LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.317 | 375 | 379 | 387 | rBV | 111807 | 140304 | 2.06% | 0.285% |
| 2 | 4.975 | 481 | 491 | 494 | rBV | 3887630 | 6795595 | 100.00% | 13.799% |
| 3 | 5.381 | 557 | 560 | 572 | rBV | 301778 | 337323 | 4.96% | 0.685% |
| 4 | 6.264 | 705 | 710 | 714 | rBV2 | 70288 | 102101 | 1.50% | 0.207% |
| 5 | 6.387 | 727 | 731 | 747 | rBV | 1693031 | 1616232 | 23.78% | 3.282% |
| 6 | 6.522 | 750 | 754 | 757 | rBV | 774107 | 671867 | 9.89% | 1.364% |
| 7 | 6.746 | 789 | 792 | 800 | rBV | 1776022 | 1403932 | 20.66% | 2.851% |
| 8 | 6.905 | 815 | 819 | 822 | rBV | 4448068 | 3677148 | 54.11% | 7.467% |
| 9 | 7.311 | 883 | 888 | 891 | rBV | 2684683 | 2576909 | 37.92% | 5.233% |
| 10 | 7.458 | 908 | 913 | 917 | rBV | 733143 | 562547 | 8.28% | 1.142% |
| 11 | 7.522 | 922 | 924 | 927 | rBV | 86237 | 75815 | 1.12% | 0.154% |
| 12 | 8.028 | 1007 | 1010 | 1013 | rBV | 1987392 | 1768769 | 26.03% | 3.592% |
| 13 | 9.116 | 1191 | 1195 | 1198 | rBV | 6405052 | 5525063 | 81.30% | 11.219% |
| 14 | 9.240 | 1213 | 1216 | 1219 | rVB | 201892 | 182144 | 2.68% | 0.370% |
| 15 | 9.310 | 1225 | 1228 | 1232 | rVB2 | 102285 | 90396 | 1.33% | 0.184% |
| 16 | 9.510 | 1259 | 1262 | 1265 | rBV | 1050597 | 759647 | 11.18% | 1.543% |
| 17 | 9.746 | 1298 | 1302 | 1307 | rBV | 187260 | 338742 | 4.98% | 0.688% |
| 18 | 9.793 | 1307 | 1310 | 1314 | rVV | 2682424 | 2293817 | 33.75% | 4.658% |
| 19 | 9.828 | 1314 | 1316 | 1319 | rVB | 161879 | 121309 | 1.79% | 0.246% |
| 20 | 9.999 | 1342 | 1345 | 1349 | rVB | 102259 | 83231 | 1.22% | 0.169% |
| 21 | 10.346 | 1401 | 1404 | 1408 | rBV | 124448 | 97602 | 1.44% | 0.198% |
| 22 | 10.387 | 1408 | 1411 | 1417 | rBV2 | 71601 | 107037 | 1.58% | 0.217% |
| 23 | 10.440 | 1417 | 1420 | 1423 | rVV | 93175 | 78945 | 1.16% | 0.160% |
| 24 | 10.587 | 1442 | 1445 | 1450 | rBV | 280078 | 246515 | 3.63% | 0.501% |
| 25 | 10.640 | 1450 | 1454 | 1461 | rBV | 297745 | 309648 | 4.56% | 0.629% |
| 26 | 10.704 | 1461 | 1465 | 1469 | rBV | 487975 | 459906 | 6.77% | 0.934% |
| 27 | 11.152 | 1537 | 1541 | 1546 | rBV3 | 158284 | 239496 | 3.52% | 0.486% |
| 28 | 11.293 | 1561 | 1565 | 1568 | rBV | 3066995 | 2470438 | 36.35% | 5.016% |
| 29 | 11.316 | 1568 | 1569 | 1572 | rVV | 193354 | 97451 | 1.43% | 0.198% |
| 30 | 11.363 | 1574 | 1577 | 1580 | rVB2 | 114117 | 109999 | 1.62% | 0.223% |
| 31 | 12.357 | 1743 | 1746 | 1758 | rBV | 656286 | 970976 | 14.29% | 1.972% |
| 32 | 12.516 | 1770 | 1773 | 1777 | rVB | 240442 | 223159 | 3.28% | 0.453% |
| 33 | 12.563 | 1778 | 1781 | 1783 | rBV | 234667 | 184187 | 2.71% | 0.374% |
| 34 | 12.746 | 1810 | 1812 | 1815 | rVB | 214992 | 195879 | 2.88% | 0.398% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.899 | 1834 | 1838 | 1841 | rBV | 6766412 | 6076166 | 89.41% | 12.338% |
| 36 | 13.087 | 1867 | 1870 | 1873 | rVB | 71303 | 69746 | 1.03% | 0.142% |
| 37 | 13.146 | 1874 | 1880 | 1883 | rBV4 | 120397 | 226497 | 3.33% | 0.460% |
| 38 | 13.763 | 1982 | 1985 | 1988 | rVB | 87544 | 85602 | 1.26% | 0.174% |
| 39 | 13.816 | 1988 | 1994 | 2002 | rBV3 | 415700 | 893879 | 13.15% | 1.815% |
| 40 | 13.963 | 2014 | 2019 | 2022 | rBV2 | 2941160 | 2914831 | 42.89% | 5.919% |
| 41 | 14.145 | 2047 | 2050 | 2054 | rBV2 | 76169 | 70342 | 1.04% | 0.143% |
| 42 | 14.451 | 2099 | 2102 | 2105 | rBV | 171780 | 155695 | 2.29% | 0.316% |
| 43 | 14.763 | 2152 | 2155 | 2162 | rVB | 170870 | 200688 | 2.95% | 0.408% |
| 44 | 14.840 | 2165 | 2168 | 2173 | rVB | 91928 | 102482 | 1.51% | 0.208% |
| 45 | 15.010 | 2194 | 2197 | 2206 | rVB | 113605 | 216329 | 3.18% | 0.439% |
| 46 | 15.098 | 2209 | 2212 | 2219 | rVV2 | 181584 | 229701 | 3.38% | 0.466% |
| 47 | 15.310 | 2245 | 2248 | 2255 | rVB | 80134 | 104602 | 1.54% | 0.212% |
| 48 | 15.369 | 2255 | 2258 | 2264 | rVV | 109322 | 160388 | 2.36% | 0.326% |
| 49 | 15.440 | 2265 | 2270 | 2274 | rVV | 1902499 | 2383049 | 35.07% | 4.839% |
| 50 | 15.481 | 2275 | 2277 | 2290 | rVB | 146608 | 238132 | 3.50% | 0.484% |
| 51 | 15.922 | 2348 | 2352 | 2360 | rBV | 113919 | 205234 | 3.02% | 0.417% |

