

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
 Data File : BF093174.D
 Acq On : 25 Feb 2017 6:32
 Operator : SJ/MA
 Sample : I1973-15
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-B1-B2-BASE-5

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	5.001	252	255	269	rBV	1301182	1943358	42.13%	5.220%
2	5.436	290	293	295	rBV	3753075	4612563	100.00%	12.391%
3	6.384	374	376	381	rVB	39034	49668	1.08%	0.133%
4	6.476	381	384	387	rBV	3412535	4480946	97.15%	12.037%
5	6.602	393	395	398	rBV	4019056	3910400	84.78%	10.504%
6	6.830	413	415	418	rBV	964153	856013	18.56%	2.299%
7	6.990	427	429	431	rBV	3471316	3105068	67.32%	8.341%
8	7.402	462	465	468	rBV	2031715	2773631	60.13%	7.451%
9	8.122	526	528	530	rBV	1349672	1103798	23.93%	2.965%
10	9.196	620	622	625	rBV	2905406	4116712	89.25%	11.059%
11	9.596	655	657	659	rBV	1047460	838289	18.17%	2.252%
12	9.871	679	681	684	rBV	741232	1000841	21.70%	2.689%
13	10.282	715	717	718	rBV	67325	57674	1.25%	0.155%
14	10.671	748	751	753	rBV	1599898	1873091	40.61%	5.032%
15	10.785	759	761	765	rVB	48055	82223	1.78%	0.221%
16	11.231	797	800	801	rBV	69665	70700	1.53%	0.190%
17	11.356	809	811	814	rBV2	720516	848579	18.40%	2.280%
18	11.596	829	832	835	rBV4	33092	58552	1.27%	0.157%
19	11.654	835	837	839	rBV	109842	89239	1.93%	0.240%
20	12.065	871	873	875	rVB	37206	49057	1.06%	0.132%
21	12.568	915	917	920	rBV	71710	109114	2.37%	0.293%
22	12.797	932	937	940	rBV2	70208	126436	2.74%	0.340%
23	12.945	948	950	953	rBV	2307747	2517633	54.58%	6.763%
24	13.848	1026	1029	1034	rBV2	95274	136504	2.96%	0.367%
25	13.997	1040	1042	1044	rBV	674590	899796	19.51%	2.417%
26	14.465	1081	1083	1086	rBV2	28783	59996	1.30%	0.161%
27	15.025	1129	1132	1136	rBV	71362	135191	2.93%	0.363%
