LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

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-BF031115.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 | 1.047 | 10 | 14 | 16 | rVB2 | 19898 | 34782 | 1.72% | 0.276% |
| 2 | 1.310 | 34 | 37 | 39 | rBV | 64367 | 63821 | 3.16% | 0.507% |
| 3 | 1.401 | 42 | 45 | 48 | rVB | 184654 | 339037 | 16.80% | 2.692% |
| 4 | 1.573 | 57 | 60 | 63 | rVB | 212956 | 276563 | 13.71% | 2.196% |
| 5 | 1.664 | 66 | 68 | 75 | rVB2 | 22312 | 42369 | 2.10% | 0.336% |
| 6 | 1.767 | 75 | 77 | 85 | rBV | 96335 | 135595 | 6.72% | 1.076% |
| 7 | 1.893 | 85 | 88 | 91 | rVB | 16754 | 24169 | 1.20% | 0.192% |
| 8 | 2.361 | 126 | 129 | 133 | rBV | 210983 | 346436 | 17.17% | 2.750% |
| 9 | 4.190 | 287 | 289 | 294 | rVB2 | 16893 | 26431 | 1.31% | 0.210% |
| 10 | 4.876 | 347 | 349 | 352 | rBV | 42749 | 63628 | 3.15% | 0.505% |
| 11 | 4.944 | 352 | 355 | 362 | rVB | 9825 | 23869 | 1.18% | 0.189% |
| 12 | 5.413 | 394 | 396 | 399 | rBV | 546879 | 568506 | 28.18% | 4.513% |
| 13 | 6.567 | 495 | 497 | 500 | rBV | 23959 | 34193 | 1.69% | 0.271% |
| 14 | 6.704 | 507 | 509 | 511 | rBV | 361216 | 355129 | 17.60% | 2.819% |
| 15 | 6.842 | 518 | 521 | 523 | rBV | 1101702 | 1101525 | 54.59% | 8.745% |
| 16 | 7.127 | 543 | 546 | 548 | rBV | 273767 | 258711 | 12.82% | 2.054% |
| 17 | 7.310 | 560 | 562 | 565 | rVB | 1123392 | 1012743 | 50.19% | 8.040% |
| 18 | 7.825 | 604 | 607 | 609 | rBV | 773887 | 815838 | 40.43% | 6.477% |
| 19 | 8.396 | 653 | 657 | 664 | rBV3 | 36994 | 72040 | 3.57% | 0.572% |
| 20 | 8.705 | 681 | 684 | 686 | rVB | 341828 | 352021 | 17.45% | 2.795% |
| 21 | 10.053 | 799 | 802 | 804 | rBV | 1849632 | 1739032 | 86.19% | 13.806% |
| 22 | 10.876 | 872 | 874 | 876 | rVB | 317911 | 413810 | 20.51% | 3.285% |
| 23 | 11.848 | 957 | 959 | 962 | rBV | 952799 | 1002023 | 49.66% | 7.955% |
| 24 | 12.705 | 1032 | 1034 | 1037 | rBV | 450057 | 438830 | 21.75% | 3.484% |
| 25 | 14.705 | 1206 | 1209 | 1211 | rBV | 2059693 | 2017766 | 100.00% | 16.018% |
| 26 | 15.882 | 1309 | 1312 | 1317 | rBV2 | 37870 | 58495 | 2.90% | 0.464% |
| 27 | 15.985 | 1319 | 1321 | 1324 | rBV | 405081 | 493189 | 24.44% | 3.915% |
| 28 | 17.746 | 1472 | 1475 | 1478 | rBV | 431181 | 485948 | 24.08% | 3.858% |

