

Molecular fingerprints

Education in Chemistry

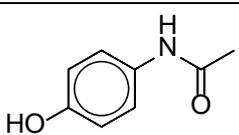
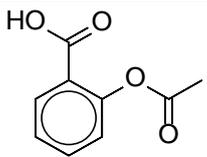
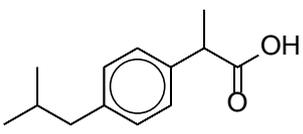
September 2017

rsc.li/EiC517-know-your-poison

This activity accompanies the above article 'Know your poison'.

The team at Bath have found lots of different substances mixed in with their drugs samples. Legal drugs such as painkillers are commonly found in the samples.

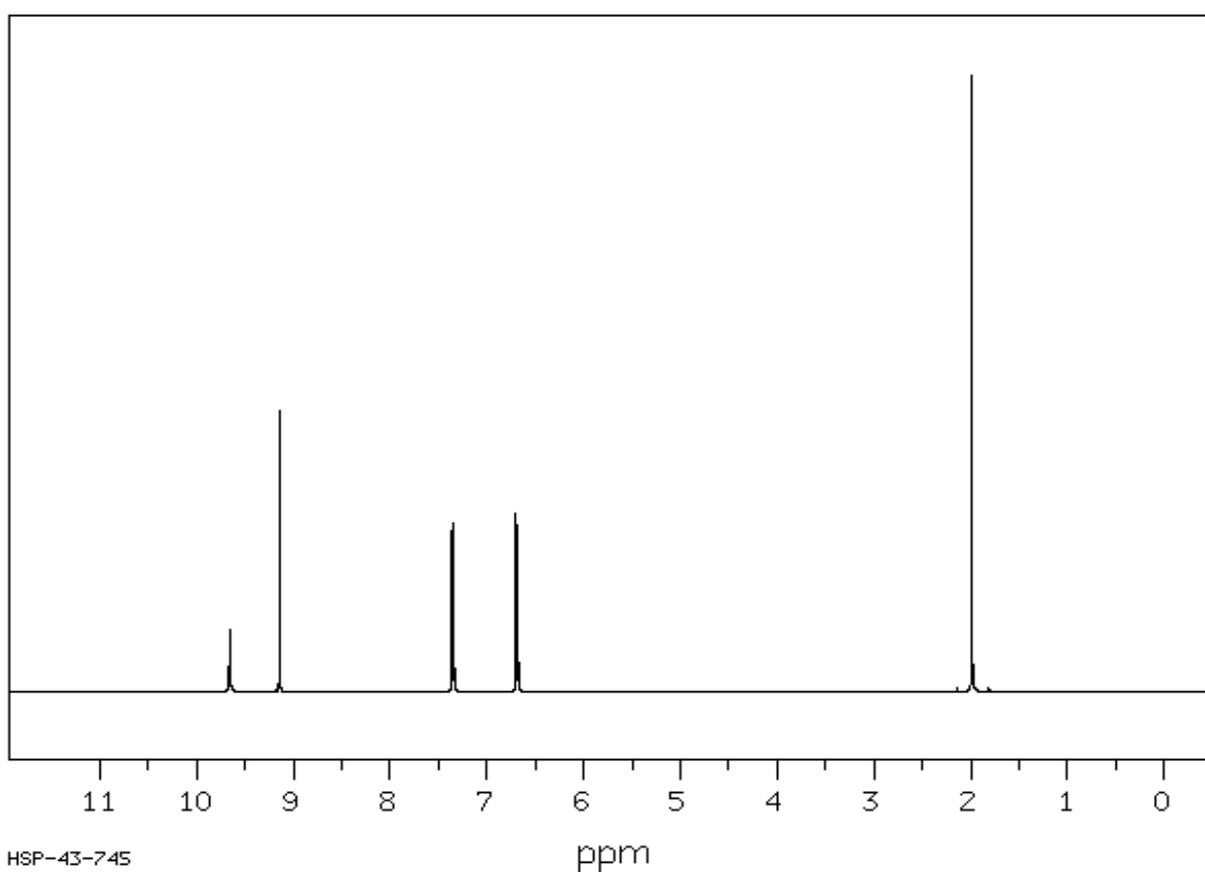
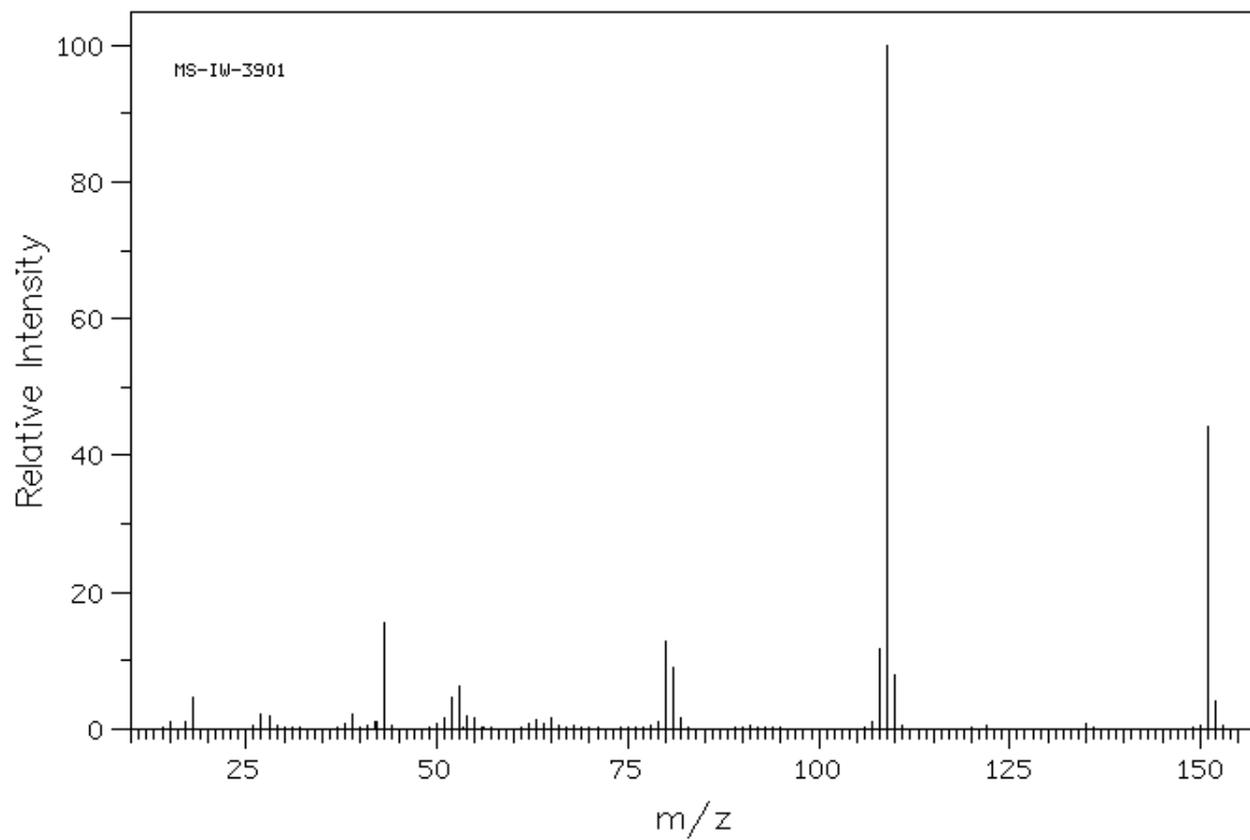
Note down the molecular formula, relative molecular mass (M_r) and functional groups for paracetamol, aspirin and ibuprofen. This will help you in the next part of the exercise.

