

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF123115\
 Data File : BF084213.D
 Acq On : 31 Dec 2015 23:44
 Operator : UM/SJ
 Sample : PB86817BL
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB86817BL

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	2.213	9	11	27	rVB2	100874	300991	3.74%	0.451%
2	5.093	260	263	274	rBV	1423760	2016535	25.07%	3.019%
3	5.504	296	299	301	rBV	6907602	6929355	86.16%	10.374%
4	6.522	385	388	391	rBV	5544534	6354525	79.01%	9.513%
5	6.670	398	401	403	rBV	6218351	7340863	91.27%	10.990%
6	6.899	419	421	423	rBV	2287221	1831087	22.77%	2.741%
7	7.059	432	435	437	rBV	5844486	5656889	70.34%	8.469%
8	7.459	467	470	473	rBV	4126696	4232350	52.62%	6.336%
9	8.179	531	533	536	rVB	1864049	2339261	29.09%	3.502%
10	9.265	625	628	630	rBV	8317950	8042583	100.00%	12.041%
11	9.939	684	687	690	rBV	2909956	2650420	32.95%	3.968%
12	10.728	753	756	758	rBV	5094856	4937506	61.39%	7.392%
13	11.425	814	817	819	rBV	3049708	2678314	33.30%	4.010%
14	12.842	938	941	943	rBV	239421	223209	2.78%	0.334%
15	13.014	953	956	958	rBV	8062871	7661249	95.26%	11.470%
16	13.539	1000	1002	1005	rBV	127084	155511	1.93%	0.233%
17	14.054	1045	1047	1050	rBV	2075700	1993296	24.78%	2.984%
18	15.494	1170	1173	1176	rBV	1168733	1451167	18.04%	2.173%

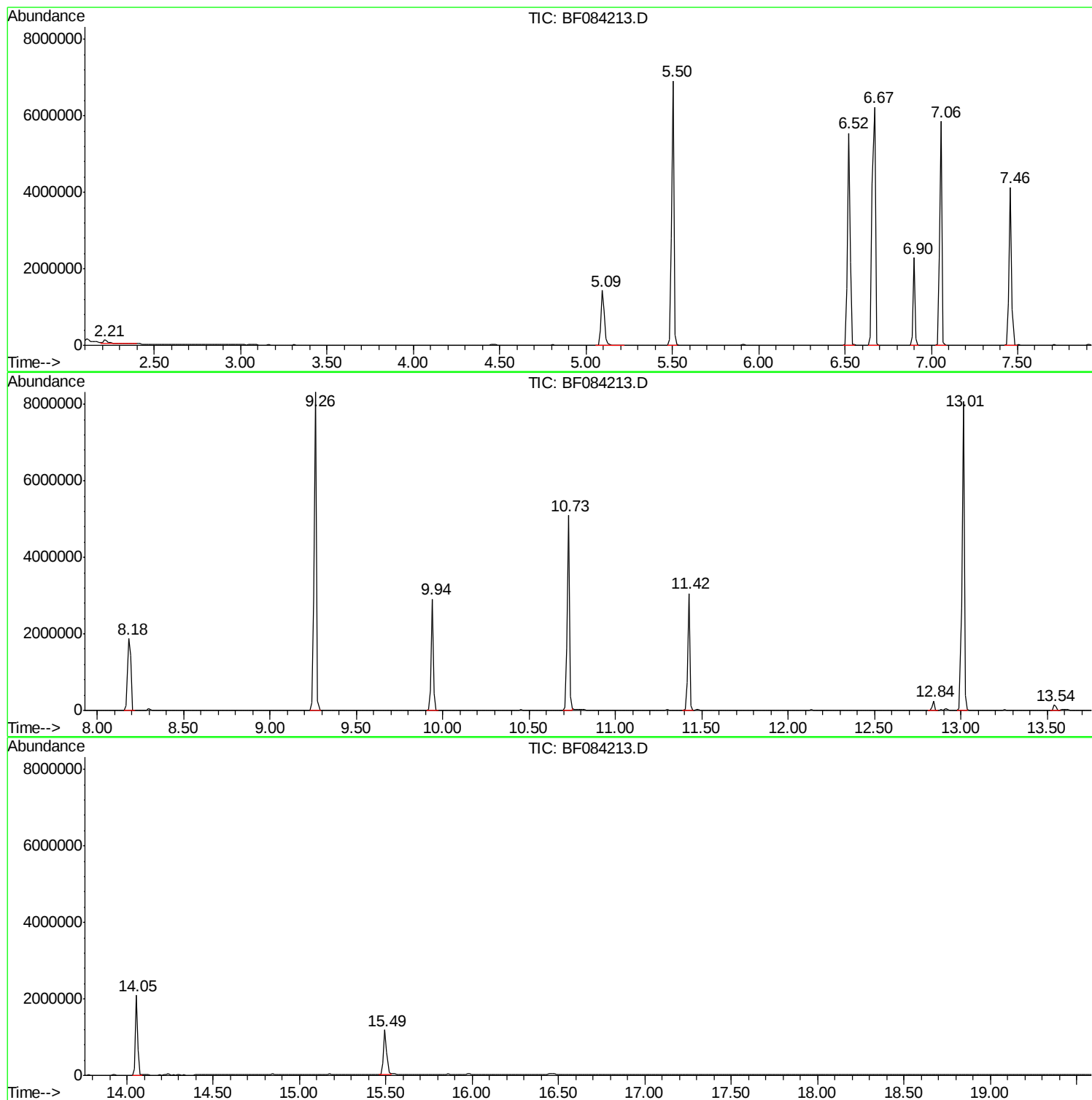
