LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029314.D
Acq On : 17 Oct 2017 23:30
Operator : SJ/JU
Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-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-BG101617.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	5.244	327	333	341	rBV	79781	122818	1.22%	0.337%
2	5.720	407	414	426	rBV	452568	728565	7.25%	1.999%
3	7.318	678	686	694	rBV	309684	525908	5.24%	1.443%
4	7.700	743	751	763	rBV	824857	1427322	14.21%	3.916%
5	8.170	824	831	836	rBV	238456	408882	4.07%	1.122%
6	8.223	836	840	847	rVB	83066	131614	1.31%	0.361%
7	8.493	878	886	897	rBV	987878	1758469	17.51%	4.825%
8	9.333	1018	1029	1039	rBV	865390	1585445	15.78%	4.350%
9	10.984	1302	1310	1319	rBV	382689	688715	6.86%	1.890%
10	13.417	1716	1724	1733	rBV	2542048	4094193	40.76%	11.234%
11	14.786	1950	1957	1967	rBV2	634521	1026496	10.22%	2.817%
12	16.266	2202	2209	2226	rBV	1326418	2042457	20.33%	5.604%
13	17.524	2416	2423	2433	rBV2	824459	1255231	12.50%	3.444%
14	18.916	2655	2660	2666	rBV	66737	127690	1.27%	0.350%
15	19.562	2765	2770	2781	rBV	448980	662959	6.60%	1.819%
16	20.009	2840	2846	2856	rBV	7072909	10044537	100.00%	27.560%
17	20.115	2859	2864	2876	rVB	4158536	5730456	57.05%	15.723%
18	20.808	2978	2982	2986	rBV	161911	183799	1.83%	0.504%
19	21.172	3036	3044	3051	rBV2	131333	257593	2.56%	0.707%
20	21.531	3101	3105	3116	rVB2	85361	155124	1.54%	0.426%
21	21.795	3144	3150	3162	rVB2	860642	1400627	13.94%	3.843%
22	22.112	3199	3204	3213	rBV2	84625	143903	1.43%	0.395%
23	23.276	3396	3402	3409	rBV2	71680	167576	1.67%	0.460%
24	24.098	3536	3542	3553	rBV3	69175	173899	1.73%	0.477%
25	25.103	3703	3713	3726	rVB2	485102	1488690	14.82%	4.085%
26	25.867	3837	3843	3854	rVB7	36065	112792	1.12%	0.309%

Sum of corrected areas: 36445760

LSC Report - Integrated Chromatogram

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Data File : BG029314.D
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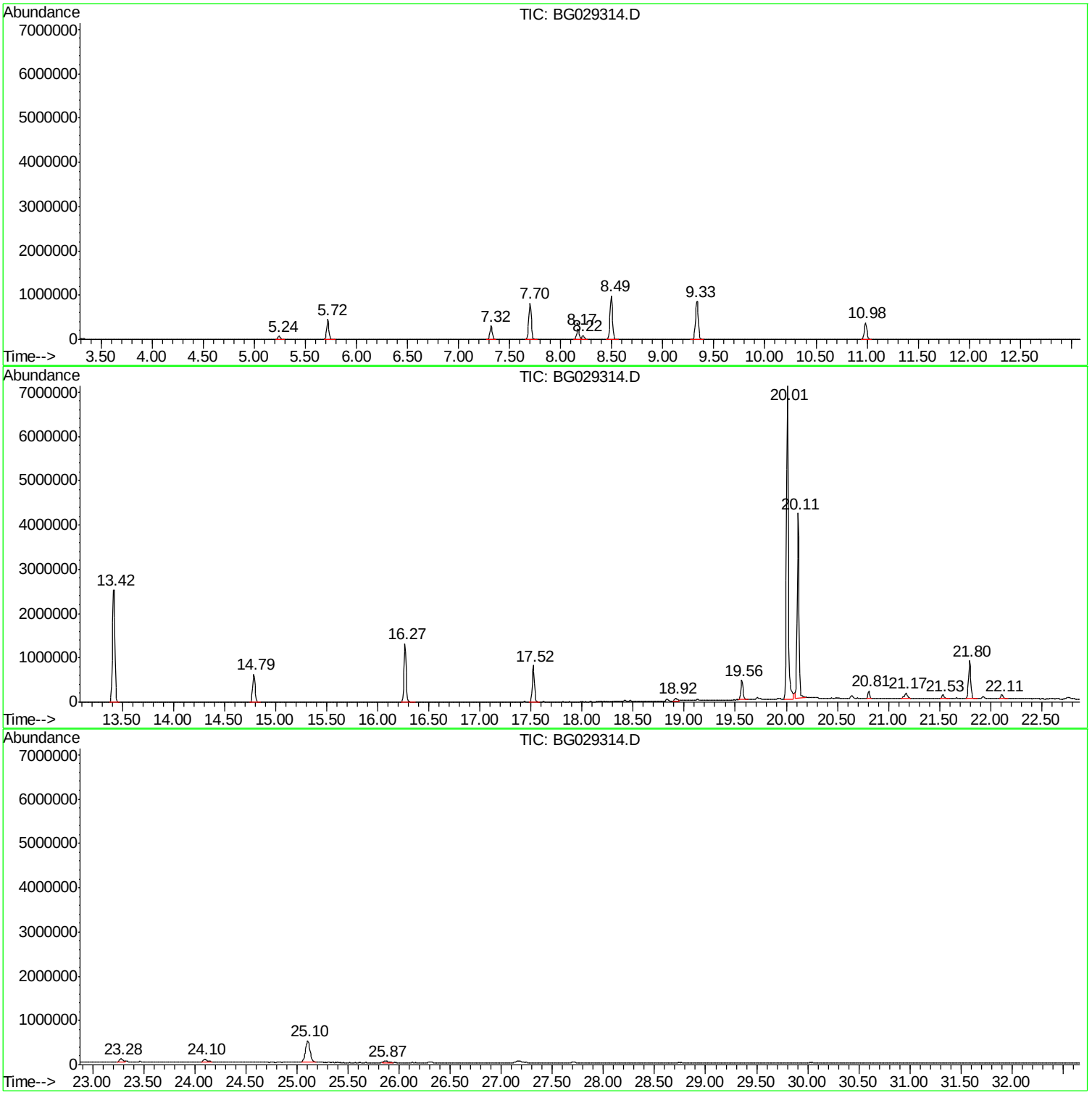
Operator : SJ/JU
Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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

