Supplementary information

Melt polycondensation of 2,5-tetrahydrofurandimethanol with various dicarboxylic acids towards a variety of biobased polyesters

Chenhao Jin[a], Lipeng Liu[a], Zhu Tu[a], Bo Wang[b], Pei Wang[c], Zhiyong Wei[a,*]

[a] *Department of Polymer Science and Engineering, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, China*

[b] *School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China*

[c] *College of Transportation Engineering, Dalian Maritime University, Dalian 116024, China*

*Corresponding author, E-mail address: zywei@dlut.edu.cn (Z. Wei).

Table S1 Feeding amount of diols reacting with FDCA

Diols	Molar (mol)		Mass (g)		TBT (g)
	Diols	FDCA	Diols	FDCA	
EG	0.400	0.004	24.819	0.624	0.0136
DEG	0.400	0.004	42.448	0.624	0.0136
BDO	0.400	0.004	36.048	0.624	0.0136
ODO	0.400	0.004	58.492	0.624	0.0136
THFDM	0.400	0.004	52.832	0.624	0.0136
CHDM	0.400	0.004	57.684	0.624	0.0136

Table S2 Feeding amount of DEG-based and THFDM-based homopolymers

Samples	Diacids	Molar (mol)		Mass (g)		TBT (g)
		Diacids	Diols	Diacids	Diols	
DEG based	SA	0.6	0.96	70.85	101.88	0.68

polyesters	AA	0.6	0.96	87.68	101.88	0.68
	PTA	0.6	0.96	99.68	101.88	0.68
	FDCA	0.6	0.96	93.65	101.88	0.68
THFDM based polyesters	SA	0.6	0.96	70.85	126.82	0.68
	AA	0.6	0.96	87.68	126.82	0.68
	PTA	0.6	0.96	99.68	126.82	0.68
	FDCA	0.6	0.96	93.65	126.82	0.68

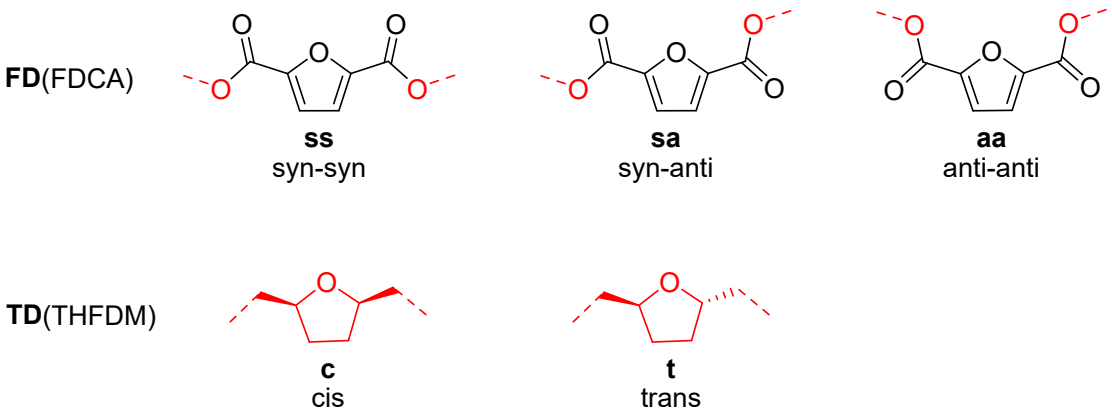

Figure S1. Possible conformations for subunit FDCA (FD) and configurations for THFDM (TD)

