

Electronic supplementary information

Greenness Assessment and Synthesis for the Bio-Based Production of the Solvent 2,2,5,5-Tetramethyloxolane (TMO)

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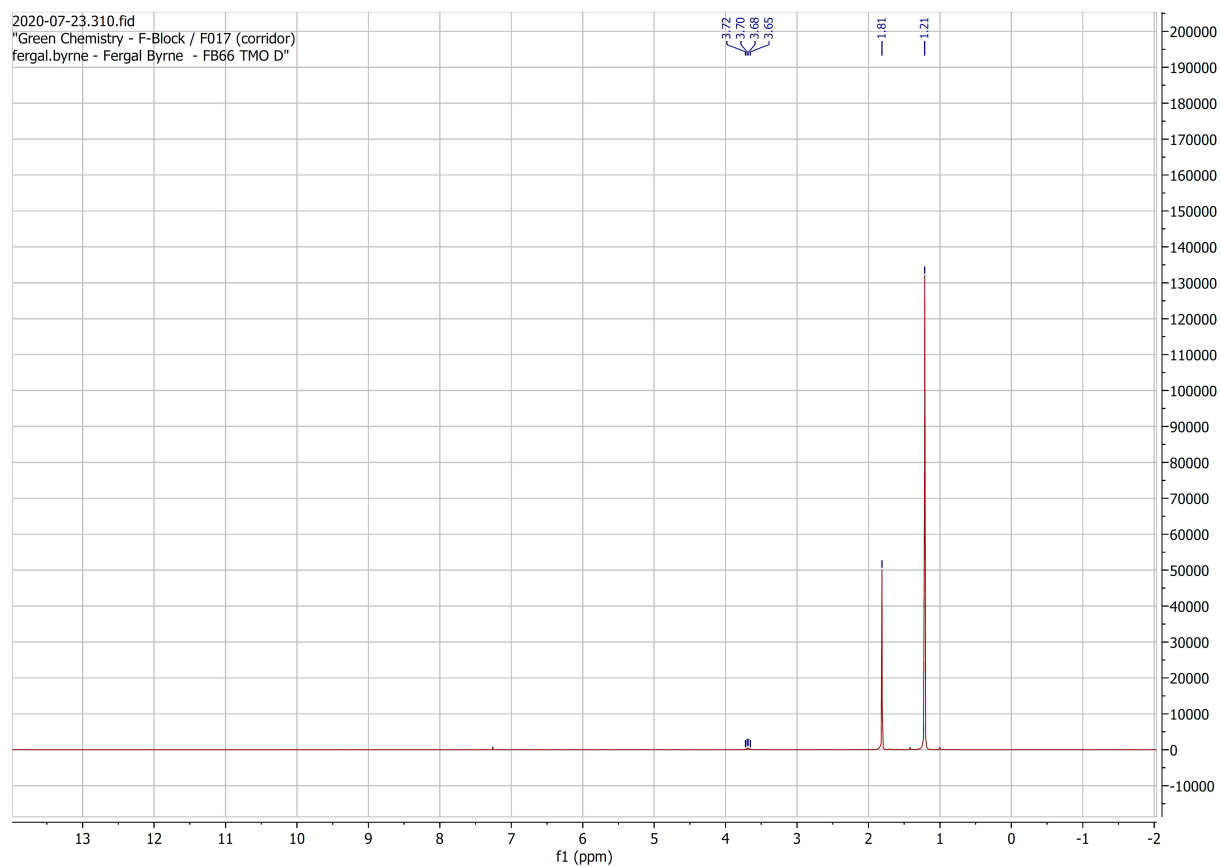


Figure S1. ^1H NMR spectrum of partially bio-based 2,2,5,5-tetramethyloxolane (TMO) produced by Route 1. CDCl_3 solvent.