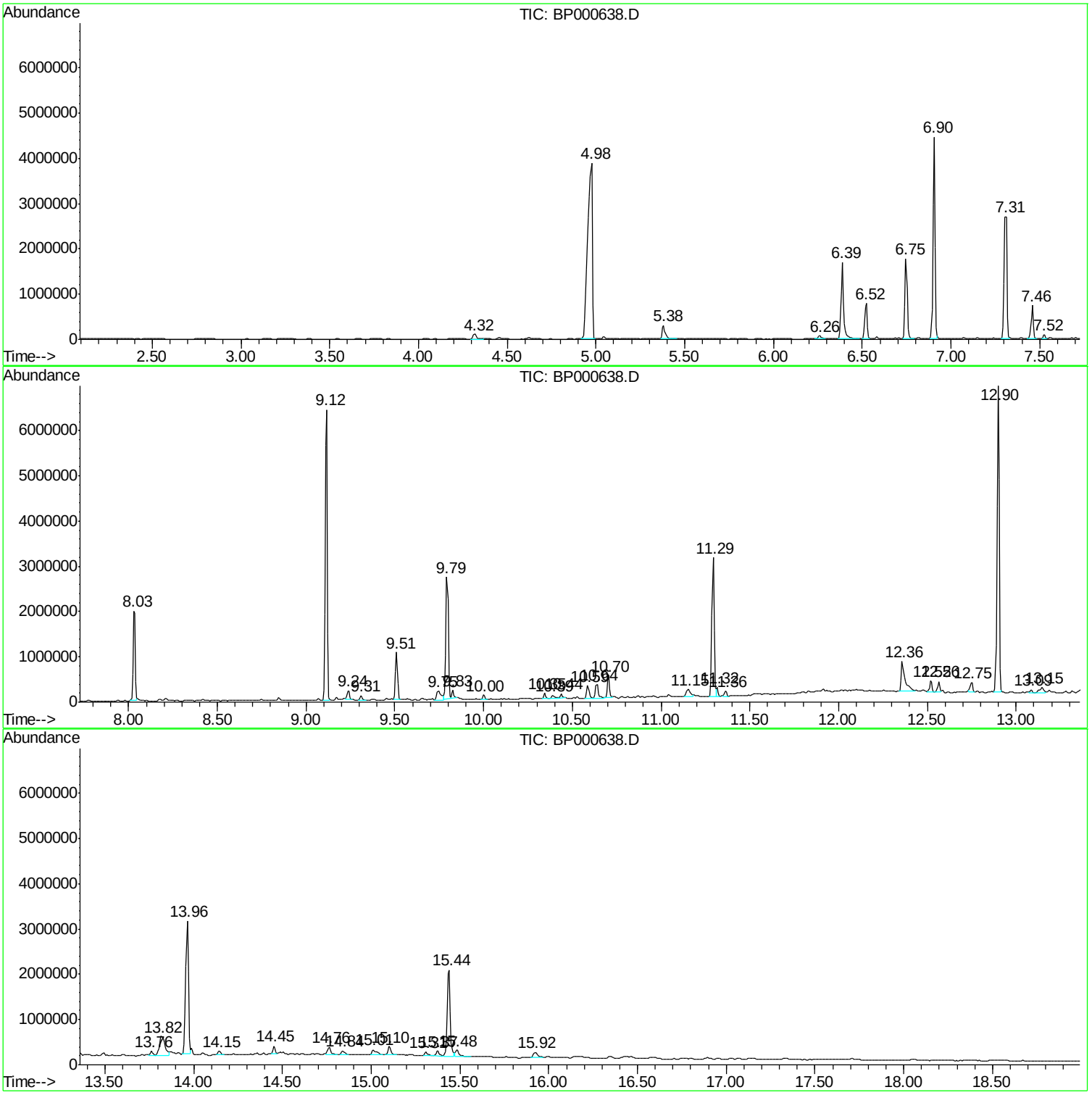
Sum of corrected areas: 49247492

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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 P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

