

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092217\
 Data File : BG028883.D
 Acq On : 22 Sep 2017 20:40
 Operator : SJ/JU
 Sample : I5301-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170609-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	5.381	299	305	314	rBV3	24713	40651	1.09%	0.306%
2	5.845	378	384	397	rBV	257853	436288	11.74%	3.288%
3	7.431	647	654	664	rBV2	173718	325294	8.76%	2.452%
4	7.813	710	719	729	rBV	421050	751642	20.23%	5.665%
5	8.278	791	798	805	rBV	90408	157014	4.23%	1.183%
6	8.601	846	853	864	rVB	373847	688902	18.54%	5.192%
7	9.447	989	997	1007	rBV	314958	589388	15.87%	4.442%
8	11.092	1270	1277	1287	rBV	110492	216371	5.82%	1.631%
9	13.513	1681	1689	1702	rBV	968310	1540942	41.48%	11.614%
10	14.893	1917	1924	1931	rBV2	216791	352223	9.48%	2.655%
11	16.386	2170	2178	2186	rBV	1114956	1750847	47.13%	13.196%
12	17.643	2385	2392	2403	rBV	388278	622598	16.76%	4.693%
13	18.283	2495	2501	2506	rBV4	128700	171702	4.62%	1.294%
14	19.094	2634	2639	2644	rBV4	26778	39991	1.08%	0.301%
15	19.887	2769	2774	2781	rVB	165389	191941	5.17%	1.447%
16	20.228	2826	2832	2842	rBV	2779043	3714992	100.00%	28.000%
17	21.962	3119	3127	3136	rBV2	442072	781640	21.04%	5.891%
18	23.160	3324	3331	3340	rVB3	66283	125349	3.37%	0.945%
19	25.410	3703	3714	3727	rVB	247281	770147	20.73%	5.805%

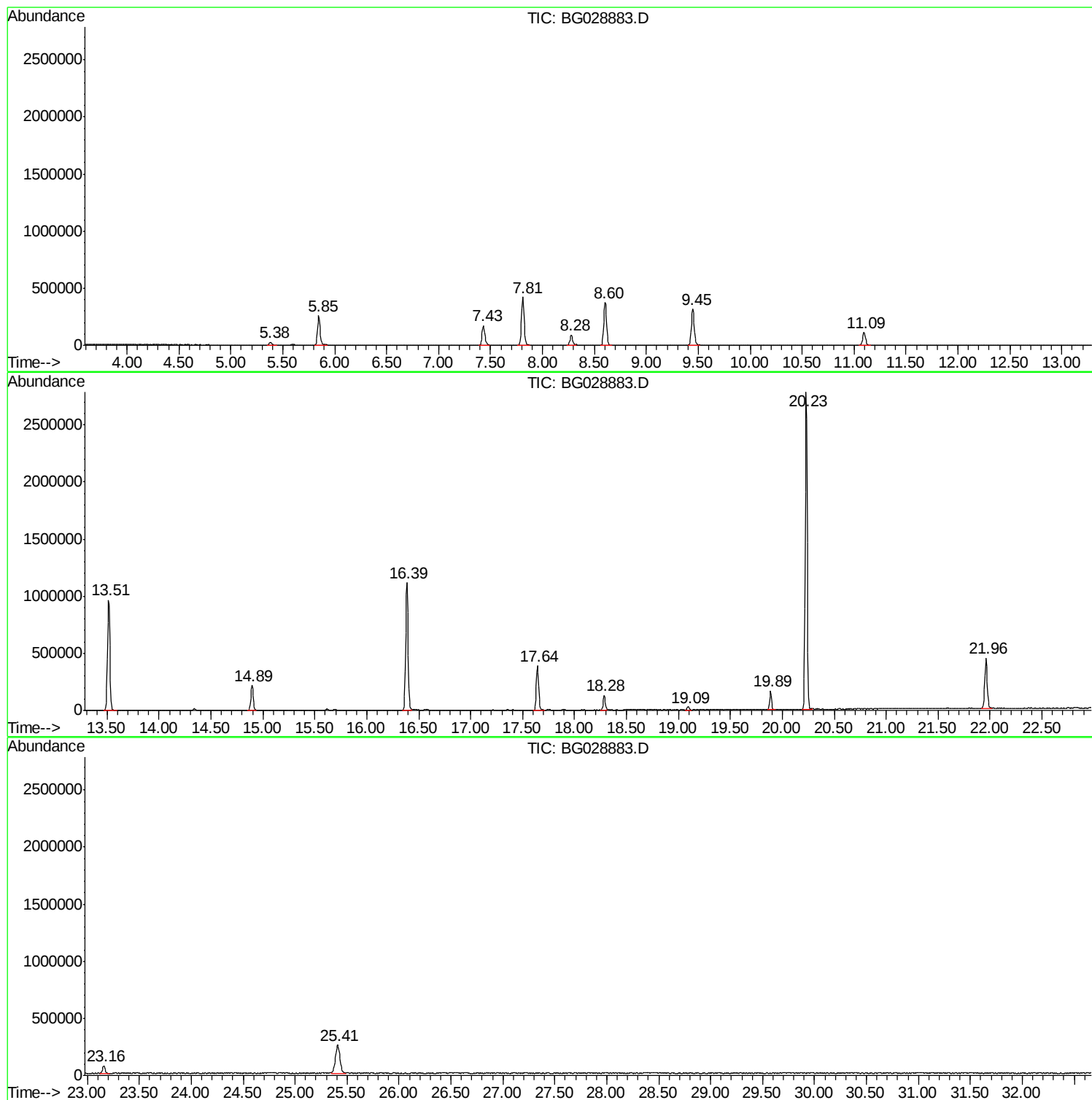
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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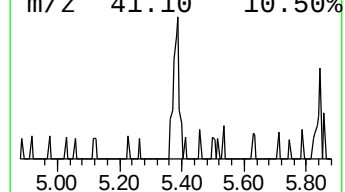
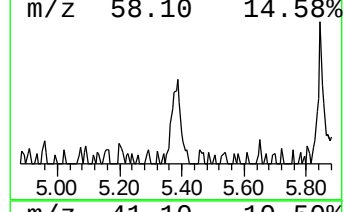
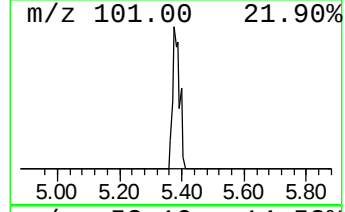
