LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021219\
Data File : BM018787.D
Acq On : 12 Feb 2019 23:56
Operator : JU/SJ
Sample : K1458-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GW-7

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 | 5.304 | 371 | 377 | 395 | rBV | 3027936 | 4318884 | 17.47% | 3.597% |
| 2 | 6.887 | 637 | 646 | 663 | rBV | 1758764 | 3059039 | 12.38% | 2.548% |
| 3 | 7.245 | 700 | 707 | 722 | rBV | 5752554 | 9210080 | 37.26% | 7.672% |
| 4 | 7.710 | 779 | 786 | 793 | rBV | 1279545 | 2028492 | 8.21% | 1.690% |
| 5 | 8.028 | 833 | 840 | 851 | rBV | 4917318 | 8136821 | 32.92% | 6.778% |
| 6 | 8.881 | 976 | 985 | 998 | rBV | 4257808 | 7113494 | 28.78% | 5.925% |
| 7 | 10.504 | 1253 | 1261 | 1274 | rBV | 1672319 | 2835964 | 11.47% | 2.362% |
| 8 | 12.980 | 1674 | 1682 | 1704 | rBV | 10974380 | 15985817 | 64.67% | 13.315% |
| 9 | 13.827 | 1820 | 1826 | 1838 | rBV | 270666 | 442678 | 1.79% | 0.369% |
| 10 | 14.363 | 1908 | 1917 | 1926 | rBV2 | 2416329 | 3779560 | 15.29% | 3.148% |
| 11 | 15.863 | 2165 | 2172 | 2188 | rBV | 9098175 | 13039182 | 52.75% | 10.861% |
| 12 | 17.115 | 2379 | 2385 | 2397 | rBV | 3164938 | 4607553 | 18.64% | 3.838% |
| 13 | 18.004 | 2531 | 2536 | 2546 | rBV | 600456 | 872896 | 3.53% | 0.727% |
| 14 | 19.433 | 2773 | 2779 | 2784 | rBV | 6469499 | 7338331 | 29.69% | 6.112% |
| 15 | 19.750 | 2827 | 2833 | 2838 | rBV | 20515036 | 24719034 | 100.00% | 20.590% |
| 16 | 21.009 | 3043 | 3047 | 3058 | rBV | 742105 | 939160 | 3.80% | 0.782% |
| 17 | 21.303 | 3092 | 3097 | 3106 | rBV | 4336303 | 5387002 | 21.79% | 4.487% |
| 18 | 21.874 | 3191 | 3194 | 3198 | rBV | 279982 | 341016 | 1.38% | 0.284% |
| 19 | 22.339 | 3270 | 3273 | 3279 | rVB | 365463 | 451233 | 1.83% | 0.376% |