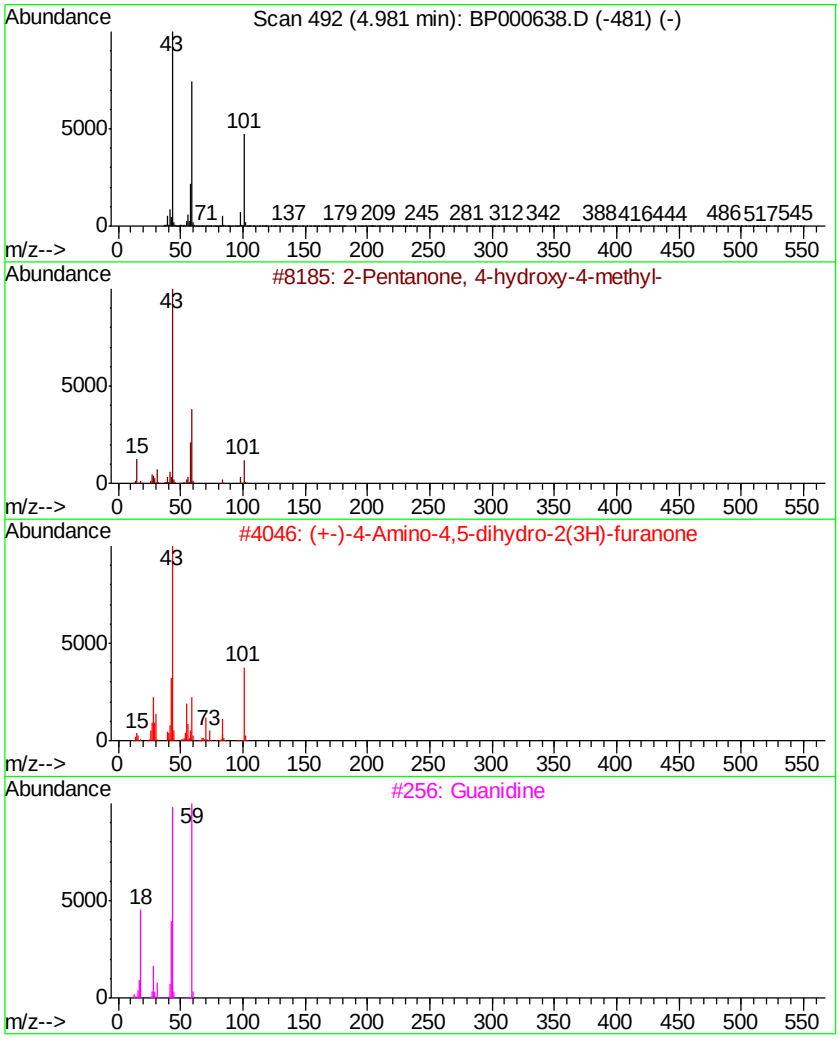
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

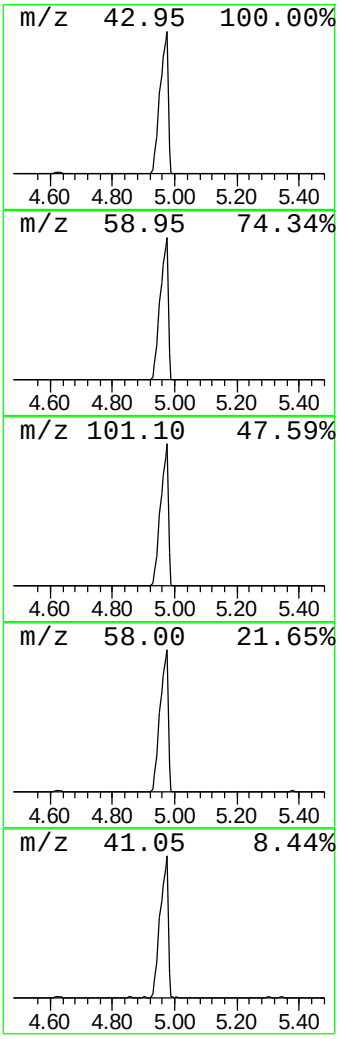
**********

Peak Number 1 unknown4.98 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.98 | 96.81 ng | 6795600 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 43 |
| 3 | Guanidine | 59 | CH5N3 | 000113-00-8 | 38 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 12 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 12 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

