

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
 Data File : BF092978.D
 Acq On : 16 Feb 2017 6:00
 Operator : SJ/MA
 Sample : I1790-02
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38-WCS021017-0-15

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_F\METHODS\8270-BF013017.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	2.578	30	43	45	rVB2	21903	115703	2.29%	0.261%
2	2.716	53	55	63	rVB	201426	276149	5.47%	0.622%
3	4.419	201	204	209	rBV	718830	1044418	20.70%	2.354%
4	5.070	258	261	271	rBV	1391497	2270875	45.00%	5.118%
5	5.482	294	297	300	rBV	3639382	4766578	94.45%	10.743%
6	6.522	384	388	390	rBV	3249935	4867070	96.44%	10.969%
7	6.590	392	394	396	rVB	209194	162336	3.22%	0.366%
8	6.647	396	399	401	rBV	4465849	5046642	100.00%	11.374%
9	6.876	416	419	421	rBV	946613	1049854	20.80%	2.366%
10	7.025	430	432	435	rBV	2940487	3840088	76.09%	8.655%
11	7.436	465	468	471	rBV	2283865	3490850	69.17%	7.868%
12	8.156	528	531	533	rBV	1634422	1443088	28.60%	3.252%
13	9.231	622	625	628	rBV	4820955	4858301	96.27%	10.950%
14	9.905	681	684	686	rBV	1692445	1441318	28.56%	3.248%
15	10.694	750	753	756	rBV	2391145	2537761	50.29%	5.720%
16	11.391	811	814	816	rBV	1355868	1270986	25.18%	2.865%
17	12.979	950	953	955	rBV	3748029	4146243	82.16%	9.345%
18	14.020	1042	1044	1047	rBV	900707	892999	17.69%	2.013%
19	15.460	1167	1170	1177	rBV	640709	848100	16.81%	1.911%

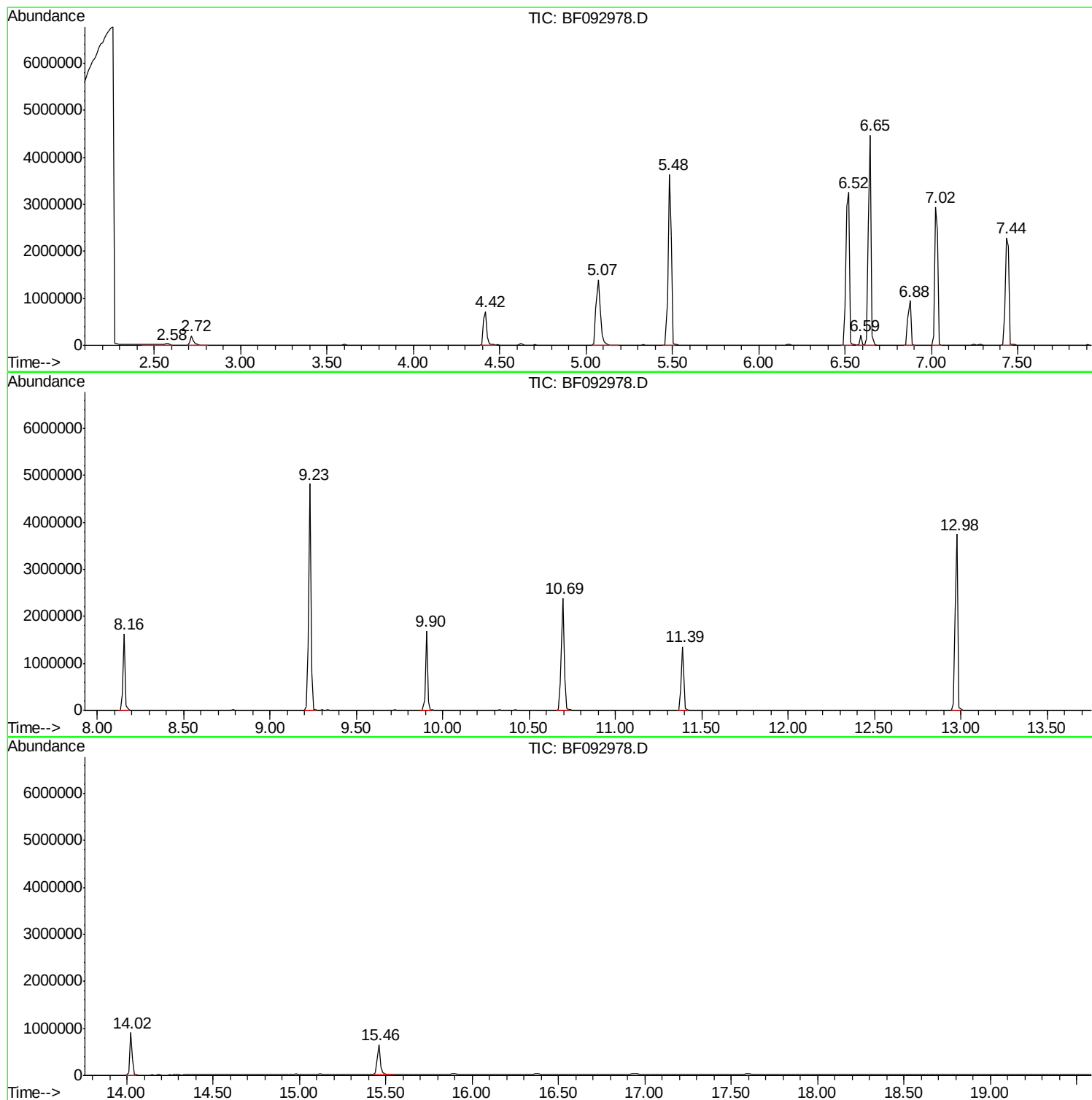
