LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046814.D
Acq On : 8 Oct 2020 14:06
Operator : CG/JU
Sample : L4293-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B-2-MW-1

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_G\METHODS\8270-BG092220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046814.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.667 | 389 | 396 | 406 | rBV | 613330 | 997111 | 16.72% | 4.175% |
| 2 | 7.254 | 659 | 666 | 677 | rBV | 395033 | 678272 | 11.38% | 2.840% |
| 3 | 8.106 | 801 | 811 | 818 | rBV | 279450 | 484380 | 8.12% | 2.028% |
| 4 | 9.269 | 1001 | 1009 | 1019 | rVB | 986808 | 1720452 | 28.85% | 7.204% |
| 5 | 10.920 | 1280 | 1290 | 1297 | rBV | 352865 | 668639 | 11.21% | 2.800% |
| 6 | 13.358 | 1697 | 1705 | 1711 | rBV | 2308618 | 3619978 | 60.71% | 15.159% |
| 7 | 13.564 | 1734 | 1740 | 1745 | rBV | 128204 | 202774 | 3.40% | 0.849% |
| 8 | 13.617 | 1745 | 1749 | 1755 | rVB | 55812 | 84053 | 1.41% | 0.352% |
| 9 | 14.175 | 1838 | 1844 | 1848 | rBV | 75481 | 118153 | 1.98% | 0.495% |
| 10 | 14.727 | 1932 | 1938 | 1946 | rBV2 | 564732 | 950727 | 15.94% | 3.981% |
| 11 | 16.214 | 2184 | 2191 | 2199 | rBV | 1936414 | 3008931 | 50.46% | 12.600% |
| 12 | 16.449 | 2225 | 2231 | 2240 | rVB4 | 48369 | 101763 | 1.71% | 0.426% |
| 13 | 17.471 | 2399 | 2405 | 2415 | rBV | 723512 | 1096769 | 18.39% | 4.593% |
| 14 | 18.358 | 2550 | 2556 | 2564 | rBV | 409174 | 633526 | 10.62% | 2.653% |
| 15 | 19.622 | 2767 | 2771 | 2781 | rBV | 299715 | 424523 | 7.12% | 1.778% |
| 16 | 20.080 | 2843 | 2849 | 2854 | rBV | 4610362 | 5962731 | 100.00% | 24.969% |