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Instrument : BNA_G
ClientSampleId : HW-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

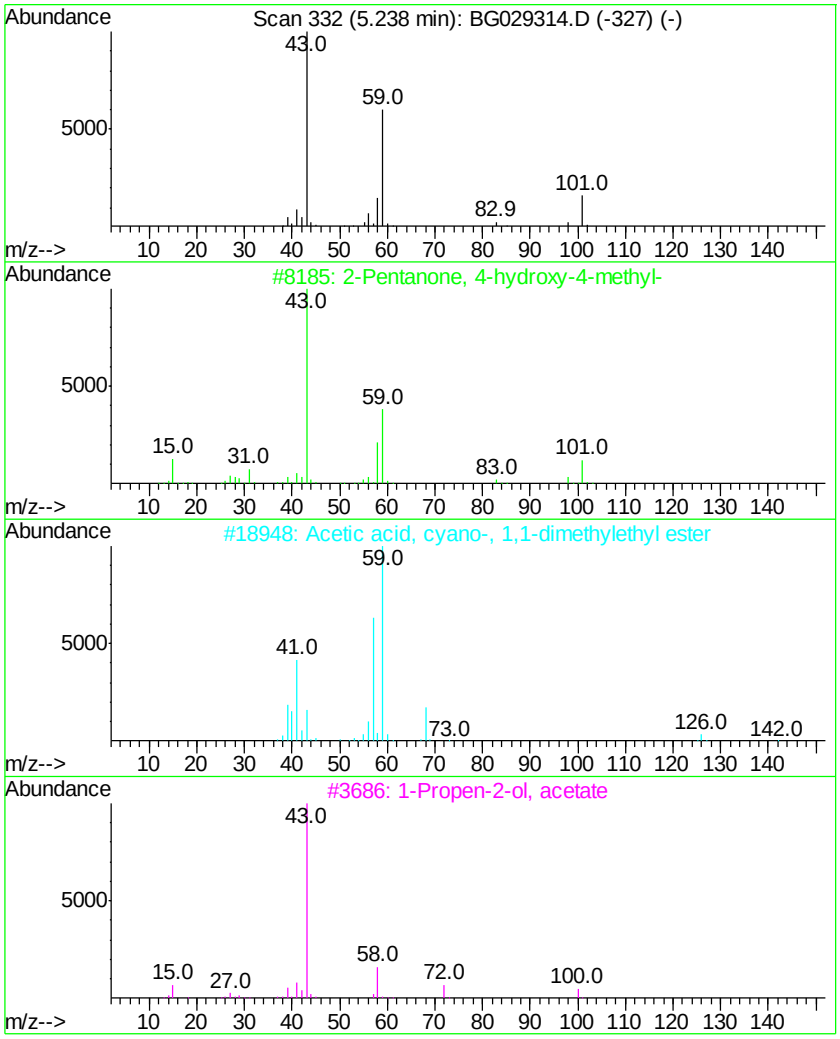
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

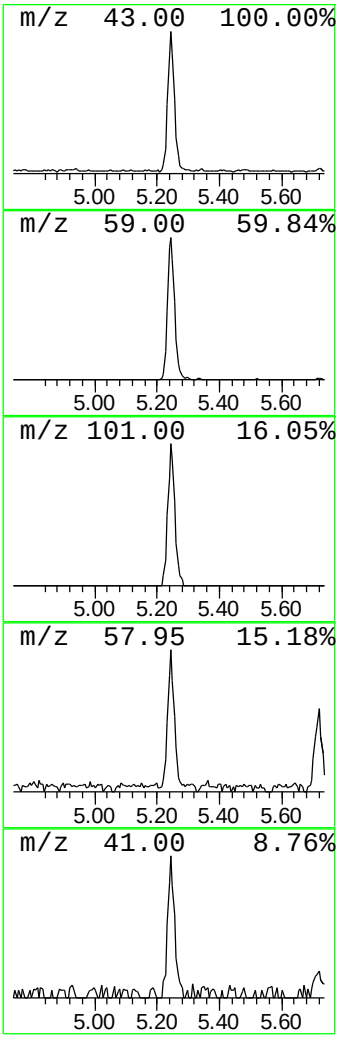
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	6.01 ng	122818	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/JU
Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

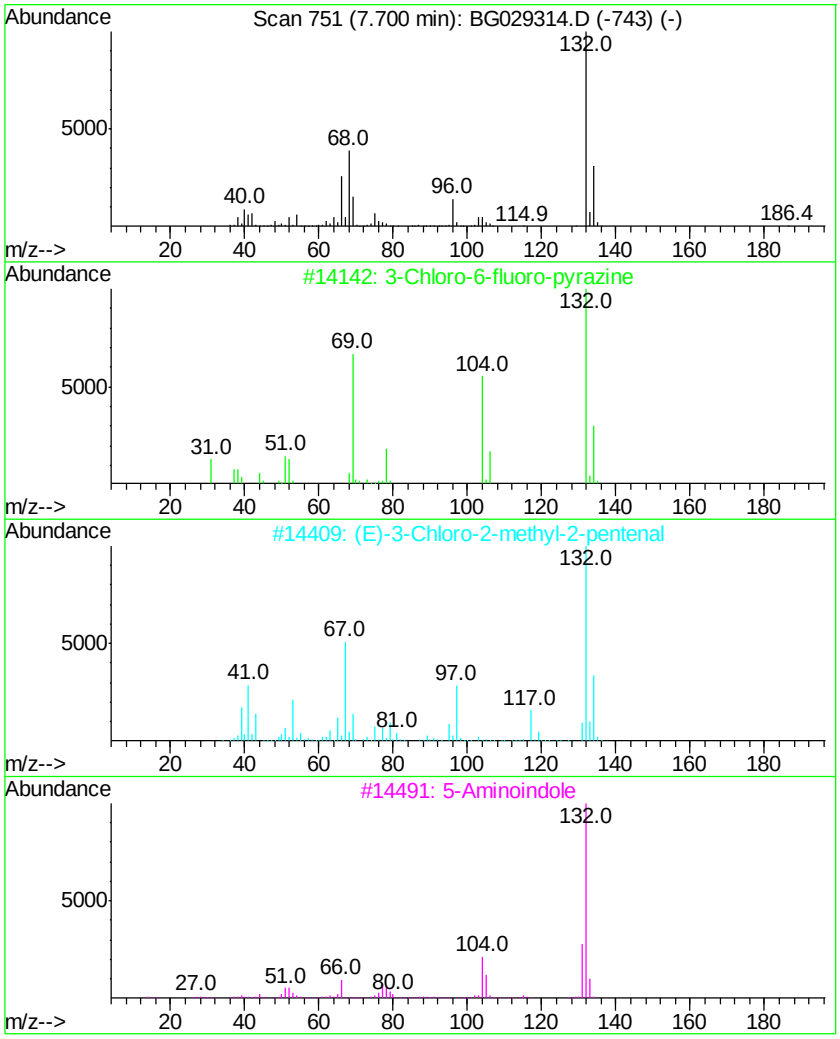
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

