LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

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-BP052720.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 | 5.158 | 381 | 386 | 391 | rBV | 142459 | 199447 | 3.40% | 0.354% |
| 2 | 5.222 | 391 | 397 | 405 | rVV | 1802097 | 2607247 | 44.39% | 4.630% |
| 3 | 5.628 | 459 | 466 | 474 | rBV | 185782 | 295181 | 5.03% | 0.524% |
| 4 | 6.793 | 657 | 664 | 678 | rVB | 1899671 | 3092155 | 52.64% | 5.491% |
| 5 | 7.605 | 795 | 802 | 810 | rBV | 1337240 | 2057438 | 35.03% | 3.653% |
| 6 | 7.922 | 849 | 856 | 864 | rBV | 1628030 | 2573339 | 43.81% | 4.569% |
| 7 | 8.746 | 989 | 996 | 1005 | rBV | 1256476 | 1995388 | 33.97% | 3.543% |
| 8 | 10.269 | 1248 | 1255 | 1262 | rBV | 119041 | 190506 | 3.24% | 0.338% |
| 9 | 10.375 | 1266 | 1273 | 1290 | rVV | 1704793 | 2943138 | 50.10% | 5.226% |
| 10 | 12.869 | 1690 | 1697 | 1709 | rBV | 3105354 | 4609372 | 78.47% | 8.185% |
| 11 | 13.710 | 1834 | 1840 | 1849 | rBV | 486818 | 690863 | 11.76% | 1.227% |
| 12 | 14.251 | 1925 | 1932 | 1939 | rBV2 | 2478524 | 3733684 | 63.56% | 6.630% |
| 13 | 14.316 | 1939 | 1943 | 1951 | rVB | 78250 | 122766 | 2.09% | 0.218% |
| 14 | 15.304 | 2107 | 2111 | 2116 | rVB | 43209 | 61904 | 1.05% | 0.110% |
| 15 | 15.745 | 2180 | 2186 | 2195 | rBV | 2192309 | 3119510 | 53.11% | 5.539% |
| 16 | 15.822 | 2195 | 2199 | 2210 | rVB | 46292 | 97400 | 1.66% | 0.173% |
| 17 | 16.375 | 2288 | 2293 | 2298 | rVB2 | 138635 | 210551 | 3.58% | 0.374% |
| 18 | 16.439 | 2298 | 2304 | 2310 | rBV6 | 54175 | 112013 | 1.91% | 0.199% |
| 19 | 16.504 | 2311 | 2315 | 2324 | rBV | 62138 | 89813 | 1.53% | 0.159% |
| 20 | 16.628 | 2331 | 2336 | 2341 | rBV | 232209 | 284449 | 4.84% | 0.505% |
| 21 | 16.792 | 2359 | 2364 | 2367 | rBV | 215151 | 270683 | 4.61% | 0.481% |
| 22 | 16.898 | 2378 | 2382 | 2386 | rVB2 | 45202 | 59789 | 1.02% | 0.106% |
| 23 | 17.010 | 2395 | 2401 | 2405 | rBV | 2856320 | 4181949 | 71.19% | 7.426% |
| 24 | 17.051 | 2405 | 2408 | 2414 | rVB | 234624 | 318078 | 5.41% | 0.565% |
| 25 | 17.139 | 2420 | 2423 | 2429 | rVB | 75899 | 103064 | 1.75% | 0.183% |
| 26 | 17.939 | 2554 | 2559 | 2565 | rBV2 | 259167 | 387268 | 6.59% | 0.688% |
| 27 | 18.075 | 2578 | 2582 | 2586 | rBV3 | 80068 | 113323 | 1.93% | 0.201% |
| 28 | 18.910 | 2720 | 2724 | 2732 | rVB2 | 86205 | 129184 | 2.20% | 0.229% |
| 29 | 19.033 | 2740 | 2745 | 2750 | rVB | 653969 | 866475 | 14.75% | 1.539% |
| 30 | 19.104 | 2753 | 2757 | 2762 | rBV | 208223 | 255980 | 4.36% | 0.455% |
| 31 | 19.381 | 2797 | 2804 | 2808 | rBV | 608347 | 958159 | 16.31% | 1.701% |
| 32 | 19.592 | 2835 | 2840 | 2850 | rVB | 4689822 | 5874133 | 100.00% | 10.431% |
| 33 | 20.828 | 3047 | 3050 | 3053 | rBV | 1240655 | 1507575 | 25.66% | 2.677% |
| 34 | 20.857 | 3053 | 3055 | 3066 | rVB3 | 539371 | 699436 | 11.91% | 1.242% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

