Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Time: Nov 17 11:14:23 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616_[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration

| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| Internal Standards | | | | | |
| 1) 1,4-Dichlorobenzene-d4 | 5.081 | 152 | 437063 | 20.00 ug/mL | 0.00 |
| 3) Naphthalene-d8 | 6.457 | 136 | 1959311 | 20.00 ug/mL | 0.00 |
| 5) Acenaphthene-d10 | 8.216 | 164 | 1035065 | 20.00 ug/mL | 0.00 |
| 10) Phenanthrene-d10 | 9.681 | 188 | 1614628 | 20.00 ug/mL | 0.00 |
| 11) Chrysene-d12 | 13.963 | 240 | 935301 | 20.00 ug/mL | 0.00 |
| 12) Perylene-d12 | 16.798 | 264 | 539612 | 20.00 ug/mL | 0.00 |
| System Monitoring Compounds | | | | | |
| 7) 2-Fluorobiphenyl | 7.581 | 172 | 1075546 | 16.91 ug/mL | 0.00 |
| Spiked Amount 12.500 | Range 25 - 150 | | Recovery = ~~135.28%~~ | | |
| Target Compounds | | | | | Qvalue |
| 2) MCHM | 0.000 | | 0 | N.D. | |
| 4) PPH | 0.000 | | 0 | N.D. | |
| 6) 1,4-CHDM | 0.000 | | 0 | N.D. d | |
| 8) DM-1,4-CHDC | 0.000 | | 0 | N.D. | |
| 9) di-PPH | 0.000 | | 0 | N.D. d | |

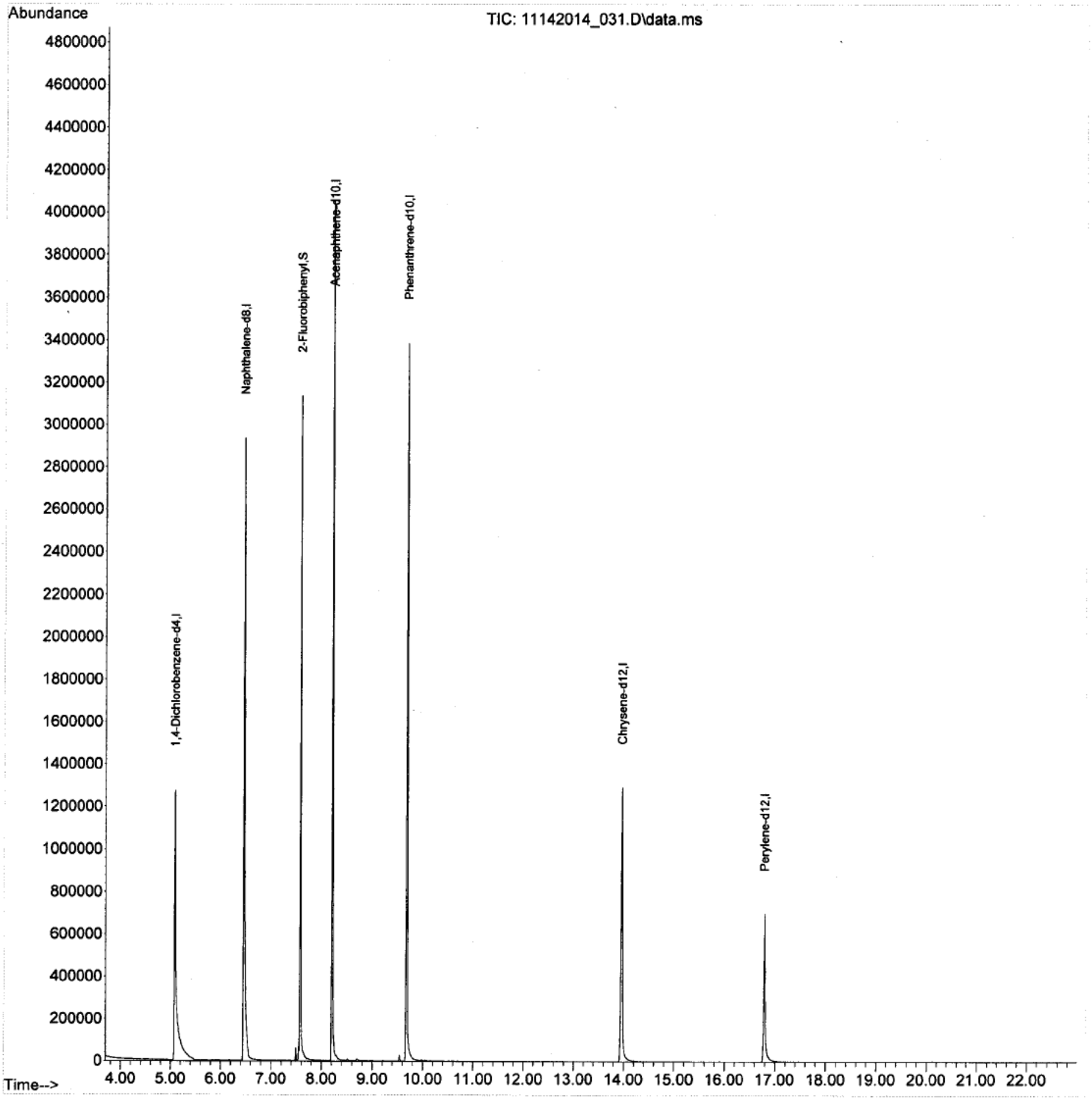
See Analyst Narrative, Surrogate Recovery [redacted] 1/7/15

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Time: Nov 17 11:14:23 2014
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration



# Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Time: Dec 01 13:01:57 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| Internal Standards | | | | | |
| 1) 1,4-Dichlorobenzene-d4 | 5.081 | 150 | 753828 | 20.00 ug/mL | 0.00 |
| 13) Naphthalene-d8 | 6.457 | 136 | 1959311 | 20.00 ug/mL | 0.00 |
| 24) Acenaphthene-d10 | 8.216 | 164 | 1035065 | 20.00 ug/mL | 0.00 |
| 37) Phenanthrene-d10 | 9.681 | 188 | 1616301 | 20.00 ug/mL | 0.00 |
| 49) Chrysene-d12 | 13.963 | 240 | 937777 | 20.00 ug/mL | -0.01 |
| 58) Perylene-d12 | 16.798 | 264 | 542067 | 20.00 ug/mL | -0.01 |

| Target Compounds | | | | Qvalue |
|---|---|---|---|---|
| 2) Bis(2-chloroethyl) ether | 0.000 | | 0 | N.D. |
| 3) n-Decane | 0.000 | | 0 | N.D. d |
| 4) 1,3-Dichlorobenzene | 0.000 | | 0 | N.D. |
| 5) 1,4-Dichlorobenzene | 0.000 | | 0 | N.D. |
| 6) 1,2-Dichlorobenzene | 0.000 | | 0 | N.D. |
| 7) Benzyl Alcohol | 0.000 | | 0 | N.D. d |
| 8) Bis(2-chloroisopropyl)... | 0.000 | | 0 | N.D. |
| 9) Hexachloroethane | 0.000 | | 0 | N.D. d |
| 10) N-Nitrosodi-N-propylamine | 0.000 | | 0 | N.D. |
| 11) Nitrobenzene | 0.000 | | 0 | N.D. d |
| 12) 4-Methylcyclohexanecar... | 0.000 | | 0 | N.D. d |
| 14) n-Dodecane | 0.000 | | 0 | N.D. d |
| 15) Isophorone | 0.000 | | 0 | N.D. d |
| 16) Bis(2-chloroethoxy) me... | 0.000 | | 0 | N.D. d |
| 17) 1,2,4-Trichlorobenzene | 0.000 | | 0 | N.D. |
| 18) Napthalene | 0.000 | | 0 | N.D. |
| 19) Hexachlorobutadiene | 0.000 | | 0 | N.D. |
| 20) 2-Methylnapthalene | 0.000 | | 0 | N.D. d |
| 21) Hexachlorocyclopentadiene | 0.000 | | 0 | N.D. |
| 22) 2-Chloronapthalene | 0.000 | | 0 | N.D. d |
| 23) n-Tetradecane | 0.000 | | 0 | N.D. d |
| 25) Dimethly Phthalate | 0.000 | | 0 | N.D. d |
| 26) Acenaphthylene | 0.000 | | 0 | N.D. d |
| 27) 2,6-Dinitrotoluene | 0.000 | | 0 | N.D. d |
| 28) Acenaphthene | 0.000 | | 0 | N.D. d |
| 29) Dibenzofuran | 0.000 | | 0 | N.D. |
| 30) 2,4-Dinitrotoluene | 0.000 | | 0 | N.D. d |
| 31) n-Hexadecane | 0.000 | | 0 | N.D. d |
| 32) Fluorene | 0.000 | | 0 | N.D. |
| 33) Diethyl Phthalate | 0.000 | | 0 | N.D. d |
| 34) 4-Chlorophenylphenyl E... | 0.000 | | 0 | N.D. d |
| 35) N-Nitrosodiphenylamine | 0.000 | | 0 | N.D. |
| 36) Azobenzene | 0.000 | | 0 | N.D. |
| 38) 4-Bromophenylphenyl Ether | 0.000 | | 0 | N.D. |
| 39) Hexachlorobenzene | 0.000 | | 0 | N.D. |
| 40) n-Octadecane | 0.000 | | 0 | N.D. d |
| 41) Phenanthrene | 0.000 | | 0 | N.D. d |
| 42) Anthracene | 0.000 | | 0 | N.D. d |
| 43) Carbazole | 0.000 | | 0 | N.D. d |
| 44) Dibutyl Phthalate | 0.000 | | 0 | N.D. d |
| 45) n-Eicosane | 0.000 | | 0 | N.D. |

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Time: Dec 01 13:01:57 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

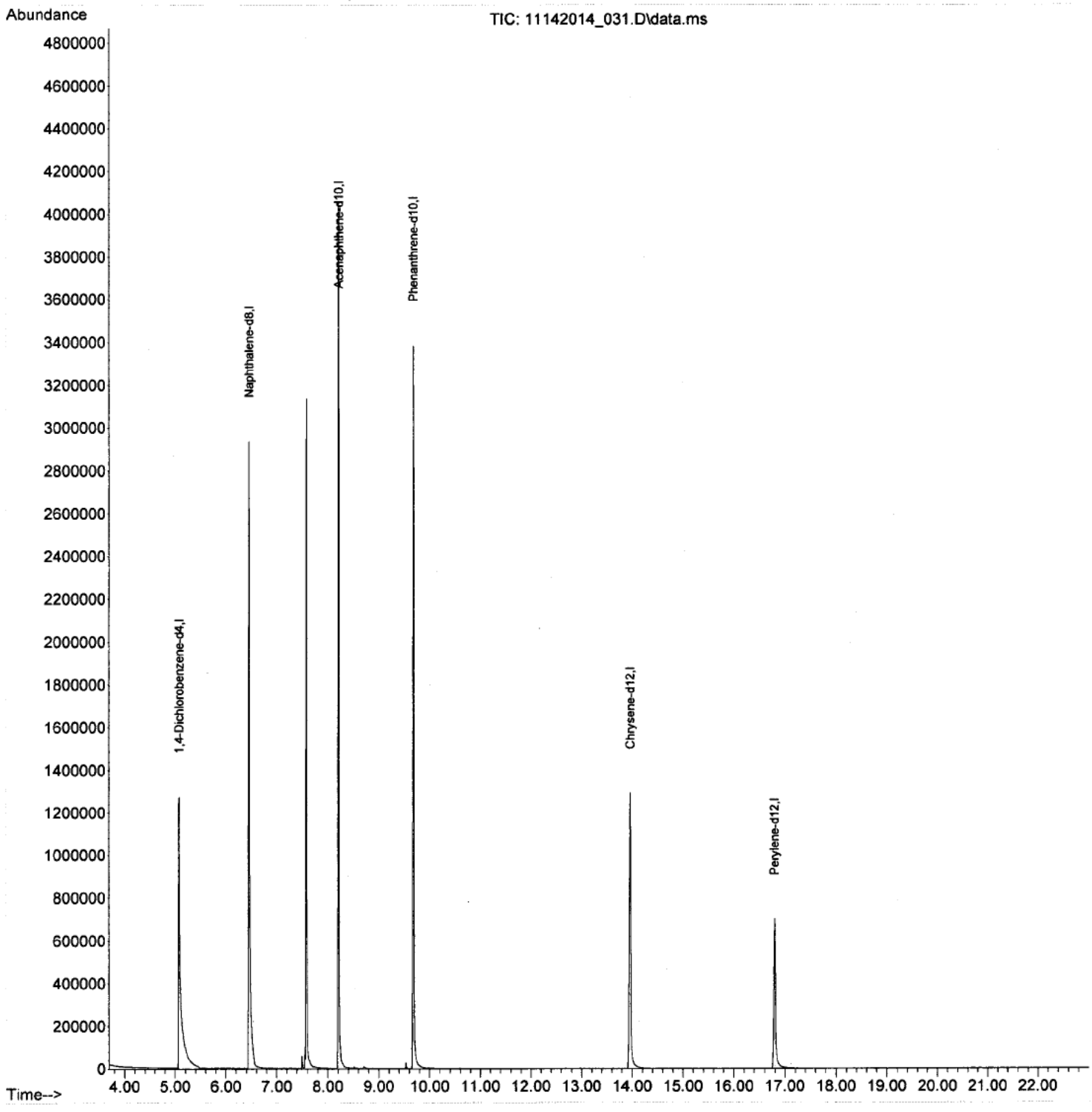
| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| 46) Fluoranthene | 0.000 | | 0 | N.D. | |
| 47) Pyrene | 0.000 | | 0 | N.D. | |
| 48) n-Docosane | 0.000 | | 0 | N.D. | |
| 50) Benzyl Butyl Phthalate | 0.000 | | 0 | N.D. | |
| 51) n-Tetracosane | 0.000 | | 0 | N.D. | |
| 52) n-Hexacosane | 0.000 | | 0 | N.D. d | |
| 53) n-Octacosane | 0.000 | | 0 | N.D. | |
| 54) Benz[a]anthracene | 0.000 | | 0 | N.D. d | |
| 55) Chrysene | 0.000 | | 0 | N.D. d | |
| 56) Bis(2-ethylhexyl) Phth... | 0.000 | | 0 | N.D. d | |
| 57) Di-n-octyl Phthalate | 0.000 | | 0 | N.D. | |
| 59) Benzo[b]fluoranthene | 0.000 | | 0 | N.D. | |
| 60) Benzo(k)fluoranthene | 0.000 | | 0 | N.D. | |
| 61) Benz[a]pyrene | 0.000 | | 0 | N.D. d | |
| 62) Indo[1,2,3-cd]pyrene | 0.000 | | 0 | N.D. | |
| 63) Dibenz[a,h]anthracene | 0.000 | | 0 | N.D. | |
| 64) Benzo[g,h,i]perylene | 0.000 | | 0 | N.D. | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Time: Dec 01 13:01:57 2014
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration



# LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 0

Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Title : RP1616-MCHM Compounds

Signal : TIC: 11142014_031.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.063 | 61 | 64 | 87 | rVB6 | 2963 | 15439 | 0.34% | 0.063% |
| 2 | 4.857 | 197 | 199 | 215 | rVB6 | 1446 | 4330 | 0.09% | 0.018% |
| 3 | 5.081 | 227 | 237 | 313 | rVB | 1270758 | 3283778 | 71.92% | 13.475% |
| 4 | 5.851 | 357 | 368 | 369 | rVV5 | 1521 | 3855 | 0.08% | 0.016% |
| 5 | 5.928 | 369 | 381 | 385 | rVV5 | 1694 | 6626 | 0.15% | 0.027% |
| 6 | 5.975 | 385 | 389 | 401 | rVV6 | 1321 | 4539 | 0.10% | 0.019% |
| 7 | 6.116 | 407 | 413 | 427 | rVB5 | 1226 | 4617 | 0.10% | 0.019% |
| 8 | 6.234 | 427 | 433 | 449 | rVB6 | 1262 | 5942 | 0.13% | 0.024% |
| 9 | 6.457 | 461 | 471 | 519 | rBV | 2934320 | 4273161 | 93.59% | 17.534% |
| 10 | 7.363 | 623 | 625 | 641 | rBV5 | 1329 | 3696 | 0.08% | 0.015% |
| 11 | 7.492 | 641 | 647 | 653 | rVV | 59437 | 50540 | 1.11% | 0.207% |
| 12 | 7.581 | 653 | 662 | 739 | rVV | 3134634 | 3416297 | 74.82% | 14.018% |
| 13 | 8.210 | 761 | 769 | 809 | rBV | 4054383 | 4565817 | 100.00% | 18.735% |
| 14 | 8.516 | 809 | 821 | 845 | rVV7 | 7510 | 25633 | 0.56% | 0.105% |
| 15 | 8.704 | 845 | 853 | 871 | rVV5 | 8459 | 19816 | 0.43% | 0.081% |
| 16 | 9.539 | 987 | 995 | 1005 | rBV | 26126 | 30098 | 0.66% | 0.124% |
| 17 | 9.681 | 1005 | 1019 | 1061 | rVV2 | 3384020 | 4363010 | 95.56% | 17.903% |
| 18 | 9.981 | 1061 | 1070 | 1079 | rVV5 | 5151 | 18580 | 0.41% | 0.076% |
| 19 | 10.057 | 1079 | 1083 | 1105 | rVV6 | 3668 | 11206 | 0.25% | 0.046% |
| 20 | 10.586 | 1165 | 1173 | 1185 | rBV | 2688 | 5364 | 0.12% | 0.022% |
| 21 | 12.422 | 1473 | 1485 | 1493 | rVB3 | 916 | 3744 | 0.08% | 0.015% |
| 22 | 13.963 | 1729 | 1747 | 1799 | rVV | 1293967 | 2654132 | 58.13% | 10.891% |
| 23 | 14.280 | 1799 | 1801 | 1811 | rVV5 | 2114 | 5807 | 0.13% | 0.024% |
| 24 | 14.357 | 1811 | 1814 | 1827 | rVV5 | 1377 | 4579 | 0.10% | 0.019% |
| 25 | 14.457 | 1827 | 1831 | 1847 | rVV4 | 1010 | 4109 | 0.09% | 0.017% |
| 26 | 16.710 | 2195 | 2214 | 2215 | rBV3 | 829 | 3966 | 0.09% | 0.016% |
| 27 | 16.798 | 2215 | 2229 | 2283 | rBV | 699973 | 1553307 | 34.02% | 6.374% |
| 28 | 17.127 | 2283 | 2285 | 2297 | rVV5 | 1860 | 4572 | 0.10% | 0.019% |
| 29 | 18.951 | 2589 | 2595 | 2605 | rVV5 | 1011 | 3422 | 0.07% | 0.014% |
| 30 | 19.121 | 2615 | 2624 | 2629 | rBV5 | 1656 | 4000 | 0.09% | 0.016% |
| 31 | 19.809 | 2731 | 2741 | 2755 | rBV6 | 1116 | 4674 | 0.10% | 0.019% |
| 32 | 21.074 | 2943 | 2956 | 2959 | rVB5 | 1395 | 4678 | 0.10% | 0.019% |
| 33 | 21.109 | 2959 | 2962 | 2973 | rBV4 | 1100 | 3375 | 0.07% | 0.014% |
| 34 | 22.115 | 3129 | 3133 | 3143 | rBV3 | 1124 | 3523 | 0.08% | 0.014% |

LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 0

Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Title : RP1616-MCHM Compounds

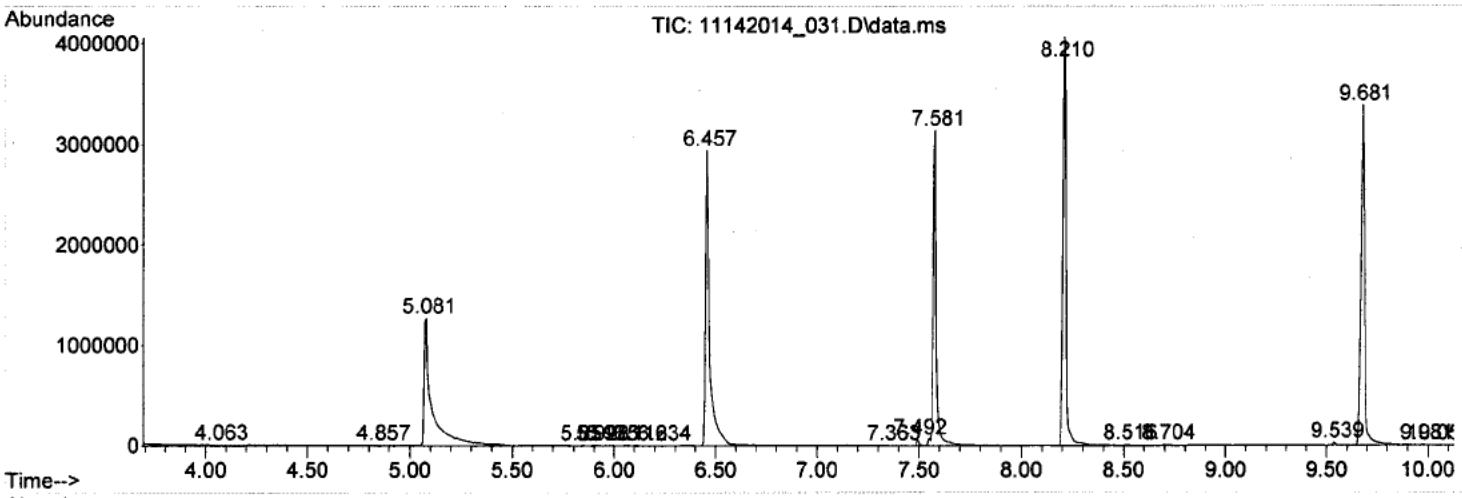
Sum of corrected areas: 24370232

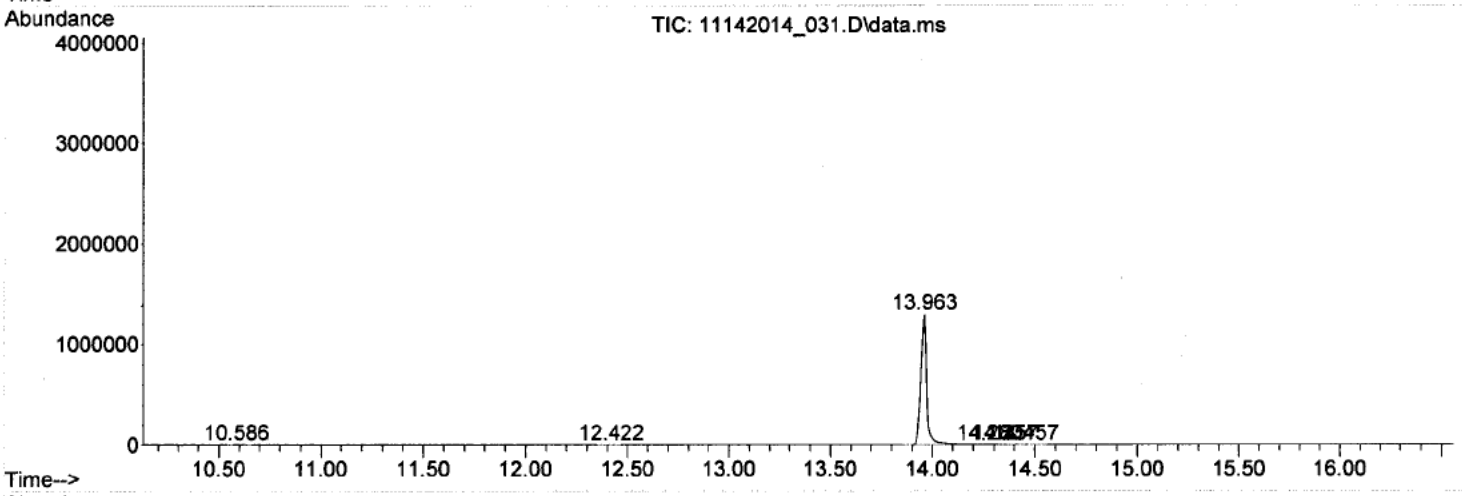
LSC Report - Integrated Chromatogram

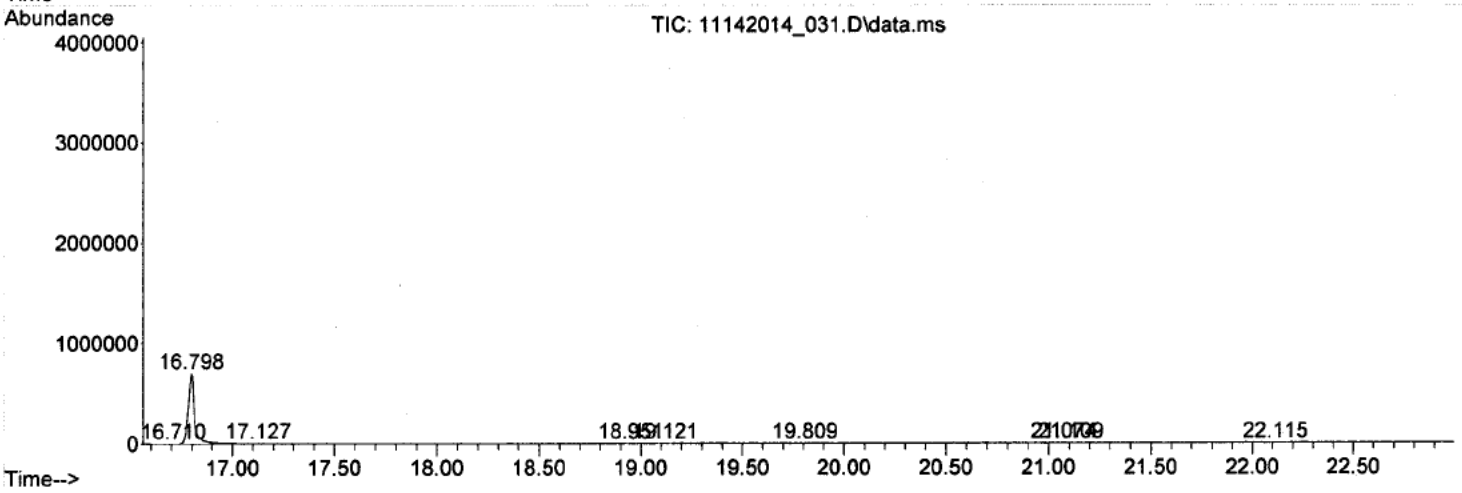
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

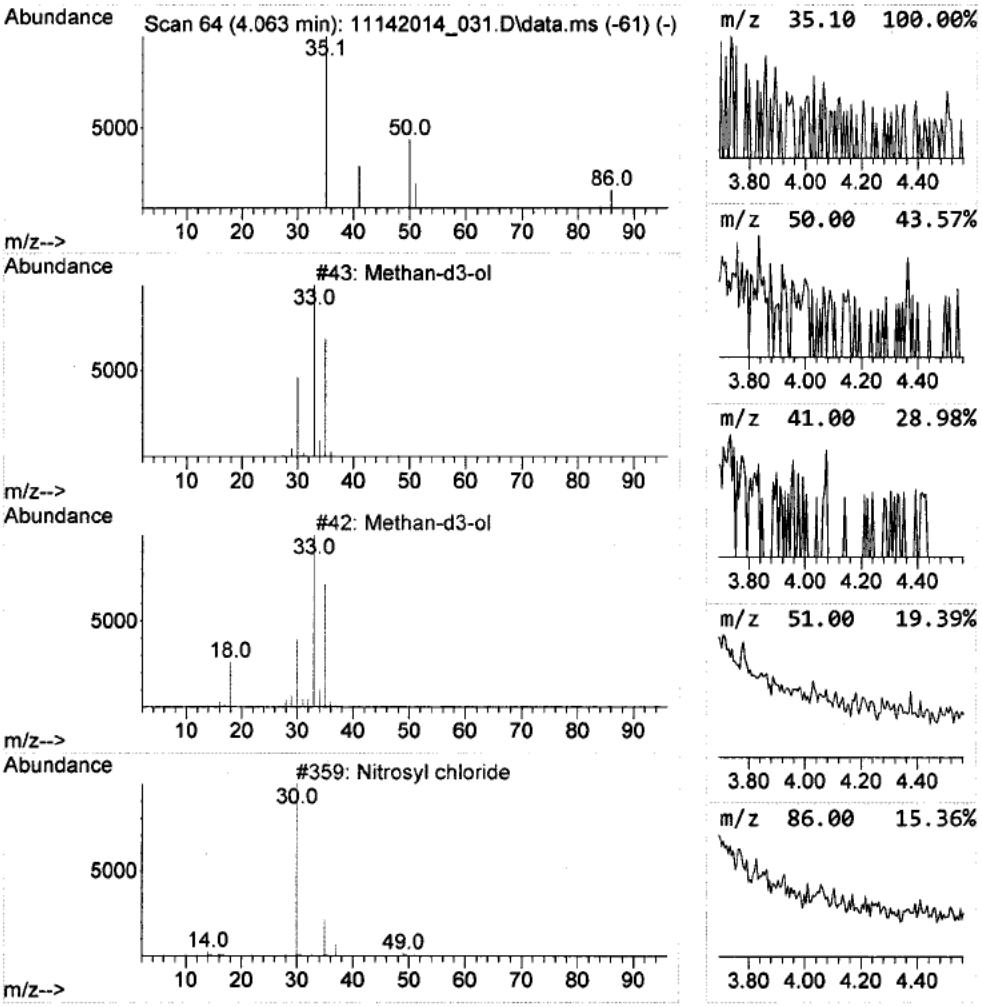
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 1 Methan-d3-ol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.063 | 0.09 ug/mL | 15439 | 1,4-Dichlorobenzene-d4 | 5.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methan-d3-ol | 35 | CHD3O | 001849-29-2 | 3 |
| 2 | Methan-d3-ol | 35 | CHD3O | 001849-29-2 | 3 |
| 3 | Nitrosyl chloride | 65 | ClNO | 002696-92-6 | 2 |
| 4 | Oxygen difluoride | 54 | F2O | 007783-41-7 | 1 |
| 5 | 1,3-Diamino-2-propanol | 90 | C3H10N2O | 000616-29-5 | 1 |



