LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071724\
Data File : BM046698.D
Acq On : 18 Jul 2024 11:09
Operator : MA/JU
Sample : P3246-26
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
WC-CTW2-BL-06

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-BM071724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046698.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.363 | 60 | 64 | 69 | rBV | 41252 | 57305 | 1.77% | 0.351% |
| 2 | 4.687 | 283 | 289 | 294 | rBV | 46758 | 66956 | 2.07% | 0.410% |
| 3 | 5.134 | 359 | 365 | 373 | rBV | 903365 | 1265126 | 39.10% | 7.738% |
| 4 | 6.687 | 622 | 629 | 639 | rBV | 905100 | 1361062 | 42.06% | 8.325% |
| 5 | 7.487 | 758 | 765 | 772 | rBV | 304275 | 450861 | 13.93% | 2.758% |
| 6 | 8.628 | 952 | 959 | 967 | rBV | 606490 | 919556 | 28.42% | 5.624% |
| 7 | 10.245 | 1228 | 1234 | 1242 | rVB | 332999 | 551252 | 17.04% | 3.372% |
| 8 | 11.004 | 1357 | 1363 | 1369 | rBV2 | 28976 | 47401 | 1.46% | 0.290% |
| 9 | 12.745 | 1653 | 1659 | 1666 | rBV | 1393658 | 2040570 | 63.07% | 12.481% |
| 10 | 14.133 | 1887 | 1895 | 1903 | rVB | 533647 | 756895 | 23.39% | 4.629% |
| 11 | 14.386 | 1931 | 1938 | 1944 | rBV6 | 21001 | 47094 | 1.46% | 0.288% |
| 12 | 15.633 | 2143 | 2150 | 2159 | rBV | 1370946 | 1905972 | 58.91% | 11.658% |
| 13 | 16.886 | 2357 | 2363 | 2370 | rVB | 701039 | 951702 | 29.41% | 5.821% |
| 14 | 17.821 | 2516 | 2522 | 2528 | rBV | 116863 | 163074 | 5.04% | 0.997% |
| 15 | 19.115 | 2738 | 2742 | 2746 | rBV4 | 42276 | 58798 | 1.82% | 0.360% |
| 16 | 19.545 | 2809 | 2815 | 2821 | rBV | 2590803 | 3235661 | 100.00% | 19.791% |
| 17 | 20.856 | 3034 | 3038 | 3042 | rVB | 111990 | 142993 | 4.42% | 0.875% |
| 18 | 21.115 | 3077 | 3082 | 3087 | rBV | 840218 | 1108627 | 34.26% | 6.781% |
| 19 | 23.880 | 3544 | 3552 | 3561 | rVB | 534984 | 1218522 | 37.66% | 7.453% |

