LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

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-BM021119.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 | 5.269 | 364 | 371 | 388 | rBV | 3645252 | 5356318 | 77.77% | 10.041% |
| 2 | 6.846 | 632 | 639 | 663 | rBV | 3376501 | 5616094 | 81.55% | 10.528% |
| 3 | 7.204 | 692 | 700 | 713 | rBV | 3751376 | 5884520 | 85.44% | 11.031% |
| 4 | 7.669 | 772 | 779 | 786 | rBV | 690016 | 1076718 | 15.63% | 2.018% |
| 5 | 7.987 | 824 | 833 | 843 | rBV | 2578780 | 4157191 | 60.36% | 7.793% |
| 6 | 8.840 | 969 | 978 | 996 | rBV | 1876800 | 3311000 | 48.08% | 6.207% |
| 7 | 10.457 | 1245 | 1253 | 1265 | rBV | 735144 | 1318811 | 19.15% | 2.472% |
| 8 | 12.933 | 1667 | 1674 | 1696 | rBV | 3972509 | 6061797 | 88.02% | 11.364% |
| 9 | 13.792 | 1814 | 1820 | 1833 | rBV | 223994 | 377992 | 5.49% | 0.709% |
| 10 | 14.204 | 1882 | 1890 | 1902 | rBV3 | 59317 | 193529 | 2.81% | 0.363% |
| 11 | 14.322 | 1904 | 1910 | 1927 | rVB2 | 985153 | 1570938 | 22.81% | 2.945% |
| 12 | 15.821 | 2156 | 2165 | 2190 | rBV | 3103488 | 4689137 | 68.09% | 8.791% |
| 13 | 17.074 | 2373 | 2378 | 2390 | rBV2 | 992125 | 1608074 | 23.35% | 3.015% |
| 14 | 17.962 | 2524 | 2529 | 2543 | rBV | 179318 | 336584 | 4.89% | 0.631% |
| 15 | 19.251 | 2744 | 2748 | 2755 | rBV3 | 76513 | 138097 | 2.01% | 0.259% |
| 16 | 19.709 | 2821 | 2826 | 2839 | rBV | 5629338 | 6887041 | 100.00% | 12.911% |
| 17 | 20.974 | 3037 | 3041 | 3047 | rBV2 | 140858 | 196066 | 2.85% | 0.368% |
| 18 | 21.274 | 3087 | 3092 | 3102 | rBV | 1351622 | 1871276 | 27.17% | 3.508% |
| 19 | 21.839 | 3185 | 3188 | 3194 | rBV2 | 88933 | 130305 | 1.89% | 0.244% |
| 20 | 22.297 | 3264 | 3266 | 3271 | rVB | 135409 | 162450 | 2.36% | 0.305% |
| 21 | 22.803 | 3349 | 3352 | 3358 | rVB2 | 148762 | 204357 | 2.97% | 0.383% |
| 22 | 23.368 | 3445 | 3448 | 3454 | rVB3 | 145078 | 213690 | 3.10% | 0.401% |
| 23 | 23.515 | 3467 | 3473 | 3486 | rVB2 | 983960 | 1981045 | 28.76% | 3.714% |

