LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 | 5.087 | 506 | 510 | 521 | rVB | 151872 | 205331 | 13.63% | 1.398% |
| 2 | 5.481 | 572 | 577 | 580 | rBV | 1449629 | 1350162 | 89.63% | 9.193% |
| 3 | 6.492 | 743 | 749 | 759 | rBV | 1377662 | 1408418 | 93.50% | 9.590% |
| 4 | 6.628 | 768 | 772 | 775 | rBV | 1554608 | 1450306 | 96.28% | 9.875% |
| 5 | 6.857 | 808 | 811 | 815 | rBV | 487835 | 382652 | 25.40% | 2.606% |
| 6 | 7.016 | 834 | 838 | 841 | rBV | 1303979 | 1085220 | 72.05% | 7.389% |
| 7 | 7.422 | 902 | 907 | 910 | rBV | 950960 | 873552 | 57.99% | 5.948% |
| 8 | 8.139 | 1025 | 1029 | 1032 | rBV | 605578 | 483130 | 32.07% | 3.290% |
| 9 | 8.692 | 1120 | 1123 | 1126 | rBV | 106994 | 80532 | 5.35% | 0.548% |
| 10 | 9.216 | 1207 | 1212 | 1215 | rBV | 1774360 | 1506292 | 100.00% | 10.256% |
| 11 | 9.604 | 1275 | 1278 | 1286 | rBB | 88152 | 68294 | 4.53% | 0.465% |
| 12 | 9.892 | 1323 | 1327 | 1331 | rBV | 542870 | 484179 | 32.14% | 3.297% |
| 13 | 10.610 | 1445 | 1449 | 1452 | rBV | 384062 | 344475 | 22.87% | 2.346% |
| 14 | 10.686 | 1458 | 1462 | 1473 | rVB | 860023 | 814486 | 54.07% | 5.546% |
| 15 | 11.380 | 1577 | 1580 | 1583 | rBV | 503958 | 418670 | 27.79% | 2.851% |
| 16 | 11.404 | 1583 | 1584 | 1587 | rVB | 62728 | 32616 | 2.17% | 0.222% |
| 17 | 11.898 | 1661 | 1668 | 1676 | rBV4 | 68716 | 82929 | 5.51% | 0.565% |
| 18 | 11.992 | 1680 | 1684 | 1687 | rBV | 16272 | 18638 | 1.24% | 0.127% |
| 19 | 12.445 | 1755 | 1761 | 1770 | rBV4 | 35821 | 51829 | 3.44% | 0.353% |
| 20 | 12.592 | 1783 | 1786 | 1789 | rBV | 188698 | 155477 | 10.32% | 1.059% |
| 21 | 12.821 | 1819 | 1825 | 1831 | rBV | 181206 | 178546 | 11.85% | 1.216% |
| 22 | 12.963 | 1841 | 1849 | 1853 | rBV | 1218473 | 1117513 | 74.19% | 7.609% |
| 23 | 13.033 | 1857 | 1861 | 1868 | rVV4 | 12773 | 21910 | 1.45% | 0.149% |
| 24 | 13.151 | 1878 | 1881 | 1884 | rVB | 16752 | 20418 | 1.36% | 0.139% |
| 25 | 13.257 | 1894 | 1899 | 1901 | rBV2 | 19036 | 21946 | 1.46% | 0.149% |
| 26 | 13.421 | 1922 | 1927 | 1932 | rVB | 23812 | 26210 | 1.74% | 0.178% |
| 27 | 13.657 | 1961 | 1967 | 1972 | rBV | 20066 | 30874 | 2.05% | 0.210% |
| 28 | 13.768 | 1983 | 1986 | 1989 | rBV3 | 15896 | 19307 | 1.28% | 0.131% |
| 29 | 13.851 | 1997 | 2000 | 2008 | rVB3 | 101744 | 145602 | 9.67% | 0.991% |
| 30 | 14.021 | 2022 | 2029 | 2032 | rBV2 | 529470 | 586332 | 38.93% | 3.992% |
| 31 | 14.045 | 2032 | 2033 | 2038 | rVB | 109370 | 72257 | 4.80% | 0.492% |
| 32 | 14.404 | 2090 | 2094 | 2097 | rBV | 26889 | 30933 | 2.05% | 0.211% |
| 33 | 14.492 | 2105 | 2109 | 2113 | rBV6 | 17602 | 29311 | 1.95% | 0.200% |
| 34 | 14.527 | 2113 | 2115 | 2118 | rBV4 | 19855 | 24010 | 1.59% | 0.163% |

LSC Area Percent Report

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Data File : BF100935.D
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Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.857 | 2169 | 2171 | 2174 | rVB2 | 22679 | 20776 | 1.38% | 0.141% |
| 36 | 15.062 | 2201 | 2206 | 2213 | rBV | 112463 | 225695 | 14.98% | 1.537% |
| 37 | 15.362 | 2254 | 2257 | 2262 | rVB | 69227 | 85408 | 5.67% | 0.582% |
| 38 | 15.427 | 2264 | 2268 | 2274 | rBV | 101324 | 127884 | 8.49% | 0.871% |
| 39 | 15.492 | 2274 | 2279 | 2283 | rBV | 329455 | 426589 | 28.32% | 2.905% |
| 40 | 16.962 | 2525 | 2529 | 2537 | rVB | 40015 | 70511 | 4.68% | 0.480% |
| 41 | 17.127 | 2551 | 2557 | 2558 | rBV5 | 13330 | 23600 | 1.57% | 0.161% |
| 42 | 17.203 | 2565 | 2570 | 2576 | rVB9 | 14747 | 30100 | 2.00% | 0.205% |
| 43 | 17.415 | 2600 | 2606 | 2610 | rBV3 | 27203 | 53377 | 3.54% | 0.363% |

