Electronic Supplementary Material (ESI) for Green Chemistry. This journal is © The Royal Society of Chemistry 2017

### **Electronic Supporting Information**

Solvent-free implementation of two dissimilar reactions using recyclable CuO nanoparticle under ball-milling conditions: Green synthesis of new oxindole-triazole pharmacophores

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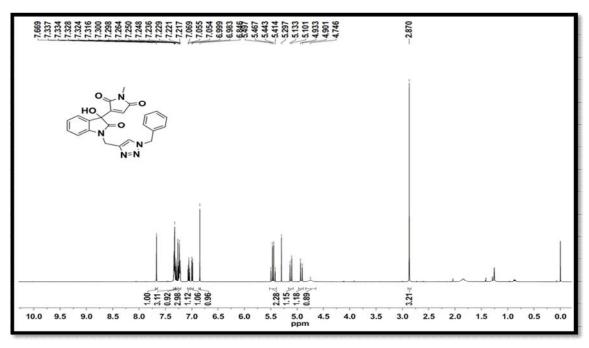
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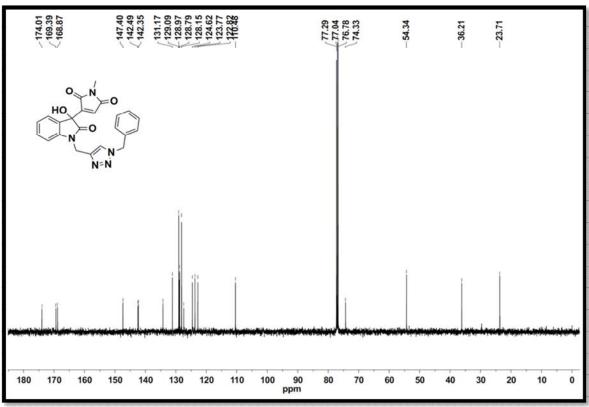
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<sup>&</sup>lt;sup>c</sup>Organic and Bioorganic Chemistry Division, CSIR-Central Leather Research Institute, Adyar, Chennai-600020, Tamil Nadu, India

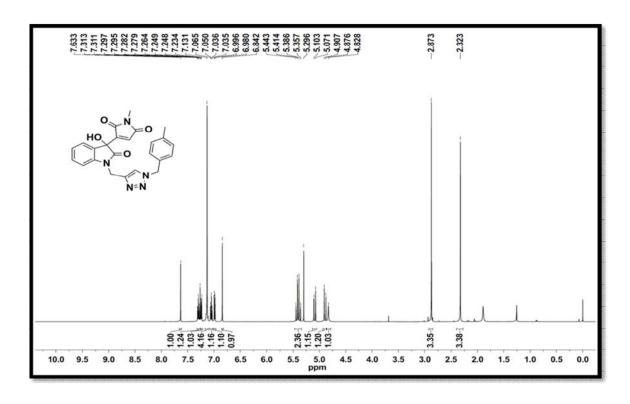
<sup>&</sup>lt;sup>d</sup>Functional Materials Division, CSIR-Central Electrochemical Research Institute, Karaikudi-630003, Tamil Nadu, India.

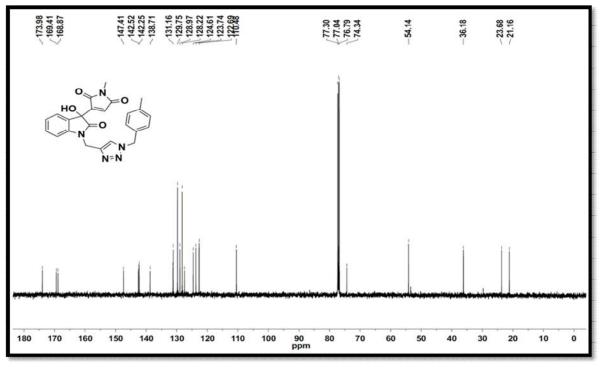
<sup>\*</sup>Email: karthiclri@gmail.com; chandrasekar.praveen@gmail.com



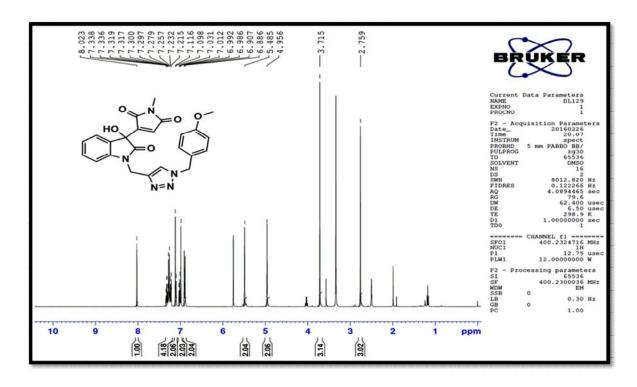


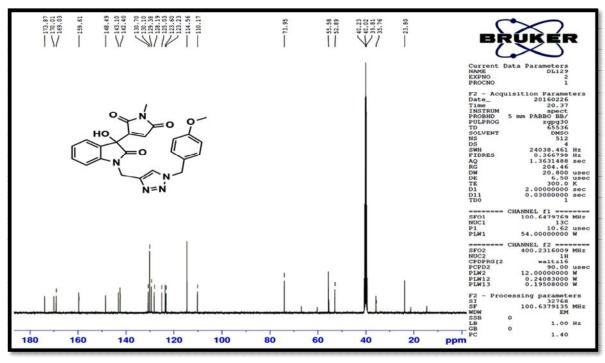
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4a (500 MHz, CDCl<sub>3</sub>)



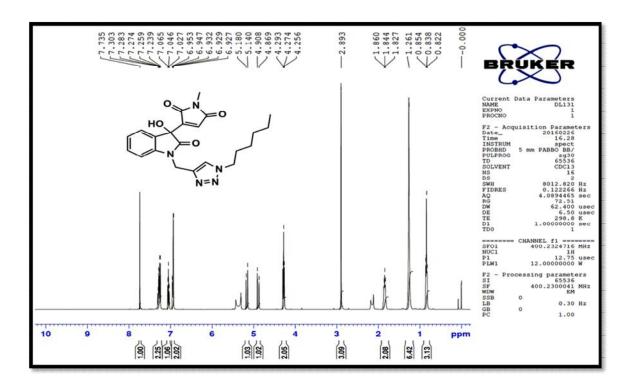


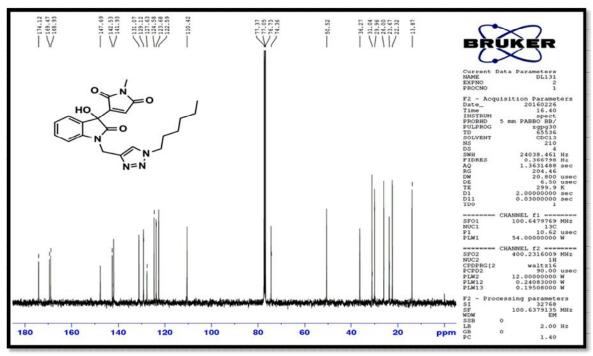
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4b (500 MHz, CDCl<sub>3</sub>)