Sum of corrected areas: 53343030

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
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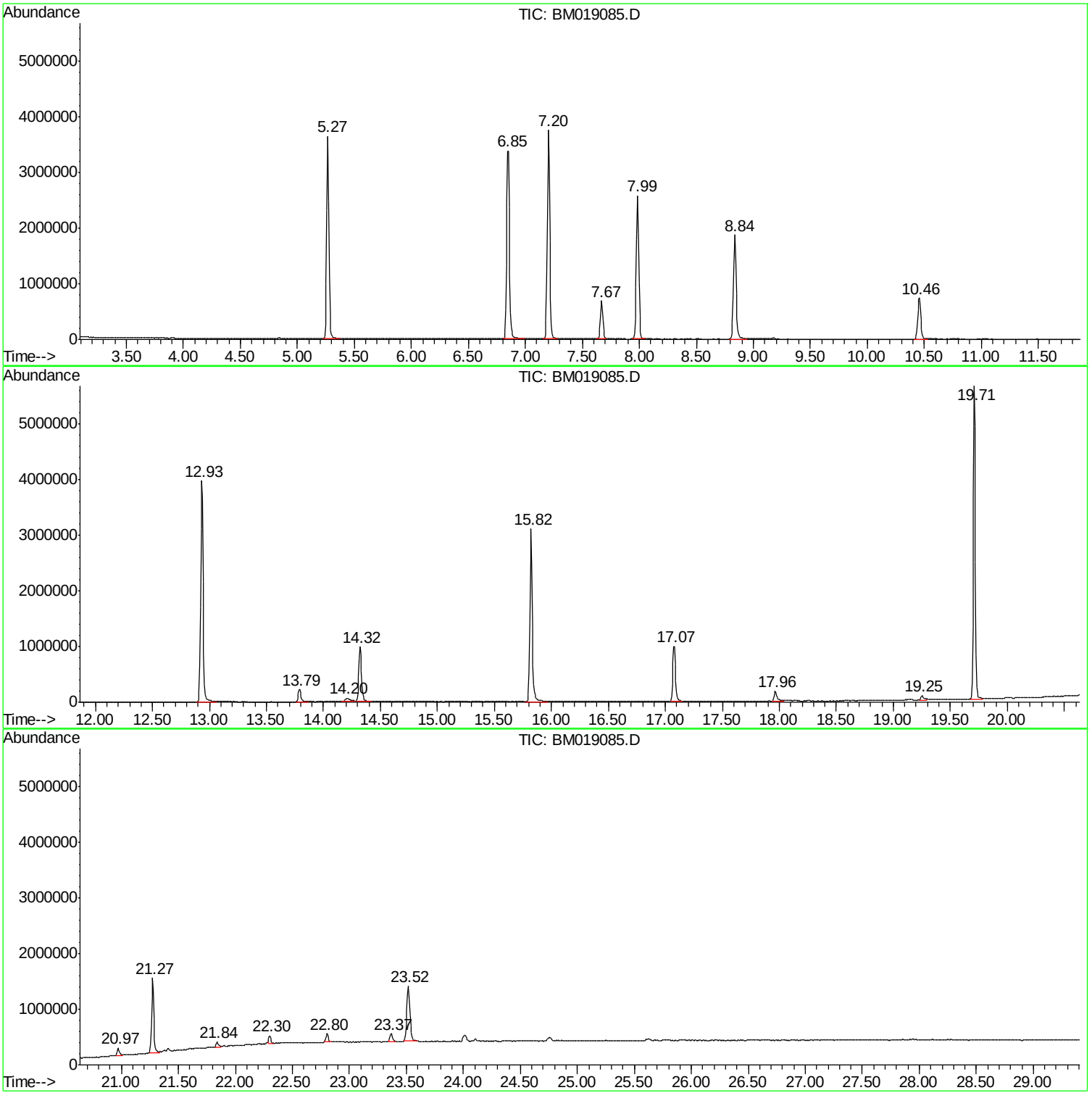
