

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092517\
 Data File : BG028911.D
 Acq On : 25 Sep 2017 17:14
 Operator : SJ/JU
 Sample : I5321-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20170611-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	5.385	301	306	318	rVB	29606	51678	1.40%	0.368%
2	5.850	378	385	396	rBV	329033	564000	15.27%	4.017%
3	7.436	648	655	667	rBV	211591	409341	11.08%	2.916%
4	7.812	712	719	734	rVB	546729	979629	26.53%	6.978%
5	8.282	790	799	805	rBV	94799	178178	4.82%	1.269%
6	8.605	846	854	862	rBV	476066	864242	23.40%	6.156%
7	9.451	990	998	1009	rBV	388698	755340	20.45%	5.380%
8	11.102	1270	1279	1289	rBV	122031	235765	6.38%	1.679%
9	13.517	1683	1690	1702	rBV	1201400	1851629	50.14%	13.189%
10	14.898	1918	1925	1932	rBV2	218808	357361	9.68%	2.546%
11	16.390	2171	2179	2194	rBV	1083453	1821447	49.32%	12.974%
12	17.647	2387	2393	2403	rVB2	341527	541621	14.67%	3.858%
13	18.294	2496	2503	2508	rBV2	156798	217080	5.88%	1.546%
14	19.892	2770	2775	2780	rBV2	178760	209871	5.68%	1.495%
15	20.239	2827	2834	2846	rBV	2674242	3692948	100.00%	26.305%
16	21.966	3121	3128	3136	rBV2	360046	670802	18.16%	4.778%
17	25.421	3705	3716	3730	rVB	196020	637827	17.27%	4.543%

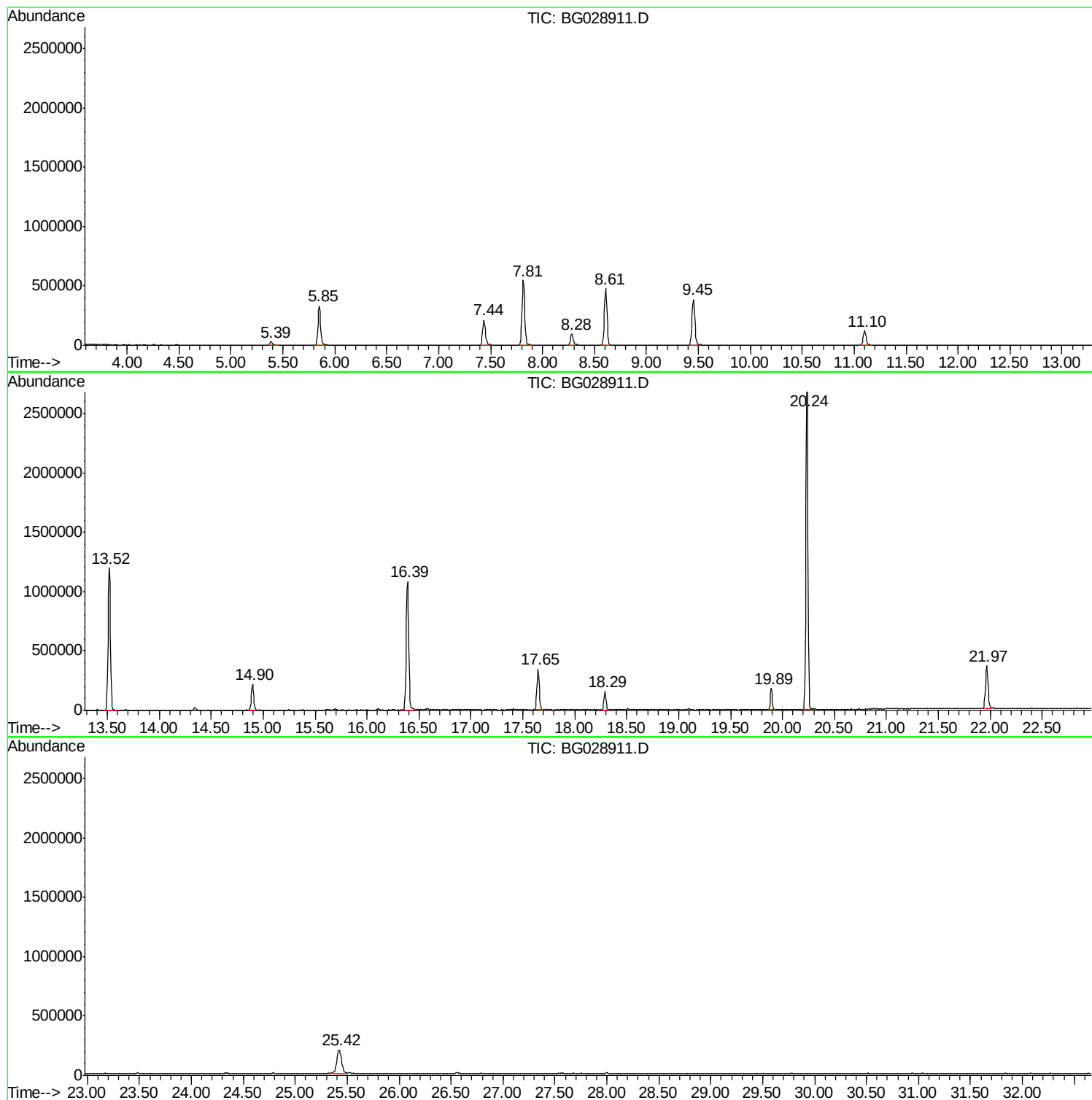
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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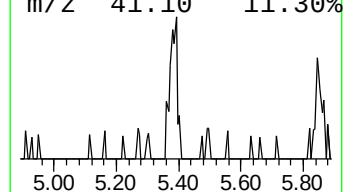
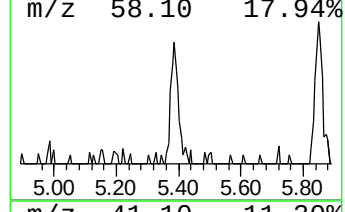
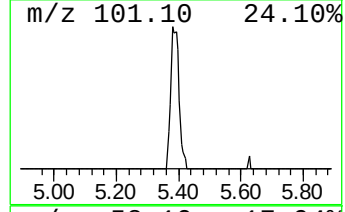