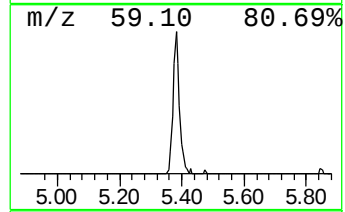
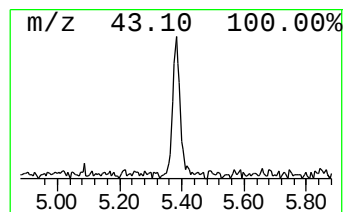
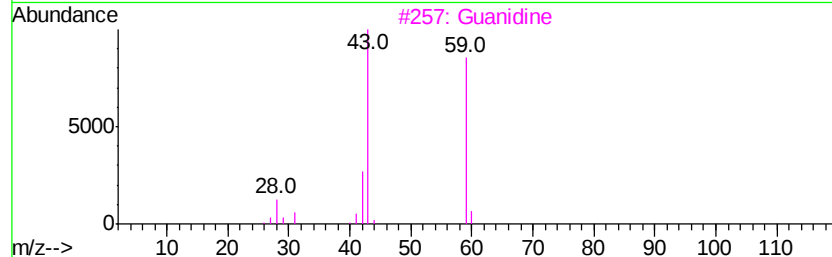
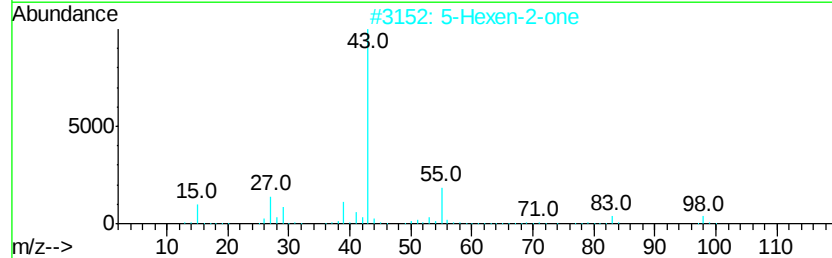
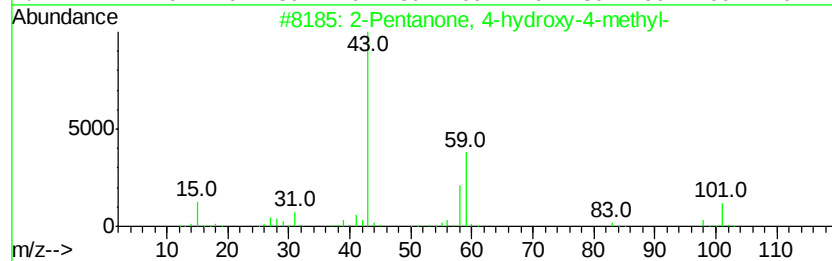
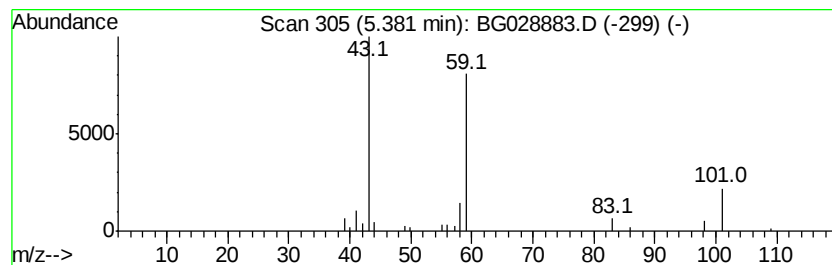
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	5.18 ng	40651	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		5-Hexen-2-one	98	C6H10O	000109-49-9	10
3		Guanidine	59	CH5N3	000113-00-8	9
4		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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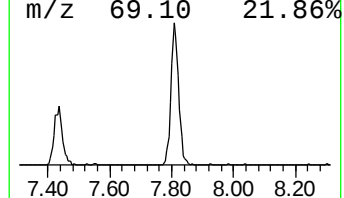
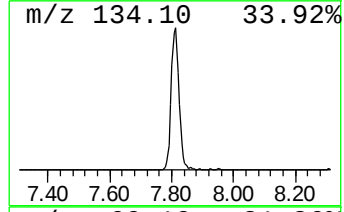
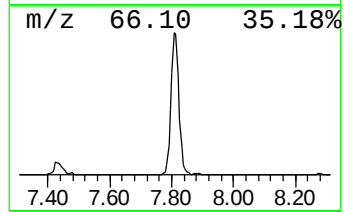
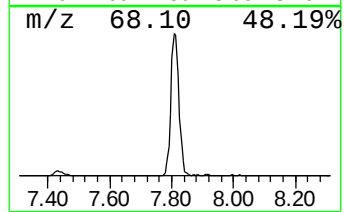
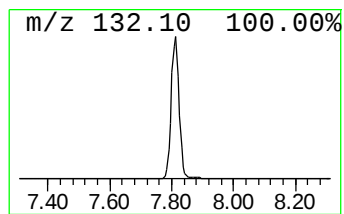
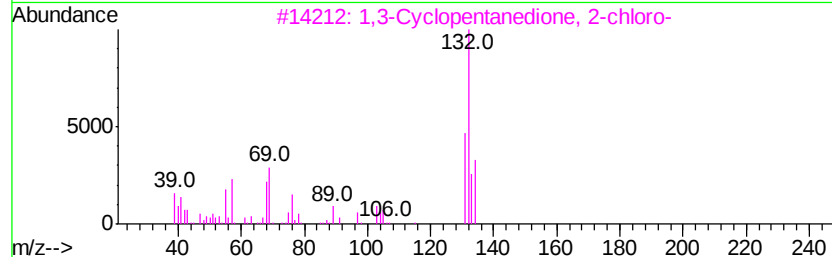
