

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
 Data File : BF093216.D
 Acq On : 27 Feb 2017 20:40
 Operator : SJ/MA
 Sample : I1996-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-AA6-SWW

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	3.150	91	93	114	rBV	33192	152198	3.16%	0.341%
2	4.990	251	254	265	rBV	1329415	2040517	42.34%	4.567%
3	5.424	290	292	295	rBV	3822630	4307590	89.38%	9.641%
4	6.464	380	383	386	rBV	3247668	4819236	100.00%	10.786%
5	6.590	391	394	396	rBV	4486456	4455144	92.45%	9.971%
6	6.819	411	414	416	rBV	869882	993572	20.62%	2.224%
7	6.967	425	427	430	rBV	2855047	3366983	69.87%	7.536%
8	7.390	460	464	466	rBV	2232825	3140184	65.16%	7.028%
9	8.099	524	526	529	rBV	1496419	1337823	27.76%	2.994%
10	9.185	617	621	623	rBV	3281799	4795092	99.50%	10.732%
11	9.573	653	655	658	rBV	995848	1040918	21.60%	2.330%
12	9.791	670	674	677	rBV	32404	56949	1.18%	0.127%
13	9.859	677	680	682	rVB	1400827	1499681	31.12%	3.356%
14	10.282	713	717	719	rBV	67664	94046	1.95%	0.210%
15	10.511	734	737	740	rBV	29542	58217	1.21%	0.130%
16	10.648	746	749	752	rBV	2304110	2663897	55.28%	5.962%
17	10.762	756	759	762	rVV	106127	139712	2.90%	0.313%
18	11.208	796	798	799	rBV	112813	102120	2.12%	0.229%
19	11.345	807	810	812	rBV	1600470	1546077	32.08%	3.460%
20	11.631	833	835	838	rBV2	55633	56469	1.17%	0.126%
21	12.191	882	884	891	rVB3	53207	84483	1.75%	0.189%
22	12.934	946	949	951	rVB	3864152	4134971	85.80%	9.254%
23	13.825	1024	1027	1034	rBV	312557	467752	9.71%	1.047%
24	13.985	1038	1041	1043	rBV	1468945	1437669	29.83%	3.218%
25	14.454	1078	1082	1086	rBV5	29779	82833	1.72%	0.185%
26	14.728	1103	1106	1109	rBV2	60316	100891	2.09%	0.226%
