Supporting Information

Benzothiazole Derivative as a Novel *Mycobacterium tuberculosis* Shikimate Kinase Inhibitor: Identification and Elucidation of its Allosteric Mode of Inhibition

Rukmankesh Mehra[#a], Vikrant Singh Rajput[#bd], Monika Gupta[a], Reena Chib[b], Amit Kumar[a], Priya Wazir[c], Inshad Ali Khan*[bd] and Amit Nargotra*[ad]

[#] Authors contributed equally

Affiliations

[a] Discovery Informatics Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

[b] Clinical Microbiology Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

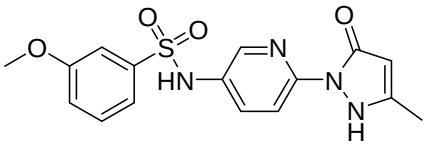
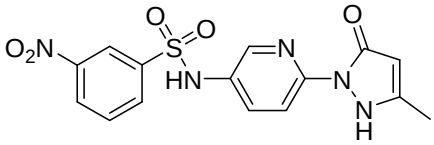
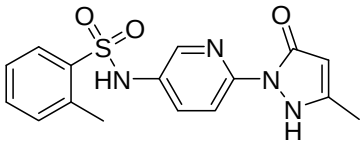
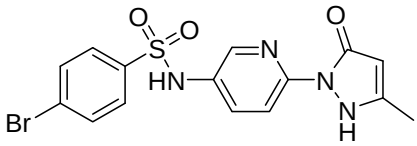
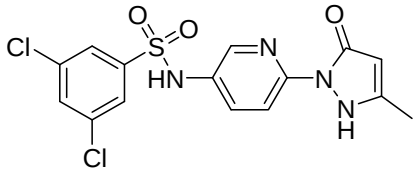
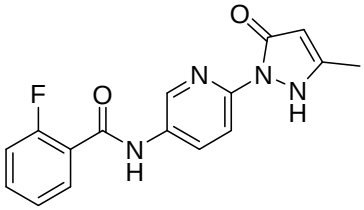
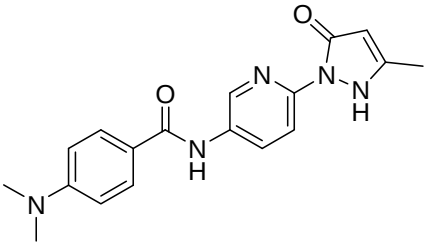
[c] Instrumentation Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

[d] Academy of Scientific and Innovative Research, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

* Corresponding authors

E-mail: anargotra@iiim.ac.in, iakhan@iiim.ac.in

Table S1. Mtb-SK inhibitors reported by Bandodkar and Schmitt (2007)

