

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
 Data File : BG028807.D
 Acq On : 18 Sep 2017 22:58
 Operator : SJ/JU
 Sample : I5259-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170601-COMP-B

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	5.858	380	386	398	rBV	270928	451575	14.11%	3.303%
2	7.445	648	656	670	rBV	176683	353354	11.04%	2.585%
3	7.821	711	720	735	rBV	478838	851729	26.61%	6.230%
4	8.291	791	800	810	rBV	103732	194385	6.07%	1.422%
5	8.614	848	855	866	rVB	431753	749100	23.40%	5.480%
6	9.460	991	999	1010	rBV	349410	643451	20.10%	4.707%
7	11.111	1273	1280	1287	rBV	140064	269245	8.41%	1.969%
8	13.526	1681	1691	1701	rBV	1110630	1754350	54.80%	12.833%
9	14.348	1824	1831	1838	rBV	34839	58935	1.84%	0.431%
10	14.413	1838	1842	1849	rVB3	29665	37228	1.16%	0.272%
11	14.906	1919	1926	1935	rBV2	260713	427366	13.35%	3.126%
12	15.294	1987	1992	1997	rBV	77458	101974	3.19%	0.746%
13	15.670	2049	2056	2060	rBV	177867	242891	7.59%	1.777%
14	16.399	2173	2180	2190	rBV	1068089	1702483	53.18%	12.453%
15	17.656	2389	2394	2406	rVB2	409224	656714	20.51%	4.804%
16	18.297	2494	2503	2510	rBV4	65806	104325	3.26%	0.763%
17	18.508	2535	2539	2547	rBV3	36408	61197	1.91%	0.448%
18	19.901	2769	2776	2782	rBV2	76083	127344	3.98%	0.932%
19	20.247	2828	2835	2843	rBV	2448766	3201244	100.00%	23.417%
20	21.411	3027	3033	3045	rBV4	28947	67759	2.12%	0.496%
21	21.557	3053	3058	3067	rBV7	29030	73435	2.29%	0.537%
22	21.980	3121	3130	3144	rBV	436826	803303	25.09%	5.876%
23	25.447	3709	3720	3733	rBV3	229472	737352	23.03%	5.394%

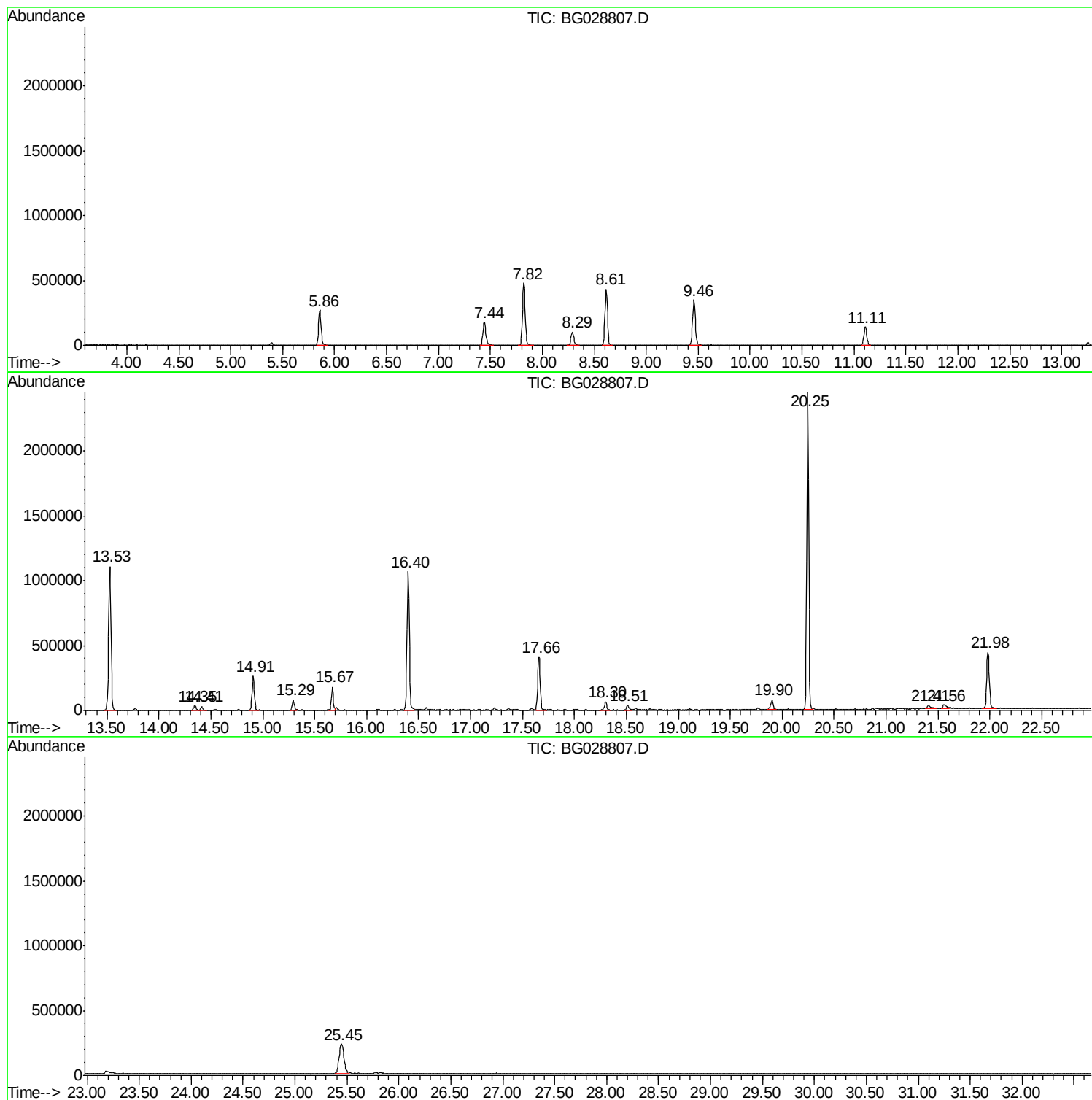
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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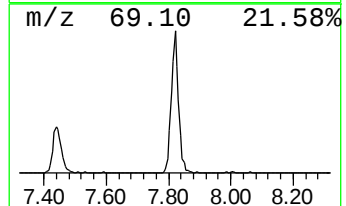
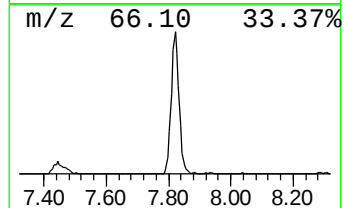