| 17 | 21.396 | 3068 | 3073 | 3082 | rVB2 | 147706 | 294171 | 4.93% | 1.232% |
| 18 | 21.749 | 3126 | 3133 | 3139 | rBV | 873600 | 1423303 | 23.87% | 5.960% |
| 19 | 25.015 | 3679 | 3689 | 3700 | rBV | 495298 | 1410198 | 23.65% | 5.905% |

Sum of corrected areas: 23880454

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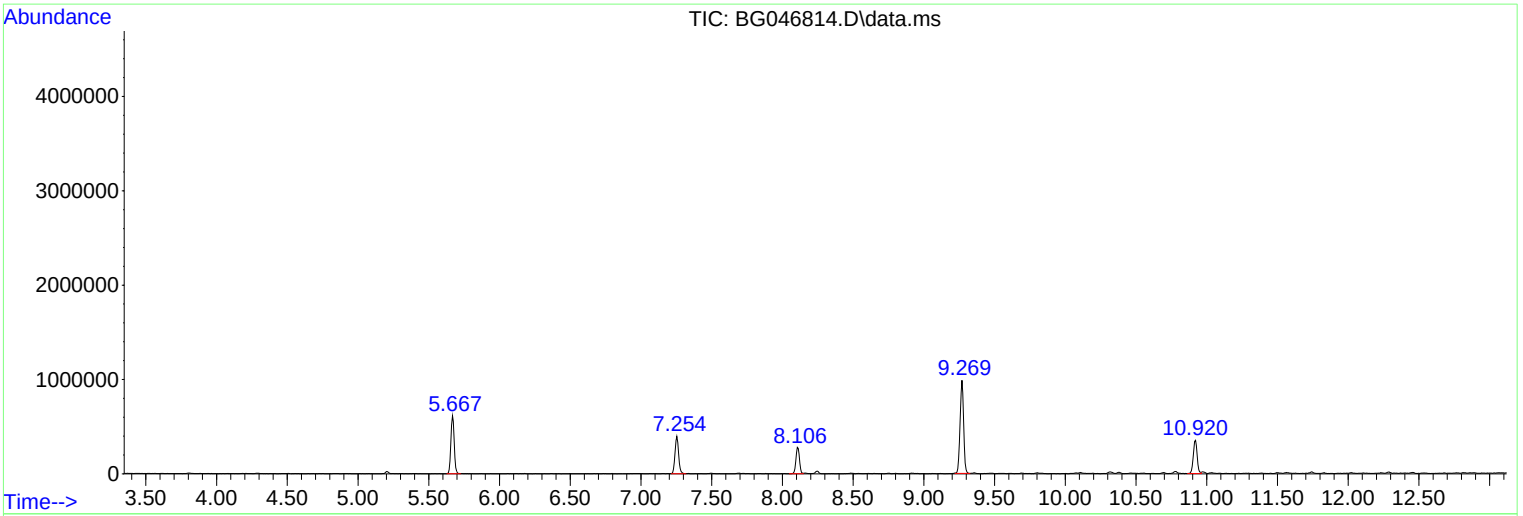
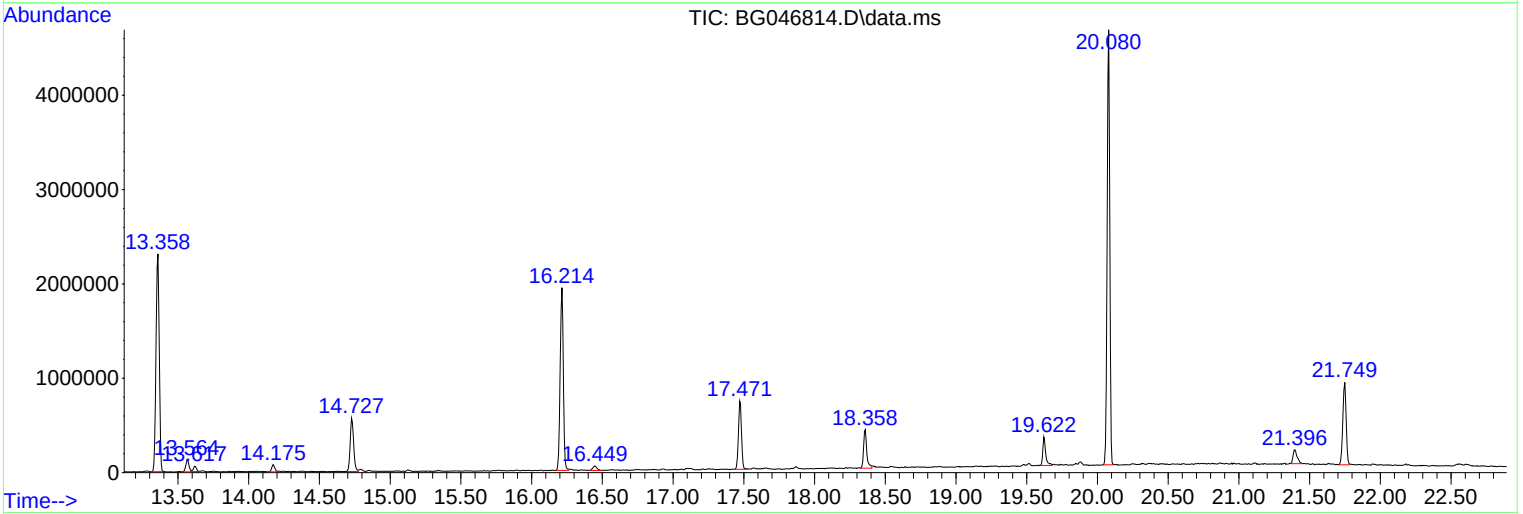
Misc :
ALS Vial : 5 Sample Multiplier: 1

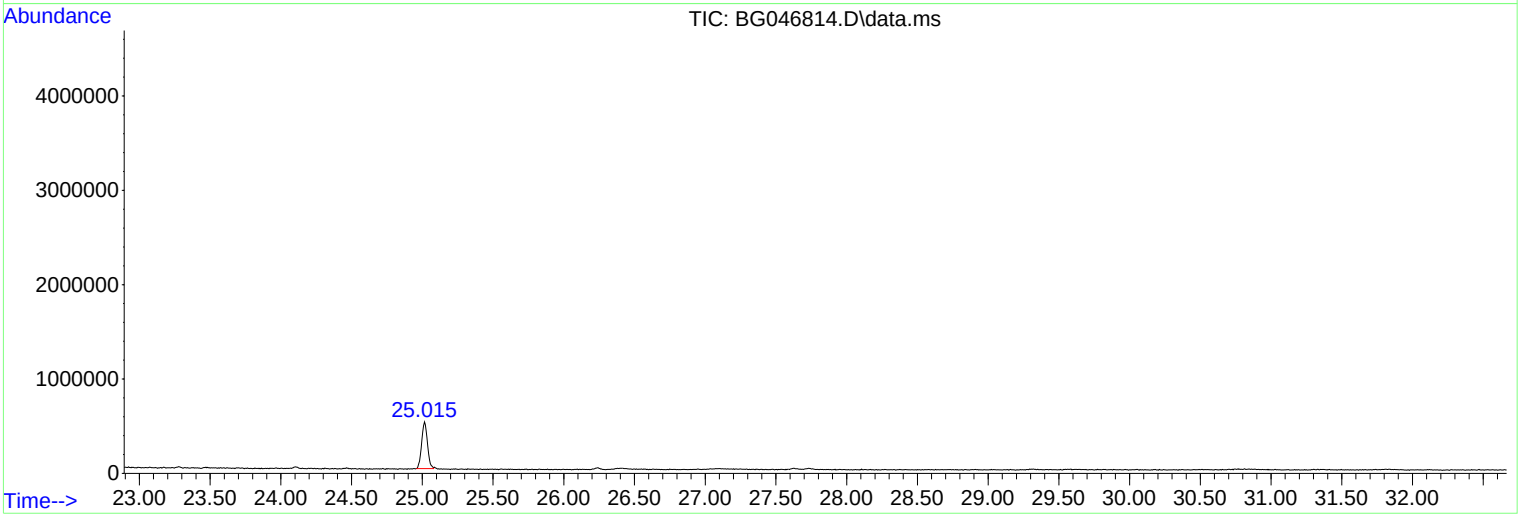
**Instrument :**
BNA_G
**ClientSampleId :**
B-2-MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.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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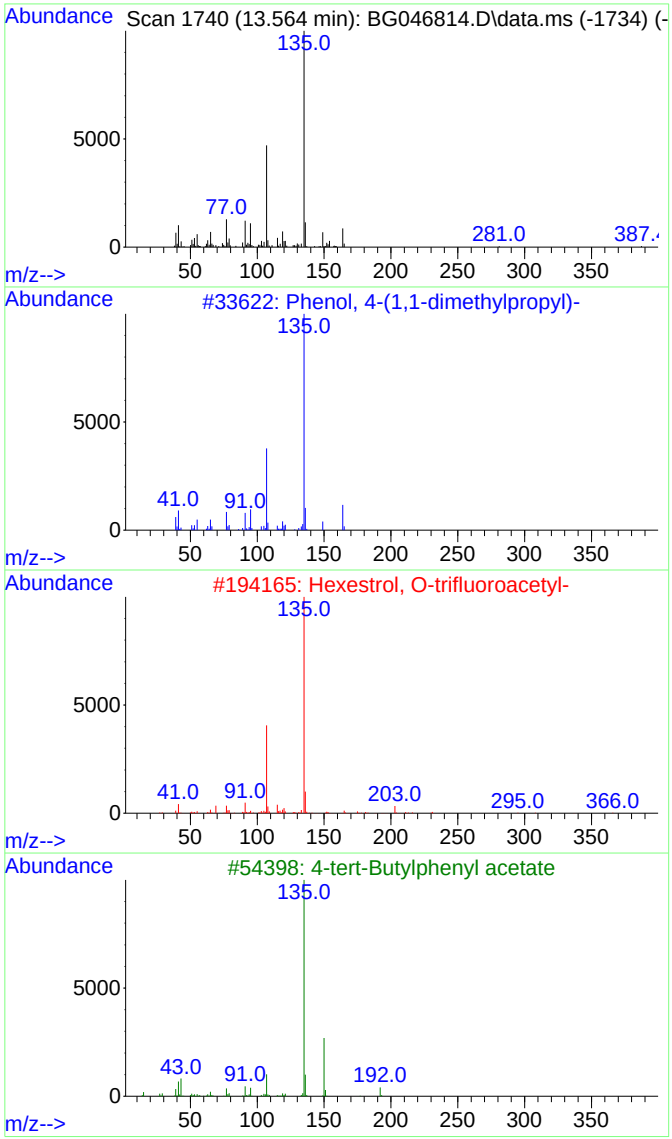
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

