LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

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_G\METHODS\8270-BG091217.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 | 5.380 | 300 | 305 | 312 | rVB2 | 27870 | 44516 | 1.16% | 0.329% |
| 2 | 5.844 | 377 | 384 | 396 | rBV | 244959 | 424510 | 11.09% | 3.141% |
| 3 | 7.431 | 648 | 654 | 665 | rBV | 177372 | 346350 | 9.05% | 2.563% |
| 4 | 7.813 | 711 | 719 | 731 | rBV | 401008 | 737917 | 19.28% | 5.460% |
| 5 | 8.277 | 791 | 798 | 803 | rBV2 | 77141 | 139527 | 3.65% | 1.032% |
| 6 | 8.600 | 846 | 853 | 864 | rVB2 | 351107 | 646981 | 16.91% | 4.787% |
| 7 | 9.446 | 989 | 997 | 1012 | rBV | 300694 | 574483 | 15.01% | 4.251% |
| 8 | 11.097 | 1270 | 1278 | 1289 | rBV | 97561 | 191426 | 5.00% | 1.416% |
| 9 | 11.896 | 1406 | 1414 | 1419 | rBV2 | 31594 | 55156 | 1.44% | 0.408% |
| 10 | 13.512 | 1678 | 1689 | 1699 | rBV | 912958 | 1511509 | 39.50% | 11.184% |
| 11 | 14.399 | 1835 | 1840 | 1847 | rVB4 | 27121 | 42938 | 1.12% | 0.318% |
| 12 | 14.893 | 1918 | 1924 | 1931 | rBV2 | 184561 | 310291 | 8.11% | 2.296% |
| 13 | 15.280 | 1984 | 1990 | 1997 | rBV2 | 85764 | 119285 | 3.12% | 0.883% |
| 14 | 15.656 | 2049 | 2054 | 2059 | rBV | 231281 | 292955 | 7.65% | 2.168% |
| 15 | 16.385 | 2170 | 2178 | 2192 | rBV | 1125487 | 1786984 | 46.69% | 13.222% |
| 16 | 17.642 | 2386 | 2392 | 2404 | rVB2 | 348156 | 552776 | 14.44% | 4.090% |
| 17 | 18.283 | 2493 | 2501 | 2508 | rBV2 | 109447 | 166516 | 4.35% | 1.232% |
| 18 | 19.887 | 2766 | 2774 | 2779 | rBV | 226335 | 285113 | 7.45% | 2.110% |
| 19 | 20.233 | 2826 | 2833 | 2840 | rBV | 2910913 | 3827072 | 100.00% | 28.317% |
| 20 | 21.391 | 3025 | 3030 | 3037 | rBV6 | 20880 | 54231 | 1.42% | 0.401% |
| 21 | 21.961 | 3119 | 3127 | 3140 | rVB2 | 403866 | 725273 | 18.95% | 5.366% |
| 22 | 25.410 | 3704 | 3714 | 3726 | rVB2 | 223606 | 679465 | 17.75% | 5.027% |

Sum of corrected areas: 13515274

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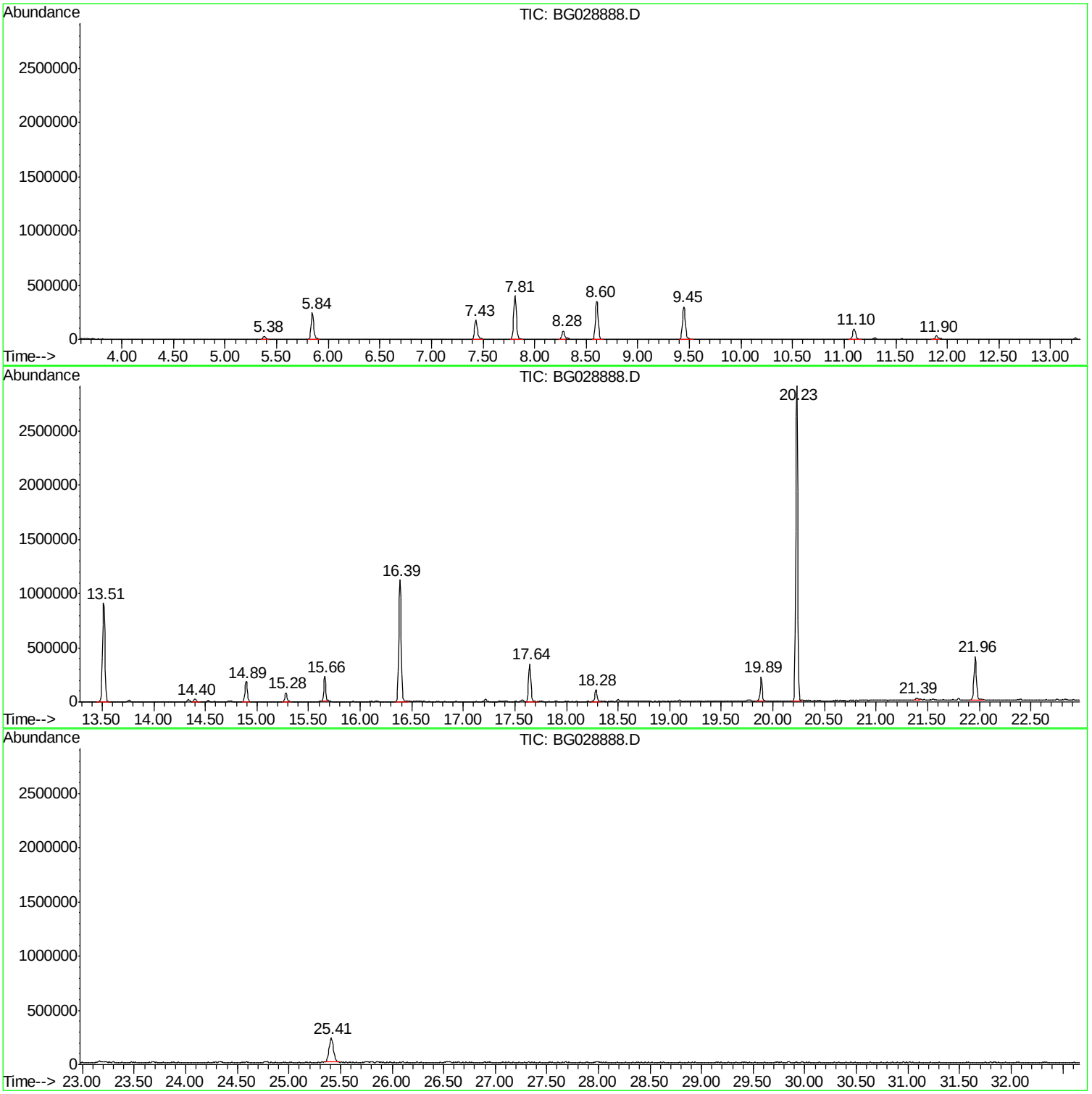
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
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**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

