Supplementary Information

In silico and Experimental Assessments Applied to Preliminary Identification of New Illicit Substances Structures

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Figure S1 was obtained with Avogadro software[1] and corresponds to the optimization geometry structure of the ten samples.

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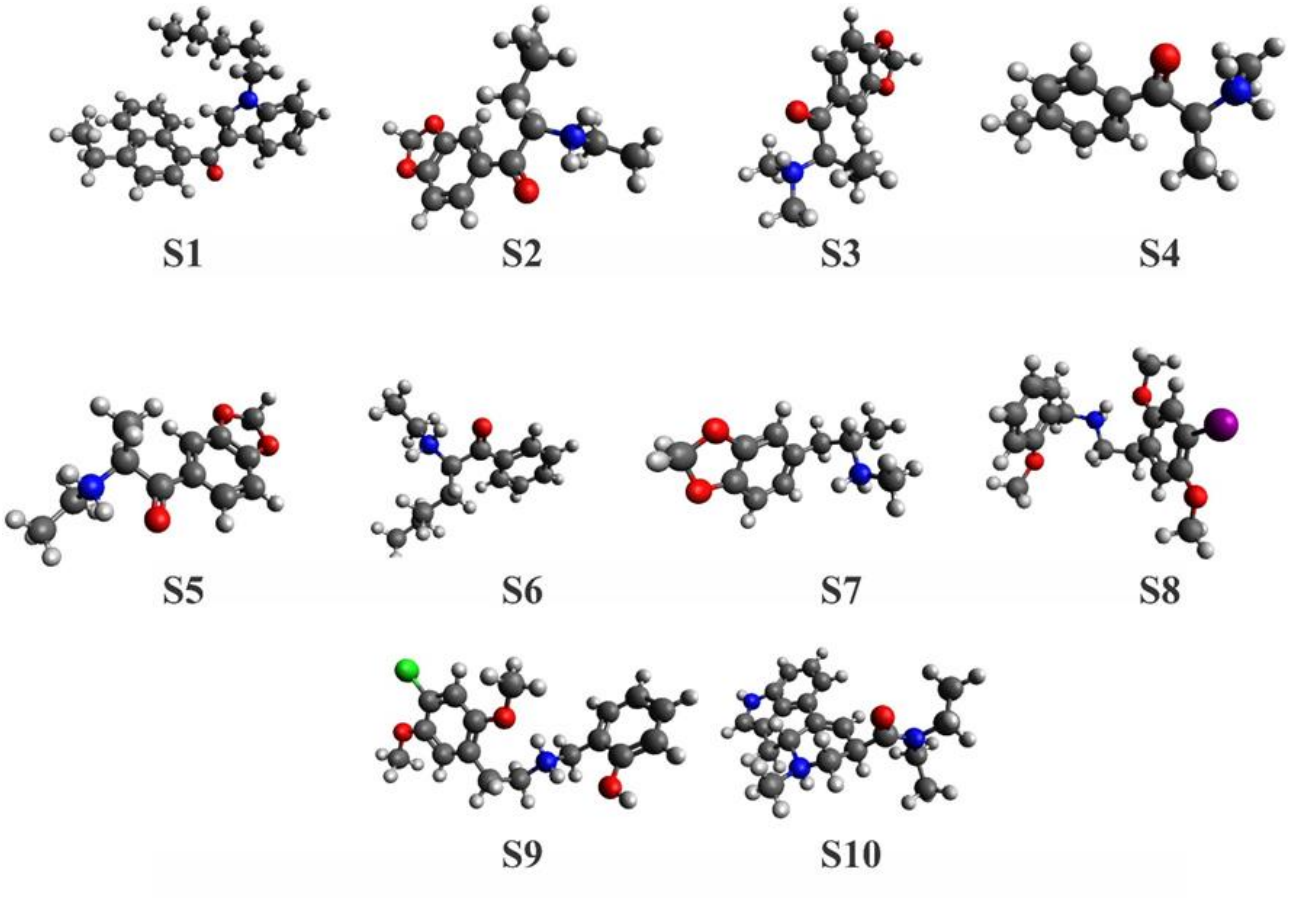

Figure S1. Sample structure with optimized geometries.

FTIR spectrum: spectra obtained from available forensic libraries such as SWGDRUG[2] and Europe Response infrared library[3]

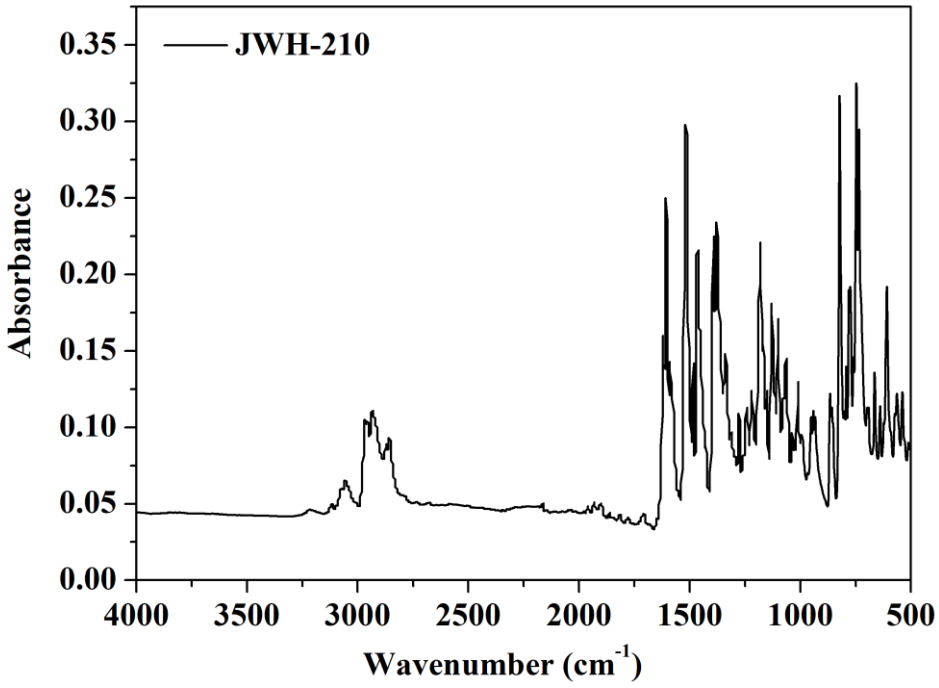

Figure S2. FTIR spectrum of compound JWH-210.

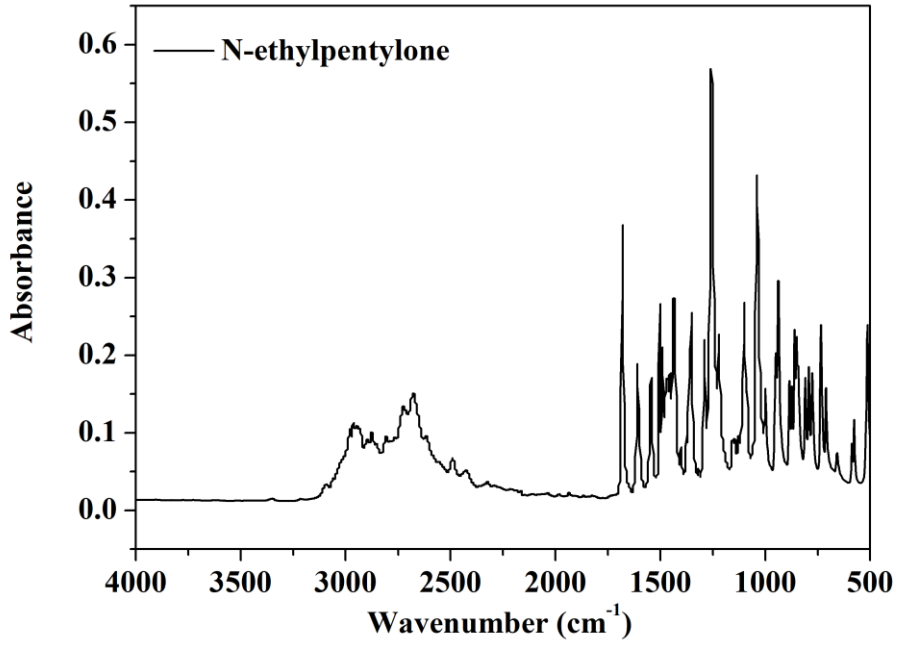

Figure S3. FTIR spectrum of compound *N*-ethylpentylone.

