Supplementary Table S4: Top docking scores of BOS with CoA substrates

Result #	Ligand	Docking score[a]	Distance [Å][b]	Angle [deg][c]	Interacting Residues
1	Oxalyl-CoA	-10.084	3.51	99	N38, K40-salt bridge
2	Oxalyl-CoA	-10.023	3.48	102.4	N38, K40-salt bridge
3	Oxalyl-CoA	-9.972	3.34	99.5	N38, K40-salt bridge
4	Oxalyl-CoA	-9.543	3.48	98.9	N38, K40-salt bridge
5	Oxalyl-CoA	-9.441	3.64	113.3	N38, K40-salt bridge
6	Acetyl-CoA	-9.436	3.2	102.1	K40-H-Bond
7	Malonyl-CoA	-11.902	4.58	59.5	R288, T168, G167
8	CoA	-9.602	-	-	-
9	CoA	-9.418	-	-	-

a. Score of the interaction between the ligand, L-DAPA and BOS calculated by 3 body docking. The more negative the score, the stronger the predicted interaction.

b. Distance between the thioester carbonyl carbon of the ligand and the nucleophilic nitrogen of L-DAPA.

c. The Büergi-Dunitz angle between the carbonyl vector and the vector defined by the L-DAPA nucleophile and the carbonyl vector.