| 20 | 22.850 | 3356 | 3360 | 3365 | rVB | 377617 | 515596 | 2.09% | 0.429% |
| 21 | 23.421 | 3454 | 3457 | 3462 | rVB | 378098 | 512187 | 2.07% | 0.427% |
| 22 | 23.568 | 3475 | 3482 | 3491 | rVB2 | 2309850 | 4421060 | 17.89% | 3.683% |

Sum of corrected areas: 120055079

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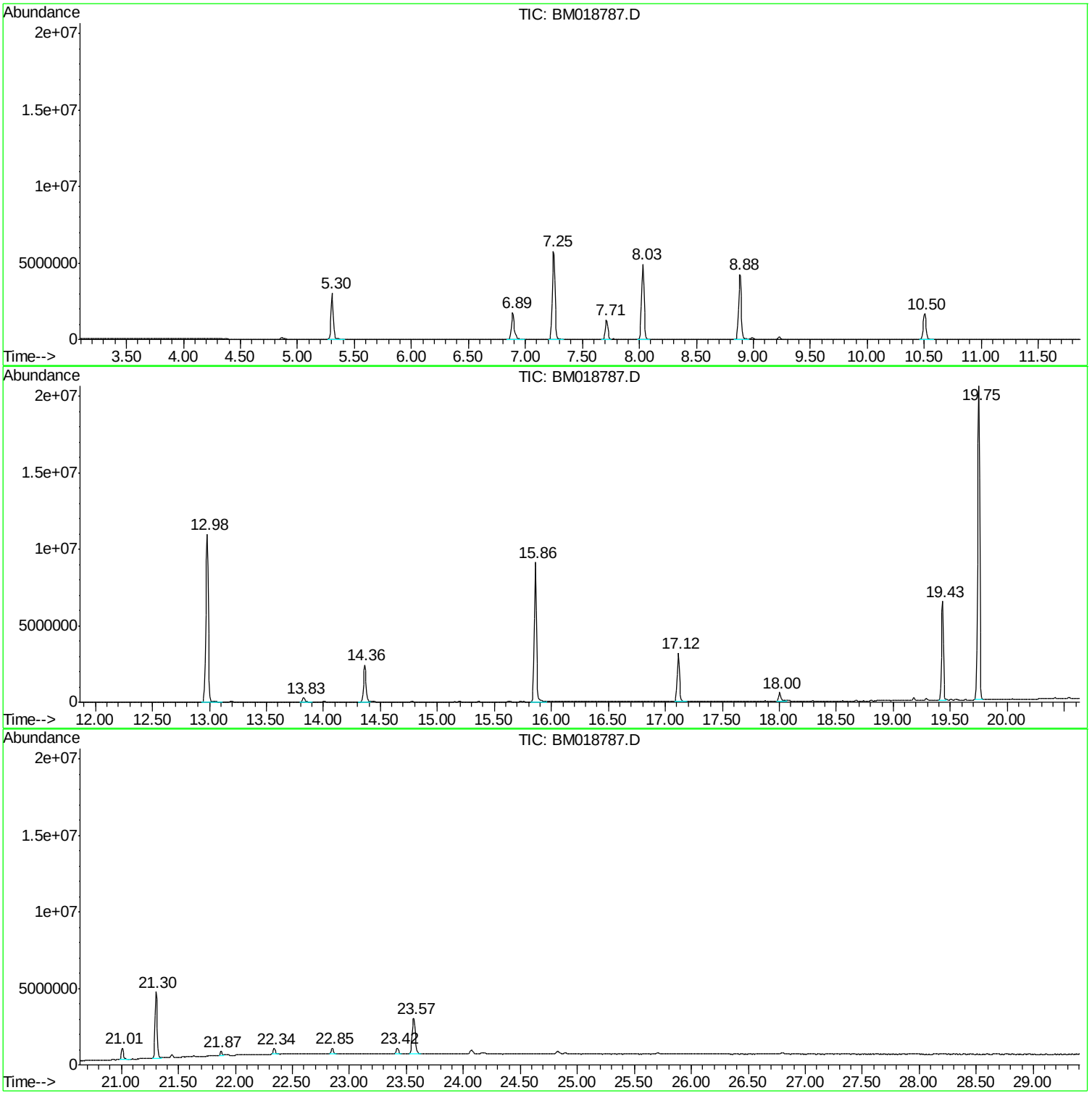
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GW-7

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\BM021219\
Data File : BM018787.D
Acq On : 12 Feb 2019 23:56
Operator : JU/SJ
Sample : K1458-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GW-7

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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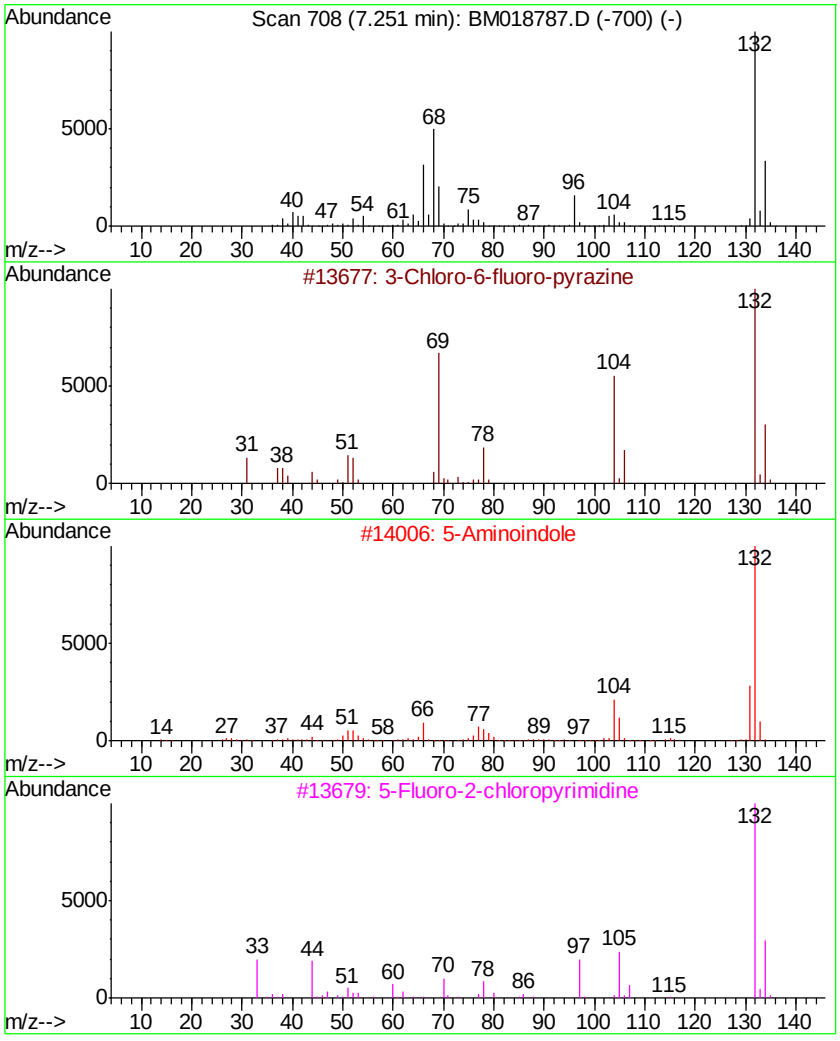
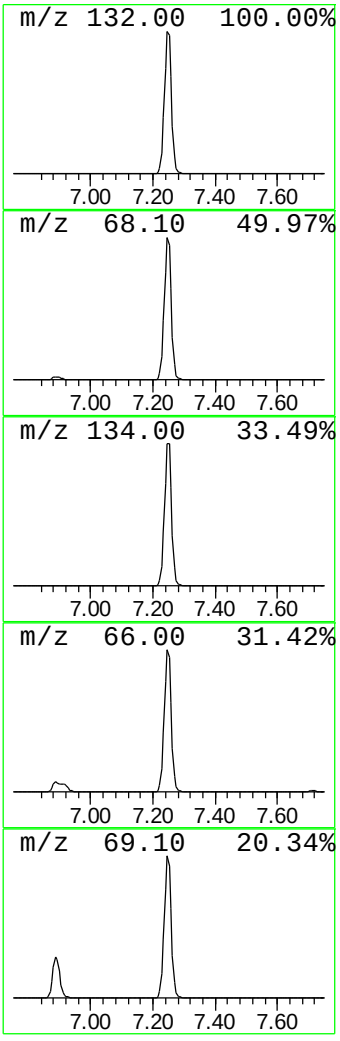
