LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088980.D
Acq On : 14 Jul 2016 2:03
Operator : UM/SJ
Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Q7-B1(0-5)C

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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 | 1.667 | 5 | 7 | 13 | rVV | 150008 | 214942 | 12.13% | 1.218% |
| 2 | 1.781 | 16 | 17 | 26 | rVV | 1007928 | 1673839 | 94.47% | 9.486% |
| 3 | 1.895 | 26 | 27 | 60 | rVB | 66027 | 277265 | 15.65% | 1.571% |
| 4 | 4.844 | 282 | 285 | 291 | rBB | 208861 | 335250 | 18.92% | 1.900% |
| 5 | 5.301 | 322 | 325 | 327 | rBV | 1141226 | 1555998 | 87.82% | 8.818% |
| 6 | 5.690 | 357 | 359 | 361 | rBB | 27370 | 23247 | 1.31% | 0.132% |
| 7 | 6.342 | 413 | 416 | 419 | rBV | 1035927 | 1552129 | 87.60% | 8.796% |
| 8 | 6.467 | 424 | 427 | 429 | rBV | 1710292 | 1669775 | 94.24% | 9.463% |
| 9 | 6.696 | 445 | 447 | 449 | rBB | 467616 | 425391 | 24.01% | 2.411% |
| 10 | 6.856 | 458 | 461 | 463 | rBB | 1001201 | 1263843 | 71.33% | 7.163% |
| 11 | 7.267 | 493 | 497 | 499 | rBV | 728027 | 1007698 | 56.87% | 5.711% |
| 12 | 7.976 | 557 | 559 | 562 | rBB | 514921 | 497088 | 28.06% | 2.817% |
| 13 | 9.062 | 651 | 654 | 656 | rBV | 1975776 | 1771778 | 100.00% | 10.041% |
| 14 | 9.450 | 686 | 688 | 691 | rBB | 239677 | 224133 | 12.65% | 1.270% |
| 15 | 9.725 | 710 | 712 | 714 | rBV2 | 446522 | 470009 | 26.53% | 2.664% |
| 16 | 10.513 | 779 | 781 | 783 | rBV | 846541 | 761469 | 42.98% | 4.315% |
| 17 | 10.651 | 791 | 793 | 796 | rVB | 18518 | 28208 | 1.59% | 0.160% |
| 18 | 11.096 | 830 | 832 | 833 | rBV | 25150 | 30372 | 1.71% | 0.172% |
| 19 | 11.199 | 839 | 841 | 845 | rVB | 355742 | 418875 | 23.64% | 2.374% |
| 20 | 11.279 | 845 | 848 | 850 | rBV | 19537 | 22258 | 1.26% | 0.126% |
| 21 | 11.519 | 866 | 869 | 876 | rVB | 19491 | 23429 | 1.32% | 0.133% |
| 22 | 11.816 | 893 | 895 | 899 | rVB | 13806 | 22079 | 1.25% | 0.125% |
| 23 | 12.411 | 945 | 947 | 949 | rBV | 140309 | 134655 | 7.60% | 0.763% |
| 24 | 12.628 | 964 | 966 | 968 | rBV | 99702 | 129384 | 7.30% | 0.733% |
| 25 | 12.788 | 978 | 980 | 982 | rVB | 1230614 | 1061392 | 59.91% | 6.015% |
| 26 | 12.856 | 982 | 986 | 990 | rVB3 | 10505 | 21197 | 1.20% | 0.120% |
| 27 | 12.959 | 990 | 995 | 997 | rBV | 20167 | 38921 | 2.20% | 0.221% |
| 28 | 13.062 | 1003 | 1004 | 1008 | rBV2 | 16466 | 21807 | 1.23% | 0.124% |
| 29 | 13.371 | 1026 | 1031 | 1034 | rBV3 | 9307 | 23493 | 1.33% | 0.133% |
| 30 | 13.462 | 1038 | 1039 | 1044 | rVB | 17212 | 20150 | 1.14% | 0.114% |
| 31 | 13.577 | 1047 | 1049 | 1050 | rBV | 18867 | 25326 | 1.43% | 0.144% |
| 32 | 13.691 | 1056 | 1059 | 1062 | rBV2 | 48853 | 76758 | 4.33% | 0.435% |
| 33 | 13.828 | 1068 | 1071 | 1075 | rBV2 | 475890 | 596441 | 33.66% | 3.380% |
| 34 | 13.931 | 1078 | 1080 | 1082 | rBV2 | 17923 | 22858 | 1.29% | 0.130% |

