LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN021918\
Data File : BN000126.D
Acq On : 20 Feb 2018 00:30
Operator : JU/SJ
Sample : J1591-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_N
**ClientSampleId :** MH-28

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:\HPCHEM1\BNA_N\METHODS\8270-BN020718.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 | 3.234 | 36 | 42 | 51 | rBV | 638380 | 1262458 | 3.55% | 0.667% |
| 2 | 3.316 | 51 | 56 | 81 | rVB | 5289364 | 8714615 | 24.54% | 4.606% |
| 3 | 5.934 | 493 | 501 | 512 | rBV | 3310962 | 5254500 | 14.79% | 2.777% |
| 4 | 7.581 | 768 | 781 | 791 | rBV | 2090499 | 3471388 | 9.77% | 1.835% |
| 5 | 7.975 | 840 | 848 | 859 | rBV | 6855749 | 11420286 | 32.16% | 6.036% |
| 6 | 8.457 | 922 | 930 | 941 | rBV | 2095861 | 3510041 | 9.88% | 1.855% |
| 7 | 8.787 | 977 | 986 | 995 | rBV | 9625917 | 16270625 | 45.81% | 8.600% |
| 8 | 9.640 | 1122 | 1131 | 1139 | rBV | 7877359 | 13329917 | 37.53% | 7.045% |
| 9 | 11.298 | 1405 | 1413 | 1422 | rBV | 3198985 | 5448021 | 15.34% | 2.880% |
| 10 | 13.698 | 1812 | 1821 | 1828 | rBV | 20767344 | 31445540 | 88.54% | 16.620% |
| 11 | 14.498 | 1952 | 1957 | 1964 | rBV | 447441 | 712411 | 2.01% | 0.377% |
| 12 | 14.928 | 2025 | 2030 | 2037 | rVB | 380145 | 476424 | 1.34% | 0.252% |
| 13 | 15.069 | 2047 | 2054 | 2062 | rVB2 | 4714204 | 7270009 | 20.47% | 3.843% |
| 14 | 15.869 | 2179 | 2190 | 2195 | rBV2 | 389560 | 698441 | 1.97% | 0.369% |
| 15 | 16.533 | 2297 | 2303 | 2320 | rBV | 9635676 | 13721408 | 38.63% | 7.252% |
| 16 | 16.716 | 2330 | 2334 | 2343 | rBV | 296072 | 467045 | 1.32% | 0.247% |
| 17 | 17.786 | 2509 | 2516 | 2528 | rBV2 | 5848612 | 8390840 | 23.63% | 4.435% |
| 18 | 18.621 | 2653 | 2658 | 2669 | rBV | 686716 | 1109861 | 3.12% | 0.587% |
| 19 | 19.874 | 2866 | 2871 | 2881 | rBV | 599674 | 983176 | 2.77% | 0.520% |
| 20 | 20.345 | 2945 | 2951 | 2963 | rBV | 28018949 | 35516182 | 100.00% | 18.772% |
| 21 | 21.568 | 3155 | 3159 | 3171 | rBV2 | 256292 | 557104 | 1.57% | 0.294% |
| 22 | 21.898 | 3209 | 3215 | 3225 | rBV | 7058265 | 9349870 | 26.33% | 4.942% |
| 23 | 24.374 | 3628 | 3636 | 3646 | rVB2 | 4851756 | 9819253 | 27.65% | 5.190% |

