

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
 Data File : BG028802.D
 Acq On : 18 Sep 2017 19:39
 Operator : SJ/JU
 Sample : I5259-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170602-COMP-C

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	5.392	302	307	313	rBV	22984	34865	1.09%	0.273%
2	5.856	379	386	399	rBV	272036	473519	14.76%	3.711%
3	7.442	649	656	667	rBV	206090	389956	12.15%	3.056%
4	7.824	714	721	731	rBV	436476	795025	24.78%	6.231%
5	8.288	793	800	809	rBV2	98959	182689	5.69%	1.432%
6	8.617	848	856	866	rVB	399704	708772	22.09%	5.555%
7	9.457	991	999	1008	rBV	329062	616911	19.23%	4.835%
8	11.108	1271	1280	1290	rBV	135522	259289	8.08%	2.032%
9	13.529	1684	1692	1700	rBV	1033038	1641493	51.16%	12.866%
10	14.910	1918	1927	1935	rBV2	239662	409890	12.77%	3.213%
11	16.396	2173	2180	2191	rBV	985241	1611690	50.23%	12.632%
12	17.660	2388	2395	2406	rVB2	401655	628074	19.57%	4.923%
13	18.300	2498	2504	2510	rBV3	45612	58387	1.82%	0.458%
14	19.904	2772	2777	2782	rBV	112172	132606	4.13%	1.039%
15	20.251	2829	2836	2847	rBV	2308288	3208826	100.00%	25.150%
16	21.573	3052	3061	3064	rBV9	13716	33185	1.03%	0.260%
17	21.984	3122	3131	3140	rBV	413847	742688	23.15%	5.821%
18	23.183	3329	3335	3344	rVB3	78057	143493	4.47%	1.125%
19	25.445	3710	3720	3735	rBV2	208726	687182	21.42%	5.386%

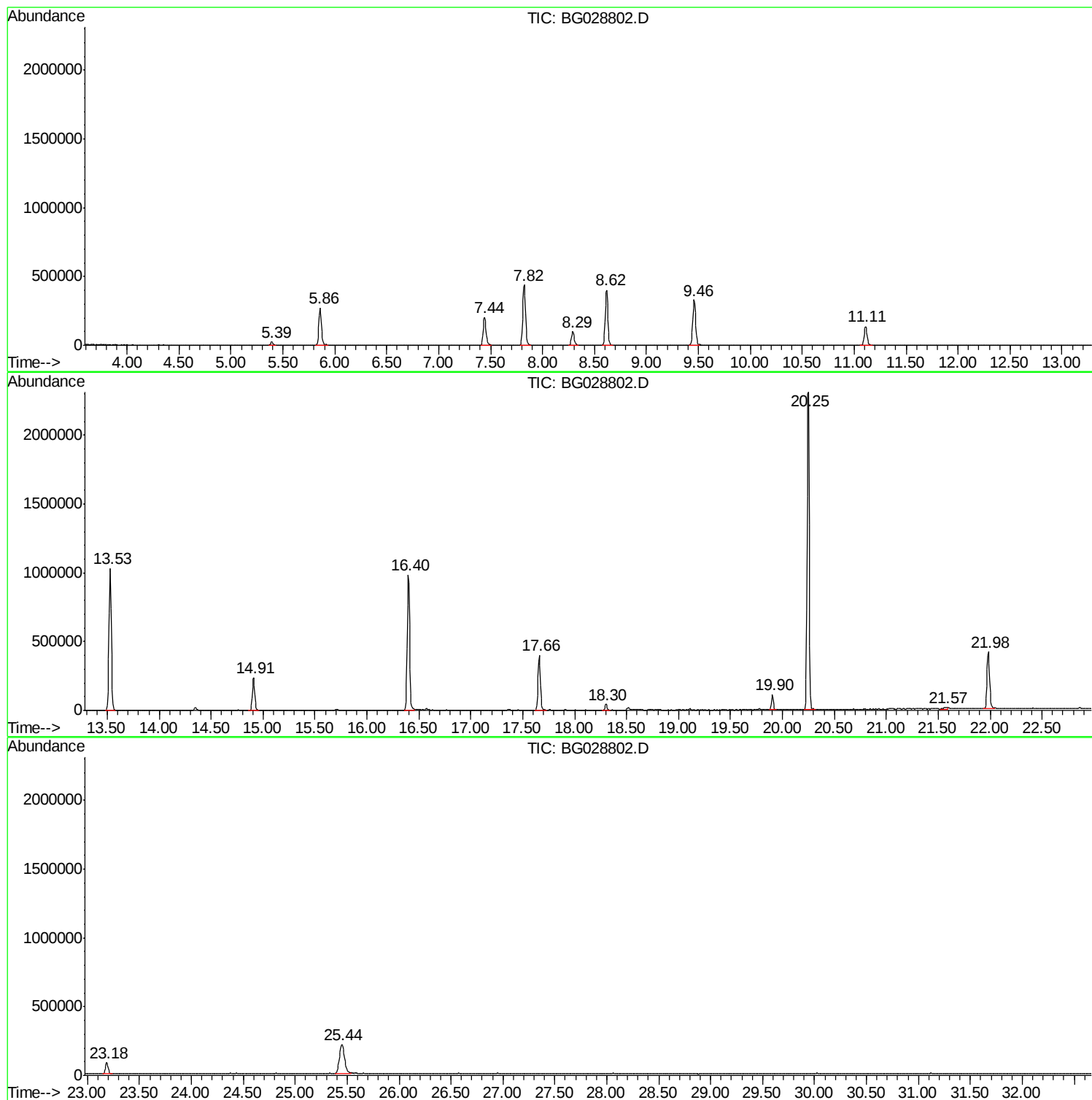
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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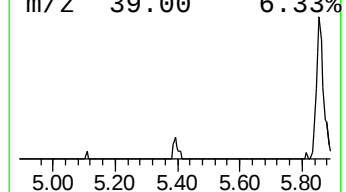
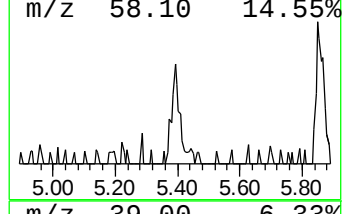