Sum of corrected areas: 14686297

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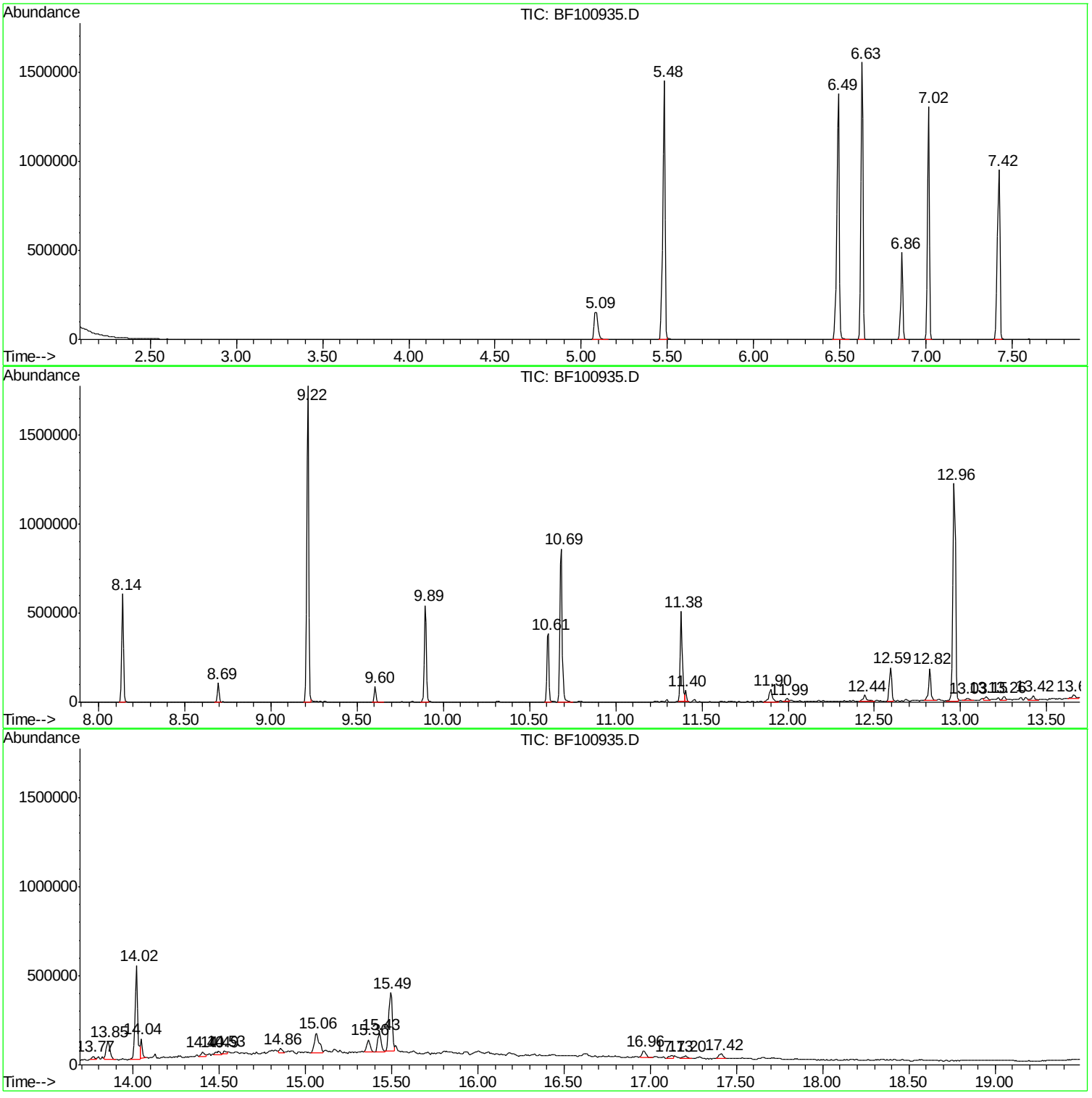
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

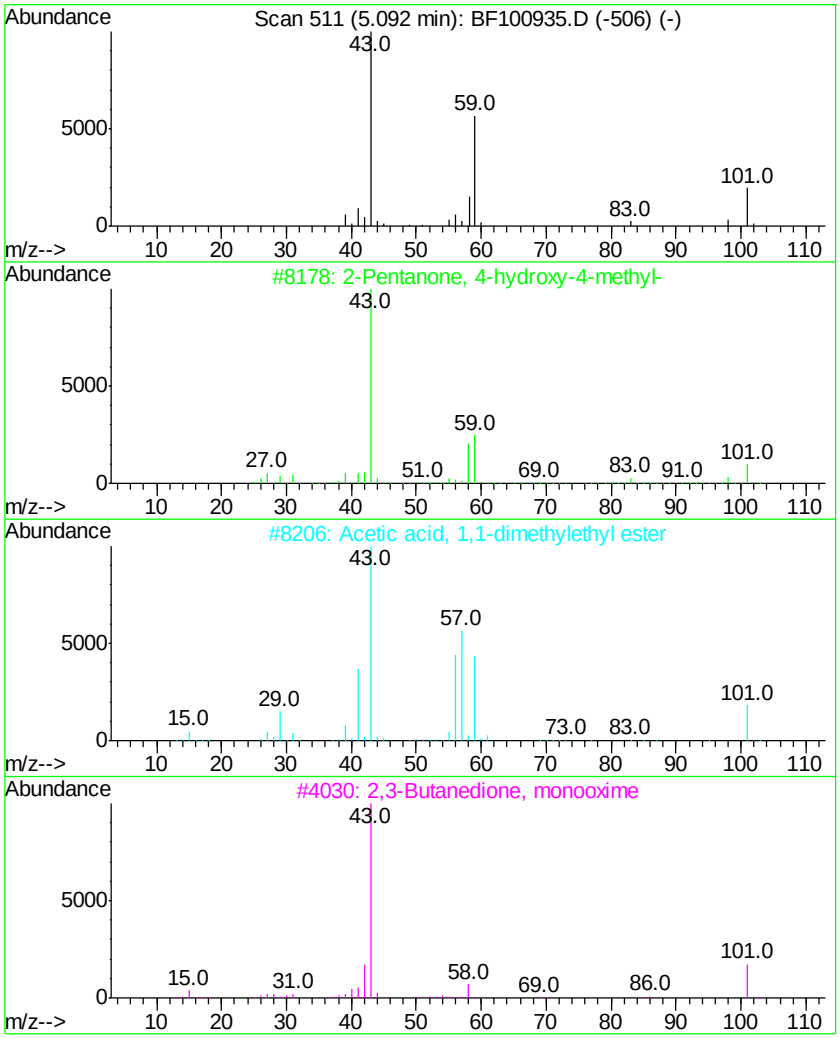
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

