LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038661.D
Acq On : 17 Dec 2018 13:45
Operator : JU/SJ
Sample : J6378-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SD007-0612-01

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.144 | 345 | 350 | 358 | rVB2 | 20472 | 34590 | 2.61% | 0.467% |
| 2 | 5.609 | 422 | 429 | 441 | rVB | 356869 | 597339 | 45.15% | 8.064% |
| 3 | 7.213 | 695 | 702 | 713 | rBV | 363735 | 686850 | 51.92% | 9.272% |
| 4 | 7.589 | 758 | 766 | 776 | rVB | 339271 | 606175 | 45.82% | 8.183% |
| 5 | 8.059 | 840 | 846 | 856 | rVB | 67107 | 115457 | 8.73% | 1.559% |
| 6 | 8.382 | 893 | 901 | 909 | rBV | 244000 | 432493 | 32.69% | 5.839% |
| 7 | 9.234 | 1039 | 1046 | 1058 | rBV | 214641 | 401378 | 30.34% | 5.419% |
| 8 | 10.879 | 1318 | 1326 | 1335 | rBV | 79945 | 152901 | 11.56% | 2.064% |
| 9 | 13.317 | 1733 | 1741 | 1752 | rBV | 467054 | 745856 | 56.38% | 10.069% |
| 10 | 14.140 | 1875 | 1881 | 1890 | rBV | 22798 | 32993 | 2.49% | 0.445% |
| 11 | 14.698 | 1969 | 1976 | 1987 | rVB2 | 131467 | 222135 | 16.79% | 2.999% |
| 12 | 16.184 | 2222 | 2229 | 2242 | rBV | 467153 | 726550 | 54.92% | 9.808% |
| 13 | 17.442 | 2437 | 2443 | 2451 | rBV2 | 196299 | 313731 | 23.72% | 4.235% |
| 14 | 18.305 | 2585 | 2590 | 2597 | rBV4 | 17130 | 30383 | 2.30% | 0.410% |
| 15 | 20.045 | 2880 | 2886 | 2897 | rVB | 1034684 | 1322915 | 100.00% | 17.859% |
| 16 | 21.320 | 3098 | 3103 | 3113 | rBV2 | 32862 | 62323 | 4.71% | 0.841% |
| 17 | 21.725 | 3165 | 3172 | 3180 | rBV | 234989 | 395521 | 29.90% | 5.339% |
| 18 | 22.477 | 3294 | 3300 | 3303 | rBV3 | 9178 | 16103 | 1.22% | 0.217% |
| 19 | 22.524 | 3303 | 3308 | 3315 | rVB7 | 9284 | 21927 | 1.66% | 0.296% |
| 20 | 23.176 | 3414 | 3419 | 3425 | rVB4 | 7743 | 14286 | 1.08% | 0.193% |
| 21 | 23.987 | 3549 | 3557 | 3567 | rVB5 | 11018 | 27062 | 2.05% | 0.365% |
| 22 | 25.021 | 3715 | 3733 | 3746 | rVB2 | 128595 | 390382 | 29.51% | 5.270% |
| 23 | 26.090 | 3906 | 3915 | 3924 | rBV8 | 5187 | 17240 | 1.30% | 0.233% |
| 24 | 32.612 | 5012 | 5025 | 5026 | rBV7 | 16917 | 40867 | 3.09% | 0.552% |