Sum of corrected areas: 12596499

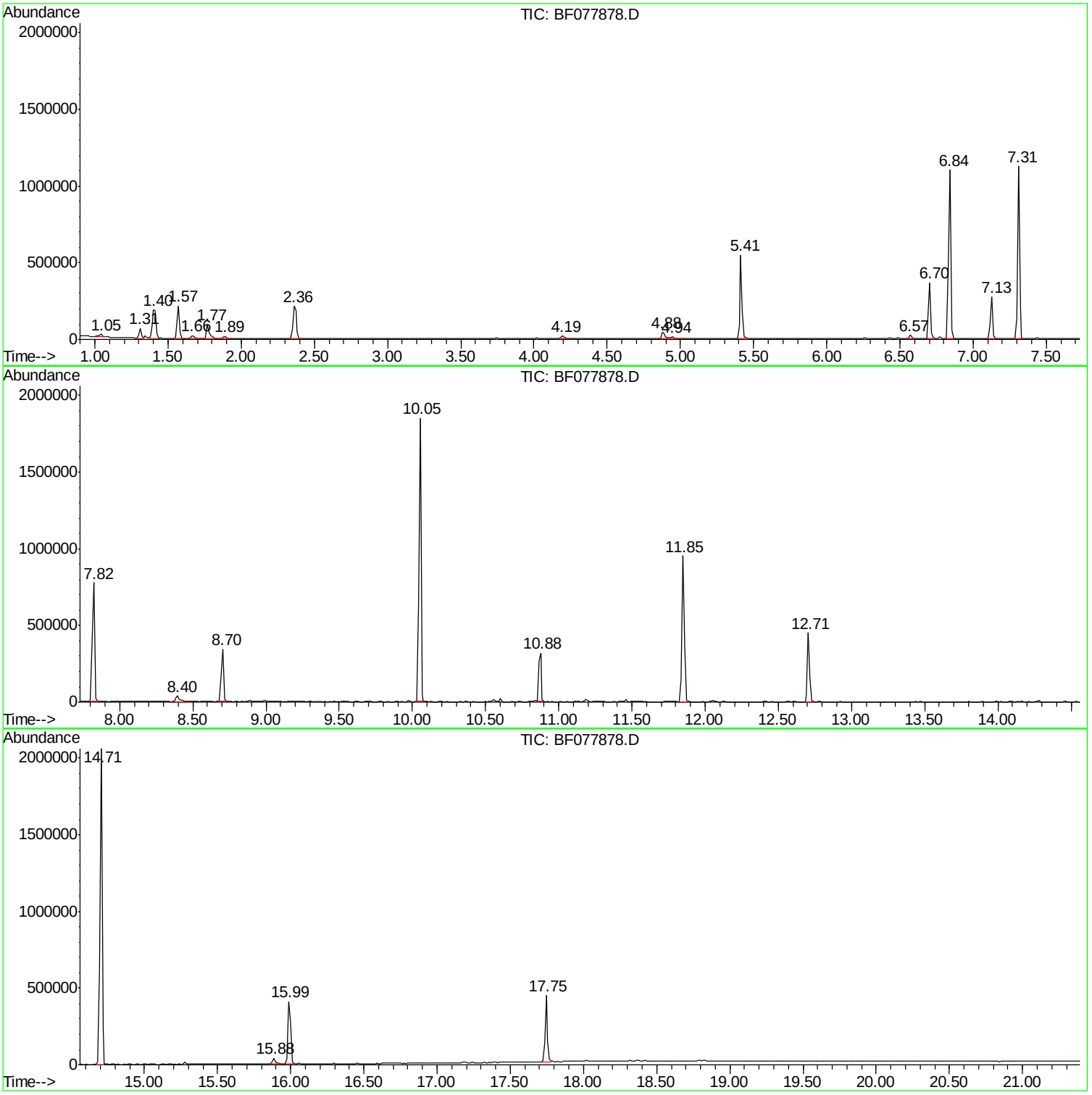
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

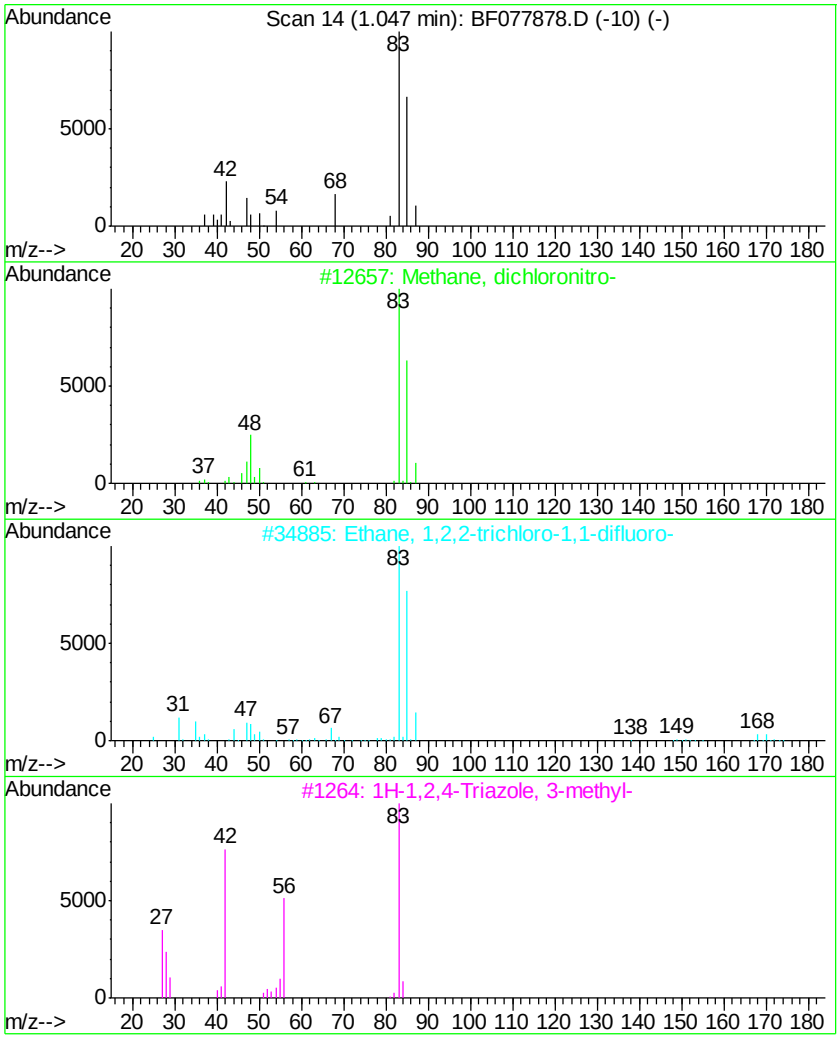
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

