

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011216\
 Data File : BF084425.D
 Acq On : 12 Jan 2016 22:43
 Operator : SJ/UM
 Sample : PB87777BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87777BL

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-BF123115.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	4.373	198	200	204	rBV	137199	165566	2.22%	0.266%
2	5.024	255	257	267	rVB	1584963	2422620	32.42%	3.886%
3	5.459	292	295	297	rBV	6510714	6839770	91.53%	10.973%
4	6.133	353	354	363	rBV	40752	75505	1.01%	0.121%
5	6.487	382	385	387	rBV	6521139	6590282	88.19%	10.572%
6	6.613	393	396	398	rBV	6973670	6394508	85.57%	10.258%
7	6.842	413	416	418	rVB	1945859	1611112	21.56%	2.585%
8	7.002	427	430	432	rBV	4858490	5355845	71.67%	8.592%
9	7.402	462	465	468	rBV	3521269	4098576	54.85%	6.575%
10	8.122	526	528	531	rBV	1725008	2003738	26.81%	3.214%
11	9.208	620	623	625	rBV	7621617	7472453	100.00%	11.988%
12	9.882	679	682	684	rBV	2590324	2310914	30.93%	3.707%
13	10.671	748	751	754	rBV	4482441	4344906	58.15%	6.970%
14	11.368	809	812	814	rBV	2389425	2293933	30.70%	3.680%
15	12.956	948	951	953	rBV	6659231	6907965	92.45%	11.082%
16	13.997	1040	1042	1045	rBV	1627358	1650833	22.09%	2.648%
