

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092517\
 Data File : BG028913.D
 Acq On : 25 Sep 2017 18:34
 Operator : SJ/JU
 Sample : I5301-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170604-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	312	rBV	32383	52063	1.36%	0.343%
2	5.846	378	384	397	rBV	336123	574827	15.01%	3.790%
3	7.438	646	655	665	rBV	224412	439843	11.49%	2.900%
4	7.814	710	719	733	rBV	557167	1000503	26.13%	6.596%
5	8.278	790	798	807	rBV	100316	182001	4.75%	1.200%
6	8.607	845	854	864	rBV	500536	892843	23.31%	5.886%
7	9.453	990	998	1007	rBV	403478	762408	19.91%	5.026%
8	11.098	1270	1278	1286	rBV	126066	243799	6.37%	1.607%
9	13.519	1683	1690	1701	rBV	1253002	1955063	51.05%	12.889%
10	14.336	1824	1829	1835	rBV	32864	55554	1.45%	0.366%
11	14.900	1917	1925	1932	rBV2	219041	369339	9.64%	2.435%
12	16.386	2171	2178	2192	rBV	1223835	1950841	50.94%	12.861%
13	17.649	2386	2393	2404	rBV2	371923	596580	15.58%	3.933%
14	18.290	2497	2502	2510	rBV4	47499	66771	1.74%	0.440%
15	19.894	2770	2775	2782	rBV	402812	458148	11.96%	3.020%
16	20.235	2827	2833	2841	rBV	2905600	3829543	100.00%	25.247%
17	21.968	3121	3128	3139	rBV	394890	728929	19.03%	4.806%
18	23.166	3324	3332	3341	rVB	166695	299740	7.83%	1.976%
19	25.417	3706	3715	3731	rVB3	216264	709570	18.53%	4.678%

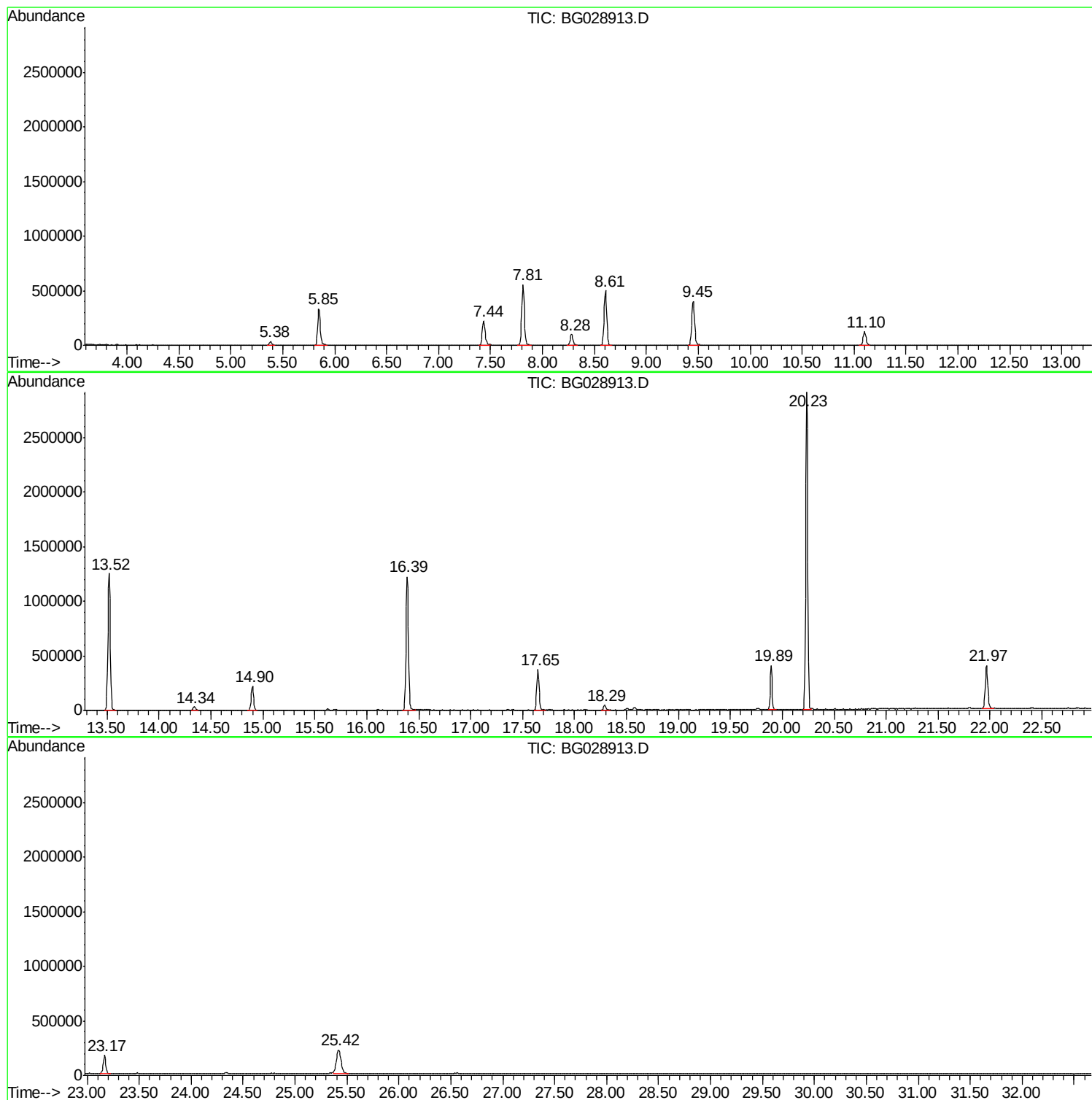
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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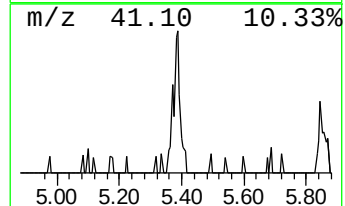
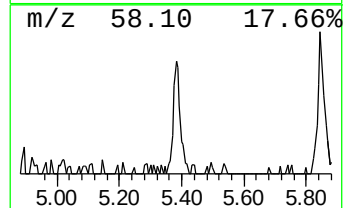
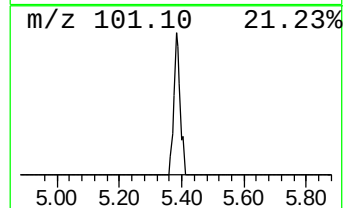