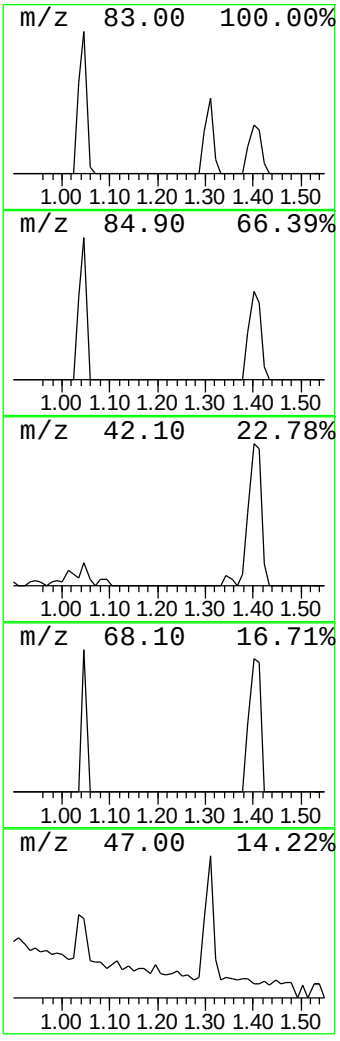
**********

Peak Number 1 unknown1.05 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.05 | 2.69 ng | 34782 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methane, dichloronitro- | 129 | CHCl2NO2 | 007119-89-3 | 38 |
| 2 | Ethane, 1,2,2-trichloro-1,1-difl... | 168 | C2HCl3F2 | 000354-21-2 | 36 |
| 3 | 1H-1,2,4-Triazole, 3-methyl- | 83 | C3H5N3 | 007170-01-6 | 5 |
| 4 | 2-Pyrrolidinone | 85 | C4H7NO | 000616-45-5 | 5 |
| 5 | Phosphoramidous difluoride | 85 | F2H2NP | 025757-74-8 | 5 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

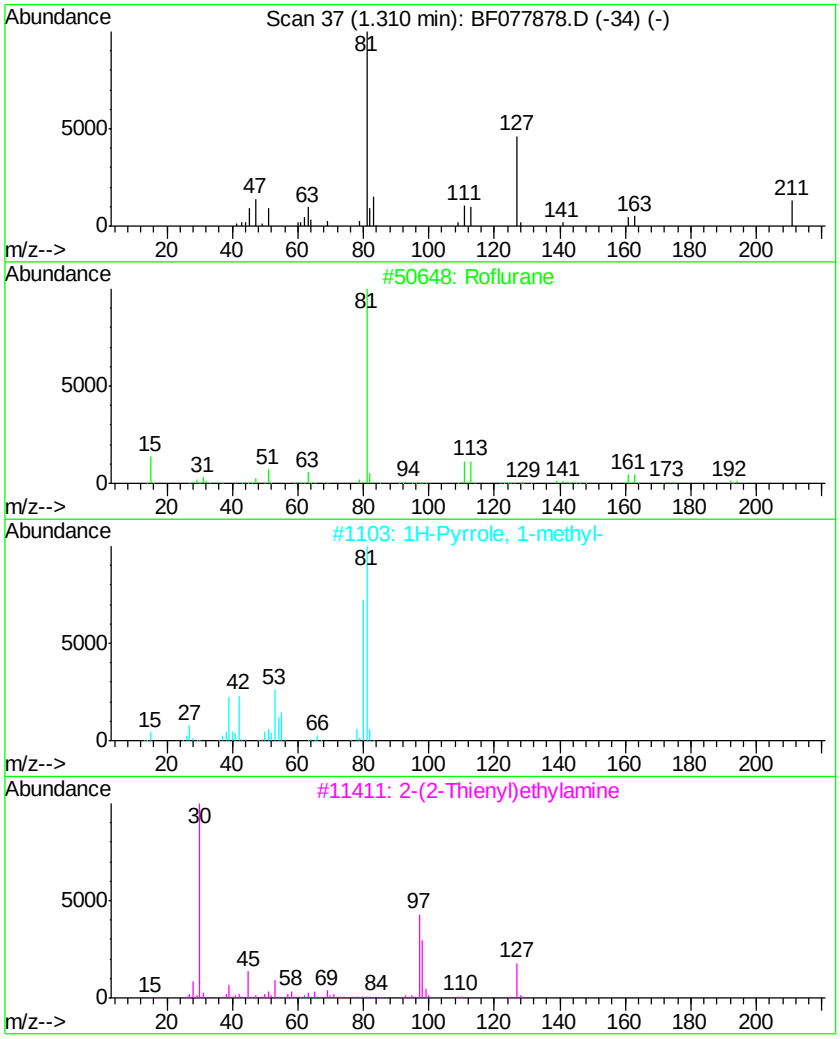
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