17	15.425	1164	1167	1170	rBV	1068219	1280687	17.14%	2.055%
18	16.031	1214	1220	1231	rVB	133590	515277	6.90%	0.827%

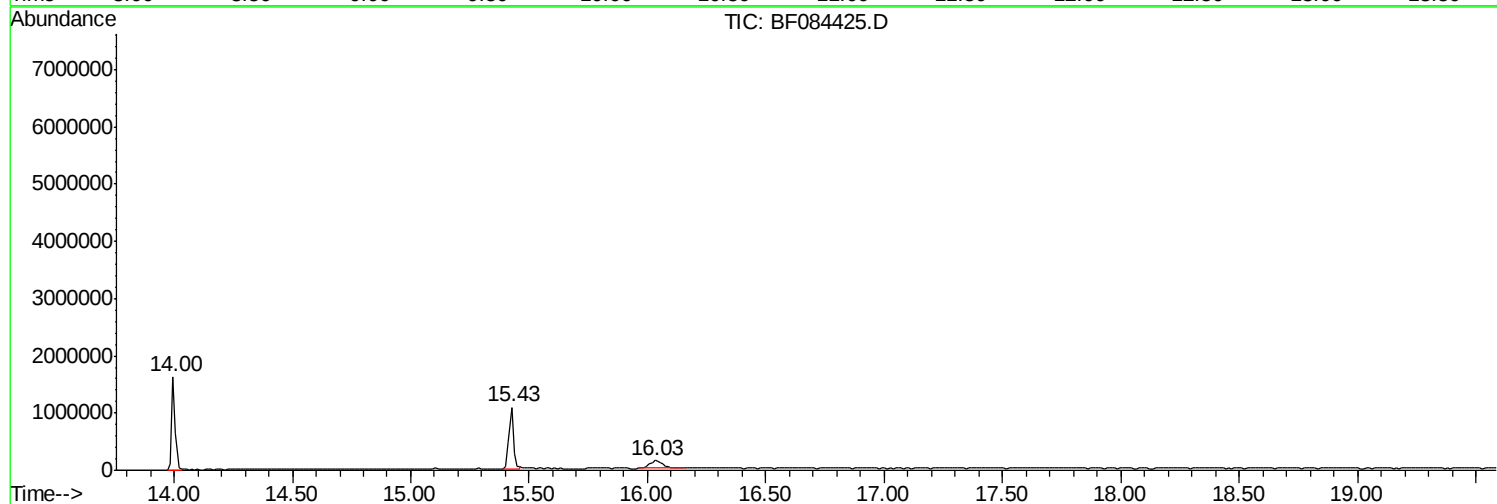
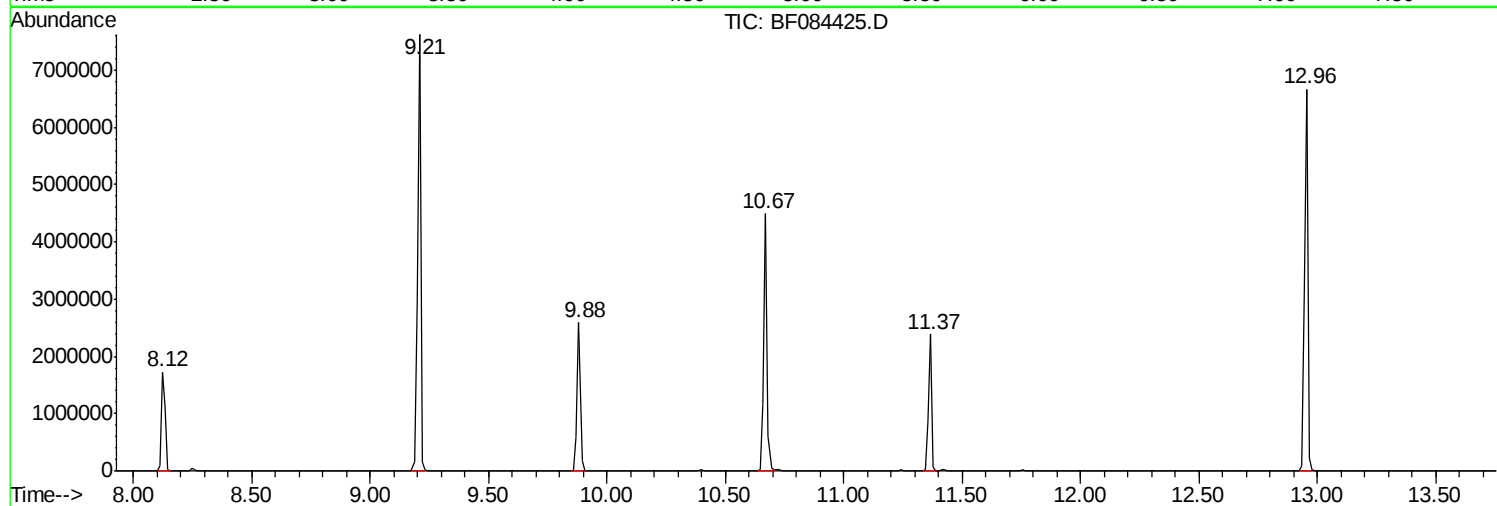
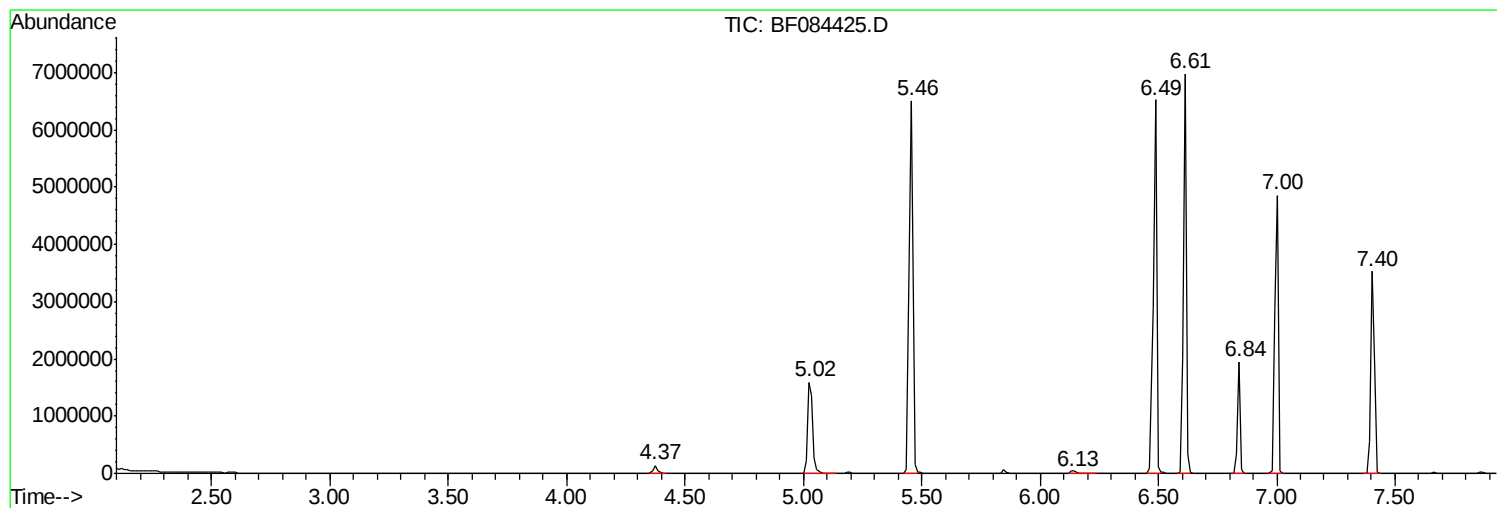
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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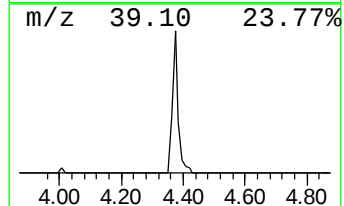
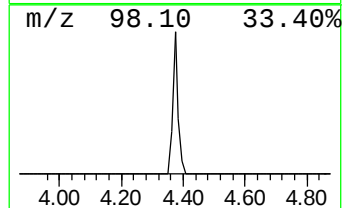
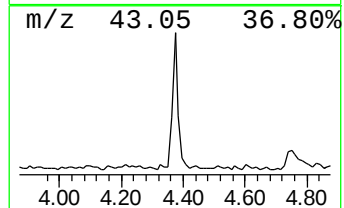
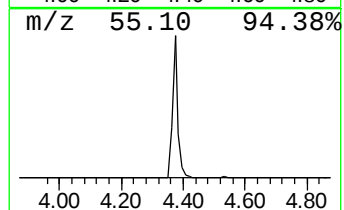
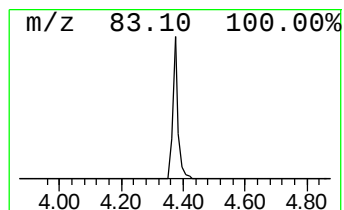
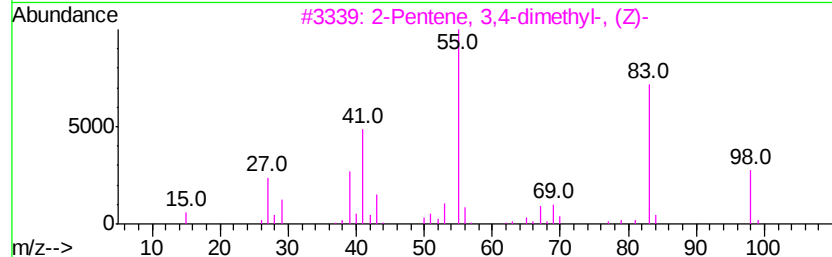