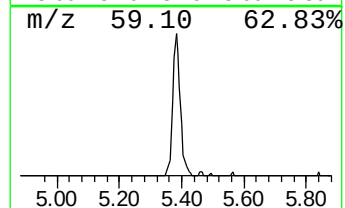
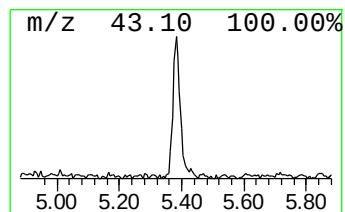
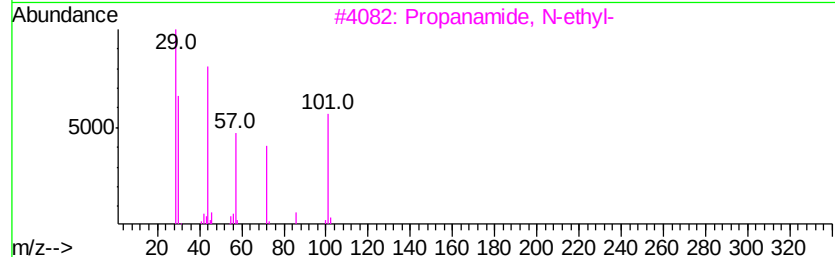
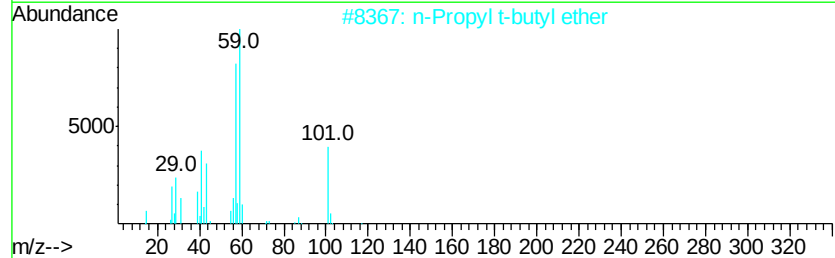
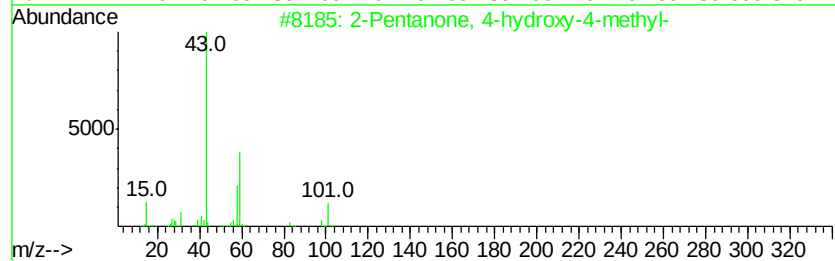
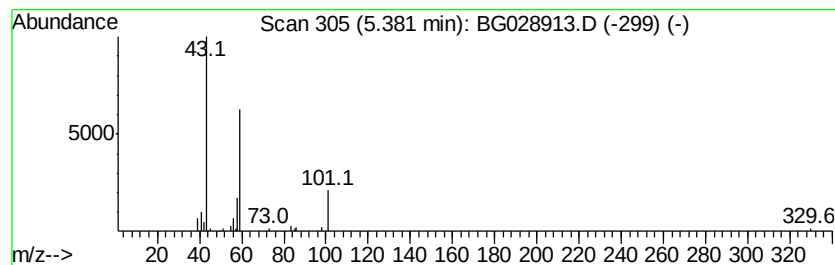
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.38	5.72 ng	52063	1,4-Dichlorobenzene-d4	8.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9
4	Pentanamide	101	C5H11NO	000626-97-1	9
5	Pentanal, oxime	101	C5H11NO	000628-79-5	9



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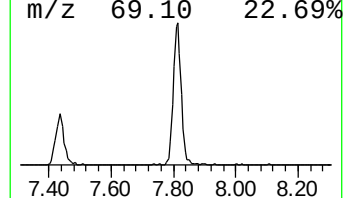
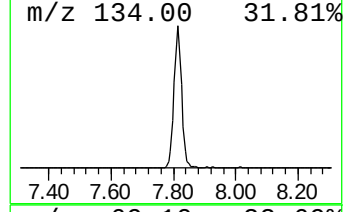
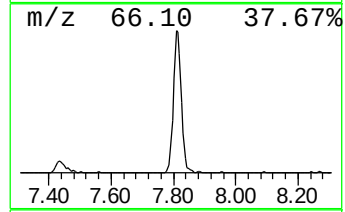
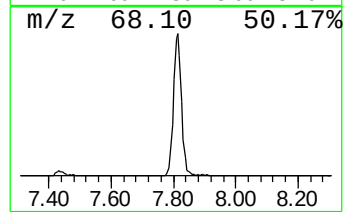
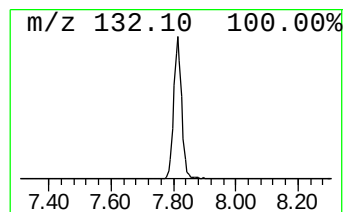
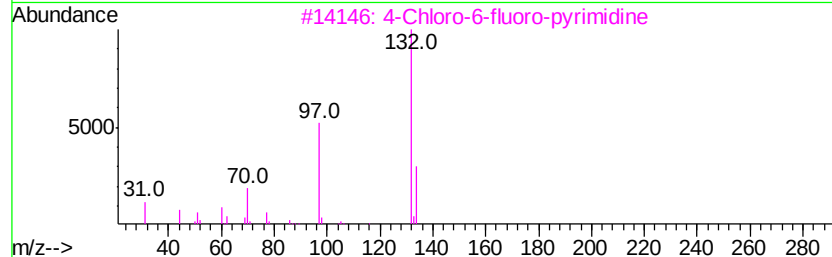
