

Understanding the Impact of Lignin Fractionation: Insights from NMR Relaxometry

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Abstract

Lignin is a promising feedstock for sustainable development. In this study, molecular dynamics of lignin fractions were investigated using NMR relaxometry. It was observed that Lg fractions had variable diameters ranging between 2000-6000 μm . The relaxometry data for all fractions fitted better in biexponential fitting models. All fractions had higher T1 values than T2 values, indicating variable proton environment.

Key words: Lignin, Fractionation, Relaxometry, NMR

Introduction

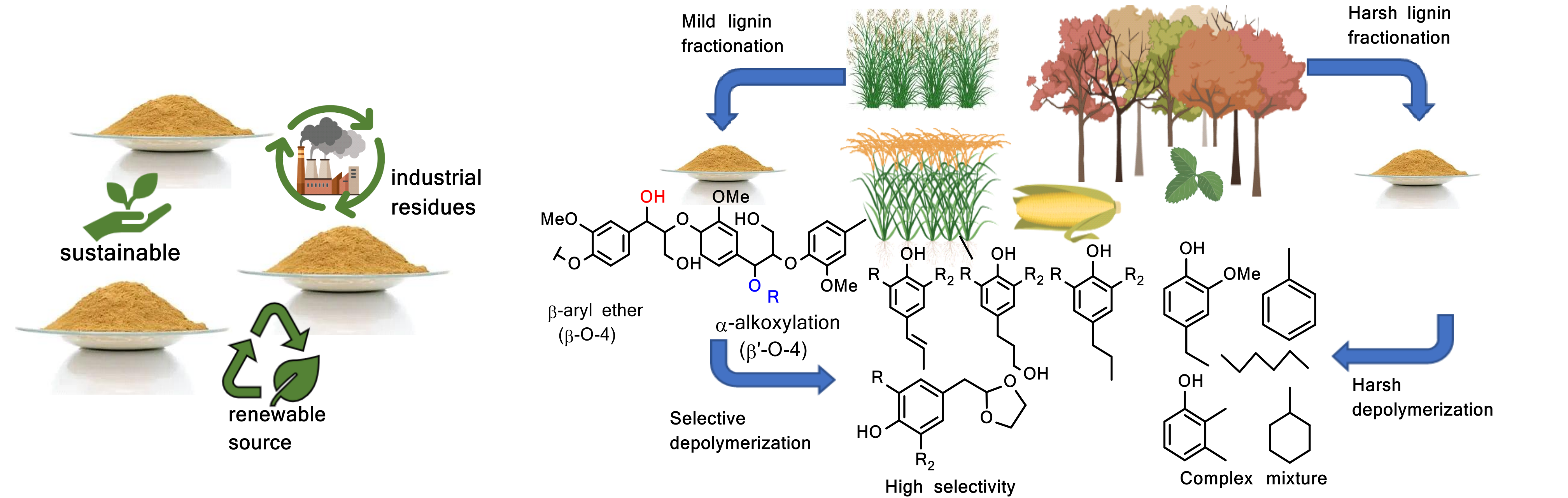


Figure 1: Lignin as a sustainable renewable resource and its separation to value added compounds