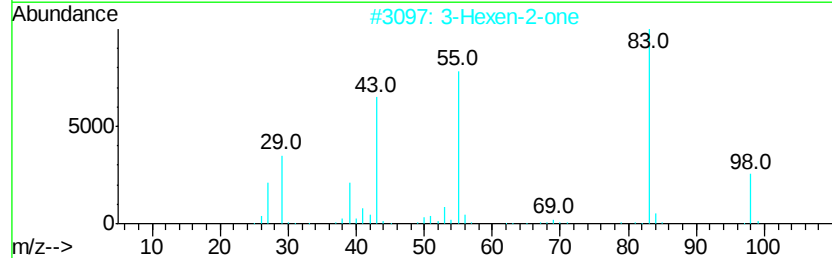
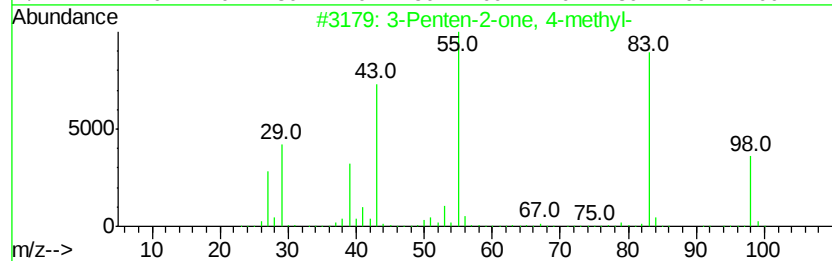
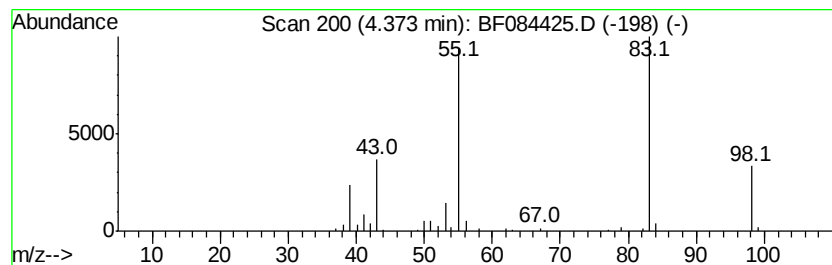
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	2.06 ng	165566	1,4-Dichlorobenzene-d4	6.84

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	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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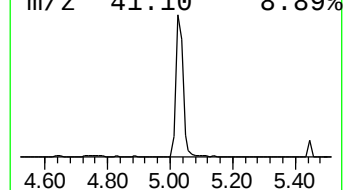
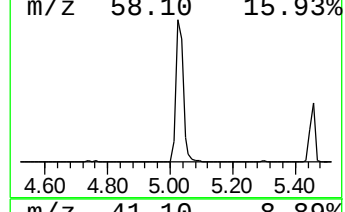
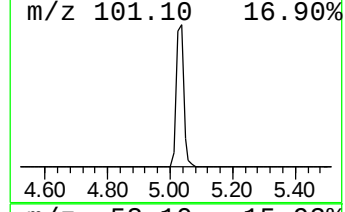
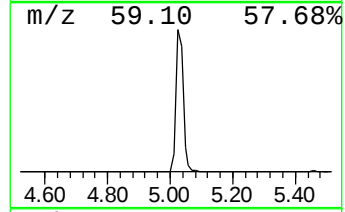
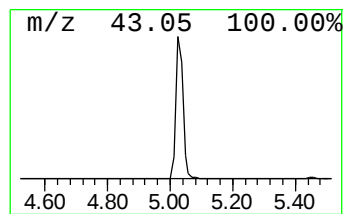
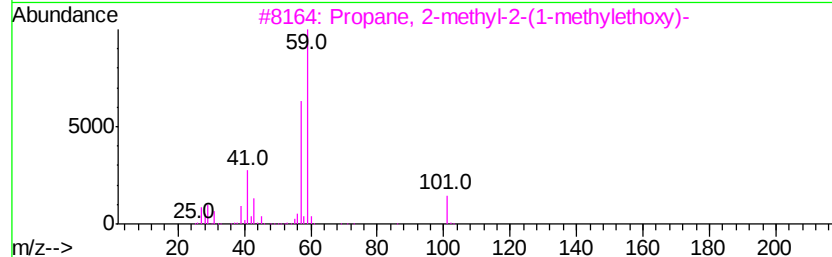