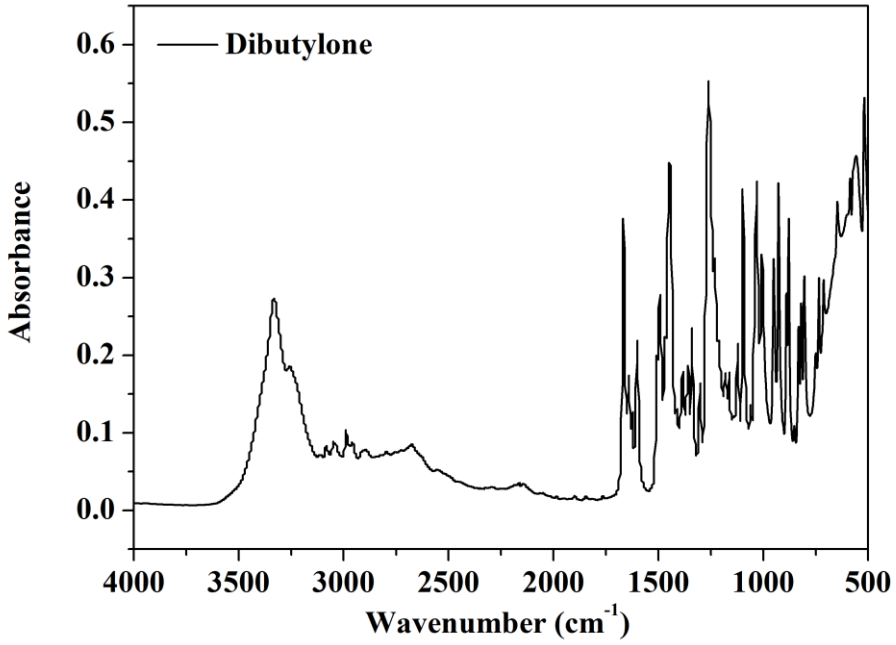

Figure S4. FTIR spectrum of compound dibutylone.

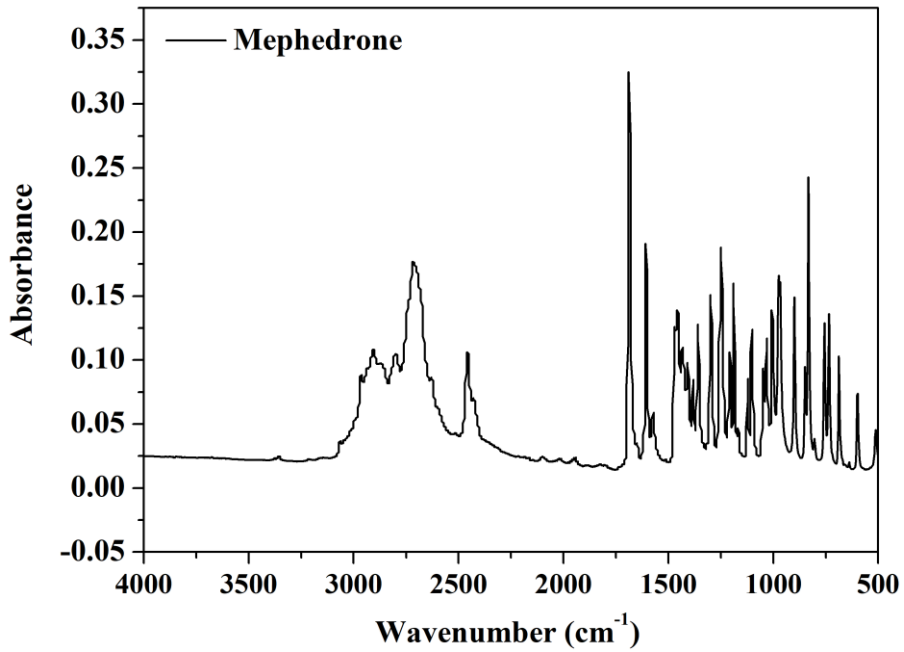

Figure S5. FTIR spectrum of compound mephedrone.

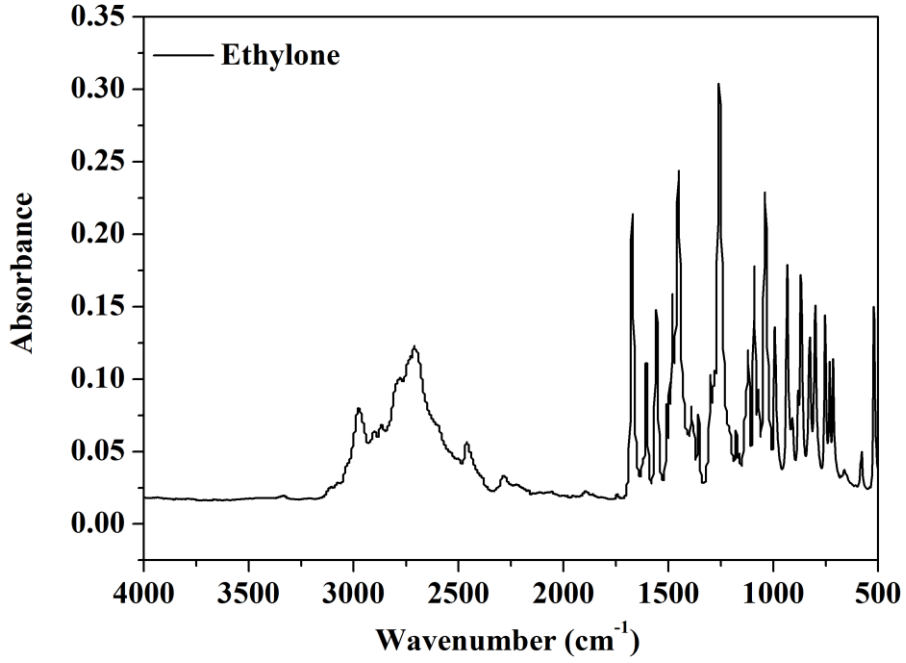

Figure S6. FTIR spectrum of compound ethylone.

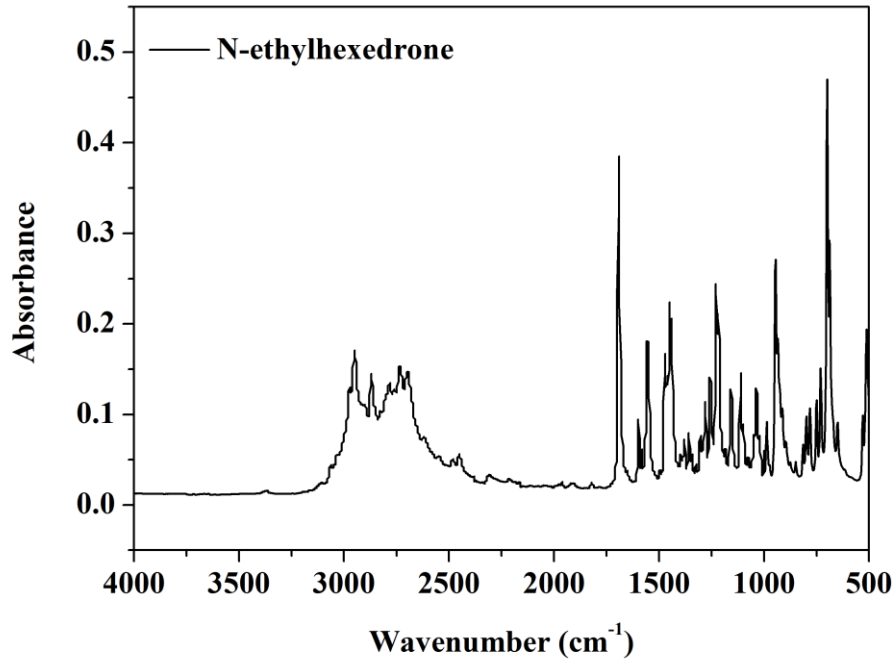

Figure S7. FTIR spectrum of compound *N*-ethylhexedrone.

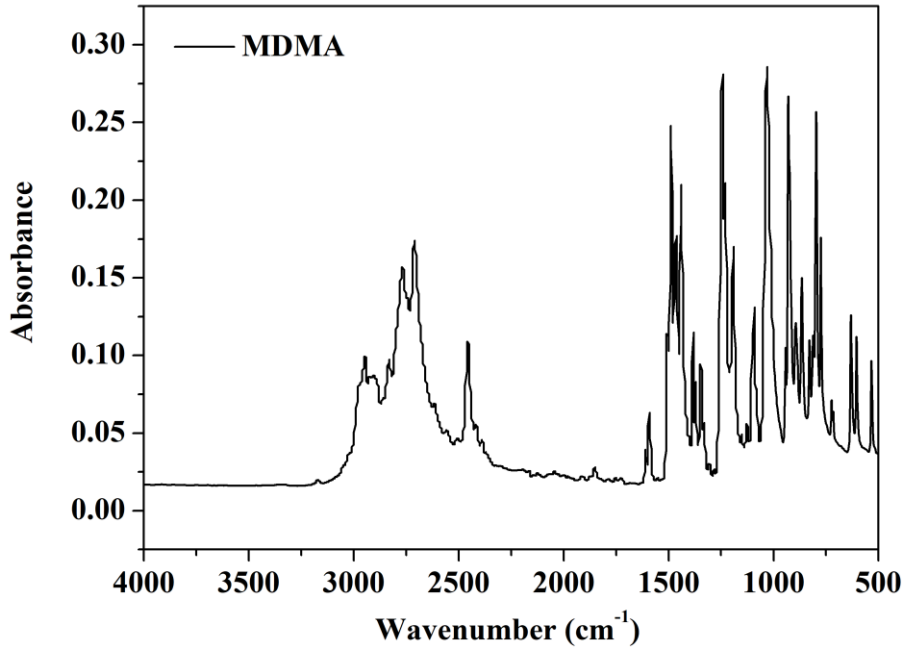

Figure S8. FTIR spectrum of compound MDMA.