Sum of corrected areas: 7407457

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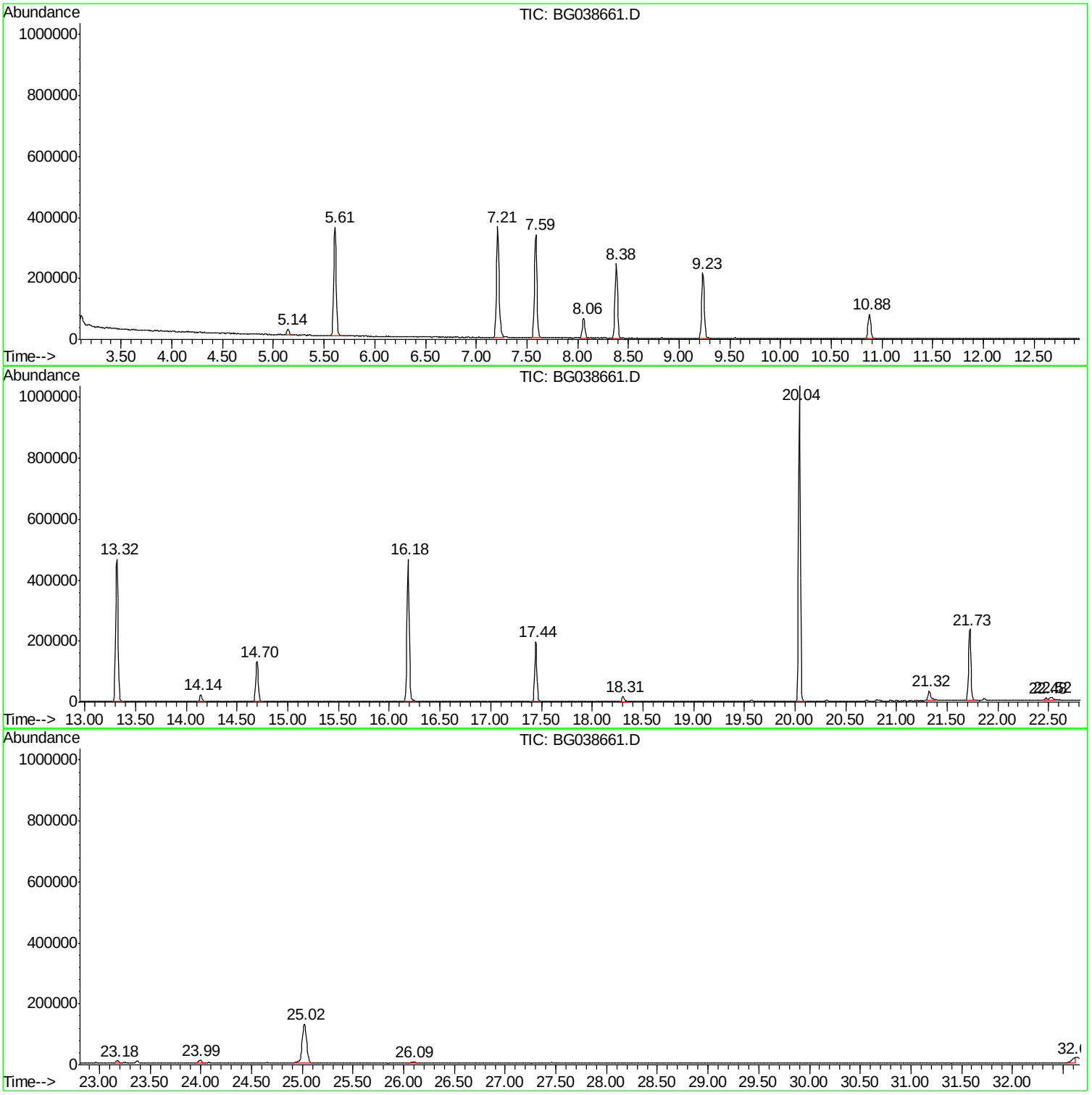
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SD007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038661.D
Acq On : 17 Dec 2018 13:45
Operator : JU/SJ
Sample : J6378-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SD007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

