LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** GBNK2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

Signal : TIC: BM037735.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.434 | 4 | 8 | 12 | rBV | 45313 | 63256 | 0.65% | 0.072% |
| 2 | 3.475 | 12 | 15 | 19 | rVB2 | 25350 | 34958 | 0.36% | 0.040% |
| 3 | 3.881 | 81 | 84 | 98 | rBV | 152696 | 313339 | 3.21% | 0.359% |
| 4 | 4.111 | 120 | 123 | 129 | rVB | 23529 | 34255 | 0.35% | 0.039% |
| 5 | 4.211 | 137 | 140 | 149 | rVB2 | 20532 | 34040 | 0.35% | 0.039% |
| 6 | 4.328 | 156 | 160 | 165 | rBV | 24124 | 32384 | 0.33% | 0.037% |
| 7 | 5.181 | 301 | 305 | 311 | rVB7 | 7666 | 17108 | 0.18% | 0.020% |
| 8 | 5.569 | 367 | 371 | 374 | rBV4 | 8393 | 13285 | 0.14% | 0.015% |
| 9 | 7.258 | 650 | 658 | 665 | rVB | 221800 | 347294 | 3.56% | 0.398% |
| 10 | 7.428 | 679 | 687 | 698 | rBV | 827613 | 1259372 | 12.91% | 1.442% |
| 11 | 7.634 | 714 | 722 | 729 | rBV | 747827 | 1169015 | 11.99% | 1.339% |
| 12 | 7.722 | 732 | 737 | 740 | rBV6 | 6091 | 10654 | 0.11% | 0.012% |
| 13 | 8.110 | 796 | 803 | 810 | rBV | 883926 | 1362251 | 13.97% | 1.560% |
| 14 | 8.816 | 916 | 923 | 934 | rBV | 612103 | 971861 | 9.96% | 1.113% |
| 15 | 9.281 | 993 | 1002 | 1009 | rBV | 1085994 | 1736889 | 17.81% | 1.989% |
| 16 | 9.510 | 1037 | 1041 | 1047 | rBV2 | 8588 | 12641 | 0.13% | 0.014% |
| 17 | 10.004 | 1117 | 1125 | 1133 | rBV | 761929 | 1216431 | 12.47% | 1.393% |
| 18 | 10.222 | 1156 | 1162 | 1170 | rBV2 | 52478 | 91606 | 0.94% | 0.105% |
| 19 | 10.546 | 1208 | 1217 | 1226 | rBV | 1125956 | 1806428 | 18.52% | 2.069% |
| 20 | 10.934 | 1275 | 1283 | 1291 | rVB | 1263030 | 2111712 | 21.65% | 2.419% |
| 21 | 11.063 | 1298 | 1305 | 1318 | rBV | 1039684 | 1725750 | 17.69% | 1.977% |
| 22 | 11.404 | 1357 | 1363 | 1370 | rBV | 221628 | 347653 | 3.56% | 0.398% |
| 23 | 11.451 | 1370 | 1371 | 1380 | rVB8 | 8645 | 14227 | 0.15% | 0.016% |
| 24 | 11.698 | 1408 | 1413 | 1423 | rVB8 | 10965 | 28567 | 0.29% | 0.033% |
| 25 | 12.175 | 1487 | 1494 | 1499 | rBV | 69345 | 112219 | 1.15% | 0.129% |
| 26 | 12.228 | 1499 | 1503 | 1509 | rVB8 | 8375 | 15727 | 0.16% | 0.018% |
| 27 | 12.510 | 1546 | 1551 | 1558 | rBV3 | 57960 | 102401 | 1.05% | 0.117% |
| 28 | 13.010 | 1631 | 1636 | 1641 | rBV | 68279 | 99665 | 1.02% | 0.114% |
| 29 | 13.098 | 1647 | 1651 | 1656 | rVB5 | 5835 | 11412 | 0.12% | 0.013% |
| 30 | 13.275 | 1678 | 1681 | 1688 | rVB | 16277 | 22275 | 0.23% | 0.026% |
| 31 | 13.628 | 1733 | 1741 | 1747 | rBV | 93293 | 150788 | 1.55% | 0.173% |
| 32 | 14.139 | 1820 | 1828 | 1837 | rBV | 2476057 | 3312903 | 33.97% | 3.794% |
| 33 | 14.434 | 1871 | 1878 | 1888 | rBV | 2647872 | 3805507 | 39.02% | 4.358% |
| 34 | 14.616 | 1902 | 1909 | 1912 | rBV8 | 6314 | 11530 | 0.12% | 0.013% |
| 35 | 14.686 | 1915 | 1921 | 1923 | rBV5 | 13080 | 15940 | 0.16% | 0.018% |
| 36 | 14.734 | 1923 | 1929 | 1937 | rVB | 2012917 | 2944140 | 30.19% | 3.372% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 14.916 | 1954 | 1960 | 1969 | rBV | 207956 | 330129 | 3.38% | 0.378% |
| 38 | 15.128 | 1991 | 1996 | 2004 | rBV | 145283 | 224077 | 2.30% | 0.257% |
| 39 | 15.622 | 2072 | 2080 | 2085 | rBV3 | 24894 | 37611 | 0.39% | 0.043% |
| 40 | 15.722 | 2088 | 2097 | 2109 | rBV | 3515671 | 4848847 | 49.71% | 5.553% |
| 41 | 15.828 | 2109 | 2115 | 2123 | rBV | 693790 | 919633 | 9.43% | 1.053% |
| 42 | 15.963 | 2131 | 2138 | 2145 | rVB10 | 17030 | 37419 | 0.38% | 0.043% |
| 43 | 16.075 | 2153 | 2157 | 2161 | rBV7 | 6316 | 11310 | 0.12% | 0.013% |
| 44 | 16.263 | 2184 | 2189 | 2193 | rBV | 45364 | 58894 | 0.60% | 0.067% |
| 45 | 16.316 | 2193 | 2198 | 2202 | rBV | 108445 | 140066 | 1.44% | 0.160% |
| 46 | 16.416 | 2210 | 2215 | 2219 | rVB7 | 11034 | 16848 | 0.17% | 0.019% |
| 47 | 16.939 | 2300 | 2304 | 2310 | rVB4 | 21946 | 37729 | 0.39% | 0.043% |
| 48 | 17.063 | 2321 | 2325 | 2329 | rVB5 | 9362 | 14338 | 0.15% | 0.016% |
| 49 | 17.116 | 2329 | 2334 | 2338 | rBV2 | 50712 | 77670 | 0.80% | 0.089% |
| 50 | 17.169 | 2338 | 2343 | 2348 | rVV | 127225 | 191899 | 1.97% | 0.220% |
| 51 | 17.251 | 2348 | 2357 | 2371 | rVB | 992859 | 1490198 | 15.28% | 1.707% |
| 52 | 17.469 | 2388 | 2394 | 2405 | rBV | 2455267 | 3569693 | 36.60% | 4.088% |
| 53 | 17.569 | 2405 | 2411 | 2421 | rBV | 3999009 | 5517587 | 56.57% | 6.319% |
| 54 | 17.651 | 2421 | 2425 | 2428 | rVV5 | 32584 | 35855 | 0.37% | 0.041% |
| 55 | 17.739 | 2434 | 2440 | 2444 | rBV | 4227936 | 5100960 | 52.30% | 5.842% |
| 56 | 17.786 | 2444 | 2448 | 2453 | rVB | 8308335 | 9753429 | 100.00% | 11.171% |
| 57 | 18.016 | 2484 | 2487 | 2491 | rVB | 45484 | 53791 | 0.55% | 0.062% |
| 58 | 18.074 | 2492 | 2497 | 2504 | rBV | 135389 | 212245 | 2.18% | 0.243% |
| 59 | 18.127 | 2504 | 2506 | 2509 | rVB4 | 17424 | 15721 | 0.16% | 0.018% |
| 60 | 18.345 | 2539 | 2543 | 2547 | rBV3 | 49452 | 68683 | 0.70% | 0.079% |
| 61 | 18.380 | 2547 | 2549 | 2553 | rVV5 | 14006 | 16679 | 0.17% | 0.019% |
| 62 | 18.422 | 2553 | 2556 | 2561 | rVB | 27310 | 34754 | 0.36% | 0.040% |
| 63 | 18.604 | 2583 | 2587 | 2590 | rBV3 | 49158 | 70933 | 0.73% | 0.081% |
| 64 | 18.680 | 2593 | 2600 | 2608 | rVB | 404406 | 631676 | 6.48% | 0.723% |
| 65 | 19.045 | 2657 | 2662 | 2666 | rBV | 740552 | 831765 | 8.53% | 0.953% |
| 66 | 19.086 | 2666 | 2669 | 2681 | rVB | 1495849 | 1760196 | 18.05% | 2.016% |
| 67 | 19.416 | 2722 | 2725 | 2730 | rVB3 | 67745 | 79415 | 0.81% | 0.091% |
| 68 | 19.486 | 2732 | 2737 | 2741 | rBV | 65082 | 112519 | 1.15% | 0.129% |
| 69 | 19.610 | 2755 | 2758 | 2762 | rBV4 | 52429 | 63701 | 0.65% | 0.073% |
| 70 | 19.851 | 2790 | 2799 | 2803 | rBV | 5011206 | 6651488 | 68.20% | 7.618% |
| 71 | 19.886 | 2803 | 2805 | 2811 | rVB | 438056 | 474371 | 4.86% | 0.543% |
| 72 | 20.163 | 2848 | 2852 | 2855 | rBV | 744881 | 796495 | 8.17% | 0.912% |
| 73 | 20.198 | 2855 | 2858 | 2863 | rVB | 1393089 | 1460931 | 14.98% | 1.673% |
| 74 | 20.821 | 2962 | 2964 | 2968 | rVB | 77441 | 76917 | 0.79% | 0.088% |
| 75 | 20.974 | 2987 | 2990 | 2993 | rBV | 71357 | 73259 | 0.75% | 0.084% |
| 76 | 21.133 | 3014 | 3017 | 3019 | rBV | 225584 | 219602 | 2.25% | 0.252% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BM112322.M
Title : SVOA CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 21.163 | 3019 | 3022 | 3028 | rVB | 402724 | 465457 | 4.77% | 0.533% |
| 78 | 21.639 | 3097 | 3103 | 3109 | rBV | 2980759 | 3987459 | 40.88% | 4.567% |
| 79 | 22.033 | 3167 | 3170 | 3173 | rBV | 261267 | 297789 | 3.05% | 0.341% |
| 80 | 22.068 | 3173 | 3176 | 3180 | rVB | 490501 | 558707 | 5.73% | 0.640% |
| 81 | 23.074 | 3344 | 3347 | 3350 | rBV | 164815 | 202732 | 2.08% | 0.232% |
| 82 | 23.115 | 3350 | 3354 | 3360 | rVB | 452293 | 660947 | 6.78% | 0.757% |
| 83 | 23.968 | 3492 | 3499 | 3514 | rVB2 | 2908780 | 6158646 | 63.14% | 7.054% |
| 84 | 24.127 | 3519 | 3526 | 3538 | rVB2 | 1689060 | 3501895 | 35.90% | 4.011% |