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Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Q7-B1(0-5)C

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.011 | 1086 | 1087 | 1092 | rBV3 | 10006 | 28915 | 1.63% | 0.164% |
| 36 | 14.217 | 1102 | 1105 | 1106 | rVB | 16058 | 22360 | 1.26% | 0.127% |
| 37 | 14.331 | 1111 | 1115 | 1119 | rVV4 | 26844 | 76311 | 4.31% | 0.432% |
| 38 | 14.537 | 1132 | 1133 | 1136 | rBV3 | 9027 | 18787 | 1.06% | 0.106% |
| 39 | 14.674 | 1143 | 1145 | 1147 | rVB2 | 17871 | 21238 | 1.20% | 0.120% |
| 40 | 14.822 | 1155 | 1158 | 1162 | rBV | 111995 | 207793 | 11.73% | 1.178% |
| 41 | 14.914 | 1164 | 1166 | 1171 | rVB2 | 36735 | 64938 | 3.67% | 0.368% |
| 42 | 15.085 | 1179 | 1181 | 1184 | rVB | 63703 | 77169 | 4.36% | 0.437% |
| 43 | 15.142 | 1184 | 1186 | 1189 | rVV | 70205 | 87968 | 4.96% | 0.499% |
| 44 | 15.200 | 1189 | 1191 | 1198 | rVB | 281936 | 366137 | 20.66% | 2.075% |
| 45 | 15.634 | 1227 | 1229 | 1231 | rBV | 21986 | 36459 | 2.06% | 0.207% |
| 46 | 16.194 | 1276 | 1278 | 1285 | rVB6 | 12094 | 30705 | 1.73% | 0.174% |
| 47 | 16.320 | 1287 | 1289 | 1293 | rVB4 | 11382 | 26349 | 1.49% | 0.149% |
| 48 | 16.480 | 1300 | 1303 | 1306 | rBV2 | 32387 | 62826 | 3.55% | 0.356% |
| 49 | 16.857 | 1333 | 1336 | 1341 | rVB | 22389 | 47304 | 2.67% | 0.268% |
| 50 | 17.063 | 1351 | 1354 | 1359 | rVB4 | 12102 | 28311 | 1.60% | 0.160% |

