

Problem Set III – IR Spectroscopy

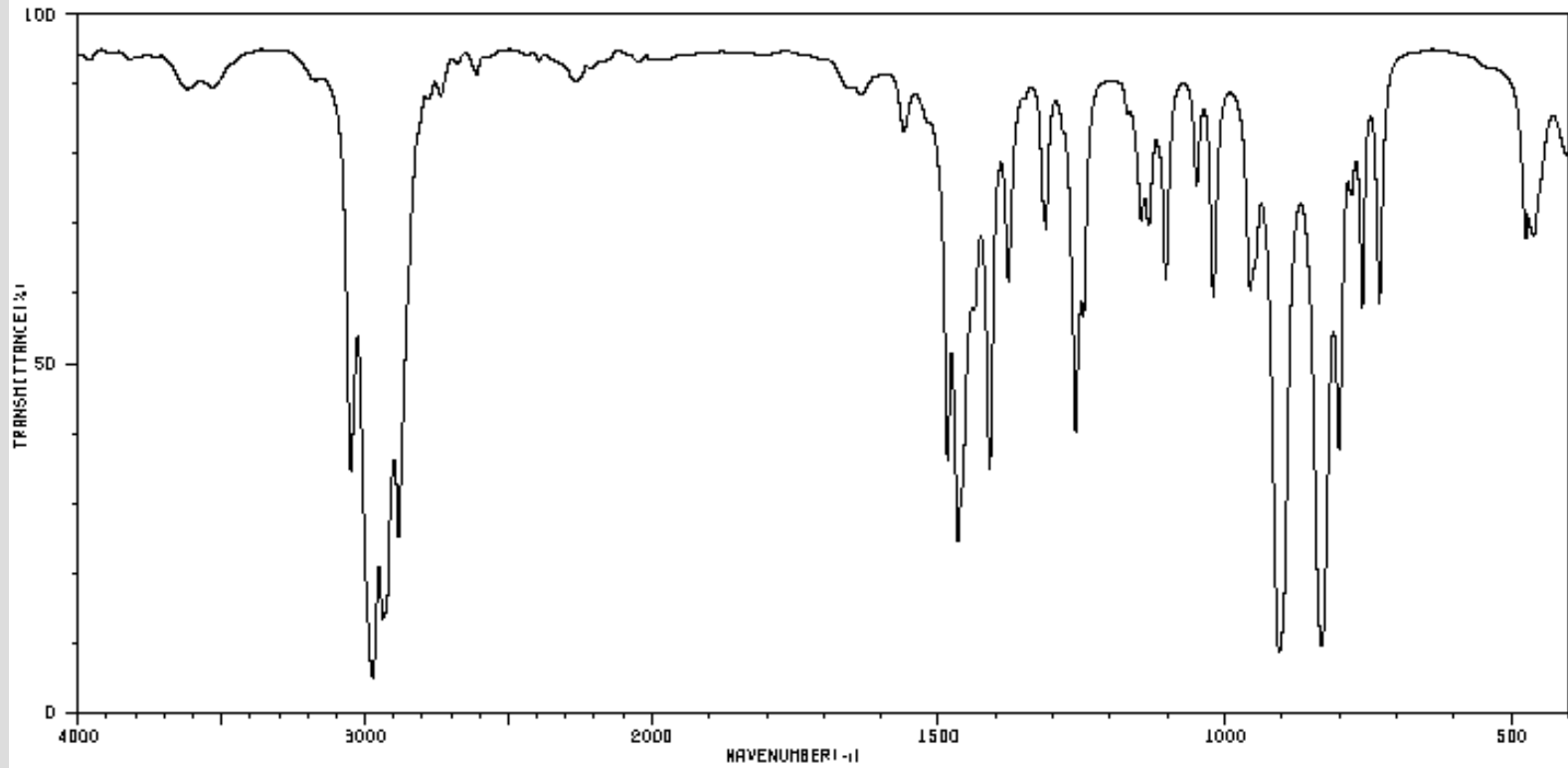


CHMBD 449 – Organic Spectral Analysis

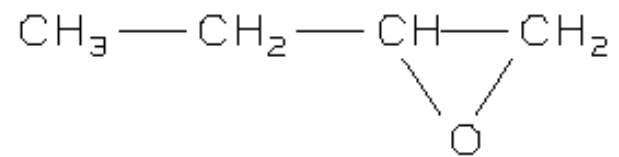
HIT-NO=1633 SCORE= () SDBS-NO=1896 IR-NIDA-04688 : LIQUID FILM

2-ETHYLOXIRANE

C₄H₈O



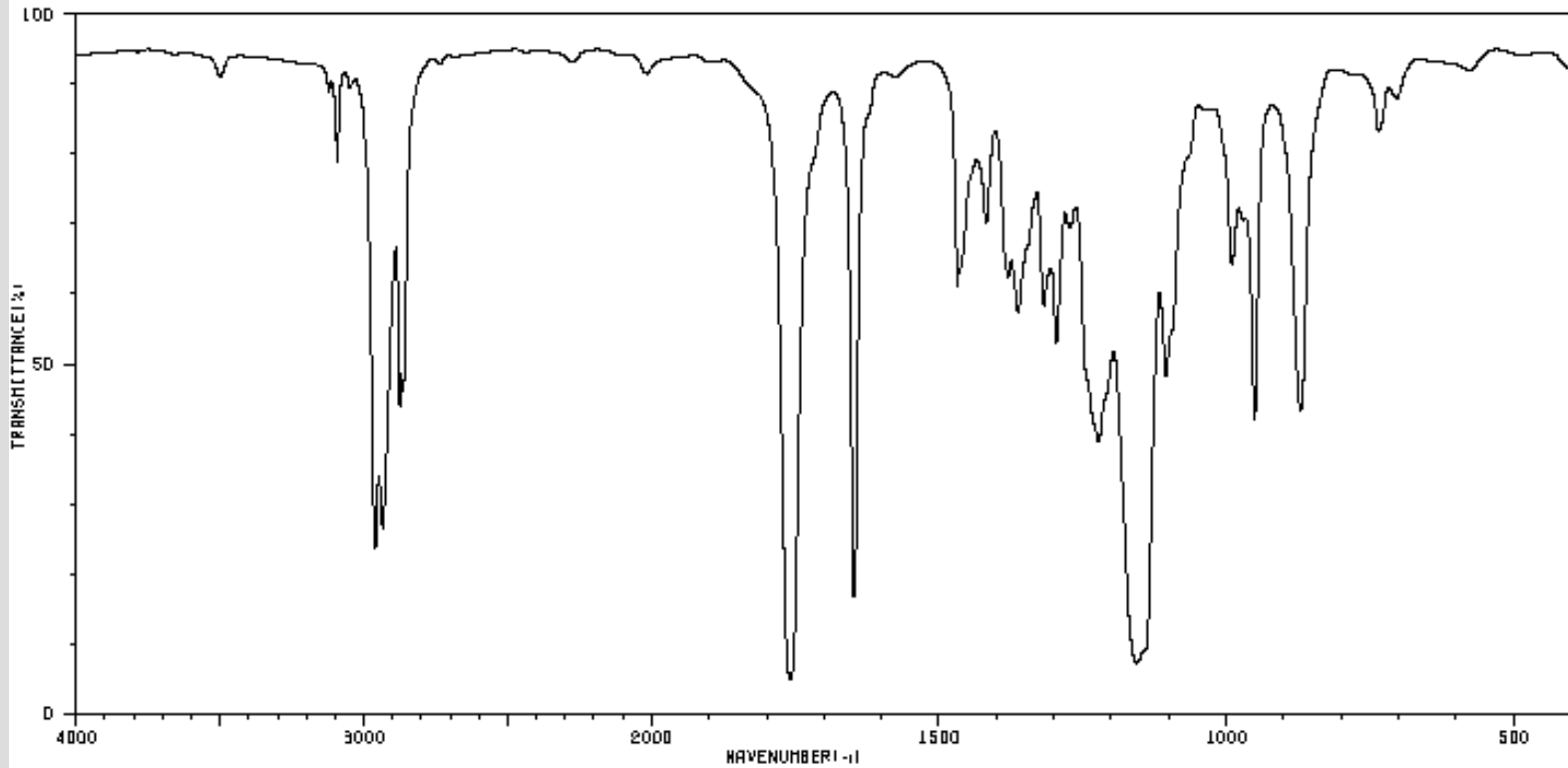
3618	86	1661	79	1247	66	949	60	476	66
3049	33	1484	35	1146	68	905	8	462	66
2973	4	1468	23	1133	86	831	9		
2939	12	1411	39	1103	80	801	36		
2884	24	1378	58	1049	72	780	70		
2736	84	1313	66	1020	57	760	55		
1643	86	1261	38	956	68	731	67		



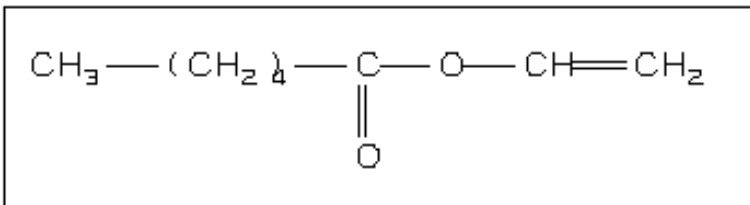
HIT-NO=2285 SCORE= () SDBS-NO=3465 IR-NIDA-01042 : LIQUID FILM

VINYL HEXANOATE

$C_8H_{14}O_2$



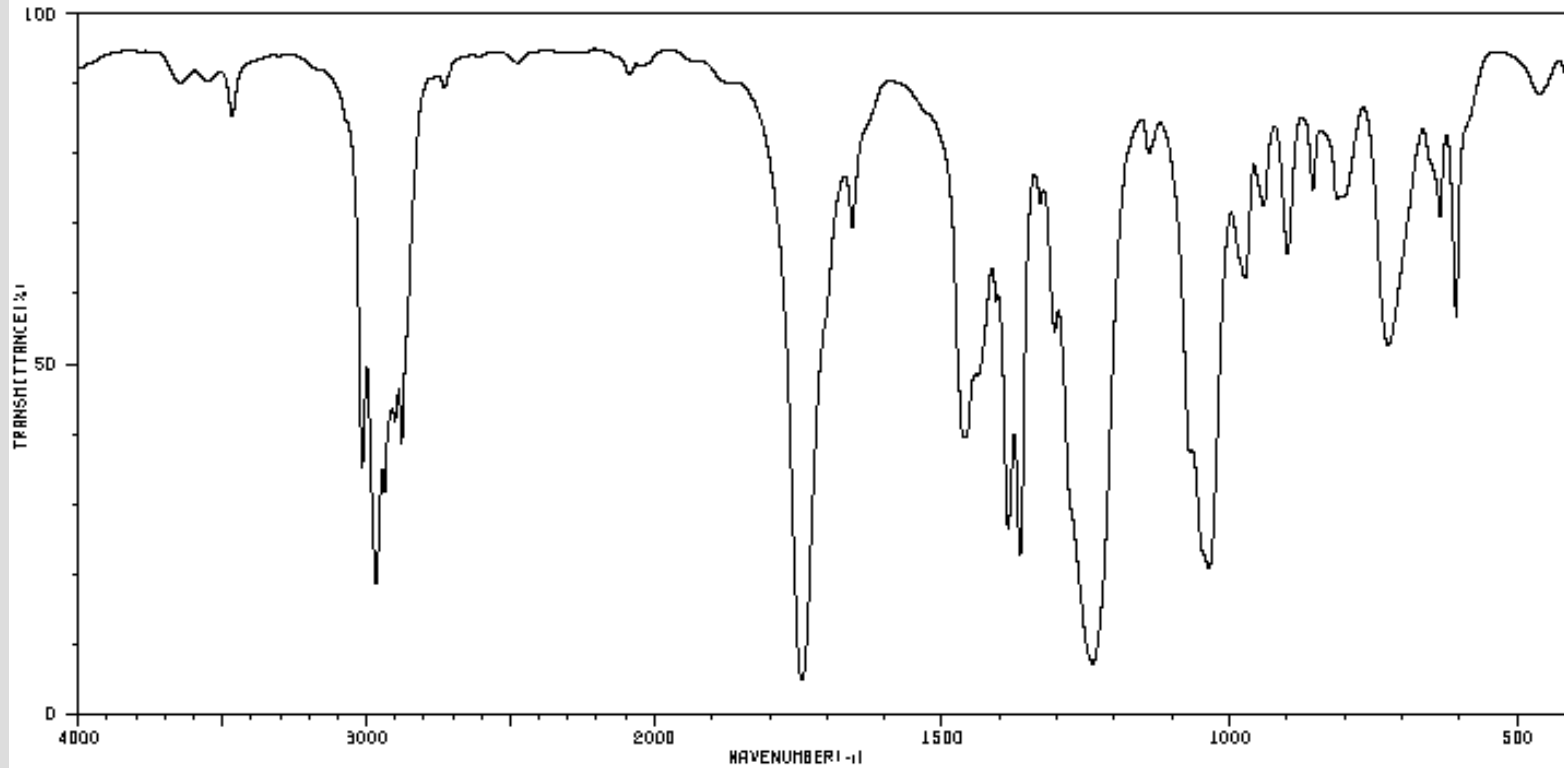
3122	84	1759	4	1296	60	961	41
3092	77	1649	16	1272	66	871	42
3048	86	1468	58	1223	37	735	79
2960	22	1418	68	1166	7	704	84
2935	25	1380	60	1145	8		
2875	42	1363	55	1105	46		
2864	44	1318	55	990	62		



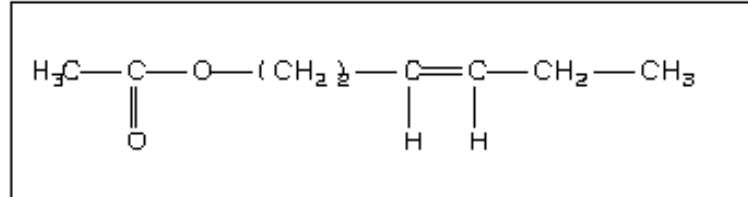
HIT-NO=4002 SCORE= () SDBS-NO=10143 IR-NIDA-05737 : LIQUID FILM

CIS-3-HEXENYL ACETATE

$C_8H_{14}O_2$



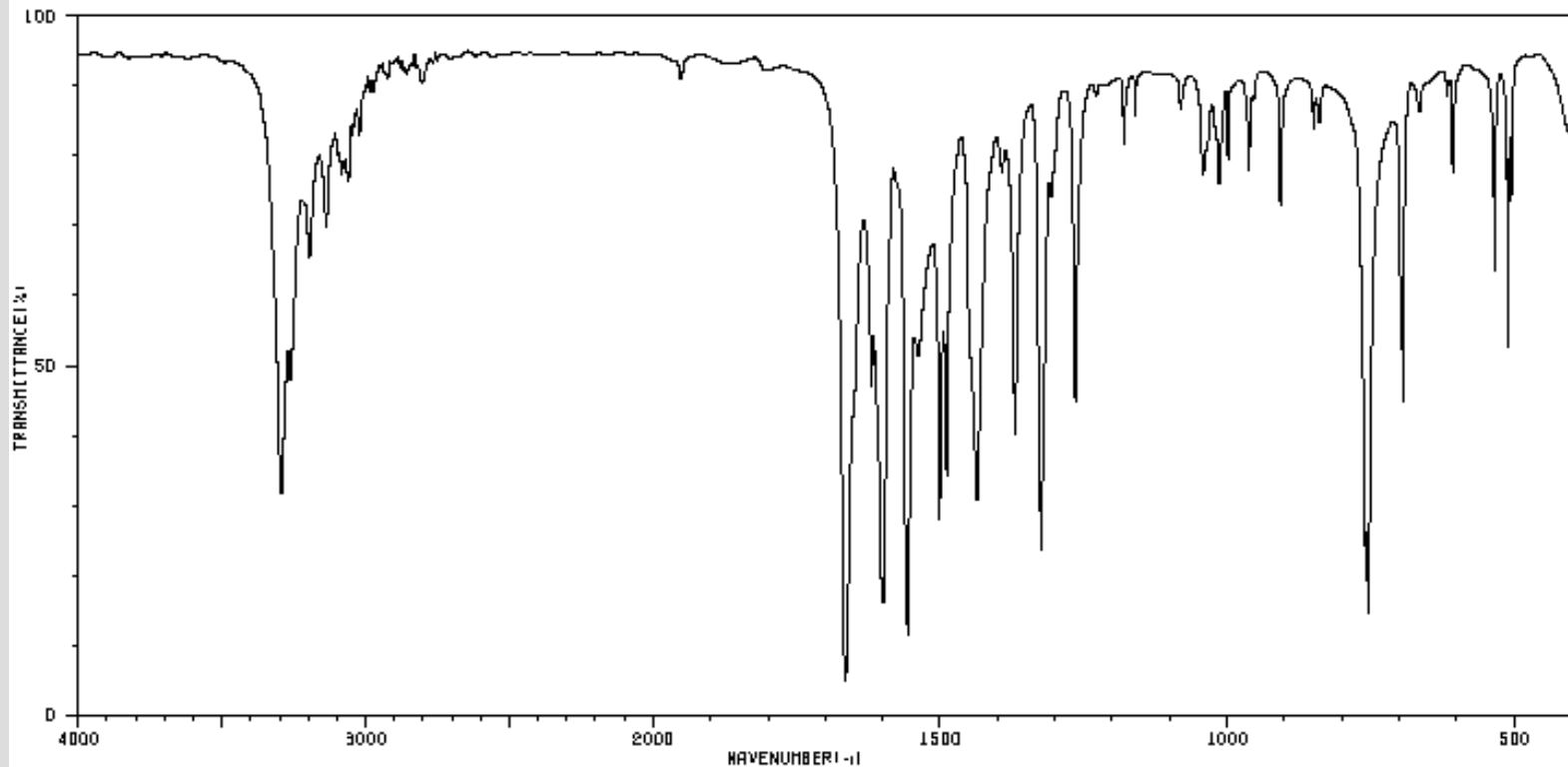
3467	81	1744	4	1238	7	866	72
3014	34	1656	66	1141	77	814	70
2966	17	1461	37	1046	21	805	70
2937	30	1386	26	1036	20	726	60
2900	39	1364	21	973	60	635	68
2877	37	1329	70	941	70	607	55
2728	86	1306	62	899	62	461	84



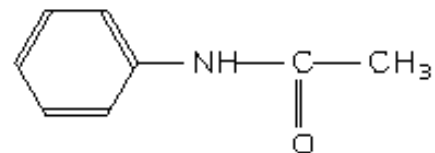
HIT-NO=1095 SCORE= () SDBS-NO=729 IR-NIDA-61373 : KBR DISC

ACETANILIDE

C₈H₉NO



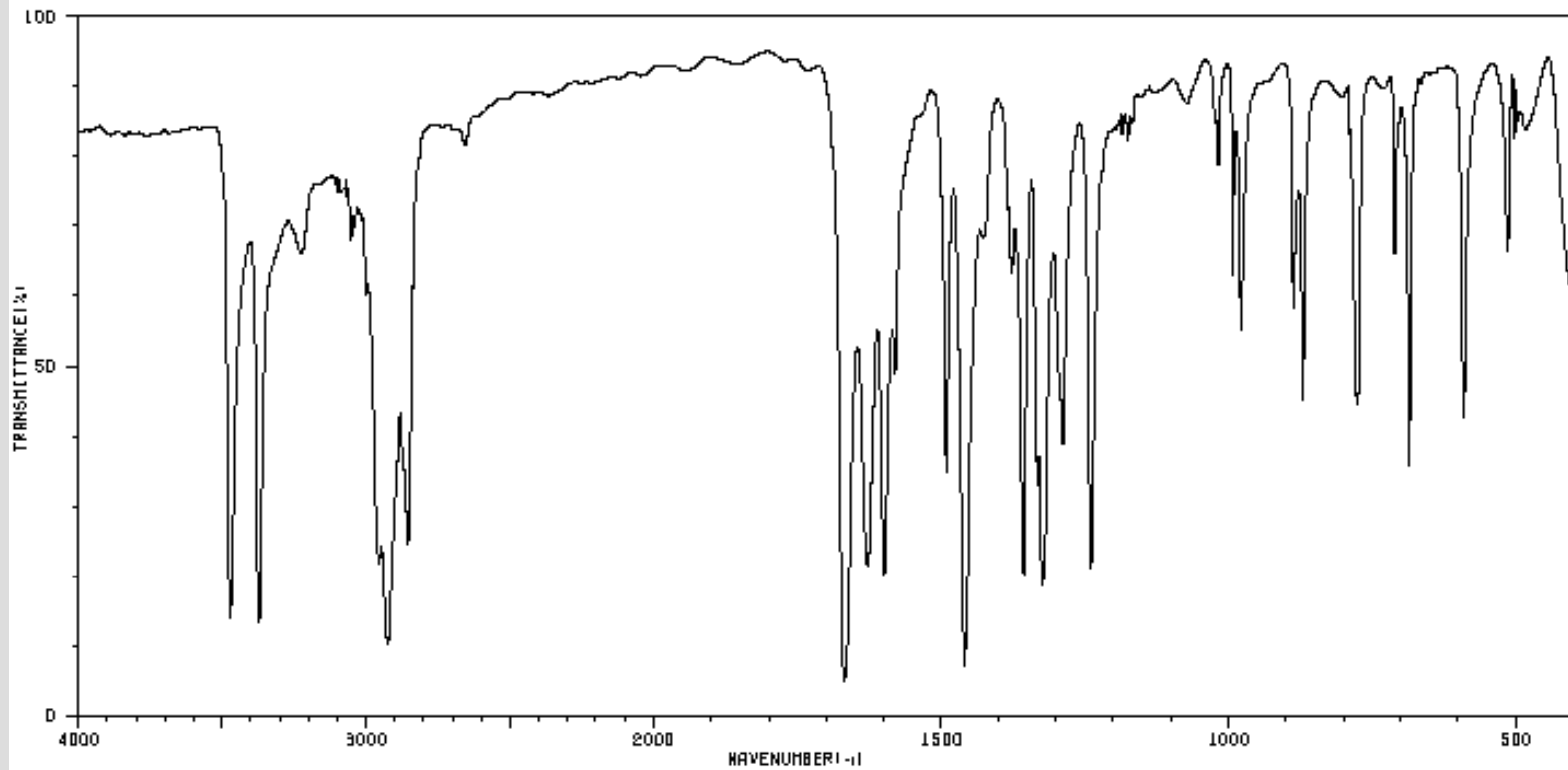
3294	30	3022	79	1489	33	1180	79	761	23
3261	46	1665	4	1436	29	1042	74	754	13
3196	82	1620	44	1393	74	1014	72	694	43
3137	66	1599	15	1369	38	999	77	607	74
3083	74	1557	10	1324	22	962	74	534	60
3059	74	1538	49	1307	72	908	70	511	50
3045	79	1501	26	1265	43	768	62	506	70