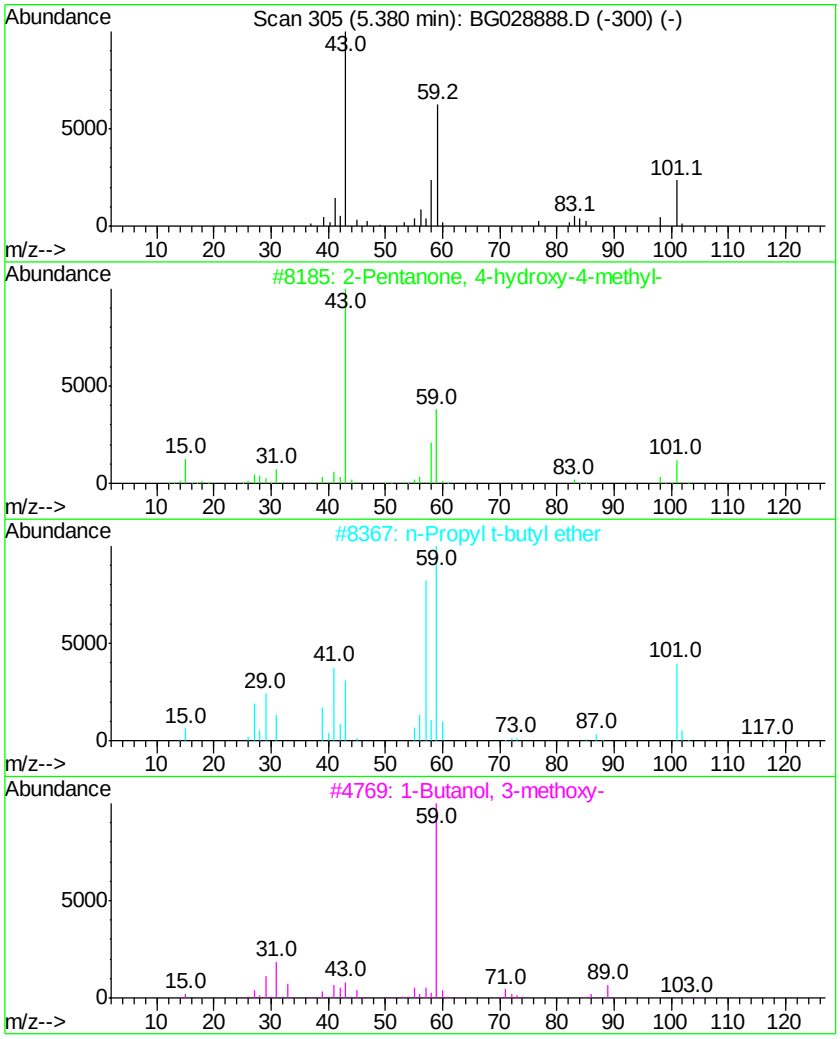
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

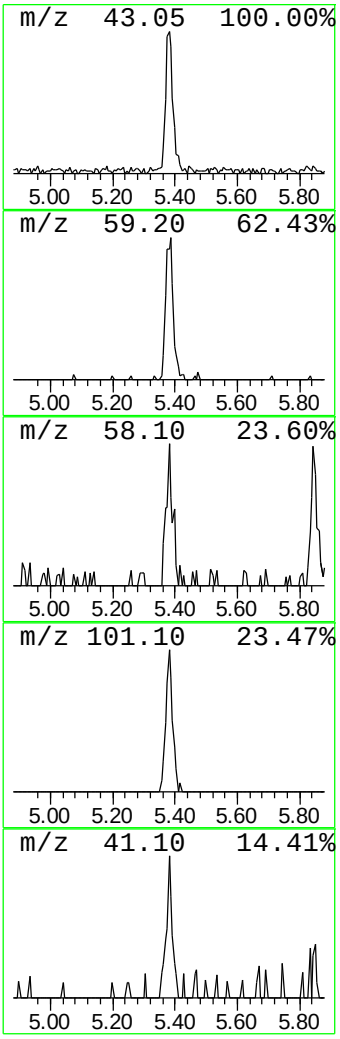
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.38 | 6.38 ng | 44516 | 1,4-Dichlorobenzene-d4 | 8.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 2 | n-Propyl t-butyl ether | 116 | C7H16O | 1000334-81-9 | 23 |
| 3 | 1-Butanol, 3-methoxy- | 104 | C5H12O2 | 002517-43-3 | 12 |
| 4 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 12 |
| 5 | 3-Pentanol | 88 | C5H12O | 000584-02-1 | 10 |



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Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

