LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031221\
Data File : BM029117.D
Acq On : 12 Mar 2021 18:44
Operator : CG/JU
Sample : M1625-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SP-1-2

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029117.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.199 | 371 | 376 | 392 | rBB | 147657 | 213786 | 68.29% | 11.268% |
| 2 | 6.816 | 646 | 651 | 668 | rBB | 139435 | 222363 | 71.03% | 11.720% |
| 3 | 7.622 | 783 | 788 | 795 | rBB | 30638 | 44796 | 14.31% | 2.361% |
| 4 | 8.792 | 981 | 987 | 1000 | rBB | 86348 | 139492 | 44.56% | 7.352% |
| 5 | 10.410 | 1256 | 1262 | 1271 | rBB | 37893 | 59528 | 19.02% | 3.138% |
| 6 | 12.898 | 1680 | 1685 | 1694 | rBB | 188180 | 268313 | 85.71% | 14.142% |
| 7 | 14.292 | 1917 | 1922 | 1928 | rBB | 51045 | 70395 | 22.49% | 3.710% |
| 8 | 15.792 | 2172 | 2177 | 2184 | rBB | 144137 | 189659 | 60.59% | 9.996% |
| 9 | 17.039 | 2384 | 2389 | 2396 | rBB | 57259 | 75749 | 24.20% | 3.992% |
| 10 | 17.939 | 2537 | 2542 | 2550 | rBV | 19369 | 29257 | 9.35% | 1.542% |
| 11 | 19.221 | 2753 | 2760 | 2773 | rBV | 35255 | 56456 | 18.03% | 2.976% |
| 12 | 19.668 | 2831 | 2836 | 2841 | rBV | 273558 | 313046 | 100.00% | 16.500% |
| 13 | 20.945 | 3048 | 3053 | 3062 | rBV | 24062 | 42857 | 13.69% | 2.259% |
| 14 | 21.221 | 3095 | 3100 | 3107 | rBV | 71012 | 84171 | 26.89% | 4.436% |
| 15 | 23.356 | 3458 | 3463 | 3470 | rVB | 52749 | 87418 | 27.92% | 4.608% |