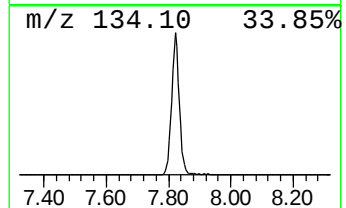
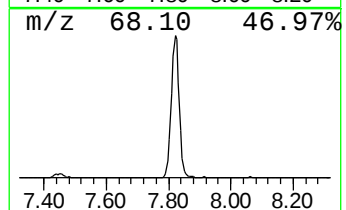
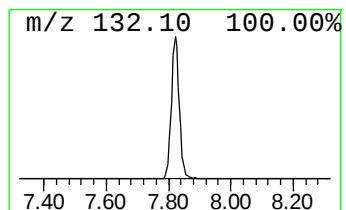
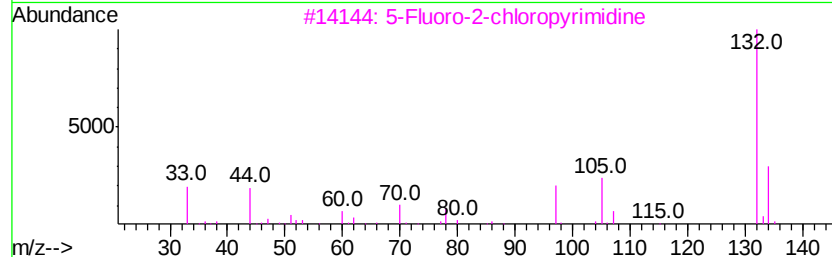
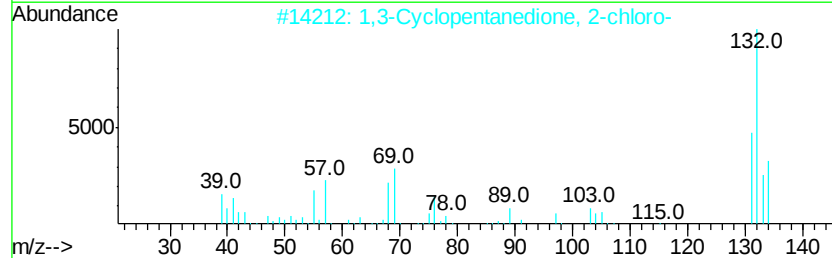
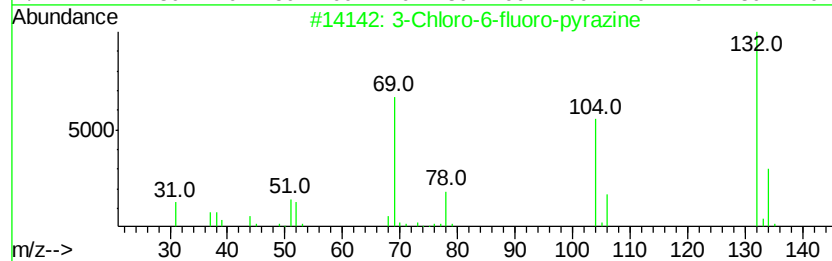
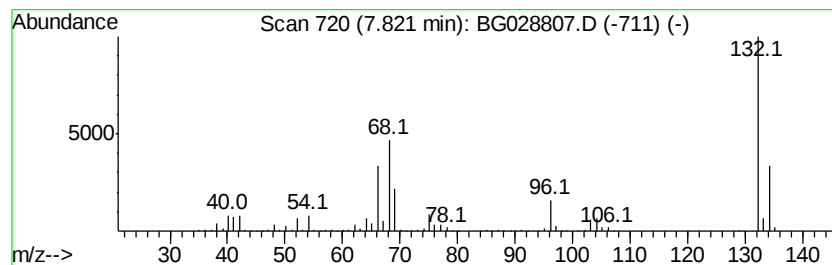
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	87.63 ng	851729	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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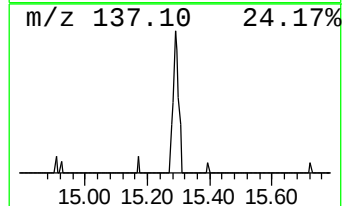
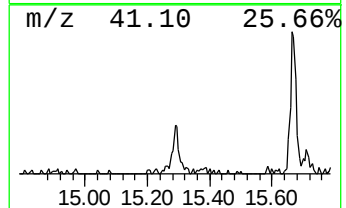
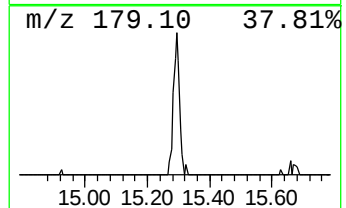
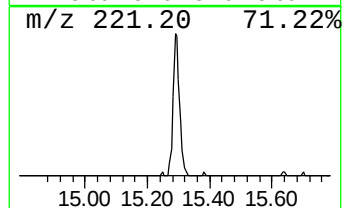
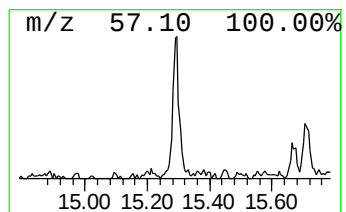
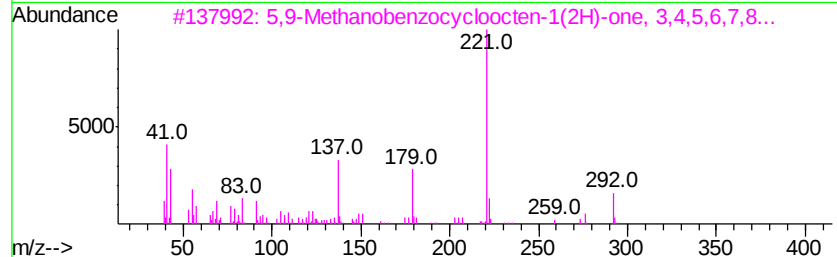
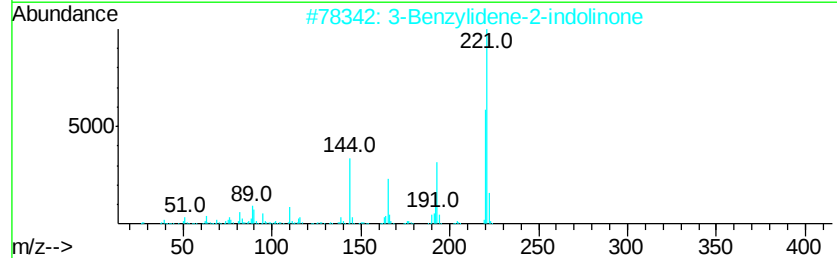
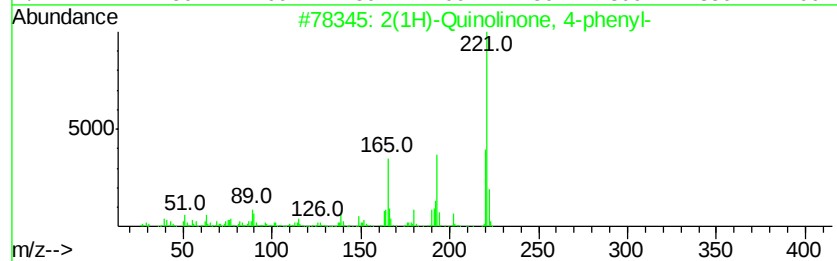
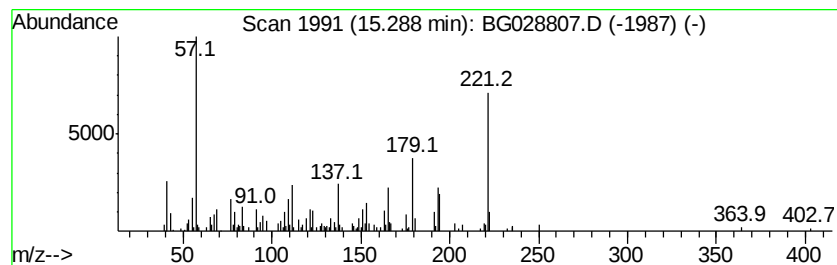