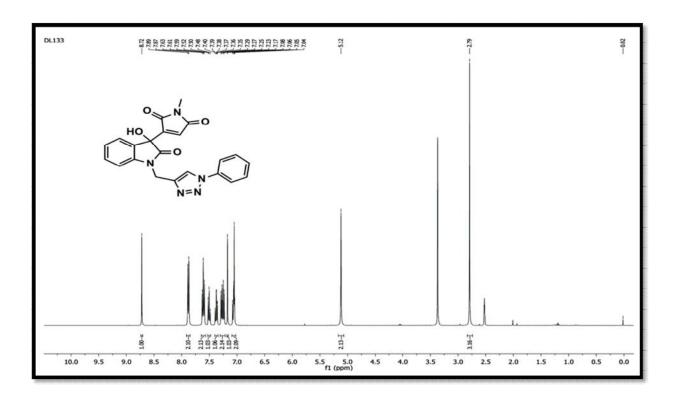


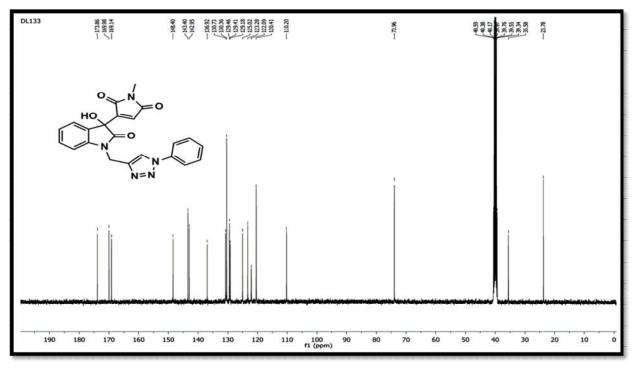
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4c (400 MHz, DMSO-d<sub>6</sub>)



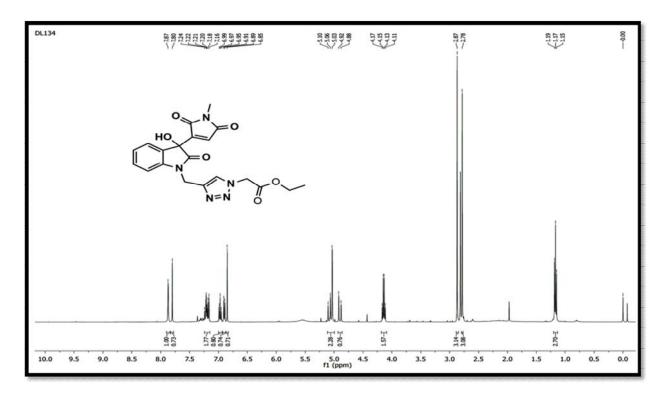


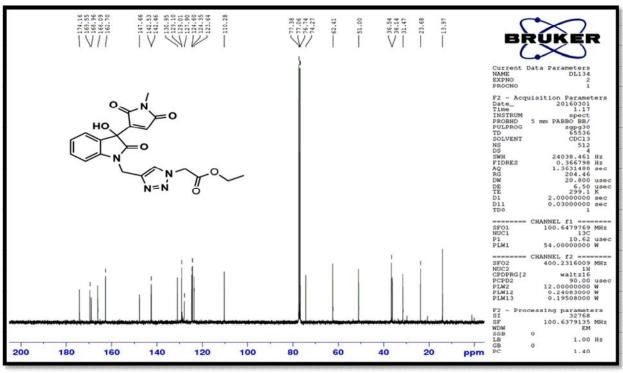
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4d (400 MHz, CDCl<sub>3</sub>)



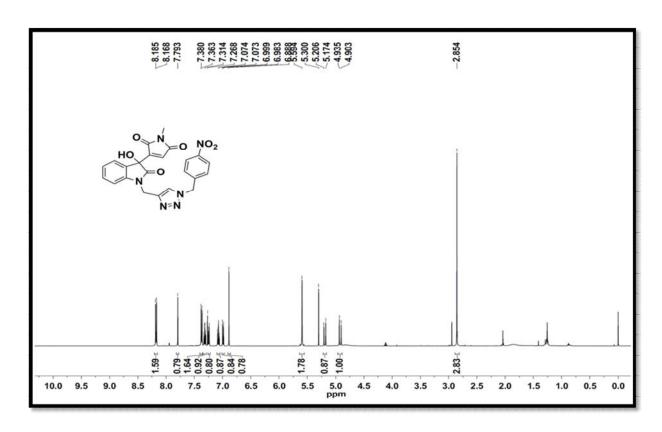


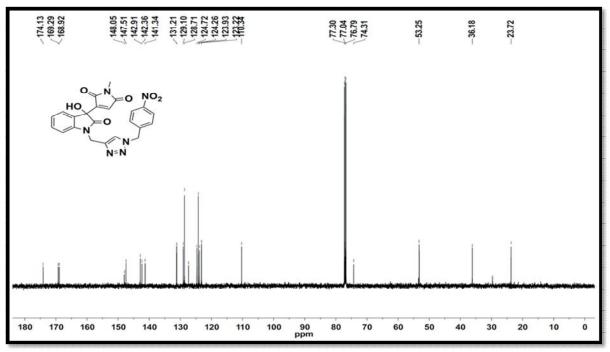
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4e (400 MHz, DMSO-d<sub>6</sub>)



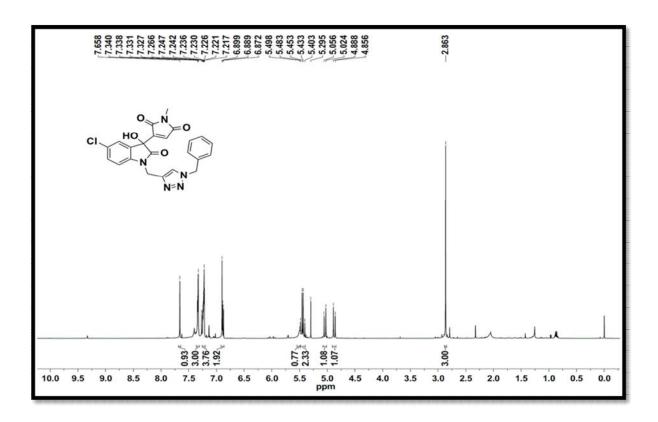


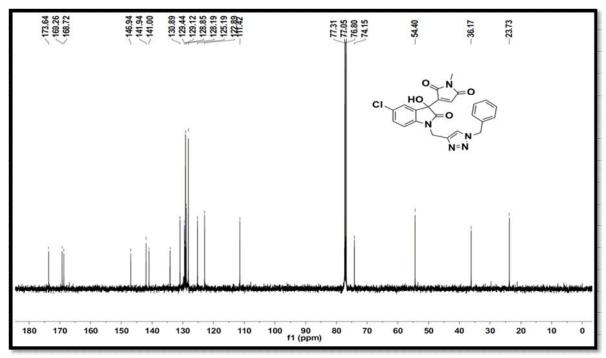
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4f (400 MHz, CDCl<sub>3</sub>)



