LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

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-BG062817.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	5.606	285	292	303	rBV	121491	199055	6.04%	1.645%
2	5.964	347	353	362	rBV	67584	115526	3.51%	0.955%
3	6.058	362	369	379	rVB	145423	246291	7.48%	2.036%
4	7.615	628	634	640	rBV	101787	177965	5.40%	1.471%
5	8.009	692	701	715	rBV	264708	495013	15.03%	4.092%
6	8.473	774	780	793	rBV	91561	189752	5.76%	1.568%
7	8.802	827	836	848	rVB	411589	764914	23.23%	6.323%
8	9.642	971	979	992	rBV	357828	687190	20.87%	5.680%
9	11.293	1252	1260	1270	rBV	155168	302790	9.19%	2.503%
10	11.881	1349	1360	1366	rBV5	19205	40858	1.24%	0.338%
11	13.685	1658	1667	1674	rBV	1134503	1789903	54.35%	14.795%
12	14.272	1762	1767	1772	rVB	26139	44403	1.35%	0.367%
13	14.337	1772	1778	1784	rBV2	25811	52479	1.59%	0.434%
14	14.684	1829	1837	1845	rVB8	12437	39069	1.19%	0.323%
15	15.060	1892	1901	1908	rBV2	258127	450137	13.67%	3.721%
16	15.512	1970	1978	1986	rBV10	17419	71292	2.16%	0.589%
17	15.859	2032	2037	2045	rVB4	39054	74388	2.26%	0.615%
18	16.311	2109	2114	2119	rBV	80048	110843	3.37%	0.916%
19	16.546	2148	2154	2163	rVB	529603	835619	25.37%	6.907%
20	16.793	2189	2196	2201	rVB7	19090	44503	1.35%	0.368%
21	16.863	2203	2208	2212	rVV	24633	34875	1.06%	0.288%
22	16.916	2212	2217	2223	rVB3	24997	50742	1.54%	0.419%
23	16.981	2223	2228	2232	rBV	26462	40597	1.23%	0.336%
24	17.051	2233	2240	2247	rVB7	14249	39201	1.19%	0.324%
25	17.809	2363	2369	2376	rVB2	353870	582247	17.68%	4.813%
26	20.389	2801	2808	2815	rBV	2424217	3293461	100.00%	27.223%
27	22.169	3104	3111	3122	rBV	358664	672120	20.41%	5.556%
28	25.782	3712	3726	3739	rBV2	202828	652806	19.82%	5.396%

Sum of corrected areas: 12098039

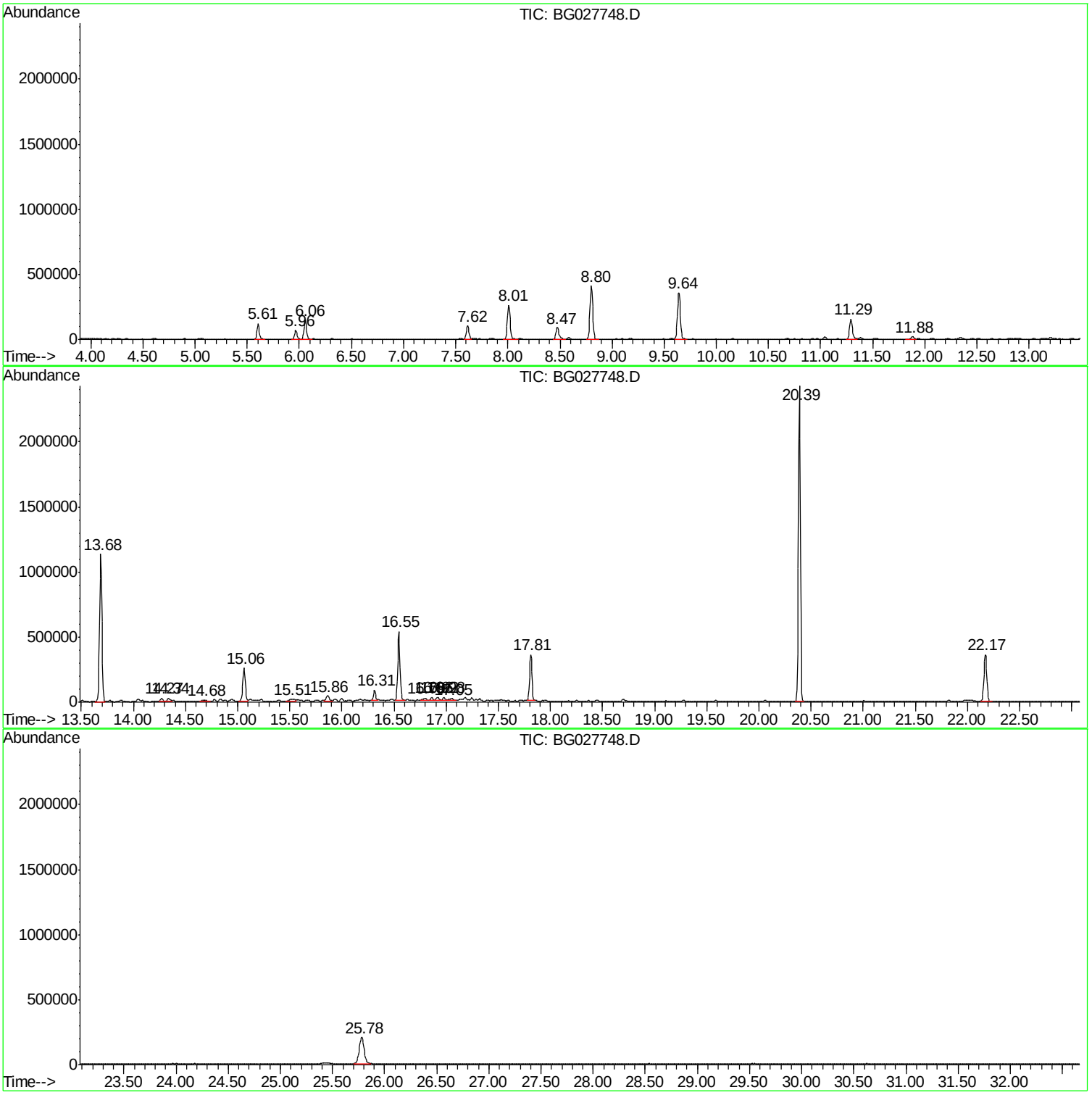
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.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 G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