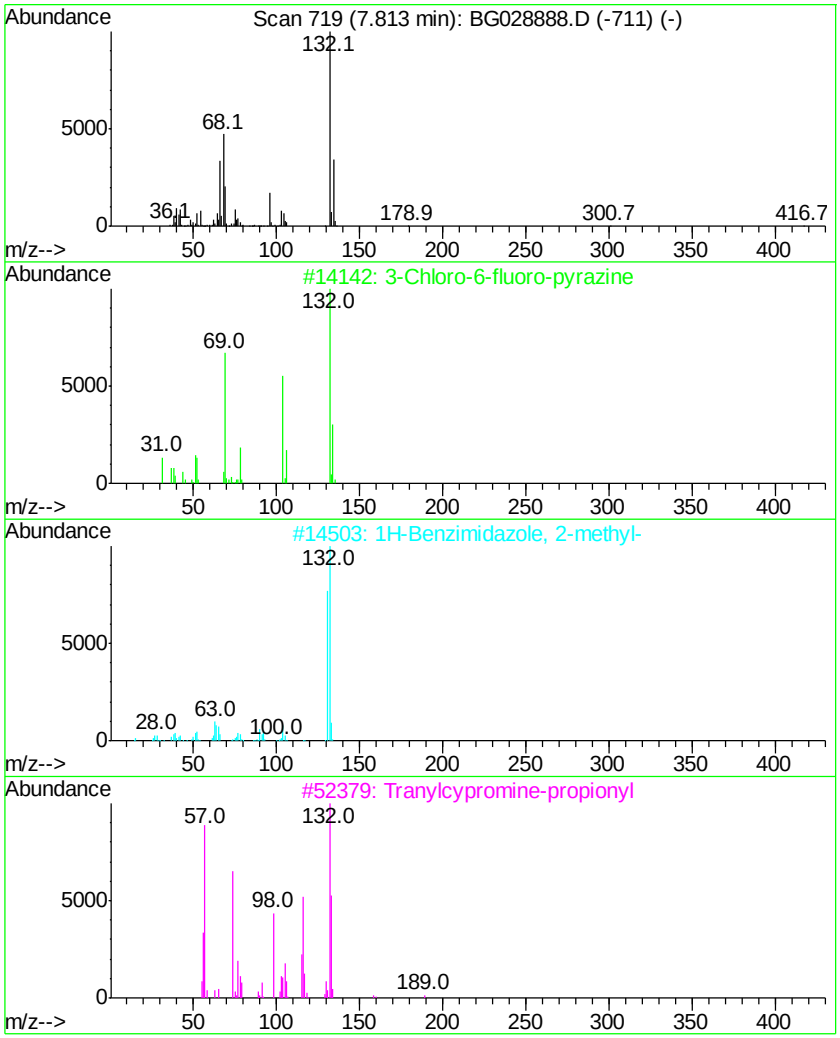
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

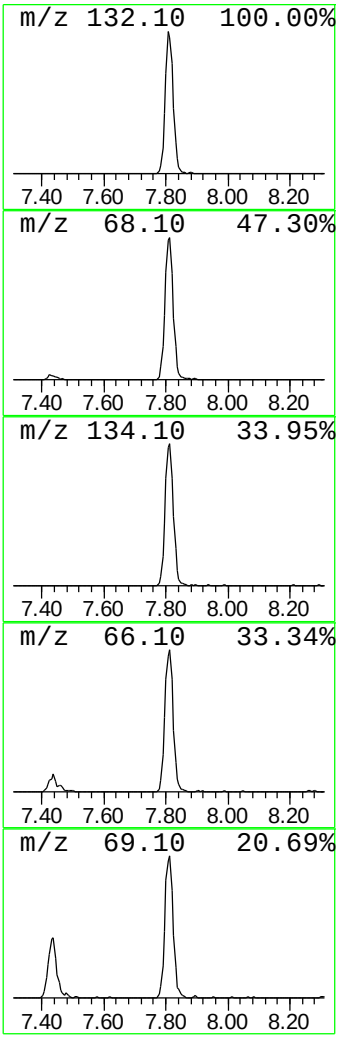
**********

Peak Number 2 unknown7.81 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.81 | 105.77 ng | 737917 | 1,4-Dichlorobenzene-d4 | 8.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 5 | 3-Ethylphenyl isocyanate | 147 | C9H9NO | 023138-58-1 | 10 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

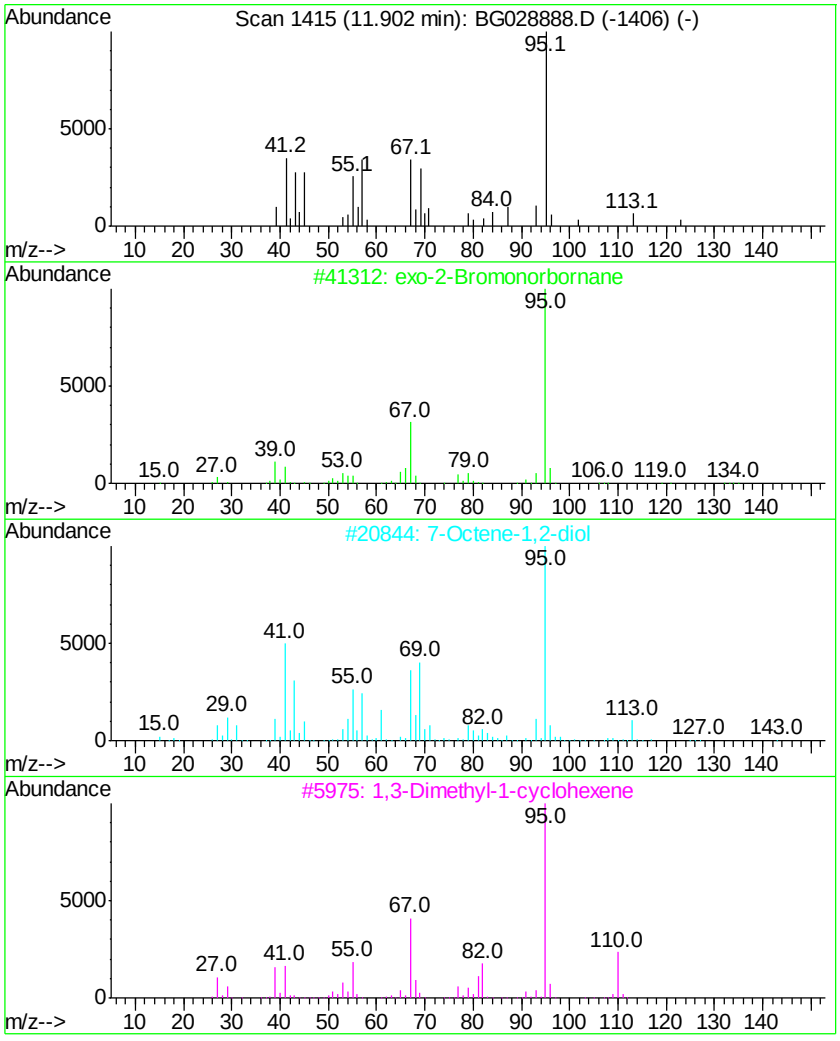
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