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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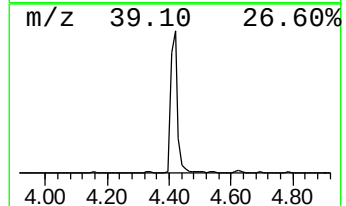
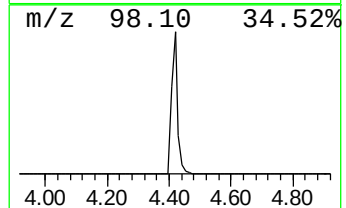
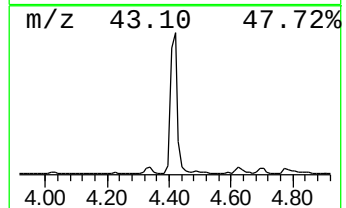
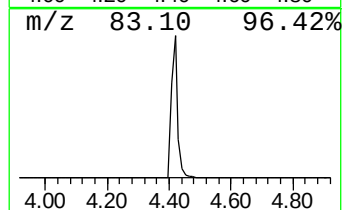
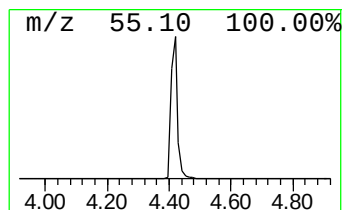
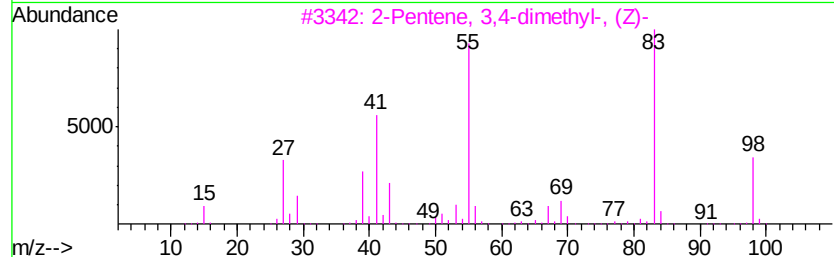
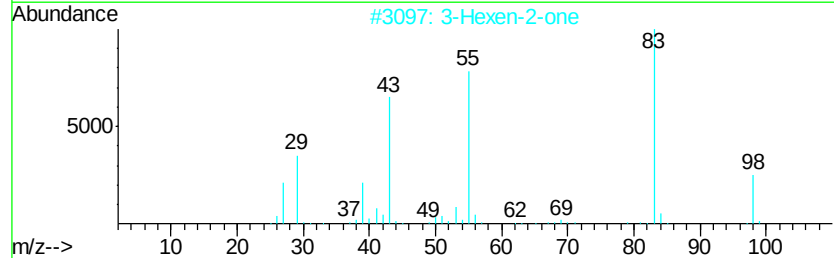
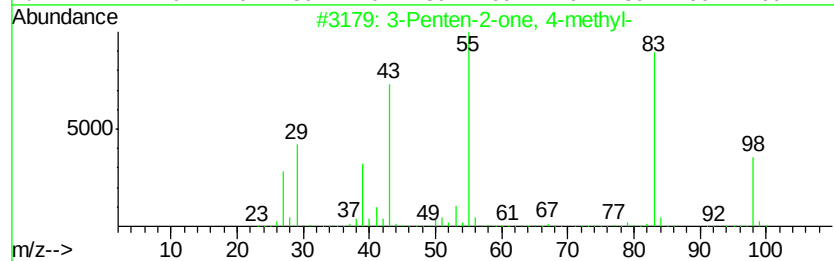
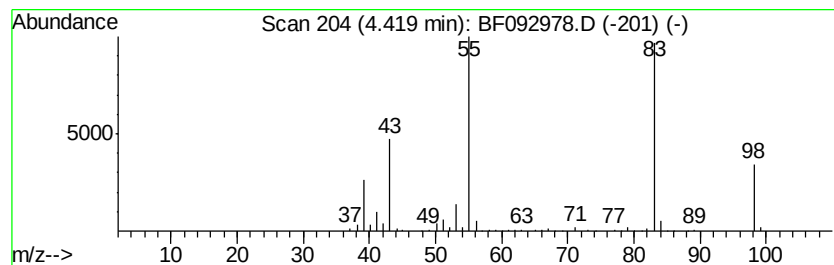
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	19.90 ng	1044420	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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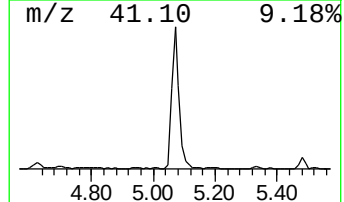
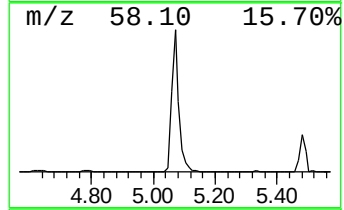