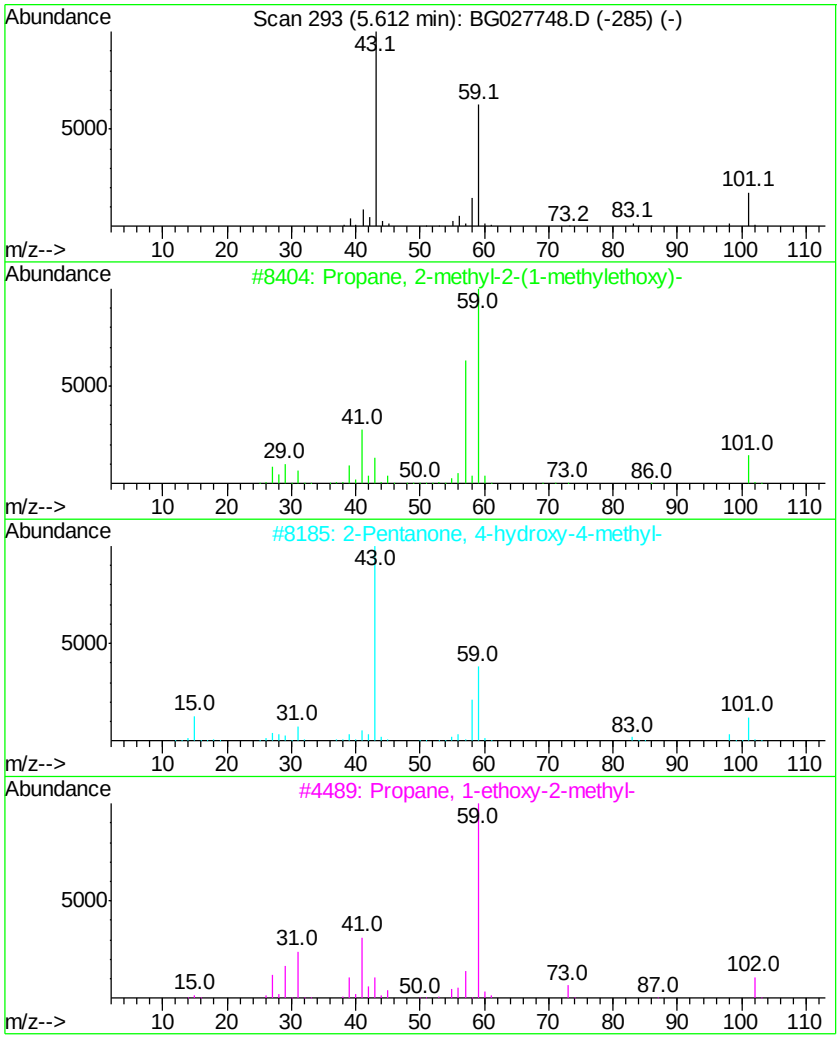
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

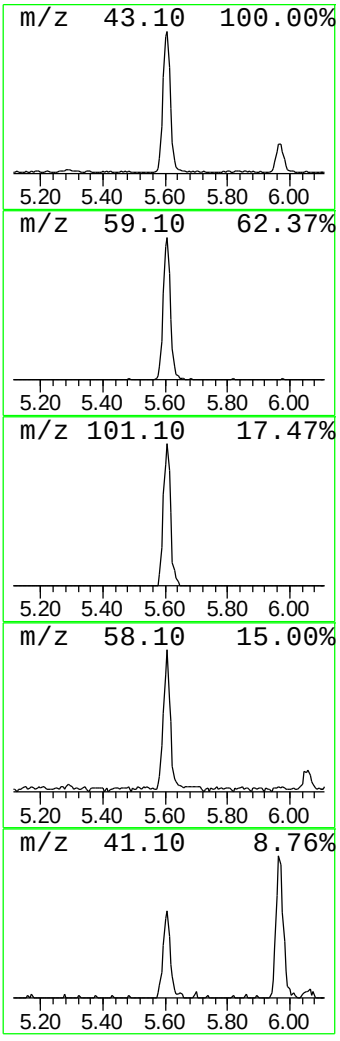
****

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	20.98 ng	199055	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	3-Hexanol	102	C6H14O	000623-37-0	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