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Peak Number 3 unknown15.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	4.77 ng	101974	Acenaphthene-d10	14.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2(1H)-Quinolinone, 4-phenyl-	221	C15H11NO	005855-57-2 46
2	3-Benzylidene-2-indolinone	221	C15H11NO	003359-49-7 27
3	5,9-Methanobenzocycloocten-1(2H)...	292	C18H28O3	054833-46-4 27
4	4(1H)-Quinolinone, 2-phenyl-	221	C15H11NO	014802-18-7 16
5	Methanone, cyclohexyl(2,5-diprop...	304	C19H28O3	076185-90-5 16



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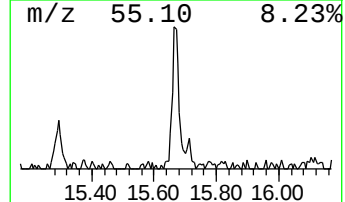
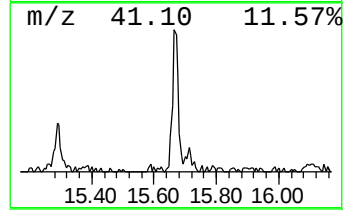
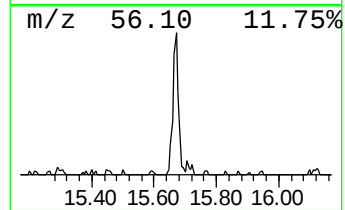
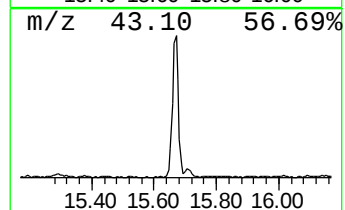
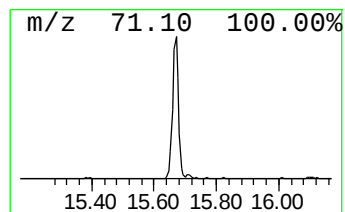
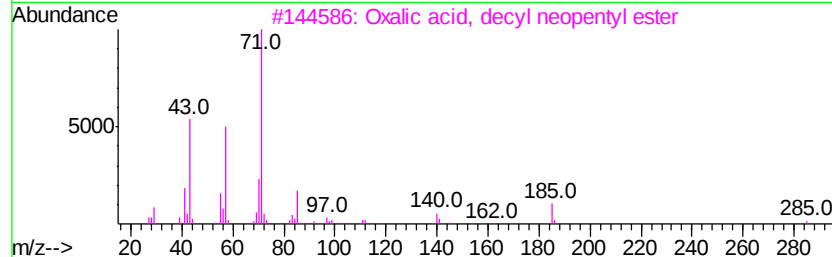
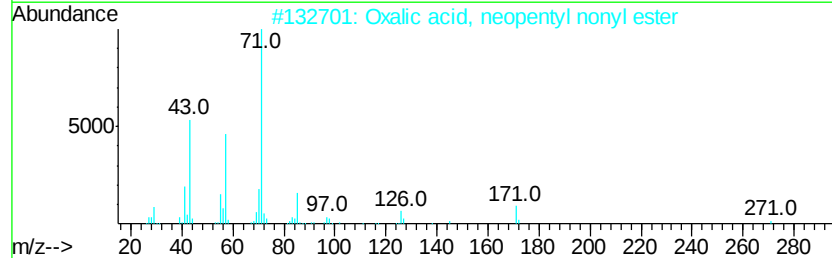
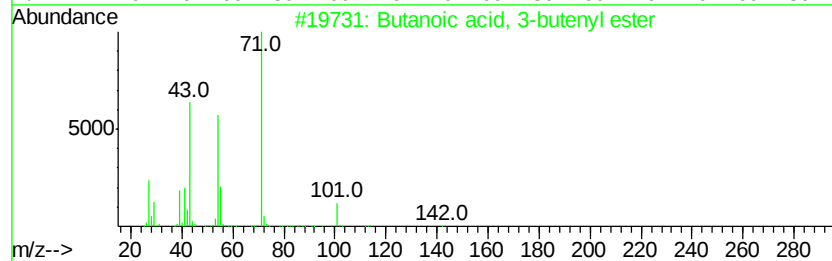