28	15.311	1155	1157	1160	rVB	37685	50229	1.09%	0.135%
29	15.380	1160	1163	1165	rVB	45776	66414	1.44%	0.178%
30	15.437	1165	1168	1175	rBV	581709	820155	17.78%	2.203%
31	15.860	1202	1205	1209	rBV	46604	76223	1.65%	0.205%
32	16.328	1244	1246	1254	rVB2	34618	79890	1.73%	0.215%
33	16.843	1287	1291	1292	rBV	21490	46475	1.01%	0.125%
34	16.888	1293	1295	1300	rVB	30324	66608	1.44%	0.179%

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35	17.540	1350	1352	1357	rVB	22992	54979	1.19%	0.148%
36	18.317	1417	1420	1427	rVB4	18235	60251	1.31%	0.162%

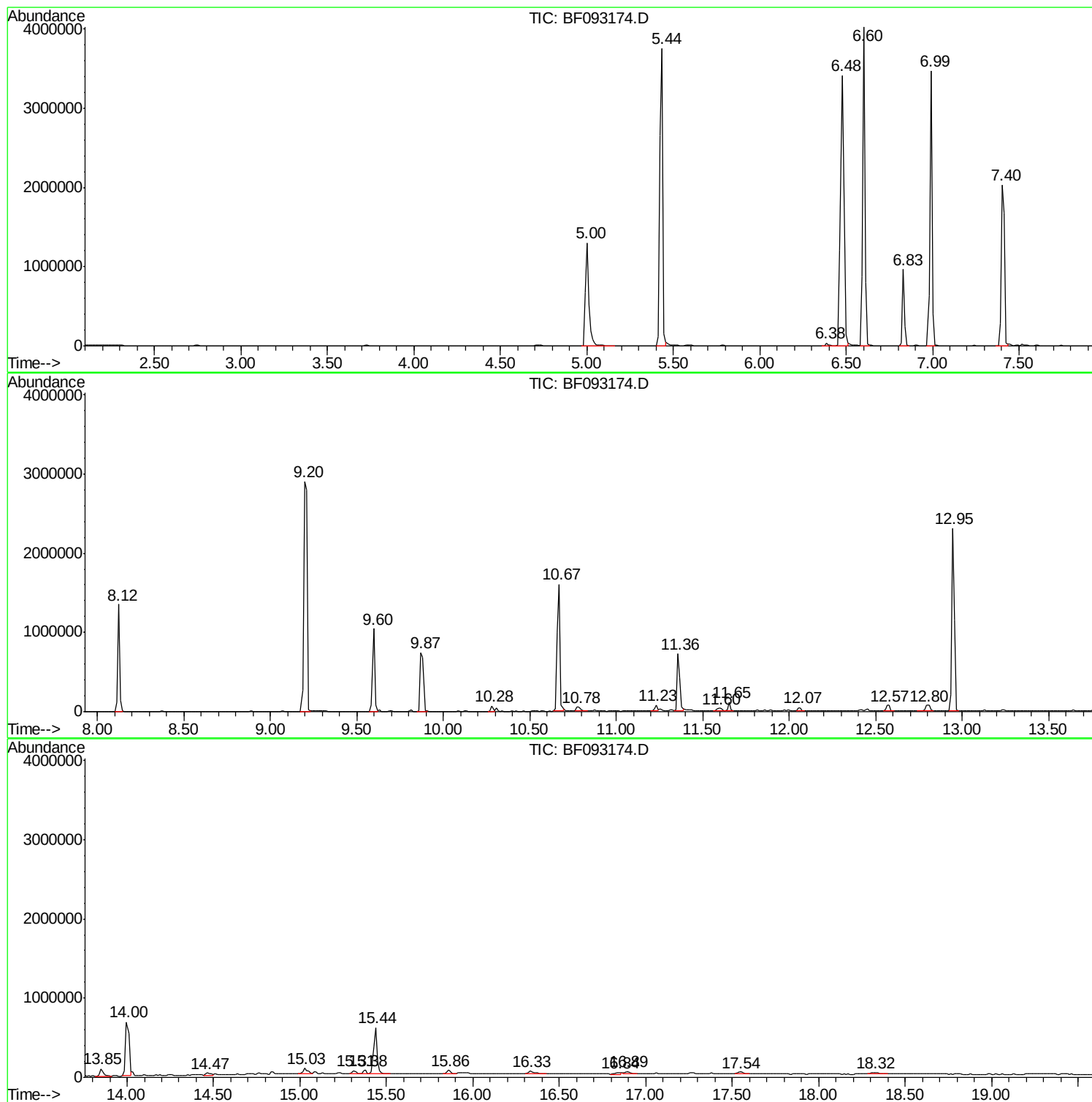
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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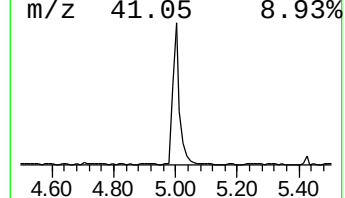
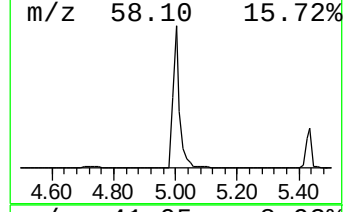
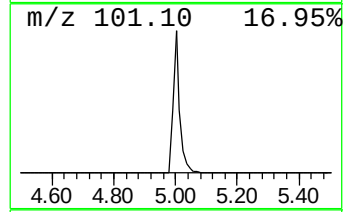
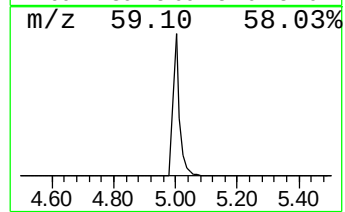
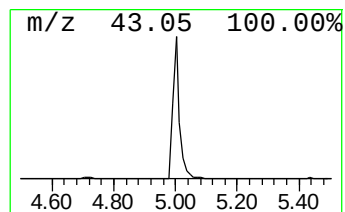