Materials and Methods

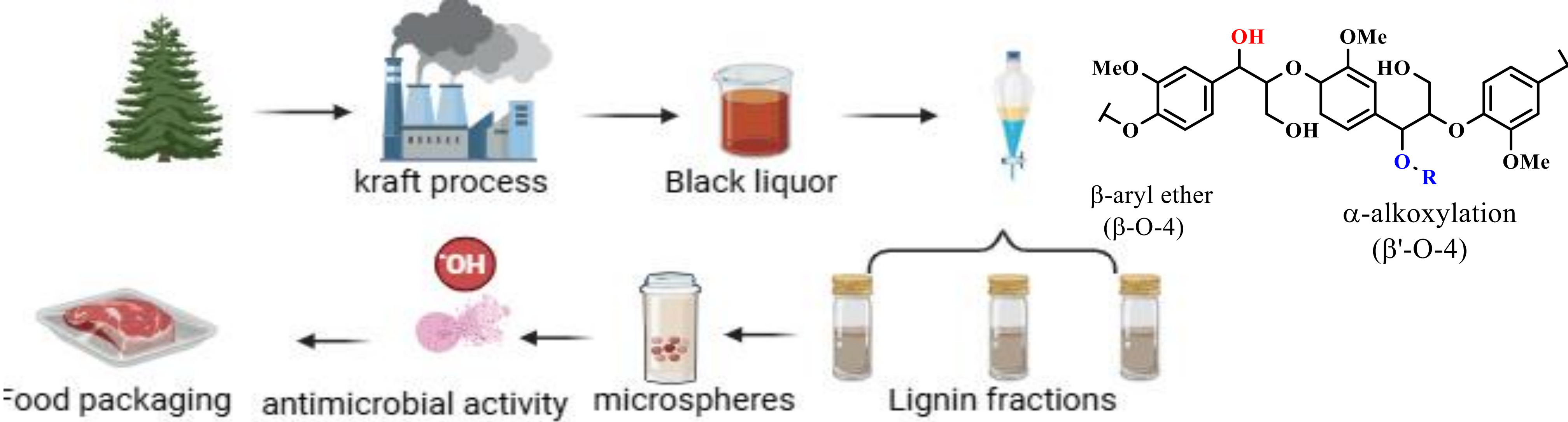


Figure 2: Fractionation of lignin using HCl, methanol and Acetone

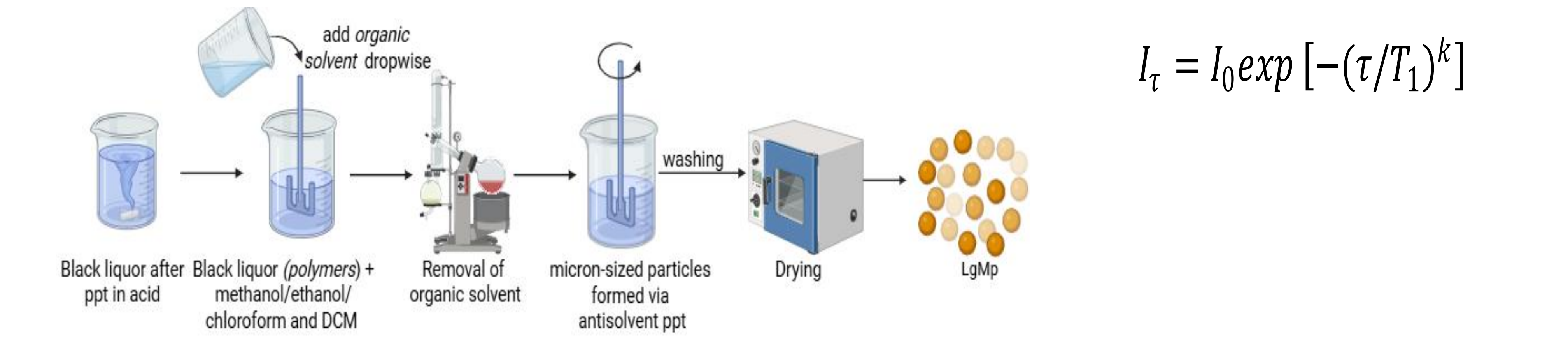


Figure 3: Fractionation of lignin using HCl, methanol, and Acetone

Results and Discussions

	LgR	LgMe	LgAc
Average Size (μm)	4.77 $\pm$ 0.14	4.18 $\pm$ 0.18	1.06 $\pm$ 0.02
Zeta potential (mV)	-0.13 $\pm$ 0.31	-0.99 $\pm$ 0.23	-4.02 $\pm$ 0.44
Polydispersibility index (PI)	0.23 $\pm$ 0.06	1 $\pm$ 0	0.61 $\pm$ 0.02
Conductivity (mS/cm)	1.72 $\pm$ 2.71e-16	12.26 $\pm$ 2.17e-15	27.57 $\pm$ 4.3e-15

