LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** FK-BPM-03-021-ABCD

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: BM029078.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.199 | 32 | 36 | 44 | rVB | 5156 | 6205 | 1.52% | 0.322% |
| 2 | 4.763 | 297 | 302 | 311 | rBB | 7356 | 10032 | 2.46% | 0.520% |
| 3 | 5.234 | 377 | 382 | 395 | rBV | 133435 | 190878 | 46.84% | 9.900% |
| 4 | 6.857 | 653 | 658 | 672 | rBV | 121412 | 196798 | 48.29% | 10.207% |
| 5 | 7.663 | 790 | 795 | 801 | rBB | 27249 | 39728 | 9.75% | 2.061% |
| 6 | 8.839 | 989 | 995 | 1004 | rBV | 76527 | 122630 | 30.09% | 6.360% |
| 7 | 10.457 | 1264 | 1270 | 1280 | rBB | 35015 | 54146 | 13.29% | 2.808% |
| 8 | 12.945 | 1687 | 1693 | 1705 | rBV | 178254 | 252256 | 61.90% | 13.083% |
| 9 | 13.221 | 1735 | 1740 | 1744 | rBB | 4308 | 5976 | 1.47% | 0.310% |
| 10 | 13.798 | 1834 | 1838 | 1844 | rBB | 5878 | 7496 | 1.84% | 0.389% |
| 11 | 14.333 | 1923 | 1929 | 1935 | rBB | 48448 | 68290 | 16.76% | 3.542% |
| 12 | 15.833 | 2179 | 2184 | 2195 | rBB | 137833 | 184179 | 45.19% | 9.553% |
| 13 | 17.080 | 2391 | 2396 | 2403 | rBV | 60193 | 79216 | 19.44% | 4.109% |
| 14 | 17.974 | 2544 | 2548 | 2555 | rBV | 8104 | 10953 | 2.69% | 0.568% |
| 15 | 18.715 | 2668 | 2674 | 2678 | rVB | 11754 | 15088 | 3.70% | 0.783% |
| 16 | 19.127 | 2739 | 2744 | 2750 | rBV | 3359 | 4559 | 1.12% | 0.236% |
| 17 | 19.256 | 2762 | 2766 | 2770 | rBV2 | 7051 | 10982 | 2.69% | 0.570% |
| 18 | 19.703 | 2837 | 2842 | 2847 | rBV | 341947 | 407530 | 100.00% | 21.137% |
| 19 | 20.980 | 3054 | 3059 | 3066 | rBV2 | 25630 | 44655 | 10.96% | 2.316% |
| 20 | 21.256 | 3101 | 3106 | 3112 | rBV | 85670 | 106963 | 26.25% | 5.548% |
| 21 | 23.409 | 3467 | 3472 | 3479 | rVB | 64010 | 109499 | 26.87% | 5.679% |