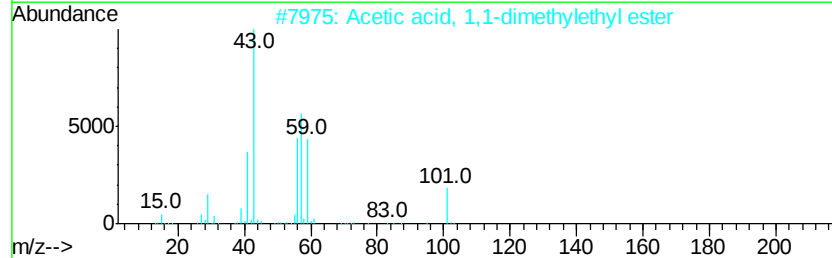
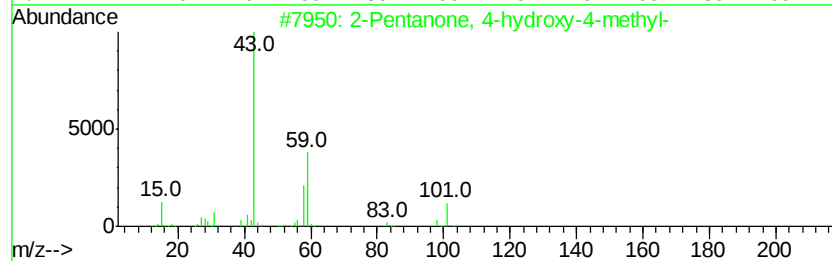
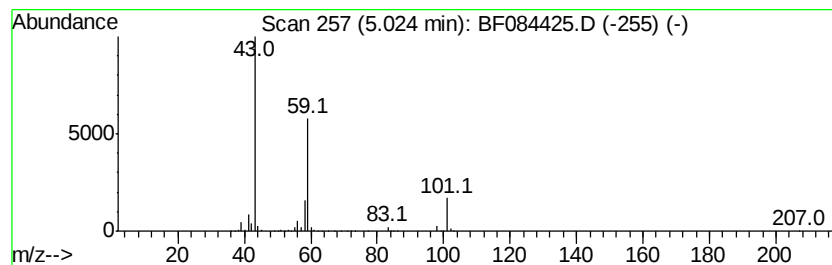
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	30.07 ng	2422620	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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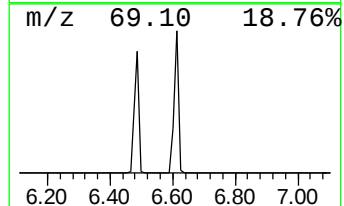
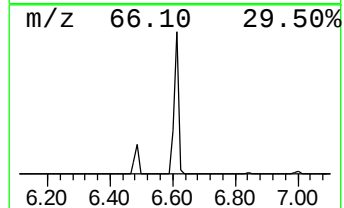
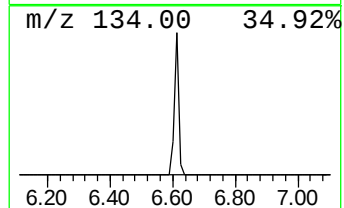
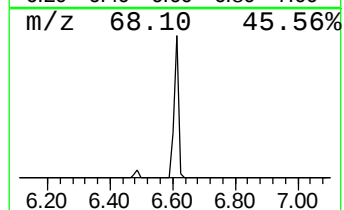
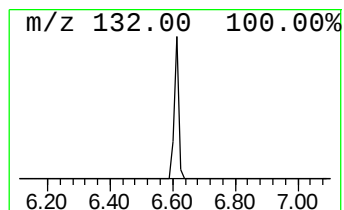
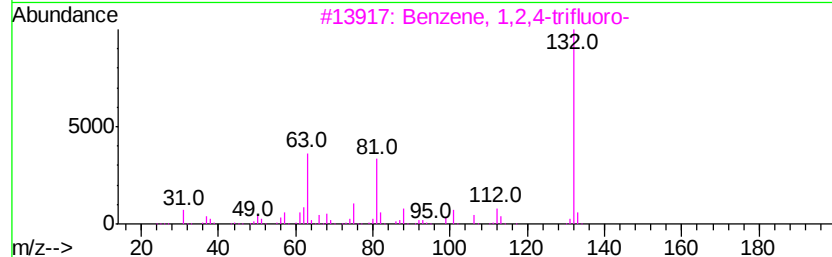
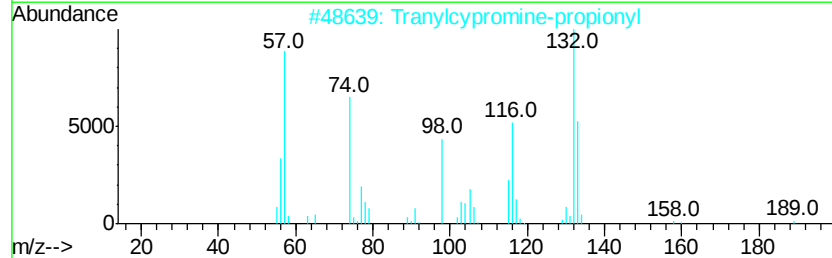