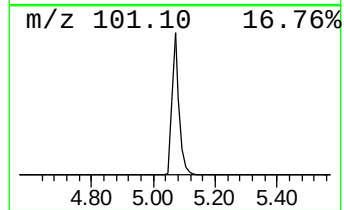
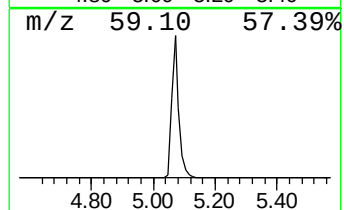
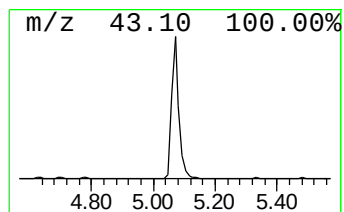
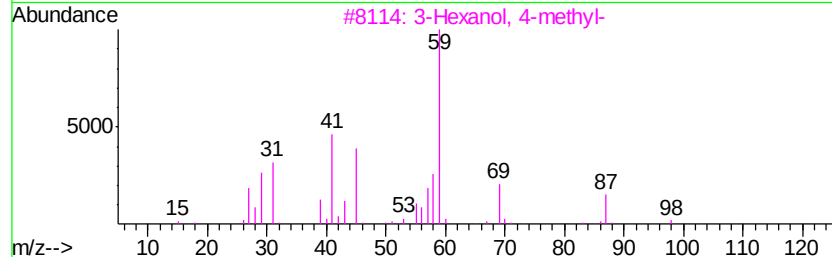
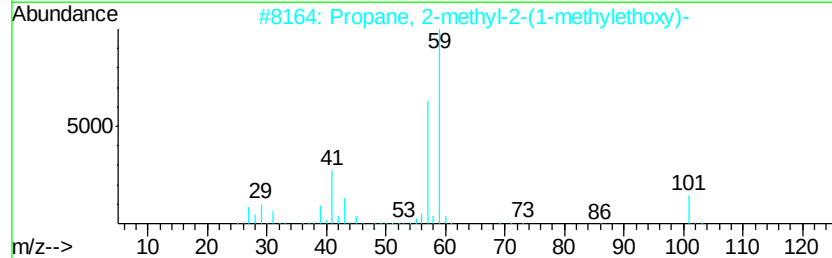
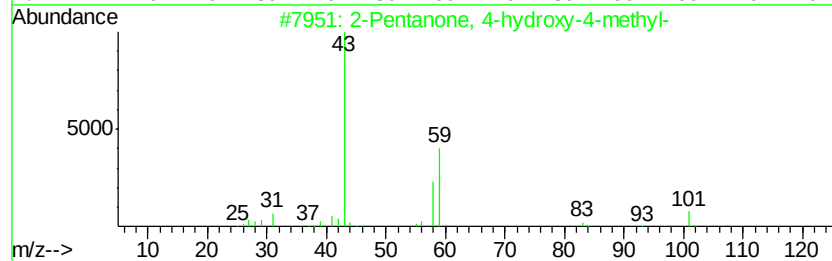
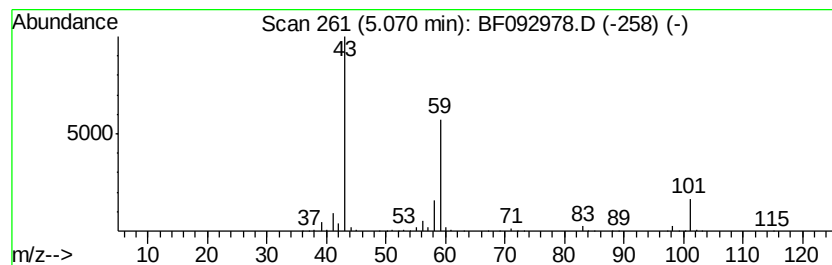
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	43.26 ng	2270880	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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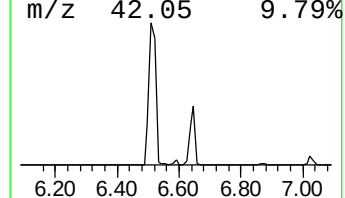
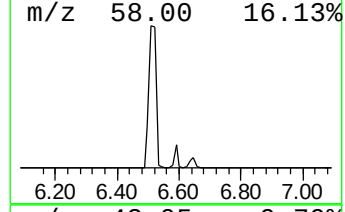
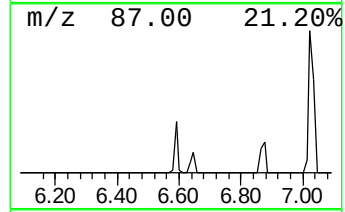
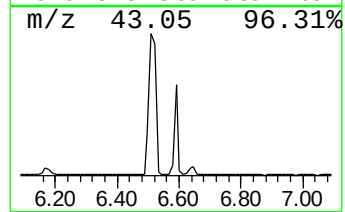
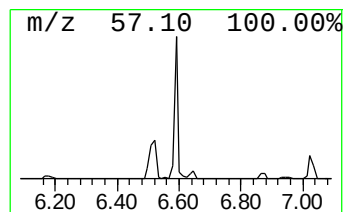
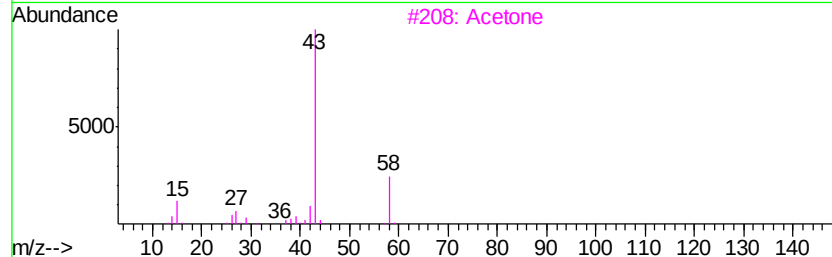