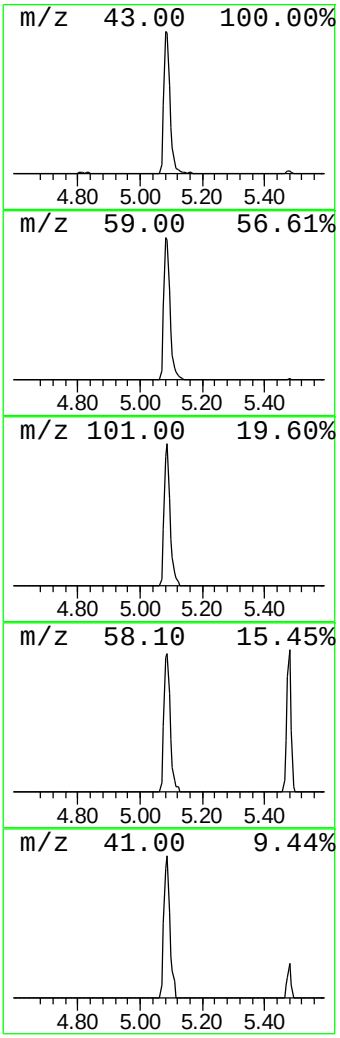
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 10.73 ng | 205331 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 4 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 28 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

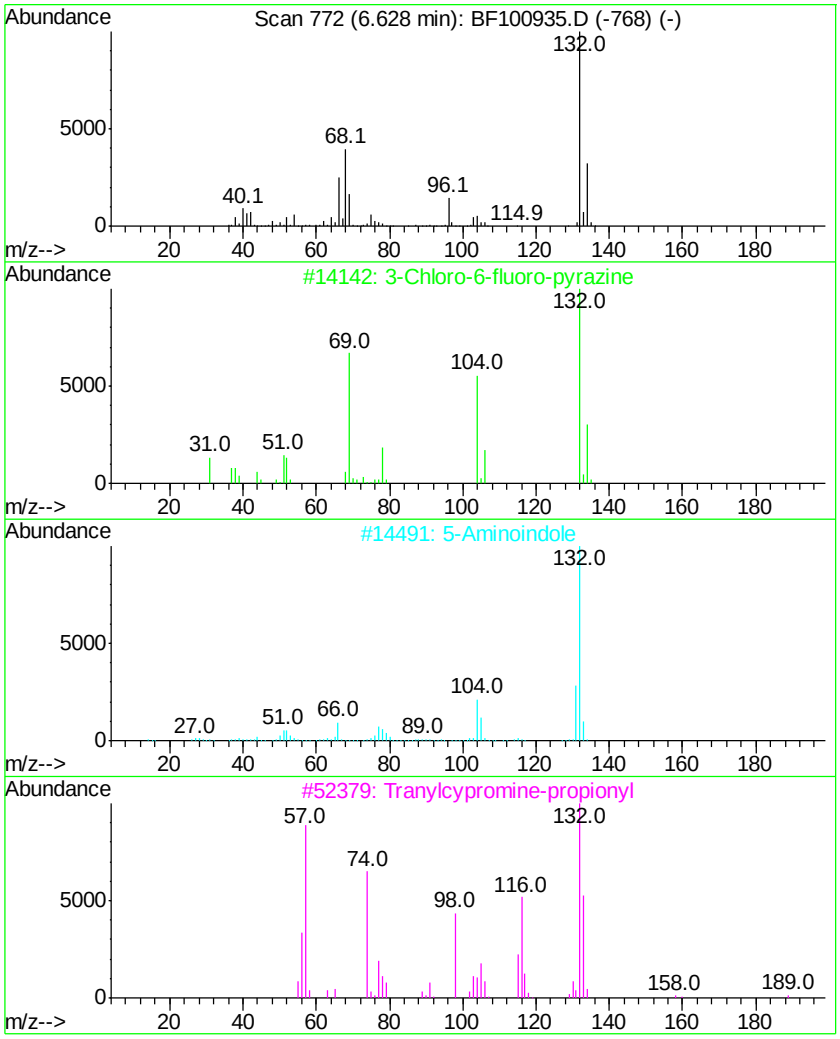
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

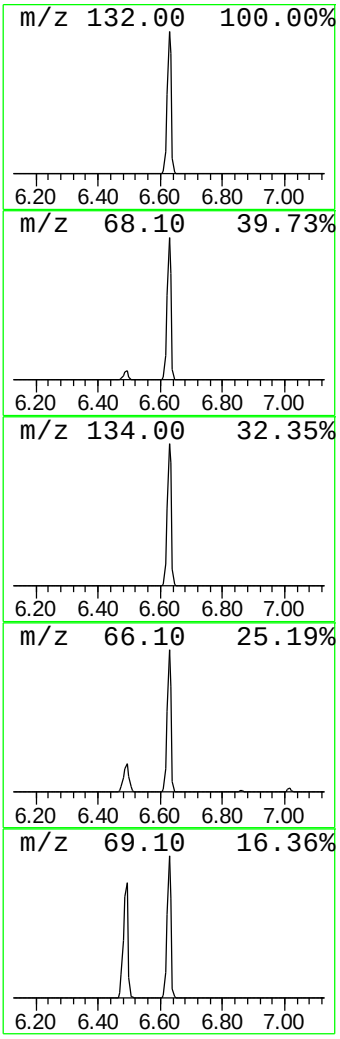
**********

Peak Number 2 unknown6.63 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 75.80 ng | 1450310 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