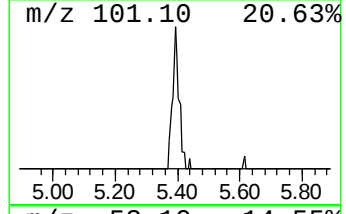
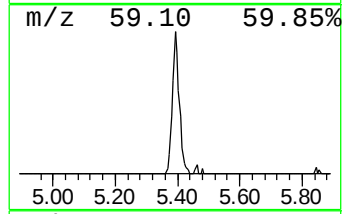
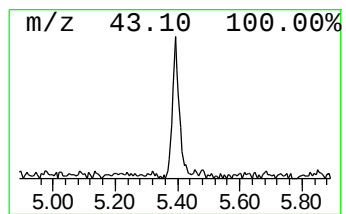
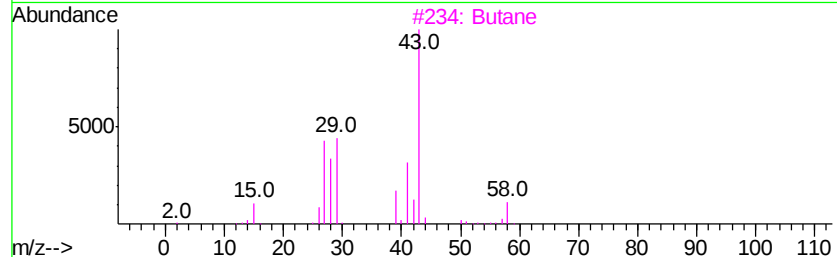
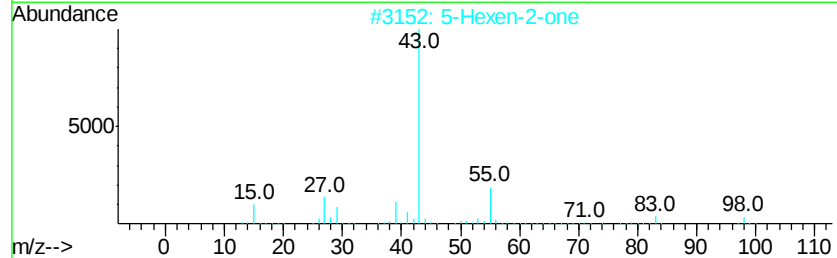
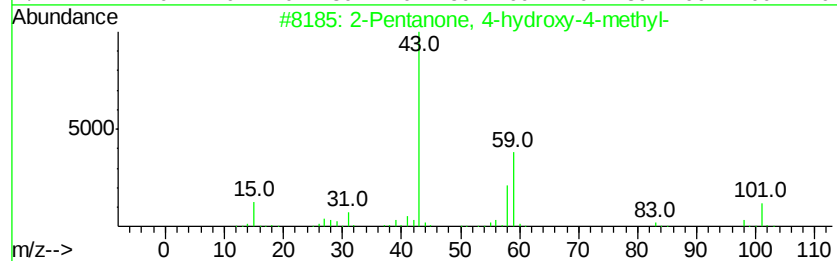
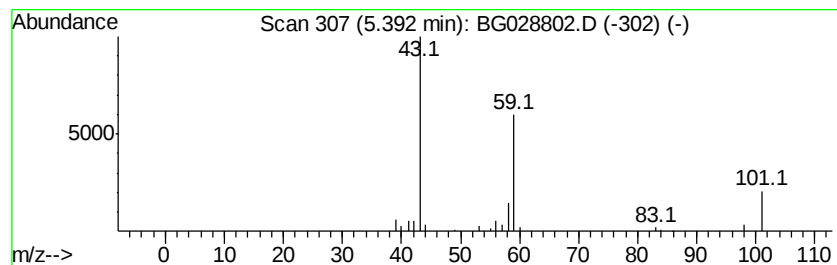
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	3.82 ng	34865	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Butane	58	C4H10	000106-97-8	9
4		Propylamine	59	C3H9N	000107-10-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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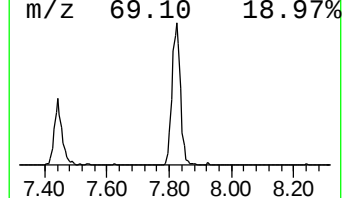
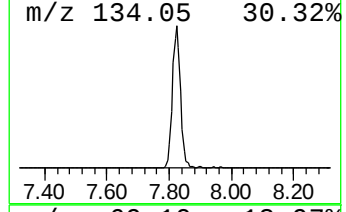
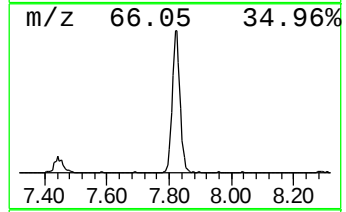
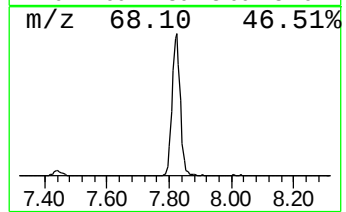
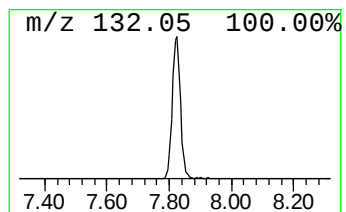