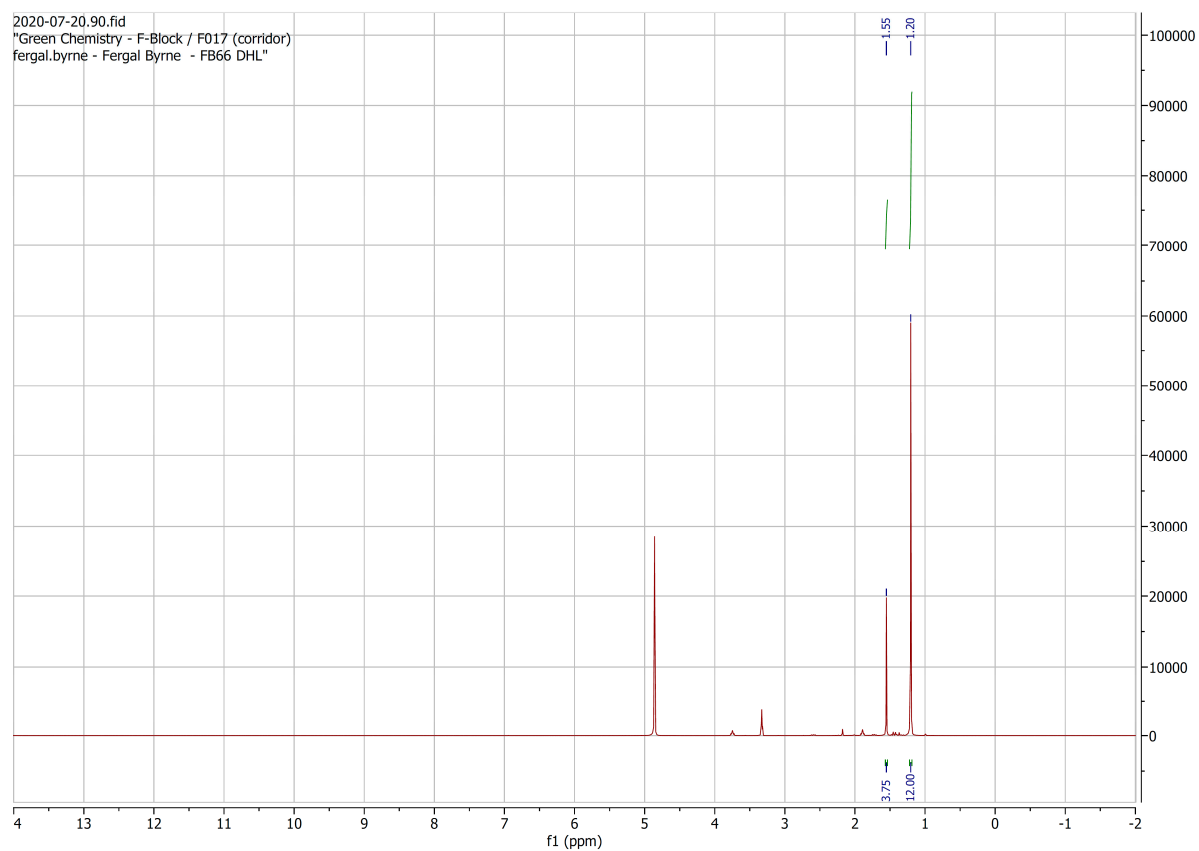


Figure S2. ^1H NMR spectrum of partially bio-based 2,5-dimethyl-2,5-hexandiol (DHL) produced by Route 1, d-MeOD solvent.

