

Supplementary Information for

A novel method to screen biodegradability for the early assessment of cellulosic rheology modifiers

Moumita Bhaumik†, Chiranjeevi Thulluri†, Arindam Roy and Harshad Ravindra Velankar*

Alt Material Innovations Private Limited (short form 'altM'), Plot no. 35, Electronic City, Phase 2, Industrial Area, Konappana Agrahara, Bengaluru, Karnataka 560100, India.

*Corresponding author: harshad@altm.bio; Tel: +91-9845808730

†These authors contributed equally

Contents

RM chemical structures of HPC, HPMC, HEMC, cet-HEC.....	S1
Chromatograms of GPC analysis (Calibration curves).....	S2
Chromatograms of GPC analysis (Test samples).....	S3
Total carbohydrate analysis (calibration curve).....	S4
Methodology for synthesis of hydroxypropyl celluloses.....	S5
Results of quantitative mathematical modeling.....	S6
Viscosity profiles of CRMs during initial phase of biodegradation.....,.....	S7

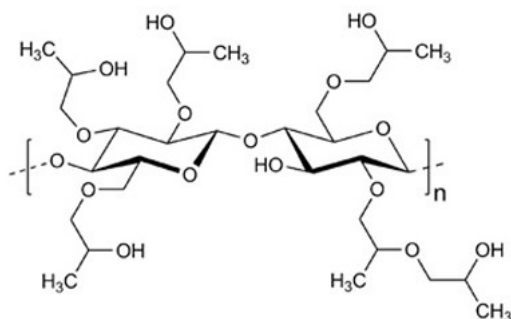
S1. Chemistry of cellulose-based rheology modifiers used in the study

CRM type	Methoxy %	Hydroxypropyl % / Hydroxyethyl %	MS	DS
HPC -J	-	8-10 %	2.5	1.8
HPC - M	-	8-10 %	3.0	2.0
HPMC*	28-30%	7 – 12%	2.2 - 7.8	2.5
HEMC**	22-30%	2 – 14%	0.8 - 1.2	2.5
Cet-HEC*	-	2-6 %	2.5	1.8

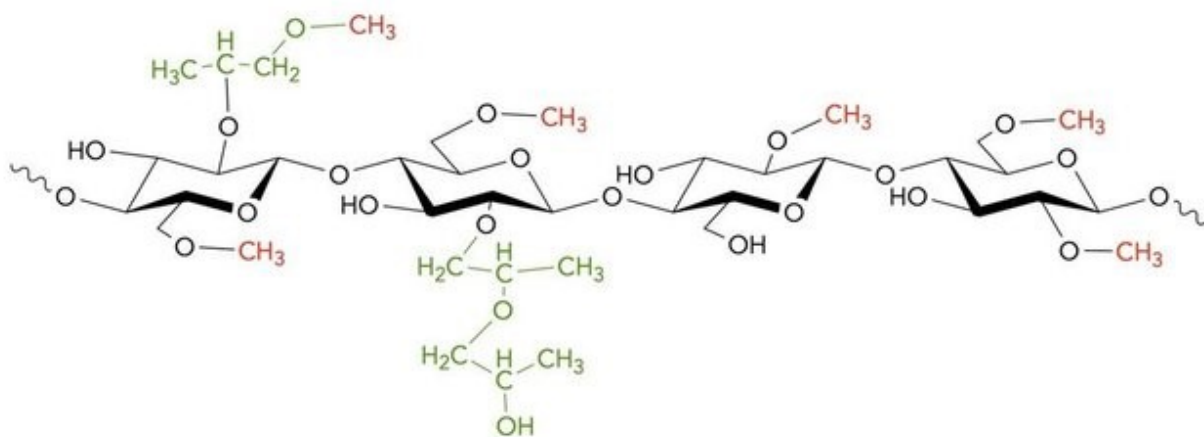
MS: Molar substitution; DS: Degree of substitution

*: HPMC: Benecel™ e4M HPMC – Technical Data Sheet,
https://www.ashland.com/file_source/Ashland/Documents/PHC19_067_Benecel_A4_081219.pdf

