LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029313.D
Acq On : 17 Oct 2017 22:50
Operator : SJ/JU
Sample : I5817-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : HW-3

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	5.245	327	333	345	rBV	69091	112042	2.02%	0.430%
2	5.721	405	414	426	rBV	375572	611694	11.04%	2.348%
3	7.319	677	686	697	rBV	249572	447969	8.09%	1.719%
4	7.701	743	751	760	rBV	723549	1257013	22.69%	4.825%
5	8.171	823	831	835	rBV	229434	395493	7.14%	1.518%
6	8.224	835	840	851	rVB	128882	211779	3.82%	0.813%
7	8.494	878	886	895	rBV	941812	1665860	30.07%	6.394%
8	9.334	1020	1029	1041	rBV	821537	1481074	26.73%	5.685%
9	10.985	1301	1310	1318	rBV	366842	657769	11.87%	2.525%
10	13.412	1715	1723	1731	rBV	2404446	3876042	69.96%	14.877%
11	14.228	1856	1862	1867	rBV	51057	73069	1.32%	0.280%
12	14.787	1949	1957	1965	rVB2	605273	990165	17.87%	3.800%
13	16.267	2201	2209	2219	rBV	1321881	1982125	35.78%	7.608%
14	17.525	2416	2423	2430	rBV	806905	1192407	21.52%	4.577%
15	18.829	2640	2645	2652	rBV	53531	85881	1.55%	0.330%
16	18.911	2655	2659	2667	rBV	66173	129040	2.33%	0.495%
17	19.569	2766	2771	2776	rBV6	28373	63494	1.15%	0.244%
18	20.016	2840	2847	2855	rBV	774615	2253352	40.67%	8.649%
19	20.116	2859	2864	2871	rVB	3929124	5540420	100.00%	21.265%
