LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** A4BR6

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP020916.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.258 | 42 | 46 | 51 | rVB | 54157 | 68292 | 1.76% | 0.110% |
| 2 | 3.534 | 90 | 93 | 102 | rBV | 42511 | 61585 | 1.59% | 0.099% |
| 3 | 3.669 | 113 | 116 | 134 | rBV | 638082 | 900966 | 23.26% | 1.447% |
| 4 | 3.981 | 164 | 169 | 174 | rVB | 24881 | 36733 | 0.95% | 0.059% |
| 5 | 4.393 | 238 | 239 | 247 | rVB7 | 3307 | 5317 | 0.14% | 0.009% |
| 6 | 4.481 | 251 | 254 | 258 | rVB4 | 3841 | 4635 | 0.12% | 0.007% |
| 7 | 4.899 | 317 | 325 | 331 | rVB2 | 17323 | 41609 | 1.07% | 0.067% |
| 8 | 5.846 | 481 | 486 | 494 | rVB | 10480 | 21261 | 0.55% | 0.034% |
| 9 | 6.381 | 570 | 577 | 579 | rBV7 | 3028 | 6748 | 0.17% | 0.011% |
| 10 | 6.916 | 659 | 668 | 682 | rBV | 870891 | 1590347 | 41.07% | 2.554% |
| 11 | 7.063 | 687 | 693 | 704 | rVV | 794249 | 1220242 | 31.51% | 1.959% |
| 12 | 7.263 | 720 | 727 | 739 | rBV | 969931 | 1618470 | 41.79% | 2.599% |
| 13 | 7.352 | 739 | 742 | 755 | rVB2 | 11811 | 28544 | 0.74% | 0.046% |
| 14 | 7.722 | 793 | 805 | 813 | rBV | 1191342 | 1993988 | 51.49% | 3.202% |
| 15 | 7.793 | 813 | 817 | 830 | rVB3 | 17334 | 38061 | 0.98% | 0.061% |