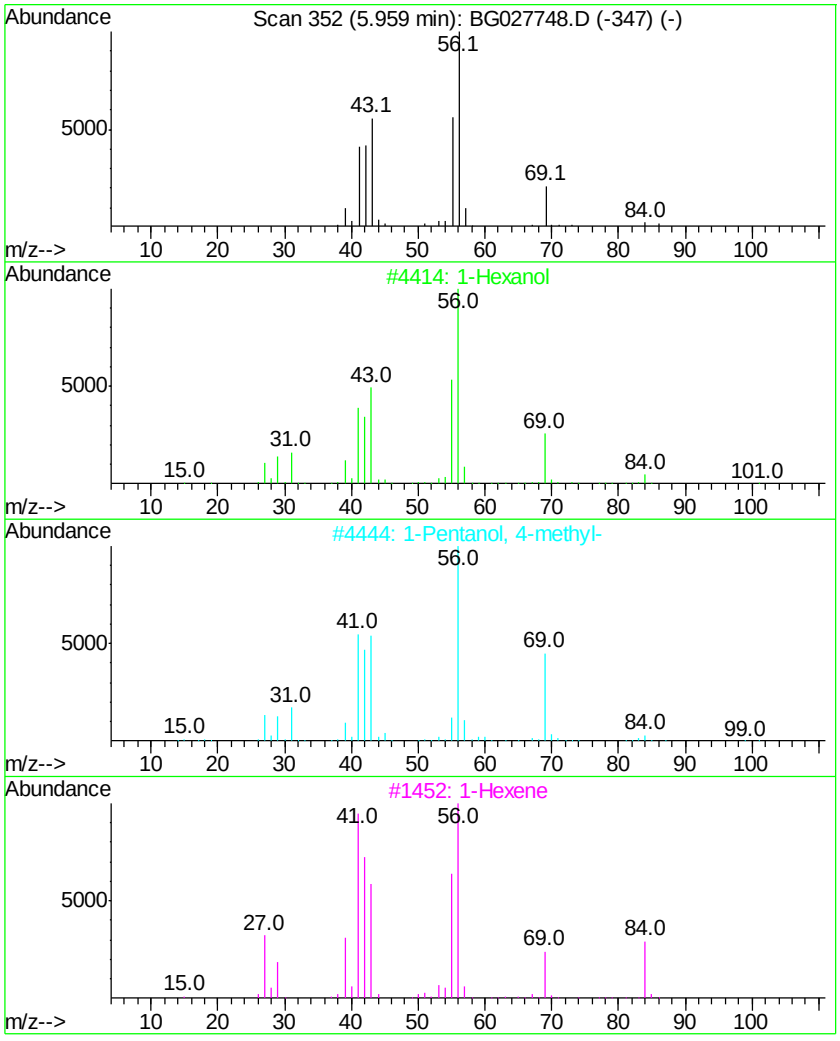
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

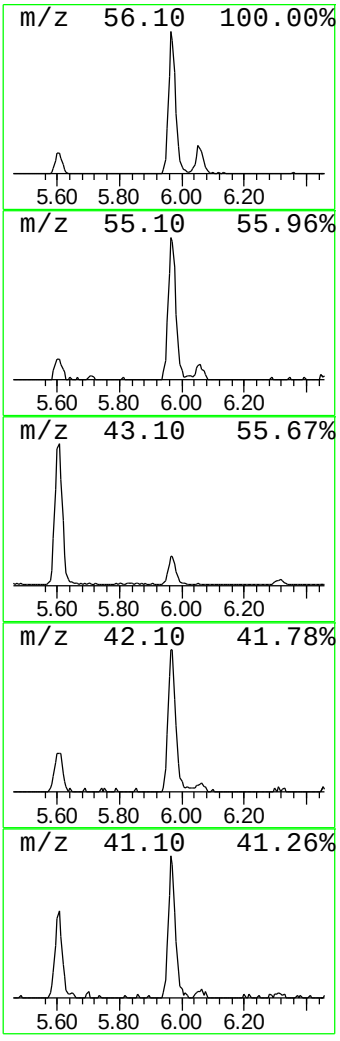
****

Peak Number 2 1-Hexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	12.18 ng	115526	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	74
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
3	1-Hexene	84	C6H12	000592-41-6	45
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	40
5	Methanamine, N-(1-methylbutylide...	99	C6H13N	022431-09-0	39