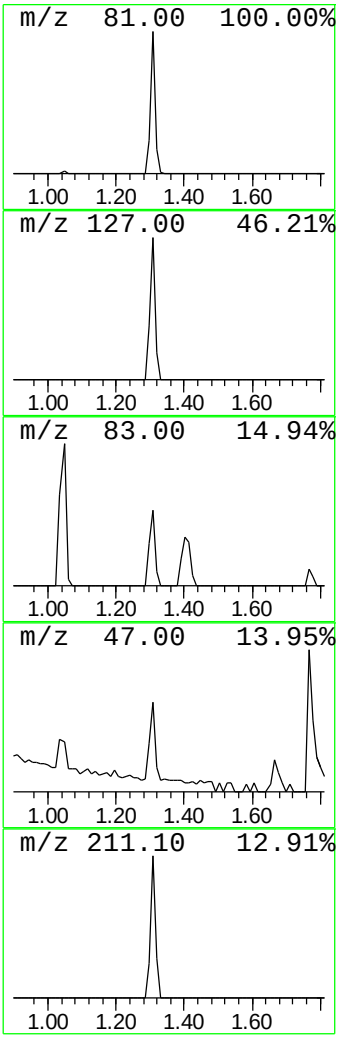
**********

Peak Number 2 Roflurane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.31 | 4.93 ng | 63821 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Roflurane | 192 | C3H4BrF3O | 000679-90-3 | 50 |
| 2 | 1H-Pyrrole, 1-methyl- | 81 | C5H7N | 000096-54-8 | 5 |
| 3 | 2-(2-Thienyl)ethylamine | 127 | C6H9NS | 030433-91-1 | 4 |
| 4 | 2,4-Decadienal, (E,E)- | 152 | C10H16O | 025152-84-5 | 4 |
| 5 | 2,4-Heptadienal, (E,E)- | 110 | C7H10O | 004313-03-5 | 4 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

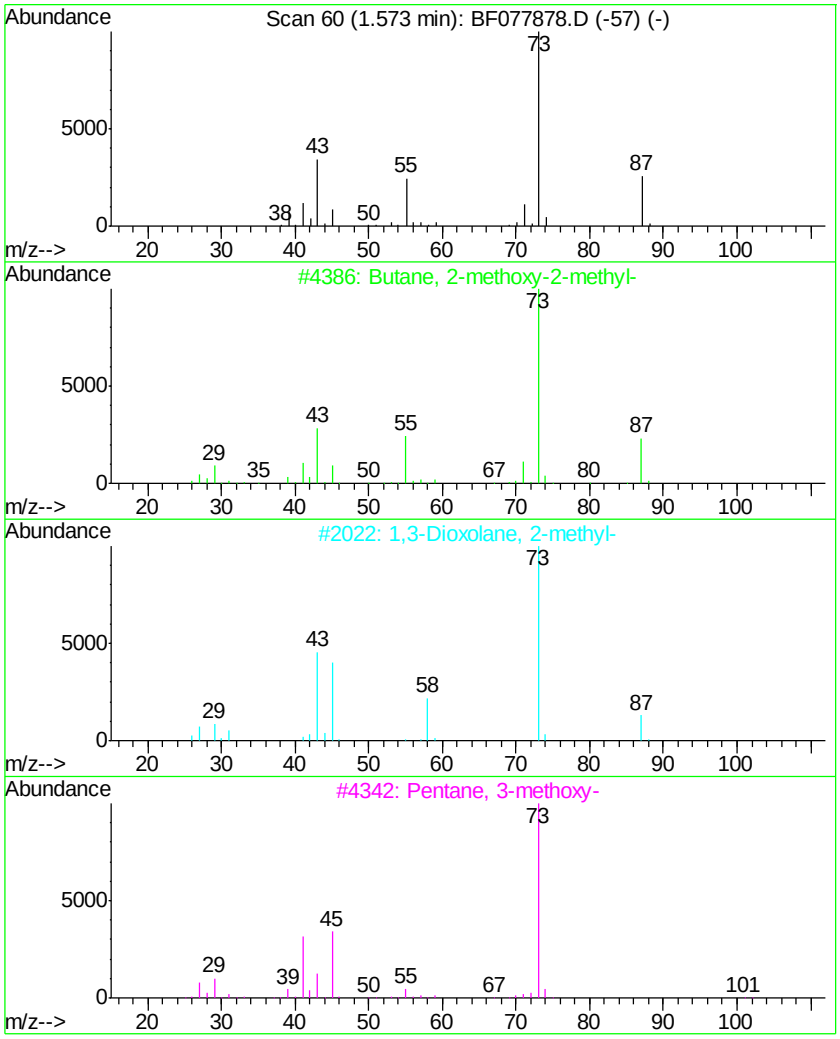
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