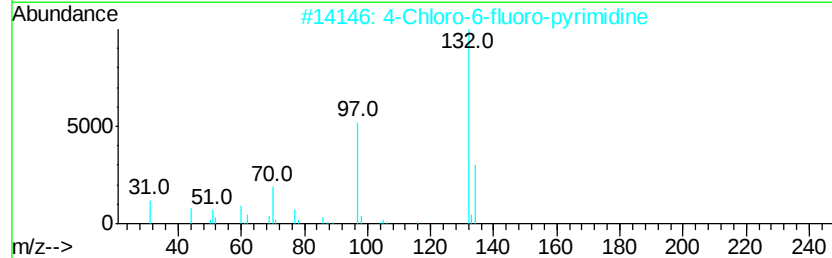
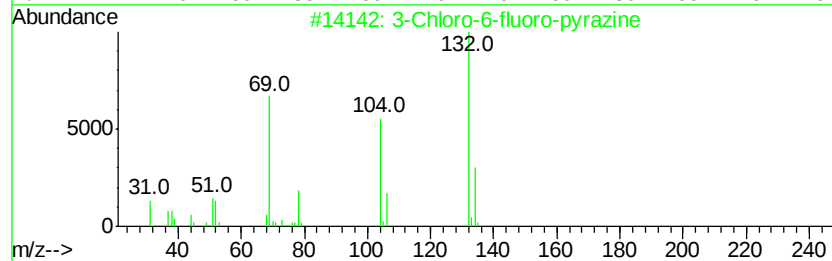
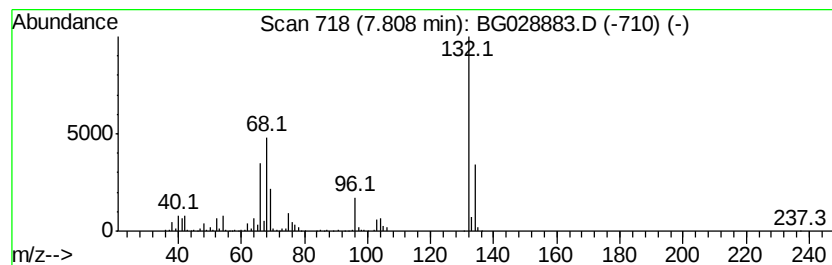
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Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	95.74 ng	751642	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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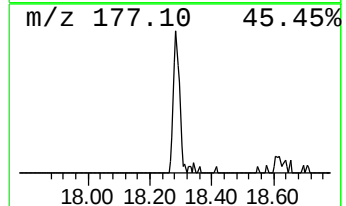
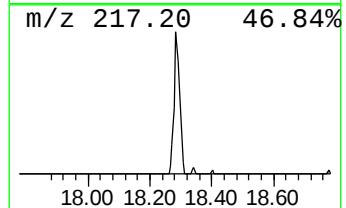
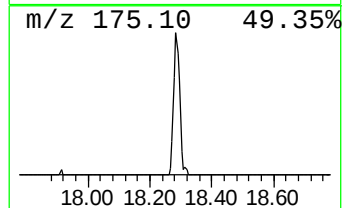
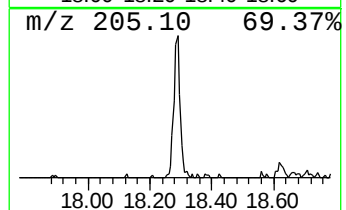
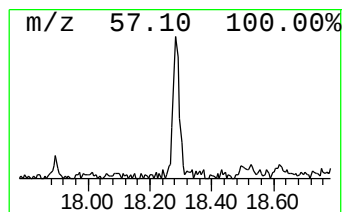
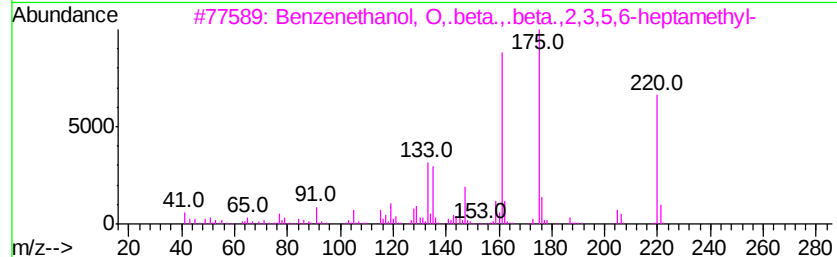
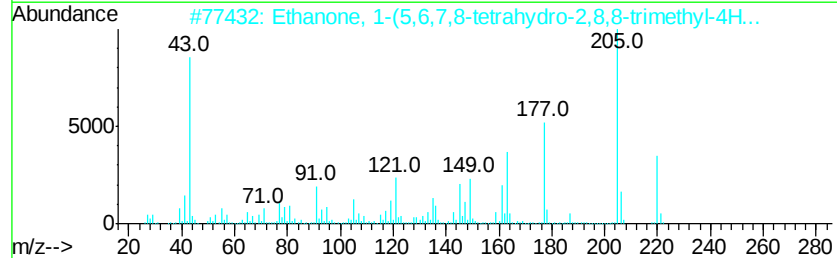
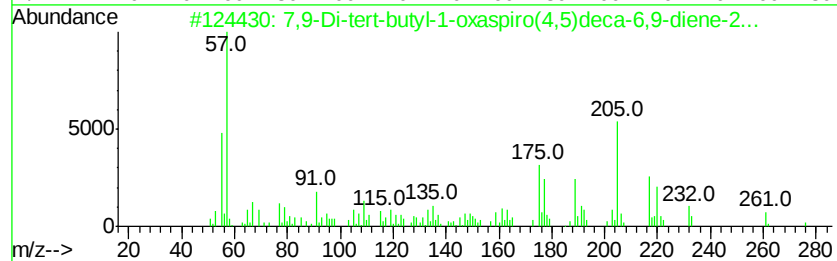
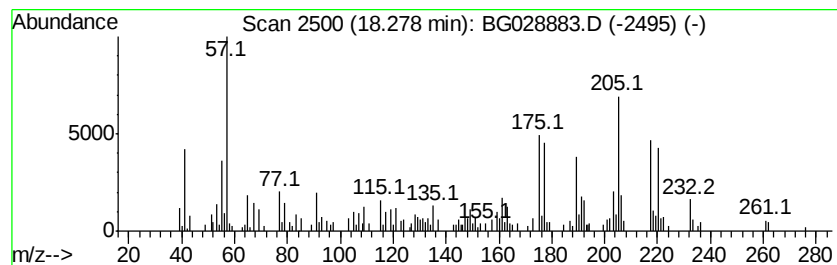