Table 1: Zeta potential and PDI of Lignin Fractions

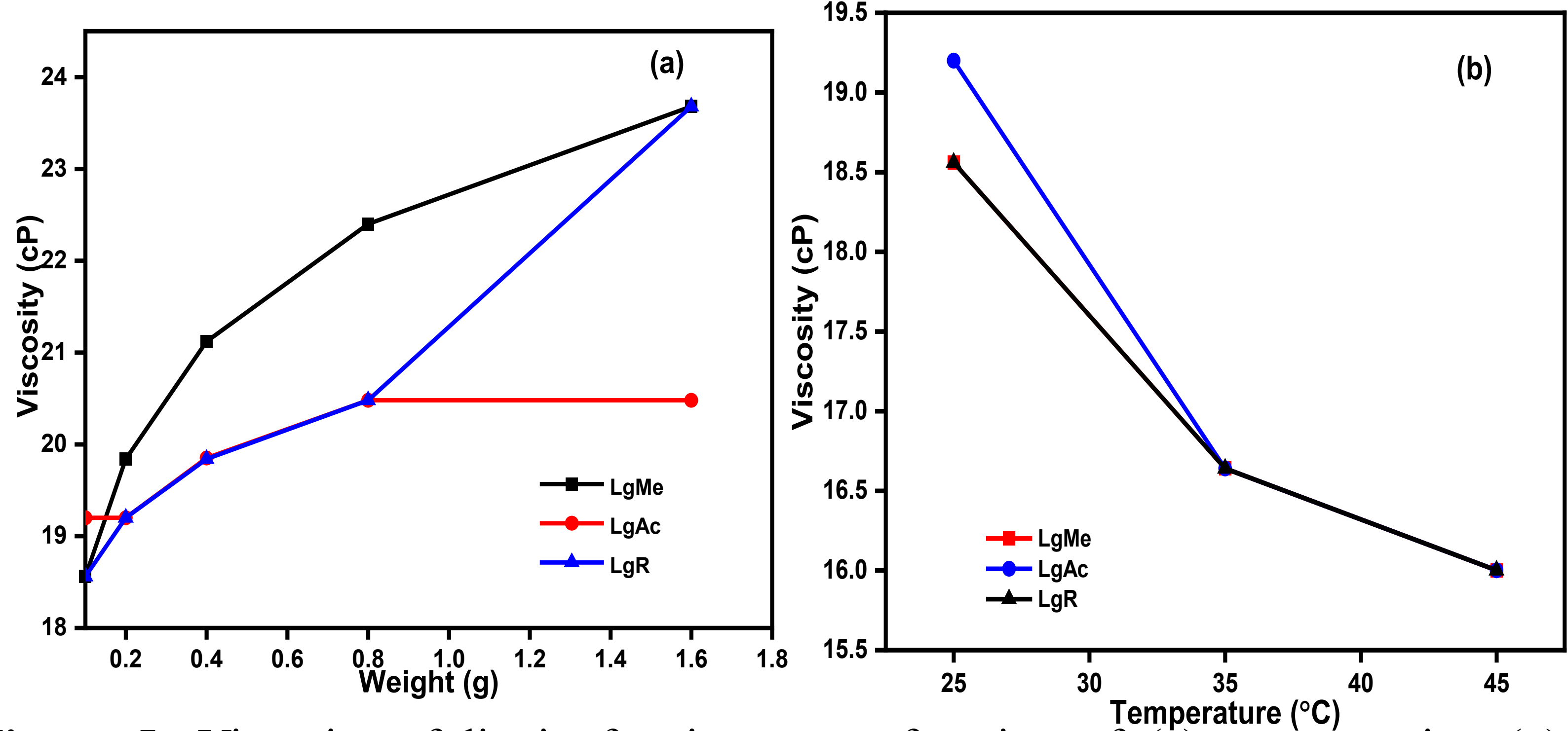


Figure 5: Viscosity of lignin fractions as a function of (a) concentration (g) (b) temperature