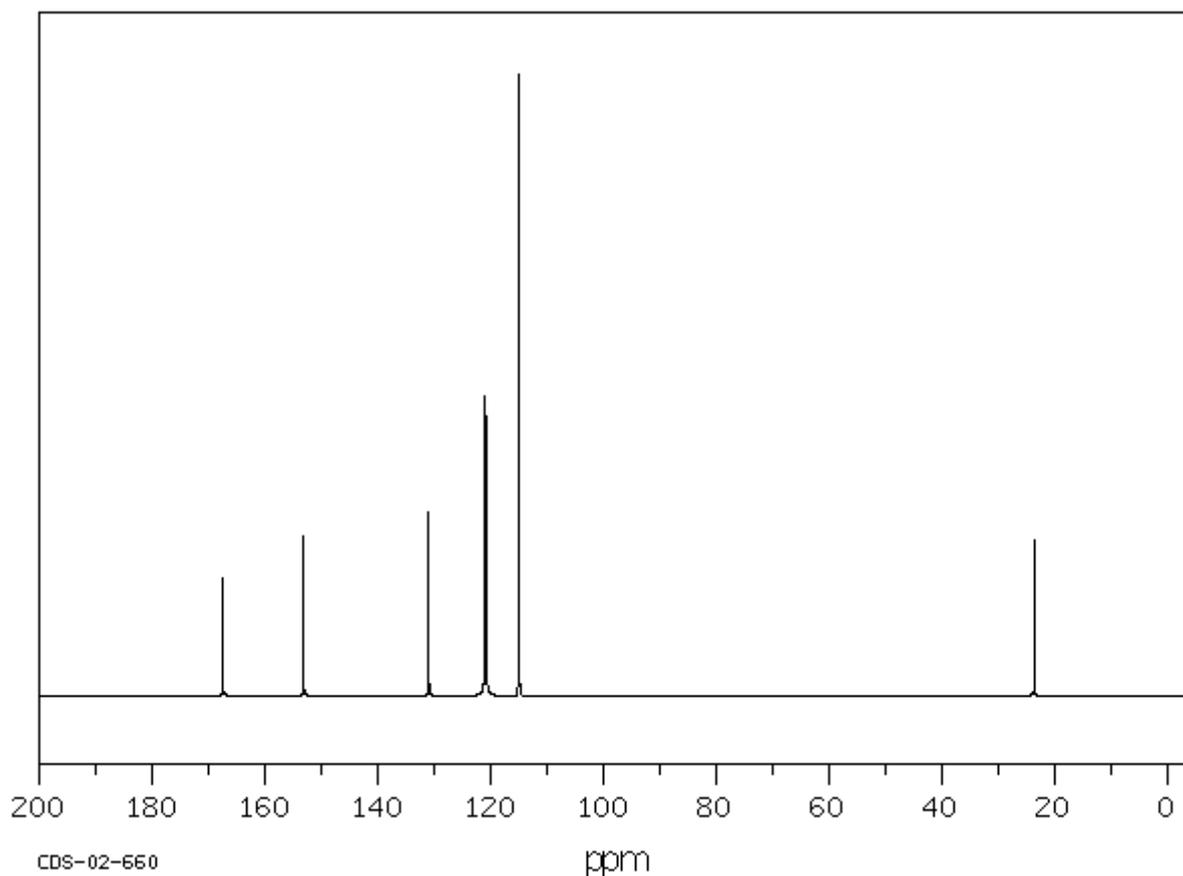
	Molecular formula and M_r	Functional groups present
 Paracetamol		
 Aspirin		
 Ibuprofen		