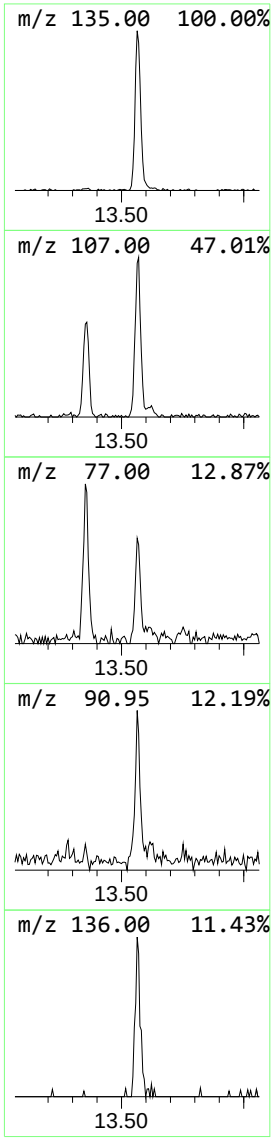
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.564 | 4.27 ng | 202774 | Acenaphthene-d10 | 14.727 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4-(1,1-dimethylpropyl)- | 164 | C11H16O | 000080-46-6 | 87 |
| 2 | Hexestrol, O-trifluoroacetyl- | 366 | C20H21F3O3 | 1000365-31-7 | 64 |
| 3 | 4-tert-Butylphenyl acetate | 192 | C12H16O2 | 003056-64-2 | 64 |
| 4 | Hexestrol | 270 | C18H22O2 | 000084-16-2 | 64 |
| 5 | Hexestrol | 270 | C18H22O2 | 005635-50-7 | 59 |



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Sample : L4293-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B-2-MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

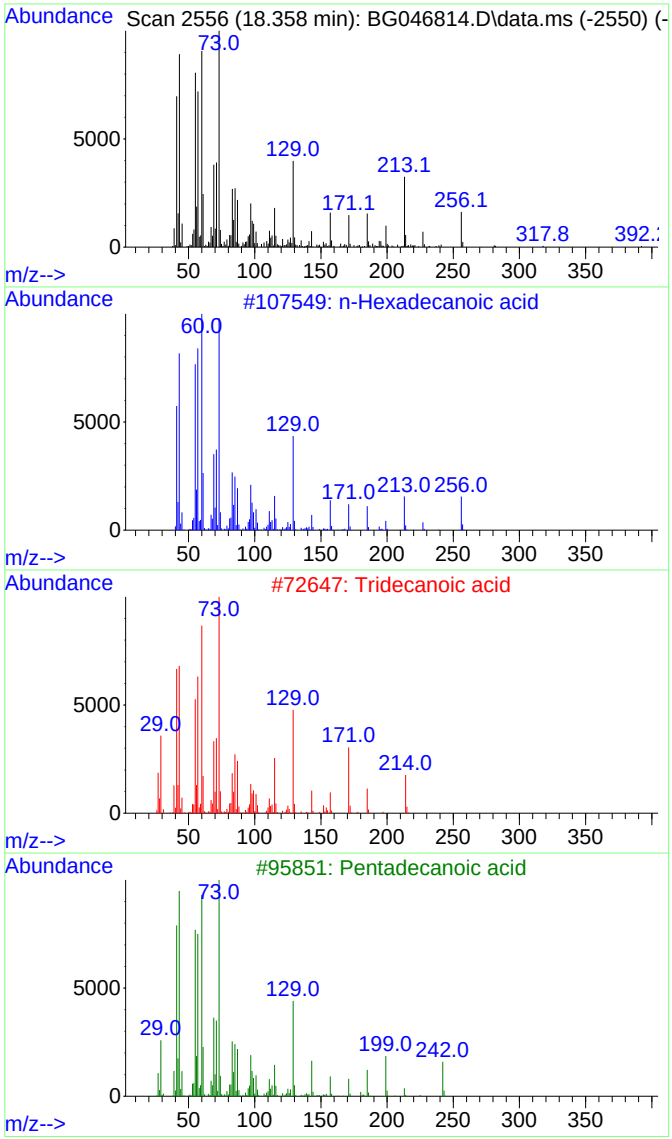
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

