

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092218\
 Data File : BG036904.D
 Acq On : 22 Sep 2018 22:43
 Operator : JU/SJ
 Sample : J5019-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 091918-JETT-E-D-B

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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	5.150	312	317	328	rBV	29845	51031	1.30%	0.343%
2	5.620	390	397	410	rBV	173780	338301	8.60%	2.276%
3	7.206	661	667	686	rBV	105784	248054	6.30%	1.669%
4	7.576	723	730	749	rBV	357087	703193	17.87%	4.731%
5	8.046	804	810	830	rBV	120312	235791	5.99%	1.586%
6	8.369	857	865	881	rBV	548935	1035504	26.31%	6.967%
7	9.210	1000	1008	1031	rBV	434172	945665	24.03%	6.362%
8	10.849	1280	1287	1302	rBV	164100	342595	8.71%	2.305%
9	13.293	1696	1703	1723	rBV	1350369	2389299	60.72%	16.075%
10	14.121	1837	1844	1852	rBV	33251	55524	1.41%	0.374%
11	14.674	1931	1938	1949	rBV2	307719	542924	13.80%	3.653%
12	15.960	2151	2157	2164	rBV	68191	96306	2.45%	0.648%
13	16.160	2183	2191	2205	rBV	718914	1255940	31.92%	8.450%
14	17.418	2399	2405	2416	rBV	432284	707405	17.98%	4.759%
15	20.026	2842	2849	2862	rBV	2758303	3935256	100.00%	26.476%
16	21.683	3124	3131	3144	rVB	476199	817771	20.78%	5.502%
17	23.358	3408	3416	3423	rBV	101843	204104	5.19%	1.373%
18	23.963	3513	3519	3529	rVB4	23731	54116	1.38%	0.364%
19	24.891	3665	3677	3690	rBV	278178	849037	21.58%	5.712%
20	26.025	3864	3870	3880	rVB6	19211	55427	1.41%	0.373%

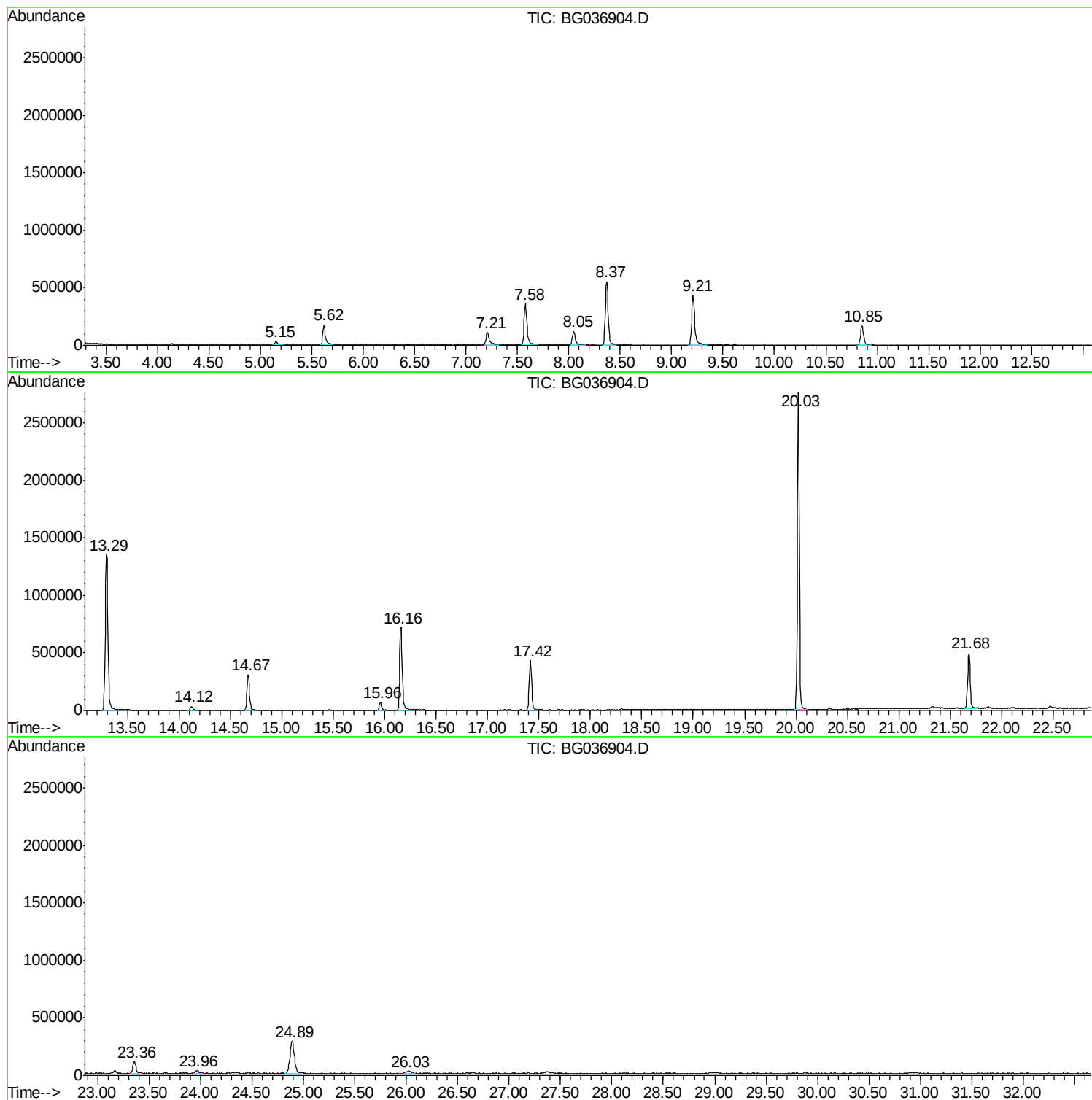
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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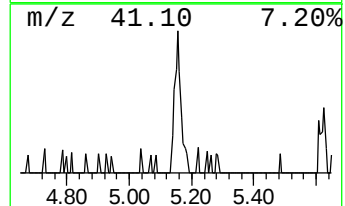