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-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 21.057 | 3085 | 3089 | 3092 | rBV | 505053 | 560116 | 9.54% | 0.995% |
| 36 | 21.110 | 3092 | 3098 | 3102 | rBV | 3312626 | 4545155 | 77.38% | 8.071% |
| 37 | 21.292 | 3125 | 3129 | 3133 | rBV2 | 408475 | 496929 | 8.46% | 0.882% |
| 38 | 21.339 | 3134 | 3137 | 3141 | rVB | 567547 | 643282 | 10.95% | 1.142% |
| 39 | 21.416 | 3147 | 3150 | 3153 | rVB2 | 214857 | 241512 | 4.11% | 0.429% |
| 40 | 21.980 | 3242 | 3246 | 3255 | rVB2 | 525958 | 787072 | 13.40% | 1.398% |
| 41 | 23.316 | 3468 | 3473 | 3489 | rVB | 2222160 | 4230363 | 72.02% | 7.512% |

Sum of corrected areas: 56315689

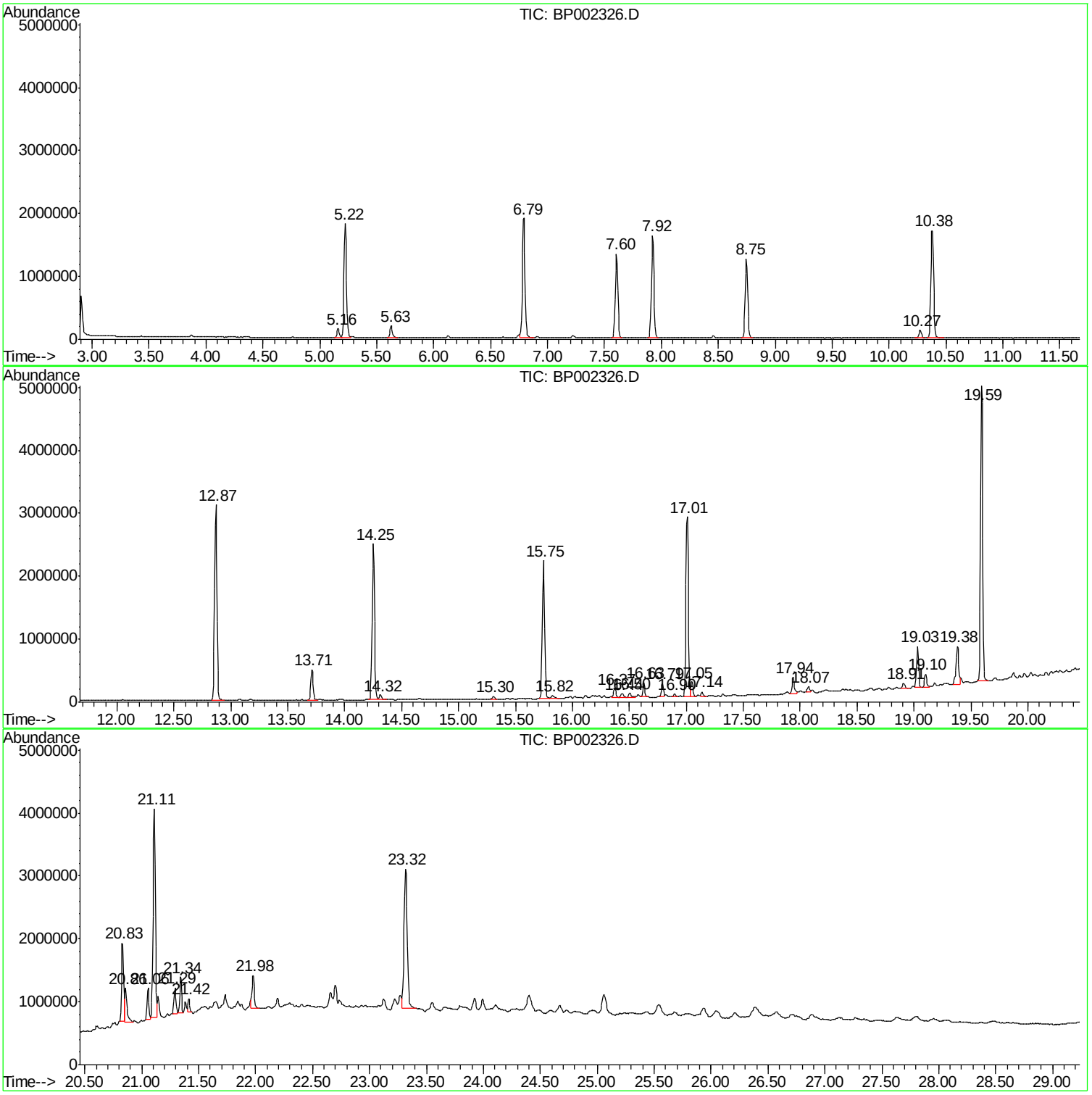
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