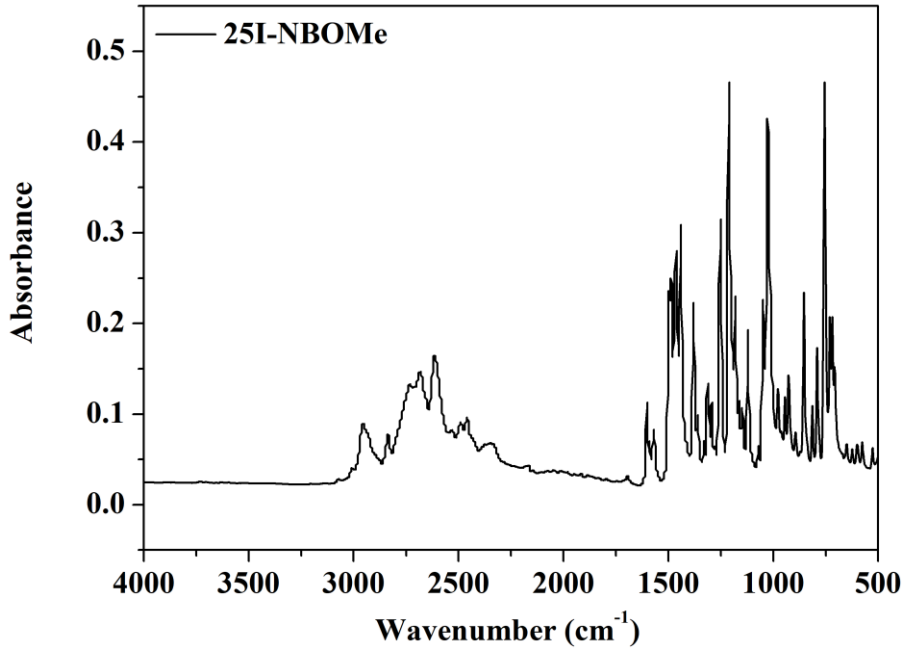

Figure S9. FTIR spectrum of compound 25I-NBOMe.

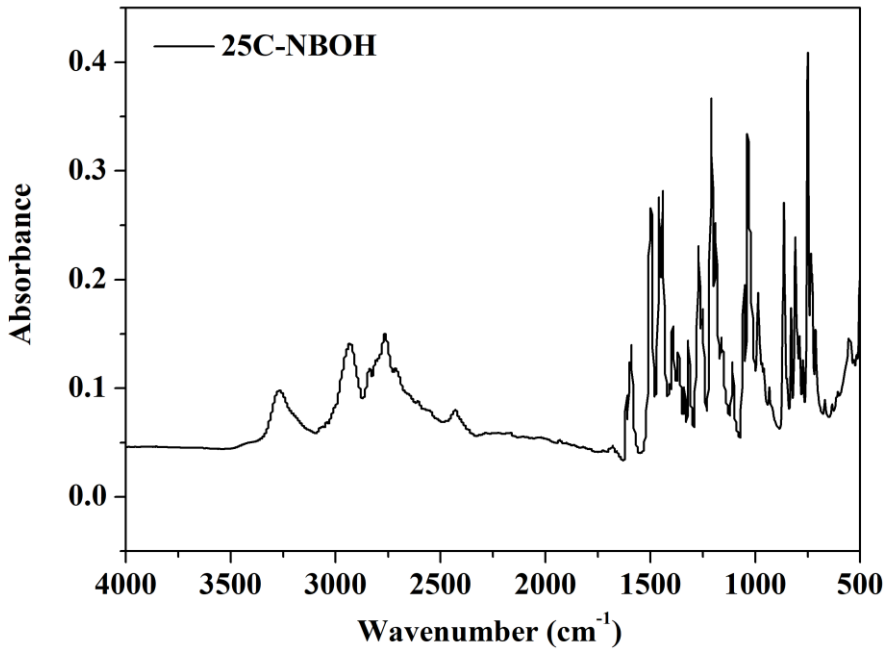

Figure S10. FTIR spectrum of compound 25C-NBOH.

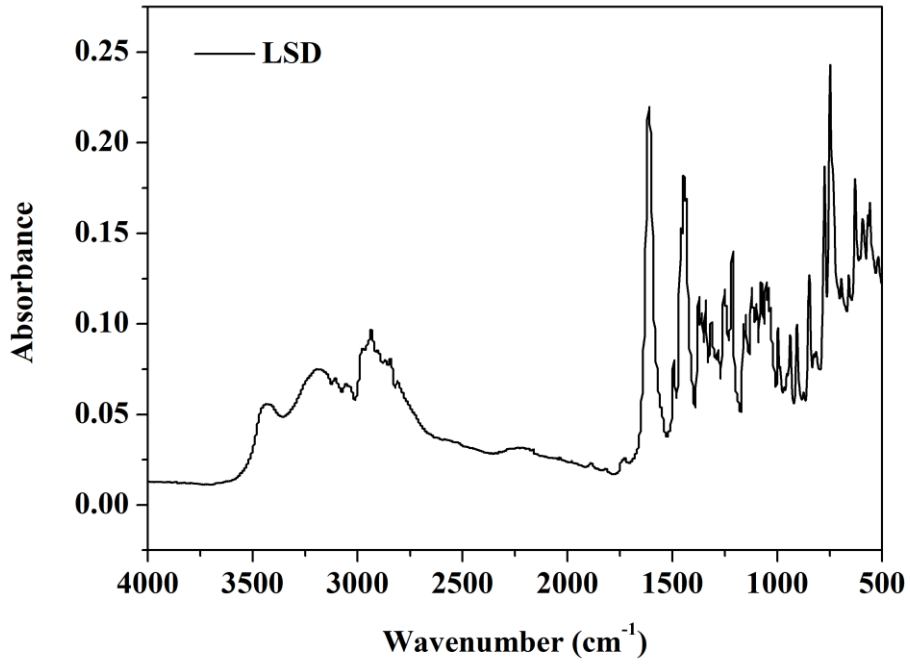

Figure S11. FTIR spectrum of compound LSD.

FTIR spectrum: spectra obtained from seized samples

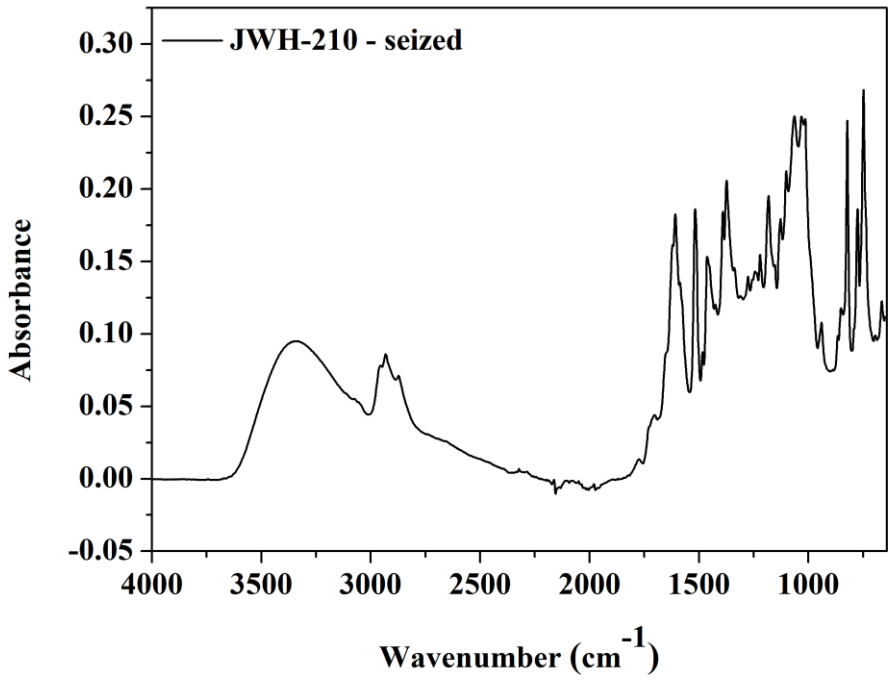

Figure S12. FTIR spectrum of sample **S**1.