Sum of corrected areas: 1897286

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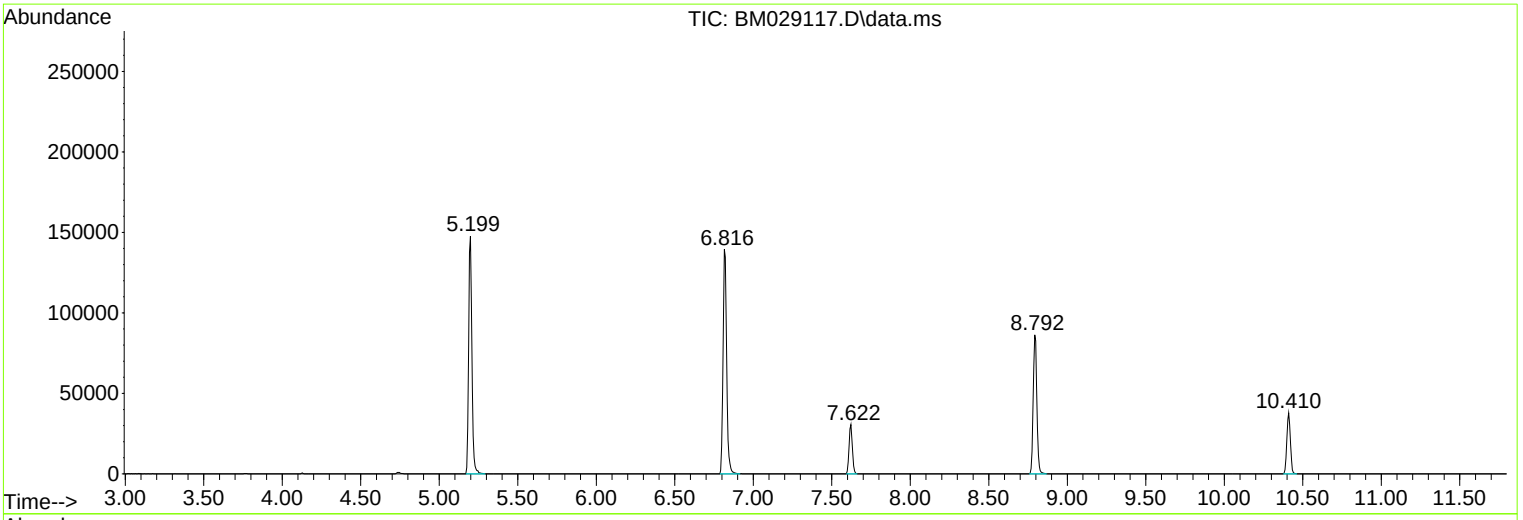
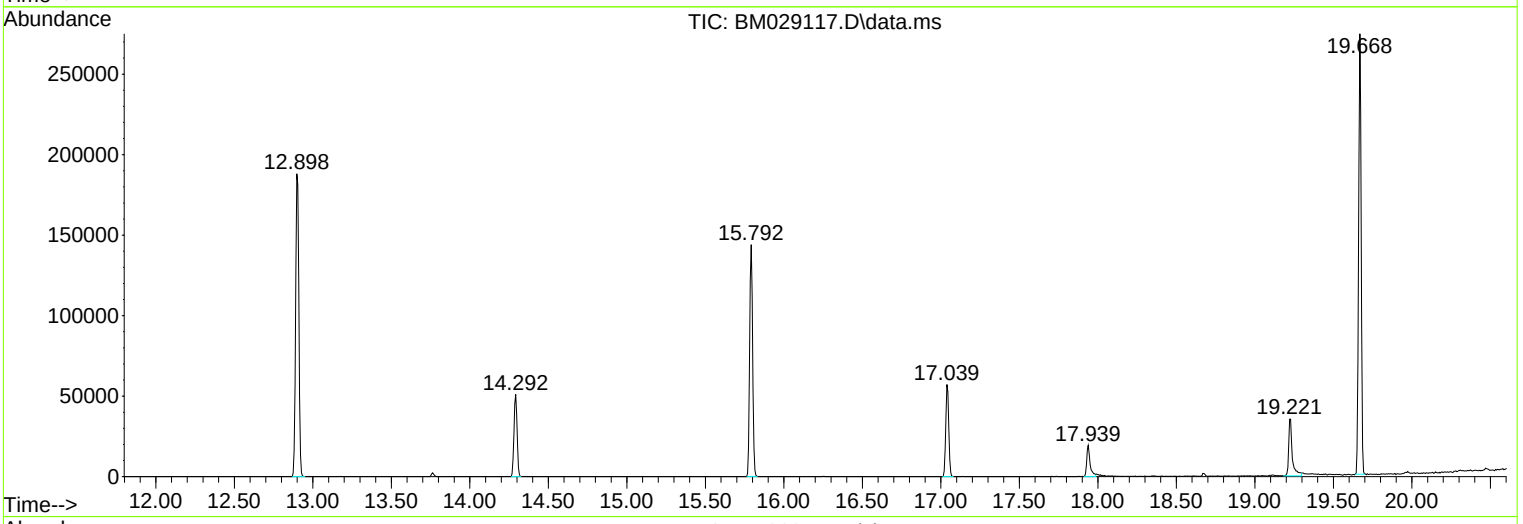
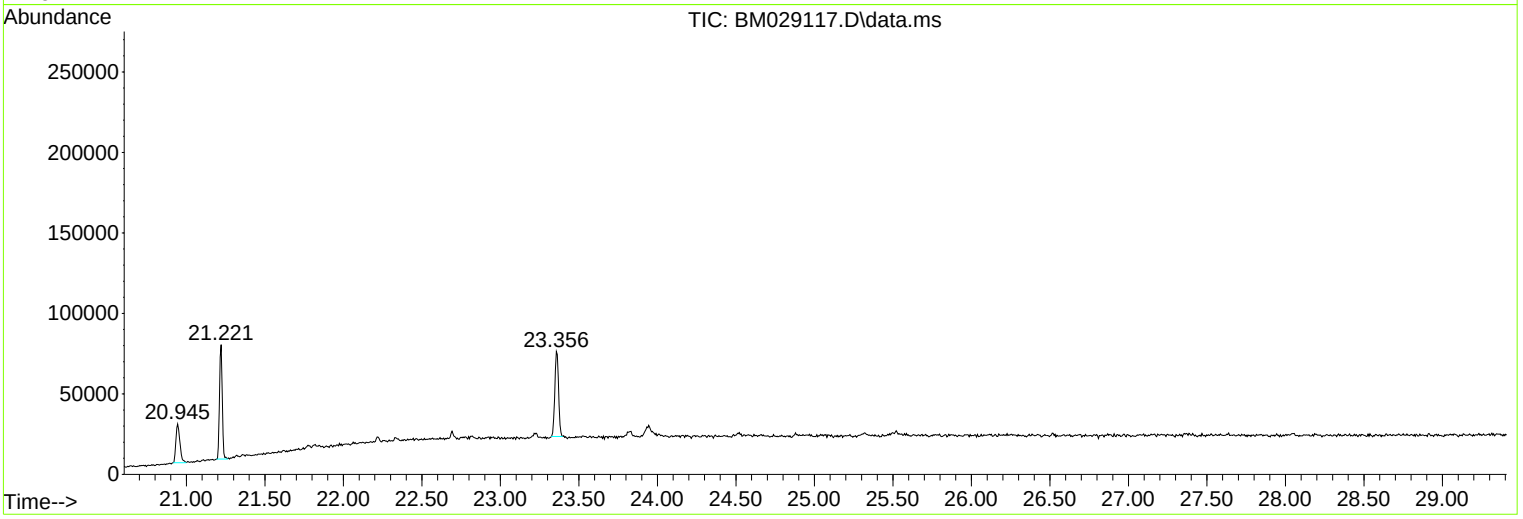
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