

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011716\
 Data File : BF084530.D
 Acq On : 17 Jan 2016 12:30
 Operator : SJ/UM
 Sample : H1148-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13

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	4.316	193	195	199	rBV	255136	305919	3.07%	0.416%
2	4.978	250	253	256	rBV	1633679	2407084	24.18%	3.270%
3	5.413	288	291	293	rBV	5091779	4608861	46.30%	6.261%
4	5.813	324	326	328	rBV	395261	409732	4.12%	0.557%
5	6.441	379	381	384	rBV	2424833	2673984	26.86%	3.633%
6	6.579	390	393	395	rBV	7684174	7809620	78.46%	10.610%
7	6.807	411	413	415	rBV	1924363	1833764	18.42%	2.491%
8	6.967	424	427	429	rBV	7101013	7713404	77.49%	10.479%
9	7.379	460	463	465	rVB	5713232	6815345	68.47%	9.259%
10	7.824	499	502	506	rBV	59306	107389	1.08%	0.146%
11	8.087	523	525	528	rBV	2079887	2313751	23.24%	3.143%
12	9.173	617	620	622	rBV	9398991	9954220	100.00%	13.523%
13	9.562	652	654	659	rVB	170418	214356	2.15%	0.291%
14	9.848	676	679	681	rBV	2834578	2800899	28.14%	3.805%
15	10.282	714	717	719	rVB2	148111	223209	2.24%	0.303%
16	10.636	745	748	751	rBV	5832836	6306443	63.35%	8.568%
17	10.750	756	758	763	rVB	105149	150944	1.52%	0.205%
18	11.322	806	808	811	rBV2	2179181	2617320	26.29%	3.556%
19	12.922	945	948	950	rBV	8734358	9850600	98.96%	13.383%
20	13.825	1024	1027	1033	rBV2	144502	280405	2.82%	0.381%
21	13.962	1036	1039	1041	rBV	2594216	2448782	24.60%	3.327%
22	14.808	1111	1113	1116	rVB	106560	107741	1.08%	0.146%