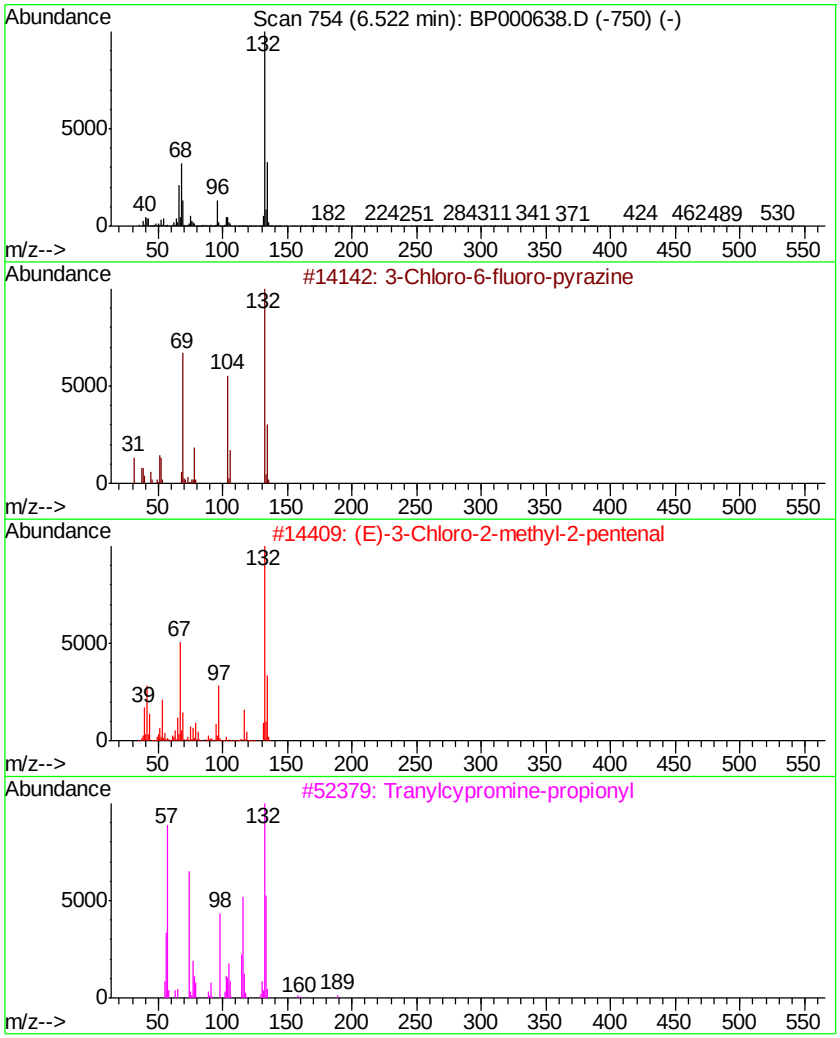
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

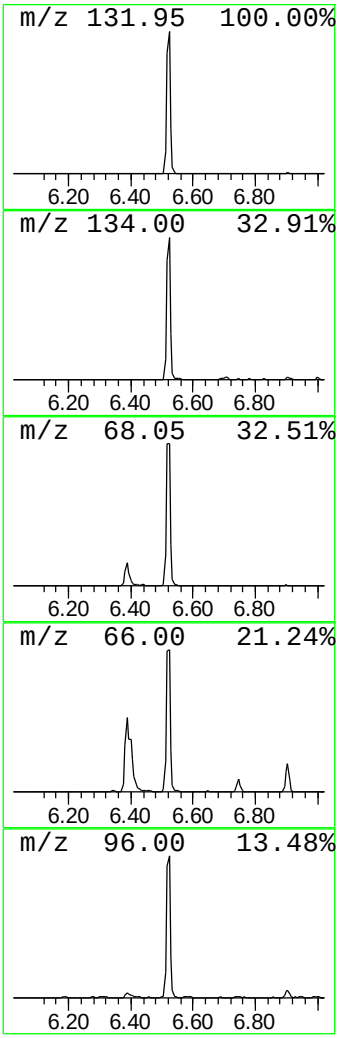
**********

Peak Number 2 unknown6.52 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.52 | 9.57 ng | 671867 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

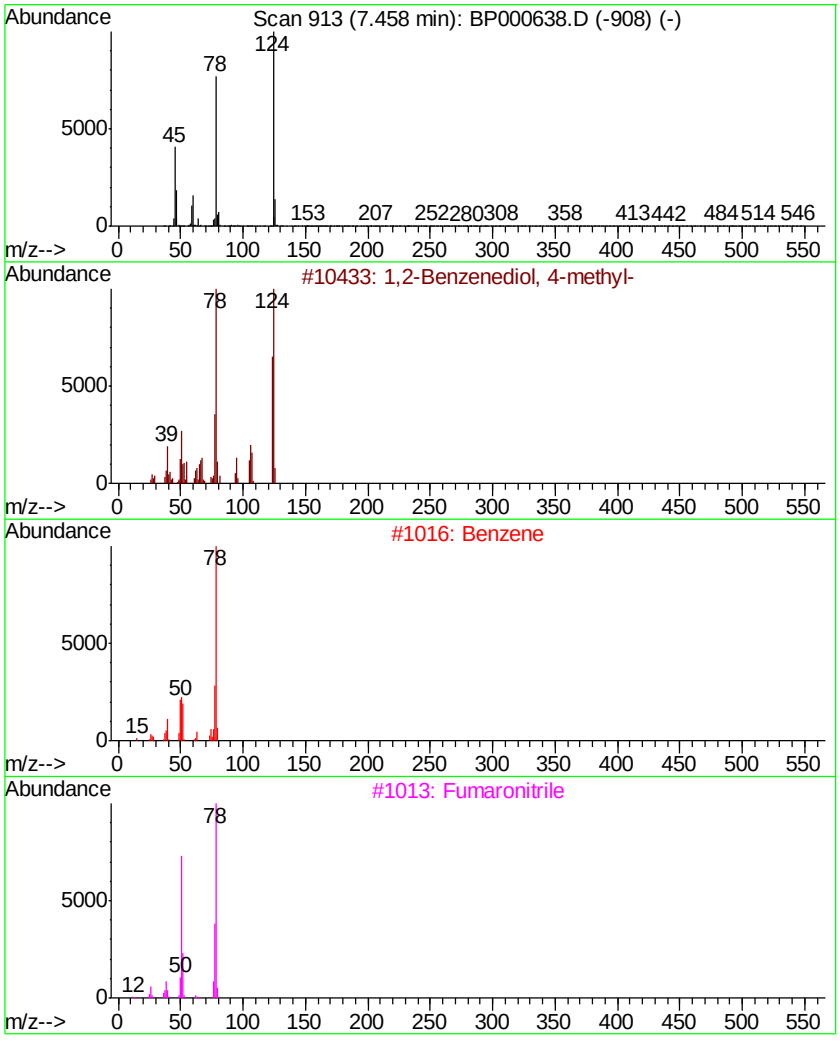
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