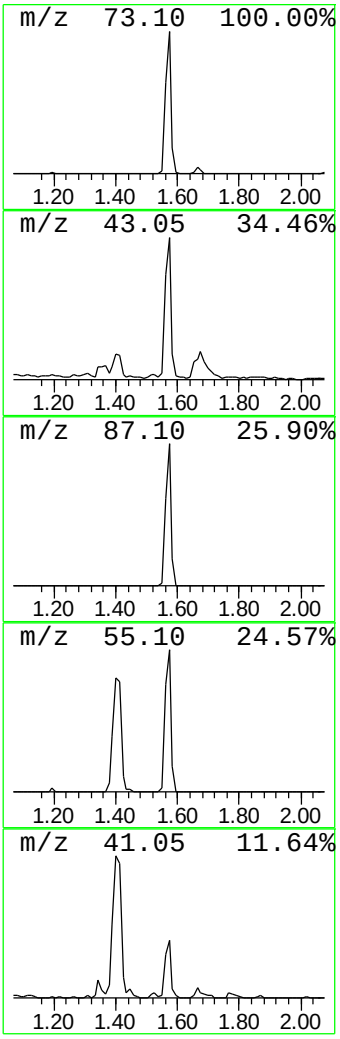
**********

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.57 | 21.38 ng | 276563 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 37 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 10 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

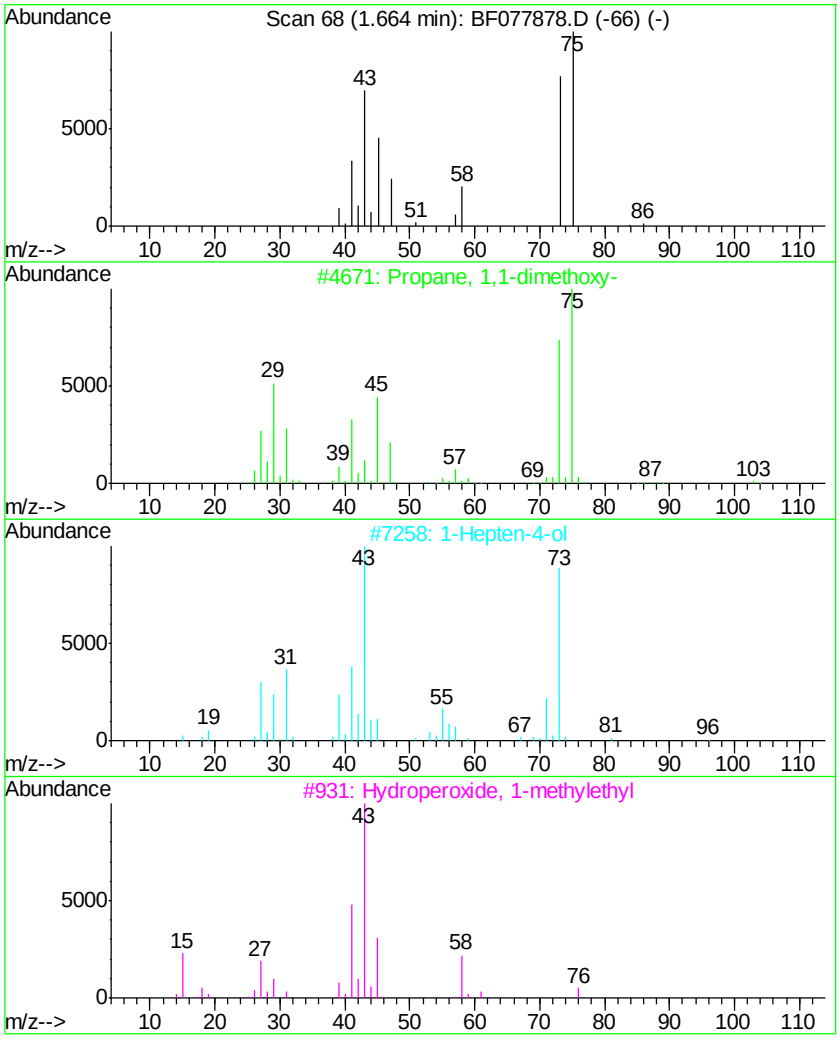
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

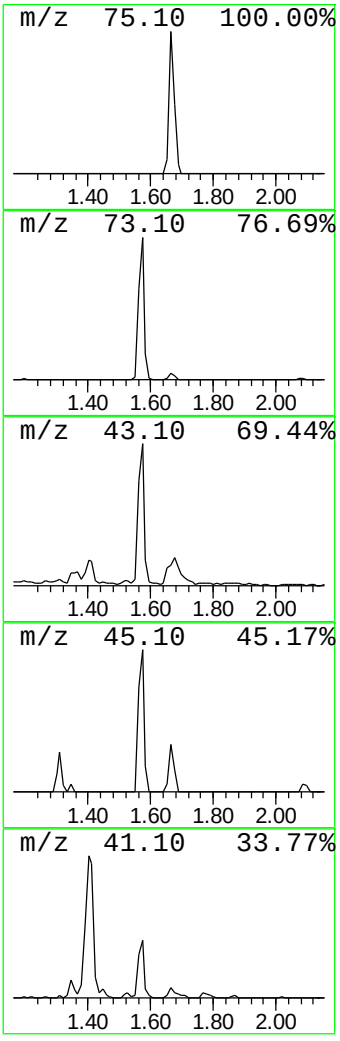
**********

Peak Number 5 unknown1.66 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.66 | 3.28 ng | 42369 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 45 |
| 2 | 1-Hepten-4-ol | 114 | C7H14O | 003521-91-3 | 9 |
| 3 | Hydroperoxide, 1-methylethyl | 76 | C3H8O2 | 003031-75-2 | 8 |
| 4 | Oxirane, trimethyl- | 86 | C5H10O | 005076-19-7 | 8 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 7 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