| 16 | 8.434 | 918 | 926 | 946 | rBV | 1124399 | 2005208 | 51.78% | 3.220% |
| 17 | 8.869 | 993 | 1000 | 1017 | rBV | 923848 | 1579590 | 40.79% | 2.536% |
| 18 | 9.010 | 1020 | 1024 | 1033 | rVB | 6634 | 16410 | 0.42% | 0.026% |
| 19 | 9.234 | 1055 | 1062 | 1070 | rBV | 22678 | 37122 | 0.96% | 0.060% |
| 20 | 9.416 | 1087 | 1093 | 1103 | rBV | 61436 | 112421 | 2.90% | 0.181% |
| 21 | 9.581 | 1113 | 1121 | 1133 | rBV | 847412 | 1366479 | 35.29% | 2.194% |
| 22 | 10.122 | 1205 | 1213 | 1232 | rBV | 1079771 | 2026471 | 52.33% | 3.254% |
| 23 | 10.487 | 1265 | 1275 | 1288 | rBV | 1696624 | 3067159 | 79.20% | 4.925% |
| 24 | 10.634 | 1291 | 1300 | 1317 | rBV | 990520 | 1965674 | 50.76% | 3.156% |
| 25 | 11.028 | 1360 | 1367 | 1382 | rBV7 | 14588 | 42181 | 1.09% | 0.068% |
| 26 | 11.234 | 1394 | 1402 | 1422 | rBV | 63597 | 204642 | 5.28% | 0.329% |
| 27 | 11.716 | 1481 | 1484 | 1486 | rBV4 | 3723 | 4112 | 0.11% | 0.007% |
| 28 | 11.887 | 1508 | 1513 | 1521 | rVB7 | 7139 | 13039 | 0.34% | 0.021% |
| 29 | 12.081 | 1541 | 1546 | 1553 | rBV | 21259 | 33435 | 0.86% | 0.054% |
| 30 | 12.322 | 1582 | 1587 | 1593 | rBV3 | 5422 | 12037 | 0.31% | 0.019% |