20	20.809	2977	2982	2986	rBV	113676	144686	2.61%	0.555%
21	21.167	3036	3043	3049	rBV	62689	115954	2.09%	0.445%
22	21.420	3082	3086	3095	rVB3	36676	62342	1.13%	0.239%
23	21.796	3143	3150	3157	rBV	830388	1347592	24.32%	5.172%
24	25.104	3702	3713	3730	rVB2	438156	1356946	24.49%	5.208%

Sum of corrected areas: 26054208

LSC Report - Integrated Chromatogram

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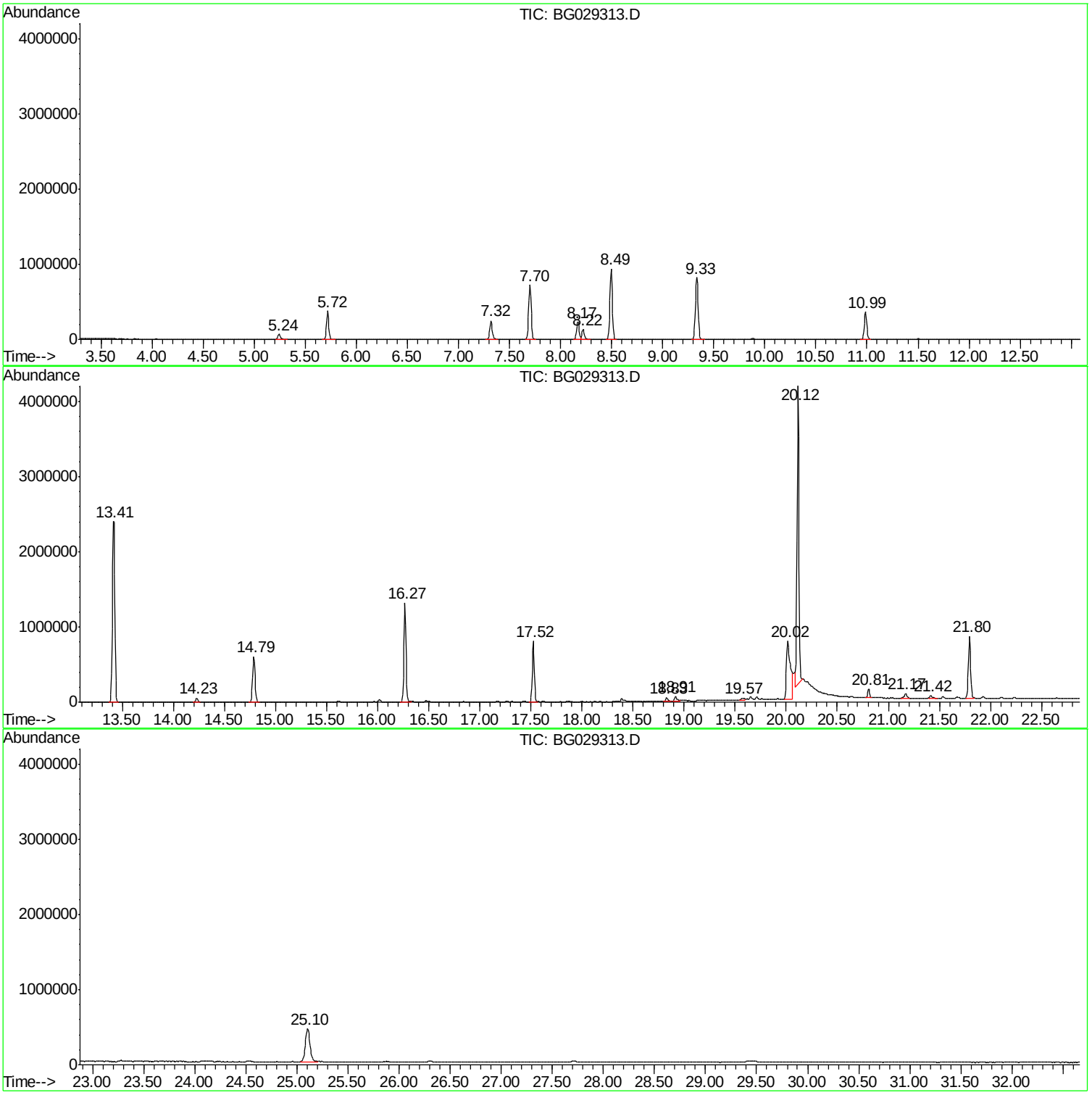
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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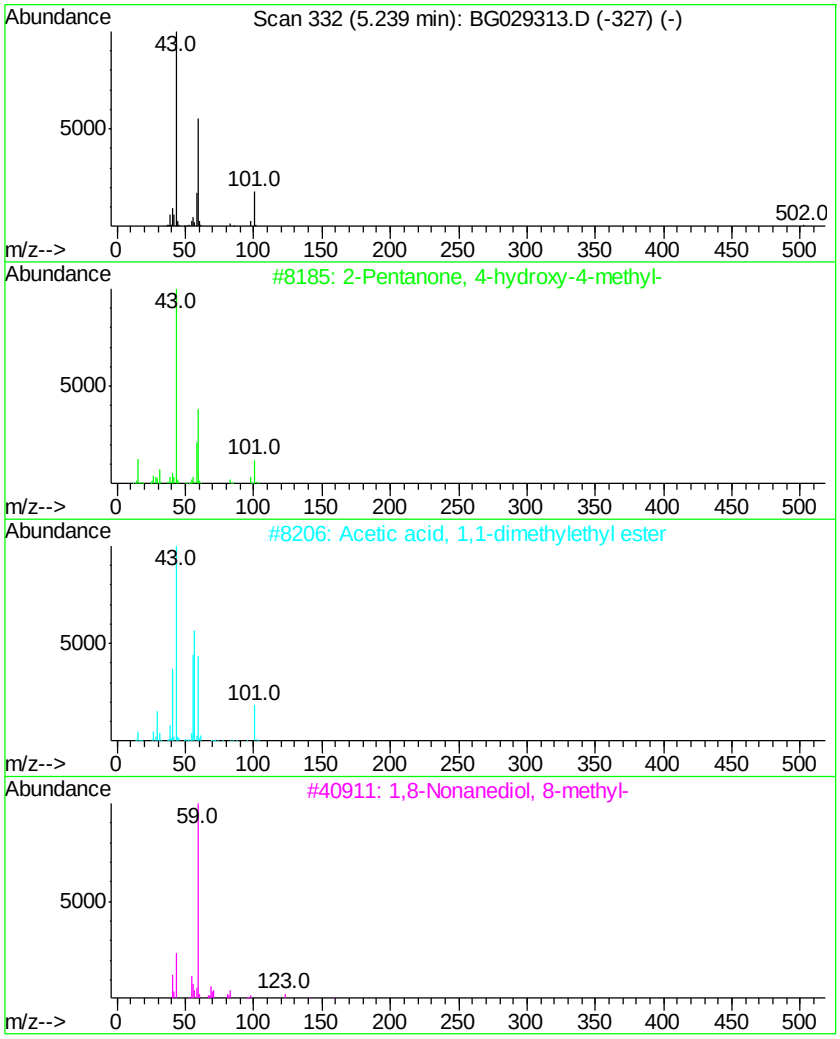
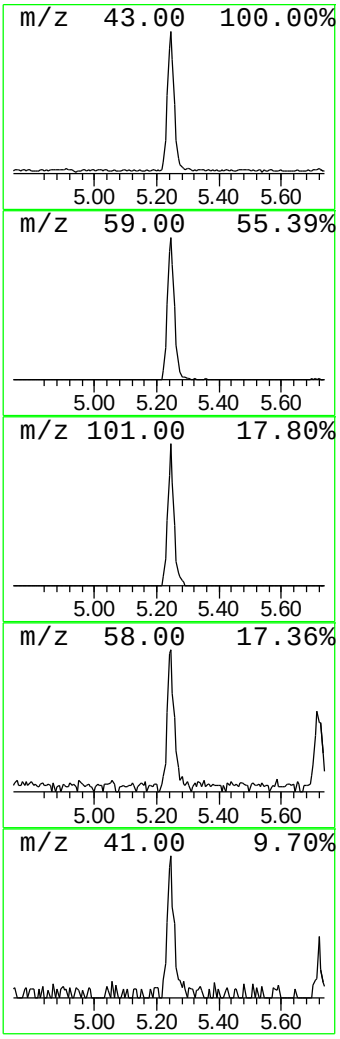
