LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
Data File : BM040233.D
Acq On : 13 Jun 2023 20:04
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

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-BM061323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040233.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.446 | 192 | 197 | 209 | rVB | 1054654 | 1389848 | 5.63% | 1.126% |
| 2 | 5.063 | 295 | 302 | 315 | rBV | 5345386 | 7121651 | 28.82% | 5.769% |
| 3 | 5.528 | 375 | 381 | 394 | rBV | 3547397 | 5001731 | 20.24% | 4.052% |
| 4 | 6.151 | 481 | 487 | 497 | rBV | 637255 | 901292 | 3.65% | 0.730% |
| 5 | 7.134 | 646 | 654 | 667 | rBV | 2117521 | 3284359 | 13.29% | 2.661% |
| 6 | 7.975 | 790 | 797 | 805 | rBV | 2266007 | 3488156 | 14.12% | 2.826% |
| 7 | 9.151 | 988 | 997 | 1009 | rBV | 6834916 | 11240921 | 45.50% | 9.106% |
| 8 | 10.792 | 1267 | 1276 | 1288 | rBV | 3014529 | 4946511 | 20.02% | 4.007% |
| 9 | 13.245 | 1685 | 1693 | 1708 | rBV | 16890900 | 24405693 | 98.78% | 19.771% |
| 10 | 14.615 | 1919 | 1926 | 1936 | rBV | 4073446 | 5719896 | 23.15% | 4.634% |
| 11 | 15.974 | 2151 | 2157 | 2164 | rBV | 244071 | 345573 | 1.40% | 0.280% |
| 12 | 16.104 | 2172 | 2179 | 2191 | rBV | 7667977 | 10618399 | 42.98% | 8.602% |
| 13 | 17.356 | 2387 | 2392 | 2403 | rVB | 4071871 | 5749678 | 23.27% | 4.658% |
| 14 | 18.251 | 2539 | 2544 | 2554 | rBV | 617967 | 1039640 | 4.21% | 0.842% |
| 15 | 19.527 | 2756 | 2761 | 2773 | rBV | 611500 | 1082219 | 4.38% | 0.877% |
| 16 | 19.980 | 2832 | 2838 | 2843 | rBV | 20444789 | 24706975 | 100.00% | 20.015% |
| 17 | 21.233 | 3048 | 3051 | 3060 | rBV3 | 390905 | 542865 | 2.20% | 0.440% |
| 18 | 21.533 | 3097 | 3102 | 3107 | rBV2 | 4351701 | 5700580 | 23.07% | 4.618% |
| 19 | 23.968 | 3510 | 3516 | 3532 | rVB | 3077610 | 6157931 | 24.92% | 4.988% |

