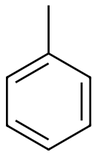
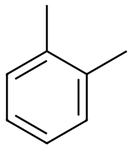
Characteristic Mono- and Di-substituted Aromatic Ring Absorptions

Mono- and disubstituted benzene rings exhibit several distinctive absorptions in the 700 to 800 cm^{-1} range. The next page lists those distinctive absorptions. Following are actual spectra of toluene (monosubstituted) and ortho-, meta-, and para-xylene and ortho-, meta-, and para-methyl nitrobenzoate. Note the characteristic absorptions are easily discerned in toluene and the xylene. In the methyl nitrobenzoates, not so much!

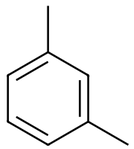
Characteristic Mono- and Di-substituted Aromatic Ring Absorptions



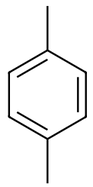
mono 700cm^{-1} 750cm^{-1}



ortho 750cm^{-1}

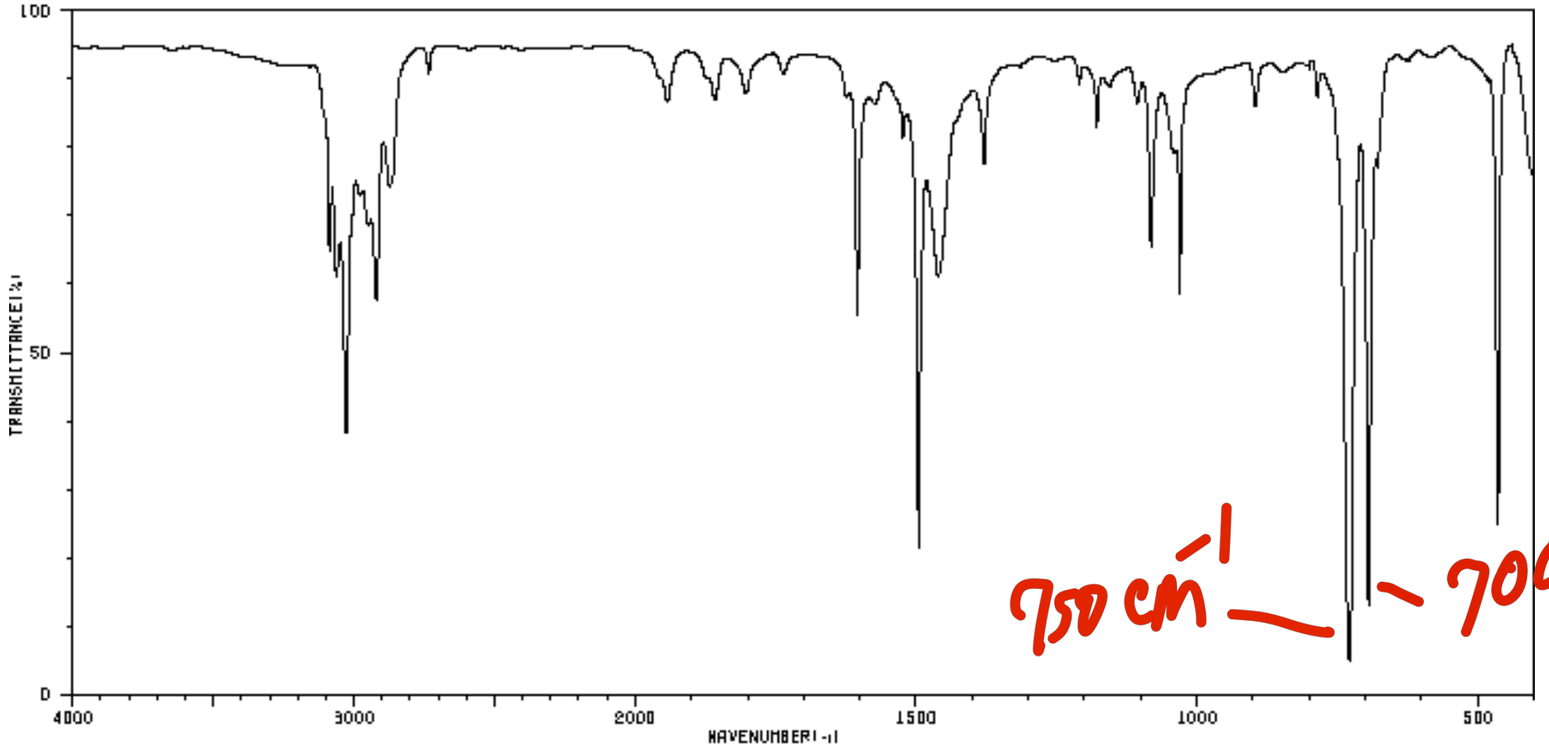


meta 700cm^{-1} 775cm^{-1}