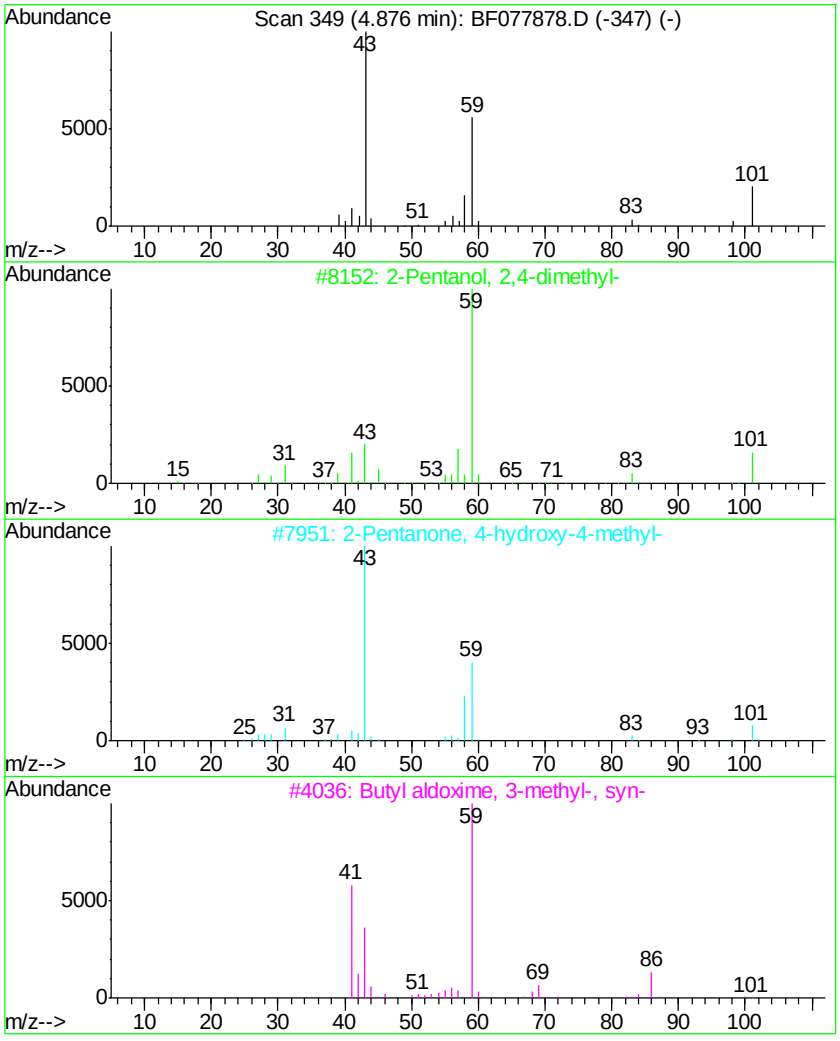
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

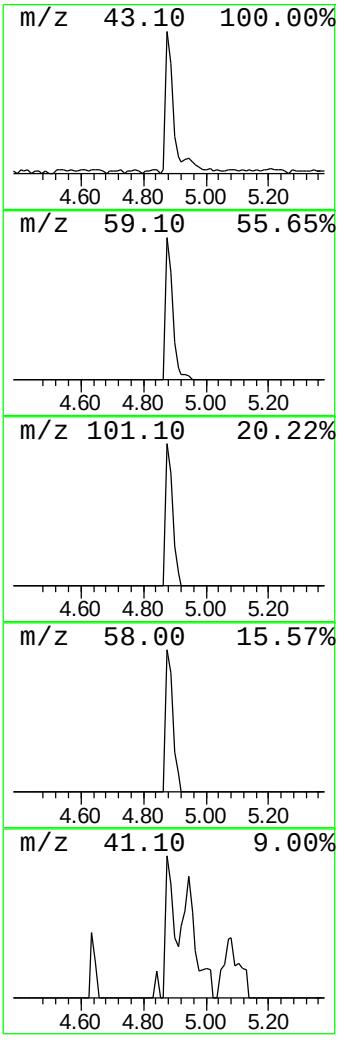
**********

Peak Number 9 unknown4.88 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.88 | 4.92 ng | 63628 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 42 |
| 2 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 3 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 17 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Propylamine | 59 | C3H9N | 000107-10-8 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