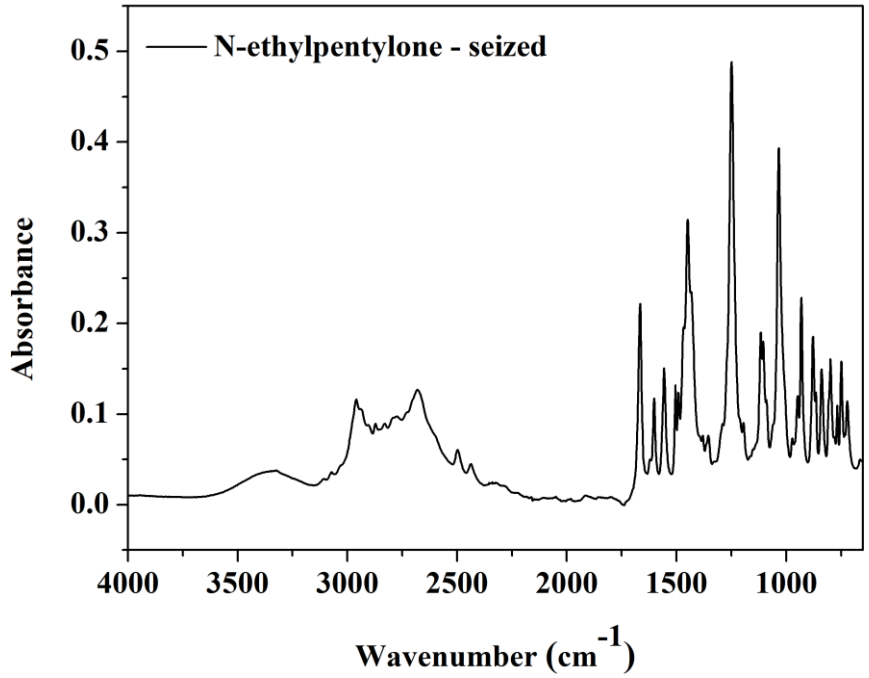

Figure S13. FTIR spectrum of sample S2.

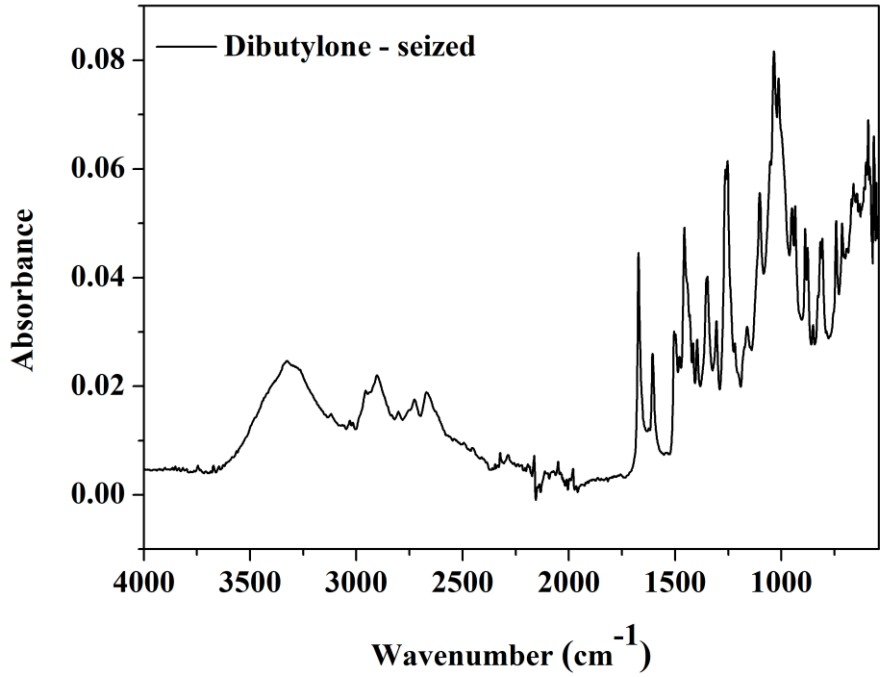

Figure S14. FTIR spectrum of sample **S**3.

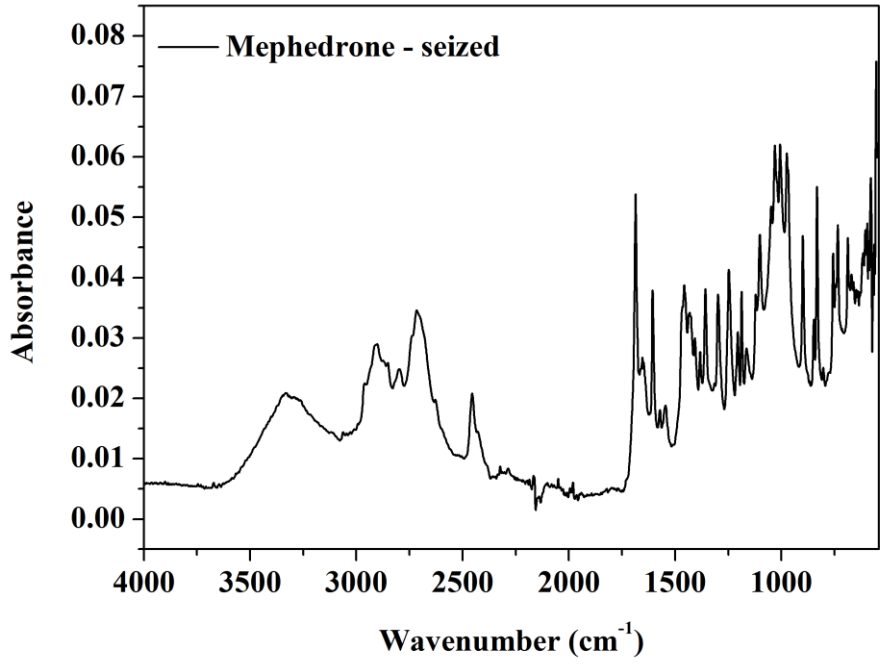

Figure S15. FTIR spectrum of sample **S**4.

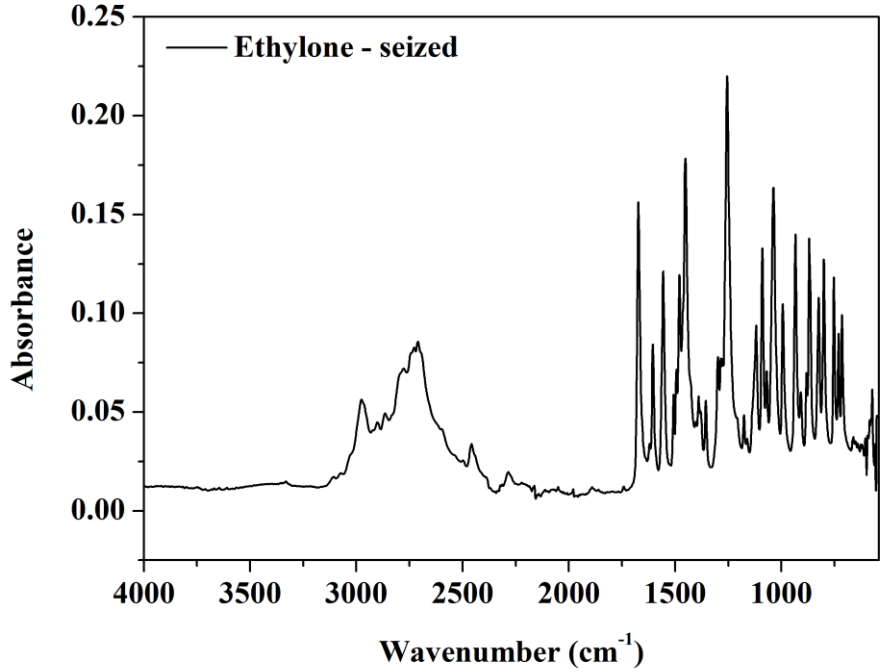

Figure S16. FTIR spectrum of sample **S**5.

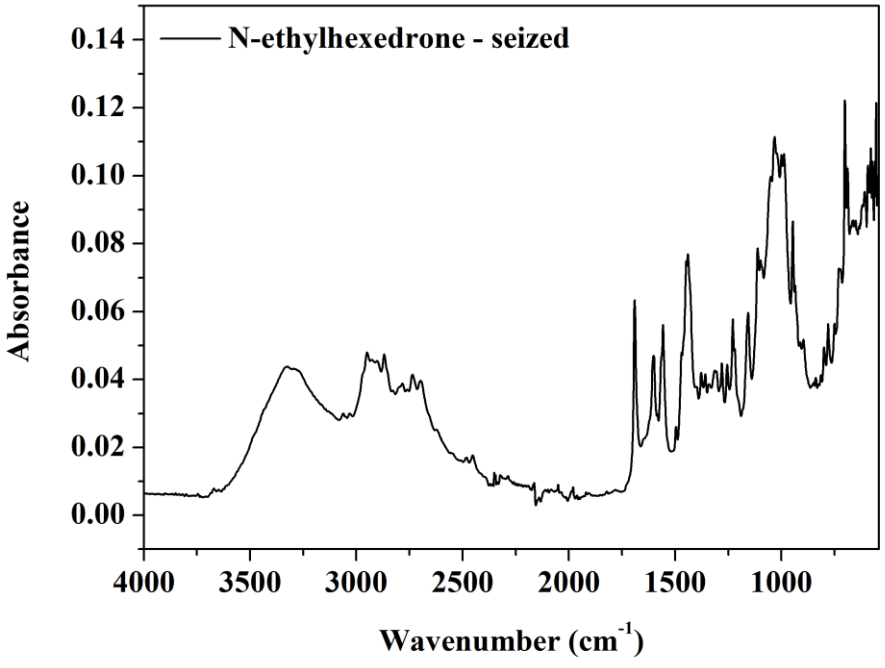

Figure S17. FTIR spectrum of sample **S**6.

