

Supporting Information for

## **Calculation of infrared spectra of organophosphorus compounds and prediction of new types of nerve agents**

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**Table S1.** Assignment to major peaks for each OP compound

Peak Assignment	Wavenumber (cm <sup>-1</sup> )					
	Experiment	M06-2X	M06-2X(Scaled)	B3LYP	B3LYP(Scaled)	
Methyldiphenylphosphine Oxide	P=O str	1169	1232	1178.9	1196	1215
	P-C str	1303	1330	1272.7	1332	1305
	C=C str (aroma)	1439	1477	1413.3	1468	1443
	C-H str	2909	3171	3034.3	3044	2940
	C-H str	2978	3199	3061.1	3132	3071
	C-H str (aroma)	3052	3227	3087.9	3188	3083
Triphenylphosphine Oxide	C-H bending	1108	1140	1090.9	1100	1106
	P=O str	1271	1316	1259.3	1295	1274
	P=O str	1439	1484	1420	1441	1470
	C=C str	1587	1660	1588.5	1583	1624
	C-H str	3063	3228	3088.9	3072	3199
tris(bromomethyl)phosphine Oxide	P=O str	1119	1148	1098.5	1120	1111
	P=O str	1182	1228	1175.1	1190	1213
	C=C str (aroma)	1311	1356	1297.6	1351	1332
	C=C str (aroma)	1438	1476	1412.4	1463	1441
	C-H str (aroma)	3056	3228	3088.9	3192	3082
Triethylphosphine Oxide	P=O str	1209	1281	1225.8	1246	1260
	C-H bending	1378	1428	1366.5	1428	1396
	C-H str	2936	3122	2987.4	3101	2994
	C-H str	3002	3192	3054.4	3171	3060
Phenylphosphonic dichloride	P=O str	1156	1211	1158.8	1183	1201
	C-H bending	1248	1281	1225.8	1274	1258
	C-H bending	1270	1295	1239.2	1295	1277
	C-H bending	1378	1414	1353.1	1414	1386

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C-H bending	1412	1456	1393.1	1456	1426
C-H bending	1457	1512	1393.2	1505	1470
C-H str	2880	3059	1446.8	3031	2929

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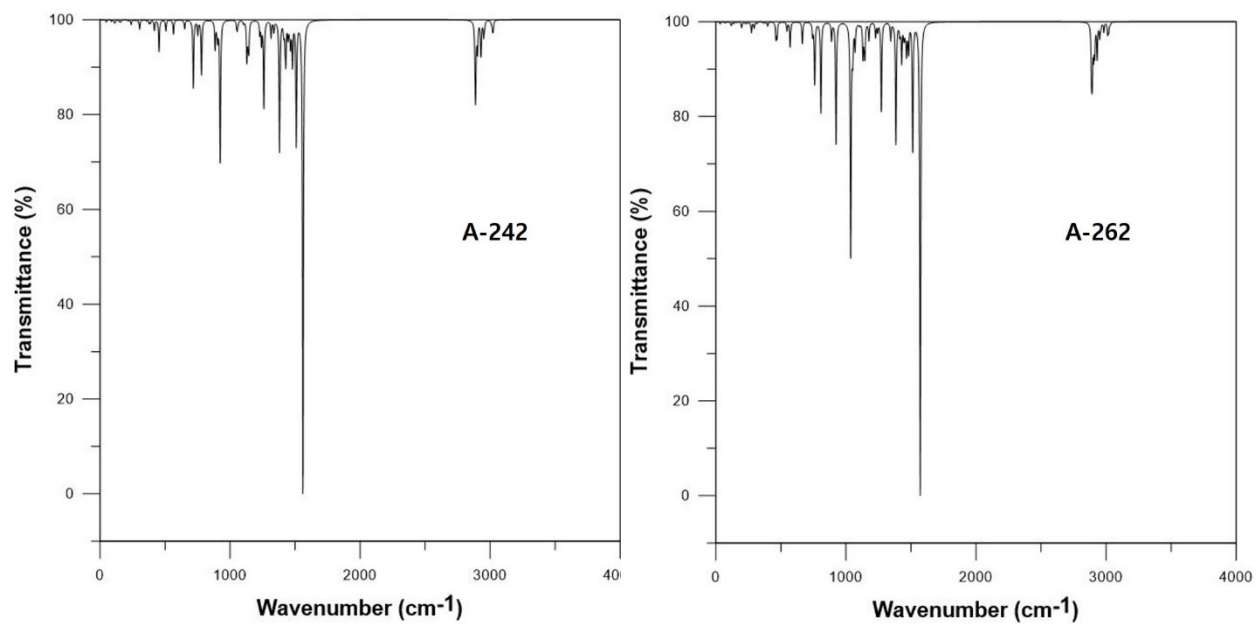
**Table S2.** Assignment to major peaks for each nerve agent

Peak Assignment	Wavenumber (cm <sup>-1</sup> )					
	Experiment	M06-2X	M06-2X(Scaled)	B3LYP	B3LYP(Scaled)	
GA(Tabun)	P-O-C str	1008.2	1008	964.6	973	1023
	P=O str	1266	1309	1252.6	1267	1270
	CH <sub>3</sub> def	1458.9	1505	1440.1	1498	1464
	CH <sub>3</sub> def	1490.1	1526	1460.2	1526	1486
	C≡N str	2201.2	2380	2277.4	2310	2234
	C-H str	2911.4	3045	2913.8	3010	2888
GB(Sarin)	P-O-C str	1034	1064	1018.1	1008	1005
	P=O str	1277	1337	1279.4	1309	1313
	P-CH <sub>3</sub> sym def	1322	1365	1306.2	1351	1339
	CH <sub>3</sub> def	1475	1512	1446.8	1512	1471
	C-H str	2928	3059	2927.2	3031	2911
	C-H str	2965	3157	3020.9	3108	2983
GD(Soman)	P-O-C str	1017	1057	1011.4	1022	1005
	P=O str	1276	1344	1286.1	1309	1312
	P-CH <sub>3</sub> sym	1321	1372	1312.9	1351	1336
	CH <sub>3</sub> def	1484	1533	1466.9	1526	1487
	C-H str	2927	3052	2920.5	3024	2902
	C-H str	2964	3143	3007.5	3087	2961
GF (Cyclosarin)	P-O-C str	1017	1106	1058.3	1022	1006
	P=O str	1278	1337	1279.4	1309	1312
	P-CH <sub>3</sub> sym	1321	1372	1312.9	1351	1339
	CH <sub>2</sub> Bending	1452	1498	1433.4	1498	1460
	C-H str	2861	3052	2920.5	3010	2892
	C-H str	2939	3108	2974	3031	2935
	C-H str	2996	3178	3041	3059	3010
VX	P-O-C str	1035	1116	1067.9	1060	1026
	P=O str	1233	1292	1236.3	1236	1262
	P-CH <sub>3</sub> sym	1300	1340	1282.2	1252	1308
	P-CH <sub>3</sub> asym	1383	1436	1374.1	1428	1392

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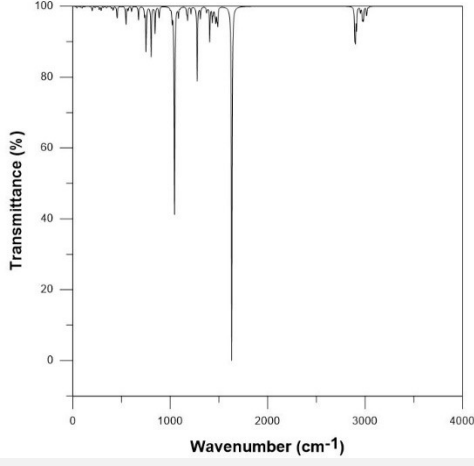
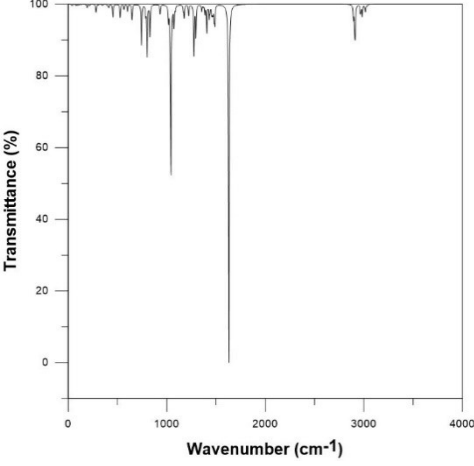
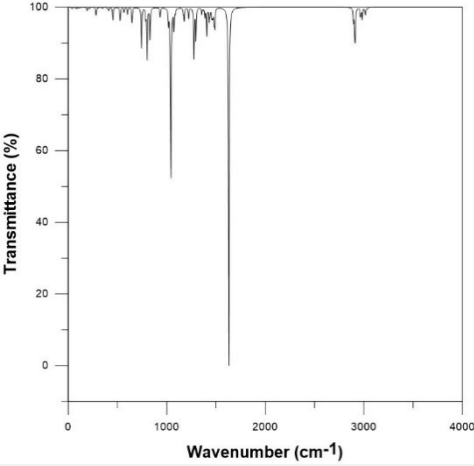
CH <sub>2</sub> bending	1477	1516	1450.7	1516	1475
C-H str	2873	3060	2928.1	3020	2897
C-H str	2967	3132	2997	3092	2964