| 31 | 12.751 | 1657 | 1660 | 1663 | rVB5 | 4003 | 4348 | 0.11% | 0.007% |
| 32 | 12.810 | 1665 | 1670 | 1673 | rVB7 | 2987 | 5471 | 0.14% | 0.009% |
| 33 | 12.851 | 1673 | 1677 | 1680 | rBV6 | 4227 | 6310 | 0.16% | 0.010% |
| 34 | 12.881 | 1680 | 1682 | 1687 | rVB6 | 3086 | 4176 | 0.11% | 0.007% |
| 35 | 12.940 | 1687 | 1692 | 1697 | rBV8 | 4285 | 10125 | 0.26% | 0.016% |
| 36 | 13.151 | 1718 | 1728 | 1732 | rBV3 | 18010 | 34421 | 0.89% | 0.055% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 13.234 | 1738 | 1742 | 1747 | rVB8 | 4539 | 7501 | 0.19% | 0.012% |
| 38 | 13.304 | 1747 | 1754 | 1759 | rBV8 | 5924 | 11828 | 0.31% | 0.019% |
| 39 | 13.528 | 1787 | 1792 | 1794 | rBV6 | 3807 | 5305 | 0.14% | 0.009% |
| 40 | 13.669 | 1811 | 1816 | 1820 | rBV8 | 3592 | 6576 | 0.17% | 0.011% |
| 41 | 13.757 | 1822 | 1831 | 1845 | rBV | 1818271 | 2741387 | 70.79% | 4.402% |
| 42 | 14.039 | 1869 | 1879 | 1897 | rBV2 | 1842025 | 3307701 | 85.41% | 5.311% |
| 43 | 14.245 | 1906 | 1914 | 1920 | rBV5 | 11623 | 19705 | 0.51% | 0.032% |
| 44 | 14.351 | 1920 | 1932 | 1941 | rBV | 2381741 | 3872668 | 100.00% | 6.219% |
| 45 | 14.434 | 1941 | 1946 | 1951 | rVB6 | 11417 | 19902 | 0.51% | 0.032% |
| 46 | 14.557 | 1957 | 1967 | 1968 | rBV | 450643 | 666718 | 17.22% | 1.071% |
