

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062415\
 Data File : BF080136.D
 Acq On : 24 Jun 2015 17:10
 Operator : TP/IZ
 Sample : G2750-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-1

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-BF061715.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	5.533	212	214	217	rBV	658345	633270	20.56%	3.122%
2	5.921	246	248	251	rBV	1531564	1757846	57.07%	8.665%
3	6.322	281	283	286	rBB	64496	55006	1.79%	0.271%
4	6.550	301	303	310	rBB	32621	42710	1.39%	0.211%
5	6.916	332	335	338	rBV	2071382	1829480	59.40%	9.018%
6	7.076	347	349	352	rBV	1897717	1887795	61.29%	9.305%
7	7.316	368	370	372	rBB	422104	372821	12.10%	1.838%
8	7.476	382	384	386	rBV	1527589	1473114	47.83%	7.261%
9	7.864	416	418	421	rBV	1021536	1162259	37.73%	5.729%
10	8.482	470	472	477	rBB	56712	46555	1.51%	0.229%
11	8.607	481	483	485	rBV	492162	502708	16.32%	2.478%
12	9.682	574	577	579	rVB	3172798	2596278	84.29%	12.798%
13	10.070	609	611	613	rBB	269277	255710	8.30%	1.260%
14	10.379	636	638	640	rBB	623019	622683	20.22%	3.069%
15	11.168	705	707	710	rBV	1738028	1567215	50.88%	7.725%
16	11.876	767	769	772	rBV	498539	688416	22.35%	3.393%
17	12.082	785	787	792	rBV	26898	47123	1.53%	0.232%
18	13.442	904	906	912	rBV	89004	98721	3.21%	0.487%
19	13.591	916	919	922	rBV	3180633	3080125	100.00%	15.182%
20	14.665	1010	1013	1026	rBV	130001	255984	8.31%	1.262%
21	14.871	1029	1031	1034	rBV	472406	683757	22.20%	3.370%
22	16.002	1128	1130	1133	rVB	29300	34107	1.11%	0.168%
23	16.768	1193	1197	1201	rBV	383398	593675	19.27%	2.926%