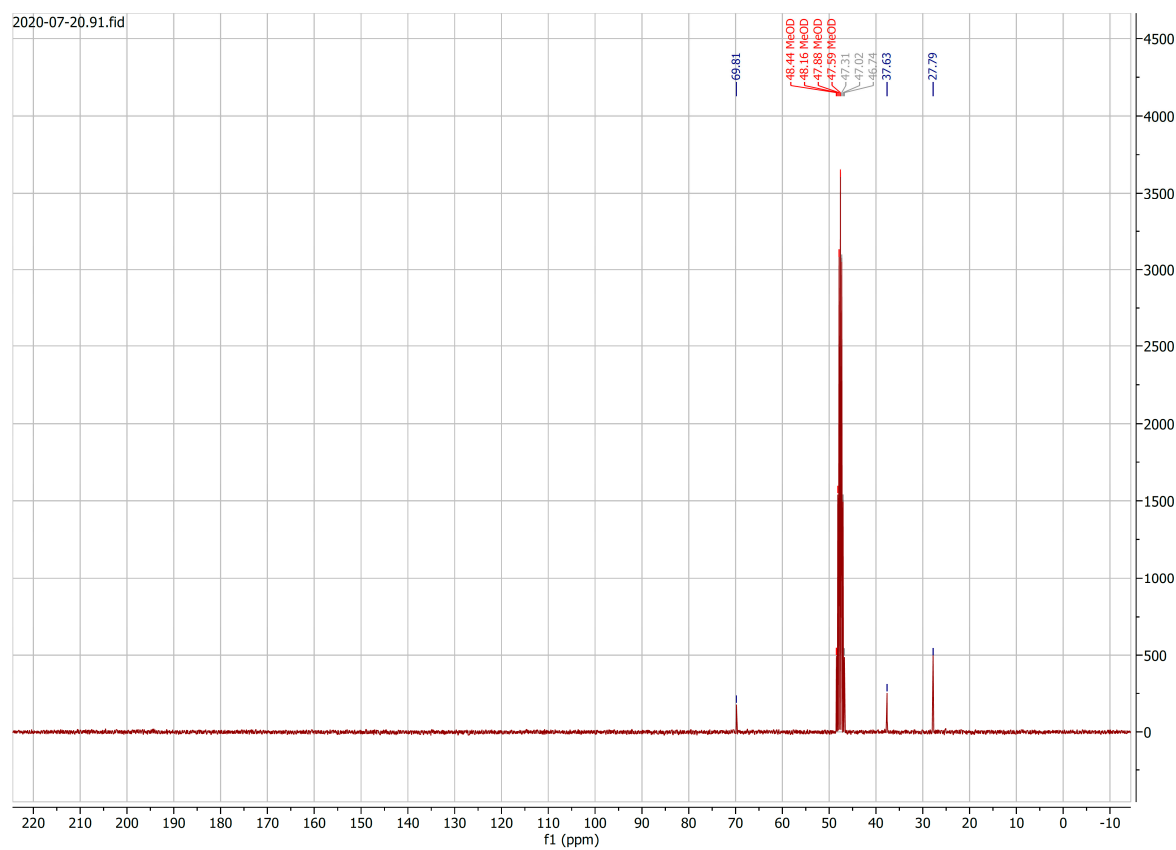


Figure S3. ^{13}C NMR spectrum of partially bio-based 2,5-dimethyl-2,5-hexandiol (DHL) produced by Route 1, d-MeOD solvent.

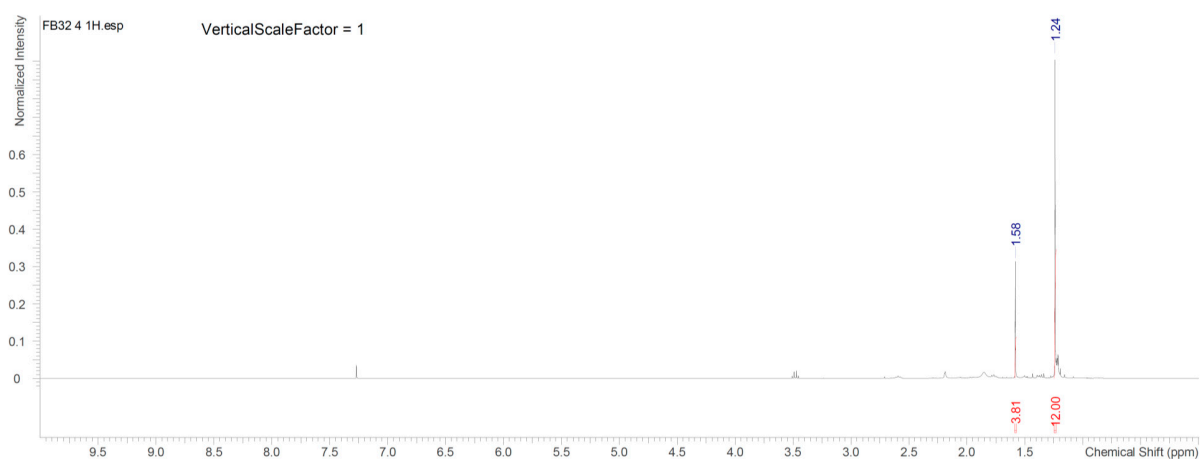


Figure S4. ^1H NMR of 2,5-dimethyl-2,5-hexanediol as produced by Route 2. CDCl_3 solvent.