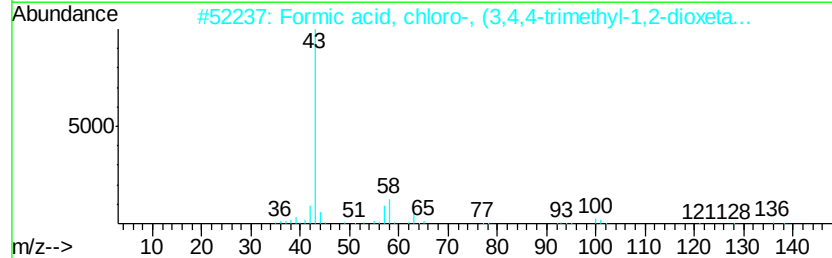
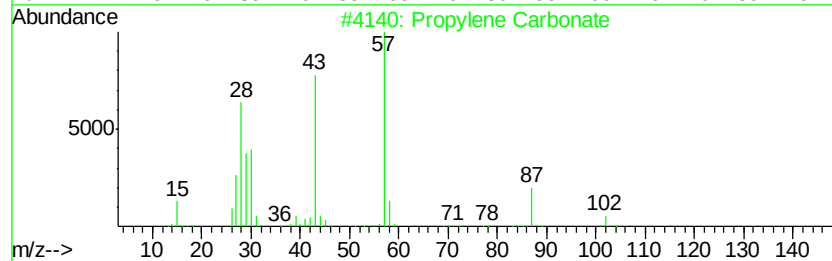
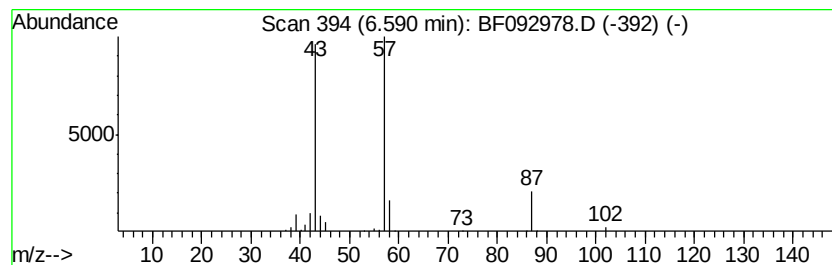
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Peak Number 5 Propylene Carbonate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	3.09 ng	162336	1,4-Dichlorobenzene-d4	6.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Propylene Carbonate	102 C4H6O3	000108-32-7 78
2		Formic acid, chloro-, (3,4,4-tri...	194 C7H11ClO4	107323-92-2 23
3		Acetone	58 C3H6O	000067-64-1 16
4		Butane	58 C4H10	000106-97-8 9
5		Formic acid, 2-propenyl ester	86 C4H6O2	001838-59-1 9



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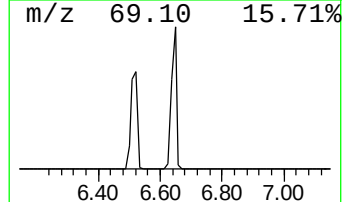