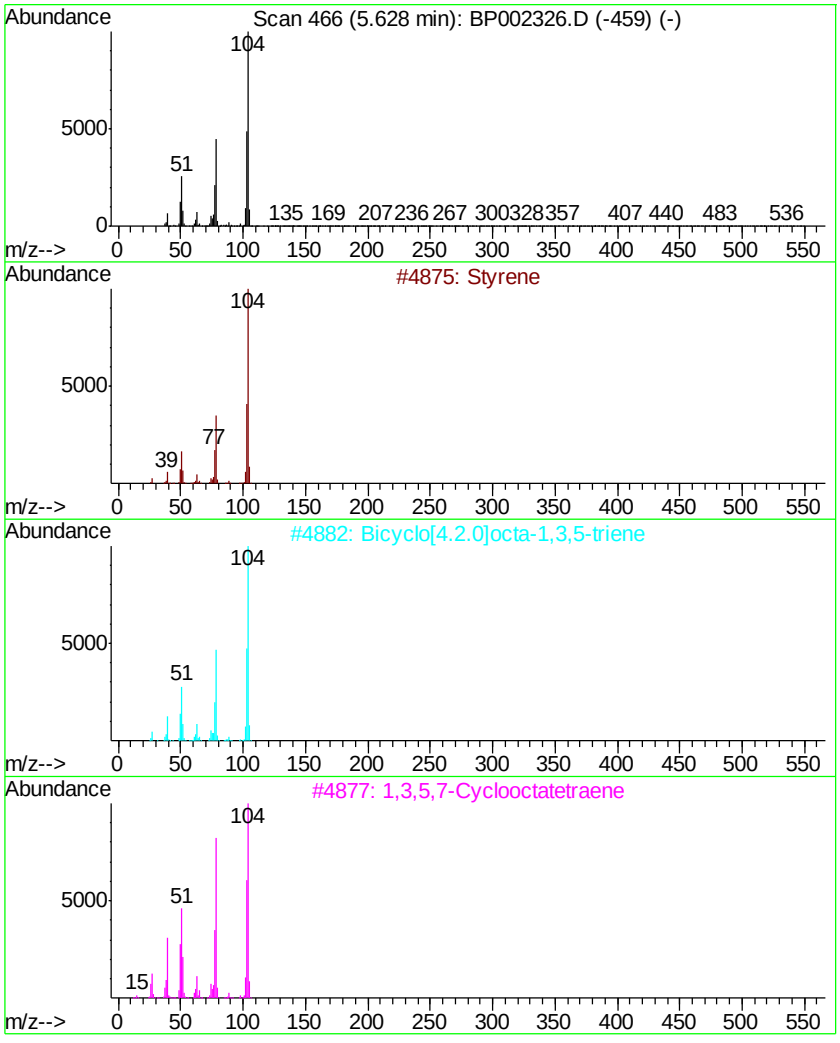
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

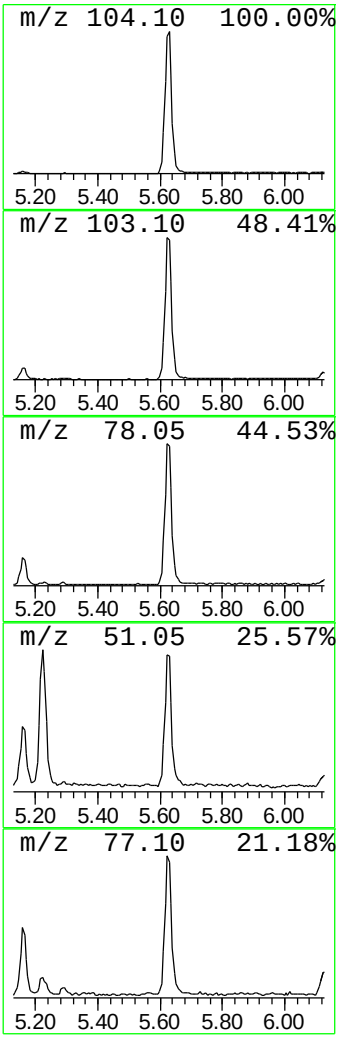
**********

Peak Number 1 Styrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.63 | 2.87 ng | 295181 | 1,4-Dichlorobenzene-d4 | 7.60 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Styrene | 104 | C8H8 | 000100-42-5 | 97 |
| 2 | Bicyclo[4.2.0]octa-1,3,5-triene | 104 | C8H8 | 000694-87-1 | 96 |
| 3 | 1,3,5,7-Cyclooctatetraene | 104 | C8H8 | 000629-20-9 | 91 |
| 4 | Butanedioic acid, phenyl- | 194 | C10H10O4 | 000635-51-8 | 64 |
| 5 | 2-Pyridinecarbonitrile | 104 | C6H4N2 | 000100-70-9 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