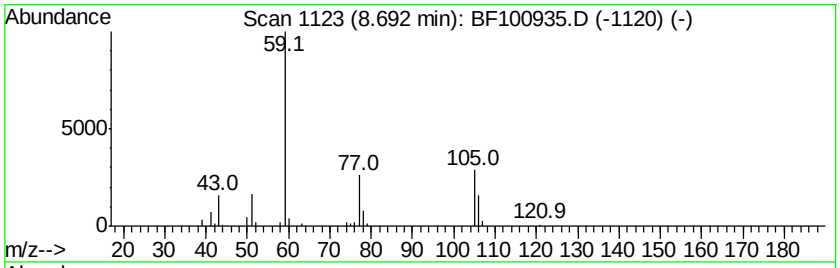
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

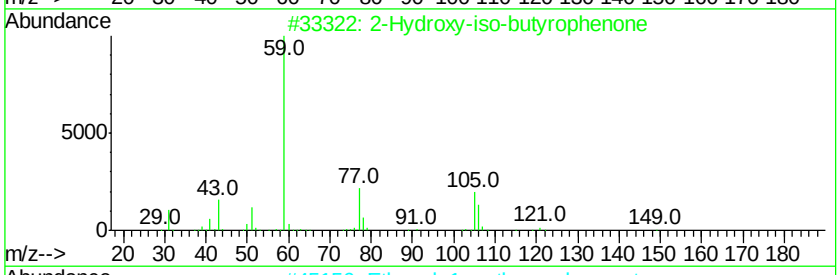
**********

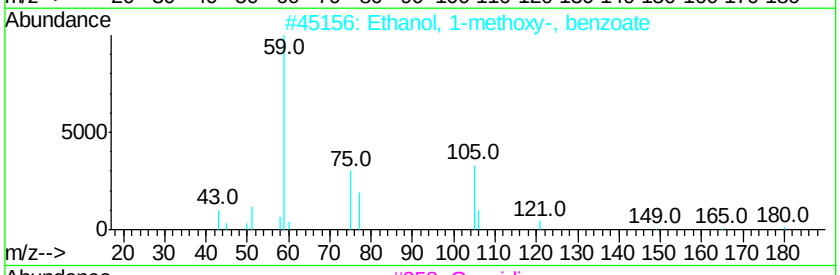
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

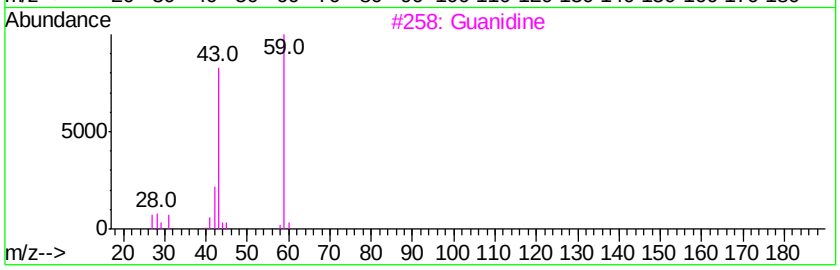
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.69 | 3.33 ng | 80532 | Naphthalene-d8 | 8.14 |

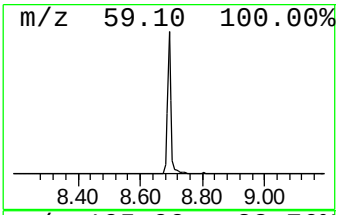
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-iso-butyrophenone | 164 | C10H12O2 | 007473-98-5 | 90 |
| 2 | Ethanol, 1-methoxy-, benzoate | 180 | C10H12O3 | 051835-44-0 | 72 |
| 3 | Guanidine | 59 | CH5N3 | 000113-00-8 | 7 |
| 4 | Formamide, N-methyl- | 59 | C2H5NO | 000123-39-7 | 5 |
| 5 | Acetamide | 59 | C2H5NO | 000060-35-5 | 5 |

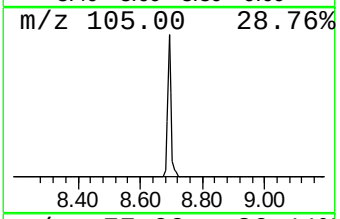


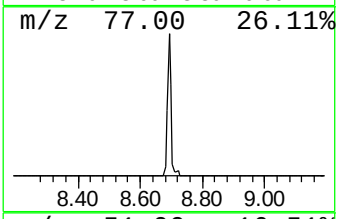



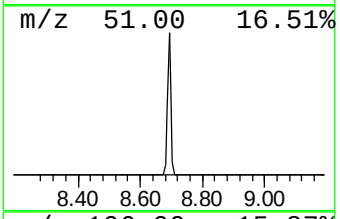



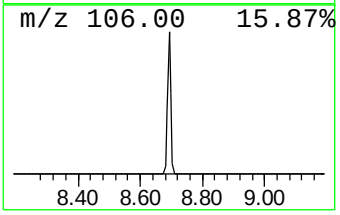



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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