Sum of corrected areas: 16349427

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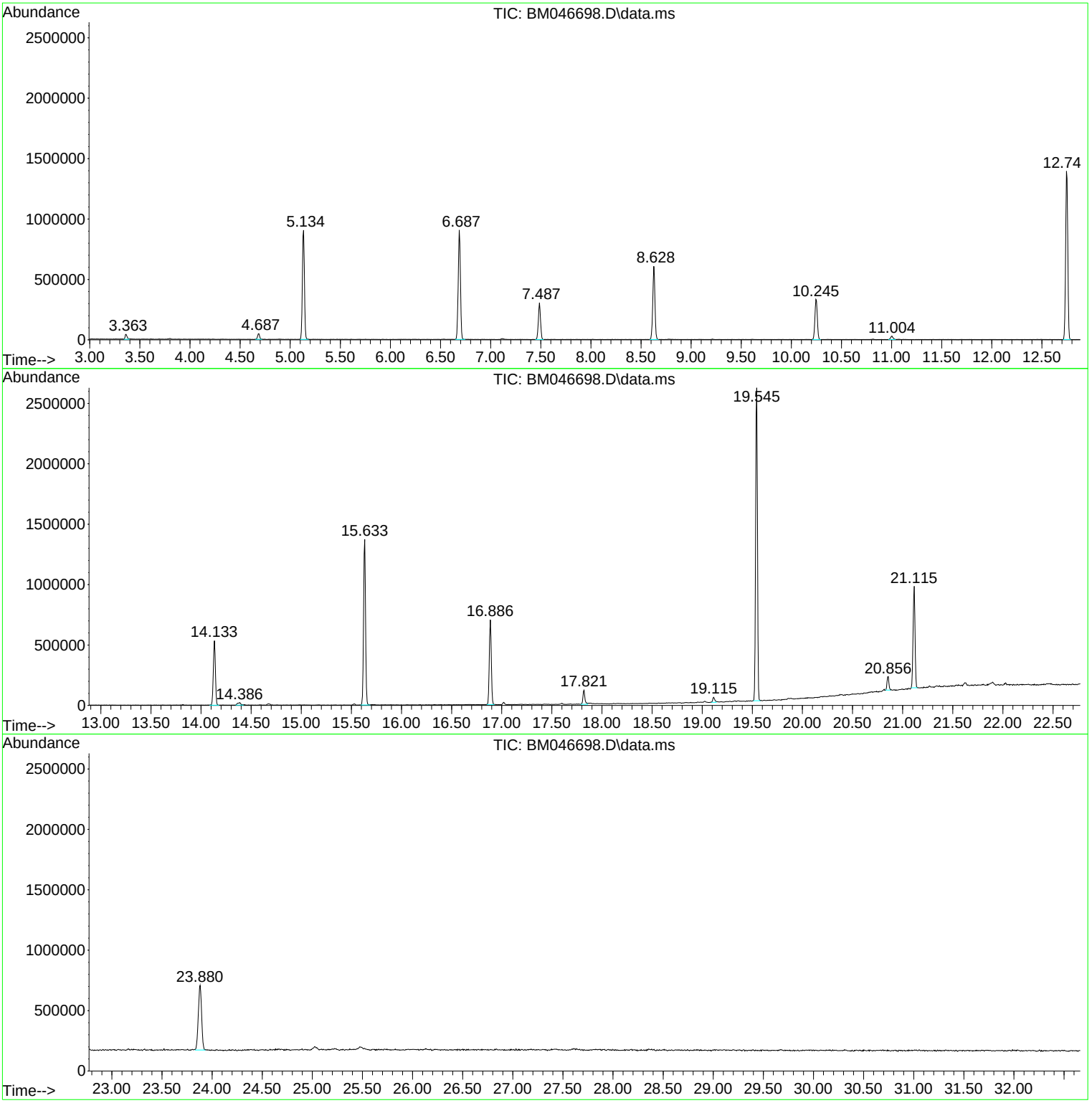
BNA_M
**ClientSampleId :**
WC-CTW2-BL-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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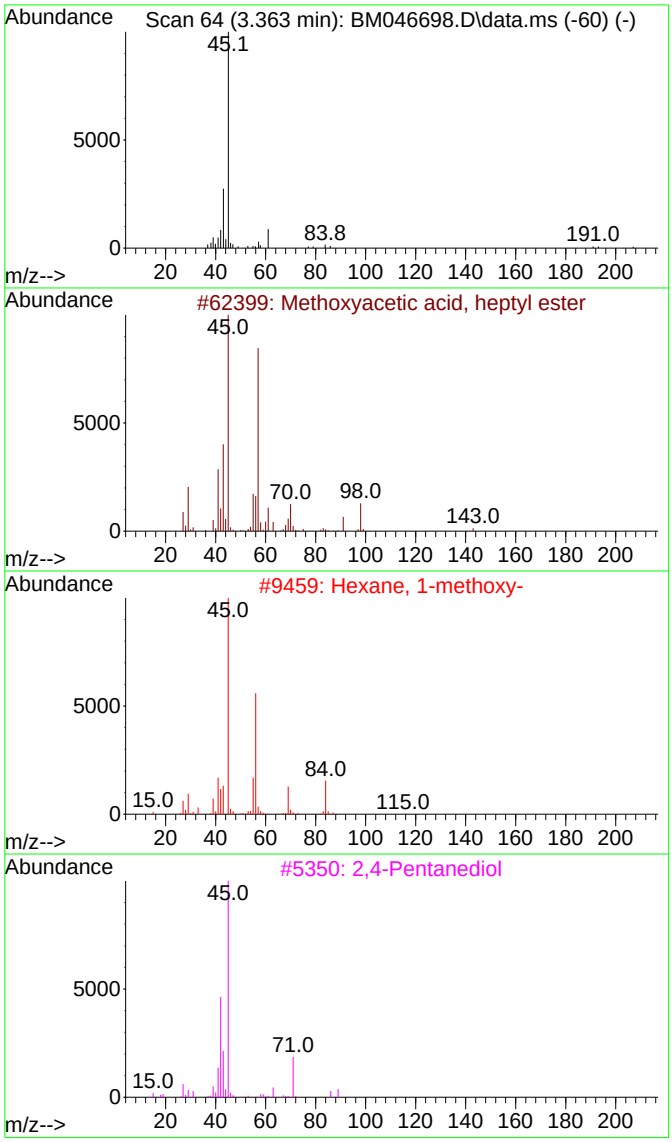
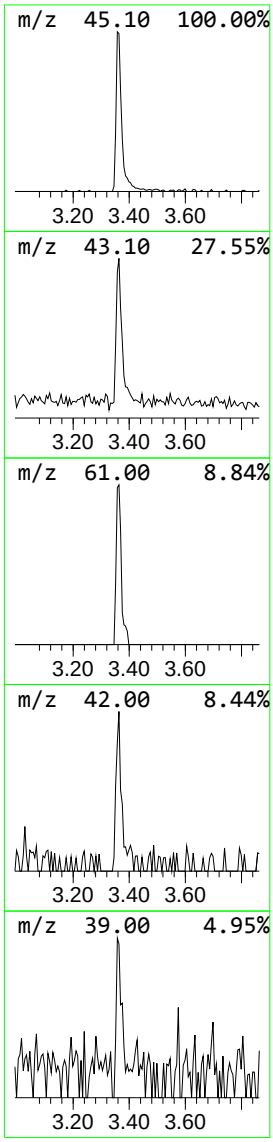
**********