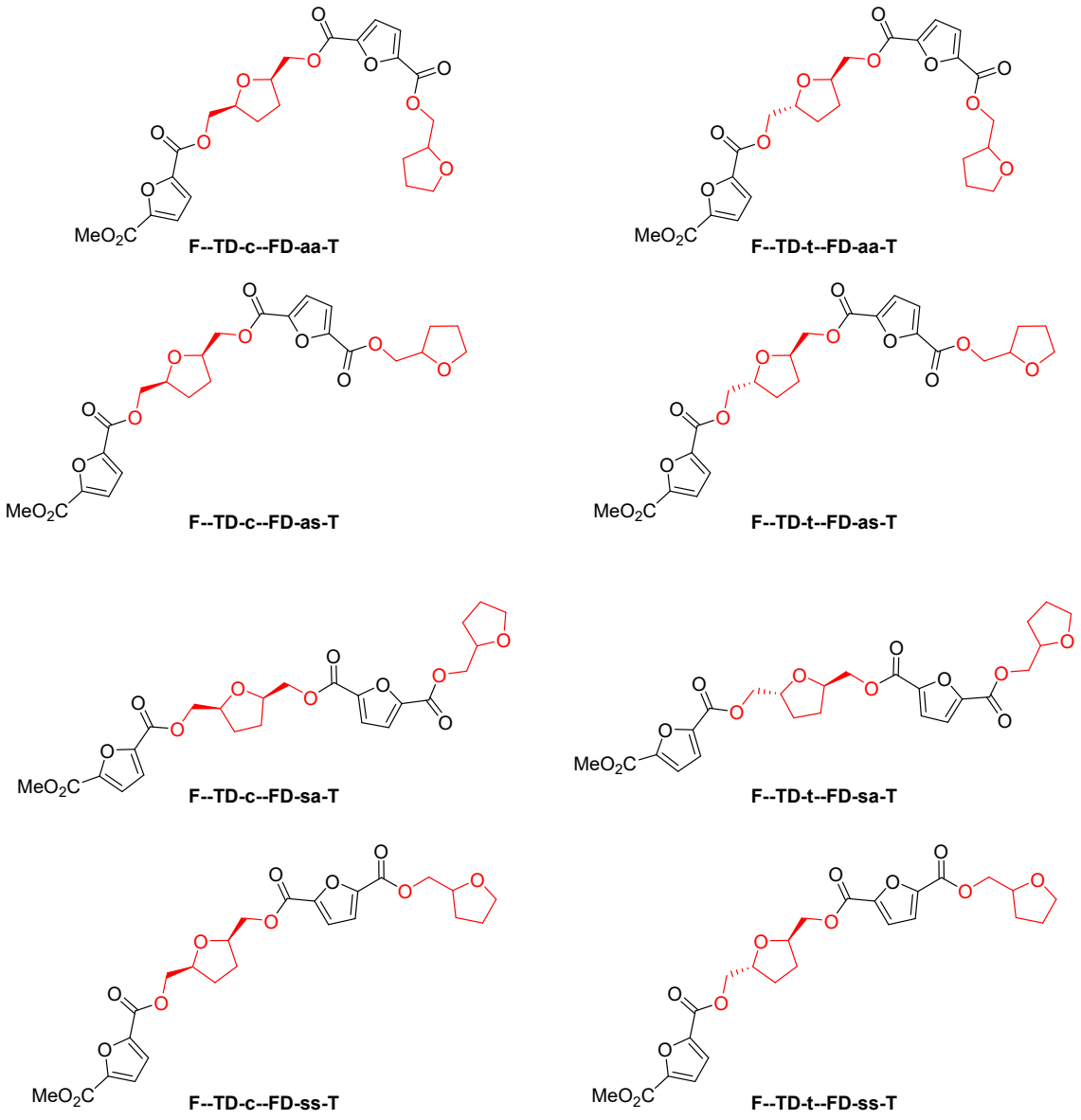

Figure S2. Eight possible combinations for FD and TD subunit in the simplified model used in the following calculations