Sum of corrected areas: 123443918

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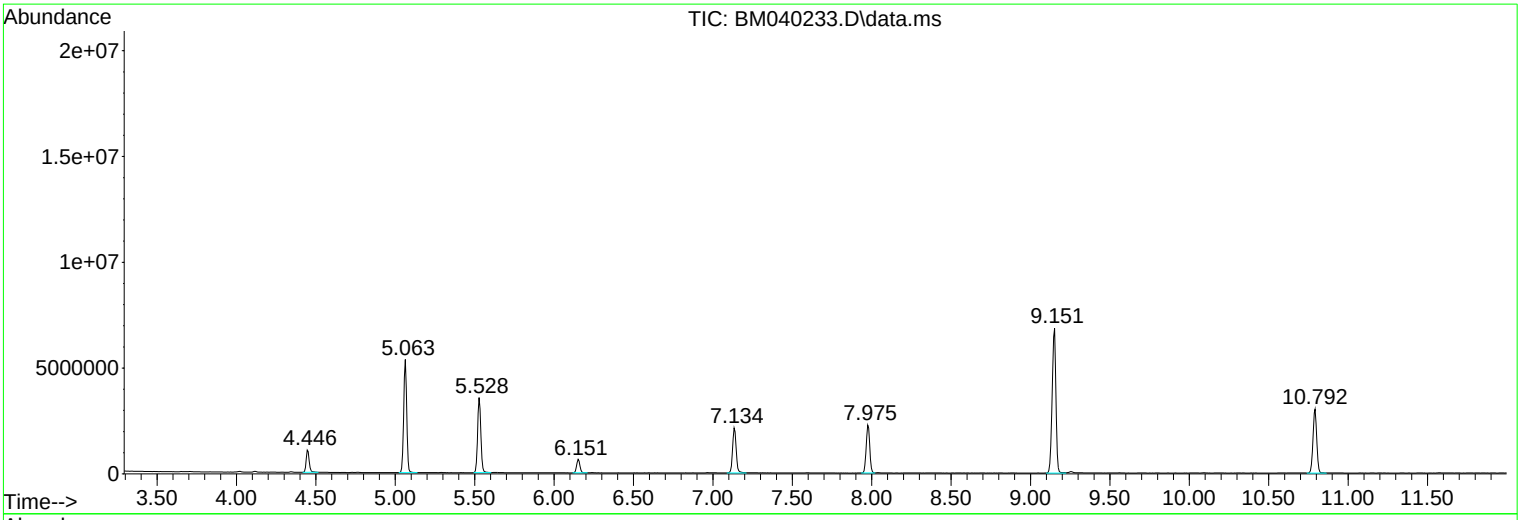
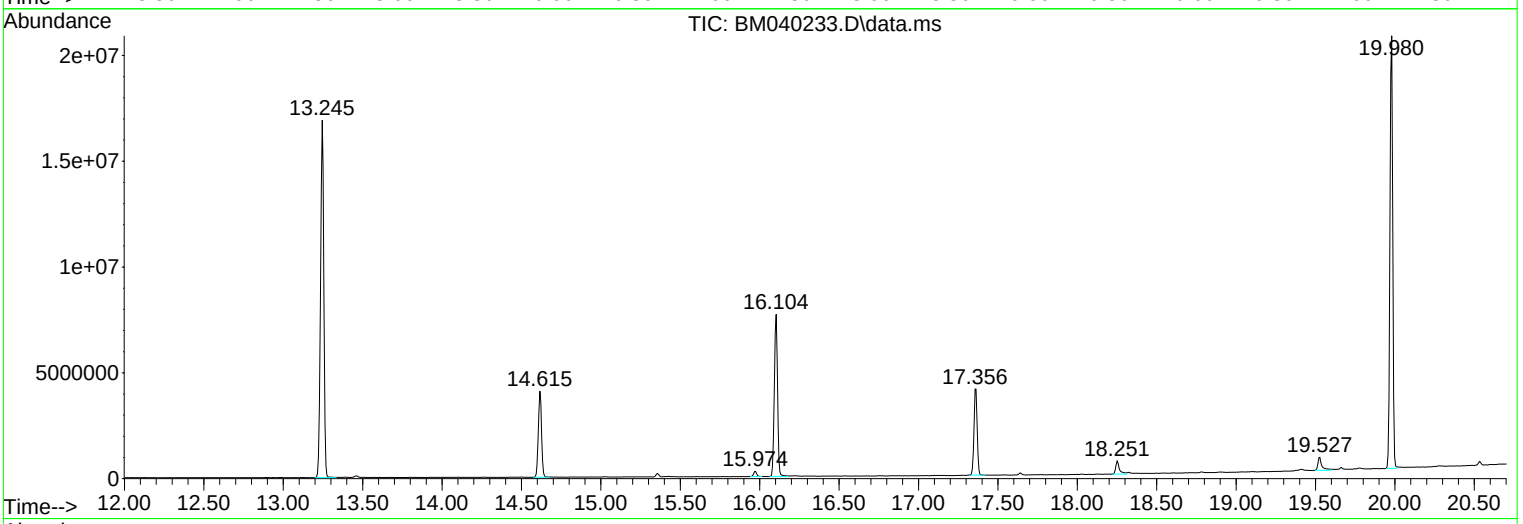
Misc :
ALS Vial : 18 Sample Multiplier: 1