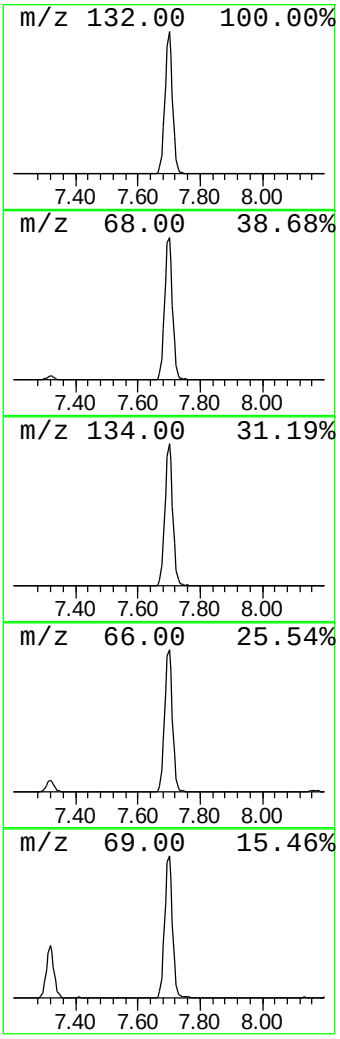
****

Peak Number 2 unknown7.70 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	69.82 ng	1427320	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
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Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

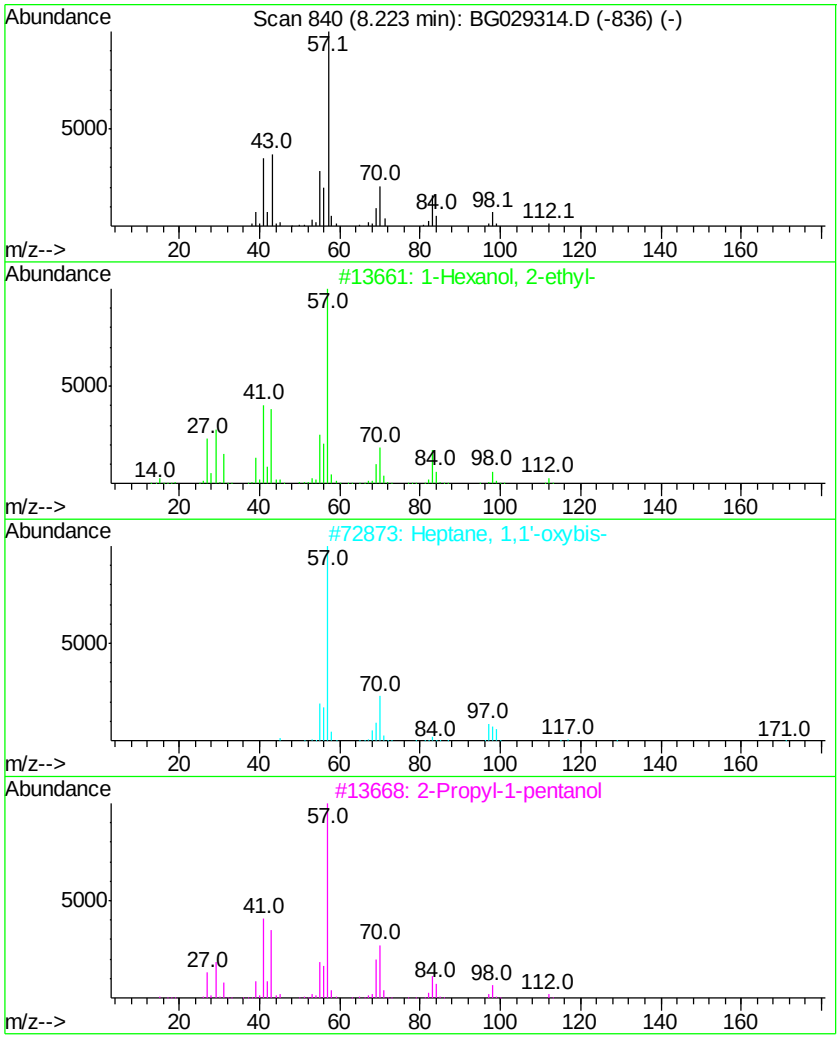
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

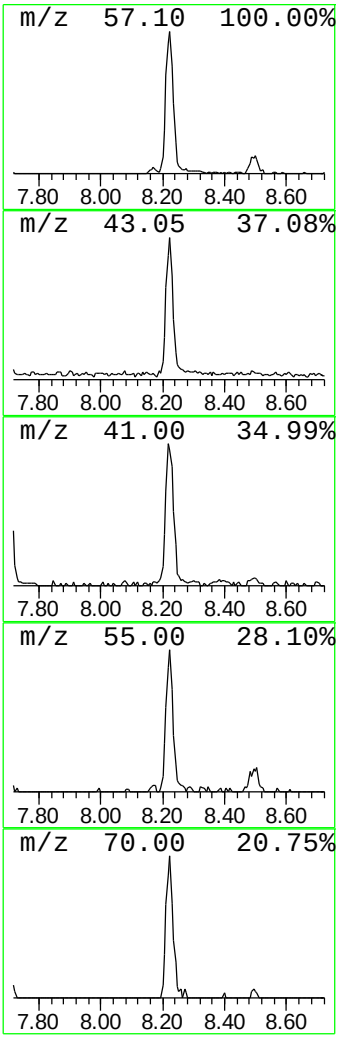
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.22	6.44 ng	131614	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50