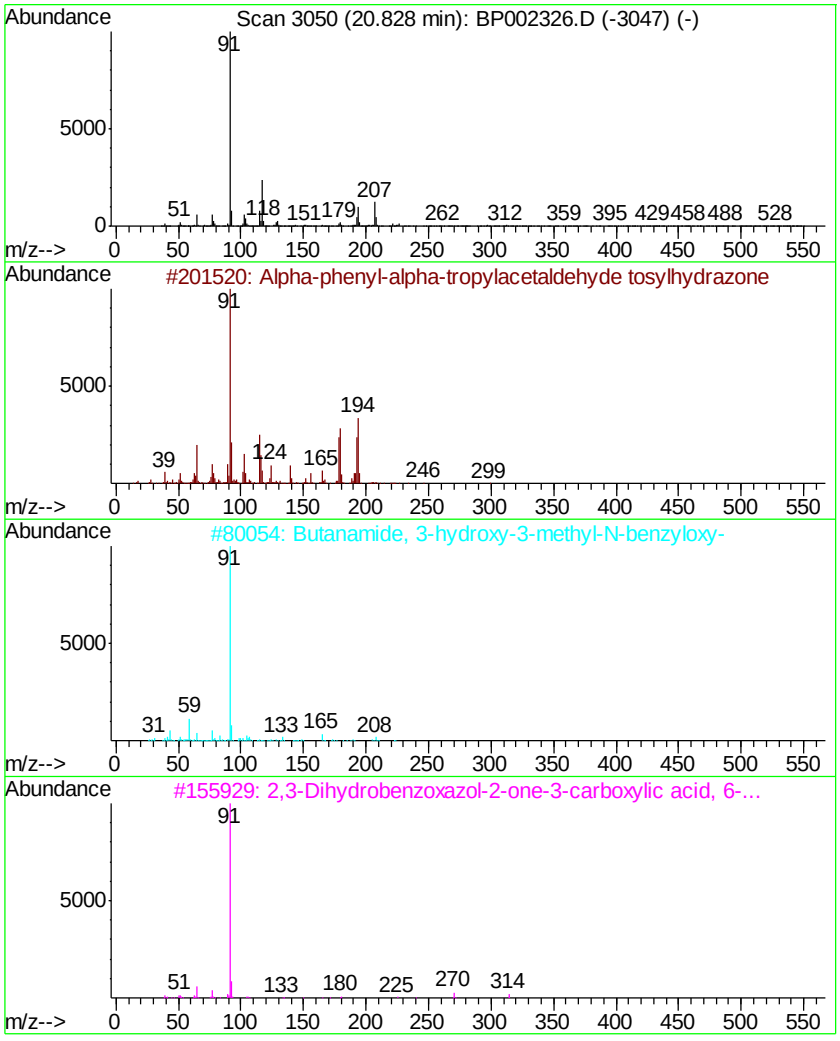
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

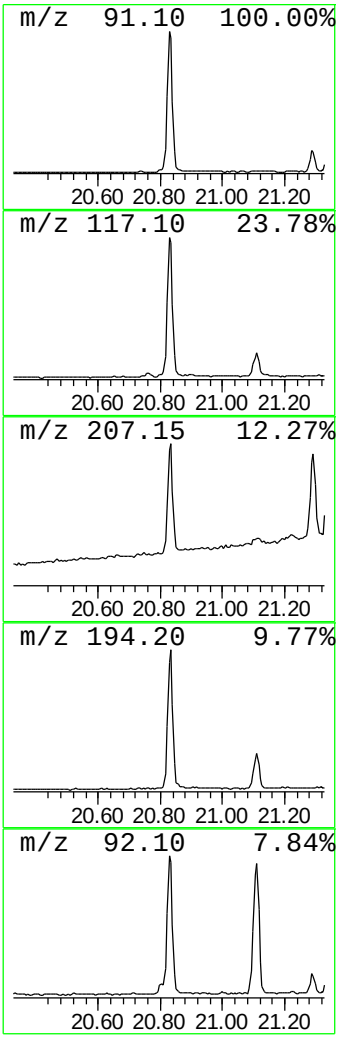
**********

Peak Number 3 unknown20.83 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.83 | 6.63 ng | 1507580 | Chrysene-d12 | 21.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Alpha-phenyl-alpha-tropylacetald... | 378 | C22H22N2O2S | 022532-16-7 | 16 |
| 2 | Butanamide, 3-hydroxy-3-methyl-N... | 223 | C12H17NO3 | 1000185-71-6 | 14 |
| 3 | 2,3-Dihydrobenzoxazol-2-one-3-ca... | 314 | C15H10N2O6 | 300808-99-5 | 10 |
| 4 | 4-Benzyloxy-3-methoxy-2-nitroben... | 303 | C15H13NO6 | 003584-32-5 | 10 |
| 5 | Piperazine-2,5-dione, 6-benzyl-3... | 288 | C12H11F3N2O3 | 1000303-24-1 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