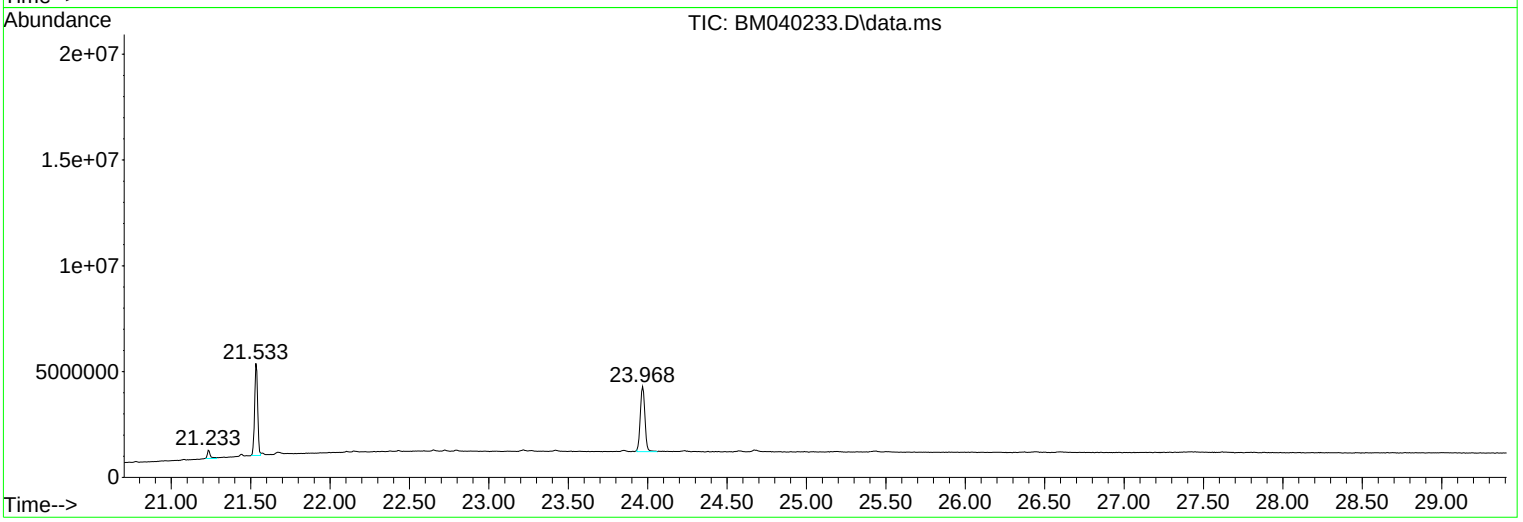
**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.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 : BM040233.D
Acq On : 13 Jun 2023 20:04
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Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

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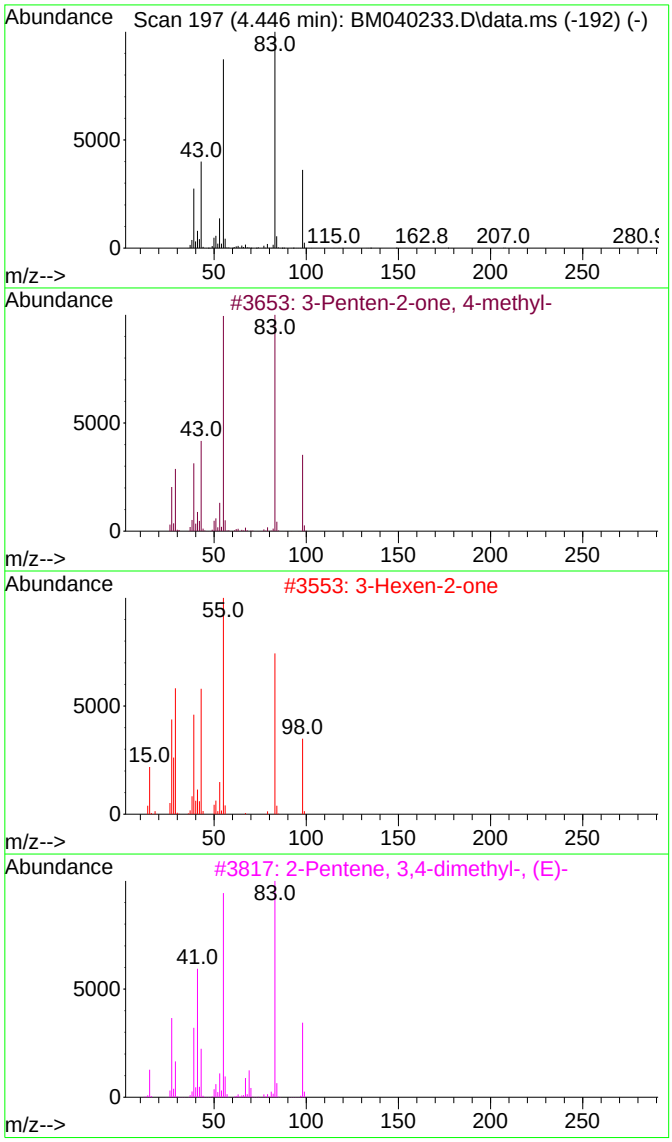
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