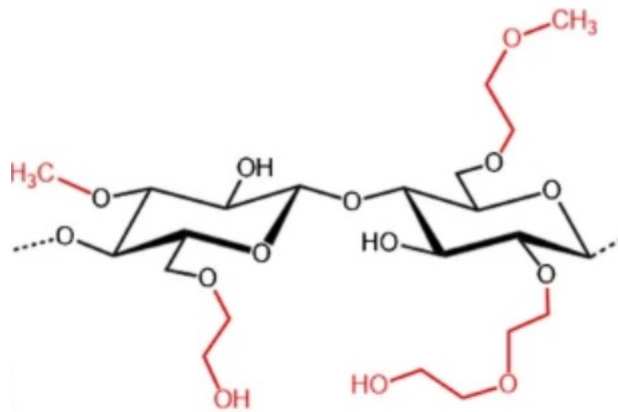
**:<https://mikazone.com/products/mikazone-cellulose-products/hydroxyethyl-methylcellulose-hemc/>



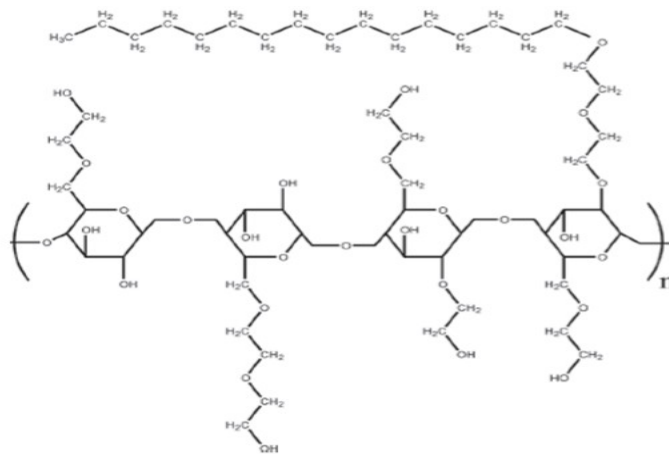
a. Hydroxypropyl cellulose (HPC)



b. Hydroxypropyl methyl cellulose (HPMC)