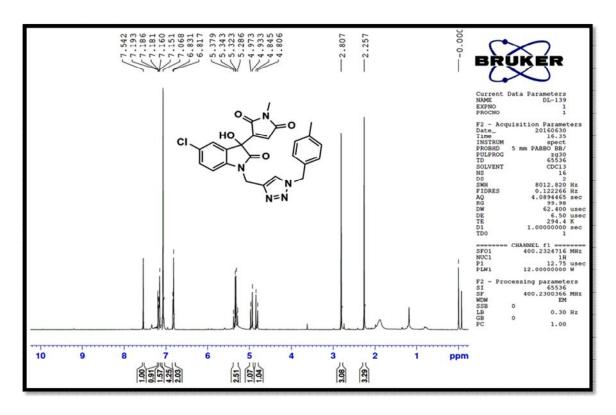


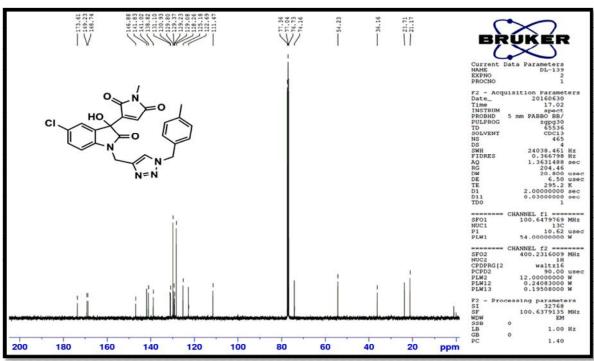
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4g (500 MHz, CDCl<sub>3</sub>)



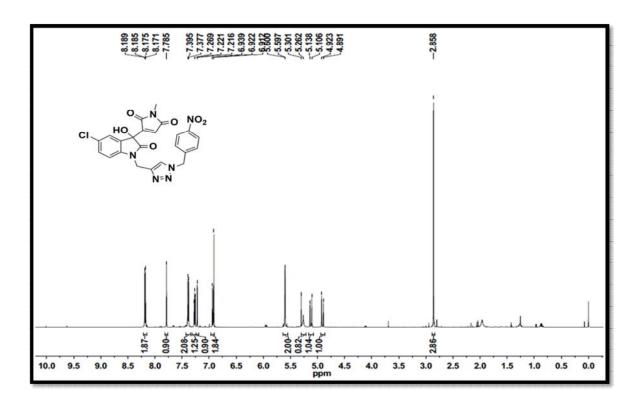


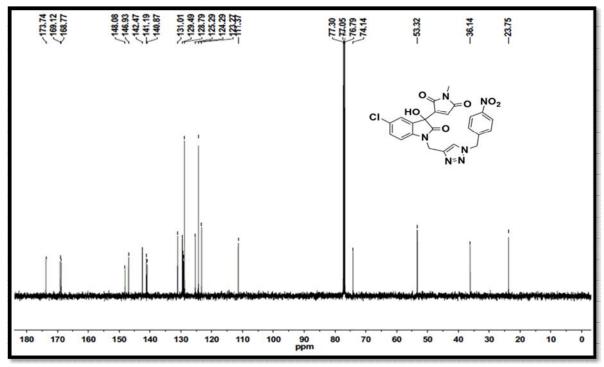
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4h (500 MHz, CDCl<sub>3</sub>)



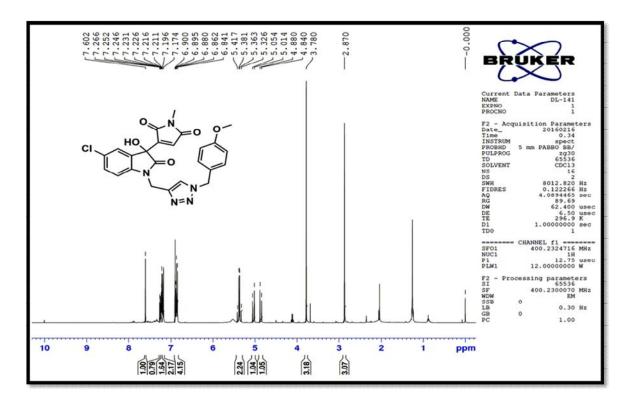


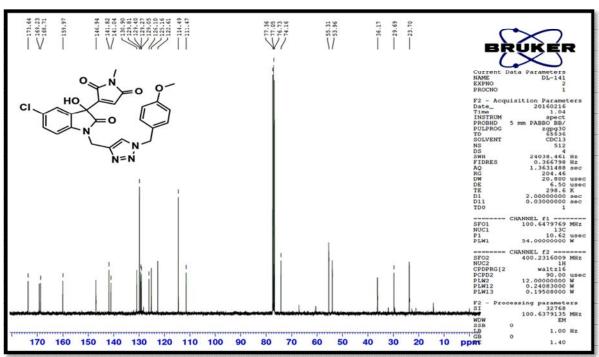
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4i (400 MHz, CDCl<sub>3</sub>)



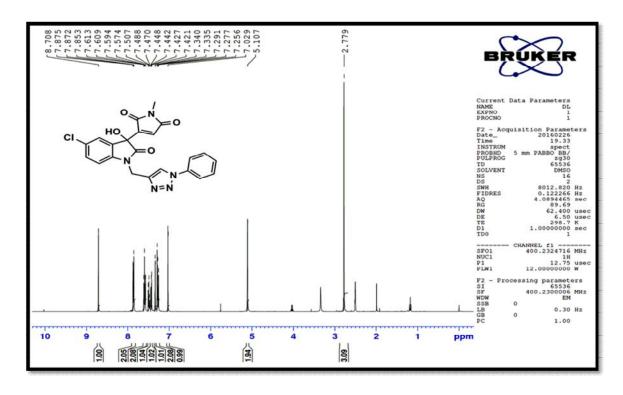


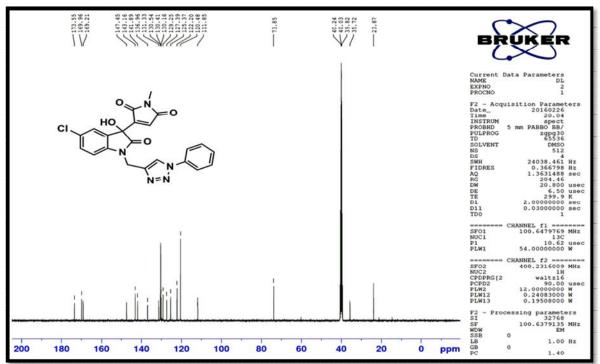
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4j (500 MHz, CDCl<sub>3</sub>)



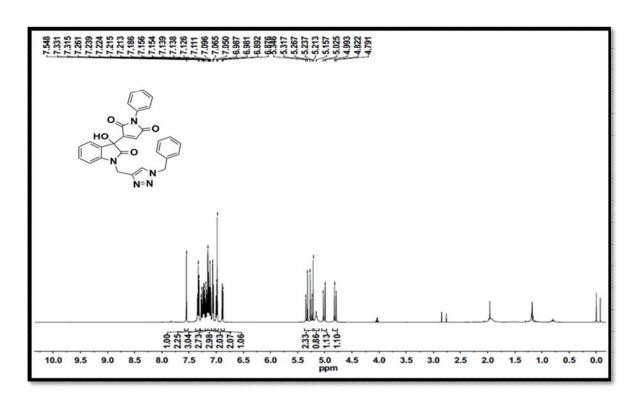


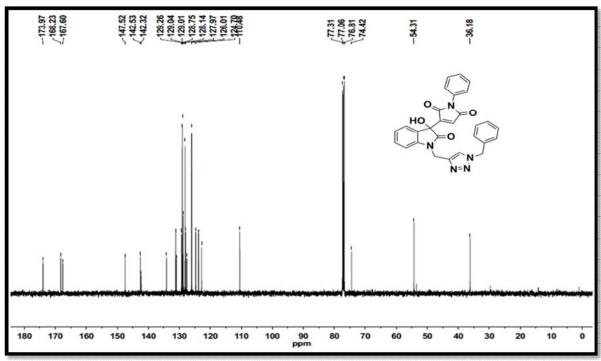
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4k (400 MHz, CDCl<sub>3</sub>)