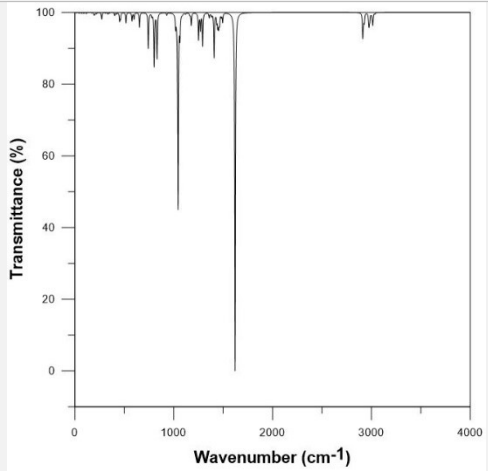
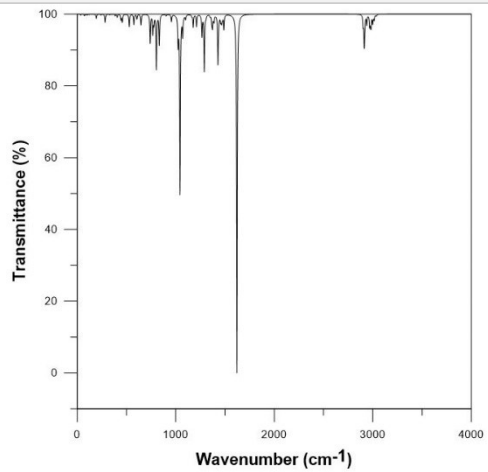
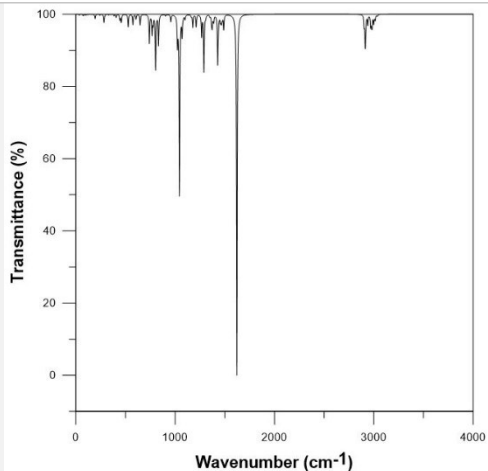
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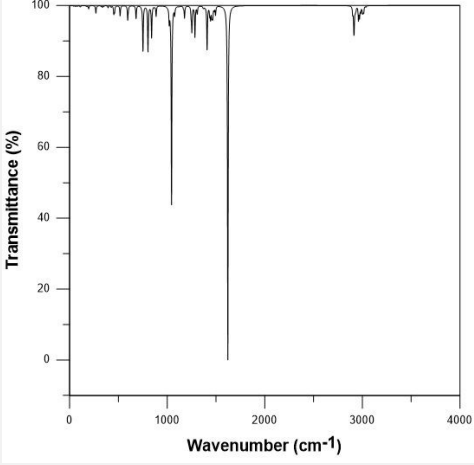
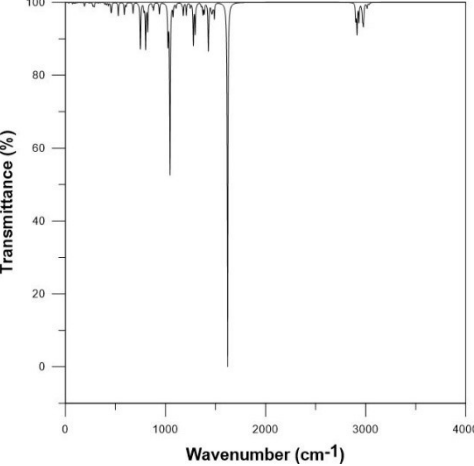
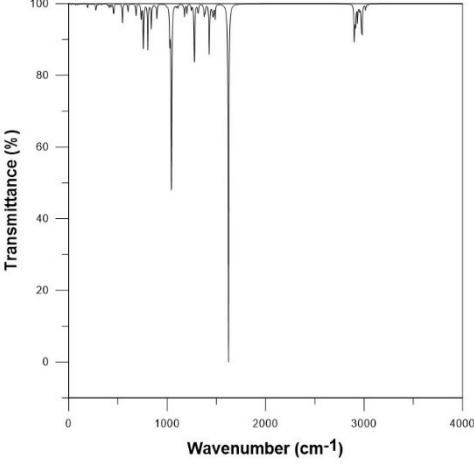
**Figure S1.** IR-spectra derived from DFT calculation for A-242 and A-262

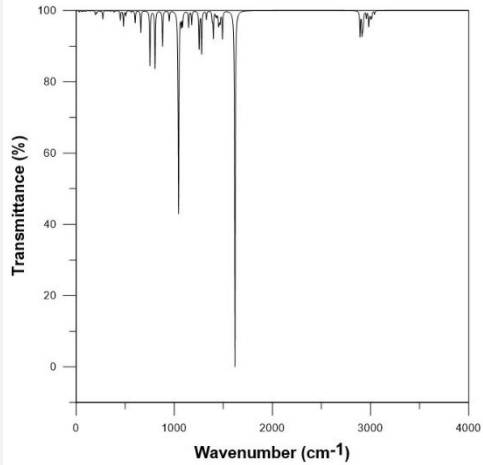
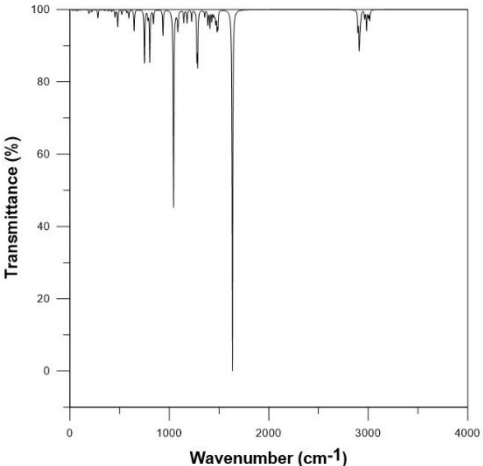
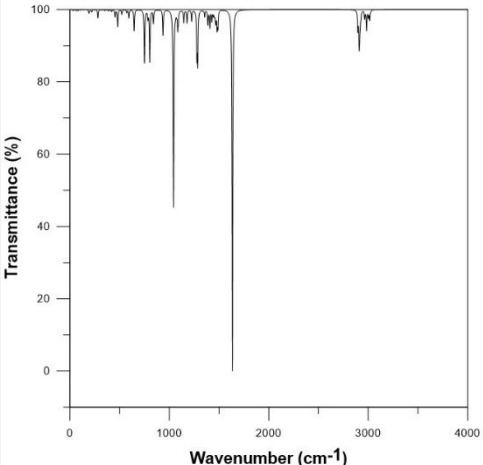
**Table S3.** Novichok candidates obtained through alkyl group substitution

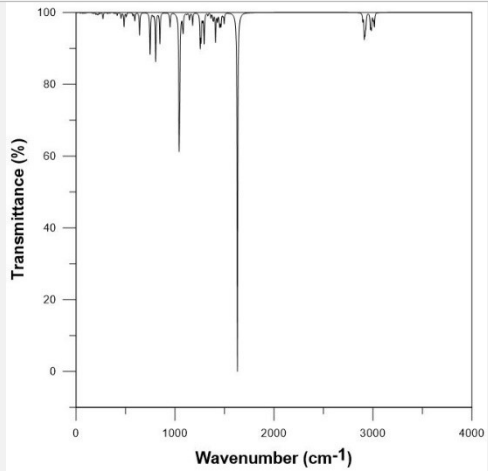
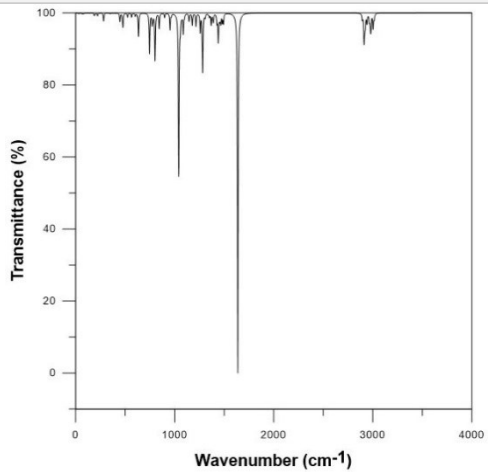
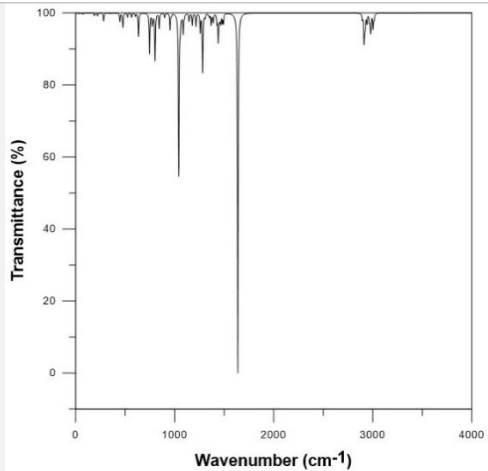
Structure Name	IR Spectra
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1112	
1113	