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	5.67 ng	112042	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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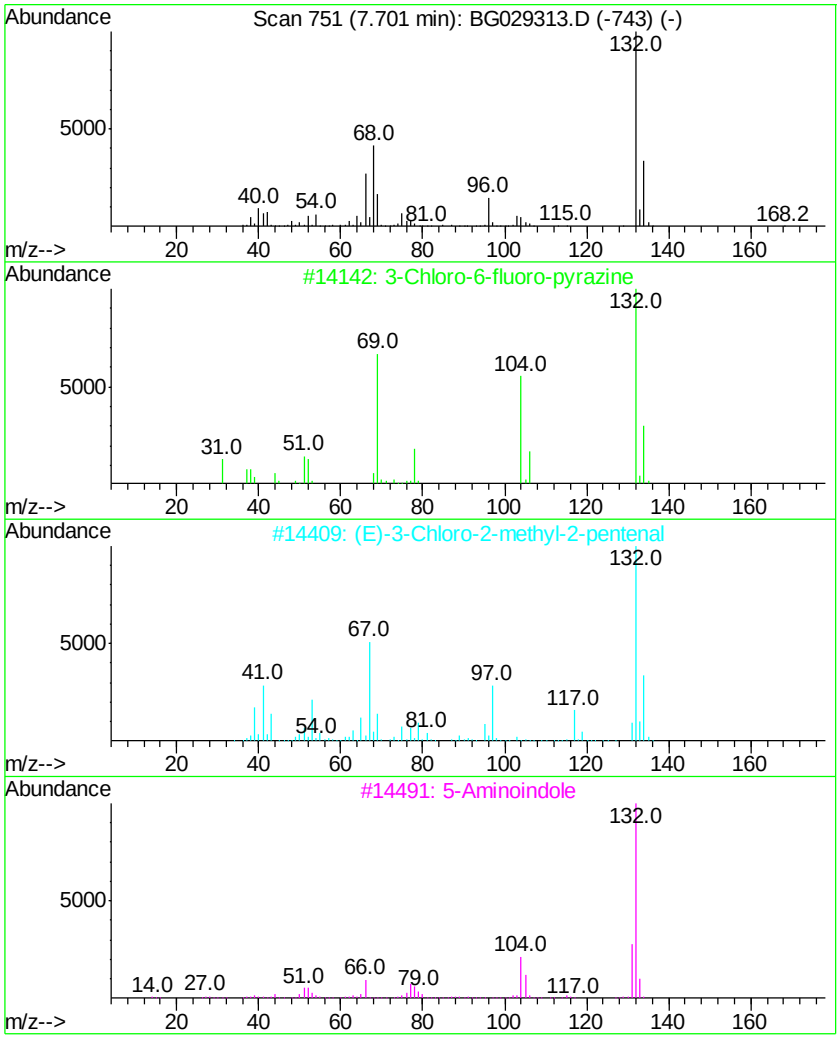
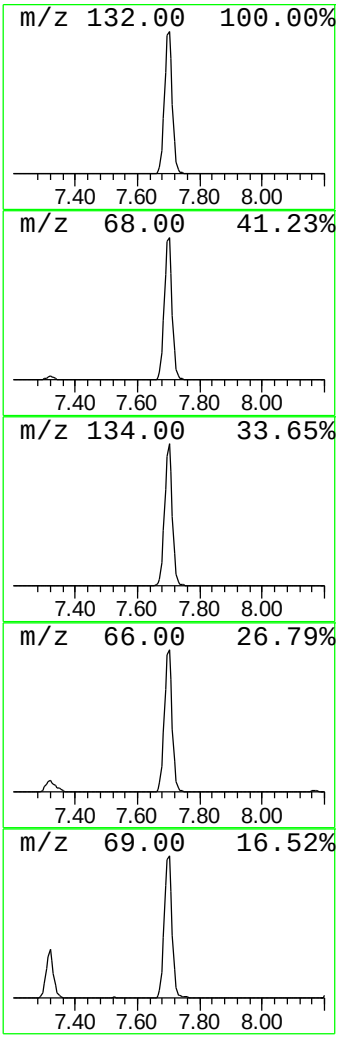
Peak Number 2 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	63.57 ng	1257010	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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Sample : I5817-06
Misc :
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Instrument : BNA_G
ClientSampleId : HW-3

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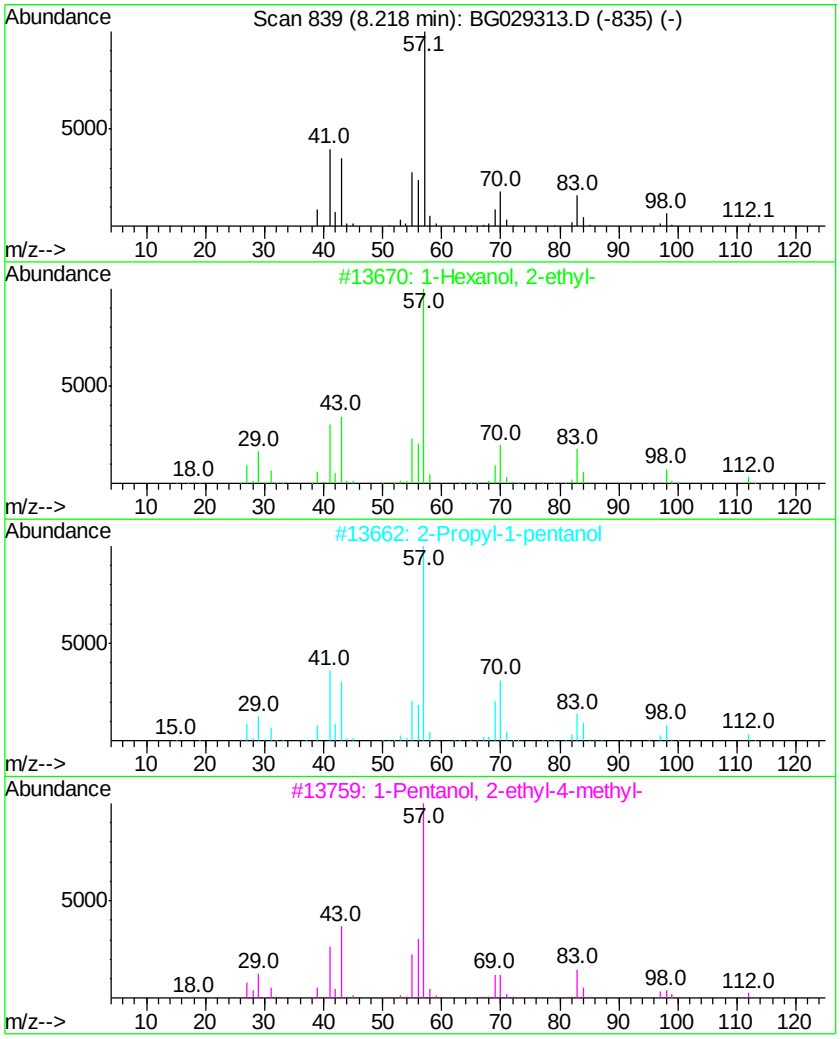