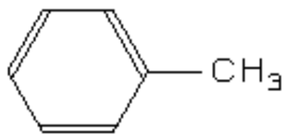
para 800cm^{-1}

HIT-NO=857	SCORE= ( )	SDBS-NO=97	IR-NIDA-63542 : LIQUID FILM
TOLUENE			
C_7H_8			

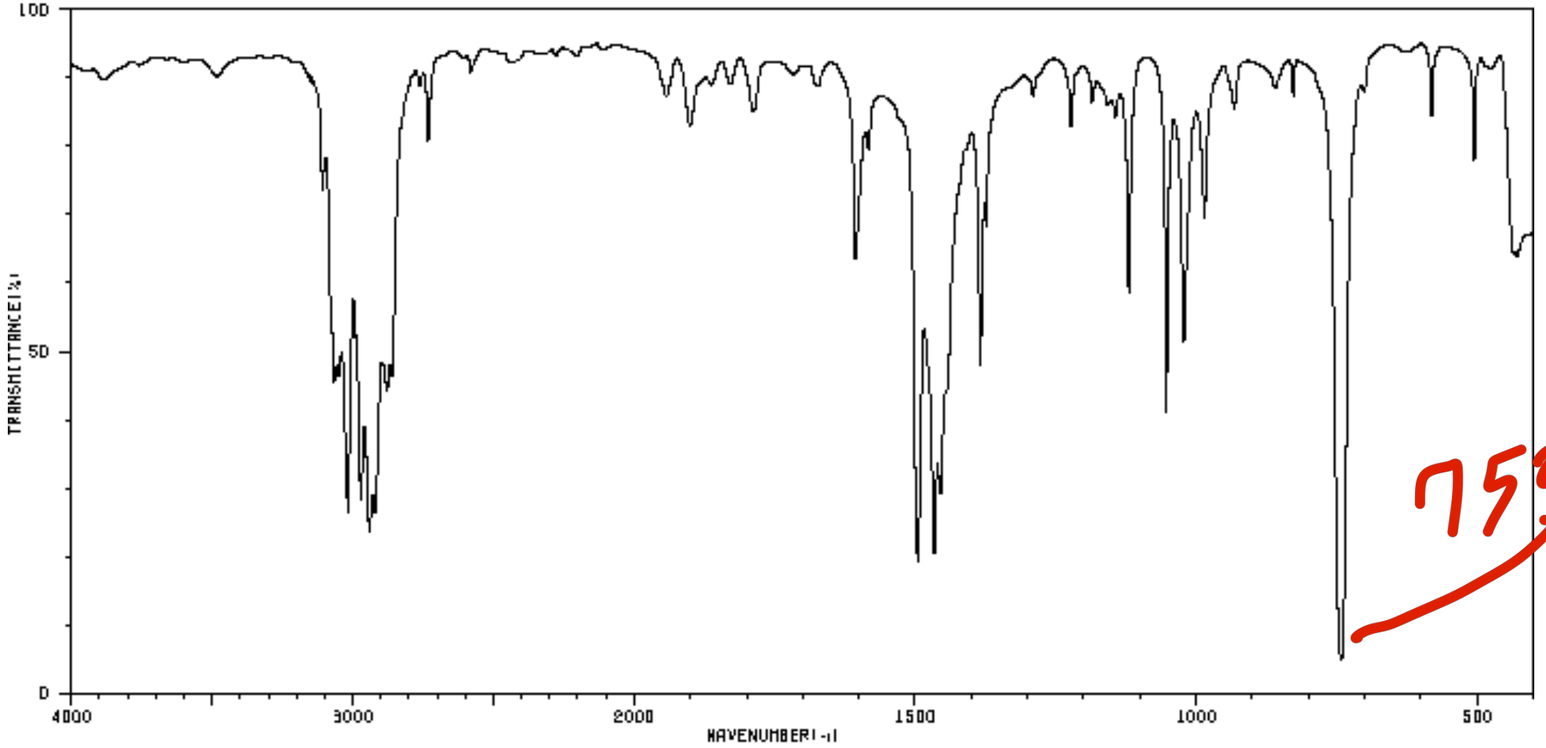


750 cm⁻¹ — 700 cm⁻¹

3087	62	1868	84	1210	86	895	81
3062	58	1803	84	1179	79	786	84
3028	37	1605	55	1156	86	729	4
2948	66	1524	79	1107	84	696	12
2920	55	1496	20	1082	62	678	74
2873	70	1461	58	1042	77	465	29
1942	84	1379	74	1030	67		

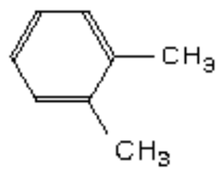