Sum of corrected areas: 1928059

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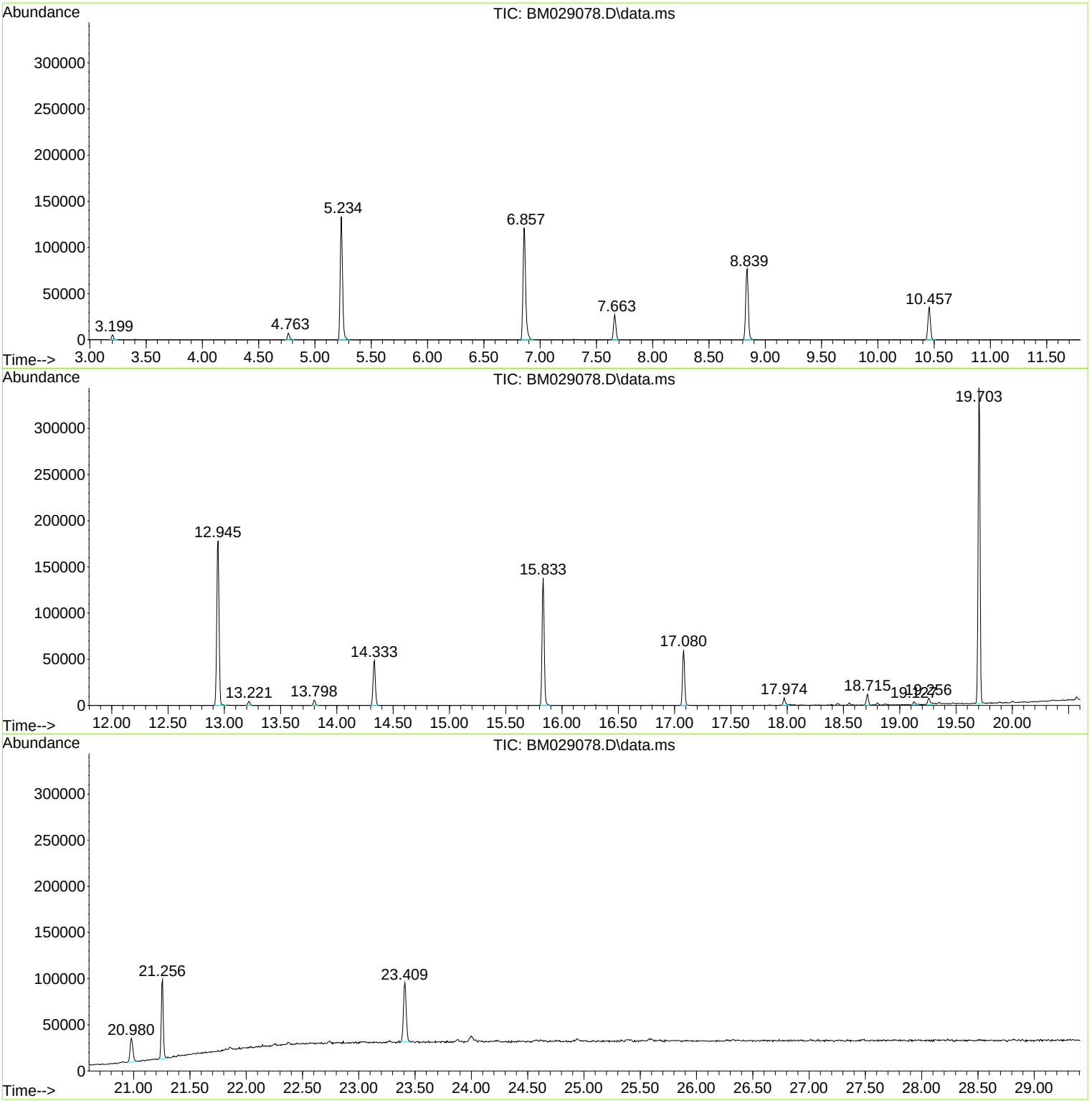
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
FK-BPM-03-021-ABCD