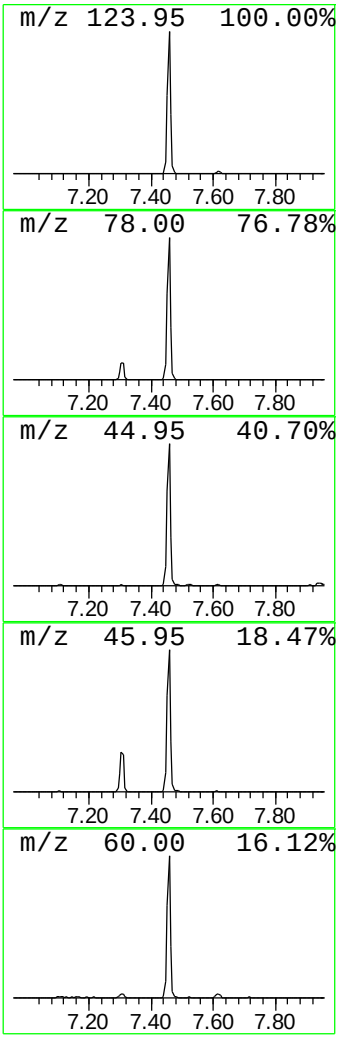
**********

Peak Number 4 1,2-Benzenediol, 4-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.46 | 6.36 ng | 562547 | Naphthalene-d8 | 8.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzenediol, 4-methyl- | 124 | C7H8O2 | 000452-86-8 | 50 |
| 2 | Benzene | 78 | C6H6 | 000071-43-2 | 9 |
| 3 | Fumaronitrile | 78 | C4H2N2 | 000764-42-1 | 9 |
| 4 | 2,4-Hexadiyne | 78 | C6H6 | 002809-69-0 | 7 |
| 5 | Propanedinitrile, methylene- | 78 | C4H2N2 | 000922-64-5 | 7 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

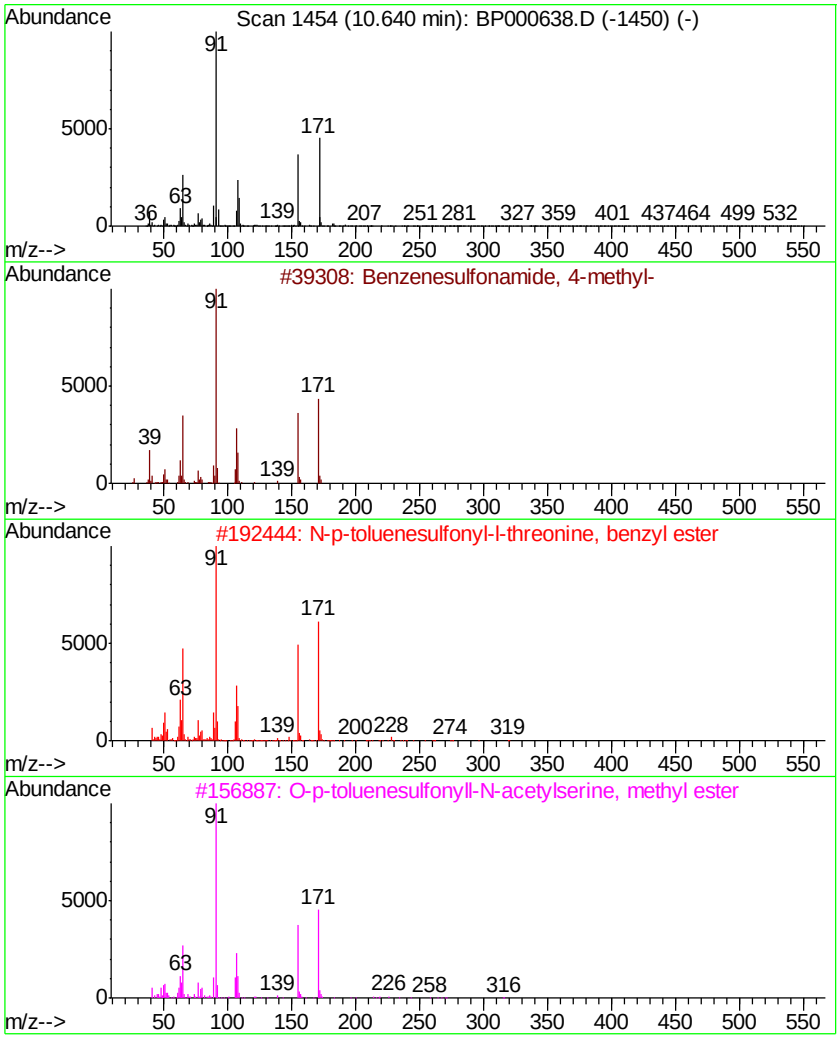
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