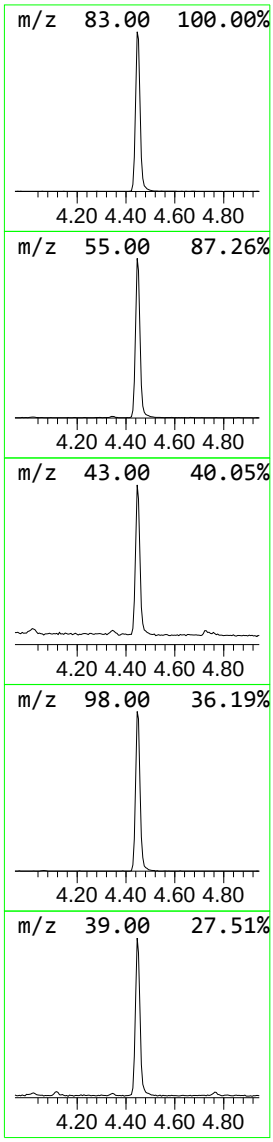
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.446 | 7.97 ng | 1389850 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 95 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 5 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 80 |



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Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

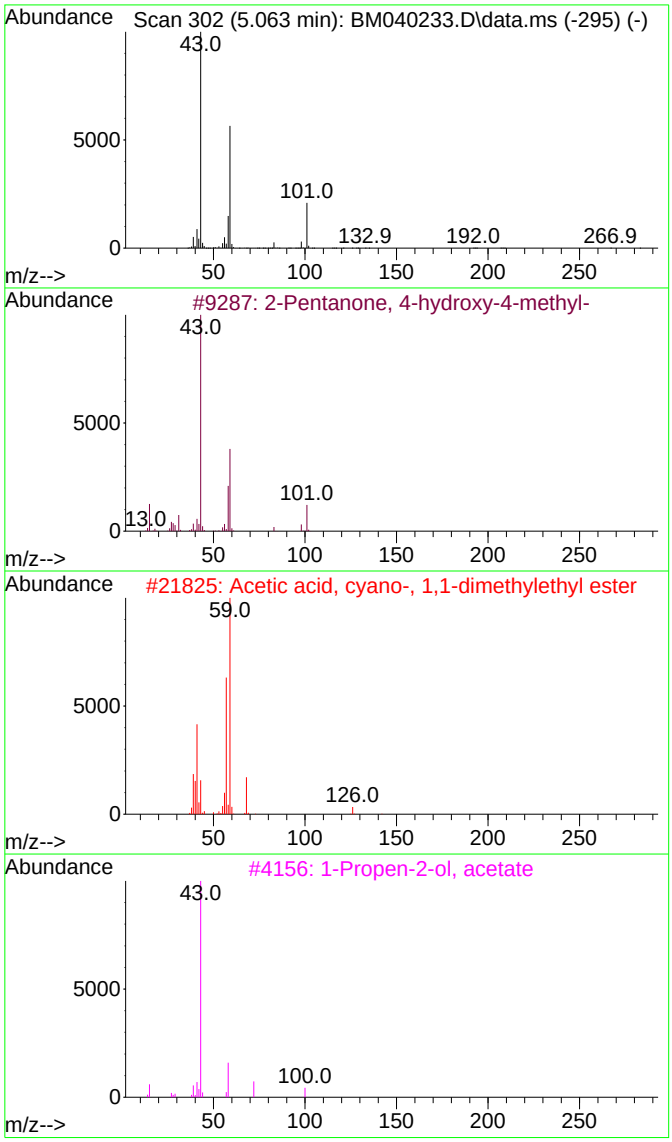
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