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

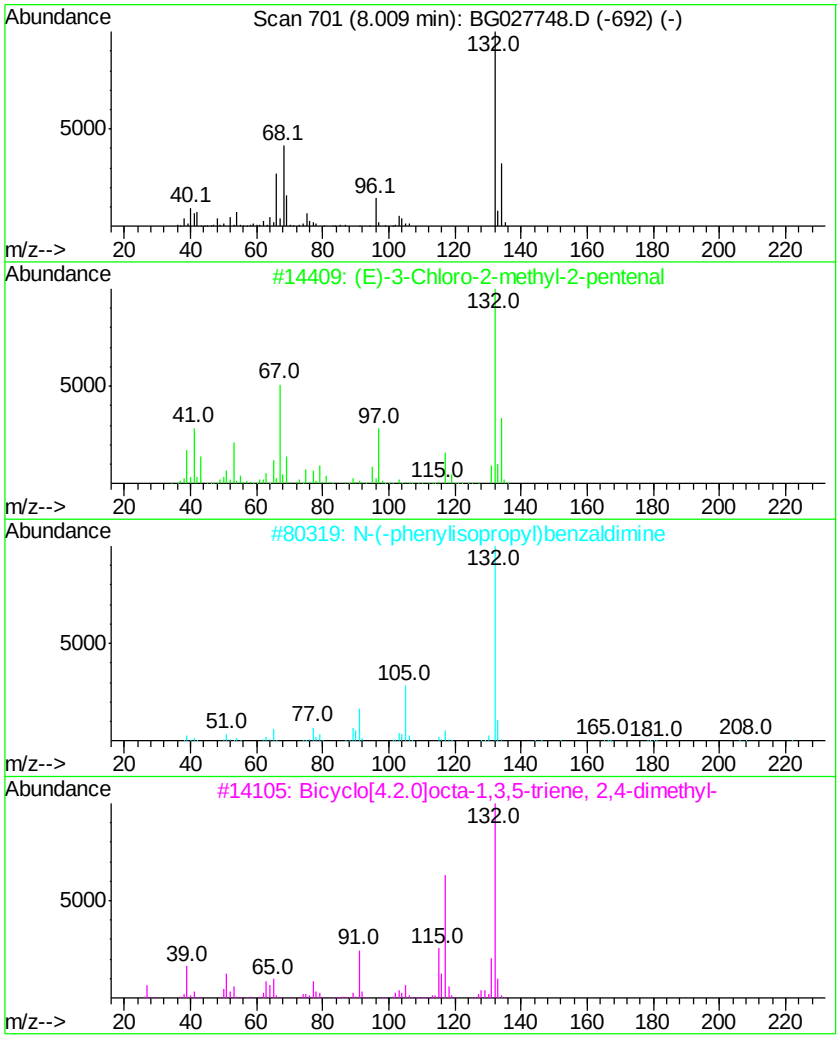
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

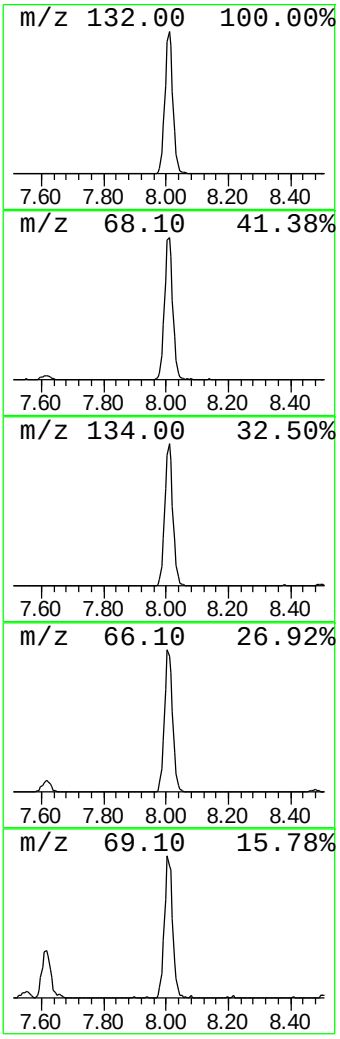
****

Peak Number 3 unknown8.01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	52.17 ng	495013	1,4-Dichlorobenzene-d4	8.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

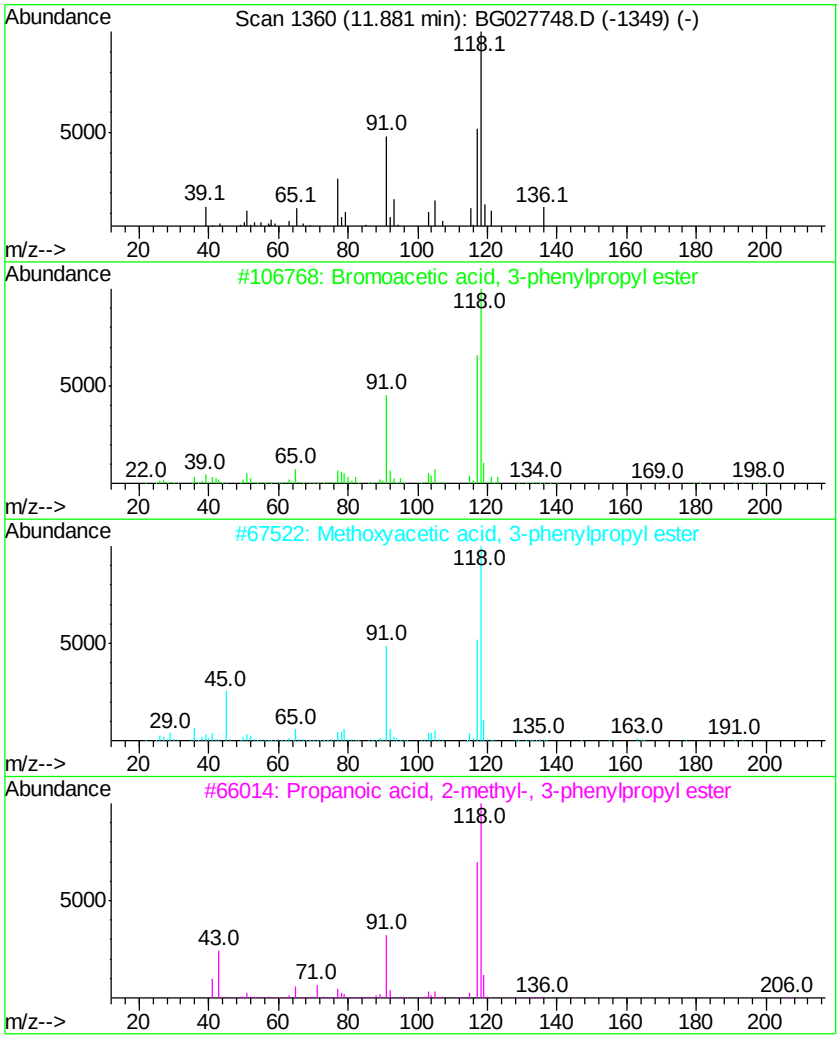
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