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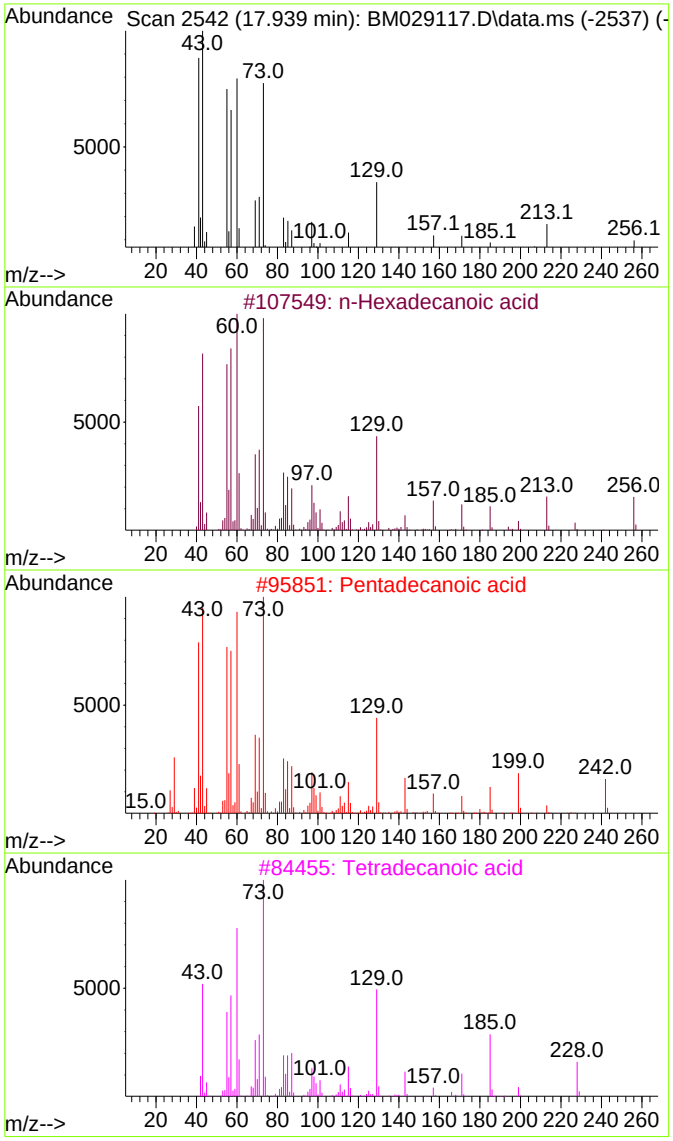
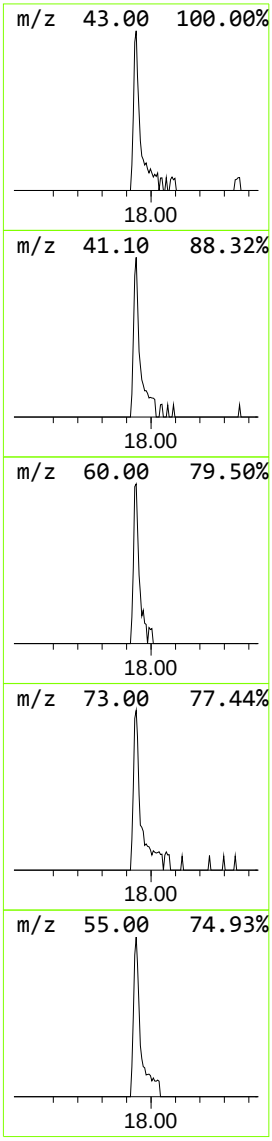
Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.939 | 7.72 ng | 29257 | Phenanthrene-d10 | 17.039 |