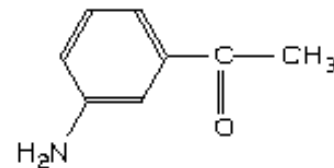
HIT-NO=610 SCORE= () SDBS-NO=1019 IR-NIDA-66954 : NUJOL MULL

3'-AMINOACETOPHENONE

C₈H₉NO



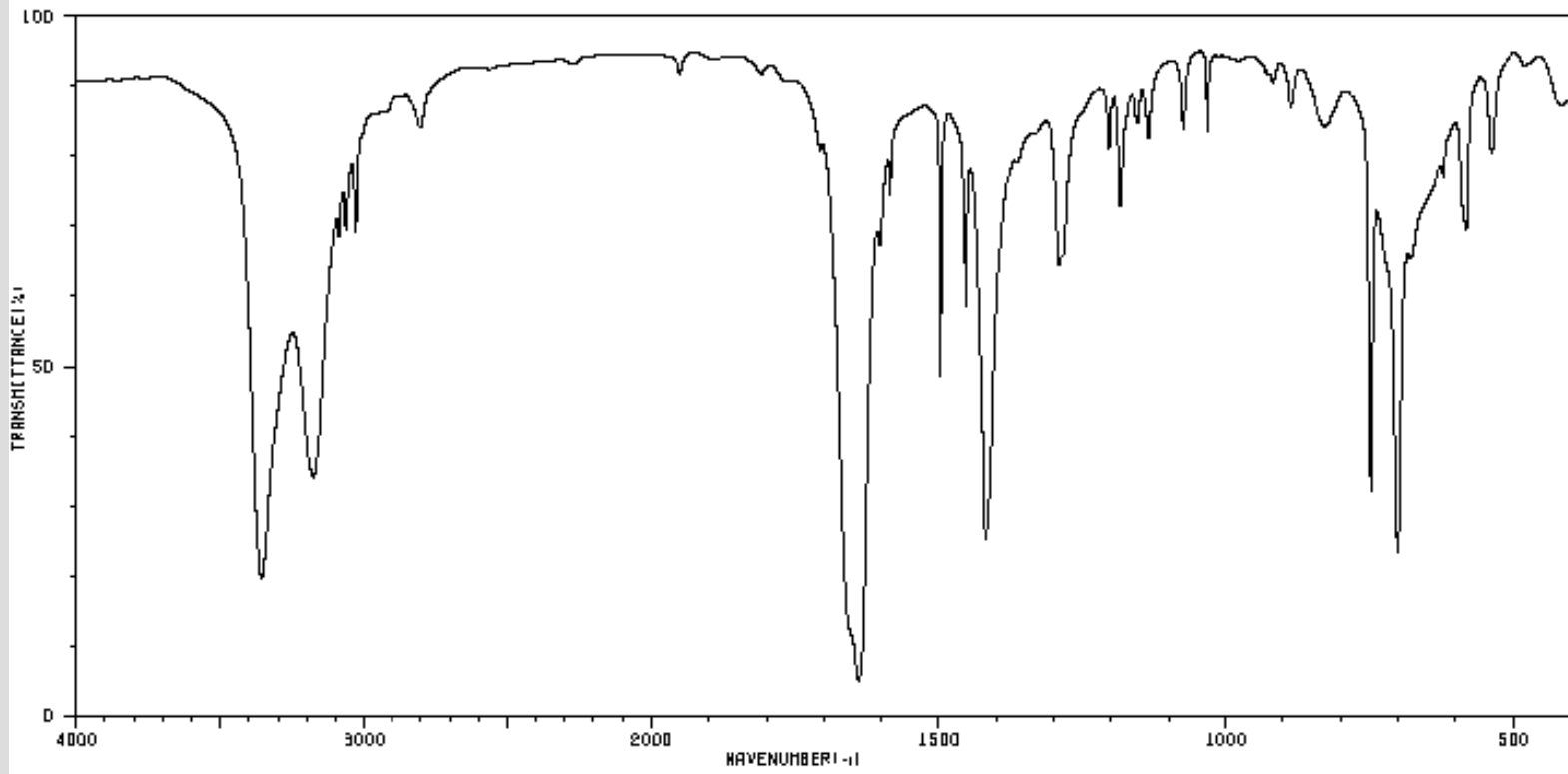
3470	13	3040	66	1600	19	1333	31	888	55
3371	12	2998	58	1580	47	1323	17	871	43
3224	84	2954	21	1492	33	1288	37	776	42
3101	72	2924	10	1460	7	1240	20	711	64
3088	72	2854	23	1426	66	1018	77	685	34
3069	72	1668	4	1377	80	993	60	591	41
3051	86	1628	20	1356	19	978	53	514	64



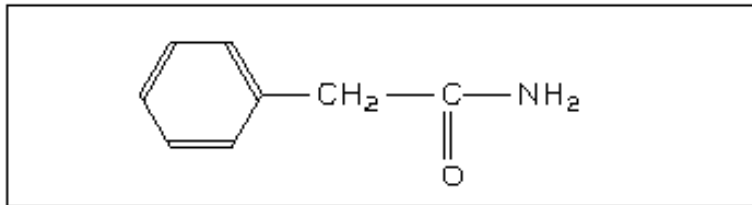
HIT-NO=2128 SCORE= () SDBS-NO=2682 IR-NIDA-03129 : KBR DISC

PHENYLACETAMIDE

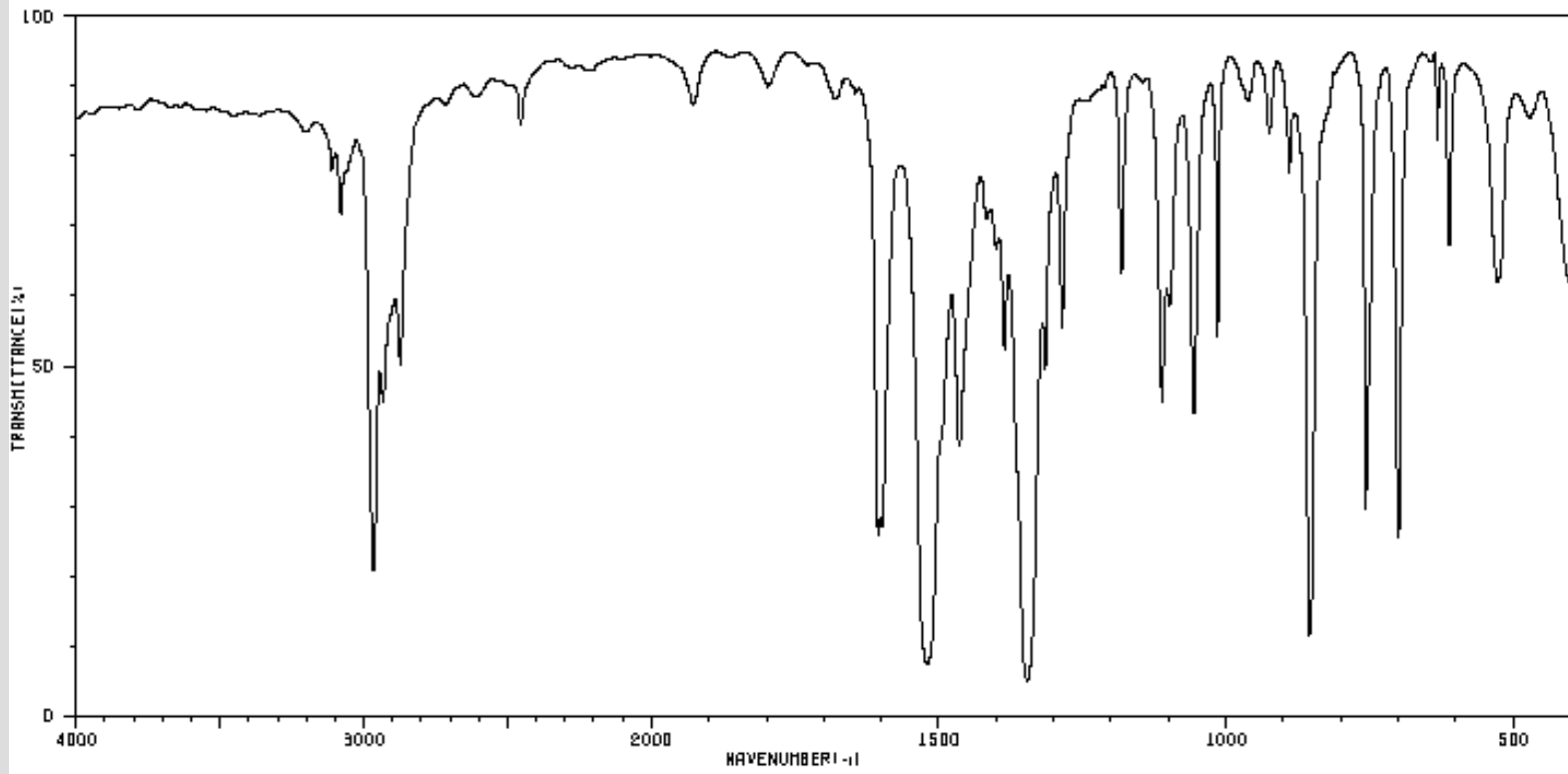
C₈H₉NO



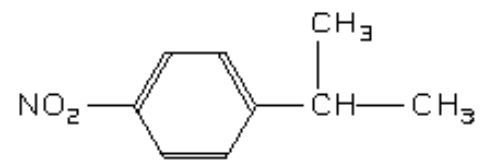
3357	18	1603	64	1205	77	828	81
3178	33	1585	72	1185	70	748	30
3088	86	1498	46	1155	81	701	22
3064	66	1464	57	1136	79	621	74
3030	66	1419	23	1074	81	589	70
2803	81	1292	62	1032	81	582	66
1639	4	1285	64	887	84	538	77



HIT-NO=5163 SCORE= () SDBS-NO=16730 IR-NIDA-75954 : LIQUID FILM
 4-NITROCUMENE
 $C_9H_{11}NO_2$



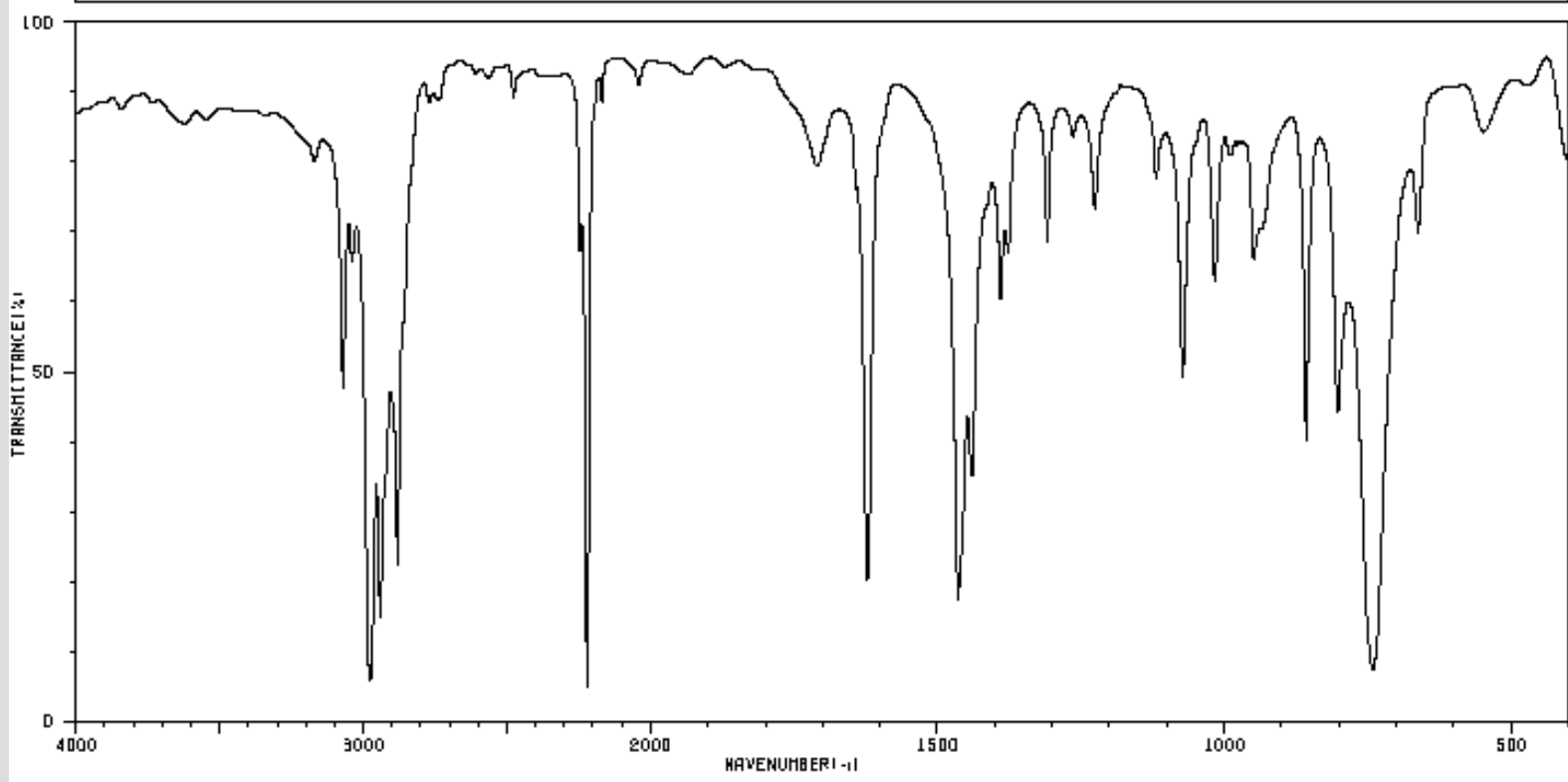
3202	79	2606	84	1417	68	1112	49	866	10
3113	74	2453	81	1400	64	1098	57	757	28
3080	86	1678	84	1386	50	1056	42	700	24
3063	74	1606	26	1347	4	1016	52	633	79
2967	20	1599	26	1315	47	960	84	612	64
2932	43	1519	7	1286	53	925	79	527	58
2873	49	1464	37	1182	60	890	74	472	81



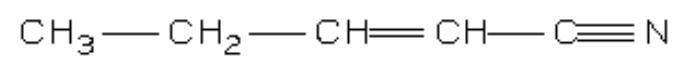
HIT-NO=2940 SCORE= () SDBS-NO=5381 IR-NIDA-09626 : LIQUID FILM

2-PENTENENITRILE

C₅H₇N



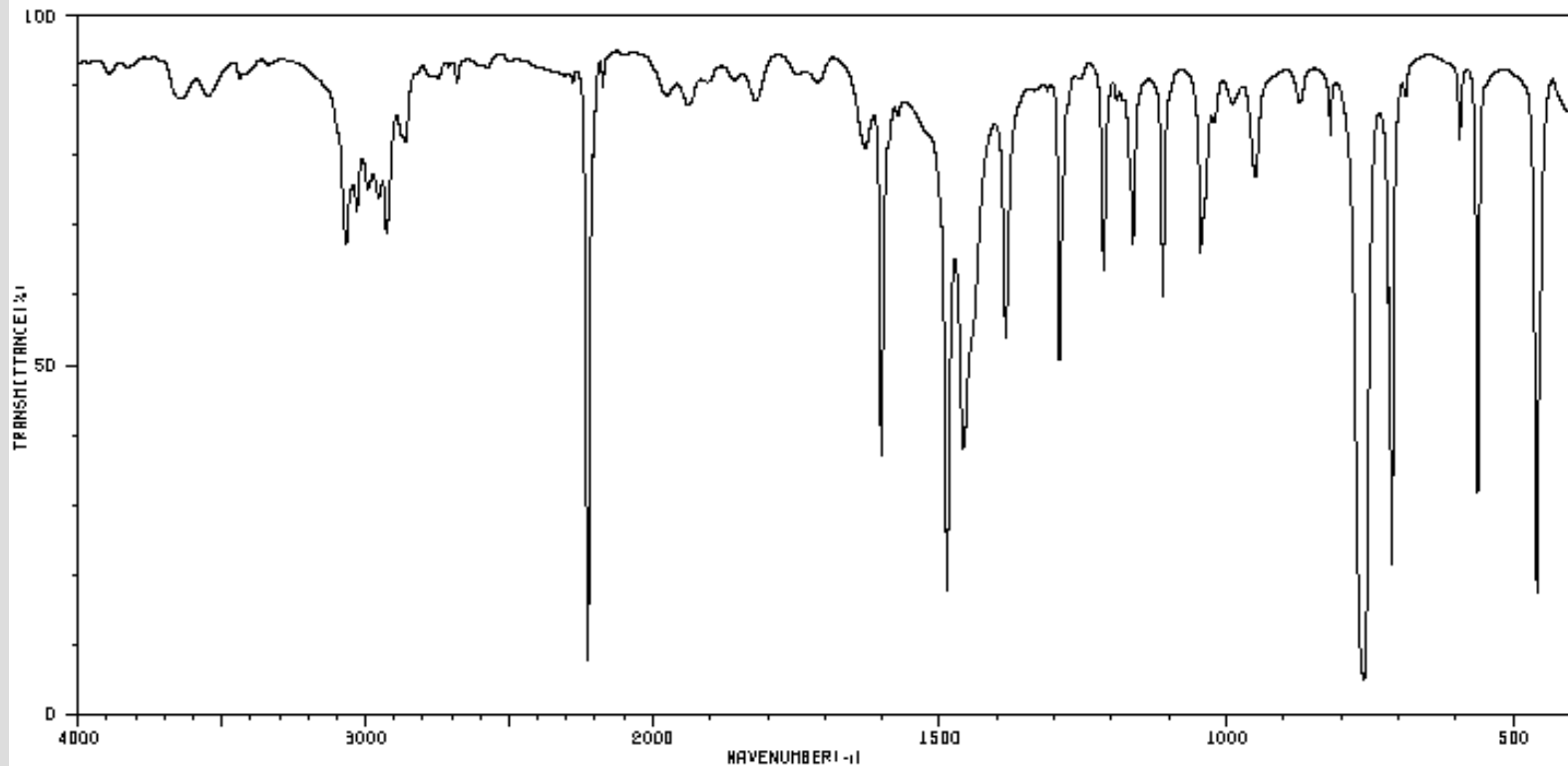
3842	84	2976	6	2170	84	1309	66	949	64
3633	81	2941	14	1709	77	1264	81	935	68
3620	81	2881	21	1622	19	1226	70	857	38
3547	81	2771	84	1464	16	1119	74	802	42
3169	77	2737	84	1441	33	1072	47	742	7
3070	46	2248	64	1390	58	1017	60	662	56
3039	62	2220	4	1377	64	990	77	549	81



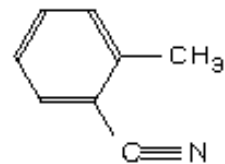
HIT-NO=1615 SCORE= () SDBS-NO=1878 IR-NIDA-04861 : LIQUID FILM

O-TOLUNITRILE

C₈H₇N

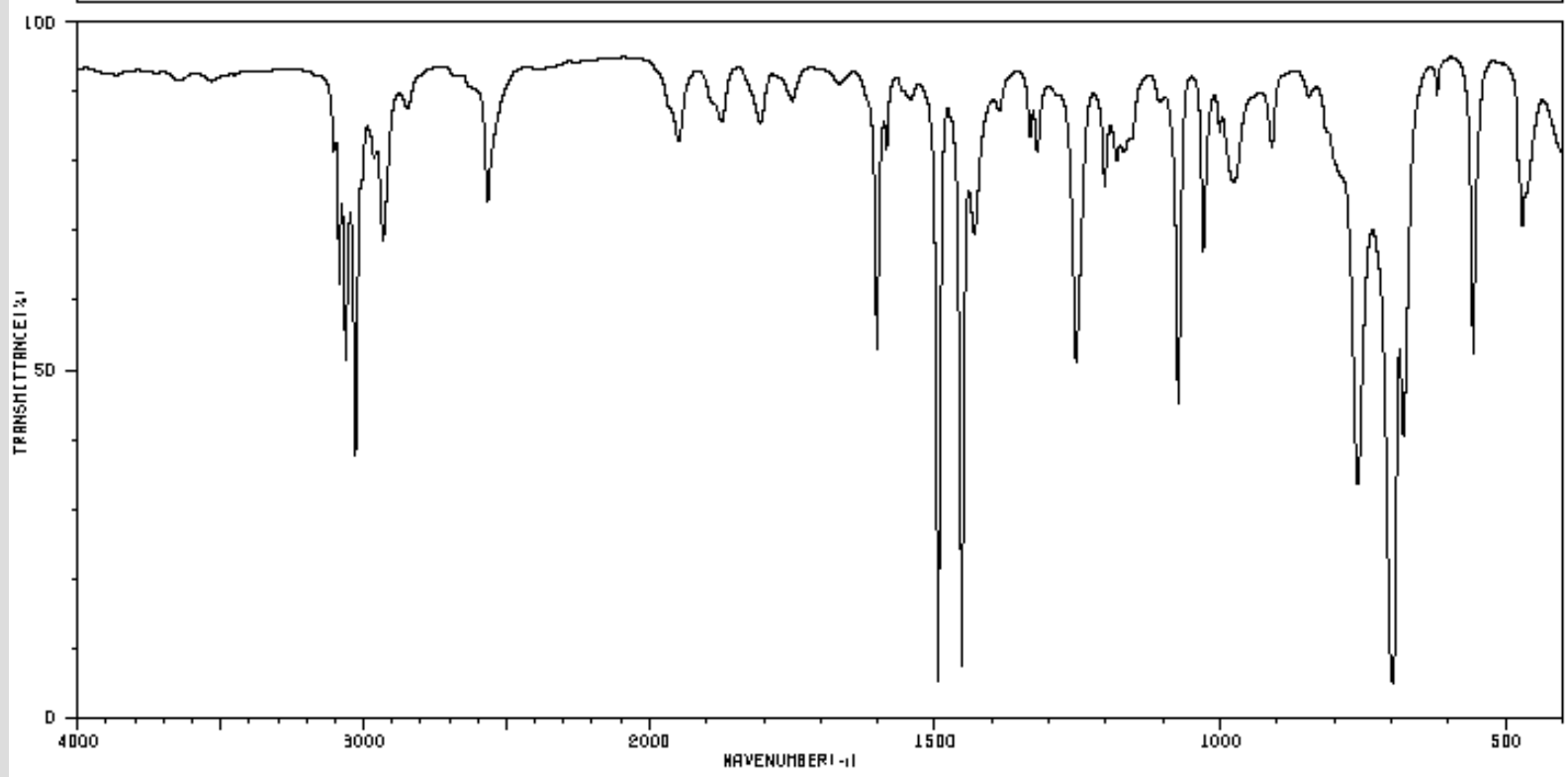


3644	84	2850	79	1602	35	1214	60	761	4
3547	84	2226	7	1591	79	1163	64	719	57
3067	84	2208	77	1574	81	1111	57	712	20
3030	70	1976	84	1487	17	1046	64	688	84
2991	72	1938	84	1460	36	990	84	594	79
2954	70	1820	84	1385	52	950	74	565	30
2926	66	1630	79	1291	49	819	78	459	16