# Library Search Compound Report

Data Path : D:[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

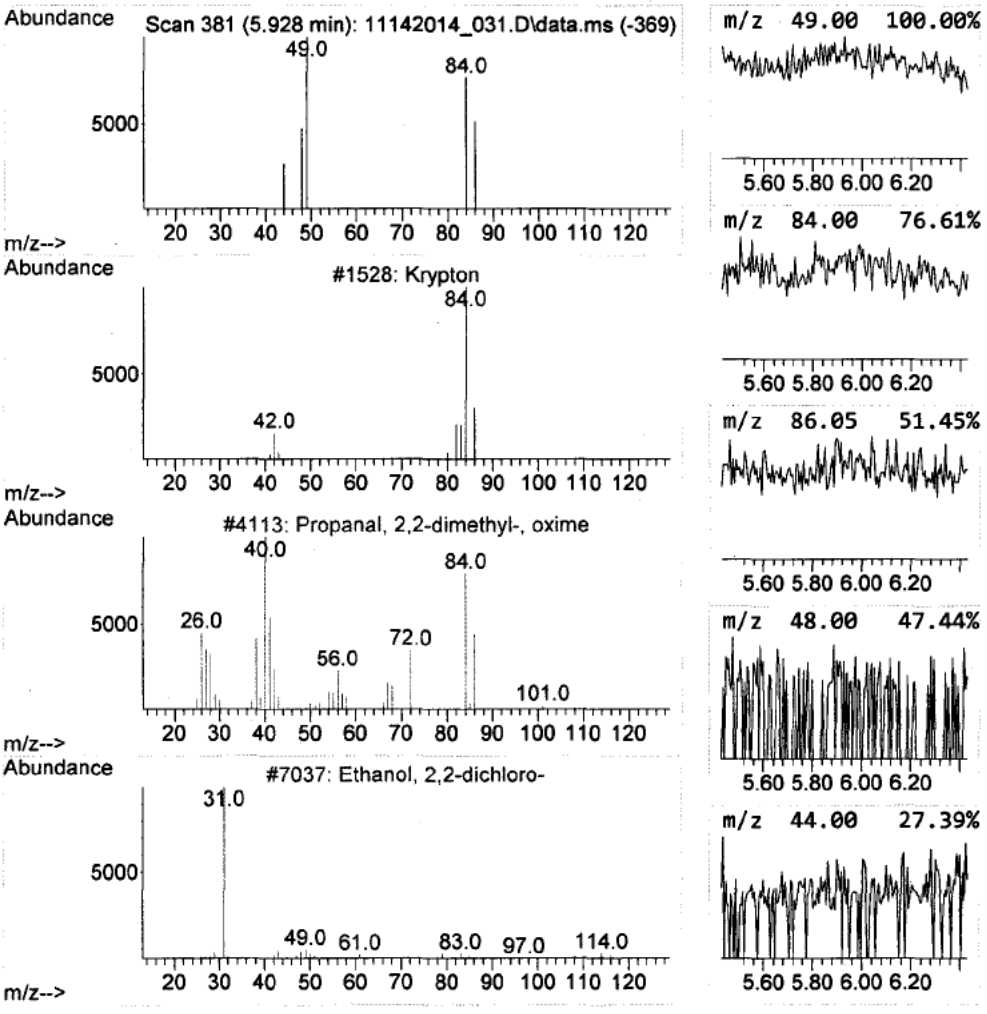
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 2 Krypton Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.928 | 0.03 ug/mL | 6626 | Naphthalene-d8 | 6.457 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Krypton | 84 | Kr | 007439-90-9 | 2 |
| 2 | Propanal, 2,2-dimethyl-, oxime | 101 | C5H11NO | 000637-91-2 | 2 |
| 3 | Ethanol, 2,2-dichloro- | 114 | C2H4Cl2O | 000598-38-9 | 1 |
| 4 | Borane, ethyldimethyl- | 70 | C4H11B | 001113-22-0 | 1 |
| 5 | 3-Butenenitrile | 67 | C4H5N | 000109-75-1 | 1 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

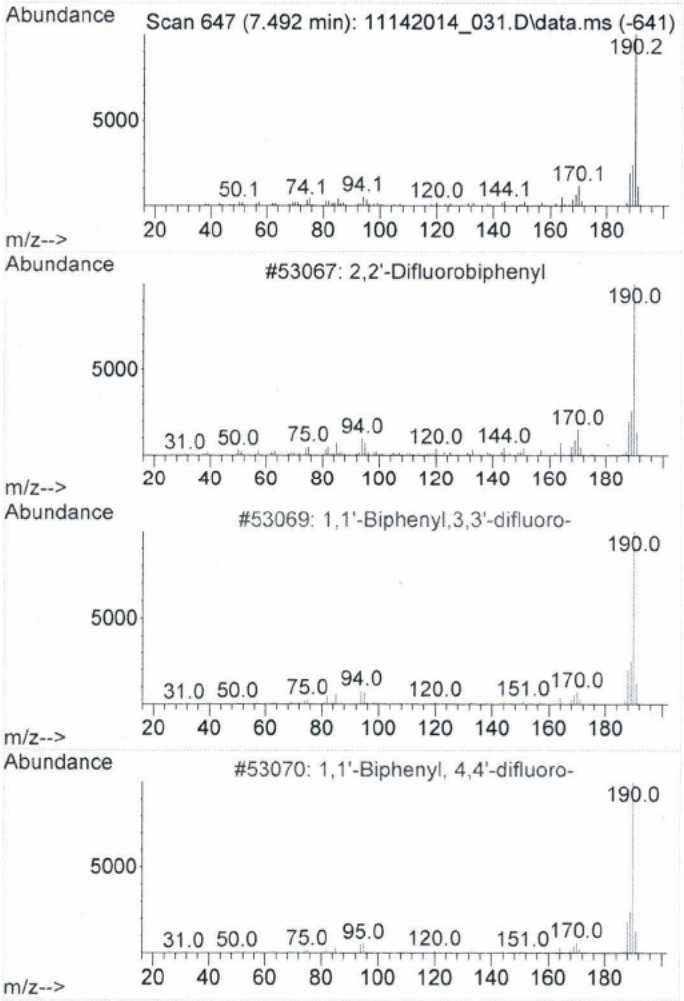
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

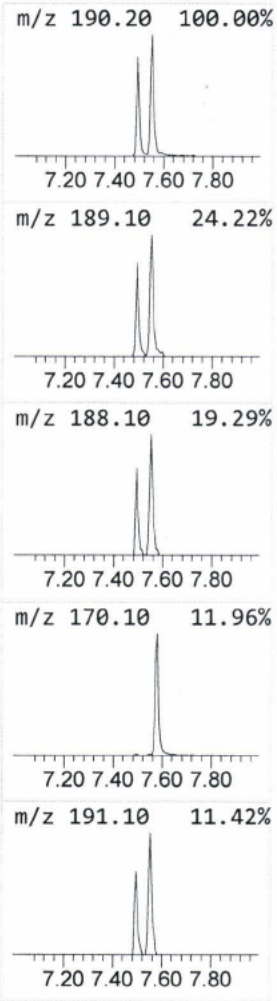
**********

Peak Number 3 2,2'-Difluorobiphenyl Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.492 | 0.22 ug/mL | 50540 | Acenaphthene-d10 | 8.216 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,2'-Difluorobiphenyl | 190 | C12H8F2 | 000388-82-9 | 96 |
| 2 | 1,1'-Biphenyl,3,3'-difluoro- | 190 | C12H8F2 | 000396-64-5 | 95 |
| 3 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 95 |
| 4 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 95 |
| 5 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 87 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

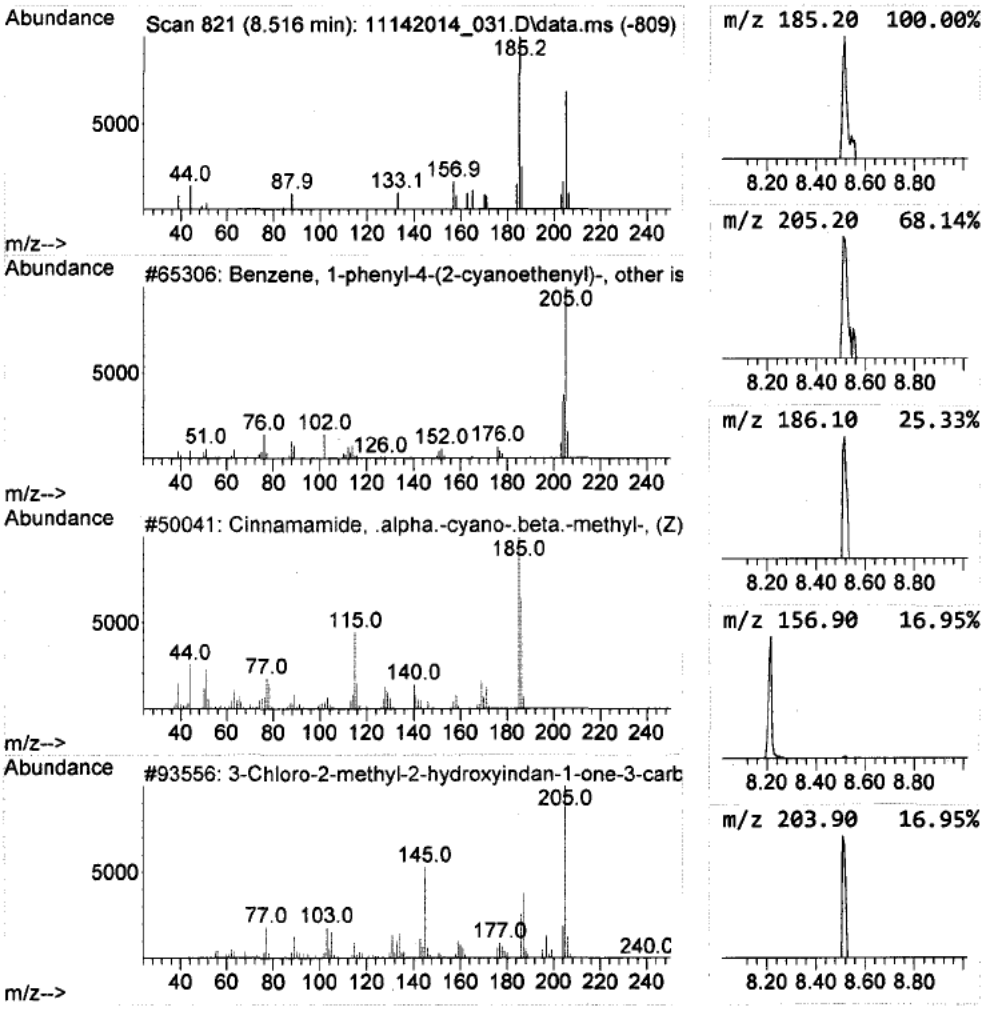
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 4 Benzene, 1-phenyl-4-(2-cyan... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.516 | 0.11 ug/mL | 25633 | Acenaphthene-d10 | 8.216 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-phenyl-4-(2-cyanoethe... | 205 | C15H11N | 1000274-65-7 | 14 |
| 2 | Cinnamamide, .alpha.-cyano-.beta... | 186 | C11H10N2O | 025327-42-8 | 12 |
| 3 | 3-Chloro-2-methyl-2-hydroxyindan... | 240 | C11H9ClO4 | 091064-12-9 | 12 |
| 4 | 4H-Benzo[def]carbazole, 4-methyl- | 205 | C15H11N | 084819-26-1 | 10 |
| 5 | 2-Aminodiphenyl ether | 185 | C12H11NO | 002688-84-8 | 9 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

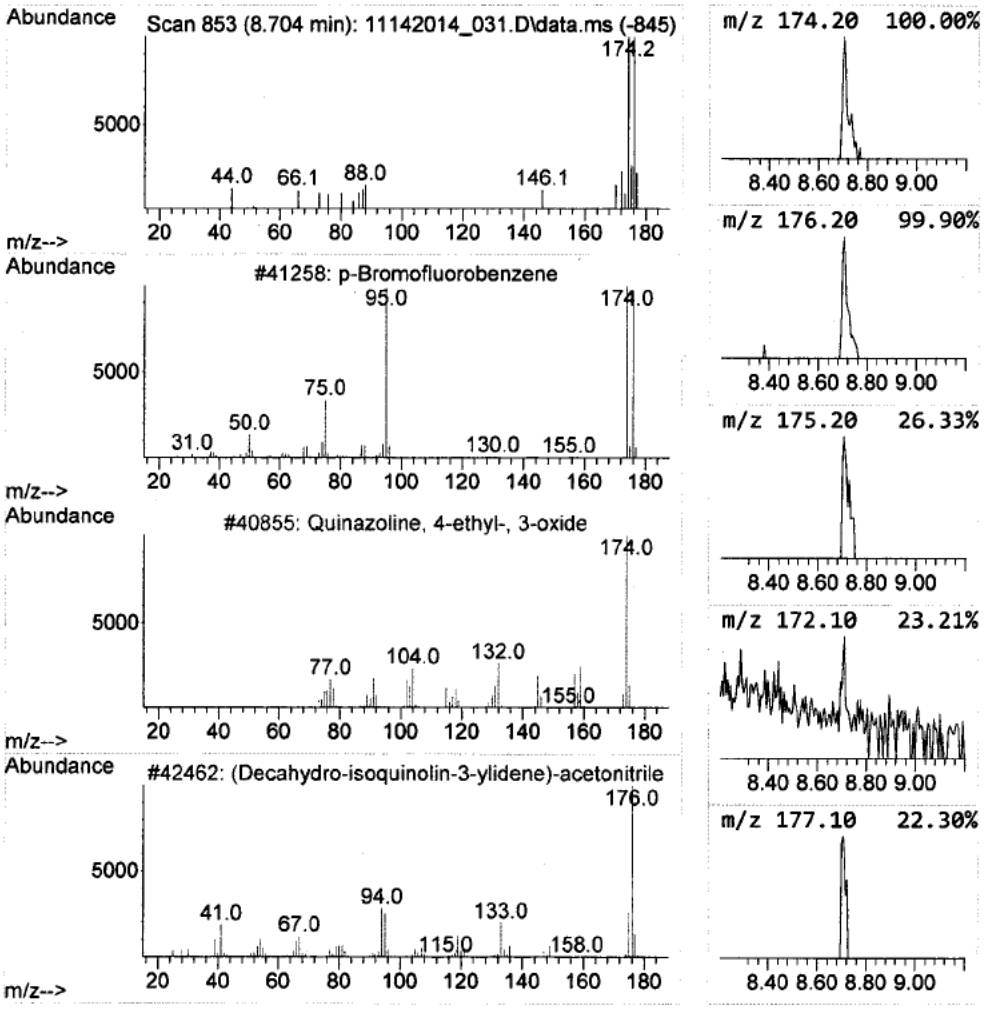
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 5 p-Bromofluorobenzene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.704 | 0.09 ug/mL | 19816 | Acenaphthene-d10 | 8.216 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | p-Bromofluorobenzene | 174 | C6H4BrF | 000460-00-4 | 42 |
| 2 | Quinazoline, 4-ethyl-, 3-oxide | 174 | C10H10N2O | 037920-74-4 | 16 |
| 3 | (Decahydro-isoquinolin-3-ylidene... | 176 | C11H16N2 | 1000185-70-0 | 9 |
| 4 | Benzene, 1,3-diisocyanato-2-methyl- | 174 | C9H6N2O2 | 000091-08-7 | 9 |
| 5 | (6,7,8,9-Tetrahydro-5H-[1,2,4]tr... | 176 | C9H12N4 | 1000302-73-1 | 9 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

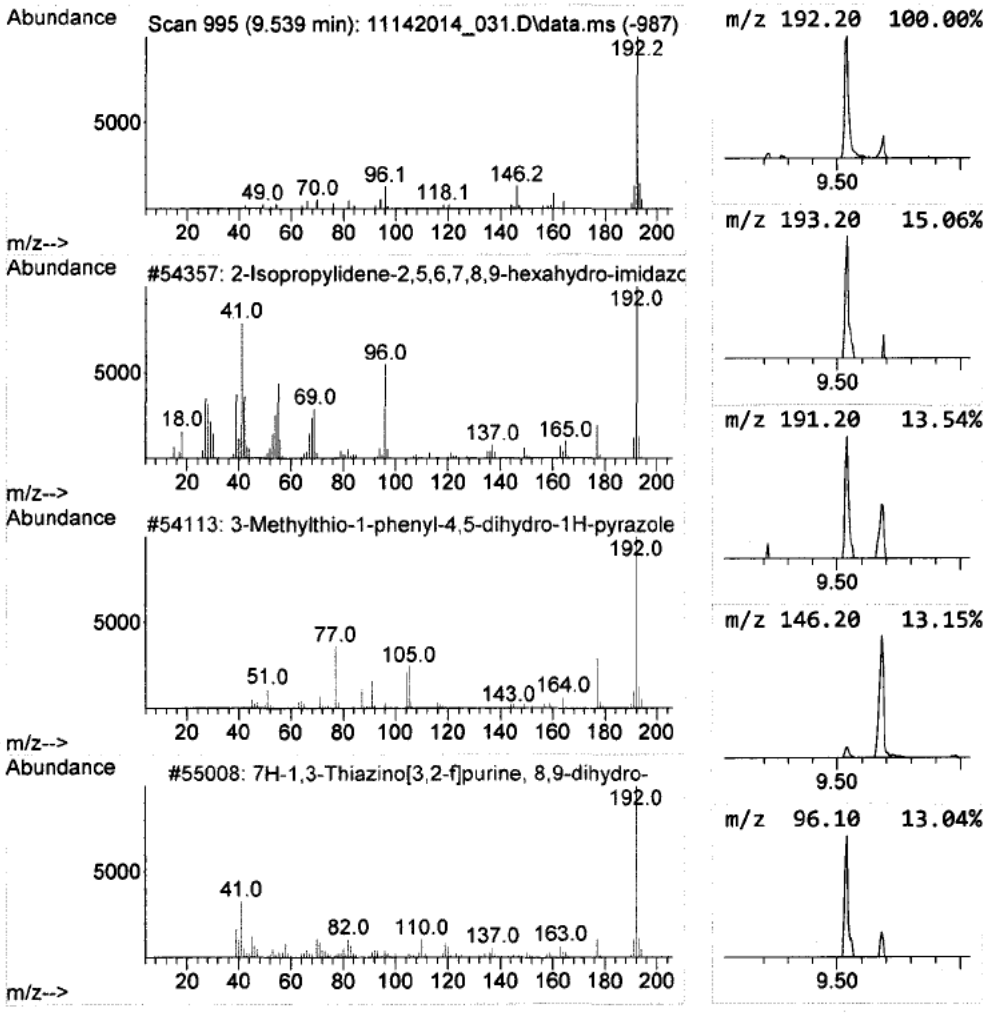
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 6 2-Isopropylidene-2,5,6,7,8,... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.539 | 0.14 ug/mL | 30098 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Isopropylidene-2,5,6,7,8,9-hex... | 192 | C11H16N2O | 172882-46-1 | 64 |
| 2 | 3-Methylthio-1-phenyl-4,5-dihydr... | 192 | C10H12N2S | 1000305-46-9 | 59 |
| 3 | 7H-1,3-Thiazino[3,2-f]purine, 8,... | 192 | C8H8N4S | 339370-55-7 | 58 |
| 4 | Phenanthrene, 9-methyl- | 192 | C15H12 | 000883-20-5 | 53 |
| 5 | Pyrido[3,4-d]pyridazine-1,5(2H,6... | 192 | C8H8N4O2 | 108480-62-2 | 47 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

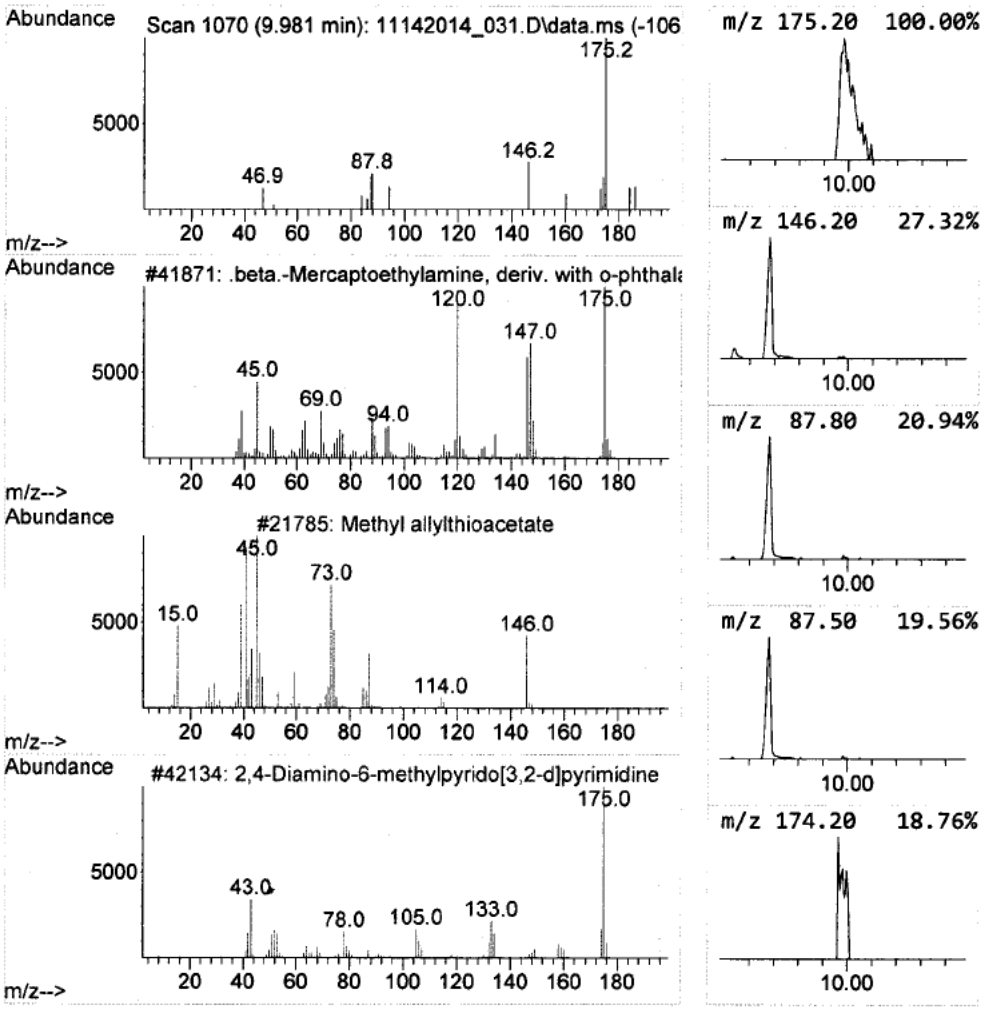
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 7 .beta.-Mercaptoethylamine, ... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.981 | 0.09 ug/mL | 18580 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .beta.-Mercaptoethylamine, deriv... | 175 | C10H9NS | 099833-29-1 | 9 |
| 2 | Methyl allylthioacetate | 146 | C6H10O2S | 072867-23-3 | 9 |
| 3 | 2,4-Diamino-6-methylpyrido[3,2-d... | 175 | C8H9N5 | 001955-57-3 | 7 |
| 4 | 5-Methoxy-2,3-dimethylindole | 175 | C11H13NO | 000828-94-4 | 7 |
| 5 | 1H-Indole-2-carboxylic acid, 1-m... | 175 | C10H9NO2 | 016136-58-6 | 5 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

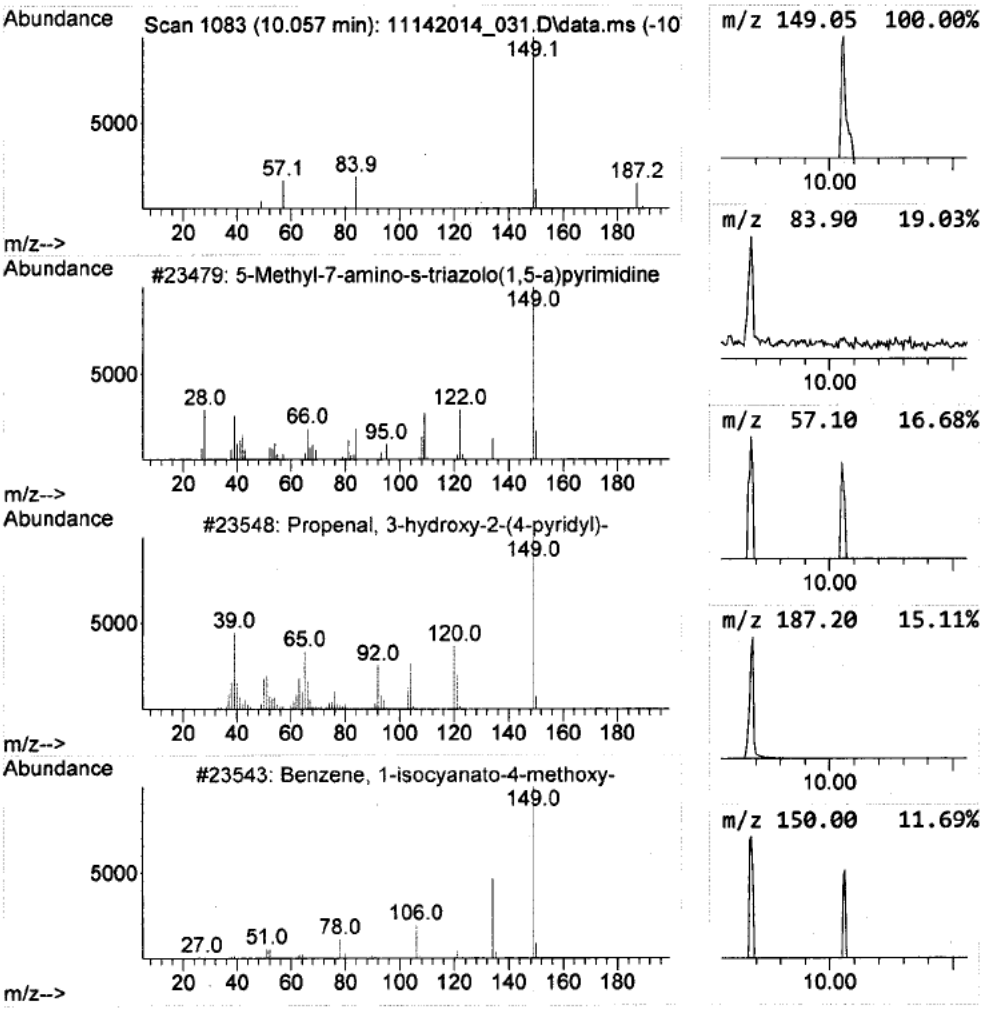
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 8 5-Methyl-7-amino-s-triazolo... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.057 | 0.05 ug/mL | 11206 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Methyl-7-amino-s-triazolo(1,5-... | 149 | C6H7N5 | 033376-96-4 | 9 |
| 2 | Propenal, 3-hydroxy-2-(4-pyridyl)- | 149 | C8H7NO2 | 026866-48-8 | 7 |
| 3 | Benzene, 1-isocyanato-4-methoxy- | 149 | C8H7NO2 | 005416-93-3 | 4 |
| 4 | Benzothiazole, 2-methyl- | 149 | C8H7NS | 000120-75-2 | 4 |
| 5 | 7-Methylthieno[3,2-b]pyridine | 149 | C8H7NS | 013362-83-9 | 4 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

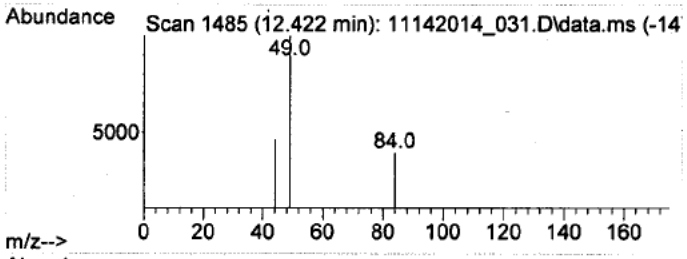
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