| 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 | 87 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 80 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 64 |



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Sample : M1625-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SP-1-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

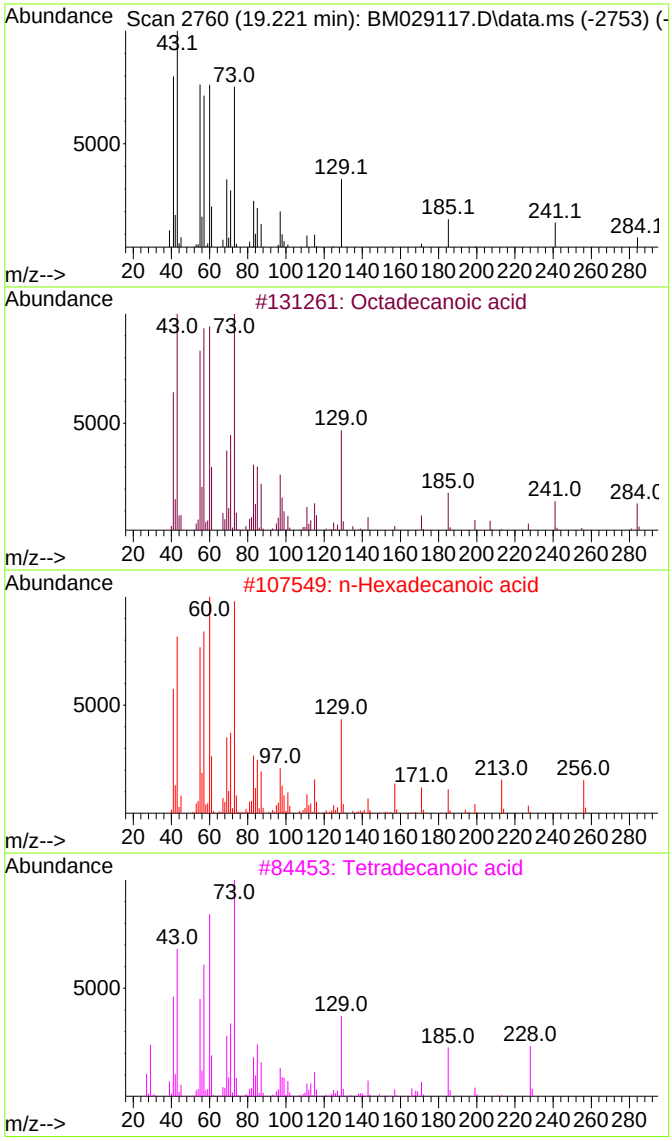
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

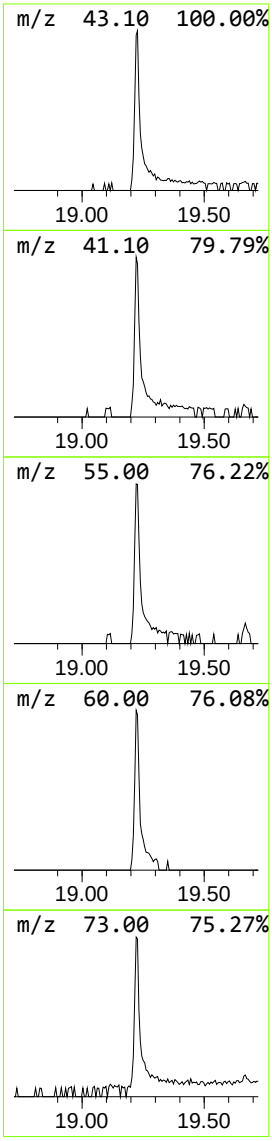
**********

Peak Number 2 Octadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.221 | 13.41 ng | 56456 | Chrysene-d12 | 21.221 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



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Operator : CG/JU
Sample : M1625-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SP-1-2