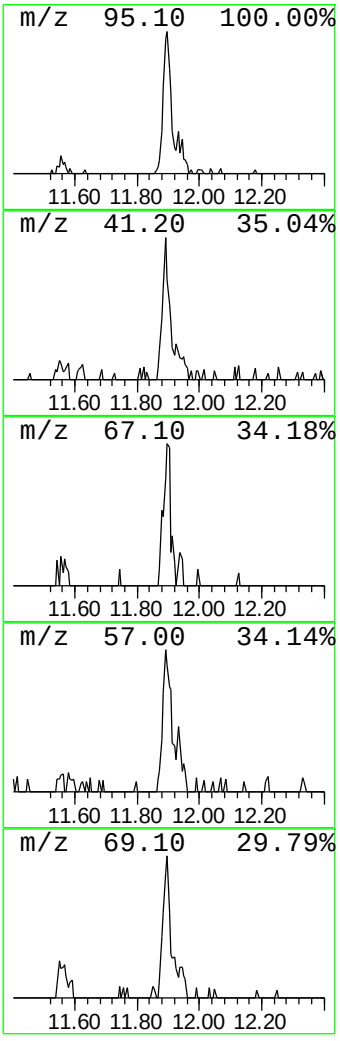
**********

Peak Number 4 unknown11.90 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.90 | 5.76 ng | 55156 | Naphthalene-d8 | 11.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | exo-2-Bromonorbornane | 174 | C7H11Br | 002534-77-2 | 47 |
| 2 | 7-Octene-1,2-diol | 144 | C8H16O2 | 085866-02-0 | 40 |
| 3 | 1,3-Dimethyl-1-cyclohexene | 110 | C8H14 | 002808-76-6 | 38 |
| 4 | 6-Methyl-2-heptyne | 110 | C8H14 | 051065-64-6 | 38 |
| 5 | 2-Norbornyl bromide | 174 | C7H11Br | 029342-65-2 | 38 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

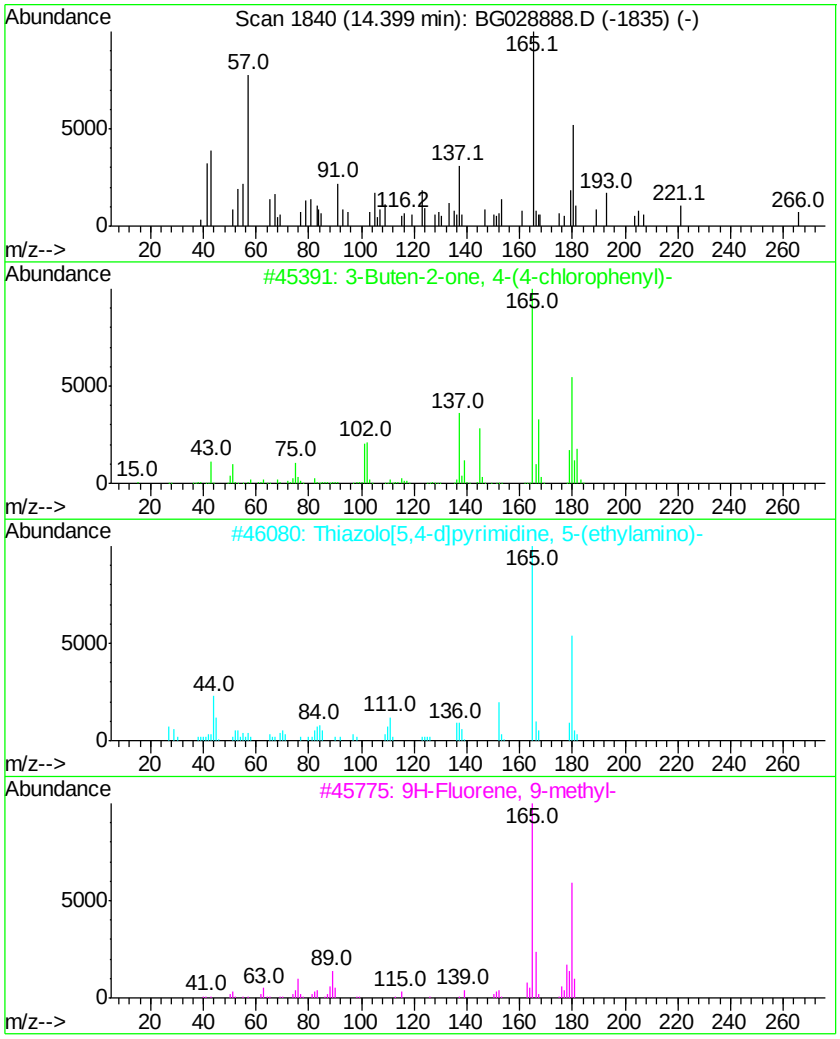
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