23	15.368	1159	1162	1165	rBV	1190416	1653309	16.61%	2.246%

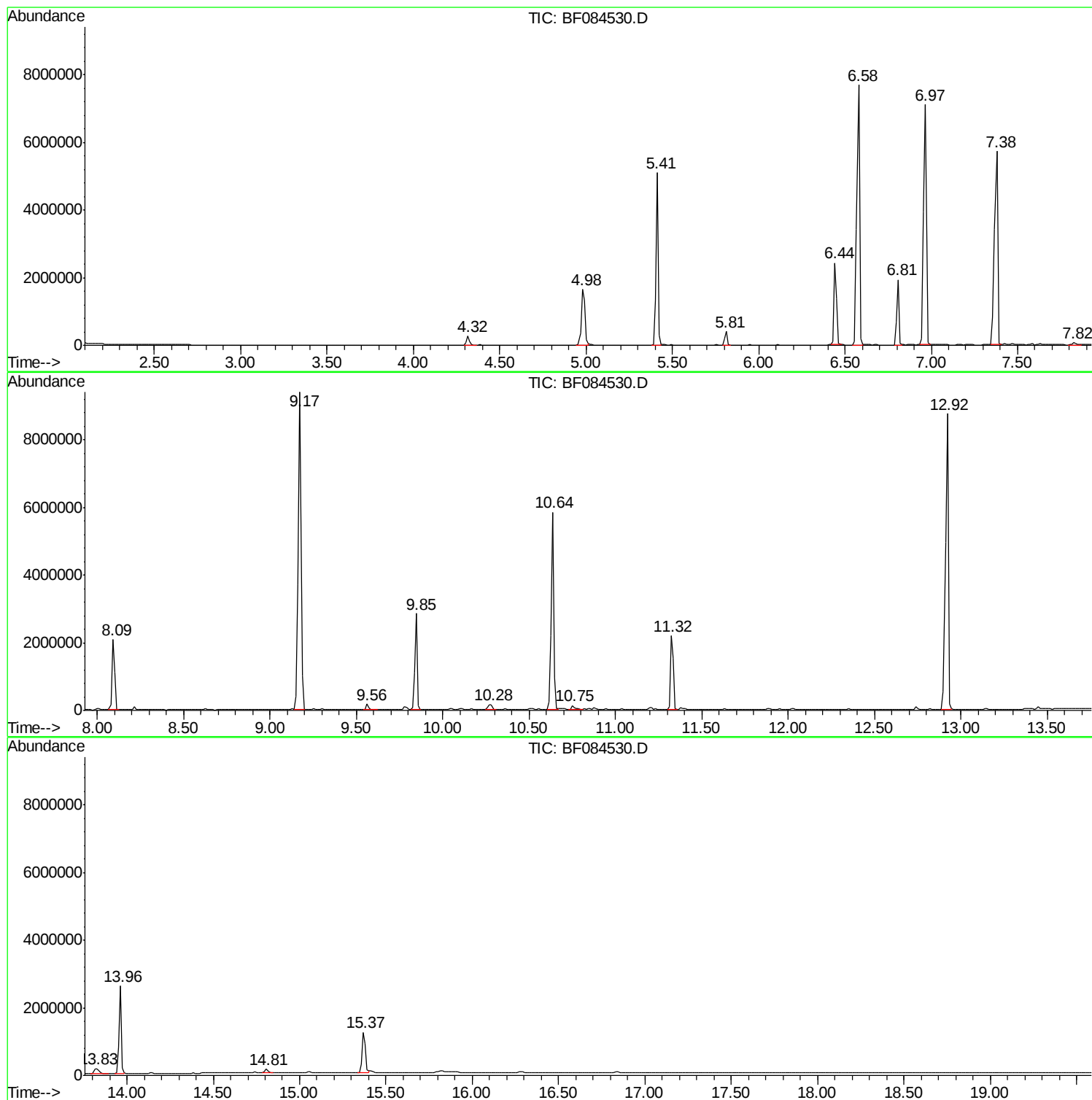
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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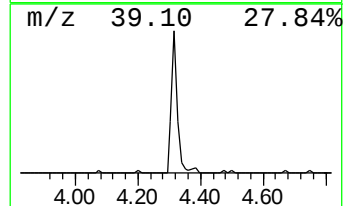
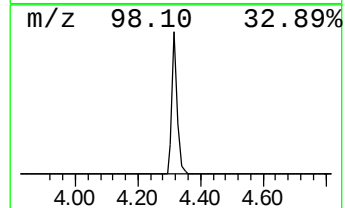
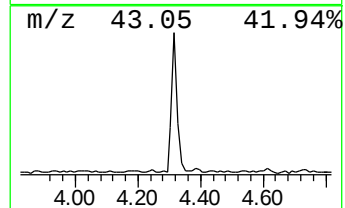
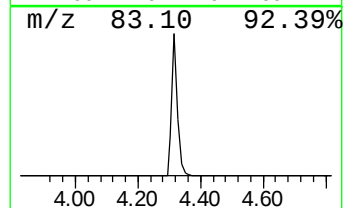
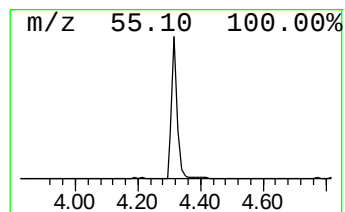
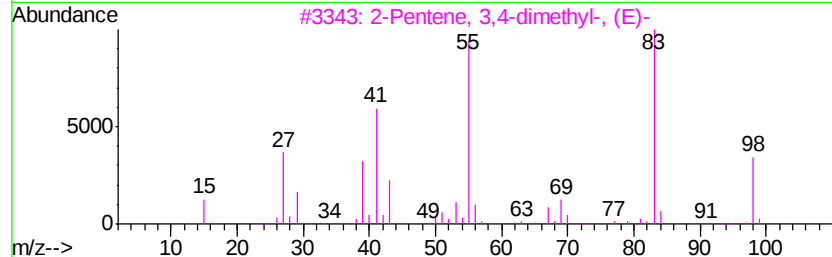
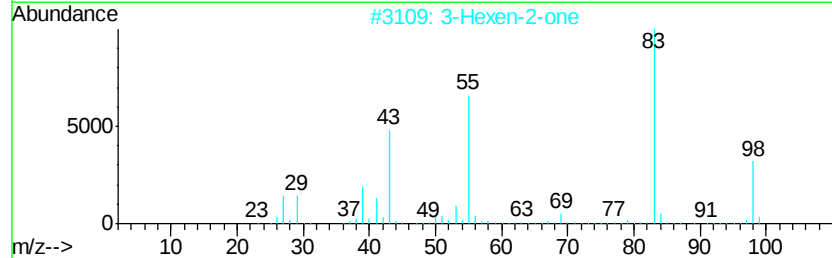
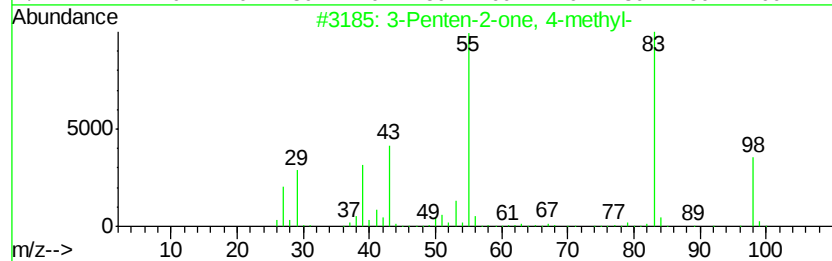
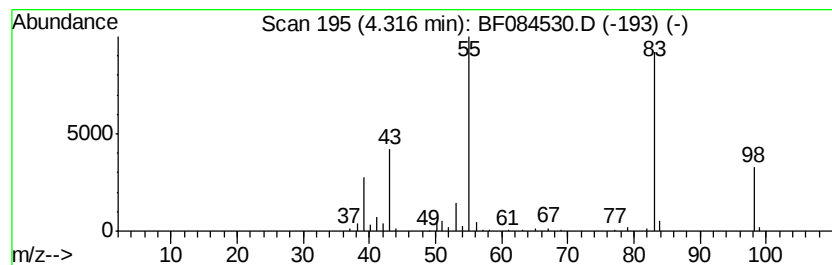
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.32	3.34 ng	305919	1,4-Dichlorobenzene-d4	6.81

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	87