| 47 | 14.575 | 1968 | 1970 | 1974 | rVV | 501509 | 787167 | 20.33% | 1.264% |
| 48 | 14.616 | 1974 | 1977 | 1986 | rVB | 340431 | 618339 | 15.97% | 0.993% |
| 49 | 14.763 | 2000 | 2002 | 2004 | rBV3 | 5117 | 5874 | 0.15% | 0.009% |
| 50 | 15.145 | 2061 | 2067 | 2071 | rBV | 18300 | 25337 | 0.65% | 0.041% |
| 51 | 15.216 | 2075 | 2079 | 2086 | rVB2 | 10339 | 14973 | 0.39% | 0.024% |
| 52 | 15.369 | 2096 | 2105 | 2112 | rBV | 2429230 | 3739858 | 96.57% | 6.005% |
| 53 | 15.510 | 2123 | 2129 | 2141 | rBV | 623506 | 886802 | 22.90% | 1.424% |
| 54 | 15.610 | 2144 | 2146 | 2153 | rVB7 | 14949 | 25606 | 0.66% | 0.041% |
| 55 | 15.739 | 2164 | 2168 | 2171 | rVB5 | 5281 | 8274 | 0.21% | 0.013% |
| 56 | 15.933 | 2197 | 2201 | 2209 | rVB10 | 10301 | 19524 | 0.50% | 0.031% |
| 57 | 16.098 | 2226 | 2229 | 2237 | rVV4 | 13559 | 30174 | 0.78% | 0.048% |
| 58 | 16.563 | 2305 | 2308 | 2311 | rBV5 | 7009 | 8037 | 0.21% | 0.013% |
| 59 | 16.916 | 2365 | 2368 | 2370 | rBV2 | 11081 | 11197 | 0.29% | 0.018% |
| 60 | 17.039 | 2387 | 2389 | 2392 | rBV3 | 9501 | 10284 | 0.27% | 0.017% |
| 61 | 17.080 | 2393 | 2396 | 2403 | rVB6 | 21574 | 30709 | 0.79% | 0.049% |