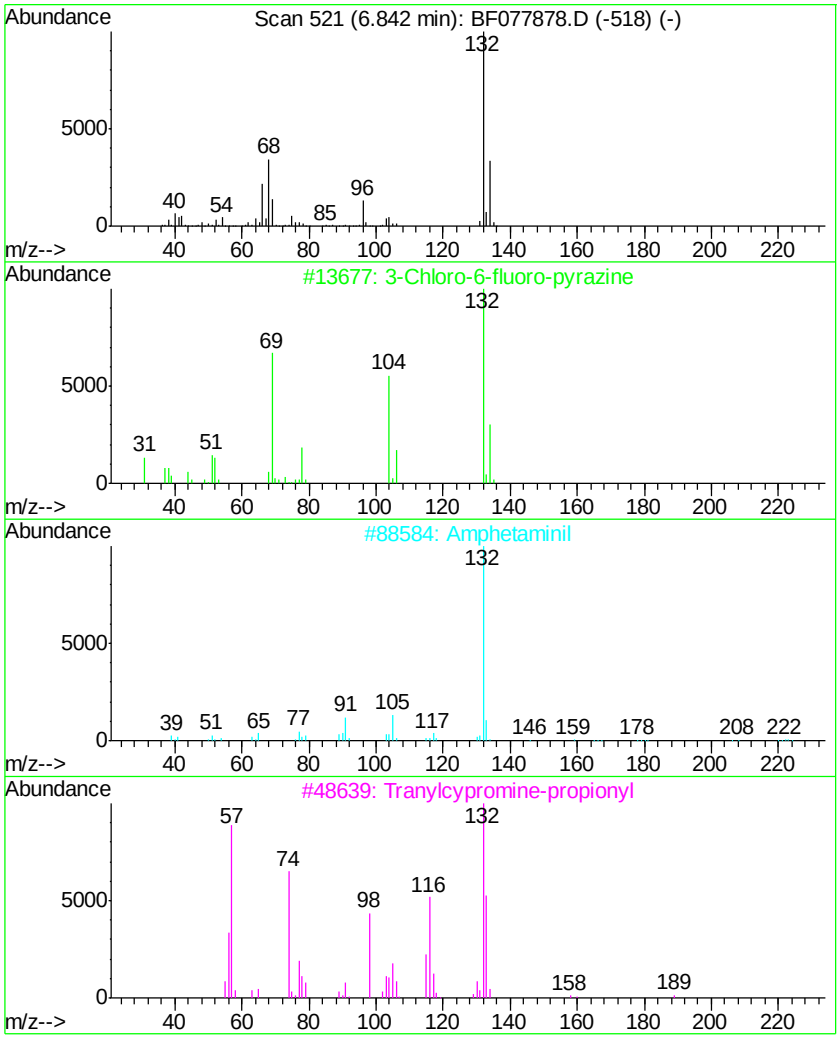
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

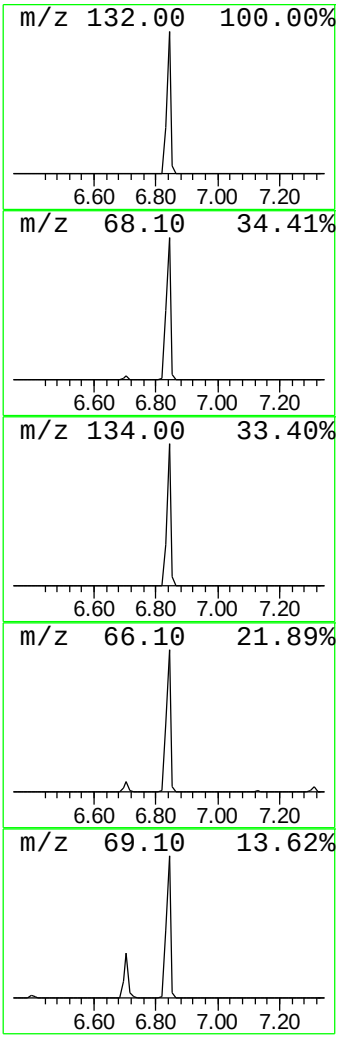
**********

Peak Number 10 unknown6.84 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.84 | 85.15 ng | 1101530 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 2 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

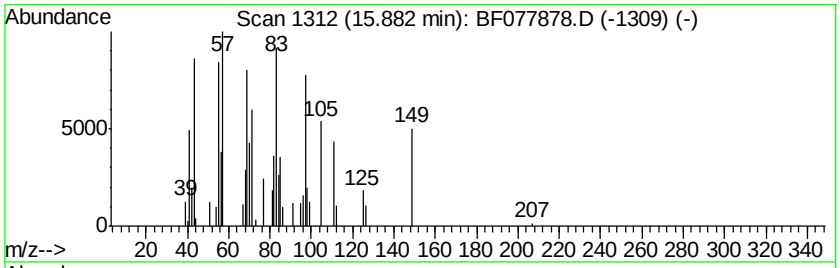
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