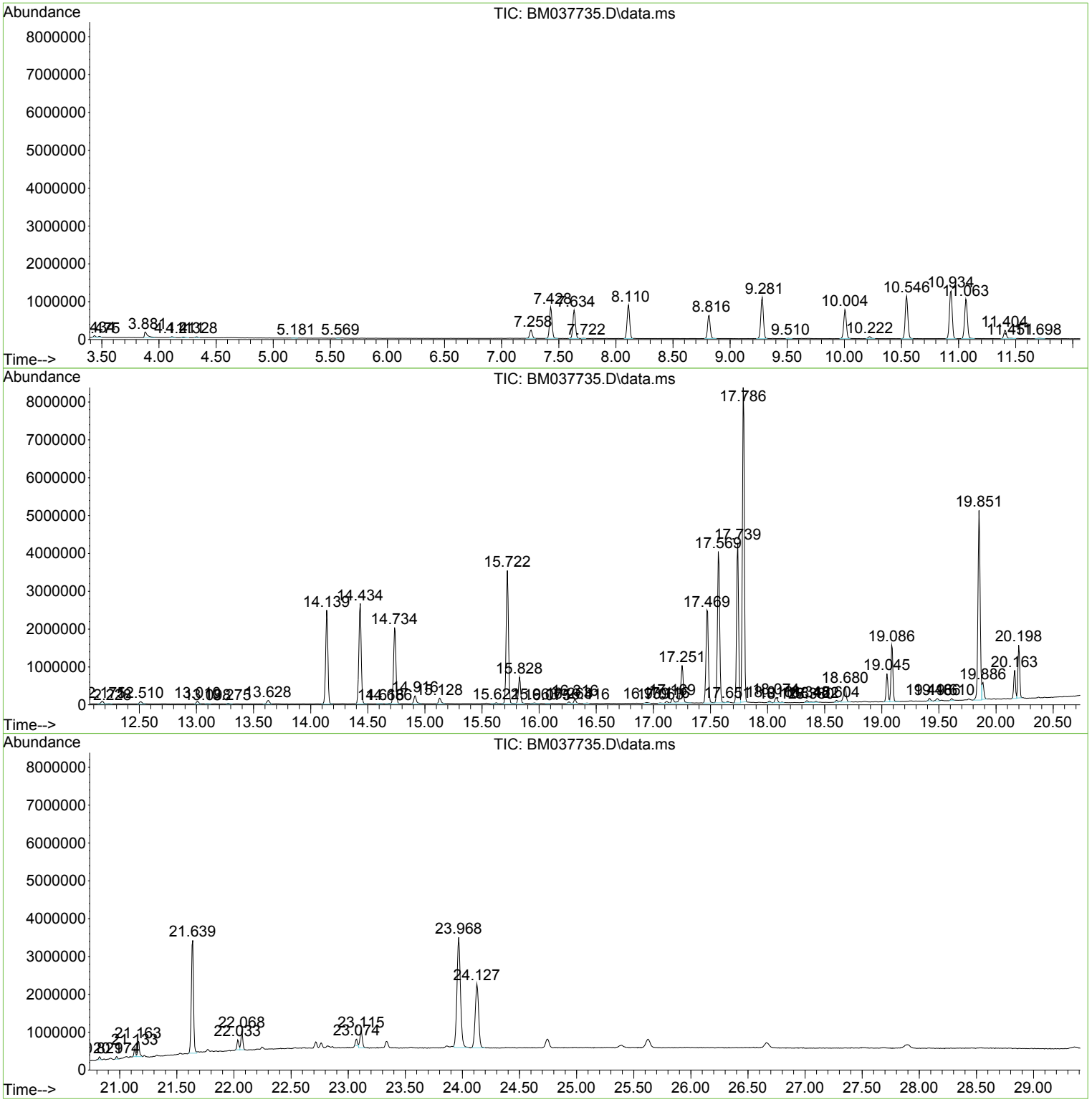
Sum of corrected areas: 87312448

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

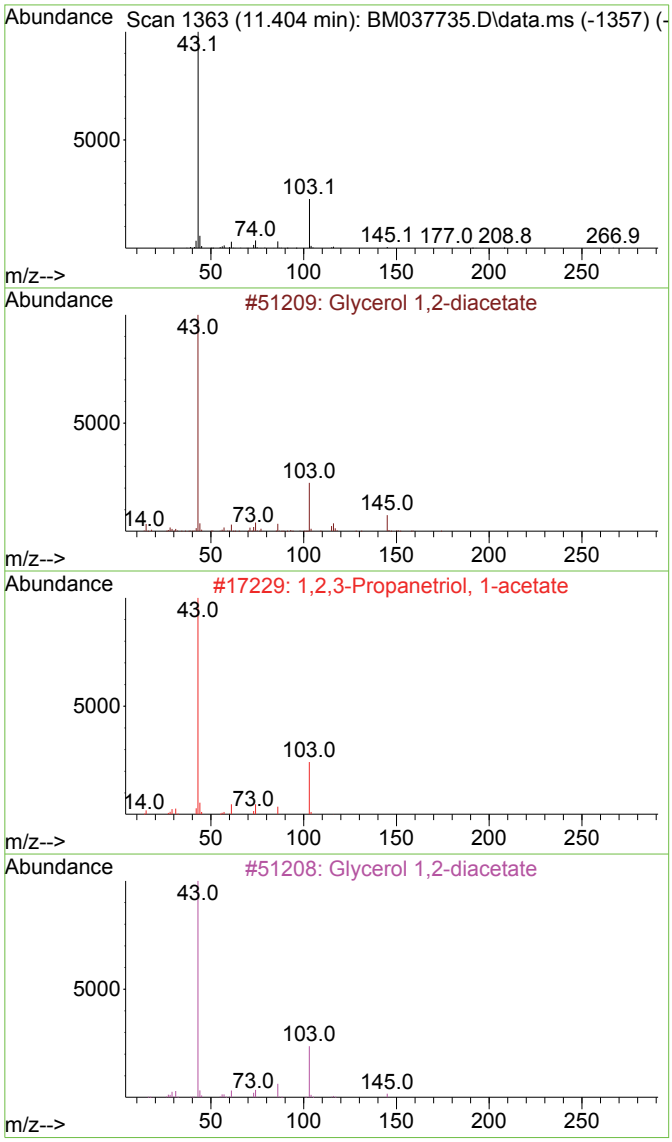
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