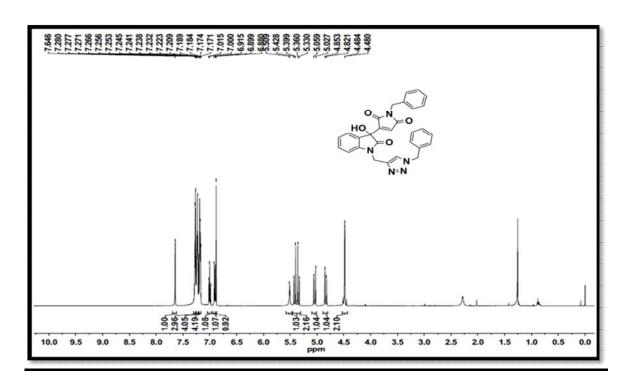


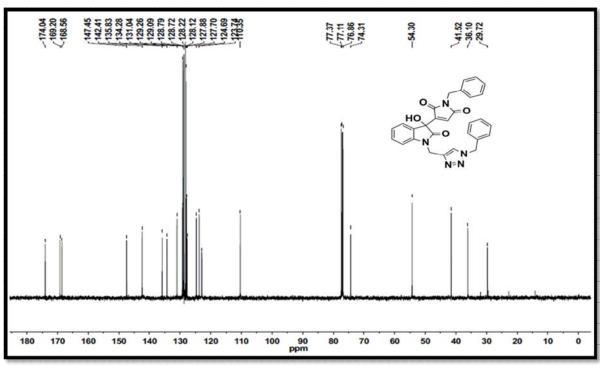
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4l (500 MHz, DMSO-d<sub>6</sub>)



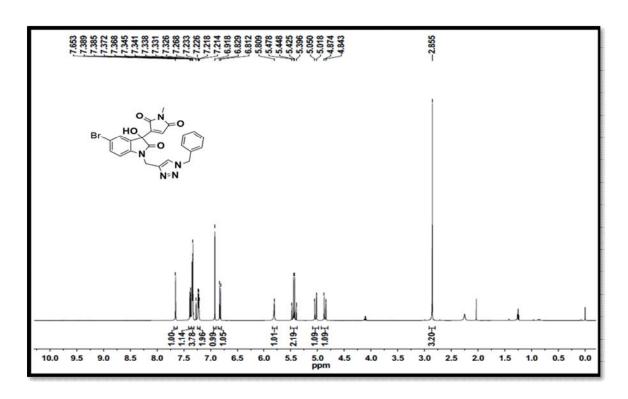


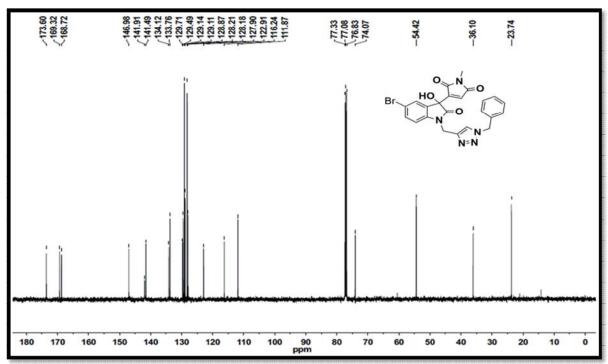
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4m (500 MHz, CDCl<sub>3</sub>)



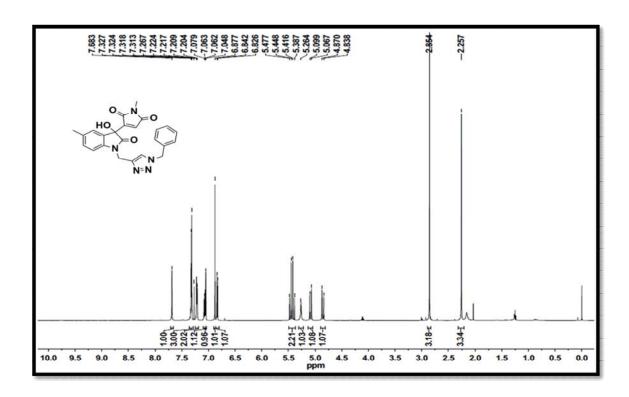


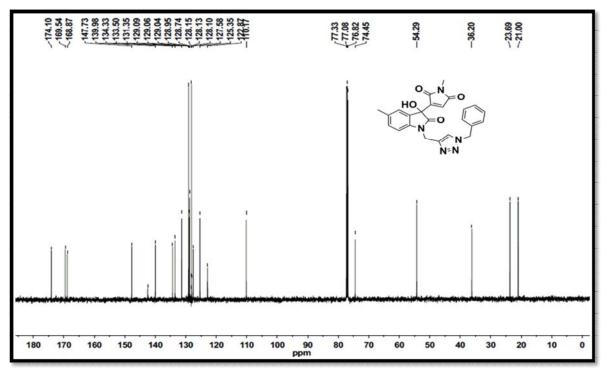
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4n (500 MHz, CDCl<sub>3</sub>)





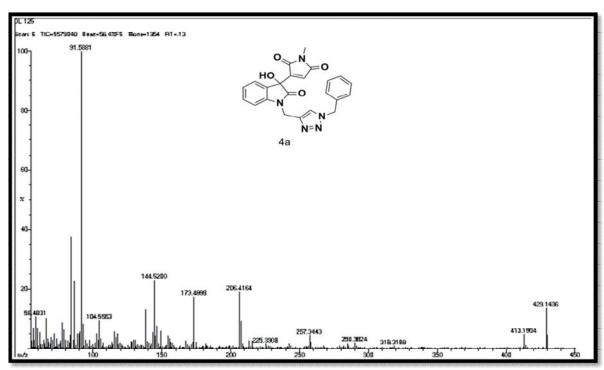
<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 40 (500 MHz, CDCl<sub>3</sub>)



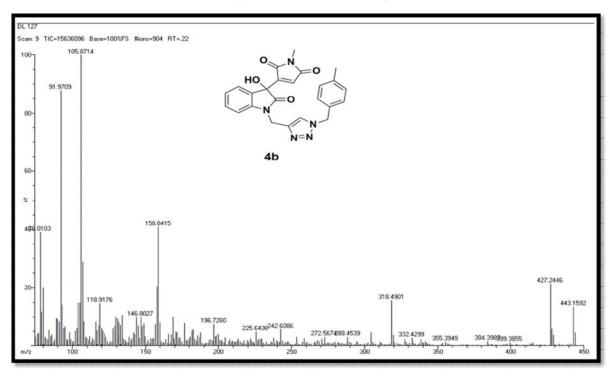


<sup>1</sup>H and <sup>13</sup>C NMR Spectrum of Compound 4p (500 MHz, CDCl<sub>3</sub>)

