | Chrysene-d12 | 21.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 87 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 87 |
| 4 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 83 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 83 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

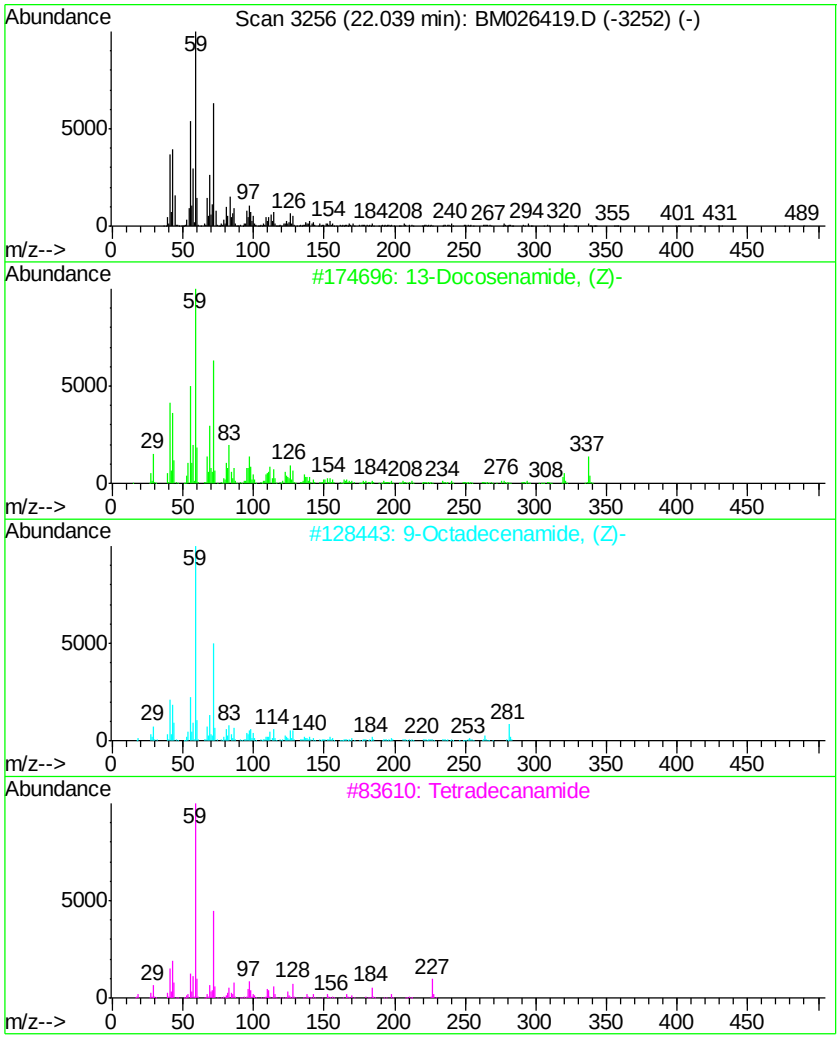
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

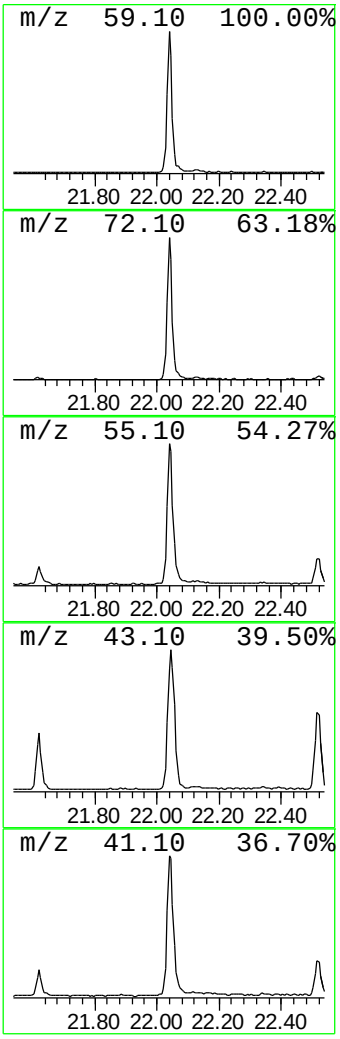
**********

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.04 | 16.53 ng | 1261510 | Chrysene-d12 | 21.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 90 |
| 2 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 62 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 59 |
| 4 | Decanamide- | 171 | C10H21NO | 002319-29-1 | 50 |
| 5 | 2-Methyl-tridecane-2,12-diol | 230 | C14H30O2 | 1000187-03-5 | 47 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