Sum of corrected areas: 189199415

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**Instrument :** BNA_N
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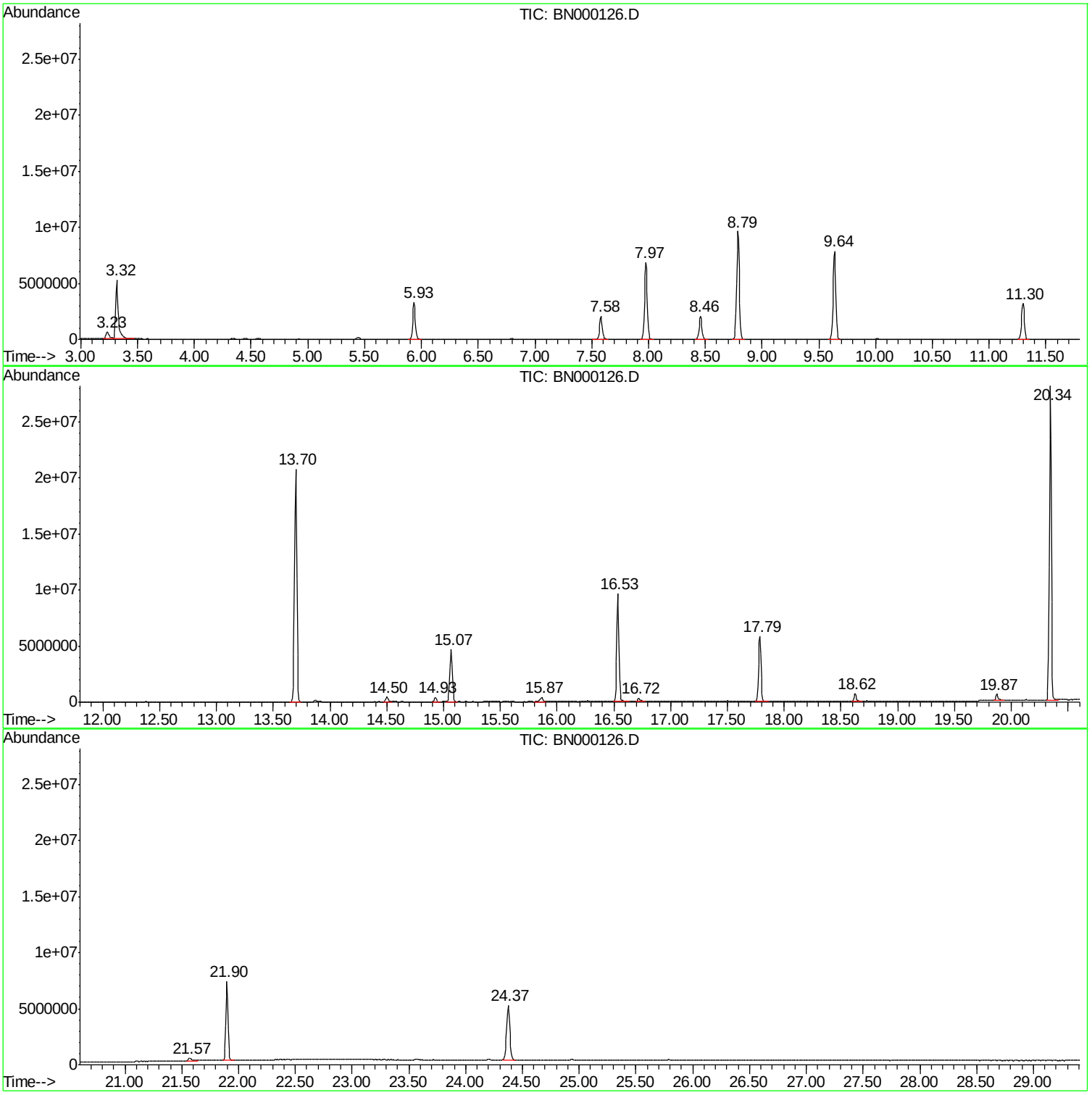
Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 16 Sample Multiplier: 1