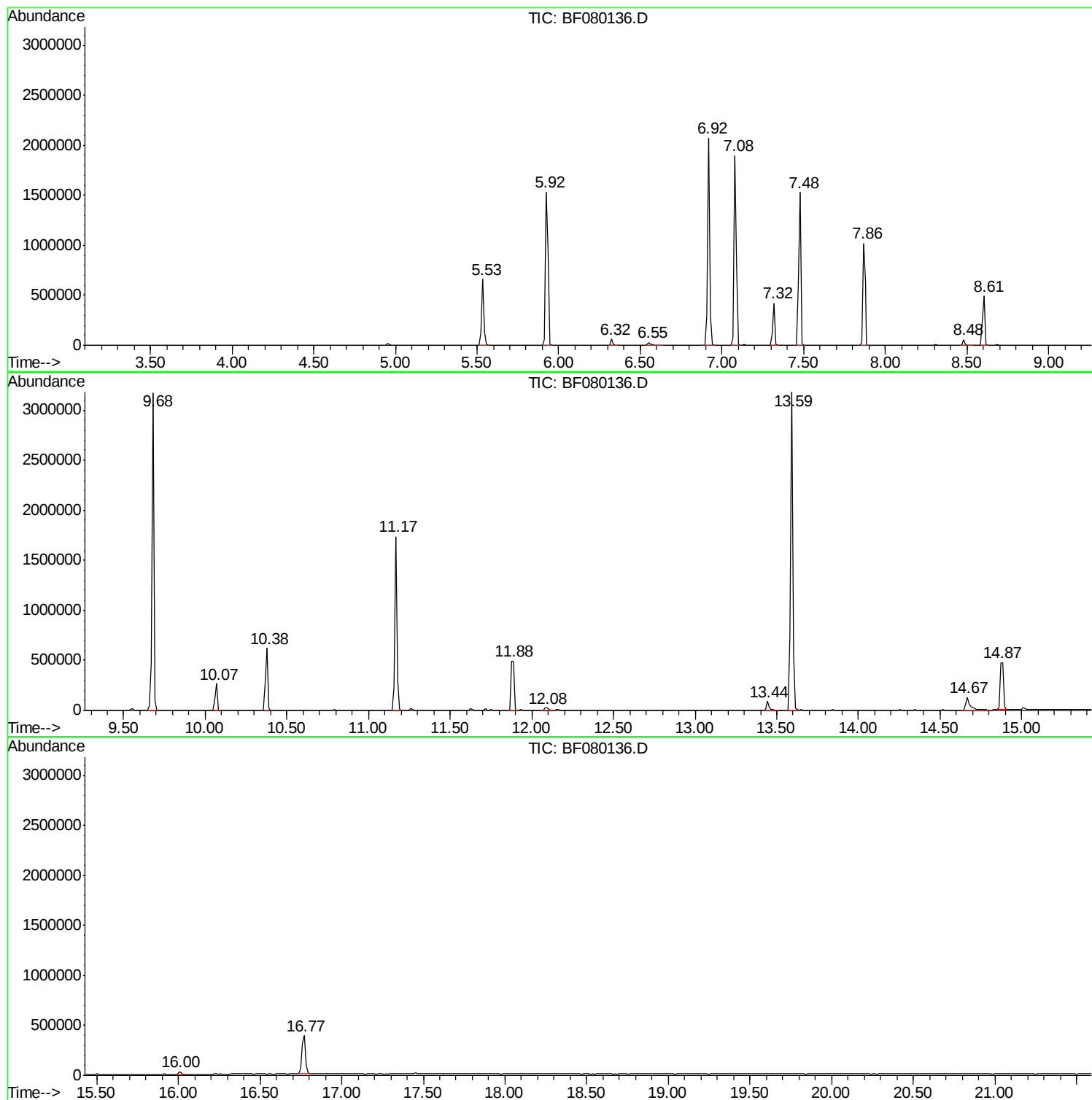
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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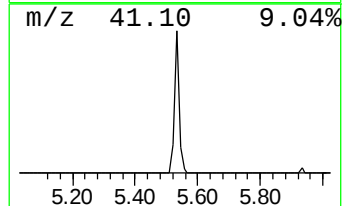
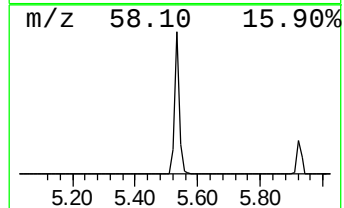
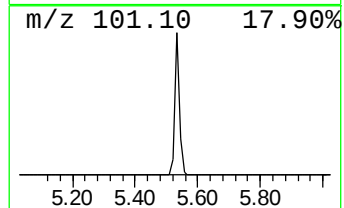
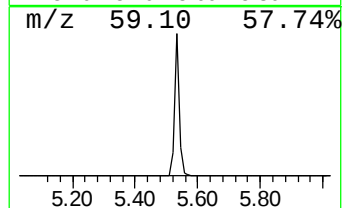
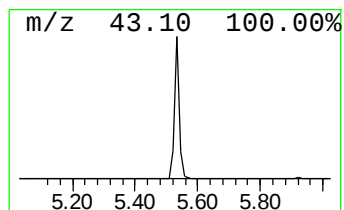
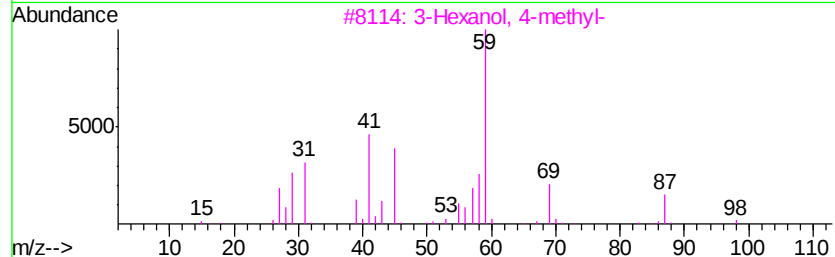
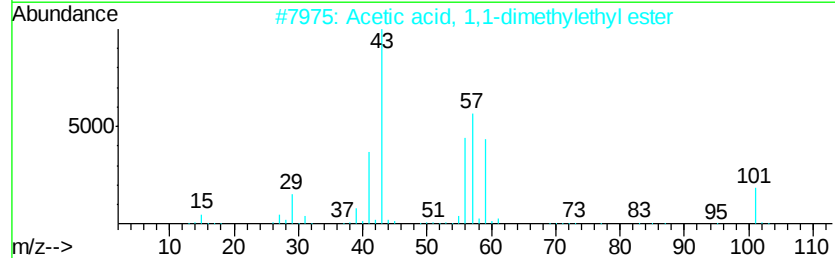
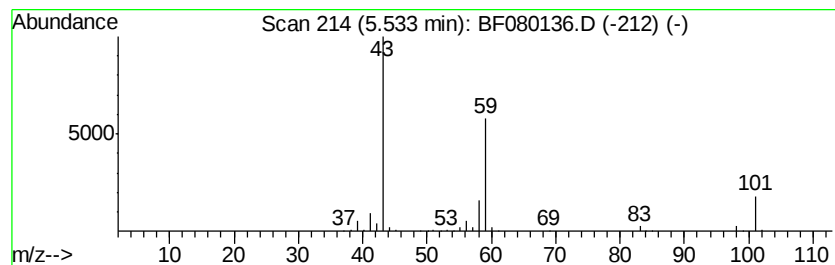
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.53	33.97 ng	633270	1,4-Dichlorobenzene-d4	7.32

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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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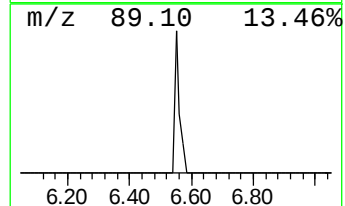