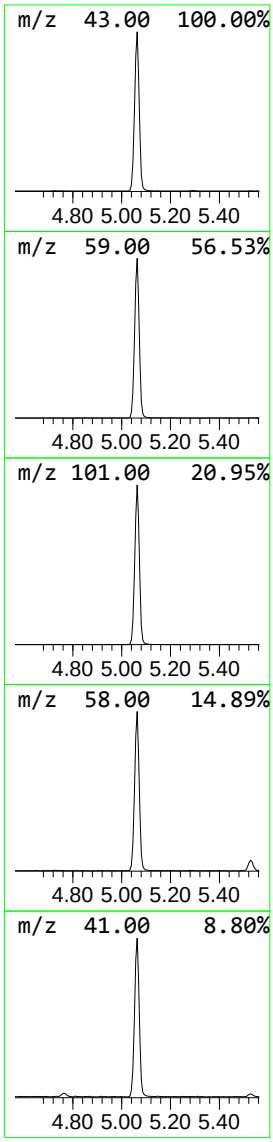
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.063 | 40.83 ng | 7121650 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
Data File : BM040233.D
Acq On : 13 Jun 2023 20:04
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

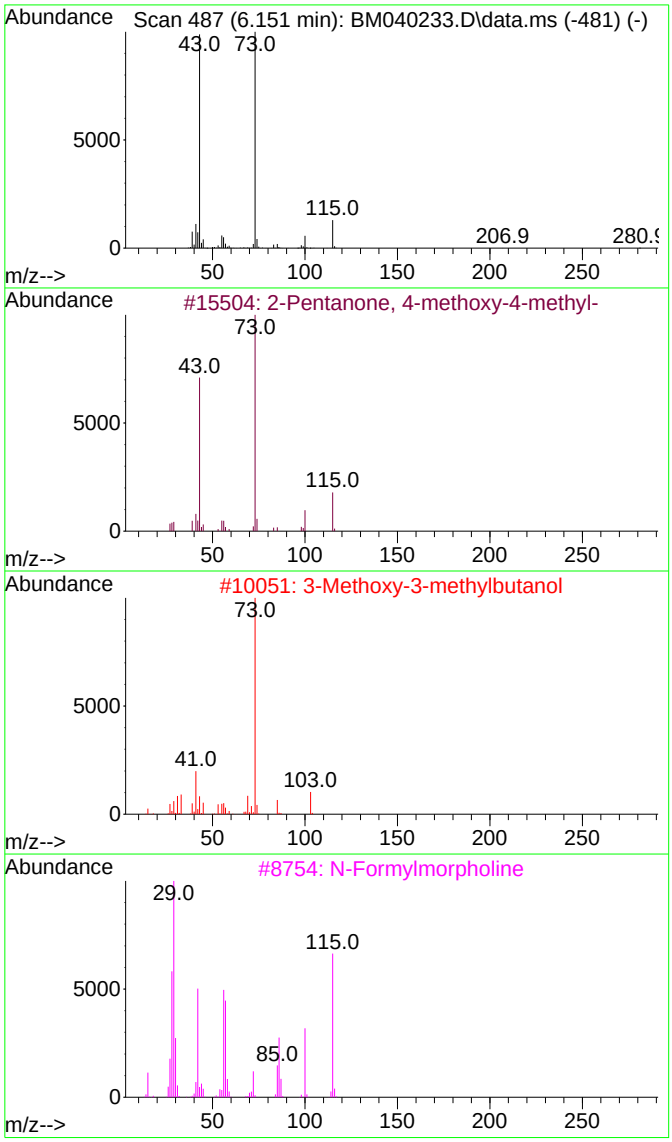
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

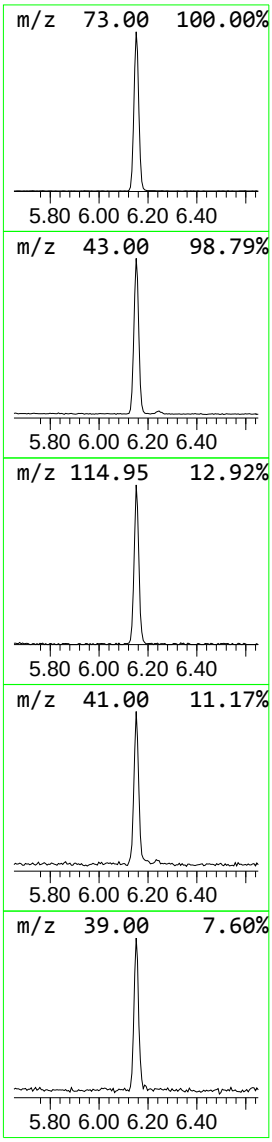
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.151 | 5.17 ng | 901292 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 83 |
| 2 | 3-Methoxy-3-methylbutanol | 118 | C6H14O2 | 056539-66-3 | 12 |
| 3 | N-Formylmorpholine | 115 | C5H9NO2 | 004394-85-8 | 10 |
| 4 | 1,3-Dioxolane, 2-(1-methylethyl)- | 116 | C6H12O2 | 000822-83-3 | 10 |
| 5 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 9 |