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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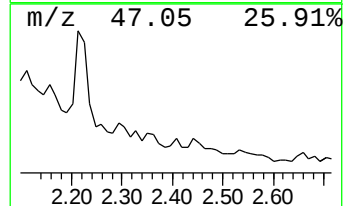
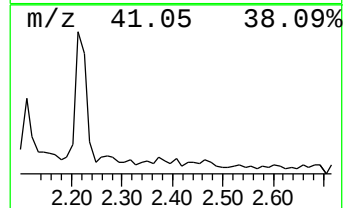
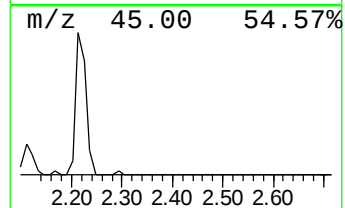
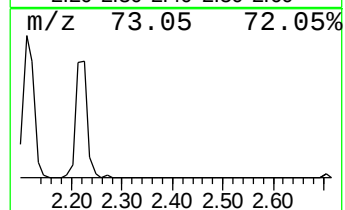
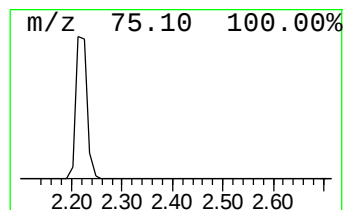
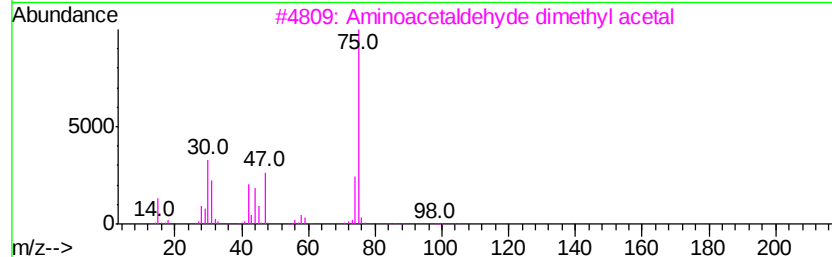
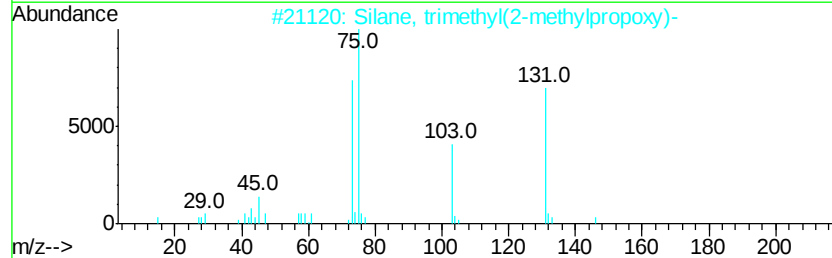
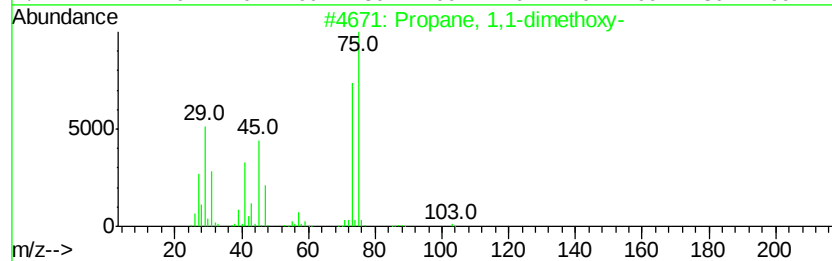
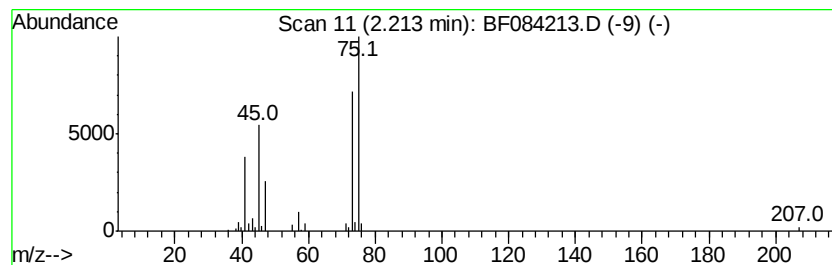
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	3.29 ng	300991	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Silane, trimethyl(2-methylpropoxy)-	146	C7H18OSi	018269-50-6	40
3		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
