

Iron is a centrally bound cofactor of specifier proteins involved in glucosinolate breakdown

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S2 Table. Evaluation of GOLD docking poses obtained with AtNSP3, Fe²⁺ and allylglucosinolate aglucone. The ten poses with lowest AtNSP3-aglucone interaction energies are included. Fulfillment of the three essential docking criteria is indicated.

Pose	Interaction energy (kJ mol ⁻¹)	Aglucone-Fe ²⁺ coordination	Sulfate group stabilization	Side chain interaction
1	-473.63	thiolate (S ⁻)	-	H394, F271
2	-463.17	thiolate (S ⁻)	-	H394, F271
3	-348.11	thiolate (S ⁻)	R237	-
4	-340.99	thiolate (S ⁻)	R237	-
5	-340.99	thiolate (S ⁻)	R237	-
6	-338.49	thiolate (S ⁻)	R237, R292	-
7	-336.39	sulfate	R237	-
8	-335.56	thiolate (S ⁻)	R237, R292	H394, F271
9	-333.05	thiolate (S ⁻)	R237, R292	H394, F271
10	-333.05	thiolate (S ⁻)	R237	F271