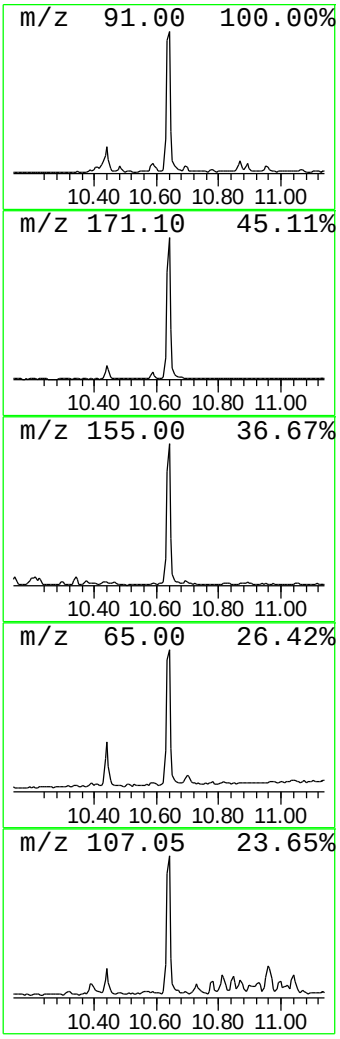
**********

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.64 | 2.51 ng | 309648 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfonamide, 4-methyl- | 171 | C7H9NO2S | 000070-55-3 | 98 |
| 2 | N-p-toluenesulfonyl-l-threonine,... | 363 | C18H21NO5S | 1000130-34-4 | 90 |
| 3 | O-p-toluenesulfonyll-N-acetylser... | 315 | C13H17NO6S | 1000126-44-8 | 64 |
| 4 | Dibenzyl phosphite | 262 | C14H15O3P | 017176-77-1 | 47 |
| 5 | N-Tosyloxy-2,2-bis(trifluorometh... | 349 | C11H9F6NO3S | 038436-38-3 | 42 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

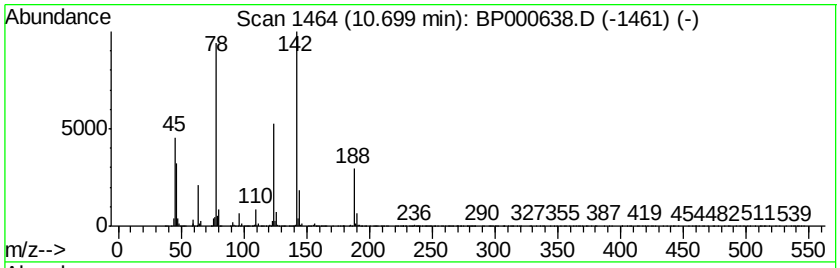
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

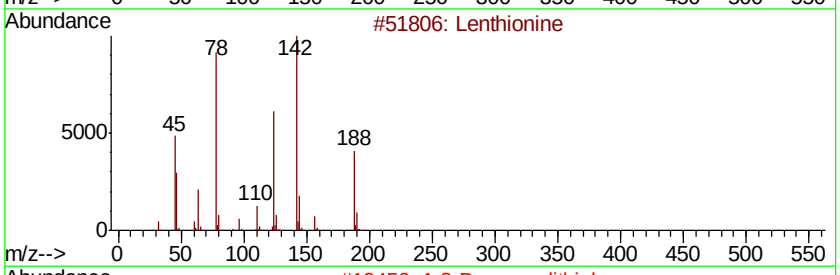
**********

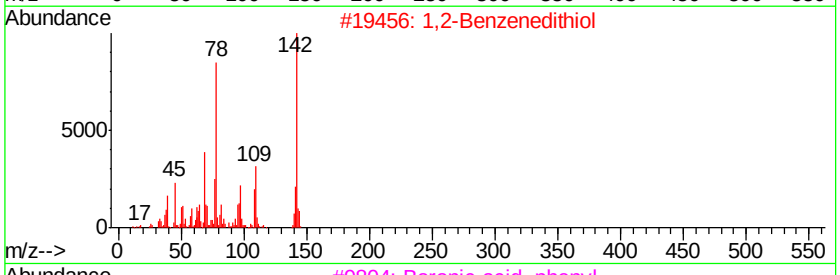
Peak Number 6 Lenthionine Concentration Rank 7

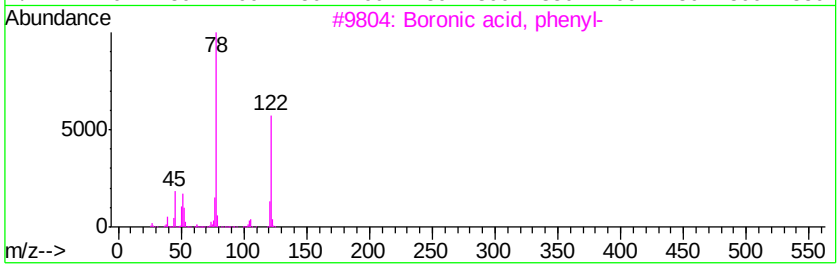
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.70 | 3.72 ng | 459906 | Phenanthrene-d10 | 11.29 |

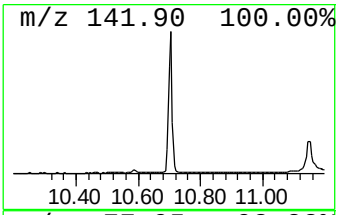
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Lenthionine | 188 | C2H4S5 | 000292-46-6 | 94 |
| 2 | 1,2-Benzenedithiol | 142 | C6H6S2 | 017534-15-5 | 9 |
| 3 | Boronic acid, phenyl- | 122 | C6H7BO2 | 000098-80-6 | 9 |
| 4 | Ehylthiophosphonamide, o-methyl ... | 139 | C3H10NOPS | 1000306-03-7 | 9 |
| 5 | 2,4-Hexadiyne | 78 | C6H6 | 002809-69-0 | 7 |