The following pages contain infrared, ^1H NMR, ^{13}C NMR and mass spectra for paracetamol, ibuprofen and aspirin. Use the structures given above and your data book to assign each of the peaks in the spectra.

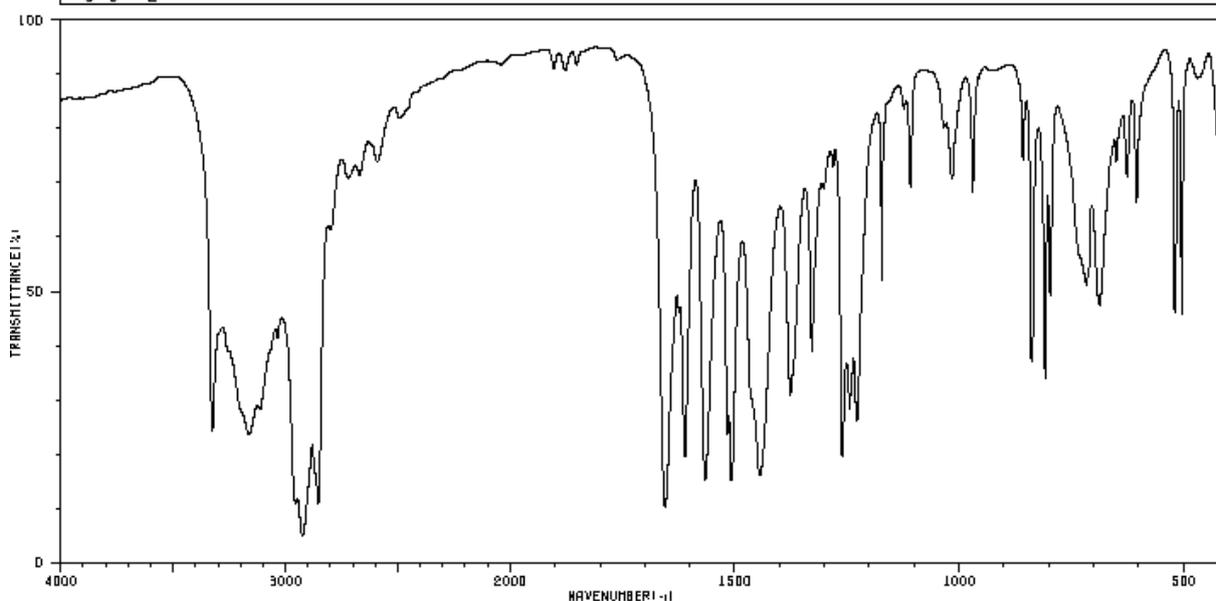
The following spectra are downloaded from SDBSWeb <http://sdb.sdb.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, accessed 22 June 2017)