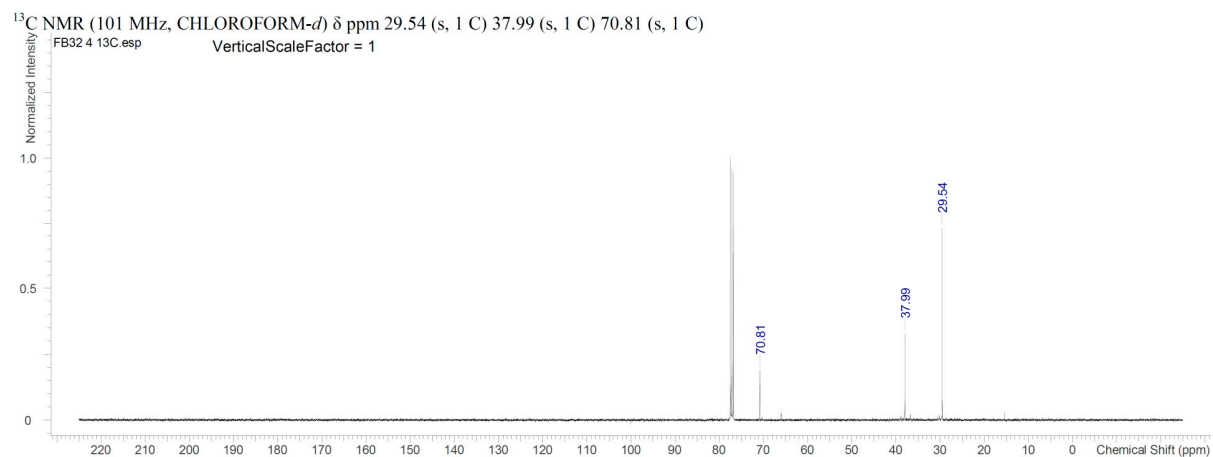


Figure S5. ¹³C NMR of 2,5-dimethyl-2,5-hexanediol as produced by Route 2, CDCl₃ solvent.