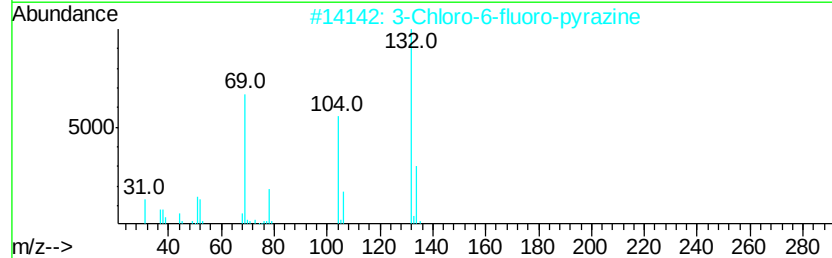
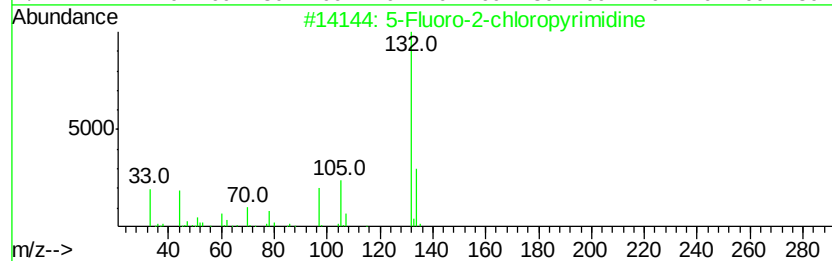
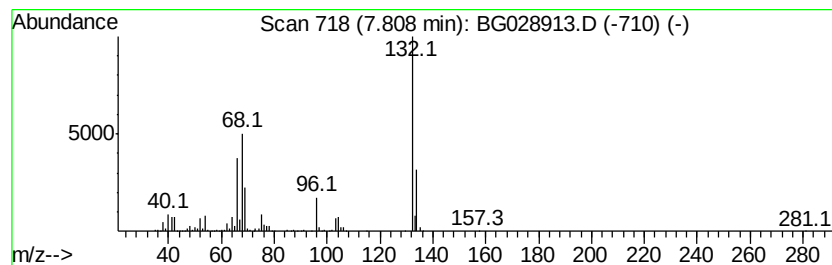
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Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	109.95 ng	1000500	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17



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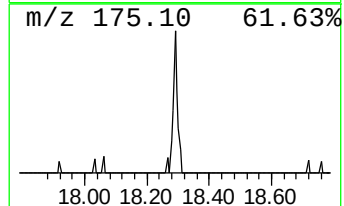
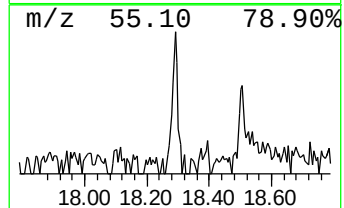
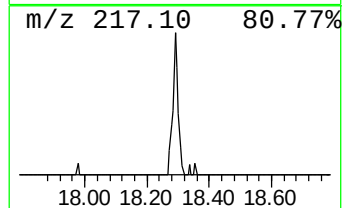
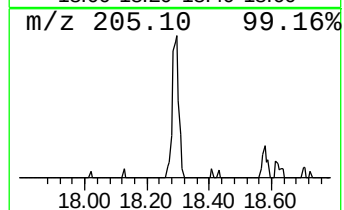
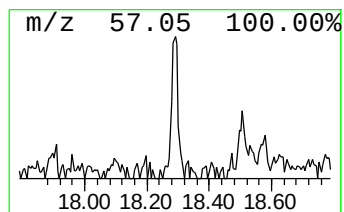
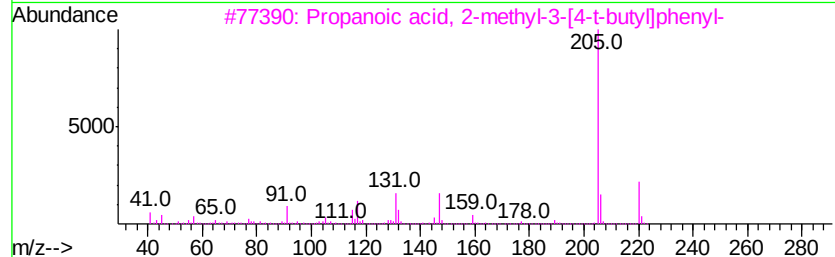
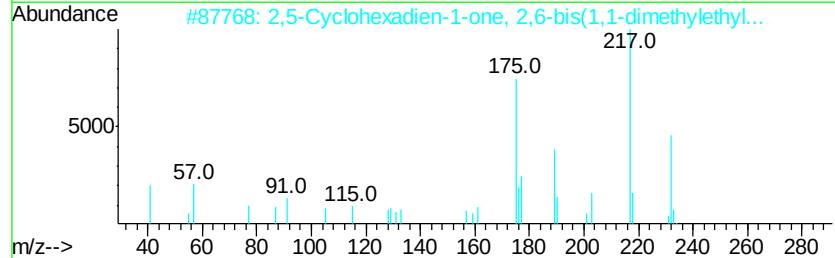
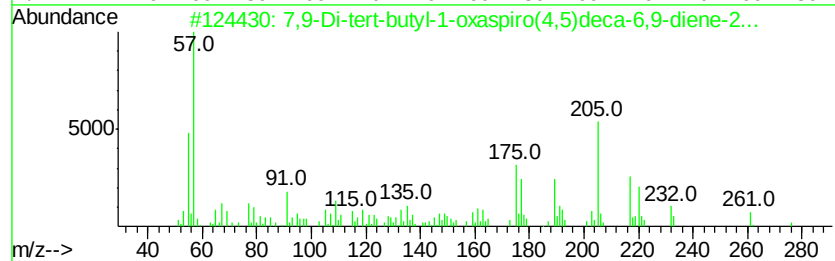
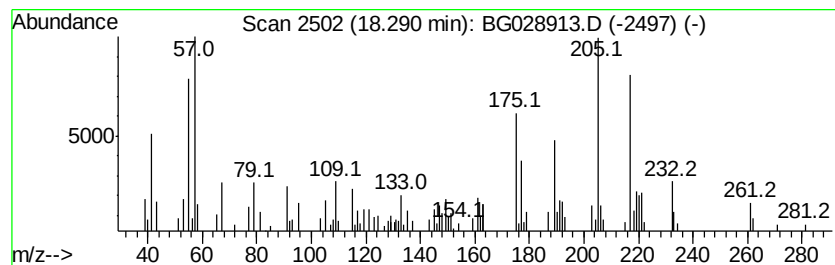