Peak Number 1 unknown7.25 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.25 | 90.81 ng | 9210080 | 1,4-Dichlorobenzene-d4 | 7.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 4 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 11 |
| 5 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 10 |



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Sample : K1458-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GW-7

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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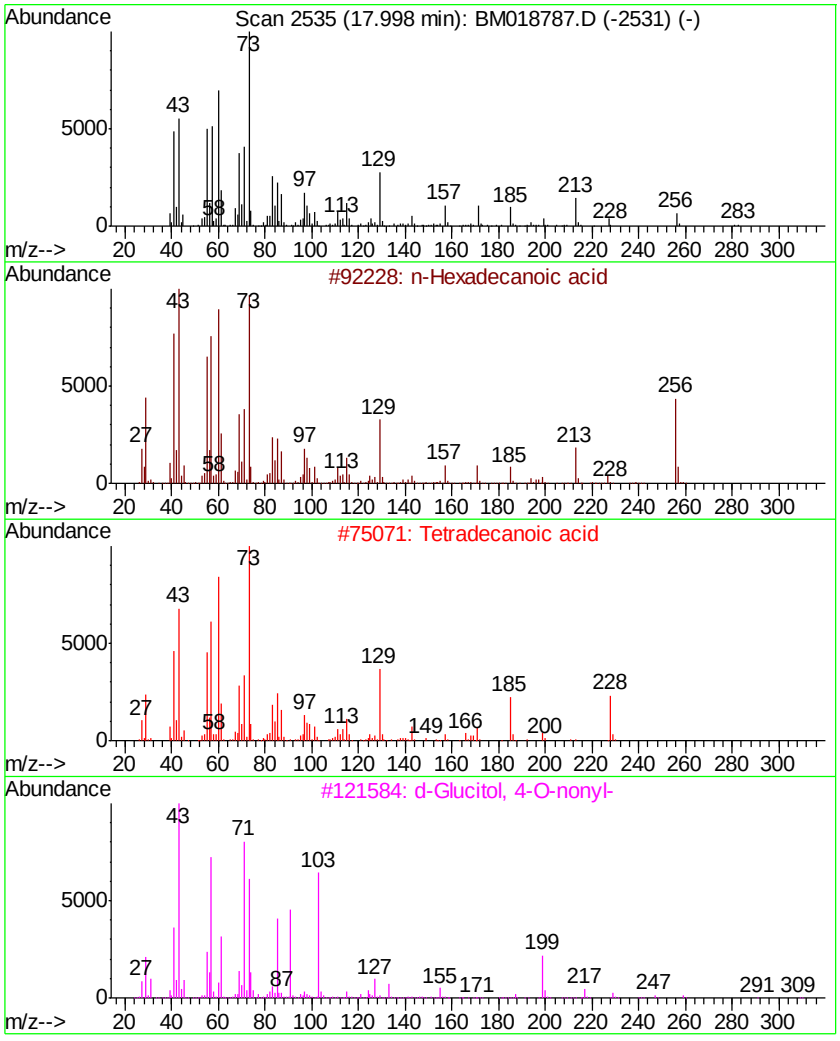
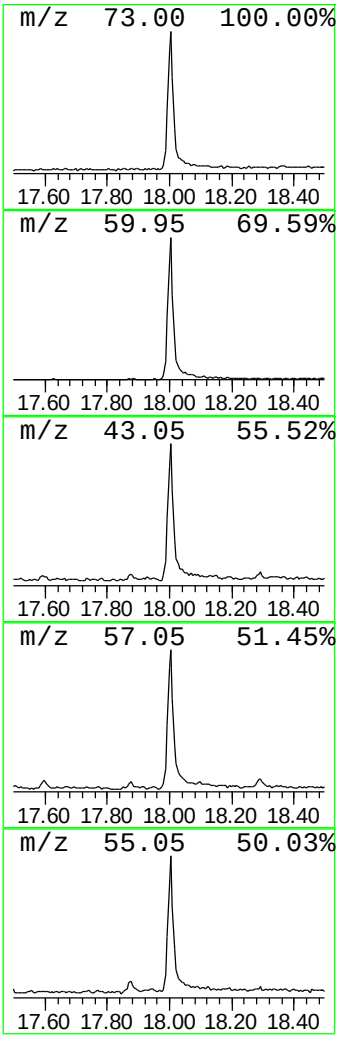
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.00 | 3.79 ng | 872896 | Phenanthrene-d10 | 17.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 3 | d-Glucitol, 4-O-nonyl- | 308 | C15H32O6 | 132591-06-1 | 27 |
| 4 | Dodecane | 170 | C12H26 | 000112-40-3 | 25 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 25 |