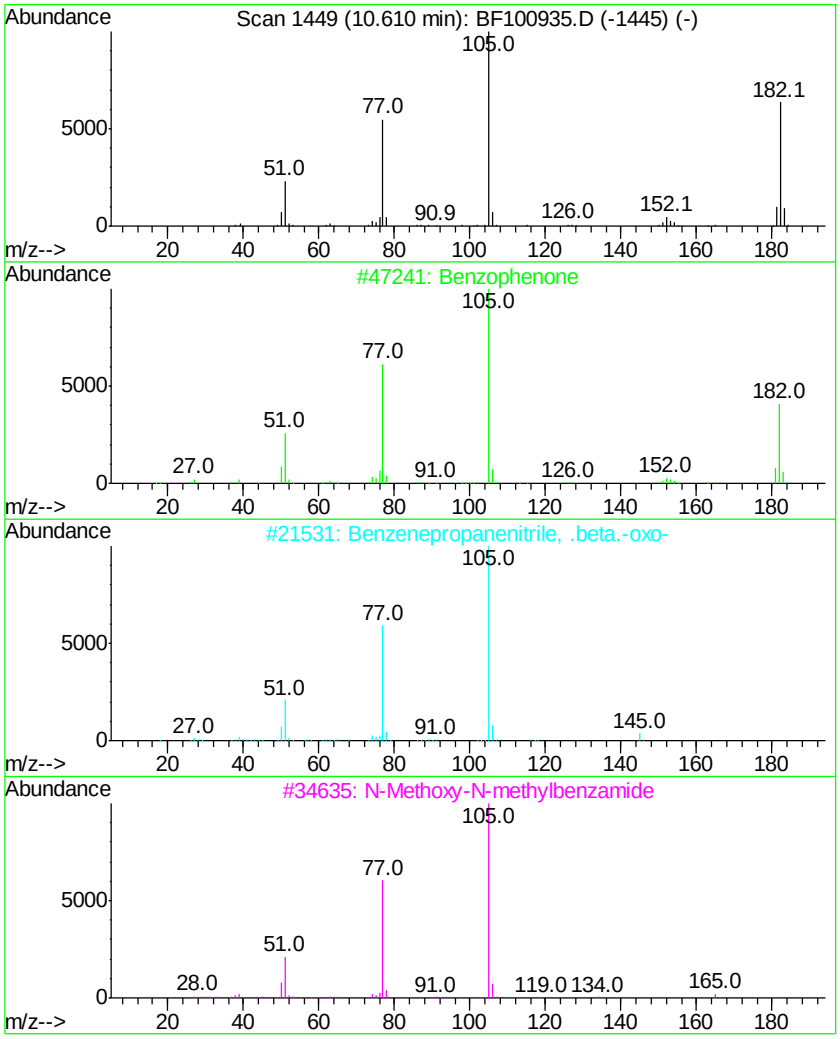
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

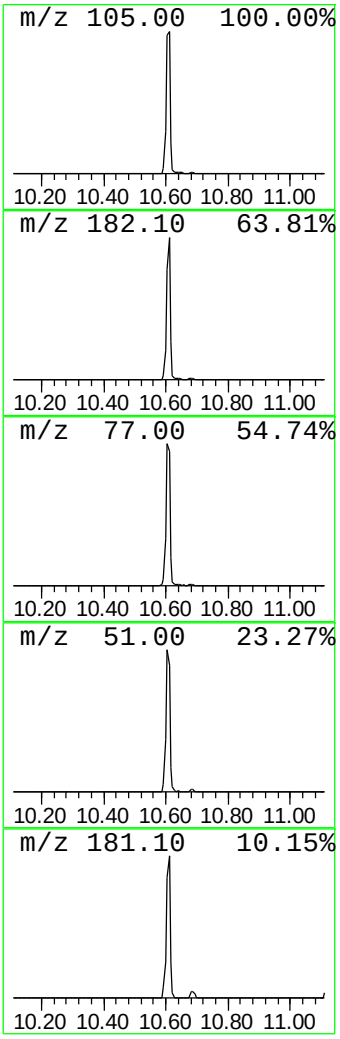
**********

Peak Number 5 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.61 | 14.23 ng | 344475 | Acenaphthene-d10 | 9.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 97 |
| 2 | Benzenepropanenitrile, .beta.-oxo- | 145 | C9H7NO | 000614-16-4 | 47 |
| 3 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 47 |
| 4 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 47 |
| 5 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 47 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
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Operator : SJ/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

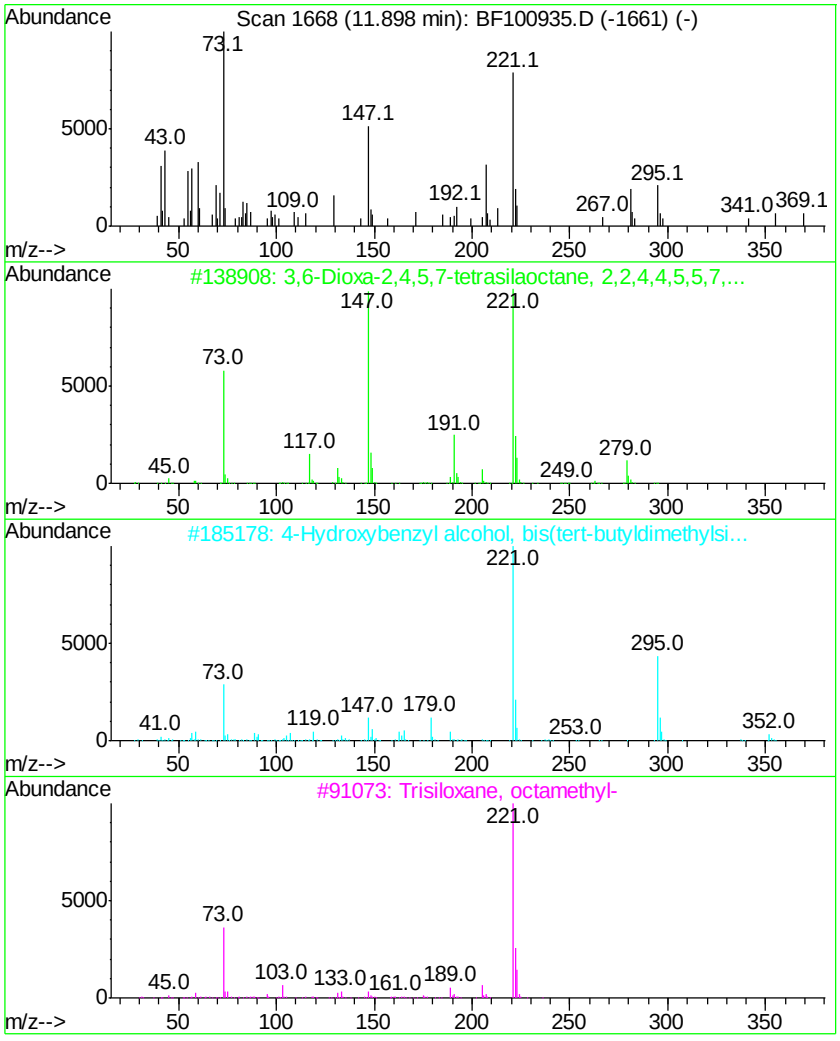
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