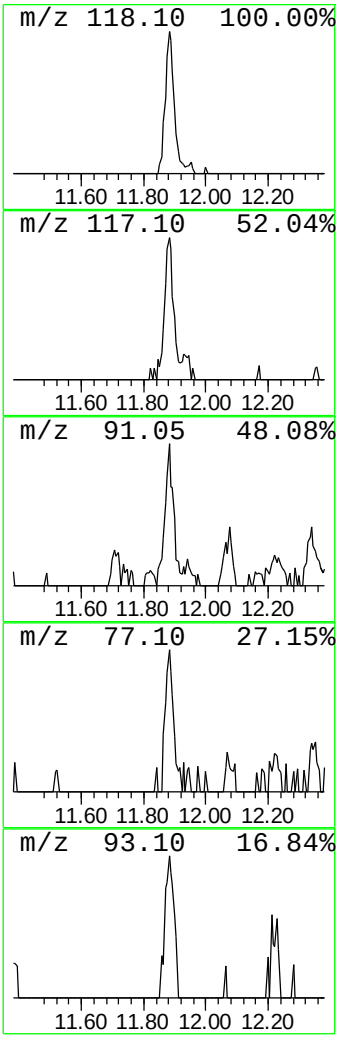
****

Peak Number 5 Bromoacetic acid, 3-phenylp... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.70 ng	40858	Naphthalene-d8	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, 3-phenylpropyl...	256	C11H13BrO2	059956-66-0	53
2	Methoxyacetic acid, 3-phenylprop...	208	C12H16O3	1000282-41-7	53
3	Propanoic acid, 2-methyl-, 3-phe...	206	C13H18O2	000103-58-2	53
4	1,3-Propanediol, 2-methyl-2-phenyl-	166	C10H14O2	024765-53-5	53
5	Dimethylmalonic acid, monochlori...	268	C14H17ClO3	1000361-84-8	53





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

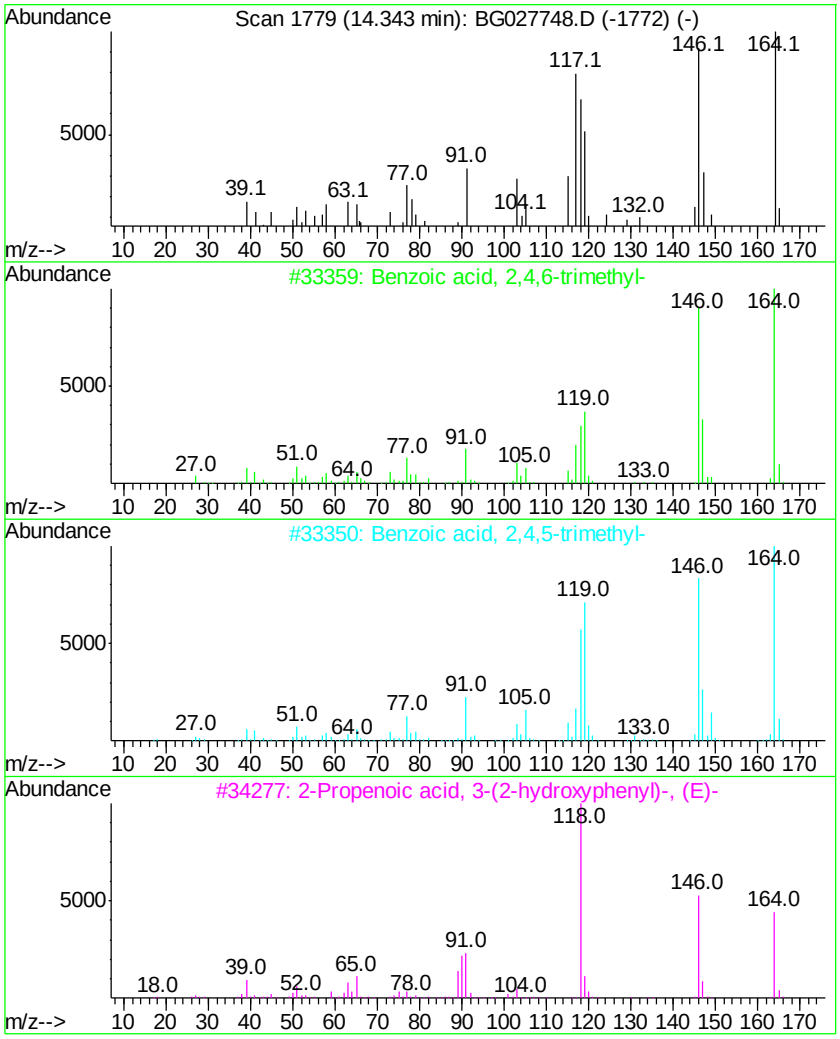
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