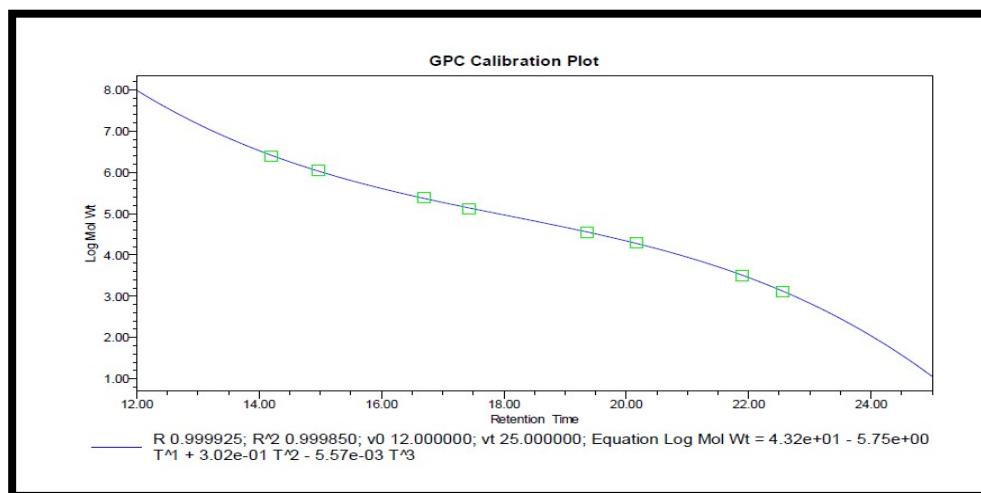
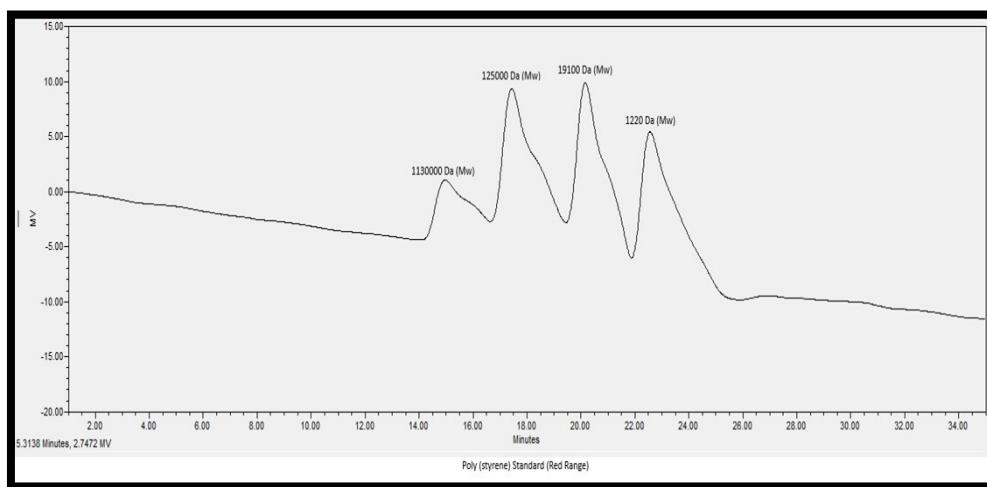
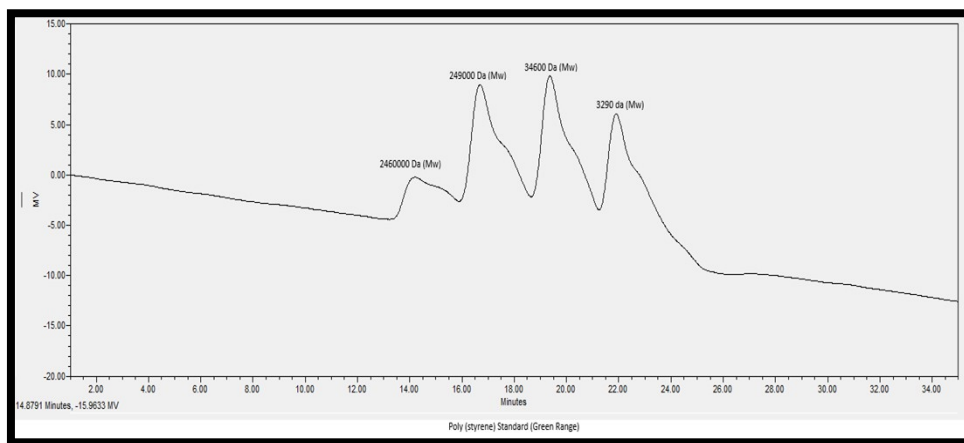


c. Hydroxyethyl methyl cellulose (HEMC)

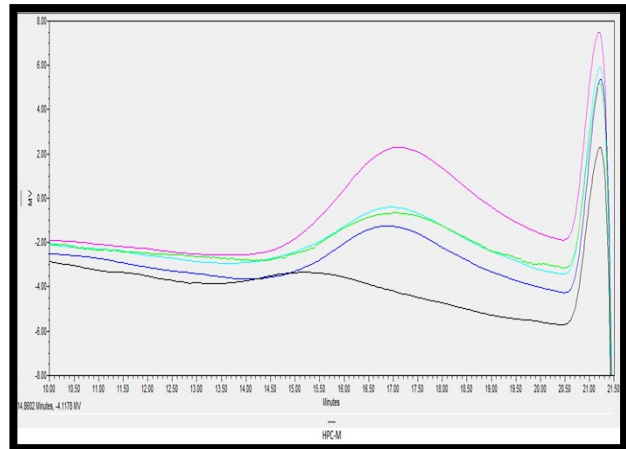


d. Cetyl-Hydroxyethyl cellulose (cet-HEC)