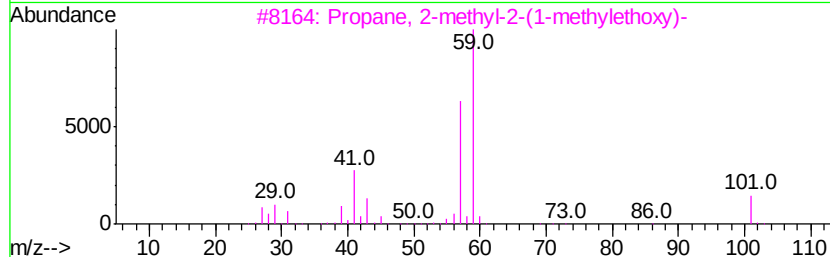
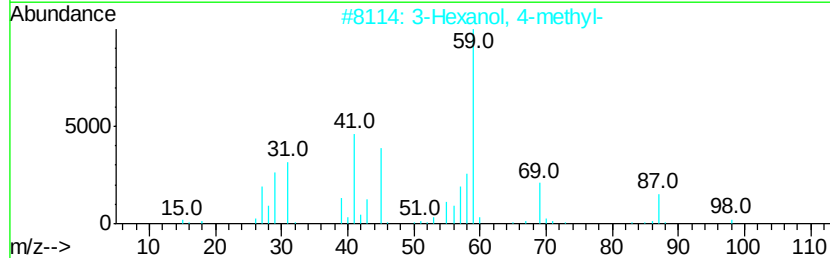
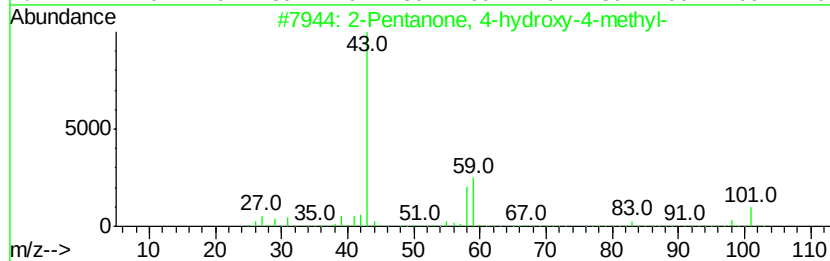
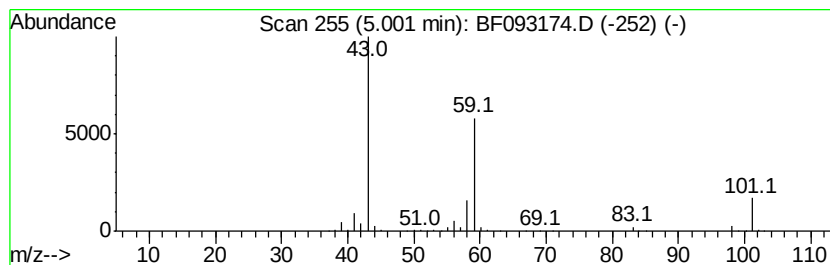
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	45.40 ng	1943360	1,4-Dichlorobenzene-d4	6.83

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



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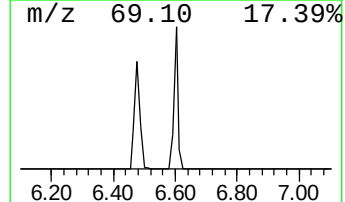
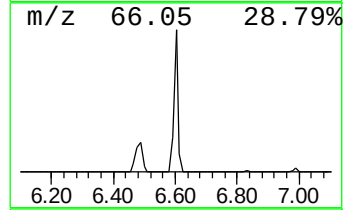
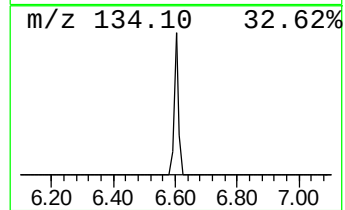
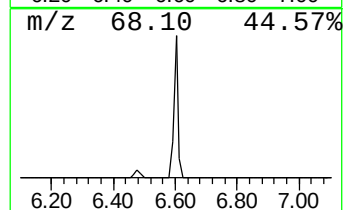
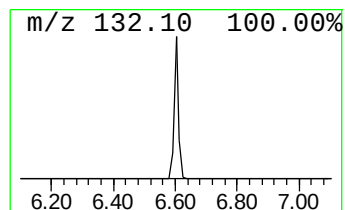
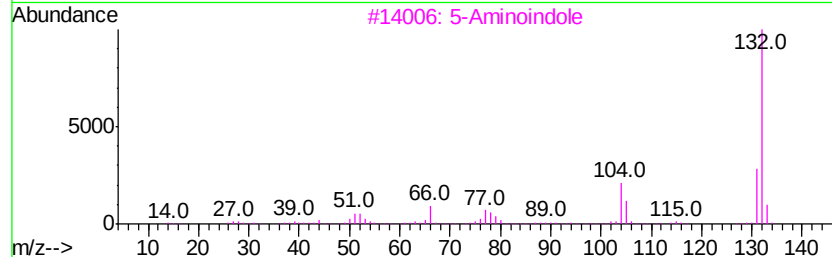
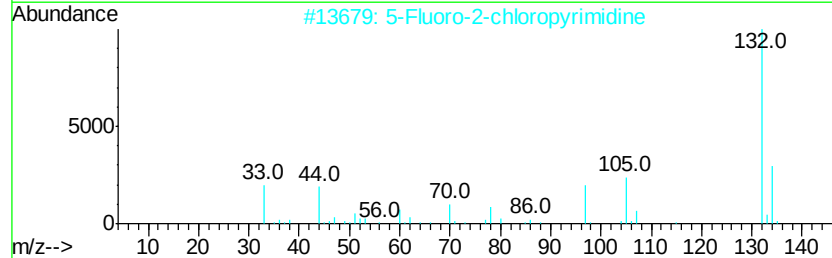
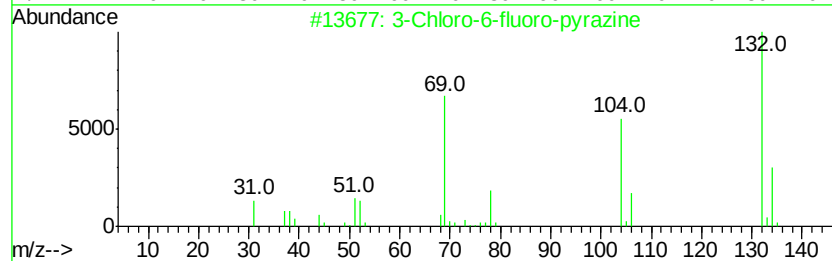
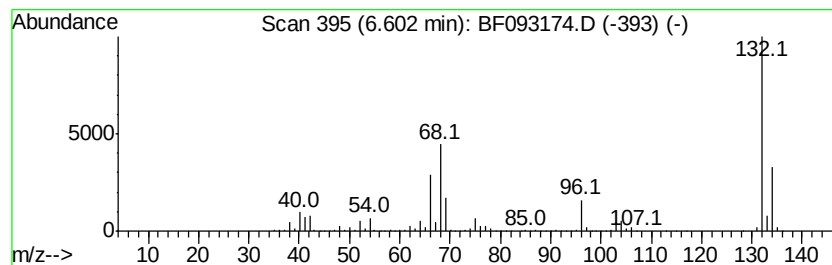
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	91.36 ng	3910400	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
