LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035254.D
Acq On : 25 May 2022 22:46
Operator : CG/JU
Sample : N2895-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
P030-SS001-1218-01

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-BM042722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035254.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.469 | 399 | 405 | 416 | rBV | 1526256 | 2252066 | 41.80% | 7.823% |
| 2 | 7.057 | 668 | 675 | 700 | rBV | 1441288 | 2348559 | 43.59% | 8.159% |
| 3 | 7.887 | 809 | 816 | 824 | rBV | 412905 | 653023 | 12.12% | 2.269% |
| 4 | 9.045 | 1005 | 1013 | 1033 | rBV | 895157 | 1509566 | 28.02% | 5.244% |
| 5 | 10.686 | 1284 | 1292 | 1302 | rBV | 506023 | 861404 | 15.99% | 2.992% |
| 6 | 13.151 | 1704 | 1711 | 1724 | rBV | 2450514 | 3559372 | 66.06% | 12.365% |
| 7 | 14.521 | 1938 | 1944 | 1961 | rVB | 771538 | 1165684 | 21.63% | 4.049% |
| 8 | 16.010 | 2191 | 2197 | 2210 | rBV | 1900035 | 2741103 | 50.87% | 9.522% |
| 9 | 17.268 | 2402 | 2411 | 2417 | rBV | 973134 | 1395087 | 25.89% | 4.846% |
| 10 | 18.174 | 2559 | 2565 | 2574 | rBV | 378532 | 549641 | 10.20% | 1.909% |
| 11 | 19.327 | 2758 | 2761 | 2770 | rVB5 | 42208 | 73085 | 1.36% | 0.254% |
| 12 | 19.445 | 2777 | 2781 | 2793 | rBV | 151603 | 239405 | 4.44% | 0.832% |
| 13 | 19.892 | 2852 | 2857 | 2863 | rBV | 4436102 | 5388292 | 100.00% | 18.718% |
| 14 | 21.174 | 3070 | 3075 | 3083 | rBV | 493966 | 723108 | 13.42% | 2.512% |
| 15 | 21.450 | 3117 | 3122 | 3128 | rBV | 1349905 | 1732941 | 32.16% | 6.020% |
| 16 | 22.703 | 3331 | 3335 | 3341 | rVB | 211003 | 295446 | 5.48% | 1.026% |
| 17 | 23.827 | 3520 | 3526 | 3536 | rVB2 | 921287 | 1820511 | 33.79% | 6.324% |
| 18 | 24.550 | 3643 | 3649 | 3661 | rVB2 | 330757 | 873649 | 16.21% | 3.035% |