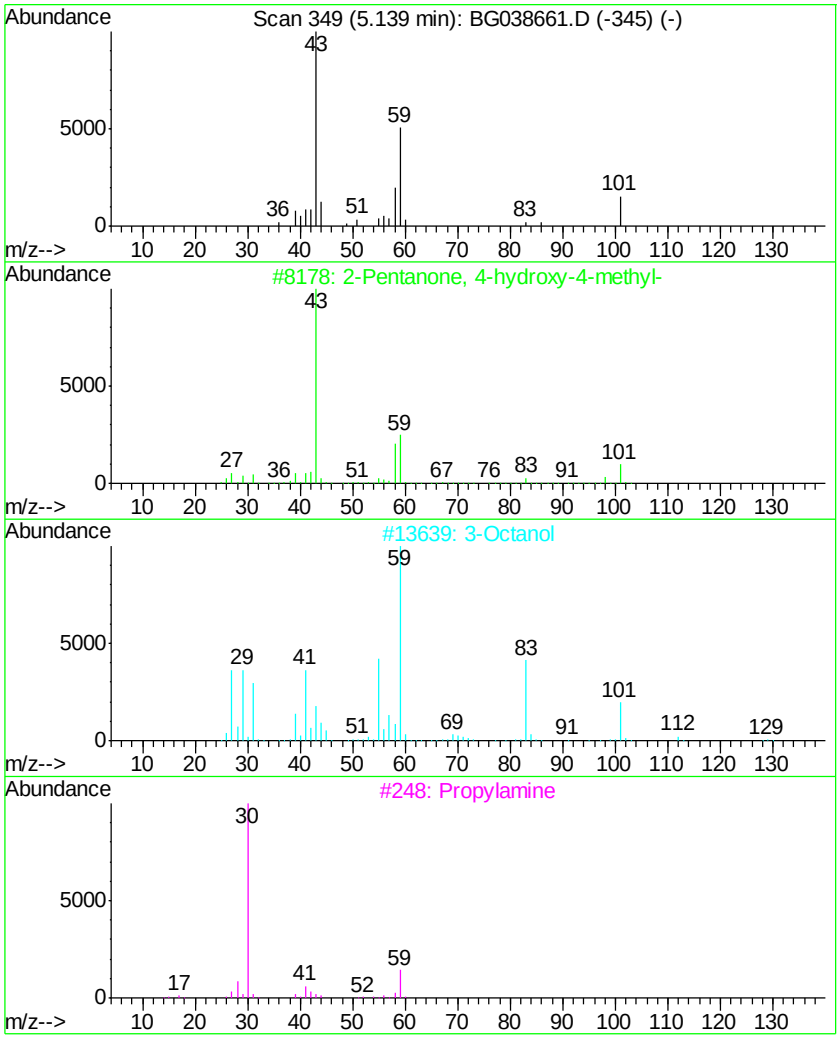
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

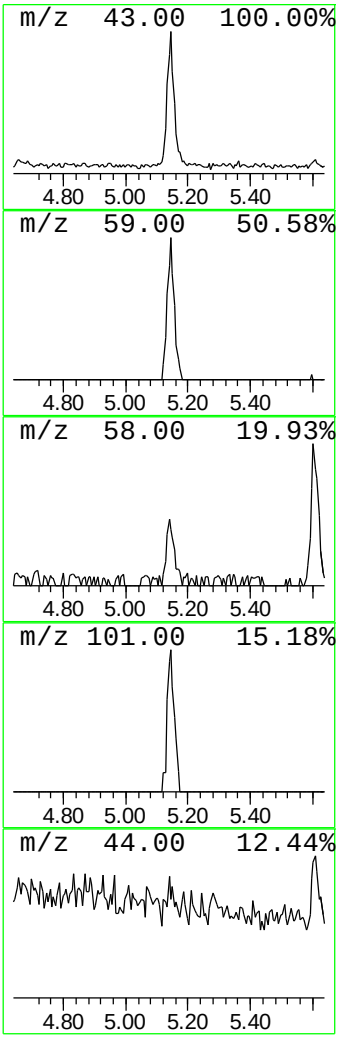
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.14 | 5.99 ng | 34590 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 36 |
| 3 | Propylamine | 59 | C3H9N | 000107-10-8 | 9 |
| 4 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 9 |
| 5 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 9 |



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Data File : BG038661.D
Acq On : 17 Dec 2018 13:45
Operator : JU/SJ
Sample : J6378-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SD007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

