Electronic Supplementary Material (ESI) for RSC Advances.

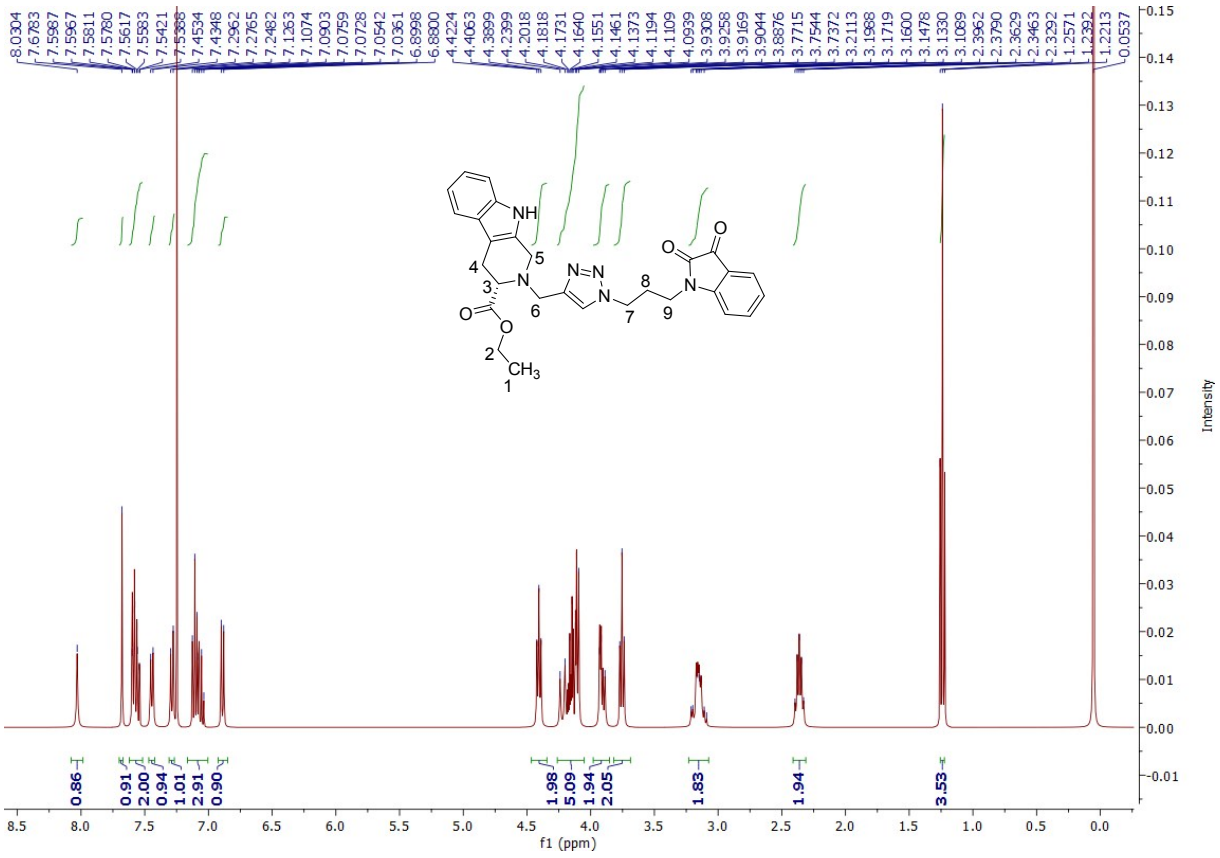
Diastereoselective approach to rationally designed tetrahydro-β-carboline-isatin conjugates as Potential SERMs against breast cancer

Bharvi Sharma[a], Amandeep Singh[a], Liang Gu[b], Sourav Taru Saha[b], Ashona Singh-Pillay[c], Nosipho Cele[c], Parvesh Singh[c], Mandeep Kaur[b]*, Vipan Kumar[a]*