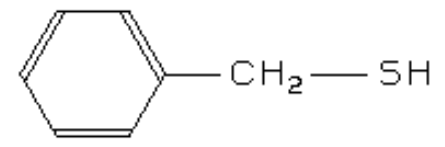


HIT-NO=4232 SCORE= () SDBS-NO=10642 IR-NIDA-03430 : LIQUID FILM
 ALPHA-TOLUENETHIOL

C₇H₈S



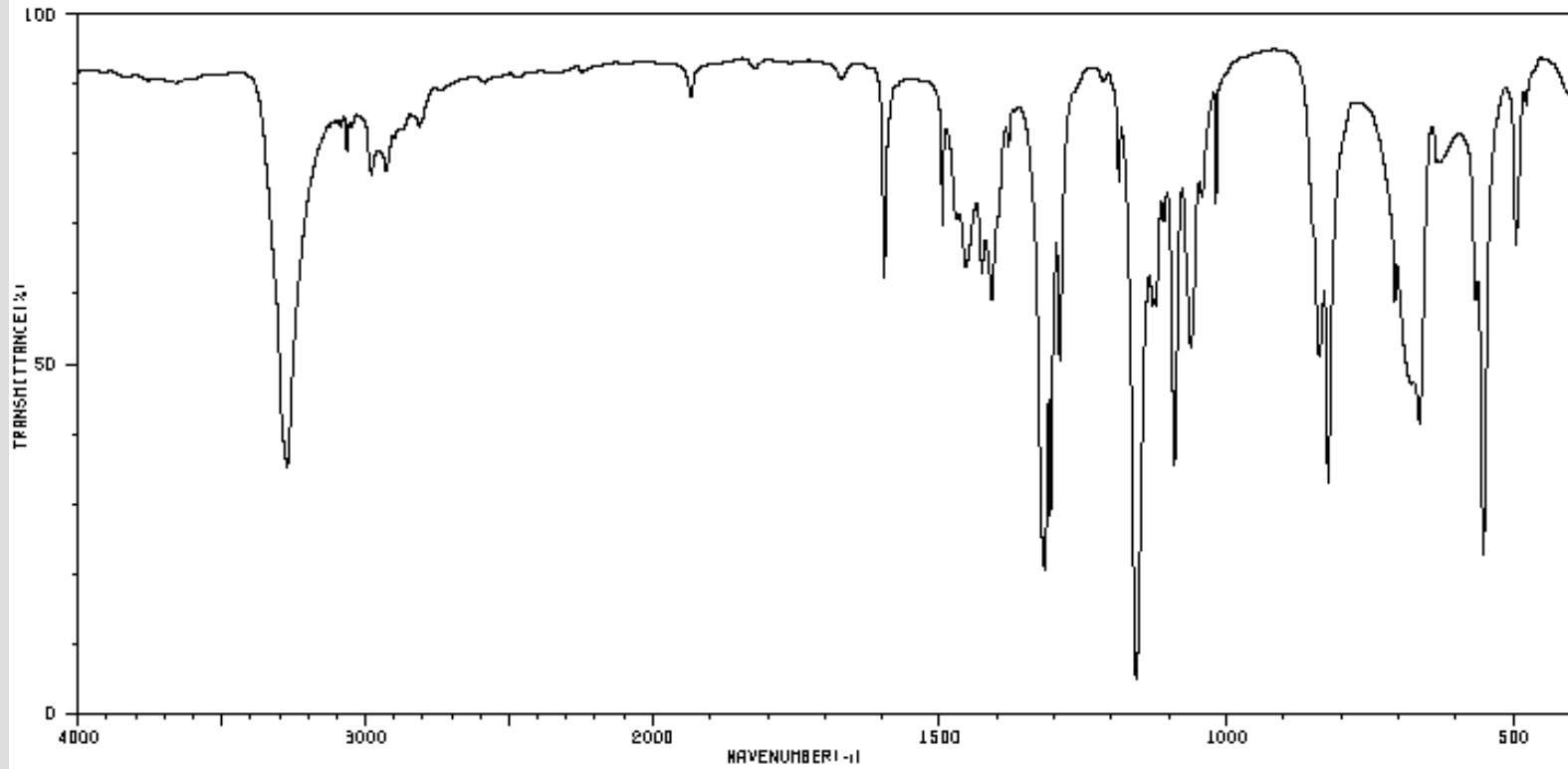
3103	79	1949	79	1496	4	1203	74	910	79
3085	60	1887	84	1453	7	1183	77	845	86
3063	49	1873	81	1431	86	1169	79	760	32
3029	36	1806	81	1387	84	1074	49	699	4
2931	66	1750	84	1334	81	1030	64	680	38
2845	84	1601	50	1321	79	1002	81	557	50
2666	72	1586	79	1253	49	976	74	472	68



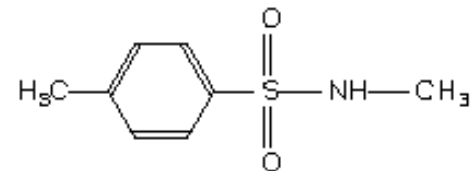
HIT-NO=7568 SCORE= () SDBS-NO=15557 IR-NIDA-23870 : KBR DISC

N-METHYL-P-TOLUENESULFONAMIDE

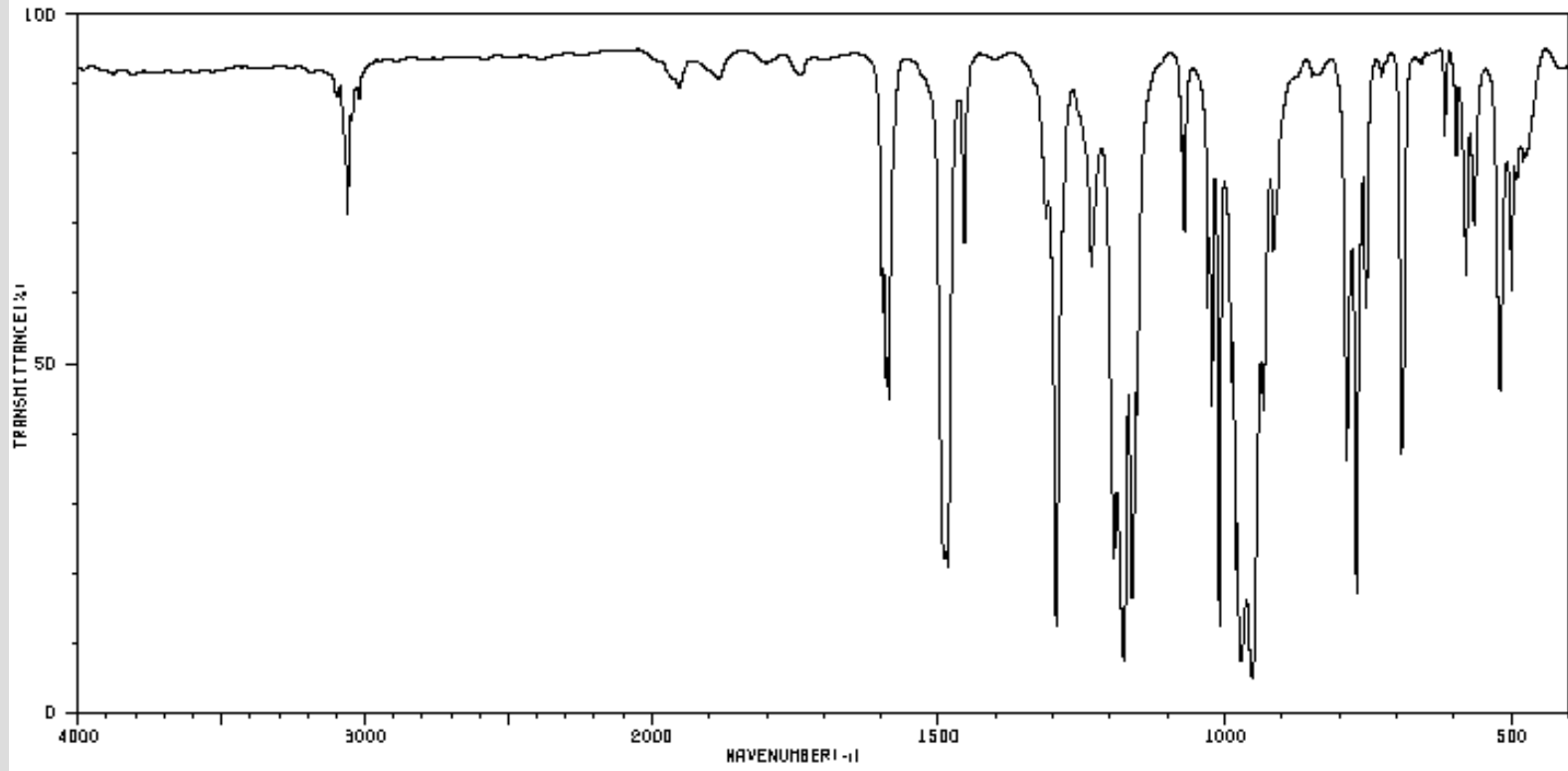
$C_8H_{11}NO_2S$



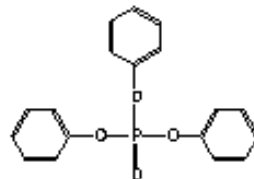
3273	34	1697	60	1318	20	1109	68	707	67
3065	77	1495	68	1308	27	1091	34	679	46
3047	81	1454	62	1291	49	1063	50	664	39
2979	74	1427	60	1188	72	1043	72	629	77
2955	77	1420	66	1158	4	1018	70	586	57
2929	74	1410	57	1128	57	838	49	553	21
2811	81	1380	79	1123	57	823	32	497	64



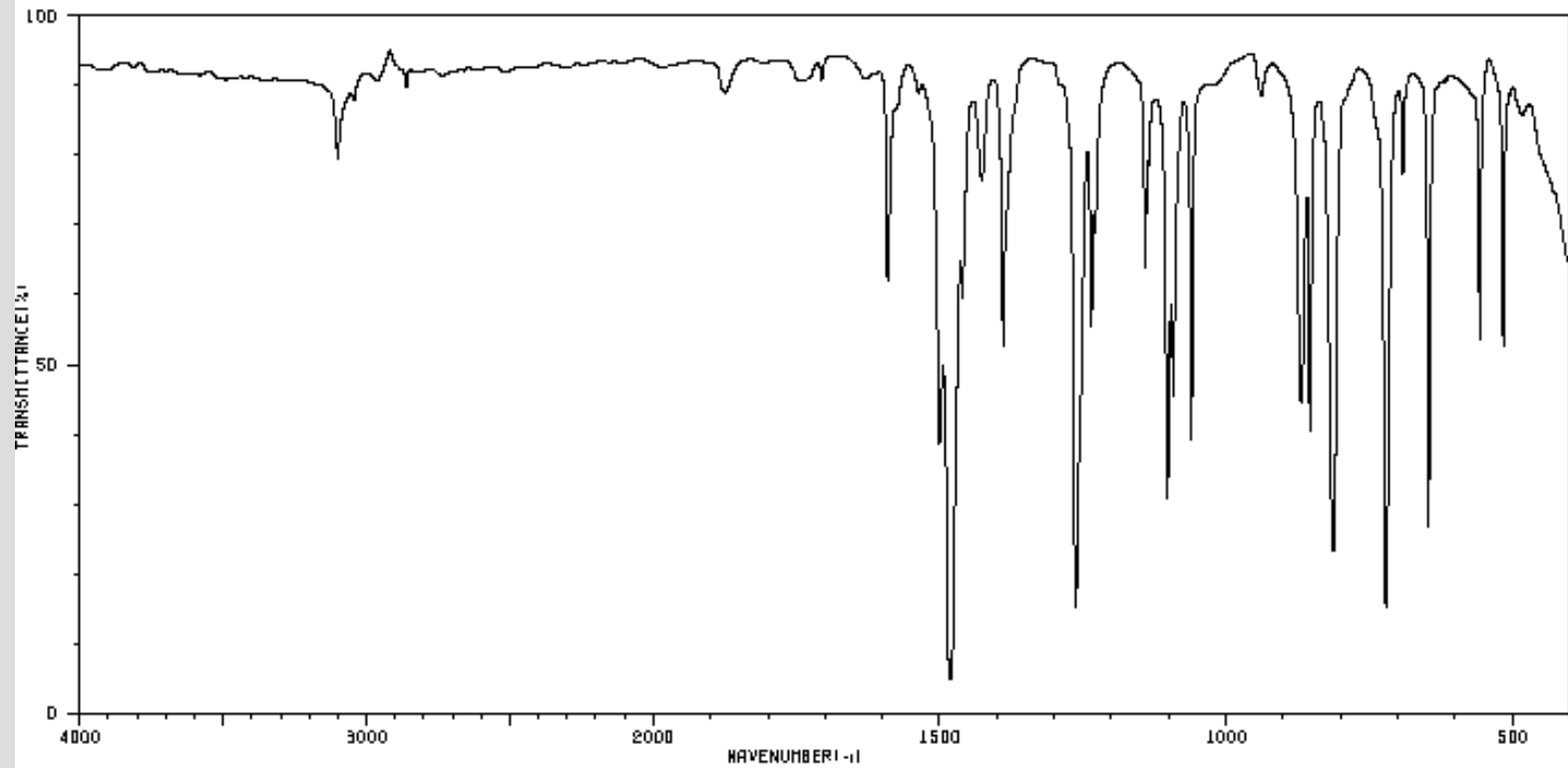
HIT-NO=2221 SCORE= () SDBS-NO=2915 IR-NIDA-30048 : KBR DISC
 TRIPHENYL PHOSPHATE
 $C_{18}H_{15}O_4P$



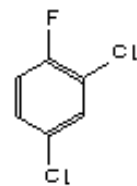
3060	66	1296	12	1071	66	963	4	697	77
1598	55	1233	60	1030	55	933	41	580	60
1567	43	1194	21	1022	42	916	64	566	66
1490	21	1177	7	1010	12	788	34	521	44
1484	20	1163	15	989	46	770	16	500	58
1455	64	1153	41	961	19	753	55	491	74
1313	68	1077	77	972	7	693	36	481	77



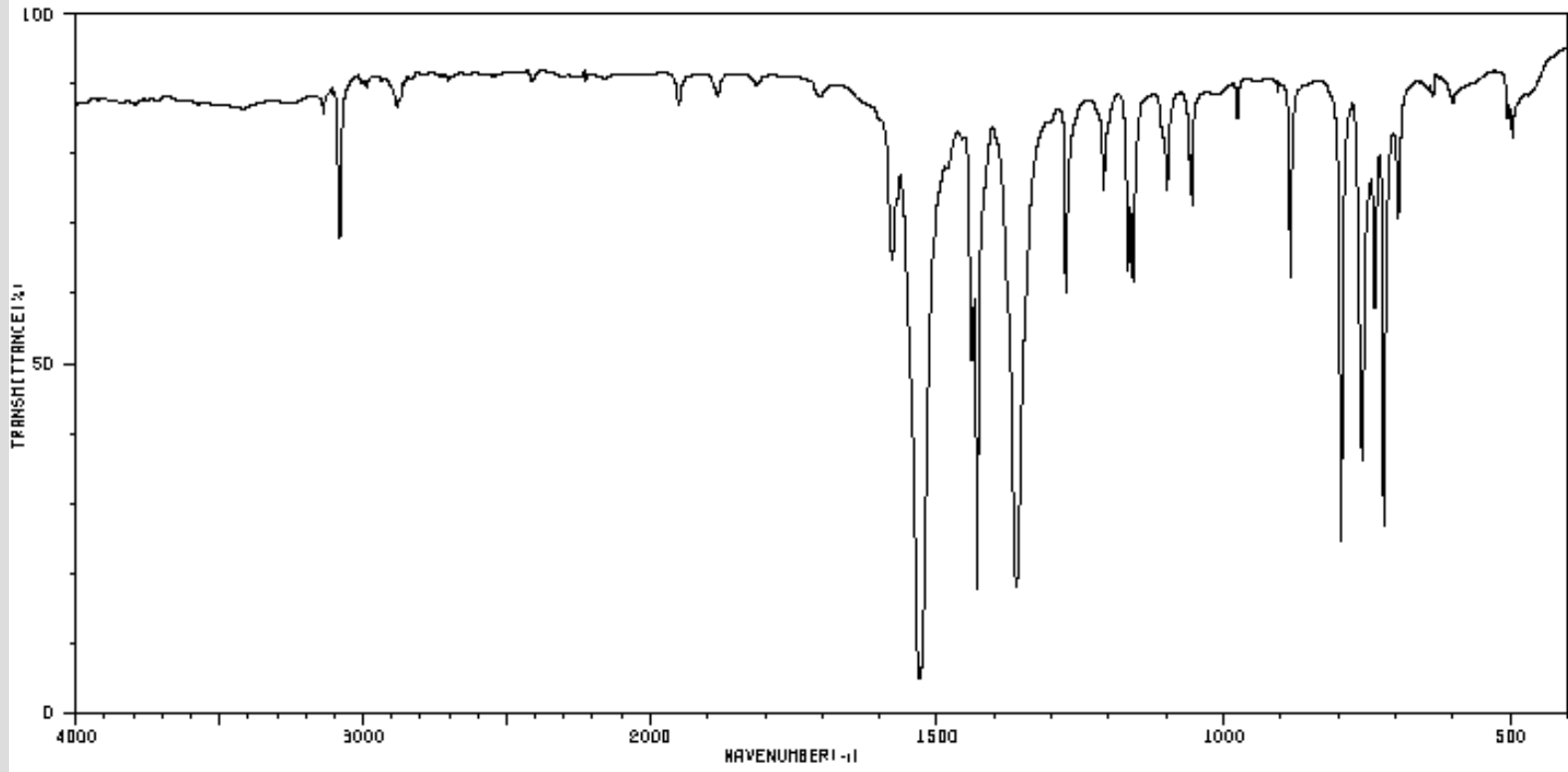
HIT-NO=4351	SCORE= ()	SDBS-NO=11529	IR-NIDA-58033 : LIQUID FILM
2,4-DICHLORO-1-FLUOROBENZENE			
C ₆ H ₃ Cl ₂ F			



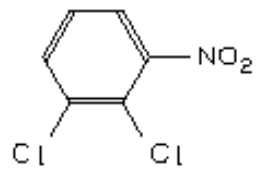
3099	77	1482	4	1142	62	864	39	617	50
2860	86	1461	57	1136	77	819	22	483	81
1873	86	1427	74	1105	30	721	14		
1691	60	1389	50	1092	43	692	74		
1578	84	1263	14	1061	37	647	26		
1538	86	1238	59	939	84	572	86		
1500	37	1229	66	869	43	567	52		



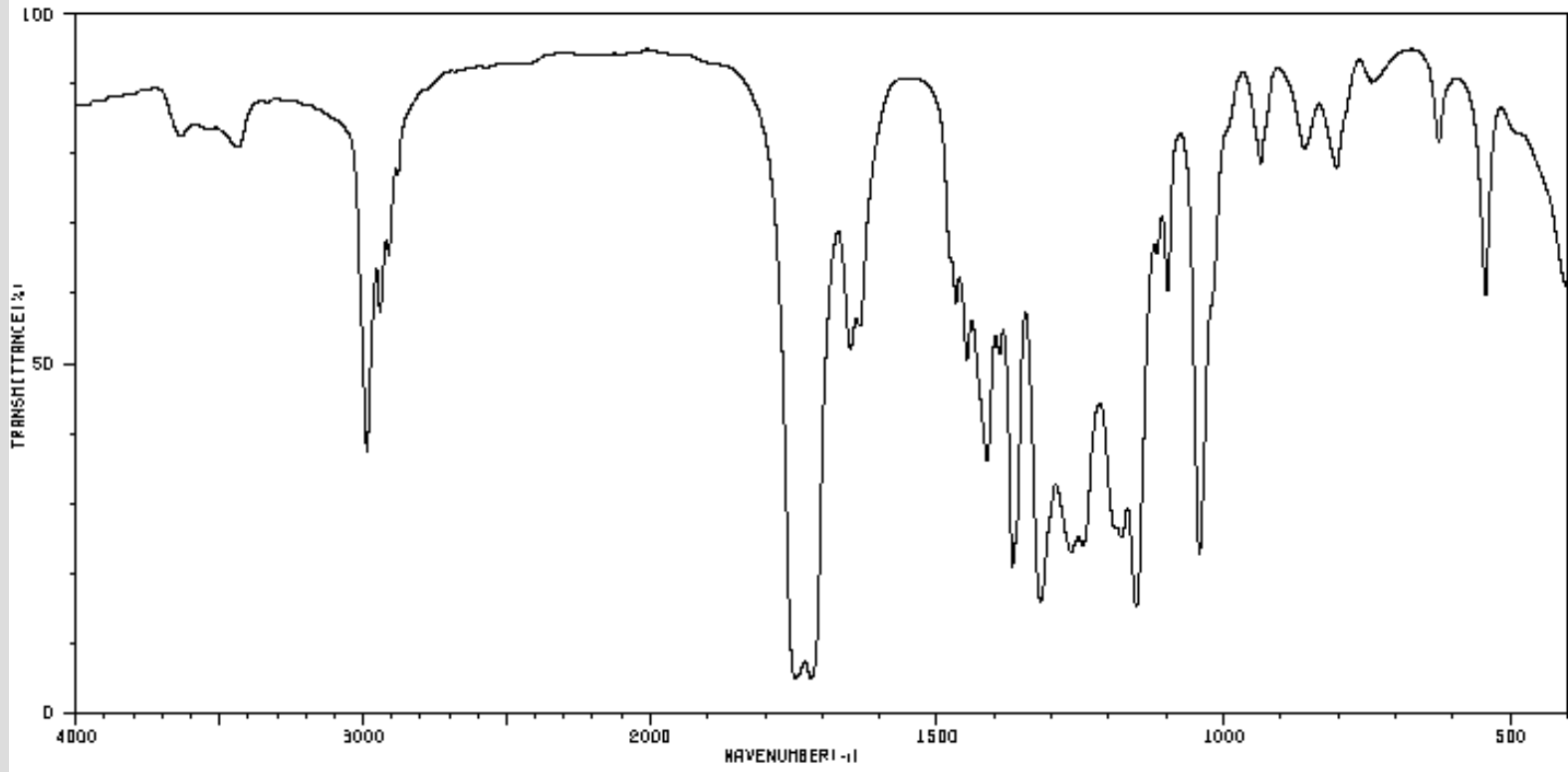
HIT-NO=2169	SCORE= ()	SDBS-NO=2753	IR-NIDA-26624 : KBR DISC
1,2-DICHLORO-3-NITROBENZENE			
C ₆ H ₃ CL ₂ NO ₂			