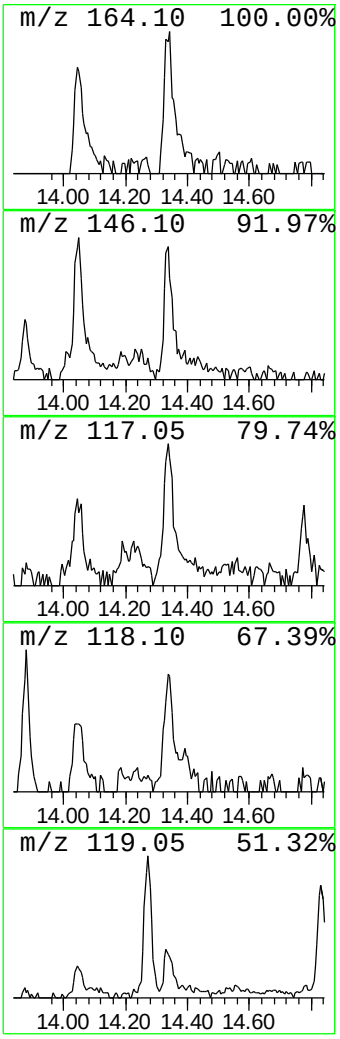
****

Peak Number 6 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.33 ng	52479	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	81
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	52
3	2-Propenoic acid, 3-(2-hydroxyph...	164	C9H8O3	000614-60-8	46
4	2-Propenoic acid, 3-(3-hydroxyph...	164	C9H8O3	014755-02-3	43
5	1H-Indole, 2,3-dihydro-5-nitro-	164	C8H8N2O2	032692-19-6	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

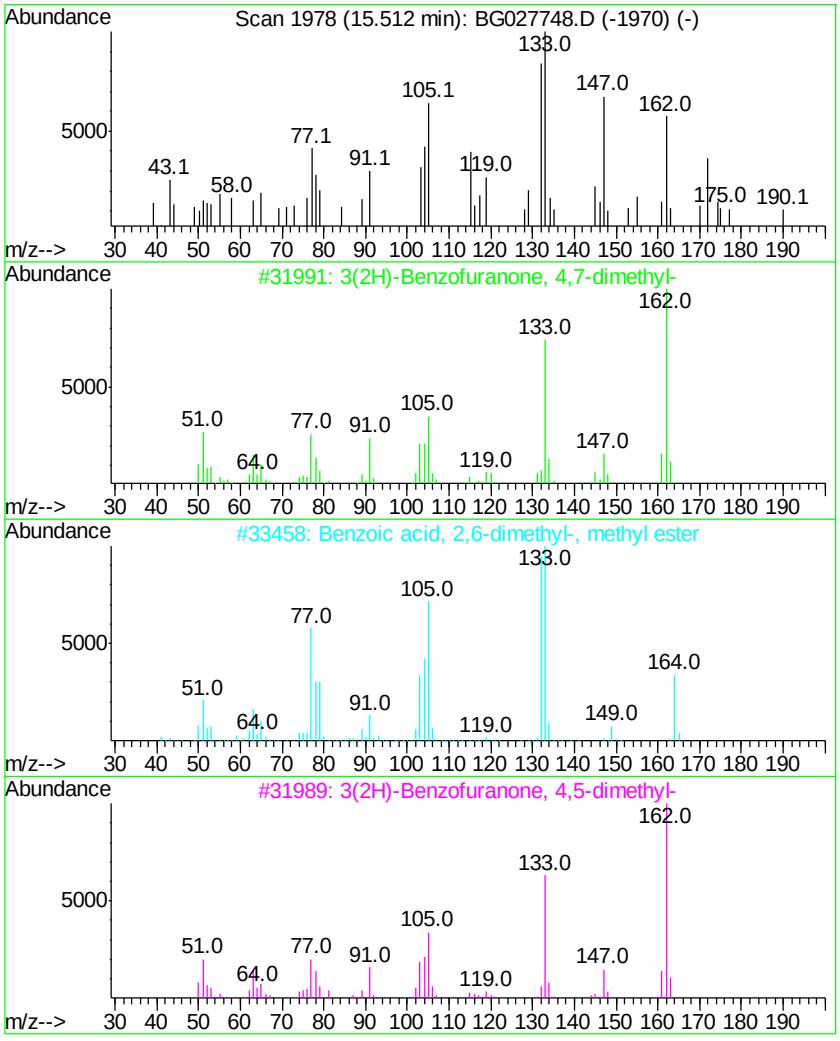
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

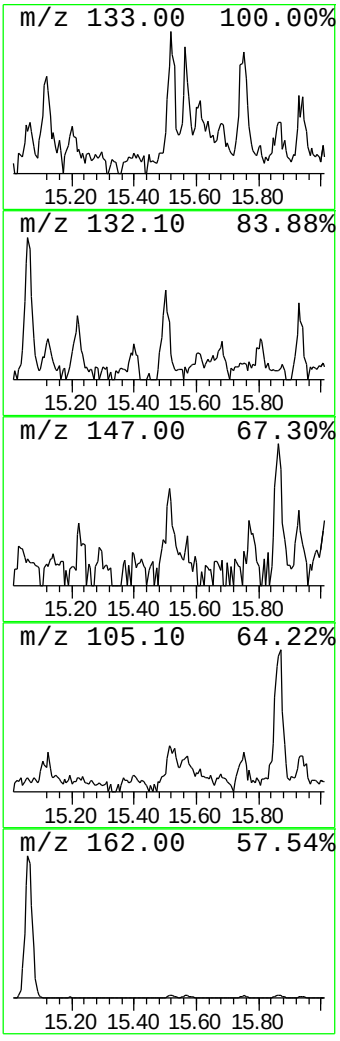
****

Peak Number 7 3(2H)-Benzofuranone, 4,7-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	3.17 ng	71292	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Benzofuranone, 4,7-dimethyl-	162	C10H10O2	020895-45-8	50
2	Benzoic acid, 2,6-dimethyl-, met...	164	C10H12O2	014920-81-1	46
3	3(2H)-Benzofuranone, 4,5-dimethyl-	162	C10H10O2	020895-42-5	46
4	2-Propanamine, N-(phenylmethylene)-	147	C10H13N	006852-56-8	41
5	1H-Indole, 4-methoxy-	147	C9H9NO	004837-90-5	38