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

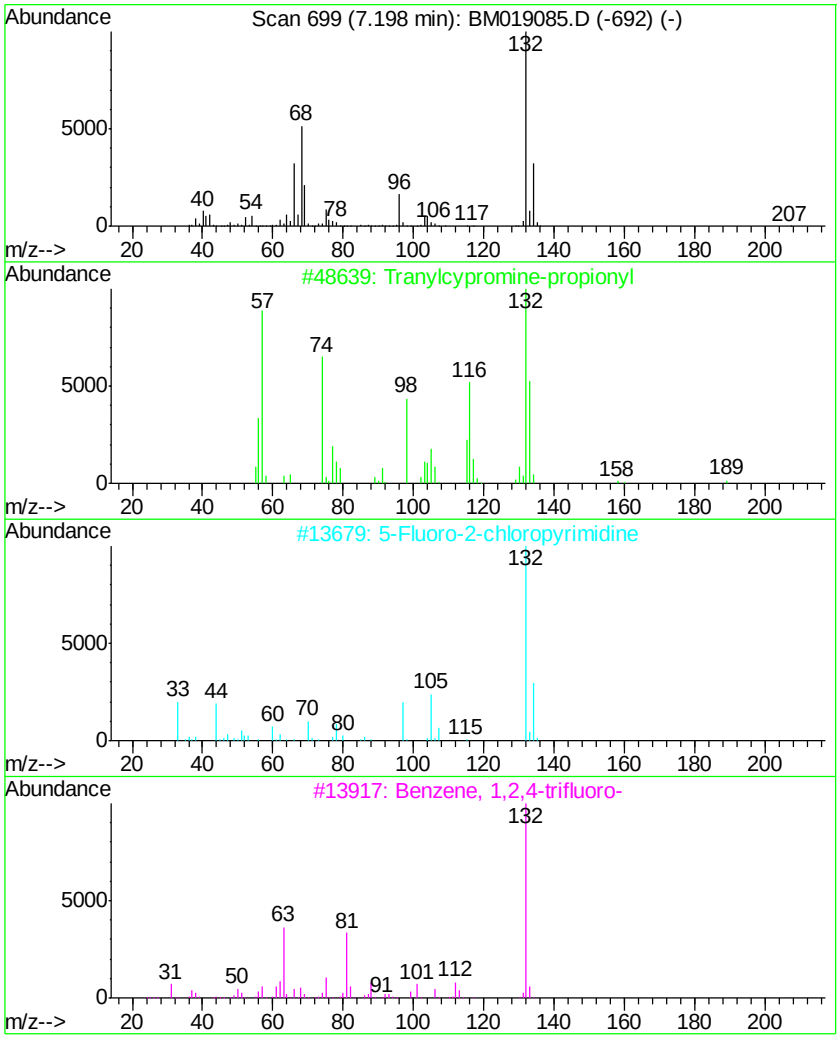
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