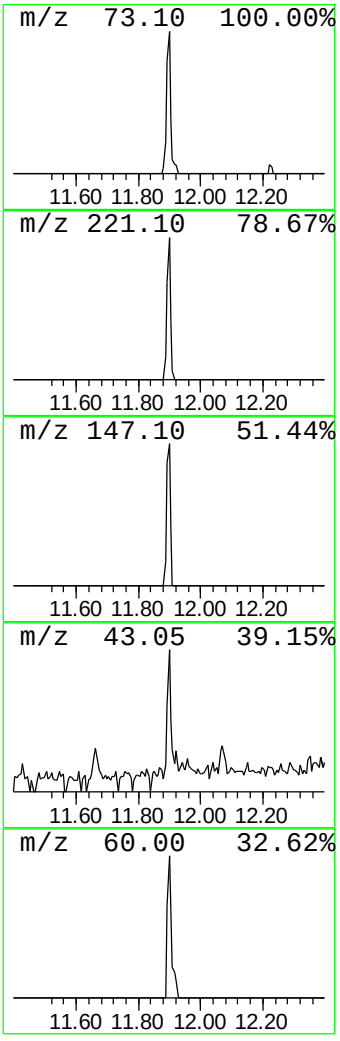
**********

Peak Number 6 Tris(trimethylsilyl)borate1... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.90 | 3.96 ng | 82929 | Phenanthrene-d10 | 11.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,6-Dioxa-2,4,5,7-tetrasilaoctan... | 294 | C10H30O2Si4 | 004342-25-0 | 47 |
| 2 | 4-Hydroxybenzyl alcohol, bis(ter... | 352 | C19H36O2Si2 | 1000364-43-9 | 38 |
| 3 | Trisiloxane, octamethyl- | 236 | C8H24O2Si3 | 000107-51-7 | 32 |
| 4 | 2-tert-Butyl-6-methylphenol, tri... | 236 | C14H24OSi | 1000333-48-3 | 32 |
| 5 | Tris(trimethylsilyl)borate | 278 | C9H27BO3Si3 | 004325-85-3 | 32 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

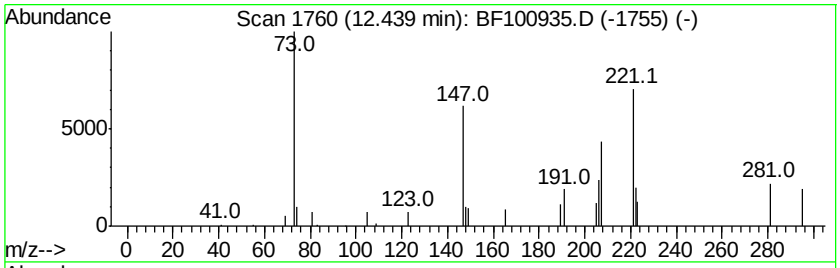
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

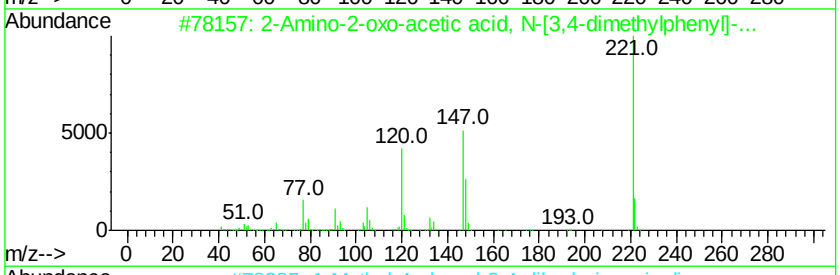
**********

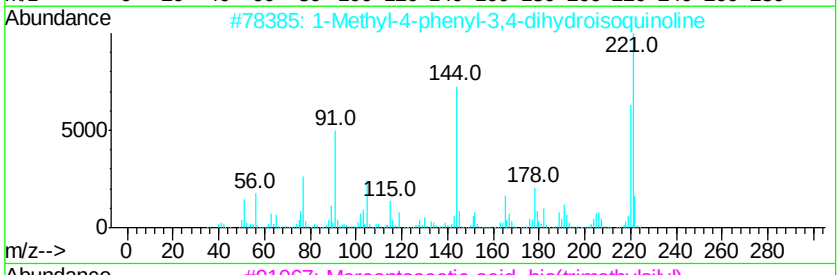
Peak Number 7 unknown12.44 Concentration Rank 9

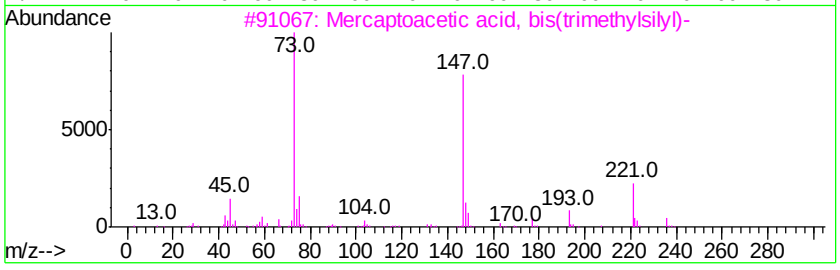
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.44 | 2.48 ng | 51829 | Phenanthrene-d10 | 11.38 |