| 62 | 17.169 | 2404 | 2411 | 2418 | rBV | 2327974 | 3802407 | 98.19% | 6.106% |
| 63 | 17.269 | 2422 | 2428 | 2439 | rVV | 2532956 | 3330398 | 86.00% | 5.348% |
| 64 | 17.633 | 2487 | 2490 | 2494 | rBV5 | 12738 | 19463 | 0.50% | 0.031% |
| 65 | 17.792 | 2512 | 2517 | 2523 | rVB | 43021 | 72626 | 1.88% | 0.117% |
| 66 | 17.863 | 2526 | 2529 | 2533 | rBV3 | 20063 | 25730 | 0.66% | 0.041% |
| 67 | 18.092 | 2563 | 2568 | 2579 | rBV | 178498 | 350857 | 9.06% | 0.563% |
| 68 | 18.275 | 2596 | 2599 | 2603 | rBV3 | 39449 | 48407 | 1.25% | 0.078% |
| 69 | 18.333 | 2607 | 2609 | 2614 | rVB5 | 25911 | 30139 | 0.78% | 0.048% |
| 70 | 18.569 | 2646 | 2649 | 2654 | rBV5 | 23195 | 36576 | 0.94% | 0.059% |
| 71 | 19.092 | 2735 | 2738 | 2742 | rVB4 | 47168 | 58261 | 1.50% | 0.094% |
| 72 | 19.310 | 2772 | 2775 | 2779 | rVB | 38474 | 45177 | 1.17% | 0.073% |
| 73 | 19.439 | 2794 | 2797 | 2807 | rBV5 | 67097 | 158738 | 4.10% | 0.255% |
| 74 | 19.657 | 2828 | 2834 | 2843 | rVB | 2403626 | 3712570 | 95.87% | 5.961% |
| 75 | 20.021 | 2889 | 2896 | 2906 | rVB5 | 223654 | 704125 | 18.18% | 1.131% |
| 76 | 20.404 | 2955 | 2961 | 2969 | rBV2 | 407232 | 1205090 | 31.12% | 1.935% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 21.286 | 3107 | 3111 | 3121 | rVB3 | 280341 | 451537 | 11.66% | 0.725% |