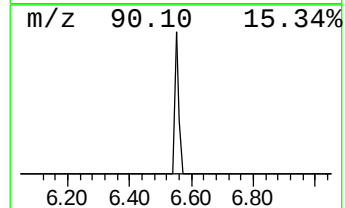
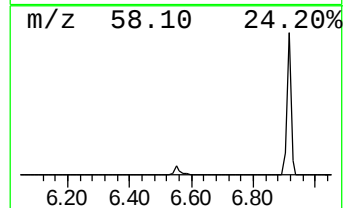
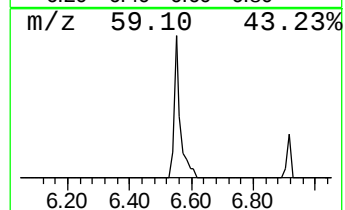
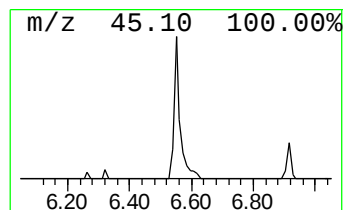
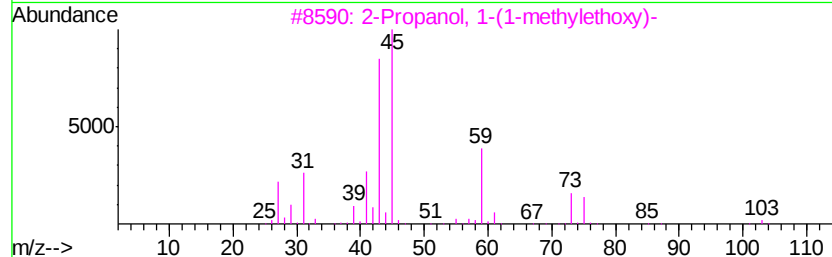
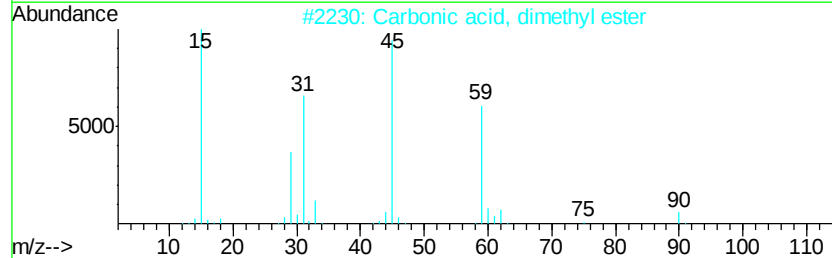
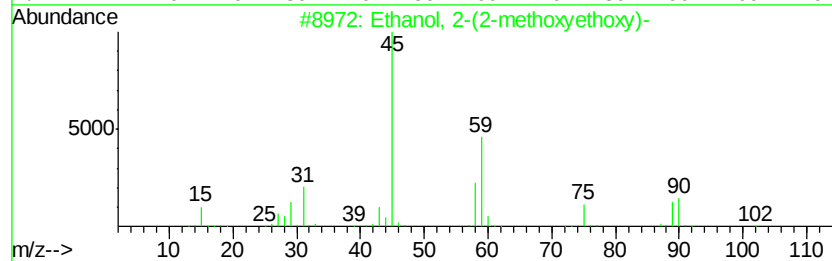
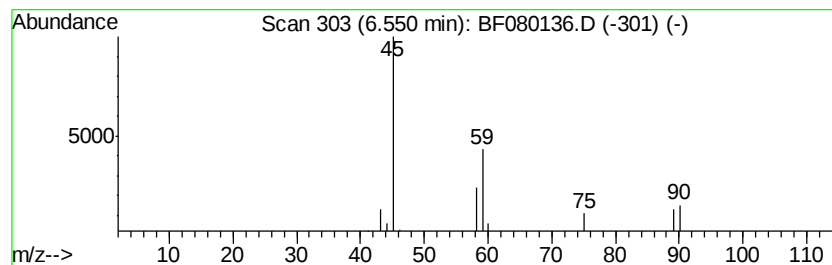
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Peak Number 3 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	2.29 ng	42710	1,4-Dichlorobenzene-d4	7.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2		Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
3		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4		Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	9
5		Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	9