Compounds	Structure
1	
2	
3	
4	
5	
6	
7	

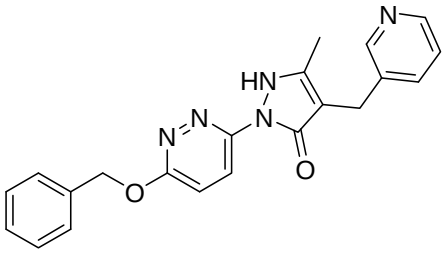
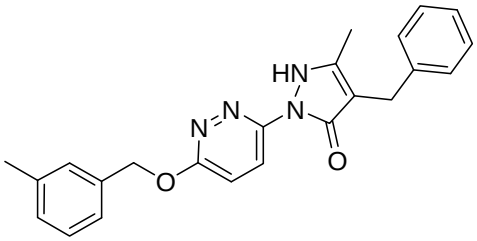
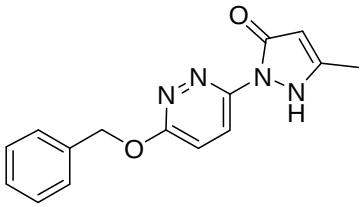
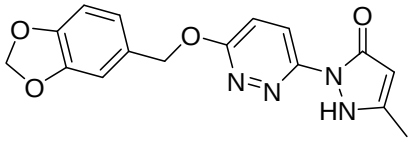
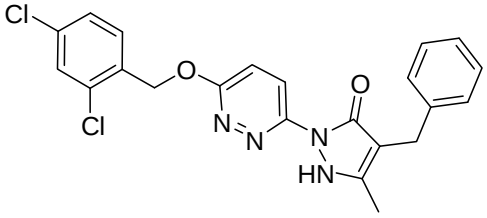
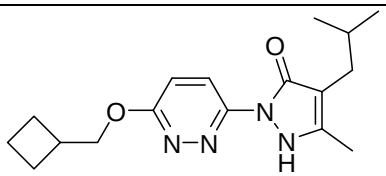
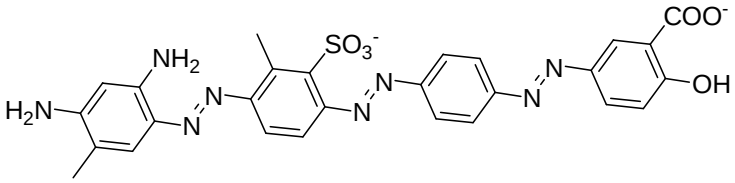
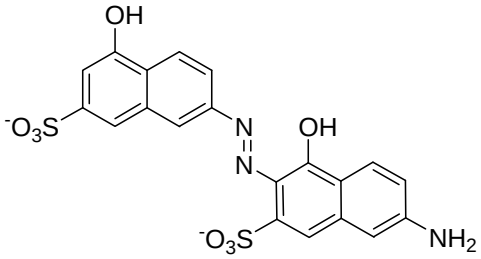
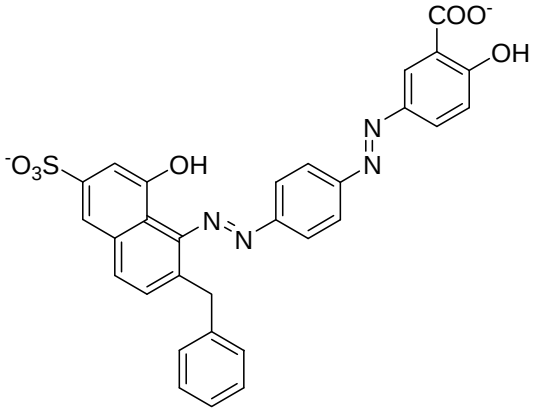
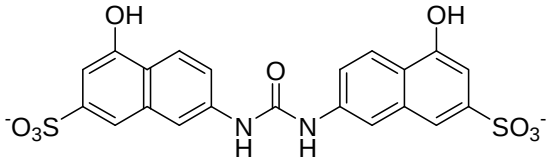
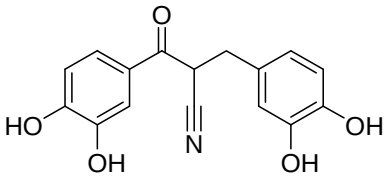
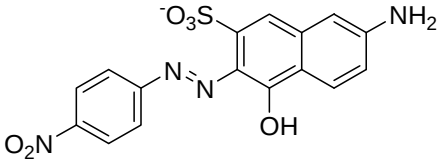
8	
9	
10	
11	
12	
13	

Table S2. Mtb-SK inhibitors reported by Hsu et al (2012)

Compound	Structure	Mtb-SK IC_{50} (µM)
NSC45611		1.5
NSC162535		1.6
NSC45612		2.8
NSC45174		2.8
AG538		0.4
NSC45547		3.4