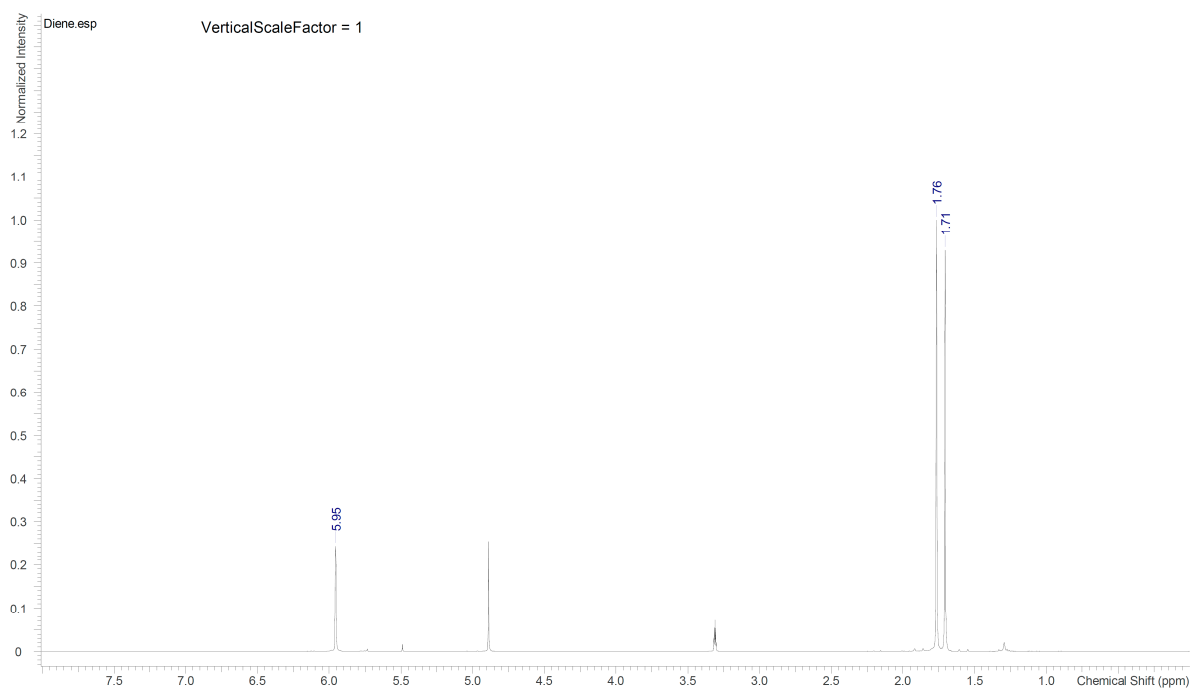


Figure S6. ¹H NMR spectrum of 2,5-dimethylhexane-2,4-diene, d-MeOD solvent.

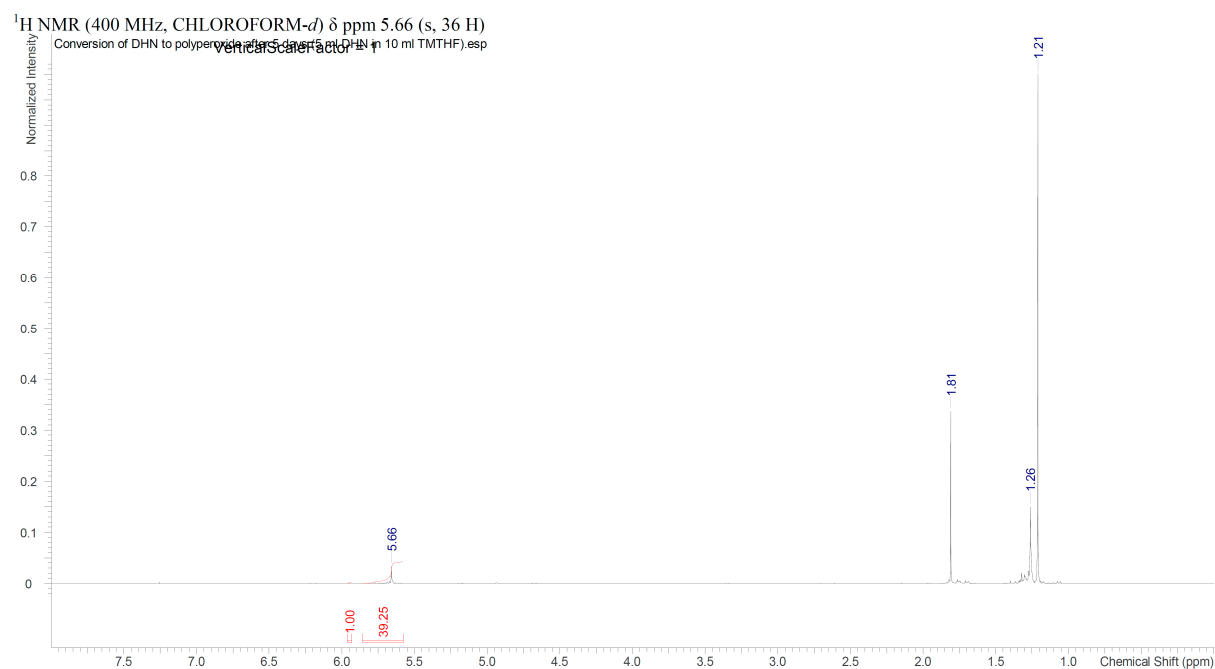
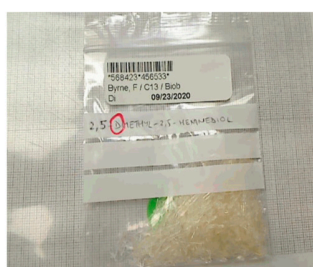


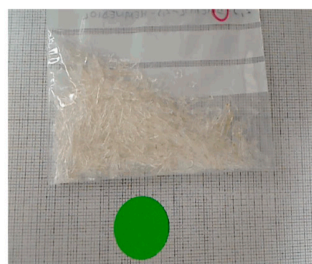
Figure S7. ¹H NMR spectrum of the polyperoxide of 2,5-dimethylhexane-2,4-diene (DHN polyperoxide). CDCl₃ solvent.