Peak Number 1 unknown3.363 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.363 | 2.54 ng | 57305 | 1,4-Dichlorobenzene-d4 | 7.487 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methoxyacetic acid, heptyl ester | 188 | C10H20O3 | 168920-36-3 | 40 |
| 2 | Hexane, 1-methoxy- | 116 | C7H16O | 004747-07-3 | 39 |
| 3 | 2,4-Pentanediol | 104 | C5H12O2 | 000625-69-4 | 39 |
| 4 | 1-Butene, 4-methoxy | 86 | C5H10O | 004696-30-4 | 9 |
| 5 | Isoamyl lactate | 160 | C8H16O3 | 019329-89-6 | 9 |



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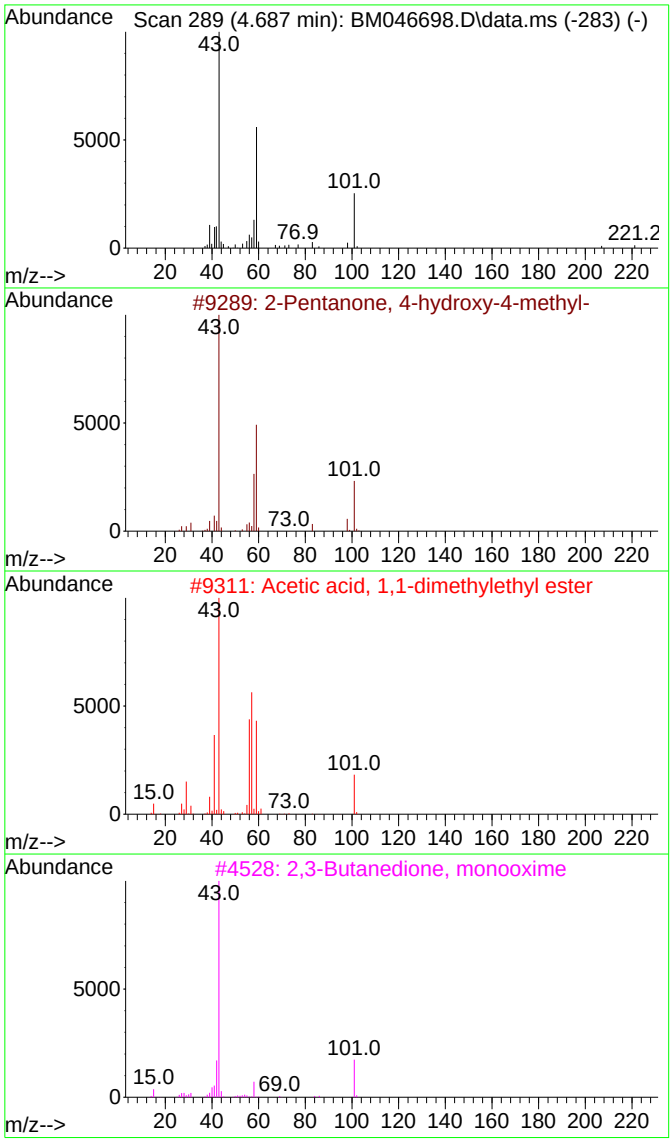
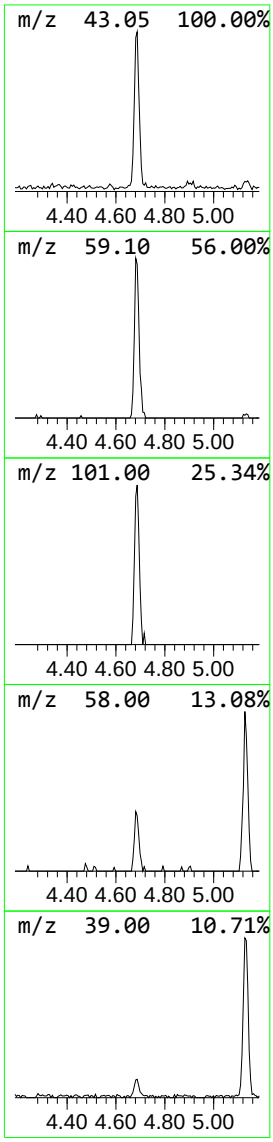
**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.687 | 2.97 ng | 66956 | 1,4-Dichlorobenzene-d4 | 7.487 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 4 | 2-Nonanone, 9-hydroxy- | 158 | C9H18O2 | 025368-56-3 | 28 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 23 |