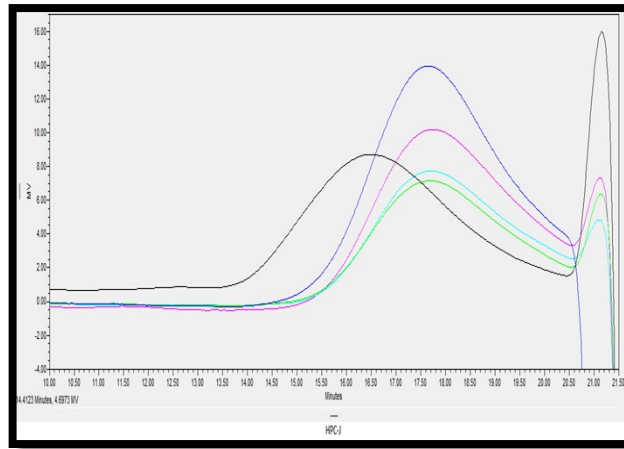
S2. GPC analysis (polystyrene standards) calibration curves



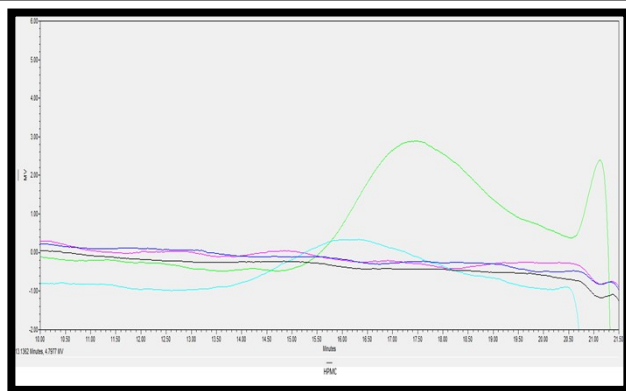
S3. GPC chromatograms of the test samples obtained during biodegradability assessment



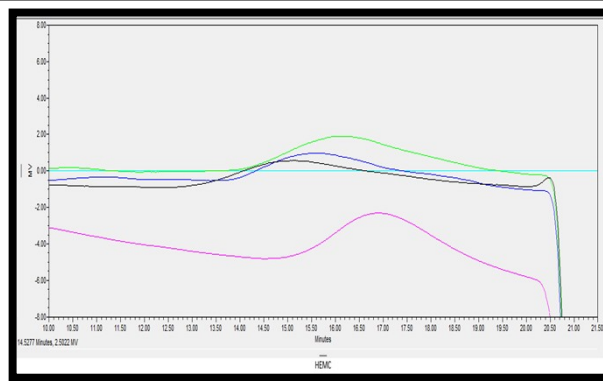
a. HPC-M (0-8 weeks)



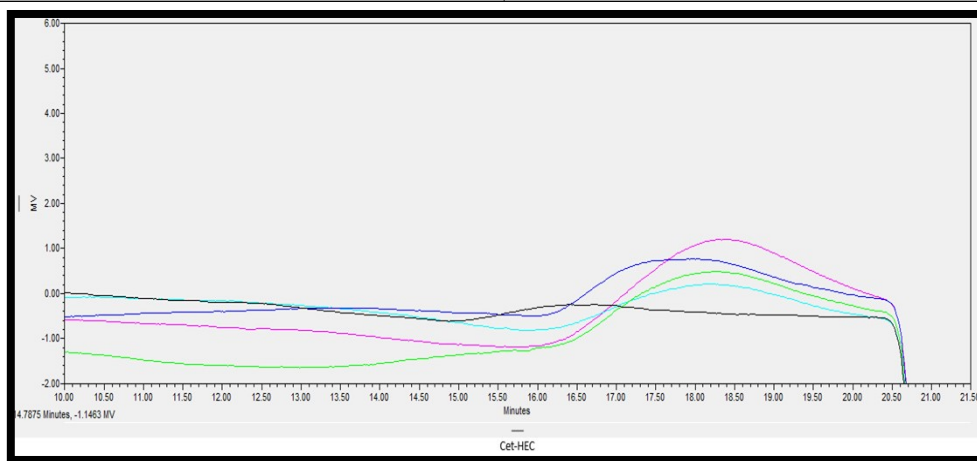
b. HPC-J (0-8 weeks)



c. HPMC (0-8 weeks)