| 19 | 25.768 | 3852 | 3856 | 3865 | rVB2 | 260925 | 604396 | 11.22% | 2.100% |

Sum of corrected areas: 28786338

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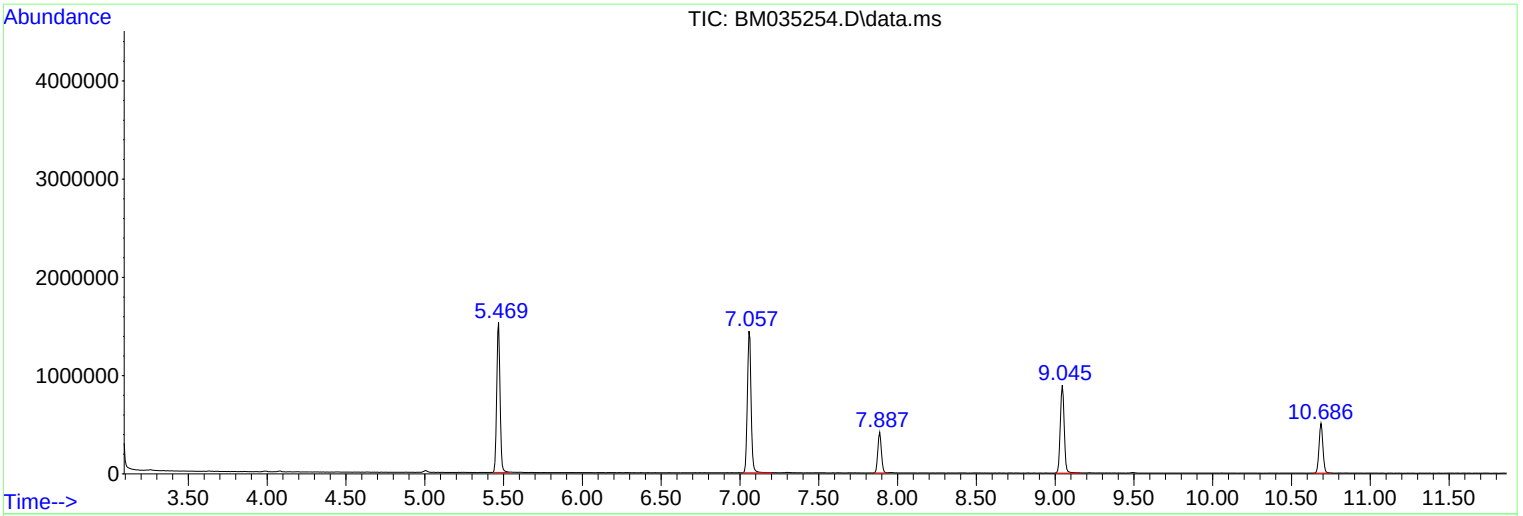
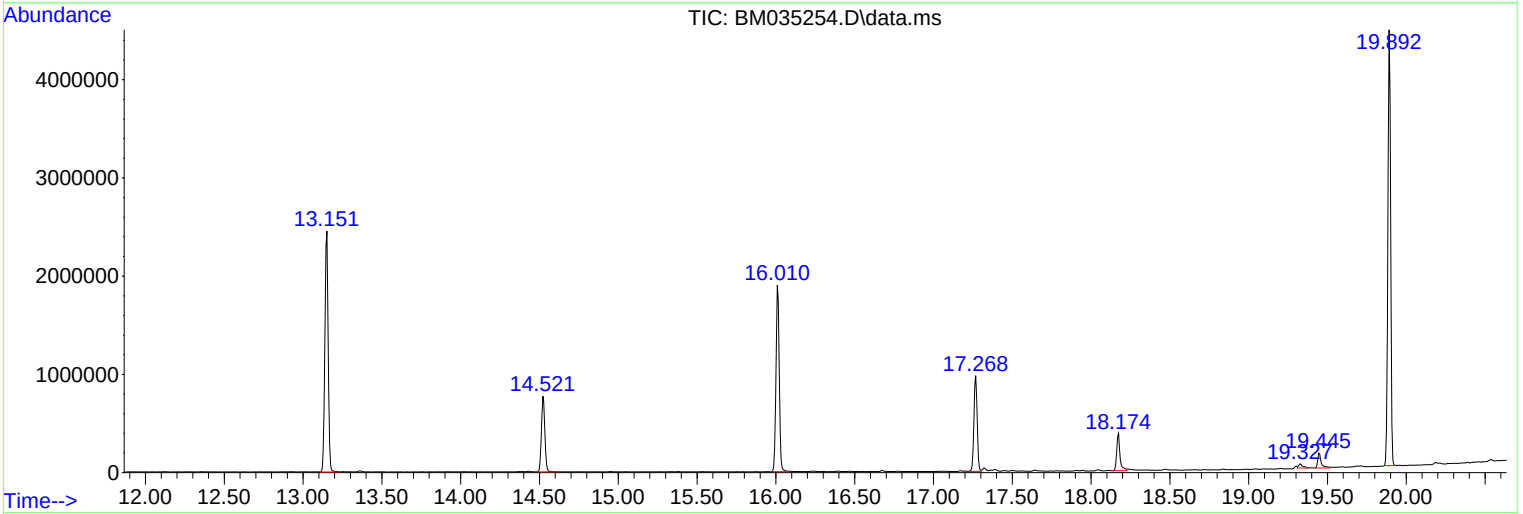
ALS Vial : 12 Sample Multiplier: 1

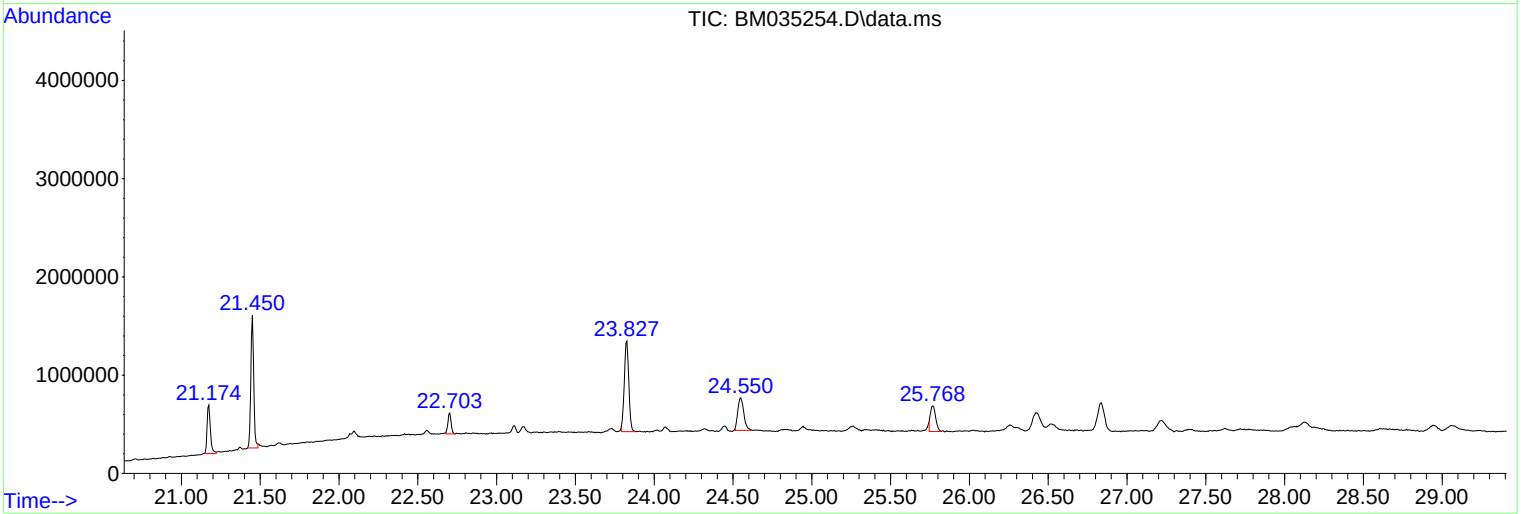
**Instrument :**
BNA_M
**ClientSampleId :**
P030-SS001-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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Data File : BM035254.D
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**ClientSampleId :**
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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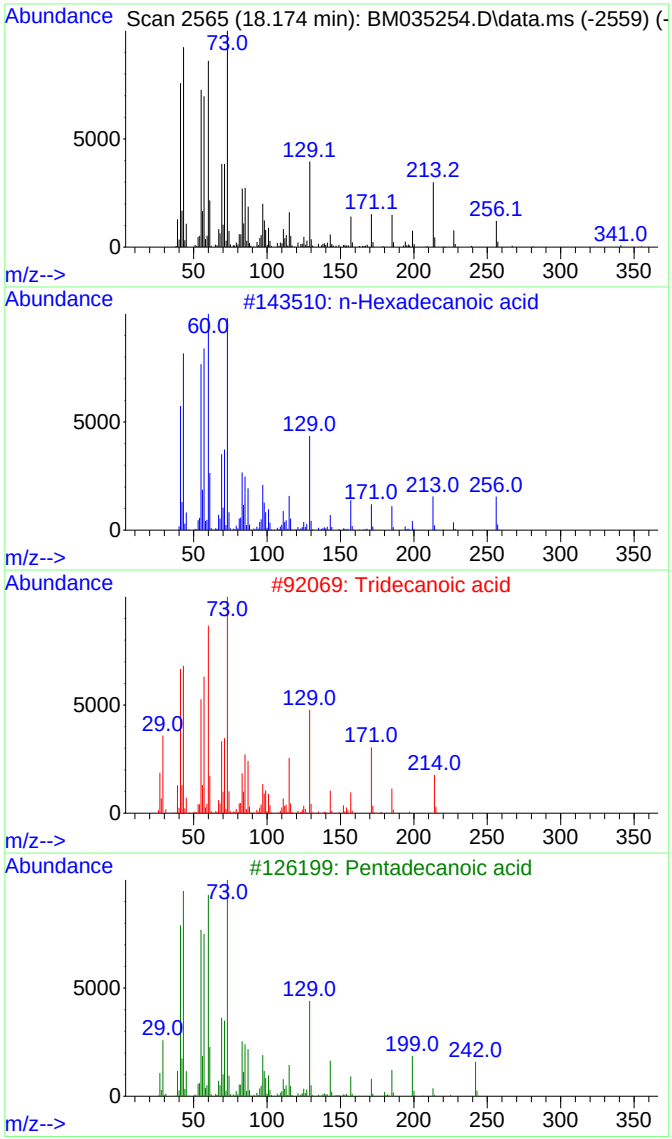
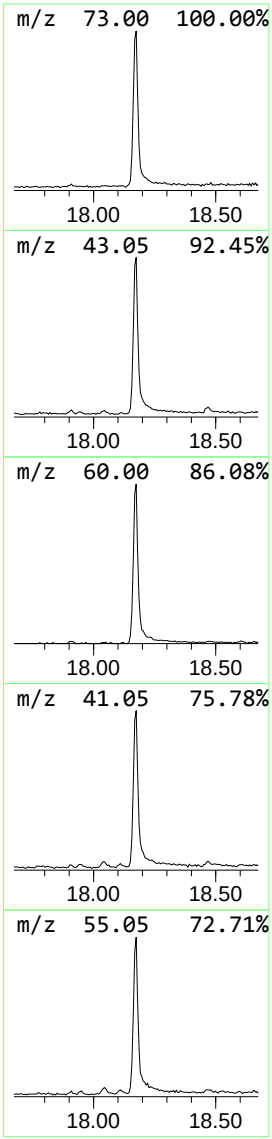
Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.174 | 7.88 ng | 549641 | Phenanthrene-d10 | 17.268 |