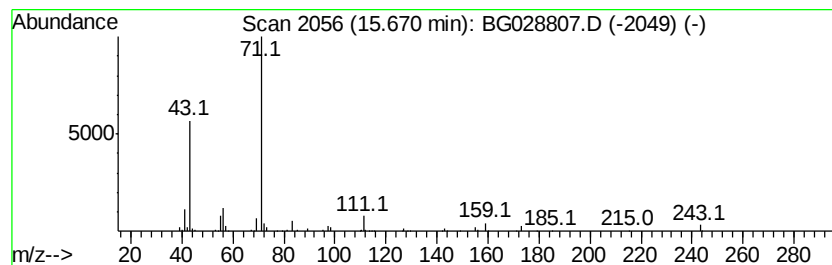
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Peak Number 4 Butanoic acid, 3-butenyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	11.37 ng	242891	Acenaphthene-d10	14.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 3-butenyl ester	142	C8H14O2	021698-32-8	53
2		Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	50
3		Oxalic acid, decyl neopentyl ester	300	C17H32O4	1000309-73-4	42
4		Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	42
5		Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	39



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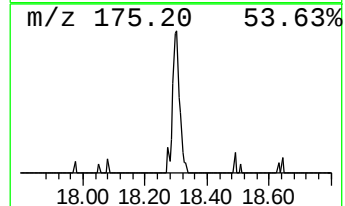
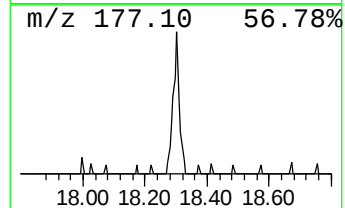
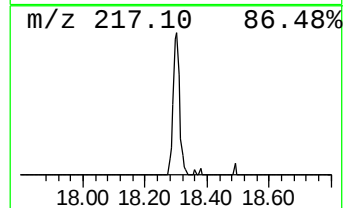
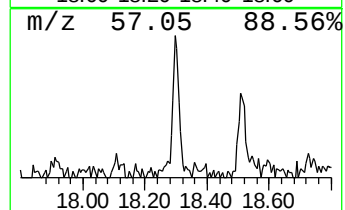
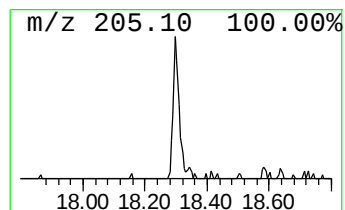
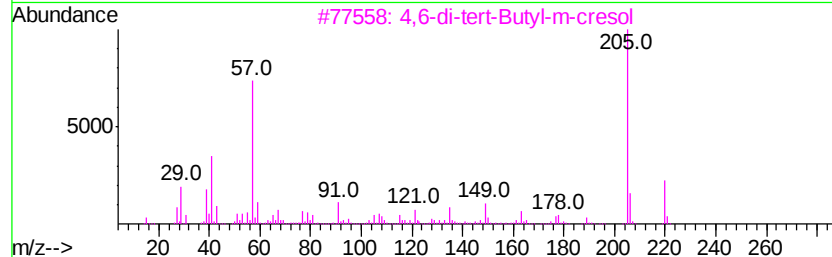
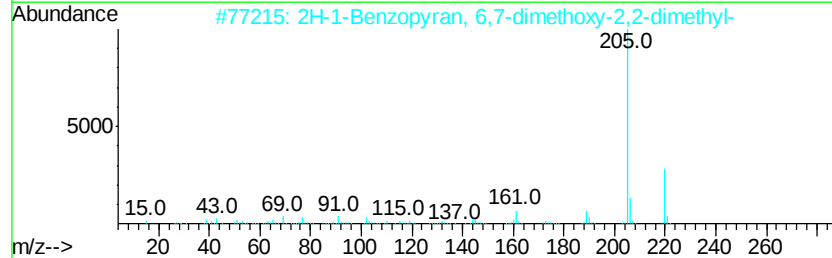
