1

REMARK VINA RESULT:			-3.0	2.759		4.705
REMARK 6 active torsions:						
REMARK status:		('A' for Active; T for Inactive)				
REMARK		I	between atoms:	C2_2	and	N1_4
REMARK	1	A	between atoms:	N1_4	and	C3_5
REMARK	2	A	between atoms:	C4_6	and	06_15
REMARK	3	A	between atoms:	C5_7	and	05_14
REMARK	4	A	between atoms:	C6_8	and	C8_12
REMARK	5	A	between atoms:	C7_10	and	03_11
REMARK	6	A	between atoms:	C8_12	and	04_13

2

3 **Table S5a. 6M0J Vina Autodock results.**

4

5

REMARK VINA RESULT			-3.6	2.021		3.190
REMARK 6 active torsions:						
REMARK status:		('A' for Active; T for Inactive)				
REMARK		I	between atoms:	C2_2	and	N1_4
REMARK	1	A	between atoms:	N1_4	and	C3_5
REMARK	2	A	between atoms:	C4_6	and	06_15
REMARK	3	A	between atoms:	C5_7	and	05_14
REMARK	4	A	between atoms:	C6_8	and	C8_12
REMARK	5	A	between atoms:	C7_10	and	03_11
REMARK	6	A	between atoms:	C8_12	and	04_13

6

7 **Table S5b. 6WKP Vina Autodock results.**

8

9