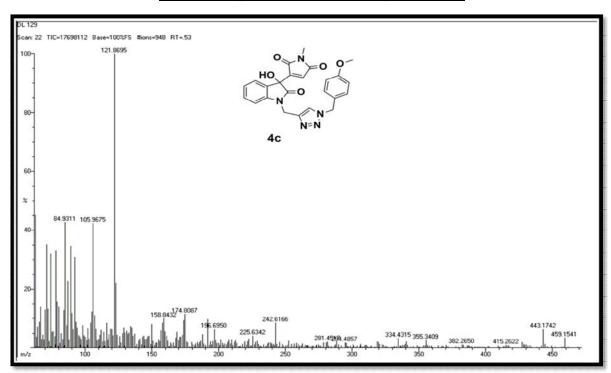
### **HRMS Spectrum of Compound 4a**



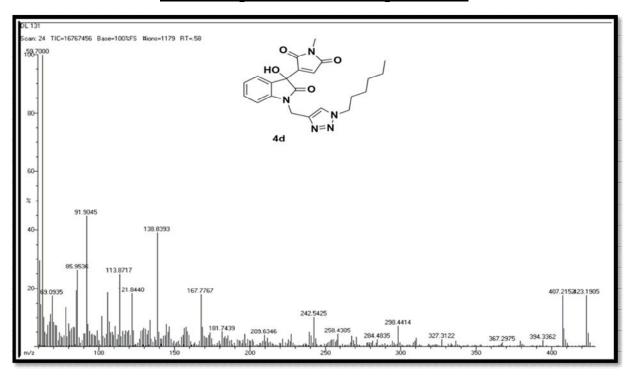
# **HRMS Spectrum of Compound 4b**



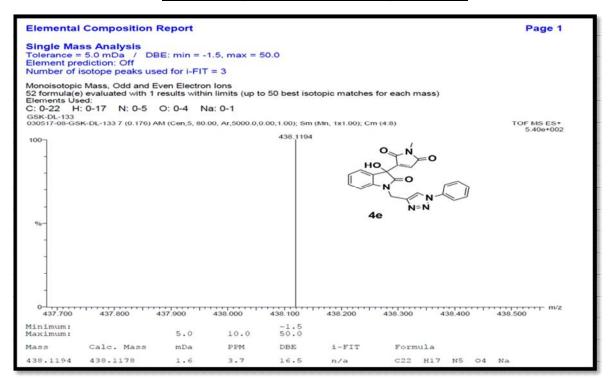
# **HRMS Spectrum of Compound 4c**



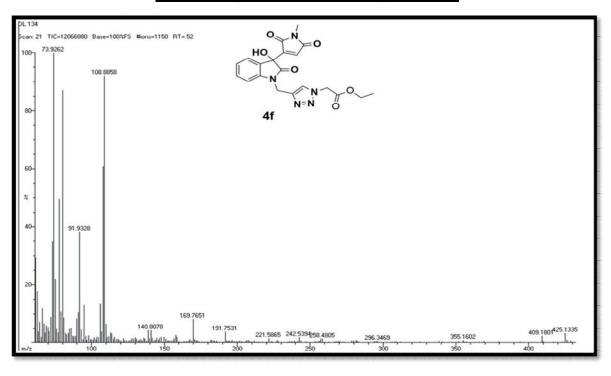
# **HRMS Spectrum of Compound 4d**



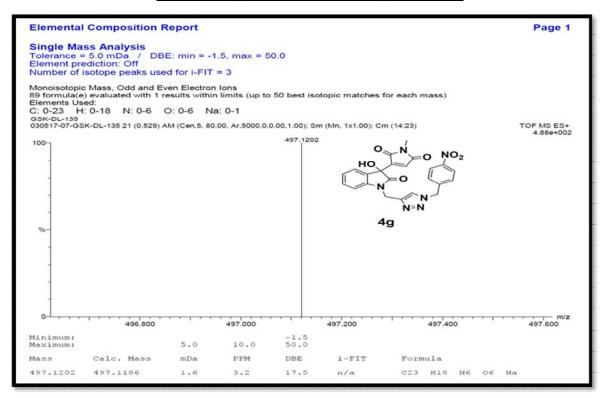
### **HRMS Spectrum of Compound 4e**



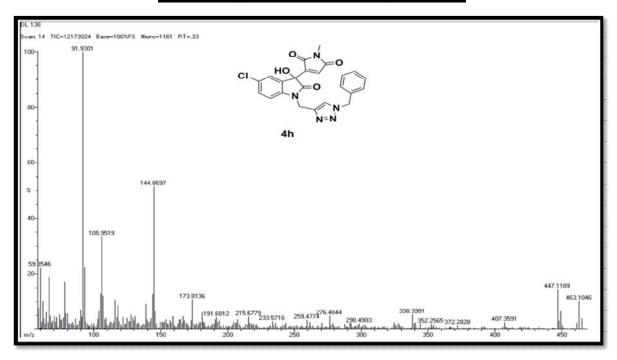
### **HRMS Spectrum of Compound 4f**



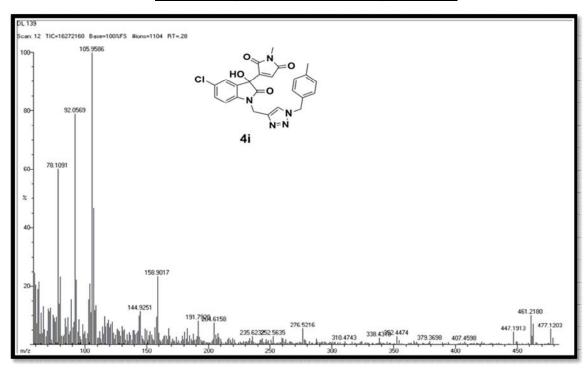
### **HRMS Spectrum of Compound 4g**



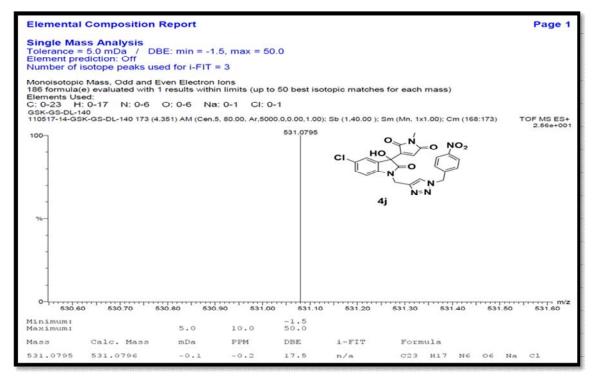
### **HRMS Spectrum of Compound 4h**



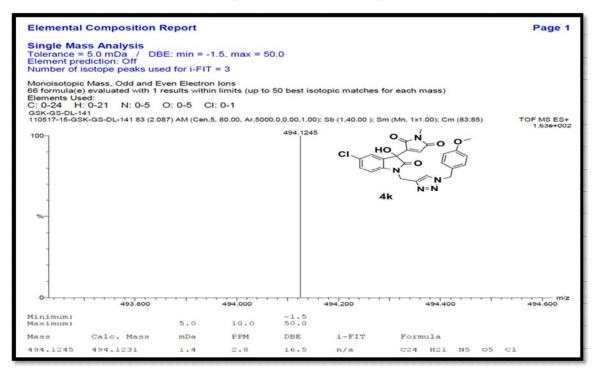
### **HRMS Spectrum of Compound 4i**



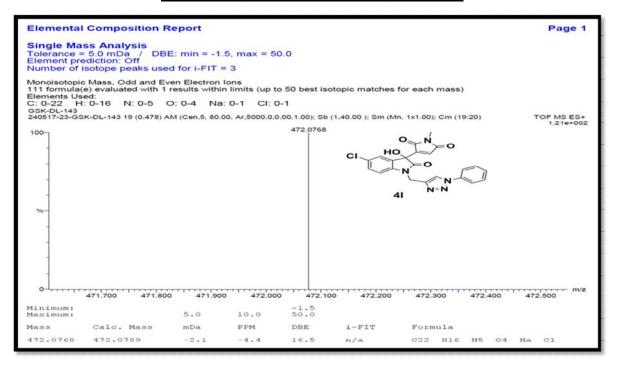
# **HRMS Spectrum of Compound 4j**



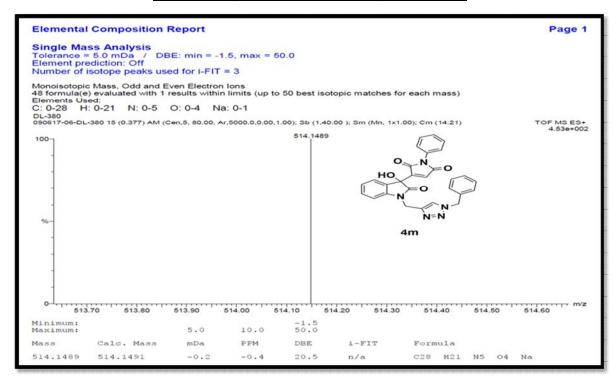
### **HRMS Spectrum of Compound 4k**



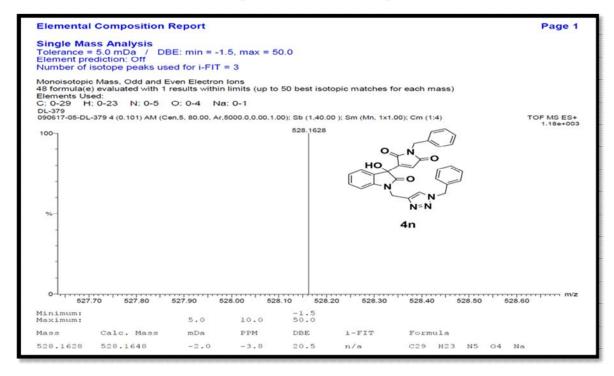
### **HRMS Spectrum of Compound 41**



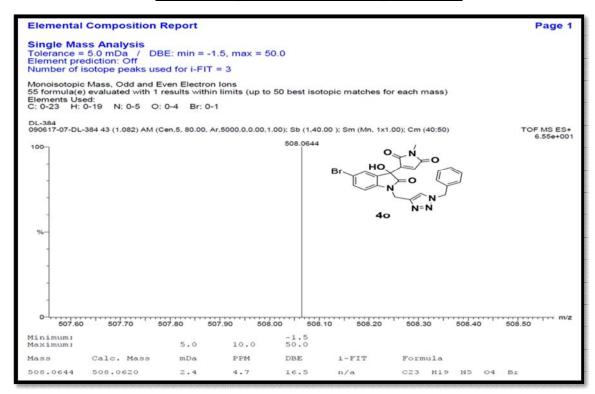