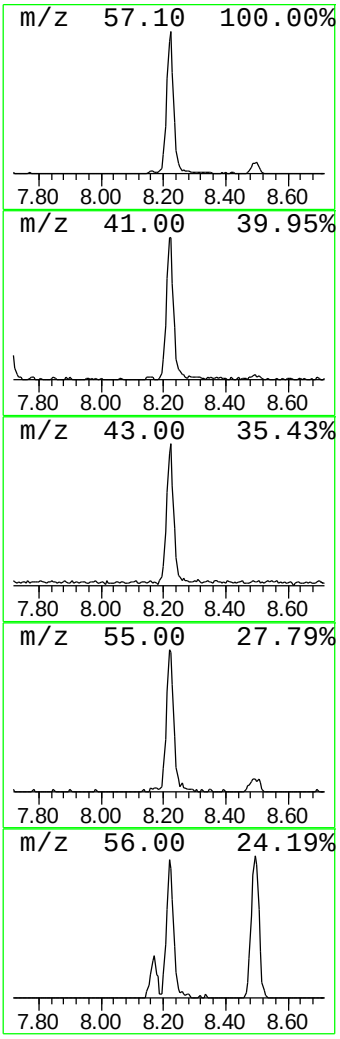
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.22	10.71 ng	211779	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	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	53
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50





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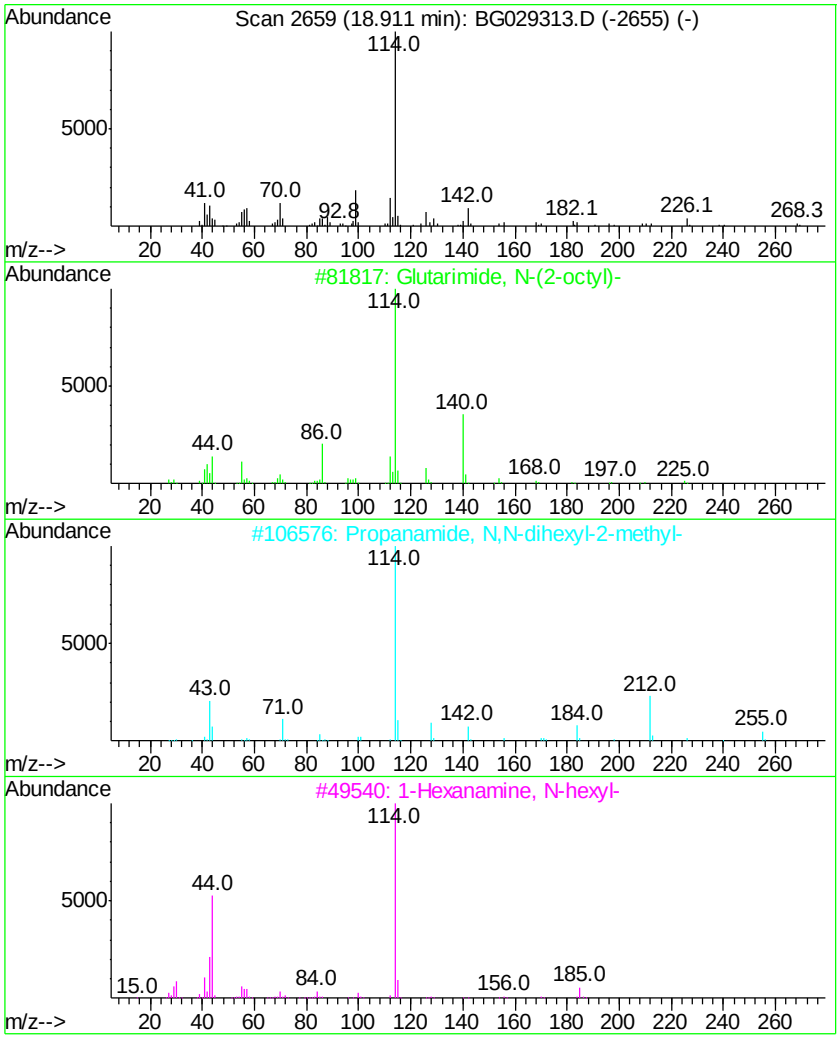
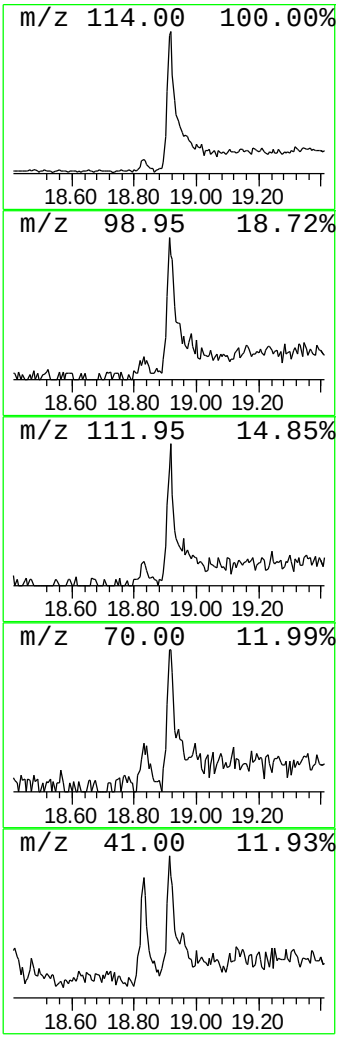
Peak Number 5 Glutarimide, N-(2-octyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.91	2.16 ng	129040	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutarimide, N-(2-octyl)-	225	C13H23NO2	1000360-86-4	53