4		3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	33
5		Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28



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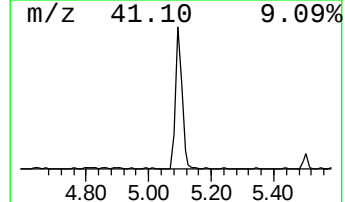
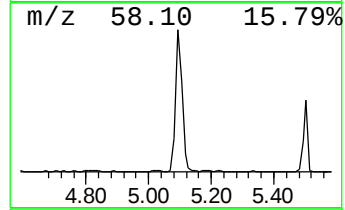
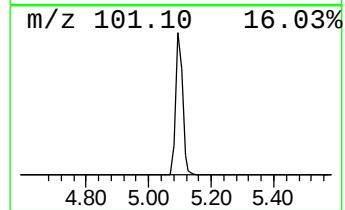
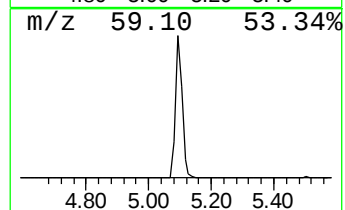
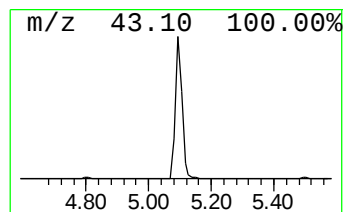
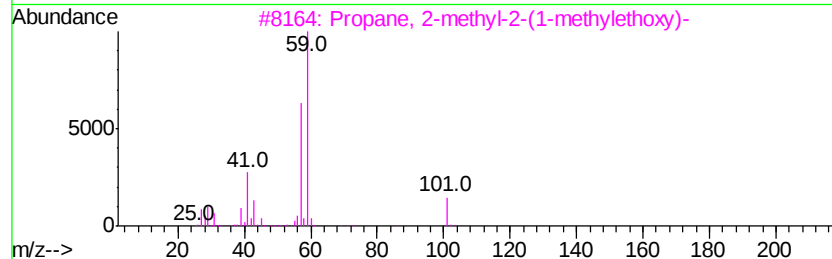
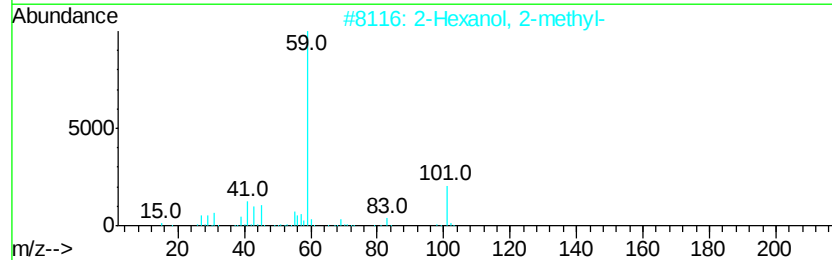
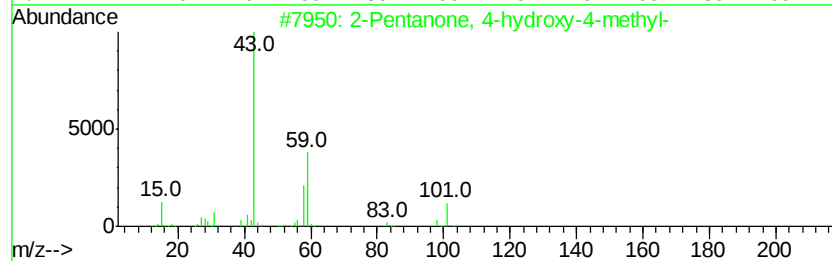
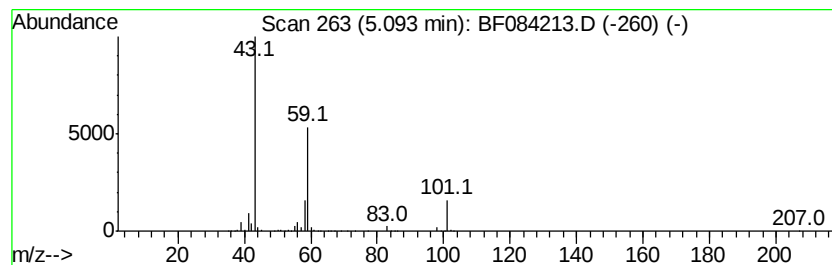
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	22.03 ng	2016540	1,4-Dichlorobenzene-d4	6.90

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