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Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

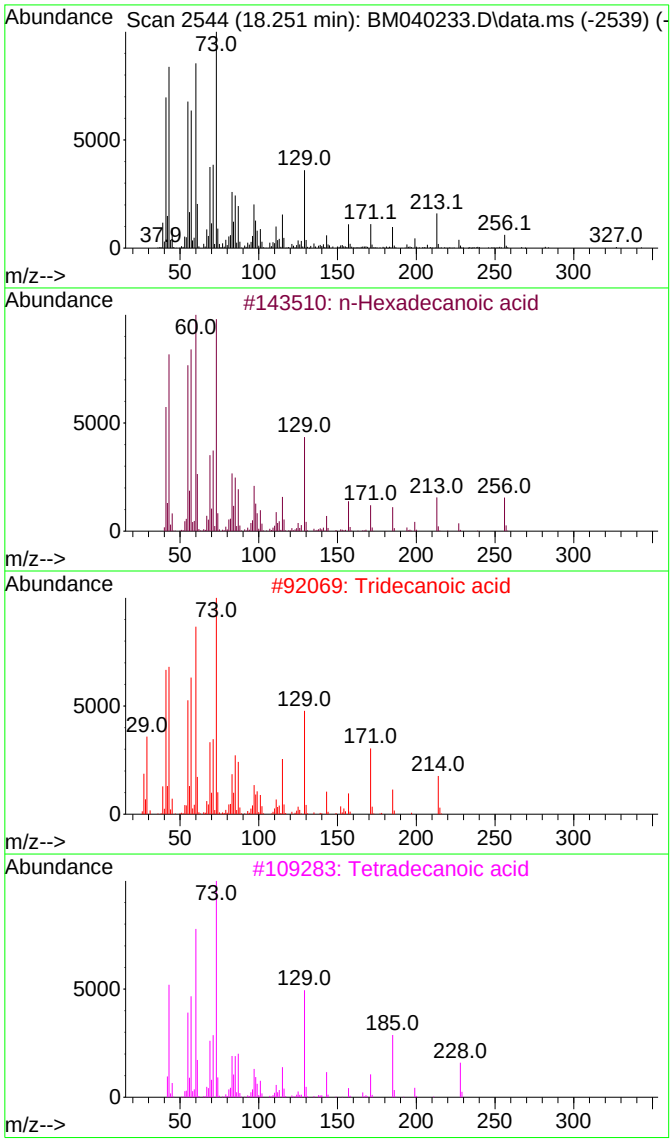
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

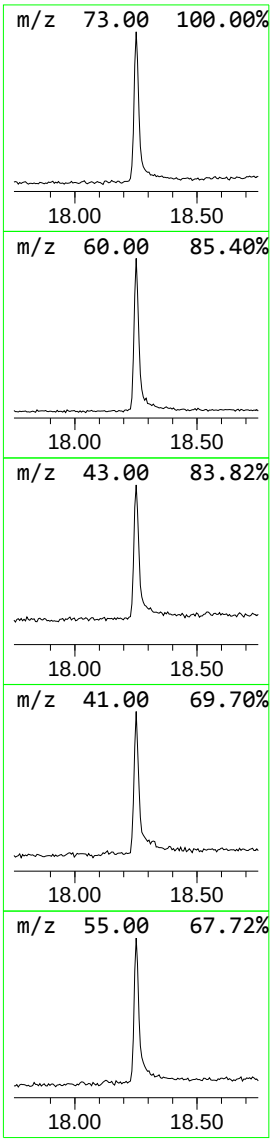
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.250 | 3.62 ng | 1039640 | Phenanthrene-d10 | 17.362 |

| 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 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 91 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |



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Data File : BM040233.D
Acq On : 13 Jun 2023 20:04
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