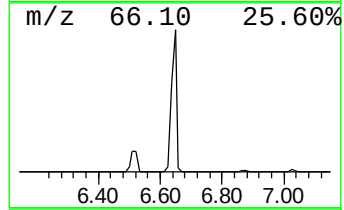
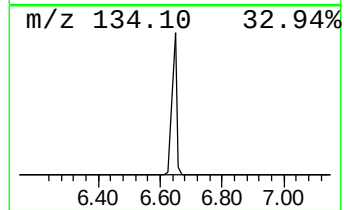
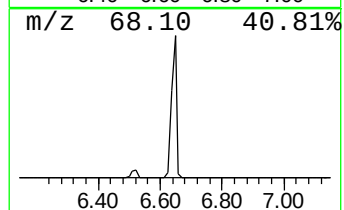
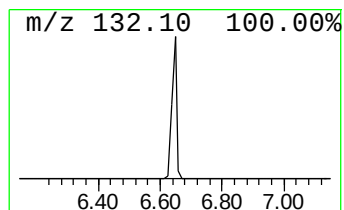
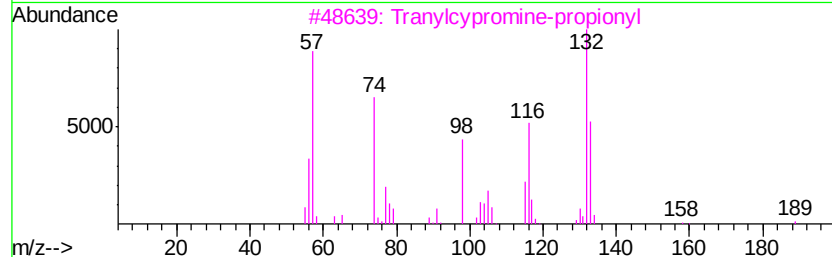
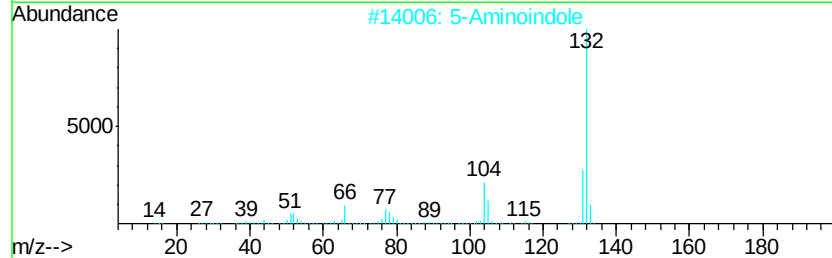
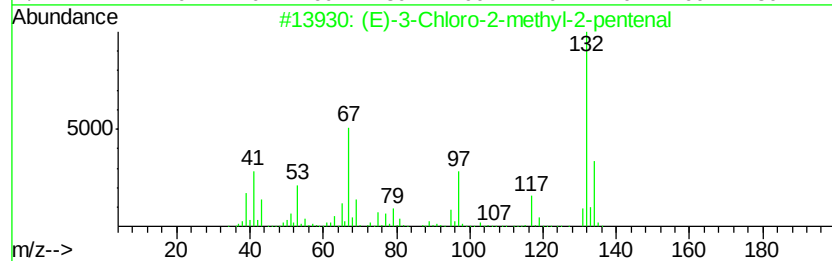
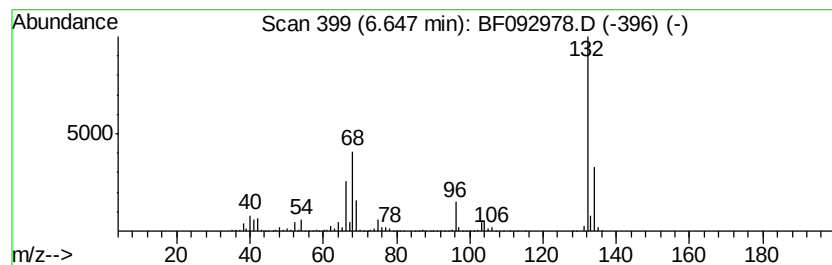
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Peak Number 6 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	96.14 ng	5046640	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.42	19.9	ng	1044420	1	6.88	1049850	20.0
2-Pentanone, 4-hy...	5.07	43.3	ng	2270880	1	6.88	1049850	20.0
Propylene Carbonate	6.59	3.1	ng	162336	1	6.88	1049850	20.0
unknown6.65	6.65	96.1	ng	5046640	1	6.88	1049850	20.0