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	Benzene, 1,3,5-trifluoro-			132	C6H3F3	000372-38-3	9



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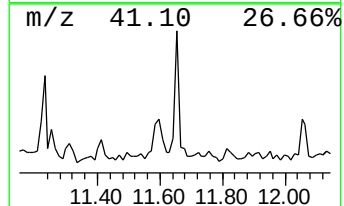
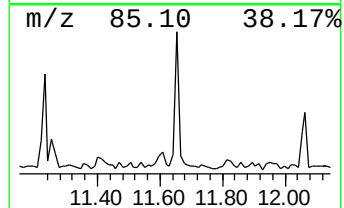
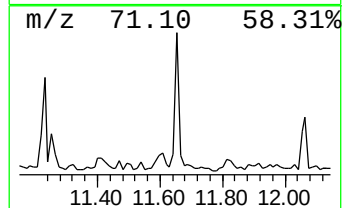
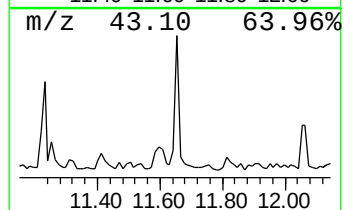
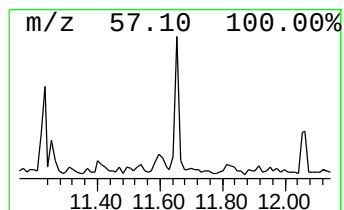
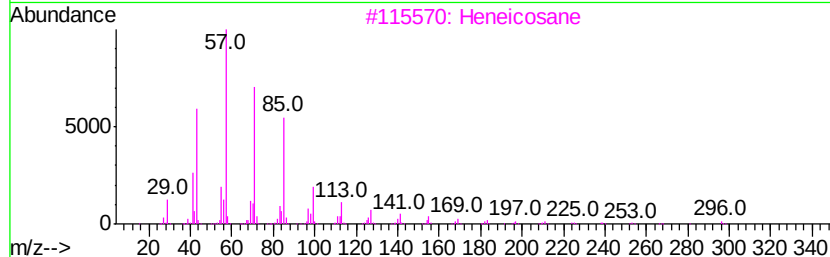
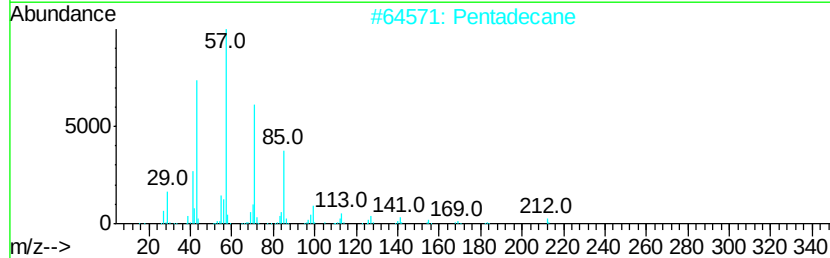
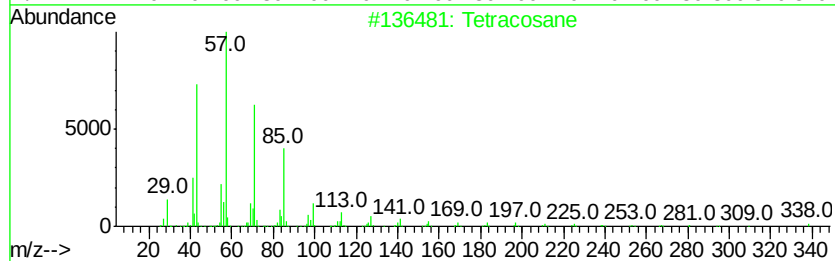
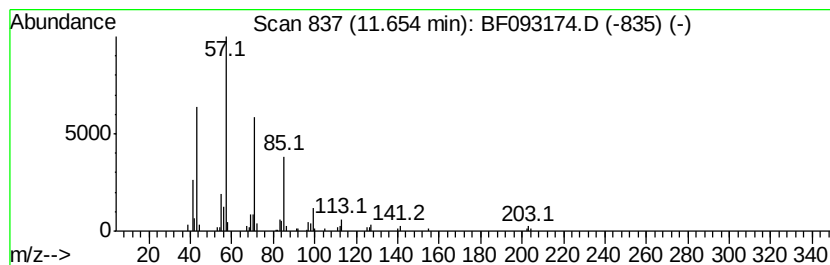
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Peak Number 4 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	2.10 ng	89239	Phenanthrene-d10	11.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Pentadecane	212	C15H32	000629-62-9	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Tetradecane	198	C14H30	000629-59-4	87