Sum of corrected areas: 17645027

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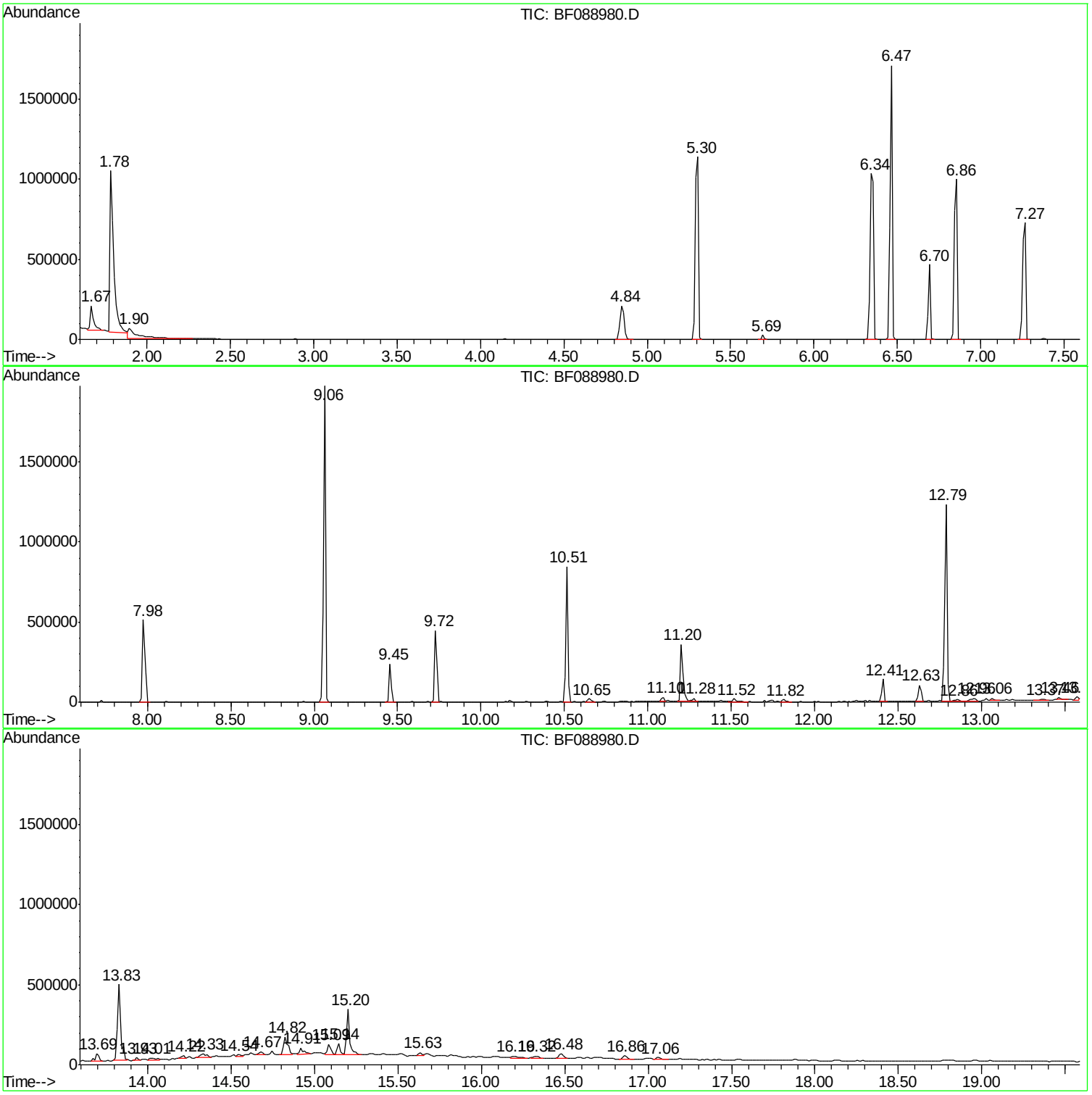
Operator : UM/SJ
Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
Q7-B1(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088980.D
Acq On : 14 Jul 2016 2:03
Operator : UM/SJ
Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Q7-B1(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

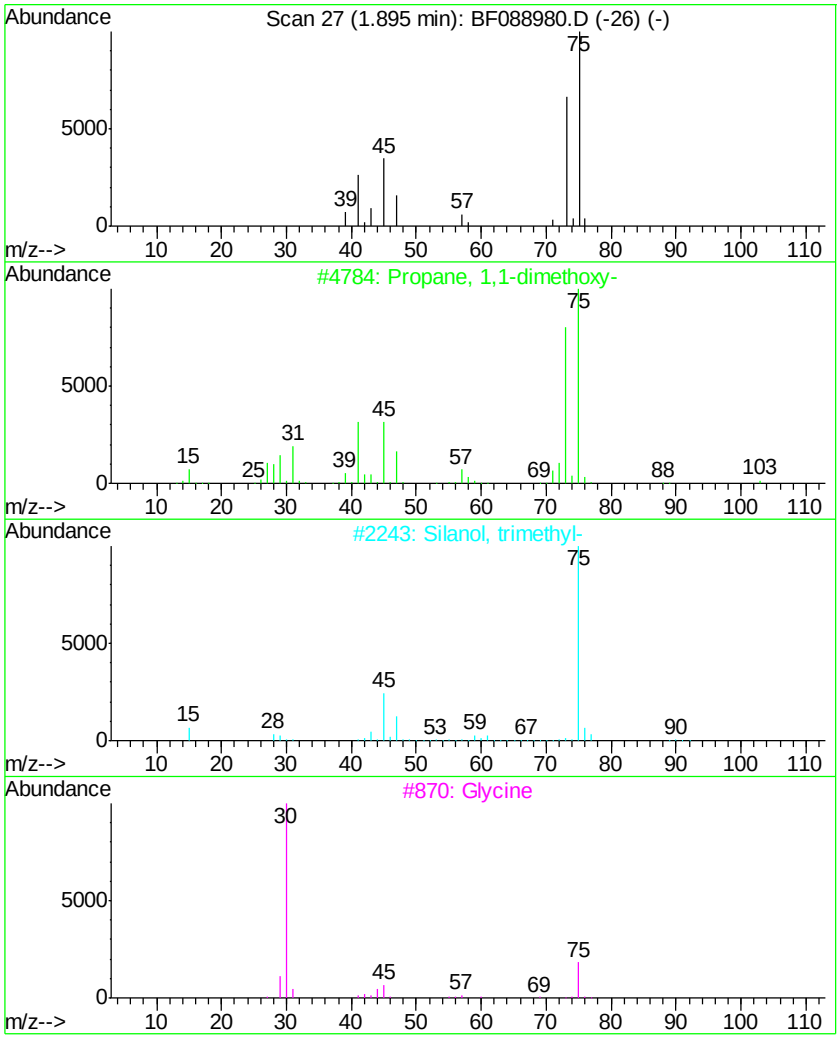
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