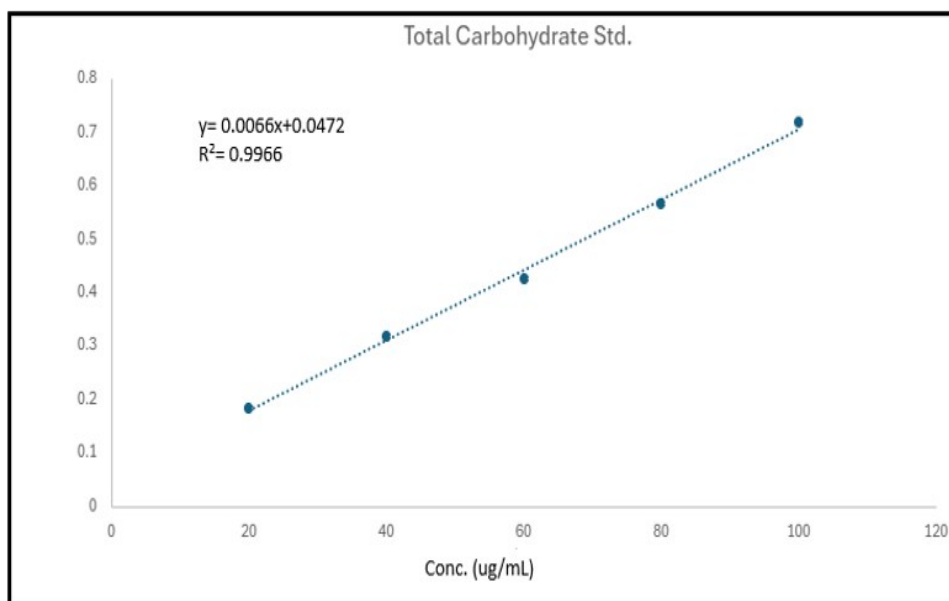


d. HEMC (0-8 weeks)



e. Cet-HEC (0-8 weeks)

S4. Calibration curve of total carbohydrate (TCC) analysis



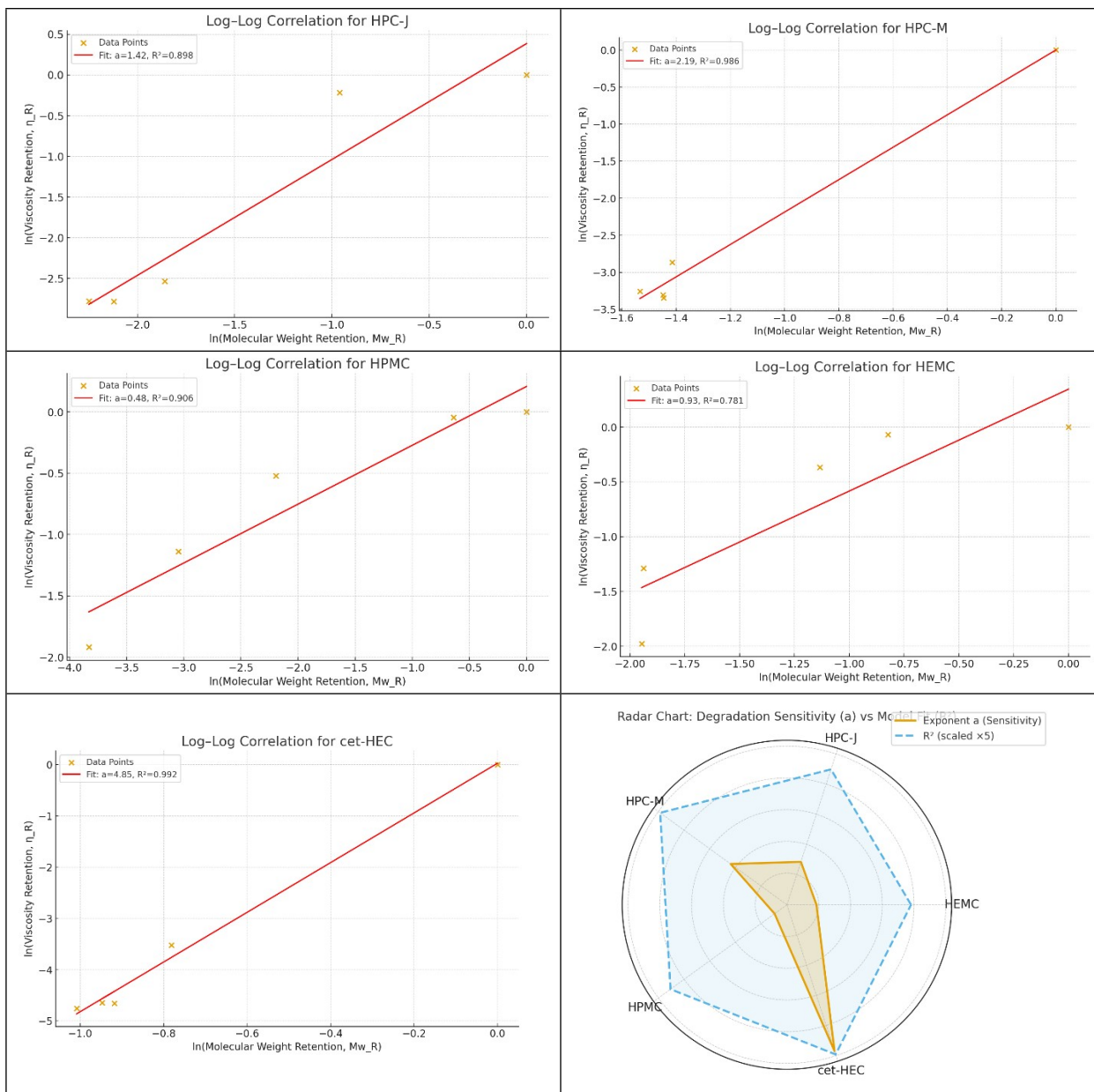
S5. Methodology for synthesis of hydroxypropyl celluloses