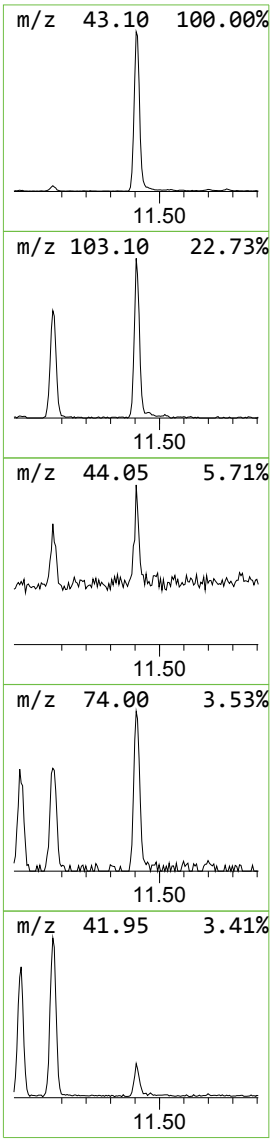
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Glycerol 1,2-diacetate Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.404 | 3.29 ng/ul | 347653 | Naphthalene-d8 | 10.934 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Glycerol 1,2-diacetate | 176 | C7H12O5 | 000102-62-5 | 56 |
| 2 | 1,2,3-Propanetriol, 1-acetate | 134 | C5H10O4 | 000106-61-6 | 50 |
| 3 | Glycerol 1,2-diacetate | 176 | C7H12O5 | 000102-62-5 | 39 |
| 4 | 1,2,3-Propanetriol, 1-acetate | 134 | C5H10O4 | 000106-61-6 | 38 |
| 5 | 1,2-Epoxy-3-propyl acetate | 116 | C5H8O3 | 006387-89-9 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

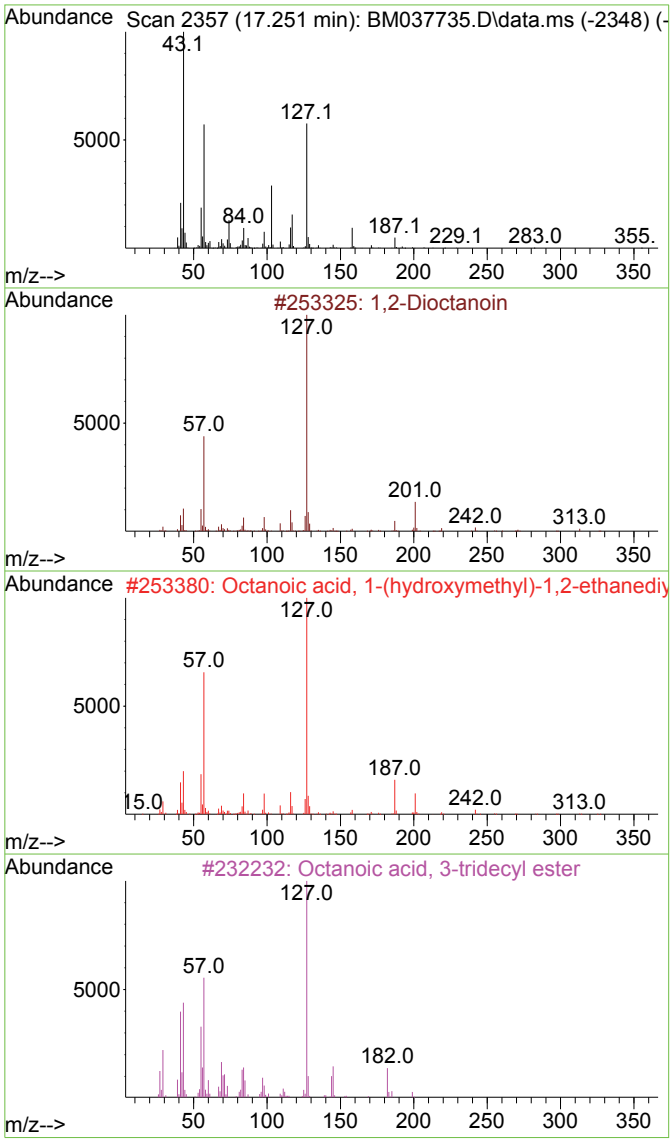
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

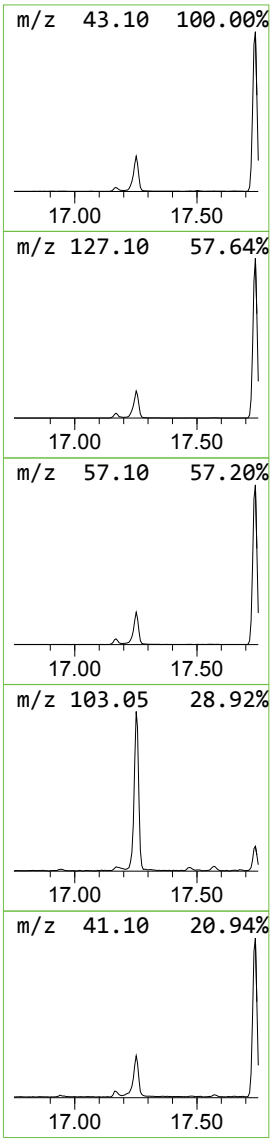
**********

Peak Number 2 unknown-01 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.251 | 8.35 ng/ul | 1490200 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Dioctanoin | 344 | C19H36O5 | 001069-87-0 | 47 |
| 2 | Octanoic acid, 1-(hydroxymethyl)... | 344 | C19H36O5 | 060514-48-9 | 40 |
| 3 | Octanoic acid, 3-tridecyl ester | 326 | C21H42O2 | 1010280-62-5 | 32 |
| 4 | 1,3,5-Triazin-2(1H)-one, 4,6-dia... | 127 | C3H5N5O | 000645-92-1 | 27 |
| 5 | 6-Azathymine | 127 | C4H5N3O2 | 000932-53-6 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

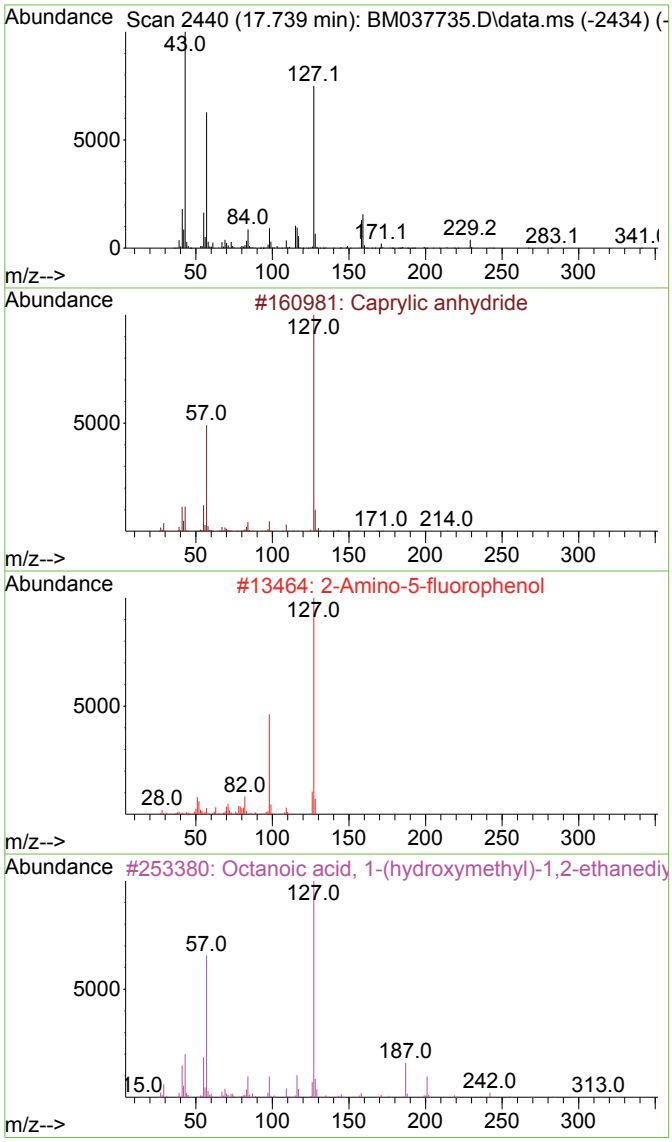
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