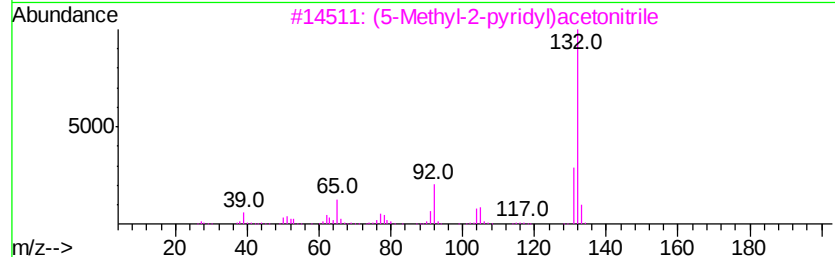
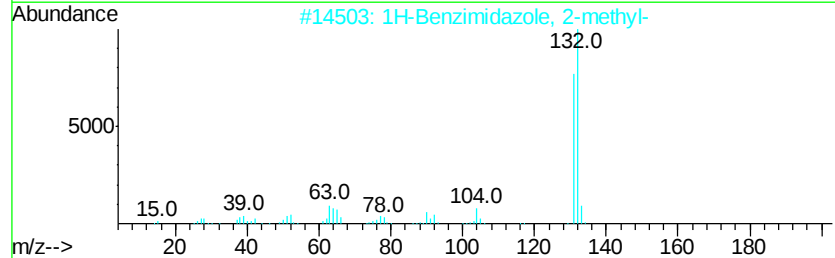
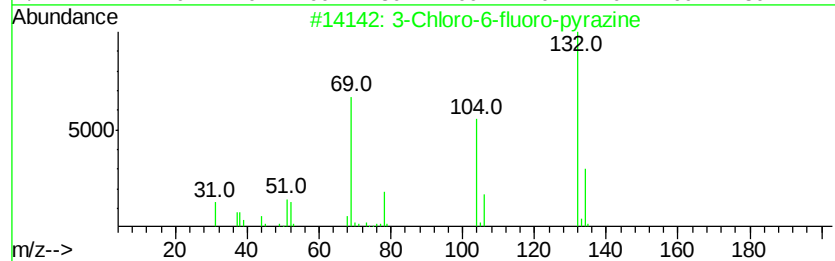
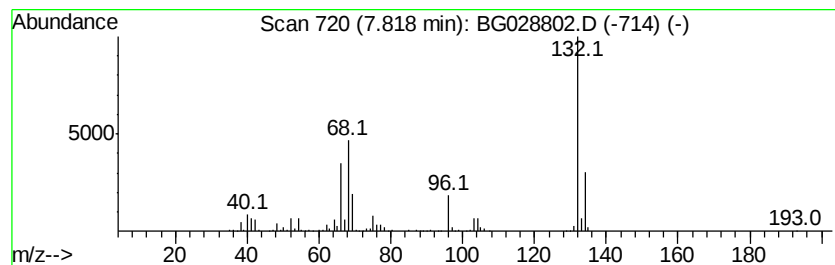
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Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	87.04 ng	795025	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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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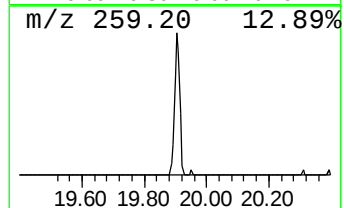
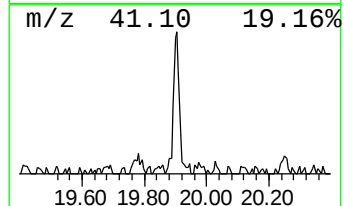
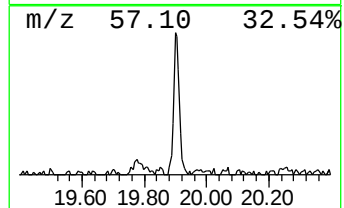
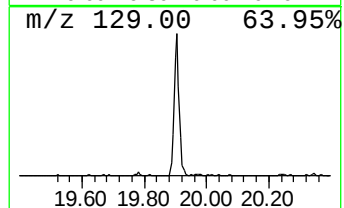
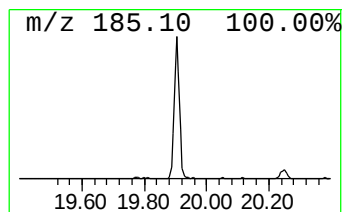
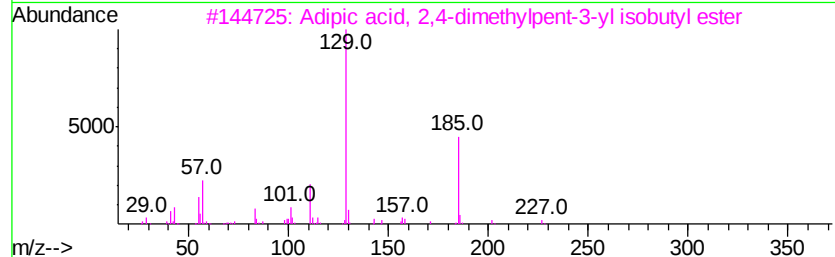
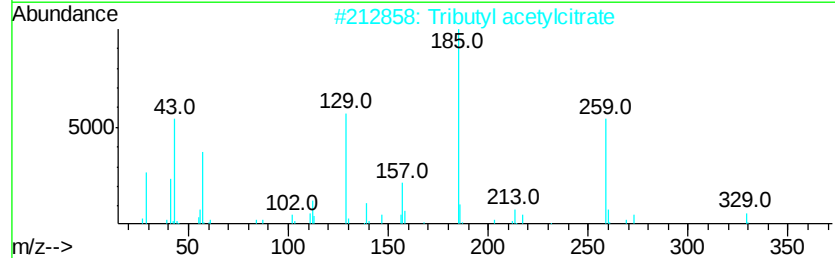