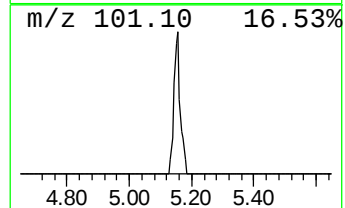
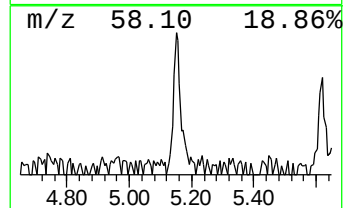
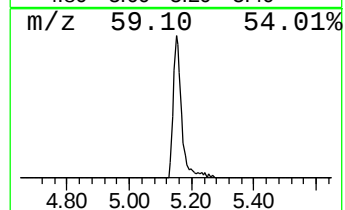
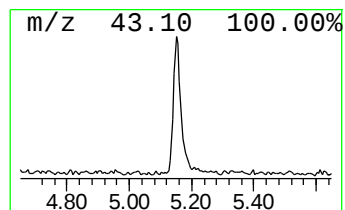
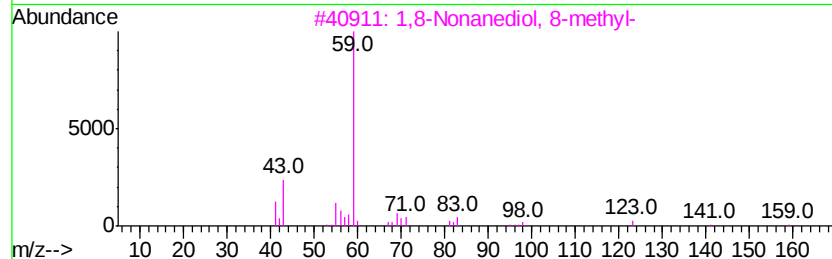
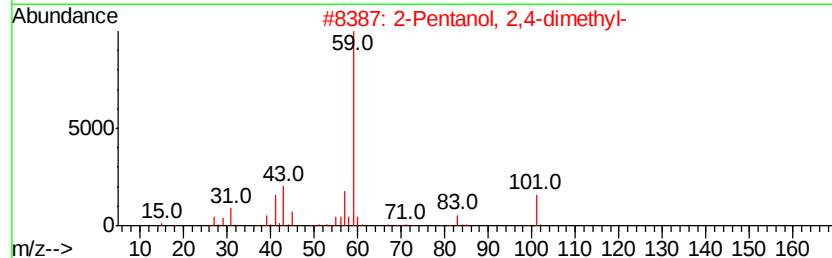
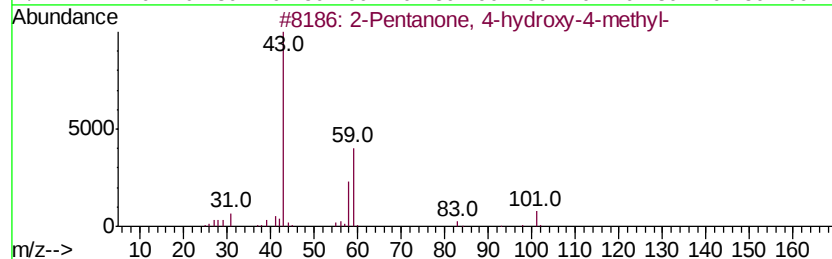
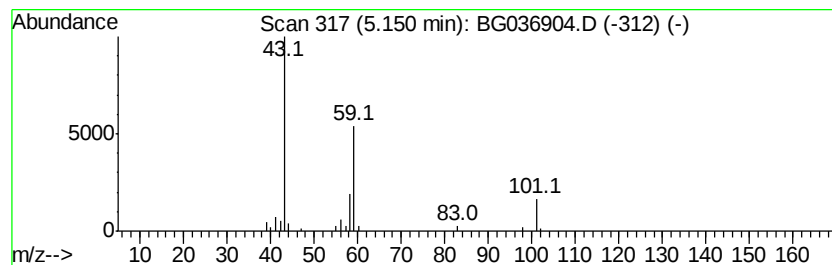
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.15	4.33 ng	51031	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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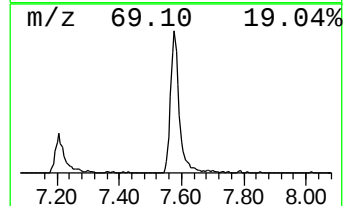
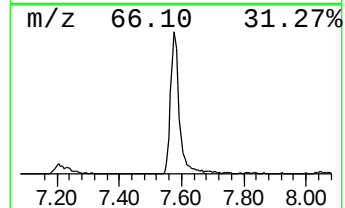
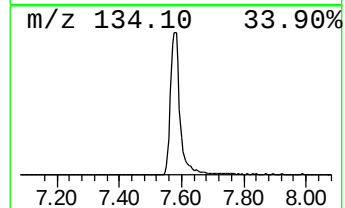
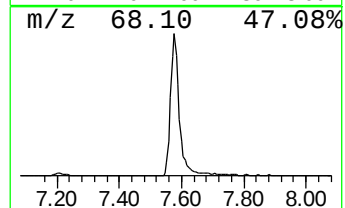
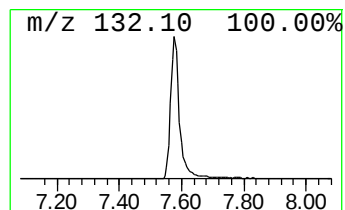