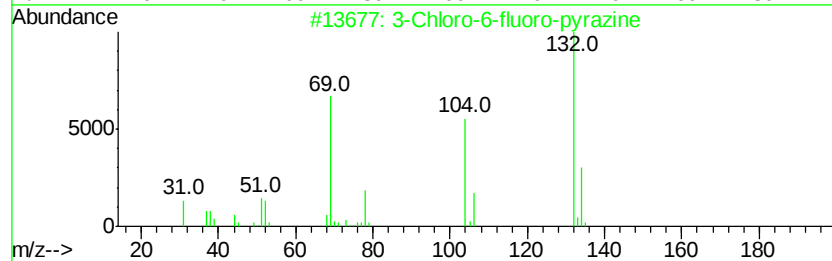
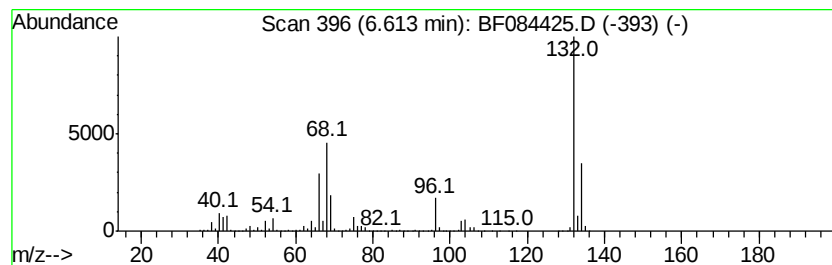
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	79.38 ng	6394510	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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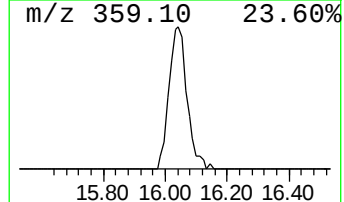
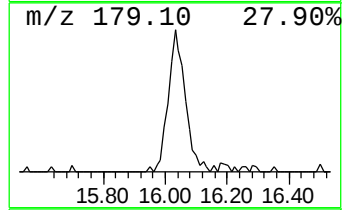
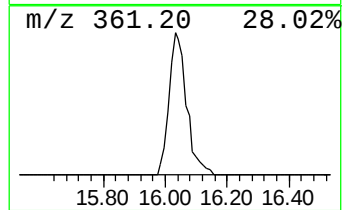
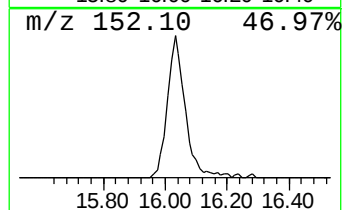
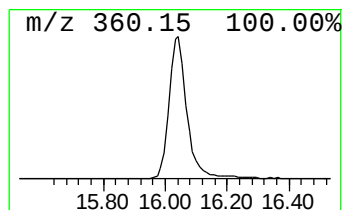
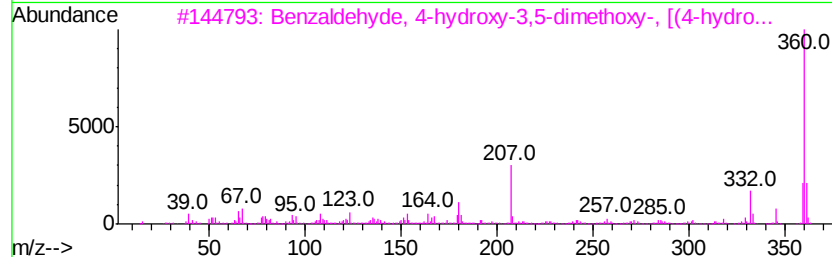
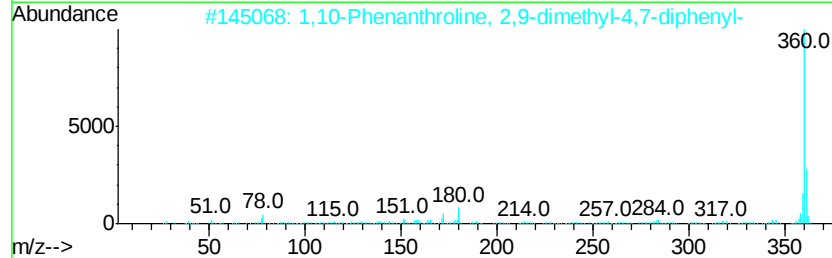
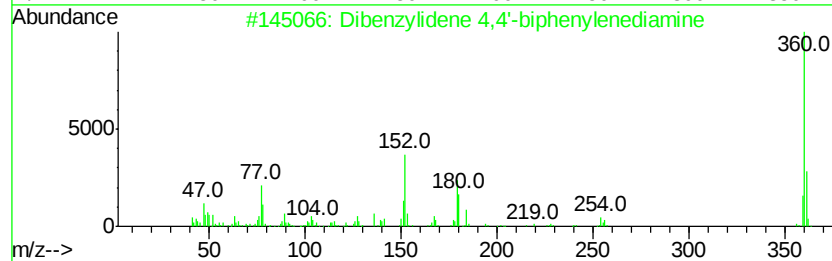
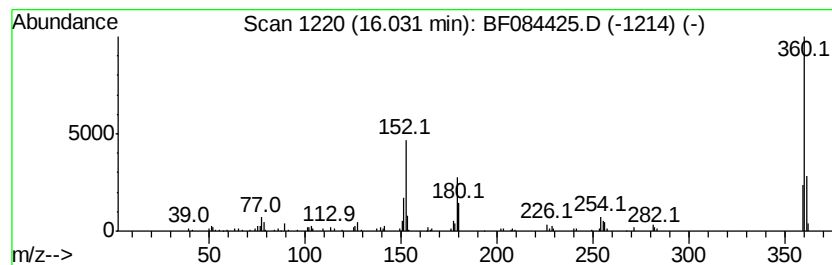
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	8.05 ng	515277	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	94
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	49
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4		Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43
5		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.37	2.1 ng		165566	1	6.84	1611110	20.0
2-Pentanone, 4-hy...	5.02	30.1 ng		2422620	1	6.84	1611110	20.0
unknown6.61	6.61	79.4 ng		6394510	1	6.84	1611110	20.0
Dibenzylidene 4,4...	16.03	8.1 ng		515277	6	15.43	1280690	20.0