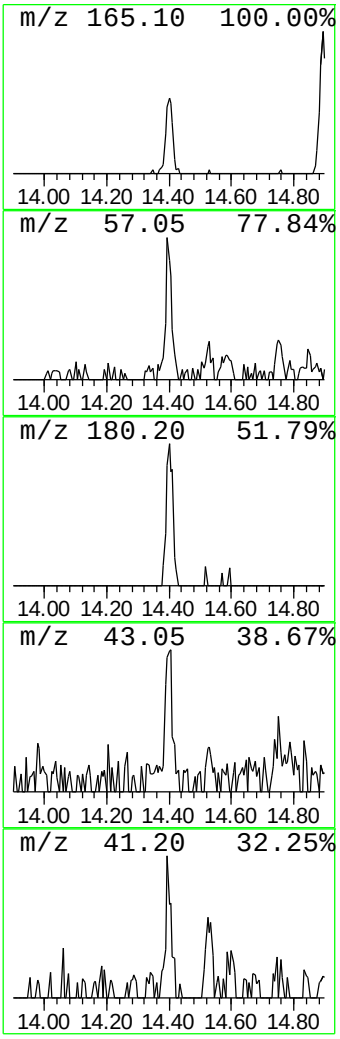
**********

Peak Number 5 3-Buten-2-one, 4-(4-chlorop... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.40 | 2.77 ng | 42938 | Acenaphthene-d10 | 14.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Buten-2-one, 4-(4-chlorophenyl)- | 180 | C10H9ClO | 003160-40-5 | 68 |
| 2 | Thiazolo[5,4-d]pyrimidine, 5-(et... | 180 | C7H8N4S | 019835-21-3 | 58 |
| 3 | 9H-Fluorene, 9-methyl- | 180 | C14H12 | 002523-37-7 | 52 |
| 4 | Ethanone, 1-(3,4-dimethoxyphenyl)- | 180 | C10H12O3 | 001131-62-0 | 50 |
| 5 | (3,3-Dimethyl-5-methylthio-3,4(2... | 180 | C9H12N2S | 1000186-20-1 | 43 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
Data File : BG028888.D
Acq On : 22 Sep 2017 23:58
Operator : SJ/JU
Sample : I5301-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

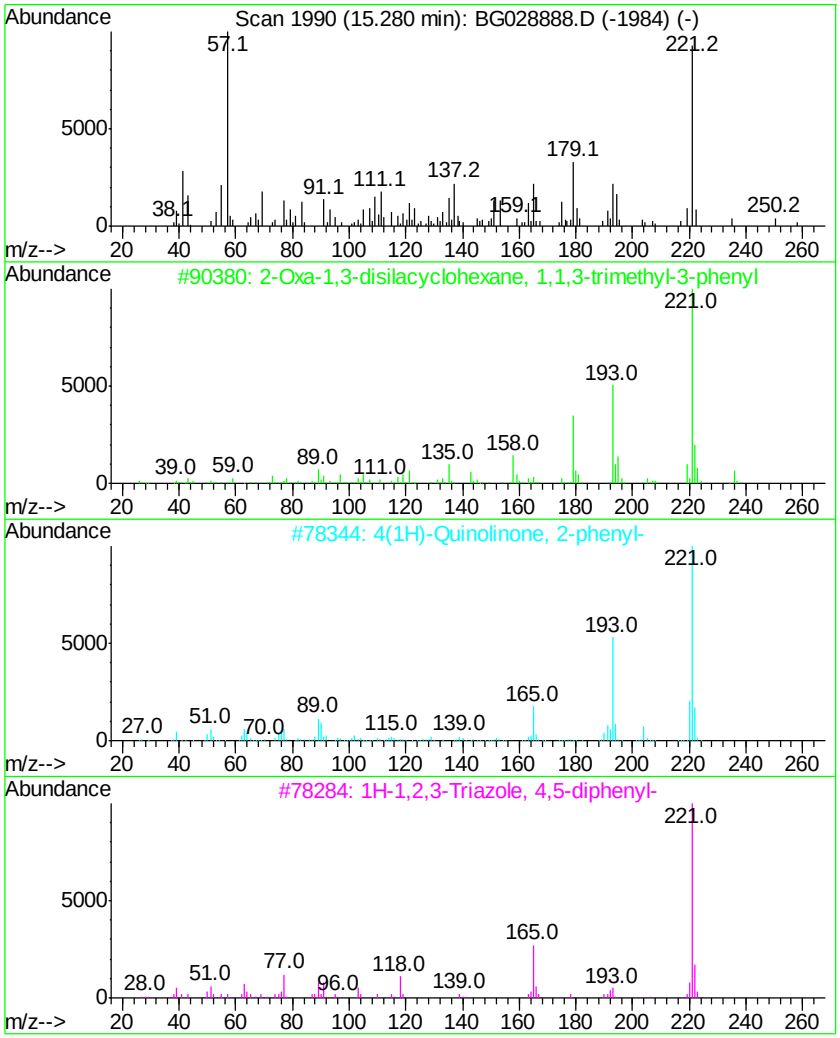
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