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

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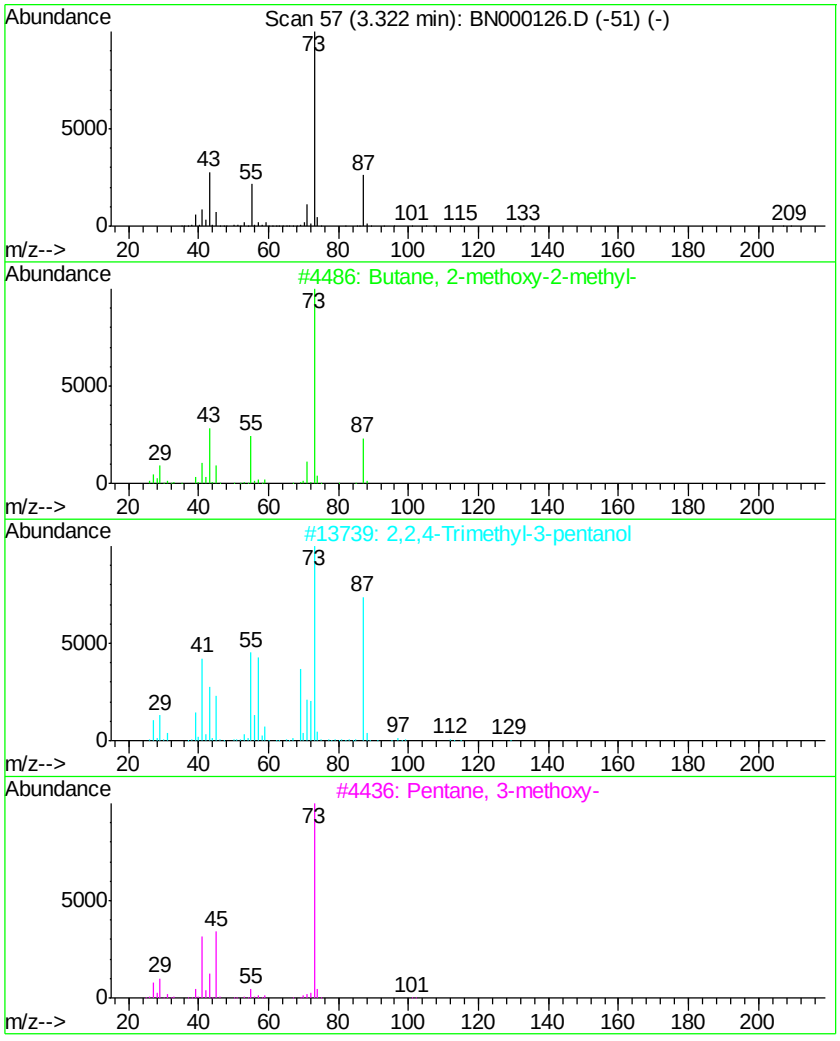
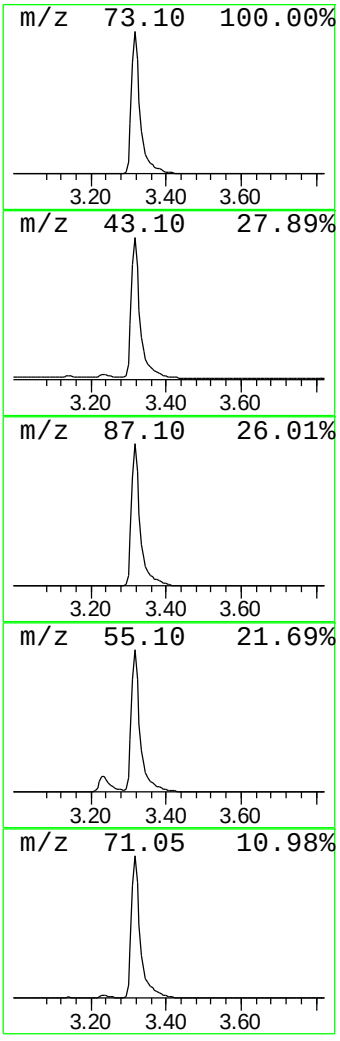
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.32 | 49.66 ng | 8714620 | 1,4-Dichlorobenzene-d4 | 8.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 43 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



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Sample : J1591-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_N
**ClientSampleId :** MH-28