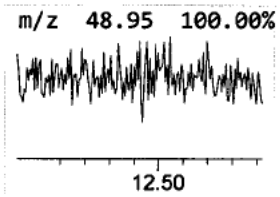
**********

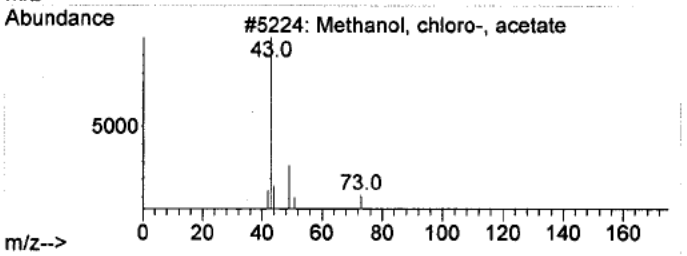
Peak Number 9 Methanol, chloro-, acetate Concentration Rank 20

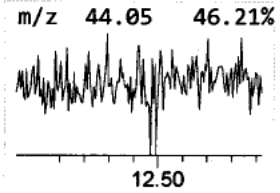
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.422 | 0.03 ug/mL | 3744 | Chrysene-d12 | 13.963 |

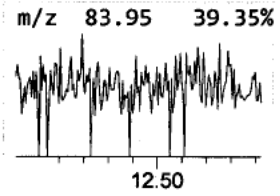
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methanol, chloro-, acetate | 108 | C3H5ClO2 | 000625-56-9 | 2 |
| 2 | Boron trifluoride | 68 | BF3 | 007637-07-2 | 1 |
| 3 | S-(Buthoxythiocarbonyl)thiohydro... | 165 | C5H11NOS2 | 035659-81-5 | 1 |
| 4 | Ethanol, 2,2,2-trifluoro- | 100 | C2H3F3O | 000075-89-8 | 1 |
| 5 | Chloroacetic acid allyl ester | 134 | C5H7ClO2 | 002916-14-5 | 1 |

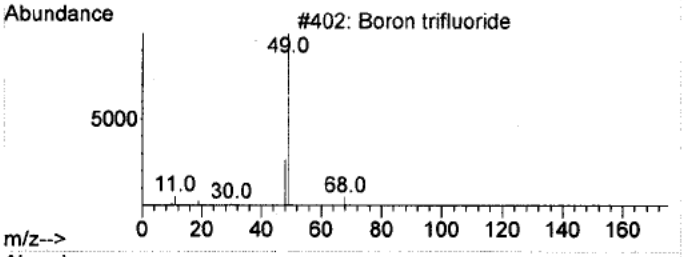


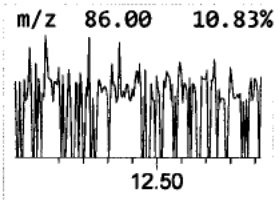



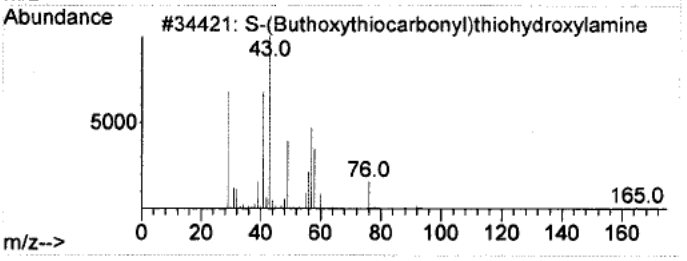



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

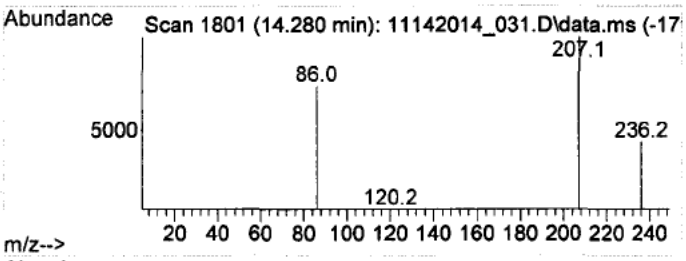
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

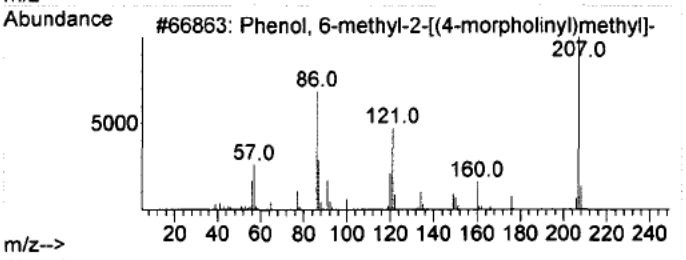
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

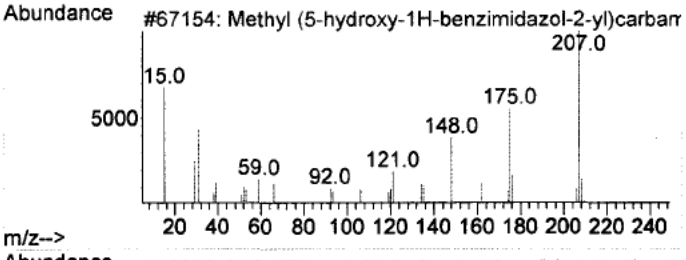
**********
Peak Number 10 Phenol, 6-methyl-2-[(4-morp... Concentration Rank 15

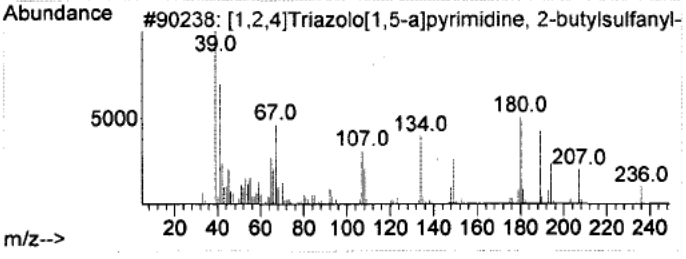
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.280 | 0.04 ug/mL | 5807 | Chrysene-d12 | 13.963 |

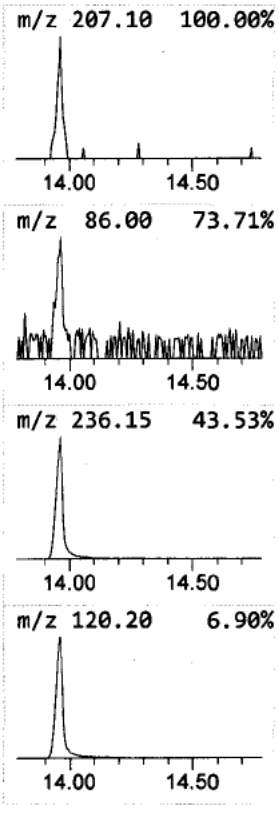
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 6-methyl-2-[(4-morpholin... | 207 | C12H17NO2 | 060460-71-1 | 5 |
| 2 | Methyl (5-hydroxy-1H-benzimidazo... | 207 | C9H9N3O3 | 022769-68-2 | 4 |
| 3 | [1,2,4]Triazolo[1,5-a]pyrimidine... | 236 | C11H16N4S | 1000304-65-4 | 4 |
| 4 | Carbonic acid, monoamide, N-meth... | 207 | C12H17NO2 | 1000339-98-1 | 4 |
| 5 | 1H-1,2,4-Triazole-5(4H)-thione, ... | 207 | C9H9N3OS | 1000277-38-2 | 4 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

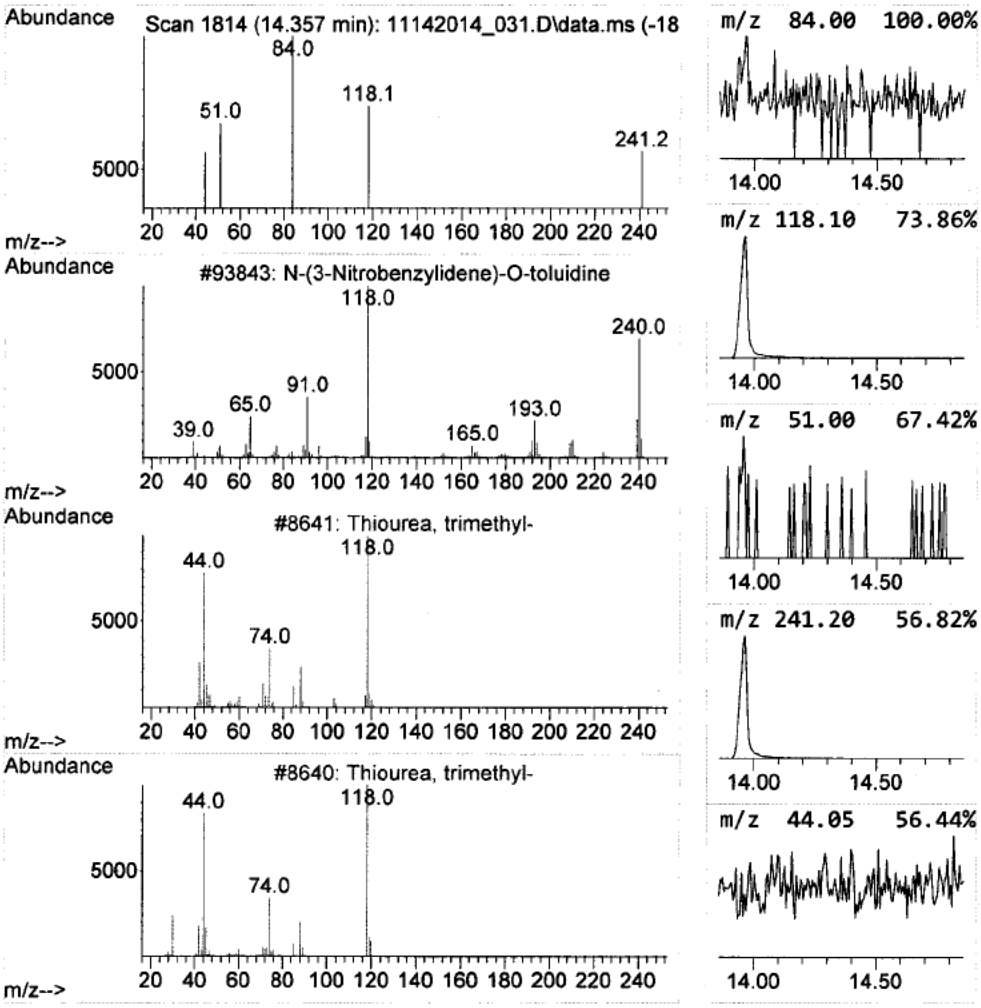
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 11 N-(3-Nitrobenzylidene)-O-to... Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.357 | 0.03 ug/mL | 4579 | Chrysene-d12 | 13.963 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | N-(3-Nitrobenzylidene)-O-toluidine | 240 | C14H12N2O2 | 017064-93-6 | 5 |
| 2 | Thiourea, trimethyl- | 118 | C4H10N2S | 002489-77-2 | 5 |
| 3 | Thiourea, trimethyl- | 118 | C4H10N2S | 002489-77-2 | 5 |
| 4 | Thiourea, trimethyl- | 118 | C4H10N2S | 002489-77-2 | 5 |
| 5 | 1-Pentanethiol, 2-methyl- | 118 | C6H14S | 001633-89-2 | 4 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

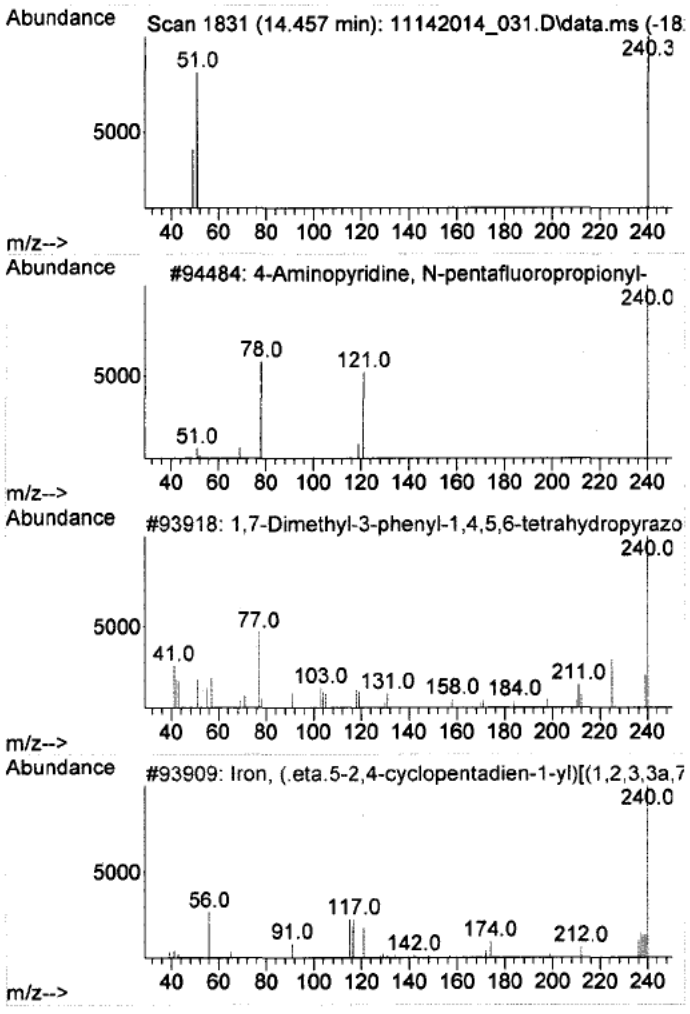
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

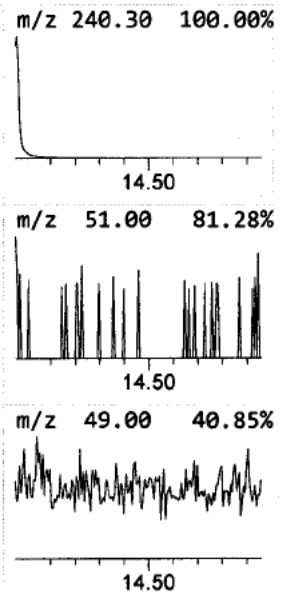
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 12 4-Aminopyridine, N-pentaflu... Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.457 | 0.03 ug/mL | 4109 | Chrysene-d12 | 13.963 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Aminopyridine, N-pentafluoropr... | 240 | C8H5F5N2O | 905417-77-8 | 3 |
| 2 | 1,7-Dimethyl-3-phenyl-1,4,5,6-te... | 240 | C14H16N4 | 1000148-10-4 | 3 |
| 3 | Iron, (.eta.5-2,4-cyclopentadien... | 240 | C14H16Fe | 033039-67-7 | 3 |
| 4 | 7-Methyl-3-phenyl-3a,6-dihydropy... | 240 | C13H12N4O | 1177783-93-5 | 3 |
| 5 | 2-Phenyl-3-amino-7-methyl-4,5(3H... | 240 | C13H12N4O | 068194-52-5 | 3 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

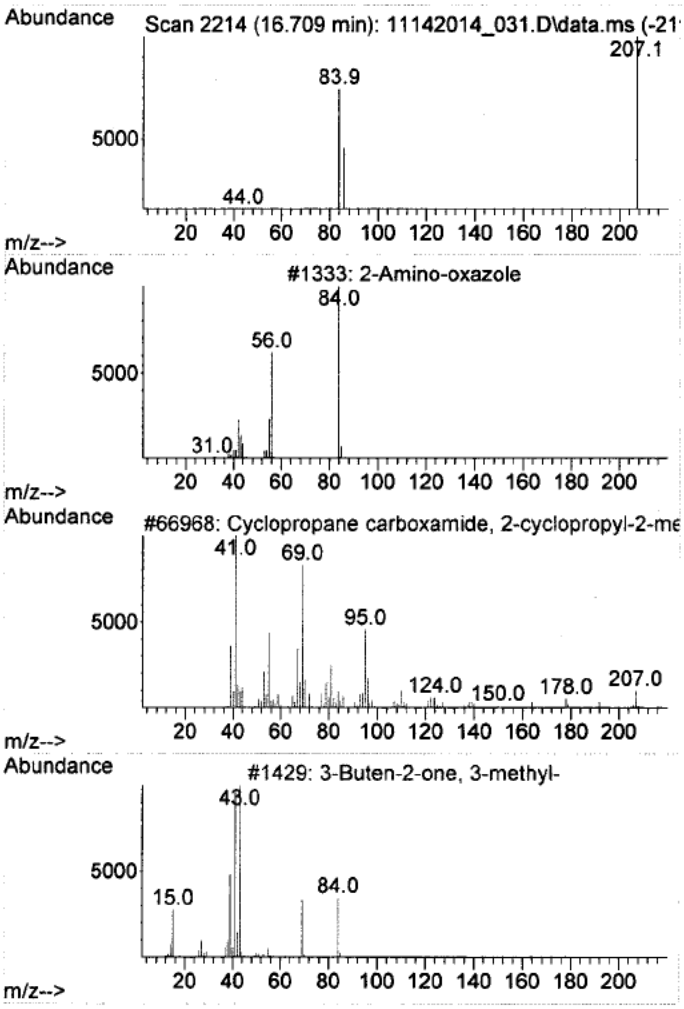
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

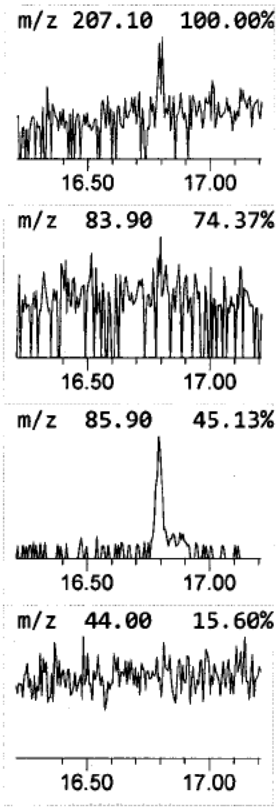
**********

Peak Number 13 2-Amino-oxazole Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.709 | 0.05 ug/mL | 3966 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Amino-oxazole | 84 | C3H4N2O | 004570-45-0 | 4 |
| 2 | Cyclopropane carboxamide, 2-cycl... | 207 | C13H21NO | 331416-19-4 | 4 |
| 3 | 3-Buten-2-one, 3-methyl- | 84 | C5H8O | 000814-78-8 | 3 |
| 4 | 4-Penten-2-one | 84 | C5H8O | 013891-87-7 | 3 |
| 5 | 2-Methyl[1,3,4]oxadiazole | 84 | C3H4N2O | 003451-51-2 | 2 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

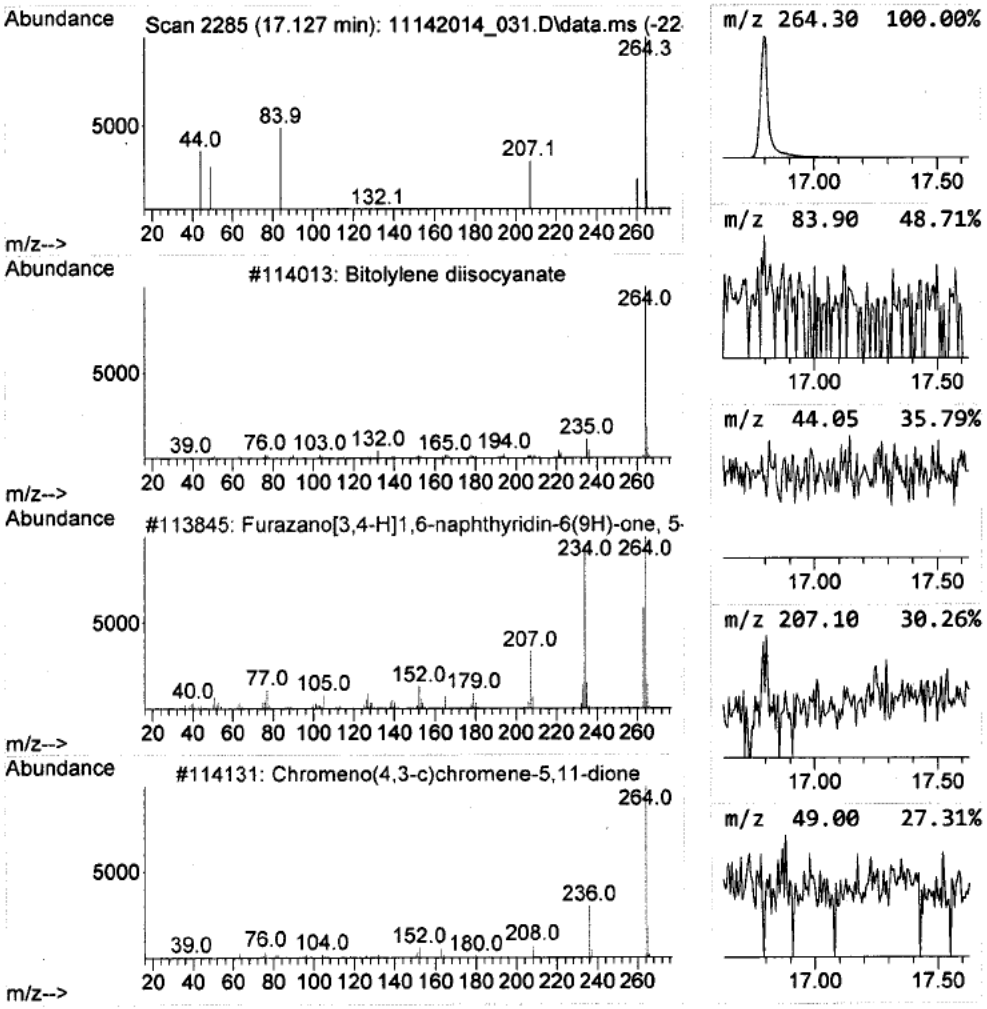
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 14 Bitolylene diisocyanate Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.127 | 0.06 ug/mL | 4572 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bitolylene diisocyanate | 264 | C16H12N2O2 | 000091-97-4 | 9 |
| 2 | Furazano[3,4-H]1,6-naphthyridin-... | 264 | C14H8N4O2 | 296245-19-7 | 9 |
| 3 | Chromeno(4,3-c)chromene-5,11-dione | 264 | C16H8O4 | 013225-81-5 | 9 |
| 4 | 1-Phosphacyclopent-2-ene, 1-meth... | 264 | C18H17P | 1000161-67-7 | 9 |
| 5 | 2-Trifluoromethyl-1,8-phenanthro... | 264 | C13H7F3N2O | 1000255-81-8 | 9 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

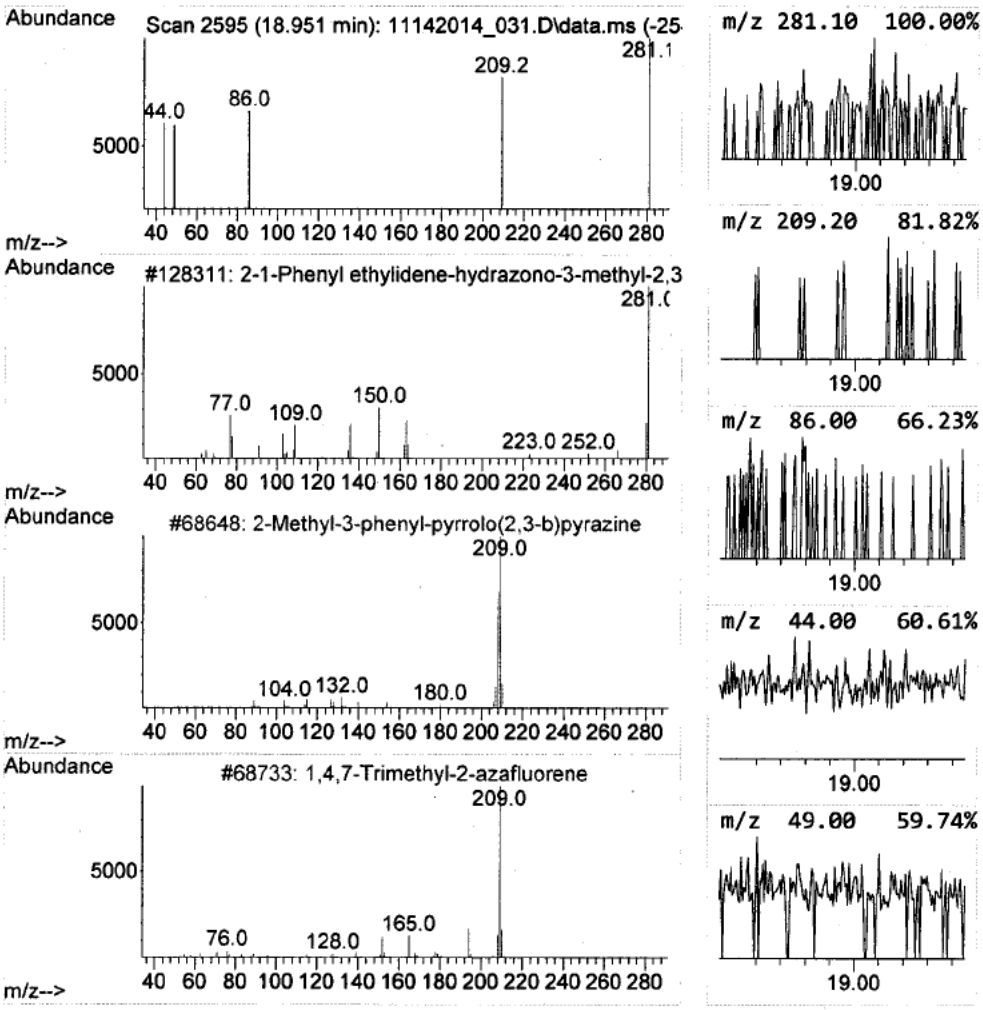
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 15 2-1-Phenyl ethylidene-hydra... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.951 | 0.04 ug/mL | 3422 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-1-Phenyl ethylidene-hydrazono-... | 281 | C16H15N3S | 1000148-55-3 | 3 |
| 2 | 2-Methyl-3-phenyl-pyrrolo(2,3-b)... | 209 | C13H11N3 | 056015-25-9 | 2 |
| 3 | 1,4,7-Trimethyl-2-azafluorene | 209 | C15H15N | 062736-78-1 | 2 |
| 4 | Proflavine | 209 | C13H11N3 | 000092-62-6 | 2 |
| 5 | 1,3-Dimethyl-2-azafluorenone | 209 | C14H11NO | 039795-66-9 | 2 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

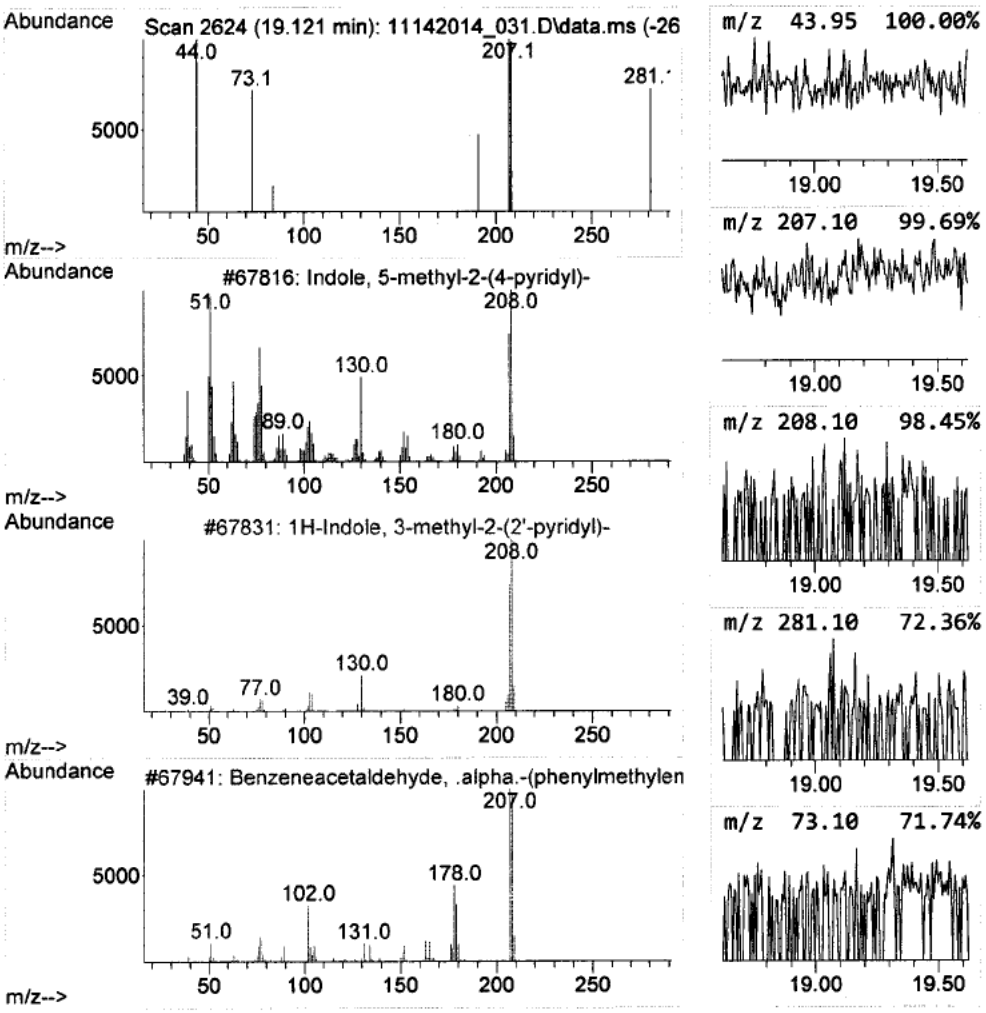
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 16 Indole, 5-methyl-2-(4-pyrid... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.121 | 0.05 ug/mL | 4000 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Indole, 5-methyl-2-(4-pyridyl)- | 208 | C14H12N2 | 107919-92-6 | 7 |
| 2 | 1H-Indole, 3-methyl-2-(2'-pyridyl)- | 208 | C14H12N2 | 000951-25-7 | 7 |
| 3 | Benzeneacetaldehyde, .alpha.-(ph... | 208 | C15H12O | 013702-35-7 | 7 |
| 4 | Benzimidazole, 7-methyl-2-phenyl- | 208 | C14H12N2 | 003659-77-6 | 7 |
| 5 | .gamma.-Cyano-3-methyl-5,10-dihy... | 208 | C14H12N2 | 1000213-00-8 | 7 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