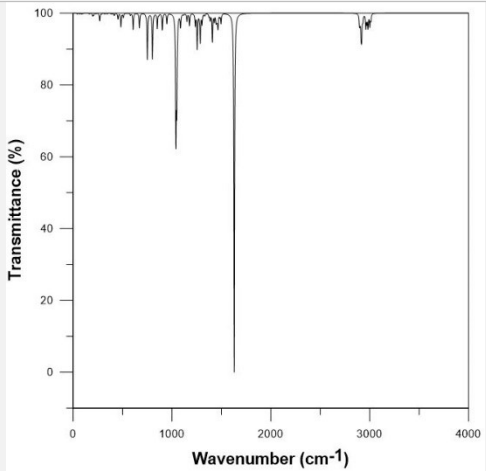
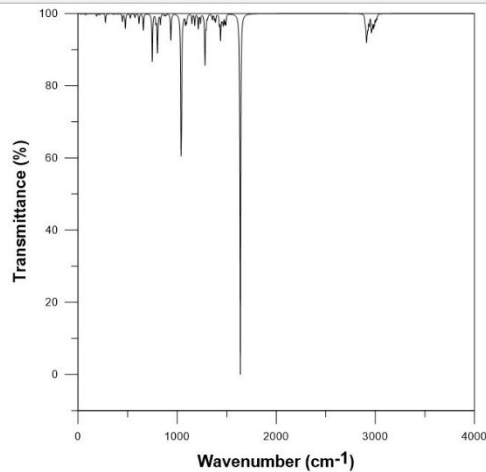
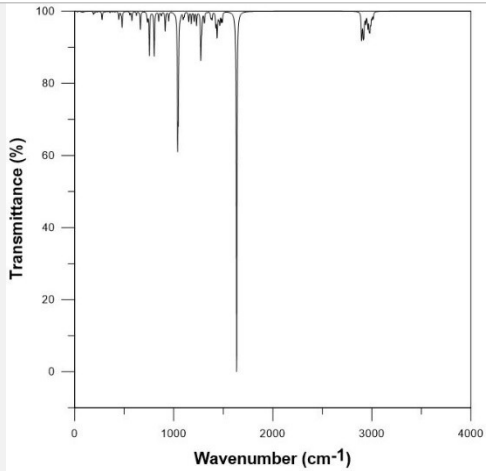
Structure Name	IR Spectra
1121	 <p>The IR spectrum for structure 1121 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
1122	 <p>The IR spectrum for structure 1122 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
1123	 <p>The IR spectrum for structure 1123 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>

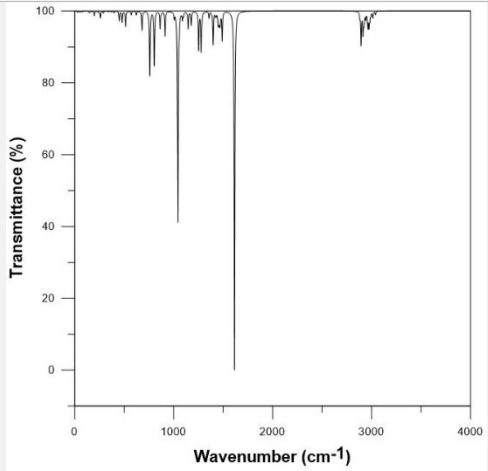
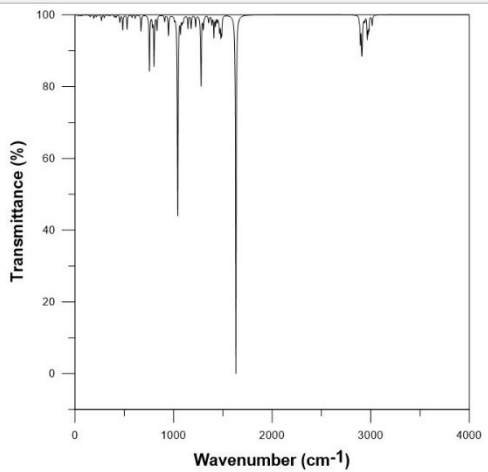
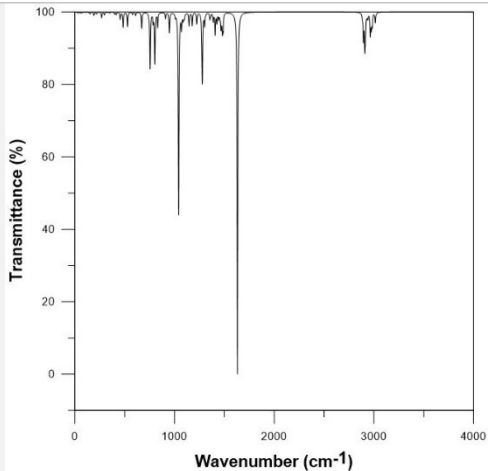


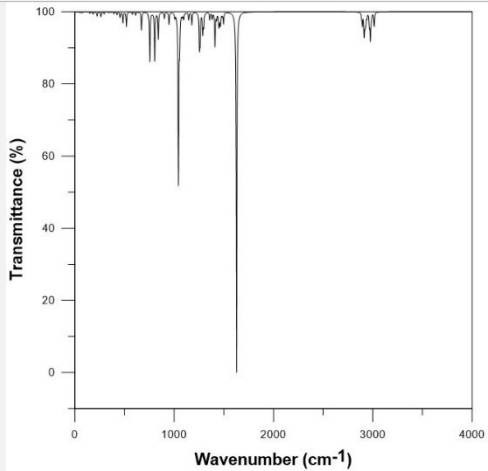
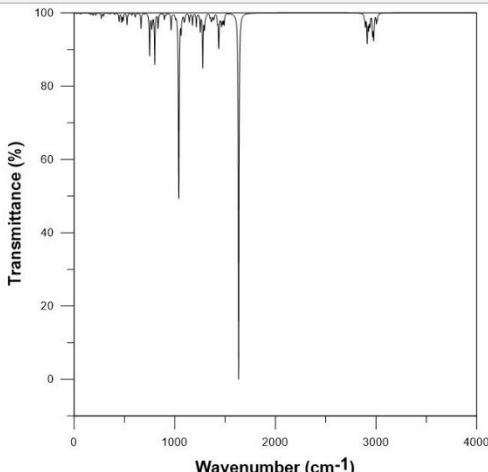
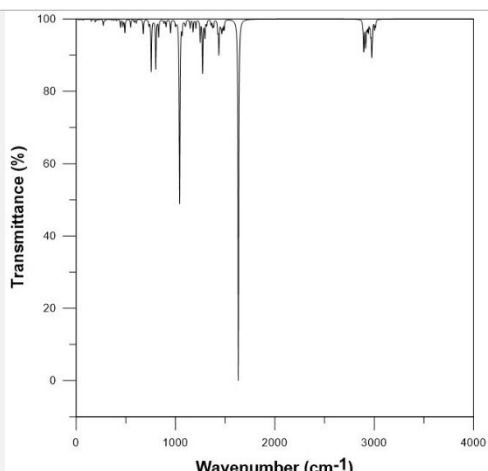
Structure Name	IR Spectra
1131	 <p>The IR spectrum for structure 1131 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1600 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are no significant peaks in the 3000-3600 cm<sup>-1</sup> range.</p>
1132	 <p>The IR spectrum for structure 1132 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1600 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are no significant peaks in the 3000-3600 cm<sup>-1</sup> range.</p>
1133	 <p>The IR spectrum for structure 1133 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1600 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are no significant peaks in the 3000-3600 cm<sup>-1</sup> range.</p>

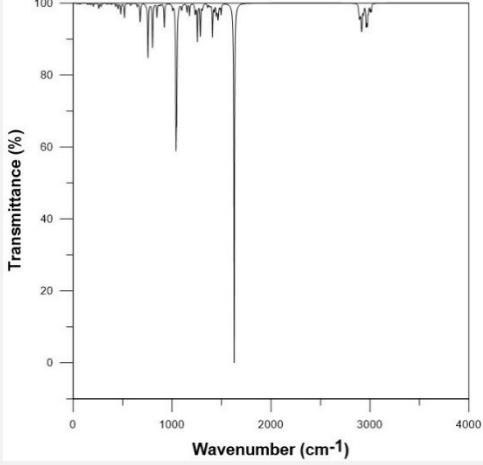
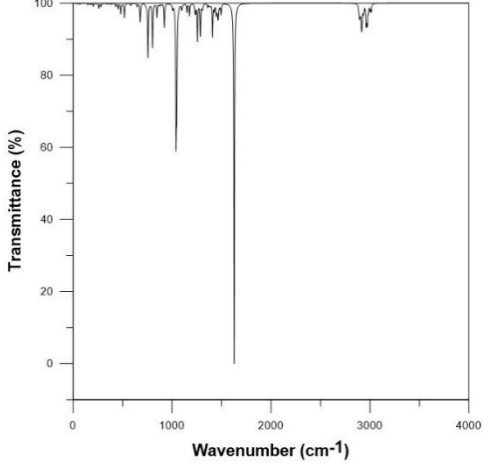
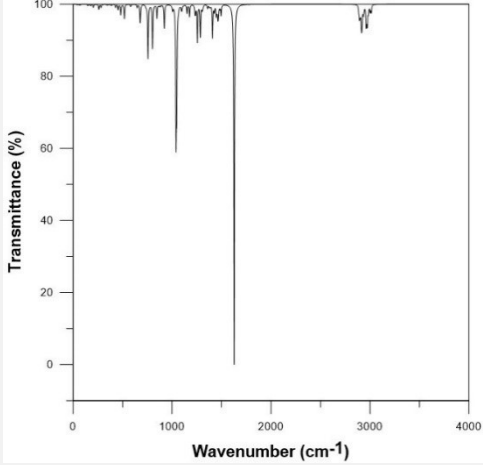
Structure Name	IR Spectra
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<b>1212</b>	
<b>1213</b>	