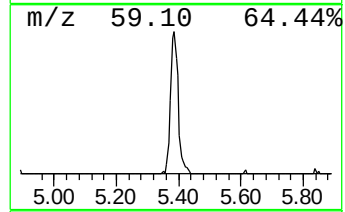
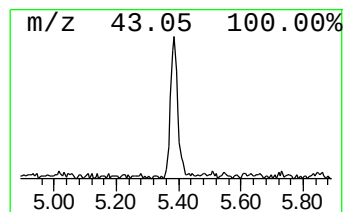
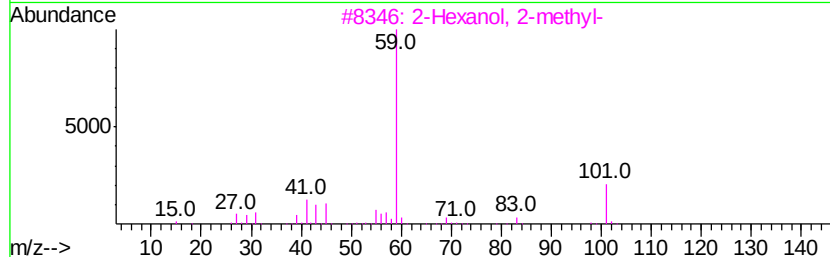
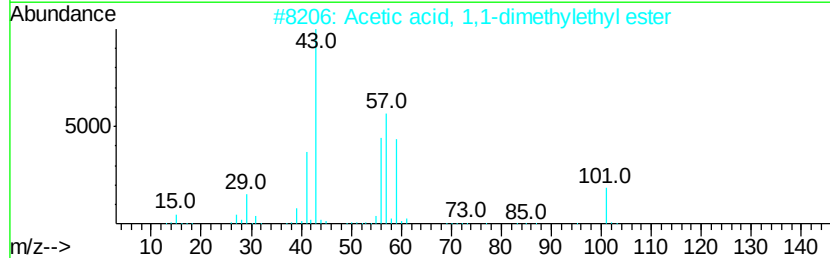
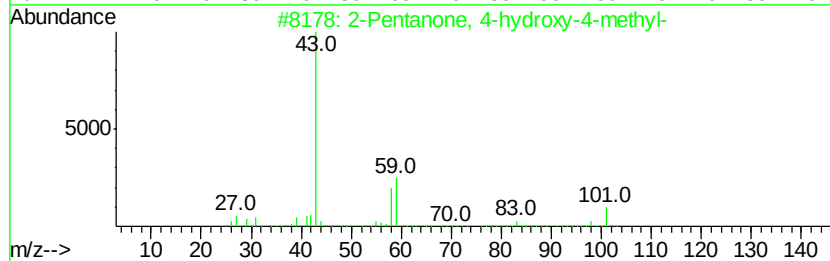
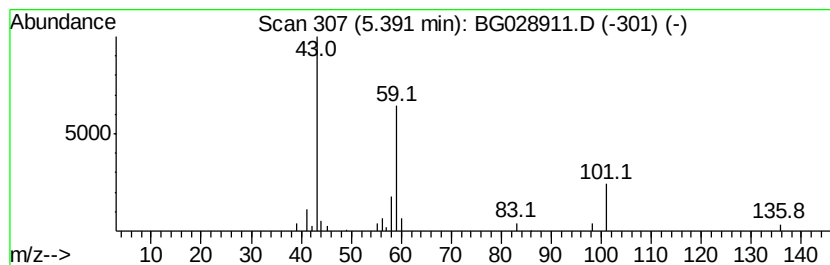
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	5.80 ng	51678	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	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25



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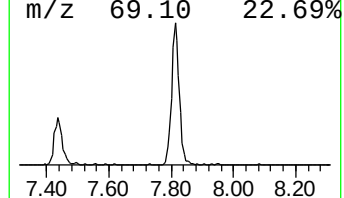
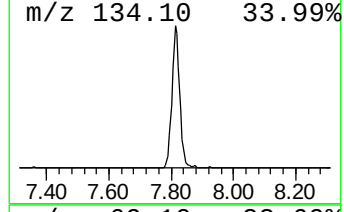
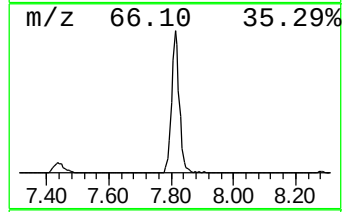
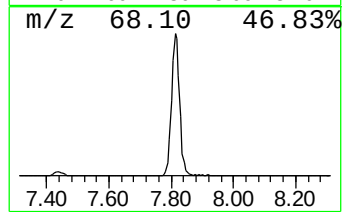
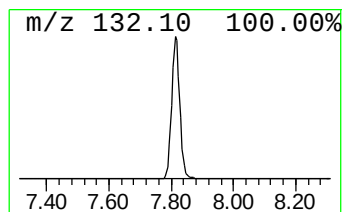
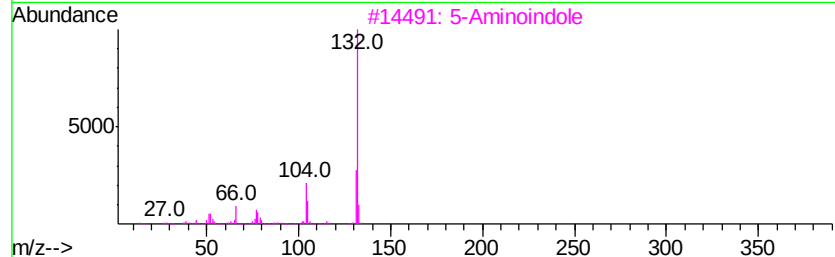
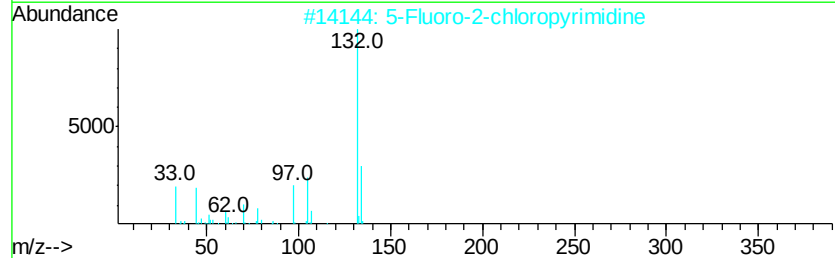