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** FK-BPM-03-021-ABCD

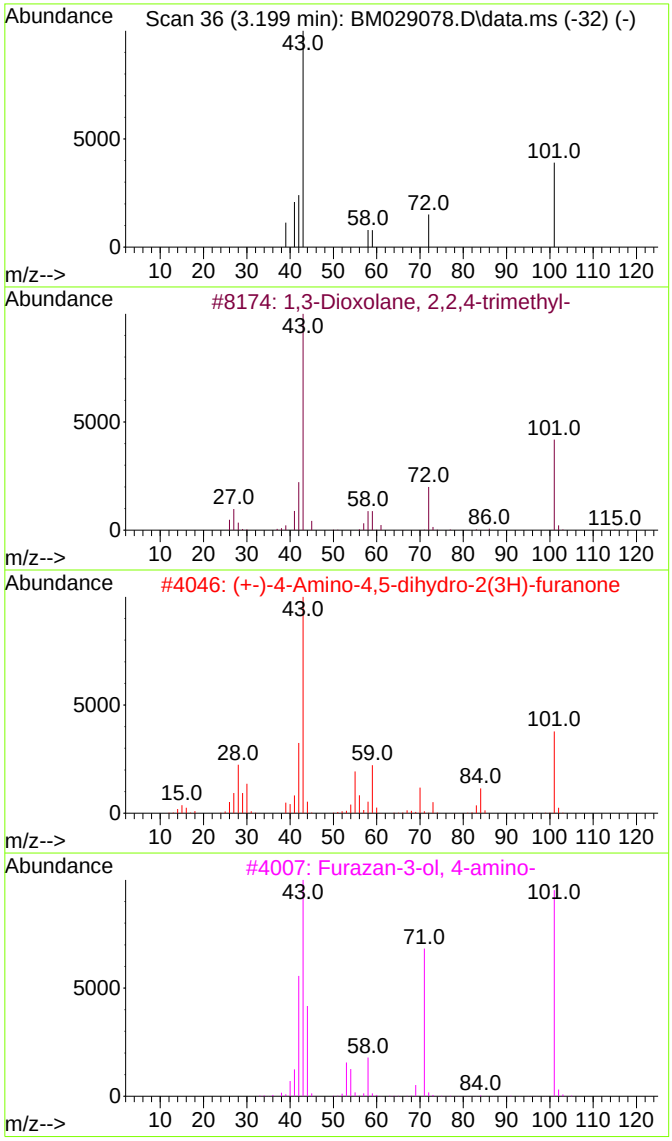
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

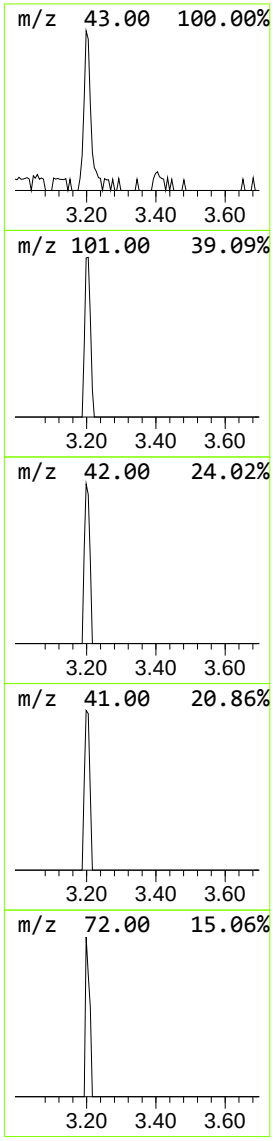
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.199 | 3.12 ng | 6205 | 1,4-Dichlorobenzene-d4 | 7.663 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Dioxolane, 2,2,4-trimethyl- | 116 | C6H12O2 | 001193-11-9 | 74 |
| 2 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 3 | Furazan-3-ol, 4-amino- | 101 | C2H3N3O2 | 159013-90-8 | 7 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 7 |
| 5 | 2-Ethylbutylamine | 101 | C6H15N | 000617-79-8 | 7 |



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Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
FK-BPM-03-021-ABCD