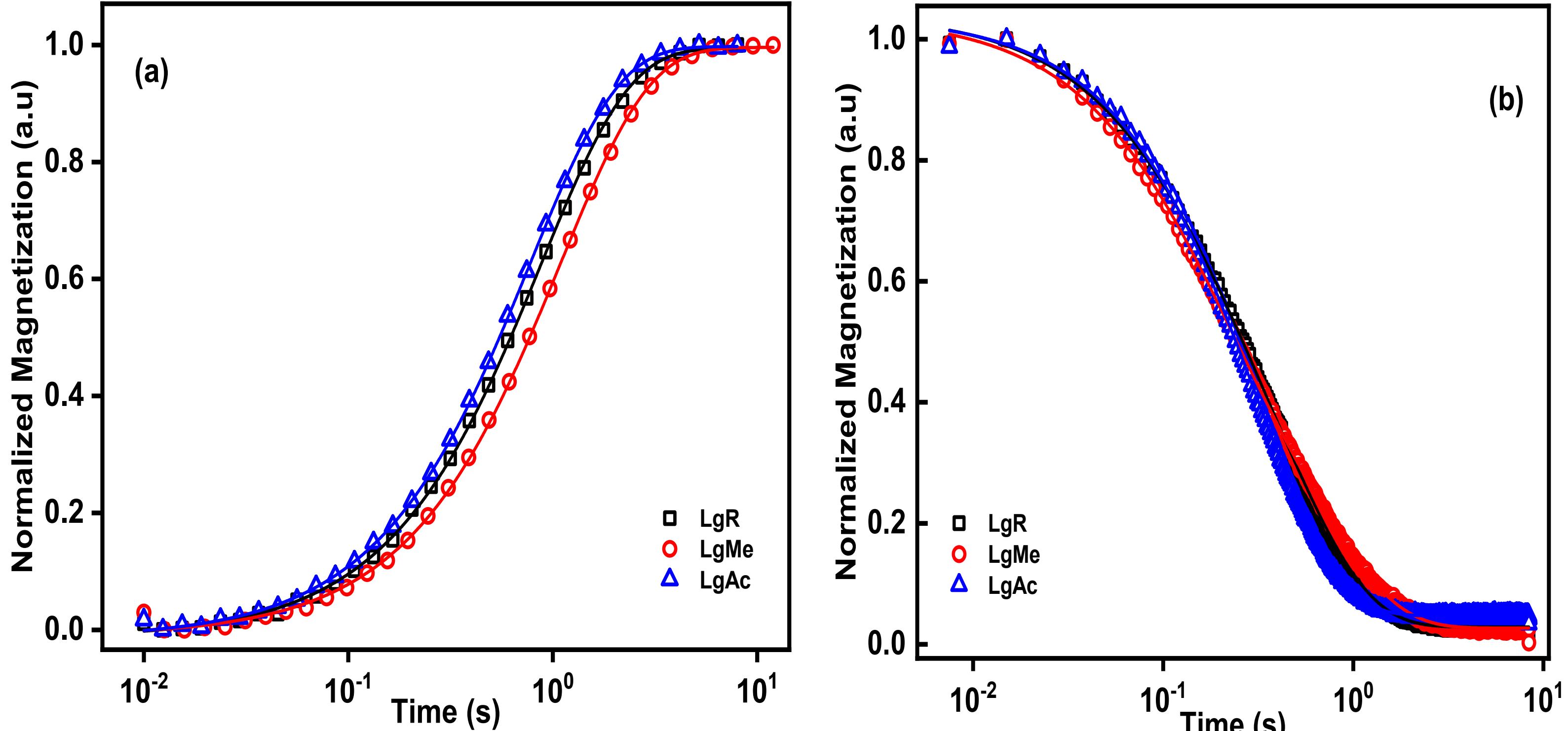


Figure 6: Magnetization curves for (a) spin lattice and (b) spin-spin relaxation for lignin fractions