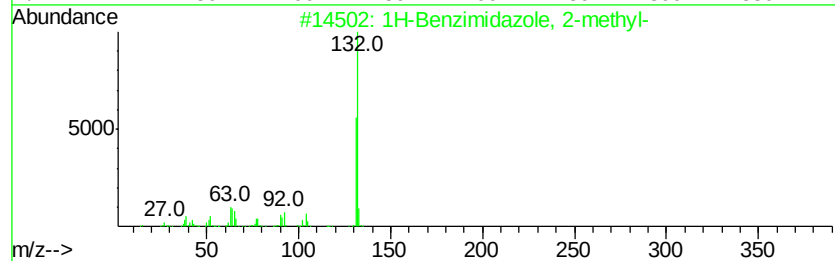
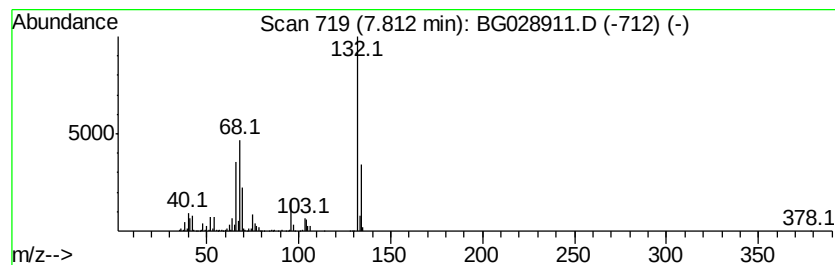
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Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	109.96 ng	979629	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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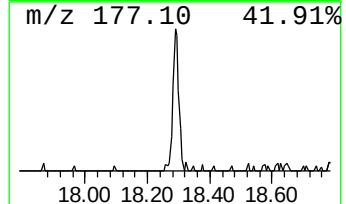
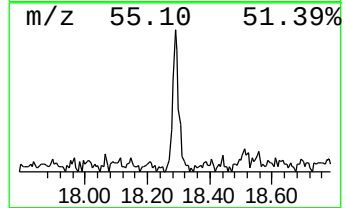
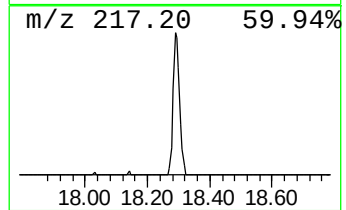
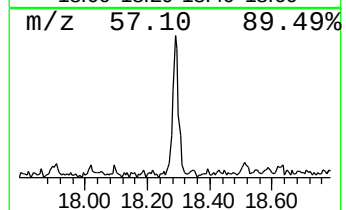
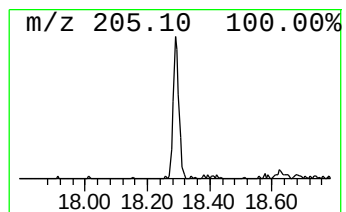
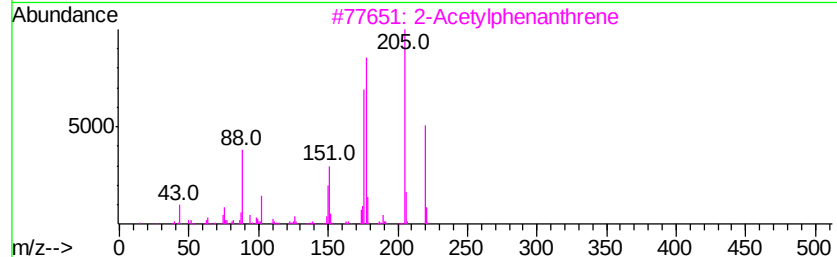
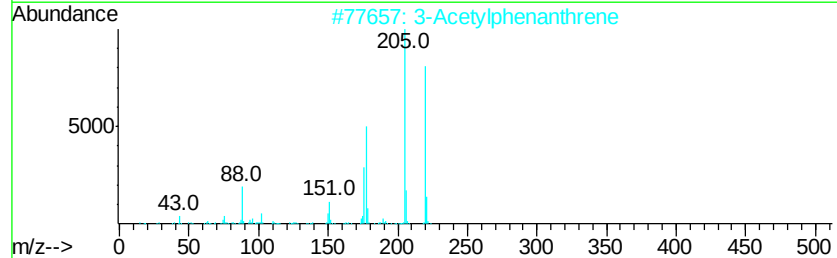
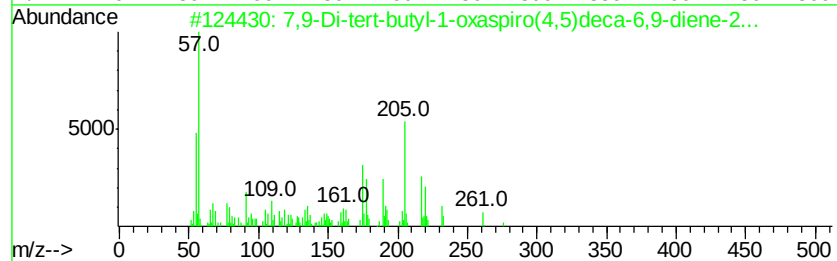
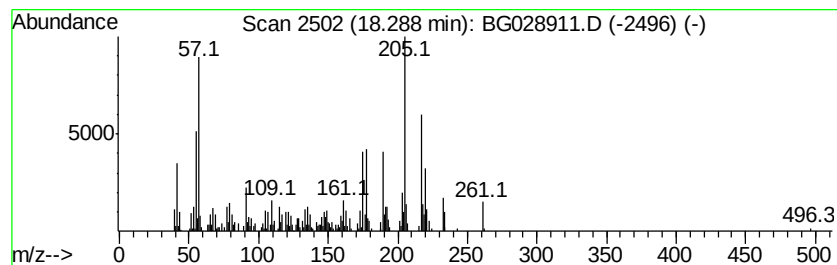