Library Search Compound Report

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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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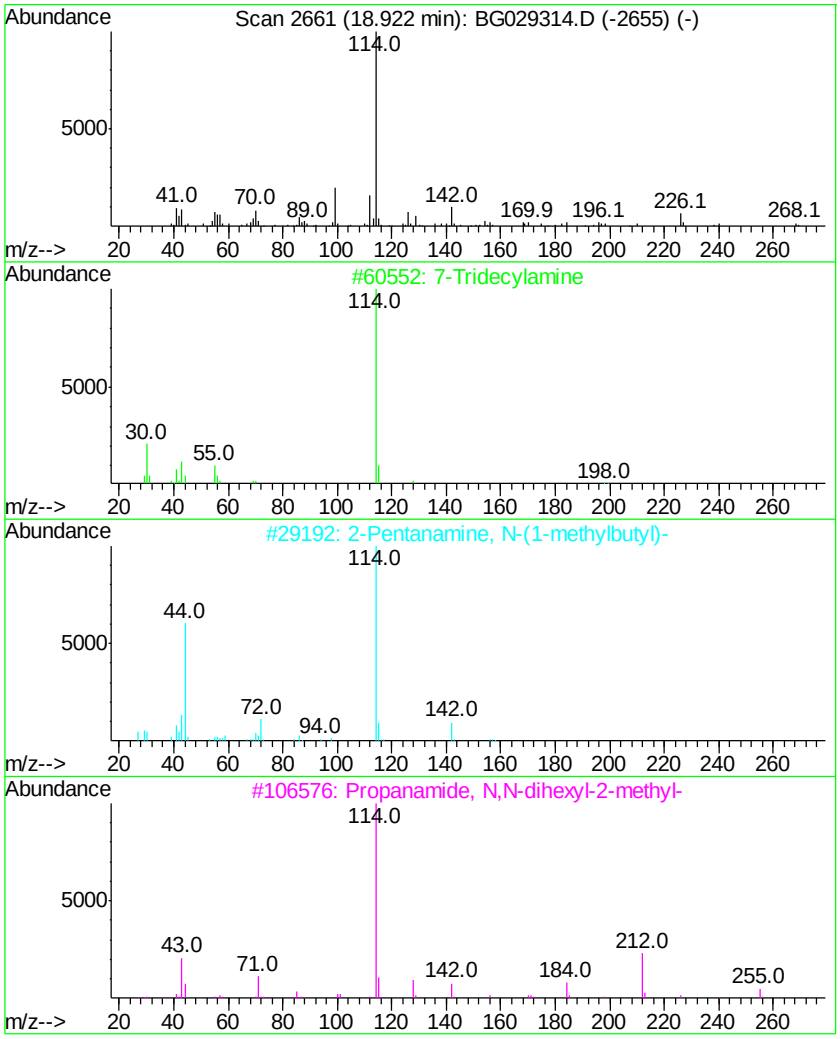
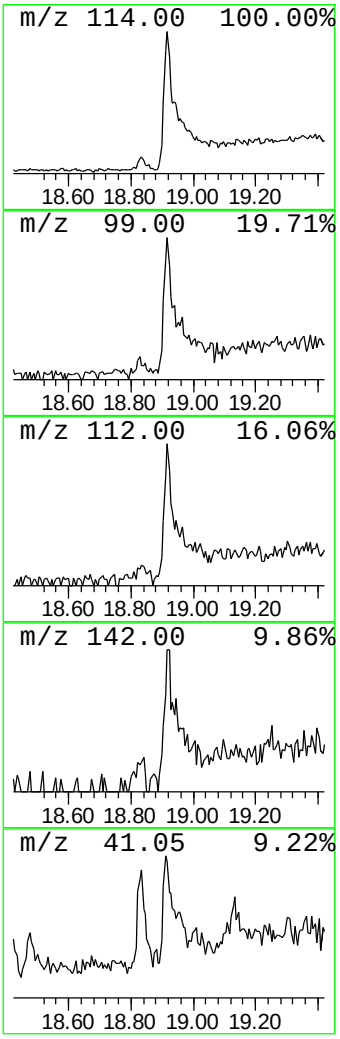
****

Peak Number 5 unknown18.92 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	2.03 ng	127690	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tridecylamine	199	C13H29N	022513-16-2	47
2	2-Pentanamine, N-(1-methylbutyl)-	157	C10H23N	040221-44-1	47
3	Propanamide, N,N-dihexyl-2-methyl-	255	C16H33NO	1000308-08-2	40
4	Oxazolidine, 2,2-diethyl-3-methyl-	143	C8H17NO	161500-43-2	38
5	Propanamide, 3-(4-morpholyl)-N-(...	346	C13H16BrClN2O2	1000266-68-9	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
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Operator : SJ/JU
Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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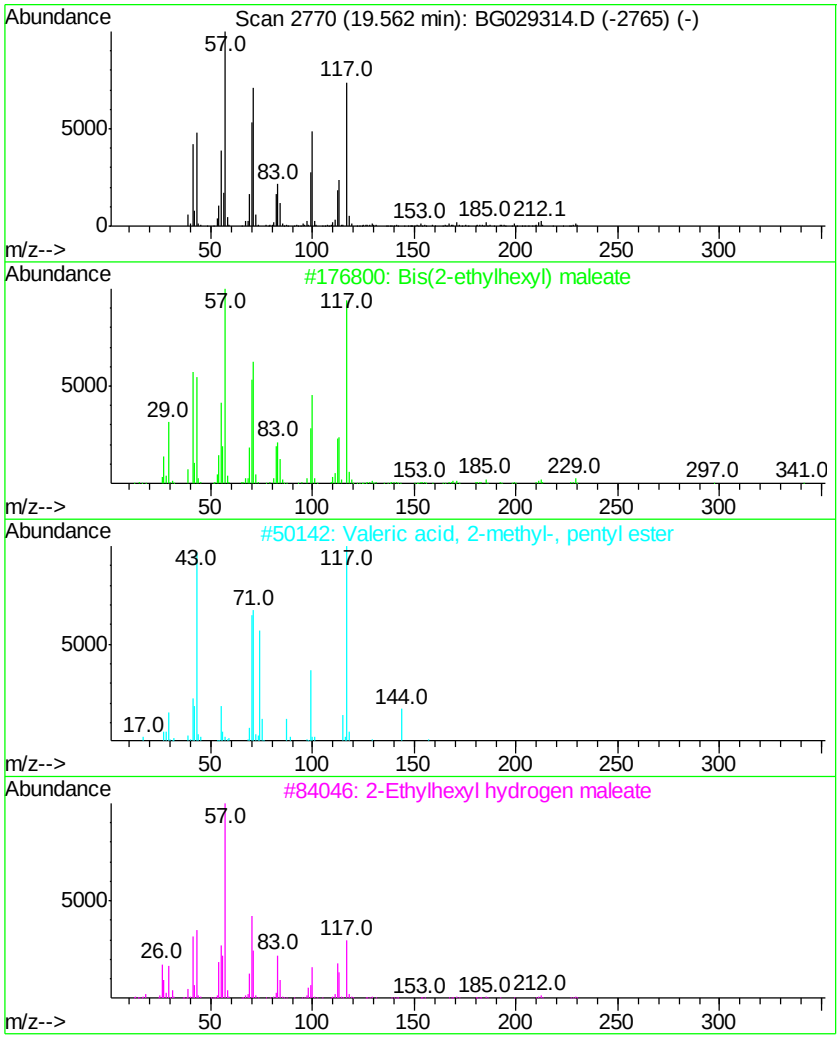
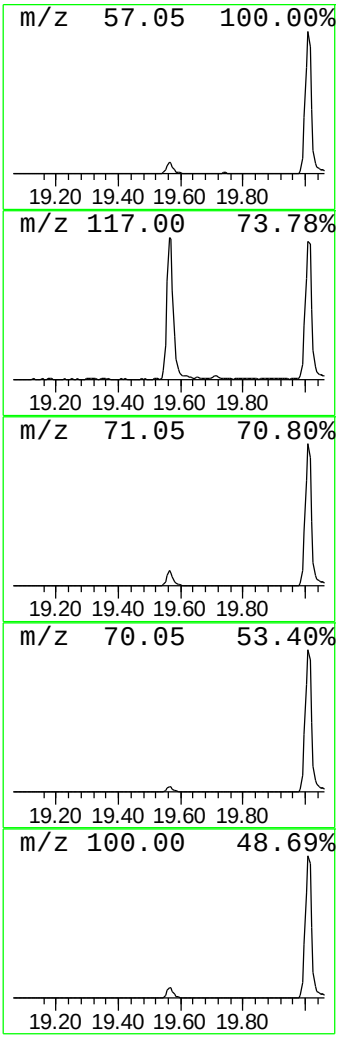
****