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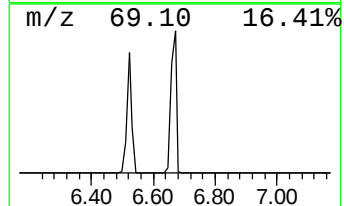
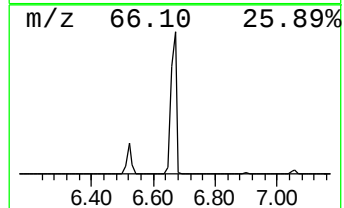
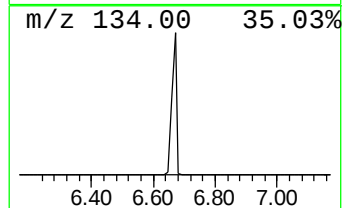
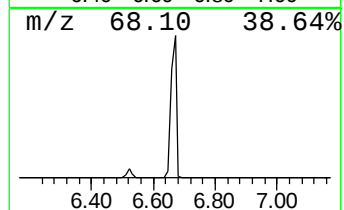
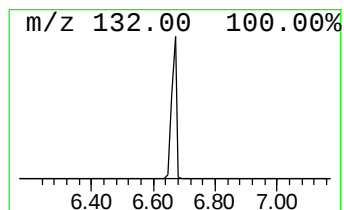
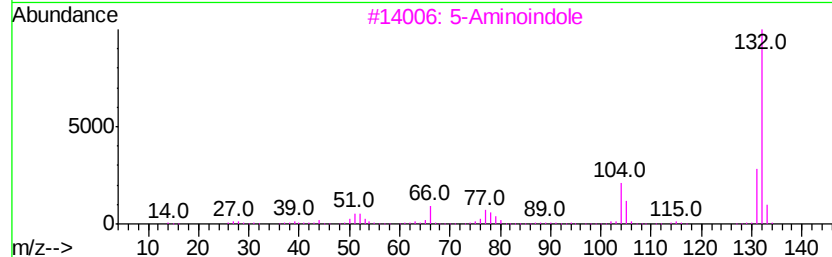
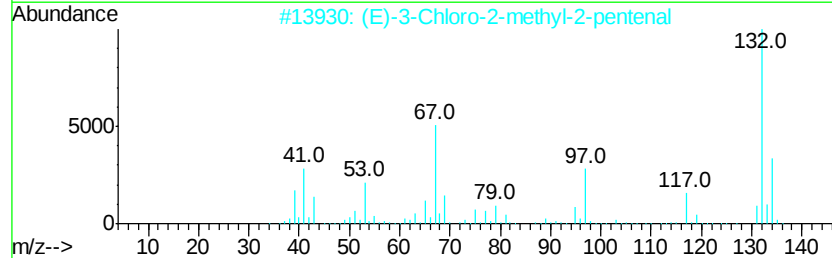
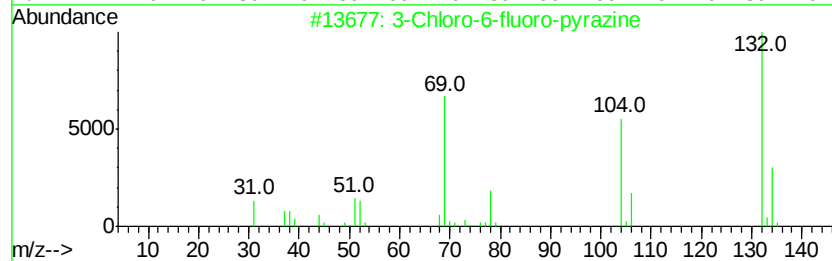
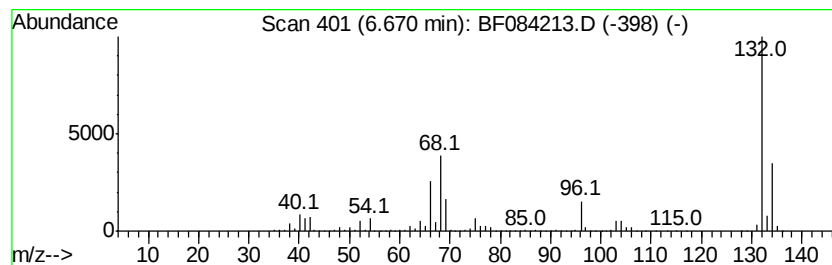
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	80.18 ng	7340860	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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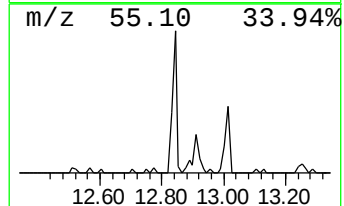
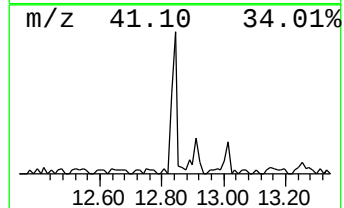