27	14.808	1111	1113	1118	rVB	38047	48365	1.00%	0.108%
28	15.414	1163	1166	1169	rBV	937273	1243644	25.81%	2.783%
29	15.825	1199	1202	1204	rBV	50613	69847	1.45%	0.156%
30	15.883	1204	1207	1210	rBV3	34205	69680	1.45%	0.156%
31	16.294	1240	1243	1250	rVB2	48844	104557	2.17%	0.234%
32	16.843	1288	1291	1297	rVB2	38283	84982	1.76%	0.190%
33	17.494	1344	1348	1353	rVB	31134	85442	1.77%	0.191%

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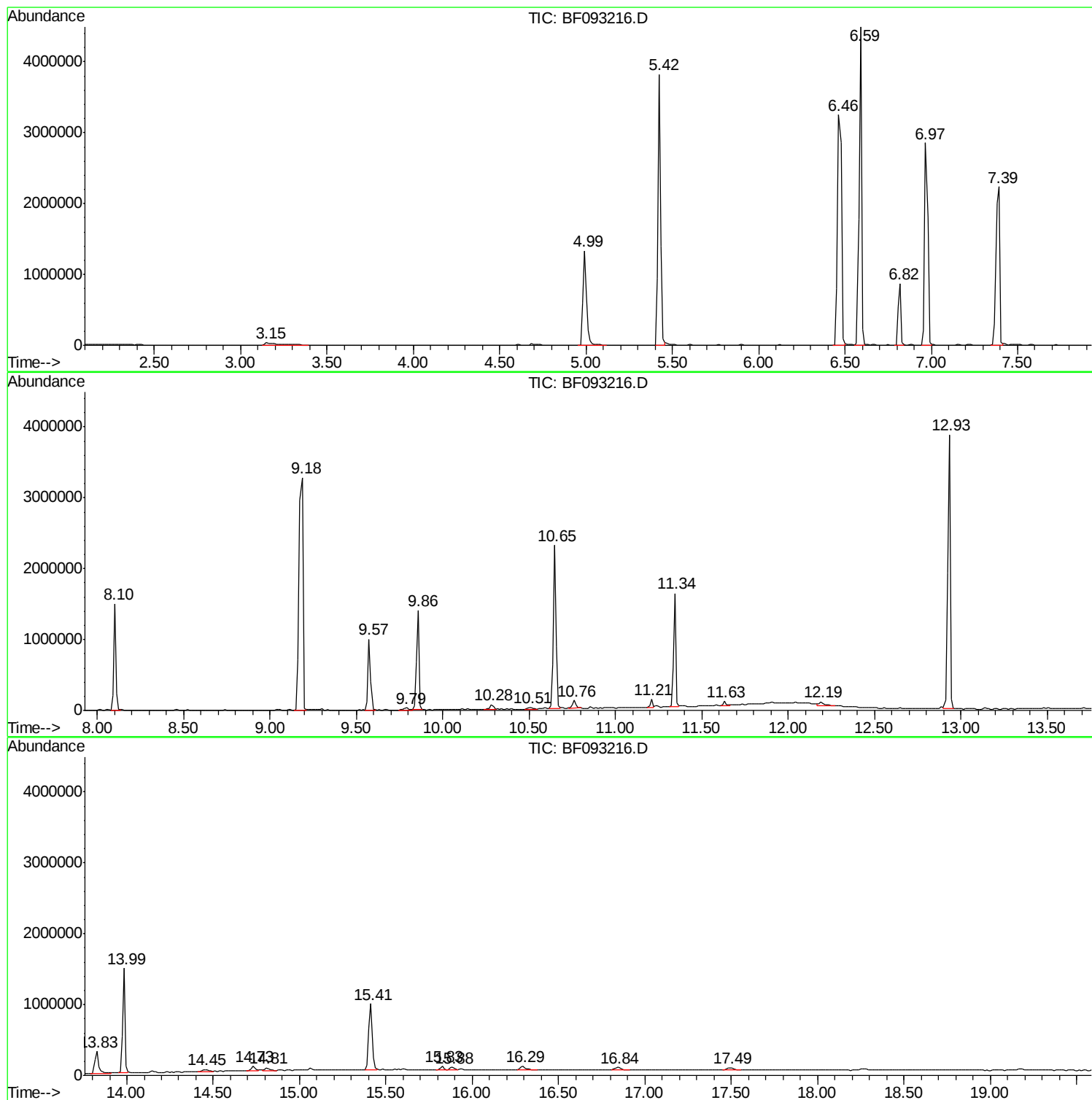
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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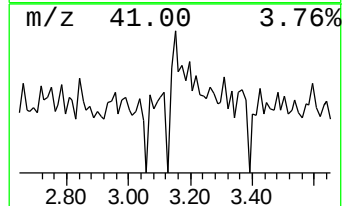
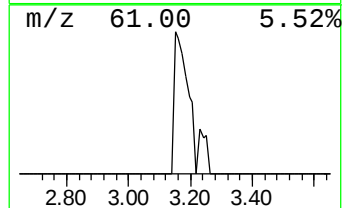
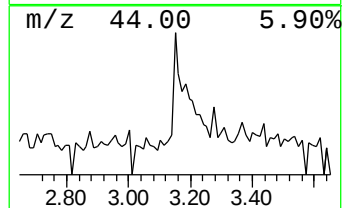
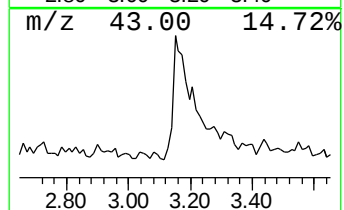
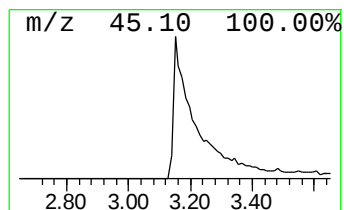