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

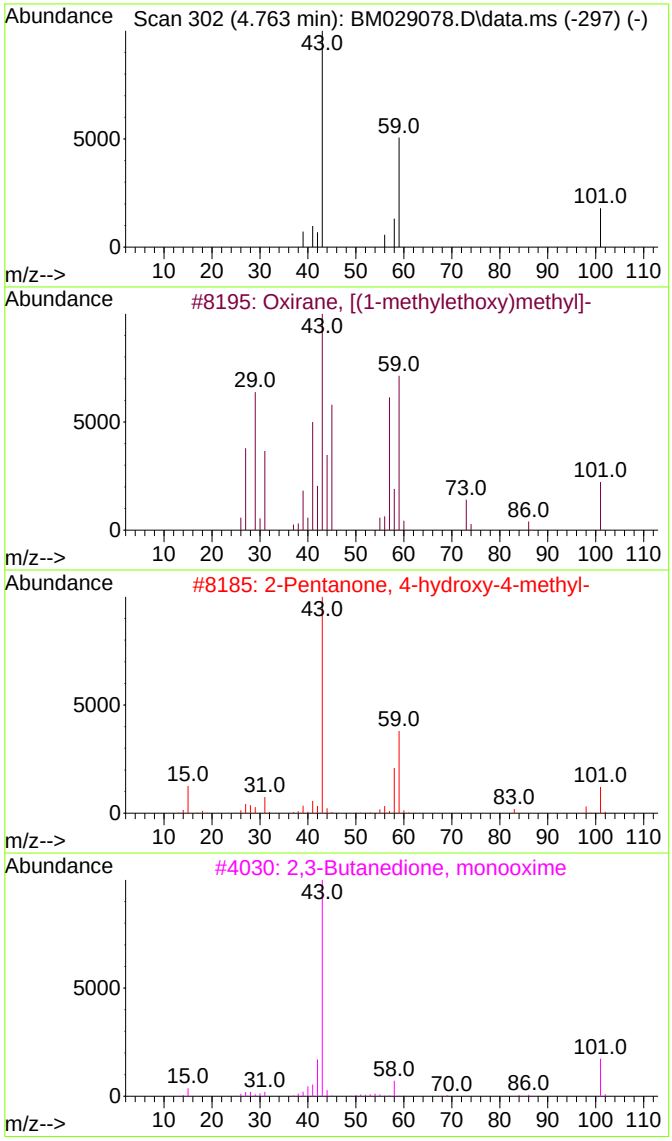
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

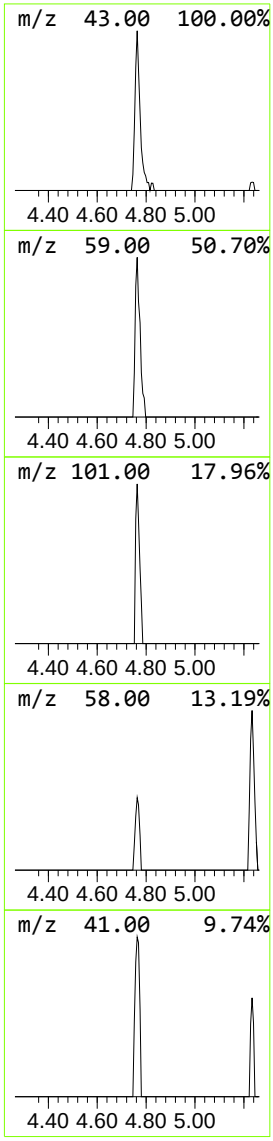
**********

Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.763 | 5.05 ng | 10032 | 1,4-Dichlorobenzene-d4 | 7.663 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxirane, [(1-methylethoxy)methyl]- | 116 | C6H12O2 | 004016-14-2 | 64 |
| 2 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 7 |
| 4 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 7 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 5 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** FK-BPM-03-021-ABCD