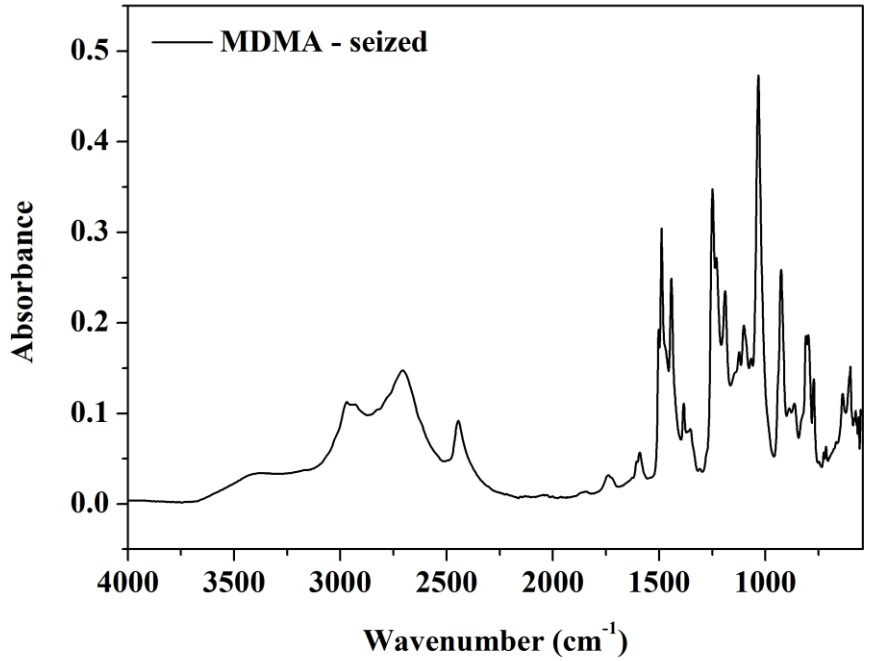

Figure S18. FTIR spectrum of sample **S**7.

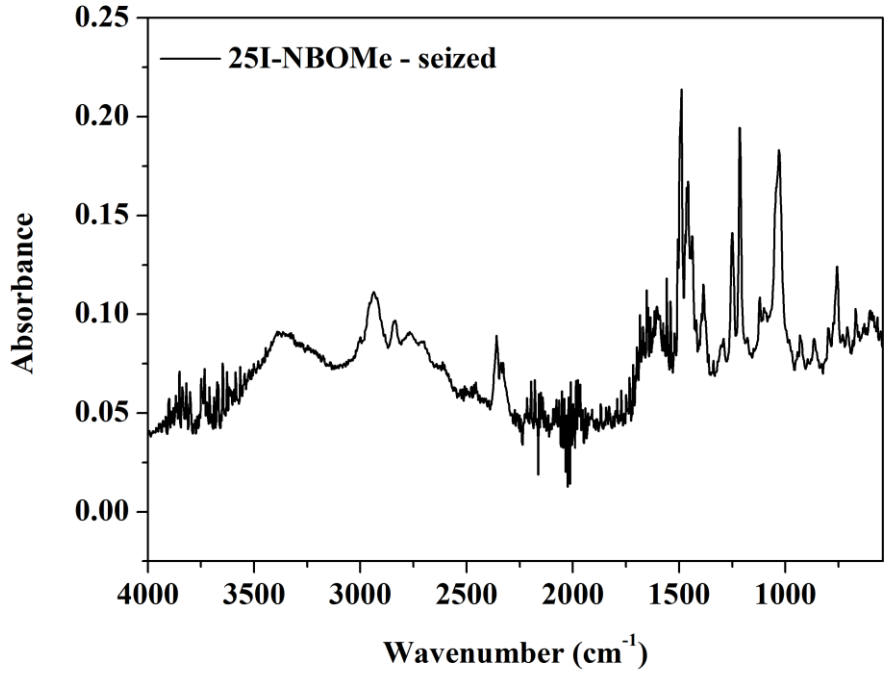

Figure S19 FTIR spectrum of sample **S**8.

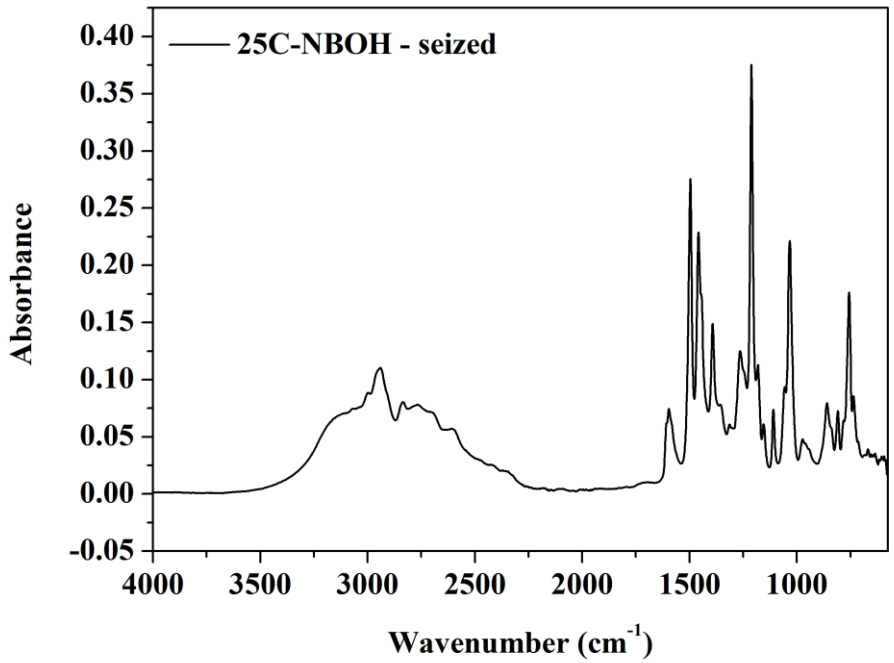

Figure S20. FTIR spectrum of sample **S**9.

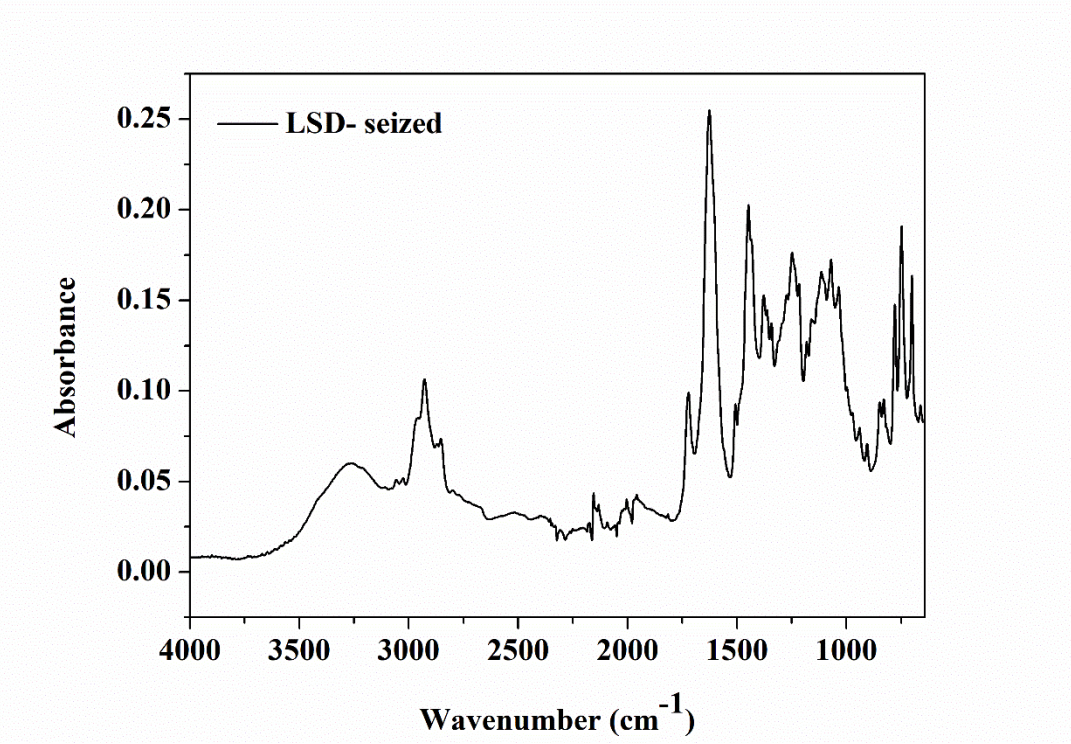

Figure S21. FTIR spectrum of sample **S**10.