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Data File : BM018787.D
Acq On : 12 Feb 2019 23:56
Operator : JU/SJ
Sample : K1458-12
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GW-7

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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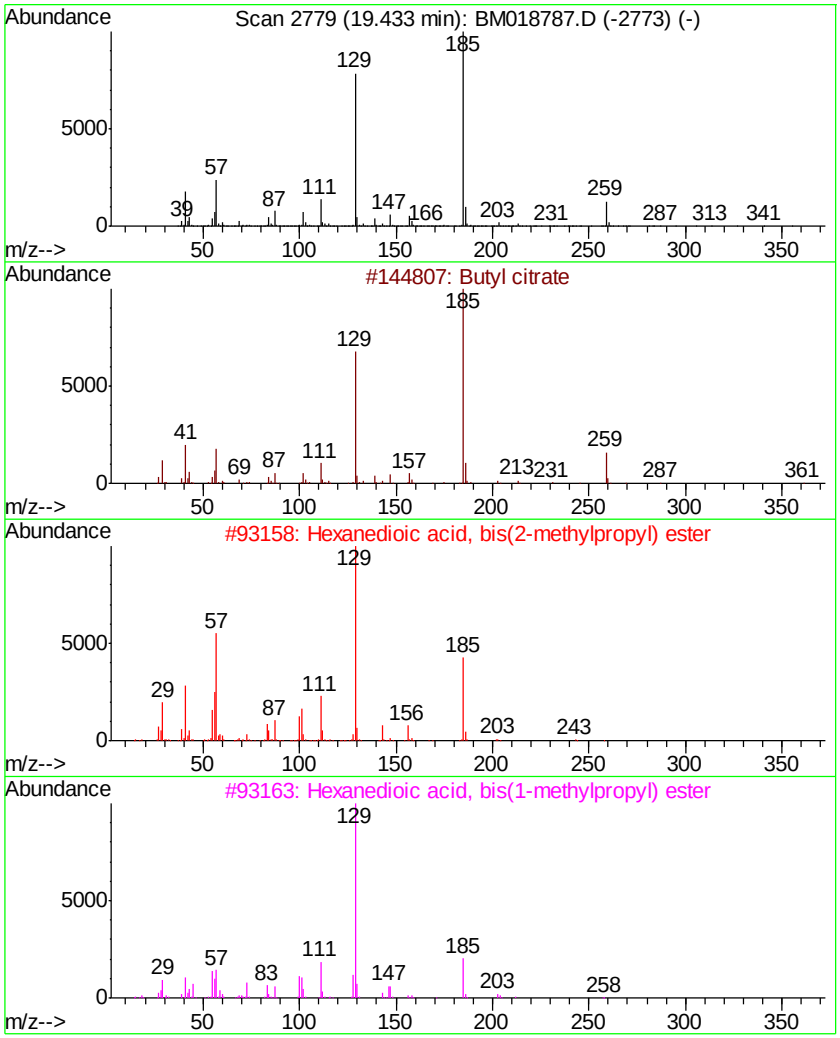
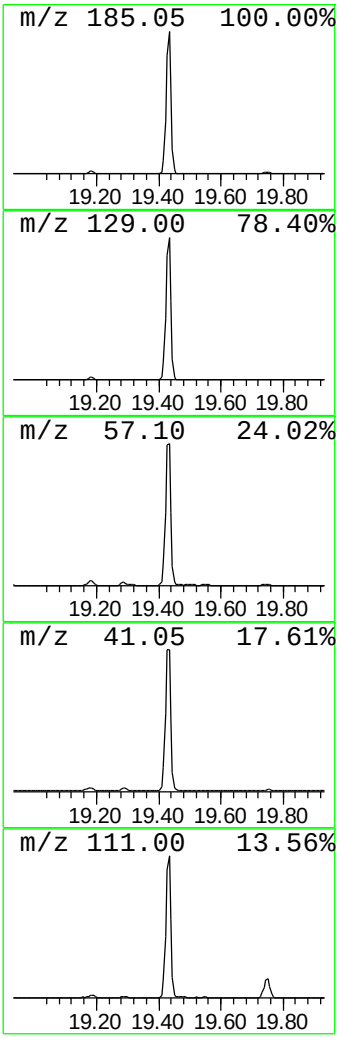
Peak Number 4 Butyl citrate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.43 | 27.24 ng | 7338330 | Chrysene-d12 | 21.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyl citrate | 360 | C18H32O7 | 000077-94-1 | 91 |
| 2 | Hexanedioic acid, bis(2-methylpr... | 258 | C14H26O4 | 000141-04-8 | 56 |
| 3 | Hexanedioic acid, bis(1-methylpr... | 258 | C14H26O4 | 038447-22-2 | 56 |
| 4 | Hexanedioic acid, dibutyl ester | 258 | C14H26O4 | 000105-99-7 | 40 |
| 5 | Butanedioic acid, 2,3-dimethyl-,... | 258 | C14H26O4 | 056051-57-1 | 39 |