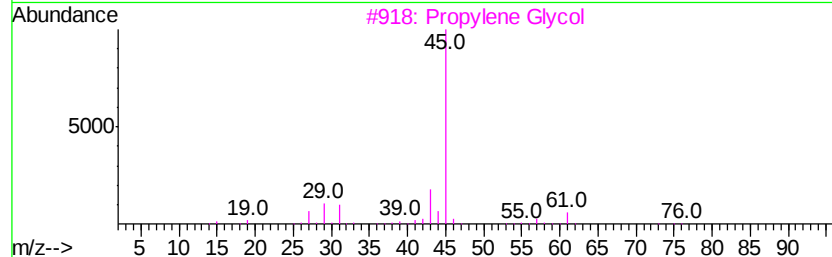
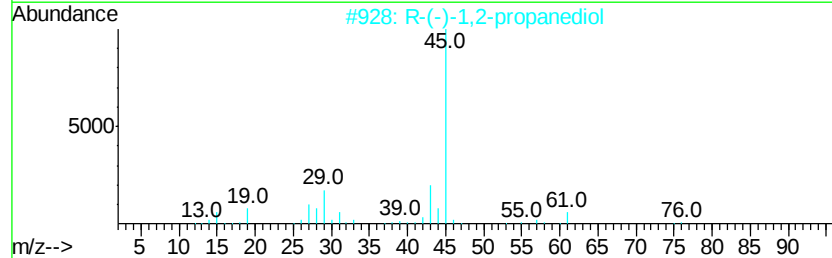
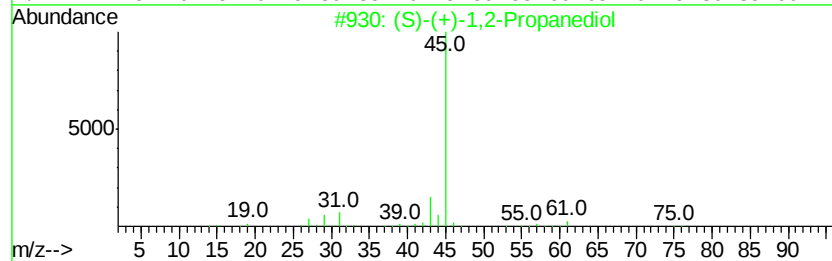
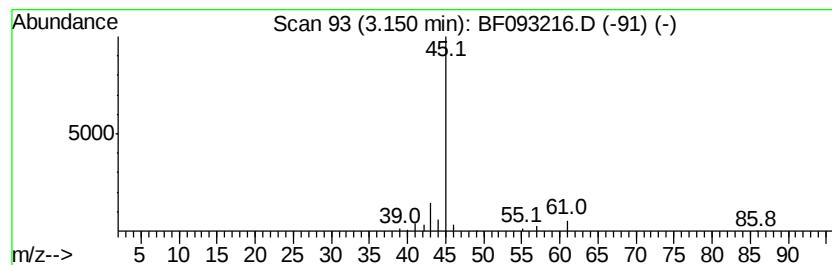
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.15	3.06 ng	152198	1,4-Dichlorobenzene-d4	6.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	2,3-Butanediol	90	C4H10O2	000513-85-9	9



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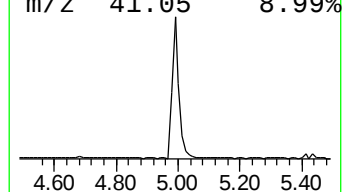
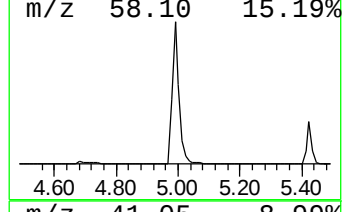
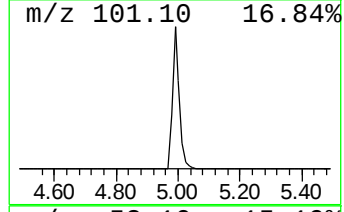
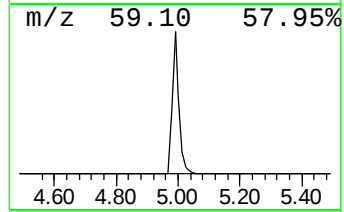
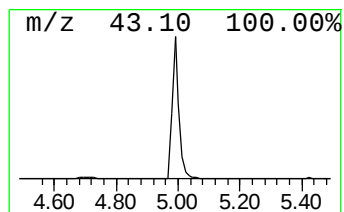
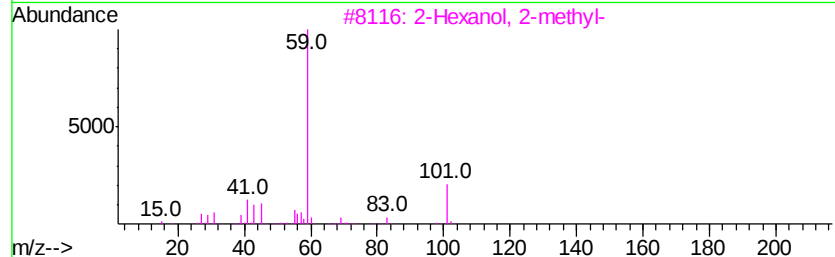
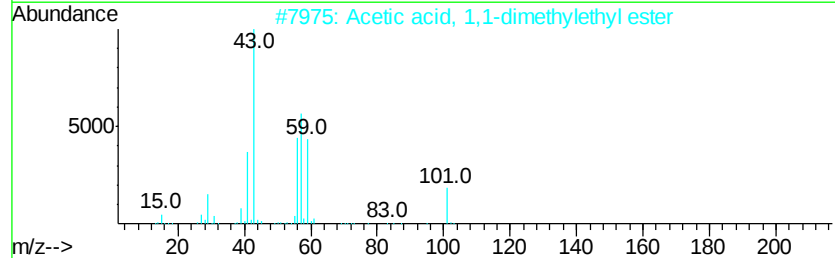
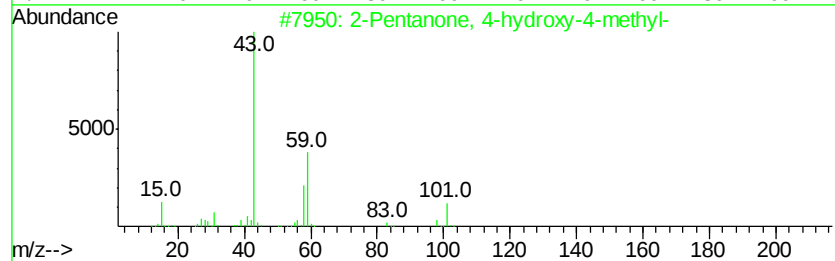
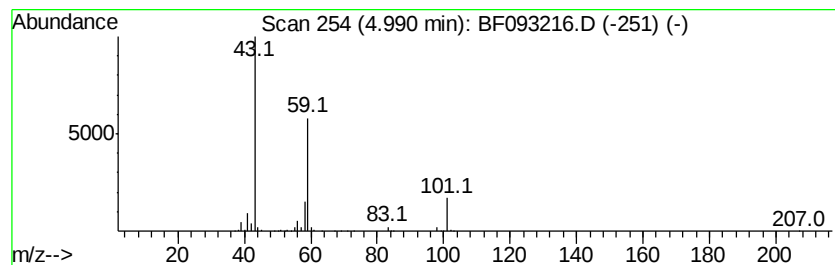