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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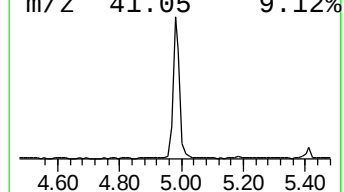
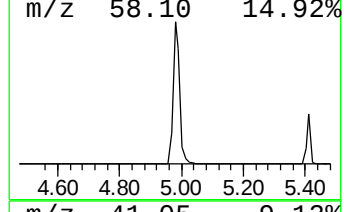
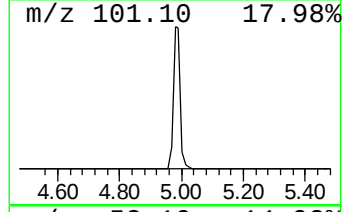
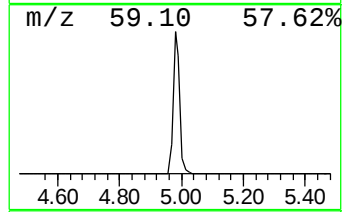
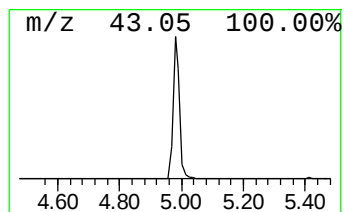
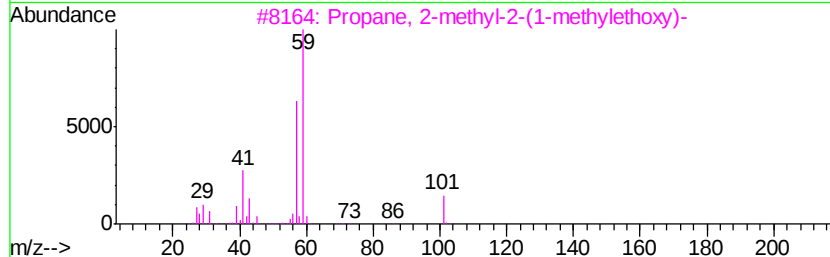
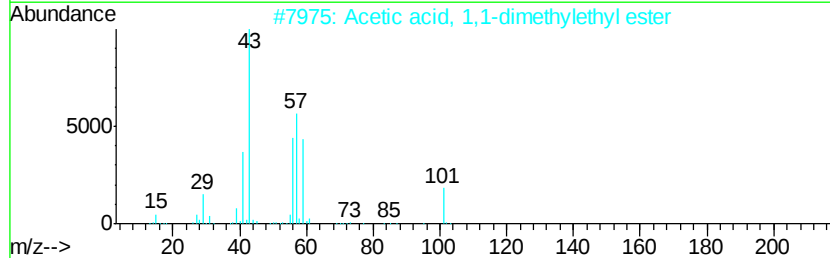
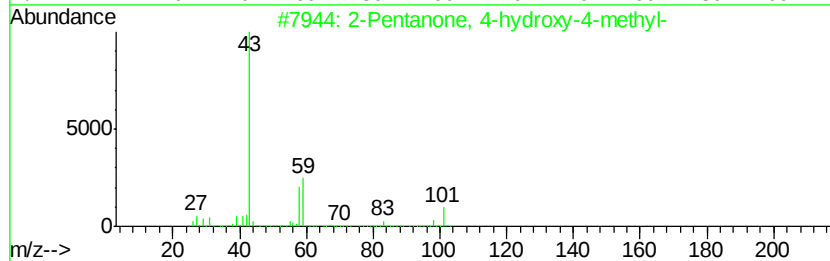
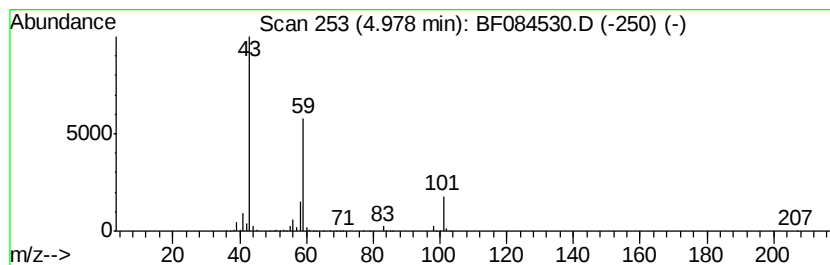
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.98	26.25 ng	2407080	1,4-Dichlorobenzene-d4	6.81

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	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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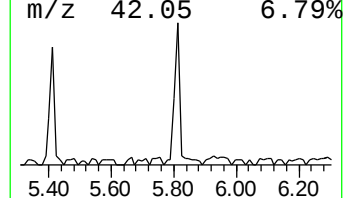