| 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 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 87 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



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Data File : BM035254.D
Acq On : 25 May 2022 22:46
Operator : CG/JU
Sample : N2895-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
P030-SS001-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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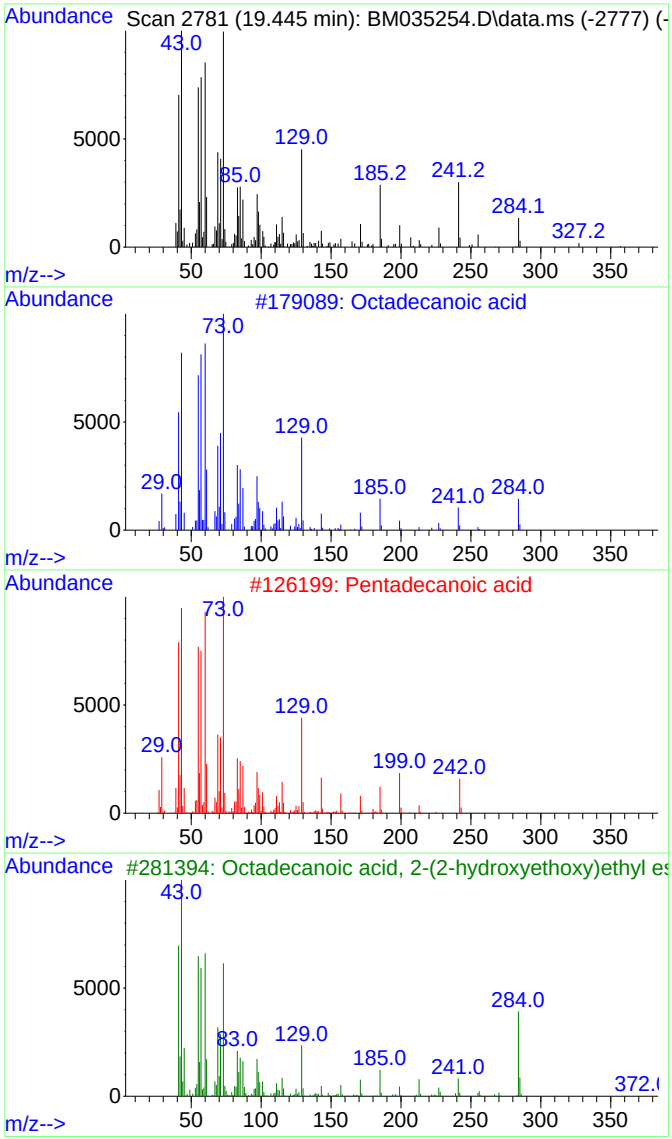
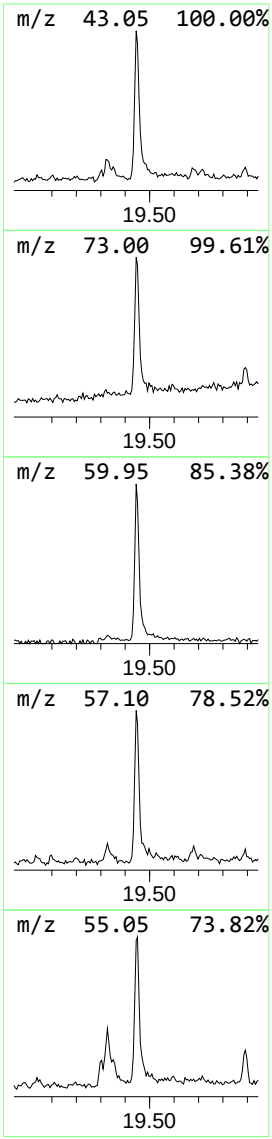
Peak Number 2 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.445 | 2.76 ng | 239405 | Chrysene-d12 | 21.450 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 3 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 5 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035254.D
Acq On : 25 May 2022 22:46