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

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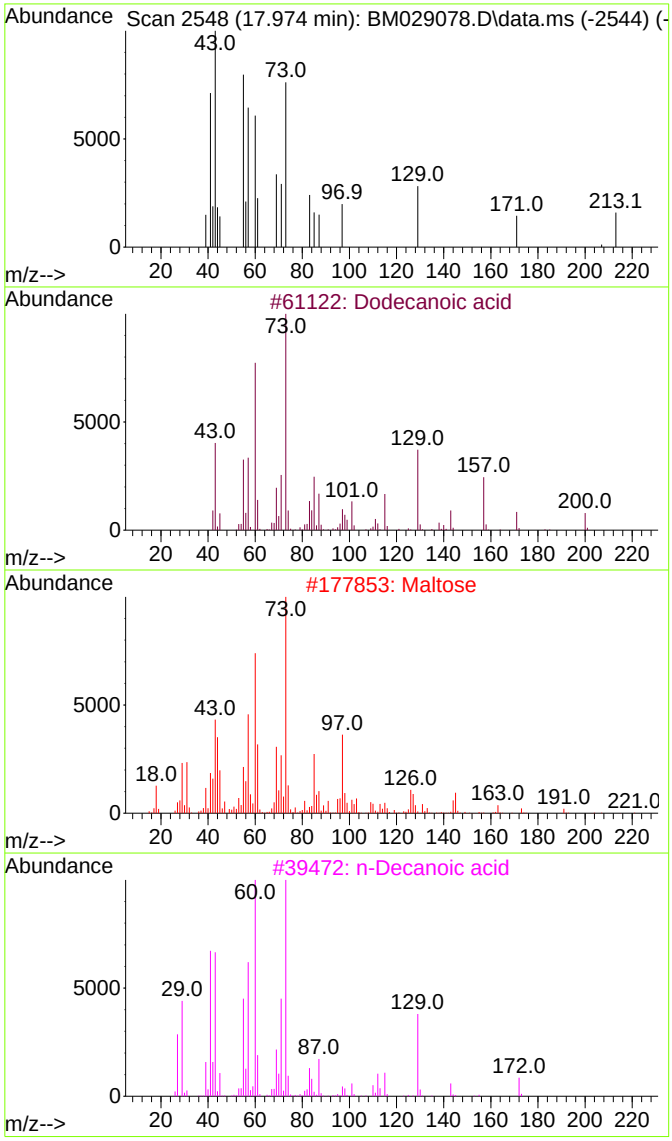
TIC Integration Parameters: LSCINT.P

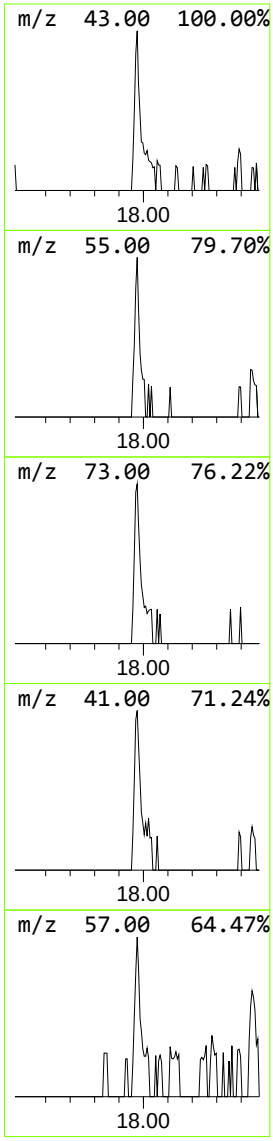
**********

Peak Number 3 Dodecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.974 | 2.77 ng | 10953 | Phenanthrene-d10 | 17.080 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 50 |
| 2 | Maltose | 342 | C12H22O11 | 000069-79-4 | 47 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 43 |
| 4 | .alpha.-D-Glucopyranoside, O-.al... | 504 | C18H32O16 | 000597-12-6 | 38 |
| 5 | l-Gala-l-ido-octose | 240 | C8H16O8 | 1000130-12-1 | 37 |



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Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
FK-BPM-03-021-ABCD