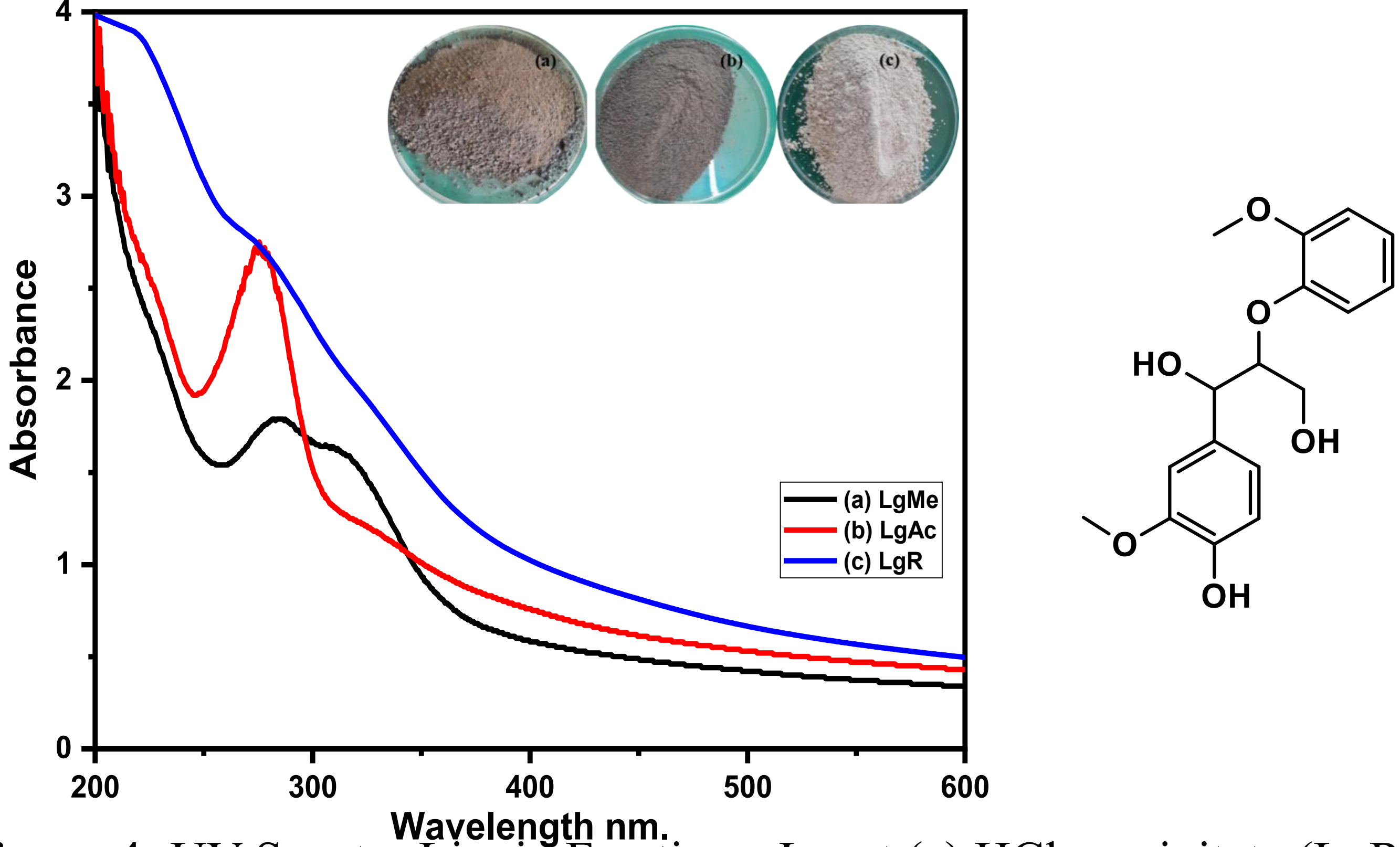


Figure 4: UV Spectra Lignin Fractions. Insert (a) HCl precipitate (LgR) (b) Methanol precipitate (LgMe) (c) acetone precipitate (LgAc)

Table 2: Spin lattice (Longitudinal) relaxation rate (T_1)

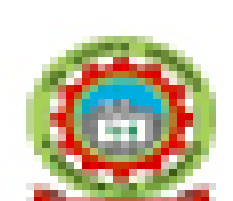
	Monoexponential Fit	Biexponential Fit			
Sample	$R_1 (s^{-1})$	$R_{fast} (s^{-1})$	$R_{slow} (s^{-1})$	A_{fast}/A_{slow}	T_1
LgR	1.14(0.01)	1.40(0.32)	0.80(0.34)	1.651594	0.71(0.16)
LgMe	0.92(0.01)	0.98(0.17)	0.51(0.78)	7.614118	1.02(0.18)
LgAc	1.29(0.01)	1.31(0.15)	0.68(3.45)	37.05435	0.76(0.09)

Table 3: Spin-spin (transverse) relaxation rate (T_2)

	Monoexponential	Biexponential Fit			
Sample	R_2	R_{fast}	R_{slow}	A_{fast}/A_{slow}	T_2
LgR	2.51(0.01)	8.76(0.19)	2.22(0.01)	0.258427	0.11(0.002)
LgMe	2.20(0.01)	7.34(0.08)	1.60(0.01)	0.69697	0.14(0.001)
LgAc	3.23(0.003)	3.25(0.005)	2.11(3.88)	0.009091	0.31(0.01)

Conclusion

The different fractions have variable particle sizes ranging between 1000 – 6000 μm , variable zeta potential and PDI. They also have varying viscosities in solution dependant on weight, temperature and RPM. Have varying relaxation profiles which have higher T1 values than T2 values indicating variable proton environments.



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