Operator : CG/JU
Sample : N2895-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
P030-SS001-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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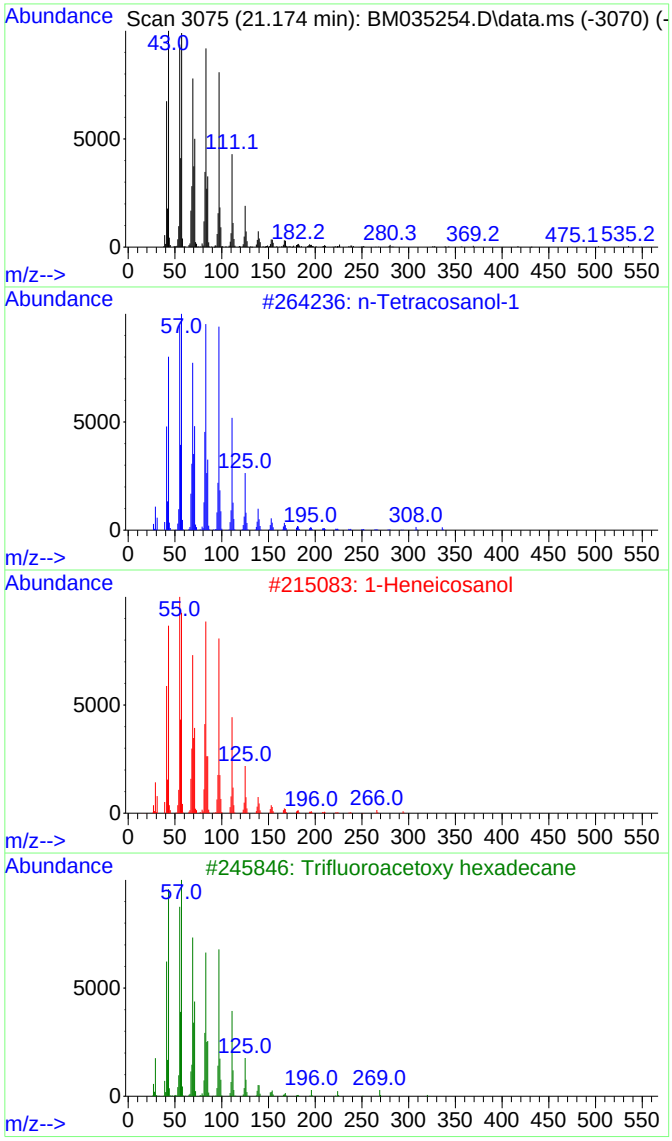
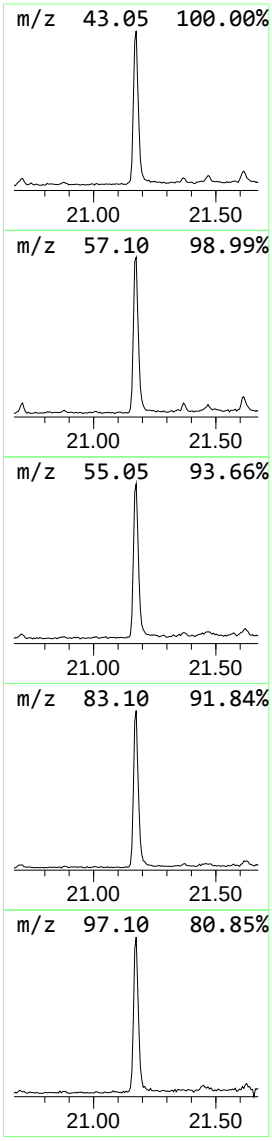
Peak Number 3 n-Tetracosanol-1 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.174 | 8.35 ng | 723108 | Chrysene-d12 | 21.450 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 95 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 4 | Pentacos-1-ene | 350 | C25H50 | 016980-85-1 | 94 |
| 5 | 1-Hexacosene | 364 | C26H52 | 018835-33-1 | 93 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052522\
Data File : BM035254.D
Acq On : 25 May 2022 22:46
Operator : CG/JU
Sample : N2895-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