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
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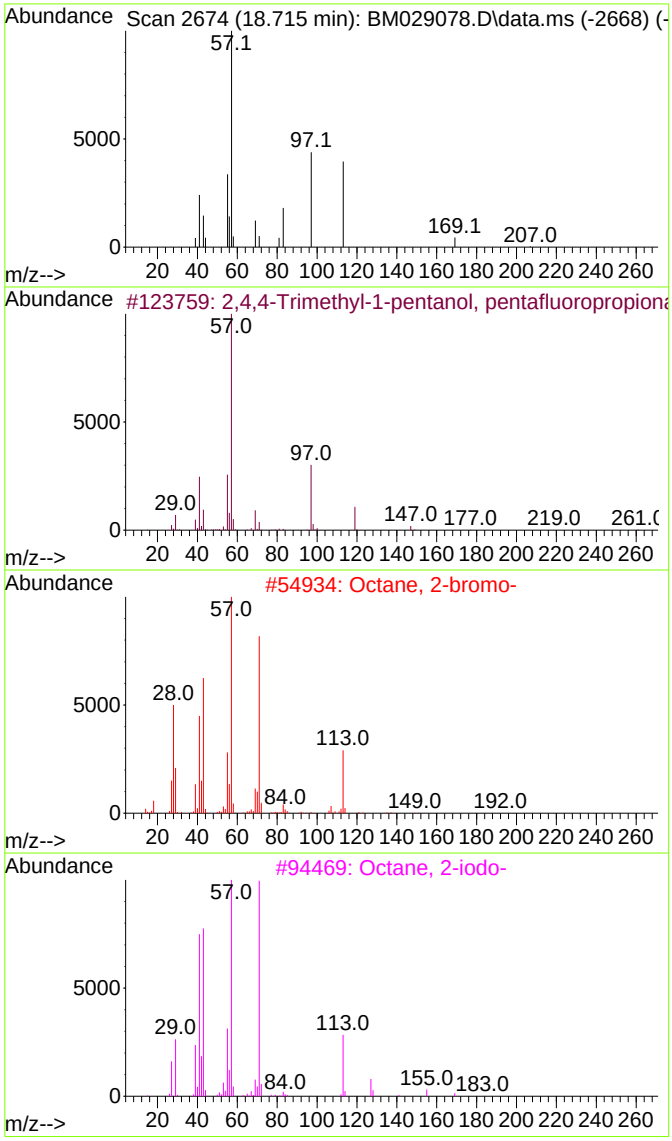
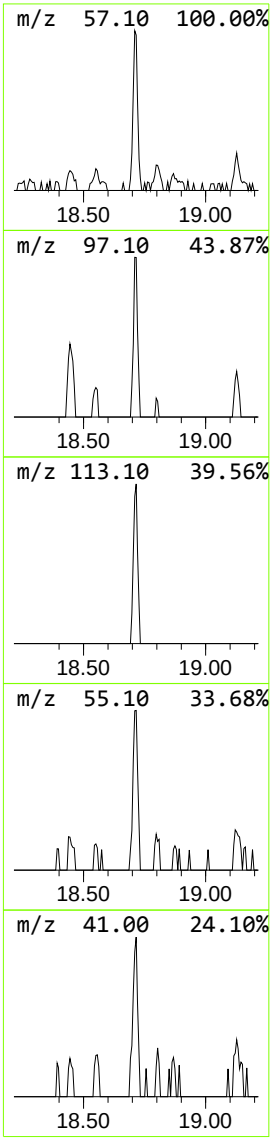
**********

Peak Number 4 unknown18.715 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.715 | 3.81 ng | 15088 | Phenanthrene-d10 | 17.080 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,4-Trimethyl-1-pentanol, pent... | 276 | C11H17F5O2 | 1000365-51-0 | 38 |
| 2 | Octane, 2-bromo- | 192 | C8H17Br | 000557-35-7 | 37 |
| 3 | Octane, 2-iodo- | 240 | C8H17I | 000557-36-8 | 28 |
| 4 | 1-Pentanol, 3-methyl-2-propyl- | 144 | C9H20O | 054004-40-9 | 28 |
| 5 | Bis(2-ethylhexyl) methylenesucci... | 354 | C21H38O4 | 002287-83-4 | 28 |



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Data File : BM029078.D
Acq On : 10 Mar 2021 20:12
Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
FK-BPM-03-021-ABCD