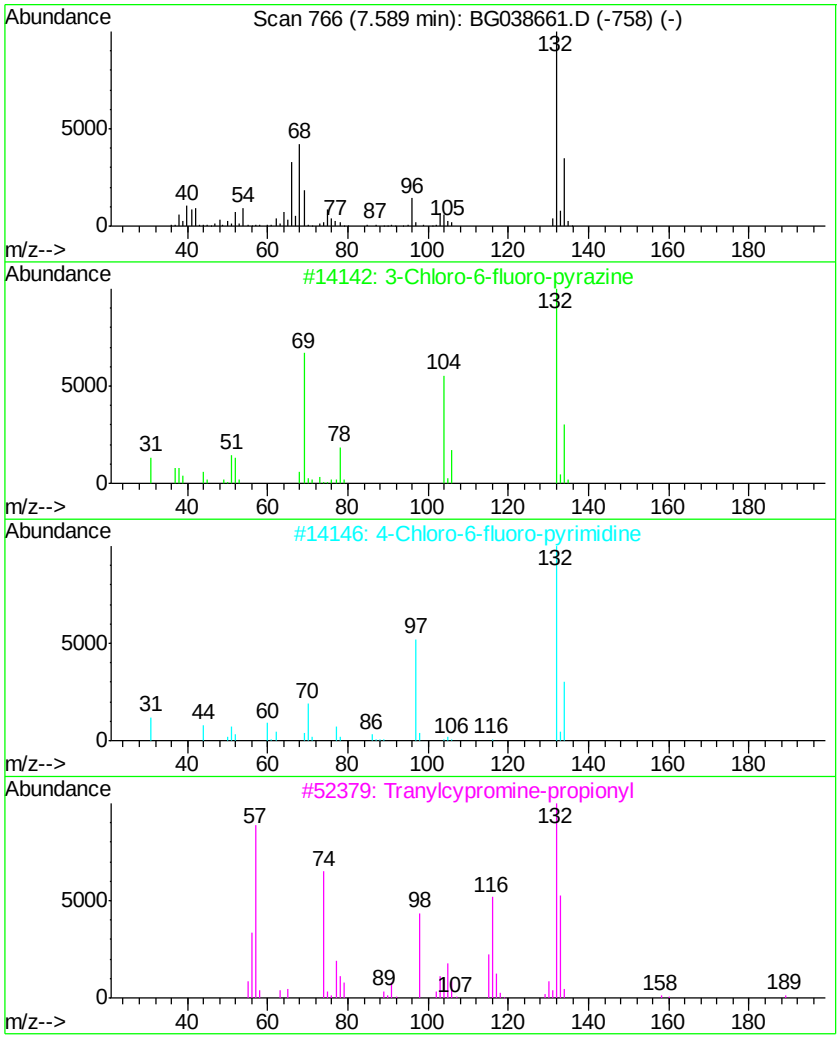
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

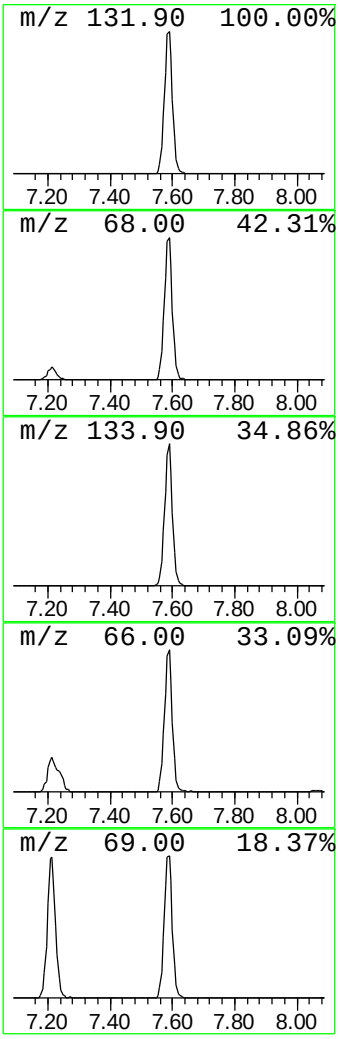
**********

Peak Number 2 unknown7.59 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.59 | 105.00 ng | 606175 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 22 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 5 | Pyrazolo(2,3-a)pyridine, 7-methyl- | 132 | C8H8N2 | 034760-58-2 | 12 |



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Operator : JU/SJ
Sample : J6378-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SD007-0612-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

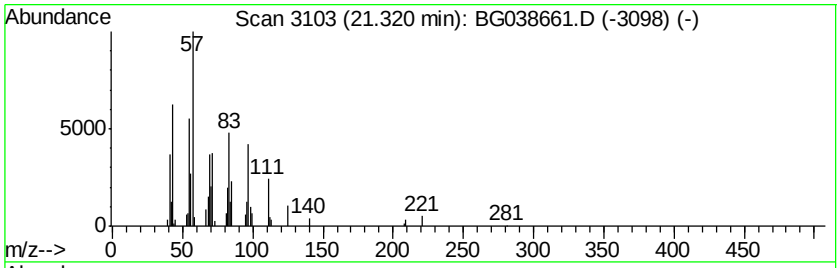
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