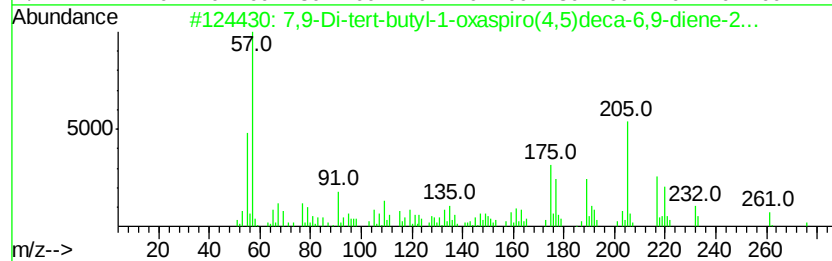
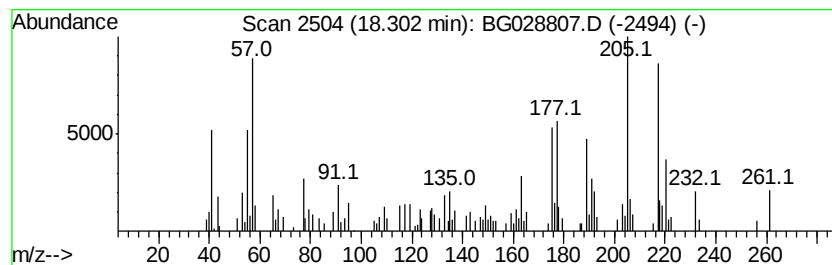
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Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.18 ng	104325	Phenanthrene-d10	17.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	96
2			2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	46
3			4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	41
4			1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	38
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38



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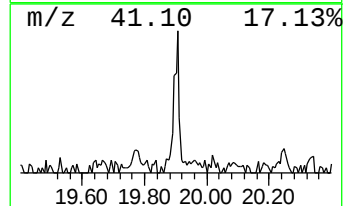
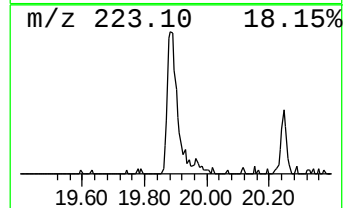
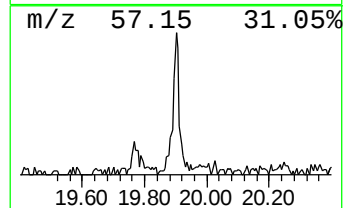
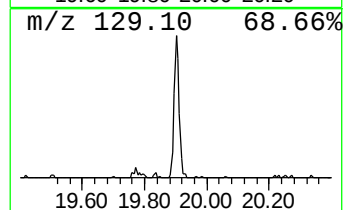
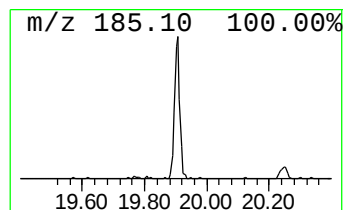
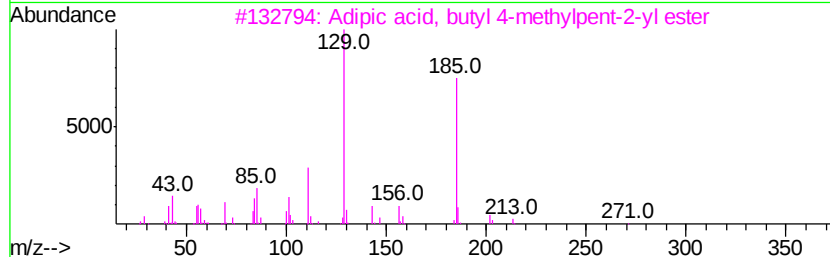
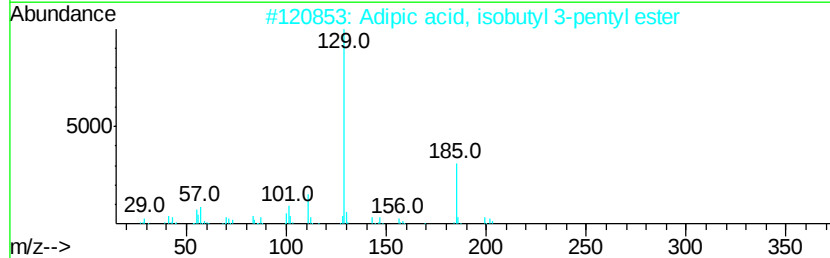
