Membrane protein native state discrimination by implicit membrane models

Olga Yuzlenko and Themis Lazaridis

City College of the City University of New York, 160 Convent Avenue, New York, New York 10031

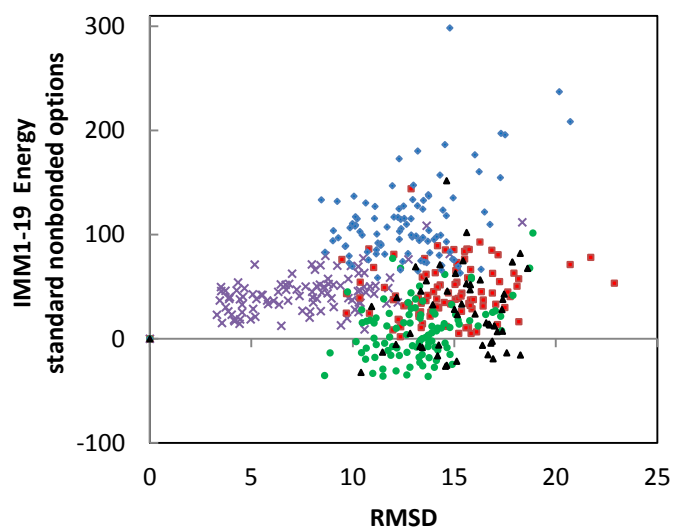Correspondence to Themis Lazaridis; email: tlazaridis@ccny.cuny.edu

Figure S1. Relative total energy in kcal/mol of the decoys obtained using IMM1 standard non-bonded options with T=27 Å vs RMSD. Purple crosses – VATP; red squares – fmr5; green dots – ltpA; blue diamonds –BRD7; black triangles –RHOD.

Table S1. Discrimination of the native structures by the implicit membrane models.

	IMM1					IMM1-p36					GBSAIM					GBSW					HDGB	Σ
T, Å	23.1	25.4	27	28.5	30.4	23.1	25.4	27	28.5	30.4	23.1	25.4	27	28.5	30.4	23.1	25.4	27	28.5	30.4	28.5	
VATP			*				*	*	*	*	*					*	*	*	*	*	*	12
fmr5		*	*			*	*	*	*	*						*	*	*	*	*	*	13
ltpA							*					*					*	*	*			5
BRD7	*	*	*	*	*	*	*	*	*	*	*	*		*	*	*	*	*	*	*	*	20
RHOD		*	*		*	*	*	*	*	*	*	*	*	*		*	*		*	*	*	16

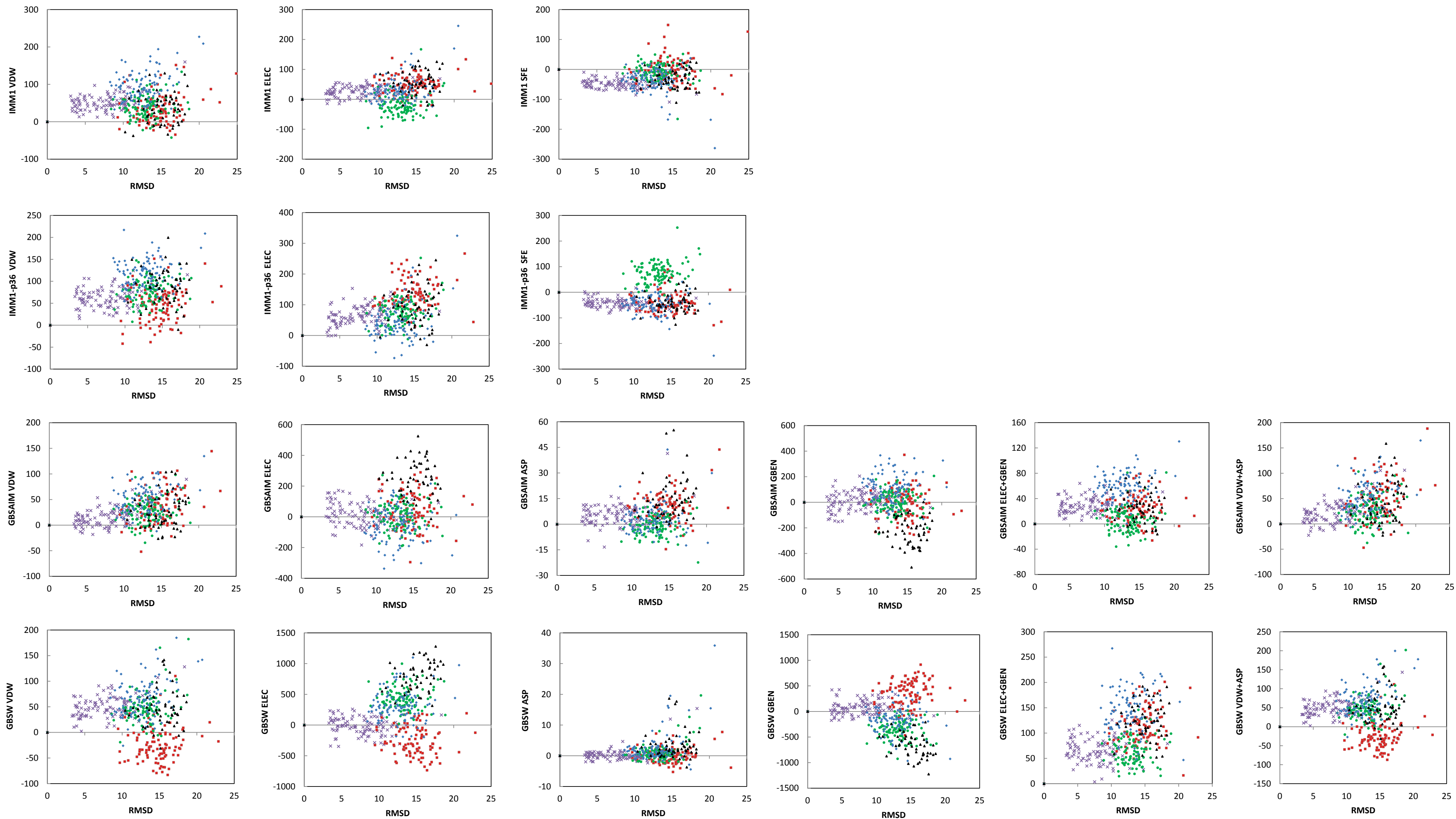[*] native structure has the lowest energy