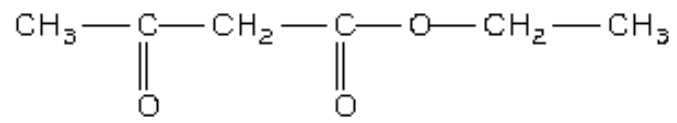
3136	81	1882	84	1430	17	1066	70	721	25
3081	66	1814	86	1362	17	976	81	696	68
2987	86	1704	84	1276	58	907	86	643	66
2900	86	1696	86	1210	72	884	60	636	84
2881	84	1578	62	1167	60	796	23	599	84
2869	84	1530	4	1158	58	759	34	506	61
1950	84	1440	49	1098	72	737	66	496	79



HIT-NO=1071 SCORE= () SDBS-NO=573 IR-NIDA-00054 : LIQUID FILM
 ETHYL ACETOACETATE
 $C_6H_{10}O_3$



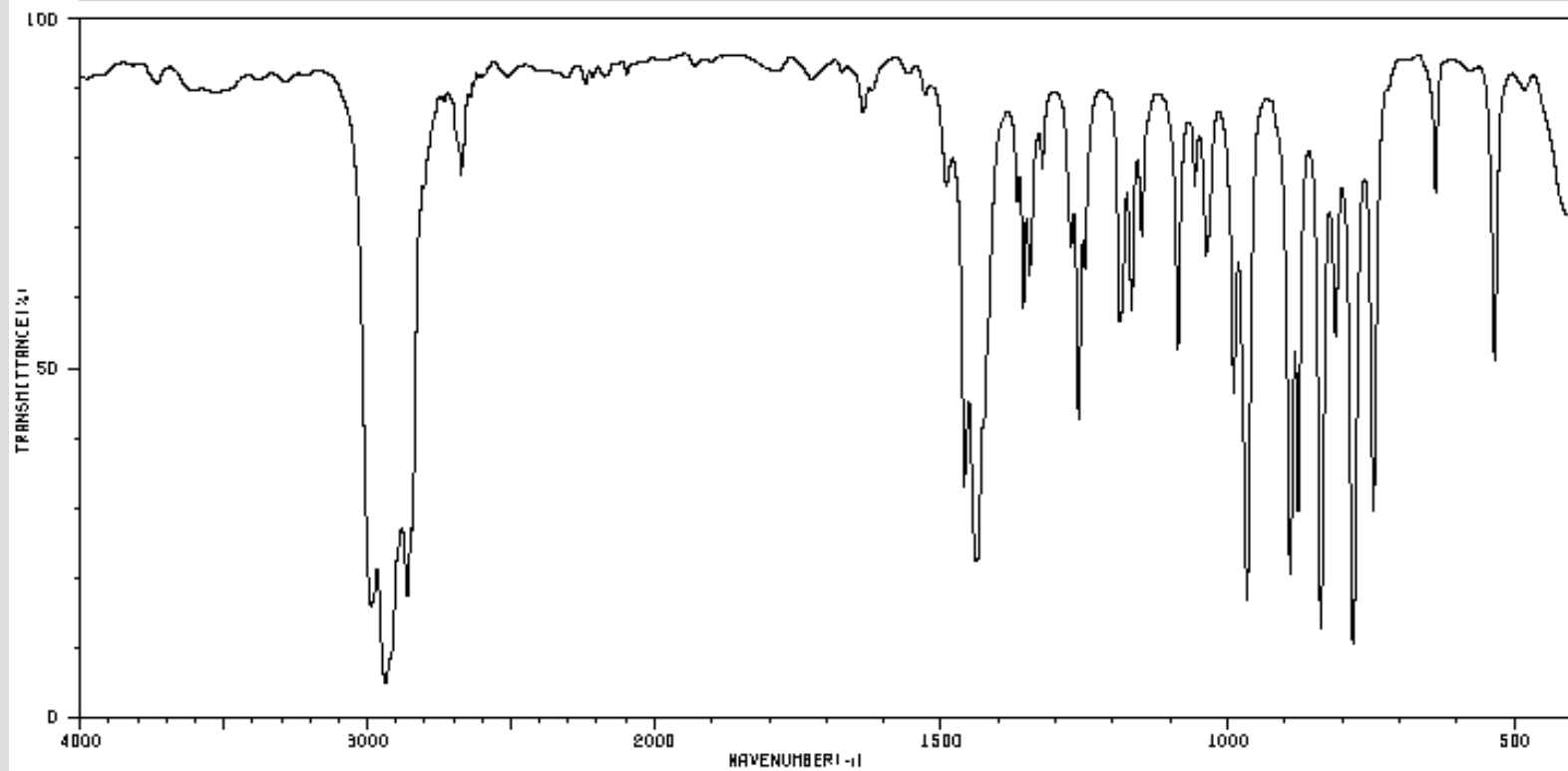
3634	79	1731	7	1391	49	1163	14	626	79
3438	77	1719	4	1368	20	1116	62	543	57
2985	35	1651	50	1319	15	1097	58		
2941	55	1634	59	1266	21	1042	21		
2910	62	1467	57	1245	23	935	77		
2878	74	1448	49	1189	25	859	77		
1746	4	1413	34	1179	23	803	74		



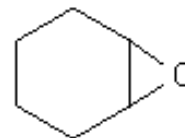
HIT-NO=1382 SCORE= () SDBS-NO=1308 IR-NIDA-61451 : LIQUID FILM

1,2-EPOXYCYCLOHEXANE

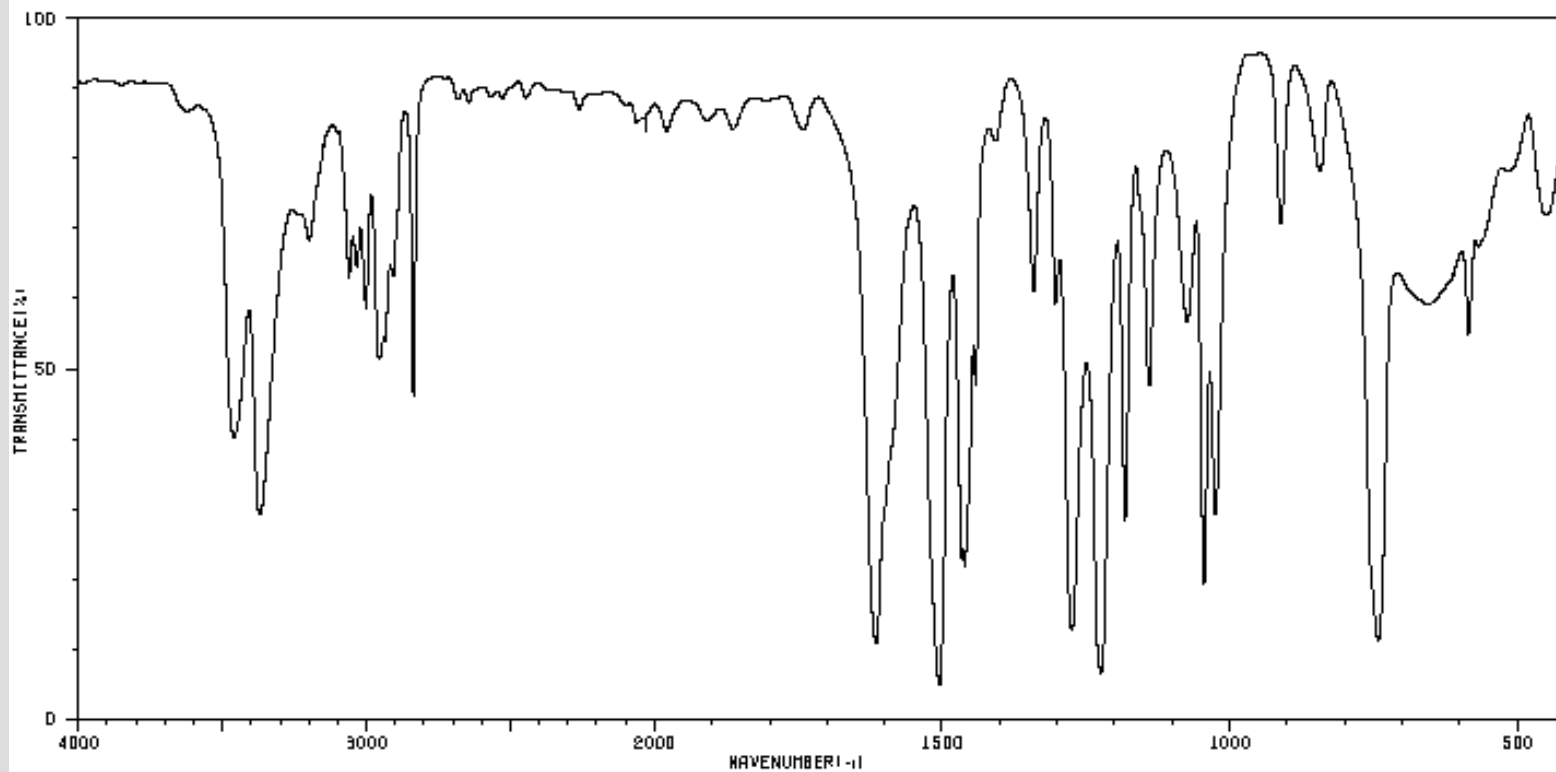
C₆H₁₀O



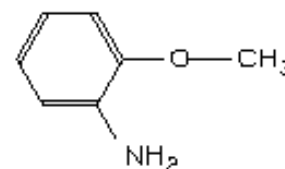
2987	16	1491	72	1323	74	1160	66	877	28
2936	4	1460	31	1274	64	1087	50	838	12
2861	16	1437	21	1260	41	1058	72	812	52
2674	74	1426	39	1249	62	1038	64	782	10
1637	84	1368	70	1189	55	990	44	746	28
1620	86	1357	57	1177	72	966	16	638	72
1628	86	1346	60	1168	67	891	20	636	49



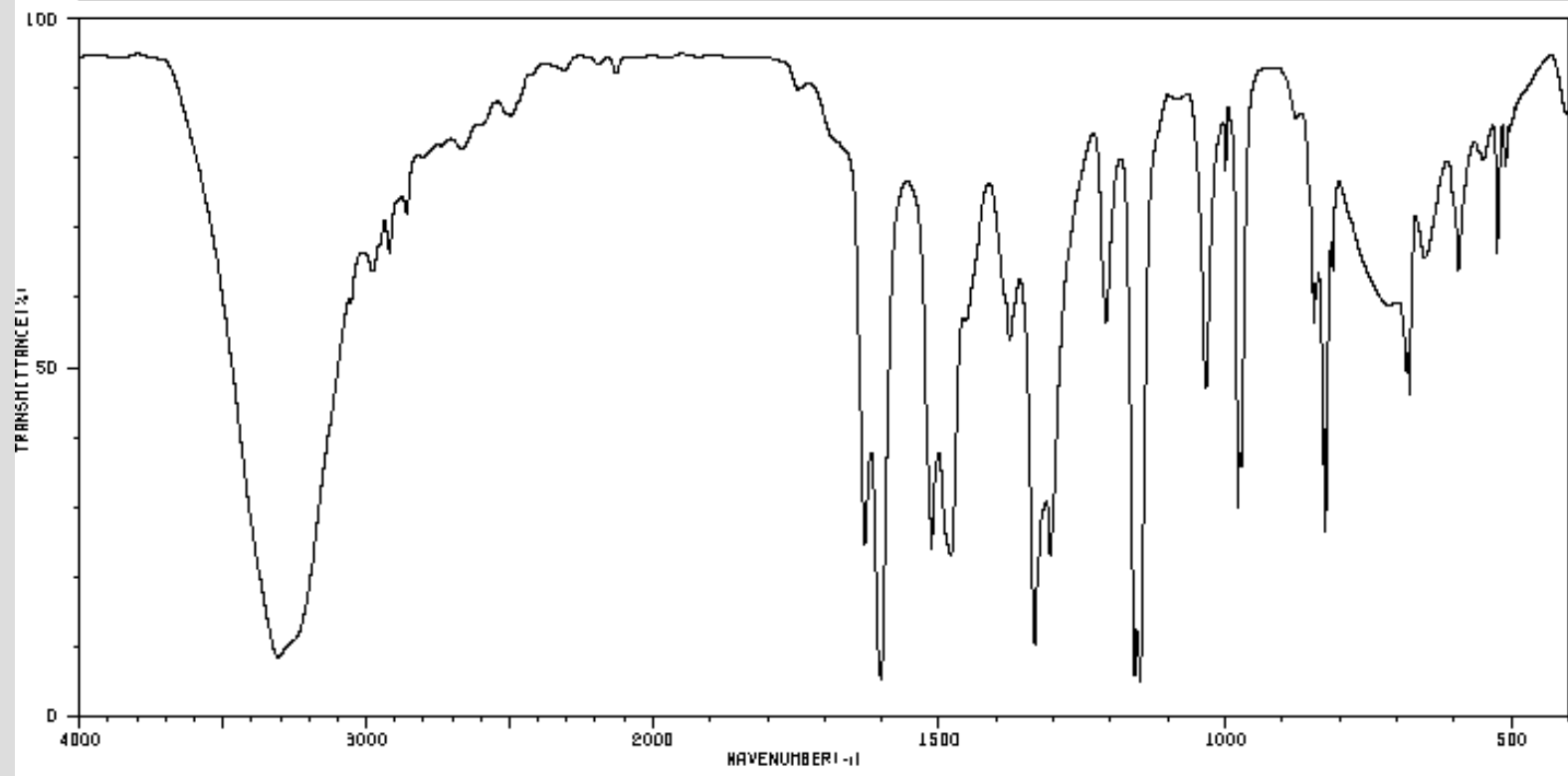
HIT-NO=1455	SCORE= ()	SDBS-NO=1475	IR-NIDA-15020 : LIQUID FILM
O-ANISIDINE			
C ₇ H ₉ NO			



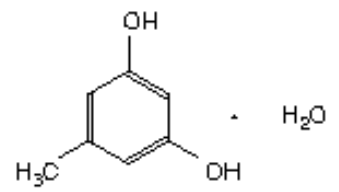
3460	39	2966	60	1460	21	1182	27	843	74
3370	28	2936	52	1442	46	1141	46	742	10
3196	86	2908	60	1408	79	1130	66	659	57
3060	80	2836	44	1341	68	1074	56	654	57
3047	66	1615	10	1303	57	1045	18	586	53
3033	82	1505	4	1275	12	1025	28	580	60
3002	67	1466	22	1226	6	911	68	460	70



HIT-NO=1517	SCORE= ()	SDBS-NO=1509	IR-NIDA-62898 : KBR DISC
5-METHYLRESORCINOL			
C ₇ H ₈ O ₂ · H ₂ O			



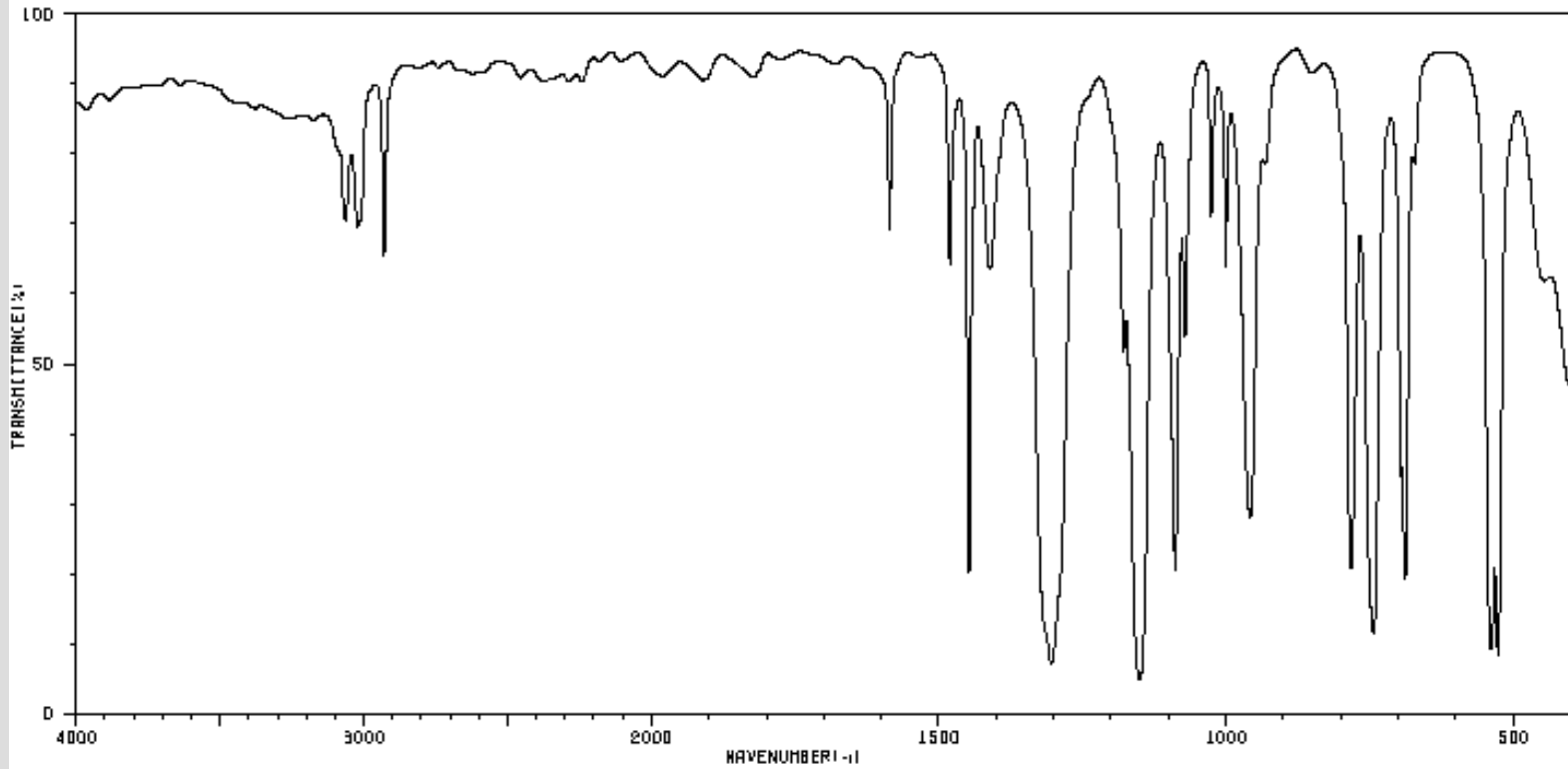
3307	6	1630	29	1209	63	846	69	661	77
2977	60	1602	5	1159	5	825	25	546	79
2920	84	1513	25	1150	4	812	62	525	64
2869	70	1479	21	1034	44	683	47	611	77
2667	79	1377	52	1000	74	678	44		
2507	84	1333	10	976	28	652	62		
2494	84	1306	22	972	34	593	62		



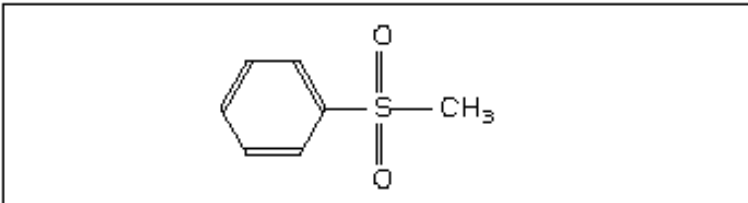
HIT-NO=1484 SCORE= () SDBS-NO=1583 IR-NIDA-00763 : LIQUID FILM

METHYL PHENYL SULFONE

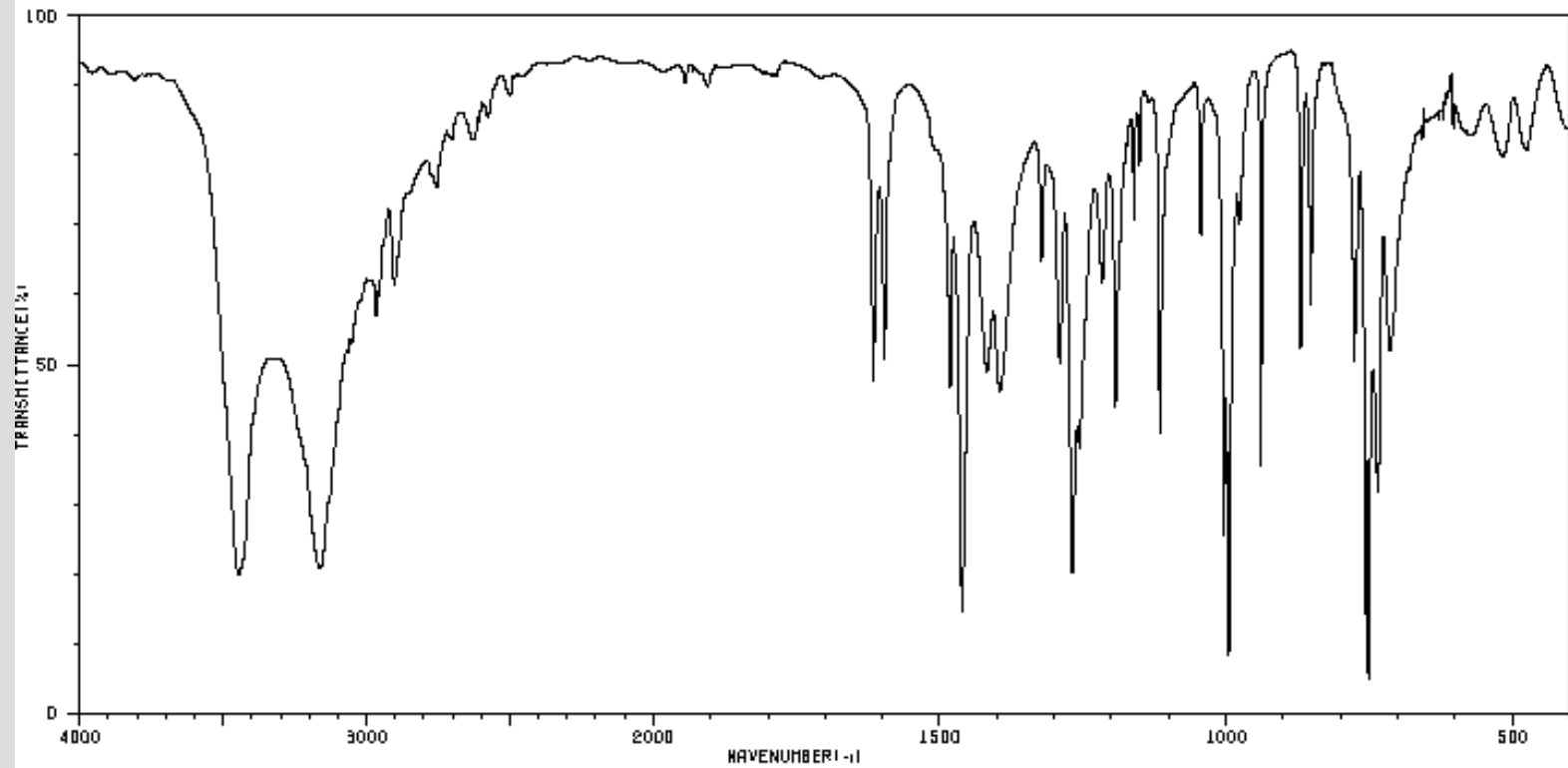
C₇H₈O₂S



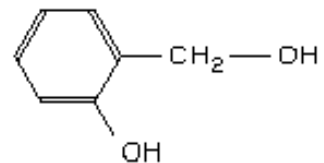
3064	68	1306	6	958	26	627	8
3022	66	1179	50	783	20		
2929	82	1151	4	744	10		
1686	66	1088	19	696	32		
1481	62	1071	52	689	18		
1447	19	1028	68	672	74		
1411	60	1000	62	639	8		