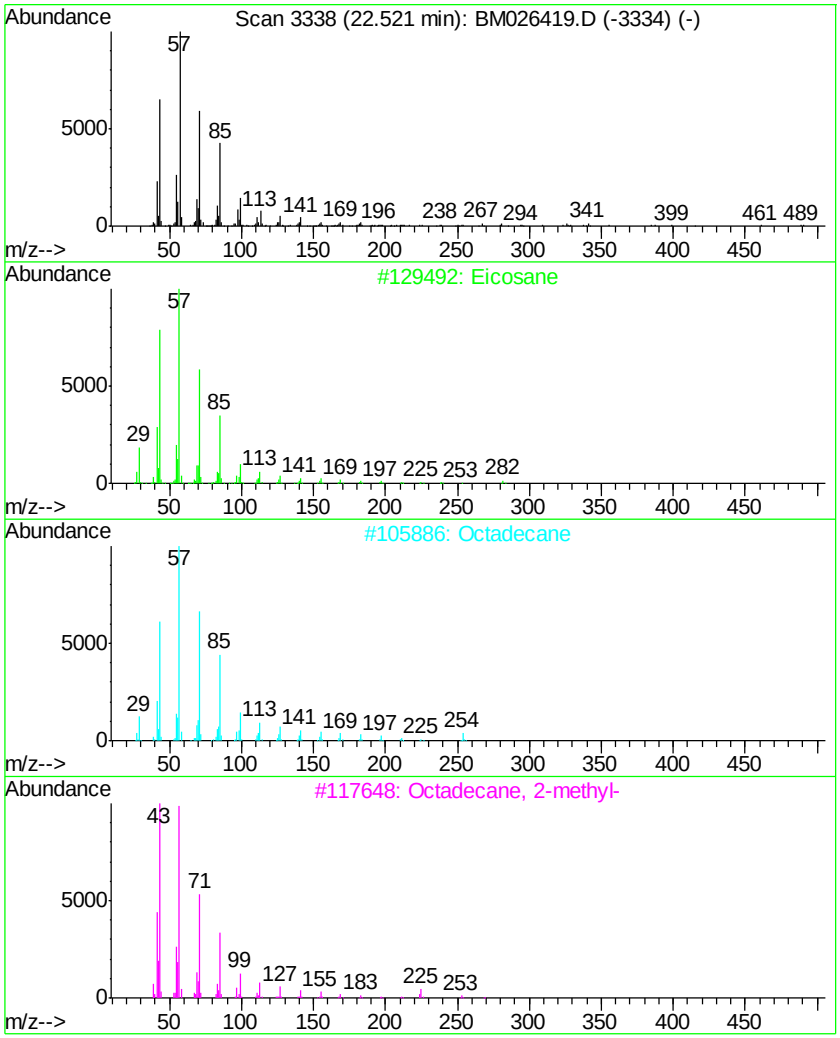
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

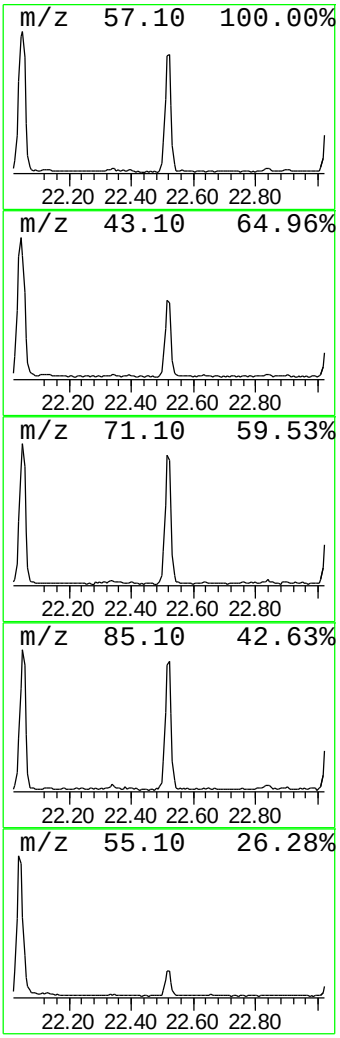
**********

Peak Number 6 Octadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.52 | 3.62 ng | 288114 | Perylene-d12 | 23.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 96 |
| 3 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 93 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