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.28	5.52 ng	171702	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-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	55
3	Benzenethanol, 0,.beta.,.beta.,2...	220	C15H24O	1000128-94-8	53
4	Silane, dichloromethylphenyl-	190	C7H8Cl2Si	000149-74-6	44
5	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	41



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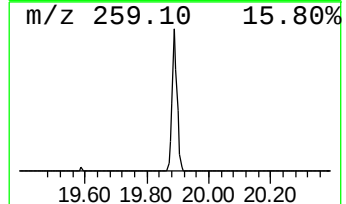
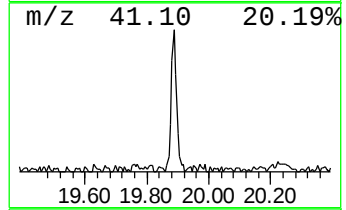
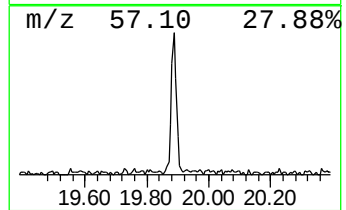
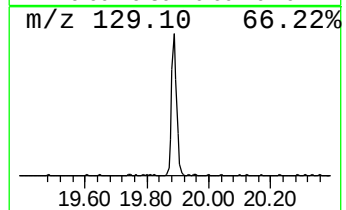
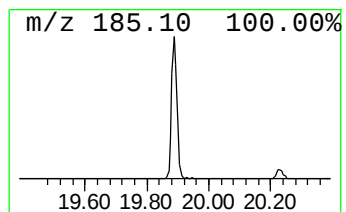
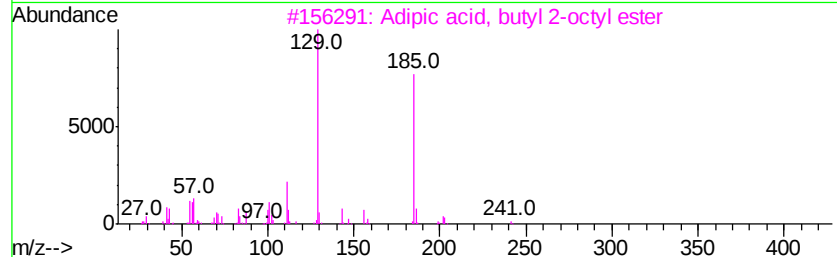
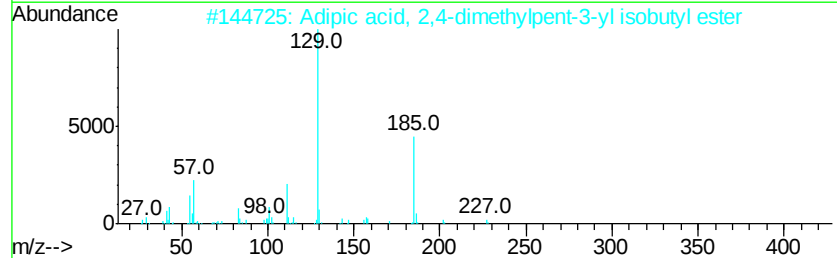
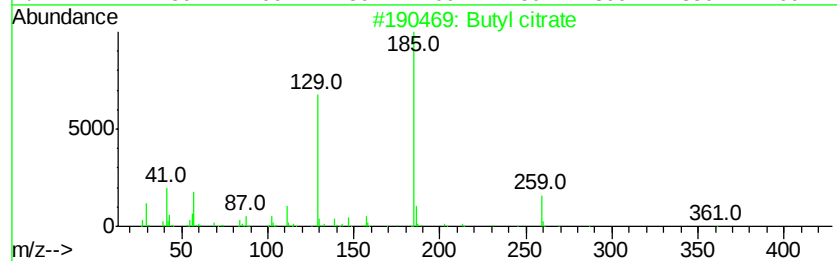
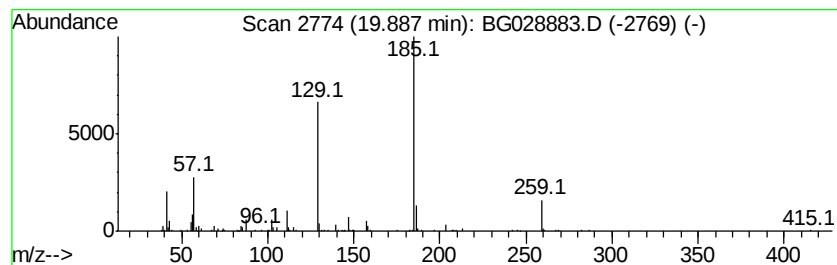