Table S3 The most stable 5 conformations of the simplified polymer model

Entry	Relative electronic energy (kcal/mol)	Relative Gibbs free energy (kcal/mol)	Absolute electronic energy (Hartree)	Absolute Gibbs free energy (Hartree)
F--TD-c--FD-aa-T-1	-1.1	*0.3*	-1833.401088	-1832.991460
F--TD-c--FD-aa-T-2	-0.4	*1.0*	-1833.400033	-1832.990367
F--TD-c--FD-aa-T-3	-1.9	*1.0*	-1833.402338	-1832.990351
F--TD-c--FD-aa-T-4	-1.8	*1.3*	-1833.402159	-1832.989955
F--TD-c--FD-aa-T-5	-1.3	*1.4*	-1833.401334	-1832.989675
F--TD-c--FD-as-T-1	-0.3	*0.8*	-1833.399774	-1832.990668
F--TD-c--FD-as-T-2	-0.6	*0.9*	-1833.400267	-1832.990499
F--TD-c--FD-as-T-3	-1.2	*2.0*	-1833.401275	-1832.988820
F--TD-c--FD-as-T-4	-1.3	*2.2*	-1833.401347	-1832.988395
F--TD-c--FD-as-T-5	0.2	*3.0*	-1833.399033	-1832.987201
F--TD-c--FD-sa-T-1	-1.6	*1.3*	-1833.401817	-1832.989935
F--TD-c--FD-sa-T-2	-0.5	*1.7*	-1833.400088	-1832.989245
F--TD-c--FD-sa-T-3	-0.9	*1.7*	-1833.400715	-1832.989219
F--TD-c--FD-sa-T-4	-0.7	*2.3*	-1833.400452	-1832.988302
F--TD-c--FD-sa-T-5	-0.2	*2.5*	-1833.399614	-1832.987941
F--TD-c--FD-ss-T-1	1.0	*1.4*	-1833.397765	-1832.989733
F--TD-c--FD-ss-T-2	-0.8	*2.2*	-1833.400574	-1832.988547
F--TD-c--FD-ss-T-3	-1.6	*3.0*	-1833.401902	-1832.987182
F--TD-c--FD-ss-T-4	1.2	*3.2*	-1833.397383	-1832.986935
F--TD-c--FD-ss-T-5	0.9	*3.3*	-1833.397898	-1832.986726
F--TD-t--FD-aa-T-1	0.0	*1.4*	-1833.399376	-1832.989770
F--TD-t--FD-aa-T-2	-0.1	*1.4*	-1833.399568	-1832.989725
F--TD-t--FD-aa-T-3	-0.3	*1.9*	-1833.399850	-1832.988959
F--TD-t--FD-aa-T-4	-1.9	*2.1*	-1833.402308	-1832.988560
F--TD-t--FD-aa-T-5	0.0	*2.4*	-1833.399363	-1832.988229
F--TD-t--FD-as-T-1	-1.4	*0.4*	-1833.401517	-1832.991414
F--TD-t--FD-as-T-2	-1.2	*0.9*	-1833.401207	-1832.990477
F--TD-t--FD-as-T-3	-1.2	*0.9*	-1833.401207	-1832.990472
F--TD-t--FD-as-T-4	-1.6	*1.3*	-1833.401960	-1832.989971
F--TD-t--FD-as-T-5	1.3	*2.5*	-1833.397194	-1832.987962
F--TD-t--FD-sa-T-1	0.0	*0.0*	-1833.399331	-1832.991978
F--TD-t--FD-sa-T-2	-0.6	*0.7*	-1833.400326	-1832.990880
F--TD-t--FD-sa-T-3	-0.6	*1.6*	-1833.400317	-1832.989480
F--TD-t--FD-sa-T-4	0.1	*2.0*	-1833.399126	-1832.988785
F--TD-t--FD-sa-T-5	0.7	*2.0*	-1833.398169	-1832.988715
F--TD-t--FD-ss-T-1	1.6	*3.2*	-1833.396799	-1832.986920
F--TD-t--FD-ss-T-2	-1.0	*3.2*	-1833.400969	-1832.986874
F--TD-t--FD-ss-T-3	-1.0	*3.2*	-1833.400969	-1832.986869
F--TD-t--FD-ss-T-4	2.4	*3.6*	-1833.395574	-1832.986229
F--TD-t--FD-ss-T-5	2.6	*3.8*	-1833.395142	-1832.985975