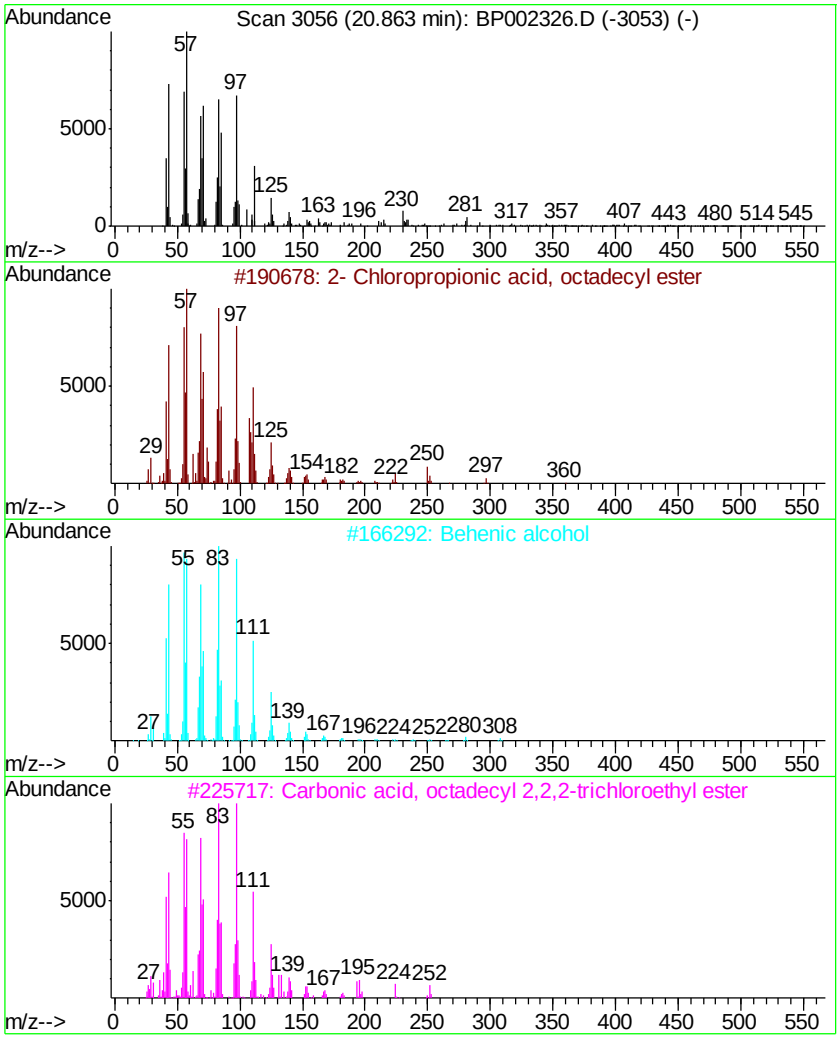
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

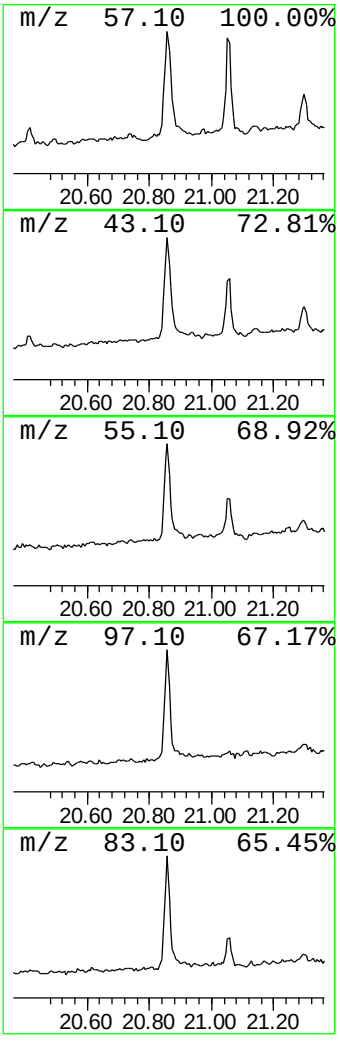
**********

Peak Number 4 2- Chloropropionic acid, oc... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.86 | 3.08 ng | 699436 | Chrysene-d12 | 21.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2- Chloropropionic acid, octadec... | 360 | C21H41ClO2 | 088104-31-8 | 96 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 91 |
| 3 | Carbonic acid, octadecyl 2,2,2-t... | 444 | C21H39Cl3O3 | 1000314-56-3 | 91 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 91 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