| 78 | 21.627 | 3163 | 3169 | 3175 | rBV2 | 2083830 | 3487633 | 90.06% | 5.600% |
| 79 | 24.745 | 3691 | 3699 | 3709 | rVB2 | 1506209 | 3834349 | 99.01% | 6.157% |
| 80 | 24.974 | 3729 | 3738 | 3748 | rVB | 1398412 | 3833283 | 98.98% | 6.155% |

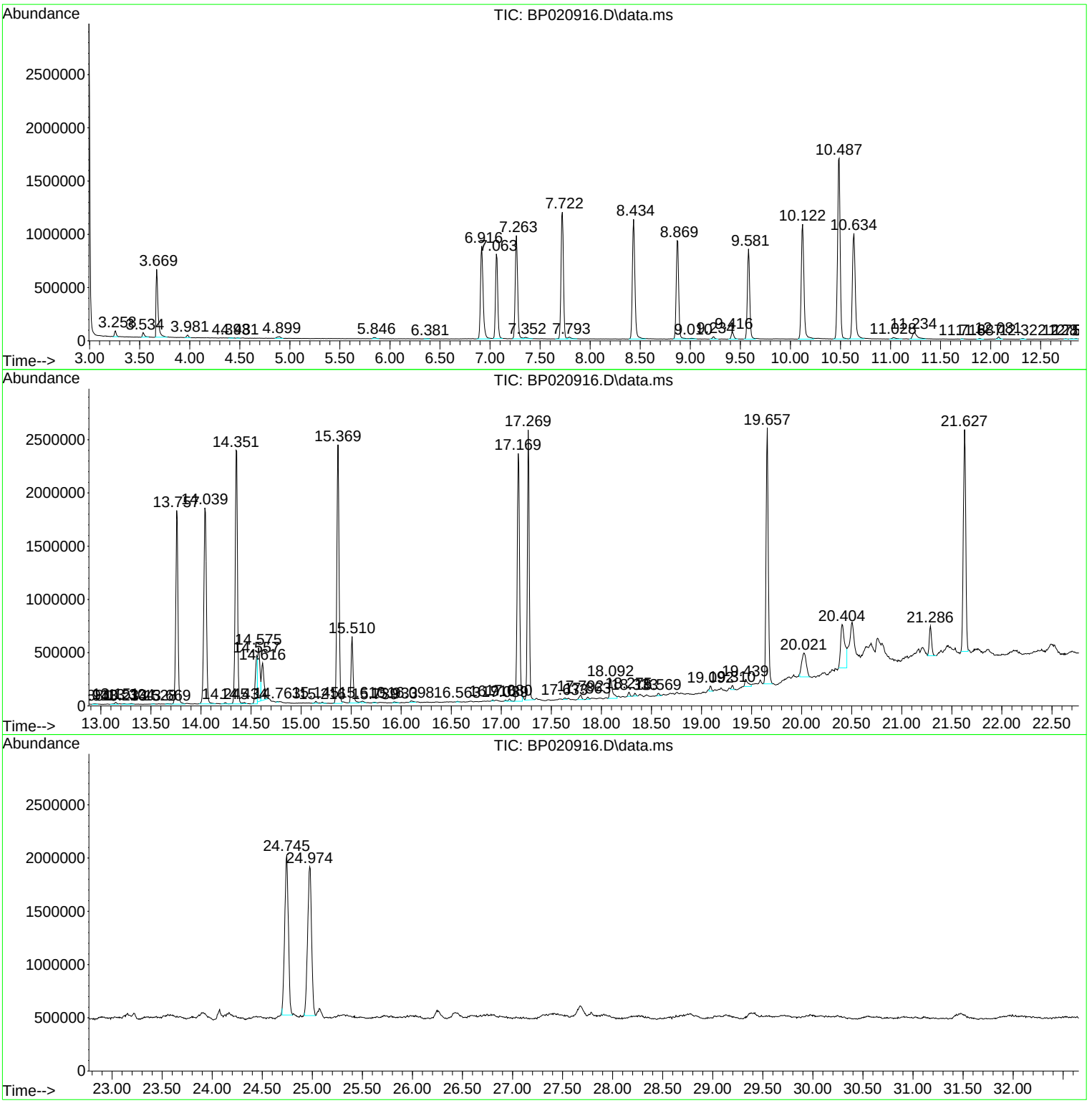
Sum of corrected areas: 62276441

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

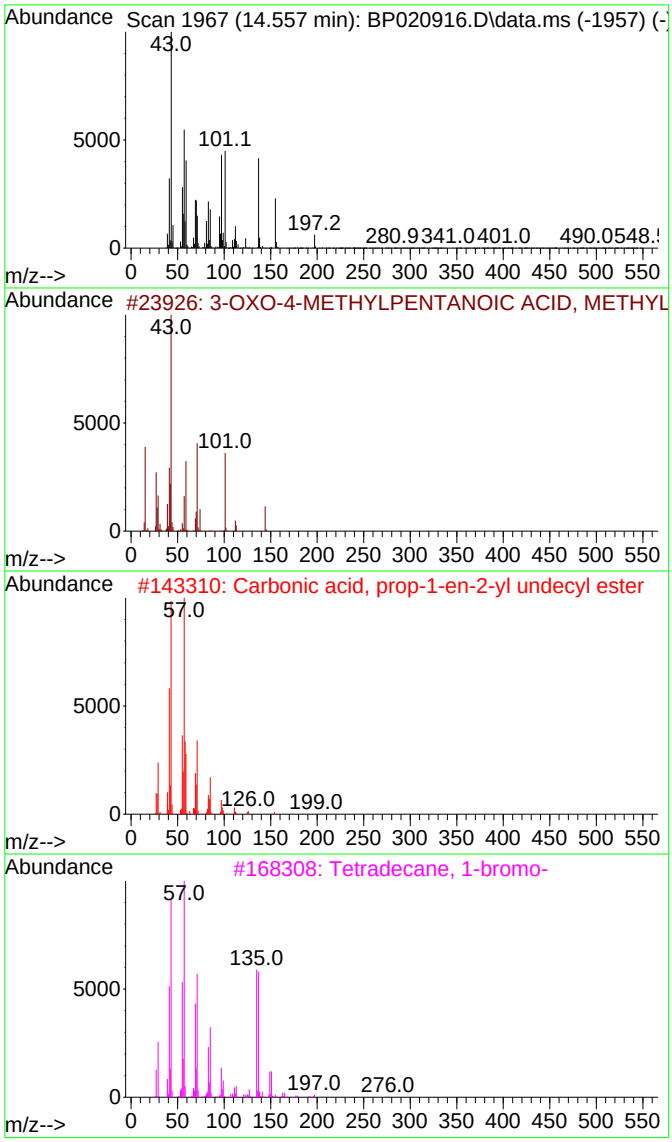
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

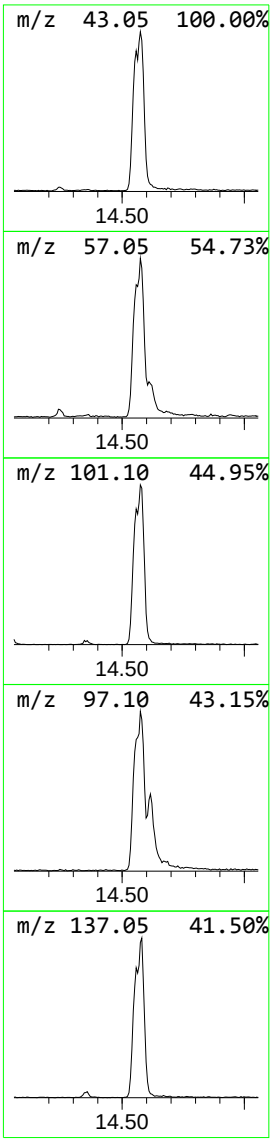
**********

Peak Number 1 unknown-01 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.557 | 3.44 ng/ul | 666718 | Acenaphthene-d10 | 14.357 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-OXO-4-METHYLPENTANOIC ACID, ME... | 144 | C7H12O3 | 042558-54-3 | 12 |
| 2 | Carbonic acid, prop-1-en-2-yl un... | 256 | C15H28O3 | 1000382-90-6 | 10 |
| 3 | Tetradecane, 1-bromo- | 276 | C14H29Br | 000112-71-0 | 10 |
| 4 | 9-Acetoxynonanal | 200 | C11H20O3 | 029541-97-7 | 10 |
| 5 | 2,2,3,4-Tetramethylhex-5-en-3-ol | 156 | C10H20O | 1010191-06-9 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

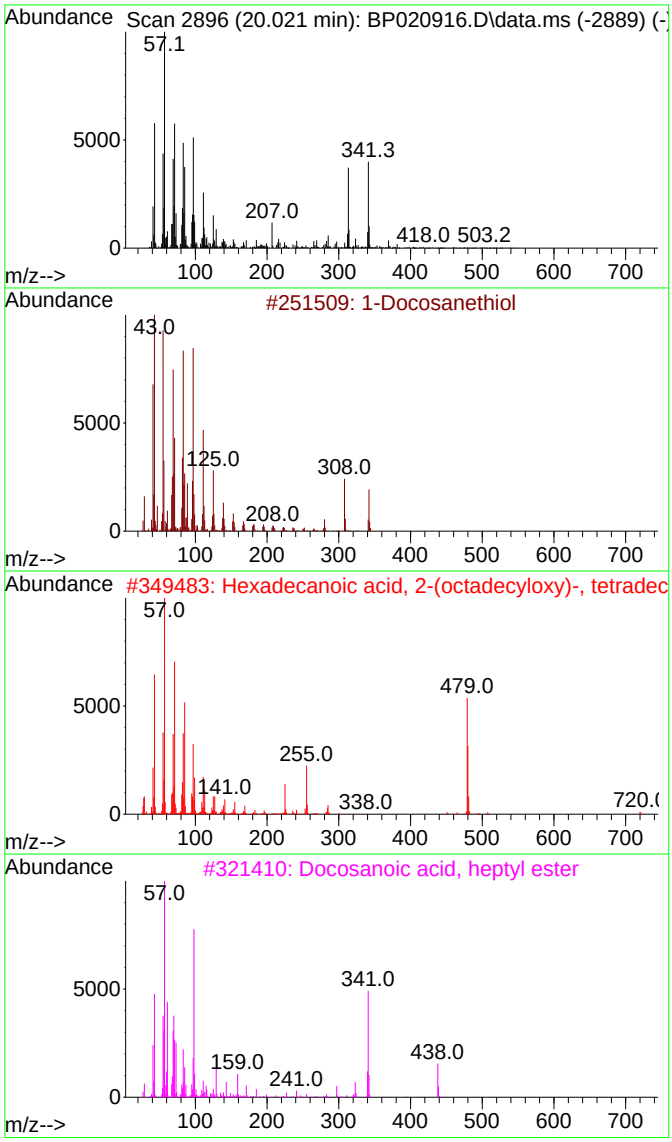
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