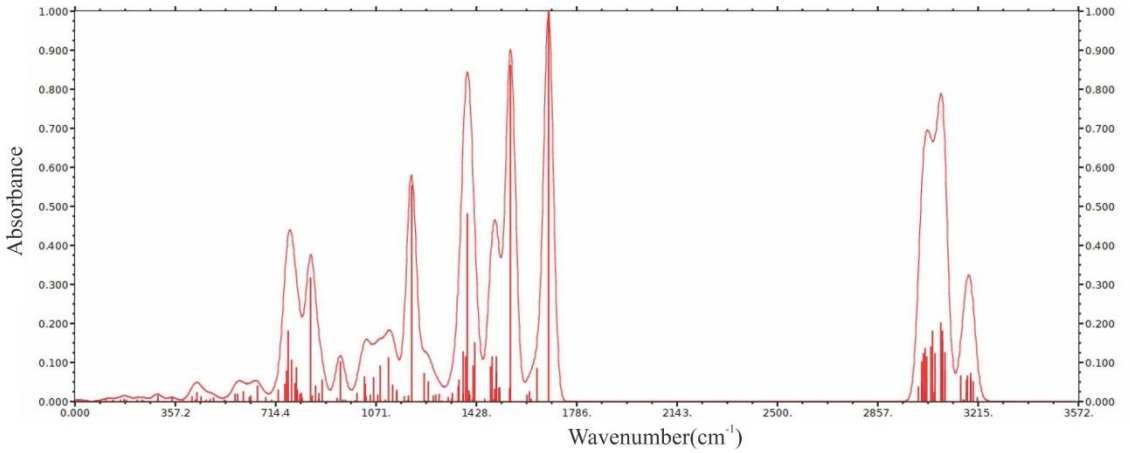

Figure S22. IR simulated of sample **S**1.

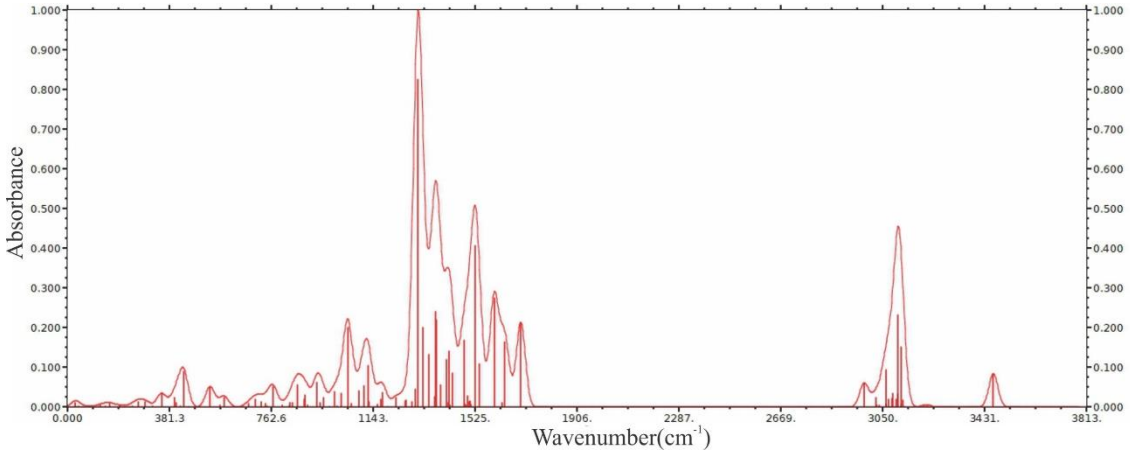

Figure S23. IR simulated of sample **S**2.

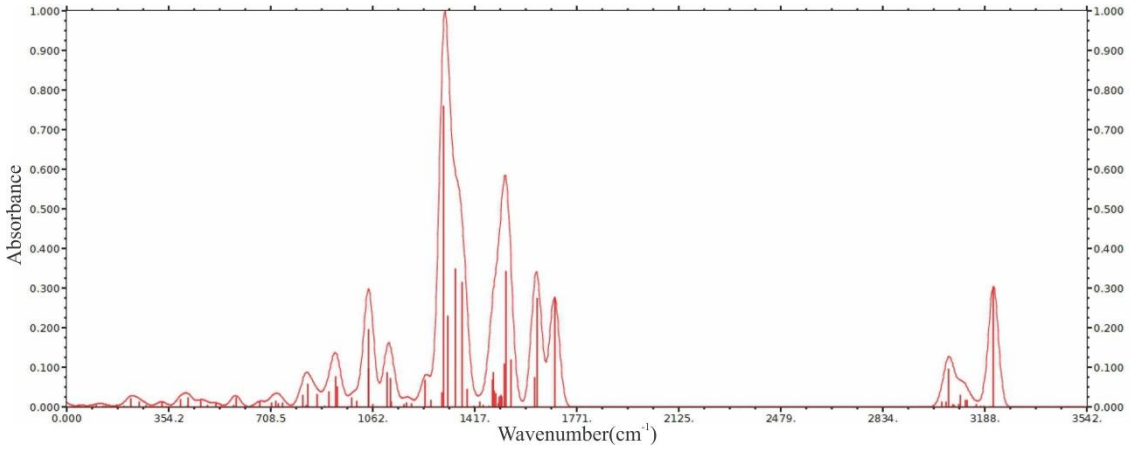

Figure S24. IR simulated of sample **S**3.

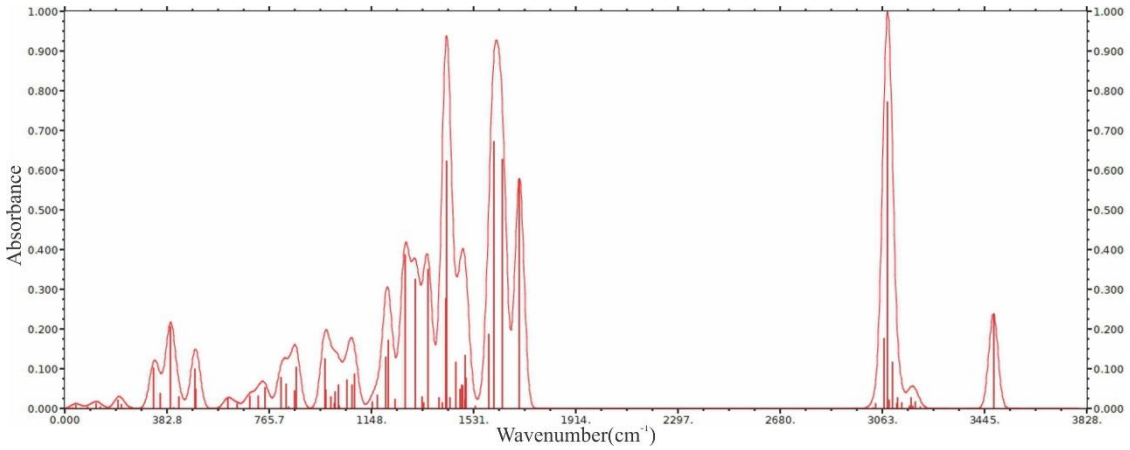

Figure S25. IR simulated of sample **S**4.

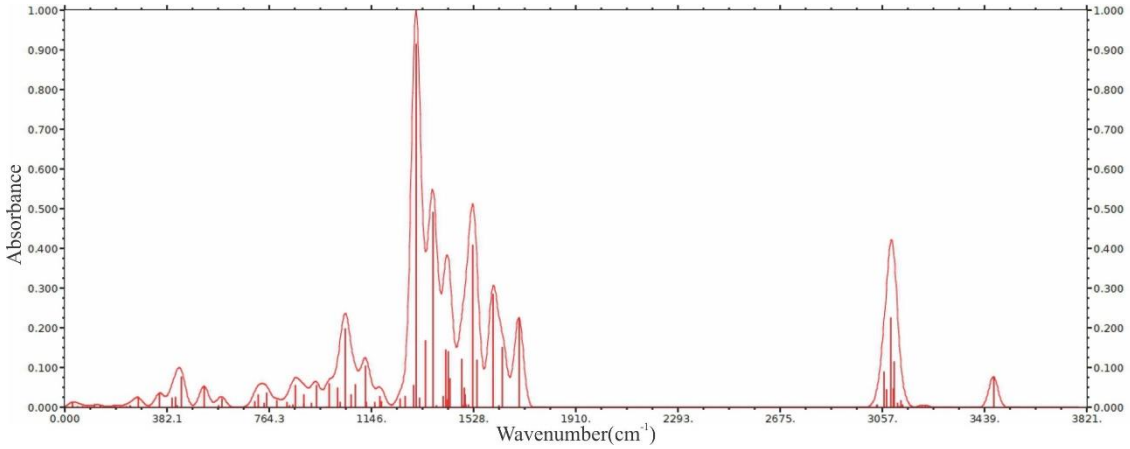

Figure S26. IR simulated of sample **S**5.