Figure S2. Relative energy contributions in kcal/mol of the decoys obtained using IMM1, IMM1-p36, GBIM, and GBSW implicit membrane models vs RMSD with membrane width 25.4 Å. Purple crosses – VATP; red squares – fmr5; green dots – ltpA; blue diamonds –BRD7; black triangles –RHOD.
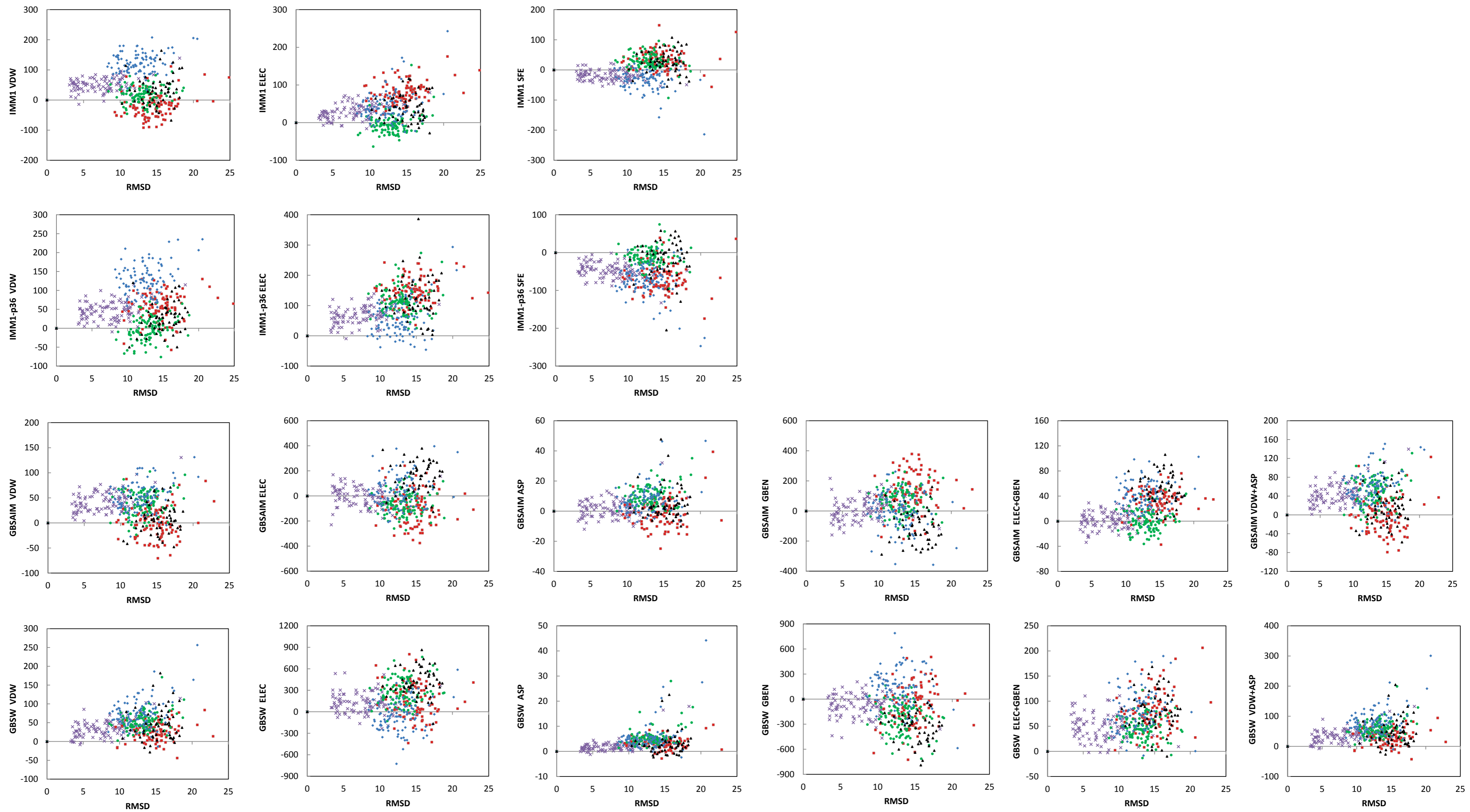
Figure S3. Relative energy contributions in kcal/mol of the decoys obtained using IMM1, IMM1-p36, GBIM, and GBSW implicit membrane models vs