Supplementary Information

Structural Determinants for the Stereoselective Hydrolysis of Chiral Substrates by Phosphotriesterase

Table S1. Structure parameters for the complexes between the G60A mutant and the R_p- and S_p-enantiomers of **1** and **2**.

Substrate	Parameters	Initial Pose					
		R_L	R_A	R_M	S_L	S_A	S_M
Compound **1**	A_L	163±7	159±7	86±7	123±14	66±6	89±6
	A_A	70±6	83.4±7	92±4	80±6	148±6	99±7
	A_M	91±9	88.5±8	163±5	128±11	104±6	150±6
	d_{PO}	3.4±0.1	3.5±0.2	3.7±0.1	3.9±0.1	3.6±0.1	4.0±0.2
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.2±0.1	2.1±0.1
Compound **2**	A_L	162±5	102±9	76±6	78±12	82±11	103±5
	A_A	72±6	144±10	93±9	156±10	157±6	86±4
	A_M	93±6	72±5	165±7	89±12	87±8	144±5
	d_{PO}	3.4±0.1	3.4±0.2	3.6±0.2	3.6±0.2	3.6±0.1	4.1±0.1
	d_{ZnO}	2.1±0.1	2.2±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1

Table S2. Structure parameters for the complexes between the GWT mutant and the R_p- and S_p-enantiomers of **1** and **2**.

Substrate	Parameters	Initial Pose					
		R_L	R_A	R_M	S_L	S_A	S_M
Compound **1**	A_L	148±9	105±11	102±9	150±8	66±6	91±6
	A_A	85±7	143±11	96±6	100±8	145±7	101±8
	A_M	97±9	71±5	144±7	77±8	113 ±7	145±6
	d_{PO}	3.8±0.2	3.5±0.1	4.1±0.1	3.6±0.2	3.6±0.1	4.1±0.1
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.2±0.1	2.1±0.1
Compound **2**	A_L	151±12	91±8	95±6	149±8	80±8	101±6
	A_A	71±6	156±9	87±4	79±7	156±8	92±4
	A_M	95±16	75±6	158±6	96 ±12	94±12	144±5
	d_{PO}	3.5±0.2	3.4±0.1	3.8±0.1	3.8±0.2	3.6±0.2	4.1±0.1
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1

Table S3. Structure parameters for the complexes between the YT mutant and the R_p- and S_p-enantiomers of **1** and **2**.

Substrate	Parameters	Initial Pose					
		R_L	R_A	R_M	S_L	S_A	S_M
Compound **1**	A_L	146±9	162±8	86±6	152±6	128±7	122±14
	A_A	86±8	85±9	91±4	91±7	120±7	89 ±5
	A_M	99±12	76±5	164±6	83±6	70±5	126±12
	d_{PO}	3.9±0.2	3.4±0.1	3.7±0.1	3.6±0.1	3.6±0.2	4.1±0.1
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1
Compound **2**	A_L	150±8	146±10	89±6	152±5	59±5	94±6
	A_A	87±8	88±6	90±4	85±7	139±7	75±5
	A_M	86±8	96±13	159±6	83±7	120±7	156±5
	d_{PO}	3.8±0.2	3.8±0.2	3.8±0.1	3.7±0.1	3.5±0.1	3.8±0.1
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1

Table S4. Structure parameters for the complexes between the GGY mutant and the R_p- and S_p-enantiomers of **1** and **2**.

Substrate	Parameters	Initial Pose					
		R_L	R_A	R_M	S_L	S_A	S_M
Compound **1**	A_L	150±5	139±6	95±7	150±9	75±6	130 ±8
	A_A	68±6	103±7	86±5	100±9	160±5	77±9
	A_M	104±9	86±13	159±6	75±7	88±7	128±8
	d_{PO}	3.5±0.1	3.8±0.3	3.7±0.1	3.6±0.1	3.6±0.1	3.9±0.2
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1
Compound **2**	A_L	130±9	88±7	78±9	144±8	65±5	97±6
	A_A	91±5	153±6	93±6	102±8	150±10	93±6
	A_M	109±9	80±7	163±6	77±6	107±12	155±5
	d_{PO}	4.2±0.2	3.7±0.2	3.6±0.2	3.8±0.2	3.5±0.1	3.9±0.1
	d_{ZnO}	2.1±0.1	2.1±0.2	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1

Table S5. Structure parameters for the complexes between the QFmutant and the R_p- and S_p-enantiomers of **1** and **2**.

Substrate	Parameters	Initial Pose					
		R_L	R_A	R_M	S_L	S_A	S_M
Compound **1**	A_L	155±7	103±7	93±8	147±9	72±11	90±6
	A_A	75±11	145±6	100±8	99 ±9	153±10	88±7
	A_M	99±7	71±4	149±6	80±6	98±15	157±7
	d_{PO}	3.6±0.2	3.5±0.1	4.1±0.1	3.7±0.2	3.5±0.2	3.9±0.2
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1
Compound **2**	A_L	166±5	91±10	88±7	150±5	68±6	76±8
	A_A	69±5	154 ±10	92±5	91±6	155±6	96±7
	A_M	89±6	73±5	161±6	84±6	105±7	156±7
	d_{PO}	3.3±0.1	3.5±0.1	3.9±0.1	3.8±0.1	3.6±0.2	3.7±0.2
	d_{ZnO}	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1	2.1±0.1