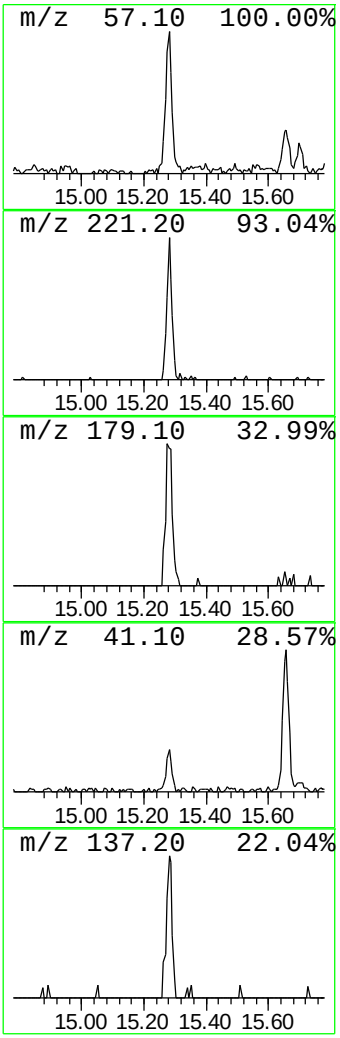
**********

Peak Number 6 unknown15.28 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.28 | 7.69 ng | 119285 | Acenaphthene-d10 | 14.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Oxa-1,3-disilacyclohexane, 1,1... | 236 | C12H20OSi2 | 1000308-85-9 | 38 |
| 2 | 4(1H)-Quinolinone, 2-phenyl- | 221 | C15H11NO | 014802-18-7 | 37 |
| 3 | 1H-1,2,3-Triazole, 4,5-diphenyl- | 221 | C14H11N3 | 005533-73-3 | 37 |
| 4 | 4-Chloro-3-trifluoromethylphenyl... | 221 | C8H3ClF3NO | 000327-78-6 | 37 |
| 5 | But-2-en-1-one, 1-(2-hydroxy-4,5... | 236 | C13H16O4 | 1000305-06-7 | 37 |



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**Instrument :** BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

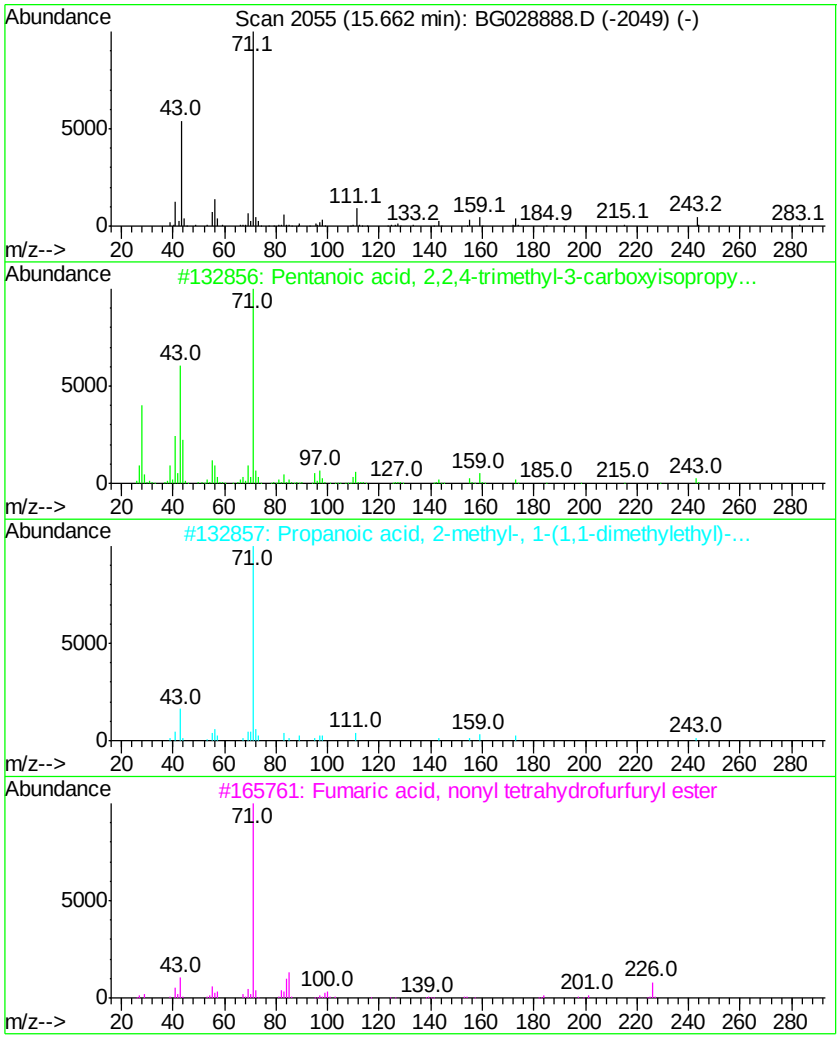
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

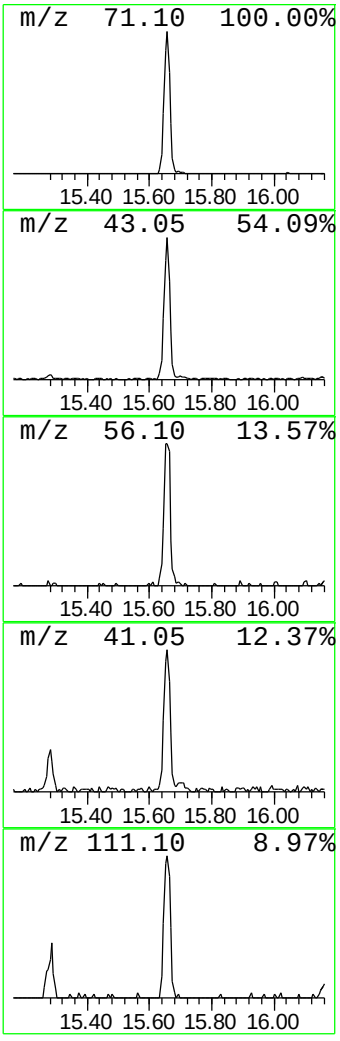
**********

Peak Number 7 Pentanoic acid, 2,2,4-trime... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.66 | 18.88 ng | 292955 | Acenaphthene-d10 | 14.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentanoic acid, 2,2,4-trimethyl-... | 286 | C16H30O4 | 1000140-77-5 | 90 |
| 2 | Propanoic acid, 2-methyl-, 1-(1,... | 286 | C16H30O4 | 074381-40-1 | 83 |
| 3 | Fumaric acid, nonyl tetrahydrofu... | 326 | C18H30O5 | 1000330-58-3 | 59 |
| 4 | Methylamine, N-(1-methylhexylide... | 127 | C8H17N | 022058-71-5 | 53 |
| 5 | 2,2,4-Trimethyl-1,3-pentanediol ... | 286 | C16H30O4 | 006846-50-0 | 50 |