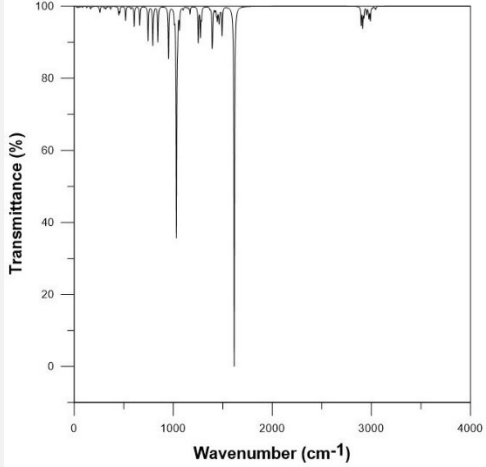
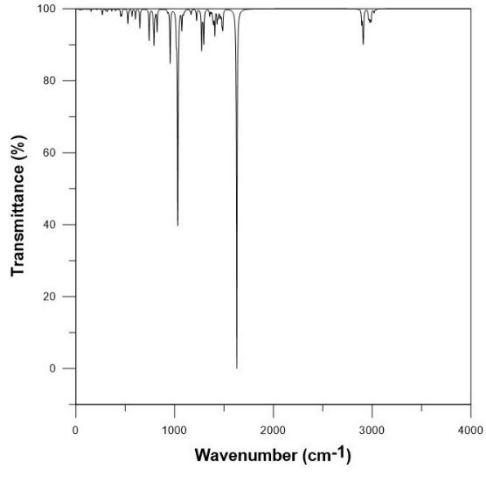
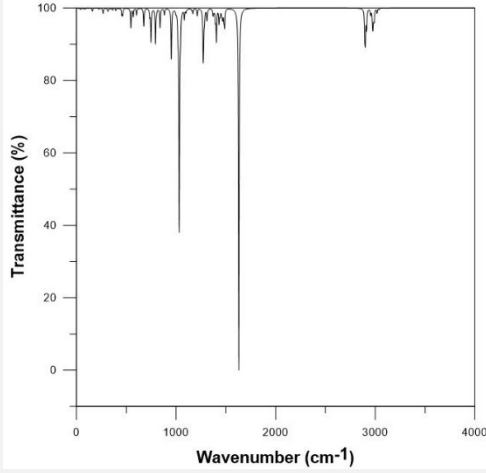
Structure Name	IR Spectra
1221	 <p>The IR spectrum for structure 1221 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and intense absorption peak at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
1222	 <p>The IR spectrum for structure 1222 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and intense absorption peak at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
1223	 <p>The IR spectrum for structure 1223 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and intense absorption peak at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>

Structure Name	IR Spectra
1231	
1232	
1233	

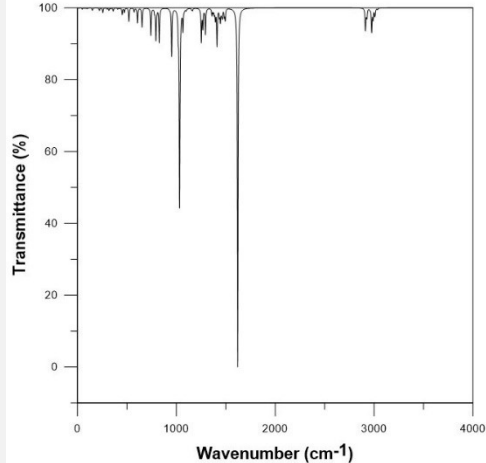
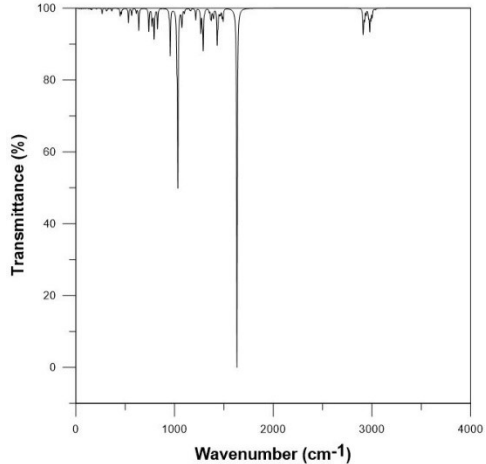
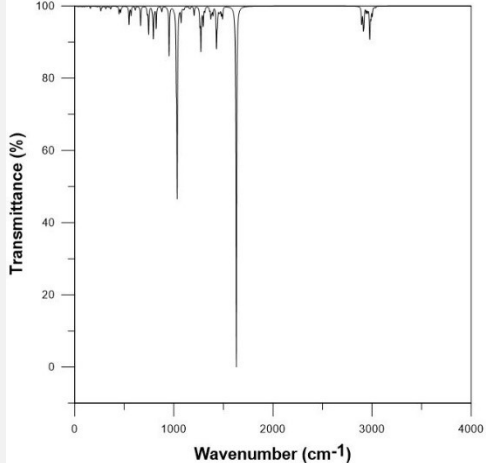
Structure Name	IR Spectra
<p style="text-align: center;"><b>1311</b></p>	 <p>The IR spectrum for structure 1311 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key absorption bands include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (aromatic C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
<p style="text-align: center;"><b>1312</b></p>	 <p>The IR spectrum for structure 1312 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key absorption bands include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (aromatic C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
<p style="text-align: center;"><b>1313</b></p>	 <p>The IR spectrum for structure 1313 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key absorption bands include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (aromatic C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>

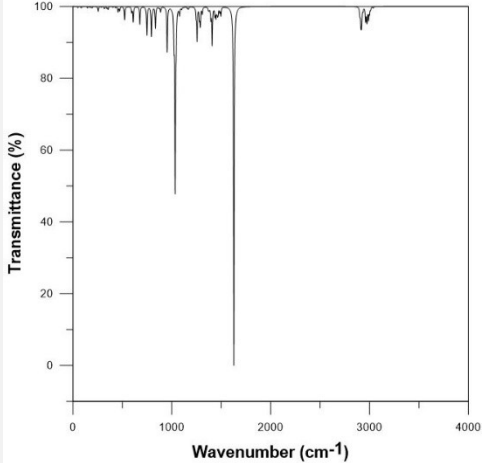
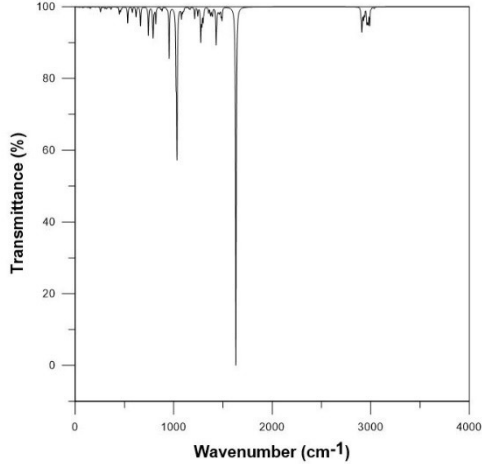
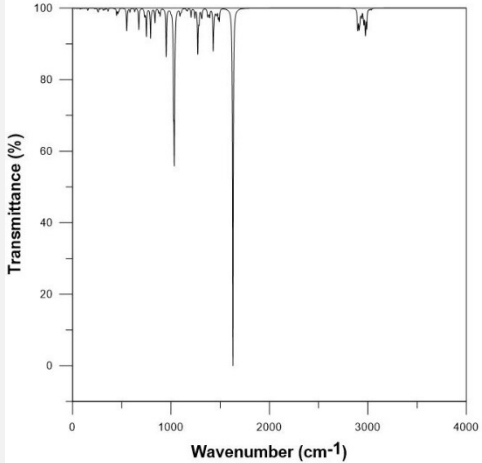
Structure Name	IR Spectra
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1322	
1323	

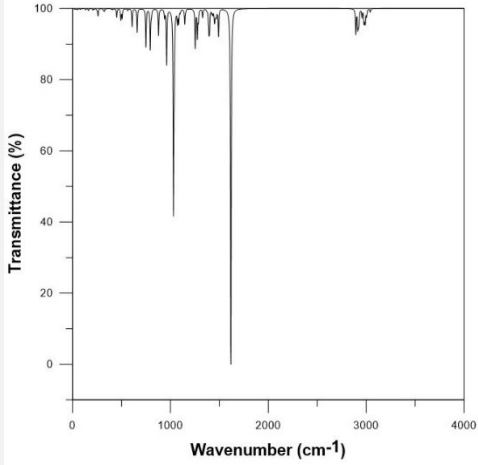
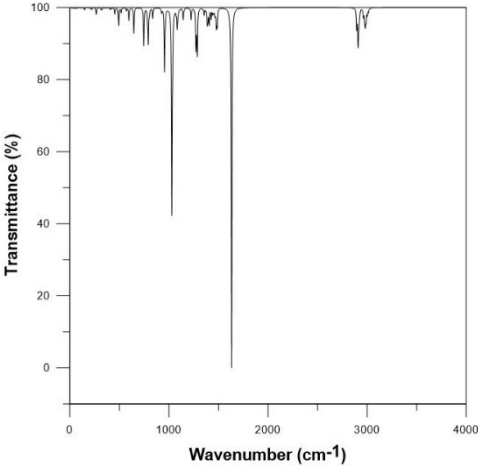
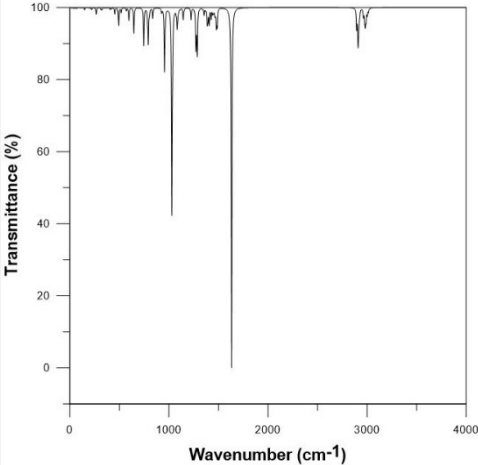
Structure Name	IR Spectra
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<b>1332</b>	
<b>1333</b>	