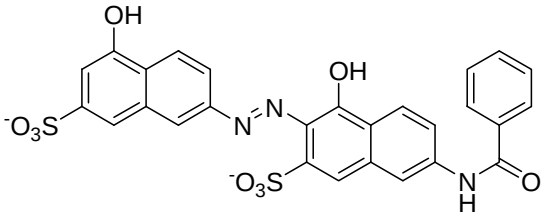
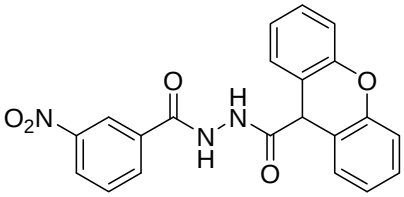
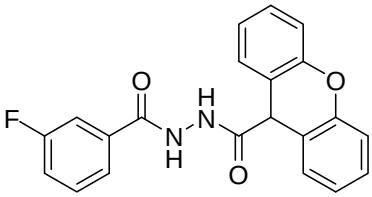
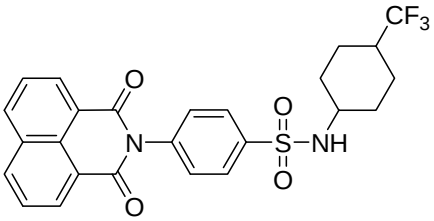
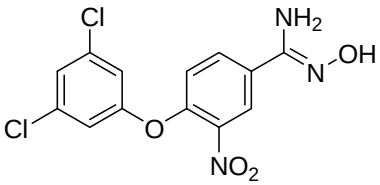
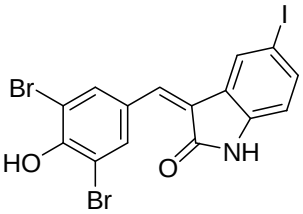
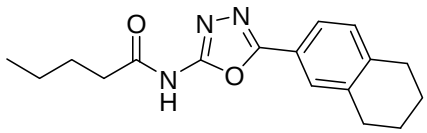
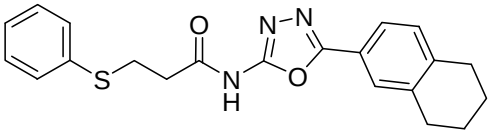
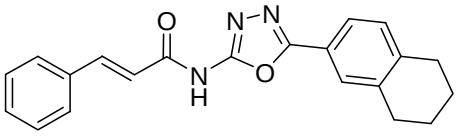
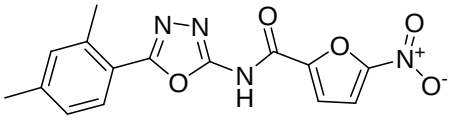
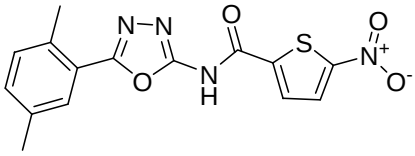
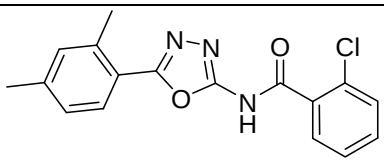
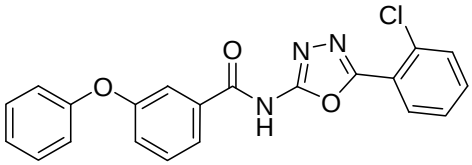
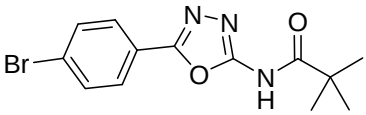
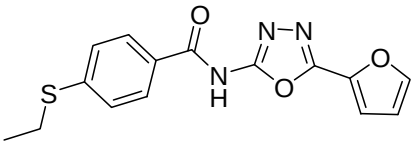
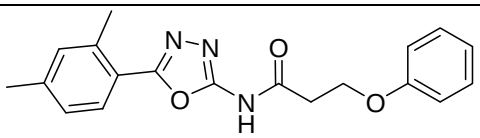
NSC45609		2.0
RH00037		<100
RH00016		<100
GK01385		<100
SPB01099		<100
GW5074		29.6

Table S3. Mtb-SK inhibitors reported by Simithy et al (2013)

Compound	Structure	Mtb-SK IC_{50} (µM)
1		32.87
2		13.81
3		3.79
4		10.35
5		13.09
6		36.04
7		3.43
8		28.36
9		20.73
10		15.14