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Misc :
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**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

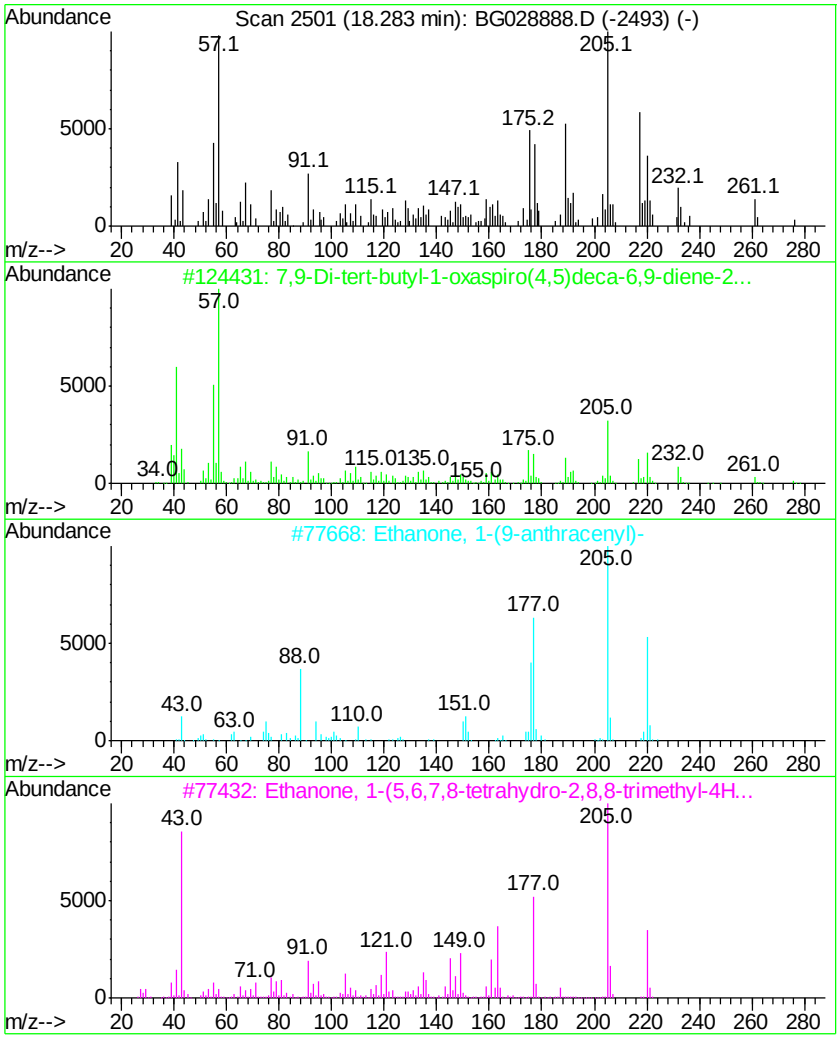
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

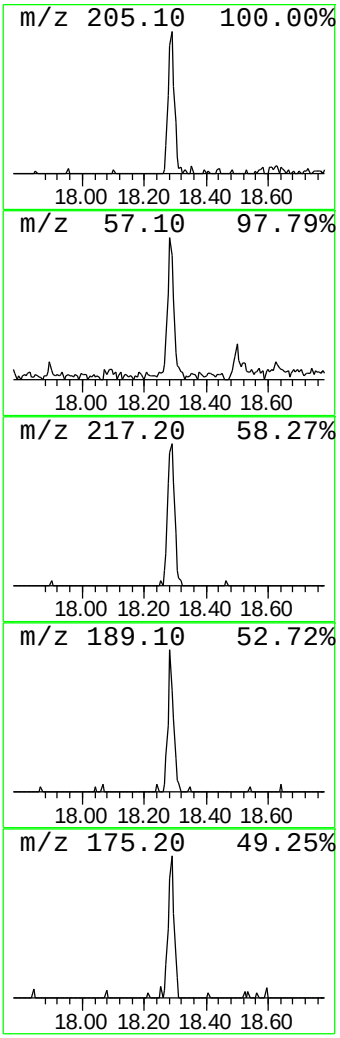
**********

Peak Number 8 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.28 | 6.02 ng | 166516 | Phenanthrene-d10 | 17.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7,9-Di-tert-butyl-1-oxaspiro(4,5... | 276 | C17H24O3 | 082304-66-3 | 93 |
| 2 | Ethanone, 1-(9-anthracenyl)- | 220 | C16H12O | 000784-04-3 | 43 |
| 3 | Ethanone, 1-(5,6,7,8-tetrahydro-... | 220 | C14H20O2 | 071596-88-8 | 38 |
| 4 | 2-Phenazinecarbonitrile | 205 | C13H7N3 | 006479-93-2 | 35 |
| 5 | 9-Acetylphenanthrene | 220 | C16H12O | 002039-77-2 | 30 |



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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