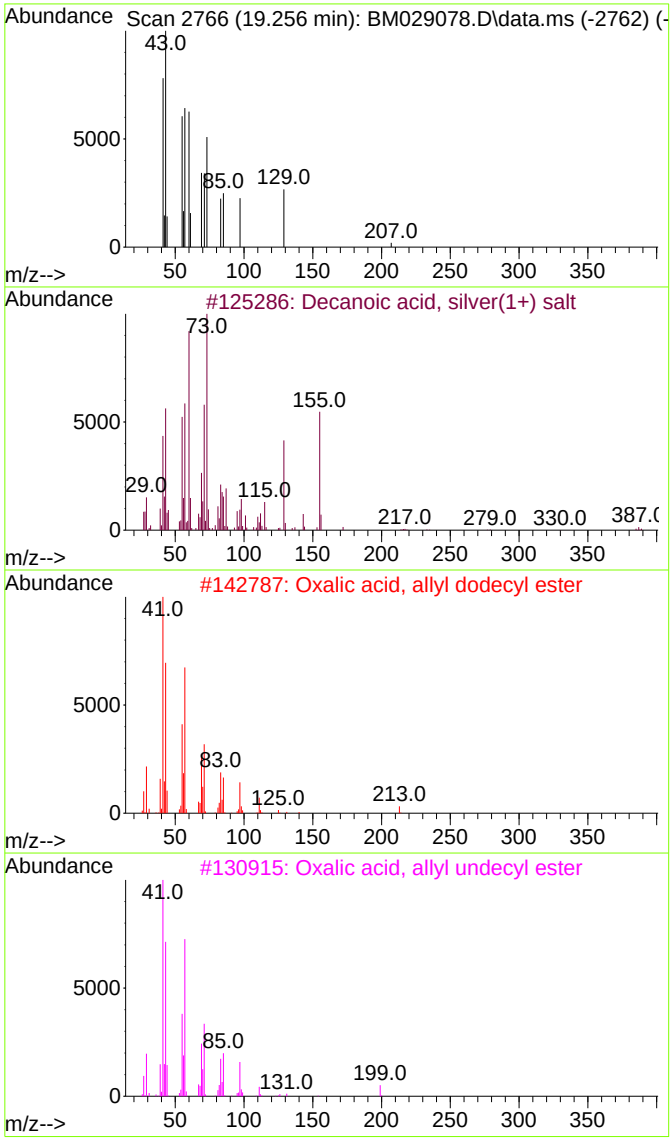
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

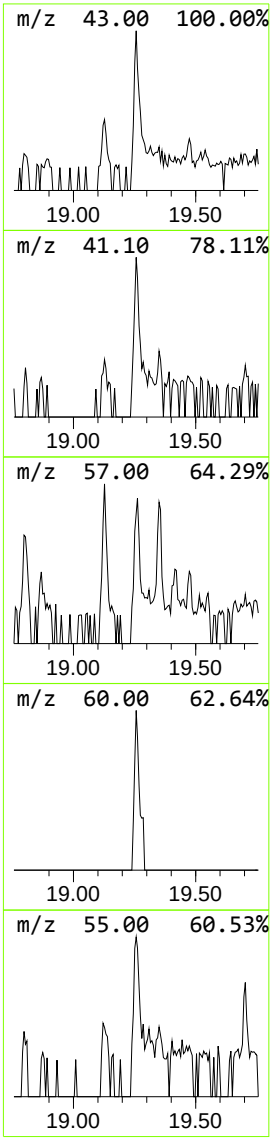
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.256 | 2.05 ng | 10982 | Chrysene-d12 | 21.256 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 50 |
| 2 | Oxalic acid, allyl dodecyl ester | 298 | C17H30O4 | 1000309-24-0 | 43 |
| 3 | Oxalic acid, allyl undecyl ester | 284 | C16H28O4 | 1000309-23-9 | 43 |
| 4 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 43 |
| 5 | Oxalic acid, allyl tridecyl ester | 312 | C18H32O4 | 1000309-24-1 | 43 |