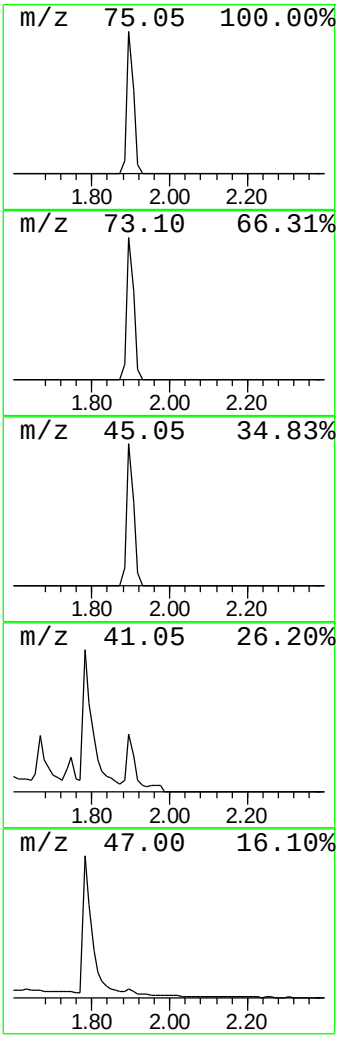
**********

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.90 | 13.04 ng | 277265 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 74 |
| 2 | Silanol, trimethyl- | 90 | C3H10OSi | 001066-40-6 | 9 |
| 3 | Glycine | 75 | C2H5NO2 | 000056-40-6 | 7 |
| 4 | 1-Propene-1-thiol | 74 | C3H6S | 000925-89-3 | 4 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 4 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088980.D
Acq On : 14 Jul 2016 2:03
Operator : UM/SJ
Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Q7-B1(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

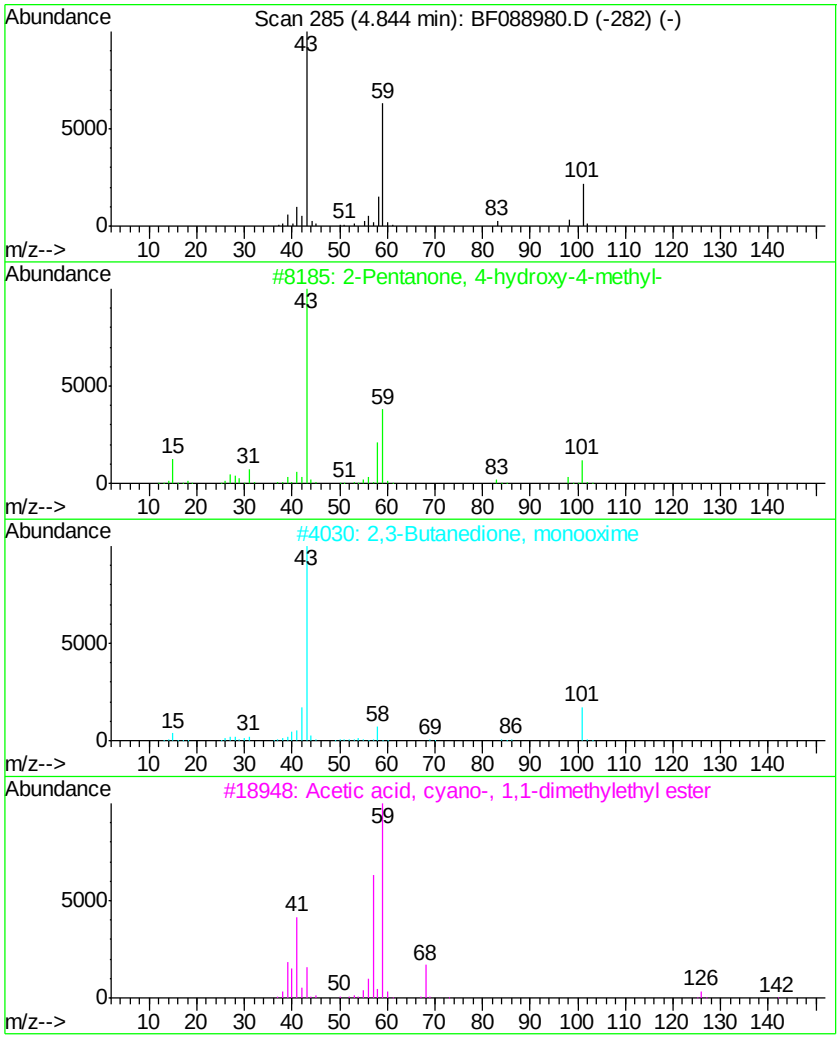
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