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ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GW-7

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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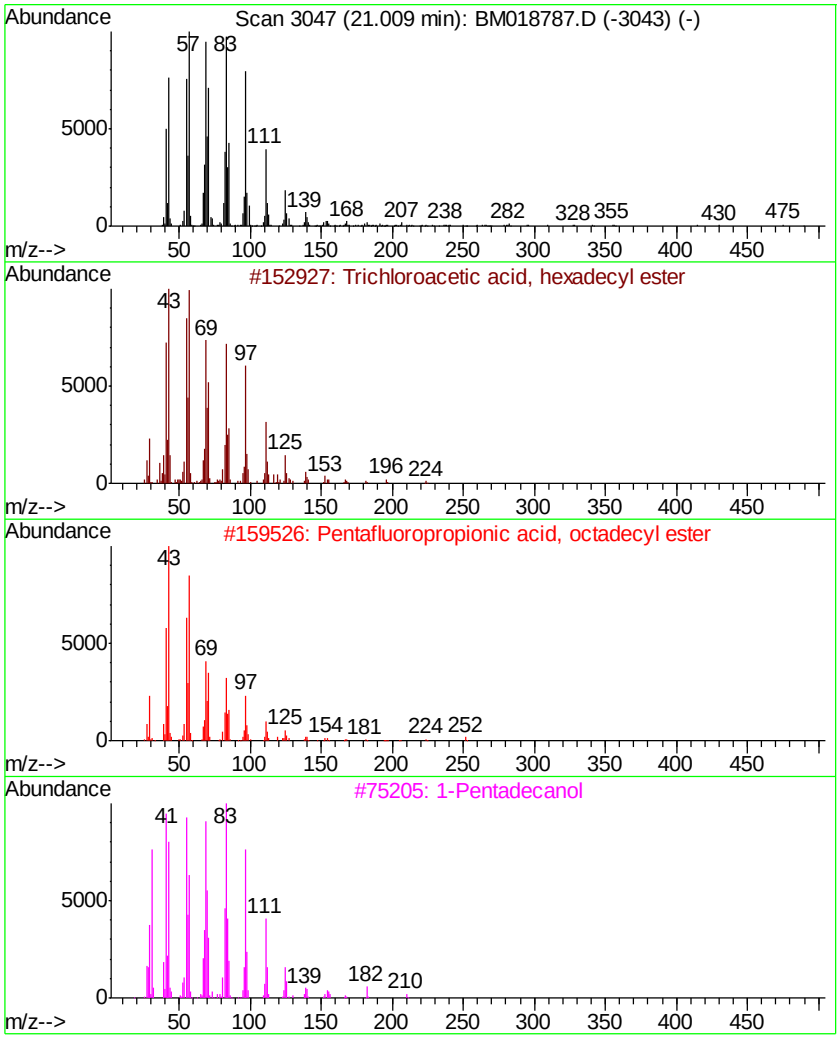
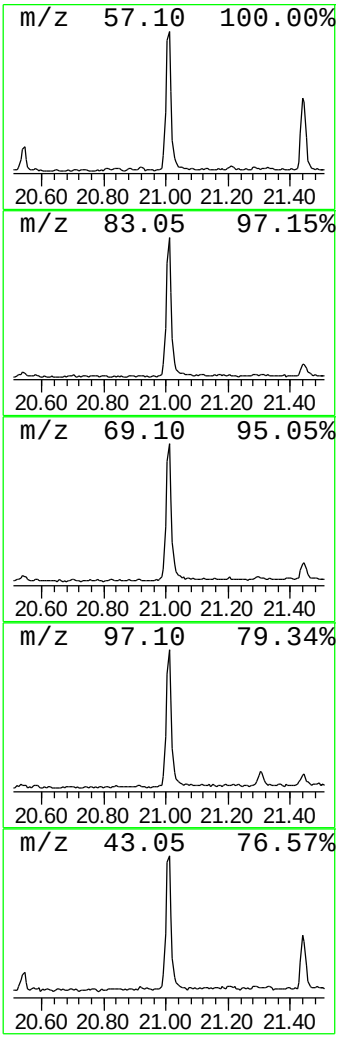
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.01 | 3.49 ng | 939160 | Chrysene-d12 | 21.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 2 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 1000280-07-7 | 91 |
| 3 | 1-Pentadecanol | 228 | C15H32O | 000629-76-5 | 90 |
| 4 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 90 |
| 5 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 87 |



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ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_M