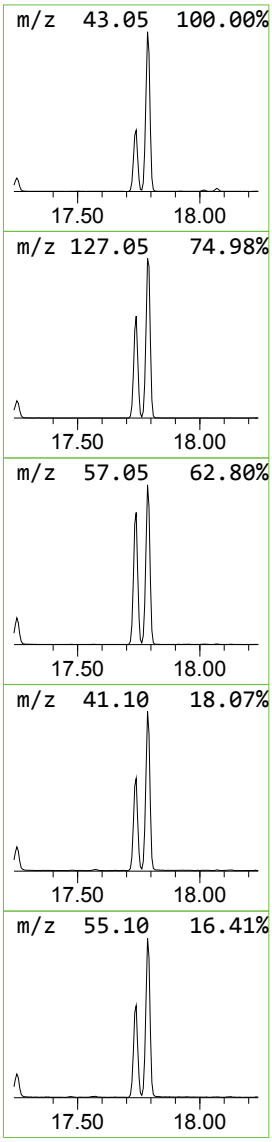
**********

Peak Number 3 Caprylic anhydride Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.739 | 28.58 ng/ul | 5100960 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Caprylic anhydride | 270 | C16H30O3 | 000623-66-5 | 50 |
| 2 | 2-Amino-5-fluorophenol | 127 | C6H6FNO | 053981-24-1 | 49 |
| 3 | Octanoic acid, 1-(hydroxymethyl)... | 344 | C19H36O5 | 060514-48-9 | 45 |
| 4 | 1,2-Dioctanoin | 344 | C19H36O5 | 001069-87-0 | 45 |
| 5 | Cyclobutylamine, N-trimethylacetyl- | 155 | C9H17NO | 1339633-43-0 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

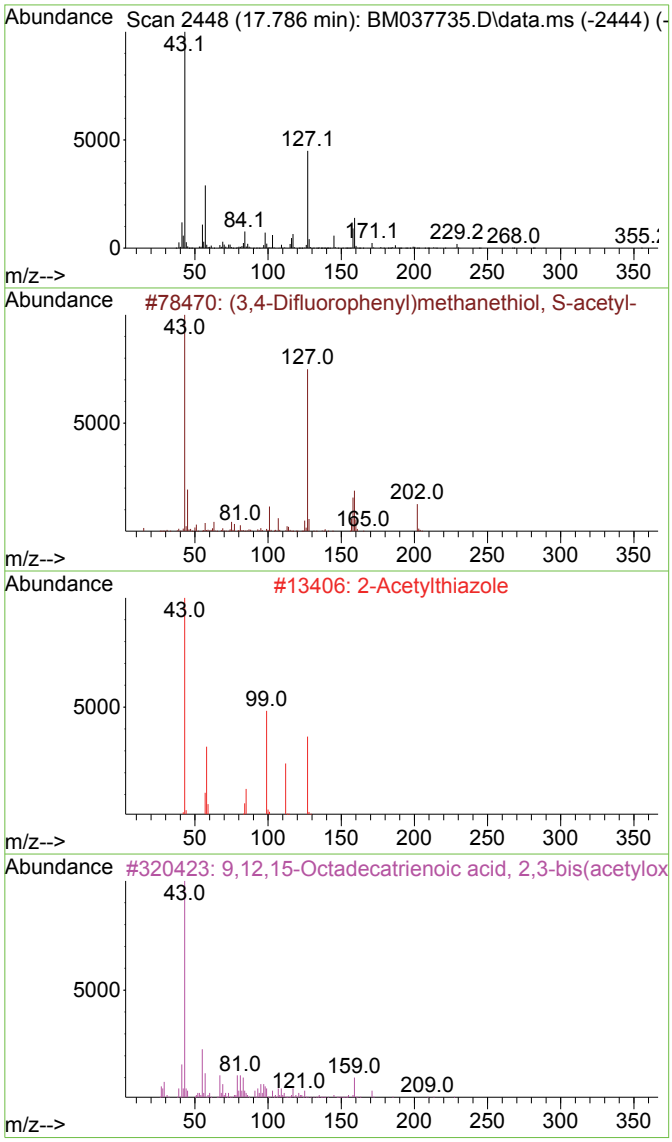
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

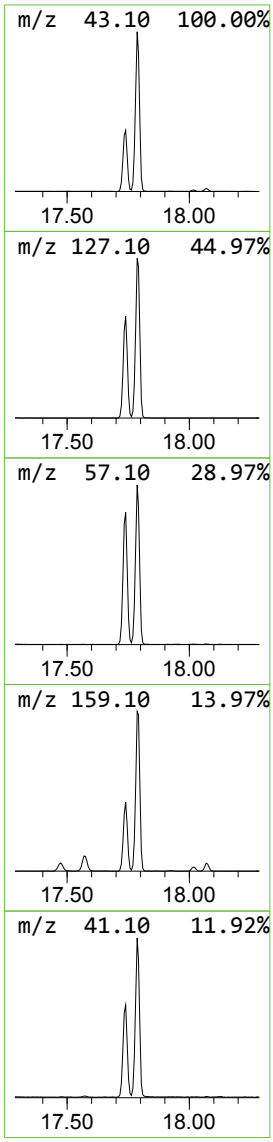
**********

Peak Number 4 unknown-02 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.786 | 54.65 ng/ul | 9753430 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (3,4-Difluorophenyl)methanethiol... | 202 | C9H8F2OS | 873463-82-2 | 33 |
| 2 | 2-Acetylthiazole | 127 | C5H5NOS | 024295-03-2 | 23 |
| 3 | 9,12,15-Octadecatrienoic acid, 2... | 436 | C25H40O6 | 055320-02-0 | 10 |
| 4 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 10 |
| 5 | N-Acetylpyrrolidone | 127 | C6H9NO2 | 000932-17-2 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

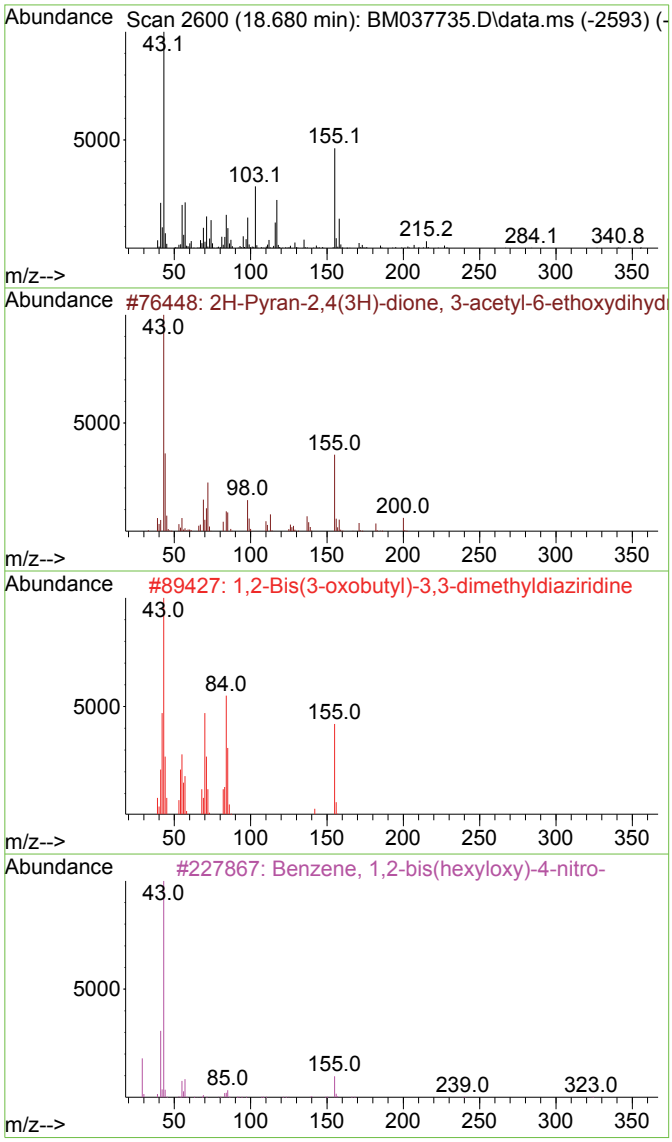
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