Paracetamol

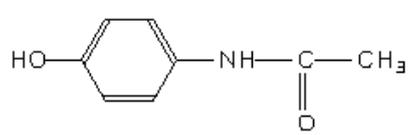




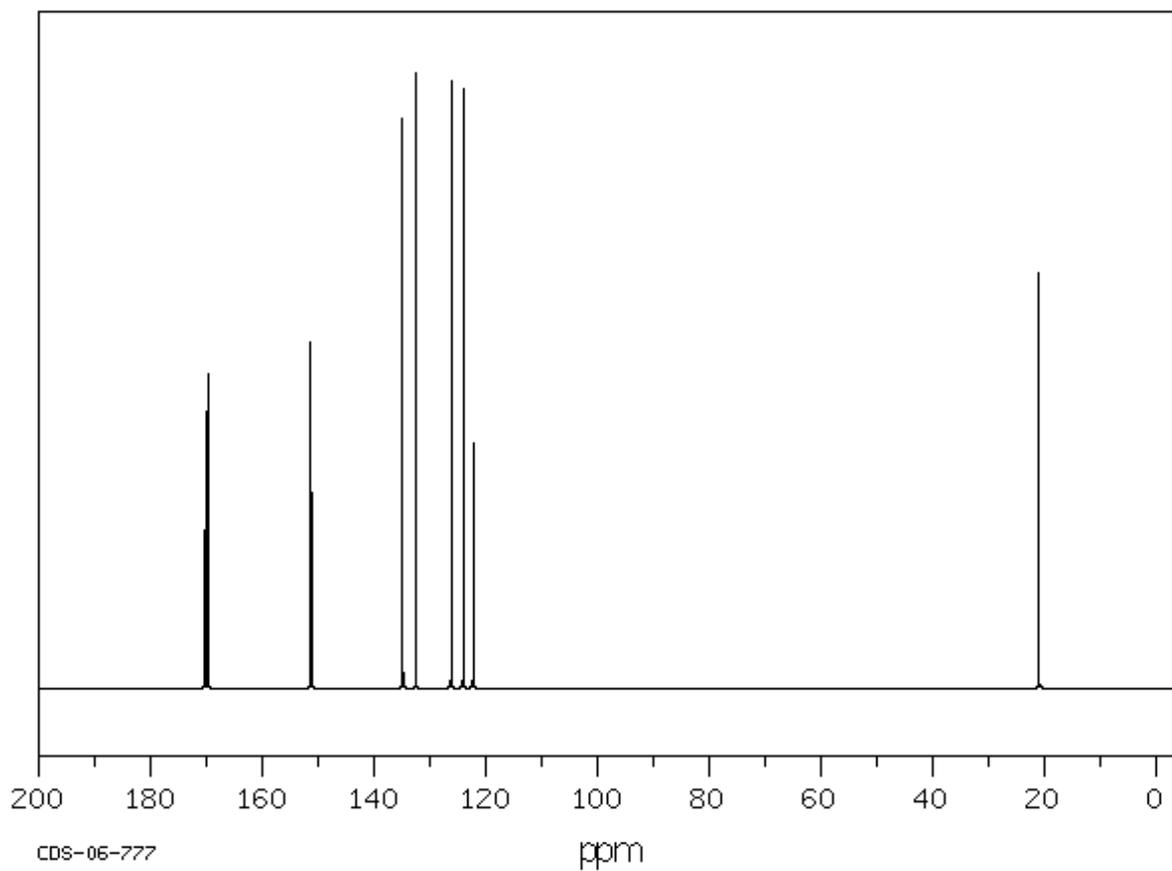
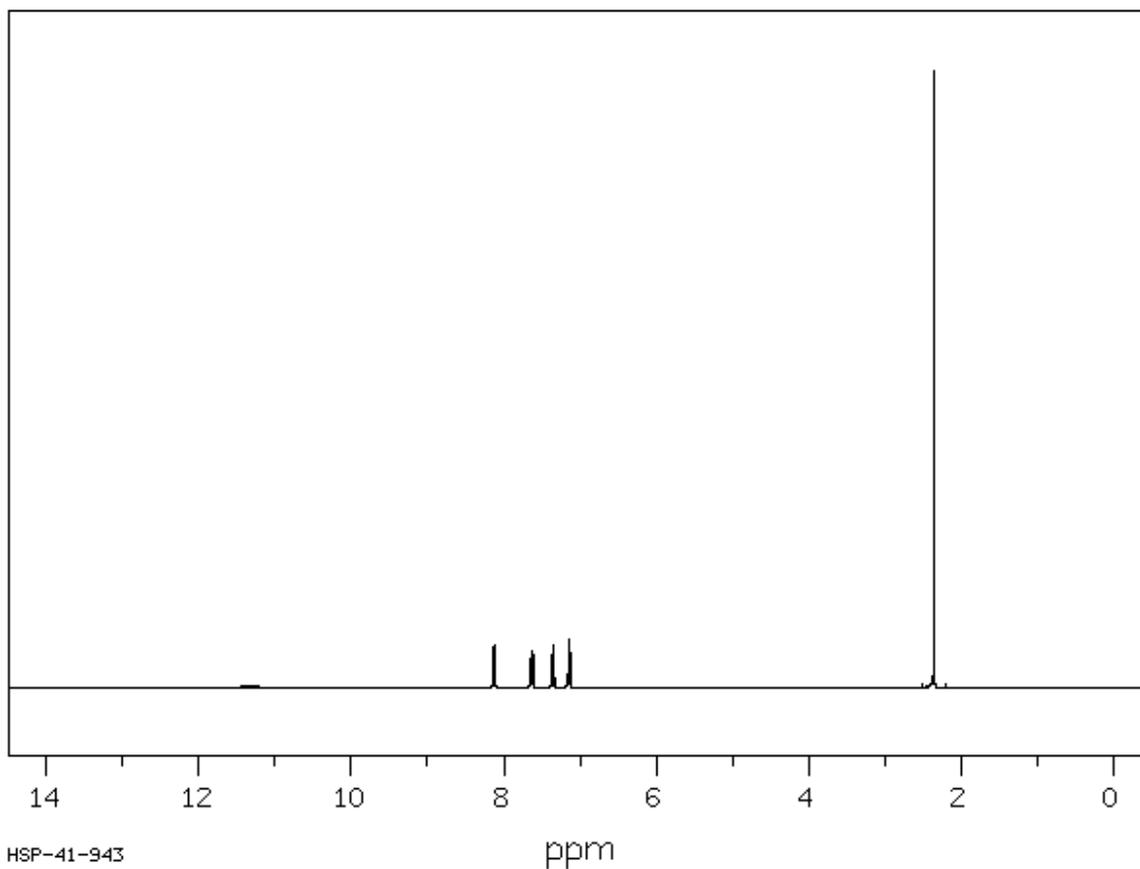
HIT-NO=1711	SCORE= ()	SDBS-NO=3290	IR-NIDA-62248 ; NUJOL MULL
4'-HYDROXYACETANILIDE			
C ₈ H ₉ NO ₂			