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.56	10.56 ng	662959	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	91
2	Valeric acid, 2-methyl-, pentyl ...	186	C11H22O2	006297-48-9	47
3	2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	46
4	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	35
5	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	27





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

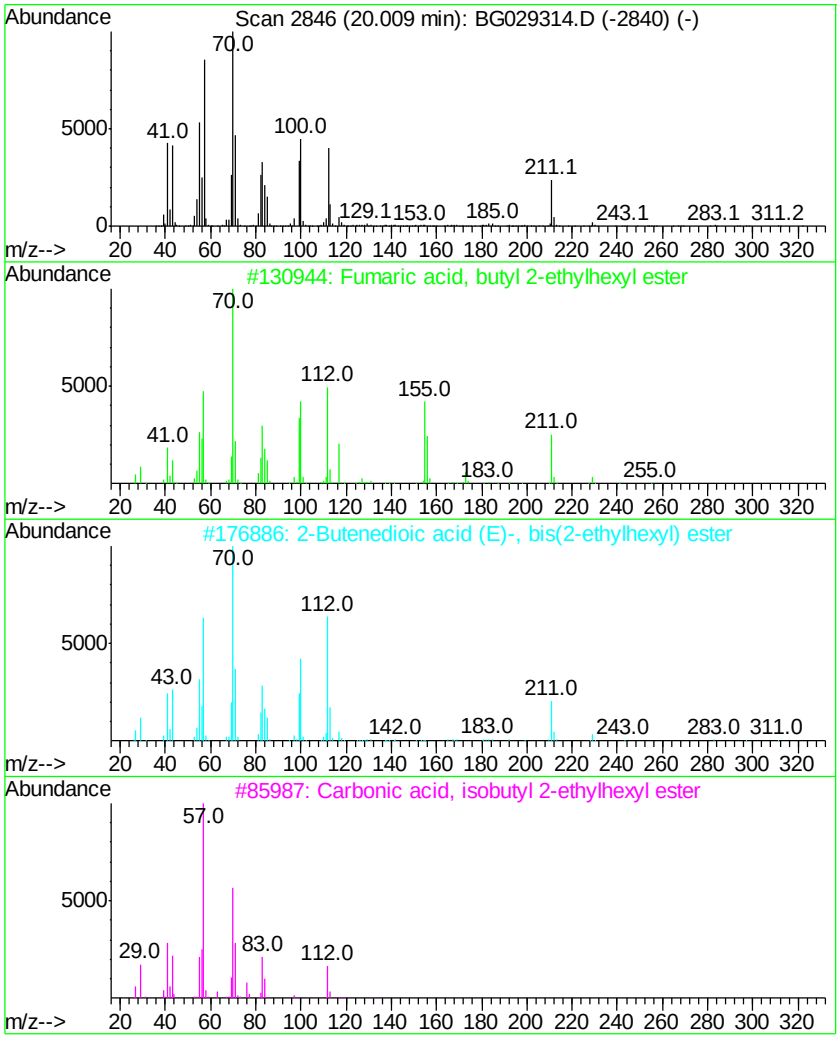
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

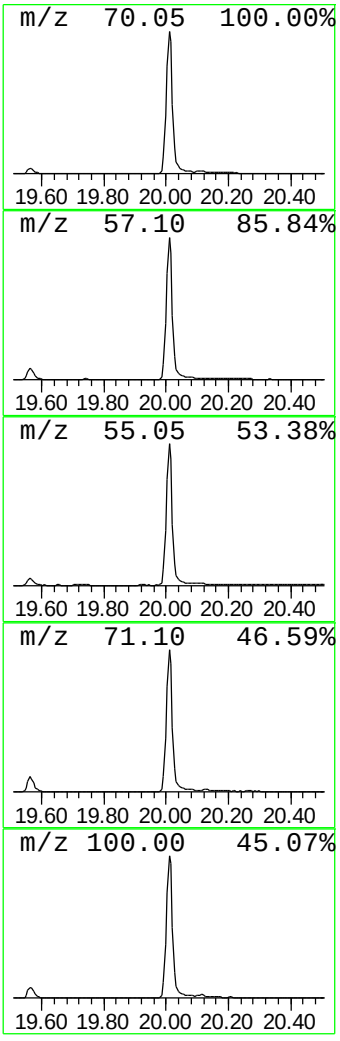
****

Peak Number 7 Fumaric acid, butyl 2-ethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.01	143.43 ng	10044500	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, butyl 2-ethylhexyl...	284	C16H28O4	1000339-13-8	86
2	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	72
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	50
4	2-Octene, (Z)-	112	C8H16	007642-04-8	38
5	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	38