2	Propanamide, N,N-dihexyl-2-methyl-	255	C16H33NO	1000308-08-2	45
3	1-Hexanamine, N-hexyl-	185	C12H27N	000143-16-8	40
4	1-[[2-[Butylamino]butyl]imino]-7...	517	C27H30Cl3N3O	144155-60-2	40
5	Propanamide, N-(2-fluorophenyl)-...	252	C13H17FN2O2	284679-89-6	40





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Instrument : BNA_G
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
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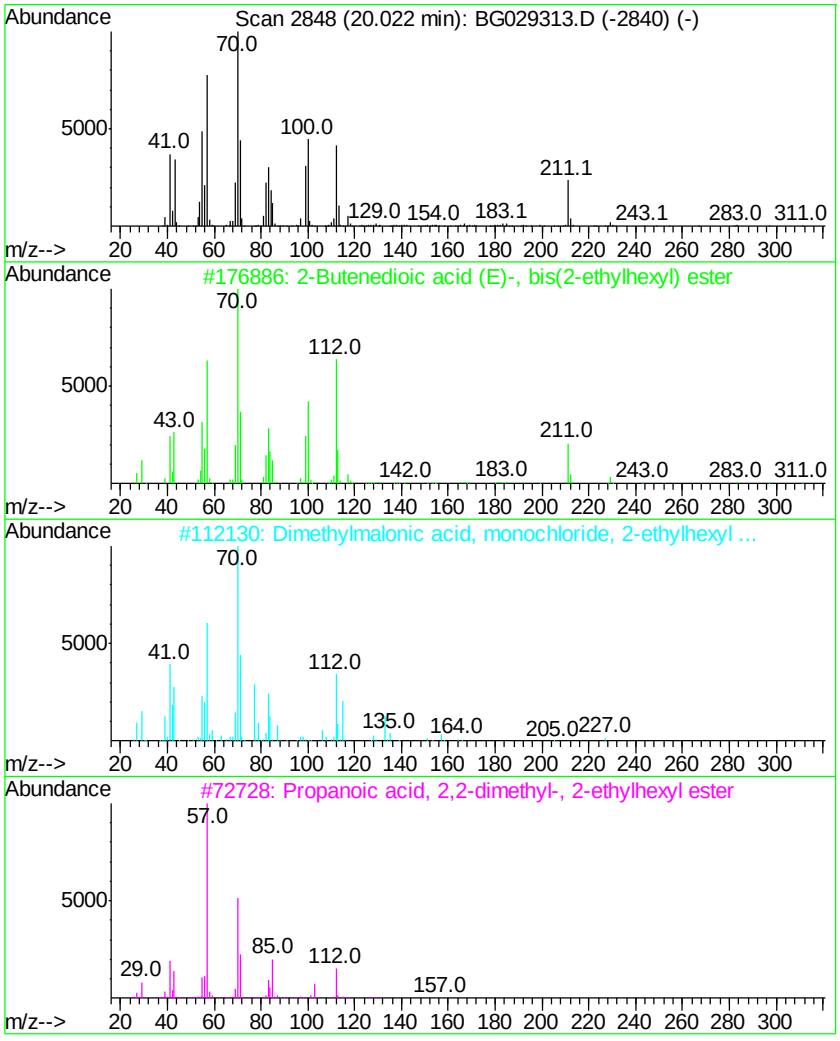
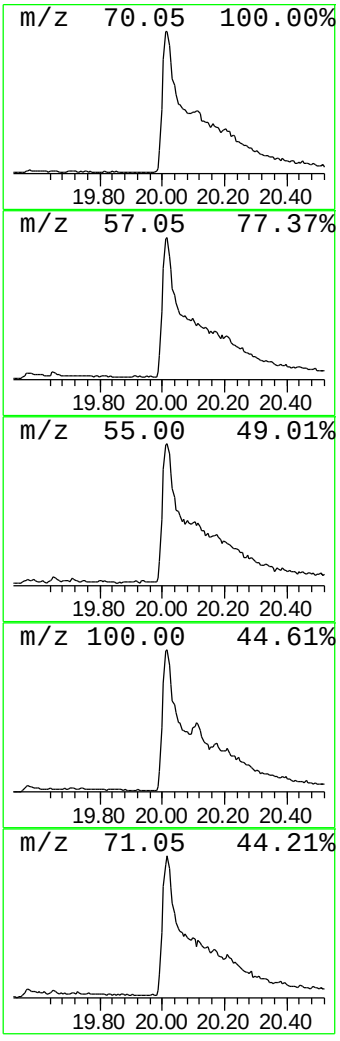
Peak Number 6 2-Butenedioic acid (E)-, bi... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.02	33.44 ng	2253350	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	87