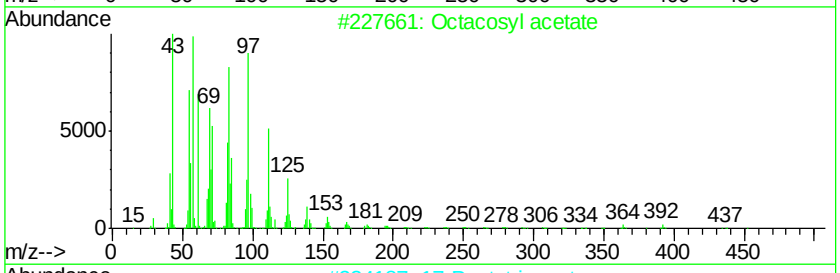
**********

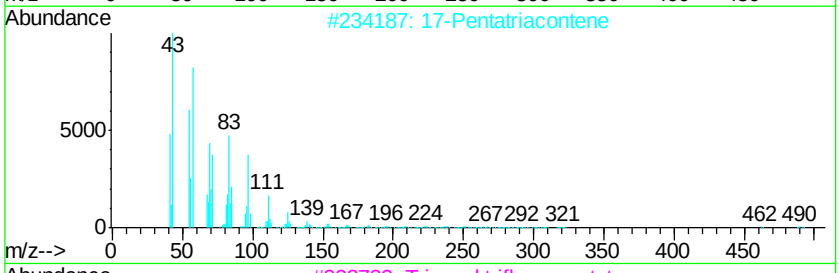
Peak Number 4 Octacosyl acetate Concentration Rank 4

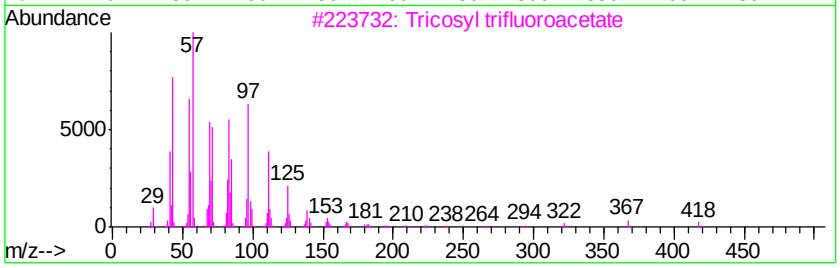
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.32 | 3.15 ng | 62323 | Chrysene-d12 | 21.73 |

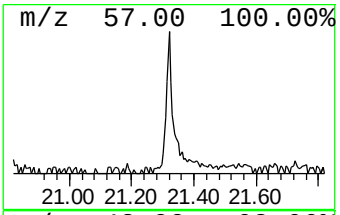
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosyl acetate | 452 | C30H60O2 | 018206-97-8 | 91 |
| 2 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 91 |
| 3 | Tricosyl trifluoroacetate | 436 | C25H47F3O2 | 1000351-75-1 | 91 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |
| 5 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 90 |