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Peak Number 5 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	4.91 ng	191941	Chrysene-d12	21.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 91
2		Adipic acid, 2,4-dimethylpent-3-...	300 C17H32O4	1000349-77-6 72
3		Adipic acid, butyl 2-octyl ester	314 C18H34O4	1000324-44-6 59
4		Adipic acid, 3,3-dimethylbut-2-v...	286 C16H30O4	1000353-66-7 50
5		Adipic acid, butyl 2-methylpent-...	286 C16H30O4	1000353-55-8 50



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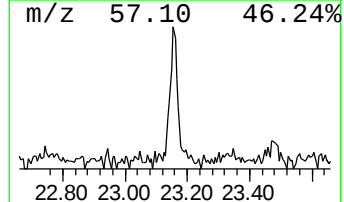
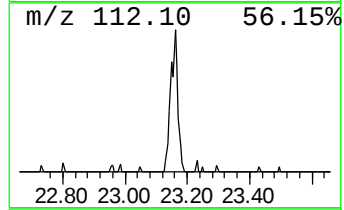
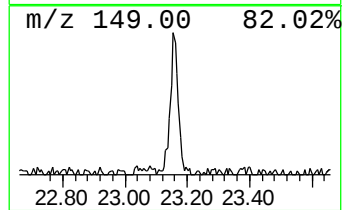
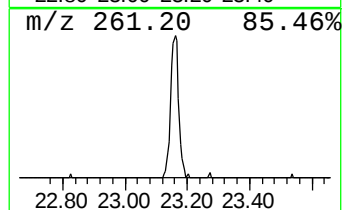
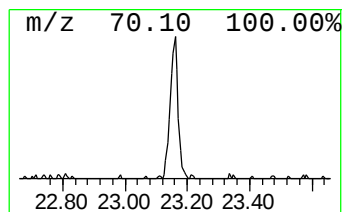
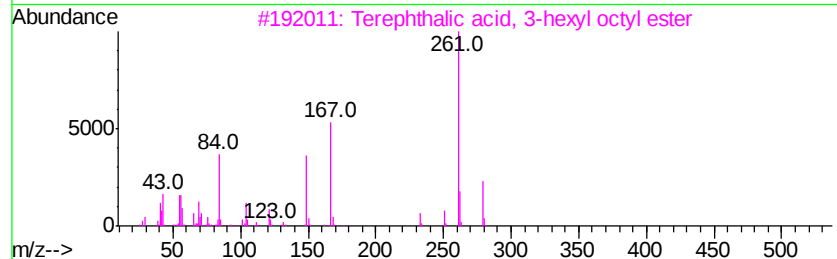
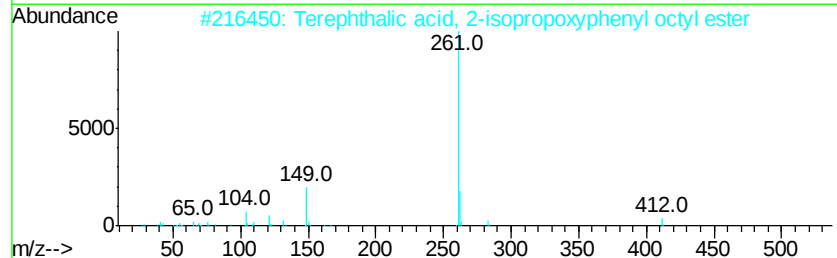
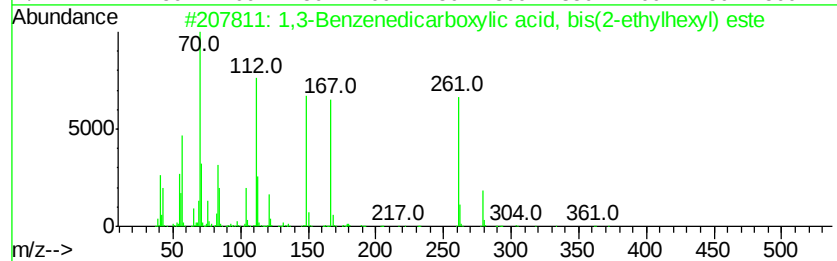