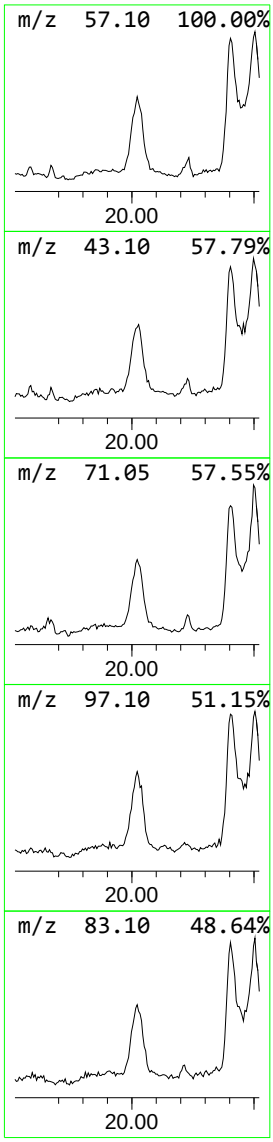
**********

Peak Number 2 1-Docosanethiol Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.022 | 4.04 ng/ul | 704125 | Chrysene-d12 | 21.627 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosanethiol | 342 | C22H46S | 007773-83-3 | 90 |
| 2 | Hexadecanoic acid, 2-(octadecylo... | 721 | C48H96O3 | 056599-98-5 | 16 |
| 3 | Docosanoic acid, heptyl ester | 438 | C29H58O2 | 1000405-21-8 | 16 |
| 4 | Docosanoic acid, isobutyl ester | 396 | C26H52O2 | 1000405-17-1 | 10 |
| 5 | Tetradecanoic acid, 2-hydroxy-, ... | 258 | C15H30O3 | 056009-40-6 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

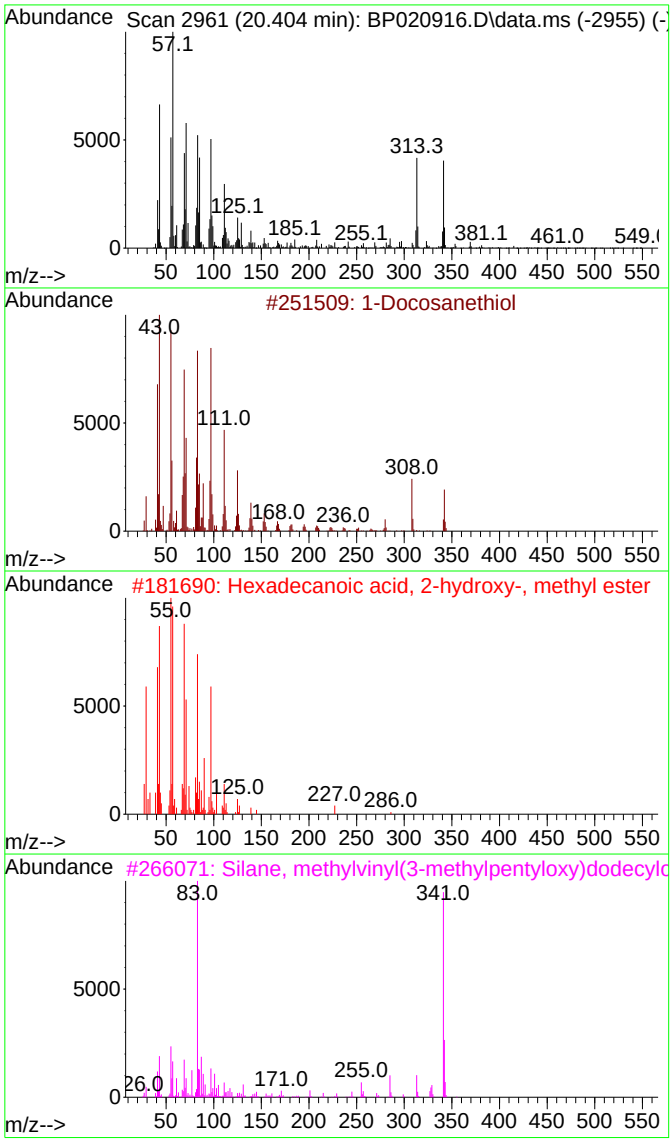
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

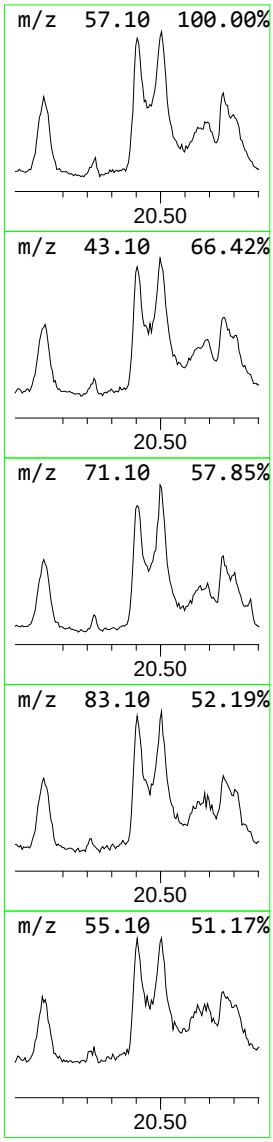
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 unknown-02 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.404 | 6.91 ng/ul | 1205090 | Chrysene-d12 | 21.627 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosanethiol | 342 | C22H46S | 007773-83-3 | 64 |
| 2 | Hexadecanoic acid, 2-hydroxy-, m... | 286 | C17H34O3 | 016742-51-1 | 14 |
| 3 | Silane, methylvinyl(3-methylpent... | 356 | C21H44O2Si | 1000421-62-5 | 10 |