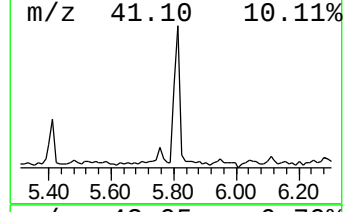
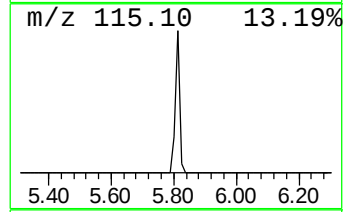
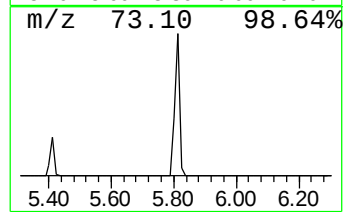
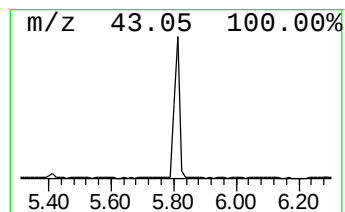
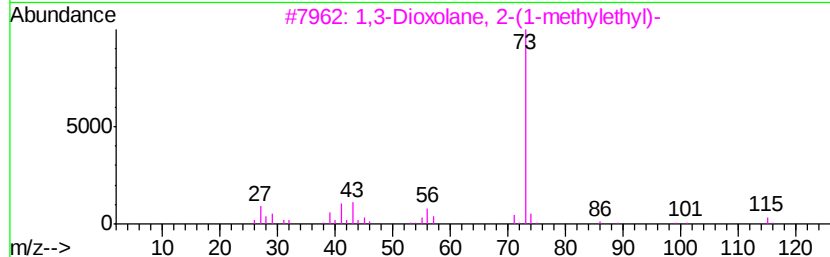
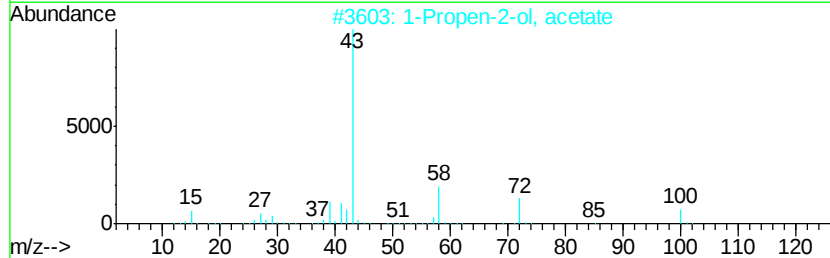
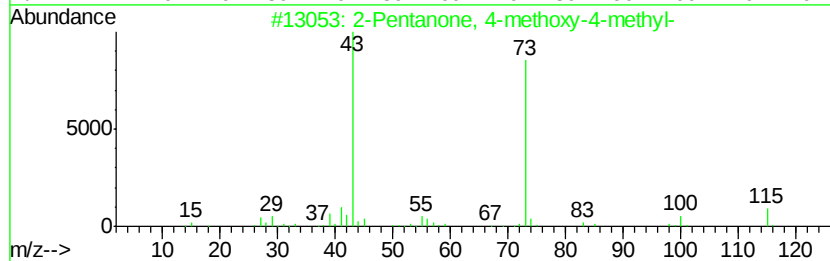
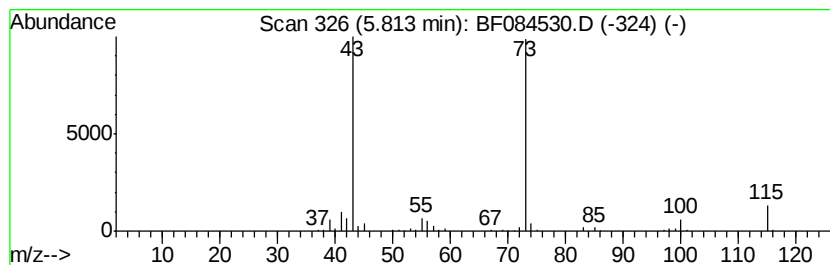
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.81	4.47 ng	409732	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9	
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	9	
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9	



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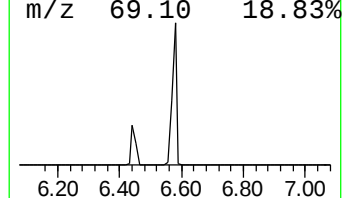
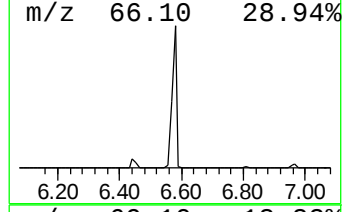