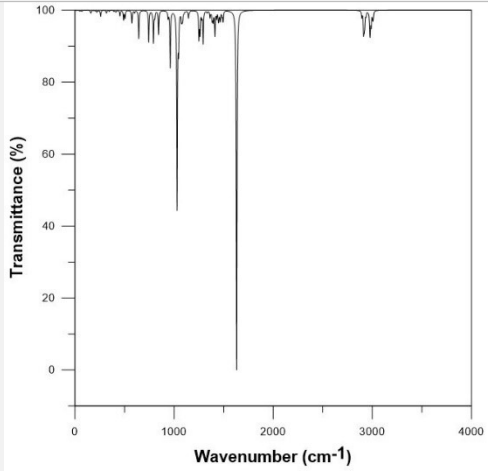
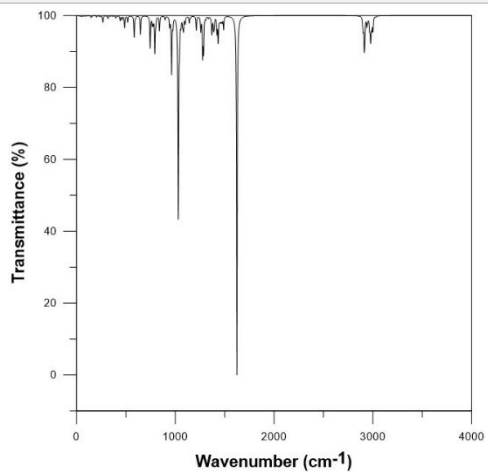
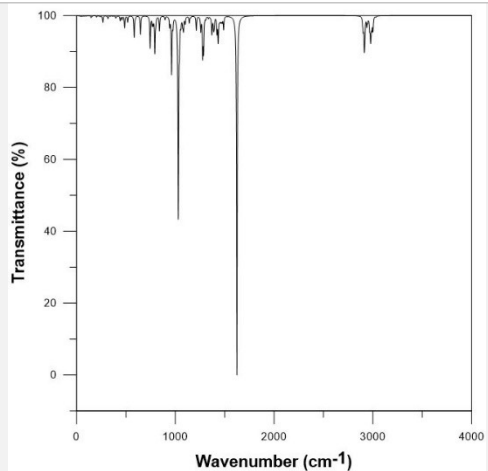
Structure Name	IR Spectra
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2112	
2113	

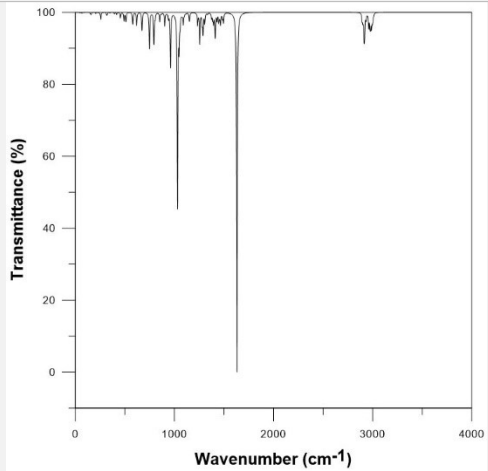
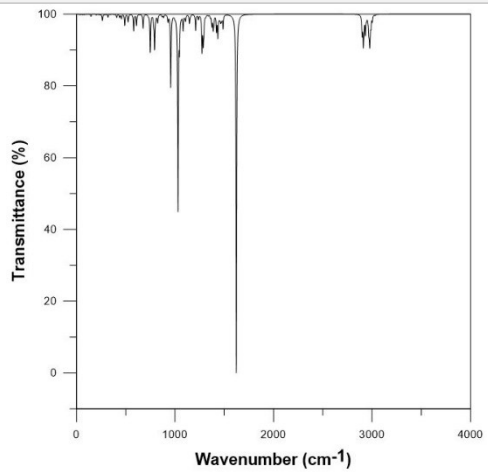
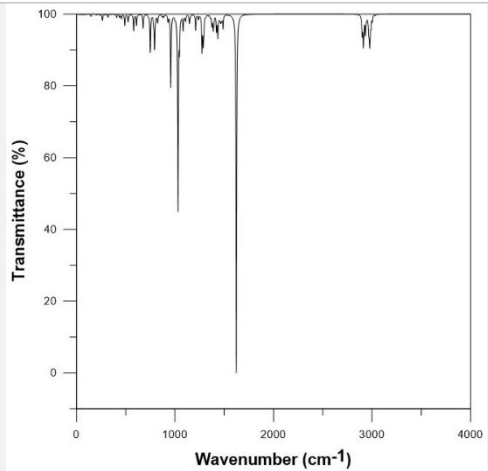


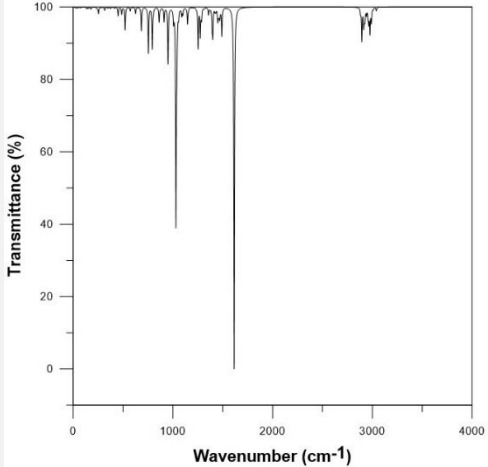
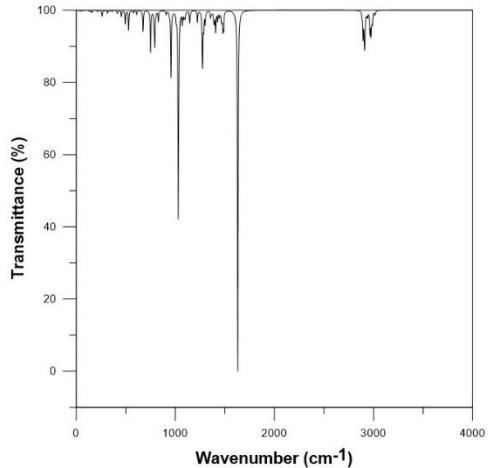
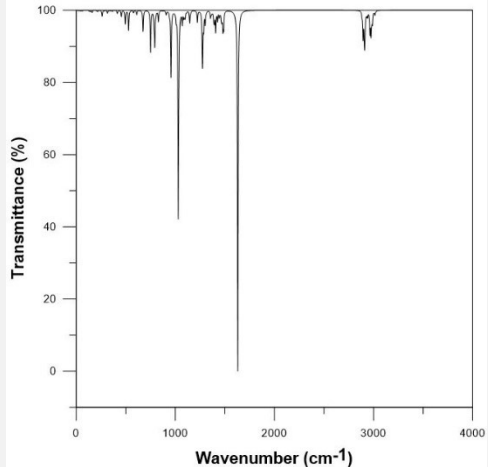
Structure Name	IR Spectra
2121	 <p>The IR spectrum for structure 2121 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Significant absorption bands are observed at approximately 1715 cm<sup>-1</sup> (strong, sharp peak), 1640 cm<sup>-1</sup> (medium peak), 1600 cm<sup>-1</sup> (medium peak), 1510 cm<sup>-1</sup> (medium peak), 1450 cm<sup>-1</sup> (medium peak), 1380 cm<sup>-1</sup> (medium peak), 1270 cm<sup>-1</sup> (medium peak), 1100 cm<sup>-1</sup> (medium peak), and 710 cm<sup>-1</sup> (medium peak). There are also several smaller peaks in the fingerprint region between 1000 and 1500 cm<sup>-1</sup>.</p>
2122	 <p>The IR spectrum for structure 2122 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Significant absorption bands are observed at approximately 1715 cm<sup>-1</sup> (strong, sharp peak), 1640 cm<sup>-1</sup> (medium peak), 1600 cm<sup>-1</sup> (medium peak), 1510 cm<sup>-1</sup> (medium peak), 1450 cm<sup>-1</sup> (medium peak), 1380 cm<sup>-1</sup> (medium peak), 1270 cm<sup>-1</sup> (medium peak), 1100 cm<sup>-1</sup> (medium peak), and 710 cm<sup>-1</sup> (medium peak). There are also several smaller peaks in the fingerprint region between 1000 and 1500 cm<sup>-1</sup>.</p>
2123	 <p>The IR spectrum for structure 2123 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Significant absorption bands are observed at approximately 1715 cm<sup>-1</sup> (strong, sharp peak), 1640 cm<sup>-1</sup> (medium peak), 1600 cm<sup>-1</sup> (medium peak), 1510 cm<sup>-1</sup> (medium peak), 1450 cm<sup>-1</sup> (medium peak), 1380 cm<sup>-1</sup> (medium peak), 1270 cm<sup>-1</sup> (medium peak), 1100 cm<sup>-1</sup> (medium peak), and 710 cm<sup>-1</sup> (medium peak). There are also several smaller peaks in the fingerprint region between 1000 and 1500 cm<sup>-1</sup>.</p>