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	41.07 ng	2040520	1,4-Dichlorobenzene-d4	6.82

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		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33



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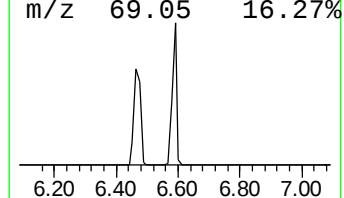
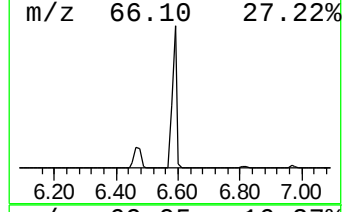
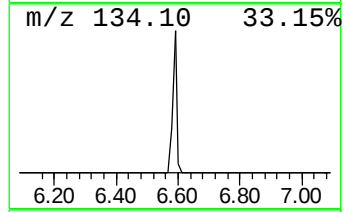
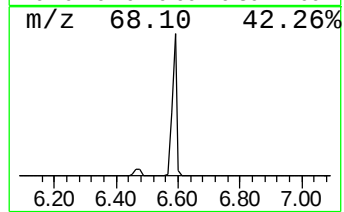
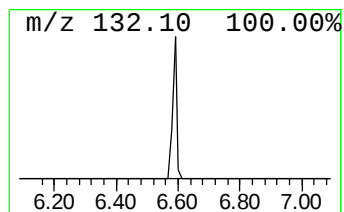
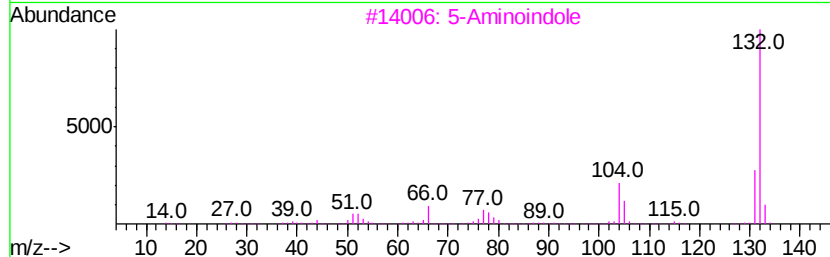
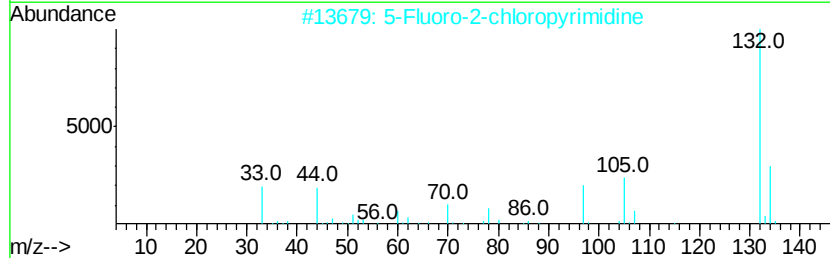
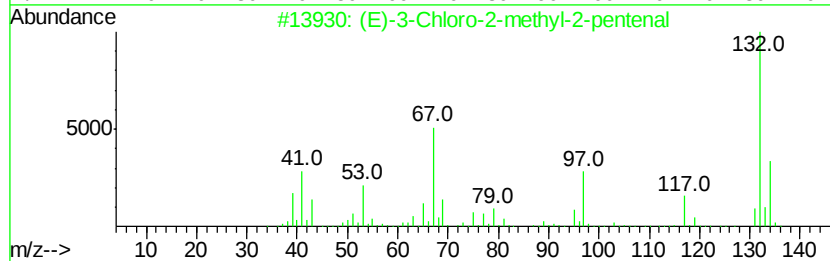
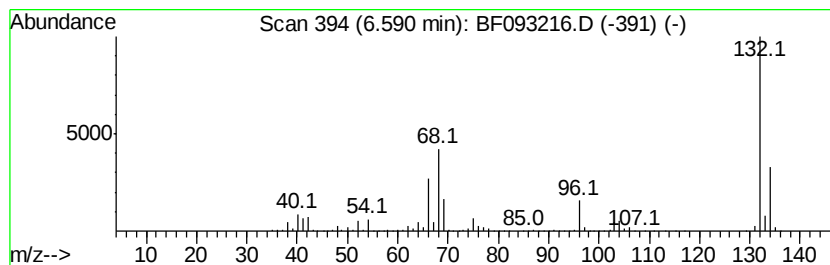
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	89.68 ng	4455140	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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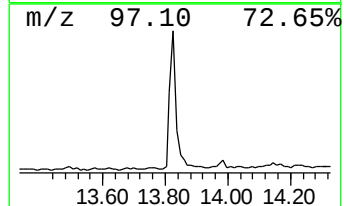