#### **HRMS Spectrum of Compound 4m**



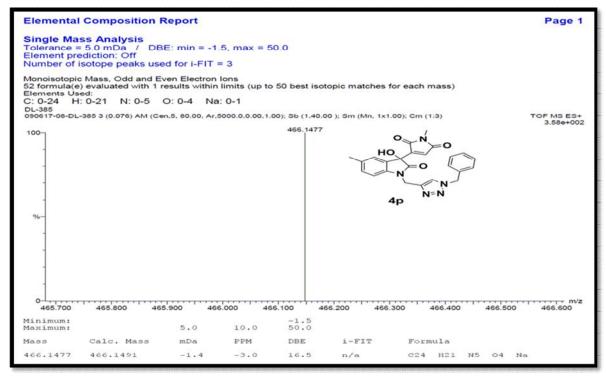
### **HRMS Spectrum of Compound 4n**



#### **HRMS Spectrum of Compound 40**



# **HRMS Spectrum of Compound 4p**



#### **Crystal parameters of Compound 4e**

Bond precision: C-C = 0.0026 A Wavelength=0.71073

Cell: a=9.7024(3) b=9.8685(3) c=12.5819(4)

alpha=80.421(1) beta=70.629(1) gamma=65.931(1)

Temperature: 296 K

Tmin'

	Calculated	Reported
Volume	1037.01(6)	1037.01(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H17 N5 O4, H2 O	C22 H19 N5 O5
Sum formula	C22 H19 N5 O5	C22 H19 N5 O5
Mr	433.42	433.42
Dx,g cm-3	1.388	1.388
Z	2	2
Mu (mm-1)	0.101	0.101
F000	452.0	452.0
F000'	452.22	
h,k,lmax	12,12,15	12,12,15
Nref	4266	4242
Tmin, Tmax	0.982,0.988	0.982,0.988

Correction method= # Reported T Limits: Tmin=0.982 Tmax=0.988 AbsCorr = MULTI-SCAN

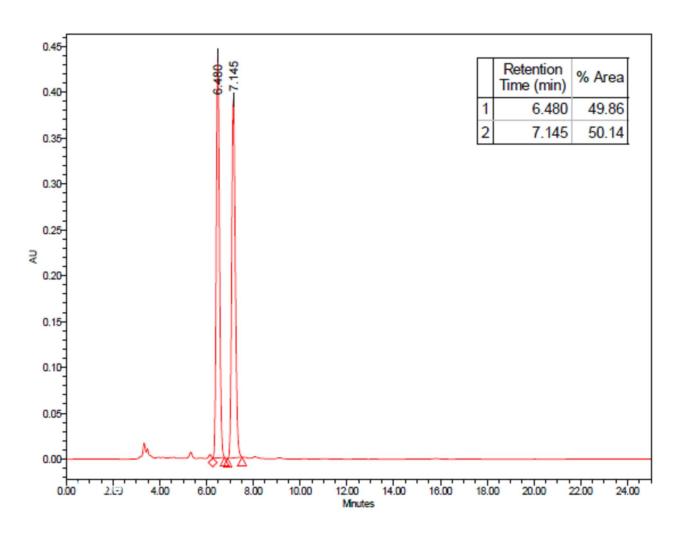
Data completeness= 0.994 Theta(max)= 26.390

0.982

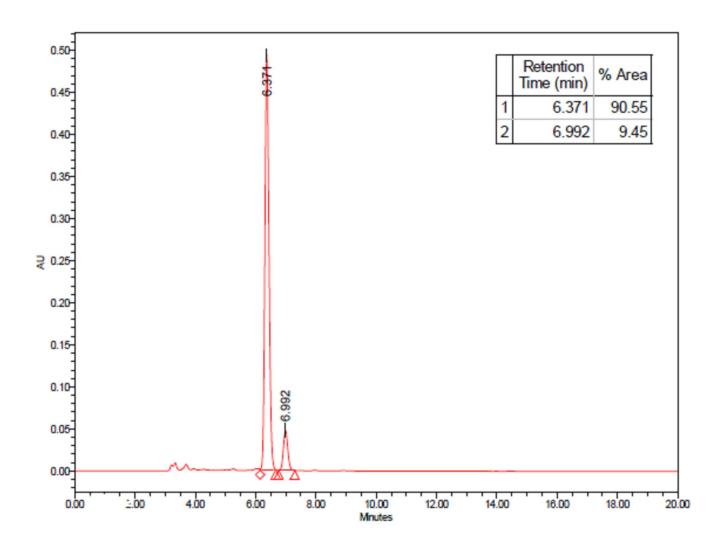
R(reflections)= 0.0382( 3447) wR2(reflections)= 0.1107( 4242)