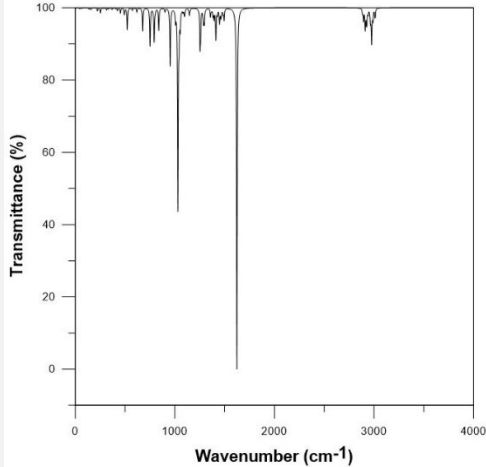
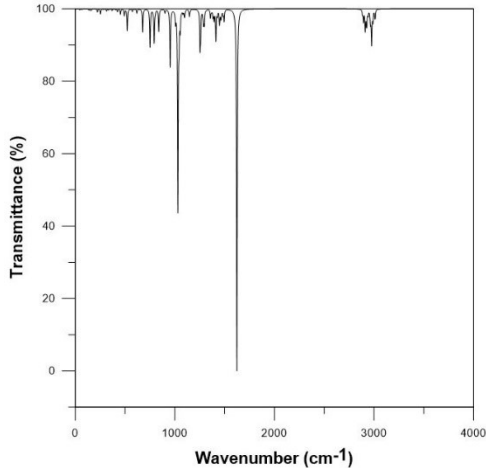
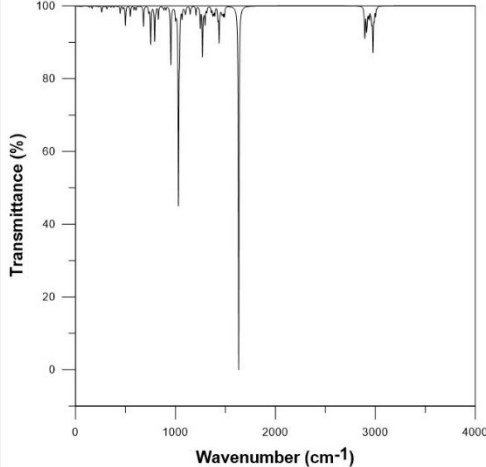
Structure Name	IR Spectra
2131	
2132	
2133	

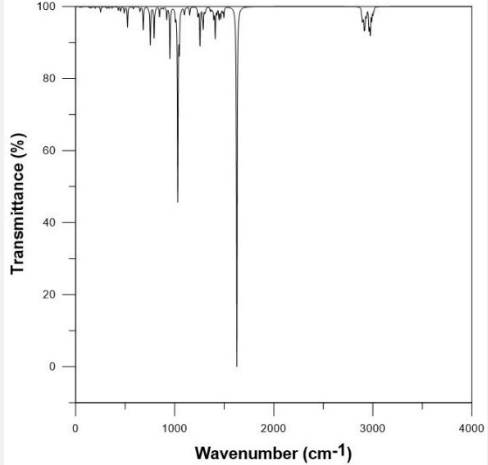
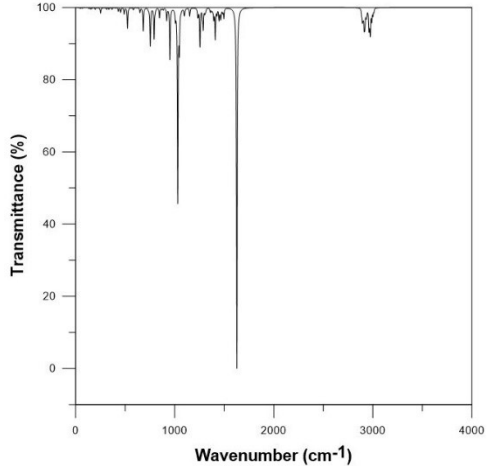
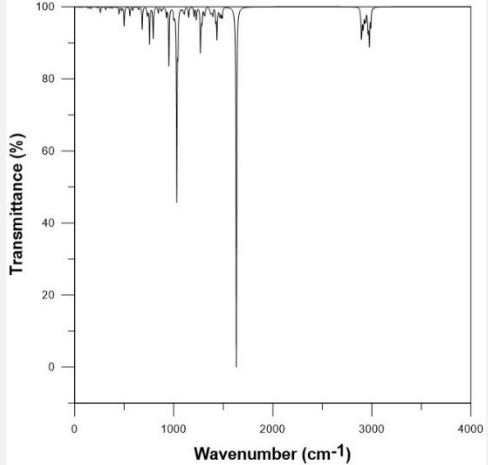
Structure Name	IR Spectra
2211	 <p>The IR spectrum for structure 2211 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and deep absorption band at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller absorption bands in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
2212	 <p>The IR spectrum for structure 2212 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and deep absorption band at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller absorption bands in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
2213	 <p>The IR spectrum for structure 2213 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. The spectrum features a very sharp and deep absorption band at approximately 1715 cm<sup>-1</sup>, characteristic of a carbonyl group. There are also several smaller absorption bands in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>

Structure Name	IR Spectra
2221	 <p>The IR spectrum for structure 2221 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Key features include a sharp peak at approximately 1700 cm<sup>-1</sup> and a broad absorption band between 3000 and 3500 cm<sup>-1</sup>.</p>
2222	 <p>The IR spectrum for structure 2222 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Key features include a sharp peak at approximately 1700 cm<sup>-1</sup> and a broad absorption band between 3000 and 3500 cm<sup>-1</sup>.</p>
2223	 <p>The IR spectrum for structure 2223 shows a transmittance plot from 0 to 4000 cm<sup>-1</sup>. The y-axis is labeled 'Transmittance (%)' and ranges from 0 to 100. The x-axis is labeled 'Wavenumber (cm<sup>-1</sup>)' and ranges from 0 to 4000. Key features include a sharp peak at approximately 1700 cm<sup>-1</sup> and a broad absorption band between 3000 and 3500 cm<sup>-1</sup>.</p>

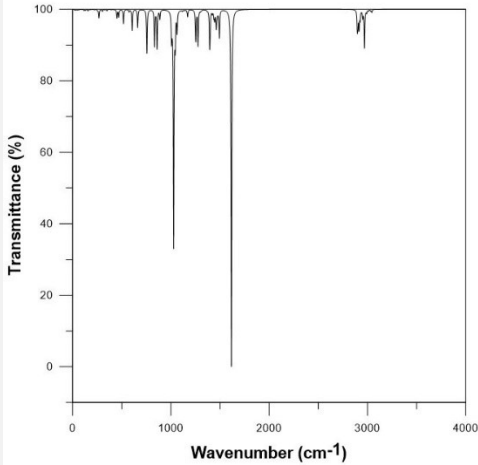
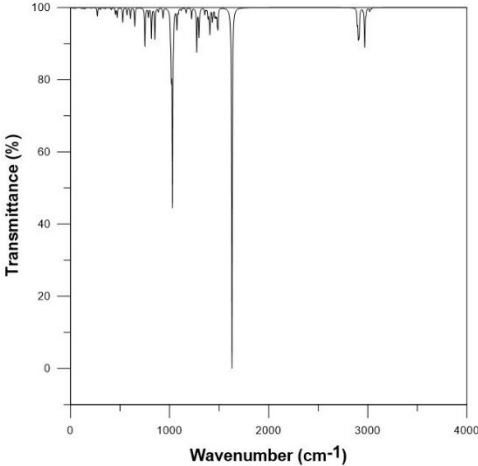
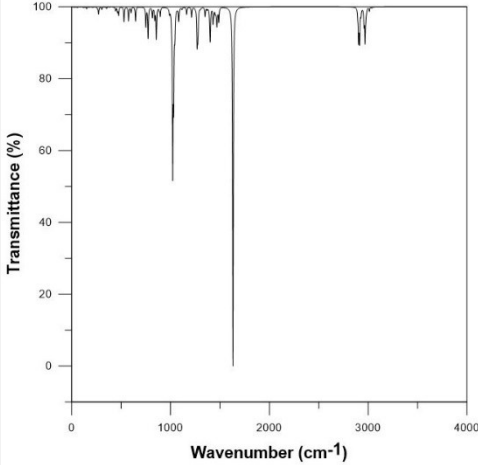
Structure Name	IR Spectra
2231	 <p>The IR spectrum for structure 2231 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a broad absorption band between 3000 and 3600 cm<sup>-1</sup> (O-H stretch). There are also several peaks in the fingerprint region below 1500 cm<sup>-1</sup>.</p>
2232	 <p>The IR spectrum for structure 2232 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a broad absorption band between 3000 and 3600 cm<sup>-1</sup> (O-H stretch). There are also several peaks in the fingerprint region below 1500 cm<sup>-1</sup>.</p>
2233	 <p>The IR spectrum for structure 2233 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a broad absorption band between 3000 and 3600 cm<sup>-1</sup> (O-H stretch). There are also several peaks in the fingerprint region below 1500 cm<sup>-1</sup>.</p>

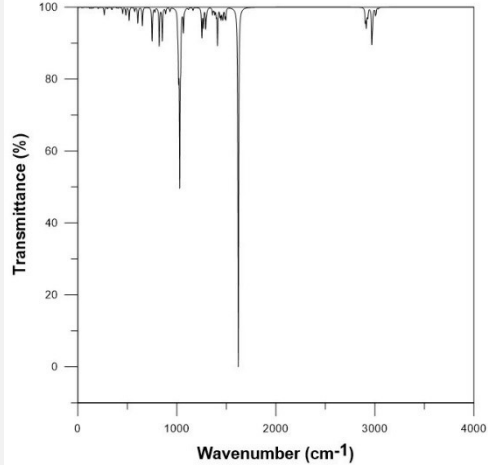
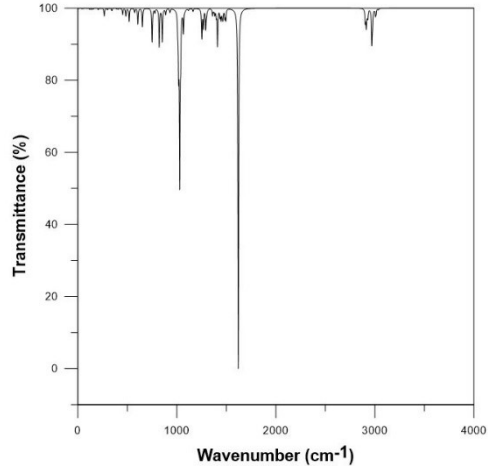
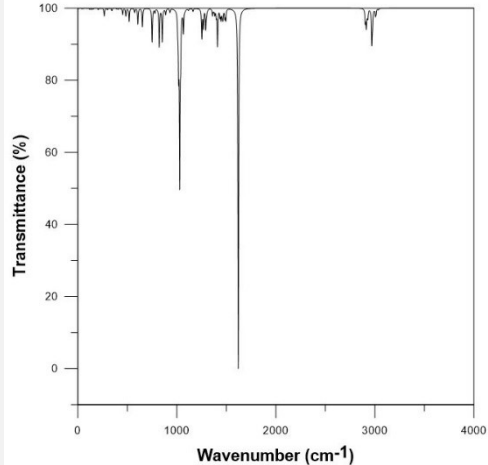
Structure Name	IR Spectra
2311	 <p>The IR spectrum for structure 2311 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>
2312	 <p>The IR spectrum for structure 2312 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>
2313	 <p>The IR spectrum for structure 2313 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>