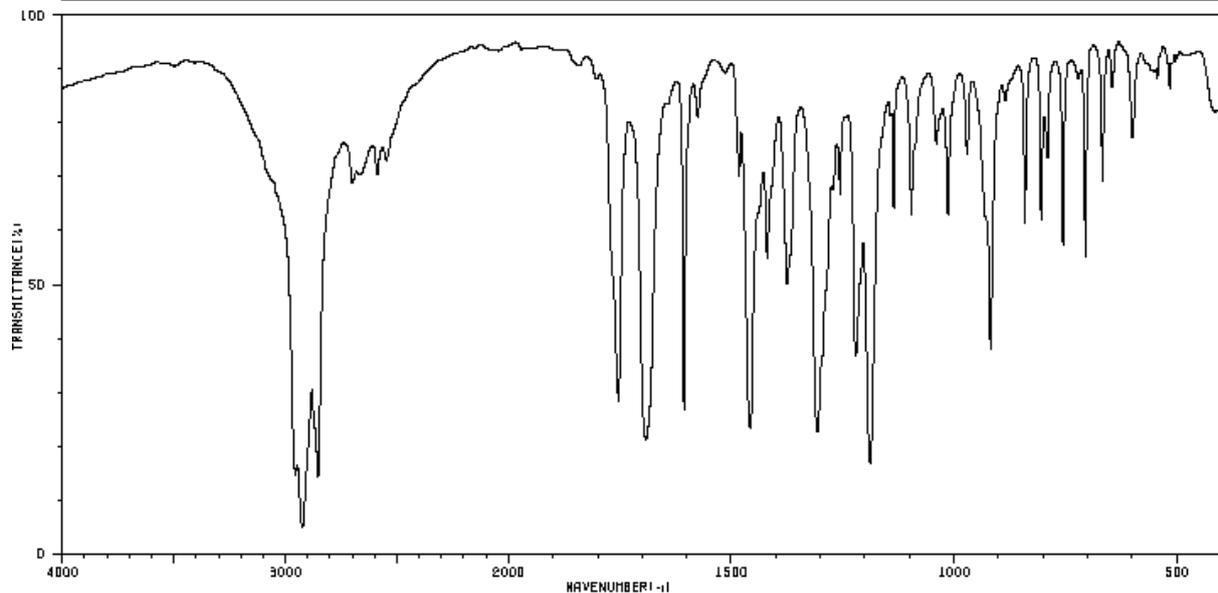
3326	23	2696	70	1608	14	1228	26	797	47
3164	22	2669	68	1444	15	1173	50	716	49
3036	39	2590	70	1376	29	1109	66	657	46
2964	10	1666	10	1329	37	1016	69	626	69
2924	4	1611	18	1281	70	970	66	605	64
2854	10	1565	14	1261	18	839	35	521	44
2720	68	1516	22	1244	27	809	32	504	44