P030-SS001-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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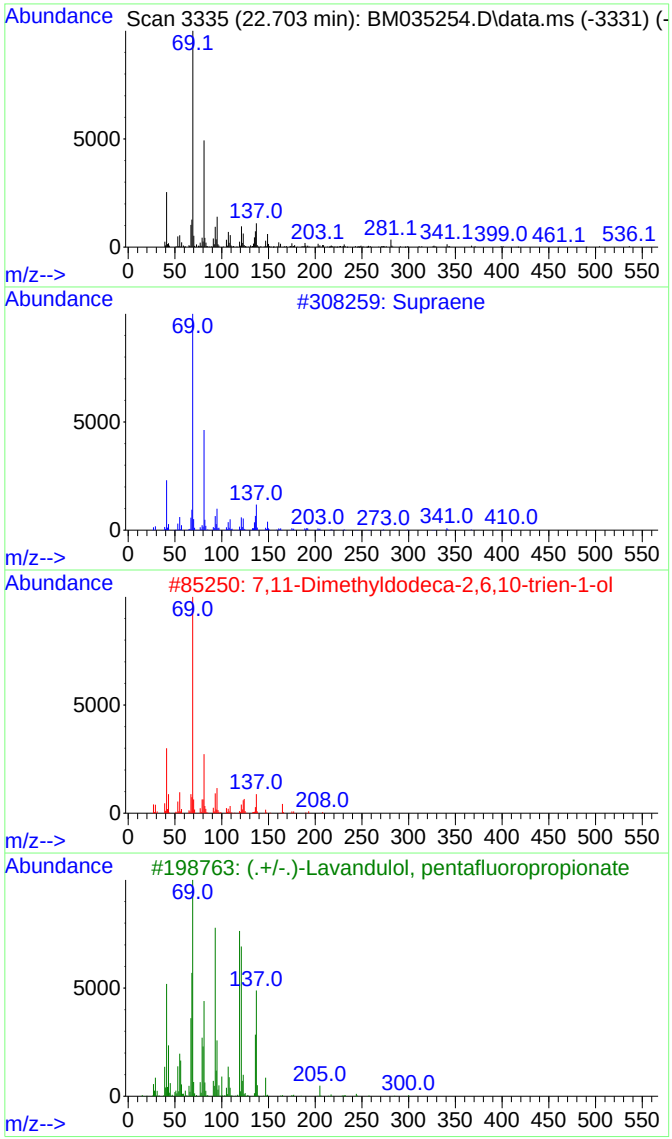
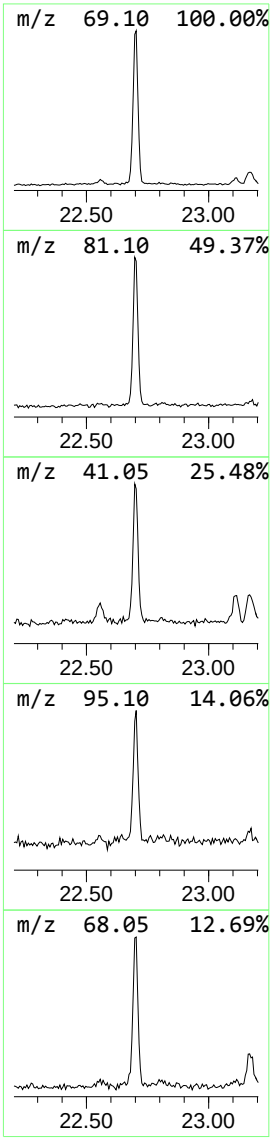
Peak Number 4 Supraene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.703 | 3.25 ng | 295446 | Perylene-d12 | 23.827 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 83 |
| 2 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 74 |
| 3 | (.+/-.)-Lavandulol, pentafluorop... | 300 | C13H17F5O2 | 1000352-63-1 | 72 |
| 4 | 1-(Phenylthio)-3,7,11-trimethyl-... | 314 | C21H30S | 028413-57-2 | 64 |
| 5 | 3,7-Dimethyl-1-phenylsulfonyl-2,... | 278 | C16H22O2S | 1000432-27-5 | 59 |



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Sample : N2895-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
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**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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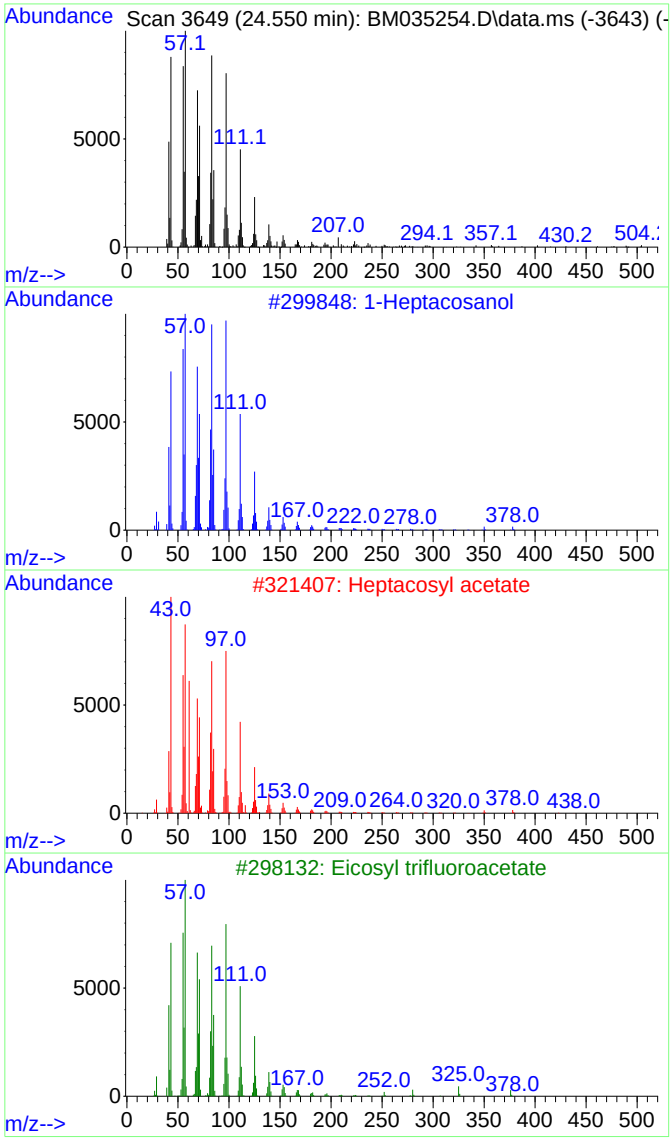