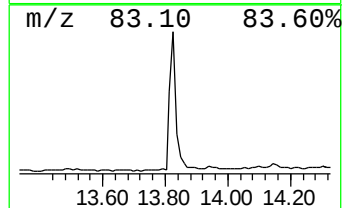
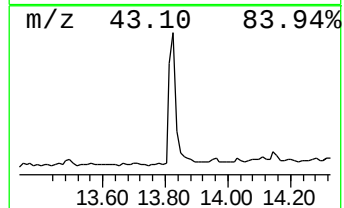
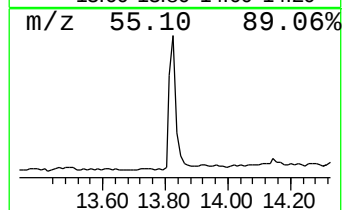
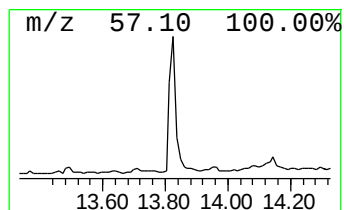
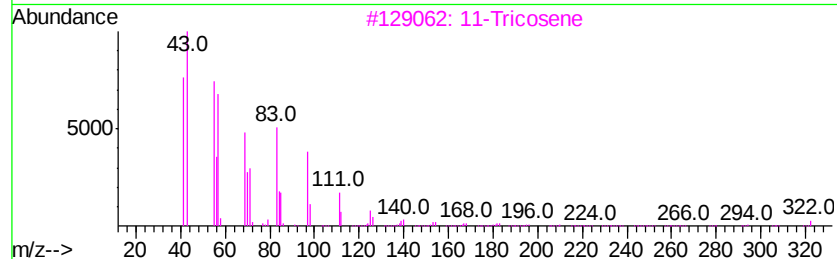
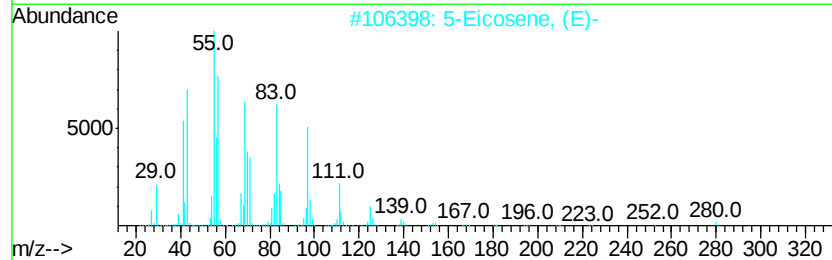
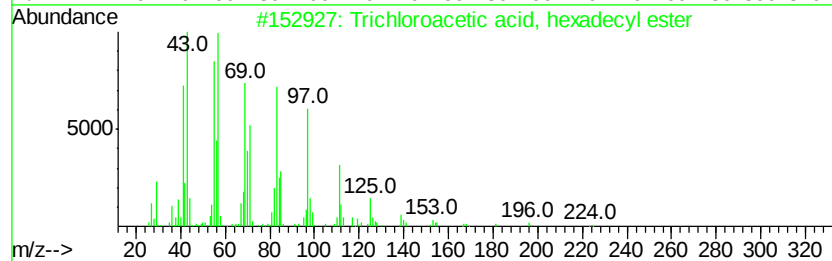
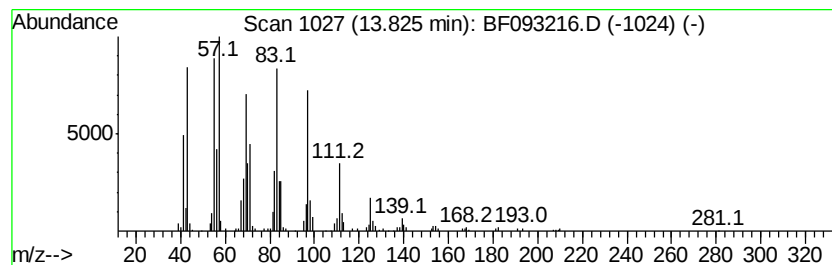
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Peak Number 5 Trichloroacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.51 ng	467752	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		11-Tricosene	322	C23H46	052078-56-5	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.15	3.1	ng	152198	1	6.82	993572	20.0
2-Pentanone, 4-hy...	4.99	41.1	ng	2040520	1	6.82	993572	20.0
unknown6.59	6.59	89.7	ng	4455140	1	6.82	993572	20.0
Trichloroacetic a...	13.83	6.5	ng	467752	5	13.99	1437670	20.0