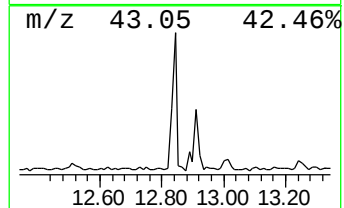
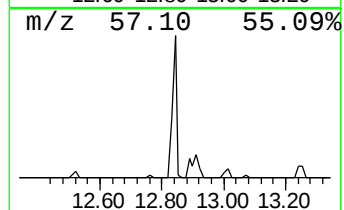
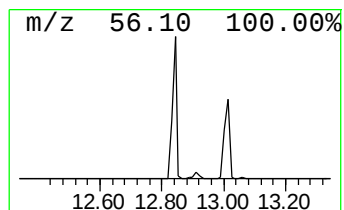
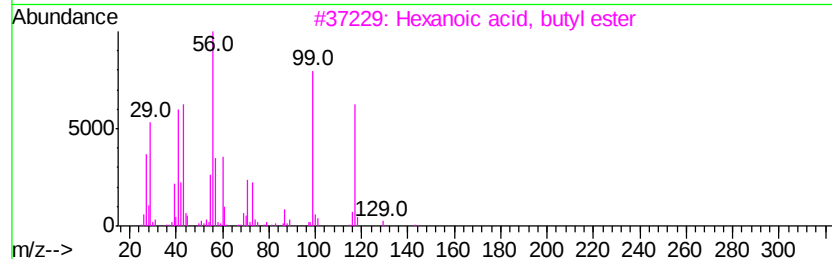
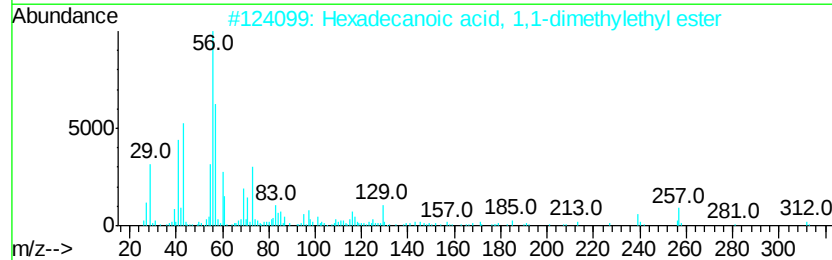
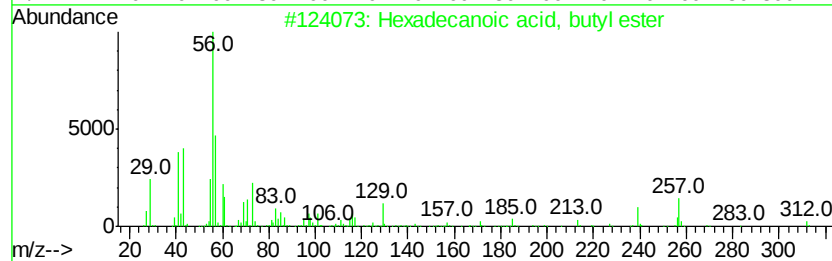
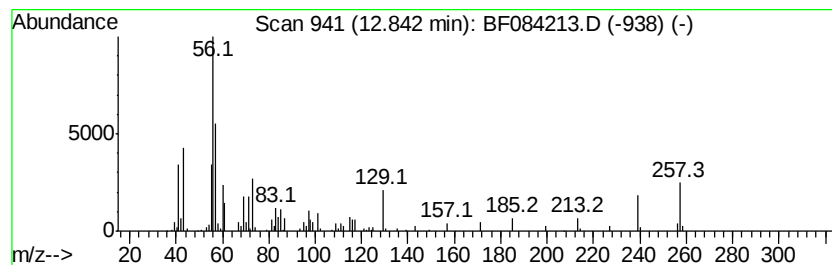
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.24 ng	223209	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	38
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.21	3.3	ng	300991	1	6.90	1831090	20.0
2-Pentanone, 4-hy...	5.09	22.0	ng	2016540	1	6.90	1831090	20.0
unknown6.67	6.67	80.2	ng	7340860	1	6.90	1831090	20.0
Hexadecanoic acid...	12.84	2.2	ng	223209	5	14.05	1993300	20.0