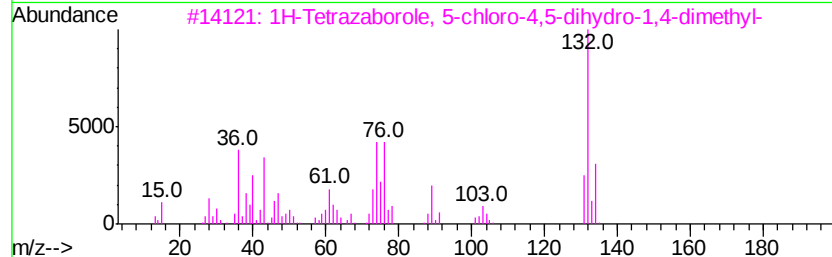
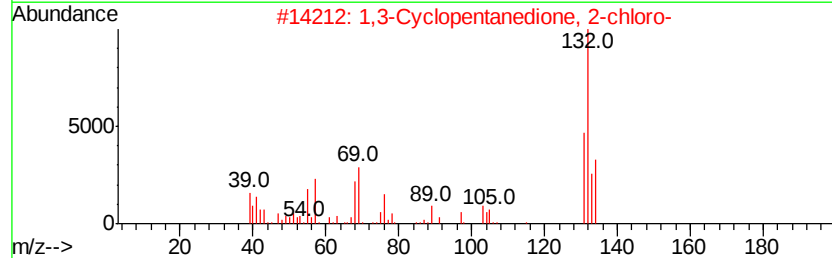
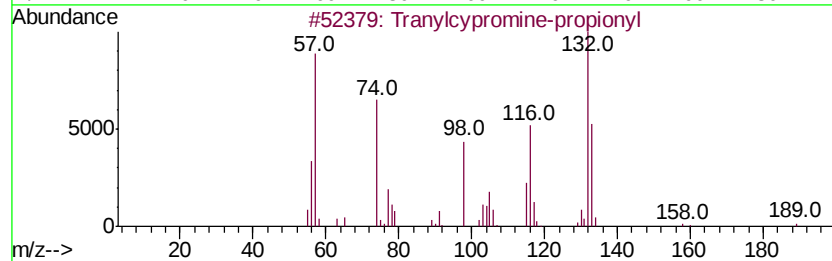
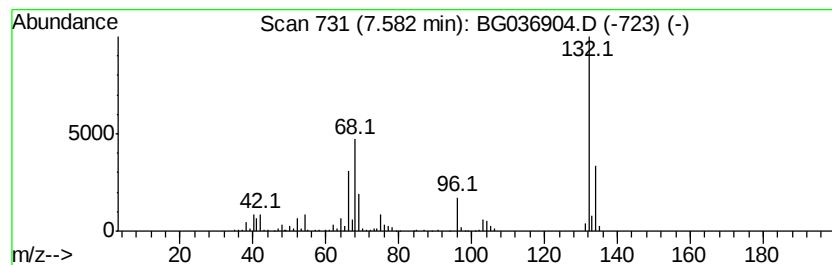
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Peak Number 2 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	59.65 ng	703193	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tranvlcyppromine-propionyl	189	C12H15NO	1000123-86-3	22
2			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3			1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	12
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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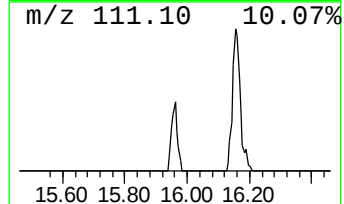
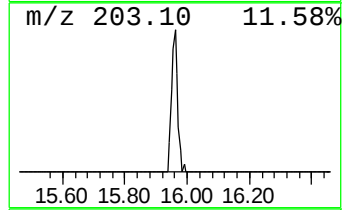
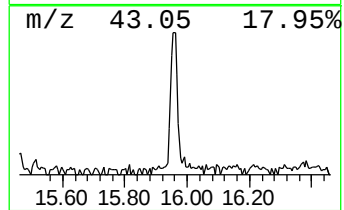