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Operator : CG/JU
Sample : M1614-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** FK-BPM-03-021-ABCD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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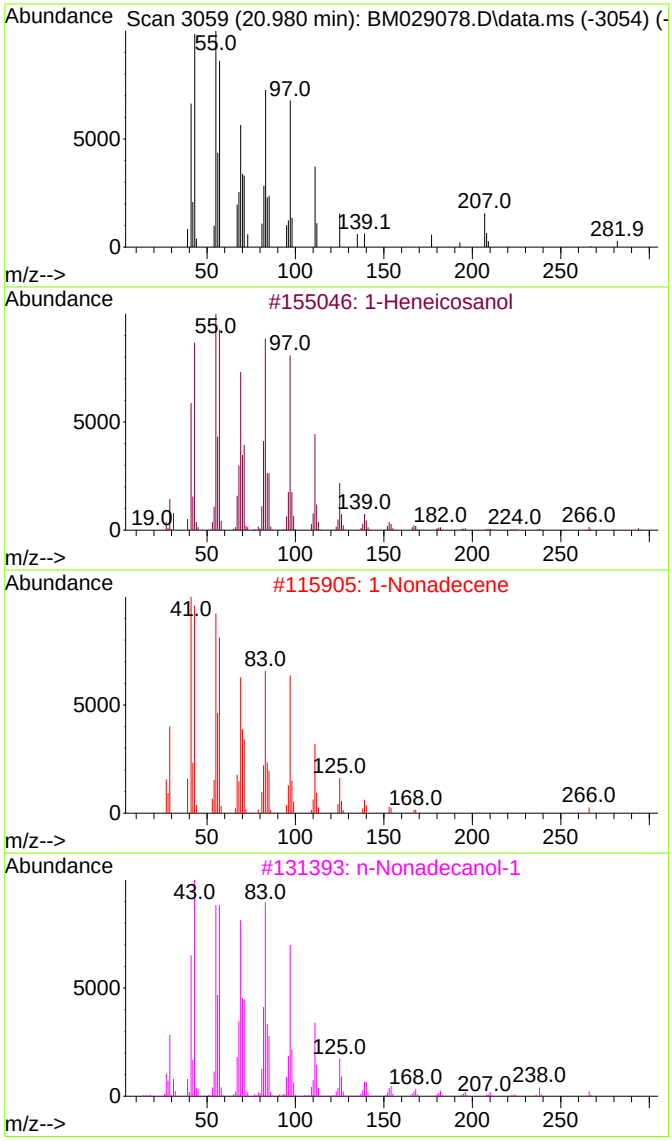
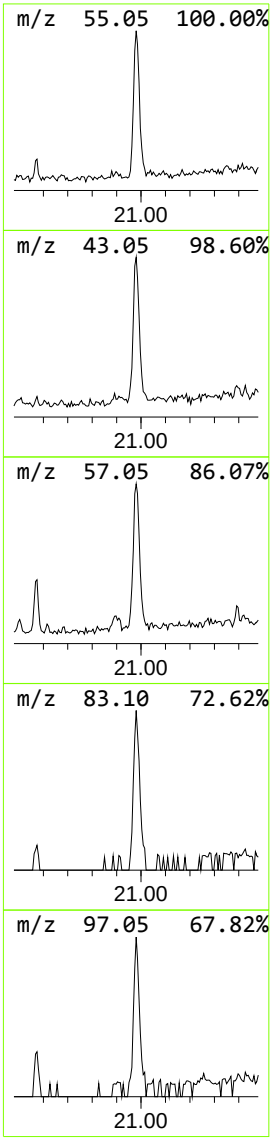
**********

Peak Number 6 1-Heneicosanol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.980 | 8.35 ng | 44655 | Chrysene-d12 | 21.256 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 93 |
| 3 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 90 |
| 4 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 90 |
| 5 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 90 |



Tentatively Identified Compound (LSC) summary

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Operator : CG/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** FK-BPM-03-021-ABCD

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 1,3-Dioxolane, ... | 3.199 | 3.1 | ng | 6205 | 1 | 7.663 | 39728 | 20.0 |
| Oxirane, [(1-me... | 4.763 | 5.0 | ng | 10032 | 1 | 7.663 | 39728 | 20.0 |
| Dodecanoic acid | 17.974 | 2.8 | ng | 10953 | 4 | 17.080 | 79216 | 20.0 |
| unknown18.715 | 18.715 | 3.8 | ng | 15088 | 4 | 17.080 | 79216 | 20.0 |
| Decanoic acid, ... | 19.256 | 2.0 | ng | 10982 | 5 | 21.256 | 106963 | 20.0 |
| 1-Heneicosanol | 20.980 | 8.3 | ng | 44655 | 5 | 21.256 | 106963 | 20.0 |