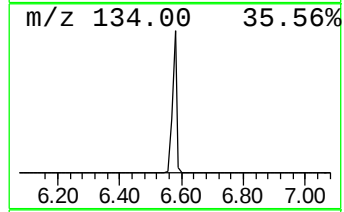
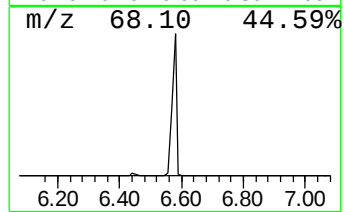
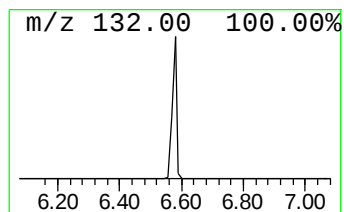
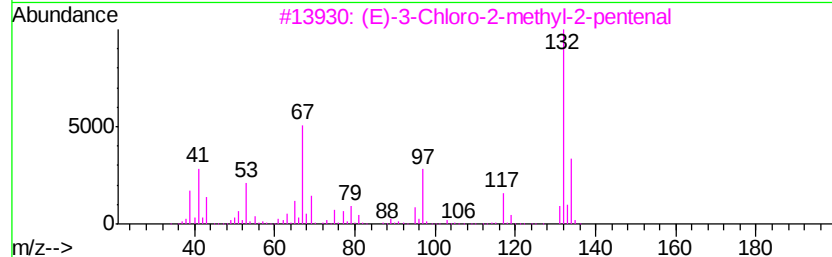
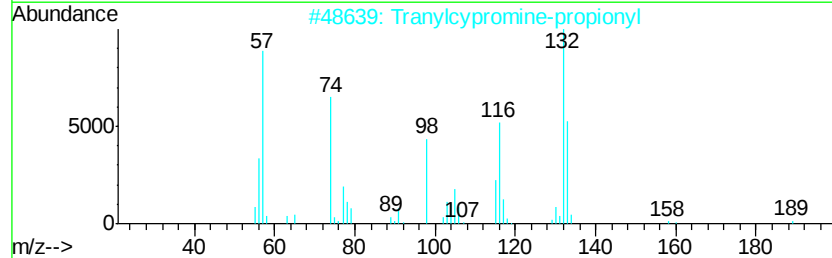
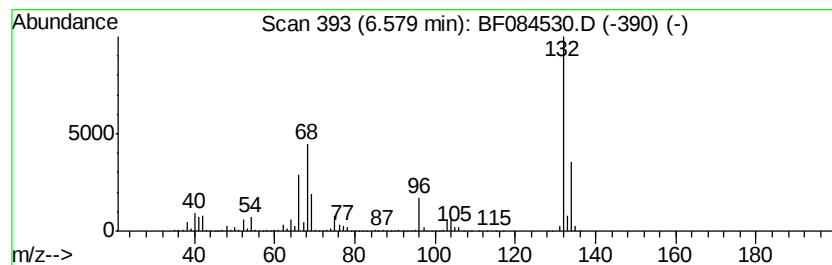
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	85.18 ng	7809620	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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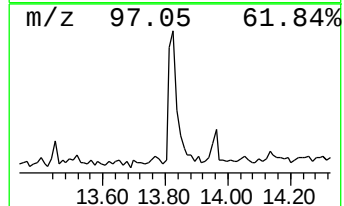
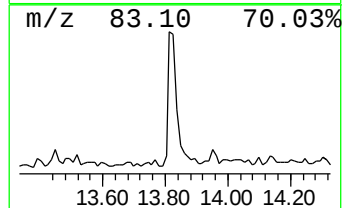
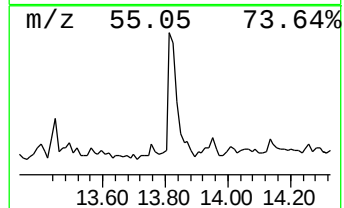
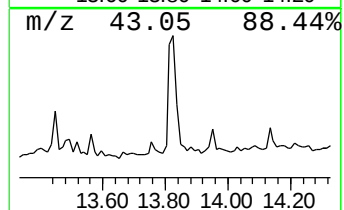
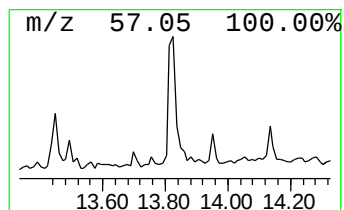
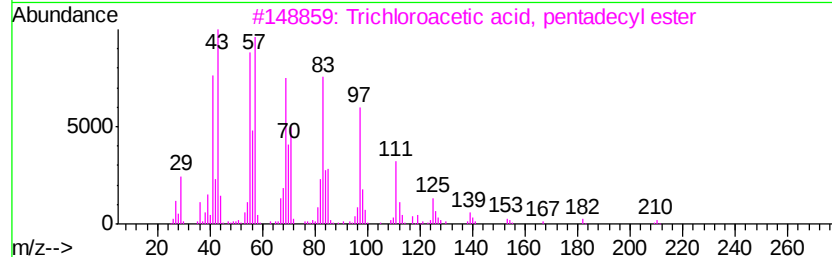
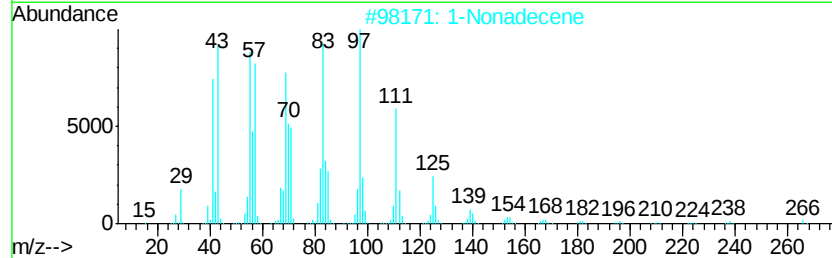