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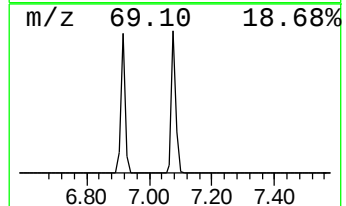
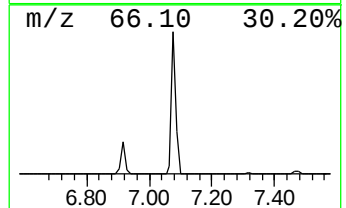
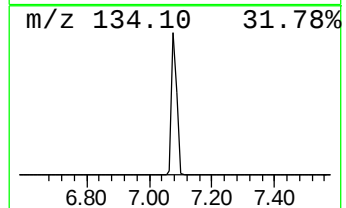
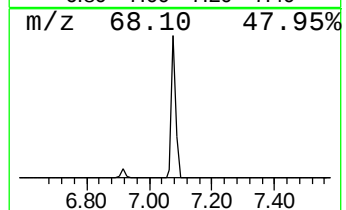
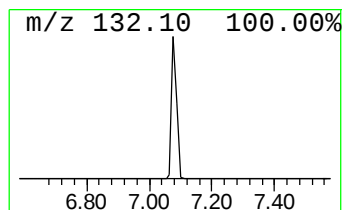
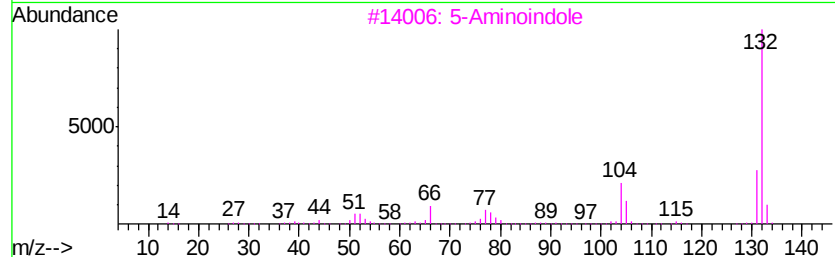
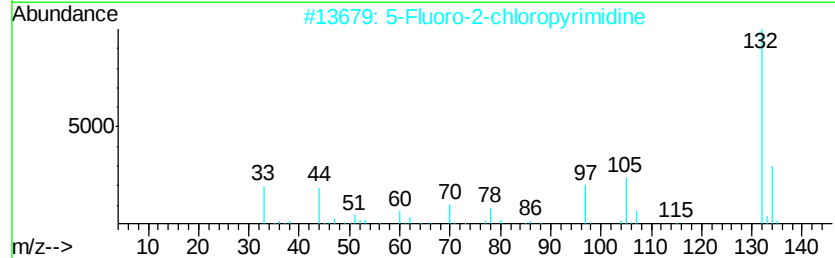
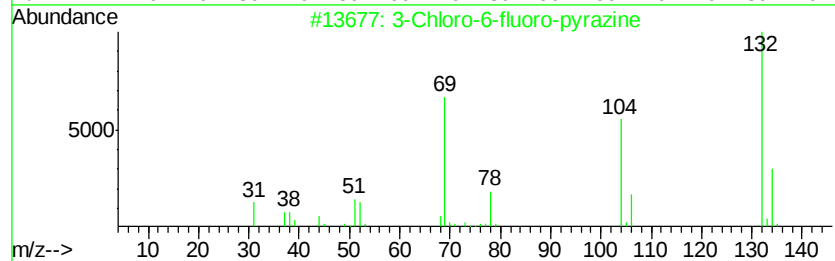
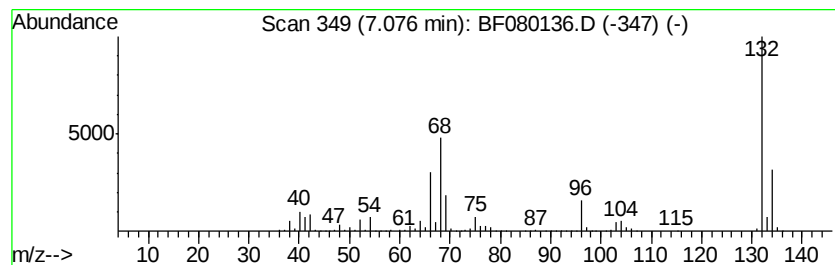
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Peak Number 4 unknown7.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	101.27 ng	1887800	1,4-Dichlorobenzene-d4	7.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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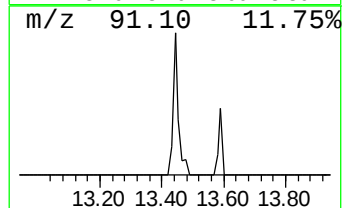
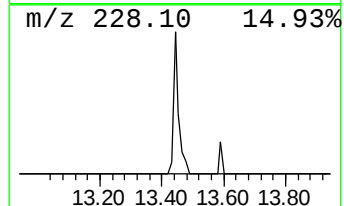