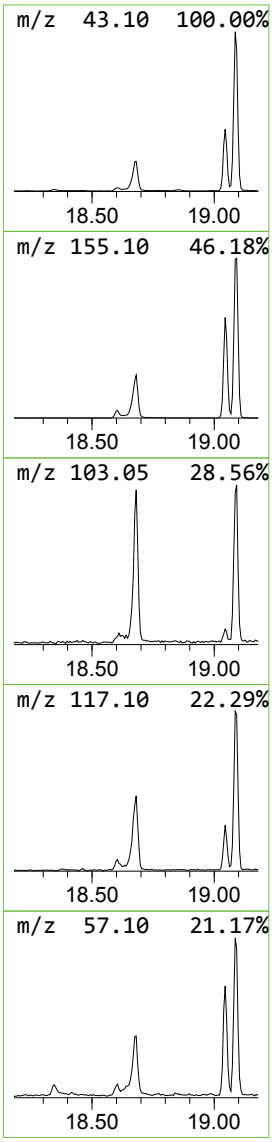
**********

Peak Number 5 unknown-03 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.680 | 3.54 ng/ul | 631676 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2H-Pyran-2,4(3H)-dione, 3-acetyl... | 200 | C9H12O5 | 1000318-74-8 | 43 |
| 2 | 1,2-Bis(3-oxobutyl)-3,3-dimethyl... | 212 | C11H20N2O2 | 1000283-18-4 | 12 |
| 3 | Benzene, 1,2-bis(hexyloxy)-4-nitro- | 323 | C18H29NO4 | 1000305-14-9 | 10 |
| 4 | 1-Pentanamine, N-(1-methylethyl)... | 158 | C8H18N2O | 028023-77-0 | 9 |
| 5 | Hexanoic acid, hexyl ester | 200 | C12H24O2 | 006378-65-0 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

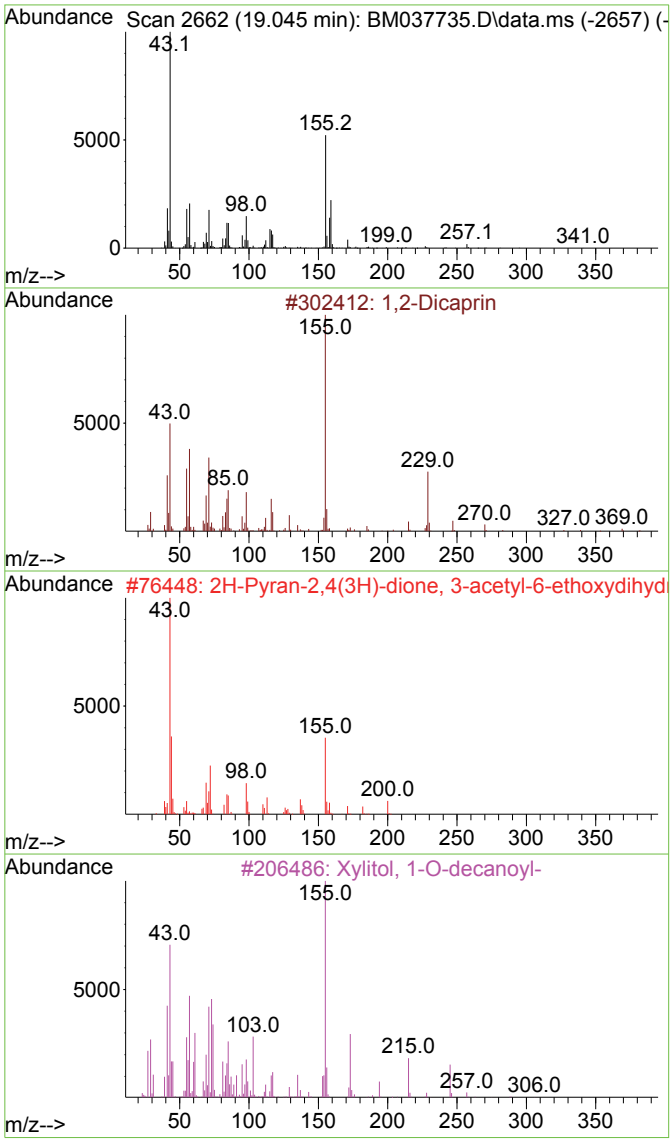
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

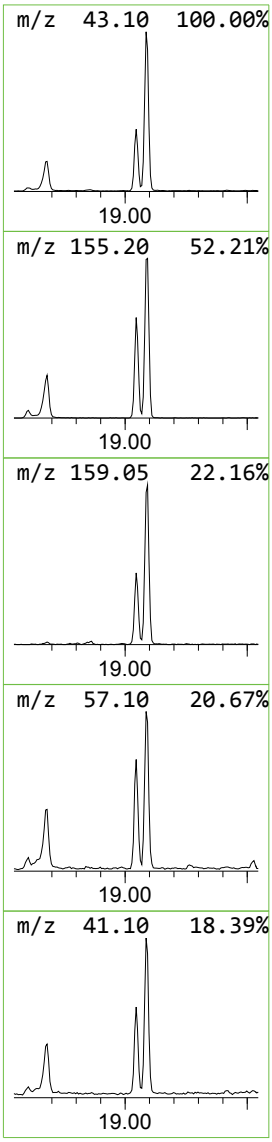
**********

Peak Number 6 1,2-Dicaprin Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.045 | 4.66 ng/ul | 831765 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Dicaprin | 400 | C23H44O5 | 017863-69-3 | 53 |
| 2 | 2H-Pyran-2,4(3H)-dione, 3-acetyl... | 200 | C9H12O5 | 1000318-74-8 | 42 |
| 3 | Xylitol, 1-O-decanoyl- | 306 | C15H30O6 | 1000155-78-0 | 40 |
| 4 | Decanoic acid, 2-hydroxy-1-(hydr... | 246 | C13H26O4 | 003376-48-5 | 40 |
| 5 | Decanoic anhydride | 326 | C20H38O3 | 002082-76-0 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

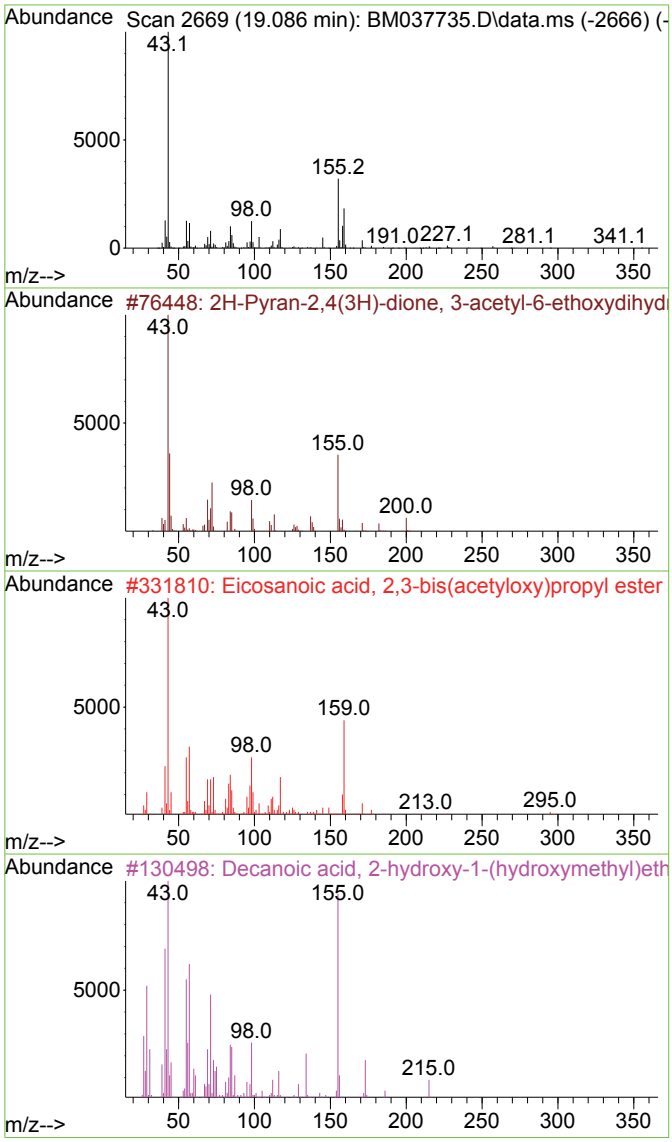
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