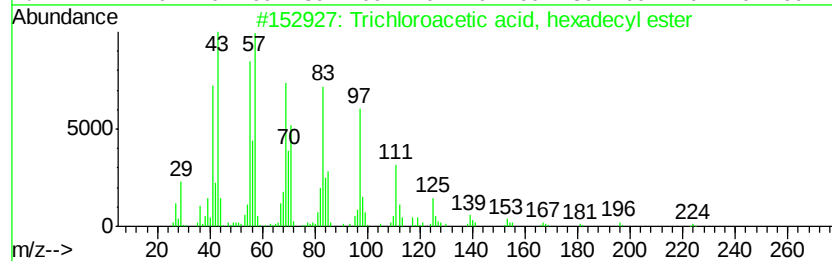
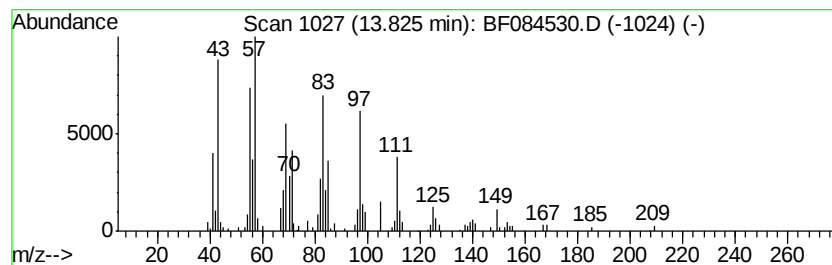
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.29 ng	280405	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
2		1-Nonadecene	266	C19H38	018435-45-5	74
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
4		Isotridecanol-	200	C13H28O	027458-92-0	74
5		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	72



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.32	3.3	ng	305919	1	6.81	1833760	20.0
2-Pentanone, 4-hy...	4.98	26.3	ng	2407080	1	6.81	1833760	20.0
2-Pentanone, 4-me...	5.81	4.5	ng	409732	1	6.81	1833760	20.0
unknown6.58	6.58	85.2	ng	7809620	1	6.81	1833760	20.0
Trichloroacetic a...	13.83	2.3	ng	280405	5	13.96	2448780	20.0