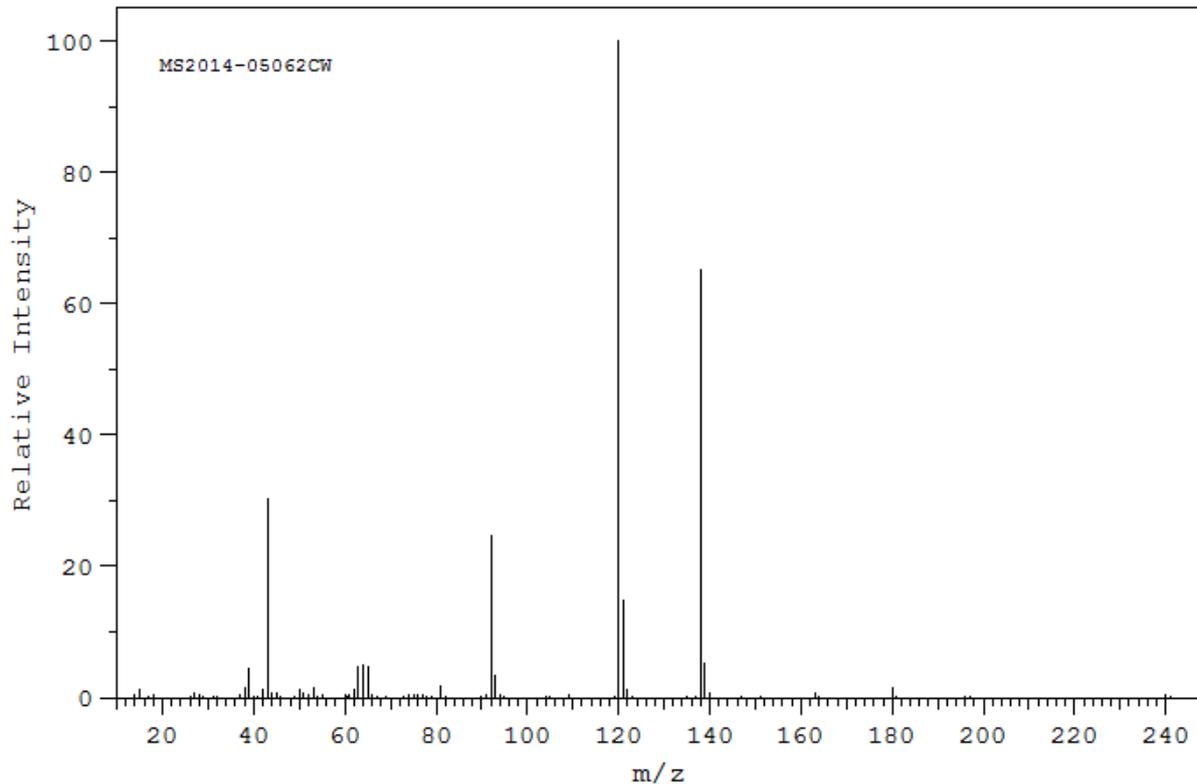
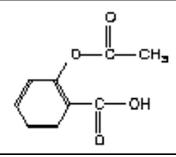
Aspirin