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Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

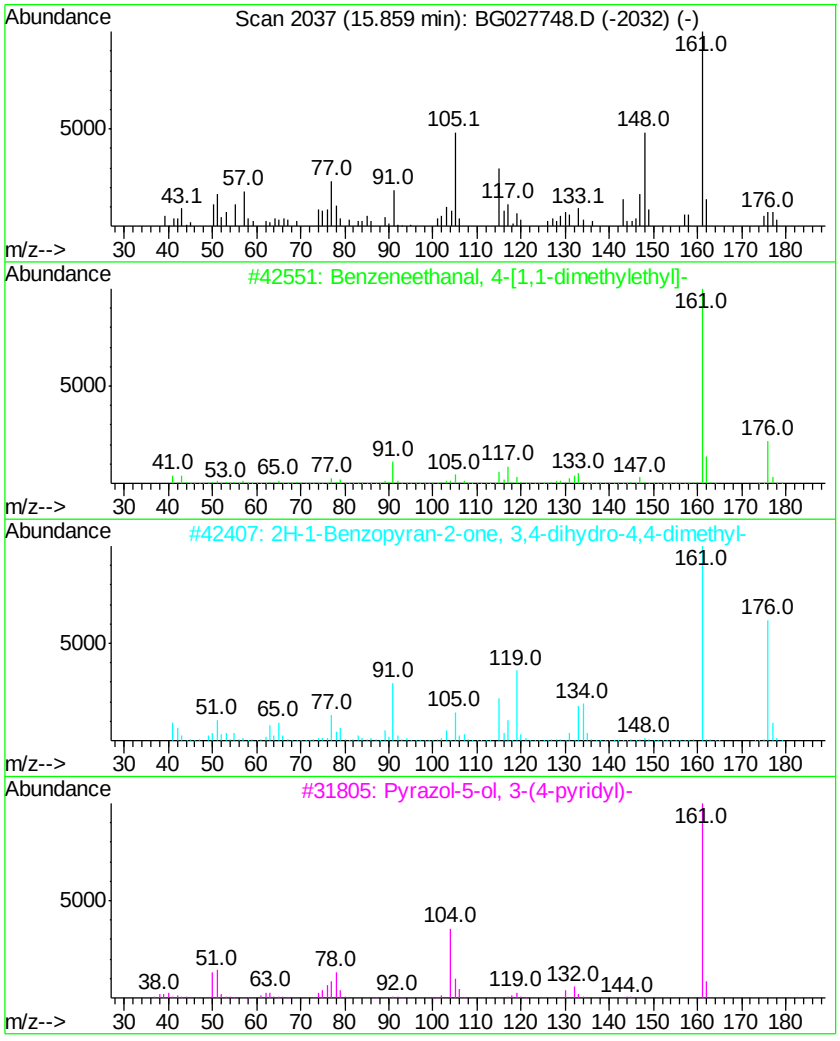
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

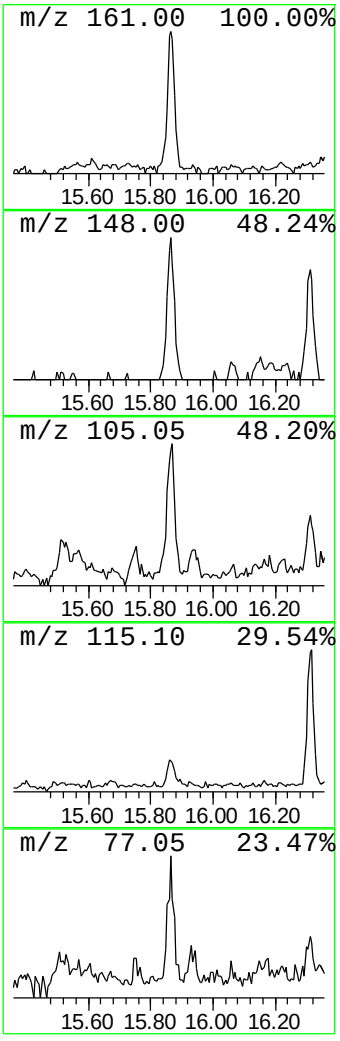
****

Peak Number 8 unknown15.86 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.31 ng	74388	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanal, 4-[1,1-dimethyle...	176	C12H16O	109347-45-7	46
2	2H-1-Benzopyran-2-one, 3,4-dihyd...	176	C11H12O2	029598-22-9	43
3	Pyrazol-5-ol, 3-(4-pyridyl)-	161	C8H7N3O	1000277-17-6	41
4	2-Quinolinol, 1-oxide	161	C9H7NO2	010285-97-9	38
5	1,3-2H-Isobenzofuranone, 3,3,7-t...	176	C11H12O2	057732-90-8	38





