Electronic Supplementary Material (ESI) for New Journal of Chemistry.

ELECTRONIC SUPPORTING INFORMATION

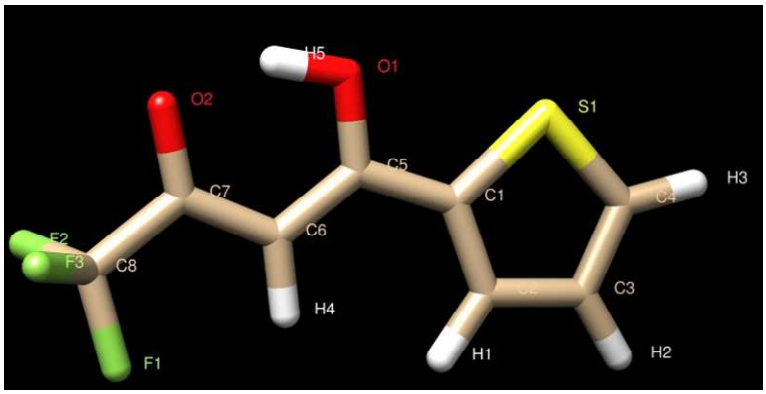

Figure S1. Schematic representation of TTA molecule with atoms

Table S1. Bonded force-field parameters

Molecules	Bonds(i-j)	K_r ($kJmol^{-1}nm^{-1}$)	r_{eq} (nm)
Tta-enol			
	S-C	104600	0.174
	C1-C5	132632.8	0.145
	C1-C2	178656.8	0.138
	C2-C3	229701.6	0.141
	C6-C7	171544	0.141
	C5-O1	133888	0.132
	C7-O2	238488	0.124
	C-F	153552.8	0.135
	C-H	142256	0.108
	O-H	231375.2	0.101
Molecules	Angles(i-j-k)	K_θ ($kJmol^{-1}rad^{-2}$)	θ_{eq} (degree)
Tta-enol			
	S-C-C	100.00	112.49
	S-C-H	209.20	119.68
	C-S-C	259.40	90.88
	C1-C5-O1	209.20	115.00
	C1-C5-C6	167.36	124.01
	C1-C2-H1	146.44	123.21
	C1-C2-C3	355.64	113.21
	C2-C1-C5	292.88	129.01
	C5-O1-H5	230.12	107.00
	C6-C7-O2	334.72	125.11
	C-C-F	209.20	110.75
	F-C-F	322.16	107.66

Table S2. Non bonded force-field parameters

molecules	site	σ (nm)	ε (kJ/mol)
tta			
	S	0.360	1.485
	C1	0.355	0.292
	C2	0.355	0.317
	C5	0.350	0.276
	C7	0.375	0.439
	O1	0.312	0.711
	O2	0.296	0.878
	H1	0.242	0.125
	H3	0.290	0.585
	H5	0.250	0.125
	F	0.295	0.221
	Eu	0.327	0.322

Table S3. Partial atomic charges on HTTA (*enol* and *enolate* forms) using Mullien atomic population analysis method.

Atom	*enol*	*enolate*
S	0.21279	0.14456
O1	-0.24717	-0.36885
O2	-0.34943	-0.33616
C1	-0.39011	-0.32152
C2	0.02586	0.03161
C3	-0.17071	-0.19762
C4	-0.16977	-0.19944
C5	0.27010	0.20764
C6	-0.18651	-0.27468
C7	0.10176	0.05297
C8	0.44059	0.36732
F	-0.15575	-0.18935
Ha	0.15068	0.1085
Hb	0.17535	0.13650