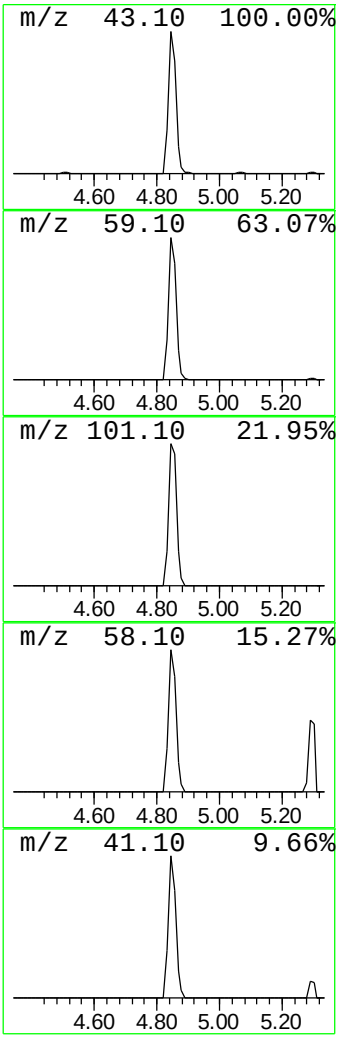
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.84 | 15.76 ng | 335250 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071316\
Data File : BF088980.D
Acq On : 14 Jul 2016 2:03
Operator : UM/SJ
Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Q7-B1(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

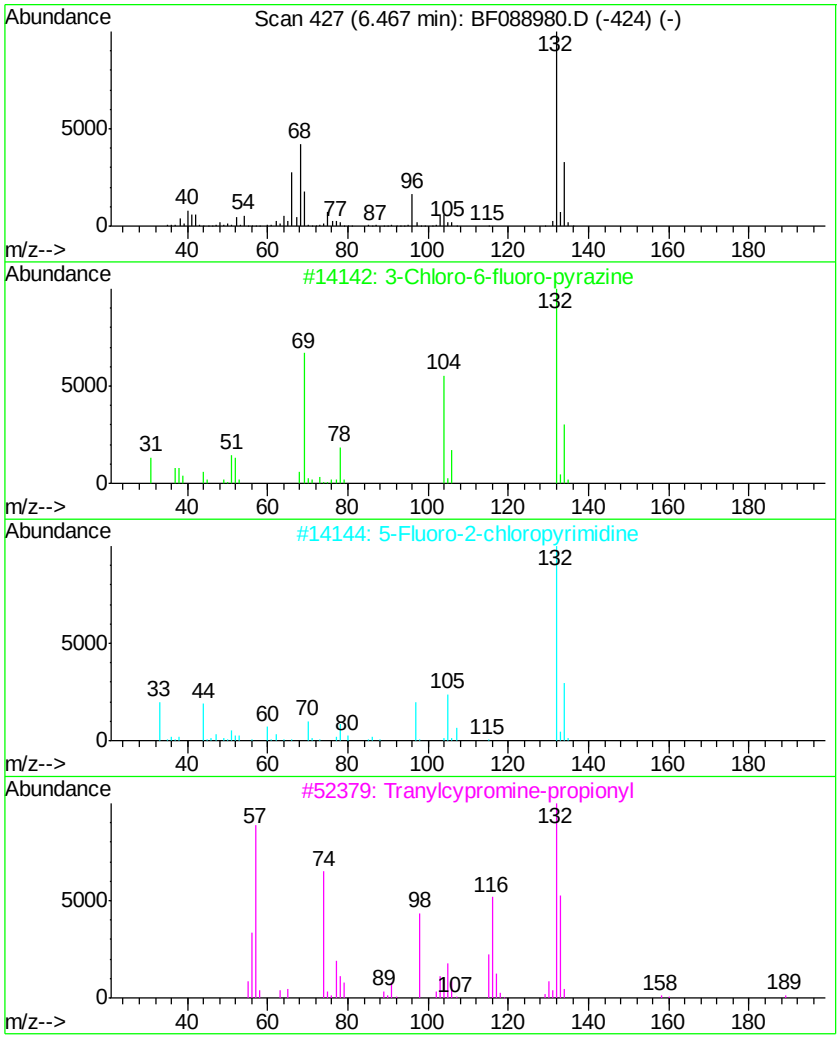
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