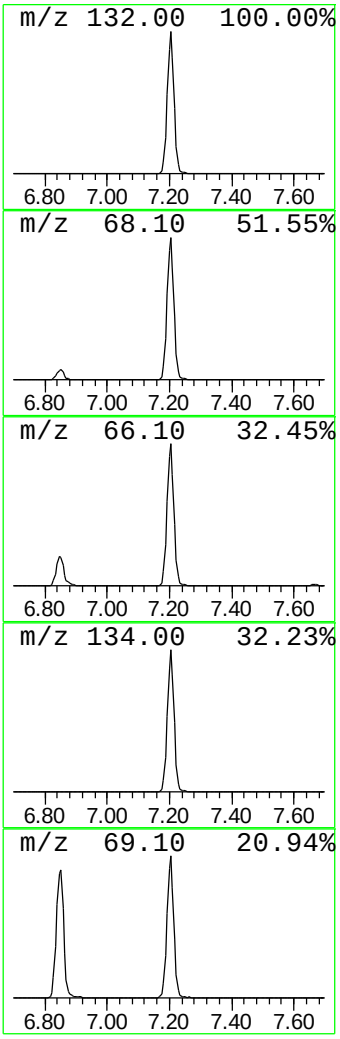
**********

Peak Number 1 unknown7.20 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.20 | 109.31 ng | 5884520 | 1,4-Dichlorobenzene-d4 | 7.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Benzene, 1,2,4-trifluoro- | 132 | C6H3F3 | 000367-23-7 | 9 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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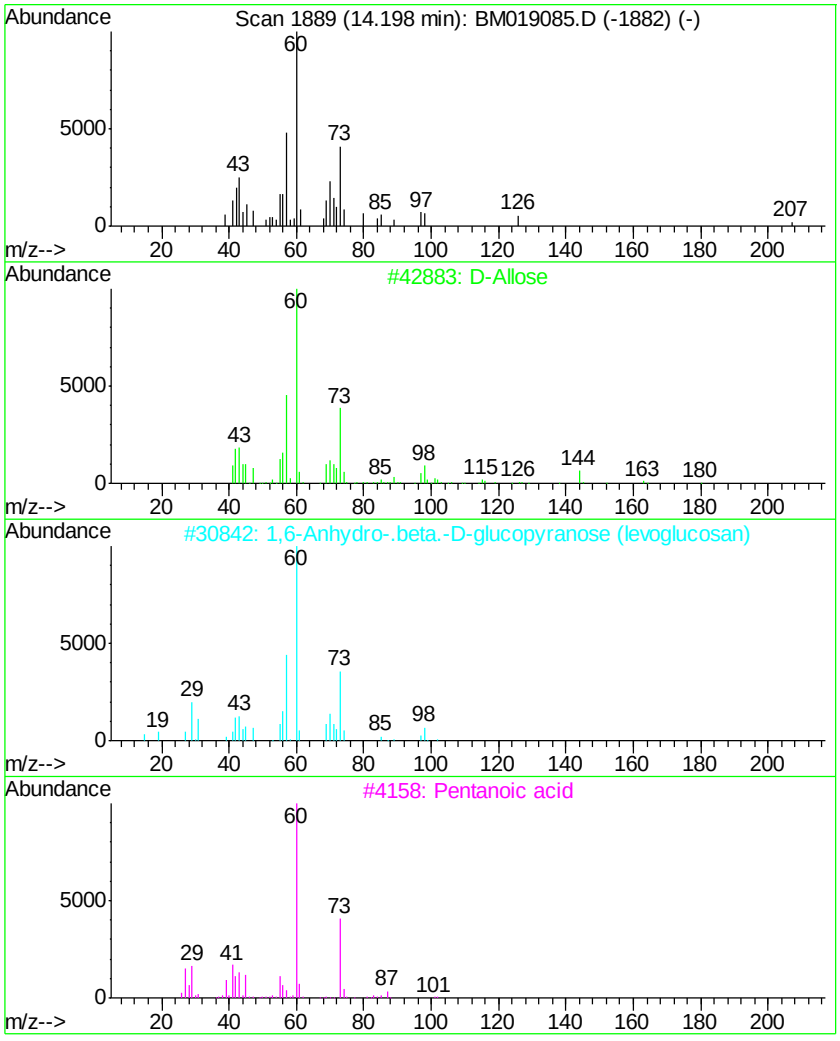
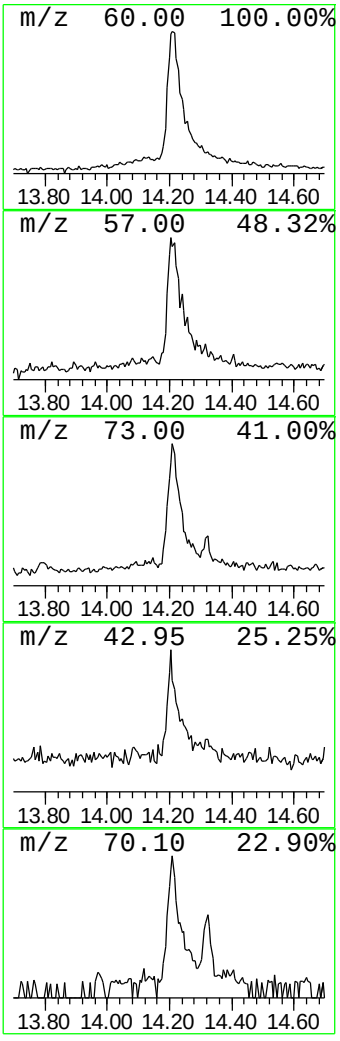
Peak Number 3 D-Allose Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.20 | 2.46 ng | 193529 | Acenaphthene-d10 | 14.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | D-Allose | 180 | C6H12O6 | 002595-97-3 | 72 |
| 2 | 1,6-Anhydro-.beta.-D-glucopyrano... | 162 | C6H10O5 | 000498-07-7 | 64 |
| 3 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 47 |
| 4 | D-Mannoheptulose | 210 | C7H14O7 | 003615-44-9 | 45 |
| 5 | 1,6-Anhydro-.beta.-d-talopyranose | 162 | C6H10O5 | 1000133-05-8 | 42 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