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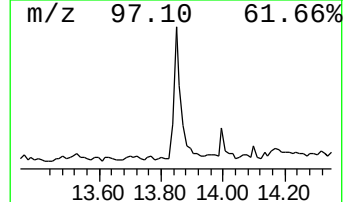
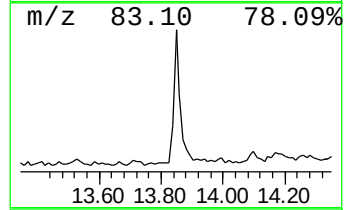
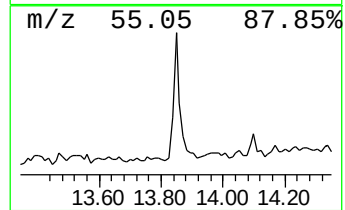
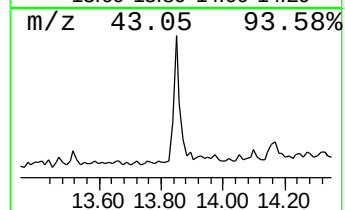
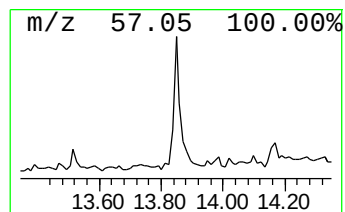
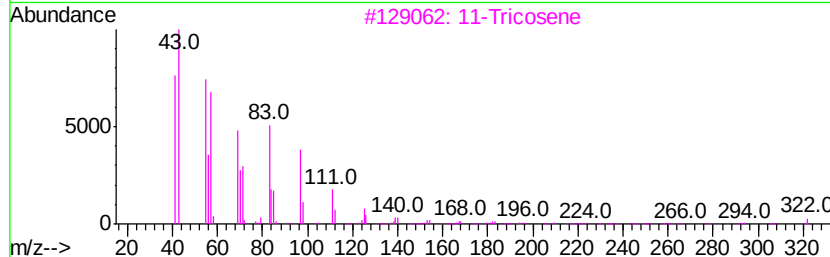
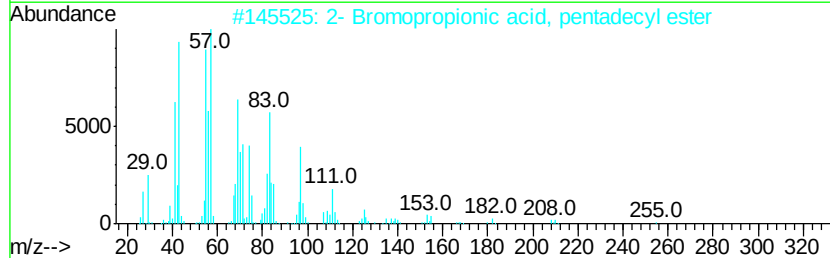
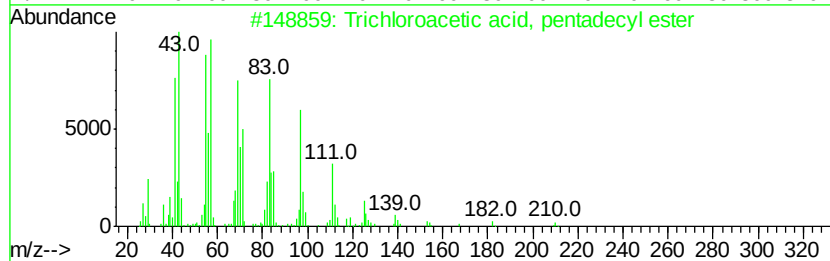
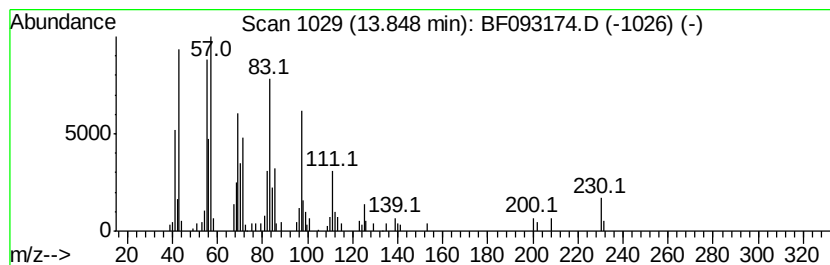
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	3.03 ng	136504	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
5	Cyclohexadecane	224	C16H32	000295-65-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	45.4	ng	1943360	1	6.83	856013	20.0
unknown6.60	6.60	91.4	ng	3910400	1	6.83	856013	20.0
Tetracosane	11.65	2.1	ng	89239	4	11.36	848579	20.0
Trichloroacetic a...	13.85	3.0	ng	136504	5	14.01	899796	20.0