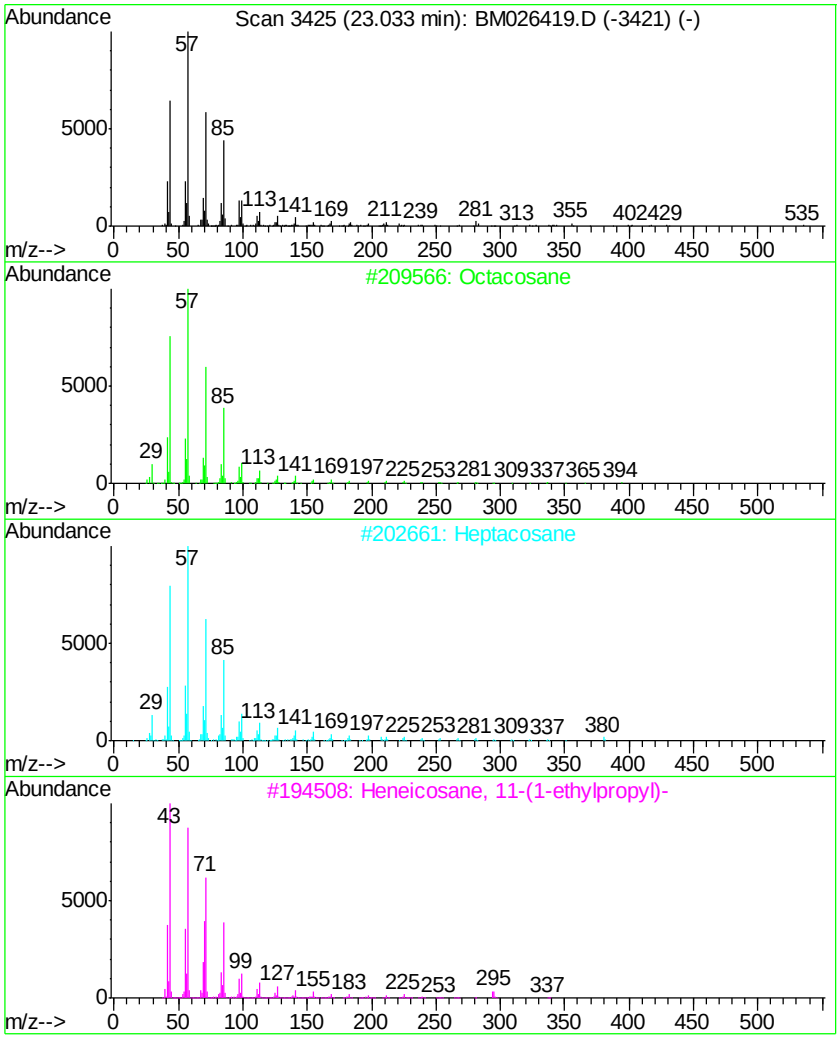
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

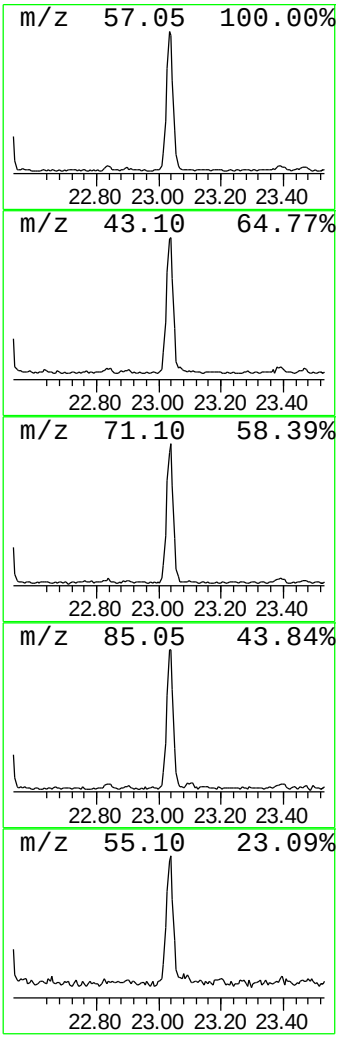
**********

Peak Number 7 Octacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.03 | 3.70 ng | 295077 | Perylene-d12 | 23.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 3 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 87 |
| 4 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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