HIT-NO=1683	SCORE= ()	SDBS-NO=1809	IR-NIDA-33479 : KBR DISC
SALICYL ALCOHOL			
C ₇ H ₈ O ₂			



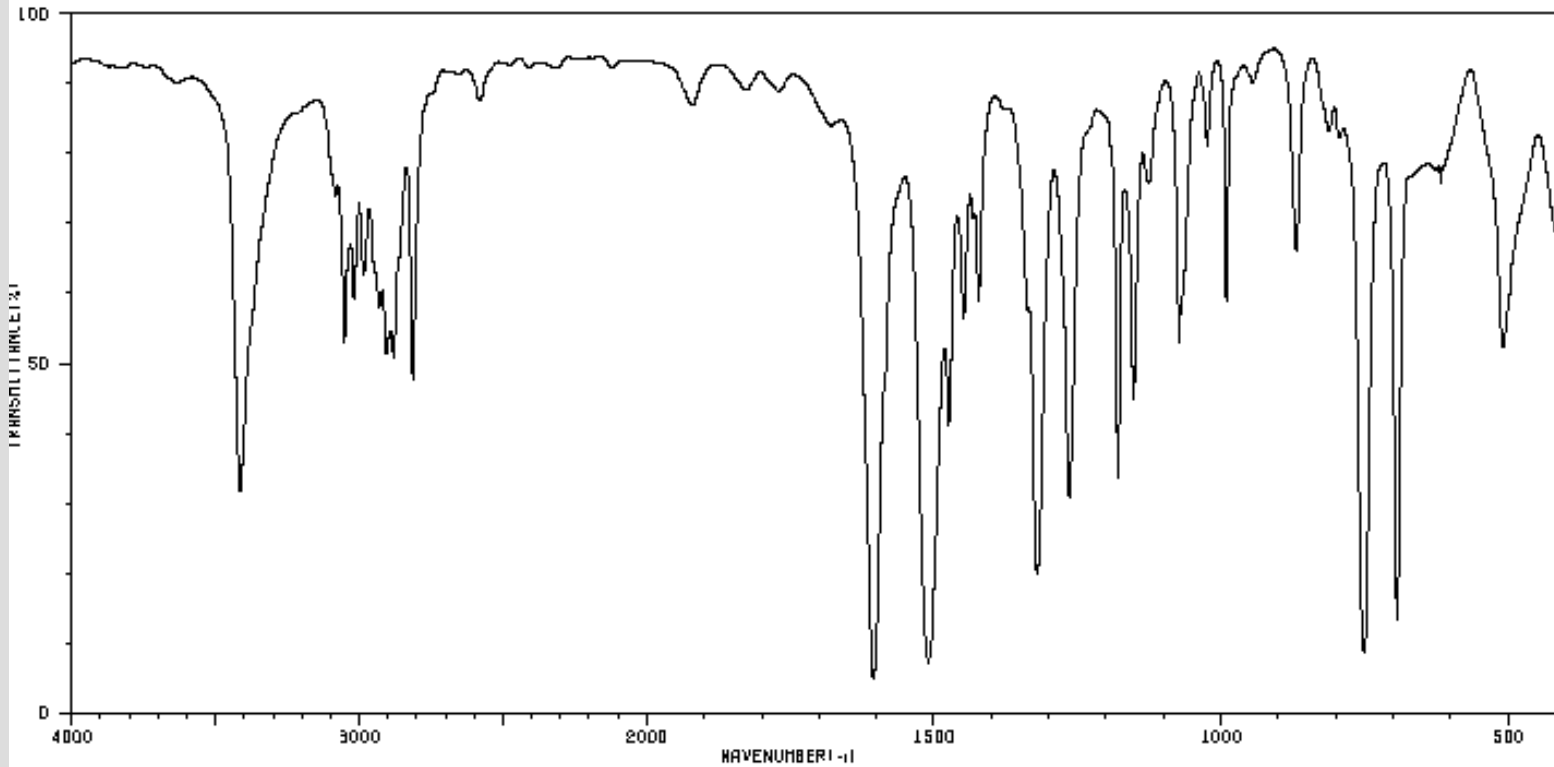
3446	18	2766	72	1322	62	1162	77	870	60
3163	20	1616	46	1291	49	1115	38	852	57
3150	21	1597	48	1269	19	1044	66	776	49
2967	66	1482	44	1267	36	1004	24	767	13
2955	57	1461	13	1217	58	995	7	752	4
2903	58	1418	47	1194	42	977	68	735	30
2773	74	1395	44	1162	68	939	34	715	60



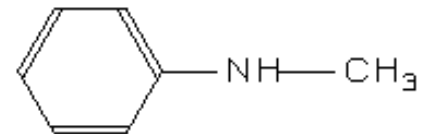
HIT-NO=1601 SCORE= () SDBS-NO=1854 IR-NIDA-64365 : LIQUID FILM

N-METHYLANILINE

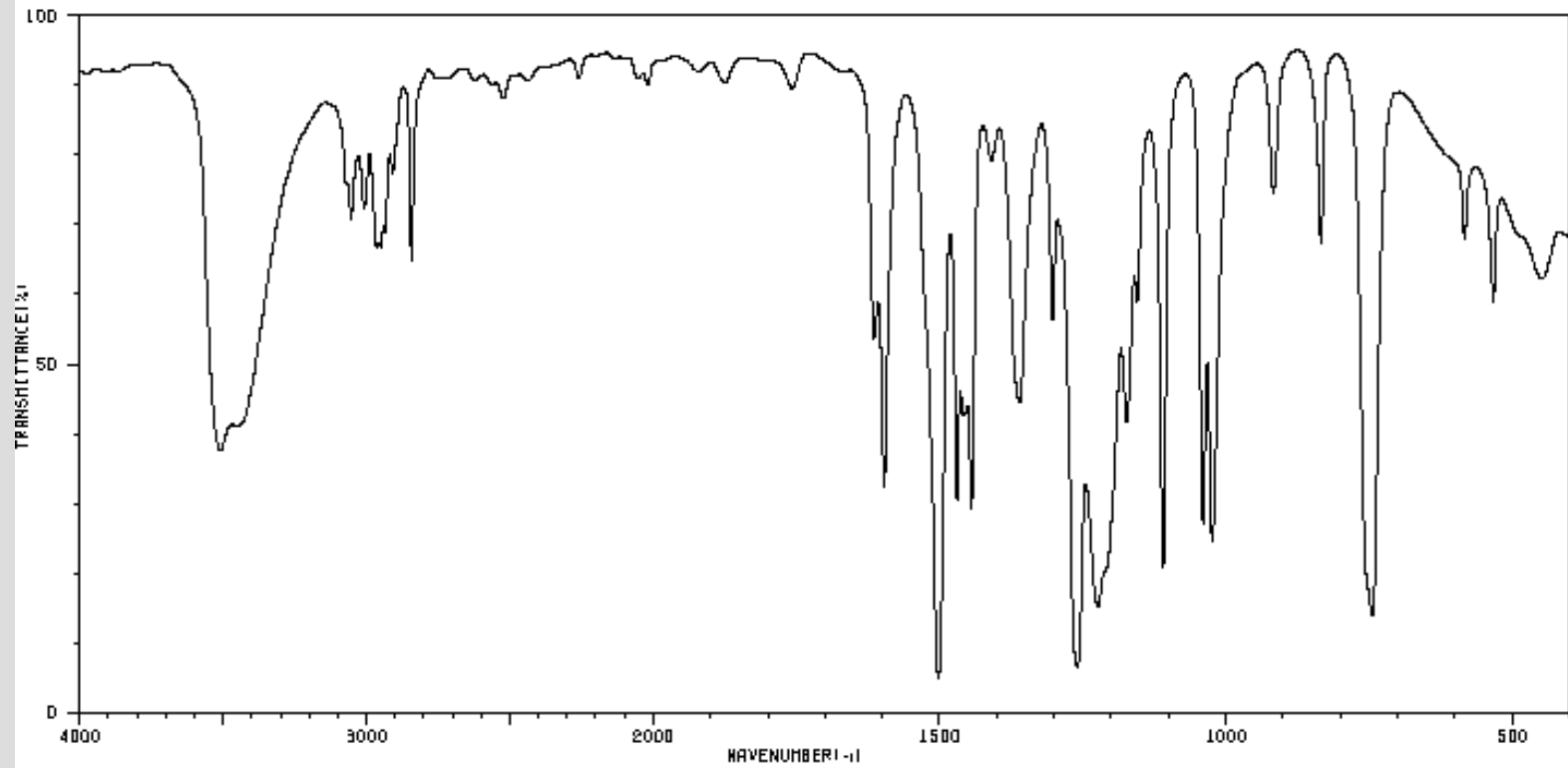
C₇H₉N



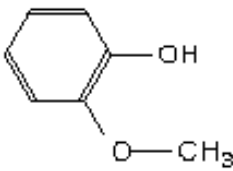
3416	31	2880	49	1610	7	1163	49	796	79
3083	72	2813	46	1474	39	1126	72	751	8
3052	52	2580	84	1448	55	1073	50	693	13
3018	67	1920	84	1422	67	1024	79	623	74
2983	60	1825	86	1320	19	991	57	617	72
2930	55	1769	86	1264	30	869	64	509	50
2905	49	1605	4	1180	32	813	79		



HIT-NO=1677	SCORE= ()	SDBS-NO=1942	IR-NIDA-00554 : LIQUID FILM
GURIACOL			
C ₇ H ₈ O ₂			



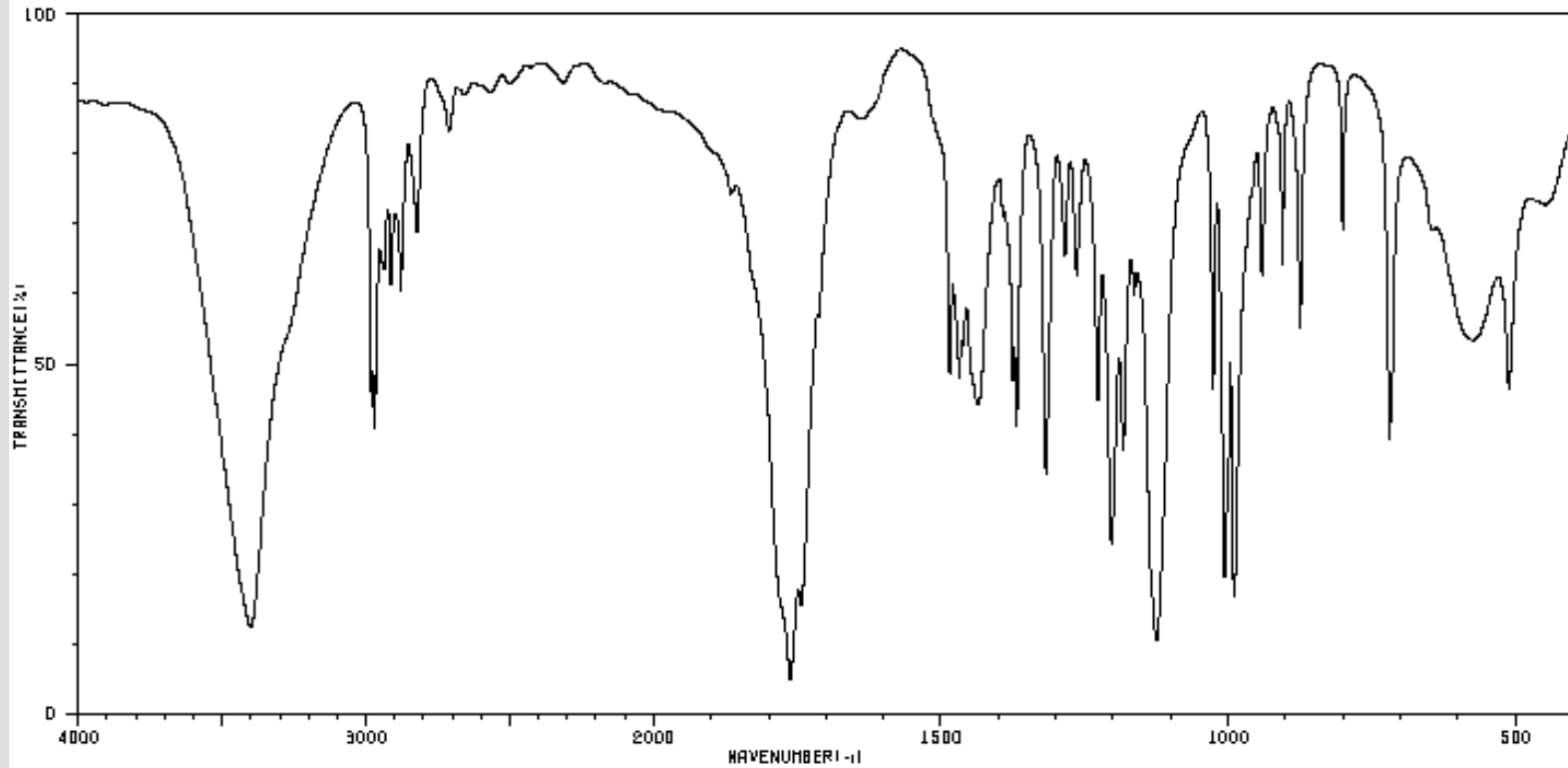
3611	36	2909	74	1470	29	1224	14	836	64
3070	72	2843	62	1457	41	1174	39	745	13
3054	88	2522	84	1444	28	1156	57	584	66
3008	70	1767	86	1410	77	1110	20	534	67
2964	64	1615	52	1361	42	1040	26	449	60
2950	64	1597	31	1305	53	1024	29		
2935	66	1502	4	1260	6	917	72		



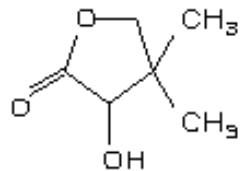
HIT-NO=1867 SCORE= () SDBS-NO=2218 IR-NIDA-00475 : KBR DISC

L-PANTOYL LACTONE

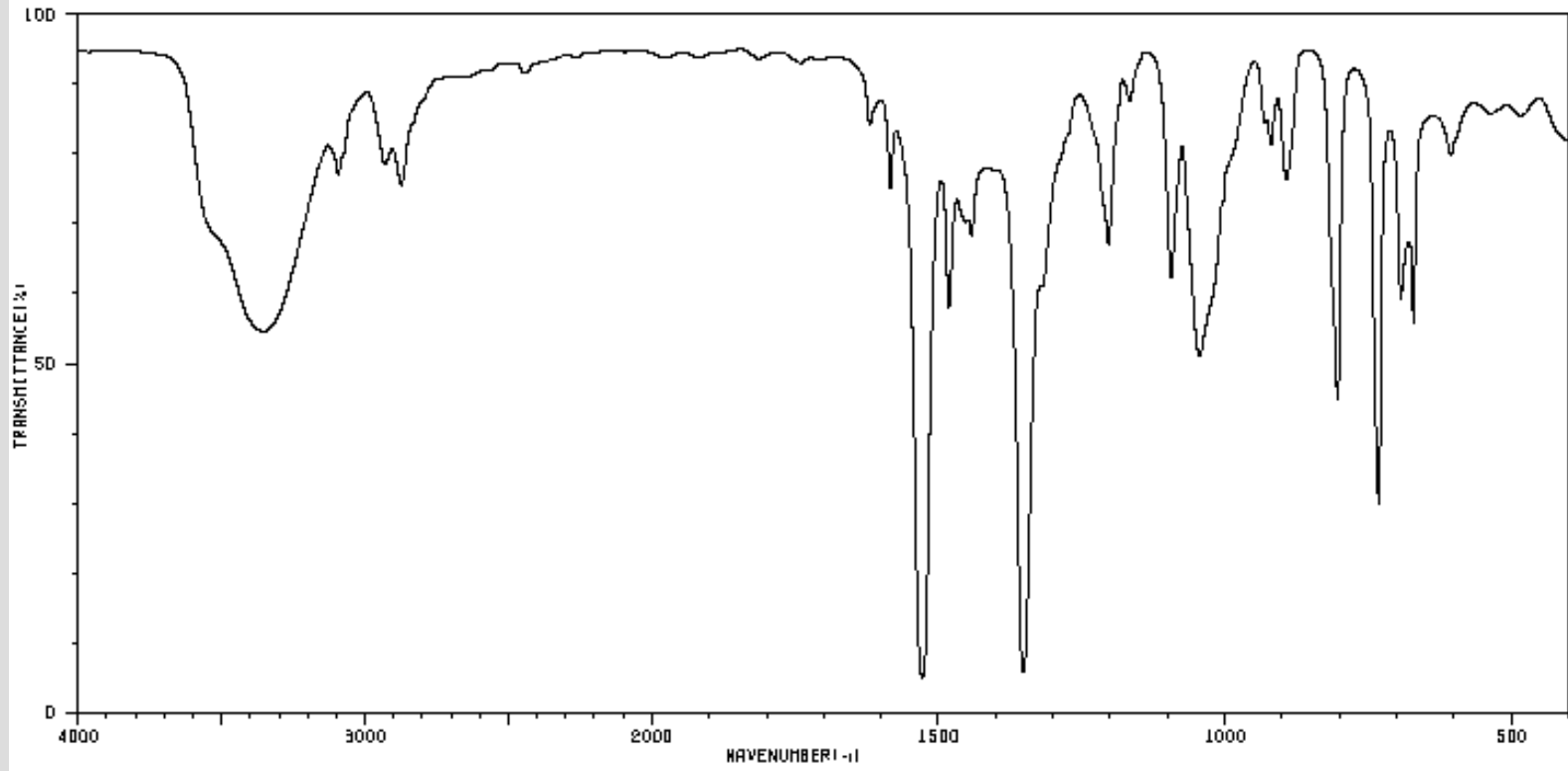
$C_6H_{10}O_3$



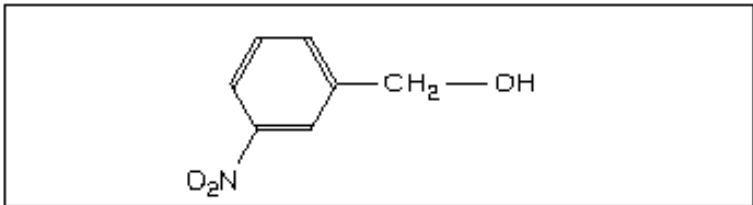
3401	12	2710	79	1436	42	1203	29	941	60
2980	42	1865	72	1375	46	1183	36	906	62
2970	39	1762	4	1368	39	1164	58	875	53
2938	60	1744	16	1318	33	1126	10	801	66
2913	58	1638	81	1285	62	1026	44	719	38
2879	58	1485	46	1264	80	1006	18	574	52
2822	66	1469	46	1228	43	990	16	511	44