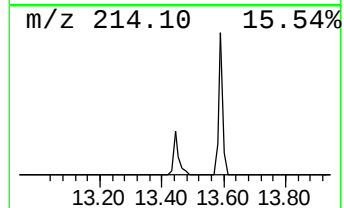
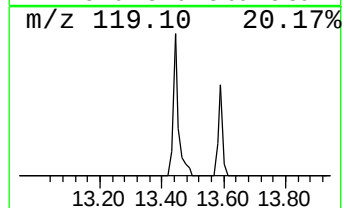
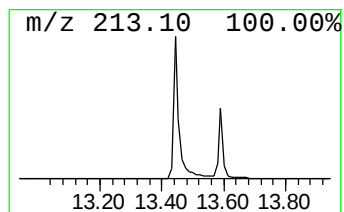
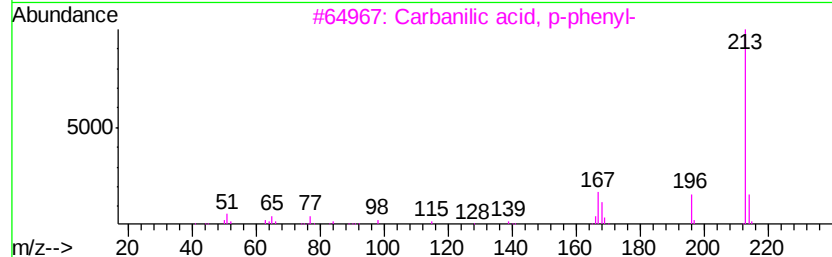
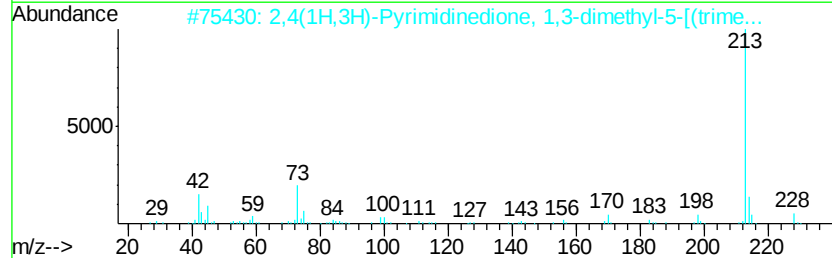
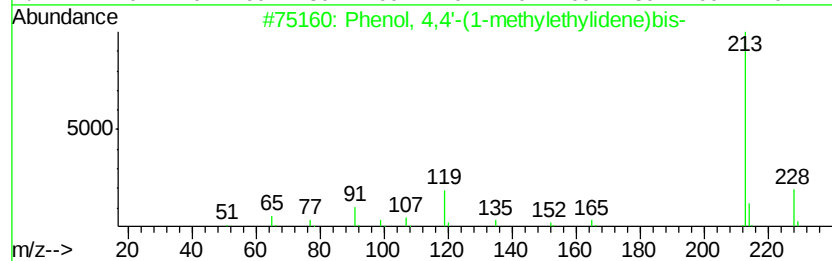
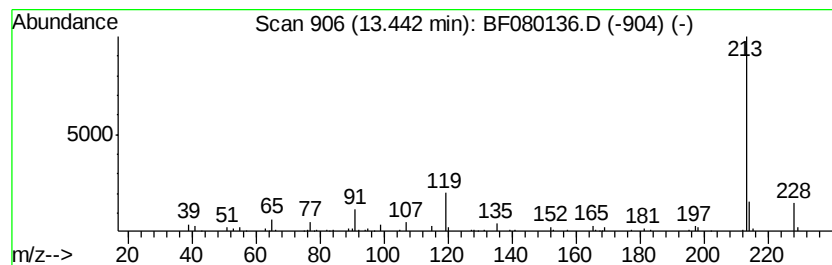
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.44	2.89 ng	98721	Chrysene-d12	14.88		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97	
2	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	53	
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47	
4	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40	
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40	



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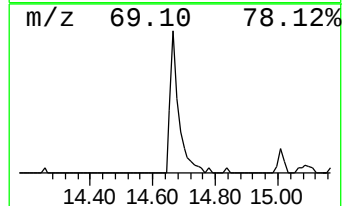