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

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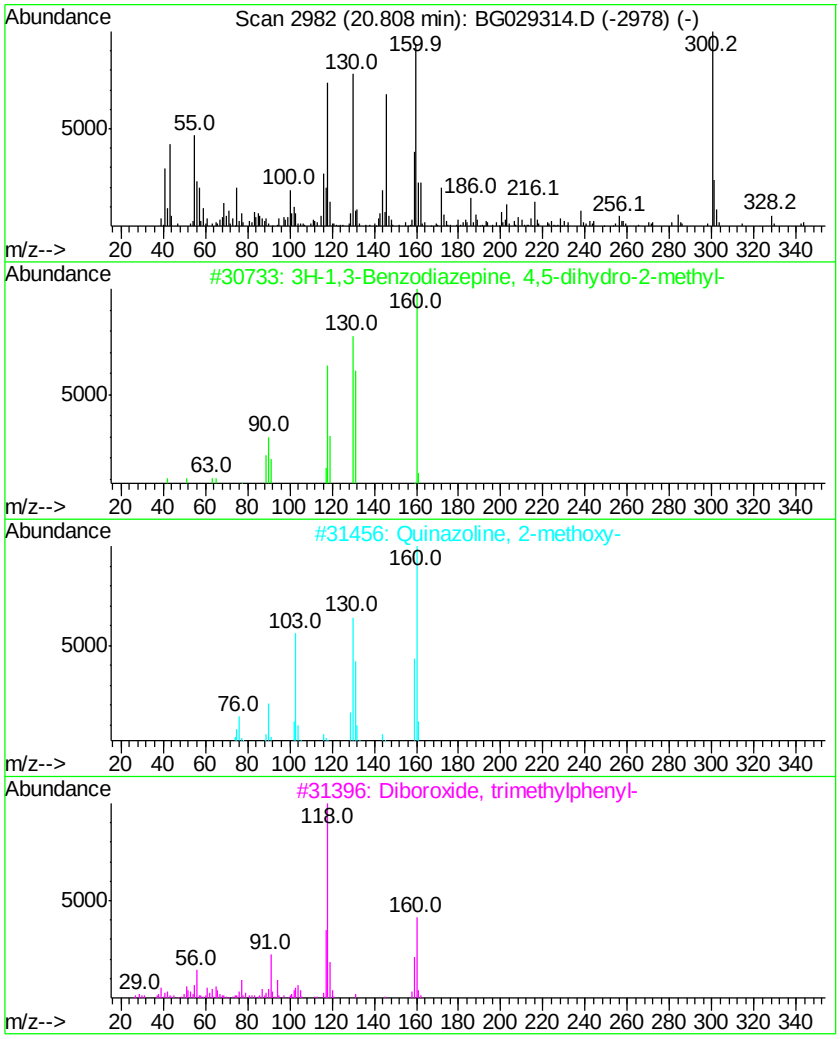
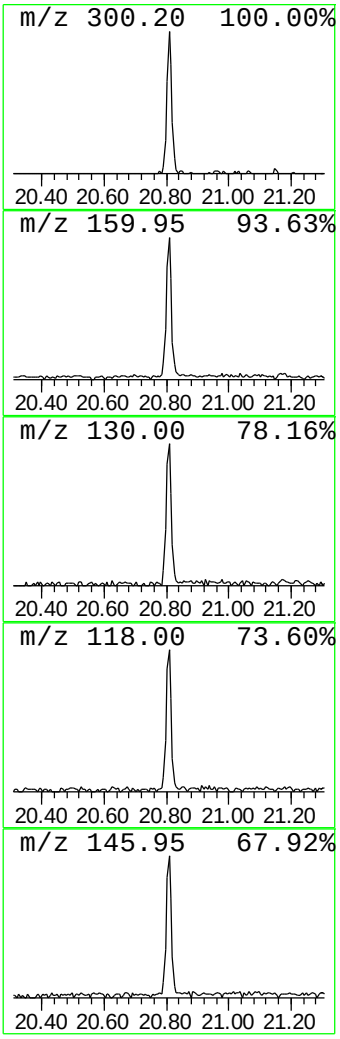
Peak Number 8 unknown20.81 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	2.62 ng	183799	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,3-Benzodiazepine, 4,5-dihyd...	160	C10H12N2	046035-38-5	38
2	Quinazoline, 2-methoxy-	160	C9H8N2O	006141-15-7	30
3	Diboroxide, trimethylphenyl-	160	C9H14B2O	1000162-60-0	27
4	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	25
5	Cyclohexylamine, N,N-dimethyl-1-...	203	C14H21N	002201-17-4	15