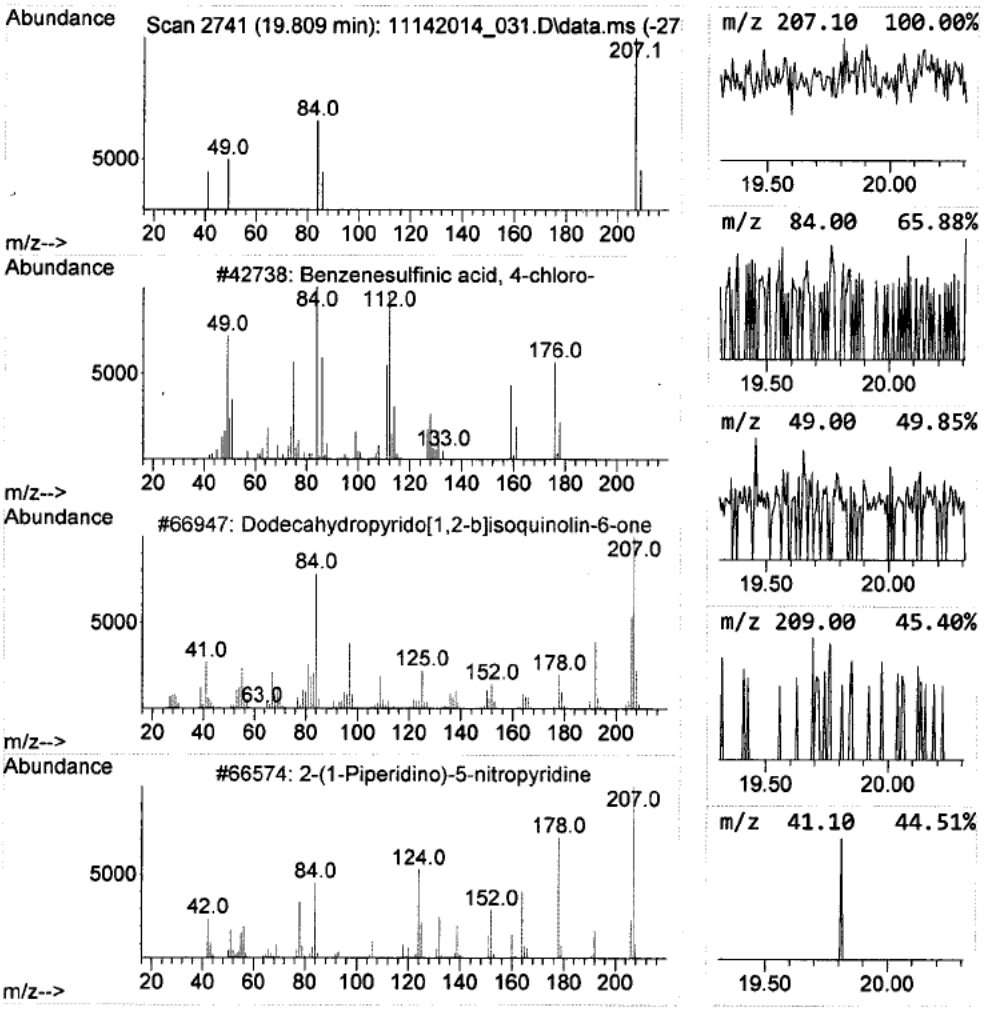
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 17 Benzenesulfinic acid, 4-chl... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.809 | 0.06 ug/mL | 4674 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfinic acid, 4-chloro- | 176 | C6H5ClO2S | 000100-03-8 | 9 |
| 2 | Dodecahydropyrido[1,2-b]isoquino... | 207 | C13H21NO | 108873-36-5 | 5 |
| 3 | 2-(1-Piperidino)-5-nitropyridine | 207 | C10H13N3O2 | 026820-61-1 | 5 |
| 4 | o-(p-Tolyl) 1-azetidinecarbothioate | 207 | C11H13NOS | 010560-24-4 | 5 |
| 5 | 4-Quinolinecarboxylic acid, 2-ch... | 207 | C10H6ClNO2 | 005467-57-2 | 5 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

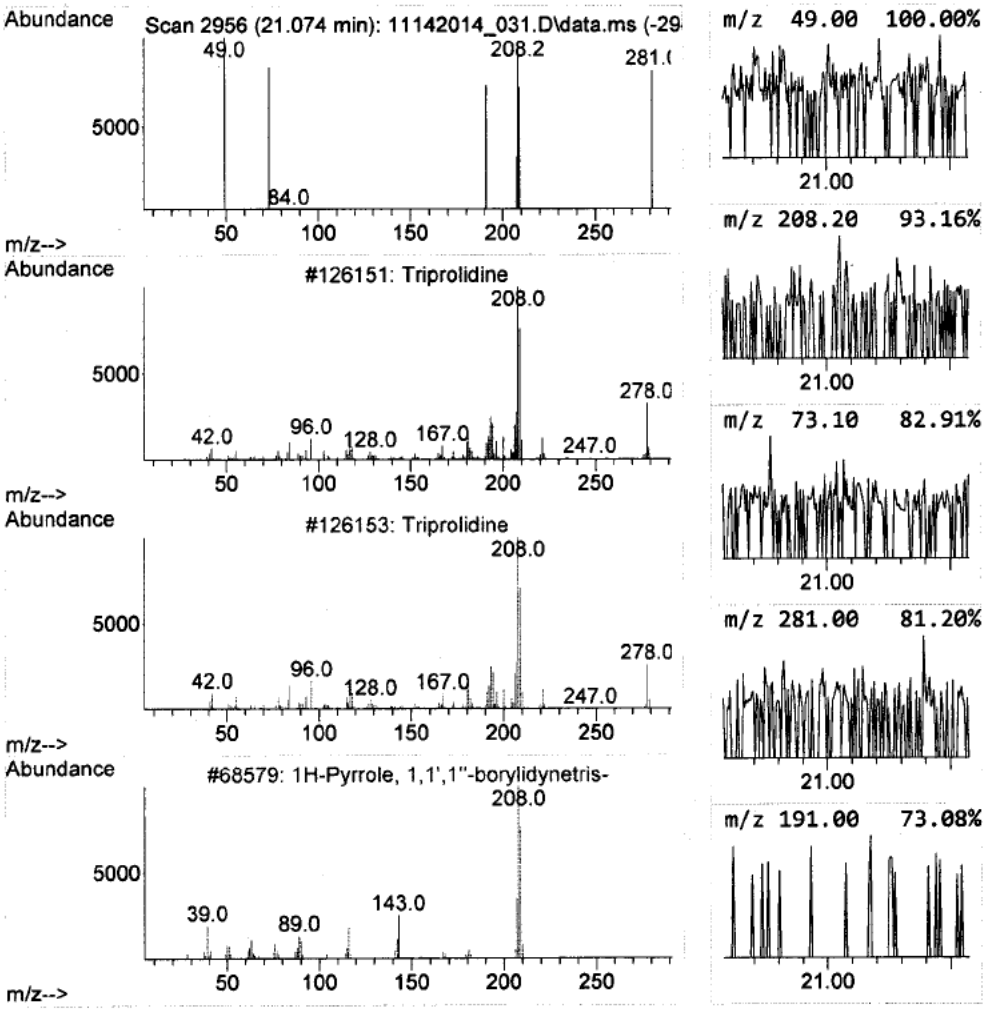
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 18 Triprolidine Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.074 | 0.06 ug/mL | 4678 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triprolidine | 278 | C19H22N2 | 000486-12-4 | 9 |
| 2 | Triprolidine | 278 | C19H22N2 | 000486-12-4 | 9 |
| 3 | 1H-Pyrrole, 1,1',1''-borylidynet... | 209 | C12H12BN3 | 018899-90-6 | 9 |
| 4 | 1H-Benzimidazol-2-amine, N-phenyl- | 209 | C13H11N3 | 021578-58-5 | 7 |
| 5 | 4-Methylbenzylidene-4-methylaniline | 209 | C15H15N | 016979-20-7 | 7 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

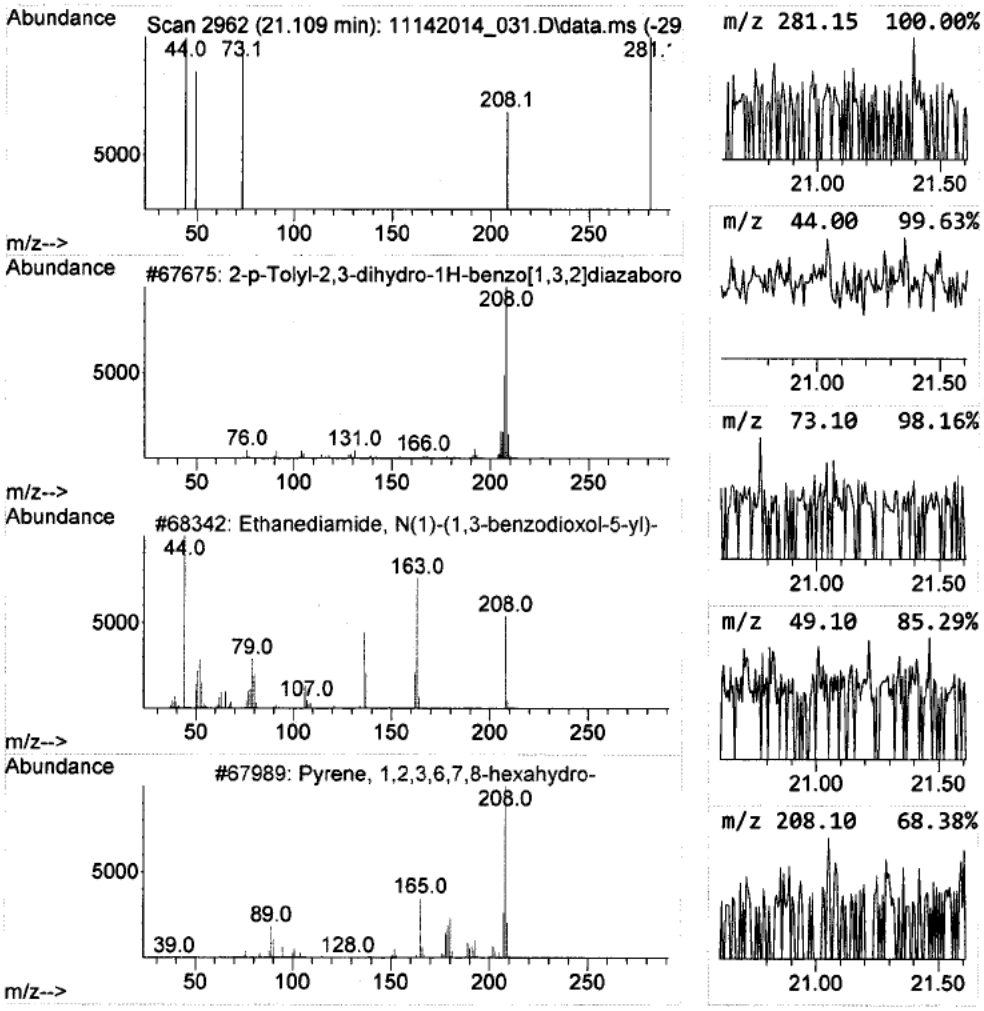
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 19 2-p-Tolyl-2,3-dihydro-1H-be... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.109 | 0.04 ug/mL | 3375 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-p-Tolyl-2,3-dihydro-1H-benzo[1... | 208 | C13H13BN2 | 1000296-11-8 | 5 |
| 2 | Ethanediamide, N(1)-(1,3-benzodi... | 208 | C9H8N2O4 | 1000351-43-9 | 5 |
| 3 | Pyrene, 1,2,3,6,7,8-hexahydro- | 208 | C16H16 | 001732-13-4 | 5 |
| 4 | 5-Methyl-3-phenyl-1H-indazole | 208 | C14H12N2 | 057614-16-1 | 5 |
| 5 | Pterin-6-carboxylic acid | 207 | C7H5N5O3 | 000948-60-7 | 3 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

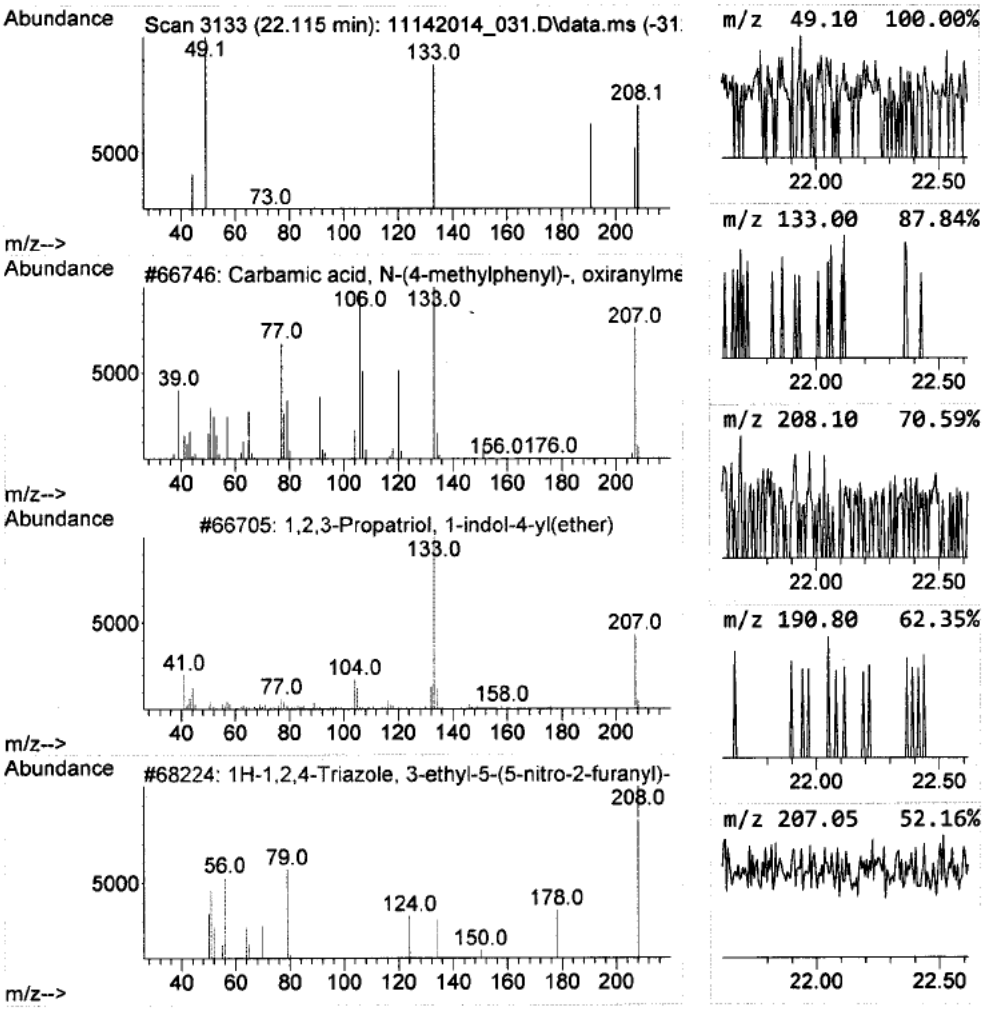
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 20 Carbamic acid, N-(4-methylp... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.115 | 0.05 ug/mL | 3523 | Perylene-d12 | 16.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Carbamic acid, N-(4-methylphenyl... | 207 | C11H13NO3 | 128897-40-5 | 5 |
| 2 | 1,2,3-Propatriol, 1-indol-4-yl(e... | 207 | C11H13NO3 | 061212-32-6 | 5 |
| 3 | 1H-1,2,4-Triazole, 3-ethyl-5-(5-... | 208 | C8H8N4O3 | 005019-57-8 | 3 |
| 4 | 1-Propene, 2-(3-methylphenyl)-1-... | 208 | C16H16 | 1000138-72-6 | 3 |
| 5 | Benzene, 1-isocyano-2-methoxy- | 133 | C8H7NO | 020771-60-2 | 2 |



Tentatively Identified Compound (LSC) summary

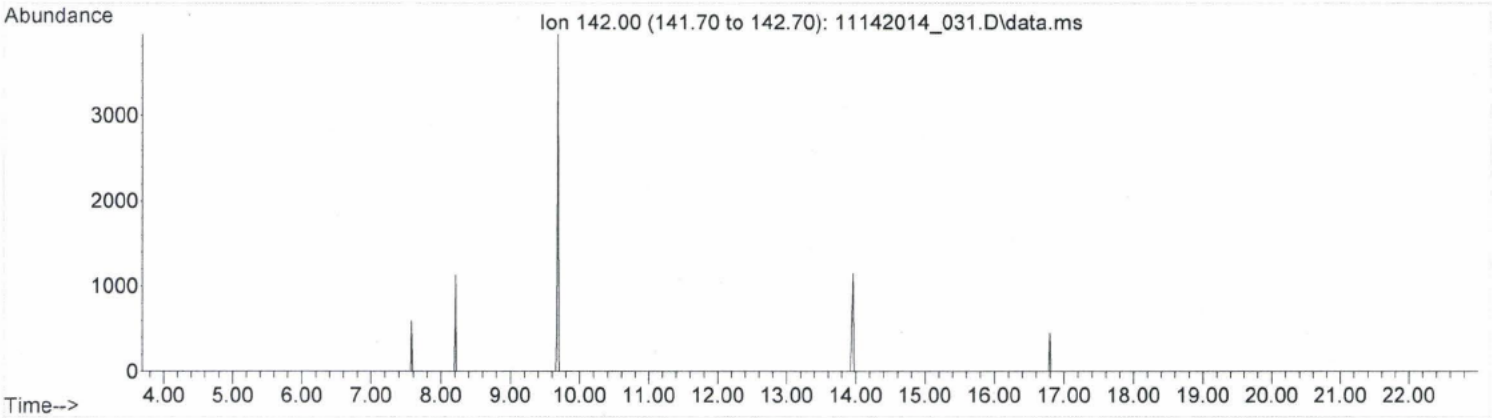
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_031.D
Acq On : 15 Nov 2014 12:31 am
Operator : [redacted]
Sample : NE36686
Misc : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 29 Sample Multiplier: 1

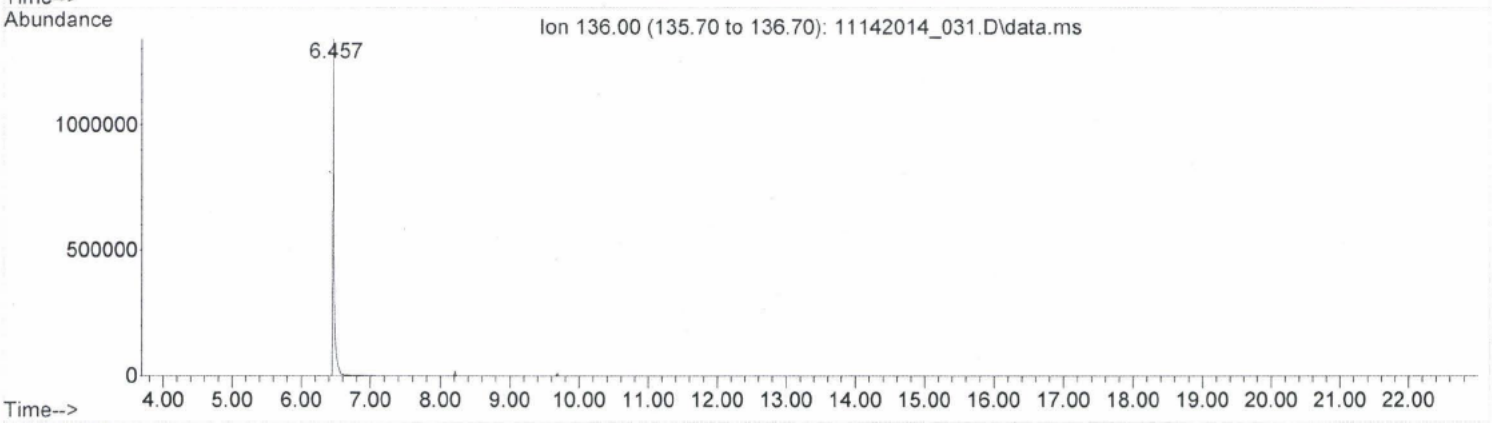
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

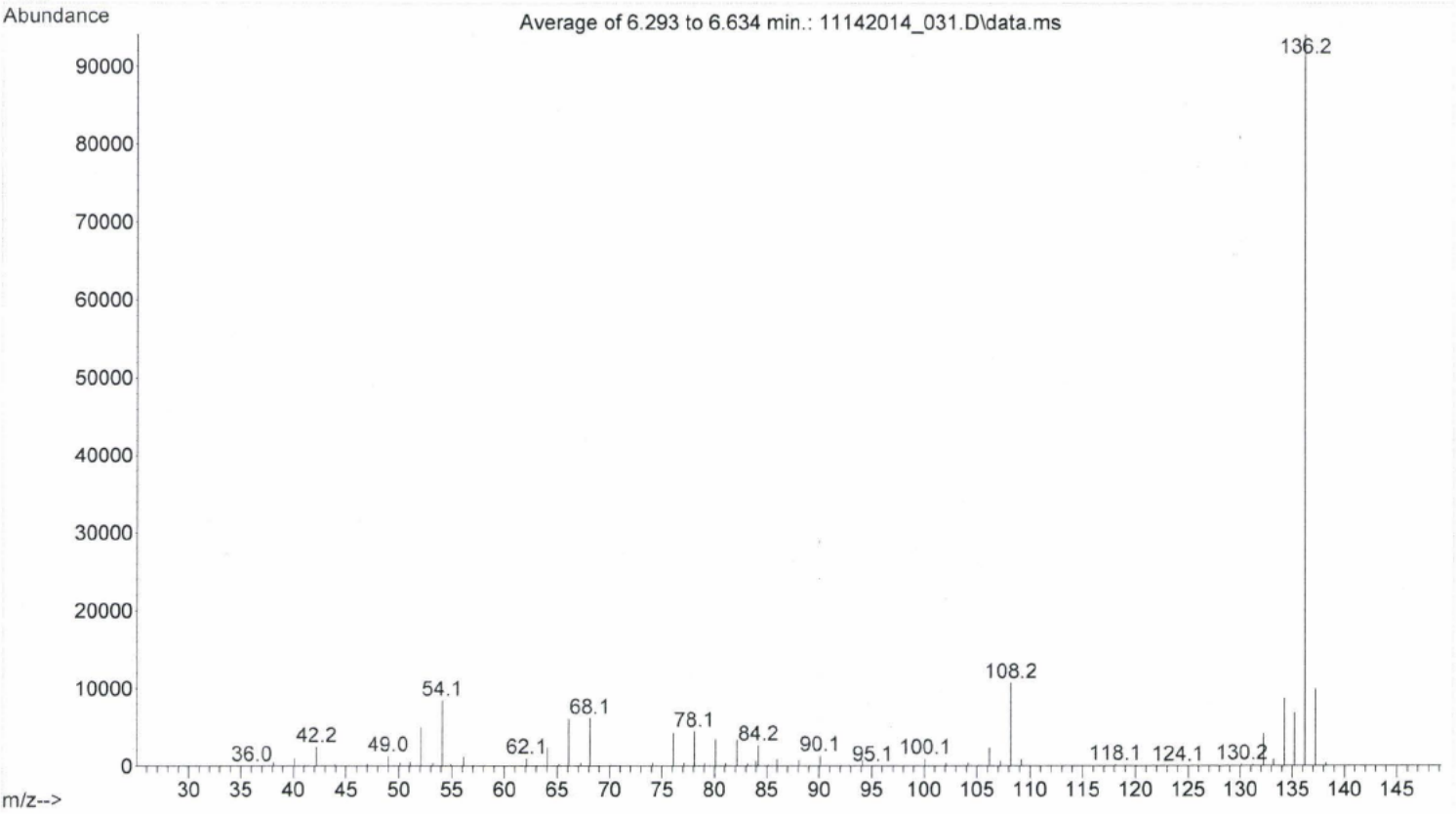
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| Methan-d3-ol | 4.063 | 0.1 | ug/mL | 15439 | 1 | 5.081 | 3283780 | 20.0 |
| Krypton | 5.928 | 0.0 | ug/mL | 6626 | 2 | 6.457 | 4273160 | 20.0 |
| 2,2'-Difluorobi... | 7.492 | 0.2 | ug/mL | 50540 | 3 | 8.216 | 4565820 | 20.0 |
| Benzene, 1-phen... | 8.516 | 0.1 | ug/mL | 25633 | 3 | 8.216 | 4565820 | 20.0 |
| p-Bromofluorobe... | 8.704 | 0.1 | ug/mL | 19816 | 3 | 8.216 | 4565820 | 20.0 |
| 2-Isopropyliden... | 9.539 | 0.1 | ug/mL | 30098 | 4 | 9.681 | 4363010 | 20.0 |
| .beta.-Mercapto... | 9.981 | 0.1 | ug/mL | 18580 | 4 | 9.681 | 4363010 | 20.0 |
| 5-Methyl-7-amin... | 10.057 | 0.1 | ug/mL | 11206 | 4 | 9.681 | 4363010 | 20.0 |
| Methanol, chlor... | 12.422 | 0.0 | ug/mL | 3744 | 5 | 13.963 | 2654130 | 20.0 |
| Phenol, 6-methy... | 14.280 | 0.0 | ug/mL | 5807 | 5 | 13.963 | 2654130 | 20.0 |
| N-(3-Nitrobenzy... | 14.357 | 0.0 | ug/mL | 4579 | 5 | 13.963 | 2654130 | 20.0 |
| 4-Aminopyridine... | 14.457 | 0.0 | ug/mL | 4109 | 5 | 13.963 | 2654130 | 20.0 |
| 2-Amino-oxazole | 16.709 | 0.1 | ug/mL | 3966 | 6 | 16.798 | 1553310 | 20.0 |
| Bitolylene diis... | 17.127 | 0.1 | ug/mL | 4572 | 6 | 16.798 | 1553310 | 20.0 |
| 2-1-Phenyl ethy... | 18.951 | 0.0 | ug/mL | 3422 | 6 | 16.798 | 1553310 | 20.0 |
| Indole, 5-methy... | 19.121 | 0.1 | ug/mL | 4000 | 6 | 16.798 | 1553310 | 20.0 |
| Benzenesulfinic... | 19.809 | 0.1 | ug/mL | 4674 | 6 | 16.798 | 1553310 | 20.0 |
| Triprolidine | 21.074 | 0.1 | ug/mL | 4678 | 6 | 16.798 | 1553310 | 20.0 |
| 2-p-Tolyl-2,3-d... | 21.109 | 0.0 | ug/mL | 3375 | 6 | 16.798 | 1553310 | 20.0 |
| Carbamic acid, ... | 22.115 | 0.0 | ug/mL | 3523 | 6 | 16.798 | 1553310 | 20.0 |

File :D:\[redacted]\RP1616\11142014_Run\11142014_031.D
Operator : [redacted]
Acquired : 15 Nov 2014 12:31 am using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36686
Misc Info : Tag # NE36686, 450 uL ext + 50 uL of CH2Cl2
Vial Number: 29