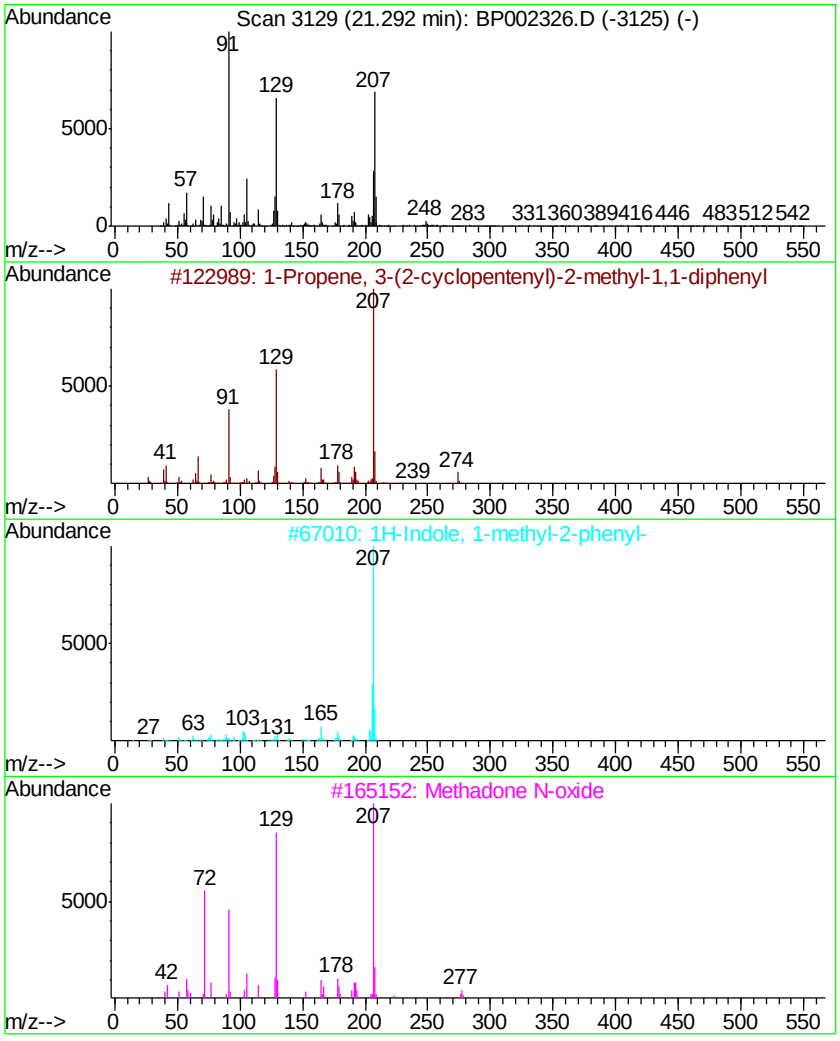
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

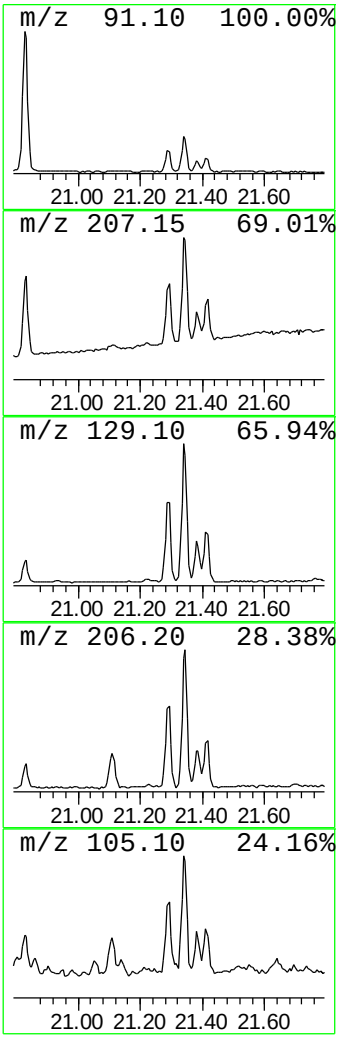
**********

Peak Number 5 unknown21.29 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.29 | 2.19 ng | 496929 | Chrysene-d12 | 21.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propene, 3-(2-cyclopentenyl)-2... | 274 | C21H22 | 1000154-23-3 | 47 |
| 2 | 1H-Indole, 1-methyl-2-phenyl- | 207 | C15H13N | 003558-24-5 | 42 |
| 3 | Methadone N-oxide | 325 | C21H27NO2 | 1000120-80-7 | 38 |
| 4 | 1H-Indole, 5-methyl-2-phenyl- | 207 | C15H13N | 013228-36-9 | 38 |
| 5 | 1H-Indole, 2-methyl-3-phenyl- | 207 | C15H13N | 004757-69-1 | 30 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

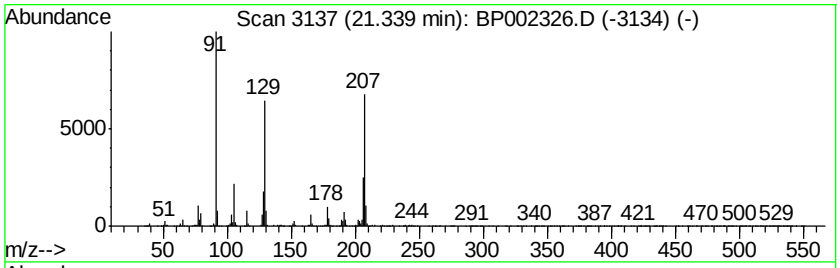
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