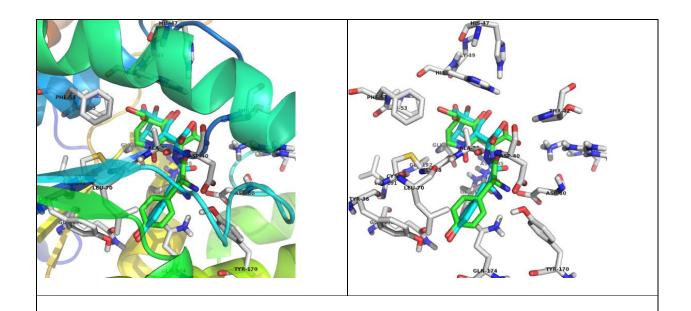
S = 1.034 Npar= 300

# **HPLC of racemic 4a**

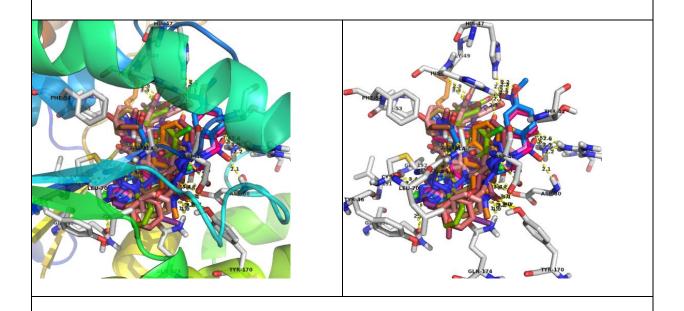


# **HPLC of enantioexcess 4a'**

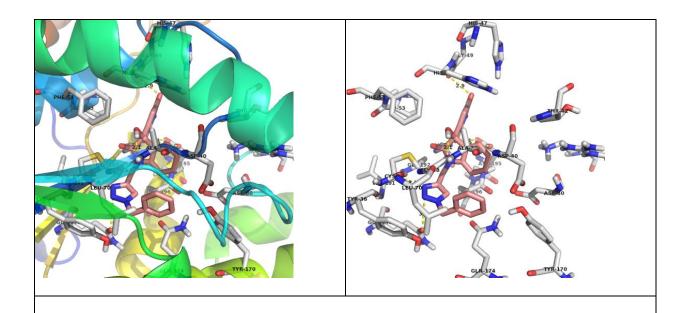




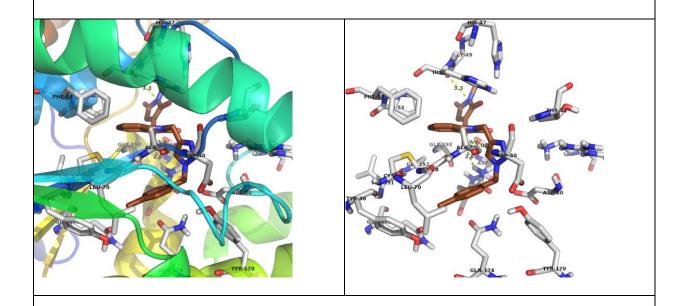
Method validation using crystallised and docked ligand with 1JIJ receptor



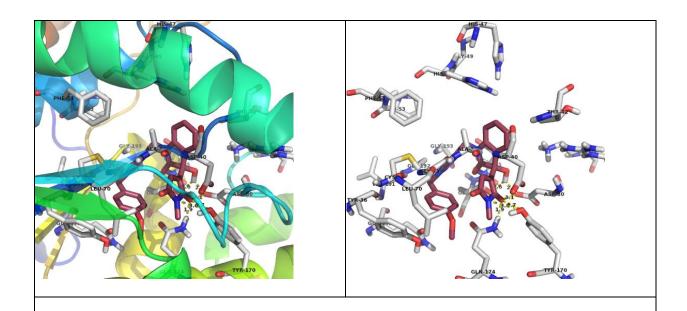
Docking mode of all the compounds in the active site of 1JIJ receptor



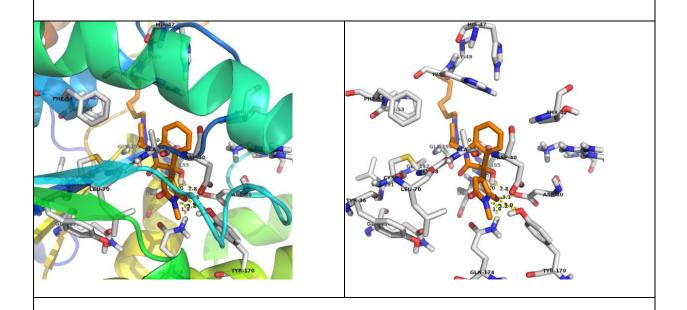
Docking mode of the compound 4a in the active site of 1JIJ



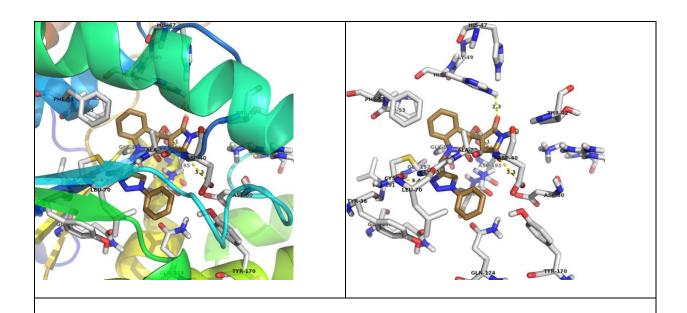
Docking mode of the compound 4b in the active site of 1JIJ



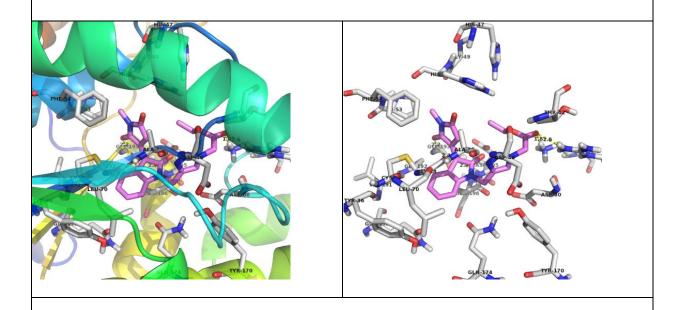
Docking mode of the compound 4c in the active site of 1JIJ



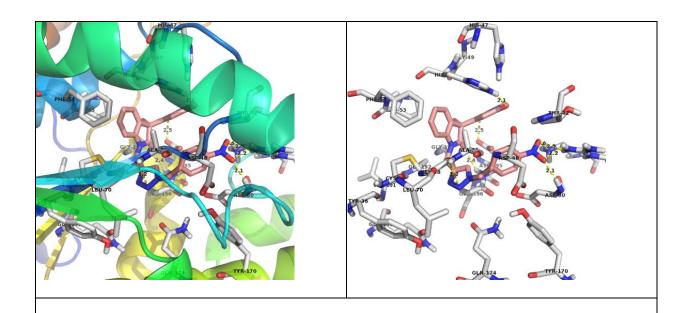
Docking mode of the compound 4d in the active site of 1JIJ