RMSD with membrane width 27 Å. Purple crosses – VATP; red squares – fmr5; green dots – ltpA; blue diamonds –BRD7; black triangles –RHOD.
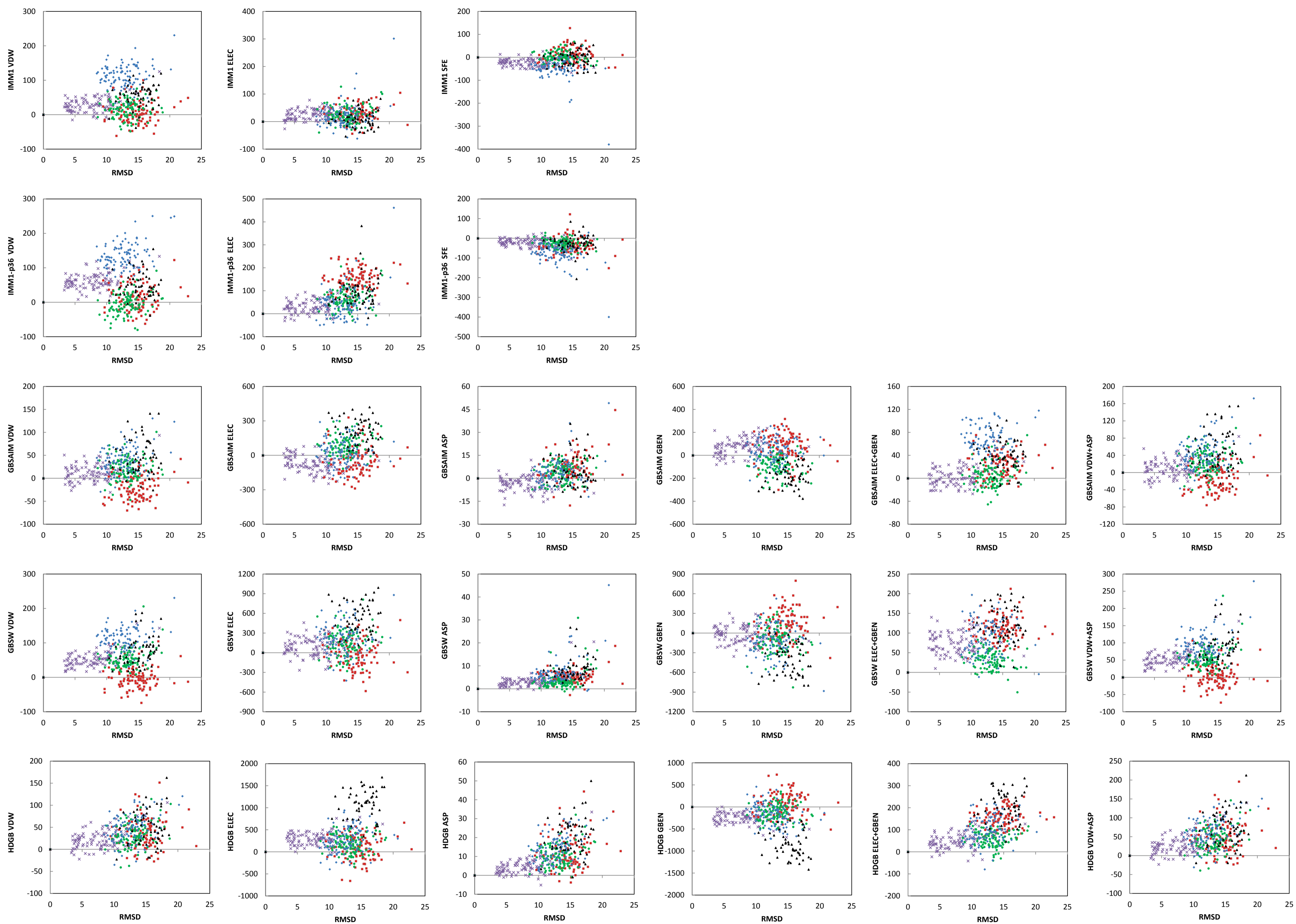
Figure S4. Relative energy contributions in kcal/mol of the decoys obtained using IMM1, IMM1-p36, GBIM, GBSW and HDGB implicit membrane models vs RMSD with membrane width 28.5 Å. Purple crosses – VATP; red squares – fmr5; green dots – ltpA; blue diamonds –BRD7; black triangles –RHOD.