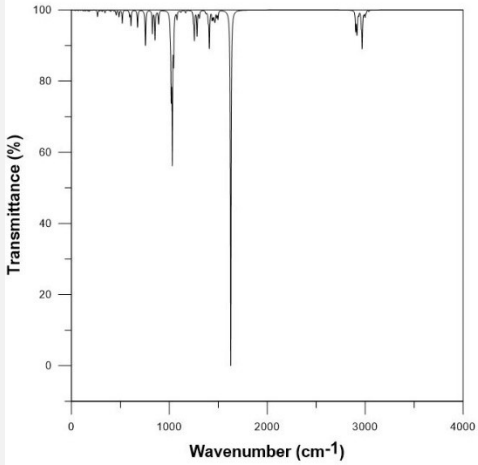
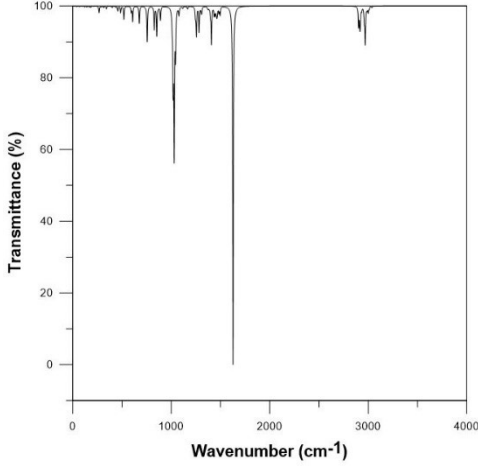
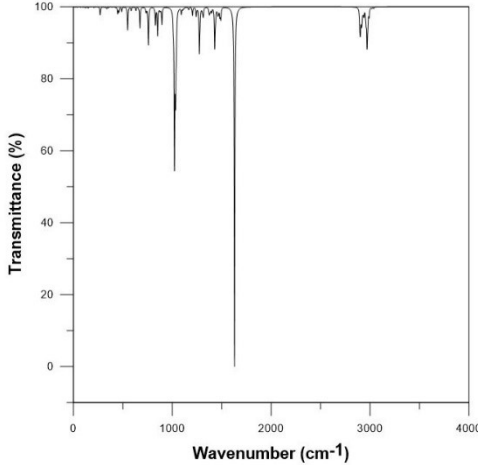
Structure Name	IR Spectra
2321	
2322	
2323	

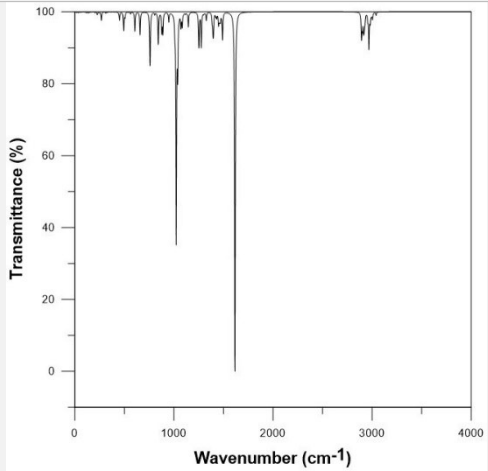
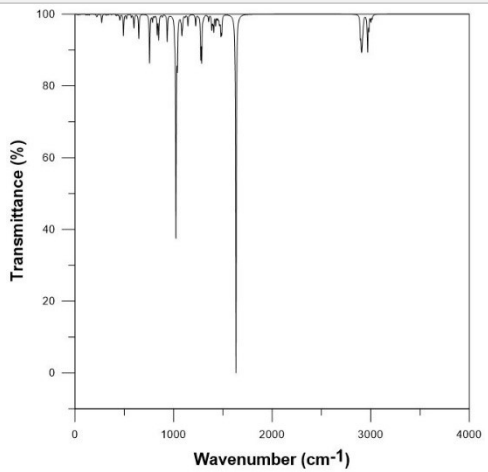
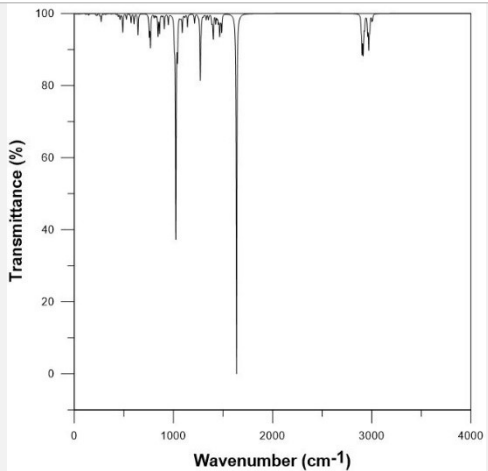
Structure Name	IR Spectra
2331	 <p>The IR spectrum for structure 2331 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>
2332	 <p>The IR spectrum for structure 2332 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>
2333	 <p>The IR spectrum for structure 2333 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1275 cm<sup>-1</sup> (C-O stretch), and a peak at approximately 1100 cm<sup>-1</sup> (C-O stretch). There are also several peaks in the fingerprint region between 1500 and 500 cm<sup>-1</sup>.</p>

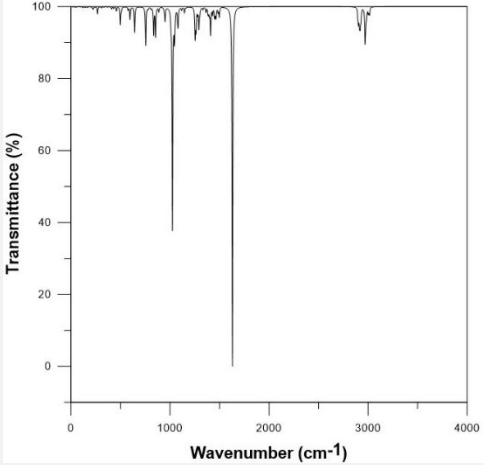
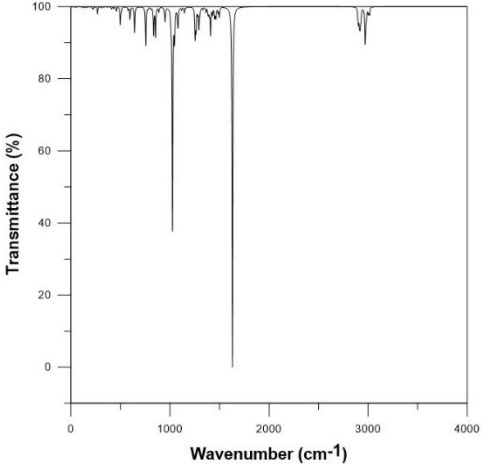
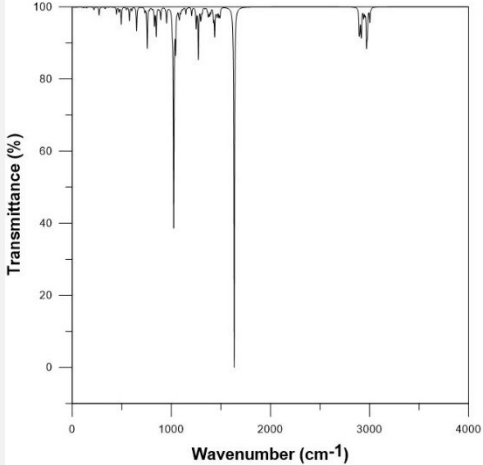


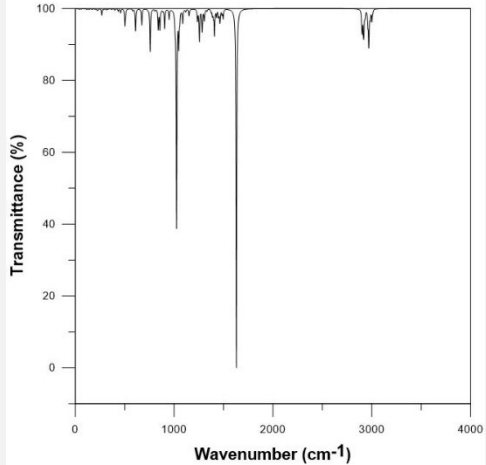
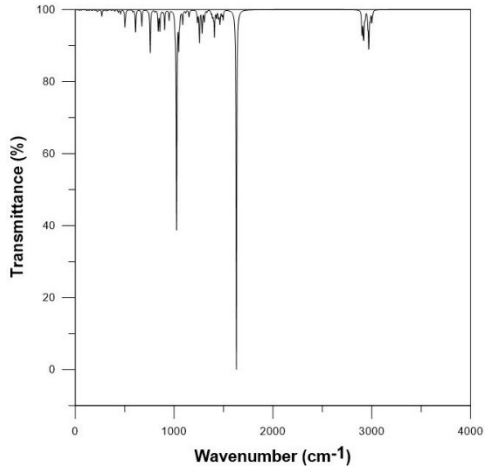
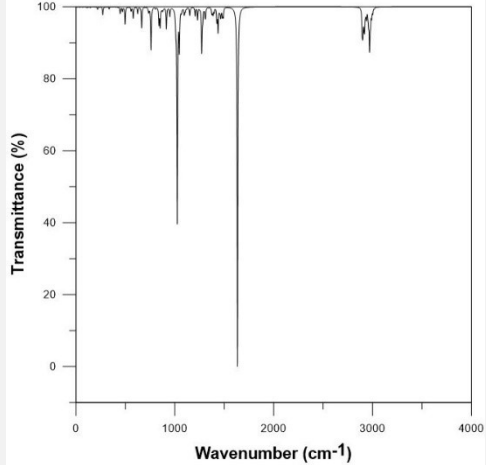
Structure Name	IR Spectra
3111	 <p>The IR spectrum for structure 3111 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are also small peaks around 3000 cm<sup>-1</sup>.</p>
3112	 <p>The IR spectrum for structure 3112 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are also small peaks around 3000 cm<sup>-1</sup>.</p>
3113	 <p>The IR spectrum for structure 3113 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a very strong and sharp peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>. There are also small peaks around 3000 cm<sup>-1</sup>.</p>