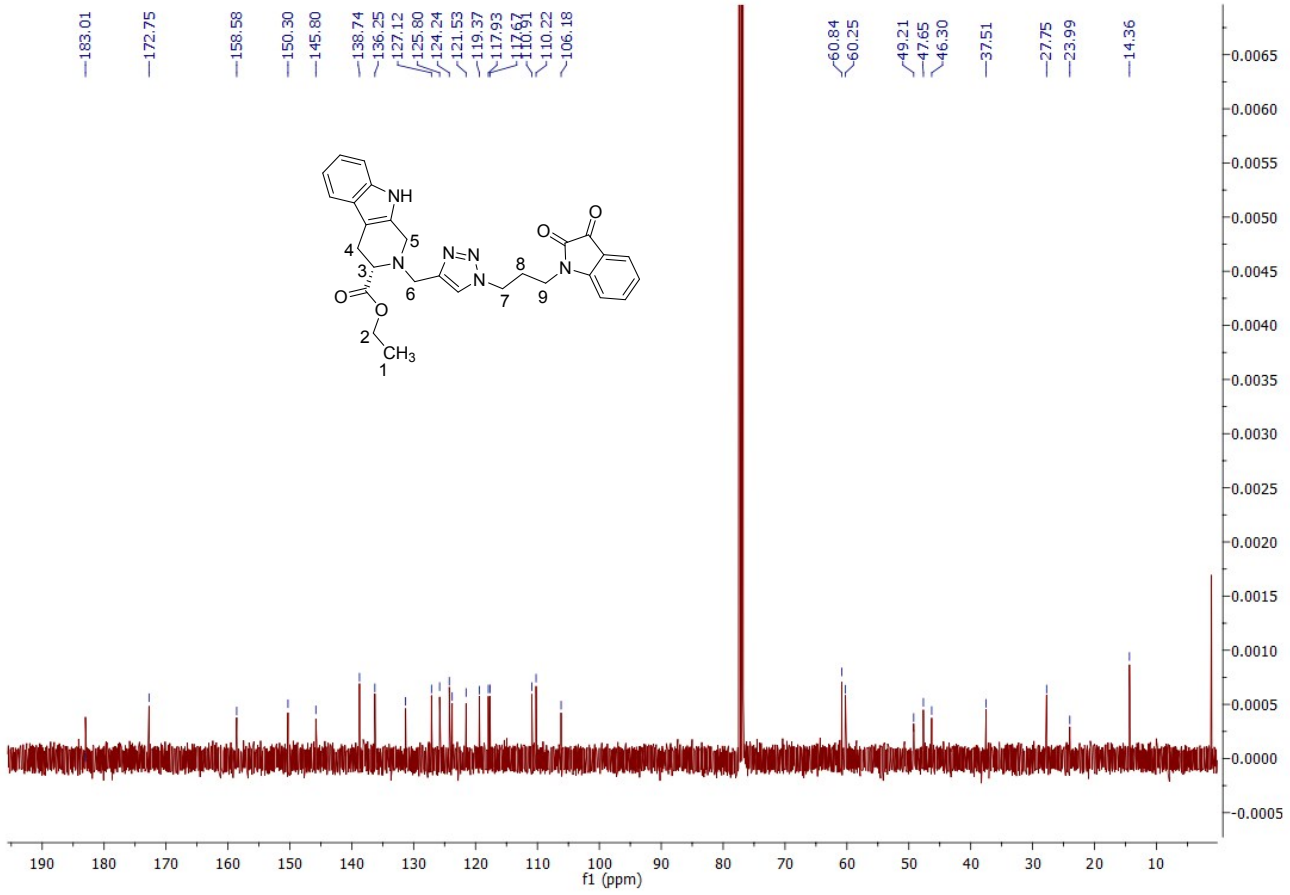
[a] Department of Chemistry, Guru Nanak Dev University, Amritsar 143005, India
[b] School of Molecular and Cell Biology, University of the Witwatersrand, Private Bag 3, Wits, 2050 Johannesburg, South Africa
[c] School of Chemistry and Physics, University of KwaZulu Natal, P/Bag X54001,Westville, Durban 4000, South Africa
*Corresponding Author. Tel: +91 183 2258802-09*3320 (V.K.); Fax: +91 183 2258819-20, Email address: vipan_org@yahoo.com (V. Kumar)

Scanned ^{1}H and ^{13}C NMR spectra of representative compounds

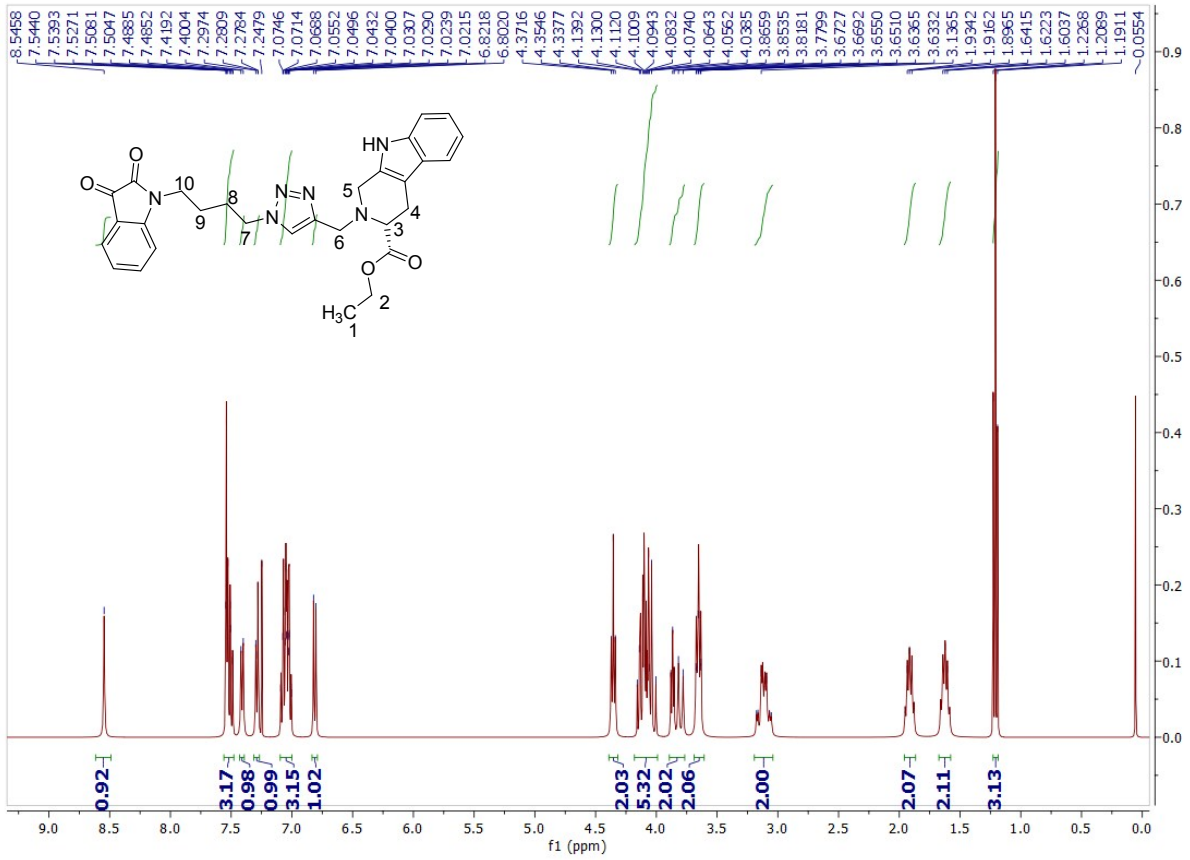
^{1}H NMR of 2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H–β-carboline-3-carboxylic acid ethyl ester **(8b)**