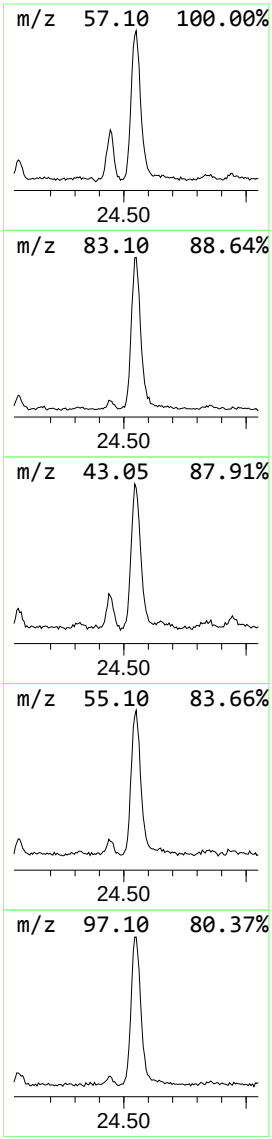
Peak Number 5 1-Heptacosanol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.550 | 9.60 ng | 873649 | Perylene-d12 | 23.827 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 95 |
| 2 | Heptacosyl acetate | 438 | C29H58O2 | 1000351-78-2 | 95 |
| 3 | Eicosyl trifluoroacetate | 394 | C22H41F3O2 | 1000351-75-2 | 94 |
| 4 | Octacosyl acetate | 452 | C30H60O2 | 018206-97-8 | 94 |
| 5 | Heptacos-1-ene | 378 | C27H54 | 015306-27-1 | 94 |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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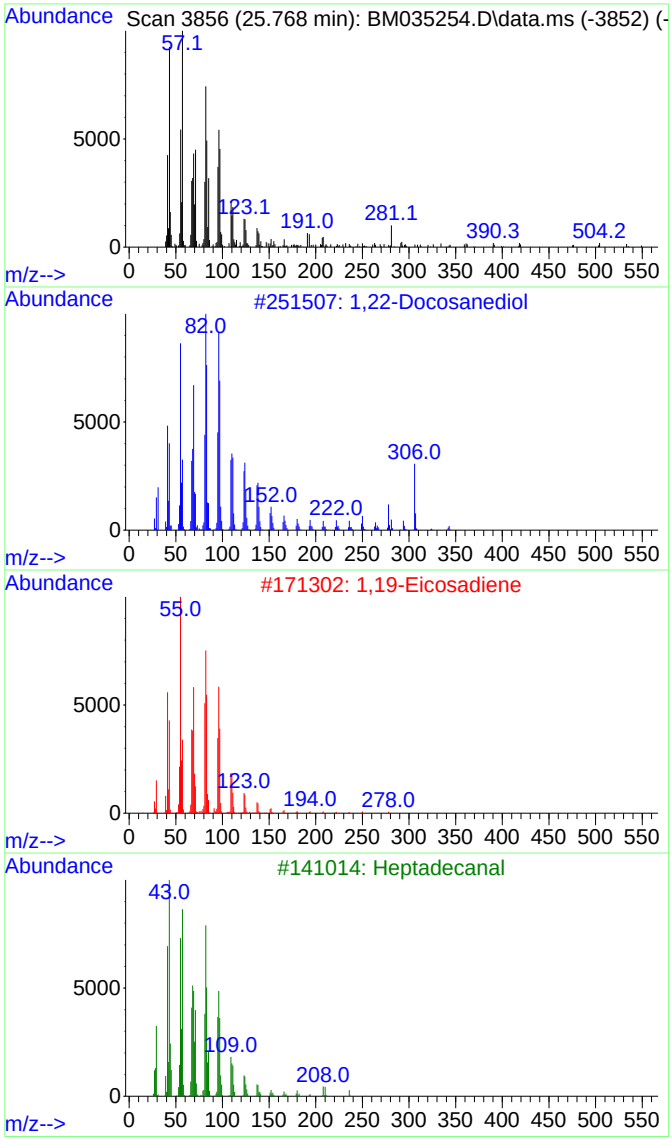
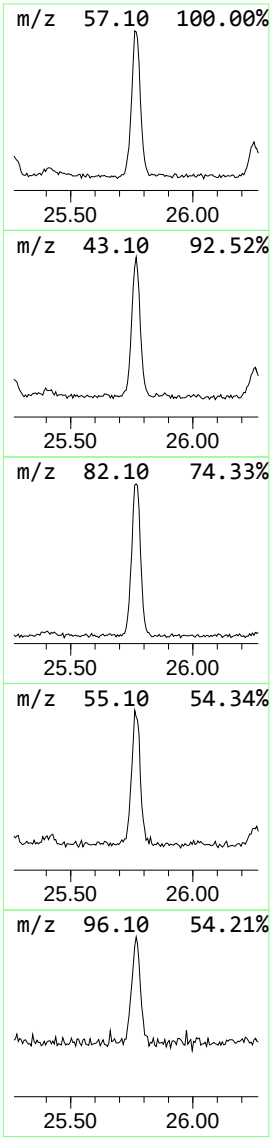