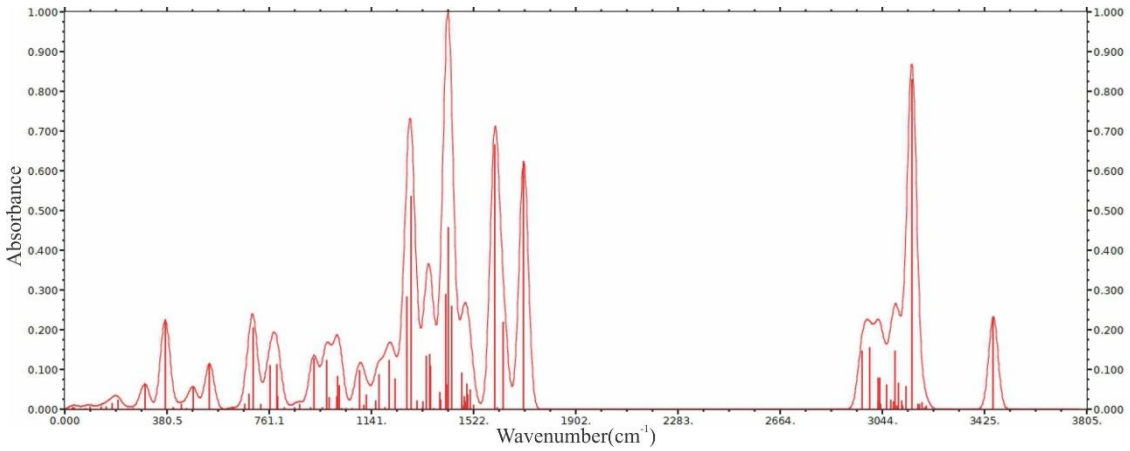

Figure S27. IR simulated of sample **S**6.

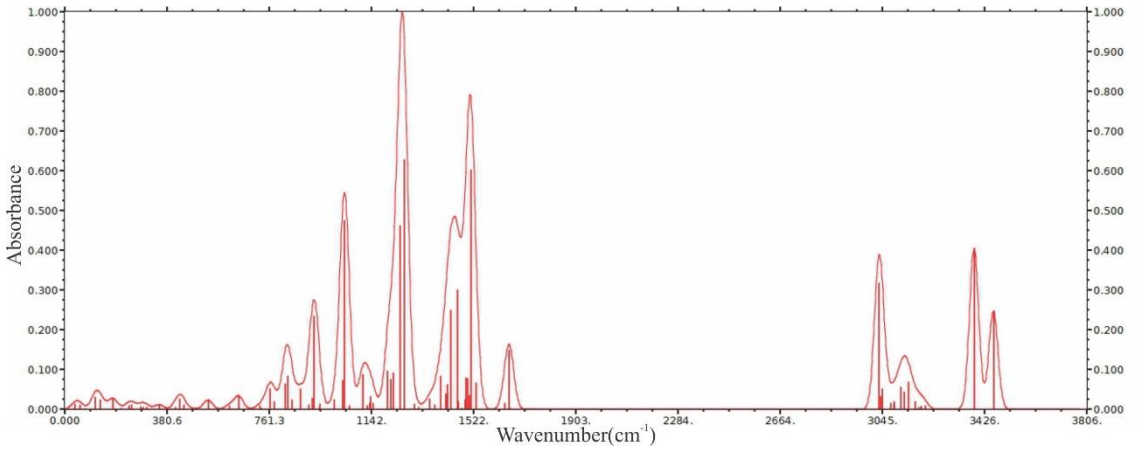

Figure S28. IR simulated of sample **S**7.

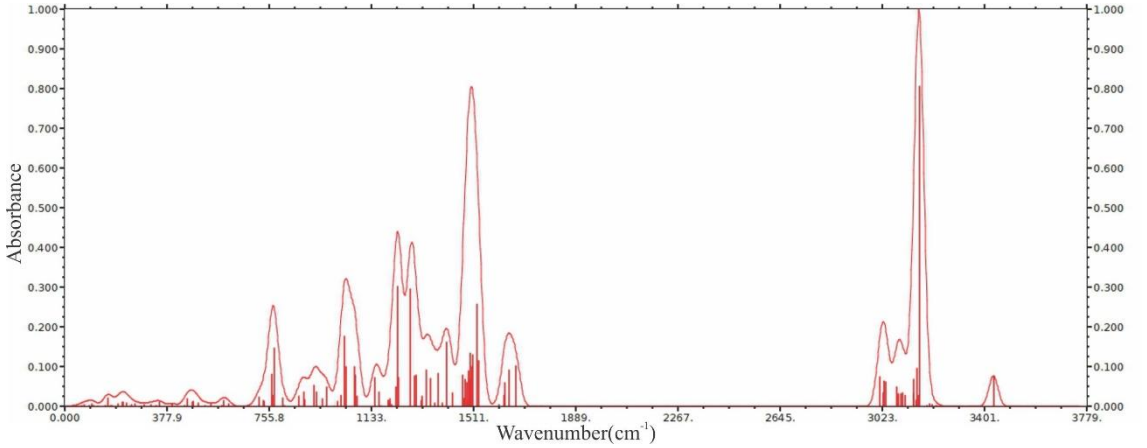

Figure S29. IR simulated of sample **S**8.

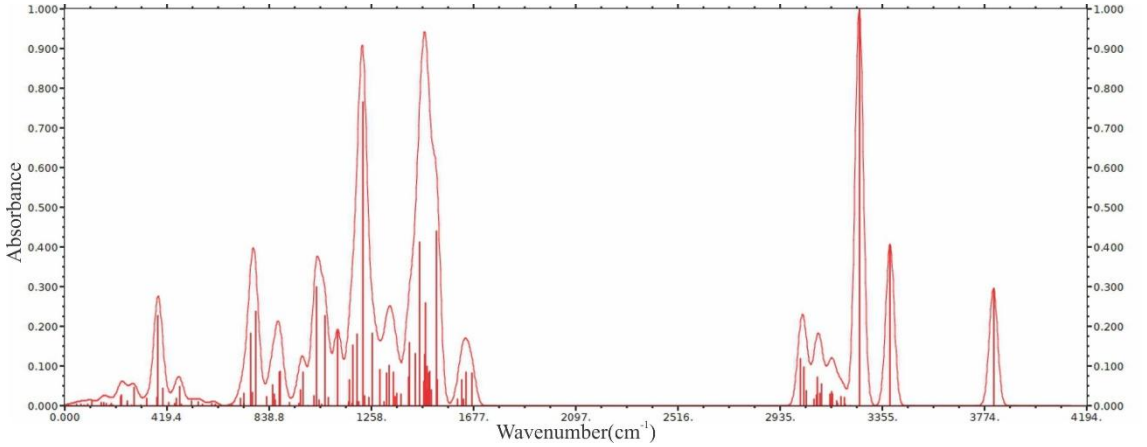

Figure S30. IR simulated of sample **S**9.

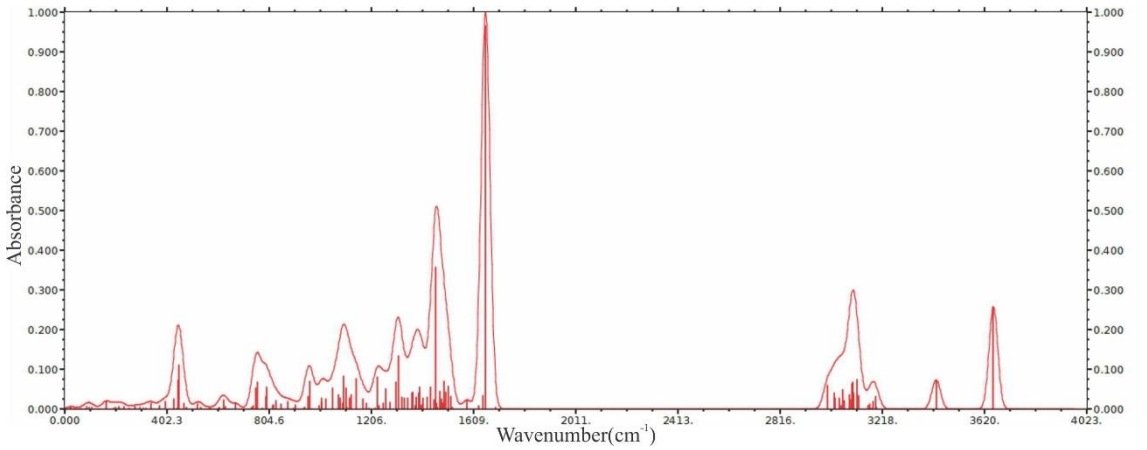

Figure S31. IR simulated of sample **S**10.