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

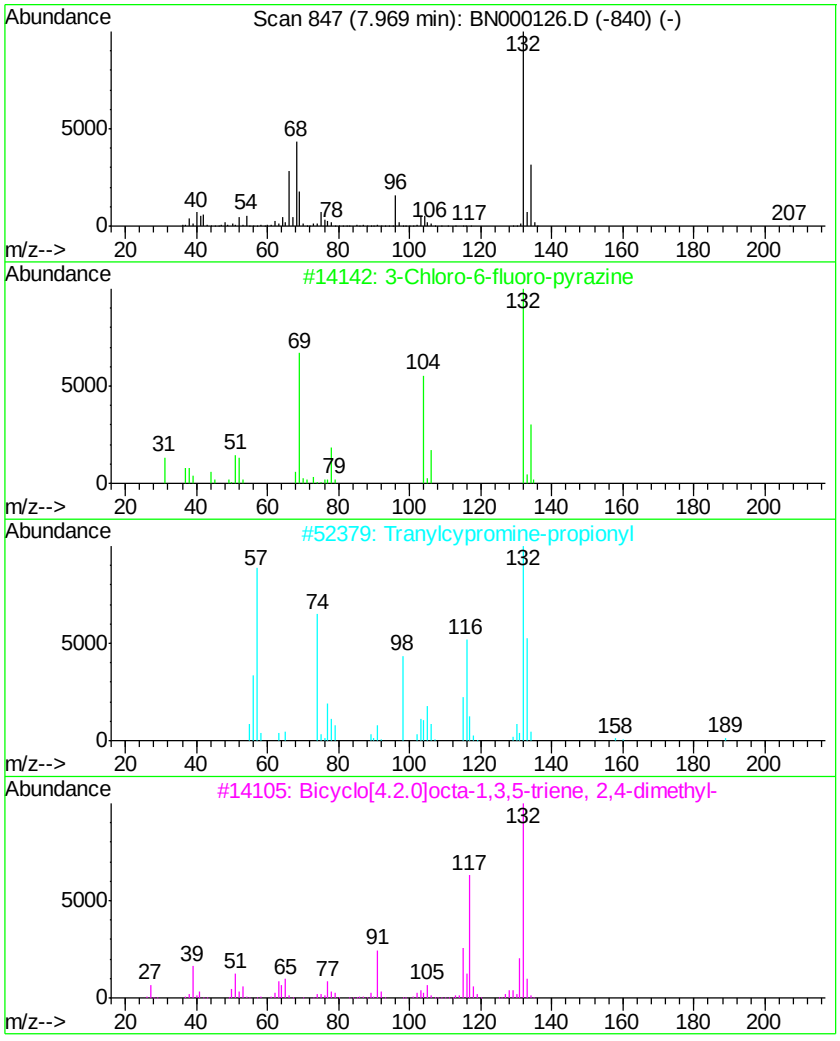
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

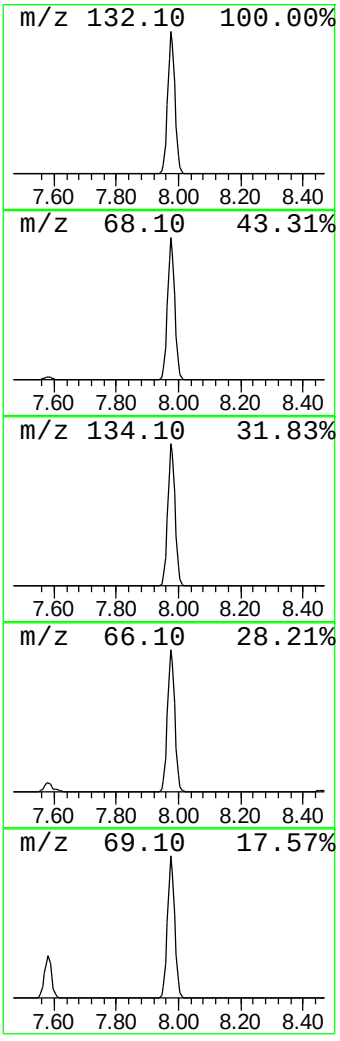
**********

Peak Number 3 unknown7.97 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.97 | 65.07 ng | 11420300 | 1,4-Dichlorobenzene-d4 | 8.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 4 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA N\DATA\BN021918\
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Acq On : 20 Feb 2018 00:30
Operator : JU/SJ
Sample : J1591-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_N
**ClientSampleId :** MH-28