[redacted] RP1616 12/17/14

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Time: Nov 17 11:15:13 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration

| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| Internal Standards | | | | | |
| 1) 1,4-Dichlorobenzene-d4 | 5.081 | 152 | 404778 | 20.00 ug/mL | 0.00 |
| 3) Naphthalene-d8 | 6.457 | 136 | 1808248 | 20.00 ug/mL | 0.00 |
| 5) Acenaphthene-d10 | 8.210 | 164 | 998933 | 20.00 ug/mL | 0.00 |
| 10) Phenanthrene-d10 | 9.681 | 188 | 1511629 | 20.00 ug/mL | 0.00 |
| 11) Chrysene-d12 | 13.963 | 240 | 928526 | 20.00 ug/mL | 0.00 |
| 12) Perylene-d12 | 16.804 | 264 | 568834 | 20.00 ug/mL | 0.01 |
| System Monitoring Compounds | | | | | |
| 7) 2-Fluorobiphenyl | 7.575 | 172 | 885360 | 14.42 ug/mL | 0.00 |
| Spiked Amount 12.500 | Range 25 - 150 | | Recovery = ~~115.36%~~ | | |
| Target Compounds | | | | | Qvalue |
| 2) MCHM | 0.000 | | 0 | N.D. | |
| 4) PPH | 0.000 | | 0 | N.D. | |
| 6) 1,4-CHDM | 0.000 | | 0 | N.D. d | |
| 8) DM-1,4-CHDC | 0.000 | | 0 | N.D. | |
| 9) di-PPH | 0.000 | | 0 | N.D. d | |

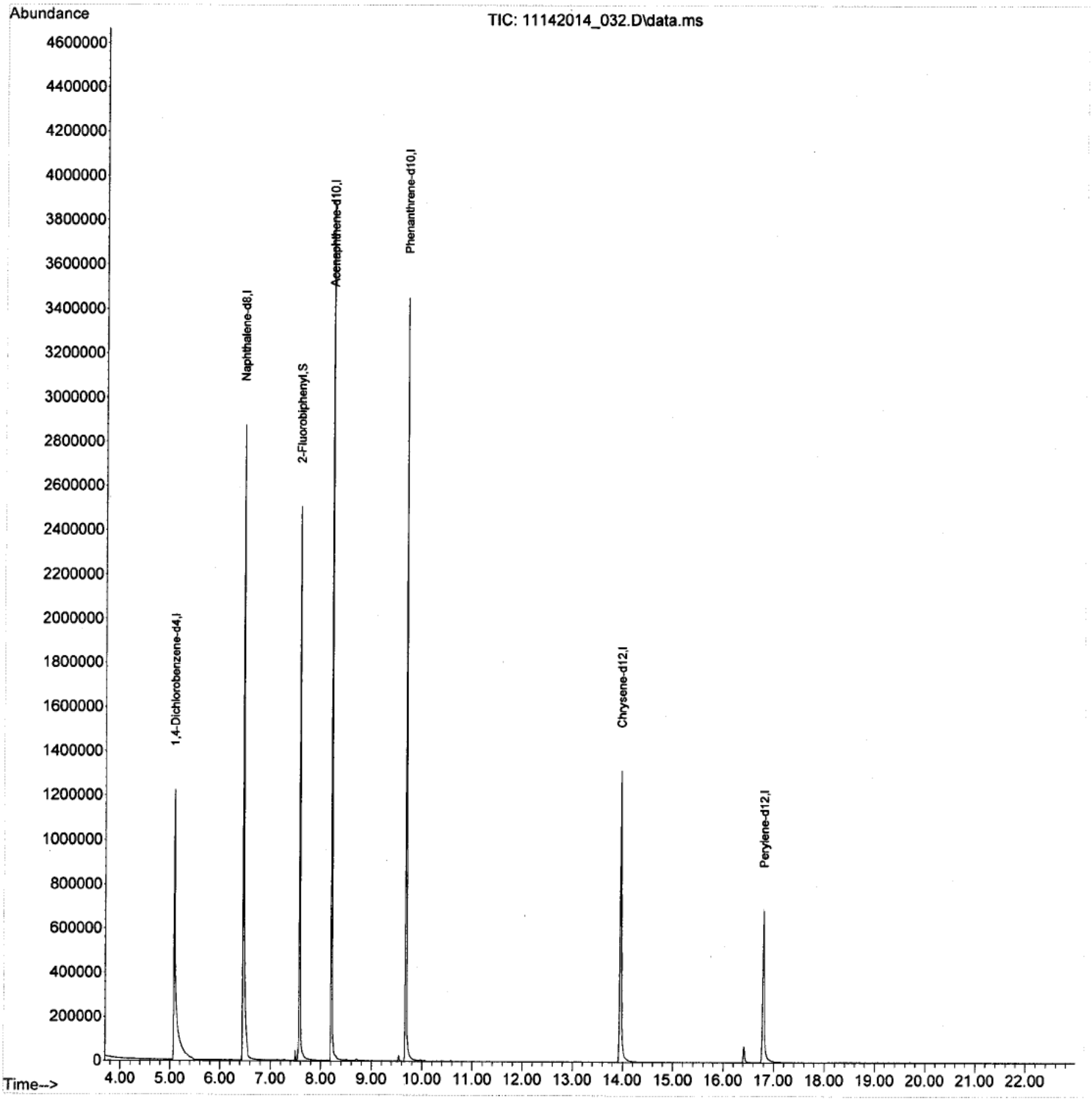
see Analyst Narrative, Surrogate Recovery [redacted] 1/5/15

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Time: Nov 17 11:15:13 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds
QLast Update : Wed Nov 12 16:18:43 2014
Response via : Initial Calibration



Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Time: Dec 01 13:05:54 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| Internal Standards | | | | | |
| 1) 1,4-Dichlorobenzene-d4 | 5.081 | 150 | 700802 | 20.00 ug/mL | 0.00 |
| 13) Naphthalene-d8 | 6.457 | 136 | 1808248 | 20.00 ug/mL | 0.00 |
| 24) Acenaphthene-d10 | 8.210 | 164 | 998933 | 20.00 ug/mL | 0.00 |
| 37) Phenanthrene-d10 | 9.681 | 188 | 1512494 | 20.00 ug/mL | 0.00 |
| 49) Chrysene-d12 | 13.963 | 240 | 930258 | 20.00 ug/mL | -0.01 |
| 58) Perylene-d12 | 16.804 | 264 | 570430 | 20.00 ug/mL | 0.00 |

| Target Compounds | | | Qvalue |
|---|---|---|---|
| 2) Bis(2-chloroethyl) ether | 0.000 | 0 | N.D. |
| 3) n-Decane | 0.000 | 0 | N.D. d |
| 4) 1,3-Dichlorobenzene | 0.000 | 0 | N.D. d |
| 5) 1,4-Dichlorobenzene | 0.000 | 0 | N.D. d |
| 6) 1,2-Dichlorobenzene | 0.000 | 0 | N.D. d |
| 7) Benzyl Alcohol | 0.000 | 0 | N.D. d |
| 8) Bis(2-chloroisopropyl)... | 0.000 | 0 | N.D. |
| 9) Hexachloroethane | 0.000 | 0 | N.D. d |
| 10) N-Nitrosodi-N-propylamine | 0.000 | 0 | N.D. |
| 11) Nitrobenzene | 0.000 | 0 | N.D. d |
| 12) 4-Methylcyclohexanecar... | 0.000 | 0 | N.D. d |
| 14) n-Dodecane | 0.000 | 0 | N.D. d |
| 15) Isophorone | 0.000 | 0 | N.D. d |
| 16) Bis(2-chloroethoxy) me... | 0.000 | 0 | N.D. d |
| 17) 1,2,4-Trichlorobenzene | 0.000 | 0 | N.D. |
| 18) Napthalene | 0.000 | 0 | N.D. |
| 19) Hexachlorobutadiene | 0.000 | 0 | N.D. |
| 20) 2-Methylnapthalene | 0.000 | 0 | N.D. d |
| 21) Hexachlorocyclopentadiene | 0.000 | 0 | N.D. |
| 22) 2-Chloronapthalene | 0.000 | 0 | N.D. d |
| 23) n-Tetradecane | 0.000 | 0 | N.D. d |
| 25) Dimethly Phthalate | 0.000 | 0 | N.D. d |
| 26) Acenaphthylene | 0.000 | 0 | N.D. d |
| 27) 2,6-Dinitrotoluene | 0.000 | 0 | N.D. d |
| 28) Acenaphthene | 0.000 | 0 | N.D. d |
| 29) Dibenzofuran | 0.000 | 0 | N.D. d |
| 30) 2,4-Dinitrotoluene | 0.000 | 0 | N.D. d |
| 31) n-Hexadecane | 0.000 | 0 | N.D. d |
| 32) Fluorene | 0.000 | 0 | N.D. |
| 33) Diethyl Phthalate | 0.000 | 0 | N.D. d |
| 34) 4-Chlorophenylphenyl E... | 0.000 | 0 | N.D. d |
| 35) N-Nitrosodiphenylamine | 0.000 | 0 | N.D. |
| 36) Azobenzene | 0.000 | 0 | N.D. |
| 38) 4-Bromophenylphenyl Ether | 0.000 | 0 | N.D. |
| 39) Hexachlorobenzene | 0.000 | 0 | N.D. |
| 40) n-Octadecane | 0.000 | 0 | N.D. d |
| 41) Phenanthrene | 0.000 | 0 | N.D. d |
| 42) Anthracene | 0.000 | 0 | N.D. d |
| 43) Carbazole | 0.000 | 0 | N.D. d |
| 44) Dibutyl Phthalate | 0.000 | 0 | N.D. d |
| 45) n-Eicosane | 0.000 | 0 | N.D. d |

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Time: Dec 01 13:05:54 2014
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration

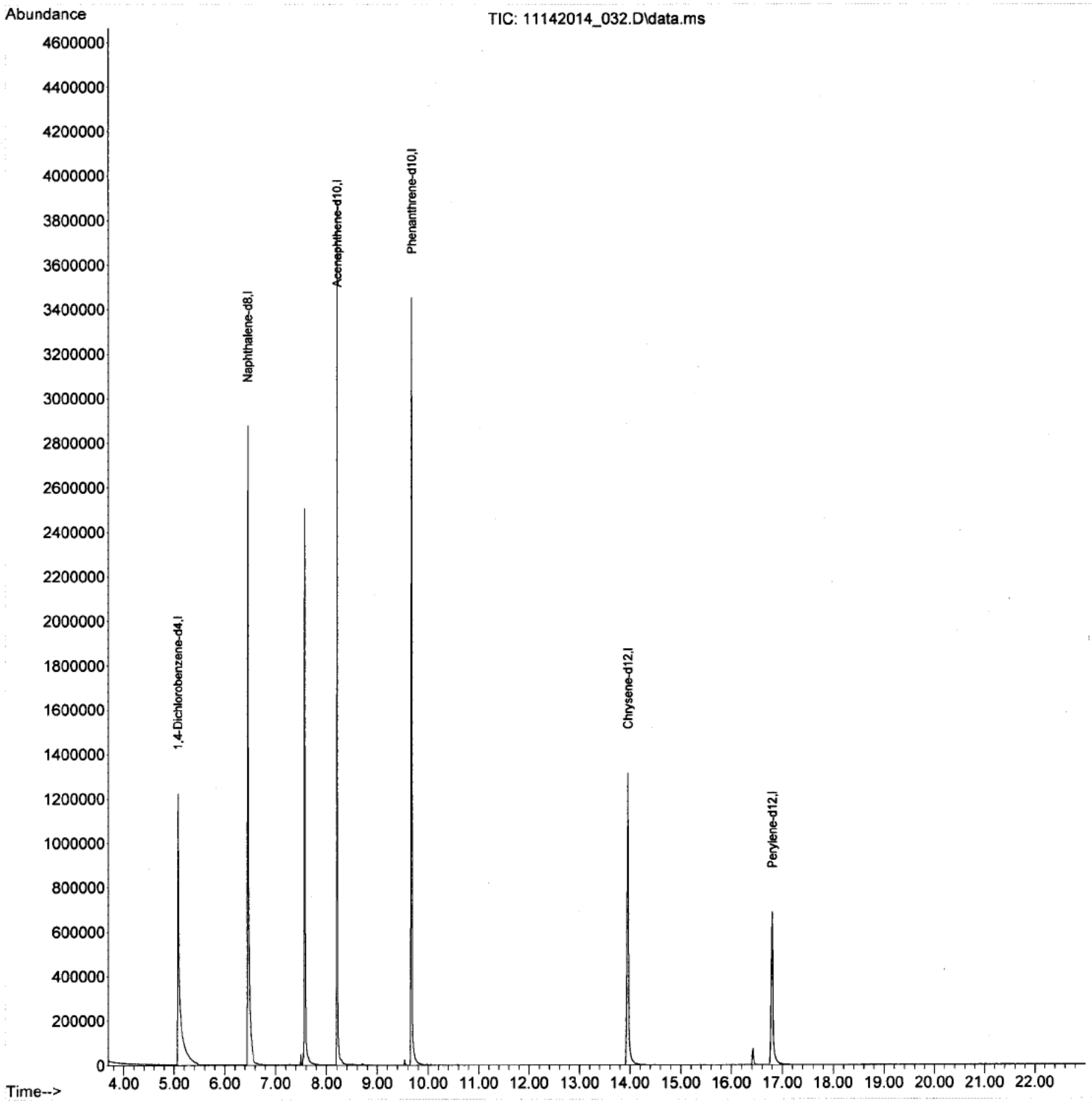
| Compound | R.T. | QIon | Response | Conc Units | Dev(Min) |
|---|---|---|---|---|---|
| 46) Fluoranthene | 0.000 | | 0 | N.D. | |
| 47) Pyrene | 0.000 | | 0 | N.D. | |
| 48) n-Docosane | 0.000 | | 0 | N.D. | |
| 50) Benzyl Butyl Phthalate | 0.000 | | 0 | N.D. | |
| 51) n-Tetracosane | 0.000 | | 0 | N.D. | |
| 52) n-Hexacosane | 0.000 | | 0 | N.D. | d |
| 53) n-Octacosane | 0.000 | | 0 | N.D. | d |
| 54) Benz[a]anthracene | 0.000 | | 0 | N.D. | d |
| 55) Chrysene | 0.000 | | 0 | N.D. | d |
| 56) Bis(2-ethylhexyl) Phth... | 0.000 | | 0 | N.D. | d |
| 57) Di-n-octyl Phthalate | 0.000 | | 0 | N.D. | |
| 59) Benzo[b]fluoranthene | 0.000 | | 0 | N.D. | |
| 60) Benzo(k)fluoranthene | 0.000 | | 0 | N.D. | |
| 61) Benz[a]pyrene | 0.000 | | 0 | N.D. | d |
| 62) Indo[1,2,3-cd]pyrene | 0.000 | | 0 | N.D. | |
| 63) Dibenz[a,h]anthracene | 0.000 | | 0 | N.D. | |
| 64) Benzo[g,h,i]perylene | 0.000 | | 0 | N.D. | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Time: Dec 01 13:05:54 2014
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]c.M
Quant Title : RP1616-MCHM Compounds-C
QLast Update : Fri Nov 21 16:16:46 2014
Response via : Initial Calibration



# LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 0

Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Title : RP1616-MCHM Compounds

Signal : TIC: 11142014_032.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.999 | 49 | 53 | 59 | rVV6 | 2017 | 4449 | 0.10% | 0.019% |
| 2 | 4.046 | 59 | 61 | 69 | rVB5 | 1604 | 3513 | 0.08% | 0.015% |
| 3 | 4.216 | 83 | 90 | 111 | rVB6 | 1896 | 8276 | 0.19% | 0.036% |
| 4 | 4.528 | 139 | 143 | 163 | rVB8 | 1654 | 7216 | 0.17% | 0.031% |
| 5 | 5.081 | 229 | 237 | 333 | rVB | 1220580 | 3091751 | 71.13% | 13.455% |
| 6 | 5.828 | 359 | 364 | 371 | rBV6 | 1618 | 3519 | 0.08% | 0.015% |
| 7 | 6.457 | 463 | 471 | 531 | rBV | 2874387 | 4005744 | 92.15% | 17.433% |
| 8 | 7.140 | 583 | 587 | 597 | rVB5 | 2623 | 3519 | 0.08% | 0.015% |
| 9 | 7.287 | 597 | 612 | 621 | rVB3 | 4444 | 8883 | 0.20% | 0.039% |
| 10 | 7.493 | 635 | 647 | 653 | rBV | 46087 | 41369 | 0.95% | 0.180% |
| 11 | 7.575 | 653 | 661 | 723 | rVV | 2505183 | 2808779 | 64.62% | 12.224% |
| 12 | 7.963 | 723 | 727 | 739 | rVV7 | 1492 | 4231 | 0.10% | 0.018% |
| 13 | 8.046 | 739 | 741 | 753 | rVB7 | 1486 | 4017 | 0.09% | 0.017% |
| 14 | 8.210 | 759 | 769 | 805 | rBV | 3885913 | 4346894 | 100.00% | 18.918% |
| 15 | 8.445 | 807 | 809 | 817 | rVV5 | 2473 | 5991 | 0.14% | 0.026% |
| 16 | 8.516 | 817 | 821 | 837 | rVB7 | 5270 | 11213 | 0.26% | 0.049% |
| 17 | 8.704 | 847 | 853 | 869 | rVB2 | 7411 | 14941 | 0.34% | 0.065% |
| 18 | 9.016 | 901 | 906 | 917 | rVB6 | 1765 | 3275 | 0.08% | 0.014% |
| 19 | 9.534 | 987 | 994 | 1011 | rVV | 23919 | 28896 | 0.66% | 0.126% |
| 20 | 9.681 | 1011 | 1019 | 1063 | rVV | 3452195 | 4081514 | 93.89% | 17.763% |
| 21 | 9.975 | 1063 | 1069 | 1079 | rVV3 | 4524 | 15467 | 0.36% | 0.067% |
| 22 | 10.057 | 1079 | 1083 | 1099 | rVV2 | 4883 | 9101 | 0.21% | 0.040% |
| 23 | 10.581 | 1167 | 1172 | 1179 | rVB | 3736 | 4569 | 0.11% | 0.020% |
| 24 | 13.475 | 1661 | 1664 | 1689 | rBV4 | 696 | 3783 | 0.09% | 0.016% |
| 25 | 13.963 | 1731 | 1747 | 1793 | rVV | 1315233 | 2625267 | 60.39% | 11.425% |
| 26 | 14.257 | 1793 | 1797 | 1803 | rVV4 | 2071 | 6004 | 0.14% | 0.026% |
| 27 | 14.316 | 1803 | 1807 | 1833 | rVV5 | 1644 | 7501 | 0.17% | 0.033% |
| 28 | 16.416 | 2153 | 2164 | 2189 | rVV | 72958 | 141707 | 3.26% | 0.617% |
| 29 | 16.804 | 2205 | 2230 | 2293 | rBV | 688316 | 1658099 | 38.14% | 7.216% |
| 30 | 17.204 | 2293 | 2298 | 2305 | rVV4 | 1374 | 3777 | 0.09% | 0.016% |
| 31 | 17.992 | 2421 | 2432 | 2433 | rBV2 | 1117 | 3263 | 0.08% | 0.014% |
| 32 | 19.709 | 2717 | 2724 | 2735 | rVB6 | 1415 | 3590 | 0.08% | 0.016% |
| 33 | 19.992 | 2757 | 2772 | 2773 | rVB5 | 1143 | 4207 | 0.10% | 0.018% |
| 34 | 21.233 | 2973 | 2983 | 2989 | rVB4 | 1171 | 3626 | 0.08% | 0.016% |

LSC Area Percent Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Integration Parameters: RP1616.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.02 Max Peaks: 34
Stop Thrs : 0.01 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 0

Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Title : RP1616-MCHM Compounds

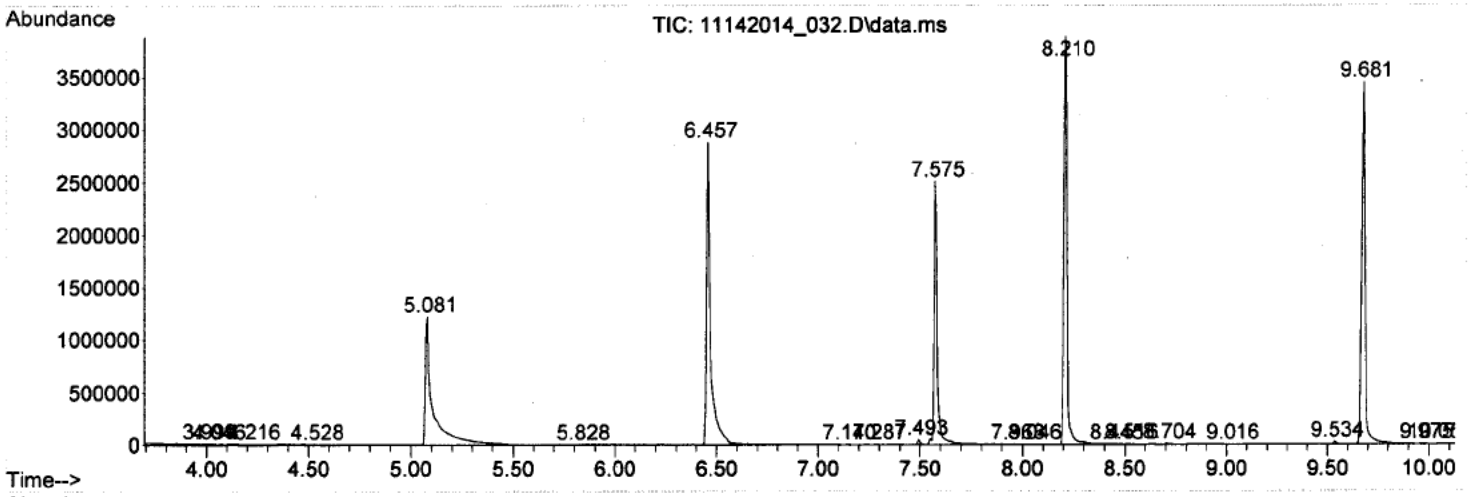
Sum of corrected areas: 22977951

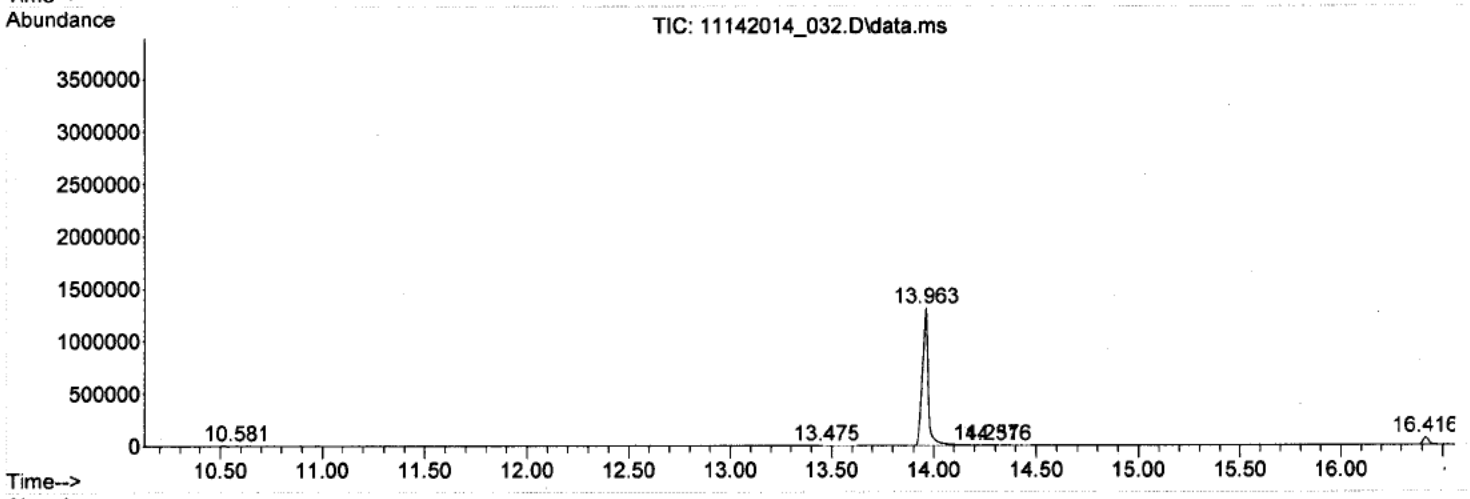
LSC Report - Integrated Chromatogram

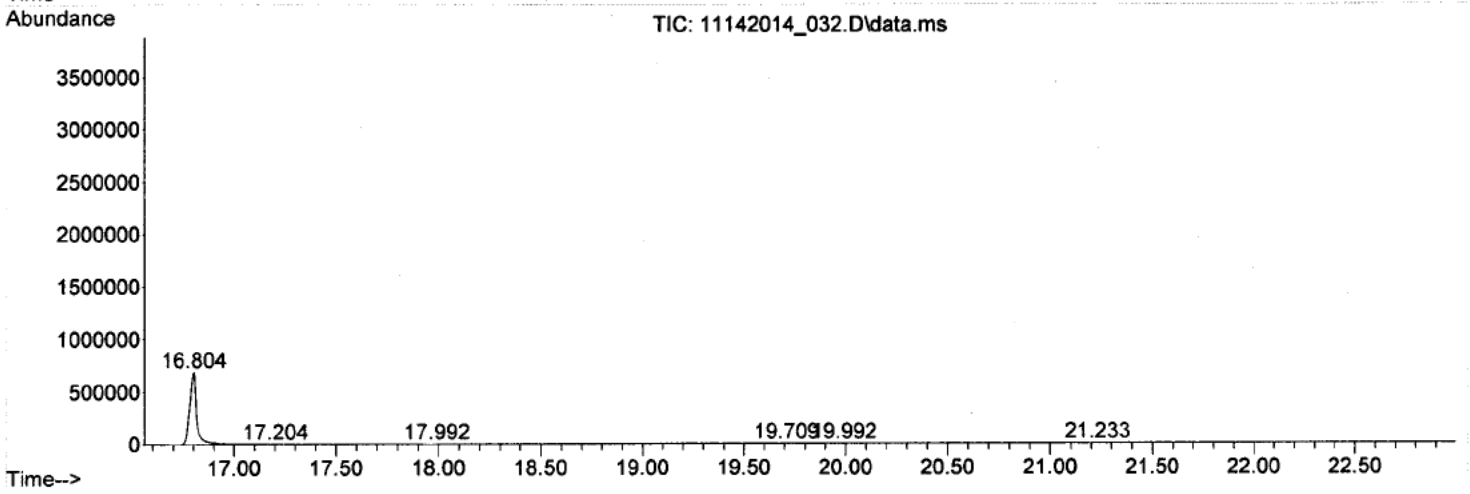
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

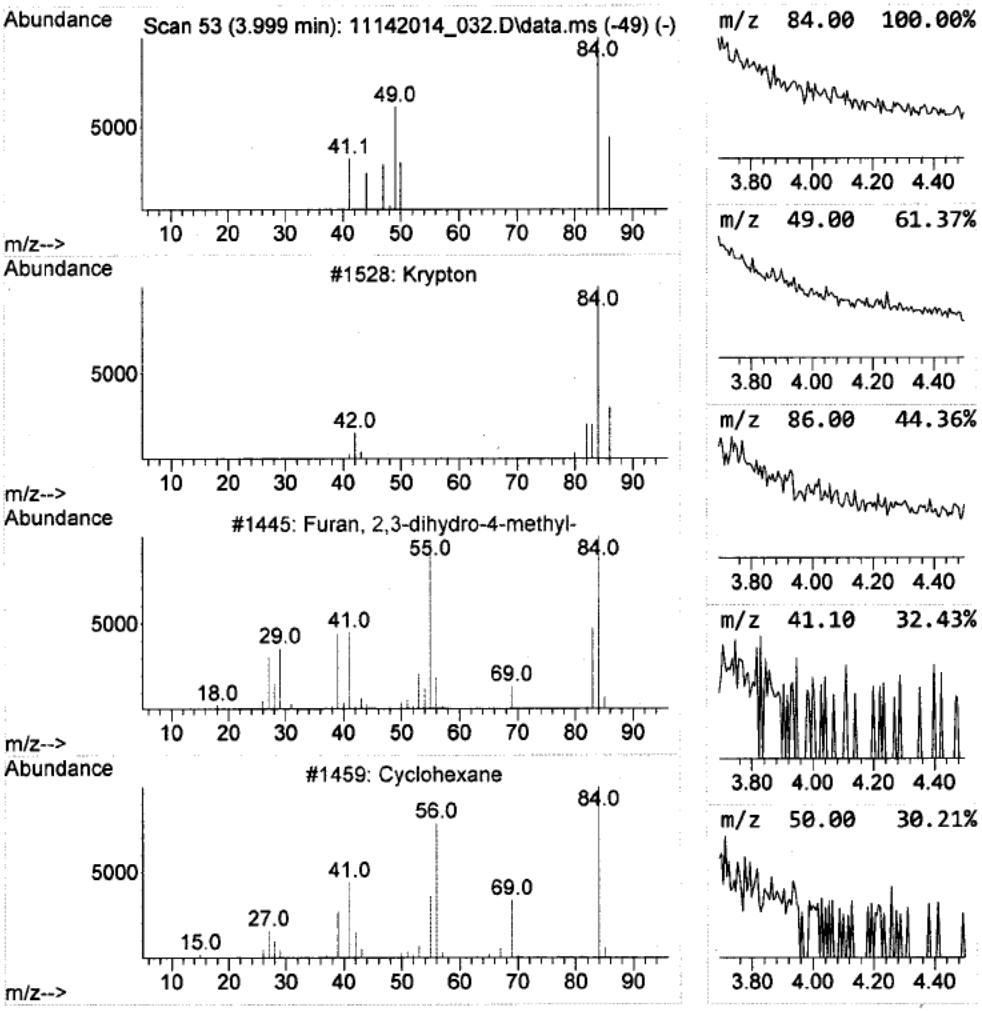
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 1 Krypton Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.999 | 0.03 ug/mL | 4449 | 1,4-Dichlorobenzene-d4 | 5.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Krypton | 84 | Kr | 007439-90-9 | 5 |
| 2 | Furan, 2,3-dihydro-4-methyl- | 84 | C5H8O | 034314-83-5 | 4 |
| 3 | Cyclohexane | 84 | C6H12 | 000110-82-7 | 4 |
| 4 | 2,3,4,5-Tetrahydropyridazine | 84 | C4H8N2 | 000694-06-4 | 4 |
| 5 | 2-Butenal, 2-methyl- | 84 | C5H8O | 001115-11-3 | 2 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