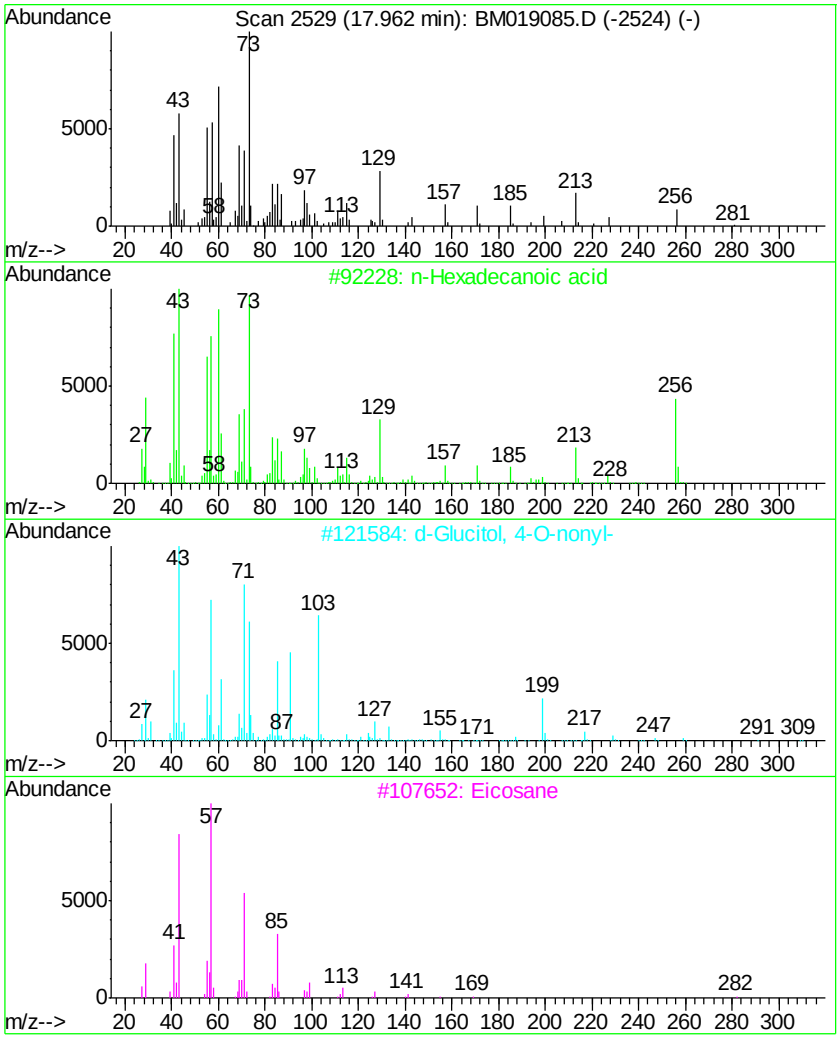
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

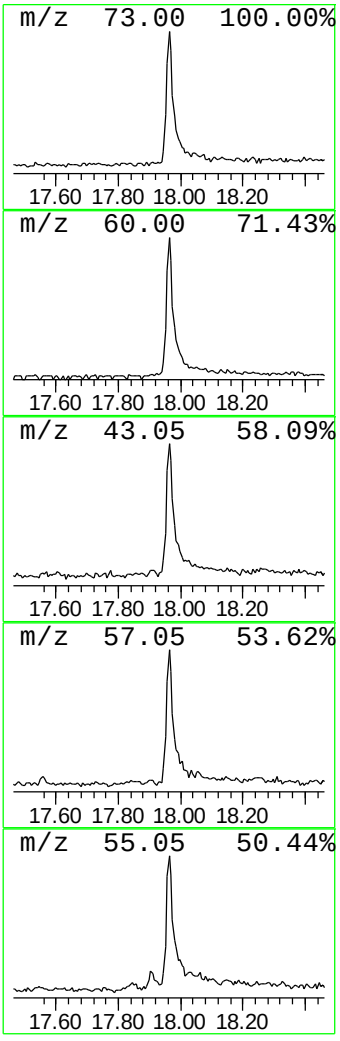
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.96 | 4.19 ng | 336584 | Phenanthrene-d10 | 17.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | d-Glucitol, 4-O-nonyl- | 308 | C15H32O6 | 132591-06-1 | 38 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 18 |
| 4 | Pentadecane | 212 | C15H32 | 000629-62-9 | 18 |
| 5 | Dodecane | 170 | C12H26 | 000112-40-3 | 18 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