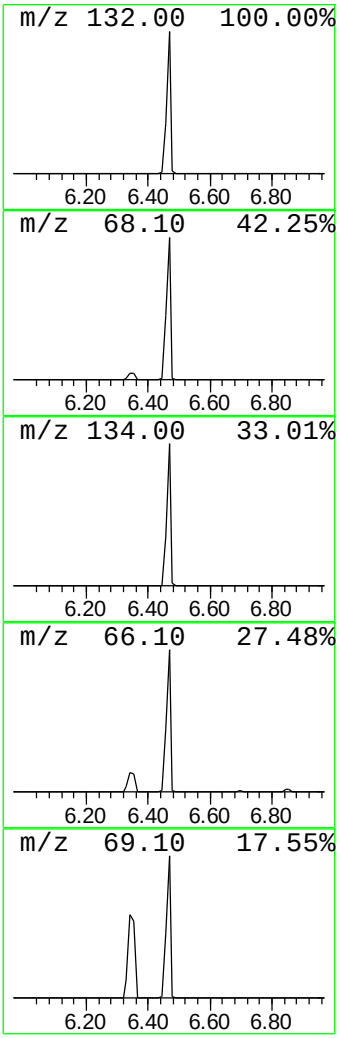
**********

Peak Number 5 unknown6.47 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.47 | 78.51 ng | 1669780 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | N-(-3,4-Methylenedioxyphenylisop... | 267 | C17H17NO2 | 1000378-96-6 | 10 |
| 5 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |



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Sample : H3946-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