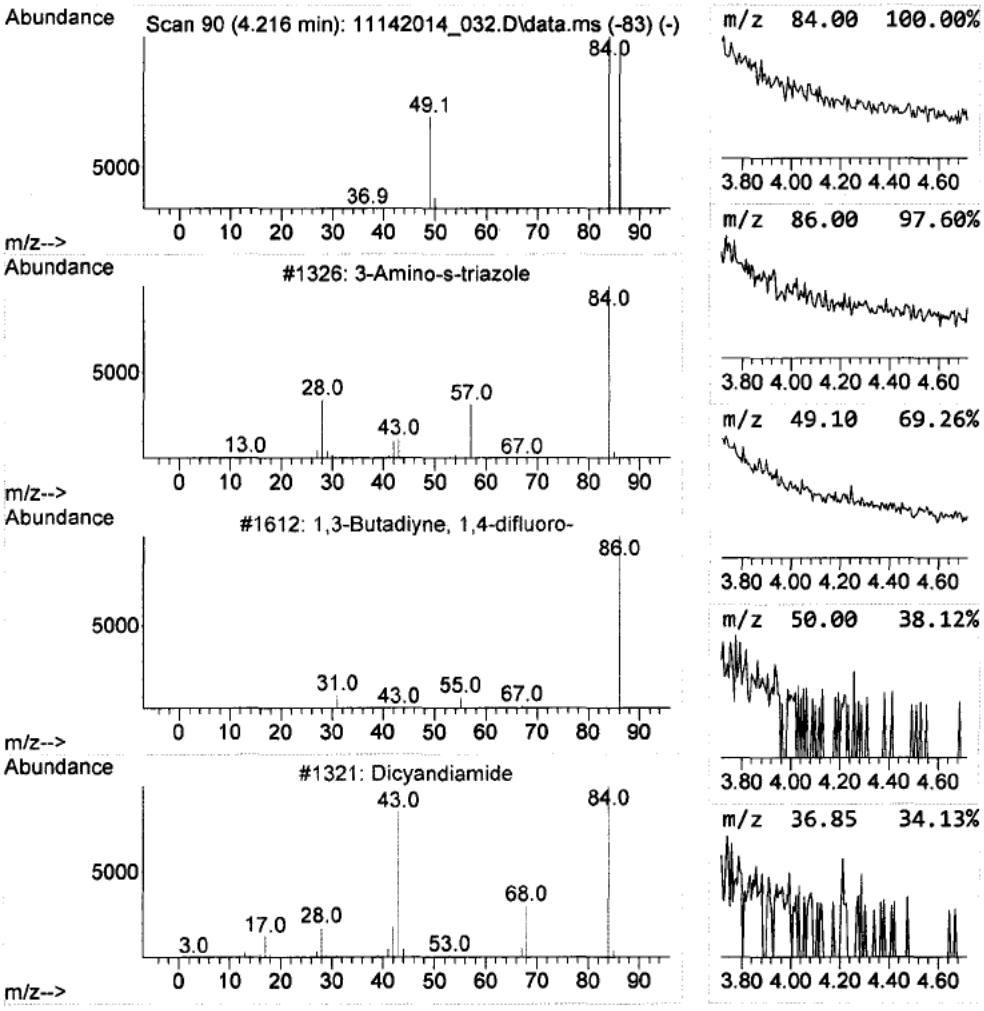
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 2 3-Amino-s-triazole Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.216 | 0.05 ug/mL | 8276 | 1,4-Dichlorobenzene-d4 | 5.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Amino-s-triazole | 84 | C2H4N4 | 000061-82-5 | 2 |
| 2 | 1,3-Butadiyne, 1,4-difluoro- | 86 | C4F2 | 064788-23-4 | 2 |
| 3 | Dicyandiamide | 84 | C2H4N4 | 000461-58-5 | 2 |
| 4 | 2-Amino-oxazole | 84 | C3H4N2O | 004570-45-0 | 2 |
| 5 | Pyridine-D5- | 84 | C5D5N | 007291-22-7 | 2 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

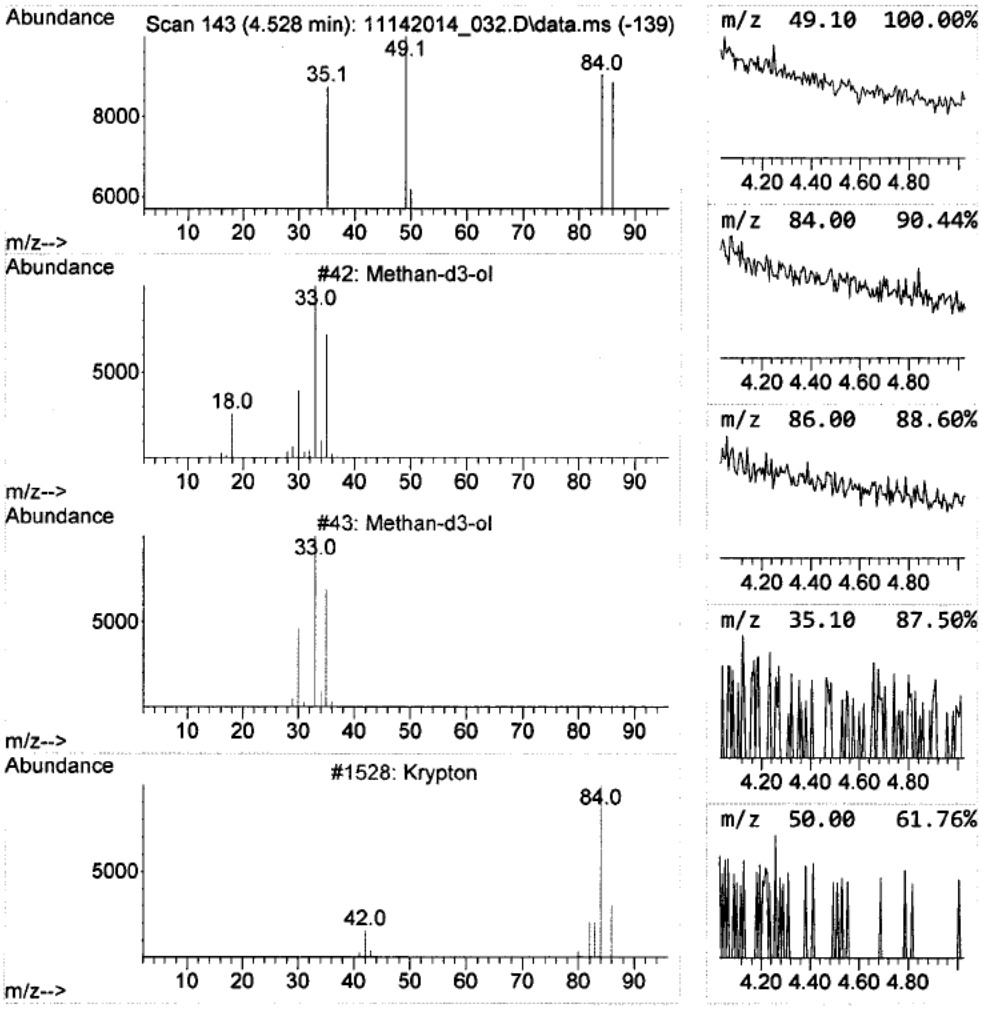
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 3 Methan-d3-ol Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.528 | 0.05 ug/mL | 7216 | 1,4-Dichlorobenzene-d4 | 5.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methan-d3-ol | 35 | CHD3O | 001849-29-2 | 3 |
| 2 | Methan-d3-ol | 35 | CHD3O | 001849-29-2 | 3 |
| 3 | Krypton | 84 | Kr | 007439-90-9 | 2 |
| 4 | Oxygen difluoride | 54 | F2O | 007783-41-7 | 1 |
| 5 | Propanoyl chloride | 92 | C3H5ClO | 000079-03-8 | 1 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

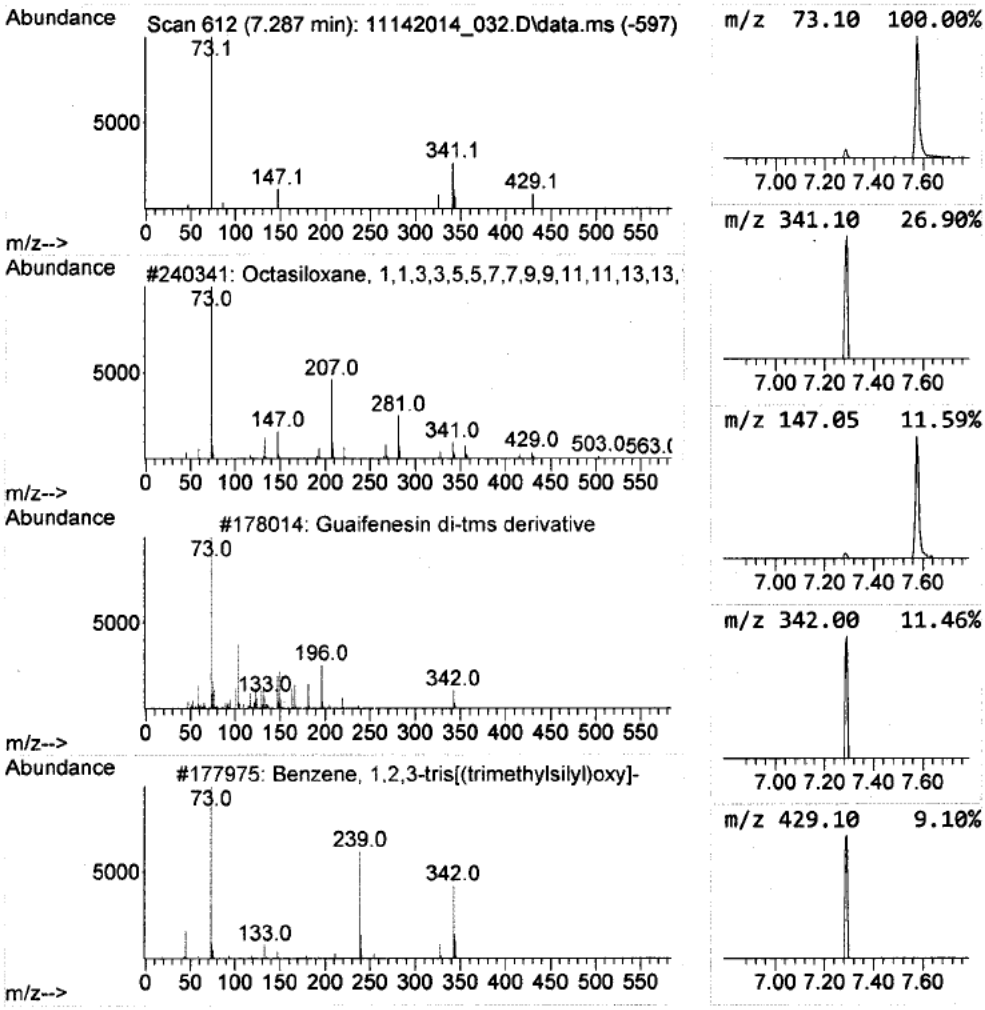
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 4 Octasiloxane, 1,1,3,3,5,5,7... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.287 | 0.04 ug/mL | 8883 | Naphthalene-d8 | 6.457 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octasiloxane, 1,1,3,3,5,5,7,7,9,... | 578 | C16H50O7Si8 | 019095-24-0 | 28 |
| 2 | Guaifenesin di-tms derivative | 342 | C16H30O4Si2 | 107966-19-8 | 7 |
| 3 | Benzene, 1,2,3-tris[(trimethylsi... | 342 | C15H30O3Si3 | 017864-23-2 | 4 |
| 4 | Benzene, 1,2,3-tris[(trimethylsi... | 342 | C15H30O3Si3 | 017864-23-2 | 4 |
| 5 | Cyclopropanecarboxamide, N-[7-(2... | 341 | C19H16FNO4 | 1000351-11-9 | 4 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

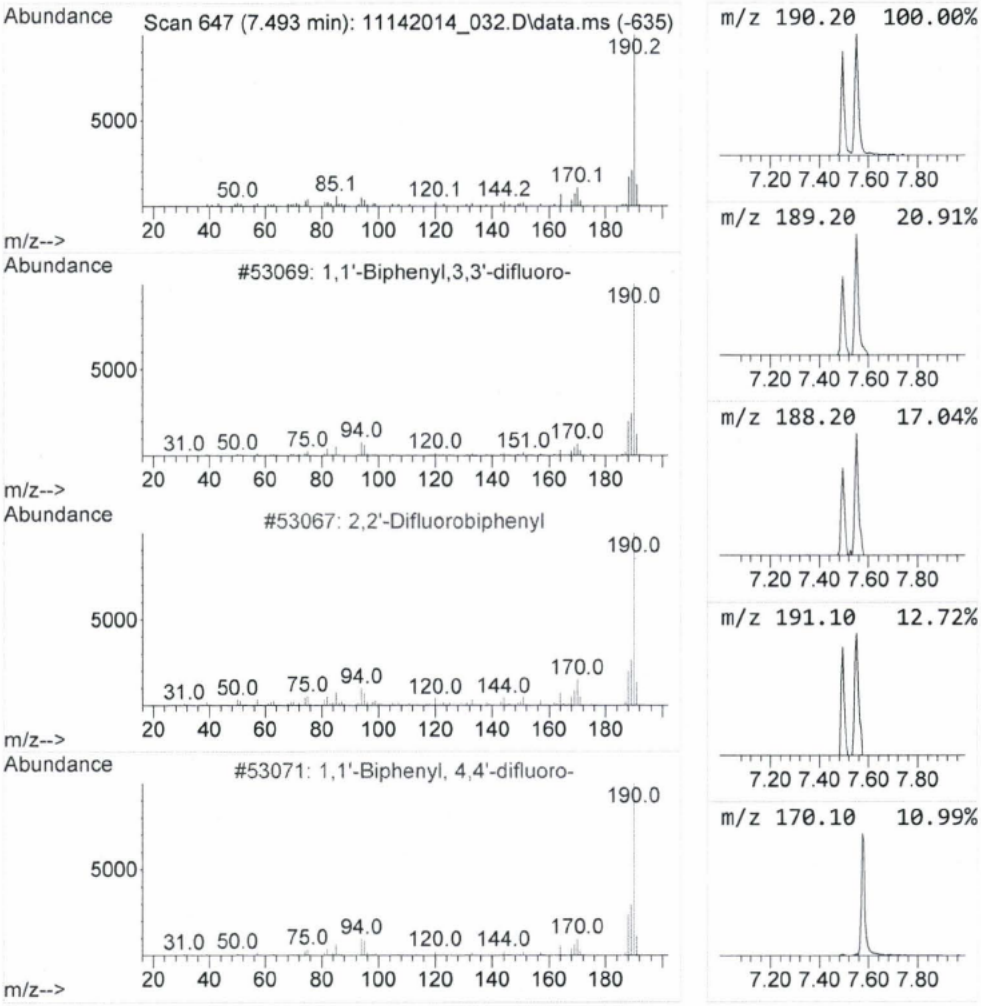
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 5 1,1'-Biphenyl,3,3'-difluoro- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.493 | 0.19 ug/mL | 41369 | Acenaphthene-d10 | 8.210 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,1'-Biphenyl,3,3'-difluoro- | 190 | C12H8F2 | 000396-64-5 | 94 |
| 2 | 2,2'-Difluorobiphenyl | 190 | C12H8F2 | 000388-82-9 | 94 |
| 3 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 93 |
| 4 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 93 |
| 5 | 1,1'-Biphenyl, 4,4'-difluoro- | 190 | C12H8F2 | 000398-23-2 | 72 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

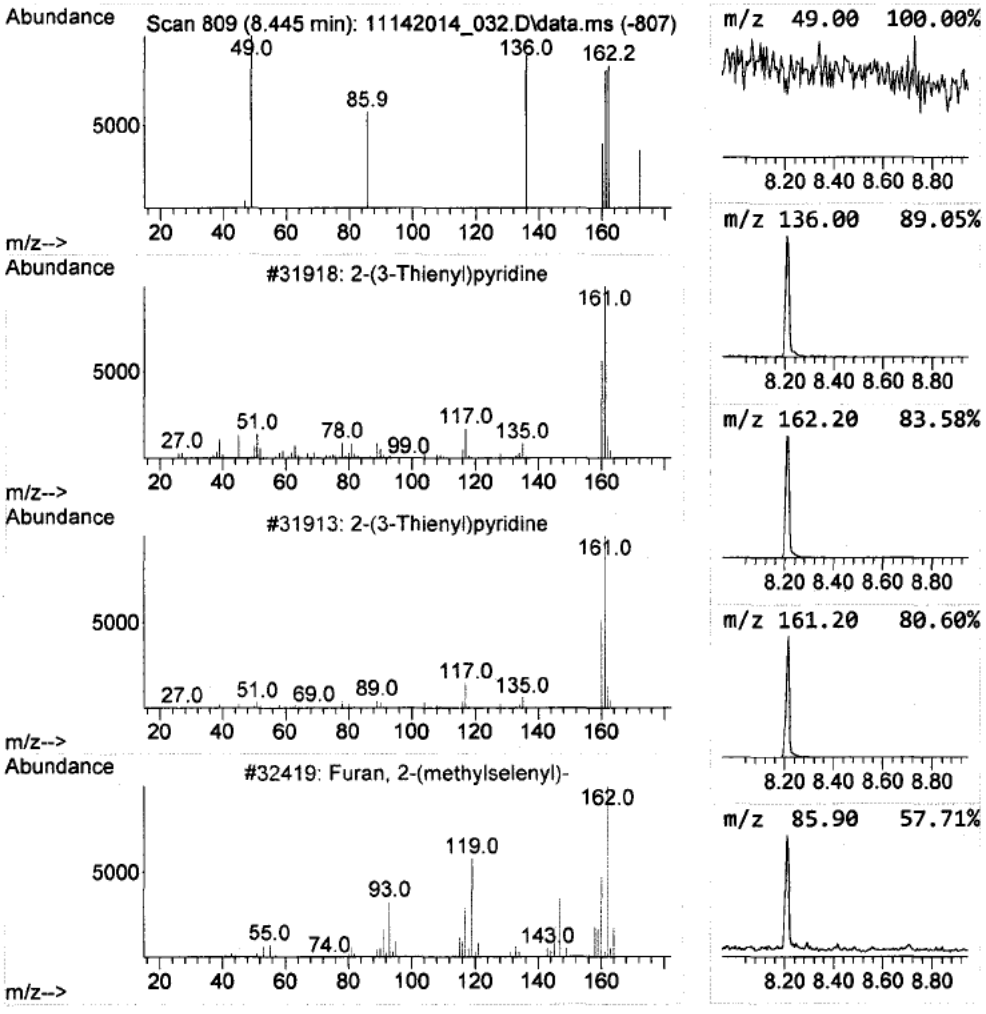
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 6 2-(3-Thienyl)pyridine Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.445 | 0.03 ug/mL | 5991 | Acenaphthene-d10 | 8.210 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-(3-Thienyl)pyridine | 161 | C9H7NS | 021298-55-5 | 9 |
| 2 | 2-(3-Thienyl)pyridine | 161 | C9H7NS | 021298-55-5 | 9 |
| 3 | Furan, 2-(methylselenyl)- | 162 | C5H6OSe | 013129-43-6 | 9 |
| 4 | Benzo[b]thiophene, 3,6-dimethyl- | 162 | C10H10S | 016587-50-1 | 5 |
| 5 | Phenylamine, 3-(pyrrolidin-1-yl)- | 162 | C10H14N2 | 1000316-72-5 | 5 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

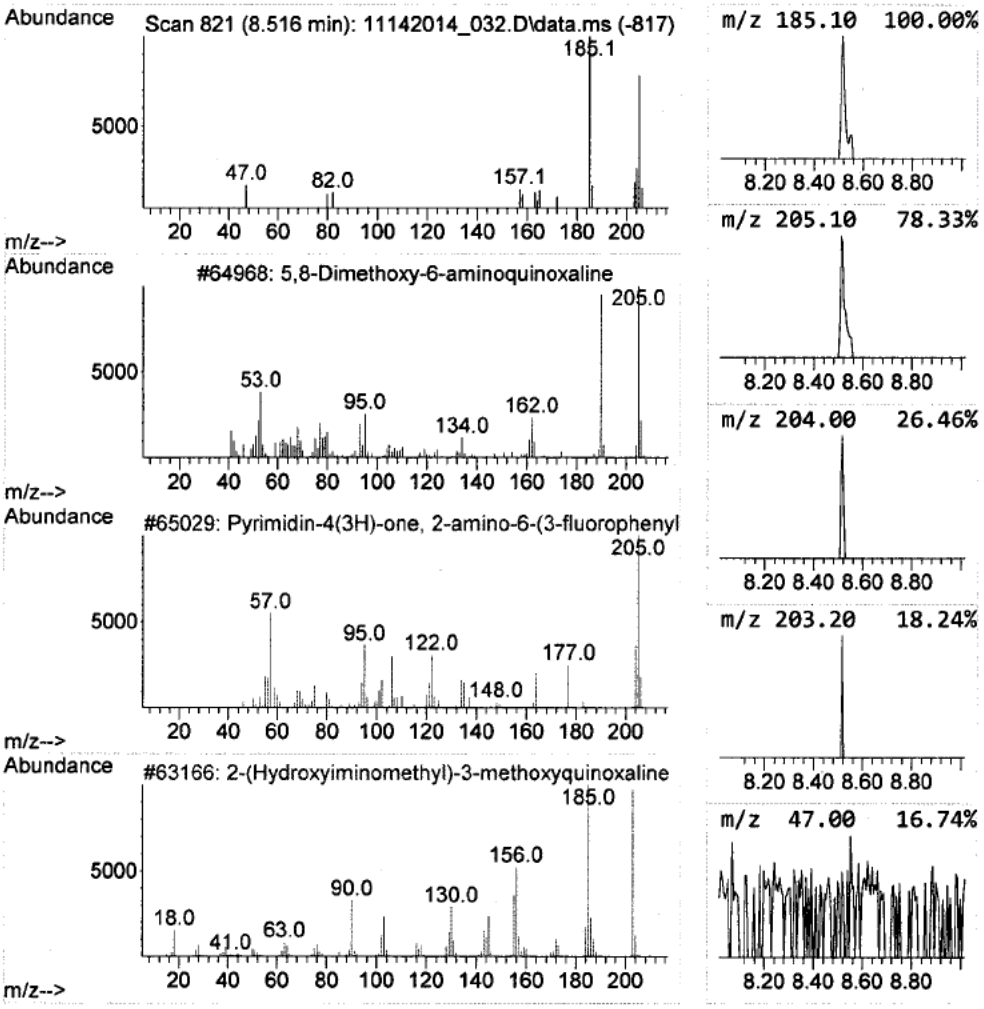
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 7 5,8-Dimethoxy-6-aminoquinox... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.516 | 0.05 ug/mL | 11213 | Acenaphthene-d10 | 8.210 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5,8-Dimethoxy-6-aminoquinoxaline | 205 | C10H11N3O2 | 056393-24-9 | 27 |
| 2 | Pyrimidin-4(3H)-one, 2-amino-6-(... | 205 | C10H8FN3O | 098305-63-6 | 27 |
| 3 | 2-(Hydroxyiminomethyl)-3-methoxy... | 203 | C10H9N3O2 | 067570-75-6 | 12 |
| 4 | Benzenamine, 3-phenoxy- | 185 | C12H11NO | 003586-12-7 | 12 |
| 5 | Quinolin-2(1H)-one, 4-hydroxy-7-... | 205 | C11H11NO3 | 074798-86-0 | 12 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

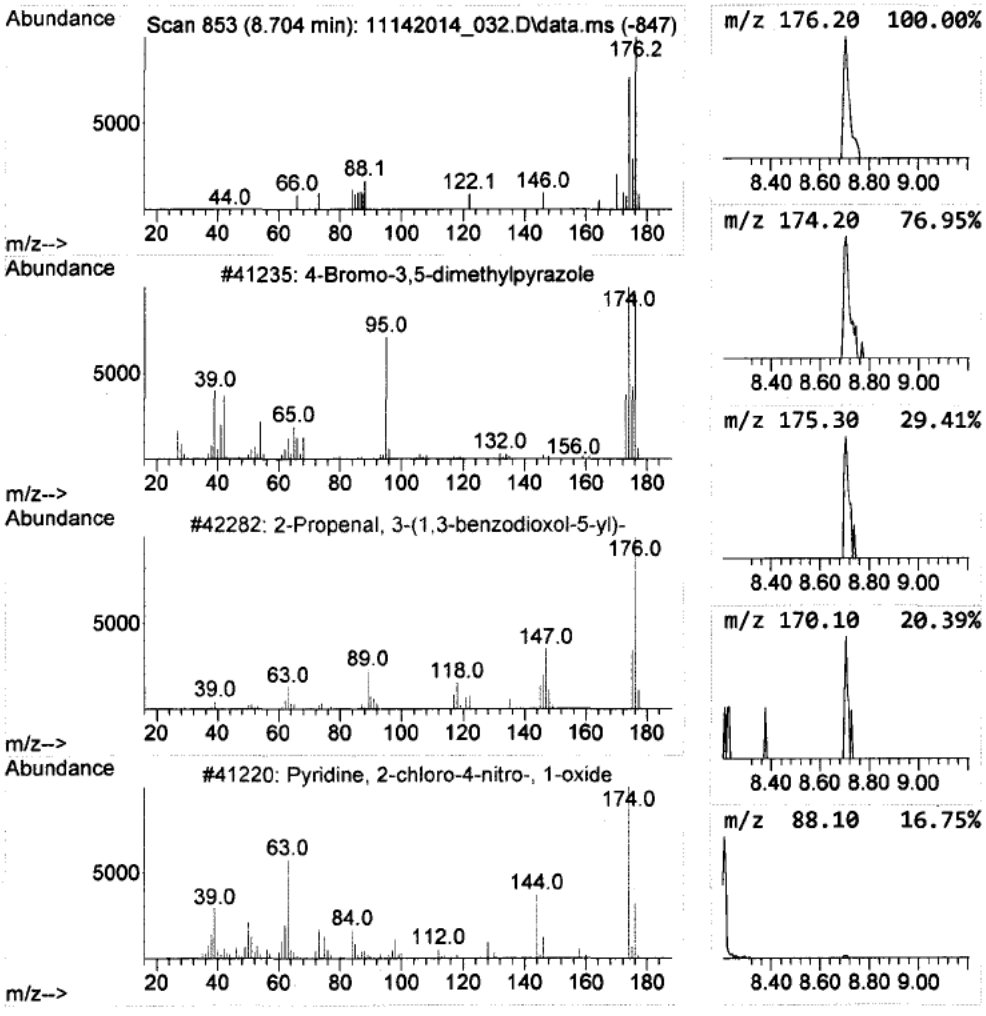
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 8 4-Bromo-3,5-dimethylpyrazole Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.704 | 0.07 ug/mL | 14941 | Acenaphthene-d10 | 8.210 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Bromo-3,5-dimethylpyrazole | 174 | C5H7BrN2 | 003398-16-1 | 42 |
| 2 | 2-Propenal, 3-(1,3-benzodioxol-5... | 176 | C10H8O3 | 014756-00-4 | 17 |
| 3 | Pyridine, 2-chloro-4-nitro-, 1-o... | 174 | C5H3ClN2O3 | 014432-16-7 | 12 |
| 4 | Furan-2(5H)-one, 5-(5-methyl-2-f... | 176 | C10H8O3 | 188576-91-2 | 12 |
| 5 | Benzene, 1-bromo-2-fluoro- | 174 | C6H4BrF | 001072-85-1 | 9 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