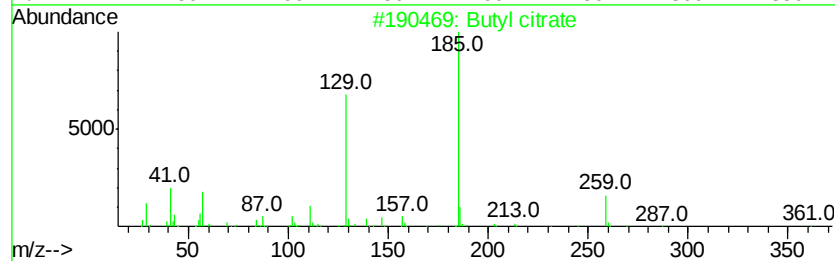
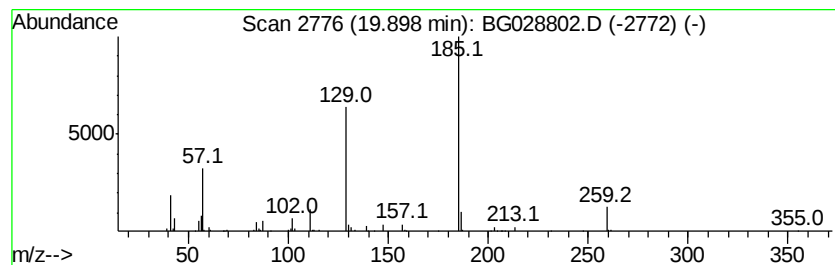
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Peak Number 4 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	3.57 ng	132606	Chrysene-d12	21.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butyl citrate	360	C18H32O7	000077-94-1	91
2		Tributyl acetylcitrate	402	C20H34O8	000077-90-7	74
3		Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	72
4		Adipic acid, 4-bromophenyl butyl...	356	C16H21BrO4	1000324-37-9	64
5		Dibutyl adipate	258	C14H26O4	000105-99-7	56



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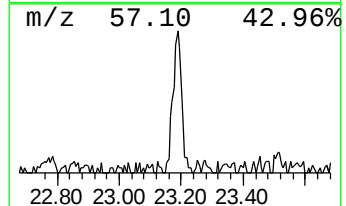
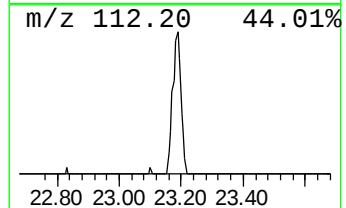
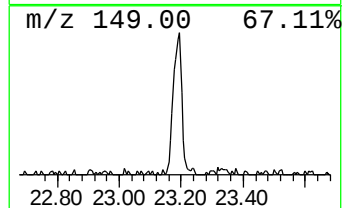
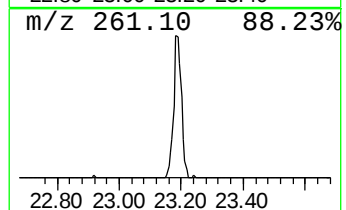