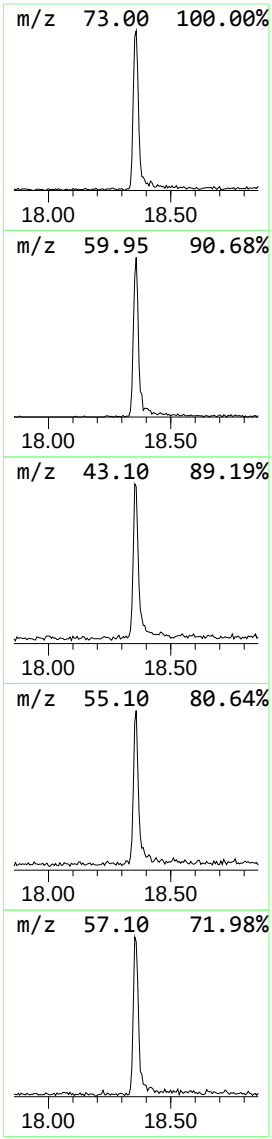
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.358 | 11.55 ng | 633526 | Phenanthrene-d10 | 17.471 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 97 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 74 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
Data File : BG046814.D
Acq On : 8 Oct 2020 14:06
Operator : CG/JU
Sample : L4293-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
B-2-MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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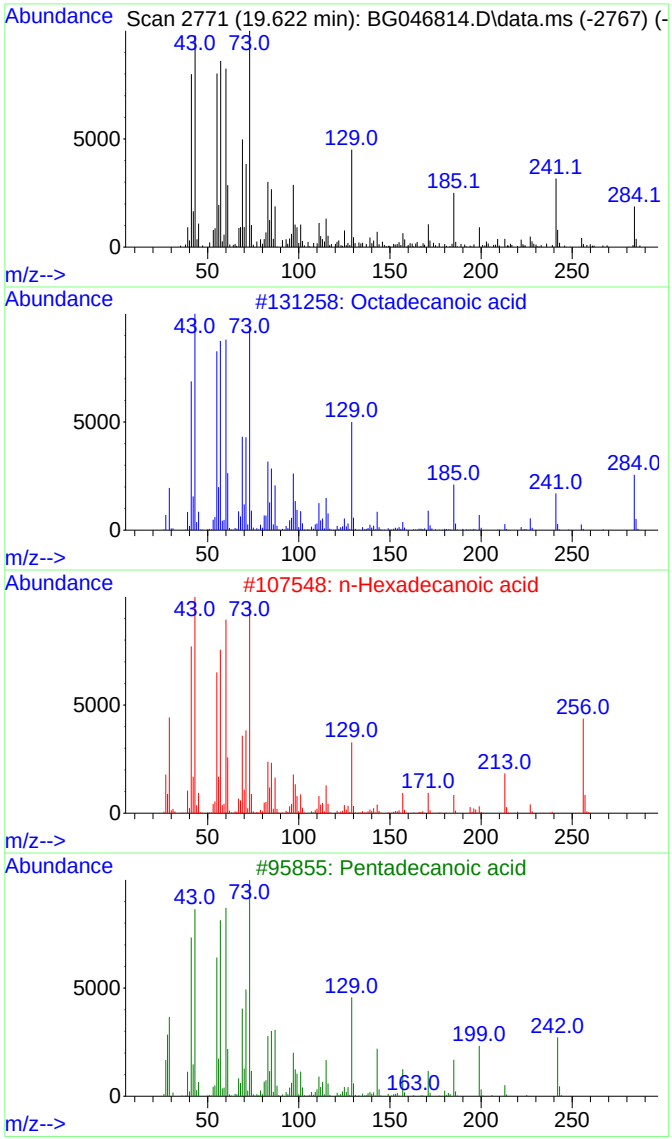
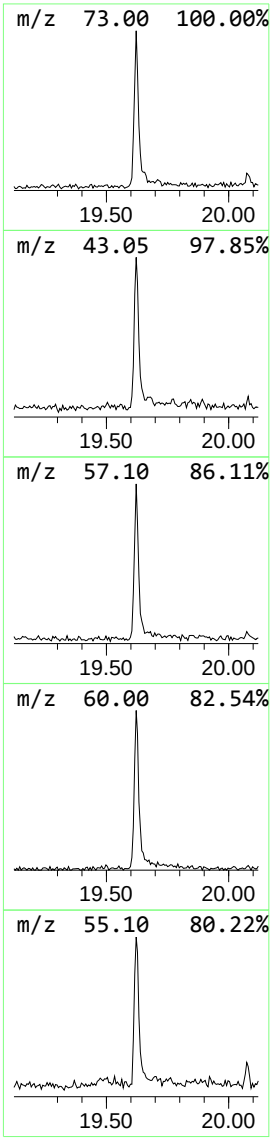
Peak Number 3 Octadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.622 | 5.97 ng | 424523 | Chrysene-d12 | 21.749 |