HIT-NO=1272	SCORE= ( )	SDBS-NO=1028	IR-NIDA-21942 : LIQUID FILM
O-XYLENE			
C_8H_{10}			



750 cm⁻¹

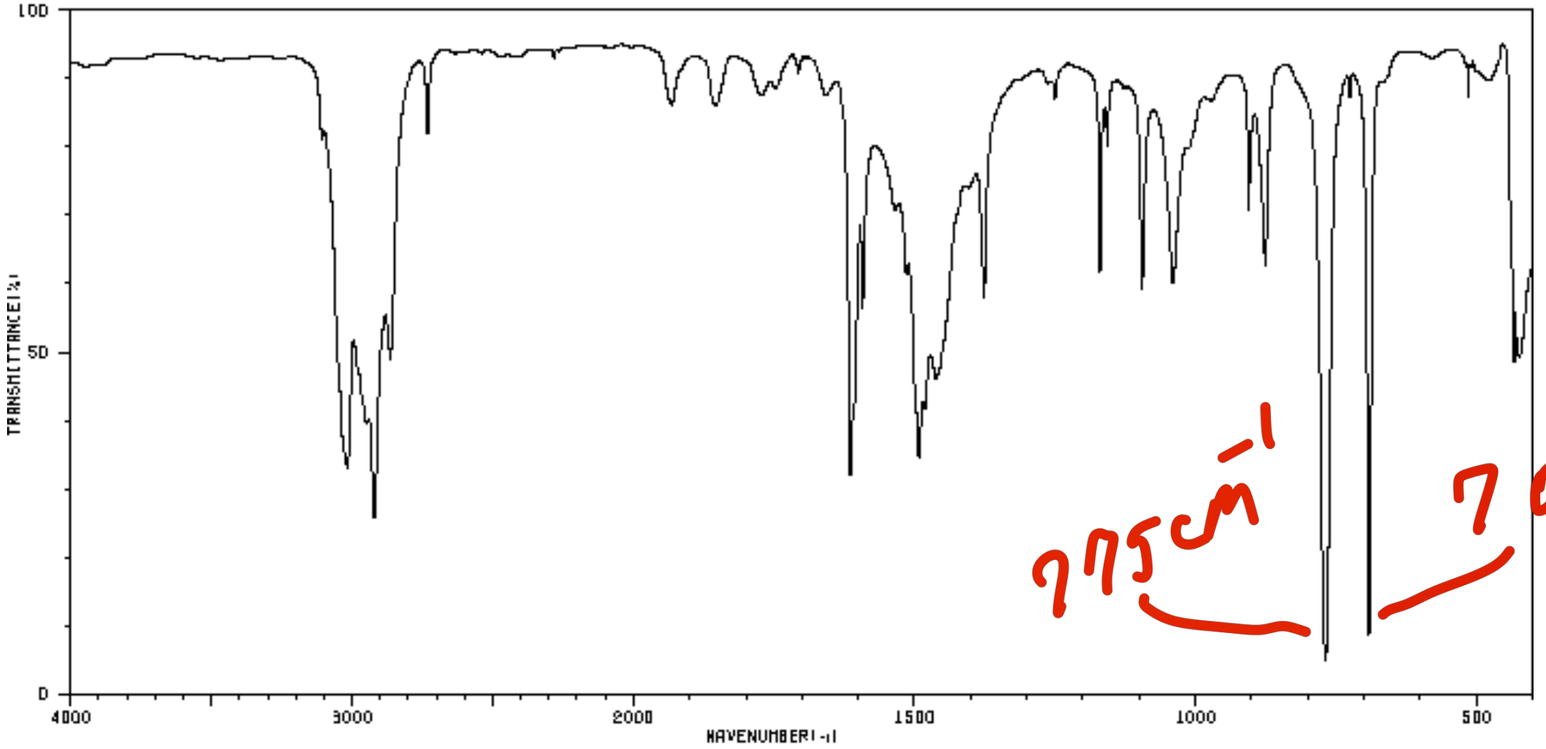
3108	70	2878	42	1583	77	1223	79	986	66
3066	43	2860	44	1495	18	1186	84	932	81
3050	44	2732	77	1467	20	1157	81	742	4
3018	25	1942	84	1456	27	1146	81	682	81
2971	26	1901	79	1384	46	1120	57	506	74
2940	22	1787	81	1374	86	1053	39	436	62
2921	25	1606	60	1291	84	1022	49	431	62