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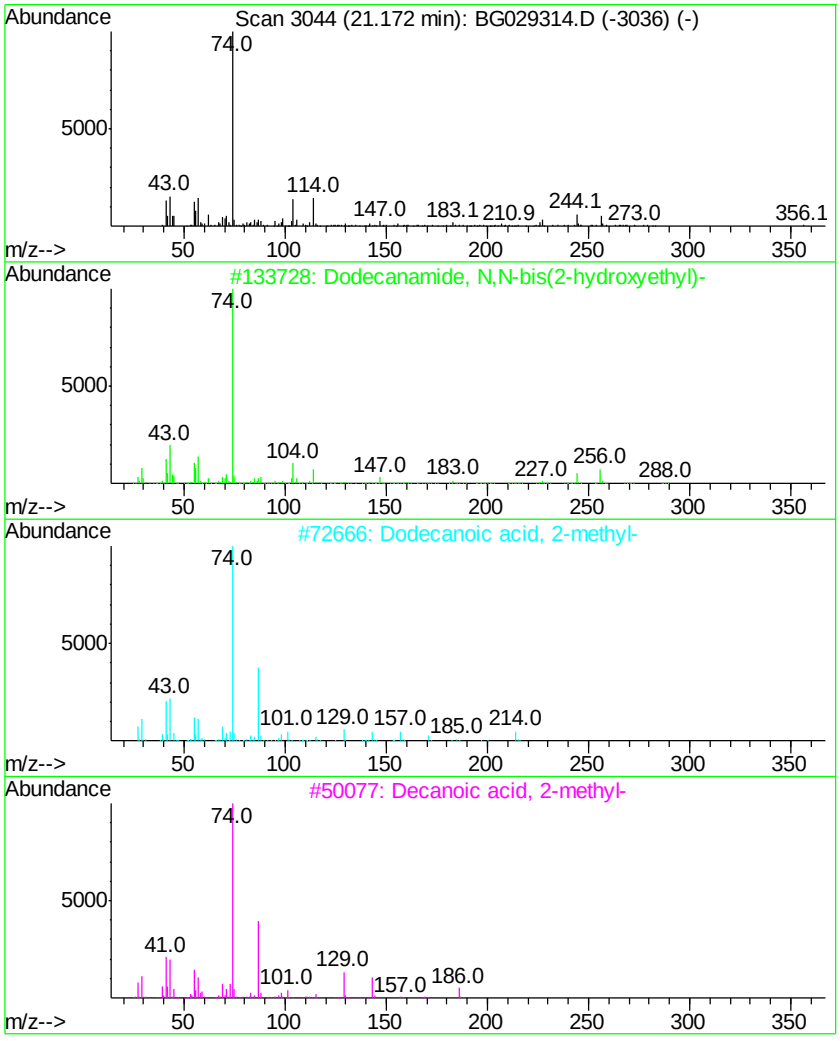
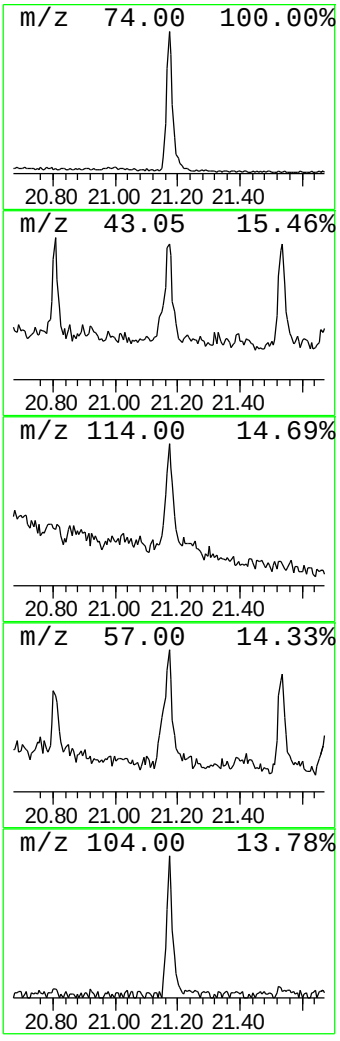
****

Peak Number 9 Dodecanamide, N,N-bis(2-hyd... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	3.68 ng	257593	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide, N,N-bis(2-hydroxye...	287	C16H33NO3	000120-40-1	80
2	Dodecanoic acid, 2-methyl-	214	C13H26O2	002874-74-0	38
3	Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	38
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	33
5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	28





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TIC Library : C:\Database\NIST11.L
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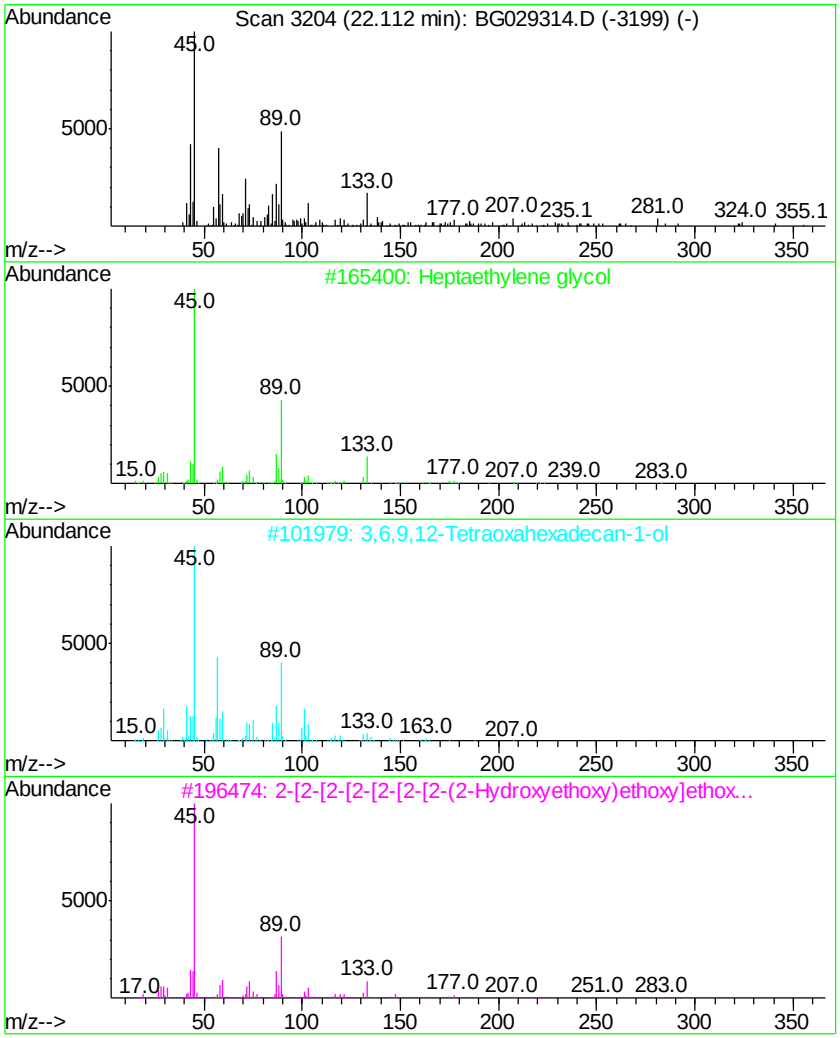
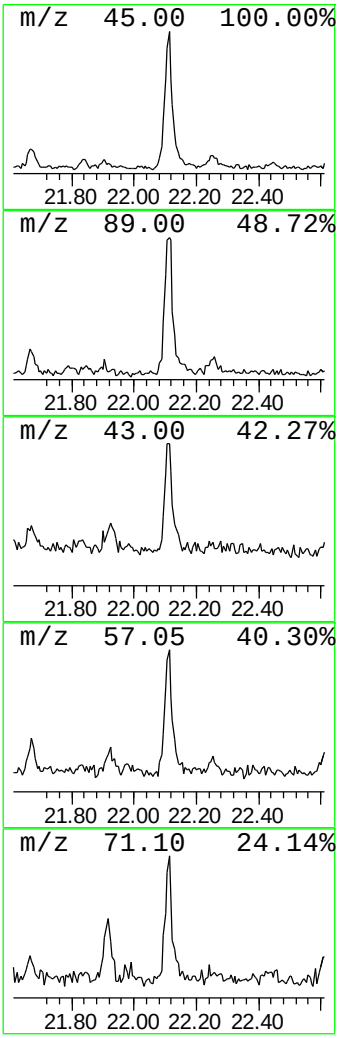
****