RESULT: 64 % Biobased Carbon Content (as a fraction of total organic carbon)

Laboratory Number	Beta-568423
Percent modern carbon (pMC)	64.34 +/- 0.2 pMC
Atmospheric adjustment factor (REF)	100.0; = pMC/1.000



Package received - labeling COC



View of content (1mm x 1mm scale)



16.8mg analyzed (1mm x 1mm scale)

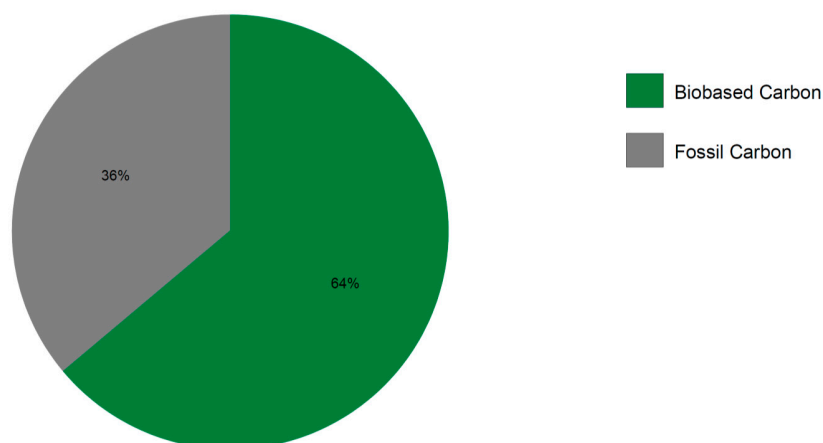
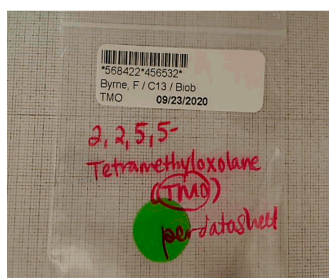


Figure S8. ASTM D6866-20 Method B for bio-based carbon testing results for 2,5-dimethyl-2,4-hexanediol.

RESULT: 64 % Biobased Carbon Content (as a fraction of total organic carbon)

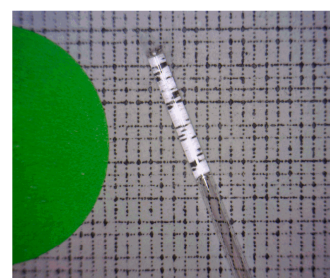
Laboratory Number	Beta-568422
Percent modern carbon (pMC)	64.44 +/- 0.21 pMC
Atmospheric adjustment factor (REF)	100.0; = pMC/1.000



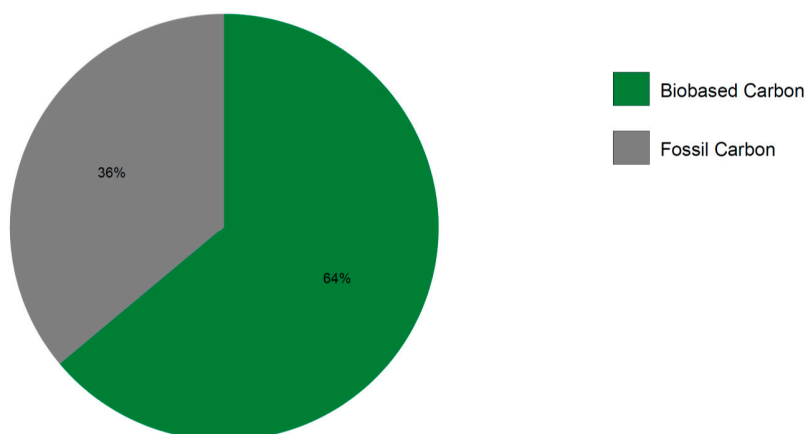
Package received - labeling COC



View of content (1mm x 1mm scale)



Representative sample analyzed (1mm x 1mm scale)



Figuer S9. ASTM D6866-20 Method B for bio-based carbon testing results for TMO.