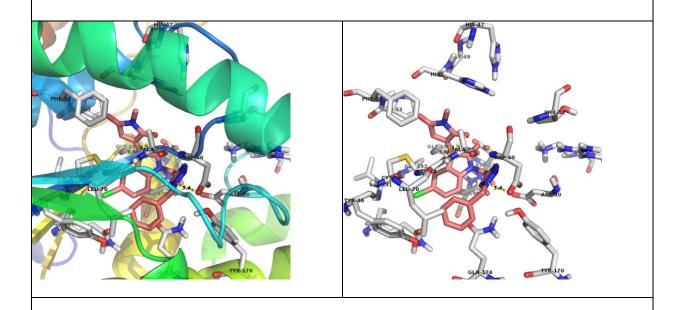
Docking mode of the compound 4e in the active site of 1JIJ



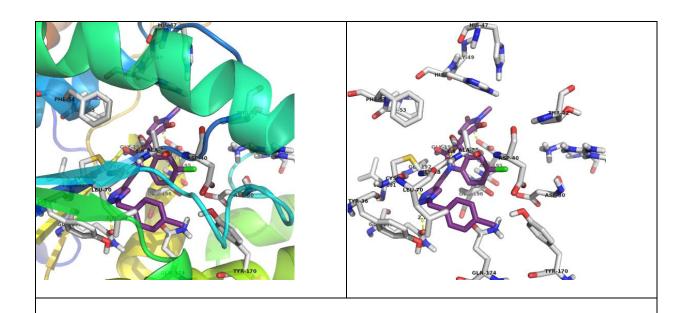
Docking mode of the compound 4f in the active site of 1JIJ



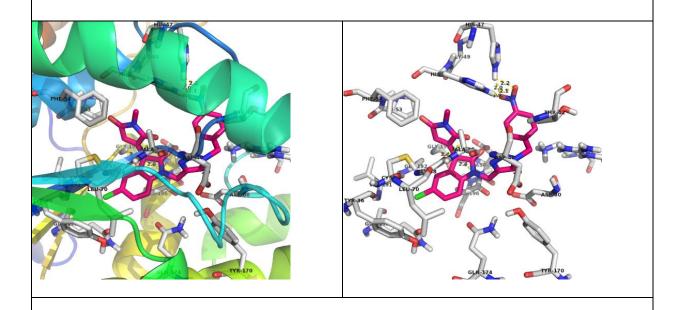
Docking mode of the compound 4g in the active site of 1JIJ



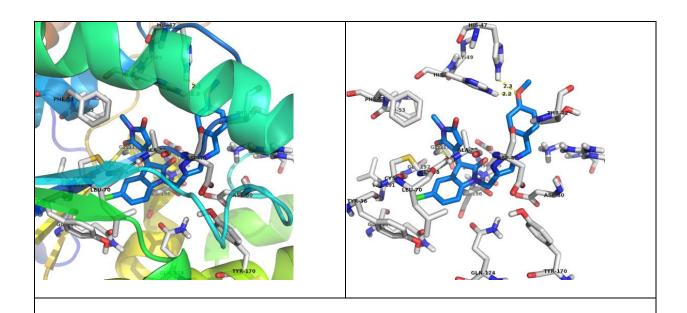
Docking mode of the compound 4h in the active site of 1JIJ



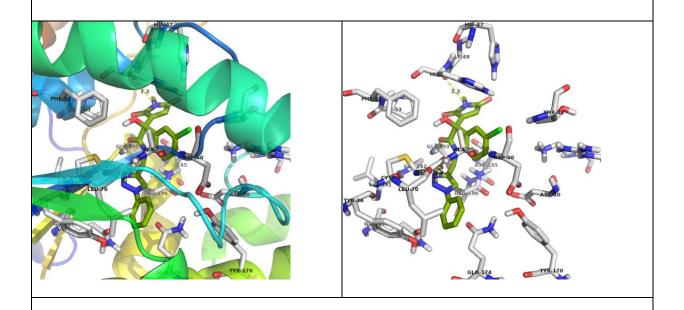
Docking mode of the compound 4i in the active site of 1JIJ



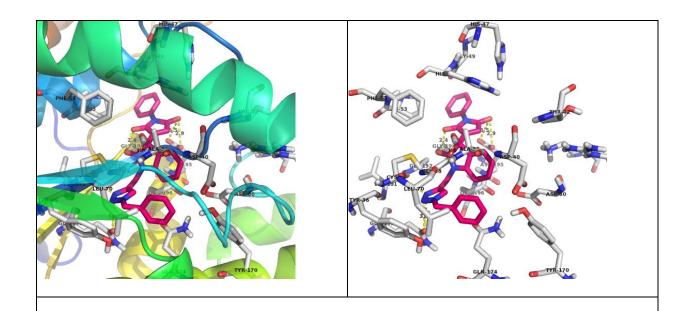
Docking mode of the compound 4j in the active site of 1JIJ



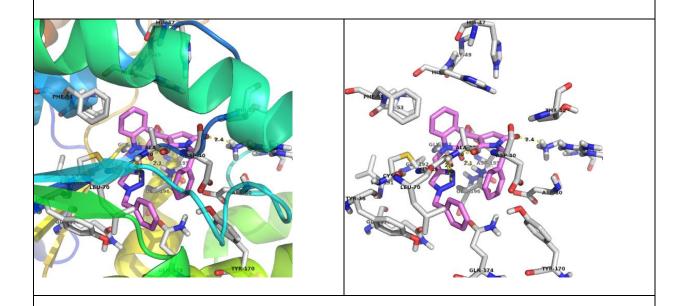
Docking mode of the compound 4k in the active site of 1JIJ



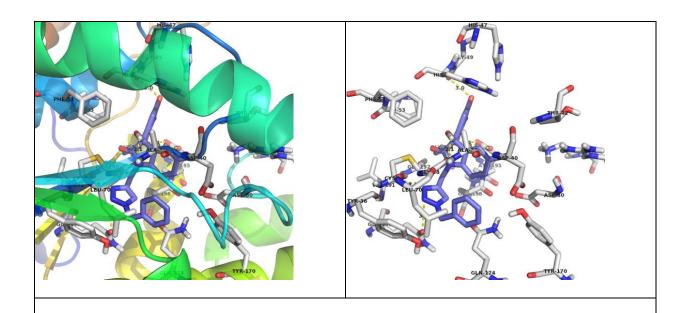
Docking mode of the compound 4l in the active site of 1JIJ



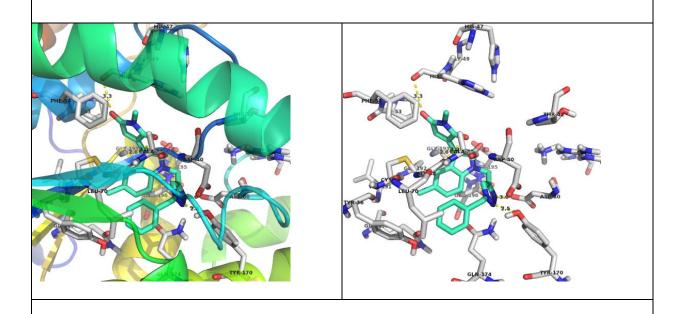
Docking mode of the compound 4min the active site of 1JIJ



Docking mode of the compound 4n in the active site of 1JIJ



Docking mode of the compound 40 in the active site of 1JIJ



Docking mode of the compound 4p in the active site of 1JIJ