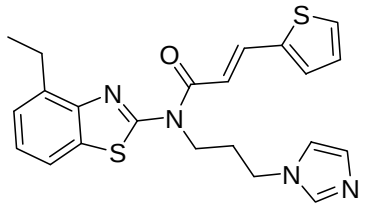
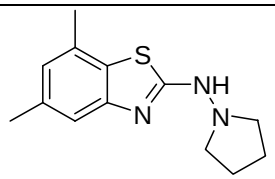
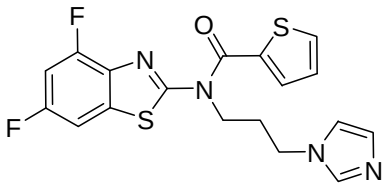
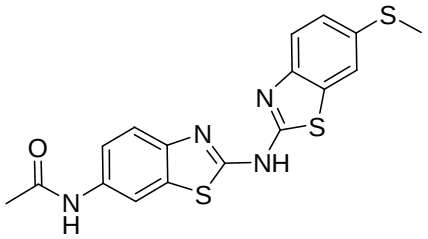
11		10.43
12		29.93
13		20.42
14		1.94

Table S4. Mtb-SK inhibitors reported by Mulabagal et al (2010)

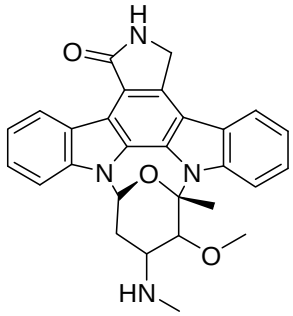
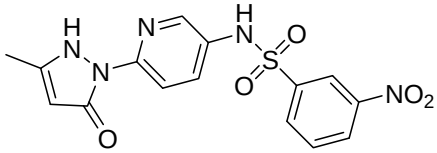
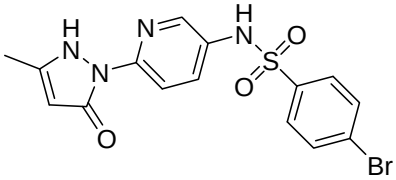
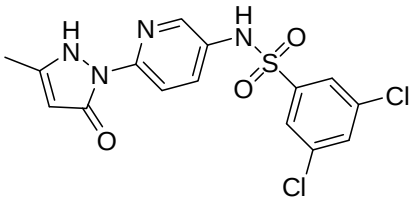
Compounds	Structure
1 (Staurosporine)	
2	
3	
4	

Table S5. Distances between different sites of ADRR hypothesis

Site1	Site2	Distance
A3	D5	3.14
A3	R7	5.593
A3	R9	4.071
D5	R7	5.601
D5	R9	3.379
R7	R9	2.254

Table S6. Angles between different sites of ADRR hypothesis

Site1	Site2	Site3	Angle
D5	A3	R7	73.8
D5	A3	R9	54
R7	A3	R9	20.1
A3	D5	R7	73.6
A3	D5	R9	77.2
R7	D5	R9	4.9
A3	R7	D5	32.6
A3	R7	R9	38.3
D5	R7	R9	7.4
A3	R9	D5	48.8
A3	R9	R7	121.7
D5	R9	R7	167.6

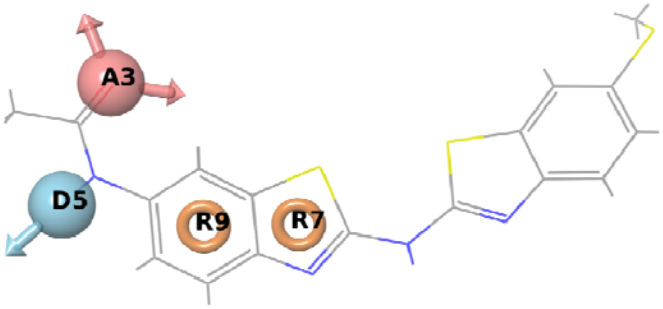


Figure S1. Features of ADRR hypothesis represented on the reference compound 14.