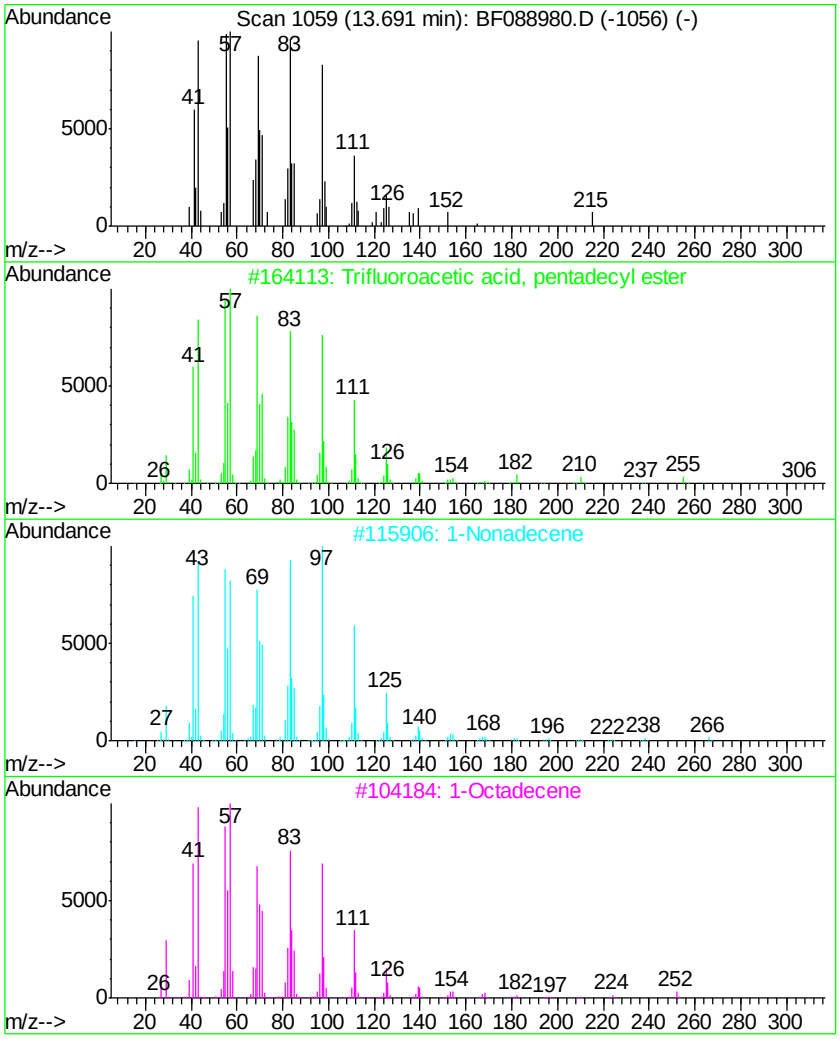
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

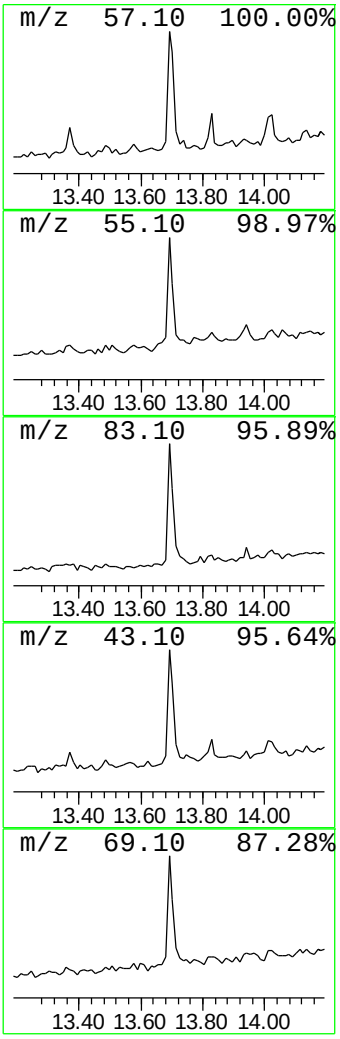
**********

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.69 | 2.57 ng | 76758 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 95 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 94 |
| 3 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 93 |
| 4 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 91 |
| 5 | Bromoacetic acid, pentadecyl ester | 348 | C17H33BrO2 | 131143-01-6 | 91 |