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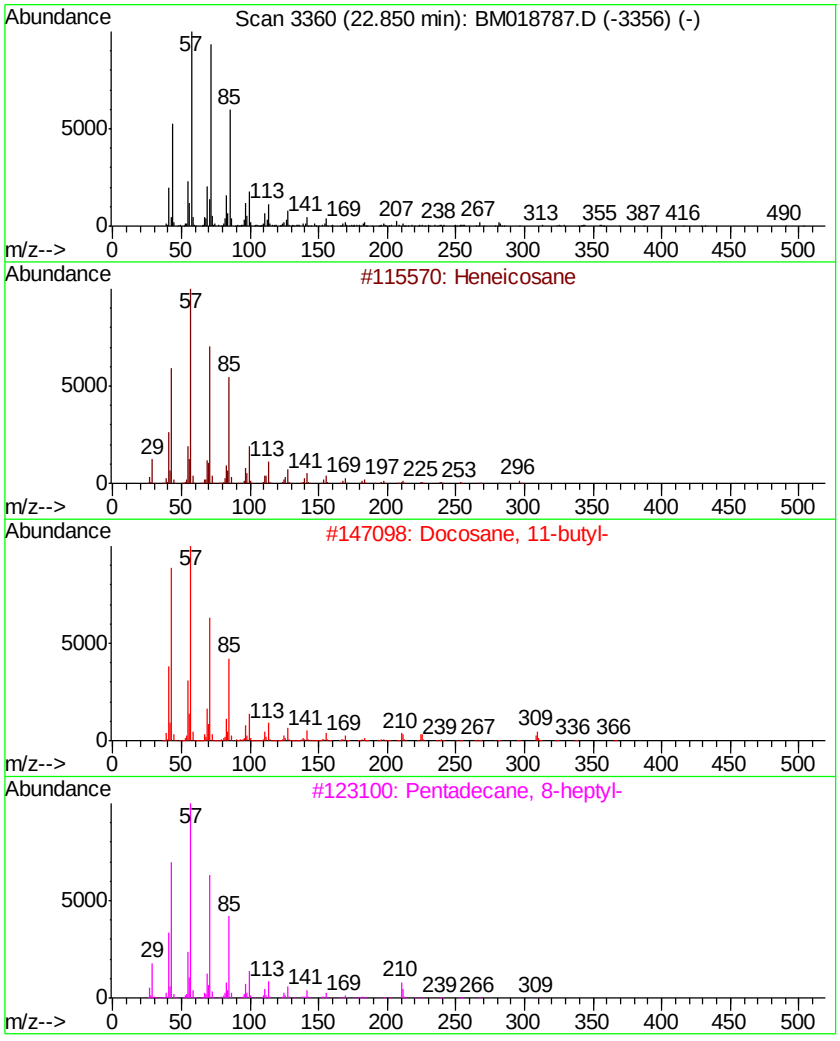
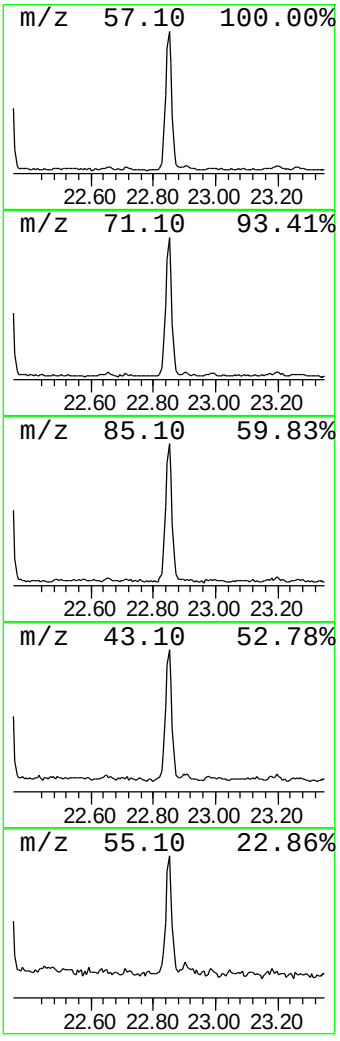
Peak Number 6 Heneicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.85 | 2.33 ng | 515596 | Perylene-d12 | 23.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 90 |
| 3 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 90 |
| 4 | Docosane, 9-butyl- | 366 | C26H54 | 055282-14-9 | 90 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 87 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown7.25 | 7.25 | 90.8 | ng | 9210080 | 1 | 7.71 | 2028490 | 20.0 |
| n-Hexadecanoic acid | 18.00 | 3.8 | ng | 872896 | 4 | 17.12 | 4607550 | 20.0 |
| Butyl citrate | 19.43 | 27.2 | ng | 7338330 | 5 | 21.30 | 5387000 | 20.0 |
| Trichloroacetic a... | 21.01 | 3.5 | ng | 939160 | 5 | 21.30 | 5387000 | 20.0 |
| Heneicosane | 22.85 | 2.3 | ng | 515596 | 6 | 23.57 | 4421060 | 20.0 |