| 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 | 90 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 83 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 74 |



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Data File : BG046814.D
Acq On : 8 Oct 2020 14:06
Operator : CG/JU
Sample : L4293-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
B-2-MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
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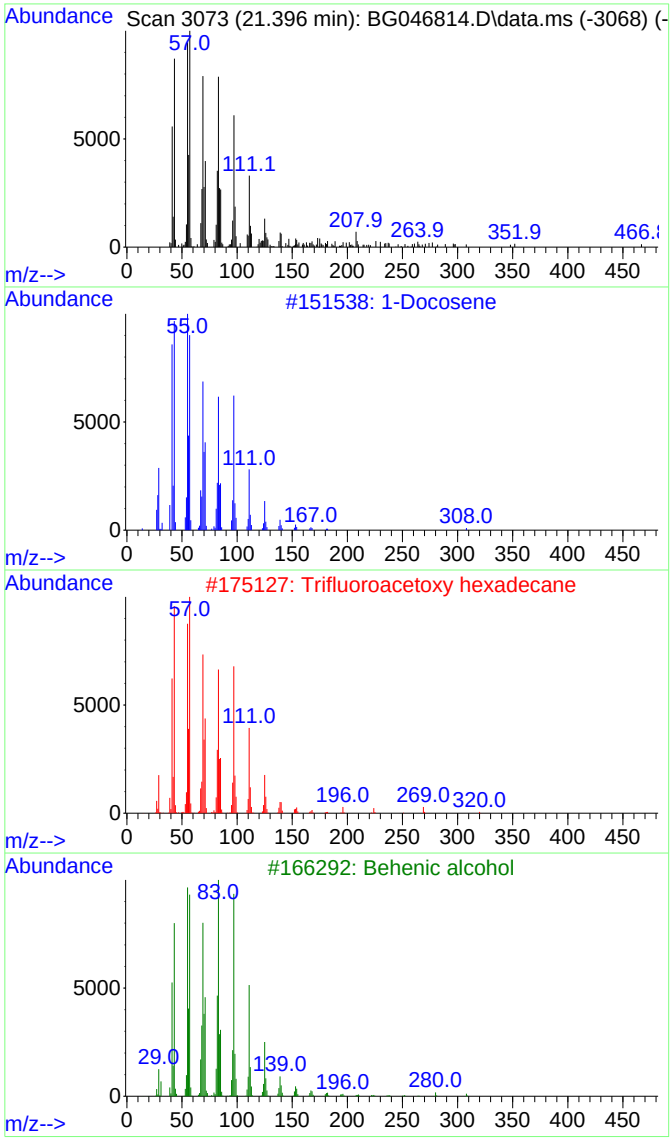
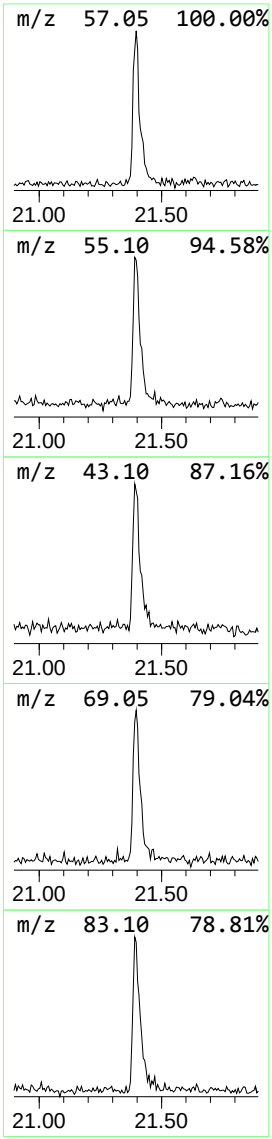
Peak Number 4 1-Docosene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.396 | 4.13 ng | 294171 | Chrysene-d12 | 21.749 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 95 |
| 2 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 93 |
| 3 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 91 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |
| 5 | Acetic acid, chloro-, octadecyl ... | 346 | C20H39ClO2 | 005348-82-3 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100820\
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Acq On : 8 Oct 2020 14:06
Operator : CG/JU
Sample : L4293-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B-2-MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.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 |
| Phenol, 4-(1,1-... | 13.564 | 4.3 | ng | 202774 | 3 | 14.727 | 950727 | 20.0 |
| n-Hexadecanoic ... | 18.358 | 11.6 | ng | 633526 | 4 | 17.471 | 1096770 | 20.0 |
| Octadecanoic acid | 19.622 | 6.0 | ng | 424523 | 5 | 21.749 | 1423300 | 20.0 |
| 1-Docosene | 21.396 | 4.1 | ng | 294171 | 5 | 21.749 | 1423300 | 20.0 |