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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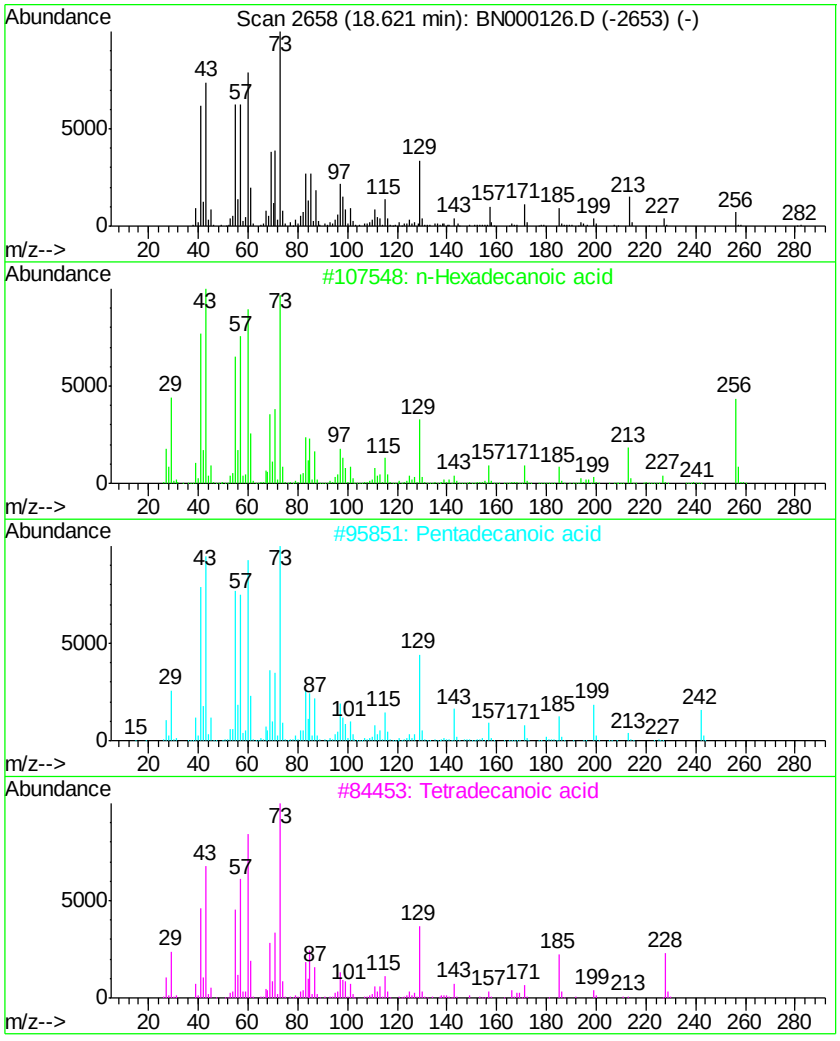
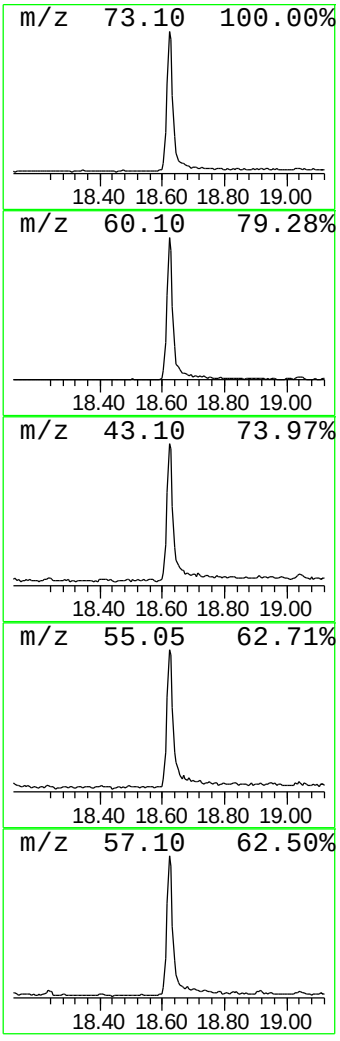
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.62 | 2.65 ng | 1109860 | Phenanthrene-d10 | 17.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 4 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 38 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 25 |



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Operator : JU/SJ
Sample : J1591-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_N
**ClientSampleId :** MH-28