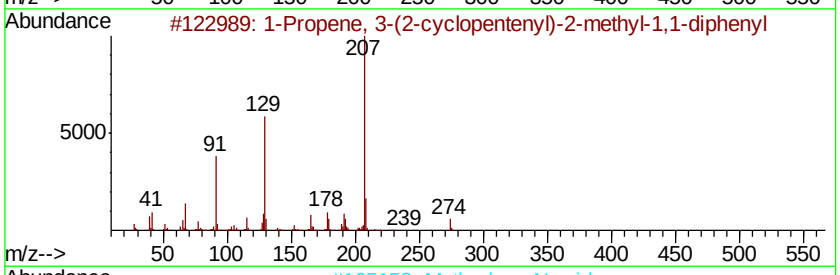
**********

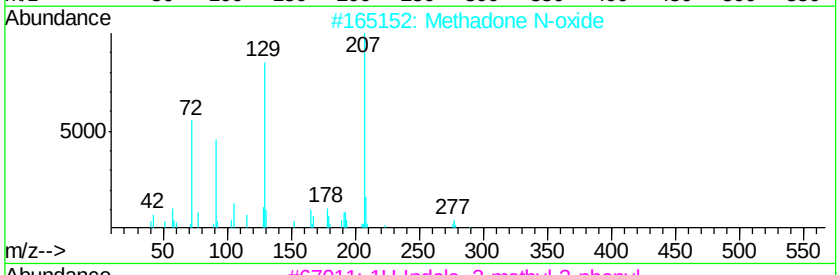
Peak Number 6 1-Propene, 3-(2-cyclopenten... Concentration Rank 6

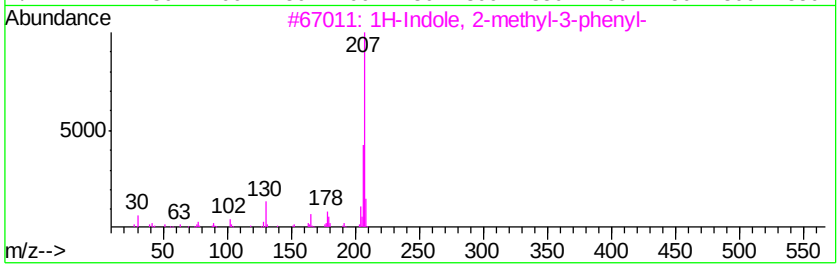
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.34 | 2.83 ng | 643282 | Chrysene-d12 | 21.11 |

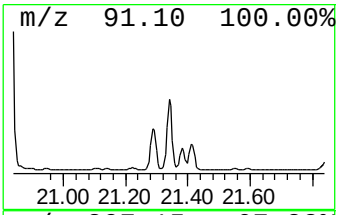
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propene, 3-(2-cyclopentenyl)-2... | 274 | C21H22 | 1000154-23-3 | 53 |
| 2 | Methadone N-oxide | 325 | C21H27NO2 | 1000120-80-7 | 52 |
| 3 | 1H-Indole, 2-methyl-3-phenyl- | 207 | C15H13N | 004757-69-1 | 46 |
| 4 | 1H-Indole, 1-methyl-2-phenyl- | 207 | C15H13N | 003558-24-5 | 42 |
| 5 | 5-Methyl-2-phenylindolizine | 207 | C15H13N | 036944-99-7 | 35 |