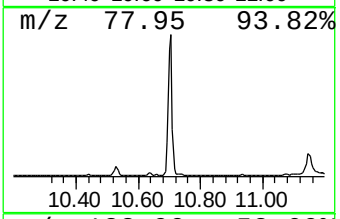


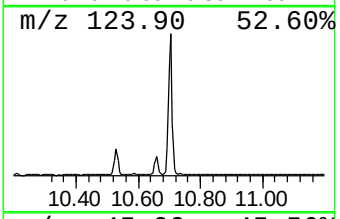



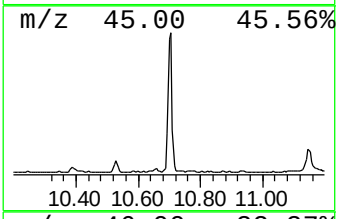



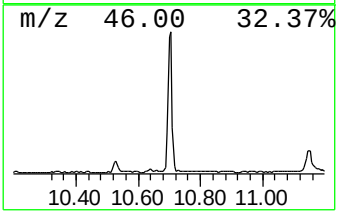



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

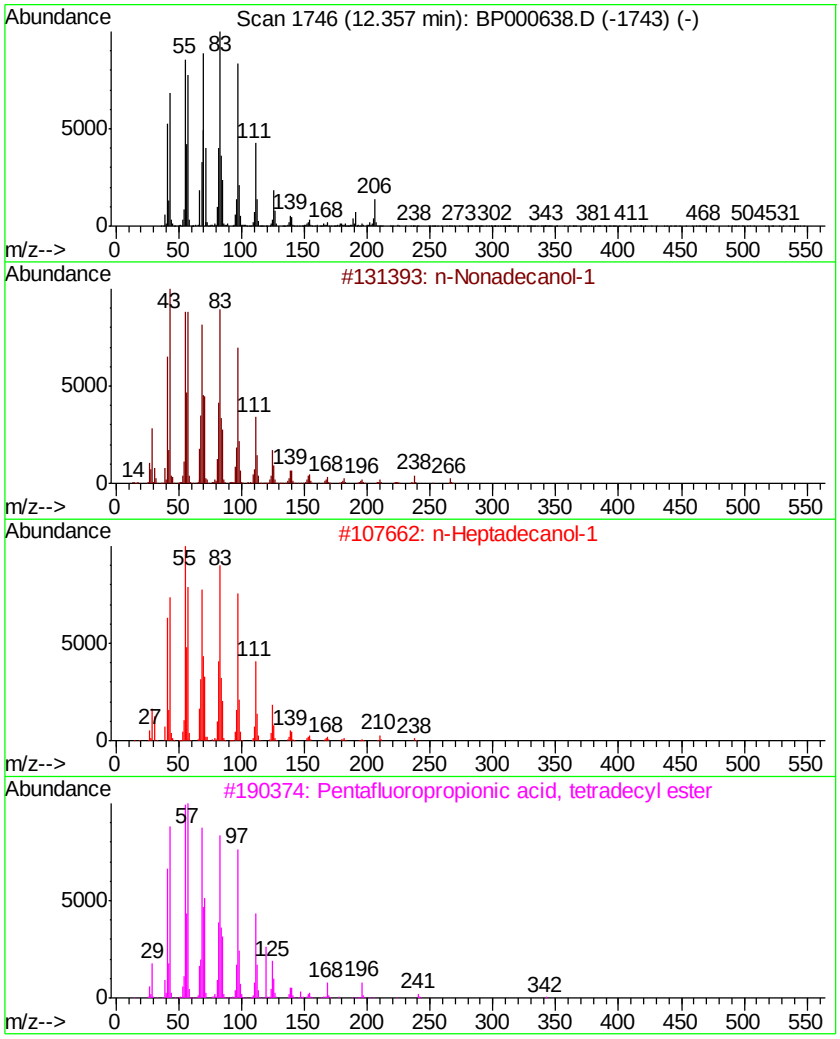
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

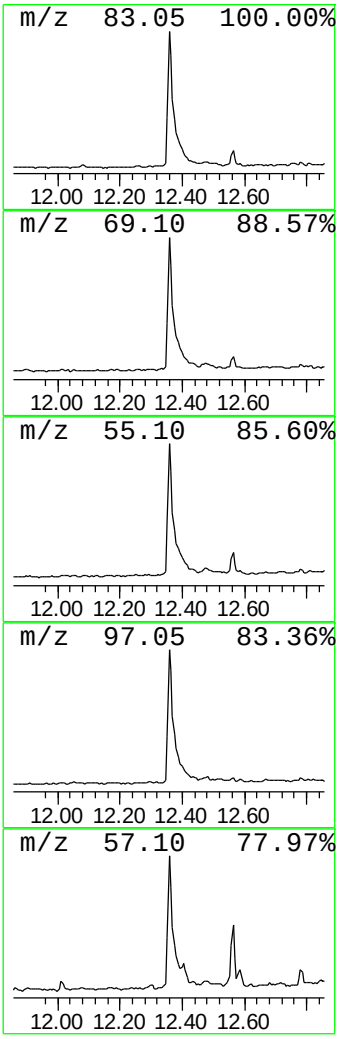
**********

Peak Number 7 n-Nonadecanol-1 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.36 | 7.86 ng | 970976 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 94 |
| 2 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 94 |
| 3 | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 91 |
| 4 | Bromoacetic acid, pentadecyl ester | 348 | C17H33BrO2 | 131143-01-6 | 91 |
| 5 | Cyclotridecane | 182 | C13H26 | 000295-02-3 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