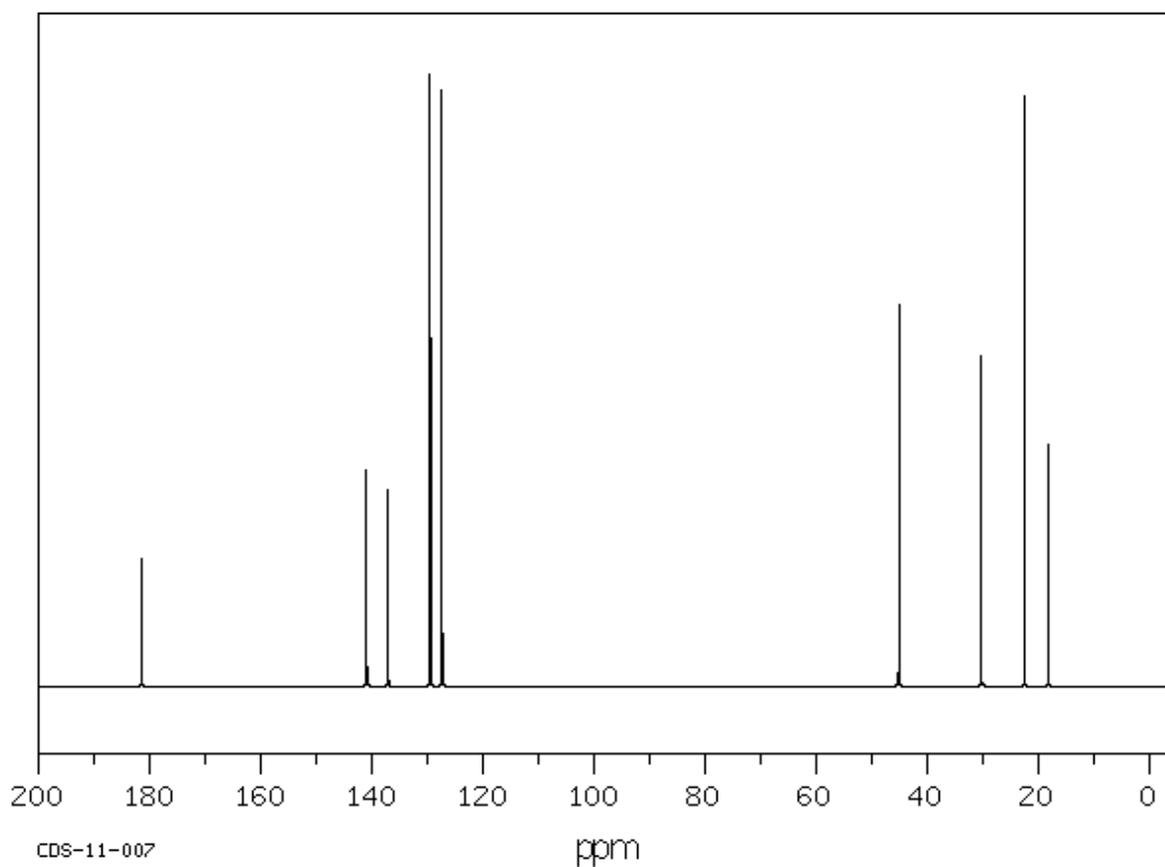
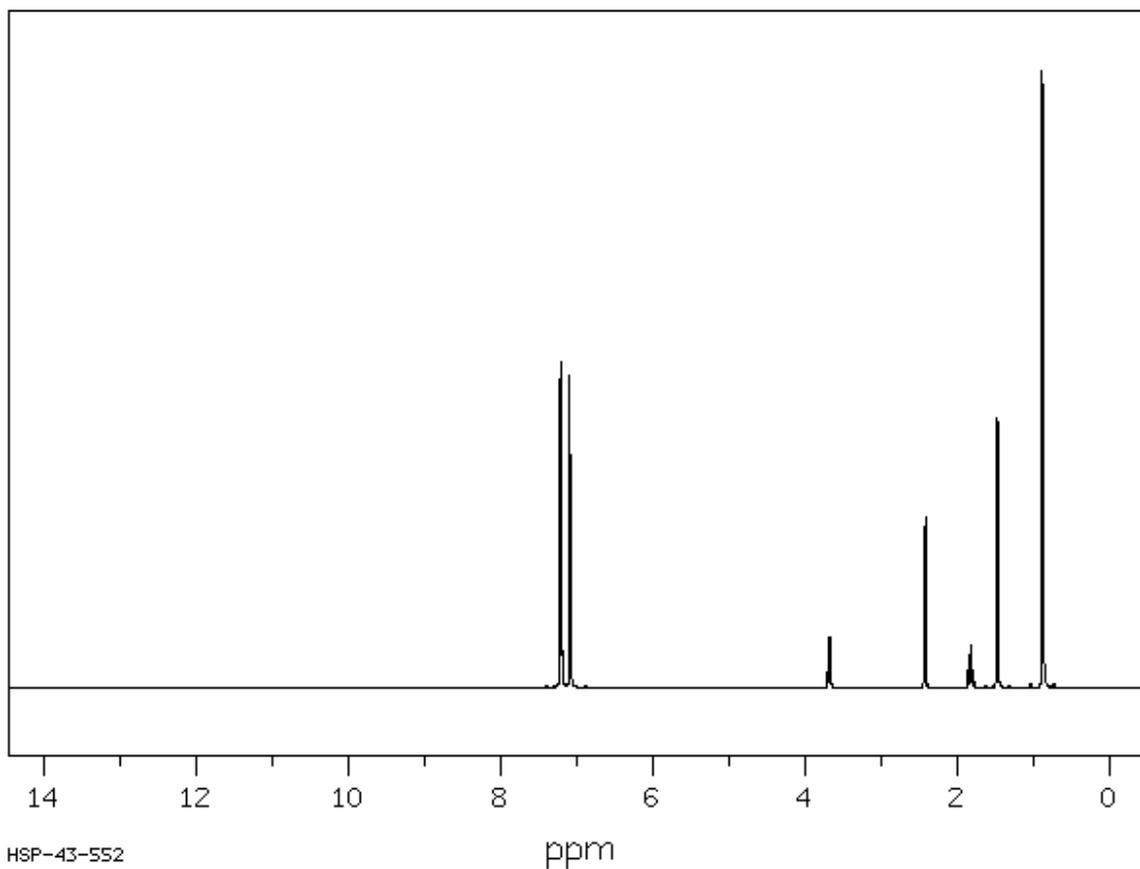
HIT-NO=411	SCORE= ()	SDBS-NO=532	IR-NIDA-63748 : NUJOL MULL
O-ACETOXYBENZOIC ACID			
C ₉ H ₈ O ₄			