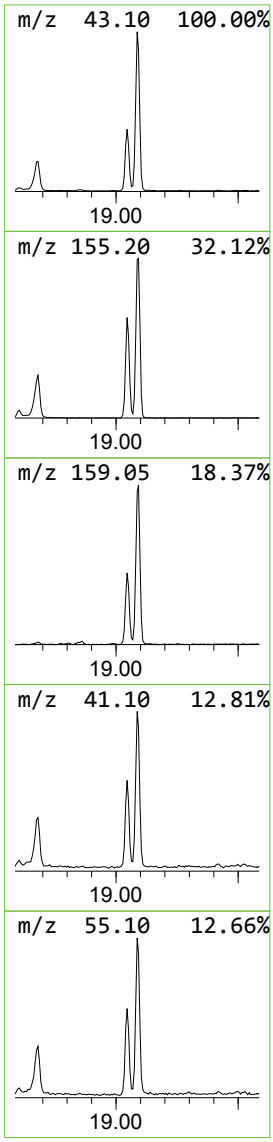
**********

Peak Number 7 unknown-04 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.086 | 9.86 ng/ul | 1760200 | Phenanthrene-d10 | 17.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2H-Pyran-2,4(3H)-dione, 3-acetyl... | 200 | C9H12O5 | 1000318-74-8 | 37 |
| 2 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 37 |
| 3 | Decanoic acid, 2-hydroxy-1-(hydr... | 246 | C13H26O4 | 003376-48-5 | 25 |
| 4 | 1,3,5-Triazin-2(1H)-one, 4-amino... | 155 | C5H9N5O | 007313-54-4 | 17 |
| 5 | Octanoic acid, 3-oxo-, methyl ester | 172 | C9H16O3 | 022348-95-4 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

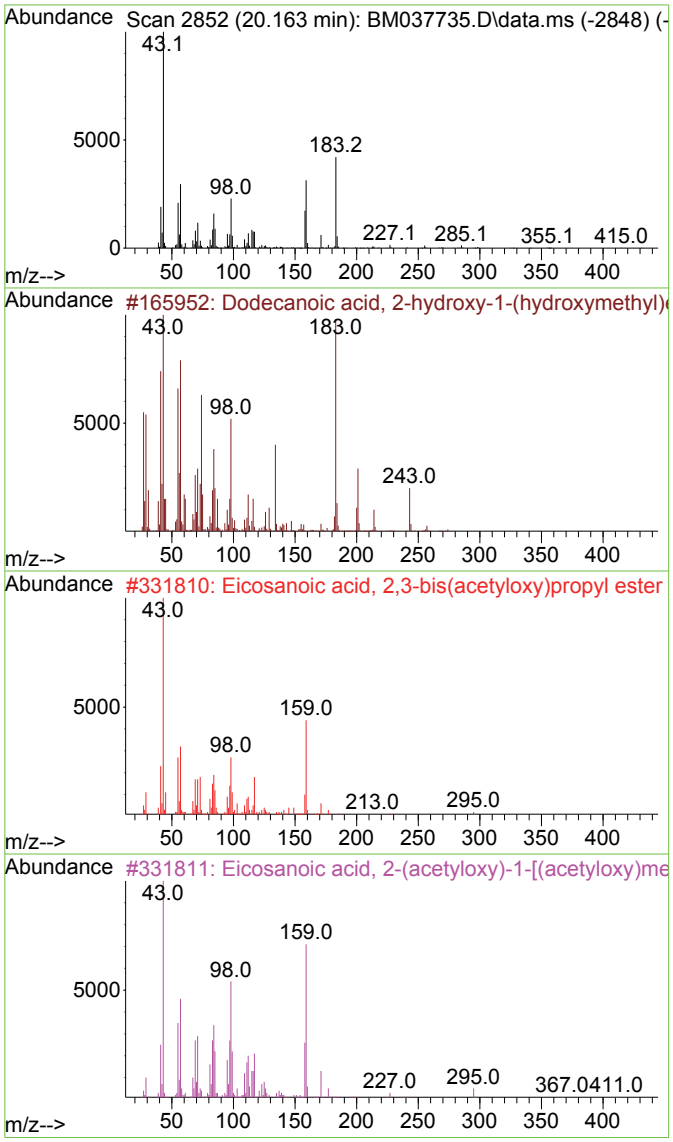
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

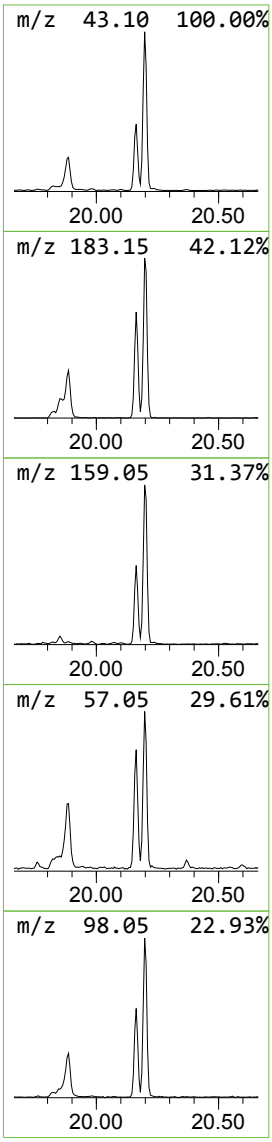
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 Dodecanoic acid, 2-hydroxy-... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.163 | 4.00 ng/ul | 796495 | Chrysene-d12 | 21.639 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid, 2-hydroxy-1-(hy... | 274 | C15H30O4 | 001678-45-1 | 50 |
| 2 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 37 |
| 3 | Eicosanoic acid, 2-(acetyloxy)-1... | 470 | C27H50O6 | 055429-68-0 | 16 |
| 4 | 9-Octadecenoic acid (Z)-, 2,3-bi... | 440 | C25H44O6 | 055401-64-4 | 10 |
| 5 | Dodecanoic acid, ethenyl ester | 226 | C14H26O2 | 002146-71-6 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

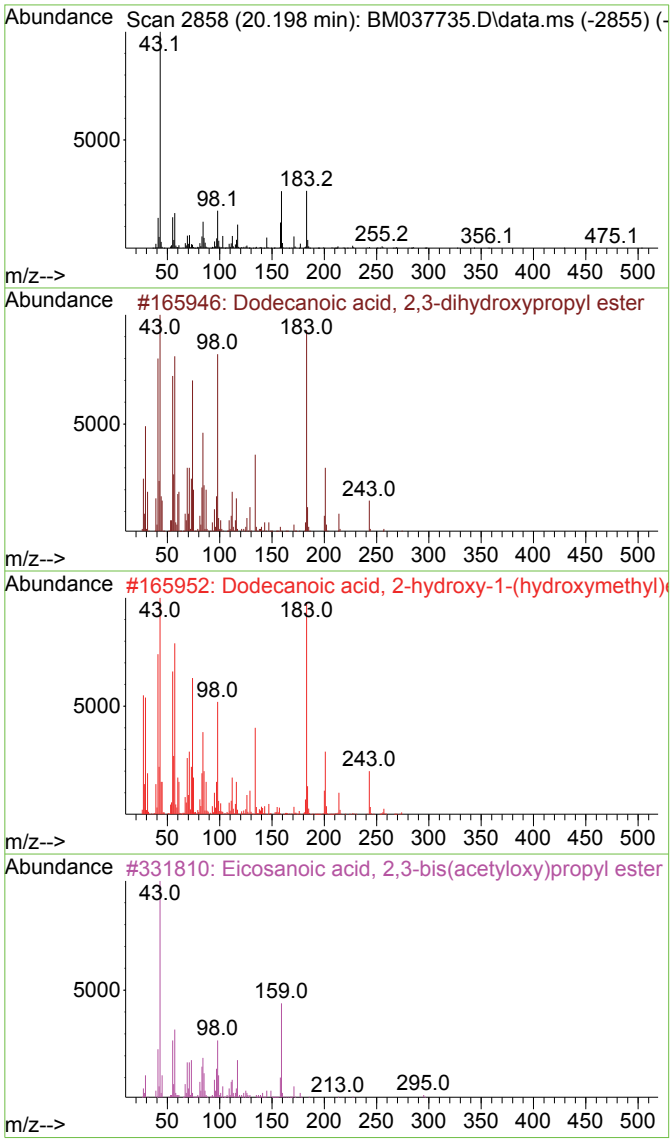
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