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Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.29	8.02 ng	217080	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	96
2	3-Acetylphenanthrene	220	C16H12O	002039-76-1	45
3	2-Acetylphenanthrene	220	C16H12O	005960-69-0	45
4	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	42
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42



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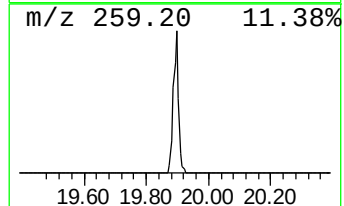
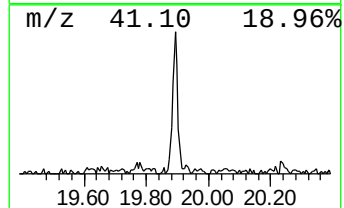
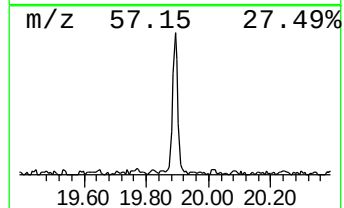
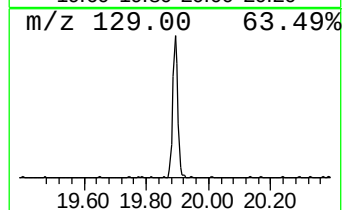
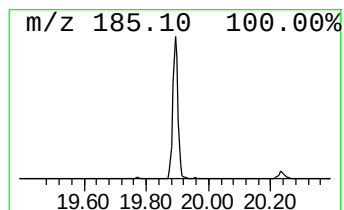
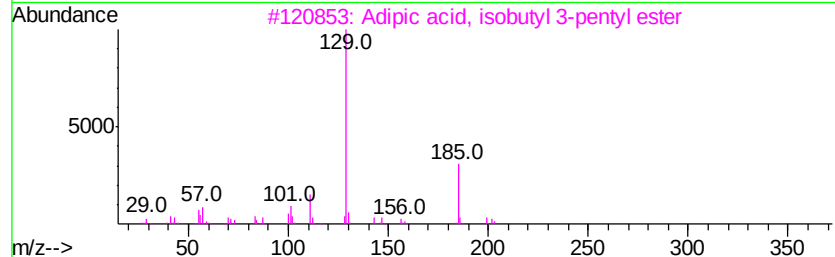
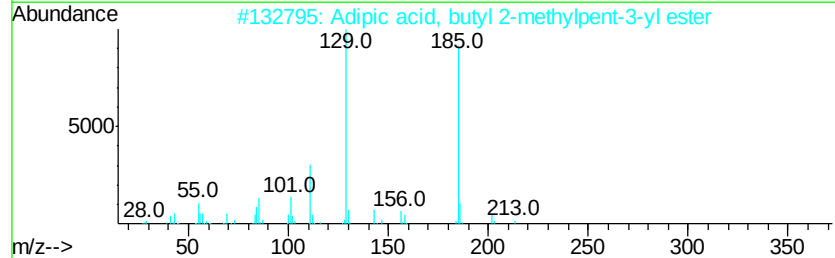
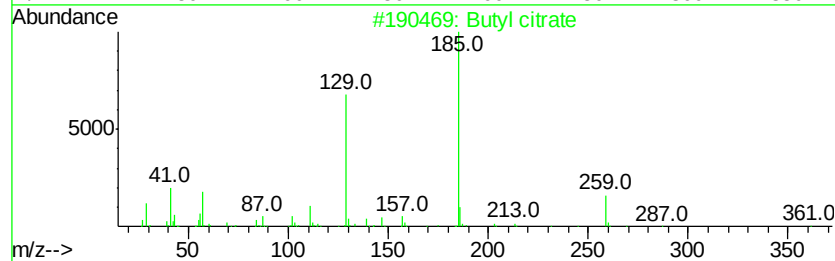
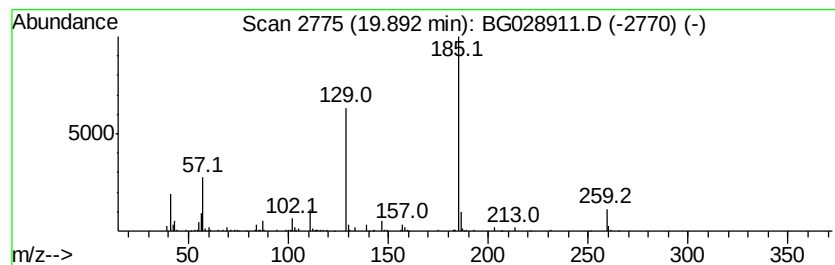
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Peak Number 5 Butyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	6.26 ng	209871	Chrysene-d12	21.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Adipic acid, butyl 2-methylpent-...	286 C16H30O4	1000353-55-8	56
3	Adipic acid, isobutyl 3-pentyl e...	272 C15H28O4	1000324-60-4	56
4	Adipic acid, 2-decyl isobutyl ester	342 C20H38O4	1000353-59-6	56
5	Adipic acid, isobutyl 2-octyl ester	314 C18H34O4	1000324-44-5	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.39	5.8	ng	51678	1	8.28	178178	20.0
unknown7.81	7.81	110.0	ng	979629	1	8.28	178178	20.0
7,9-Di-tert-butyl...	18.29	8.0	ng	217080	4	17.65	541621	20.0
Butyl citrate	19.89	6.3	ng	209871	5	21.97	670802	20.0