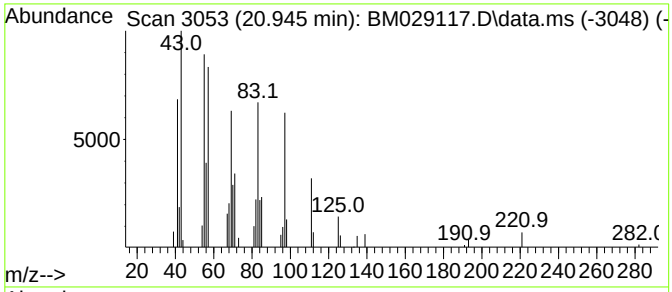
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

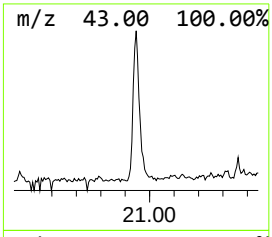
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

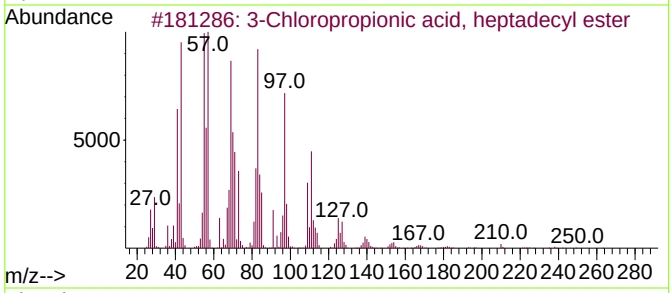
**********
Peak Number 3 3-Chloropropionic acid, hep... Concentration Rank 2

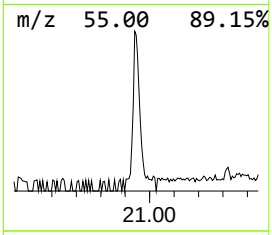
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.945 | 10.18 ng | 42857 | Chrysene-d12 | 21.221 |

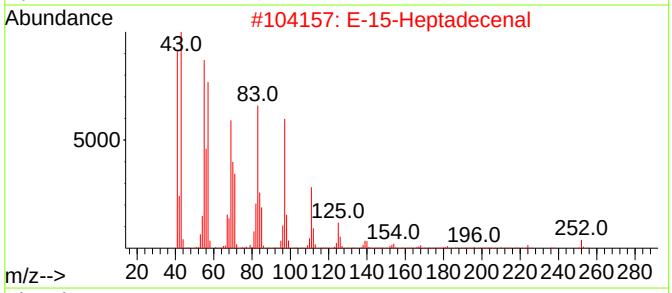
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 91 |
| 2 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 91 |
| 3 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 4 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 5 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |

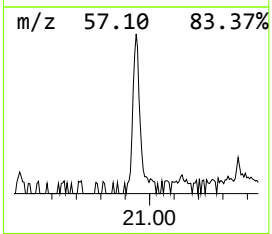


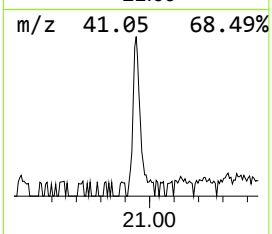



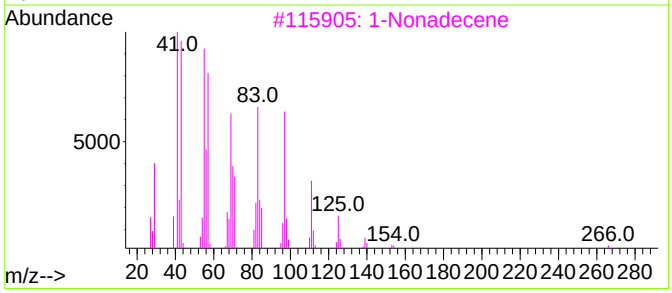



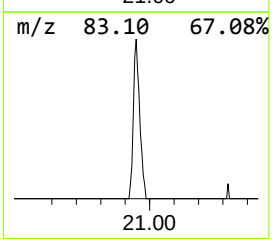



Tentatively Identified Compound (LSC) summary

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Misc :
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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| n-Hexadecanoic ... | 17.939 | 7.7 | ng | 29257 | 4 | 17.039 | 75749 | 20.0 |
| Octadecanoic acid | 19.221 | 13.4 | ng | 56456 | 5 | 21.221 | 84171 | 20.0 |
| 3-Chloropropion... | 20.945 | 10.2 | ng | 42857 | 5 | 21.221 | 84171 | 20.0 |