Peak Number 6 1,22-Docosanediol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 25.768 | 6.64 ng | 604396 | Perylene-d12 | 23.827 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,22-Docosanediol | 342 | C22H46O2 | 022513-81-1 | 94 |
| 2 | 1,19-Eicosadiene | 278 | C20H38 | 014811-95-1 | 93 |
| 3 | Heptadecanal | 254 | C17H34O | 1000376-70-0 | 91 |
| 4 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 90 |
| 5 | Tetradecanal | 212 | C14H28O | 000124-25-4 | 90 |



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 ... | 18.174 | 7.9 | ng | 549641 | 4 | 17.268 | 1395090 | 20.0 |
| Octadecanoic acid | 19.445 | 2.8 | ng | 239405 | 5 | 21.450 | 1732940 | 20.0 |
| n-Tetracosanol-1 | 21.174 | 8.3 | ng | 723108 | 5 | 21.450 | 1732940 | 20.0 |
| Supraene | 22.703 | 3.3 | ng | 295446 | 6 | 23.827 | 1820510 | 20.0 |
| 1-Heptacosanol | 24.550 | 9.6 | ng | 873649 | 6 | 23.827 | 1820510 | 20.0 |
| 1,22-Docosanediol | 25.768 | 6.6 | ng | 604396 | 6 | 23.827 | 1820510 | 20.0 |