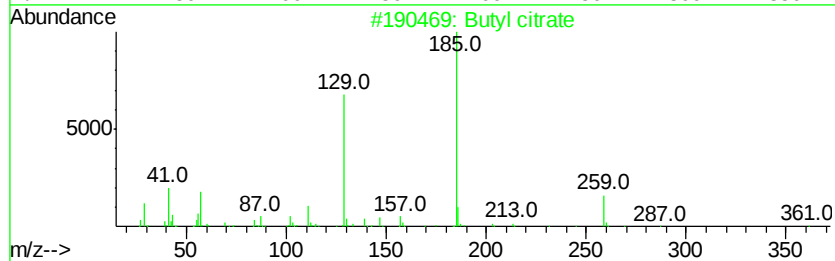
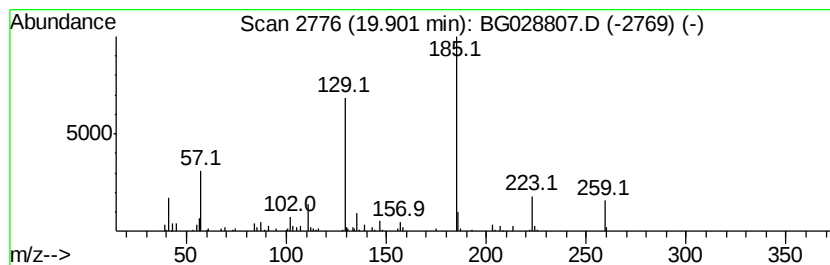
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Peak Number 6 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	3.17 ng	127344	Chrysene-d12	21.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	87
2	Adipic acid, isobutyl 3-pentyl e...	272 C15H28O4	1000324-60-4	59
3	Adipic acid, butyl 4-methylpent-...	286 C16H30O4	1000353-50-2	50
4	Adipic acid, butyl 3-pentyl ester	272 C15H28O4	1000324-60-5	50
5	Adipic acid, isobutyl 2-pentyl e...	272 C15H28O4	1000324-15-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.82	7.82	87.6	ng	851729	1	8.29	194385	20.0
unknown15.29	15.29	4.8	ng	101974	3	14.91	427366	20.0
Butanoic acid, 3-...	15.67	11.4	ng	242891	3	14.91	427366	20.0
7,9-Di-tert-butyl...	18.30	3.2	ng	104325	4	17.66	656714	20.0
Butyl citrate	19.90	3.2	ng	127344	5	21.98	803303	20.0