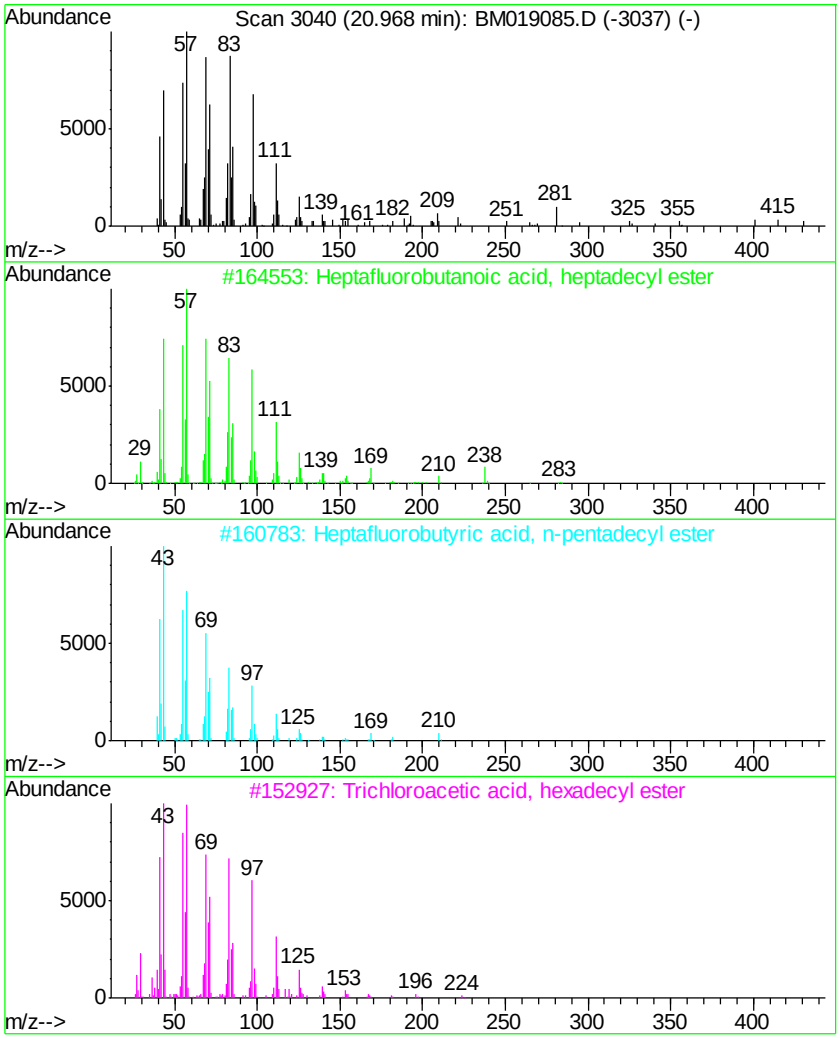
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

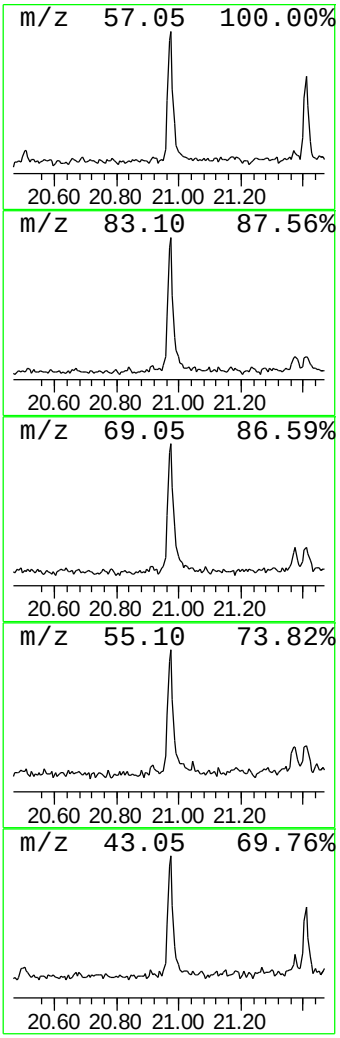
**********

Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.97 | 2.10 ng | 196066 | Chrysene-d12 | 21.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 94 |
| 2 | Heptafluorobutyric acid, n-penta... | 424 | C19H31F7O2 | 1000216-79-3 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 4 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 91 |
| 5 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |



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Data File : BM019085.D
Acq On : 08 Mar 2019 22:04
Operator : JU/SJ
Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