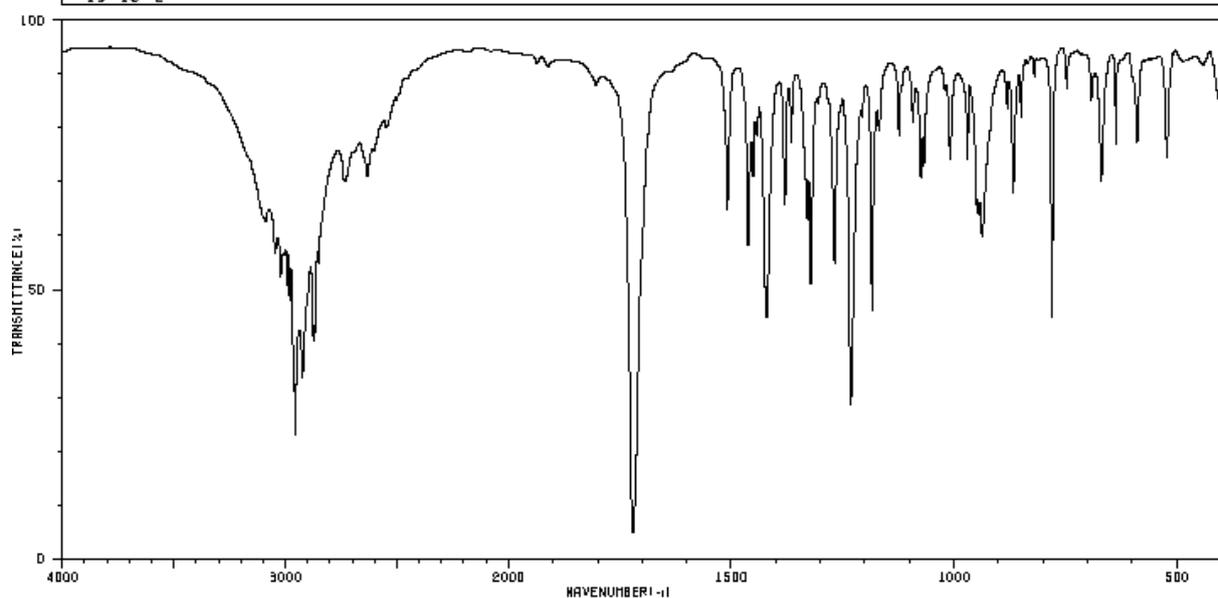
2956	13	2647	70	1420	63	1096	60	841	68
2924	4	1753	26	1375	47	1040	72	805	58
2854	13	1692	20	1307	21	1025	79	790	70
2701	66	1606	26	1257	84	1014	60	766	66
2682	68	1575	79	1221	35	971	70	705	53
2665	68	1483	68	1166	16	918	36	667	66
2688	68	1458	22	1136	62	886	81	600	74



Ibuprofen



HIT-NO=5517	SCORE= ()	SDBS-NO=10570	IR-NIDA-57772 : KBR DISC
2-(P-ISOBUTYLPHENYL)PROPIONIC ACID			
C ₁₃ H ₁₆ O ₂			



3100	60	2941	38	1609	62	1322	48	970	70
3089	60	2924	32	1463	55	1269	52	945	62
3045	55	2859	38	1451	88	1232	27	937	57
3020	60	2851	52	1442	74	1184	44	868	66
2992	49	2732	68	1421	43	1075	68	780	43
2980	46	2633	68	1381	82	1068	70	670	68
2956	22	1721	4	1329	60	1008	70	523	72