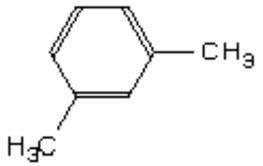
HIT-NO=1275	SCORE= ( )	SDBS-NO=1032	IR-NIDA-63601 : LIQUID FILM

M-XYLENE

C_8H_{10}



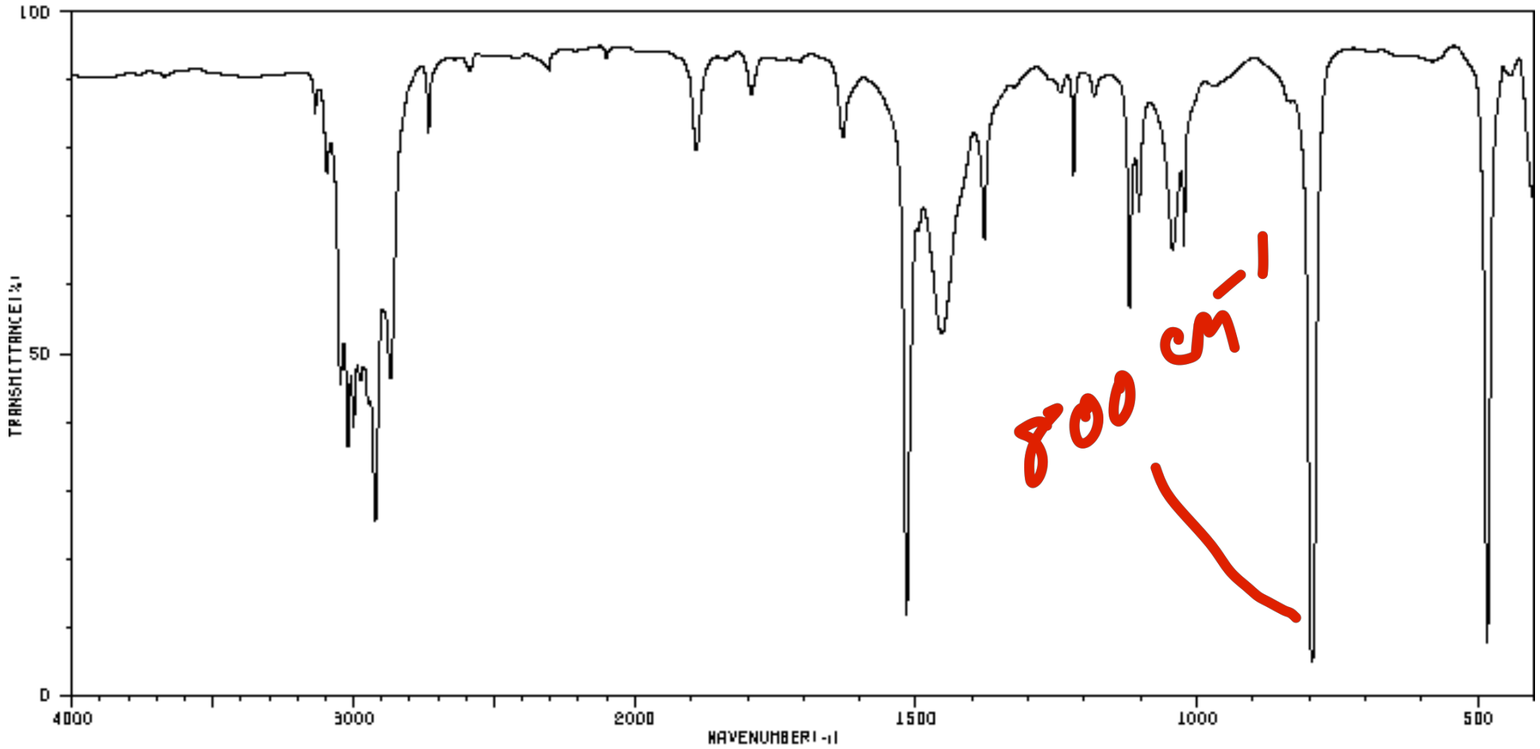
3106	79	1864	84	1492	33	1170	68	726	84
3016	32	1772	84	1482	39	1157	77	691	8
2948	37	1764	84	1462	44	1095	57	515	64
2921	24	1668	84	1376	65	1040	67	483	86
2864	47	1614	31	1263	86	905	68	478	86
2732	79	1592	59	1256	86	876	60	434	46
1932	84	1616	68	1260	84	769	4		



