

Supplementary Table S2. Results of validation of various charge models in ShaEP program.

charge model	BEDROC	EF10%
doramapimod		
EEM	0.14	3.00
Gasteiger-Marsili	0.07	2.00
dovitinib		
EEM	0.33	5.00
Gasteiger-Marsili	0.09	2.00
QEq	0.19	4.33
QTPIE	0.18	4.00
sunitinib		
EEM	0.26	5.00
Gasteiger-Marsili	0.10	3.00
QEq	0.27	5.00
QTPIE	0.27	4.67