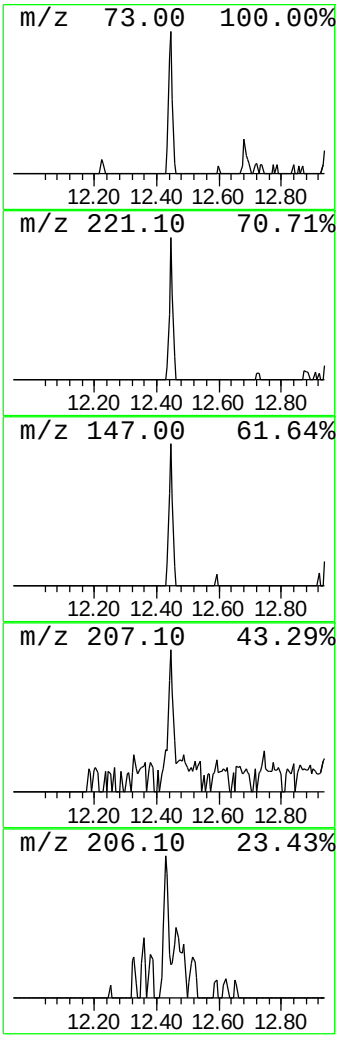
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Amino-2-oxo-acetic acid, N-[3,... | 221 | C12H15NO3 | 024451-17-0 | 43 |
| 2 | 1-Methyl-4-phenyl-3,4-dihydroiso... | 221 | C16H15N | 1000211-01-5 | 38 |
| 3 | Mercaptoacetic acid, bis(trimeth... | 236 | C8H20O2SSi2 | 006398-62-5 | 37 |
| 4 | Trisiloxane, octamethyl- | 236 | C8H24O2Si3 | 000107-51-7 | 35 |
| 5 | 4-Hydroxybenzyl alcohol, bis(ter... | 352 | C19H36O2Si2 | 1000364-43-9 | 32 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

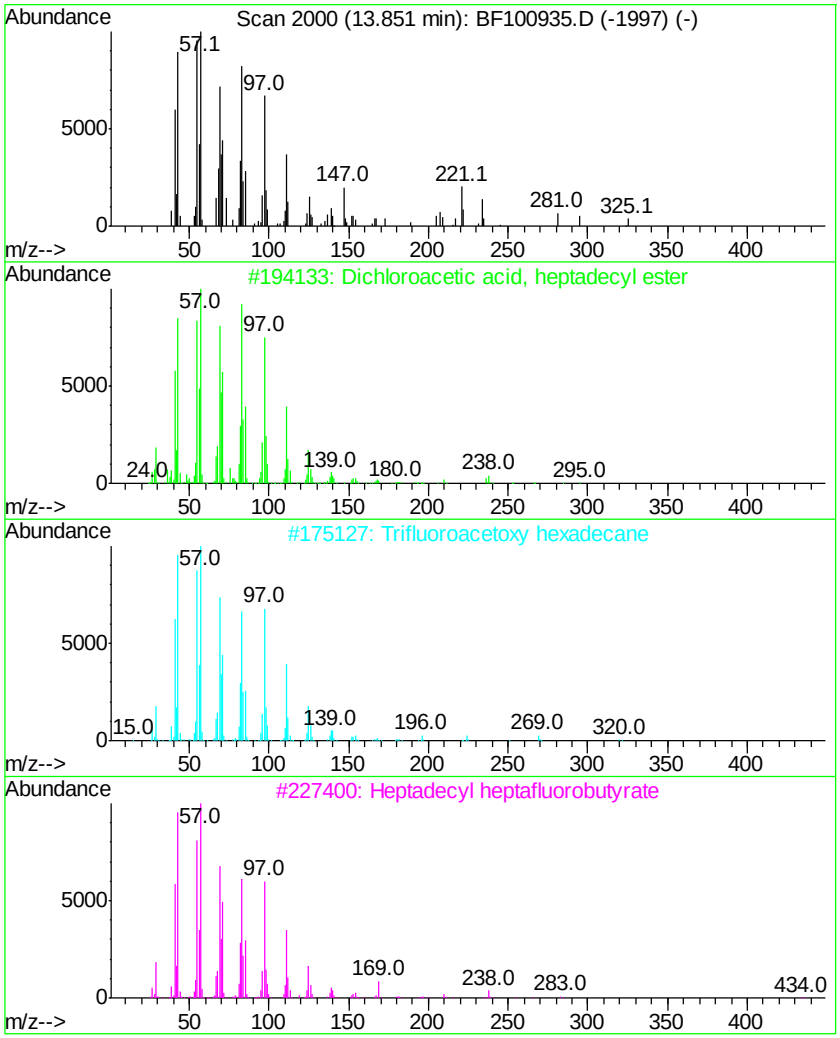
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

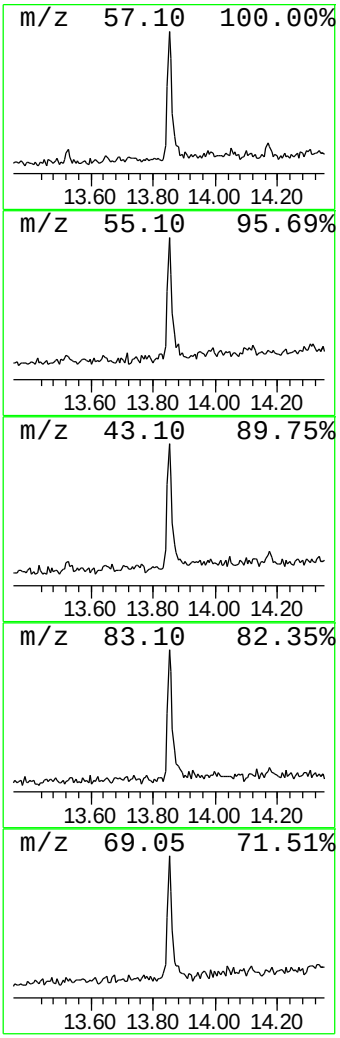
**********

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.85 | 4.97 ng | 145602 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 93 |
| 2 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 93 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 92 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 90 |
| 5 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