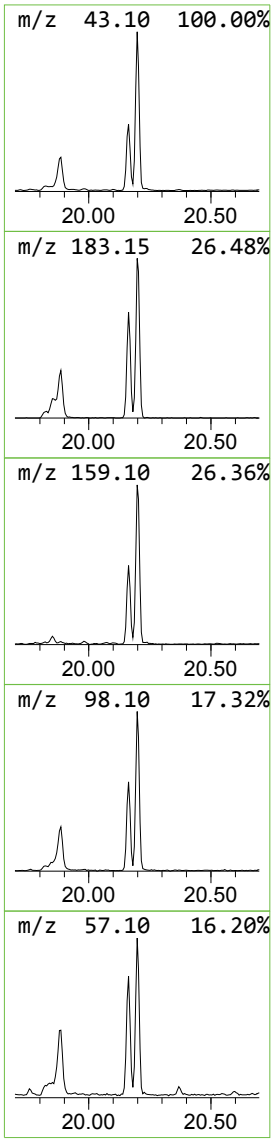
**********

Peak Number 9 unknown-05 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.198 | 7.33 ng/ul | 1460930 | Chrysene-d12 | 21.639 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid, 2,3-dihydroxypr... | 274 | C15H30O4 | 000142-18-7 | 38 |
| 2 | Dodecanoic acid, 2-hydroxy-1-(hy... | 274 | C15H30O4 | 001678-45-1 | 32 |
| 3 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 32 |
| 4 | 9-Octadecenoic acid (Z)-, 2,3-bi... | 440 | C25H44O6 | 055401-64-4 | 17 |
| 5 | Dodecanoyl chloride | 218 | C12H23ClO | 000112-16-3 | 14 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

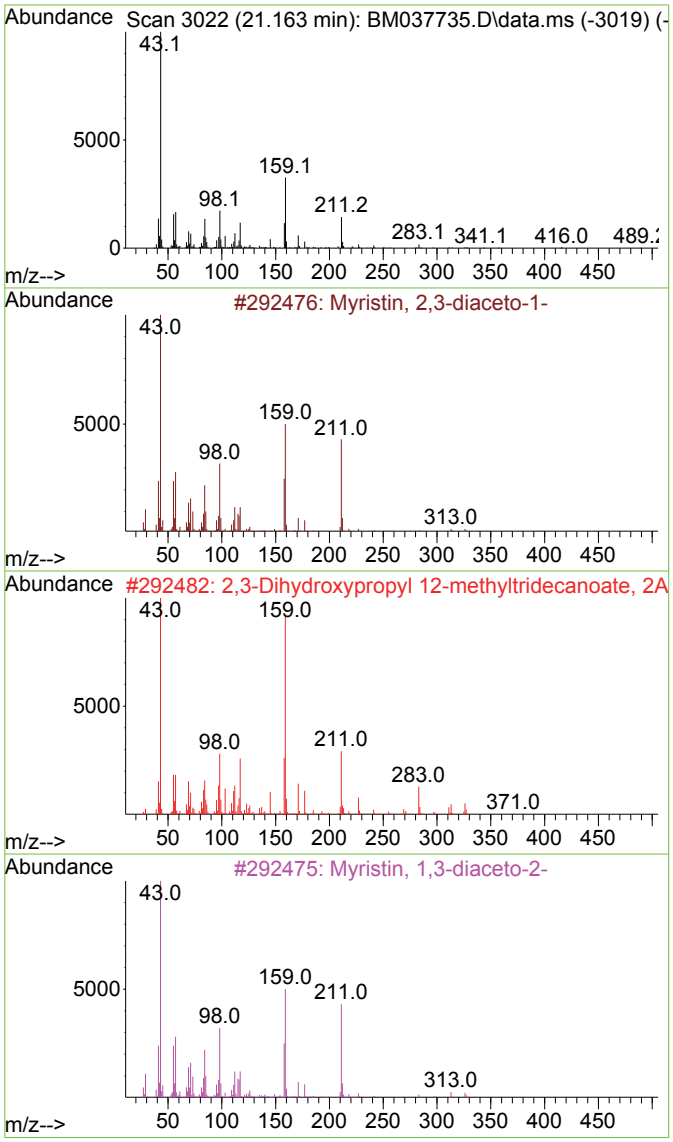
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

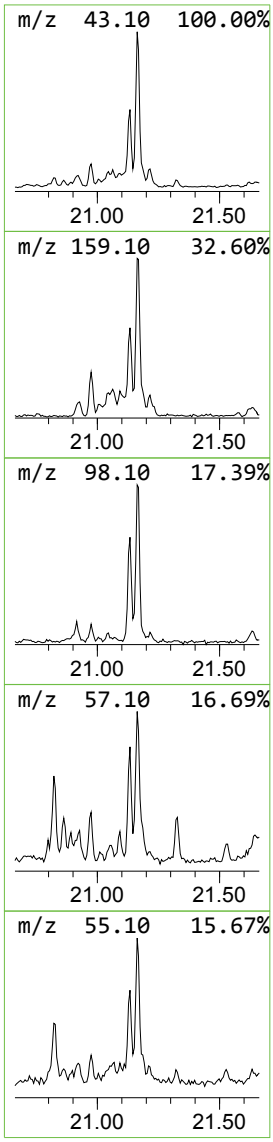
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 Myristin, 2,3-diaceto-1- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.163 | 2.33 ng/ul | 465457 | Chrysene-d12 | 21.639 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Myristin, 2,3-diaceto-1- | 386 | C21H38O6 | 014473-55-3 | 58 |
| 2 | 2,3-Dihydroxypropyl 12-methyltri... | 386 | C21H38O6 | 1000488-66-8 | 56 |
| 3 | Myristin, 1,3-diaceto-2- | 386 | C21H38O6 | 014290-23-4 | 53 |
| 4 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 43 |
| 5 | 9-Octadecenoic acid (Z)-, 2,3-bi... | 440 | C25H44O6 | 055401-64-4 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

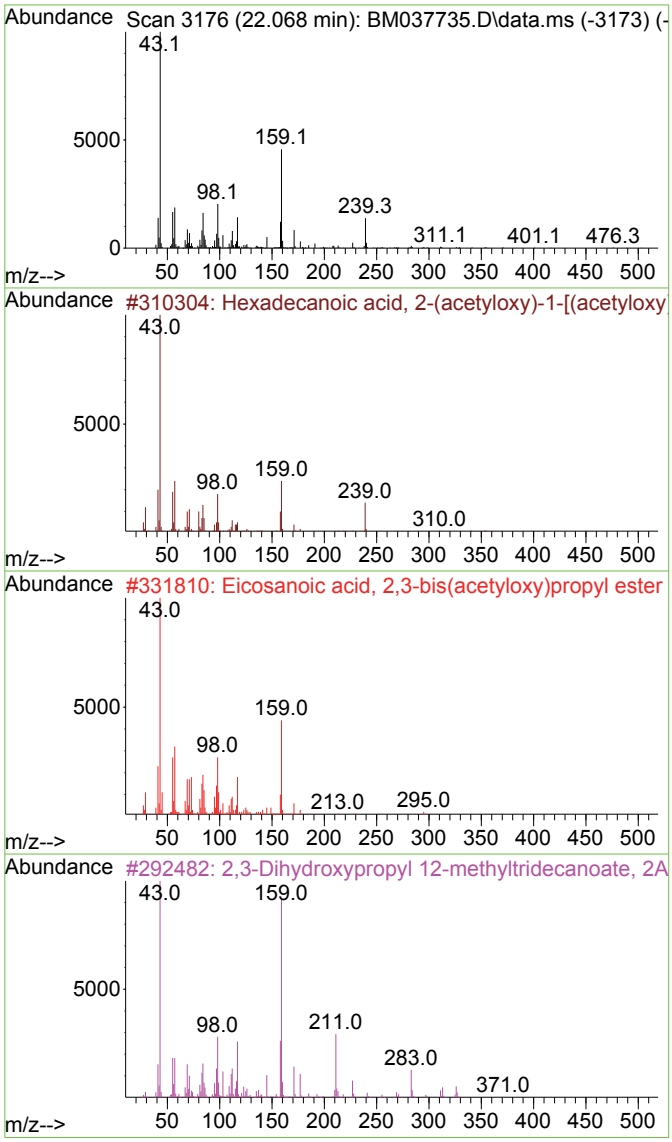
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