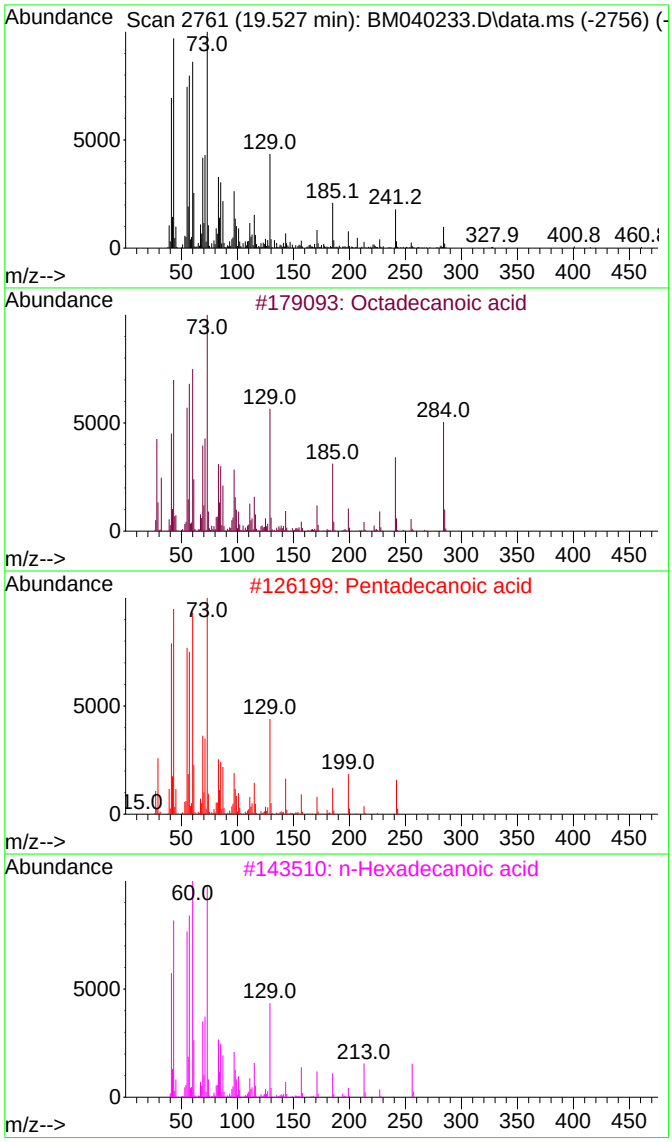
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

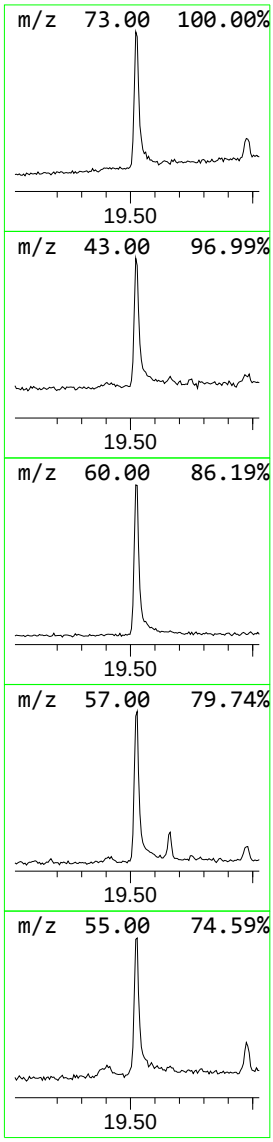
**********

Peak Number 5 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.527 | 3.80 ng | 1082220 | Chrysene-d12 | 21.533 |

| 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 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 5 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
Data File : BM040233.D
Acq On : 13 Jun 2023 20:04
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
B-45(OW)RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 3-Penten-2-one,... | 4.446 | 8.0 | ng | 1389850 | 1 | 7.975 | 3488160 | 20.0 |
| 2-Pentanone, 4-... | 5.063 | 40.8 | ng | 7121650 | 1 | 7.975 | 3488160 | 20.0 |
| 2-Pentanone, 4-... | 6.151 | 5.2 | ng | 901292 | 1 | 7.975 | 3488160 | 20.0 |
| n-Hexadecanoic ... | 18.250 | 3.6 | ng | 1039640 | 4 | 17.362 | 5749680 | 20.0 |
| Octadecanoic acid | 19.527 | 3.8 | ng | 1082220 | 5 | 21.533 | 5700580 | 20.0 |