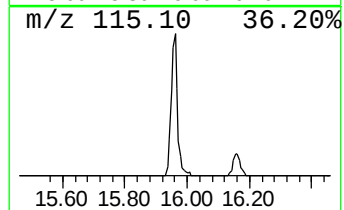
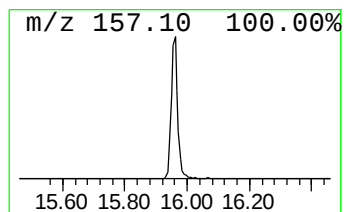
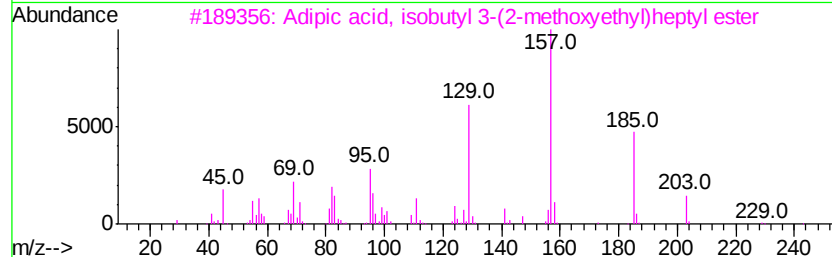
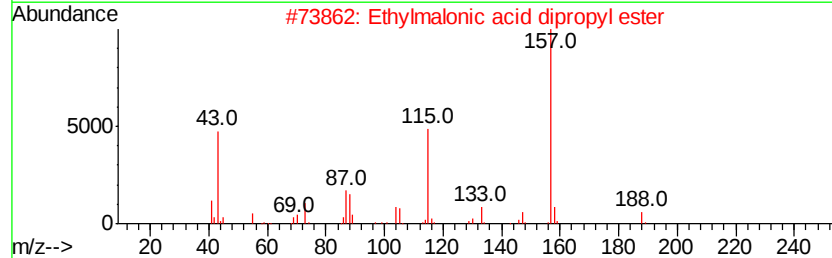
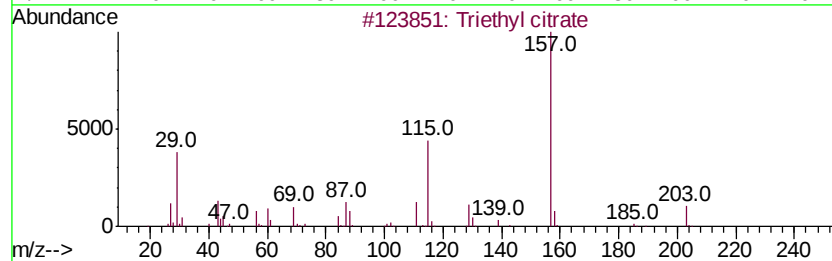
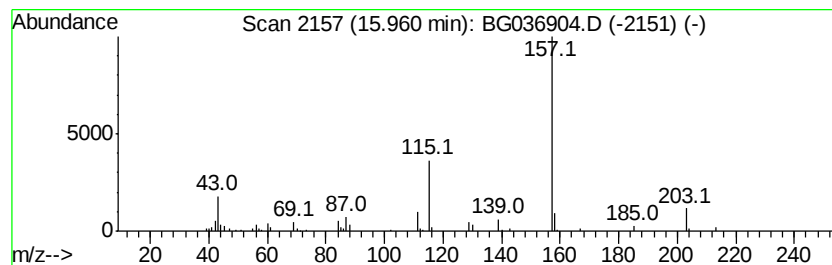
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Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.55 ng	96306	Acenaphthene-d10	14.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triethyl citrate	276	C12H20O7	000077-93-0	74
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	38
3		Adipic acid, isobutyl 3-(2-metho...	358	C20H38O5	1000324-28-7	36
4		3-Chloro2-fluorobenzoic acid, 4-...	384	C22H34ClF02	1000338-65-1	36
5		3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClF02	1000338-64-6	36