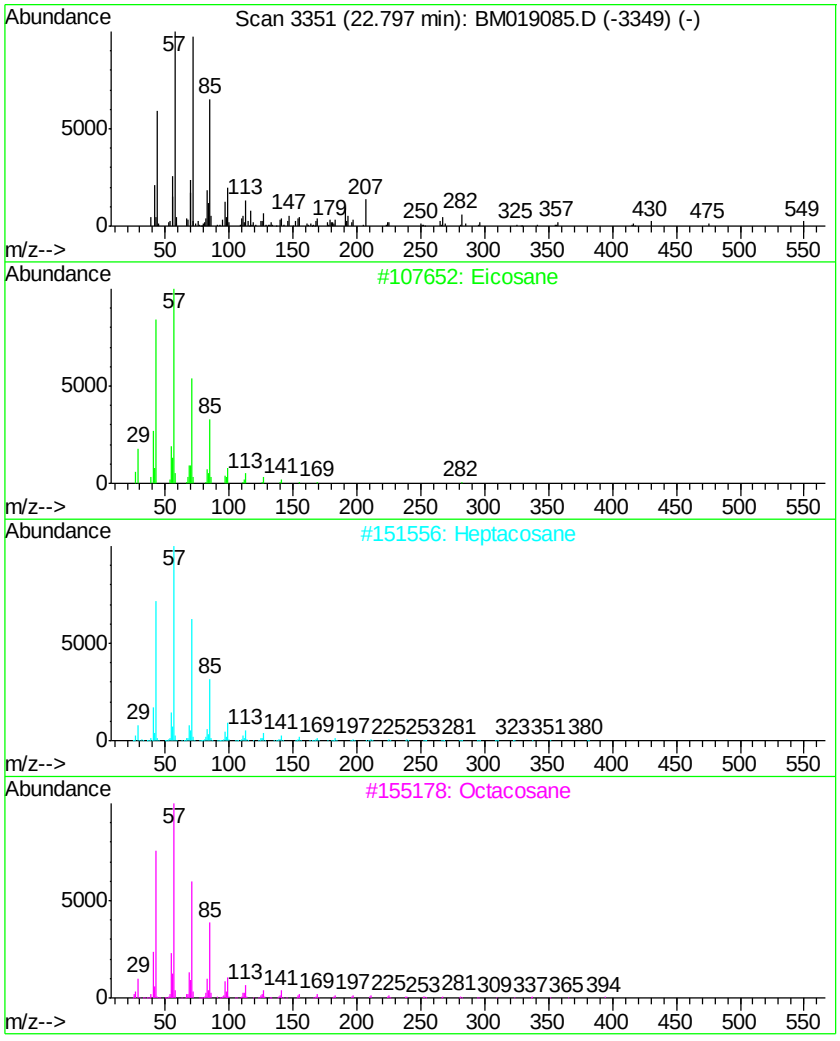
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

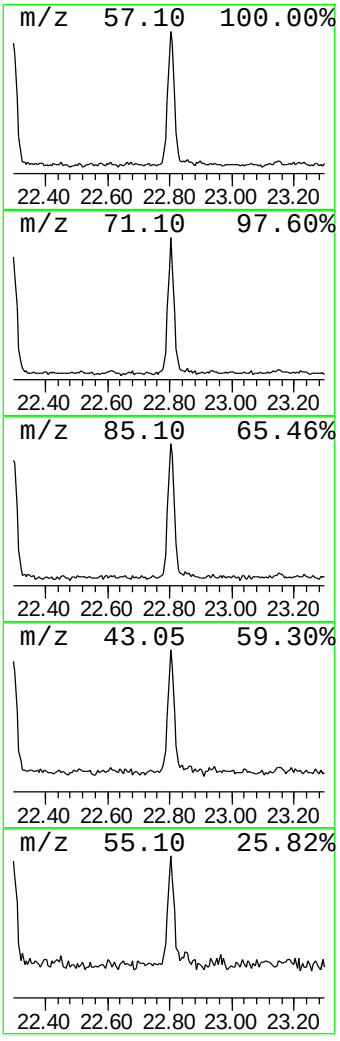
**********

Peak Number 6 Eicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.80 | 2.06 ng | 204357 | Perylene-d12 | 23.52 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 74 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 74 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 72 |
| 5 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 72 |