Table S1. Assignment and comparison of the LTD, ED and TD IR of S1

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1607	1687; 1644	1609	νC=C (aromatic) νC=C (alkene)
1515	1552	1516	νC=O
1468	1487	1465	νC=C (aromatic) δ_s CH2
1484	1503	1481	νC=C (aromatic)
1391	1425	1390	δ_s CH_3
1379	1399	1374	ν C–N
1339	1363	–	ω CH2
1187	1197	1184	τ CH2
941	949	939	ω C–H (alkene)
822	837	822	C–H out-of-plane angular deformation (tetra-substituted aromatic)
774	790	775	C–H out-of-plane angular deformation (trisubstituted alkene)
746	762	748	C–H out-of-plane angular deformation (*ortho*-disubstituted aromatic)
734	670	654	ρ CH_2

LTD: literature data; TD: theoretical data; ED: experimental data; *ν*: axial deformation; *δ*s: in-plane symmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: asymmetrical out-of-plane angular deformation; ρ: angular deformation asymmetric in the plane.

Table S2. Assignment and comparison of the LTD, ED and TD IR of S2

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1680	1695	1665	ν C=O
1609	1599	1604	ν C=C (aromatic)
1546	1521	1562	ν C=C (aromatic)
1503	1482	1505	ν C=C (aromatic)
1437	1414	1454	δ_s CH2
1355	1380	1350	δ_s CH_3
1258	1309	1250	ν_{as} O–C–O
1100	1124	1112	ν C–N
1035	1050	1033	ν_s O–C–O
937	997	934	ν_{as} O–C–O
884	934	878	C–H out-of-plane angular deformation (tri-substituted aromatic)
859	852	836	C–H out-of-plane angular deformation (tri-substituted aromatic)
812	769	799	ω N–H

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial strain; δs: symmetrical angular strain in the plane; ω: symmetrical angular strain out of the plane; τ: asymmetrical angular strain out of the plane; νas: axial strain asymmetrical; νs: symmetrical axial strain.

Table S3. Assignment and comparison of the LTD, ED and TD IR of S3

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1668	1631	1668	ν C=O
1600	1534	1607	ν C=C
1492	1473	1501	ν C=C (aromatic) δ_s CH2
1450	–	1457	δ_{as} CH_3
1384	1356	1395	δ_s CH_3
1355	–	1351	ω CH2
1258	1309	1258	ν_{as} O–C–O
1185	1240	1161	τ CH2
1098	1118	1124	ν C–N
1031	1045	1046	ν_s O–C–O
1002	936	940	ν_{as} O–C–O
890	867	886	C–H, out-of-plane angular deformation (tri-substituted aromatic)
877	831	872	C–H, out-of-plane angular deformation (tri-substituted aromatic)

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: symmetrical angular deformation in the plane; δas: asymmetrical angular deformation; ω: symmetrical angular deformation out of the plane; τ: asymmetrical angular deformation out of the plane; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S4. Assignment and comparison of the LTD, ED and TD IR of S4

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1690	1640	1687	ν C=O
1605	1609	1611	ν C=C
1570	1497	1547	ν C=C
1457	1470	1461	C=C (aromatic) δ_s CH2
–	1432	1429	δ_{as} CH_3
1379	1362	1361	δ_s CH_3
1356	1293	1297	ω CH2
1196	1211	1189	τ CH2
1095	1094	1103	ν C–N
831	815	830	C–H, out-of-plane angular deformation (para-disubstituted aromatic)

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: symmetrical angular deformation in the plane; δas: asymmetrical angular deformation; ω: symmetrical angular deformation out of the plane; τ: asymmetrical angular deformation out of the plane; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S5. Assignment and comparison of the LTD, ED and TD IR of S5

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1674	1699	1673	ν C=O
1605	1601	1607	ν C=C
1557	1530	1560	ν C=C
1452	1483	1451	C=C δ_{as} CH_3
1382	1379	1386	δ_s CH_3
1356	–	1356	ω CH2
1173	1178	1174	τ CH2
1091	1122	1092	ν C–N
1258	1312	1259	ν_{as} O–C–O
1037	1045	1040	ν_s O–C–O
993	994	992	ν_{as} O–C–O
867	860	861	C–H, out-of-plane angular deformation (tri-substituted aromatic)
800	761	796	C–H, out-of-plane angular deformation (tri-substituted aromatic)

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: symmetrical angular deformation in the plane; δas: asymmetrical angular deformation; ω: symmetrical angular deformation out of the plane; τ: asymmetrical angular deformation out of the plane; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S6. Assignment and comparison of the LTD, ED and TD IR of S6

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1690	1705	1690	ν C=O
1601	1604	1601	ν C=C
1554	–	1556	ν C=C
1445	1430	1444	C=C δ_{as} CH_3
1381	1397	1375	δ_s CH_3
1355	1354	1360	ω CH2
1228	1211	1228	τ CH2
1157	1165	1159	ν C–N
699	697	699	C=C out-of-plane angular deformation, out-of-plane ring bending

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: in-plane symmetric angular deformation; δas: asymmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: out-of-plane asymmetric angular deformation; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S7. Assignment and comparison of the LTD, ED and TD IR of S7

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1602	1656	1601	ν C=C
–	1516	–	ν C=C
1491	1495	1488	ν C=C
1463	1465	–	δ_s CH2
1441	–	1439	δ_{as} CH_3
1384	1399	1379	δ_s CH_3
1346	1353	–	ω CH2
1189	1203	1189	τ CH2
795	761	773	ω N–H
1243	1263	1248	ν_{as} O–C–O
1028	1045	1039	ν_s O–C–O
927	933	927	ν_{as} O–C–O
1095	1107	1099	ν C–N
892	879	862	C–H out of plane (trisubstituted aromatic)
865	830	810	C–H out of plane (trisubstituted aromatic)

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: in-plane symmetric angular deformation; δas: asymmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: out-of-plane asymmetric angular deformation; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S8. Assignment and comparison of the LTD, ED and TD IR of S8

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1602	1631	–	ν C=C
1570	1521	–	ν C=C
1494	1483	1488	ν C=C
1461	1464	1460	δ_s CH2
1442	1412	1440	δ_{as} CH_3
1381	1390	1386	δ_s CH_3
1316	1336	1338	ω CH2
1181	1195	1178	τ CH2
1255	1267	1251	ν_{as} O–C–O
1027	1058	1030	ν_s O–C–O
926	927	926	ν_{as} O–C–O
1120	1141	1121	ν C–N
854	877	864	C–H out of plane (tetrasubstituted aromatic)
755	763	755	C–H out of plane (orthosubstituted aromatic)
1210	1220	1217	ν C–I

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: in-plane symmetric angular deformation; δas: asymmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: out-of-plane asymmetric angular deformation; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S9. Assignment and comparison of the LTD, ED and TD IR of S9

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
–	1644	–	ν C=C
–	1628	–	ν C=C
1596	1525	1598	ν C=C
1498	1480	1499	ν C=C
1459	1458	1459	δ_s CH2
1439	1414	–	δ_{as} CH_3
1396	–	1390	δ_s CH_3
1364	1336	–	ω CH2
1189	1185	1179	τ CH2
1270	1265	1263	ν_{as} O–C–O
1038	1034	1030	ν_s O–C–O
980	973	972	ν_{as} O–C–O
1208	1224	1208	ν C–O (alcohol)
1110	1122	1110	ν C–N
862	883	859	C–H out of plane (tetrasubstituted aromatic)
750	788	757	C–H out of plane (orthosubstituted aromatic)
1059	1068	1058	ν C–Cl
732	762	731	C=C out-of-plane ring bending

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: in-plane symmetric angular deformation; δas: asymmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: out-of-plane asymmetric angular deformation; νas: asymmetrical axial strain; νs: symmetrical axial strain.

Table S10. Assignment and comparison of the LTD, ED and TD IR of S10

LTD / cm^{-1}	TD / cm^{-1}	ED / cm^{-1}	Assignment
1611	1657	1626	ν C=O
–	1510	1507	ν C=C
1493	1459	1448	ν C=C, N–H
1449	1441	–	δ_{as} CH_3
1373	1375	1376	δ_{s} CH_3
1340	1313	1337	ν C–N
1213	1224	1242	ν C–N
1153	1154	1164	τ CH2
751	756	746	C–H out of plane (trisubstituted aromatic)
846	800	831	C–H out of plane (trisubstituted alkene)
777	–	777	C=C out-of-plane ring bending

LTD: literature data; TD: theoretical data; ED: experimental data; ν: axial deformation; δs: in-plane symmetric angular deformation; δas: asymmetric angular deformation; ω: out-of-plane symmetric angular deformation; τ: out-of-plane asymmetric angular deformation; νas: asymmetrical axial strain; νs: symmetrical axial strain.

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