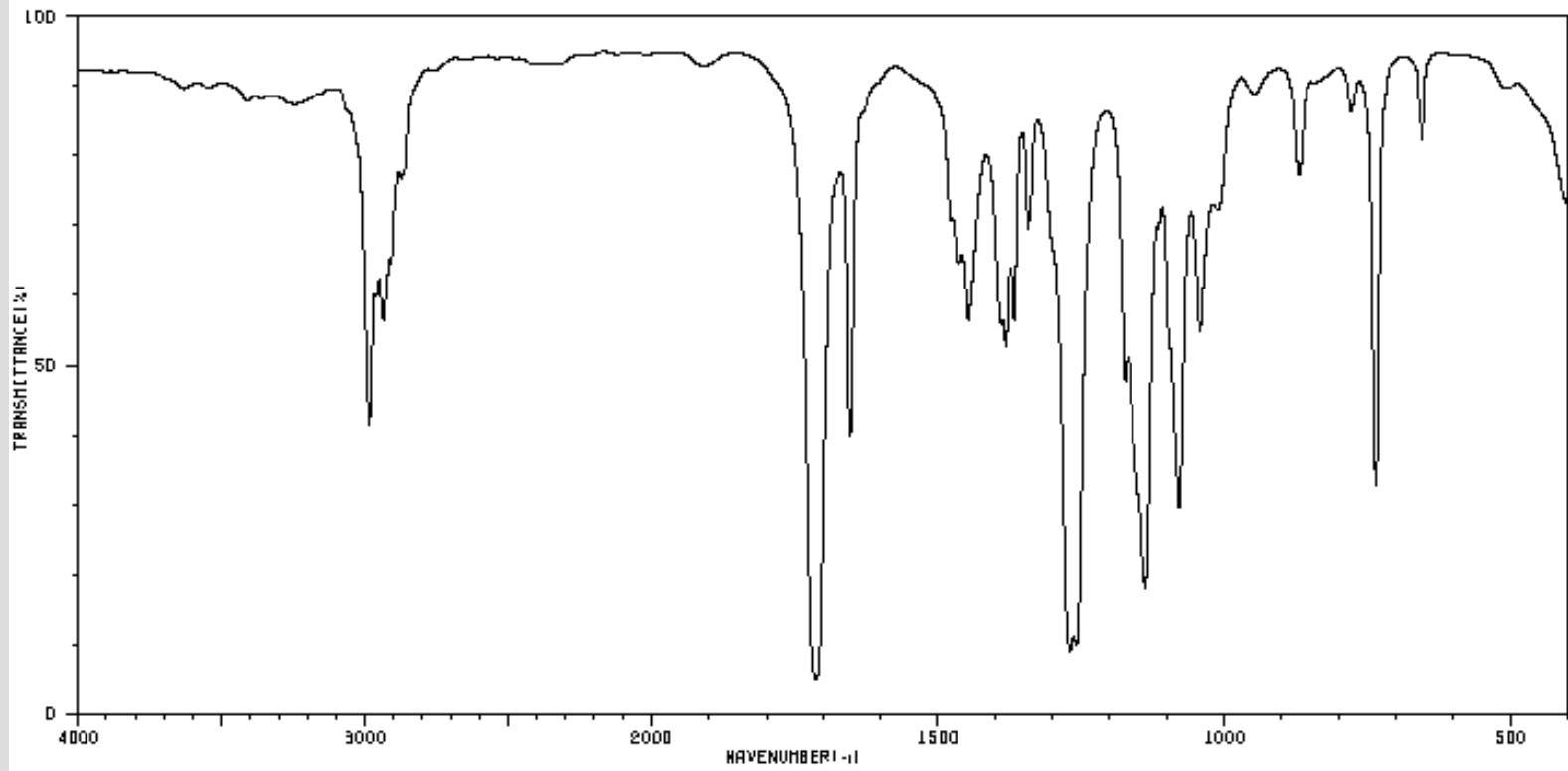
HIT-NO=2283	SCORE= ()	SDBS-NO=3433	IR-NIDA-01004 : LIQUID FILM
M-NITROBENZYL ALCOHOL			
C ₇ H ₇ NO ₃			



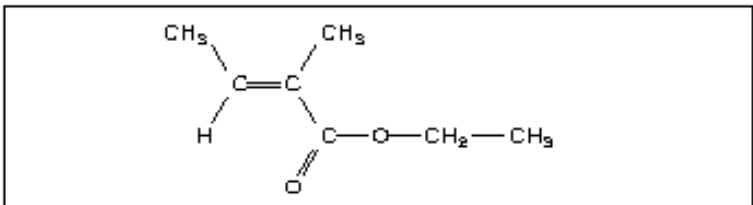
3363	62	1628	4	1094	60	693	67
3352	52	1482	55	1044	49	678	64
3092	74	1453	68	930	81	671	59
2931	74	1442	66	920	79	606	77
2872	72	1352	5	893	74	535	81
1620	81	1203	64	803	43	484	81
1584	72	1167	84	732	28		



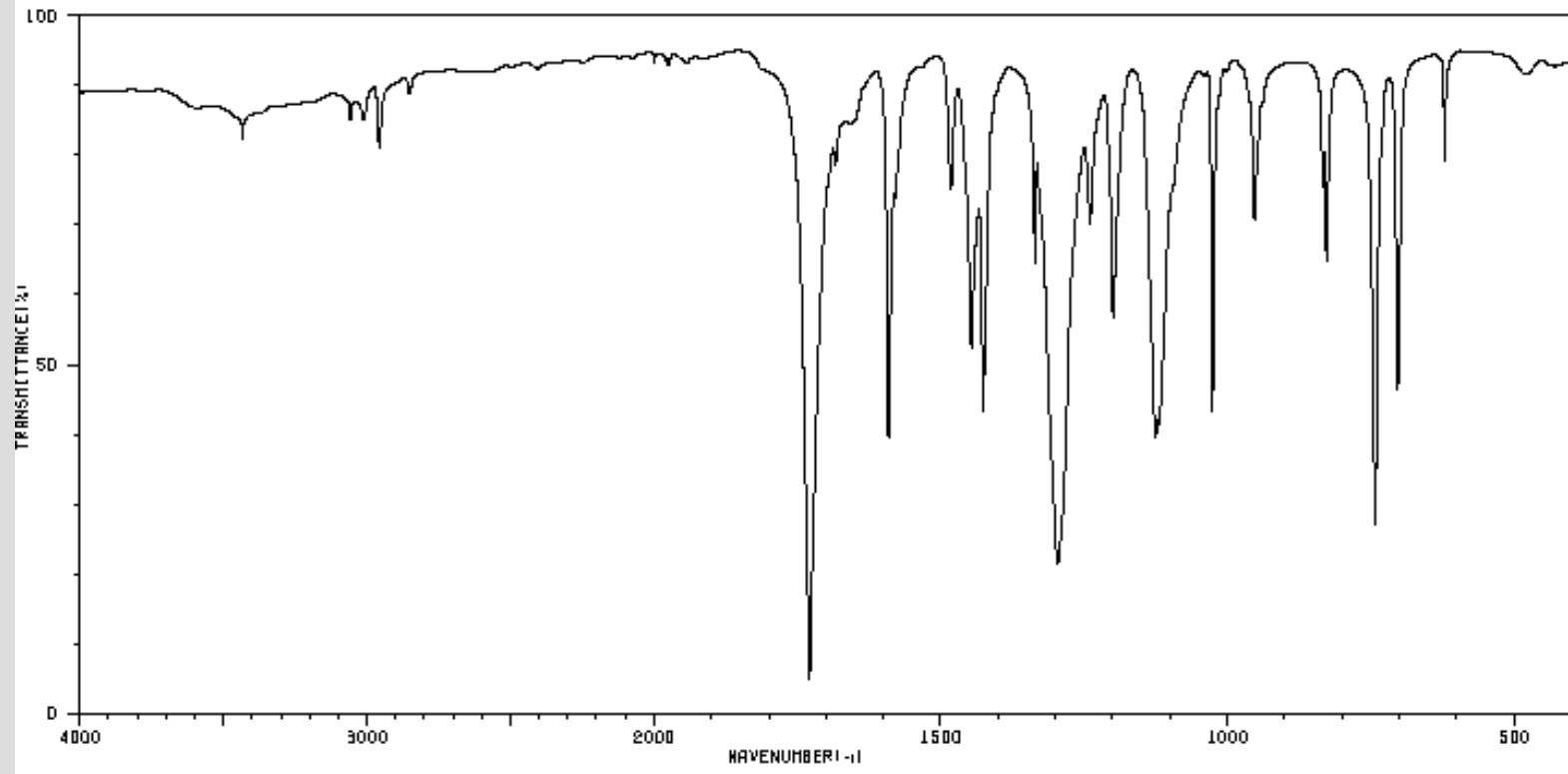
HIT-NO=2286 SCORE= () SDBS-NO=3466 IR-NIDA-01046 : LIQUID FILM
 ETHYL (E)-2-METHYL-2-BUTENOATE
 $C_7H_{12}O_2$



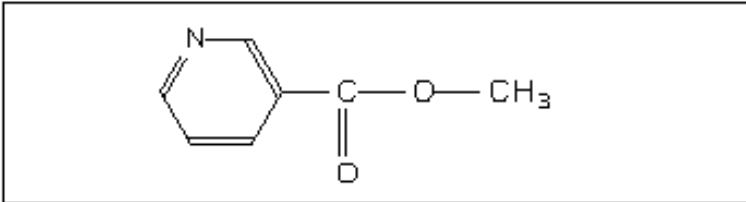
2984	39	1390	69	1138	17	666	79
2960	57	1381	50	1078	28		
2936	55	1367	53	1042	53		
1712	4	1343	66	947	86		
1654	38	1270	8	870	74		
1465	82	1259	9	778	84		
1446	63	1173	46	736	31		



HIT-NO=2603	SCORE= ()	SDBS-NO=3563	IR-NIDA-03423 : KBR DISC
METHYL NICOTINATE			
C ₇ H ₇ NO ₂			



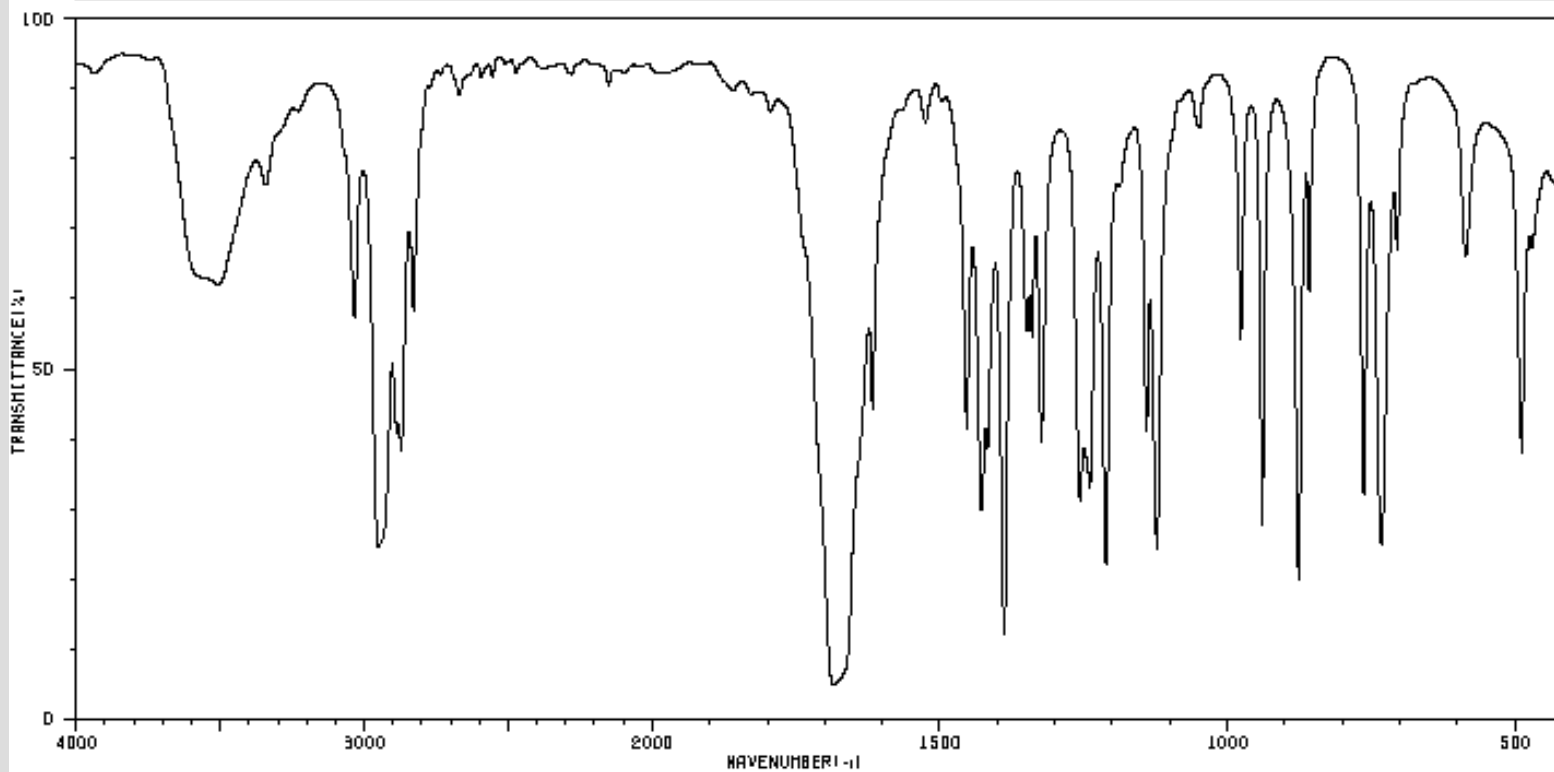
3433	79	1691	38	1240	68	834	72
3058	81	1580	70	1200	55	827	62
3010	81	1482	72	1125	37	742	26
2957	77	1446	60	1120	39	704	44
2855	86	1426	42	1026	42	622	77
1729	4	1338	62	953	88		
1683	74	1297	20	939	84		



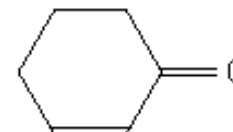
HIT-NO=2990 SCORE= () SDBS-NO=5498 IR-NIDA-09290 : LIQUID FILM

2-CYCLOHEXEN-1-ONE

C₆H₈O



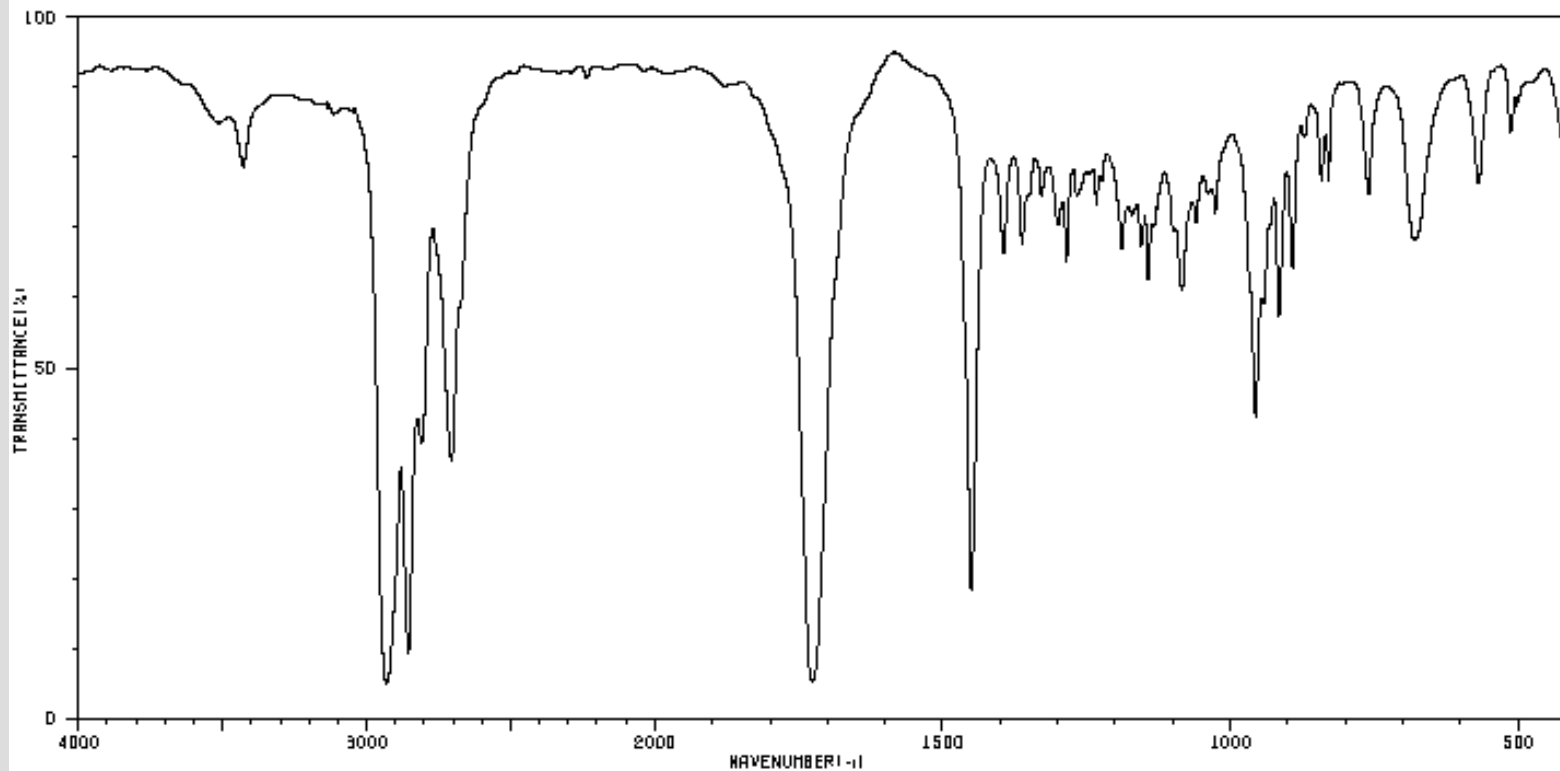
3341	72	1796	84	1388	11	1141	38	868	68
3034	55	1685	4	1349	53	1123	23	763	31
2951	23	1617	42	1340	52	1056	84	733	23
2887	38	1526	81	1324	38	1049	81	706	64
2871	36	1454	39	1257	30	977	52	586	64
2829	55	1428	28	1240	32	940	26	489	36
2670	86	1417	37	1212	21	876	18	472	64



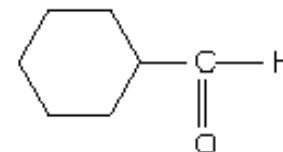
HIT-NO=3097 SCORE= () SDBS-NO=5755 IR-NIDA-58303 : LIQUID FILM

CYCLOHEXANECARBALDEHYDE

C₇H₁₂O



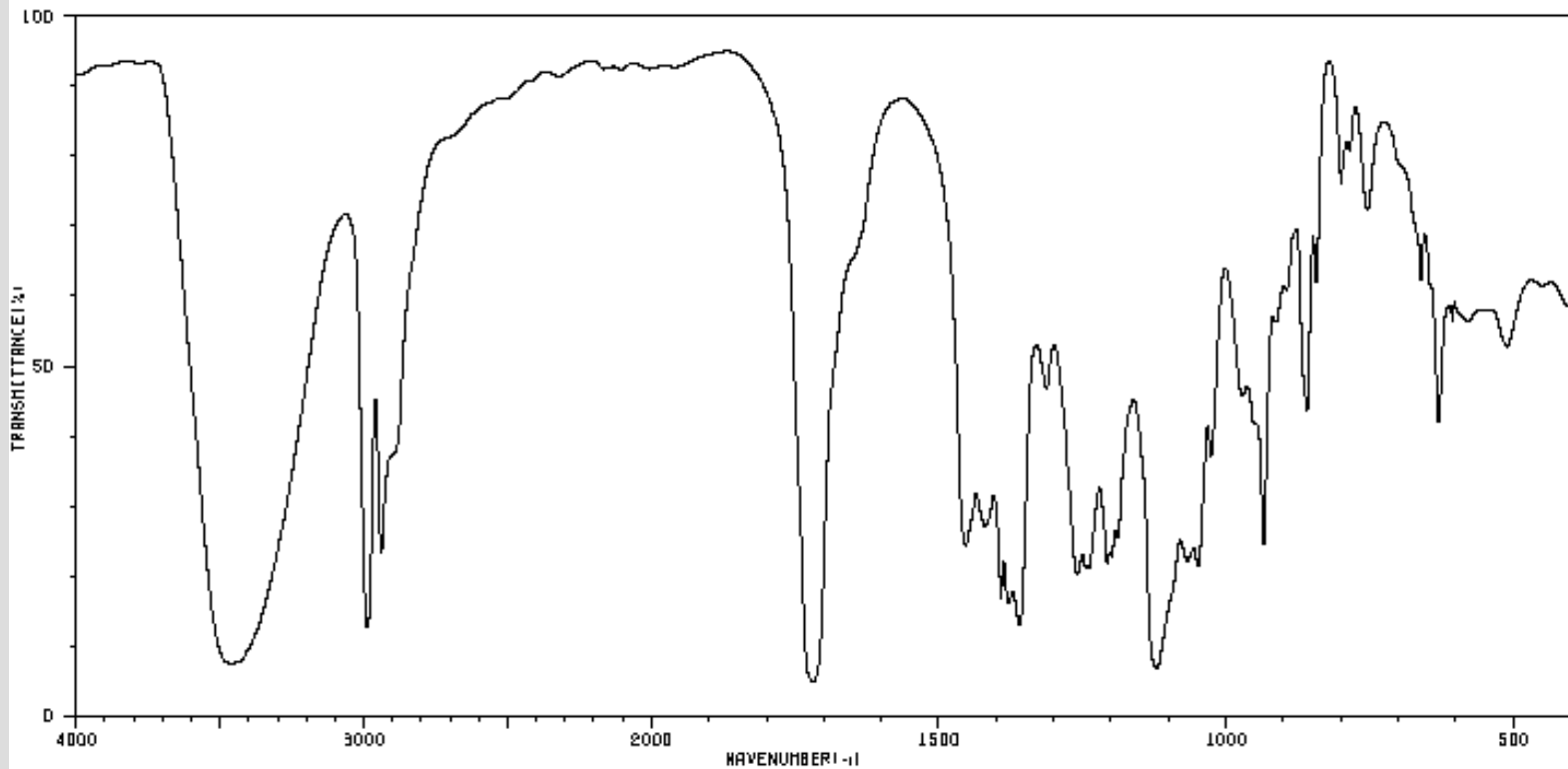
2932	4	1396	64	1233	70	1099	66	943	67
2908	13	1362	66	1224	74	1084	58	916	55
2856	6	1351	72	1189	84	1060	68	895	62
2809	37	1329	72	1170	70	1038	72	842	74
2705	35	1300	68	1156	64	1033	72	829	74
1727	5	1285	62	1144	80	1026	70	761	72
1451	17	1267	72	1133	68	967	42	681	66



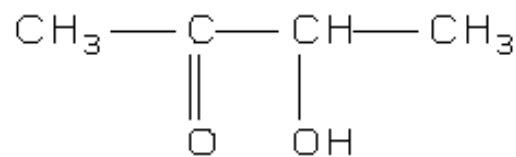
HIT-NO=1028 SCORE= () SDBS-NO=498 IR-NIDA-01733 : LIQUID FILM