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.29	2.24 ng	66771	Phenanthrene-d10	17.65		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	62	
2	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	38	
3	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	35	
4	4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	35	
5	3-isopropylphenol, trifluoroacetate	232	C11H11F3O2	1000376-49-6	18	



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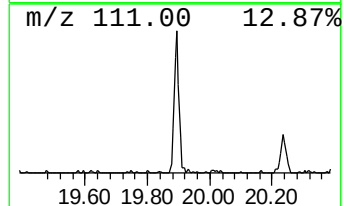
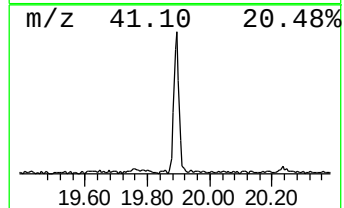
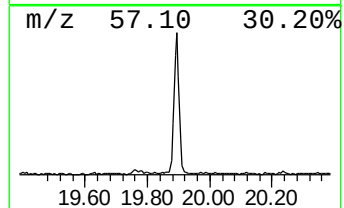
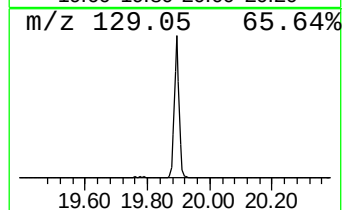
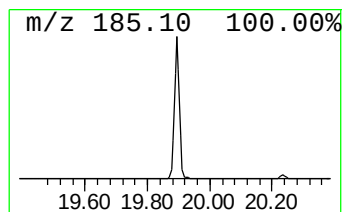
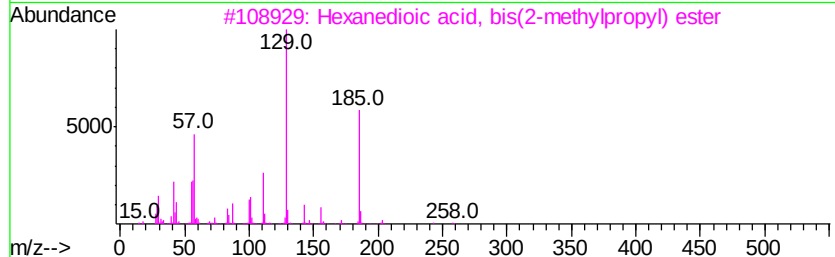
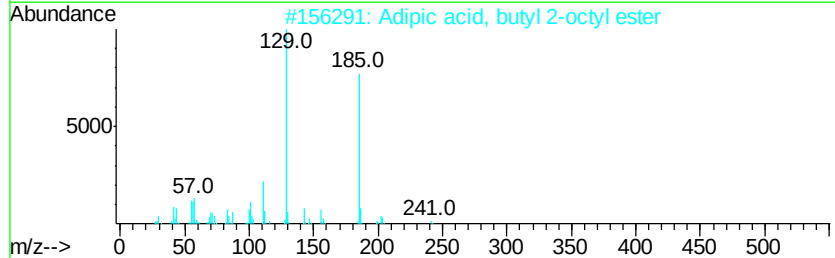
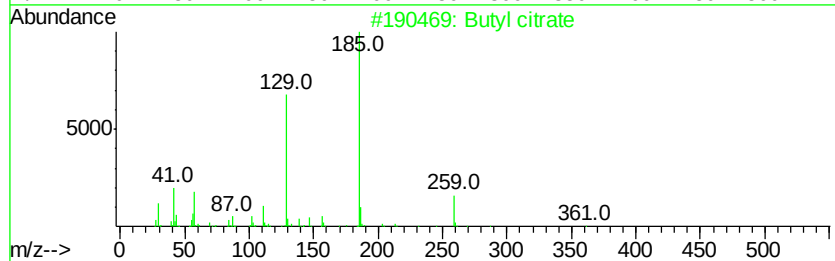
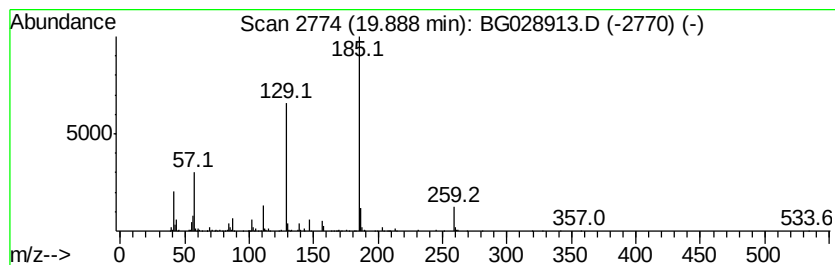