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Misc :
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**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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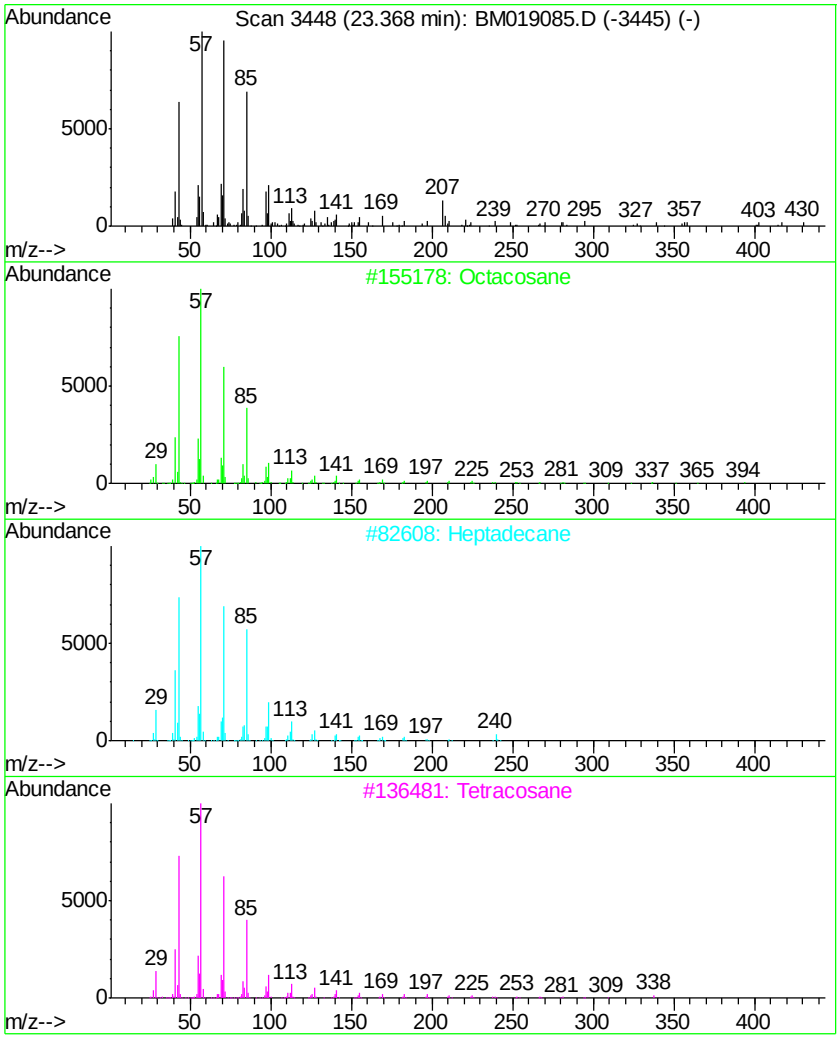
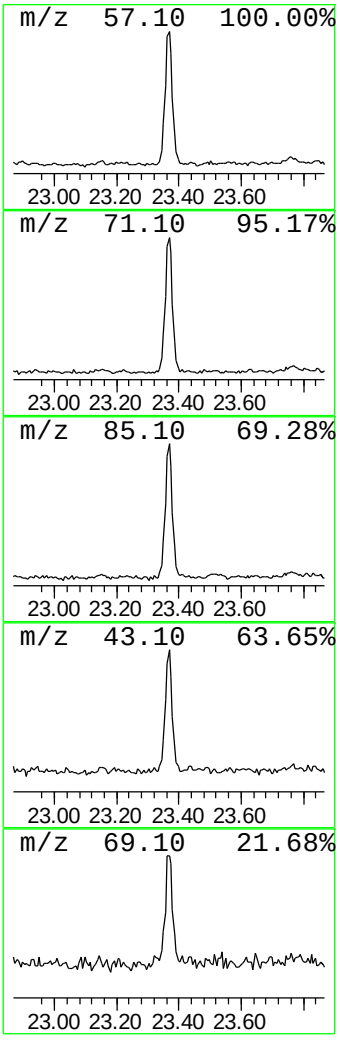
Peak Number 7 Octacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.37 | 2.16 ng | 213690 | Perylene-d12 | 23.52 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 80 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 80 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 74 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
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Sample : K1807-37
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TP-19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown7.20 | 7.20 | 109.3 | ng | 5884520 | 1 | 7.67 | 1076720 | 20.0 |
| D-Allose | 14.20 | 2.5 | ng | 193529 | 3 | 14.32 | 1570940 | 20.0 |
| n-Hexadecanoic acid | 17.96 | 4.2 | ng | 336584 | 4 | 17.07 | 1608070 | 20.0 |
| Heptafluorobutano... | 20.97 | 2.1 | ng | 196066 | 5 | 21.27 | 1871280 | 20.0 |
| Eicosane | 22.80 | 2.1 | ng | 204357 | 6 | 23.52 | 1981050 | 20.0 |
| Octacosane | 23.37 | 2.2 | ng | 213690 | 6 | 23.52 | 1981050 | 20.0 |