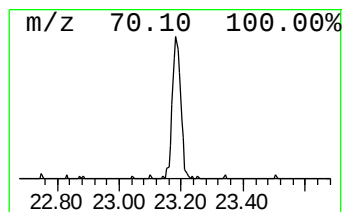
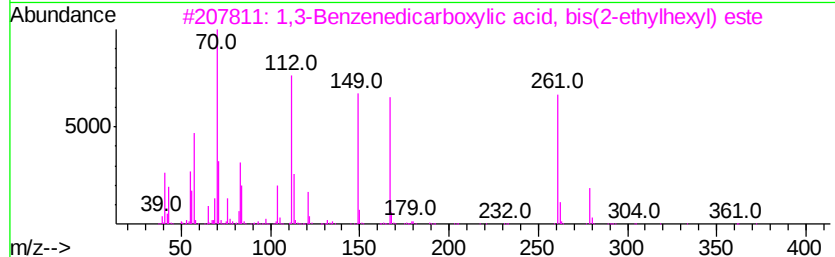
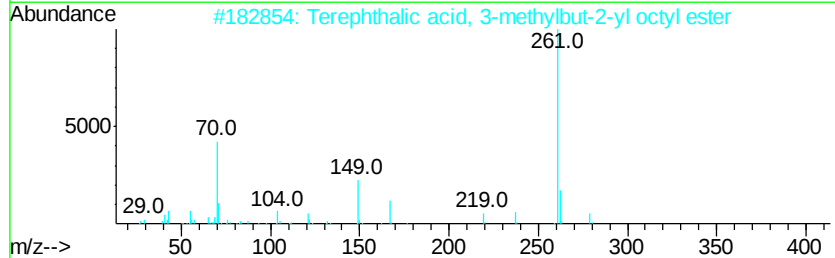
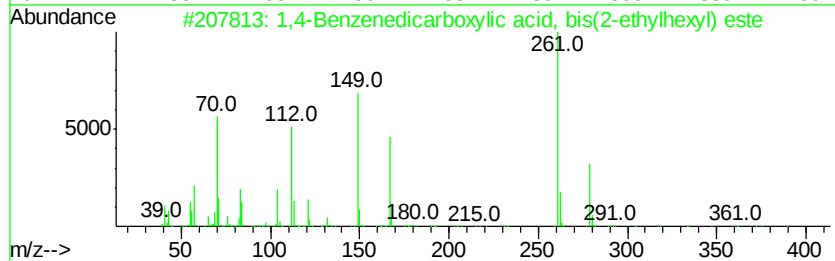
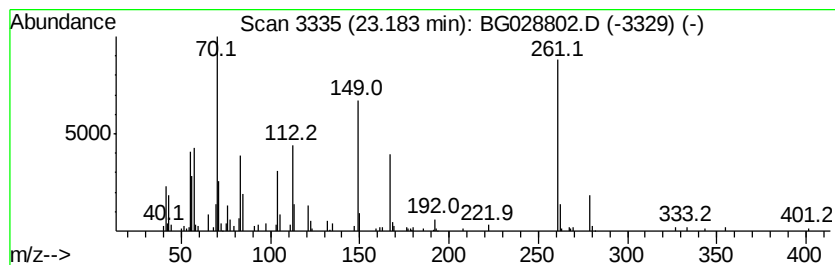
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.86 ng	143493	Chrysene-d12	21.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
2		Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
3		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
4		Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38
5		Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.39	3.8	ng	34865	1	8.29	182689	20.0
unknown7.82	7.82	87.0	ng	795025	1	8.29	182689	20.0
Butyl citrate	19.90	3.6	ng	132606	5	21.98	742688	20.0
1,4-Benzenedicarb...	23.18	3.9	ng	143493	5	21.98	742688	20.0