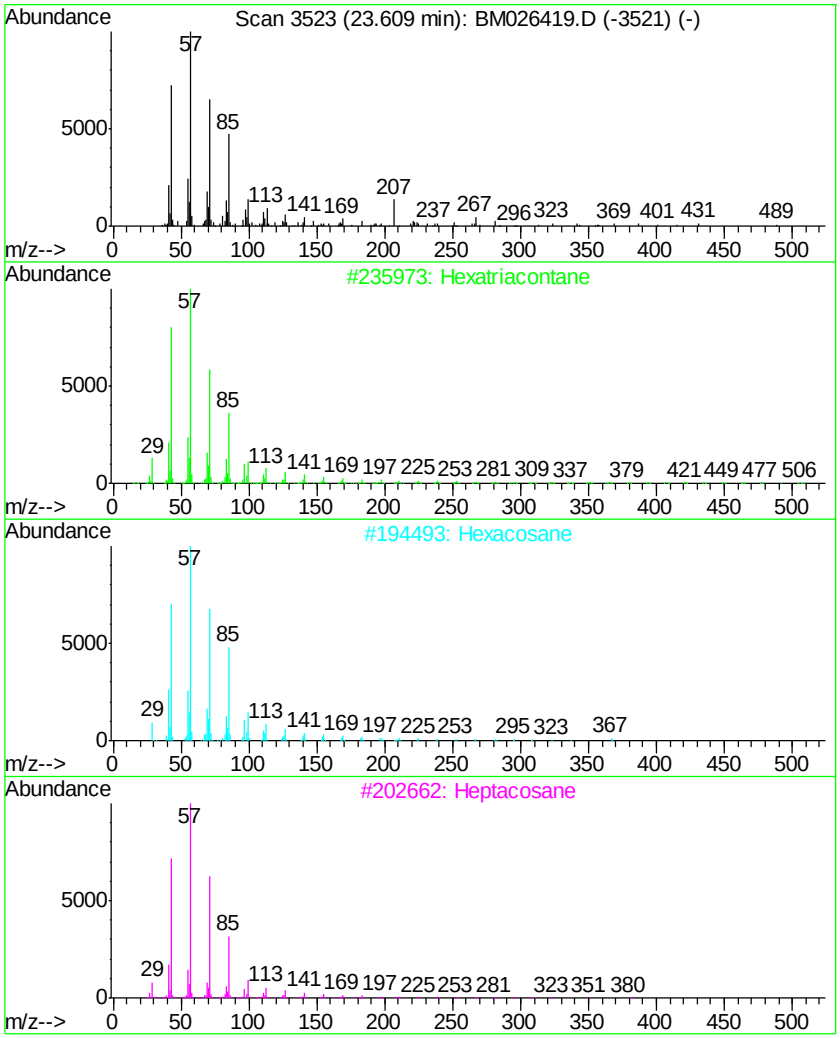
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

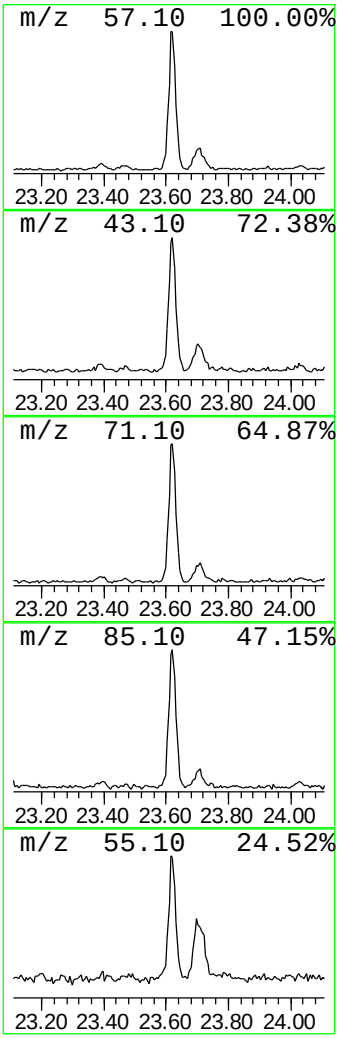
**********

Peak Number 8 Hexatriacontane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.61 | 3.09 ng | 246367 | Perylene-d12 | 23.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 90 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |
| 5 | Docosane, 11-decyl- | 451 | C32H66 | 055401-55-3 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM061620\
Data File : BM026419.D
Acq On : 16 Jun 2020 19:18
Operator : JU/CG
Sample : L3020-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** MW-24(19-21)

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 |
| Phenol, 4,4'-(1-m... | 19.28 | 5.0 | ng | 382232 | 5 | 21.01 | 1526700 | 20.0 |
| 5-Eicosene, (E)- | 20.77 | 4.4 | ng | 333273 | 5 | 21.01 | 1526700 | 20.0 |
| Eicosane | 21.62 | 2.3 | ng | 178265 | 5 | 21.01 | 1526700 | 20.0 |
| 13-Docosenamide, ... | 22.04 | 16.5 | ng | 1261510 | 5 | 21.01 | 1526700 | 20.0 |
| Octadecane | 22.52 | 3.6 | ng | 288114 | 6 | 23.10 | 1593320 | 20.0 |
| Octacosane | 23.03 | 3.7 | ng | 295077 | 6 | 23.10 | 1593320 | 20.0 |
| Hexatriacontane | 23.61 | 3.1 | ng | 246367 | 6 | 23.10 | 1593320 | 20.0 |