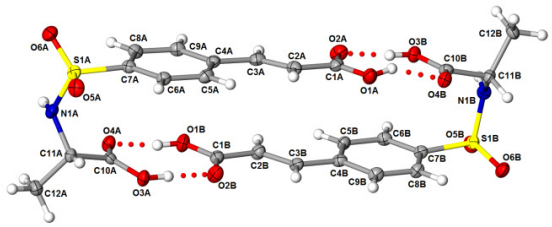
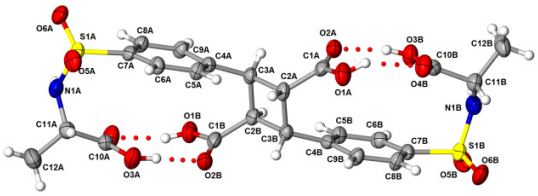
Supplementary data for





Crystal Code	recrystallization solvent	misc.
3-I	acetone	
3-IIa	2-butanone	room temp. phase of **3**-IIb
3-IIb		low temp. phase of **3**-IIa

Hydrogen-bond geometries for reactant and product phases of **3**.*

Compound	**D-H···A (Å)**	**D···A (Å)**	**D-H···A (º)**	Symmetry operator
3-I (unreacted)	O1A-H···O4B	2.639(3)	164	*x*,*y*,*z*
	O1B-H···O4a	2.7254(3)	171	*x*,*y*,*z*
	O3A-H···O2B	2.604(3)	172	*x*,*y*,*z*
	O3B-H···O2A	2.647(3)	178	*x*,*y*,*z*
	N1A-H···O4B	2.998(3)	168	*x*-1, *y*-1, *z*-1
	N1B-H···O1A	2.999(3)	167	*x*, *y*+1, *z*
	C9A-H···O5A	3.318(3)	157	*x*, *y*+1, *z*
	C9B-H···O5B	3.195(3)	153	x, y-1, z
3-I (photodimerized)	O1A-H···O4B	2.782(3)	150	*x*,*y*,*z*
	O1B-H···O4a	2.817(3)	162	*x*,*y*,*z*
	O3A-H···O2B	2.620(3)	177	*x*,*y*,*z*
	O3B-H···O2A	2.670(3)	170	*x*,*y*,*z*
	N1A-H···O4B	3.084(3)	172	*x*-1, *y*-1, *z*-1
	N1B-H···O1A	3.324(3)	148	*x*, *y*+1, *z*
	C9A-H···O5A	3.370(3)	152	*x*, *y*+1, *z*
	C9B-H···O5B	3.445(3)	153	*x*, *y*-1, *z*
3-IIa (unreacted)	O1A-H···O4B	2.645(3)	169	*x*,*y*,*z*
	O1B-H···O4a	2.693(3)	168	*x*,*y*,*z*
	O3A-H···O2B	2.676(3)	157	*x*,*y*,*z*
	O3B-H···O2A	2.702(3)	167	*x*,*y*,*z*
	N1A-H···O4B	3.055(4)	157	*x*, *y*+1, *z*-1
	N1B-H···O1A	3.154(4)	153	*x*, *y*-1, *z*
	C9A-H···O5A	3.375(4)	145	*x*, *y*-1, *z*
	C9B-H···O5B	3.188(4)	156	*x*, *y*+1, *z*
3-IIa (photodimerized)	O1A-H···O4B	2.776(7)	150	*x*,*y*,*z*
	O1B-H···O4a	2.811(8)	155	*x*,*y*,*z*
	O3A-H···O2B	2.624(7)	154	*x*,*y*,*z*
	O3B-H···O2A	2.811(8)	155	*x*,*y*,*z*
	N1A-H···O4B	3.095(6)	155	*x*-1, *y*-1, *z*-1
	N1B-H···O1A	3.325(8)	149	*x*, *y*+1, *z*
	C9A-H···O5A	3.451(8)	152	*x*, *y*-1, *z*
	C9B-H···O5B	3.364(7)	152	*x*, *y*+1, *z*

3-IIb (unreacted)	O2A-H···O3B	2.713(3)	168	*x,y,z*
	O2B-H···O3A	2.698(3)	166	*x,y,z*
	O4A-H···O1B	2.654(3)	172	*x,y,z*
	O4B-H···O1A	2.606(3)	168	*x,y,z*
	N1A-H···O6B	3.199(3)	150	*x*, *y*-1, *z*-1
	N1B-H···O1A	3.132(3)	152	*x*, *y*+1, *z*
	C9A-H···O5A	3.360(3)	150	*x*, *y*+1, *z*
	C5B-H···O5B	3.124(3)	157	*x*, *y*-1, *z*

* H atoms (for OH and NH) were located in difference Fourier synthesis and refined isotropically with O/N-H distances restrained to 0.85(2) Å.