ACETOIN

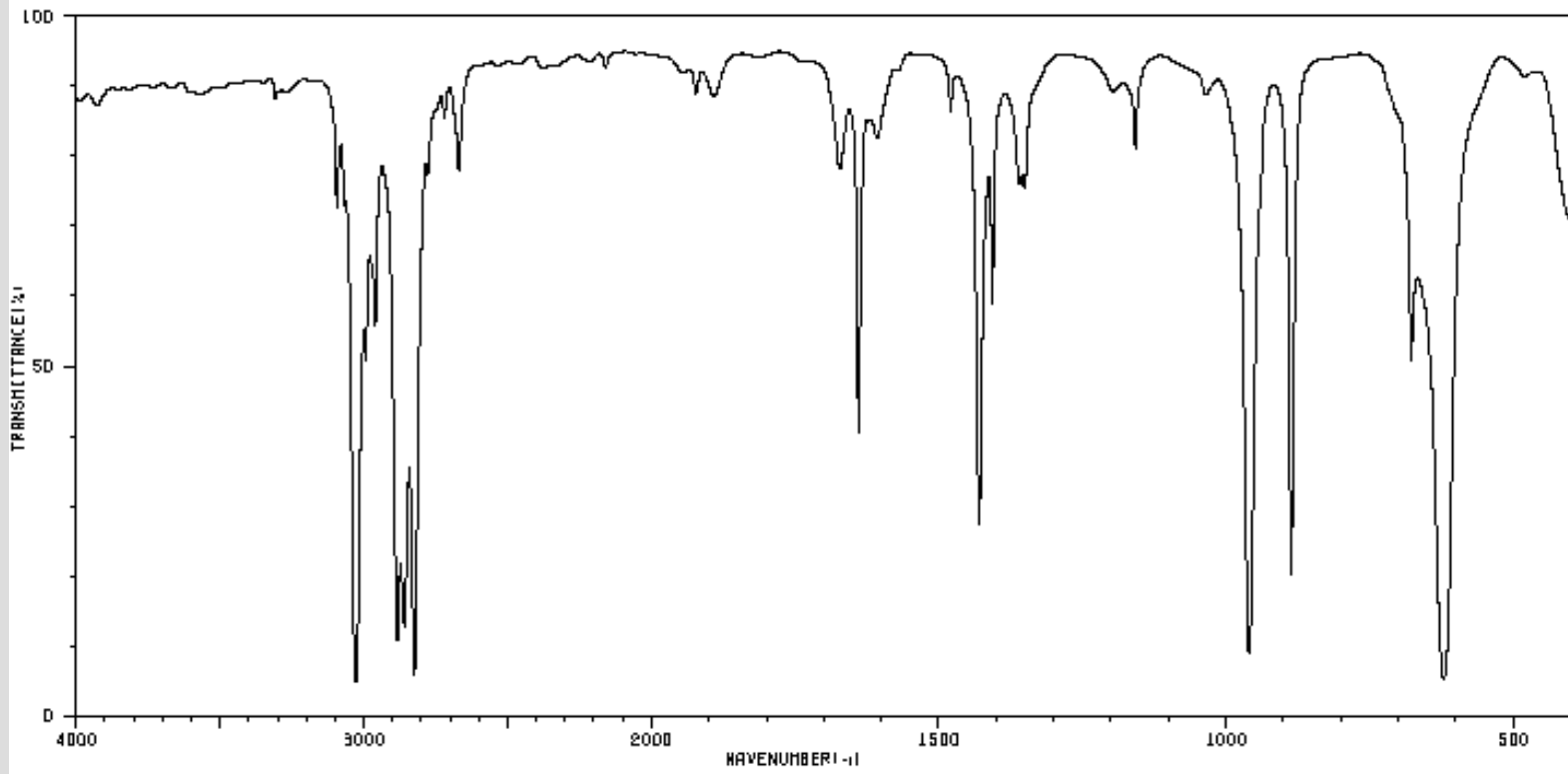
C₄H₈O₂



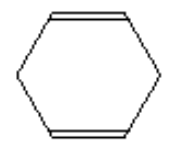
3456	7	1392	16	1207	21	1026	36	786	77
3446	7	1379	15	1200	21	971	44	754	70
2986	12	1360	12	1189	24	952	39	661	60
2938	22	1313	44	1121	6	934	29	631	41
1718	4	1259	19	1067	21	859	42	607	53
1454	23	1245	20	1060	21	843	60	580	55
1420	26	1238	20	1048	21	800	72	511	60



HIT-NO=1063	SCORE= ()	SDBS-NO=559	IR-NIDA-38491 ; LIQUID FILM
1,4-CYCLOHEXADIENE			
C ₆ H ₈			



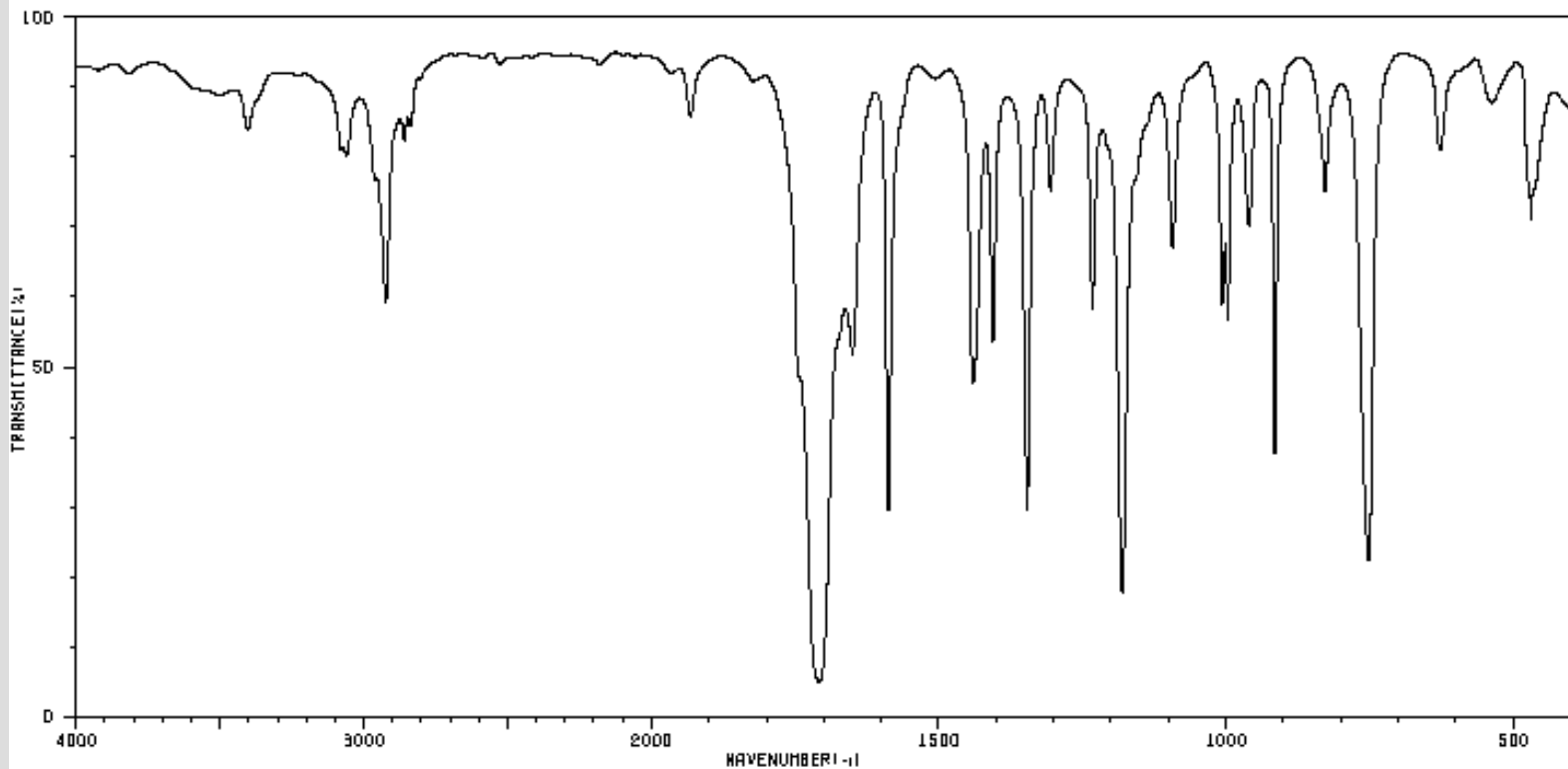
3929	84	2960	69	1922	86	1407	67	960	8
3569	86	2884	10	1891	84	1360	72	886	19
3308	84	2860	12	1872	74	1351	72	676	49
3270	86	2824	6	1640	38	1197	86	621	4
3094	70	2778	74	1607	79	1158	79		
3028	4	2719	61	1460	84	1035	66		
2993	49	2670	74	1430	26	1028	86		



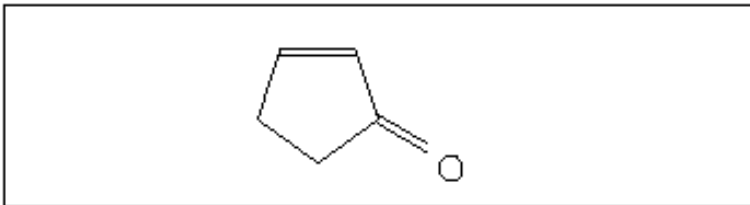
HIT-NO=980 SCORE= () SDBS-NO=382 IR-NIDA-03553 : LIQUID FILM

2-CYCLOPENTEN-1-ONE

C₅H₆O



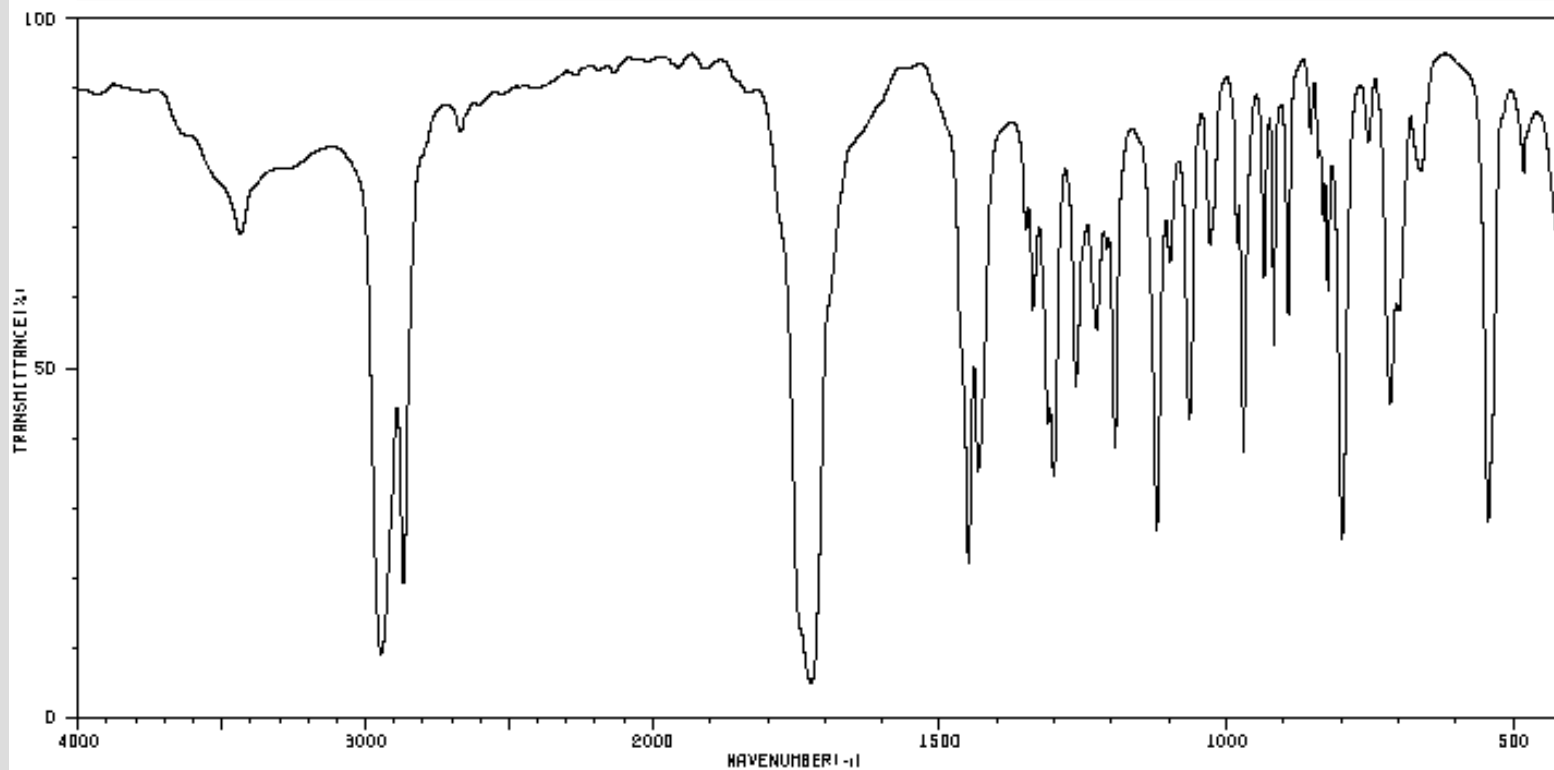
3406	81	1709	4	1239	66	828	72
3081	79	1650	50	1181	17	752	21
3059	77	1588	28	1093	84	628	79
2924	67	1441	46	1007	67	537	84
2859	79	1406	52	997	55	469	68
2837	81	1348	28	960	88		
1932	81	1306	72	916	36		



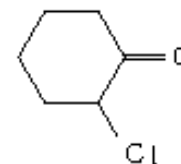
HIT-NO=4913 SCORE= () SDBS-NO=15187 IR-NIDA-24474 ; LIQUID FILM

2-CHLOROCYCLOHEXANONE

C₆H₉ClO



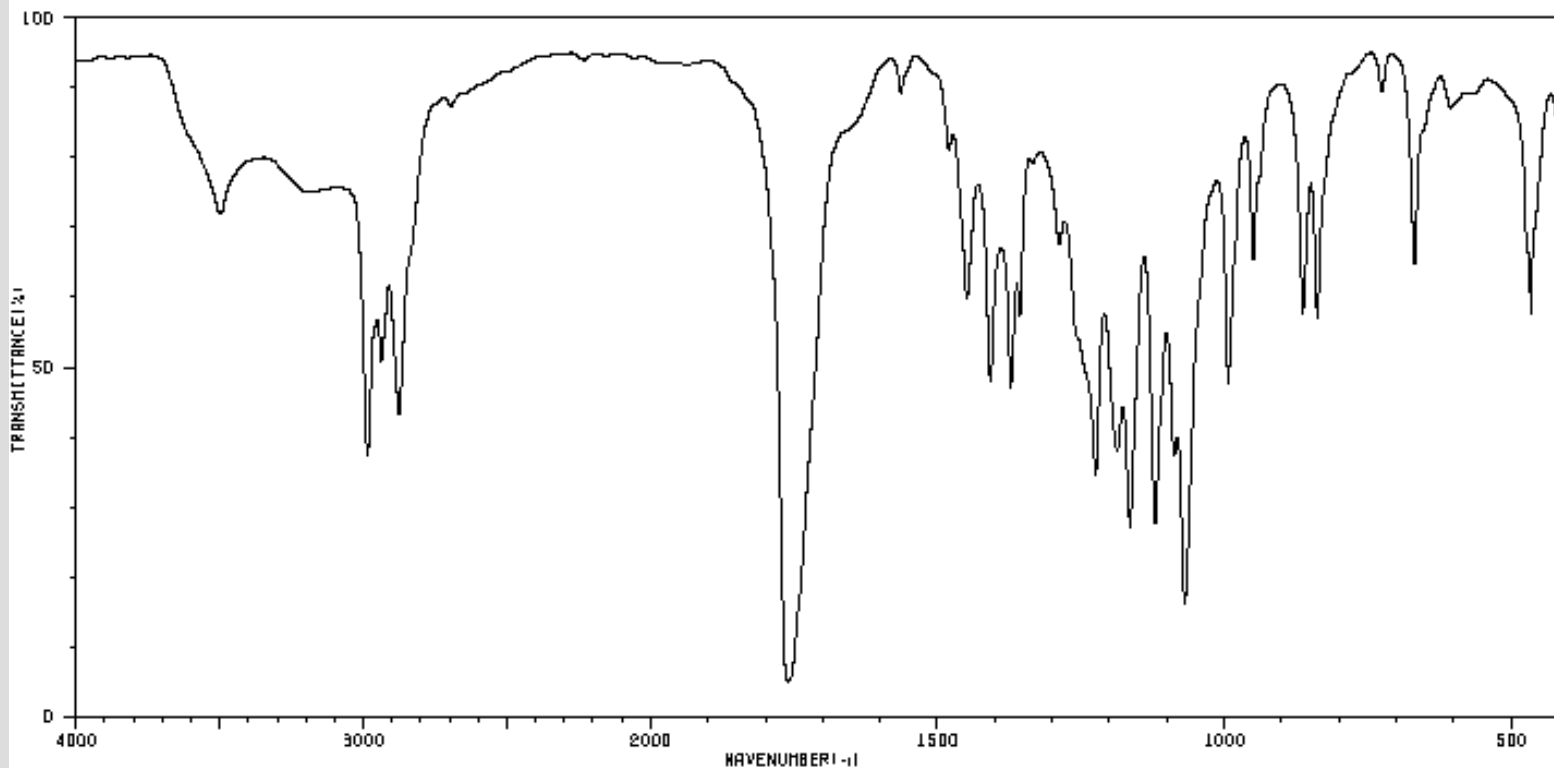
3436	66	1360	66	1196	37	936	60	763	79
2946	8	1338	55	1122	25	917	52	715	43
2867	16	1311	39	1098	62	893	55	700	55
2671	81	1302	39	1066	41	863	78	662	74
1723	4	1263	46	1029	66	831	68	544	26
1450	21	1227	59	982	66	823	58	482	74
1433	34	1209	64	971	36	798	24		



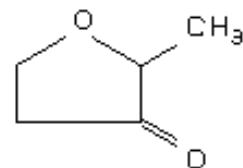
HIT-NO=5614 SCORE= () SDBS-NO=19132 IR-NIDA-62409 : LIQUID FILM

2-METHYL-4,5-DIHYDRO-3(2H)-FURANONE

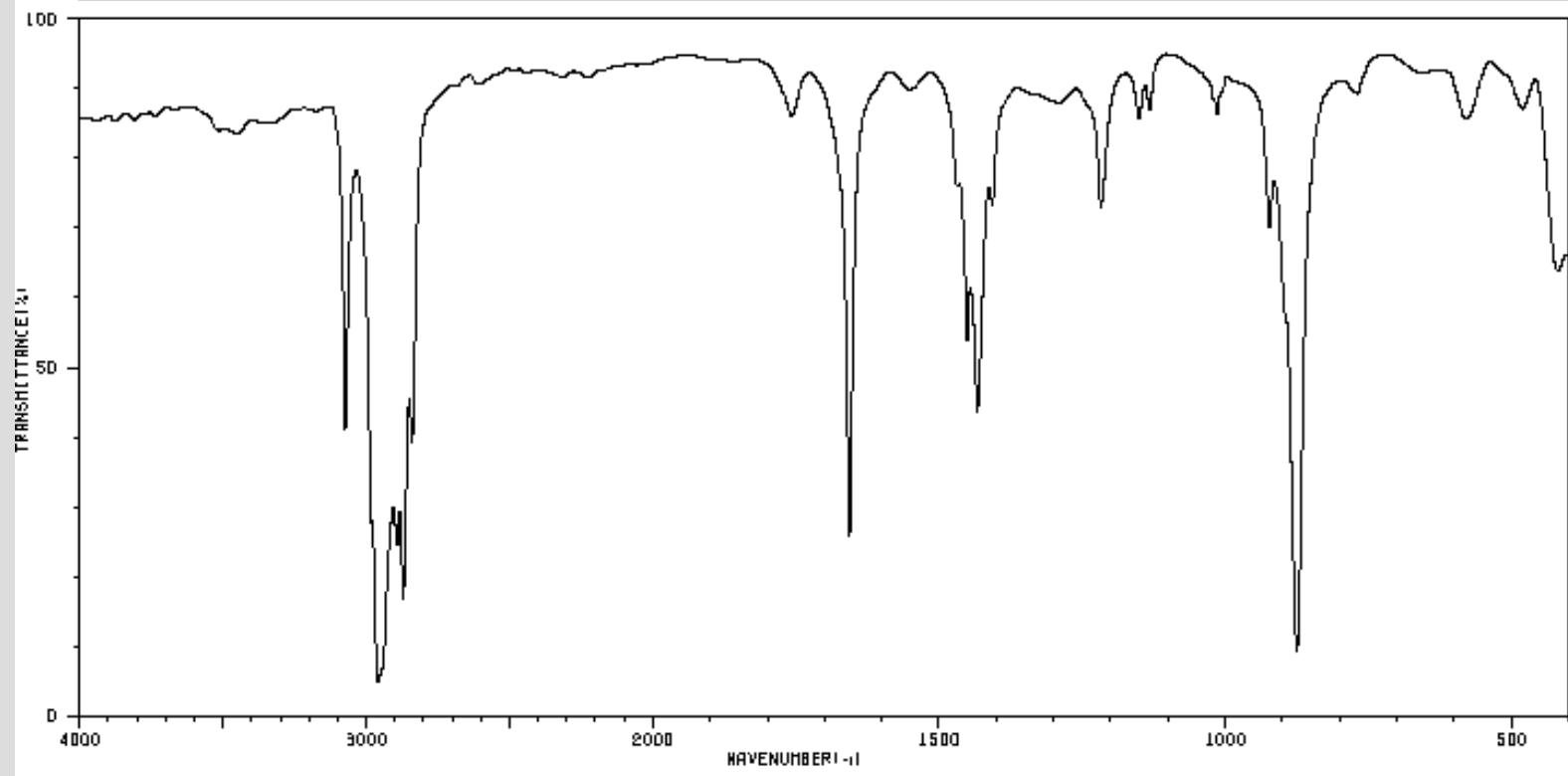
C₅H₈O₂



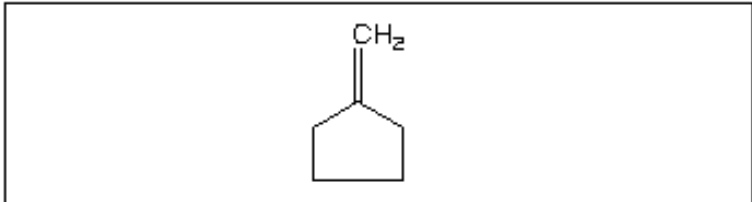
3619	72	1664	86	1225	33	960	62	466	55
3497	68	1481	77	1187	36	863	55		
2985	35	1449	57	1165	26	838	55		
2938	49	1408	46	1121	26	726	86		
2874	42	1372	44	1088	36	669	62		
2696	84	1357	55	1069	15	605	84		
1760	4	1288	66	993	46	600	84		