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ALS Vial : 38 Sample Multiplier: 1

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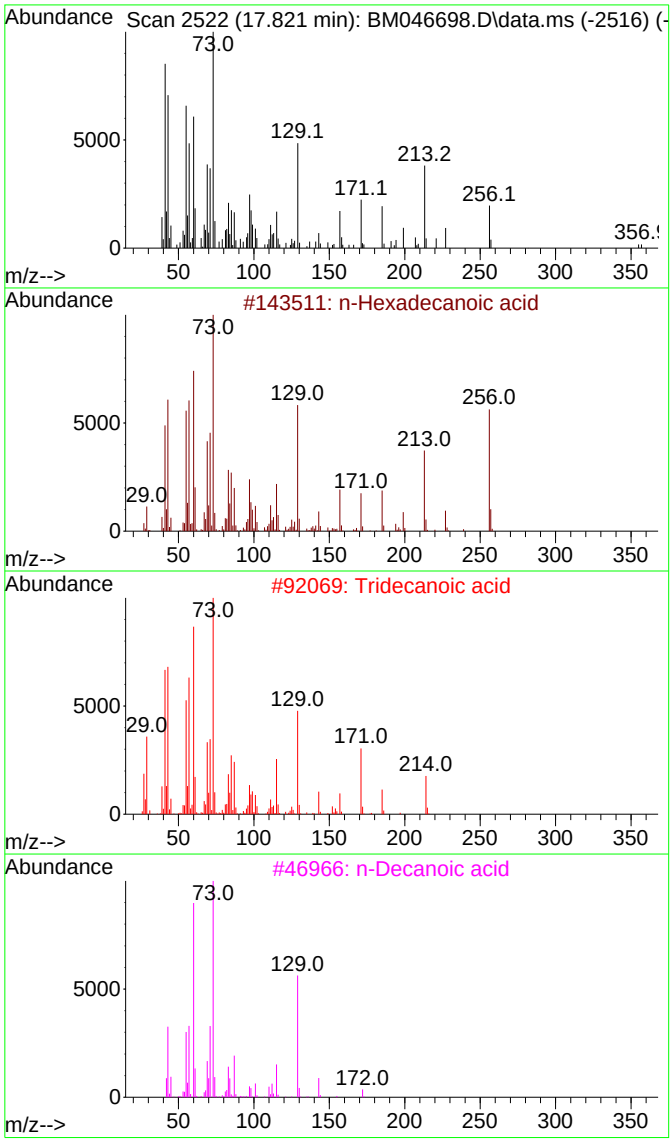
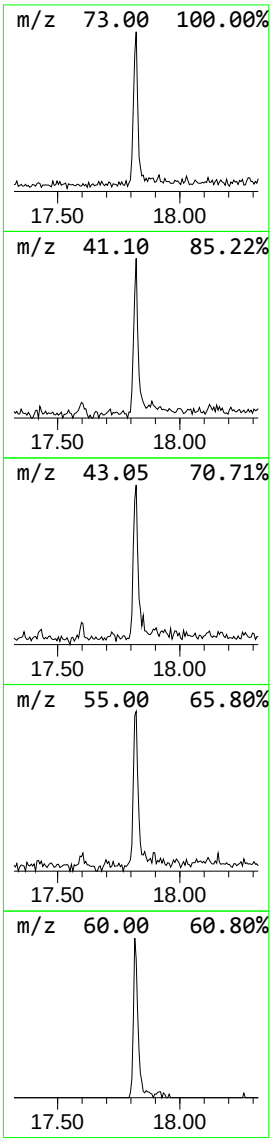
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.821 | 3.43 ng | 163074 | Phenanthrene-d10 | 16.886 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 46 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 42 |
| 4 | 3,7-Dimethyl-8-oxo-1,5-dioxa-spi... | 256 | C13H20O5 | 1000193-79-8 | 41 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 35 |