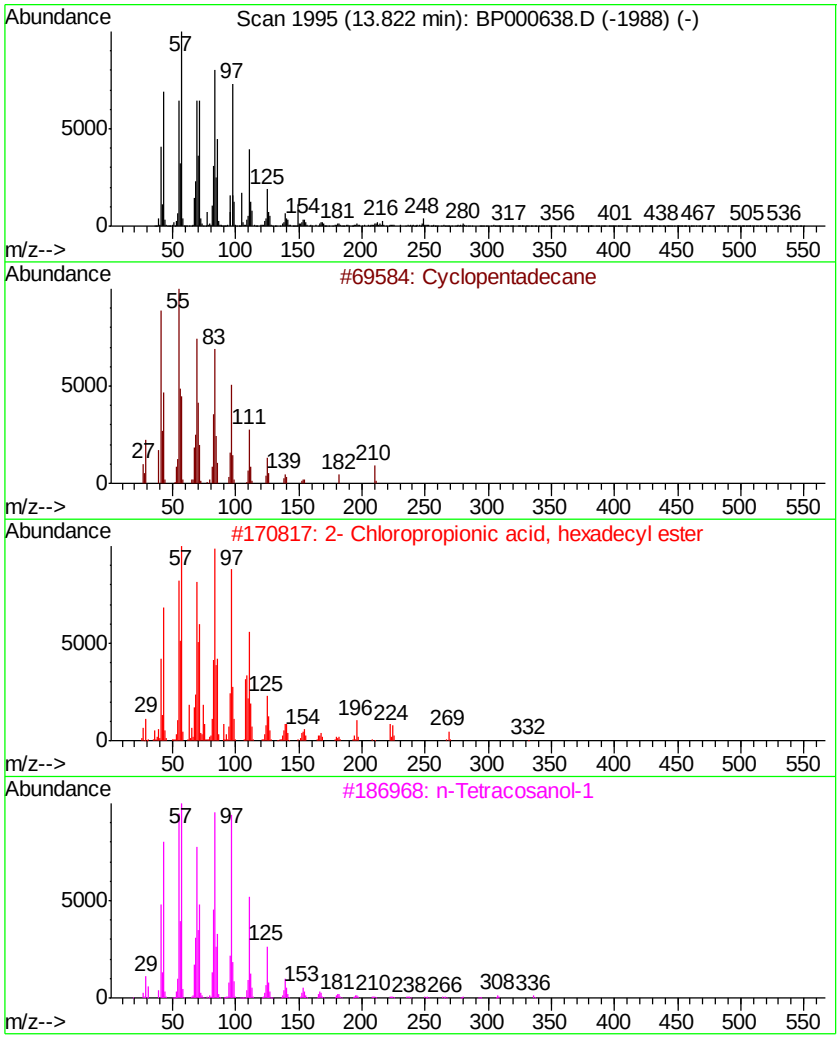
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

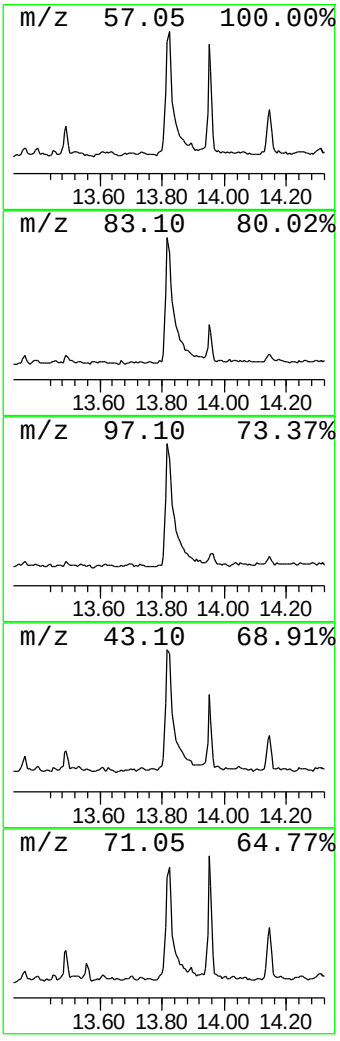
**********

Peak Number 8 Cyclopentadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.82 | 6.13 ng | 893879 | Chrysene-d12 | 13.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 94 |
| 2 | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1 | 94 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP101119\
Data File : BP000638.D
Acq On : 11 Oct 2019 17:58
Operator : JU
Sample : K5266-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 20190856-AMENDED-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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 |
| unknown4.98 | 4.98 | 96.8 | ng | 6795600 | 1 | 6.75 | 1403930 | 20.0 |
| unknown6.52 | 6.52 | 9.6 | ng | 671867 | 1 | 6.75 | 1403930 | 20.0 |
| 1,2-Benzenediol, ... | 7.46 | 6.4 | ng | 562547 | 2 | 8.03 | 1768770 | 20.0 |
| Benzenesulfonamid... | 10.64 | 2.5 | ng | 309648 | 4 | 11.29 | 2470440 | 20.0 |
| Lenthionine | 10.70 | 3.7 | ng | 459906 | 4 | 11.29 | 2470440 | 20.0 |
| n-Nonadecanol-1 | 12.36 | 7.9 | ng | 970976 | 4 | 11.29 | 2470440 | 20.0 |
| Cyclopentadecane | 13.82 | 6.1 | ng | 893879 | 5 | 13.96 | 2914830 | 20.0 |