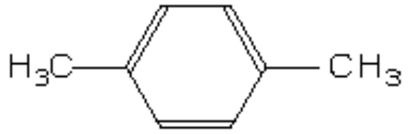
HIT-NO=1238	SCORE= ( )	SDBS-NO=899	IR-NIDA-63598 : LIQUID FILM

P-XYLENE

C_8H_{10}



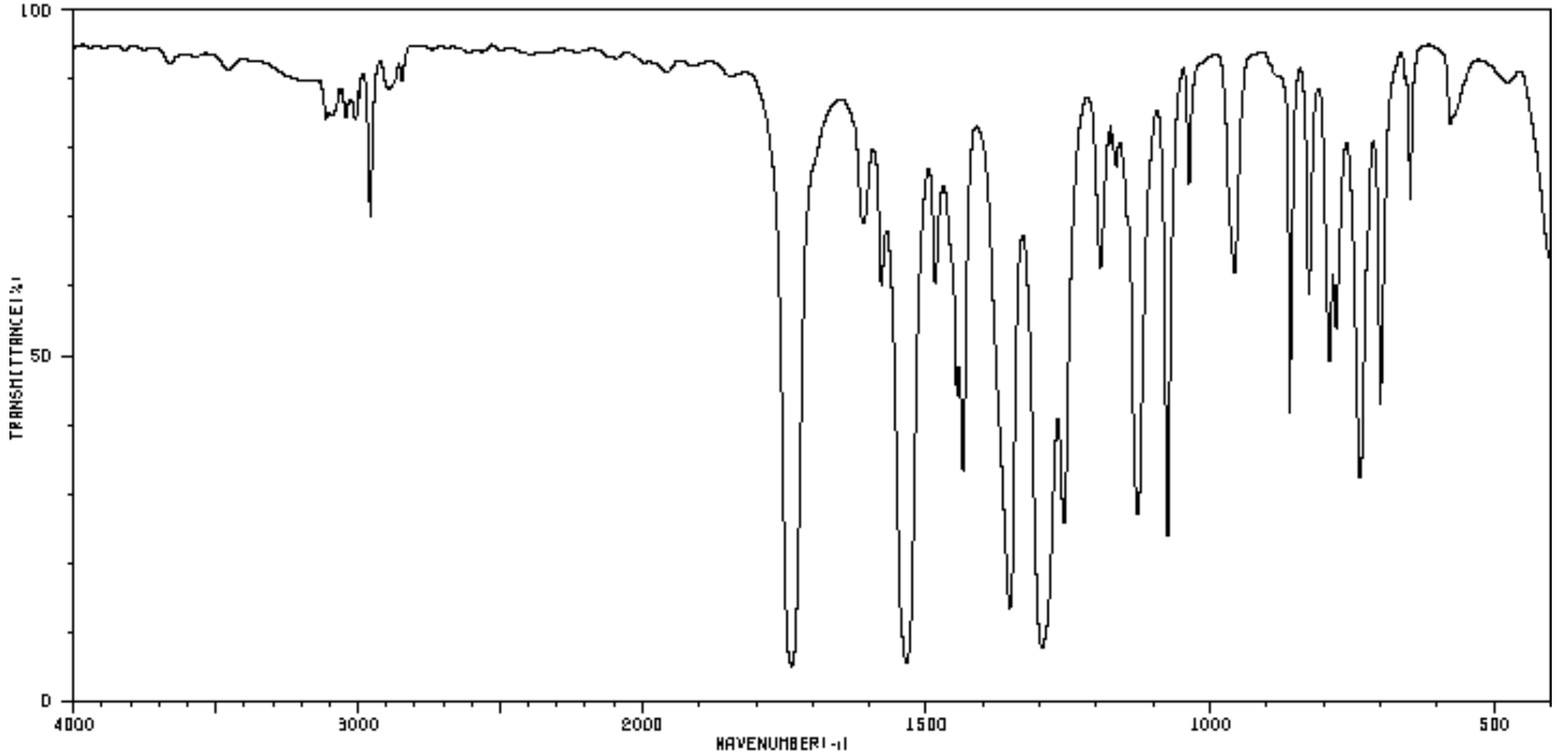
3136	81	2923	24	1464	60	1043	62
3095	74	2868	44	1378	64	1023	64
3047	43	2733	79	1243	84	795	4
3020	35	1890	77	1220	72	484	7
3000	37	1793	84	1183	84		
2976	44	1630	79	1120	55		
2945	41	1516	11	1103	68		



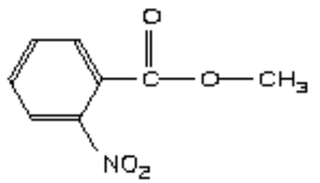
HIT-NO=3231	SCORE= ( )	SDBS-NO=6110	IR-NIDA-67155 : LIQUID FILM