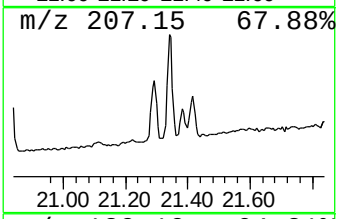


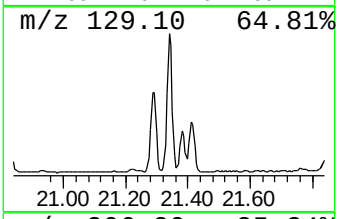



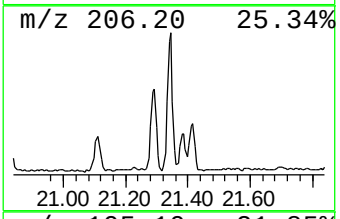



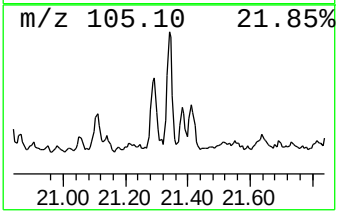



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

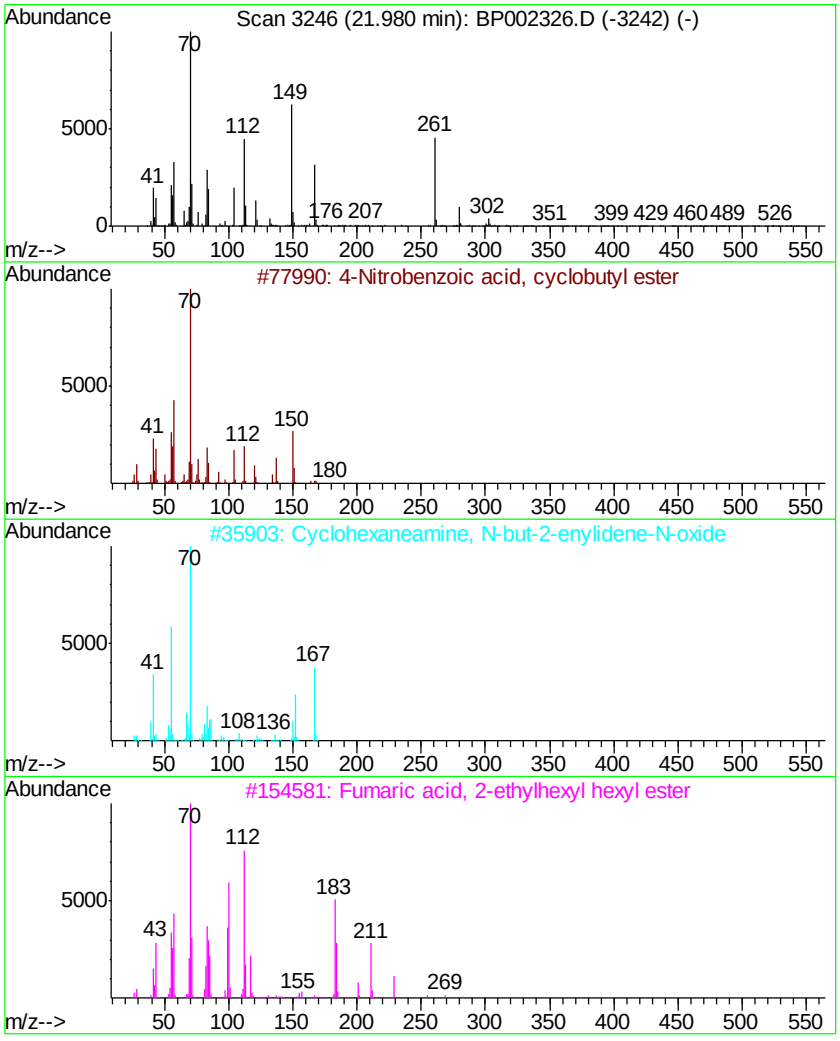
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

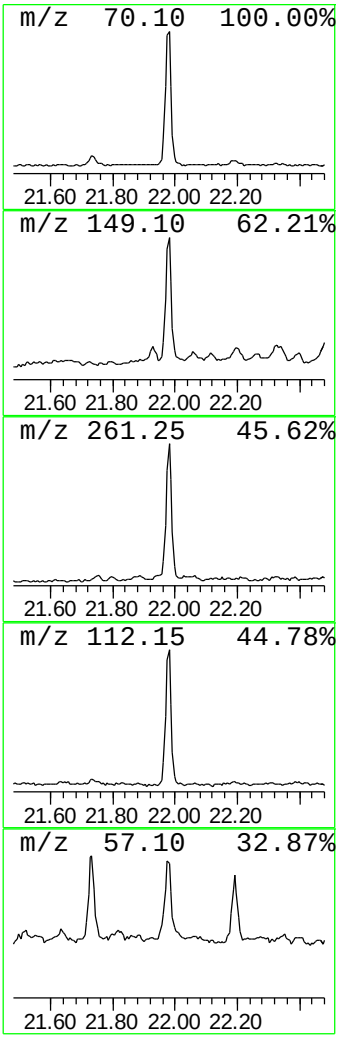
**********

Peak Number 7 unknown21.98 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.98 | 3.46 ng | 787072 | Chrysene-d12 | 21.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Nitrobenzoic acid, cyclobutyl ... | 221 | C11H11NO4 | 070335-00-1 | 27 |
| 2 | Cyclohexaneamine, N-but-2-enylid... | 167 | C10H17NO | 068048-01-1 | 22 |
| 3 | Fumaric acid, 2-ethylhexyl hexyl... | 312 | C18H32O4 | 1000339-14-1 | 22 |
| 4 | Bis(2-ethylhexyl) phthalate | 390 | C24H38O4 | 000117-81-7 | 18 |
| 5 | 1-(2-Hydroxymethylpyrrolidin-1-y... | 143 | C7H13NO2 | 1000192-83-2 | 16 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
Data File : BP002326.D
Acq On : 29 May 2020 21:27
Operator : CG/JU
Sample : L2776-04 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 225

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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 |
| Styrene | 5.63 | 2.9 | ng | 295181 | 1 | 7.60 | 2057440 | 20.0 |
| unknown20.83 | 20.83 | 6.6 | ng | 1507580 | 5 | 21.11 | 4545160 | 20.0 |
| 2- Chloropropioni... | 20.86 | 3.1 | ng | 699436 | 5 | 21.11 | 4545160 | 20.0 |
| unknown21.29 | 21.29 | 2.2 | ng | 496929 | 5 | 21.11 | 4545160 | 20.0 |
| 1-Propene, 3-(2-c... | 21.34 | 2.8 | ng | 643282 | 5 | 21.11 | 4545160 | 20.0 |
| unknown21.98 | 21.98 | 3.5 | ng | 787072 | 5 | 21.11 | 4545160 | 20.0 |