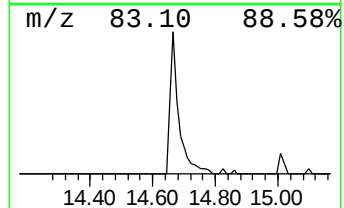
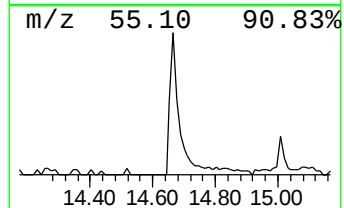
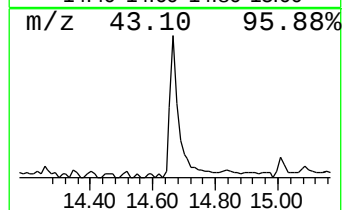
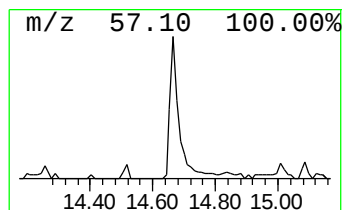
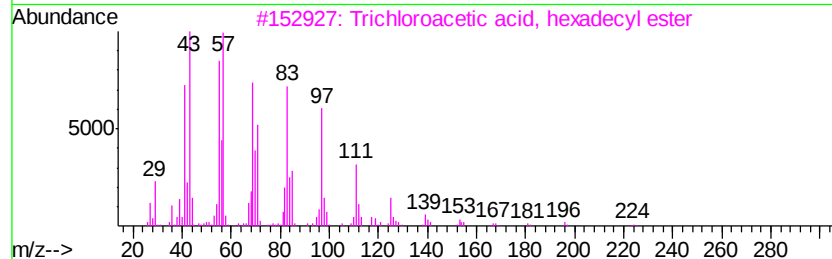
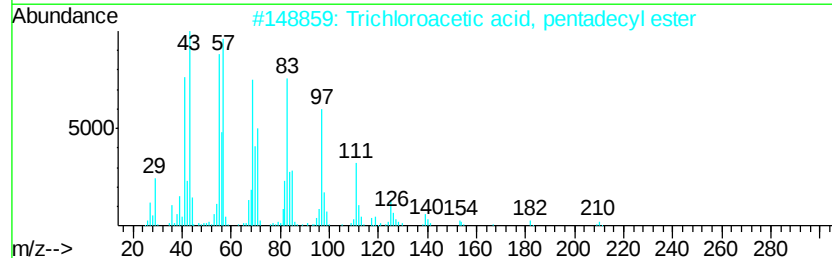
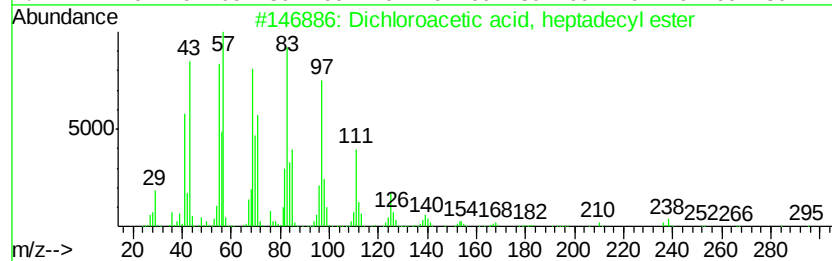
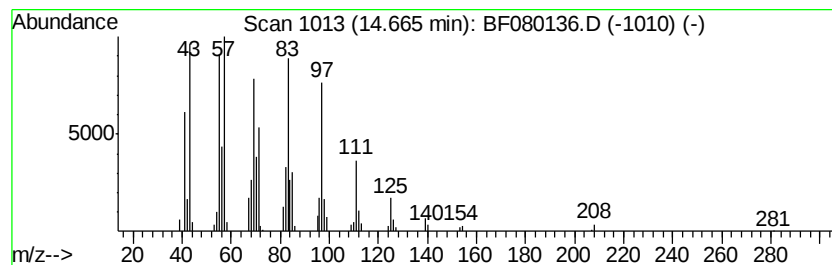
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Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	7.49 ng	255984	Chrysene-d12	14.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.53	34.0	ng	633270	1	7.32	372821	20.0
Ethanol, 2-(2-met...	6.55	2.3	ng	42710	1	7.32	372821	20.0
unknown7.08	7.08	101.3	ng	1887800	1	7.32	372821	20.0
Phenol, 4,4'-(1-m...	13.44	2.9	ng	98721	5	14.88	683757	20.0
Dichloroacetic ac...	14.67	7.5	ng	255984	5	14.88	683757	20.0