METHYL O-NITROBENZOATE

$C_8H_7NO_4$



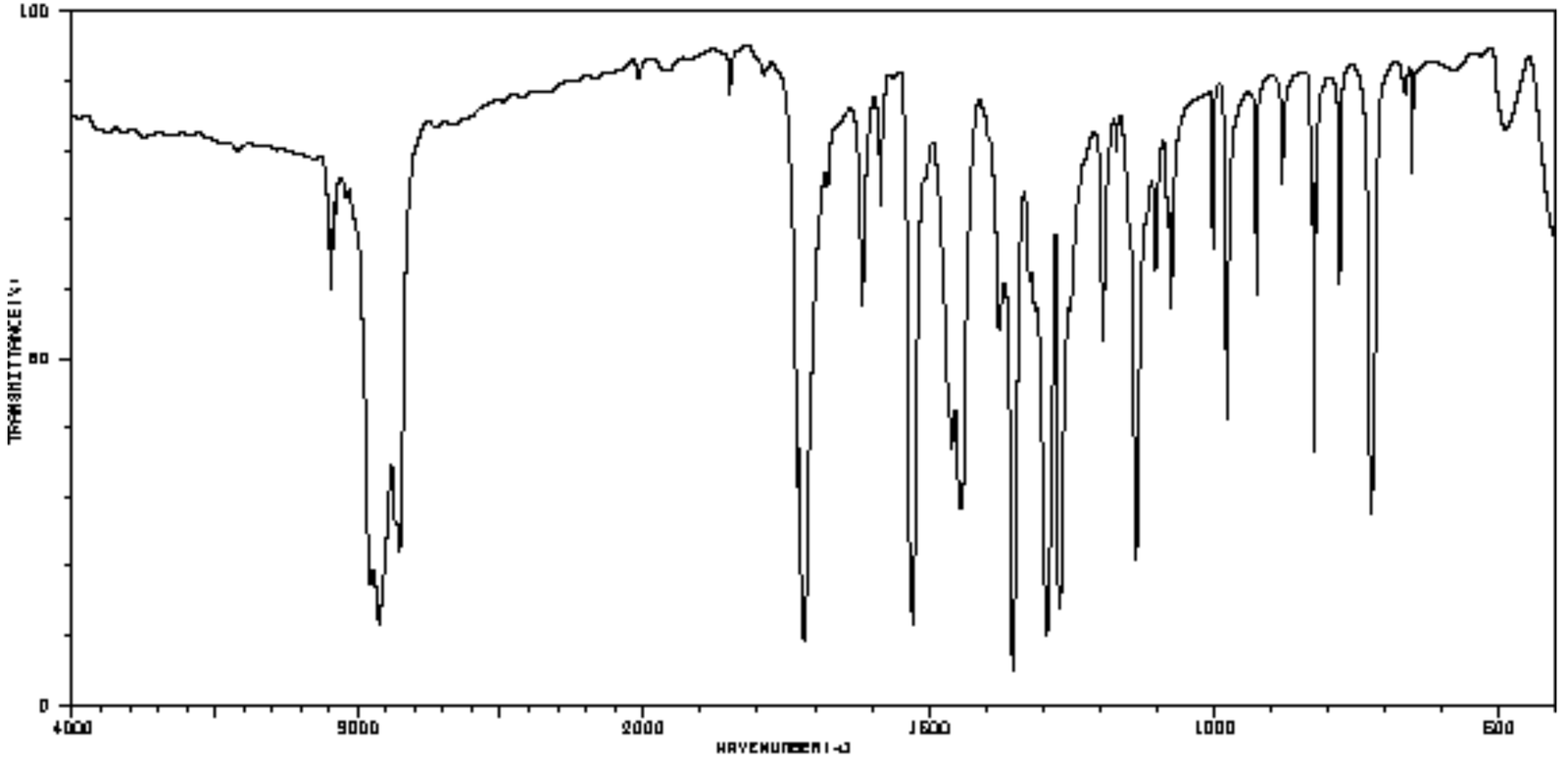
3111	81	2845	86	1436	32	1128	26	778	62
3098	81	1737	4	1353	12	1075	23	736	31
3068	81	1611	66	1296	7	1037	72	701	41
3042	81	1579	68	1267	24	967	68	648	70
3008	81	1535	5	1193	60	860	39	578	79
2956	86	1484	58	1177	77	826	57	572	61
2888	84	1446	42	1167	74	790	47	477	86



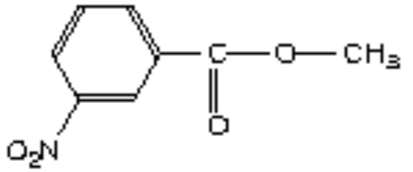
HIT-NO=1832	SCORE= ( )	SDBS-NO=3528	IR-NIDA-12590 : NUJOL MULL