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Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

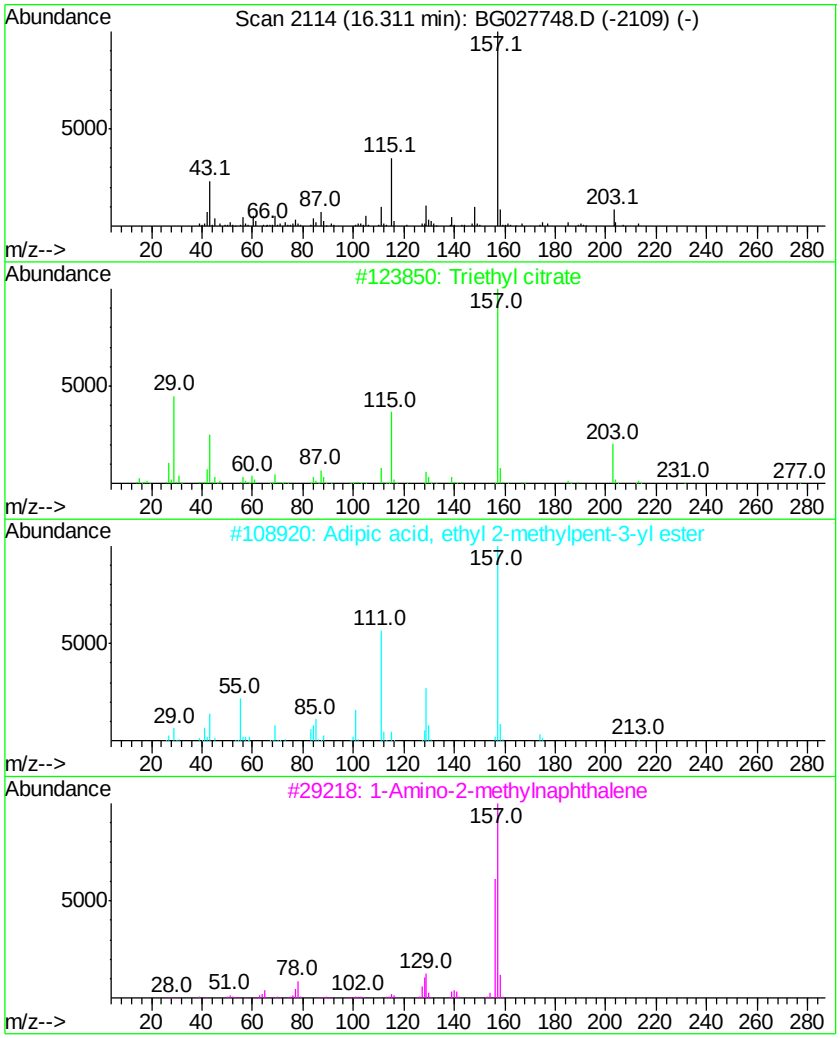
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

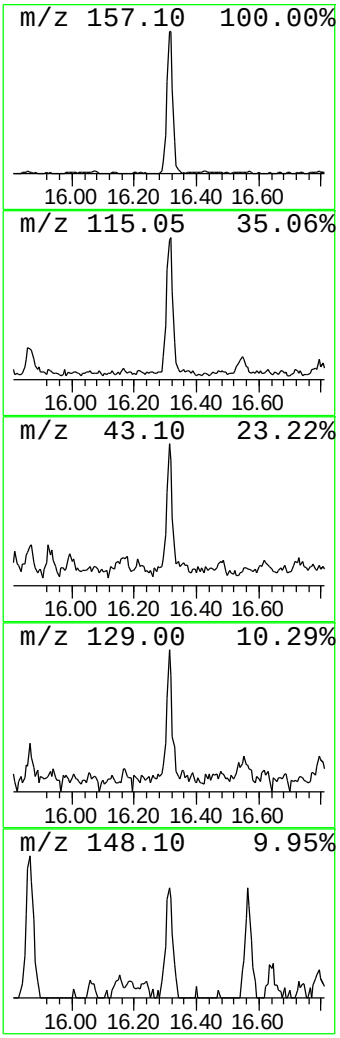
****

Peak Number 9 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	4.92 ng	110843	Acenaphthene-d10	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	Adipic acid, ethyl 2-methylpent-...	258	C14H26O4	1000353-55-5	53
3	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50
4	Adipic acid, 3,3-dimethylbut-2-y...	258	C14H26O4	1000353-66-5	50
5	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062917\
Data File : BG027748.D
Acq On : 29 Jun 2017 19:53
Operator : SJ/JU
Sample : I3938-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062817.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
Propane, 2-methyl...	5.61	21.0	ng	199055	1	8.48	189752	20.0
1-Hexanol	5.96	12.2	ng	115526	1	8.48	189752	20.0
unknown8.01	8.01	52.2	ng	495013	1	8.48	189752	20.0
Bromoacetic acid,...	11.88	2.7	ng	40858	2	11.29	302790	20.0
Benzoic acid, 2,4...	14.34	2.3	ng	52479	3	15.06	450137	20.0
3(2H)-Benzofurano...	15.51	3.2	ng	71292	3	15.06	450137	20.0
unknown15.86	15.86	3.3	ng	74388	3	15.06	450137	20.0
Triethyl citrate	16.31	4.9	ng	110843	3	15.06	450137	20.0