- Before synthesizing hydroxypropyl cellulose (HPC), cellulose isolated from sugarcane bagasse underwent a crucial preparation step. The cellulose was oven-dried overnight at $105 \pm 2^\circ\text{C}$ to remove moisture. To prevent lump formation during subsequent processing, this dried cellulosic material was then ground in a laboratory mixer, ensuring a finely disintegrated, lump-free mass ready for HPC synthesis.
- The hydroxypropylation of sugarcane bagasse cellulose was achieved using a two-stage method: alkalization followed by etherification. This heterogeneous reaction was conducted under conditions established in existing literature.
- During HPC synthesis, unavoidable and competitive side reactions consume propylene oxide, the primary reactant for alkali cellulose etherification—and can hinder the achievement of a high degree of substitution (DS). These side reactions, which can only be partially controlled, lead to major byproducts like propylene glycol and polypropylene glycol, potentially compromising the quality of the final HPC. To ensure a

high-quality product, rigorous washing steps were implemented to completely remove these byproducts from the synthesized HPC.

- The process began with alkalization using a 2.5M sodium hydroxide solution. Subsequently, the alkali cellulose underwent etherification with propylene oxide. An excess of propylene oxide (ranging from 15–40M/AGU) was used to treat the alkali cellulose for a specific duration (2–4.5 hours) at temperatures varying between 40 and 60 °C.
- Upon completion of the reaction, the mixture was cooled below room temperature and then neutralized with 5M acetic acid. The HPC was then precipitated by adding the mixture to excess acetone. The precipitated HPC was washed multiple times with 80% aqueous isopropyl alcohol solution, followed by acetone washes, to ensure complete removal of any reaction byproducts. Finally, the purified HPC was dried in a vacuum oven at 55 °C and ground into a fine powder.

S6. Quantitative mathematical modeling: Results of linear regression modelling of the viscosities and polymer molecular weight analysis across the 56-day test period



Final verified degradation sensitivity results of predictive analysis

CRM type	Exponent 'a'	R ²	p-value	Std Error
HPC-J	1.422872	0.897581	0.014364	0.277497
HPC-M	2.186259	0.986375	0.000678	0.14835
HPMC	0.480058	0.905558	0.012686	0.089507
HEMC	0.92964	0.781057	0.046727	0.28417
cet-HEC	4.84986	0.992114	0.000298	0.249635

S7. Viscosity profiles of CRMs during initial phase (week-1 & 2) of their biodegradation