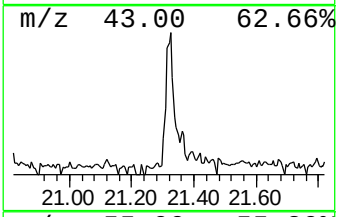


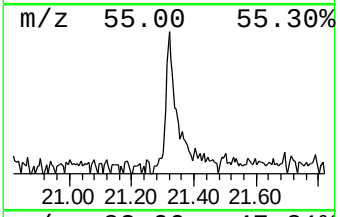



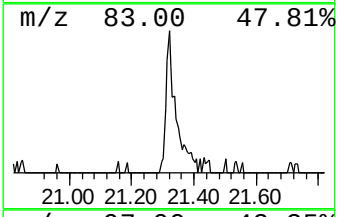



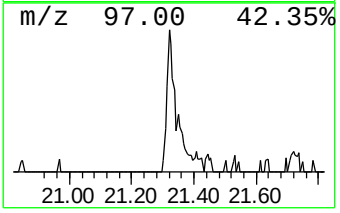



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

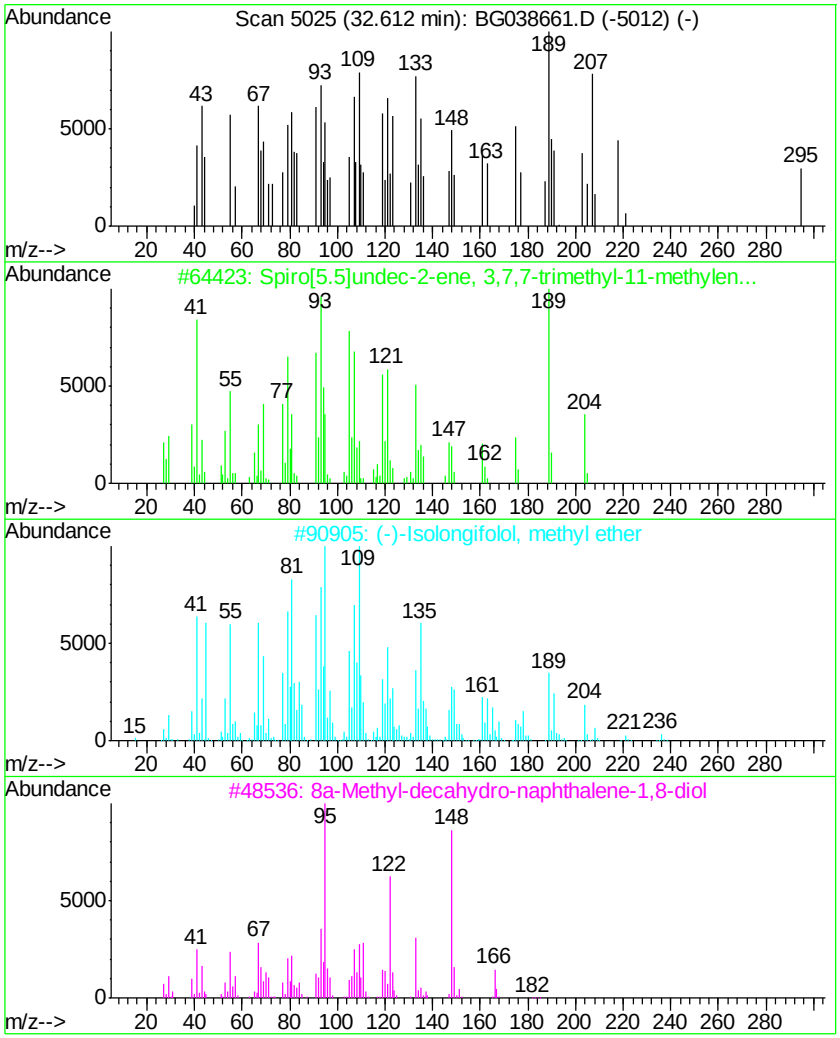
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

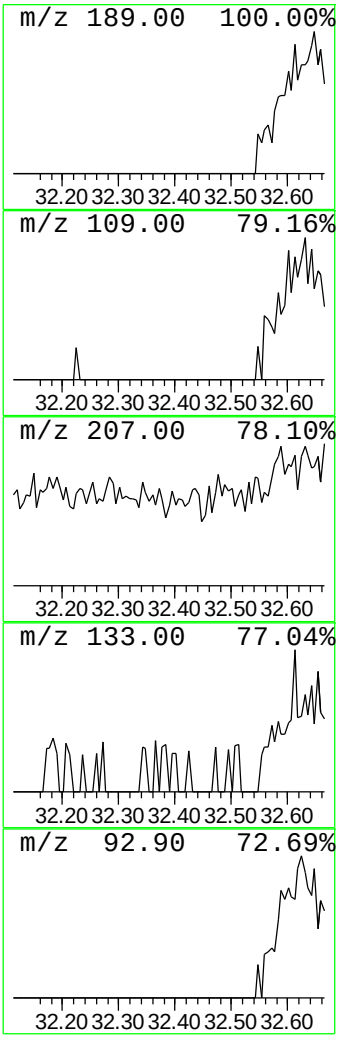
**********

Peak Number 5 unknown32.61 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 32.61 | 2.09 ng | 40867 | Perylene-d12 | 25.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Spiro[5.5]undec-2-ene, 3,7,7-tri... | 204 | C15H24 | 018431-82-8 | 22 |
| 2 | (-)-Isolongifolol, methyl ether | 236 | C16H28O | 1000333-80-8 | 22 |
| 3 | 8a-Methyl-decahydro-naphthalene-... | 184 | C11H20O2 | 1000185-34-4 | 18 |
| 4 | 3-Methylindole-2-carboxylic acid... | 207 | C12H17NO2 | 037945-37-2 | 14 |
| 5 | 1H-1,5-Benzodiazepine, 2,3,4,5-t... | 190 | C12H18N2 | 040358-38-1 | 14 |



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 |
| 2-Pentanone, 4-hy... | 5.14 | 6.0 | ng | 34590 | 1 | 8.06 | 115457 | 20.0 |
| unknown7.59 | 7.59 | 105.0 | ng | 606175 | 1 | 8.06 | 115457 | 20.0 |
| Octacosyl acetate | 21.32 | 3.1 | ng | 62323 | 5 | 21.73 | 395521 | 20.0 |
| unknown32.61 | 32.61 | 2.1 | ng | 40867 | 6 | 25.02 | 390382 | 20.0 |