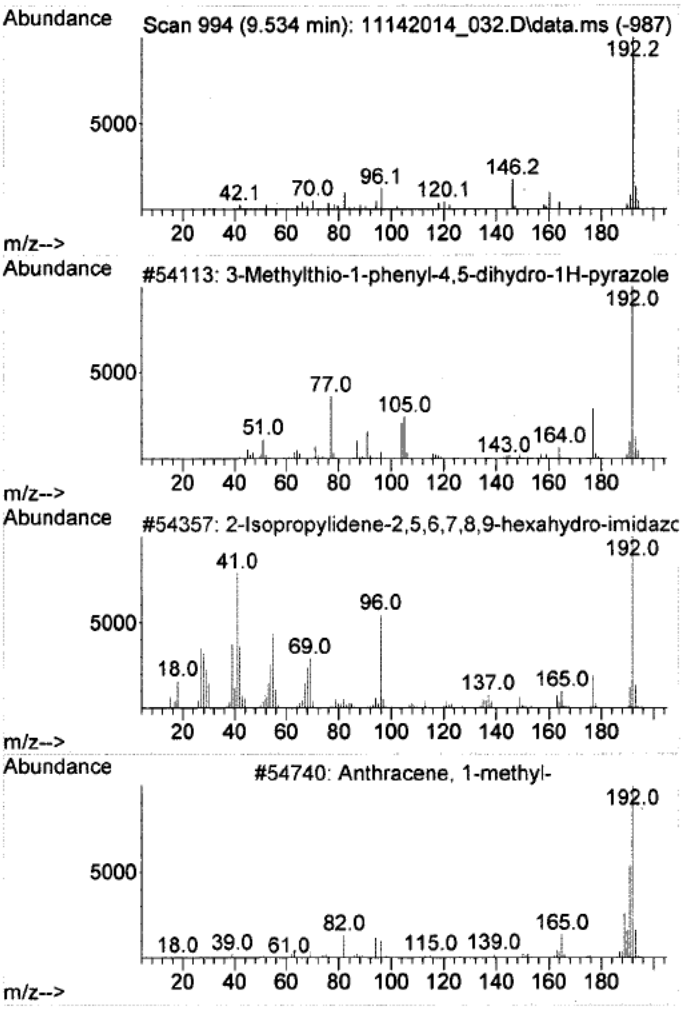
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

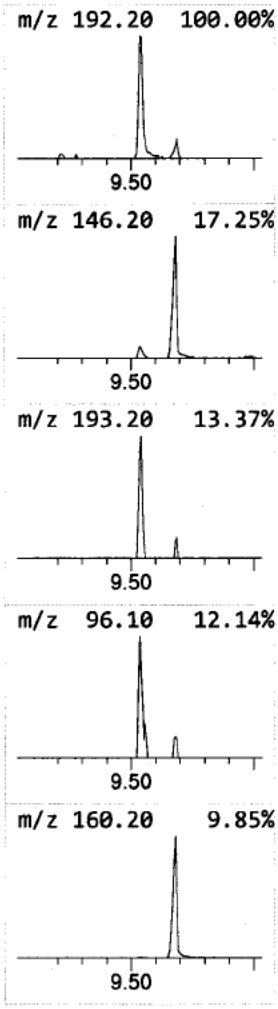
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 9 3-Methylthio-1-phenyl-4,5-d... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.534 | 0.14 ug/mL | 28896 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Methylthio-1-phenyl-4,5-dihydr... | 192 | C10H12N2S | 1000305-46-9 | 59 |
| 2 | 2-Isopropylidene-2,5,6,7,8,9-hex... | 192 | C11H16N2O | 172882-46-1 | 59 |
| 3 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 59 |
| 4 | 7H-1,3-Thiazino[3,2-f]purine, 8,... | 192 | C8H8N4S | 339370-55-7 | 58 |
| 5 | Phenanthrene, 9-methyl- | 192 | C15H12 | 000883-20-5 | 53 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

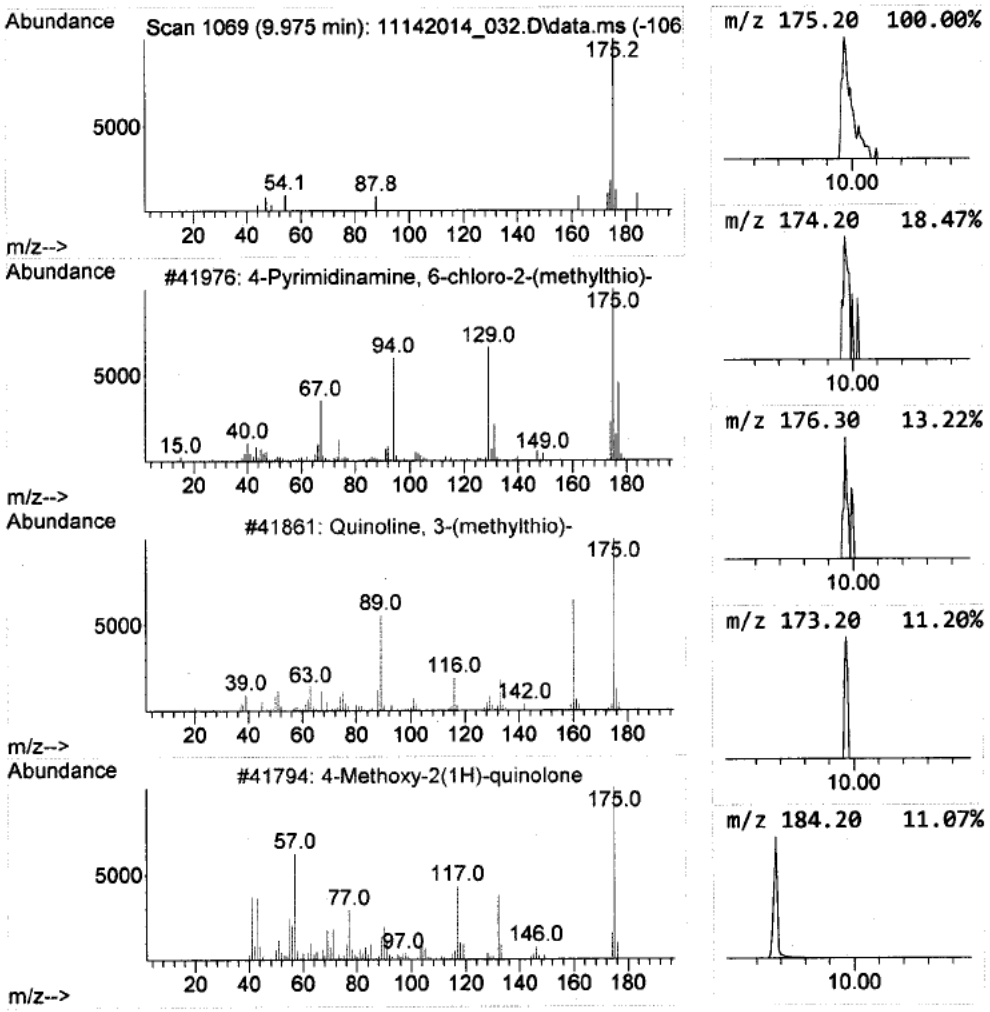
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 10 4-Pyrimidinamine, 6-chloro-... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.975 | 0.08 ug/mL | 15467 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Pyrimidinamine, 6-chloro-2-(me... | 175 | C5H6ClN3S | 001005-38-5 | 42 |
| 2 | Quinoline, 3-(methylthio)- | 175 | C10H9NS | 051934-46-4 | 9 |
| 3 | 4-Methoxy-2(1H)-quinolone | 175 | C10H9NO2 | 027667-34-1 | 9 |
| 4 | 1H-Indole-2-carboxylic acid, 1-m... | 175 | C10H9NO2 | 016136-58-6 | 9 |
| 5 | 2-Quinolinemethanol, 8-hydroxy- | 175 | C10H9NO2 | 017018-82-5 | 9 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

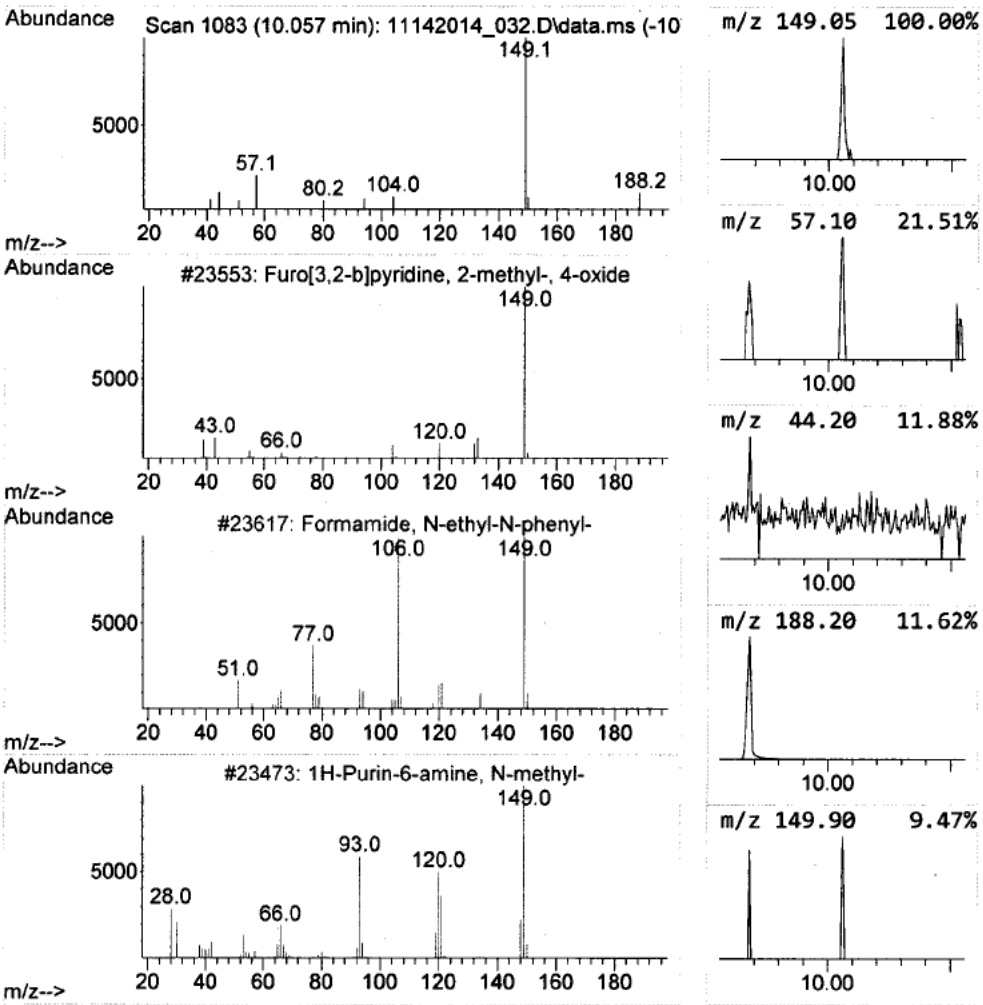
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 11 Furo[3,2-b]pyridine, 2-meth... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.057 | 0.04 ug/mL | 9101 | Phenanthrene-d10 | 9.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Furo[3,2-b]pyridine, 2-methyl-, ... | 149 | C8H7NO2 | 069022-83-9 | 50 |
| 2 | Formamide, N-ethyl-N-phenyl- | 149 | C9H11NO | 005461-49-4 | 40 |
| 3 | 1H-Purin-6-amine, N-methyl- | 149 | C6H7N5 | 000443-72-1 | 9 |
| 4 | 4-Methylthieno[2,3-b]pyridine | 149 | C8H7NS | 013362-81-7 | 9 |
| 5 | 2-Acetylbenzoic acid | 164 | C9H8O3 | 000577-56-0 | 9 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

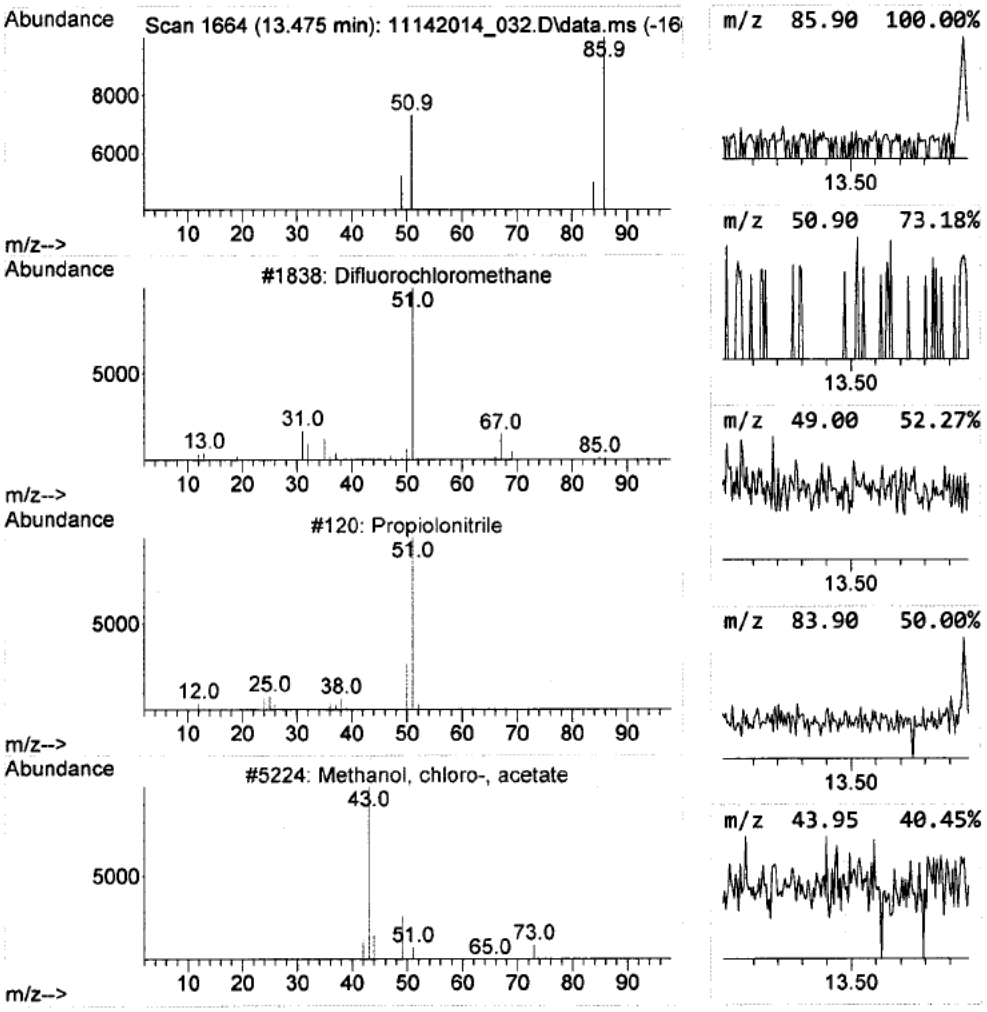
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 12 Difluorochloromethane Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.475 | 0.03 ug/mL | 3783 | Chrysene-d12 | 13.963 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Difluorochloromethane | 86 | CHClF2 | 000075-45-6 | 3 |
| 2 | Propiolonitrile | 51 | C3HN | 001070-71-9 | 3 |
| 3 | Methanol, chloro-, acetate | 108 | C3H5ClO2 | 000625-56-9 | 2 |
| 4 | 1-[4-(2,2-Difluoroacetyl)piperaz... | 242 | C8H10F4N2O2 | 1000311-46-6 | 1 |
| 5 | 2-Butyne-1,4-diol, diacetate | 170 | C8H10O4 | 001573-17-7 | 1 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

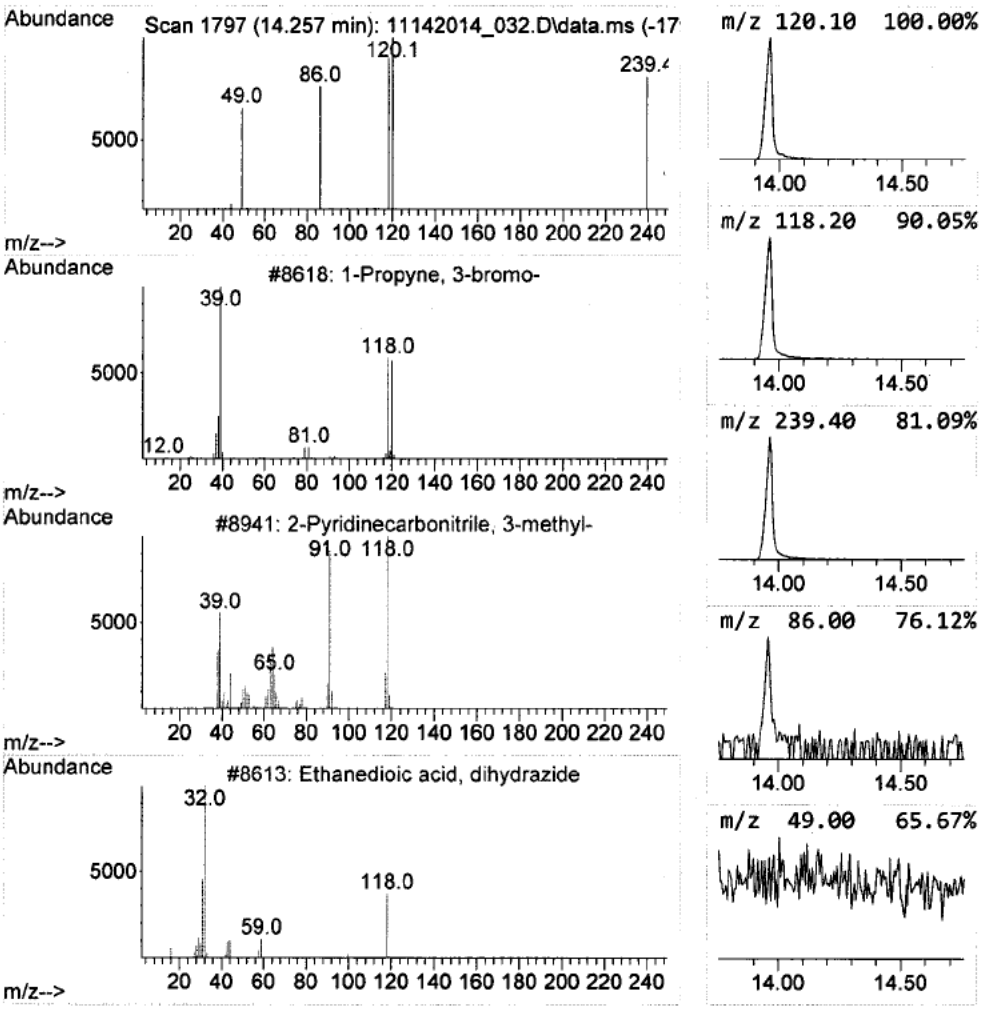
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 13 1-Propyne, 3-bromo- Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.257 | 0.05 ug/mL | 6004 | Chrysene-d12 | 13.963 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propyne, 3-bromo- | 118 | C3H3Br | 000106-96-7 | 5 |
| 2 | 2-Pyridinecarbonitrile, 3-methyl- | 118 | C7H6N2 | 1000318-76-9 | 4 |
| 3 | Ethanedioic acid, dihydrazide | 118 | C2H6N4O2 | 000996-98-5 | 4 |
| 4 | Amidinothiourea | 118 | C2H6N4S | 002114-02-5 | 4 |
| 5 | 1-Propyne, 3-bromo- | 118 | C3H3Br | 000106-96-7 | 4 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

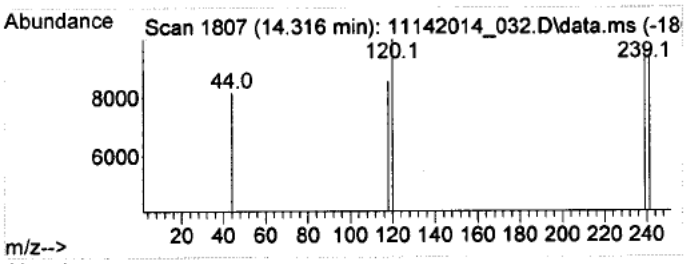
Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

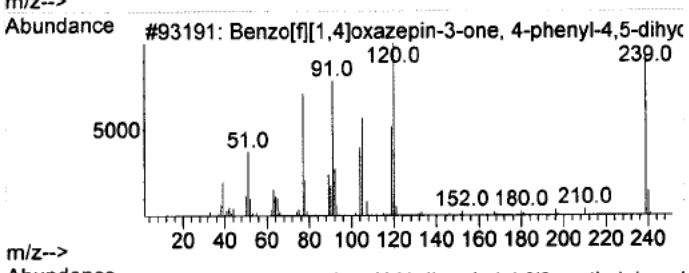
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

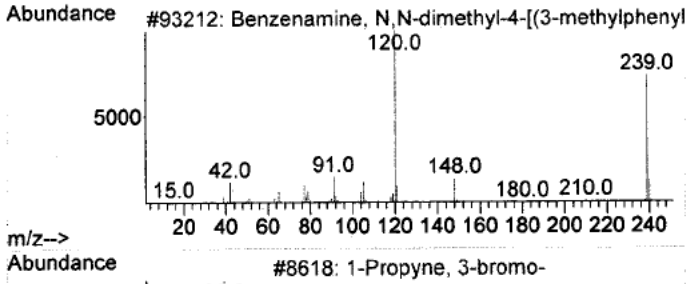
**********
Peak Number 14 Benzo[f][1,4]oxazepin-3-one... Concentration Rank 6

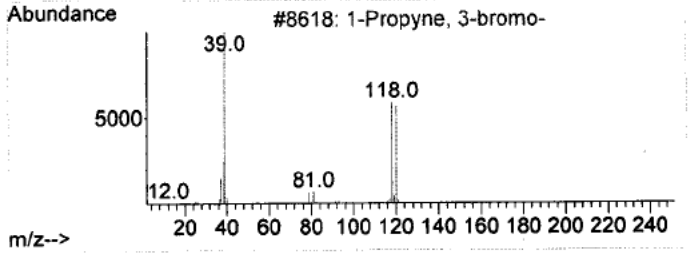
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.316 | 0.06 ug/mL | 7501 | Chrysene-d12 | 13.963 |

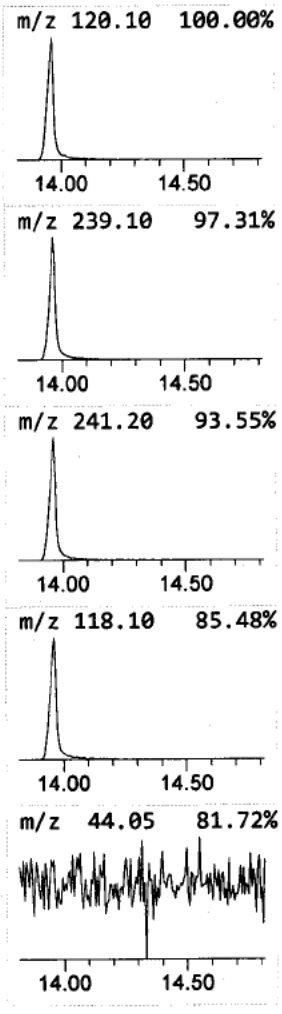
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[f][1,4]oxazepin-3-one, 4-p... | 239 | C15H13NO2 | 1000302-29-3 | 5 |
| 2 | Benzenamine, N,N-dimethyl-4-[(3-... | 239 | C15H17N3 | 000055-80-1 | 5 |
| 3 | 1-Propyne, 3-bromo- | 118 | C3H3Br | 000106-96-7 | 5 |
| 4 | 1-Propyne, 3-bromo- | 118 | C3H3Br | 000106-96-7 | 4 |
| 5 | 1-Propyne, 3-bromo- | 118 | C3H3Br | 000106-96-7 | 4 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

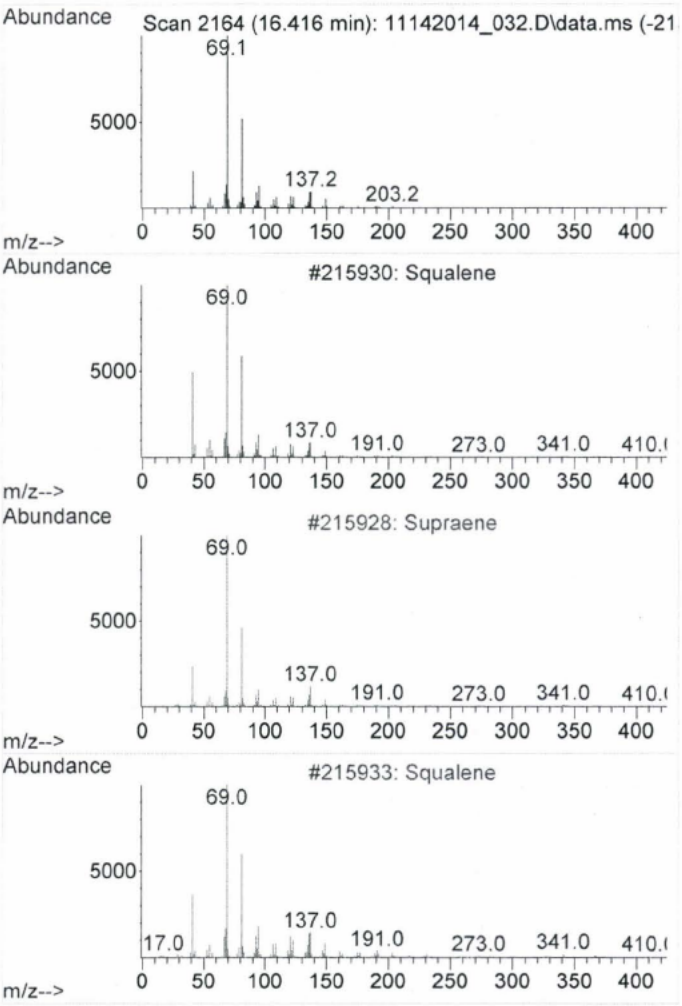
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

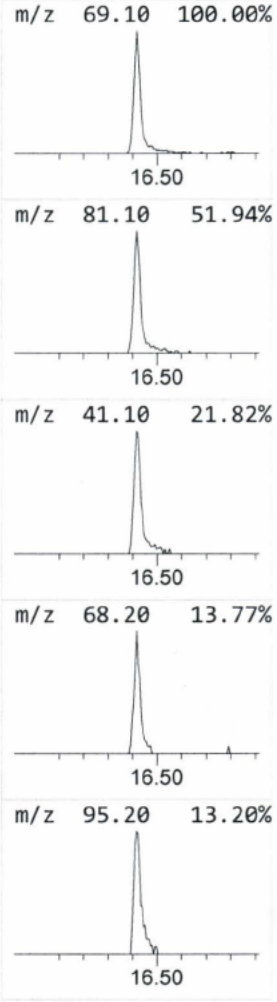
**********

Peak Number 15 Squalene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.416 | 1.71 ug/mL | 141707 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 3 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 4 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 5 | Squalene | 410 | C30H50 | 000111-02-4 | 78 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

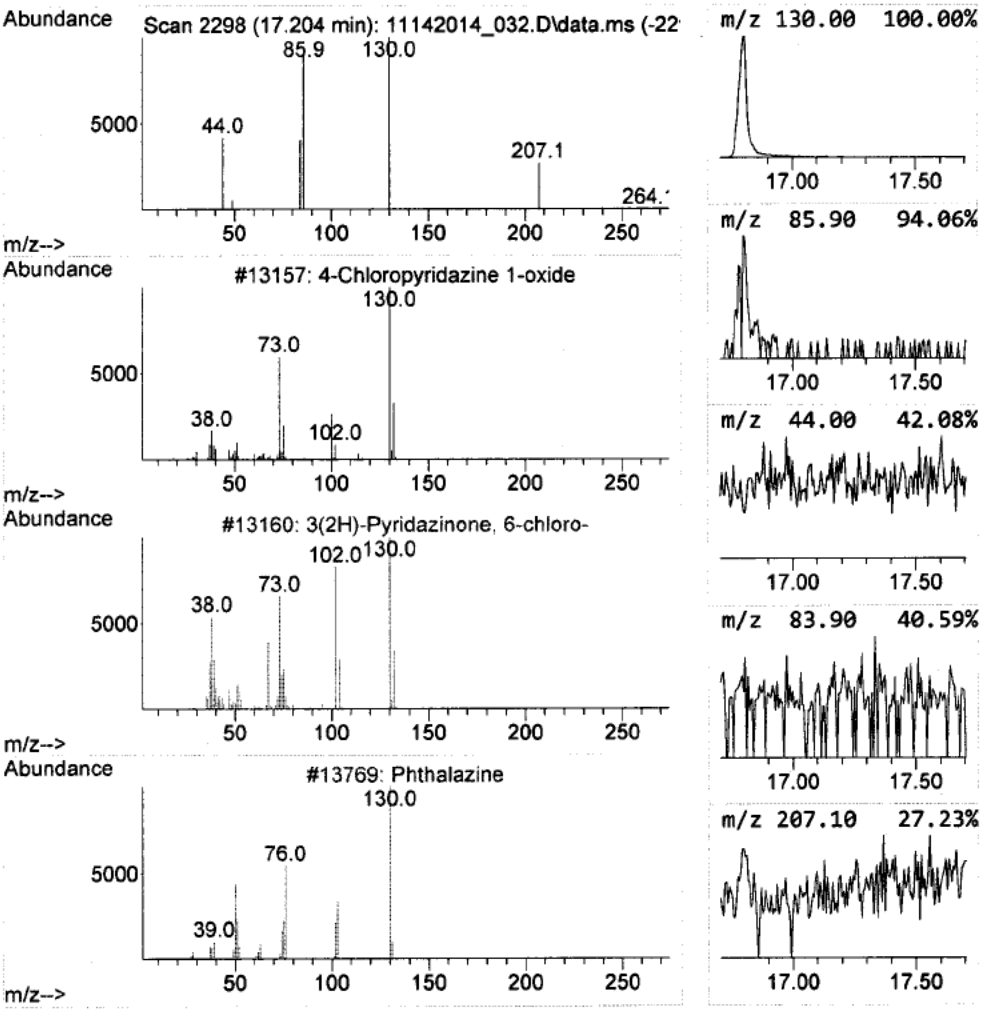
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 16 4-Chloropyridazine 1-oxide Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.204 | 0.05 ug/mL | 3777 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloropyridazine 1-oxide | 130 | C4H3ClN2O | 007217-74-5 | 4 |
| 2 | 3(2H)-Pyridazinone, 6-chloro- | 130 | C4H3ClN2O | 019064-67-6 | 4 |
| 3 | Phthalazine | 130 | C8H6N2 | 000253-52-1 | 4 |
| 4 | Quinazoline | 130 | C8H6N2 | 000253-82-7 | 4 |
| 5 | 2-Propanamine, N-(1-methylethyl)... | 130 | C6H14N2O | 000601-77-4 | 4 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