HIT-NO=6401 SCORE= () SDBS-NO=22681 IR-NIDA-38238 : LIQUID FILM
 METHYLENECYCLOPENTANE
 C_6H_{10}



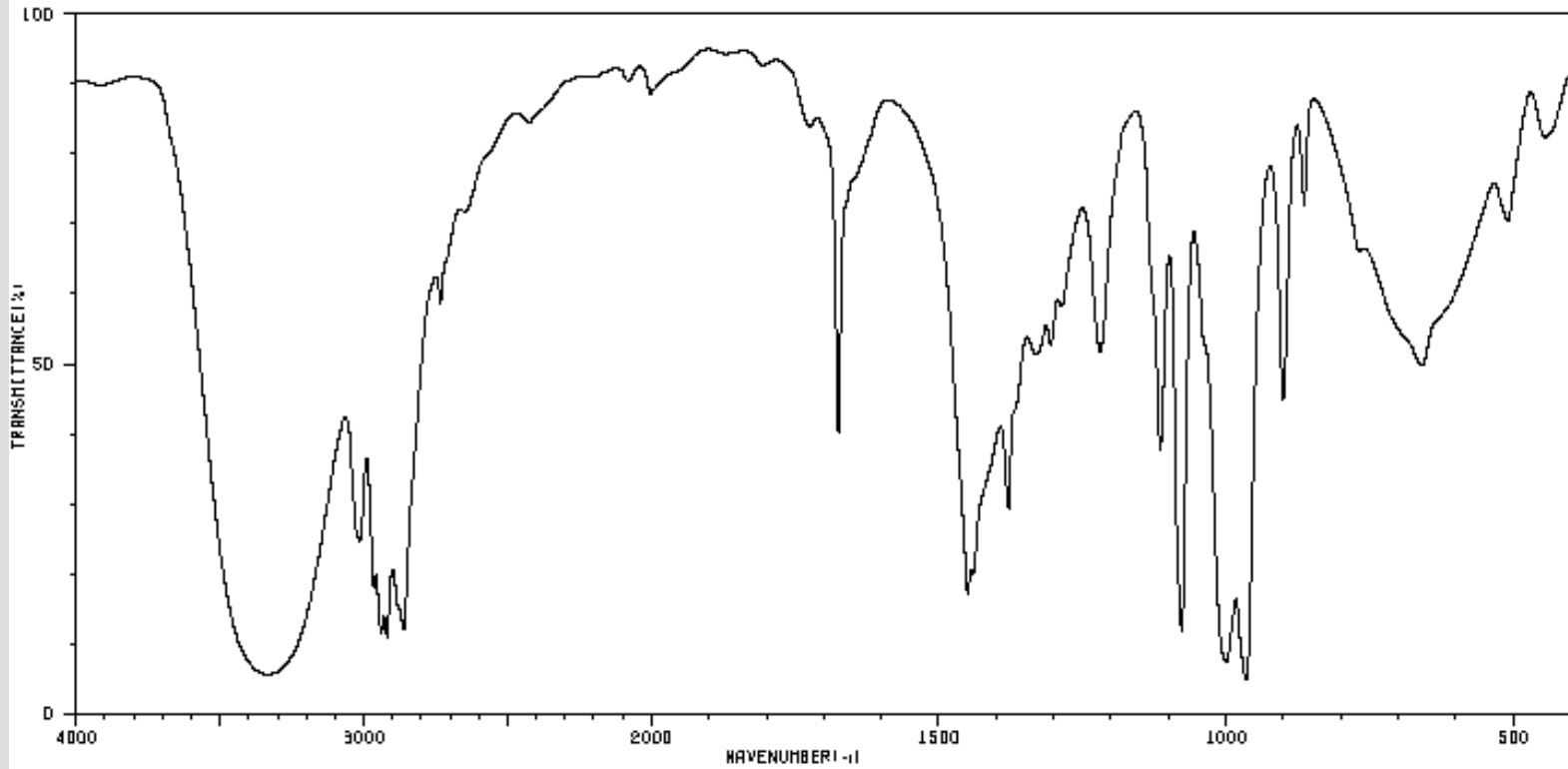
3073	39	1662	86	1023	84	481	84
2958	4	1452	52	1014	84		
2892	23	1433	42	925	88		
2871	16	1407	70	876	9		
2840	37	1218	70	775	88		
1758	84	1150	81	770	86		
1657	25	1131	84	678	81		



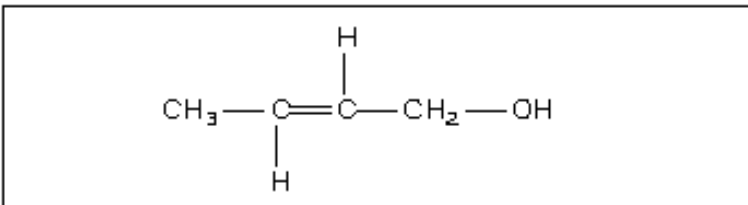
HIT-NO=1625 SCORE= () SDBS-NO=1888 IR-NIDA-03508 : LIQUID FILM

TRANS-2-BUTEN-1-OL

C₄H₈O



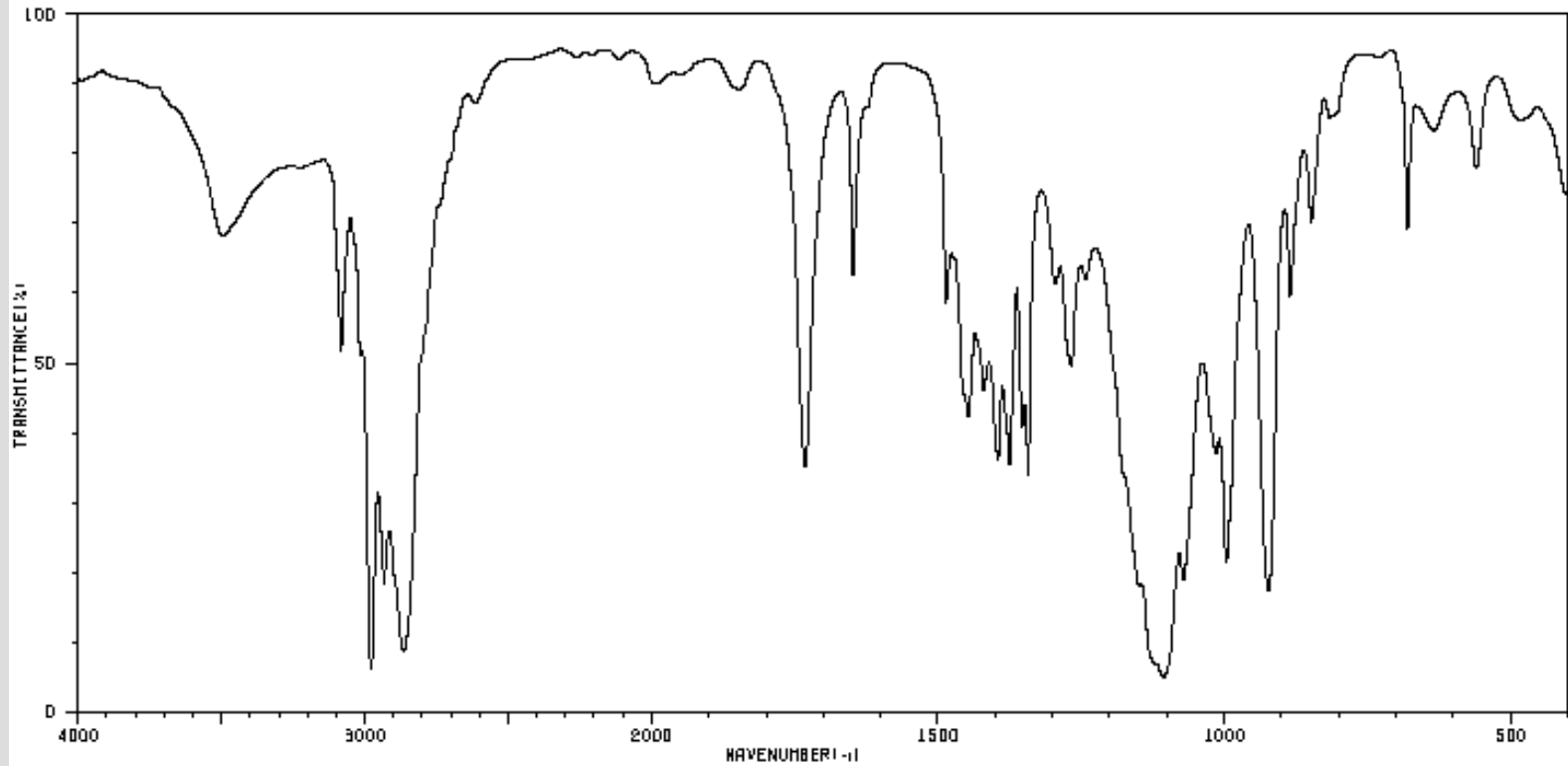
3014	23	2004	86	1330	60	900	49
2965	17	1992	86	1305	50	864	70
2940	11	1724	81	1219	50	673	50
2920	10	1676	38	1114	36	669	49
2861	12	1450	17	1077	11	511	68
2734	57	1440	19	1000	7	444	79
2426	81	1379	28	966	4		



HIT-NO=6241 SCORE= () SDBS-NO=21918 IR-NIDA-29522 : LIQUID FILM

ALLYL ETHYL ETHER

C₅H₁₀O



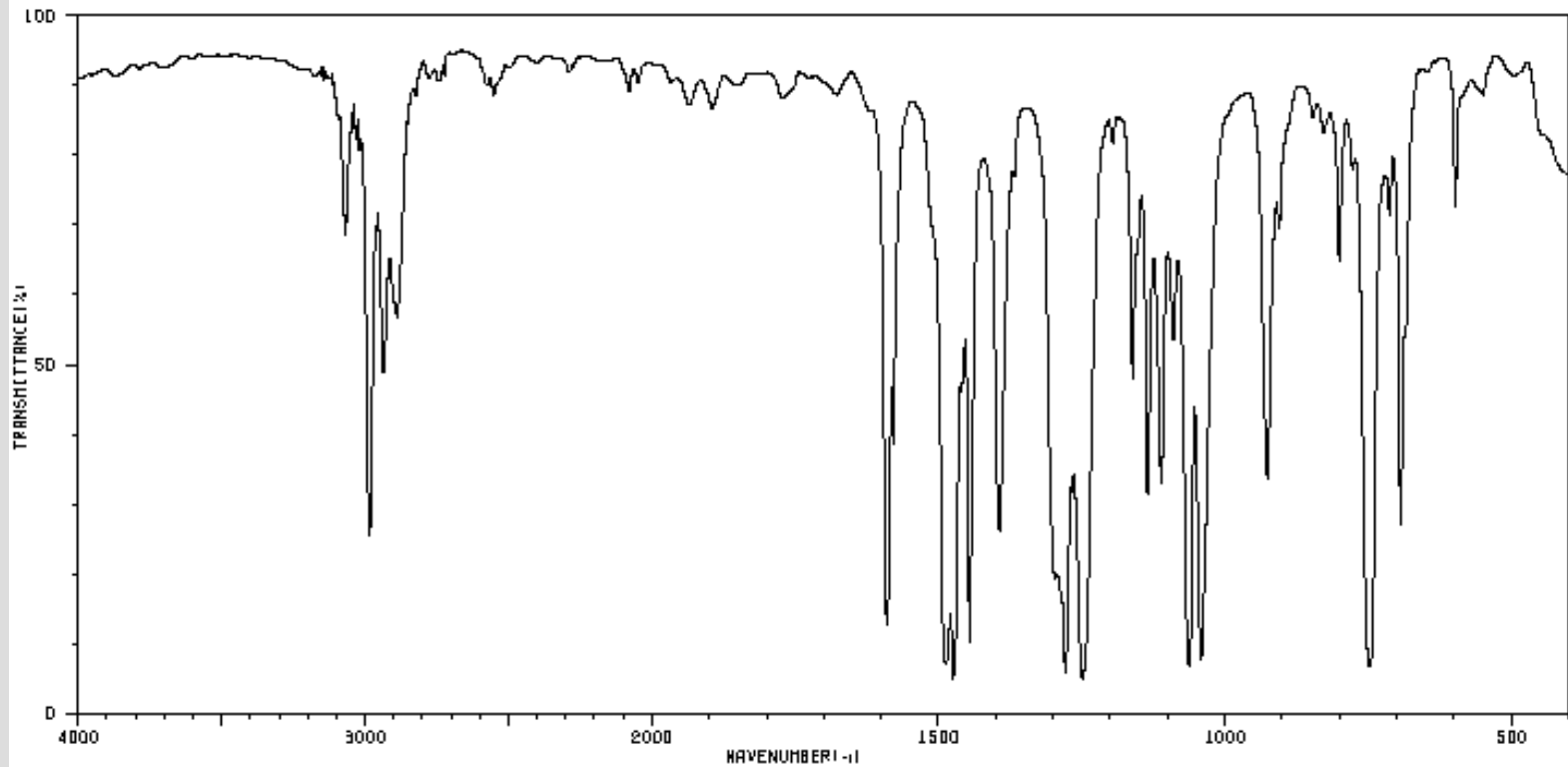
3494	66	1486	67	1343	32	1016	36	804	61
3082	49	1456	43	1296	58	996	20	680	66
2978	5	1447	41	1268	47	923	16	634	79
2932	17	1420	44	1242	60	886	57	566	79
2865	8	1396	35	1118	6	849	68	560	74
1732	34	1375	34	1106	4	816	81	485	61
1649	60	1353	38	1071	18	810	81	480	81



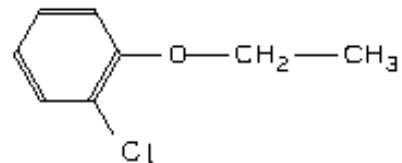
HIT-NO=3245 SCORE= () SDBS-NO=6160 IR-NIDA-58307 : LIQUID FILM

O-CHLOROPHENETOLE

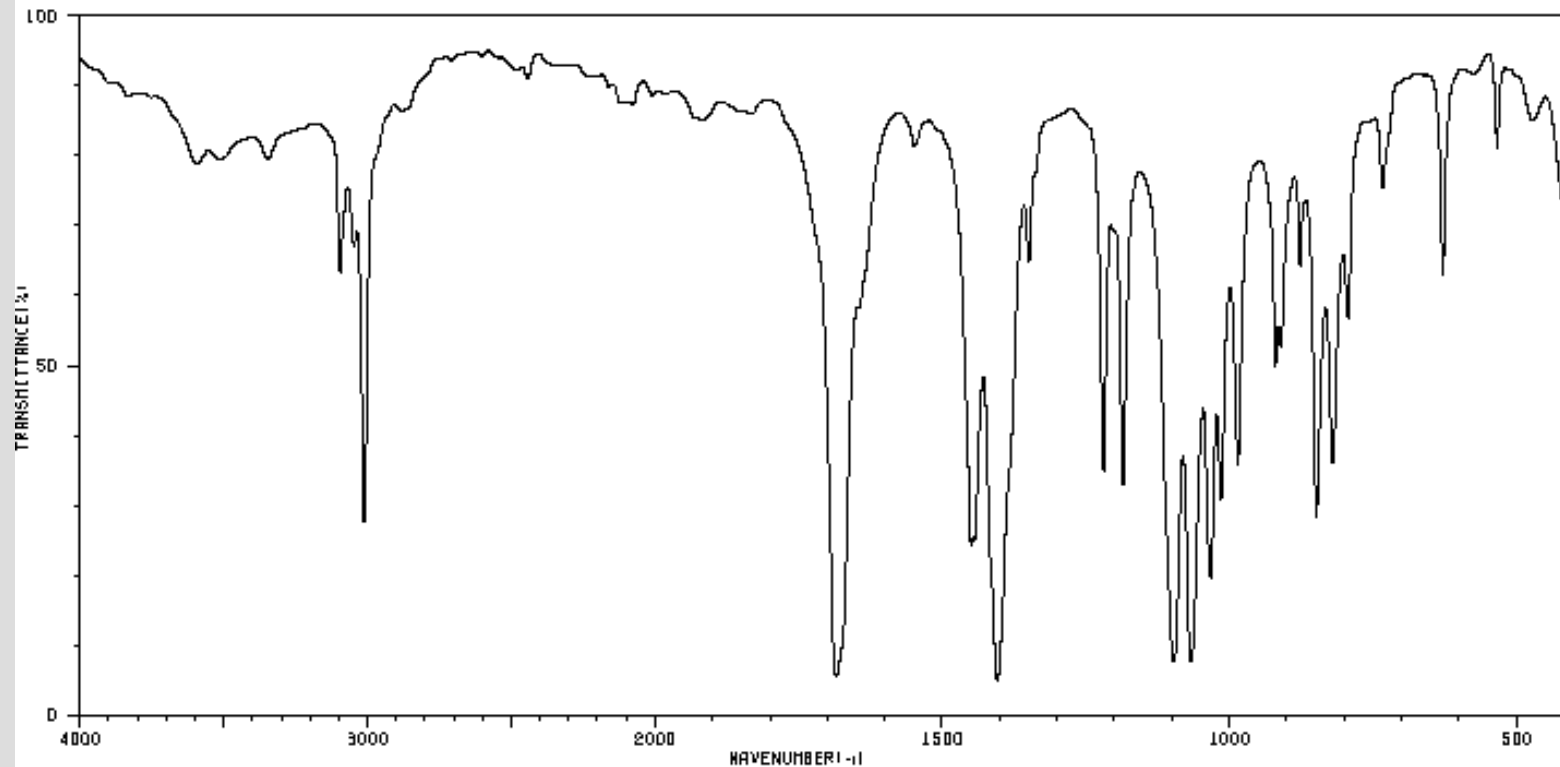
C₆H₅ClO



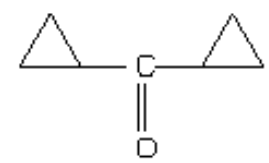
3078	74	2889	66	1394	26	1111	31	801	62
3068	66	1590	12	1298	18	1090	52	778	74
3020	77	1579	37	1279	5	1062	6	748	6
2984	24	1487	6	1249	4	1042	7	713	68
2936	47	1474	4	1196	79	926	32	693	26
2926	53	1460	44	1162	46	905	66	665	52
2899	67	1446	9	1135	30	827	78	698	70



HIT-NO=3900 SCORE= () SDBS-NO=8552 IR-NIDA-24656 : LIQUID FILM
 DICYCLOPROPYL KETONE
 $C_7H_{10}O$



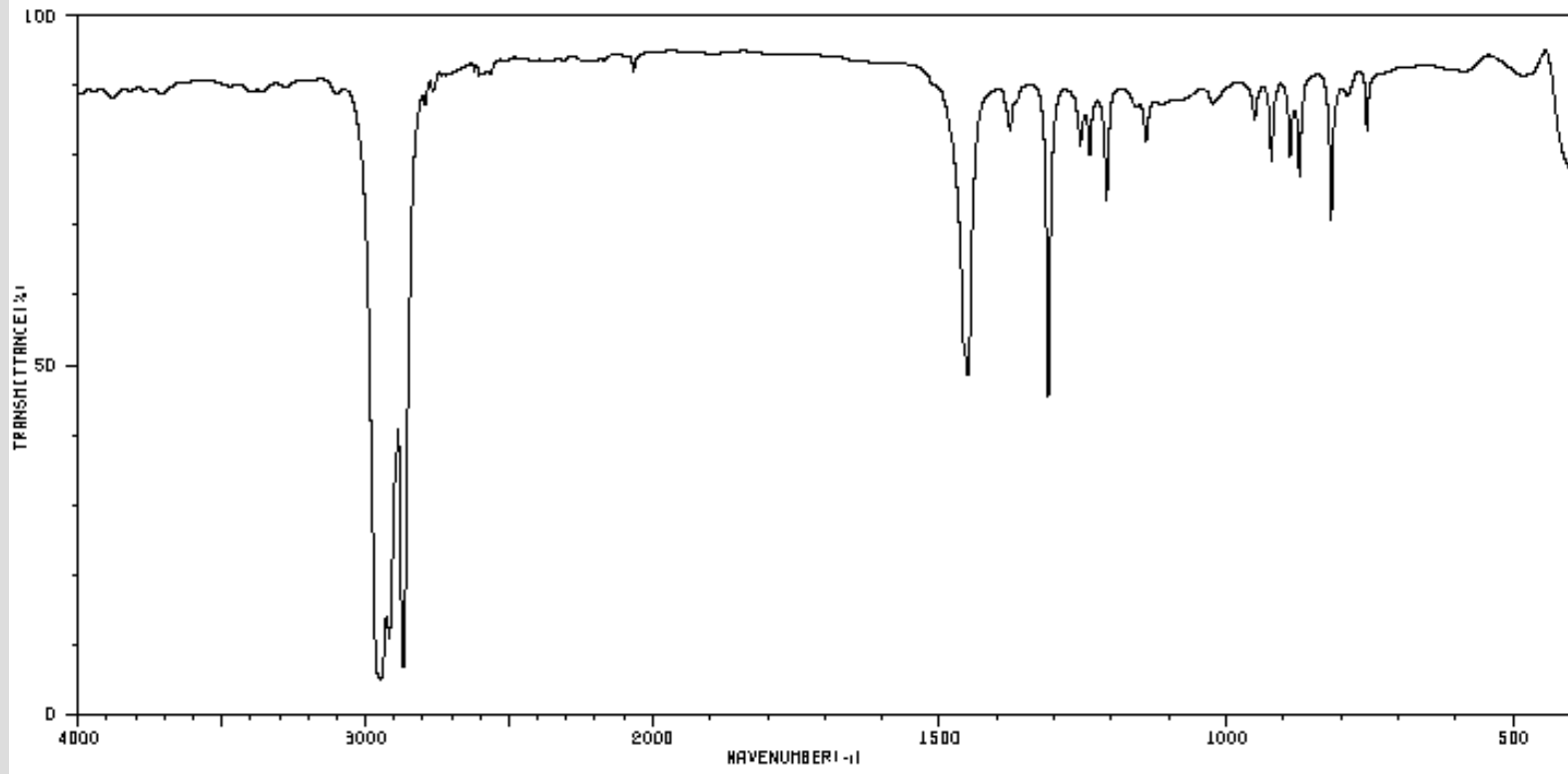
3692	77	2093	84	1444	23	1033	18	833	55
3511	77	1924	81	1404	4	1015	29	820	34
3346	77	1918	81	1349	82	985	34	794	55
3096	60	1913	81	1219	33	920	47	733	72
3046	64	1684	5	1185	32	911	50	629	60
3011	26	1548	79	1097	7	877	62	534	77
2107	84	1460	29	1067	7	849	26	472	81



HIT-NO=5762 SCORE= () SDBS-NO=13576 IR-NIDA-68177 : NUJOL MULL

NORBORNANE

C₇H₁₂



3881	84	1378	81	1140	79	873	74
2946	4	1367	84	1025	84	818	68
2917	10	1311	45	1019	84	755	78
2868	6	1266	79	1013	84		
2792	84	1246	81	951	81		
2763	86	1239	77	921	77		
1452	46	1209	70	889	77		