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Peak Number 5 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	12.57 ng	458148	Chrysene-d12	21.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl citrate	360	C18H32O7	000077-94-1	91
2		Adipic acid, butyl 2-octyl ester	314	C18H34O4	1000324-44-6	72
3		Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
4		Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	64
5		Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	64



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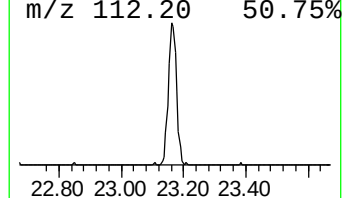
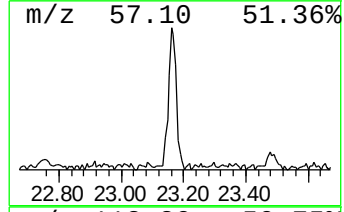
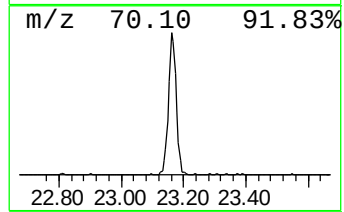
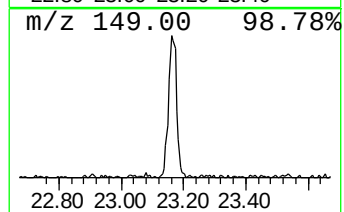
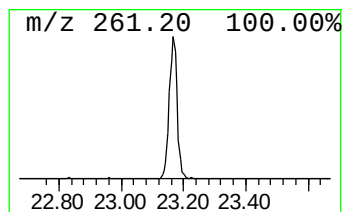
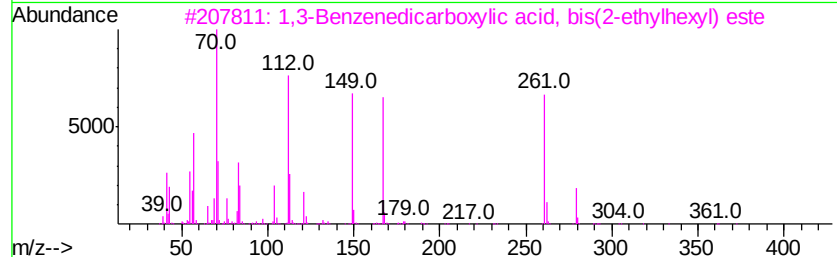
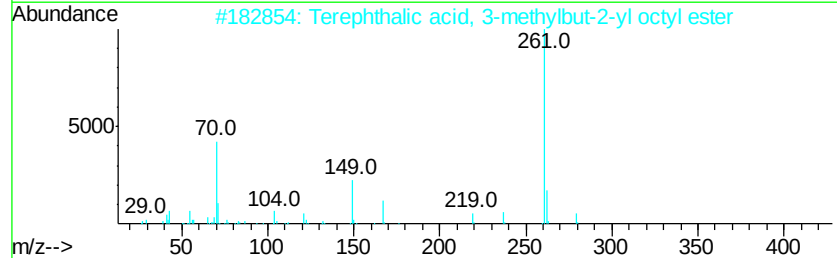