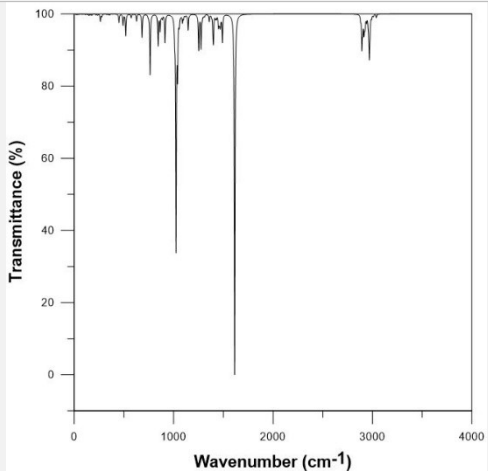
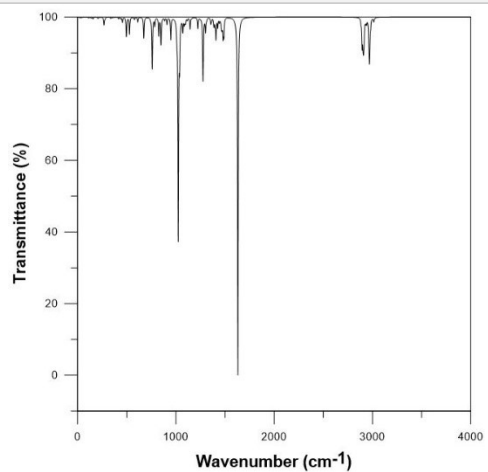
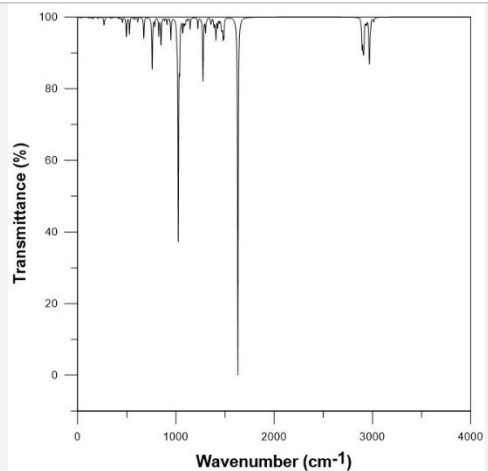
Structure Name	IR Spectra
3121	 <p>The IR spectrum for structure 3121 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
3122	 <p>The IR spectrum for structure 3122 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
3123	 <p>The IR spectrum for structure 3123 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>

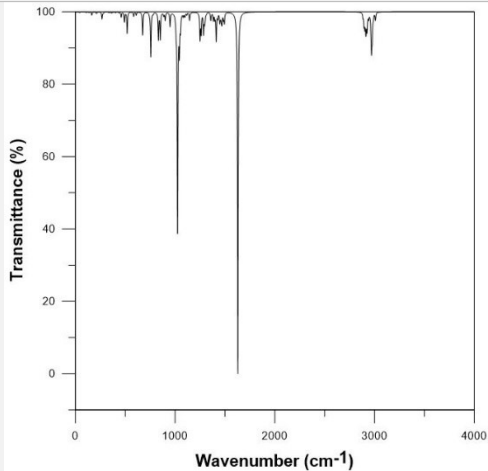
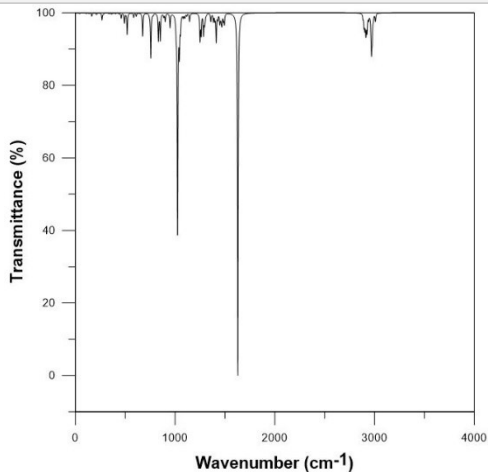
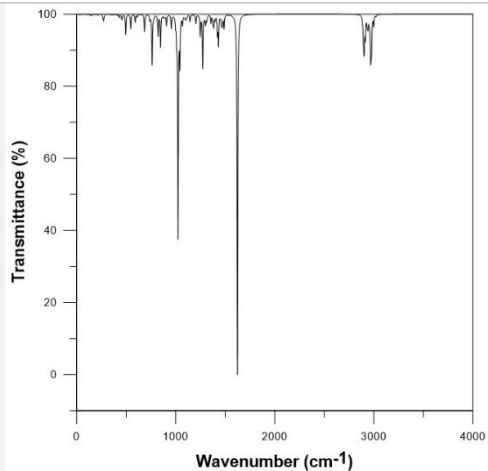
Structure Name	IR Spectra
3131	
3132	
3133	

Structure Name	IR Spectra
3211	 <p>The IR spectrum for structure 3211 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup>, a strong peak at approximately 1275 cm<sup>-1</sup>, and a cluster of peaks between 2800 and 3000 cm<sup>-1</sup>.</p>
3212	 <p>The IR spectrum for structure 3212 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup>, a strong peak at approximately 1275 cm<sup>-1</sup>, and a cluster of peaks between 2800 and 3000 cm<sup>-1</sup>.</p>
3213	 <p>The IR spectrum for structure 3213 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup>, a strong peak at approximately 1275 cm<sup>-1</sup>, and a cluster of peaks between 2800 and 3000 cm<sup>-1</sup>.</p>

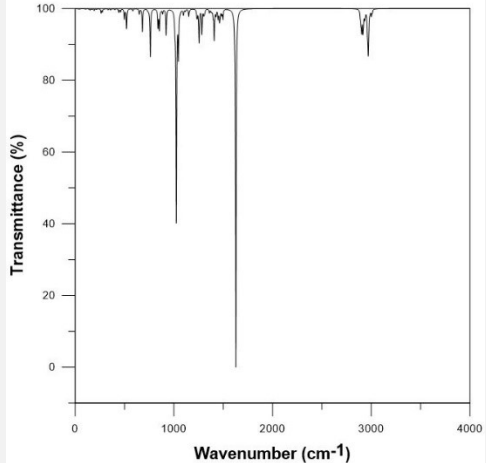
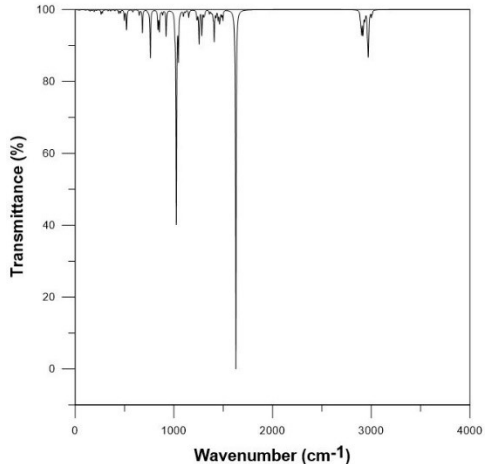
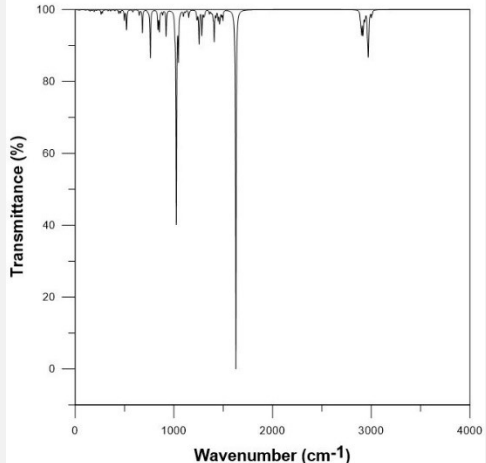
Structure Name	IR Spectra
3221	
3222	
3223	

Structure Name	IR Spectra
3231	
3232	
3233	

Structure Name	IR Spectra
3311	
3312	
3313	

Structure Name	IR Spectra
3321	
3322	
3323	



Structure Name	IR Spectra
3331	 <p>The IR spectrum for structure 3331 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
3332	 <p>The IR spectrum for structure 3332 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>
3333	 <p>The IR spectrum for structure 3333 shows transmittance (%) on the y-axis (0 to 100) and wavenumber (cm<sup>-1</sup>) on the x-axis (0 to 4000). Key features include a sharp peak at approximately 1715 cm<sup>-1</sup> (C=O stretch), a strong peak at approximately 1640 cm<sup>-1</sup> (C=C stretch), and a very strong, sharp peak at approximately 1600 cm<sup>-1</sup> (C=C stretch). There are also several peaks in the fingerprint region between 1500 and 600 cm<sup>-1</sup>.</p>