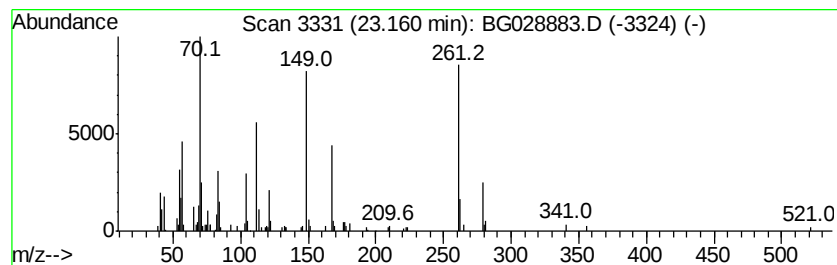
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Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	3.21 ng	125349	Chrysene-d12	21.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
2		Terephthalic acid, 2-isopropoxyph...	412	C25H32O5	1000324-07-8	38
3		Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	38
4		Isophthalic acid, octyl 3-pentyl...	348	C21H32O4	1000344-00-4	35
5		Terephthalic acid, monoamide, N-...	371	C22H26FN03	1000324-02-6	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	5.2	ng	40651	1	8.28	157014	20.0
unknown7.81	7.81	95.7	ng	751642	1	8.28	157014	20.0
7,9-Di-tert-butyl...	18.28	5.5	ng	171702	4	17.64	622598	20.0
Butyl citrate	19.89	4.9	ng	191941	5	21.96	781640	20.0
1,3-Benzenedicarb...	23.16	3.2	ng	125349	5	21.96	781640	20.0