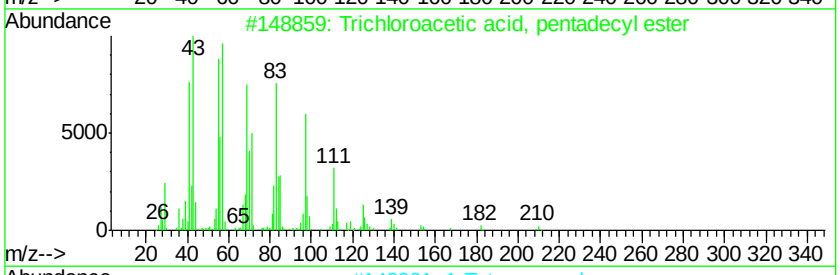
**********

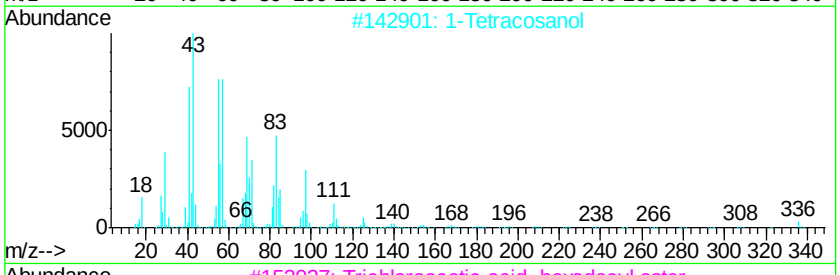
Peak Number 12 Trichloroacetic acid, penta... Concentration Rank 11

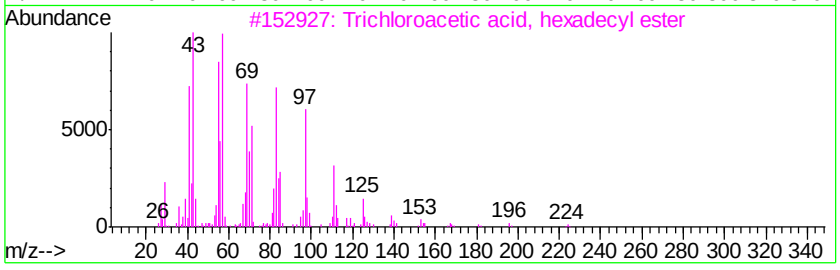
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.88 | 2.37 ng | 58495 | Chrysene-d12 | 15.99 |

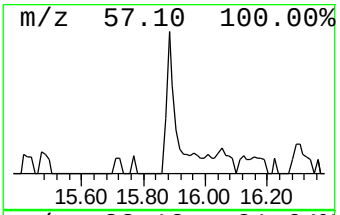
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 90 |
| 2 | 1-Tetracosanol | 354 | C24H50O | 000506-51-4 | 87 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 87 |
| 4 | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 87 |
| 5 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 87 |

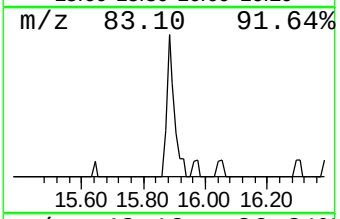


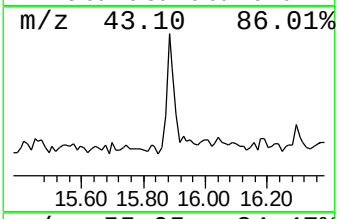



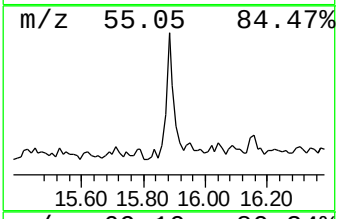



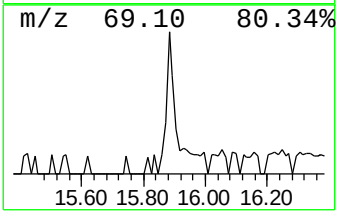



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032015\
Data File : BF077878.D
Acq On : 20 Mar 2015 22:20
Operator : TP/IZ
Sample : G1575-05
Misc : W
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-8S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown1.05 | 1.05 | 2.7 | ng | 34782 | 1 | 7.13 | 258711 | 20.0 |
| Roflurane | 1.31 | 4.9 | ng | 63821 | 1 | 7.13 | 258711 | 20.0 |
| Butane, 2-methoxy... | 1.57 | 21.4 | ng | 276563 | 1 | 7.13 | 258711 | 20.0 |
| unknown1.66 | 1.66 | 3.3 | ng | 42369 | 1 | 7.13 | 258711 | 20.0 |
| unknown4.88 | 4.88 | 4.9 | ng | 63628 | 1 | 7.13 | 258711 | 20.0 |
| unknown6.84 | 6.84 | 85.2 | ng | 1101530 | 1 | 7.13 | 258711 | 20.0 |
| Trichloroacetic a... | 15.88 | 2.4 | ng | 58495 | 5 | 15.99 | 493189 | 20.0 |