Peak Number 11 Heptaethylene glycol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	2.05 ng	143903	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
2	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	90
3	2-[2-[2-[2-[2-[2-(2-Hydroxyvet...	370	C16H34O9	005117-19-1	87
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	87
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	86





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
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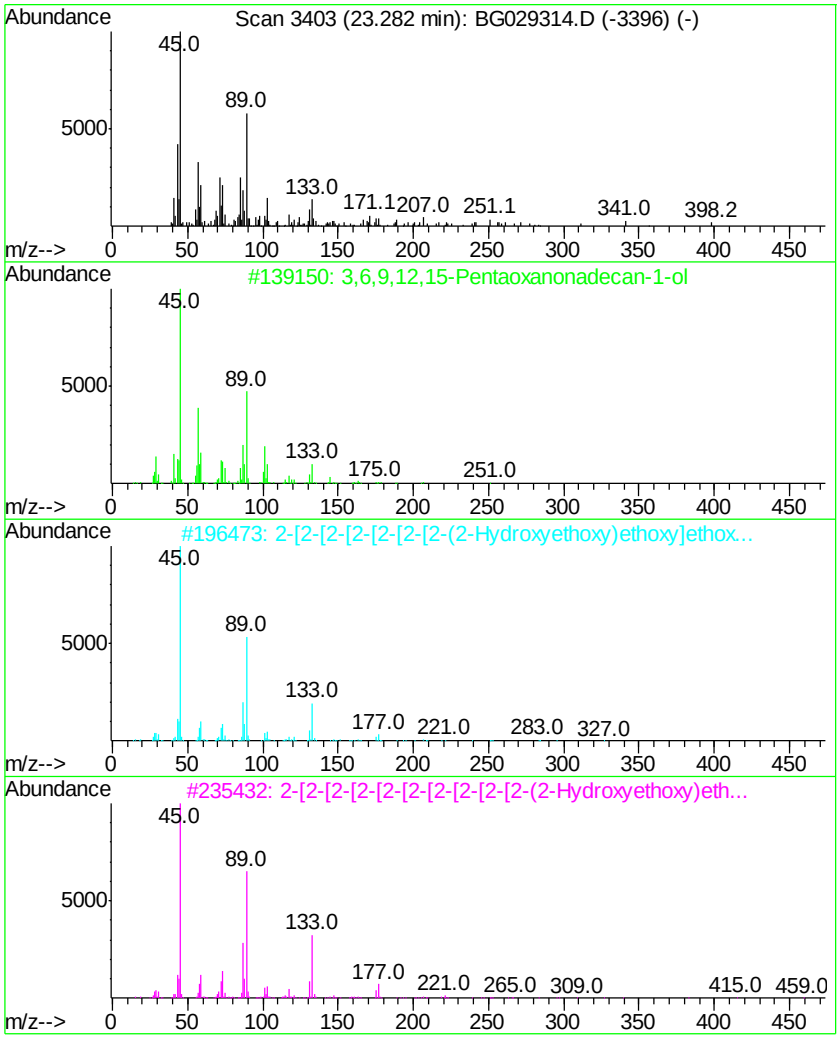
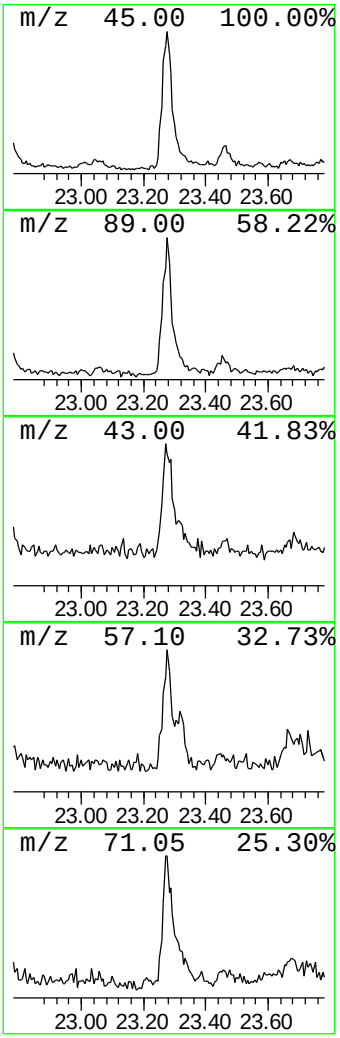
****

Peak Number 12 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	2.39 ng	167576	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	87
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	83
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	80
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101717\
Data File : BG029314.D
Acq On : 17 Oct 2017 23:30
Operator : SJ/JU
Sample : I5817-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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...	5.24	6.0	ng	122818	1	8.17	408882	20.0
unknown7.70	7.70	69.8	ng	1427320	1	8.17	408882	20.0
1-Hexanol, 2-ethyl-	8.22	6.4	ng	131614	1	8.17	408882	20.0
unknown18.92	18.92	2.0	ng	127690	4	17.52	1255230	20.0
Bis(2-ethylhexyl)...	19.56	10.6	ng	662959	4	17.52	1255230	20.0
Fumaric acid, but...	20.01	143.4	ng	10044500	5	21.80	1400630	20.0
unknown20.81	20.81	2.6	ng	183799	5	21.80	1400630	20.0
Dodecanamide, N,N...	21.17	3.7	ng	257593	5	21.80	1400630	20.0
Heptaethylene glycol	22.11	2.0	ng	143903	5	21.80	1400630	20.0
3,6,9,12,15-Penta...	23.28	2.4	ng	167576	5	21.80	1400630	20.0