| 4 | Docosanoic acid, heptyl ester | 438 | C29H58O2 | 1000405-21-8 | 10 |
| 5 | 1-(4-Iodophenyl)-5-(2-dimethylam... | 341 | C11H12IN5 | 1000144-63-0 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

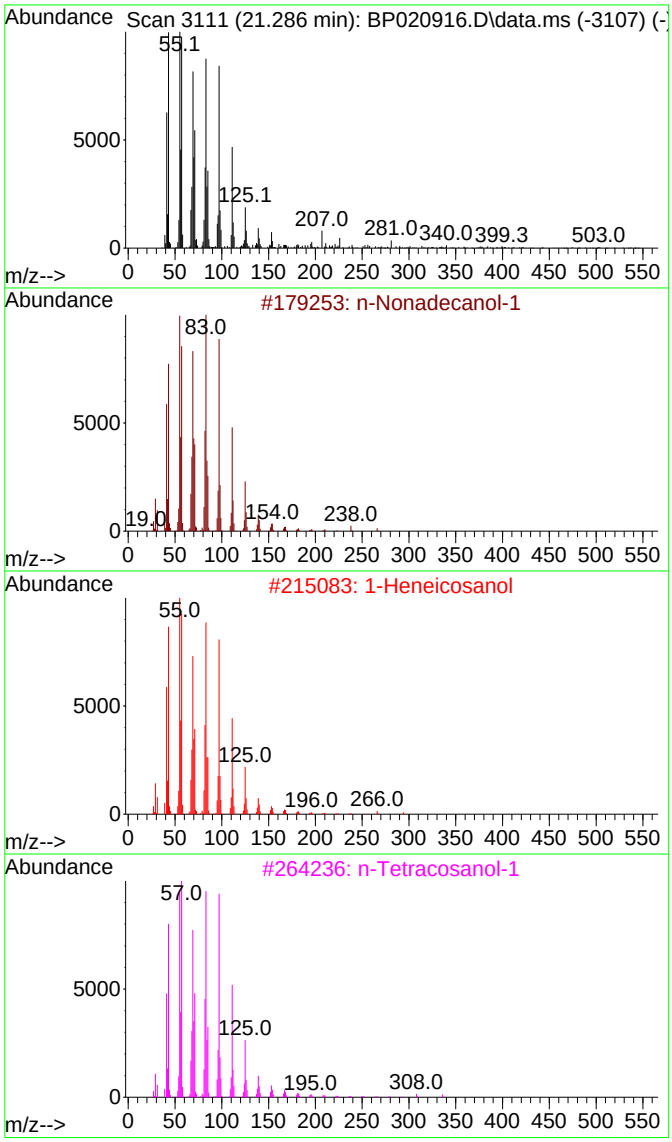
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

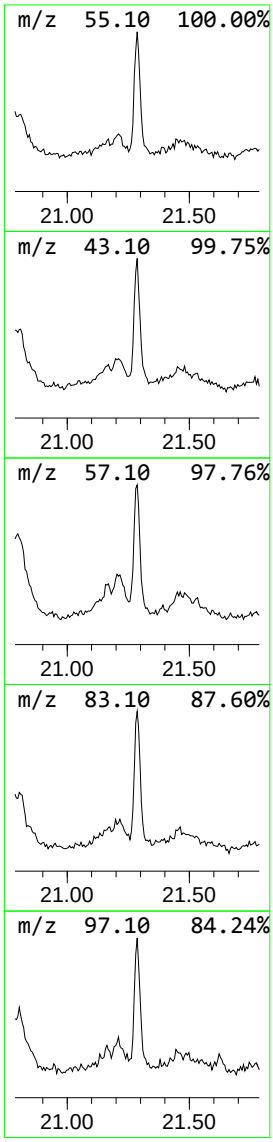
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 n-Nonadecanol-1 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.286 | 2.59 ng/ul | 451537 | Chrysene-d12 | 21.627 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 4 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071124\
Data File : BP020916.D
Acq On : 12 Jul 2024 00:41
Operator : MA/JU
Sample : P3087-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
A4BR6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.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 |
| unknown-01 | 14.557 | 3.4 | ng/ul | 666718 | 3 | 14.357 | 3872670 | 20.0 |
| 1-Docosanethiol | 20.022 | 4.0 | ng/ul | 704125 | 5 | 21.627 | 3487630 | 20.0 |
| unknown-02 | 20.404 | 6.9 | ng/ul | 1205090 | 5 | 21.627 | 3487630 | 20.0 |
| n-Nonadecanol-1 | 21.286 | 2.6 | ng/ul | 451537 | 5 | 21.627 | 3487630 | 20.0 |