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

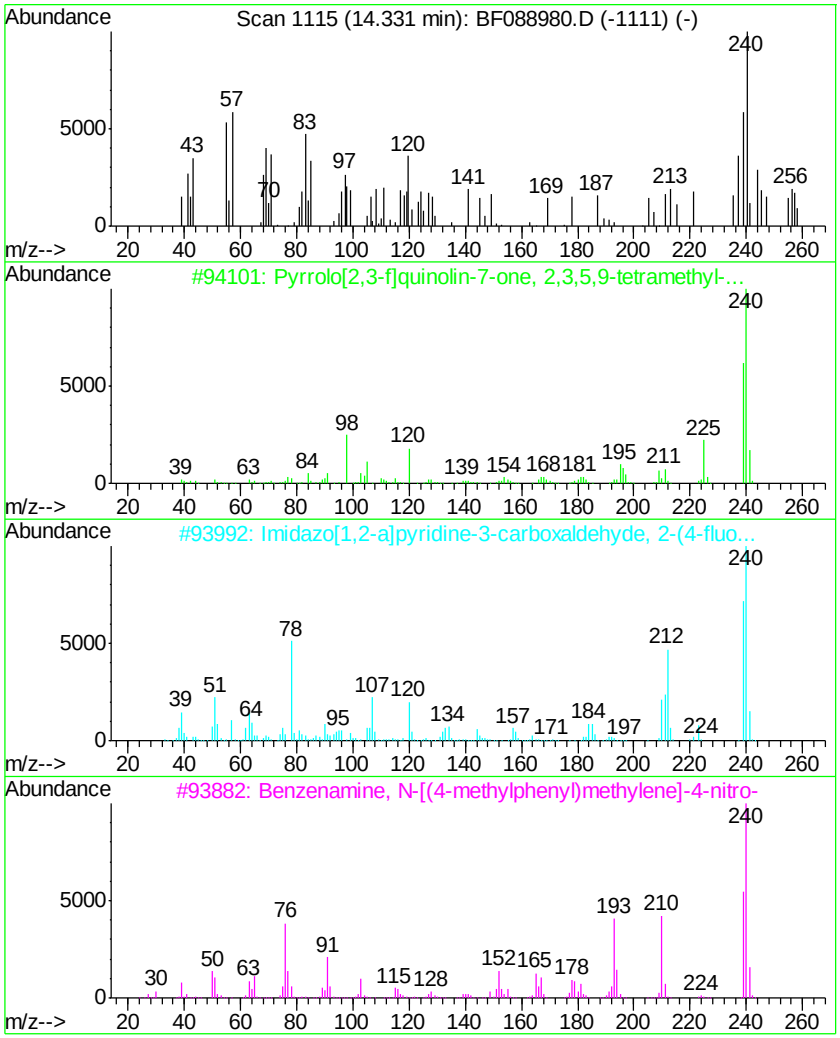
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

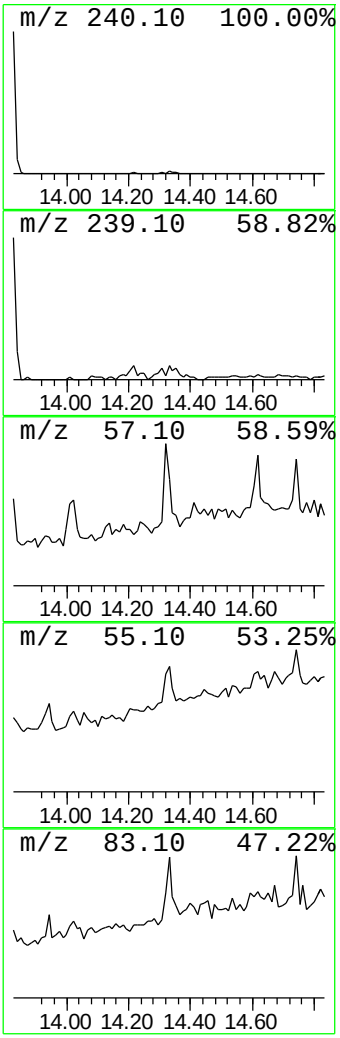
**********

Peak Number 8 unknown14.33 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.33 | 2.56 ng | 76311 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pyrrolo[2,3-f]quinolin-7-one, 2,... | 240 | C15H16N2O | 1000302-73-0 | 38 |
| 2 | Imidazo[1,2-a]pyridine-3-carboxa... | 240 | C14H9FN2O | 1000351-44-5 | 38 |
| 3 | Benzenamine, N-[(4-methylphenyl)... | 240 | C14H12N2O2 | 020192-50-1 | 38 |
| 4 | o-(p-(Dimethylamino)benzylidenea... | 240 | C15H16N2O | 023837-35-6 | 38 |
| 5 | Fumaric acid, decyl 3-oxobut-2-y... | 326 | C18H30O5 | 1000348-82-4 | 32 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Propane, 1,1-dime... | 1.90 | 13.0 | ng | 277265 | 1 | 6.70 | 425391 | 20.0 |
| 2-Pentanone, 4-hy... | 4.84 | 15.8 | ng | 335250 | 1 | 6.70 | 425391 | 20.0 |
| unknown6.47 | 6.47 | 78.5 | ng | 1669780 | 1 | 6.70 | 425391 | 20.0 |
| Trifluoroacetic a... | 13.69 | 2.6 | ng | 76758 | 5 | 13.83 | 596441 | 20.0 |
| unknown14.33 | 14.33 | 2.6 | ng | 76311 | 5 | 13.83 | 596441 | 20.0 |