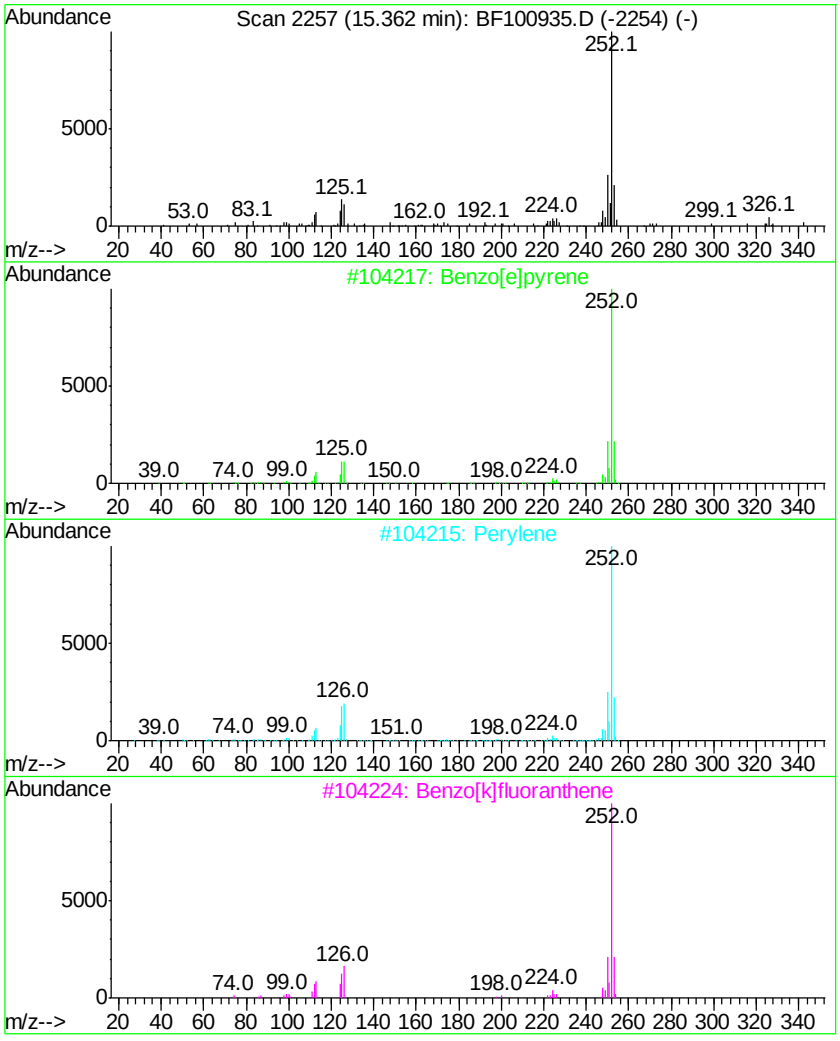
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

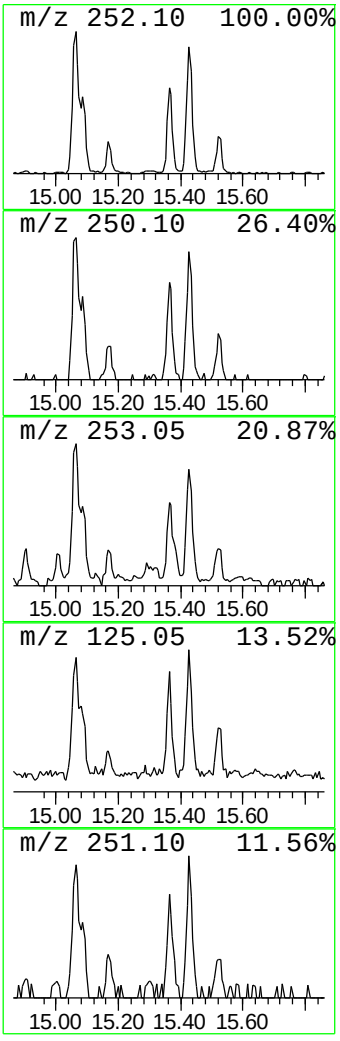
**********

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.36 | 4.00 ng | 85408 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 97 |
| 2 | Perylene | 252 | C20H12 | 000198-55-0 | 94 |
| 3 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 93 |
| 4 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 93 |
| 5 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 89 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100935.D
Acq On : 28 Nov 2017 15:48
Operator : SJ/JU
Sample : I6579-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HAR-4-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 |
| 2-Pentanone, 4-hy... | 5.09 | 10.7 | ng | 205331 | 1 | 6.86 | 382652 | 20.0 |
| unknown6.63 | 6.63 | 75.8 | ng | 1450310 | 1 | 6.86 | 382652 | 20.0 |
| 2-Hydroxy-iso-but... | 8.69 | 3.3 | ng | 80532 | 2 | 8.14 | 483130 | 20.0 |
| Benzophenone | 10.61 | 14.2 | ng | 344475 | 3 | 9.89 | 484179 | 20.0 |
| Tris(trimethylsil... | 11.90 | 4.0 | ng | 82929 | 4 | 11.38 | 418670 | 20.0 |
| unknown12.44 | 12.44 | 2.5 | ng | 51829 | 4 | 11.38 | 418670 | 20.0 |
| Dichloroacetic ac... | 13.85 | 5.0 | ng | 145602 | 5 | 14.02 | 586332 | 20.0 |
| Benzo[e]pyrene | 15.36 | 4.0 | ng | 85408 | 6 | 15.49 | 426589 | 20.0 |