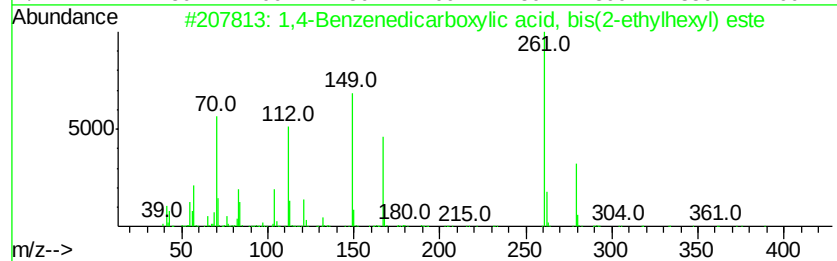
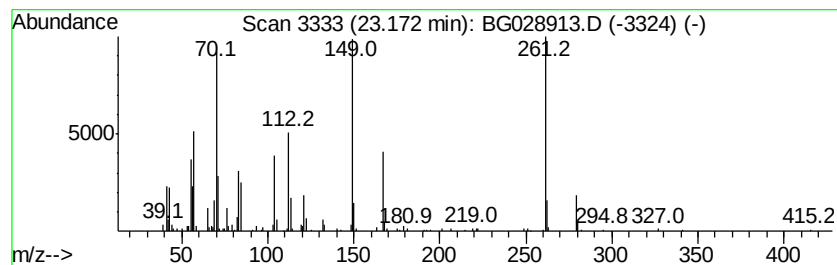
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Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	8.22 ng	299740	Chrysene-d12	21.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2		Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
4		Isophthalic acid, 4-nitrophenyl ...	399	C22H25NO6	1000344-68-5	38
5		Isophthalic acid, 2-chlorophenyl...	388	C22H25ClO4	1000344-50-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	5.7	ng	52063	1	8.28	182001	20.0
unknown7.81	7.81	110.0	ng	1000500	1	8.28	182001	20.0
7,9-Di-tert-butyl...	18.29	2.2	ng	66771	4	17.65	596580	20.0
Butyl citrate	19.89	12.6	ng	458148	5	21.97	728929	20.0
1,4-Benzenedicarb...	23.17	8.2	ng	299740	5	21.97	728929	20.0