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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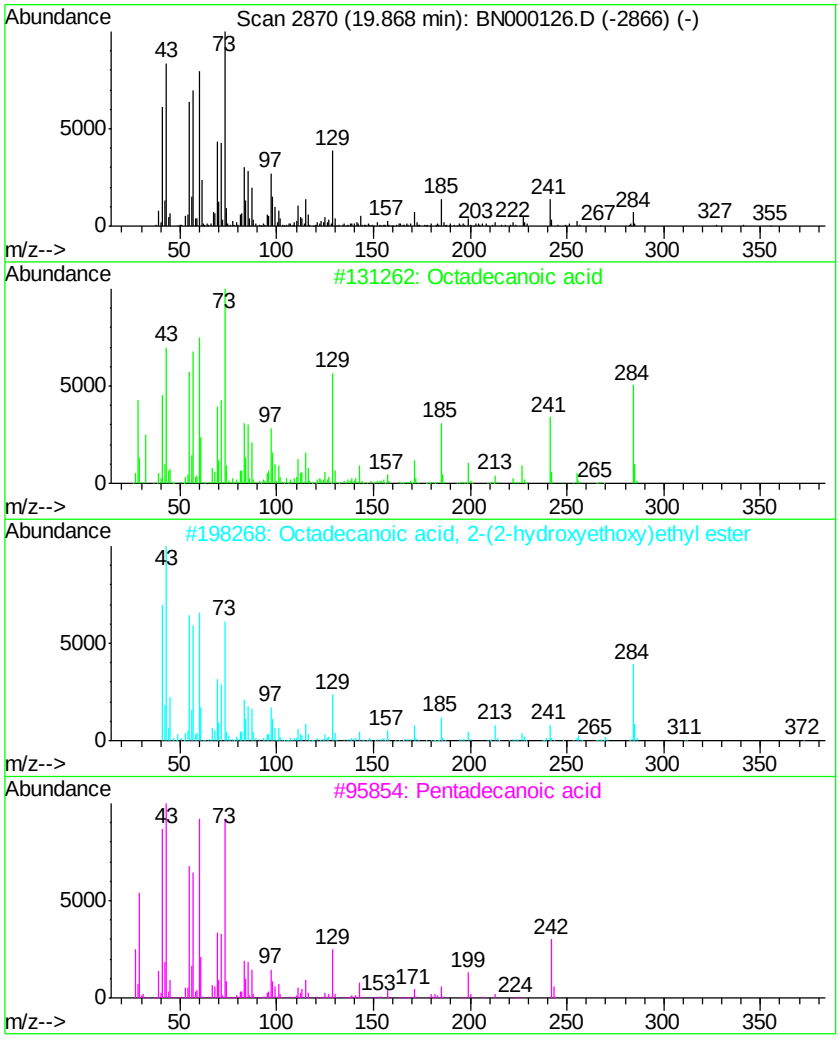
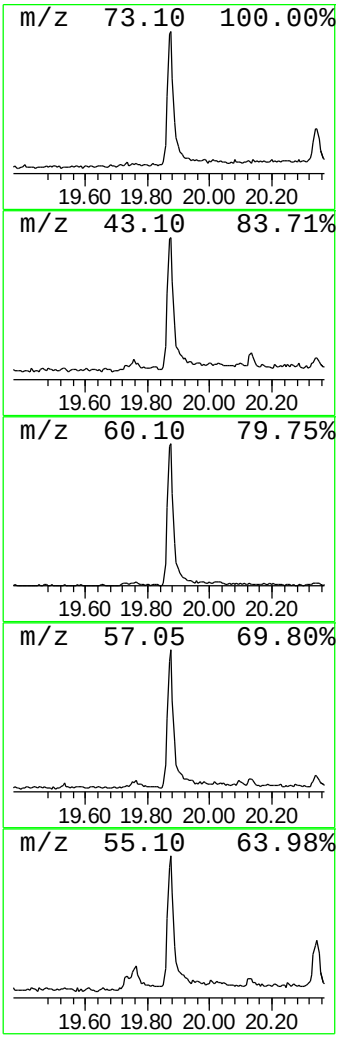
Peak Number 6 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.87 | 2.10 ng | 983176 | Chrysene-d12 | 21.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 91 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 68 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_N\DATA\BN021918\
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Sample : J1591-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_N
**ClientSampleId :**
MH-28

Quant Method : Z:\HPCHEM1\BNA_N\METHODS\8270-BN020718.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 |
| Butane, 2-methoxy... | 3.32 | 49.7 | ng | 8714620 | 1 | 8.46 | 3510040 | 20.0 |
| unknown7.97 | 7.97 | 65.1 | ng | 11420300 | 1 | 8.46 | 3510040 | 20.0 |
| n-Hexadecanoic acid | 18.62 | 2.6 | ng | 1109860 | 4 | 17.79 | 8390840 | 20.0 |
| Octadecanoic acid | 19.87 | 2.1 | ng | 983176 | 5 | 21.90 | 9349870 | 20.0 |