2	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	50
3	Propanoic acid, 2,2-dimethyl-, 2...	214	C13H26O2	016387-18-1	47
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	38
5	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	35





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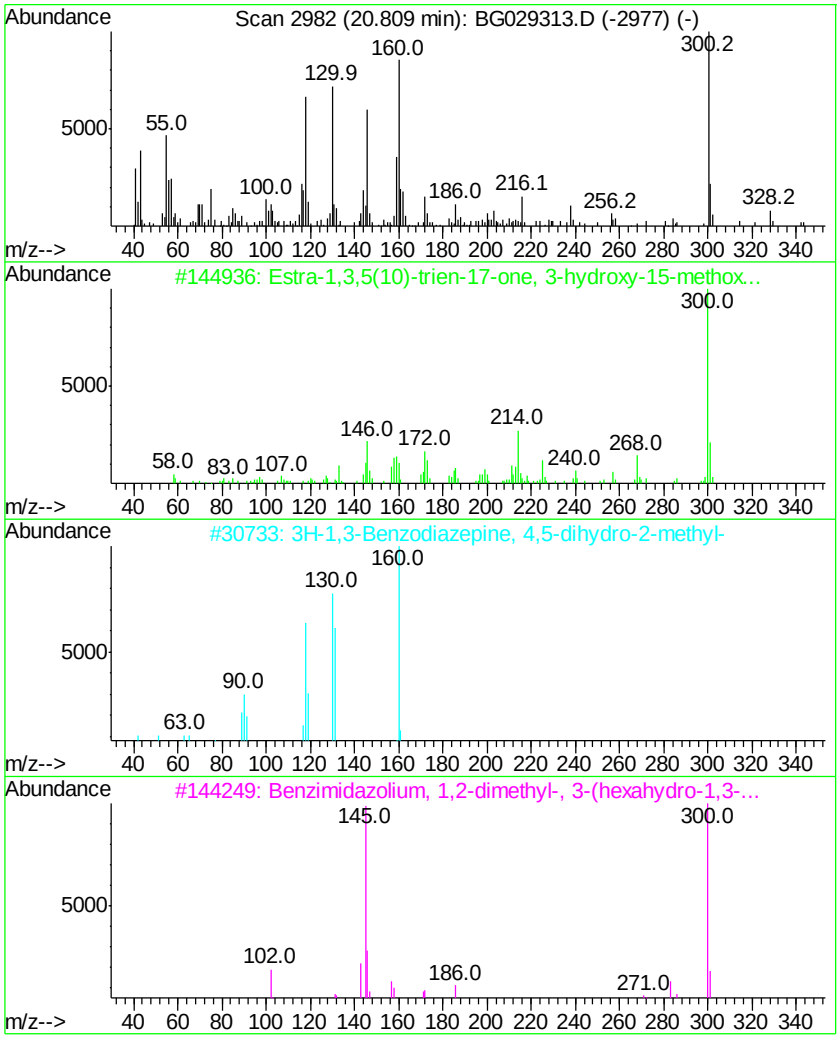
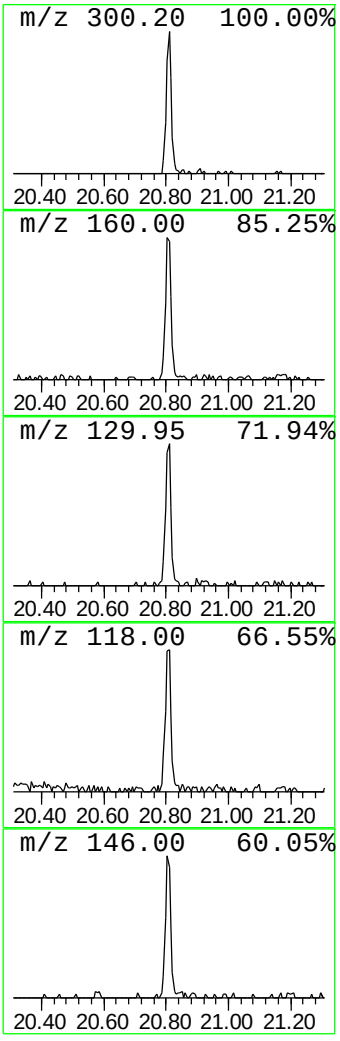
Peak Number 7 unknown20.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	2.15 ng	144686	Chrysene-d12	21.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estra-1,3,5(10)-trien-17-one, 3-...	300	C19H24O3	074299-15-3	38
2	3H-1,3-Benzodiazepine, 4,5-dihyd...	160	C10H12N2	046035-38-5	35
3	Benzimidazolium, 1,2-dimethyl-, ...	300	C15H16N4O3	027355-95-9	27
4	Quinazoline, 2-methoxy-	160	C9H8N2O	006141-15-7	25
5	Fluorenone, 2,3,4,7-tetramethoxy-	300	C17H16O5	127825-92-7	18





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	5.7	ng	112042	1	8.17	395493	20.0
unknown7.70	7.70	63.6	ng	1257010	1	8.17	395493	20.0
1-Hexanol, 2-ethyl-	8.22	10.7	ng	211779	1	8.17	395493	20.0
Glutarimide, N-(2...	18.91	2.2	ng	129040	4	17.52	1192410	20.0
2-Butenedioic aci...	20.02	33.4	ng	2253350	5	21.80	1347590	20.0
unknown20.81	20.81	2.1	ng	144686	5	21.80	1347590	20.0