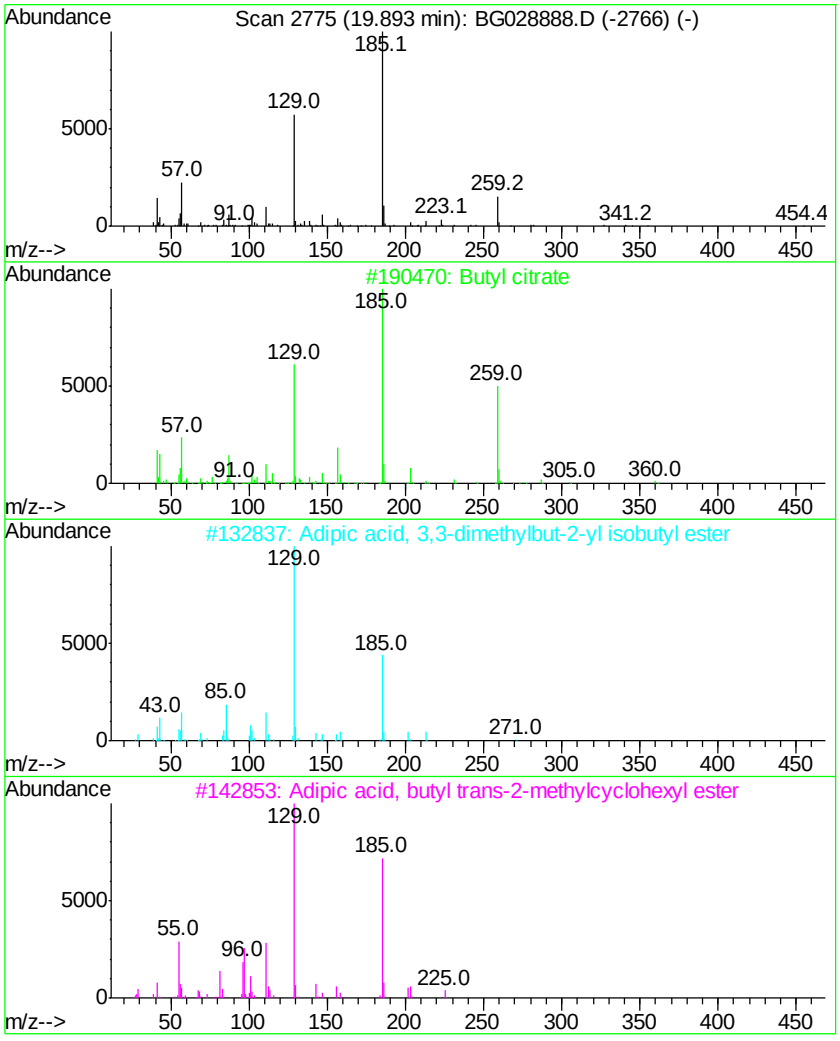
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

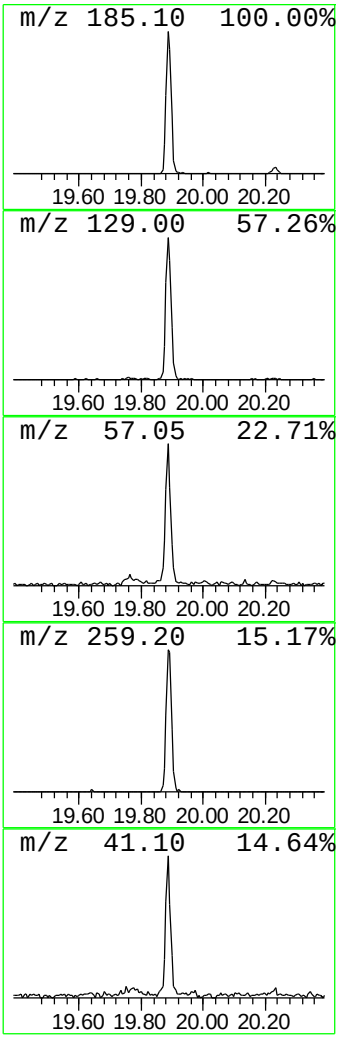
**********

Peak Number 9 Butyl citrate Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.89 | 7.86 ng | 285113 | Chrysene-d12 | 21.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyl citrate | 360 | C18H32O7 | 000077-94-1 | 72 |
| 2 | Adipic acid, 3,3-dimethylbut-2-y... | 286 | C16H30O4 | 1000353-66-7 | 64 |
| 3 | Adipic acid, butyl trans-2-methy... | 298 | C17H30O4 | 1000324-74-6 | 64 |
| 4 | Adipic acid, 2-ethylhexyl isobut... | 314 | C18H34O4 | 1000324-48-0 | 64 |
| 5 | Adipic acid, 4-heptyl isobutyl e... | 300 | C17H32O4 | 1000349-73-6 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092217\
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Operator : SJ/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 20170608-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.38 | 6.4 | ng | 44516 | 1 | 8.28 | 139527 | 20.0 |
| unknown7.81 | 7.81 | 105.8 | ng | 737917 | 1 | 8.28 | 139527 | 20.0 |
| unknown11.90 | 11.90 | 5.8 | ng | 55156 | 2 | 11.10 | 191426 | 20.0 |
| 3-Buten-2-one, 4-... | 14.40 | 2.8 | ng | 42938 | 3 | 14.90 | 310291 | 20.0 |
| unknown15.28 | 15.28 | 7.7 | ng | 119285 | 3 | 14.90 | 310291 | 20.0 |
| Pentanoic acid, 2... | 15.66 | 18.9 | ng | 292955 | 3 | 14.90 | 310291 | 20.0 |
| 7,9-Di-tert-butyl... | 18.28 | 6.0 | ng | 166516 | 4 | 17.64 | 552776 | 20.0 |
| Butyl citrate | 19.89 | 7.9 | ng | 285113 | 5 | 21.96 | 725273 | 20.0 |