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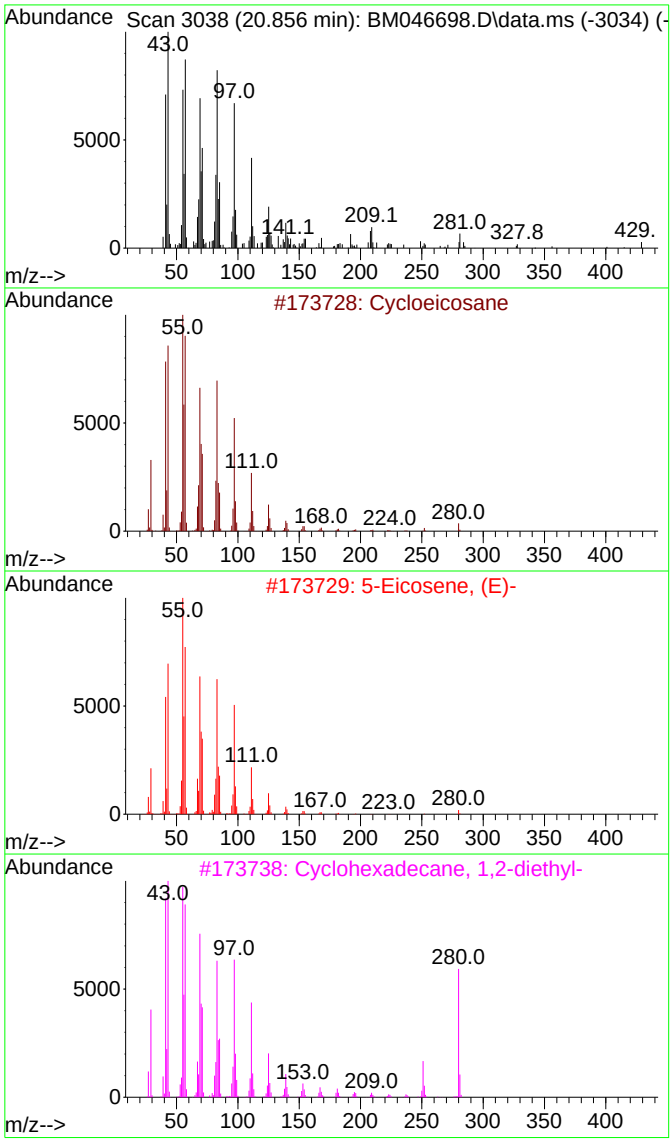
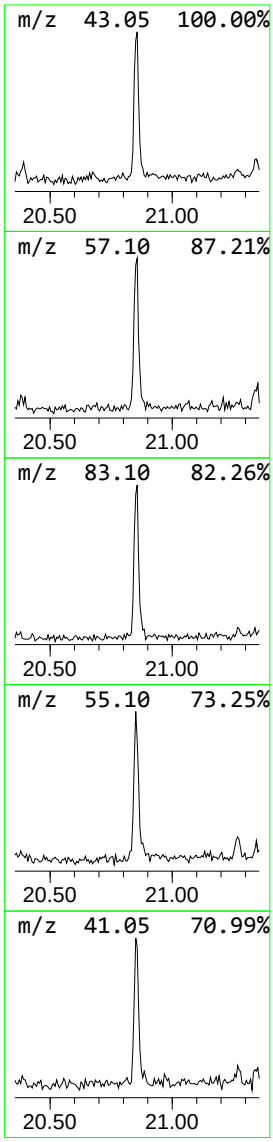
Peak Number 4 Cycloeicosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.856 | 2.58 ng | 142993 | Chrysene-d12 | 21.115 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 98 |
| 2 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 97 |
| 3 | Cyclohexadecane, 1,2-diethyl- | 280 | C20H40 | 1000155-85-3 | 95 |
| 4 | 1-Eicosene | 280 | C20H40 | 003452-07-1 | 93 |
| 5 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 93 |



Tentatively Identified Compound (LSC) summary

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Misc :
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BNA_M
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| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown3.363 | 3.363 | 2.5 | ng | 57305 | 1 | 7.487 | 450861 | 20.0 |
| 2-Pentanone, 4-... | 4.687 | 3.0 | ng | 66956 | 1 | 7.487 | 450861 | 20.0 |
| n-Hexadecanoic ... | 17.821 | 3.4 | ng | 163074 | 4 | 16.886 | 951702 | 20.0 |
| Cycloeicosane | 20.856 | 2.6 | ng | 142993 | 5 | 21.115 | 1108630 | 20.0 |