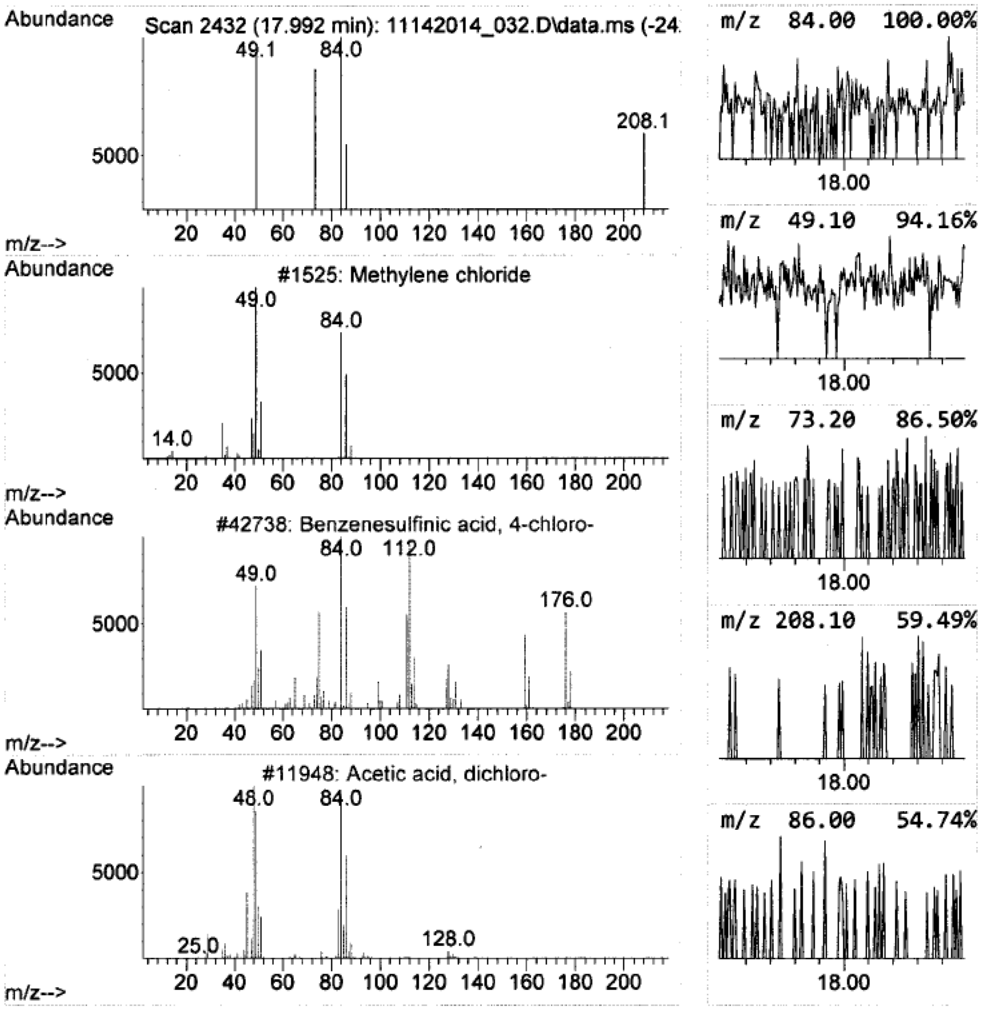
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 17 Methylene chloride Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.992 | 0.04 ug/mL | 3263 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methylene chloride | 84 | CH2Cl2 | 000075-09-2 | 64 |
| 2 | Benzenesulfinic acid, 4-chloro- | 176 | C6H5ClO2S | 000100-03-8 | 9 |
| 3 | Acetic acid, dichloro- | 128 | C2H2Cl2O2 | 000079-43-6 | 9 |
| 4 | Acetic acid, dichloro- | 128 | C2H2Cl2O2 | 000079-43-6 | 9 |
| 5 | Acetic acid, dichloro- | 128 | C2H2Cl2O2 | 000079-43-6 | 9 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

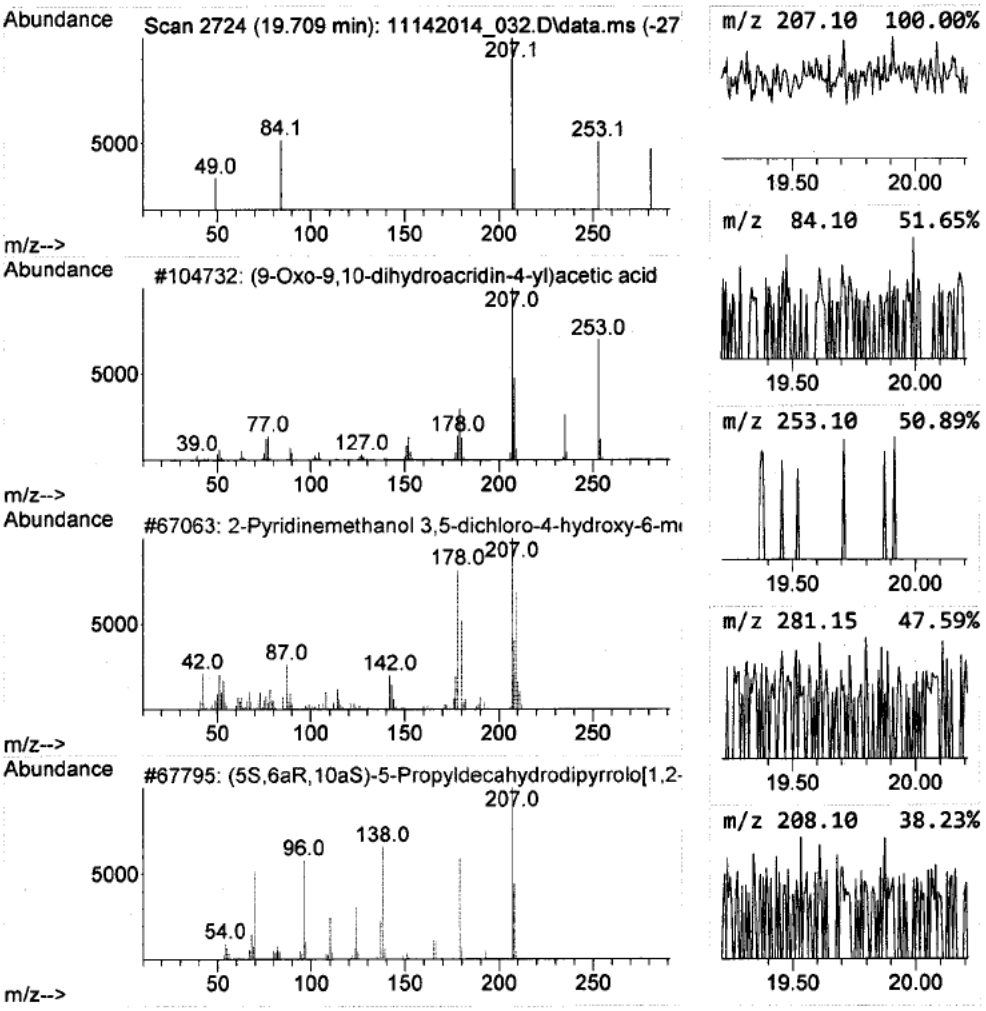
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 18 (9-Oxo-9,10-dihydroacridin-... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.709 | 0.04 ug/mL | 3590 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (9-Oxo-9,10-dihydroacridin-4-yl)... | 253 | C15H11NO3 | 145447-90-1 | 32 |
| 2 | 2-Pyridinemethanol 3,5-dichloro-... | 207 | C7H7Cl2NO2 | 055042-78-9 | 5 |
| 3 | (5S,6aR,10aS)-5-Propyldecahydrod... | 208 | C13H24N2 | 172139-30-9 | 5 |
| 4 | o-(p-Tolyl) 1-azetidinecarbothioate | 207 | C11H13NOS | 010560-24-4 | 5 |
| 5 | 2-(1-Piperidino)-5-nitropyridine | 207 | C10H13N3O2 | 026820-61-1 | 5 |



Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

Quant Method : D:\[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

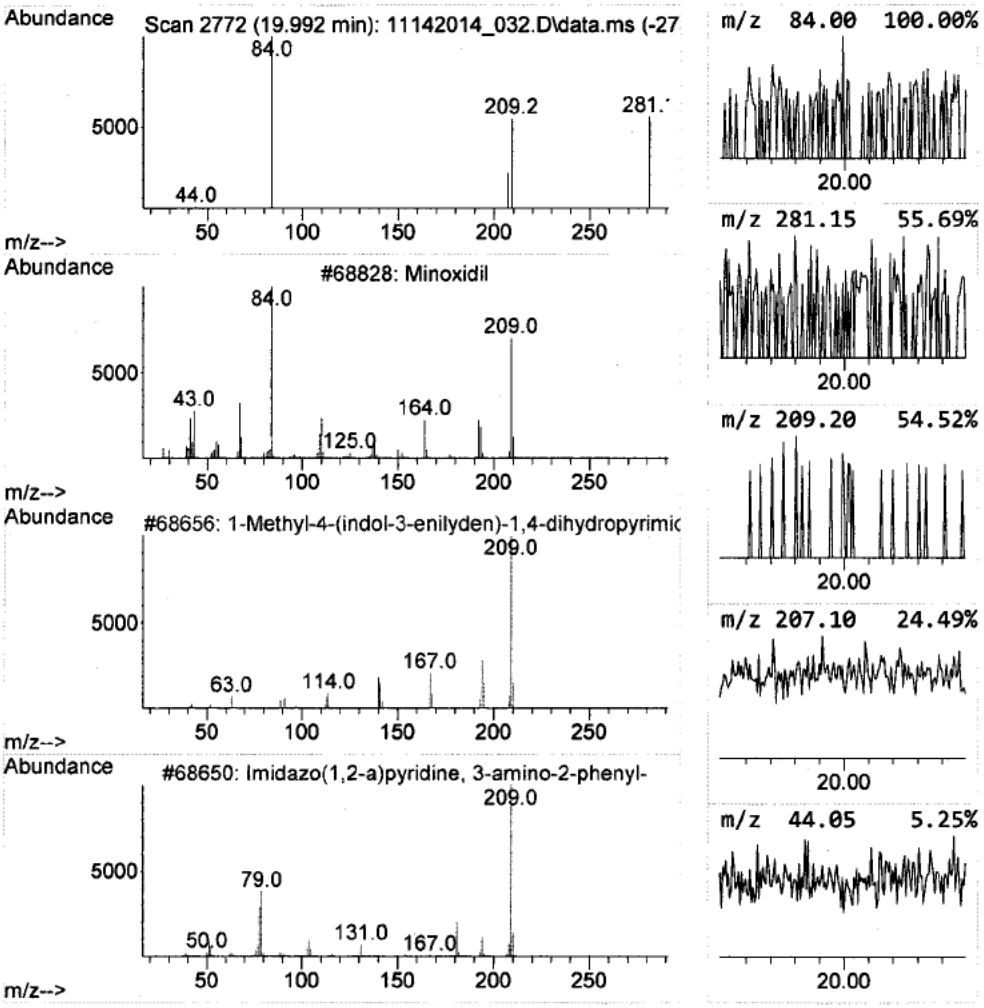
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********

Peak Number 19 Minoxidil Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.992 | 0.05 ug/mL | 4207 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Minoxidil | 209 | C9H15N5O | 038304-91-5 | 9 |
| 2 | 1-Methyl-4-(indol-3-enilyden)-1,... | 209 | C13H11N3 | 077219-01-3 | 4 |
| 3 | Imidazo(1,2-a)pyridine, 3-amino-... | 209 | C13H11N3 | 003999-29-9 | 4 |
| 4 | 1-Azatricyclo[7.3.0.0(2,7)]dodec... | 209 | C12H19NO2 | 111491-60-2 | 4 |
| 5 | Benzo[f]quinolin-1-ol, 3-methyl- | 209 | C14H11NO | 001210-03-3 | 4 |



# Library Search Compound Report

Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

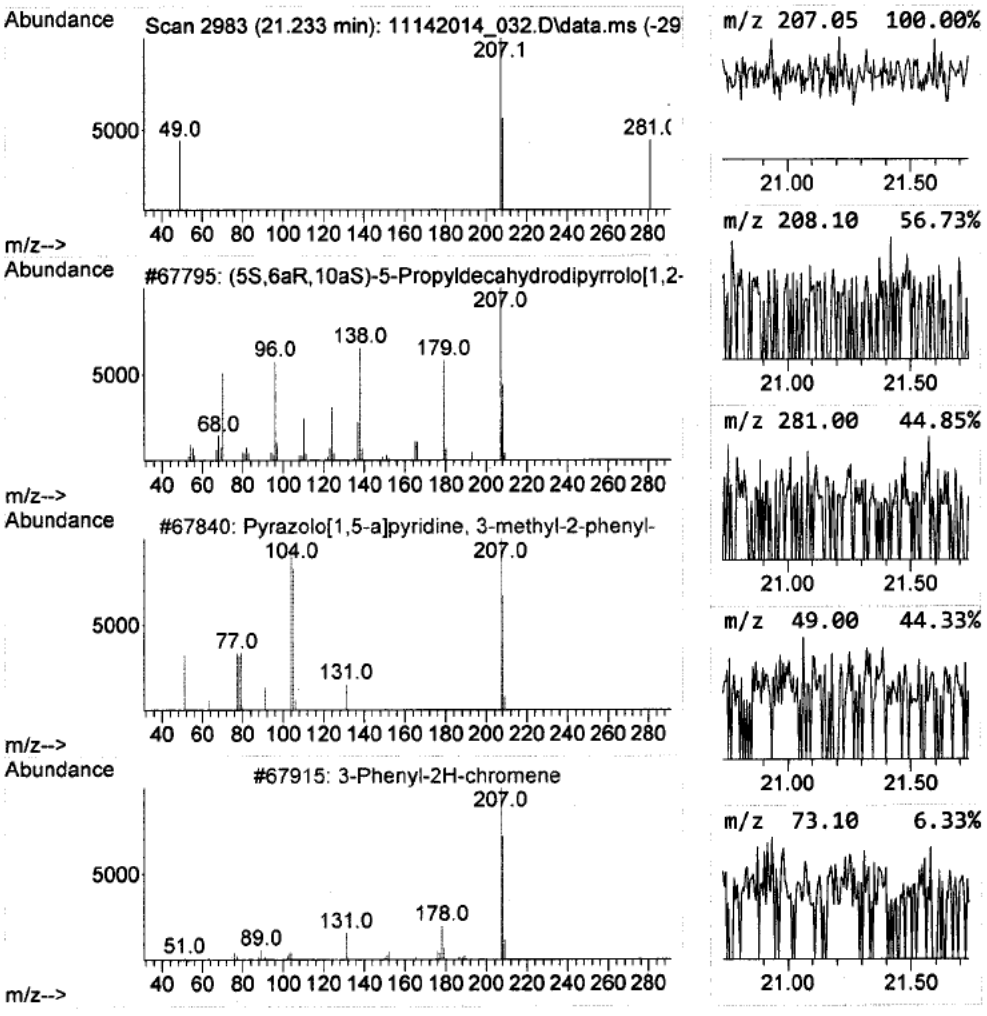
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

**********
Peak Number 20 (5S,6aR,10aS)-5-Propyldecah... Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.233 | 0.04 ug/mL | 3626 | Perylene-d12 | 16.804 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (5S,6aR,10aS)-5-Propyldecahydrod... | 208 | C13H24N2 | 172139-30-9 | 5 |
| 2 | Pyrazolo[1,5-a]pyridine, 3-methy... | 208 | C14H12N2 | 017408-32-1 | 5 |
| 3 | 3-Phenyl-2H-chromene | 208 | C15H12O | 006054-00-8 | 5 |
| 4 | Imidazo[5,4-e][1,4]diazepine-4,7... | 208 | C9H12N4O2 | 144105-22-6 | 3 |
| 5 | 1,2-Dimethoxy-4-(1-methoxy-1-pro... | 208 | C12H16O3 | 1000313-34-3 | 3 |



Tentatively Identified Compound (LSC) summary

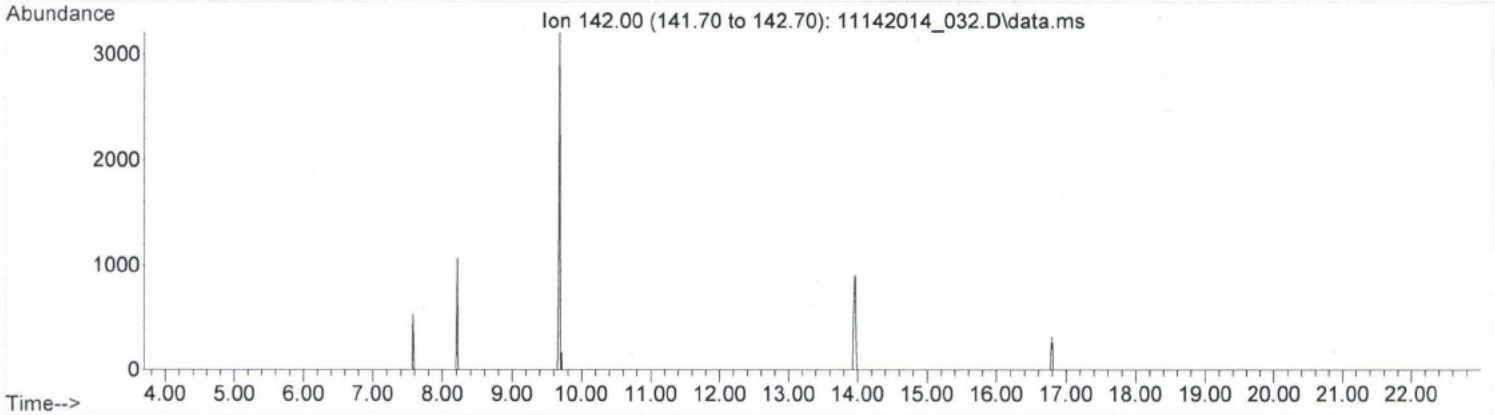
Data Path : D:\[redacted]\RP1616\11142014_Run\
Data File : 11142014_032.D
Acq On : 15 Nov 2014 01:00 am
Operator : [redacted]
Sample : NE36687
Misc : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
ALS Vial : 30 Sample Multiplier: 1

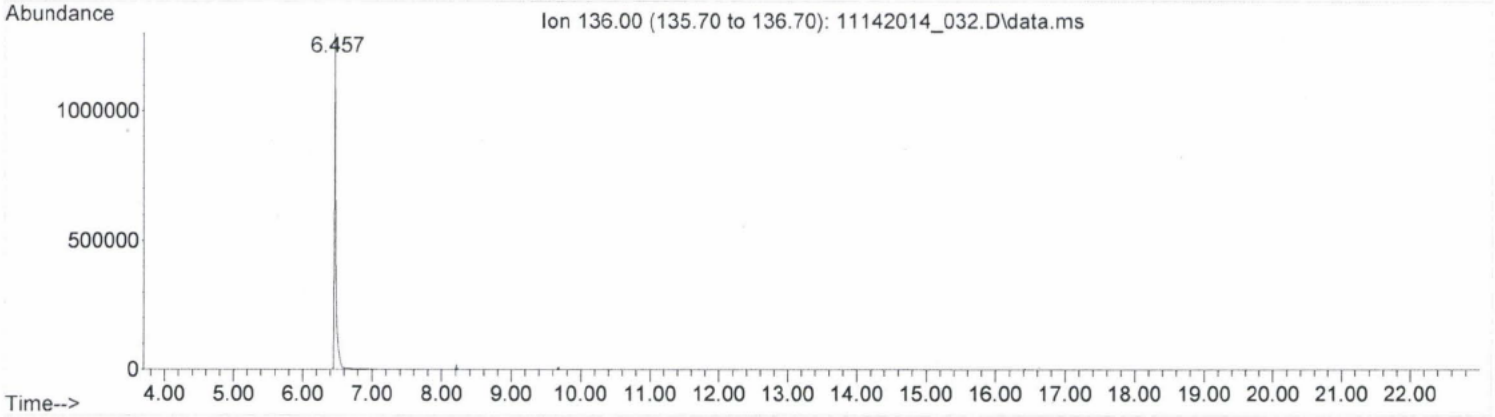
Quant Method : D:[redacted]\GCMS\1\methods\RP1616[redacted]b.M
Quant Title : RP1616-MCHM Compounds

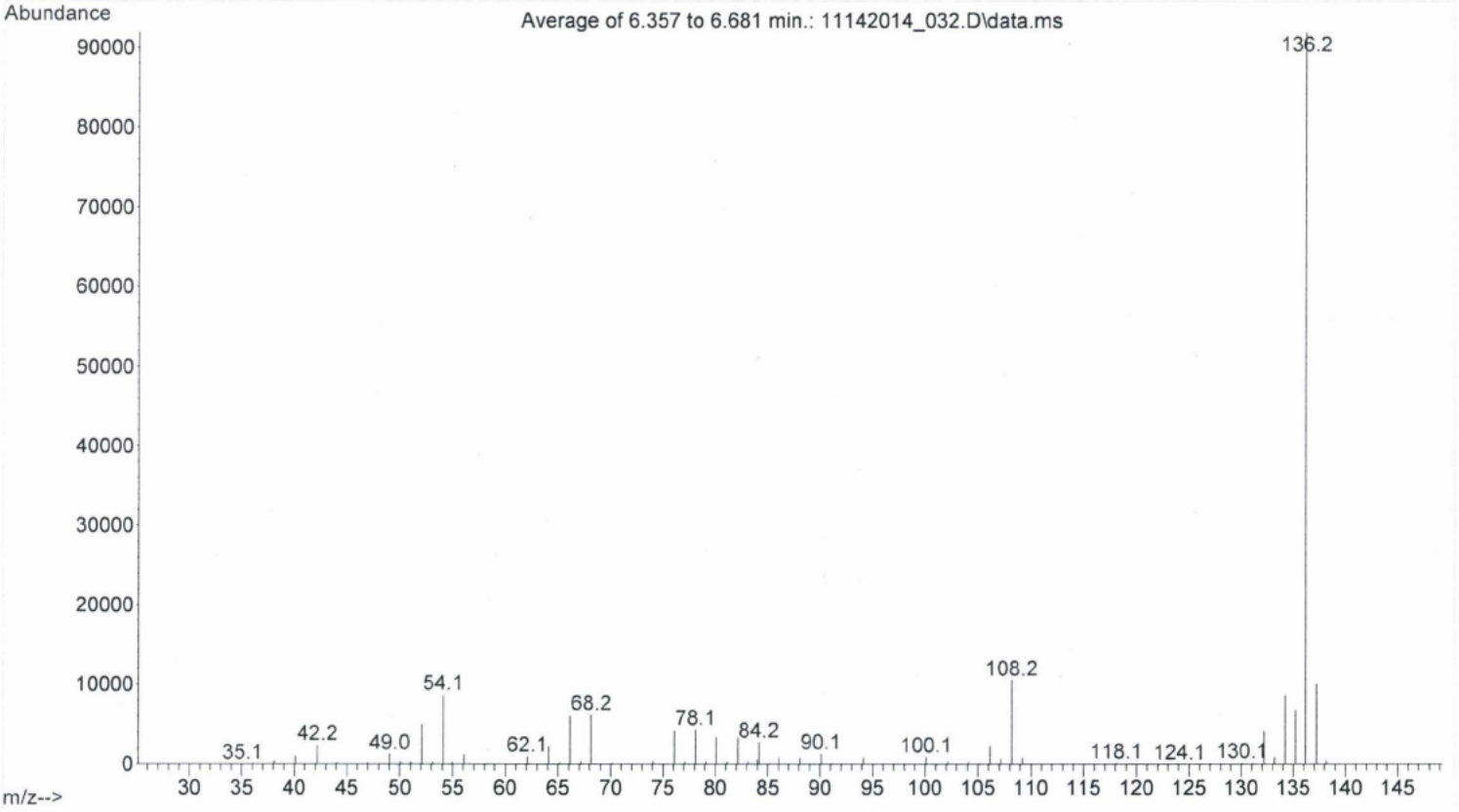
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: RP1616.P

| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| Krypton | 3.999 | 0.0 | ug/mL | 4449 | 1 | 5.081 | 3091750 | 20.0 |
| 3-Amino-s-triazole | 4.216 | 0.1 | ug/mL | 8276 | 1 | 5.081 | 3091750 | 20.0 |
| Methan-d3-ol | 4.528 | 0.0 | ug/mL | 7216 | 1 | 5.081 | 3091750 | 20.0 |
| Octasiloxane, 1... | 7.287 | 0.0 | ug/mL | 8883 | 2 | 6.457 | 4005740 | 20.0 |
| 1,1'-Biphenyl,3... | 7.493 | 0.2 | ug/mL | 41369 | 3 | 8.210 | 4346890 | 20.0 |
| 2-(3-Thienyl)py... | 8.445 | 0.0 | ug/mL | 5991 | 3 | 8.210 | 4346890 | 20.0 |
| 5,8-Dimethoxy-6... | 8.516 | 0.1 | ug/mL | 11213 | 3 | 8.210 | 4346890 | 20.0 |
| 4-Bromo-3,5-dim... | 8.704 | 0.1 | ug/mL | 14941 | 3 | 8.210 | 4346890 | 20.0 |
| 3-Methylthio-1-... | 9.534 | 0.1 | ug/mL | 28896 | 4 | 9.681 | 4081510 | 20.0 |
| 4-Pyrimidinamin... | 9.975 | 0.1 | ug/mL | 15467 | 4 | 9.681 | 4081510 | 20.0 |
| Furo[3,2-b]pyri... | 10.057 | 0.0 | ug/mL | 9101 | 4 | 9.681 | 4081510 | 20.0 |
| Difluorochlorom... | 13.475 | 0.0 | ug/mL | 3783 | 5 | 13.963 | 2625270 | 20.0 |
| 1-Propyne, 3-br... | 14.257 | 0.0 | ug/mL | 6004 | 5 | 13.963 | 2625270 | 20.0 |
| Benzo[f][1,4]ox... | 14.316 | 0.1 | ug/mL | 7501 | 5 | 13.963 | 2625270 | 20.0 |
| Squalene | 16.416 | 1.7 | ug/mL | 141707 | 6 | 16.804 | 1658100 | 20.0 |
| 4-Chloropyridaz... | 17.204 | 0.0 | ug/mL | 3777 | 6 | 16.804 | 1658100 | 20.0 |
| Methylene chloride | 17.992 | 0.0 | ug/mL | 3263 | 6 | 16.804 | 1658100 | 20.0 |
| (9-Oxo-9,10-dih... | 19.709 | 0.0 | ug/mL | 3590 | 6 | 16.804 | 1658100 | 20.0 |
| Minoxidil | 19.992 | 0.1 | ug/mL | 4207 | 6 | 16.804 | 1658100 | 20.0 |
| (5S,6aR,10aS)-5... | 21.233 | 0.0 | ug/mL | 3626 | 6 | 16.804 | 1658100 | 20.0 |

File :D:[redacted]\RP1616\11142014_Run\11142014_032.D
Operator : [redacted]
Acquired : 15 Nov 2014 01:00 am using AcqMethod RP1616[redacted].M
Instrument : EnvQnt
Sample Name: NE36687
Misc Info : Tag # NE36687, 450 uL ext + 50 uL of CH2Cl2
Vial Number: 30




[redacted] RP1616 12/17/14