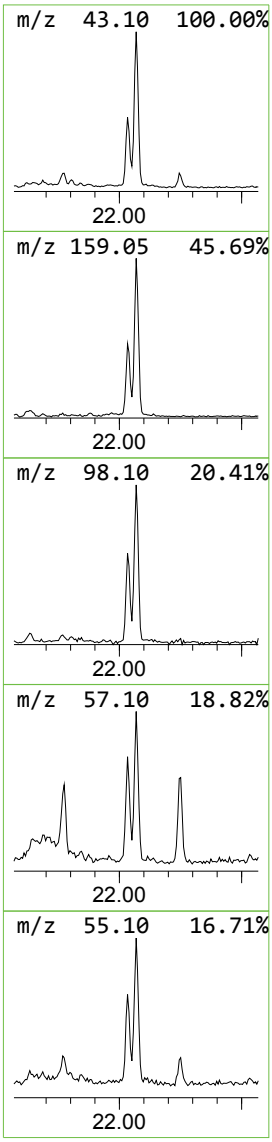
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 Hexadecanoic acid, 2-(acety... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.068 | 2.80 ng/ul | 558707 | Chrysene-d12 | 21.639 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, 2-(acetyloxy)... | 414 | C23H42O6 | 055268-69-4 | 58 |
| 2 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 50 |
| 3 | 2,3-Dihydroxypropyl 12-methyltri... | 386 | C21H38O6 | 1000488-66-8 | 25 |
| 4 | 4,5,6-Trimethyltetrahydro-1,3-ox... | 159 | C7H13NOS | 085333-98-8 | 17 |
| 5 | Thioacetic acid, S-(5-acetylthio... | 234 | C9H14O3S2 | 1000185-15-4 | 17 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

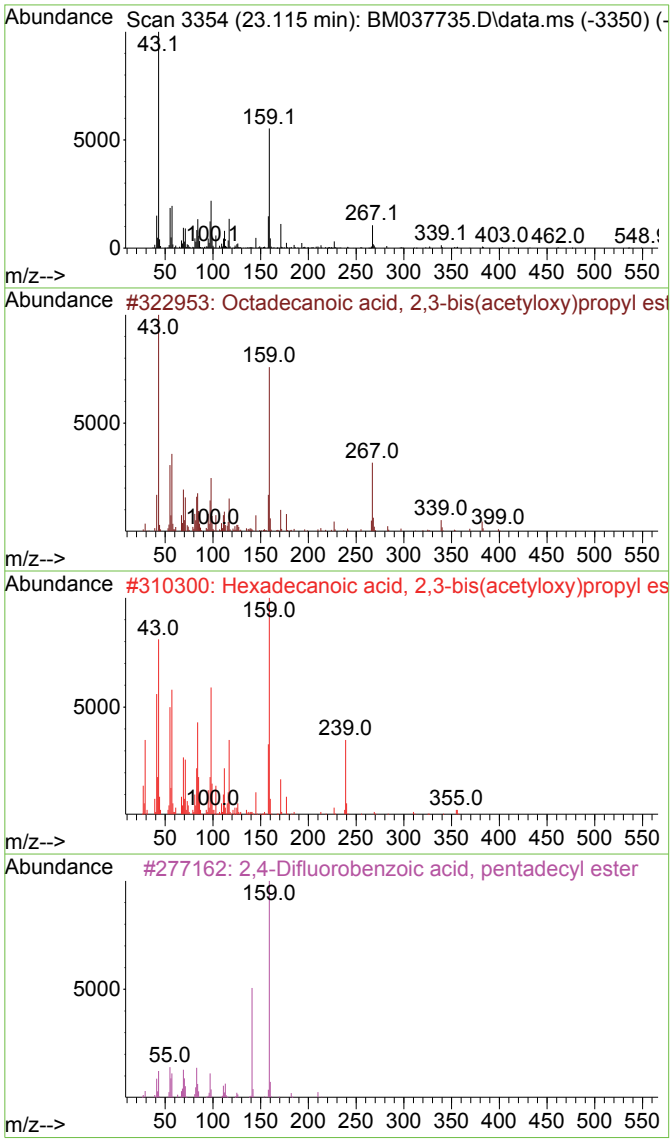
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA CALIBRATION

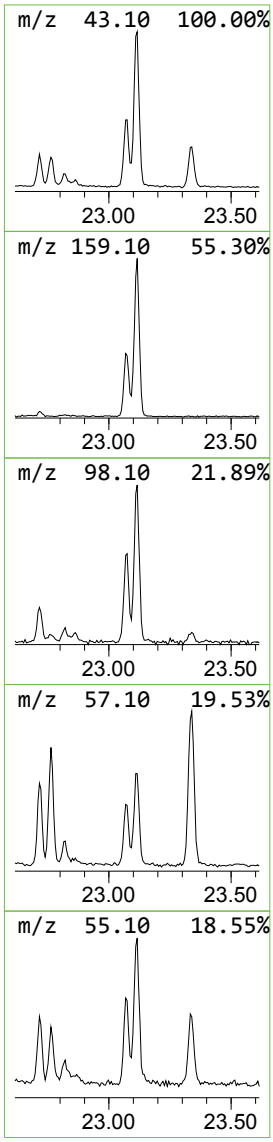
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 12 Octadecanoic acid, 2,3-bis(... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.115 | 3.77 ng/ul | 660947 | Perylene-d12 | 24.127 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid, 2,3-bis(acety... | 442 | C25H46O6 | 033599-07-4 | 83 |
| 2 | Hexadecanoic acid, 2,3-bis(acety... | 414 | C23H42O6 | 055268-70-7 | 58 |
| 3 | 2,4-Difluorobenzoic acid, pentad... | 368 | C22H34F2O2 | 1010338-79-3 | 35 |
| 4 | Eicosanoic acid, 2,3-bis(acetylo... | 470 | C27H50O6 | 055429-67-9 | 35 |
| 5 | 2,3,4-Trifluorobenzoic acid, 3-t... | 358 | C20H29F3O2 | 1000280-61-8 | 32 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112522\
Data File : BM037735.D
Acq On : 26 Nov 2022 16:15
Operator : CG/JU
Sample : N5746-02
Misc :
ALS Vial : 47 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
GBNK2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM112322.M
Quant Title : SVOA 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 |
| Glycerol 1,2-di... | 11.404 | 3.3 | ng/ul | 347653 | 2 | 10.934 | 2111710 | 20.0 |
| unknown-01 | 17.251 | 8.3 | ng/ul | 1490200 | 4 | 17.469 | 3569690 | 20.0 |
| Caprylic anhydride | 17.739 | 28.6 | ng/ul | 5100960 | 4 | 17.469 | 3569690 | 20.0 |
| unknown-02 | 17.786 | 54.6 | ng/ul | 9753430 | 4 | 17.469 | 3569690 | 20.0 |
| unknown-03 | 18.680 | 3.5 | ng/ul | 631676 | 4 | 17.469 | 3569690 | 20.0 |
| 1,2-Dicaprin | 19.045 | 4.7 | ng/ul | 831765 | 4 | 17.469 | 3569690 | 20.0 |
| unknown-04 | 19.086 | 9.9 | ng/ul | 1760200 | 4 | 17.469 | 3569690 | 20.0 |
| Dodecanoic acid... | 20.163 | 4.0 | ng/ul | 796495 | 5 | 21.639 | 3987460 | 20.0 |
| unknown-05 | 20.198 | 7.3 | ng/ul | 1460930 | 5 | 21.639 | 3987460 | 20.0 |
| Myristin, 2,3-d... | 21.163 | 2.3 | ng/ul | 465457 | 5 | 21.639 | 3987460 | 20.0 |
| Hexadecanoic ac... | 22.068 | 2.8 | ng/ul | 558707 | 5 | 21.639 | 3987460 | 20.0 |
| Octadecanoic ac... | 23.115 | 3.8 | ng/ul | 660947 | 6 | 24.127 | 3501900 | 20.0 |