METHYL M-NITROBENZOATE

$C_8H_7NO_4$



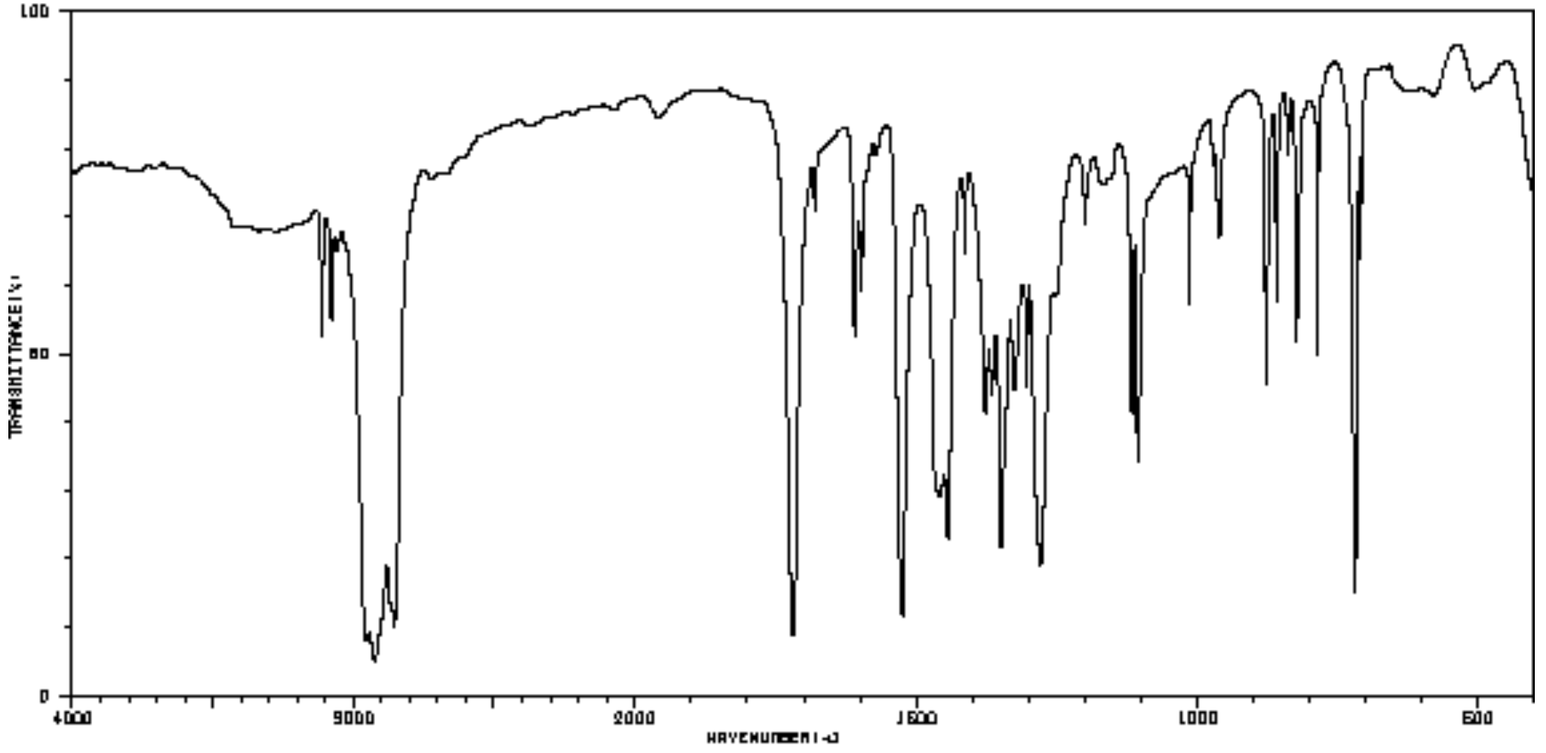
3092	68	1751	90	1480	36	1196	60	926	67
3082	86	1718	8	1444	26	1137	20	881	72
3042	70	1678	72	1377	62	1103	60	830	66
2966	17	1616	66	1362	4	1082	66	826	36
2924	11	1586	70	1293	9	1076	66	781	68
2868	26	1532	13	1272	13	1002	64	726	26
2864	21	1527	11	1269	66	978	39	663	74



HIT-NO=1346	SCORE= ( )	SDBS-NO=2583	IR-NIDA-11590 : NUJOL MULL

METHYL P-NITROBENZOATE

$C_8H_7NO_4$



3113	60	1718	8	1414	62	1279	18	960	64
3079	62	1680	88	1377	39	1199	66	878	43
3060	62	1609	60	1366	42	1163	72	869	66
2966	7	1598	67	1349	20	1166	72	823	49
2924	4	1624	11	1340	41	1117	39	786	47
2868	12	1468	27	1326	43	1106	33	719	14
2864	10	1449	21	1303	43	1014	66	709	62