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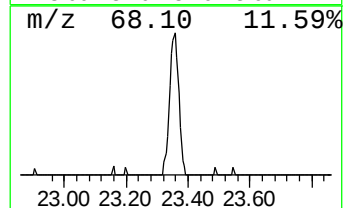
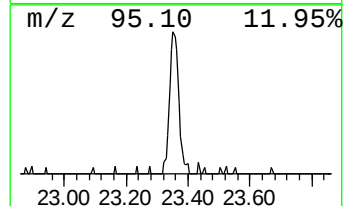
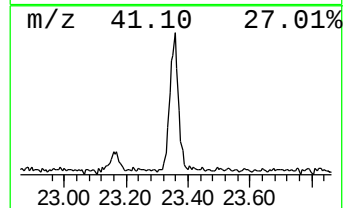
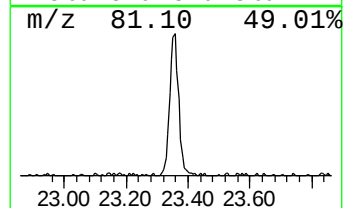
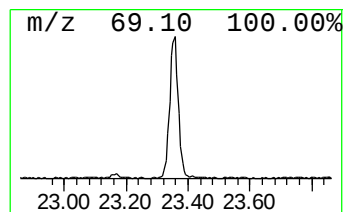
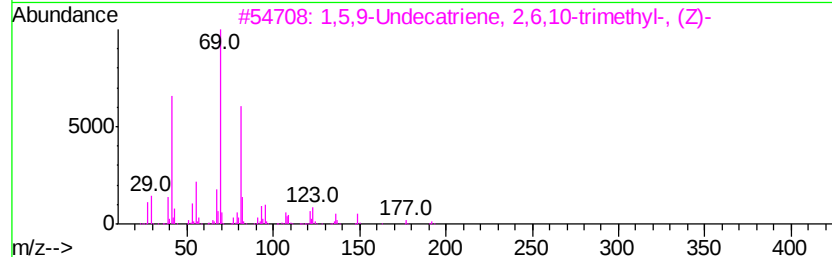
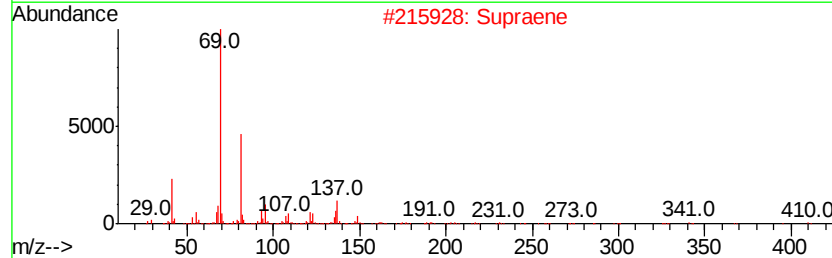
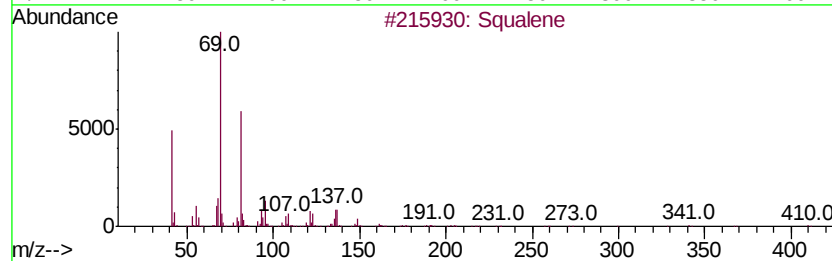
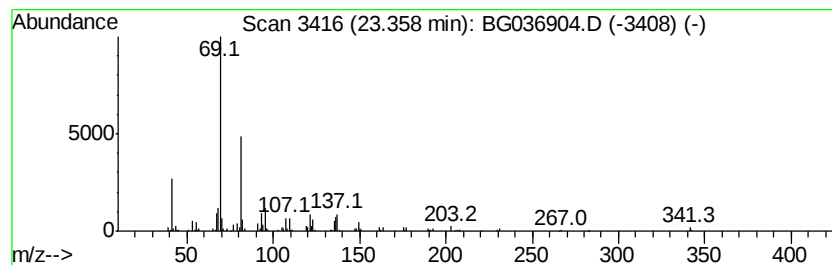
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Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	4.81 ng	204104	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	4.3	ng	51031	1	8.05	235791	20.0
unknown7.58	7.58	59.6	ng	703193	1	8.05	235791	20.0
Triethyl citrate	15.96	3.5	ng	96306	3	14.67	542924	20.0
Squalene	23.36	4.8	ng	204104	6	24.89	849037	20.0