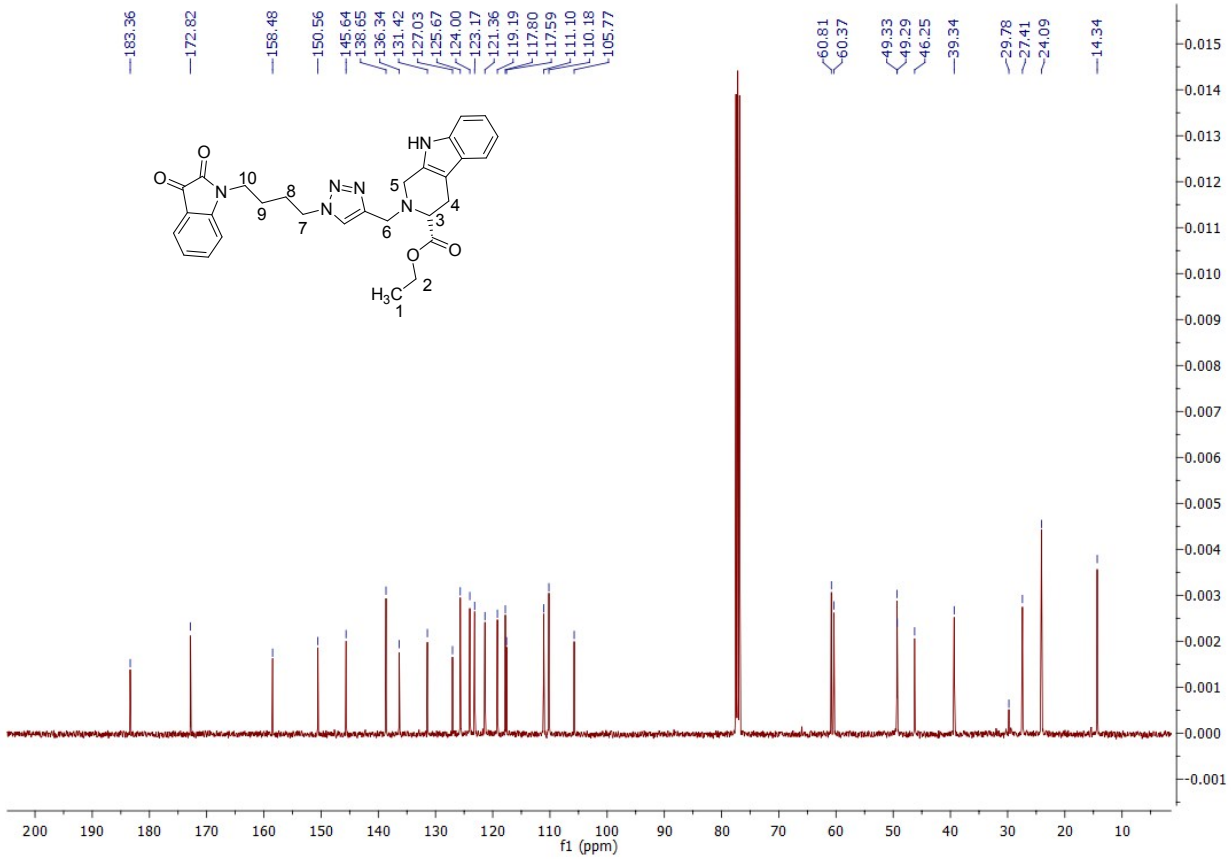
^{13}C NMR of 2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8b)**



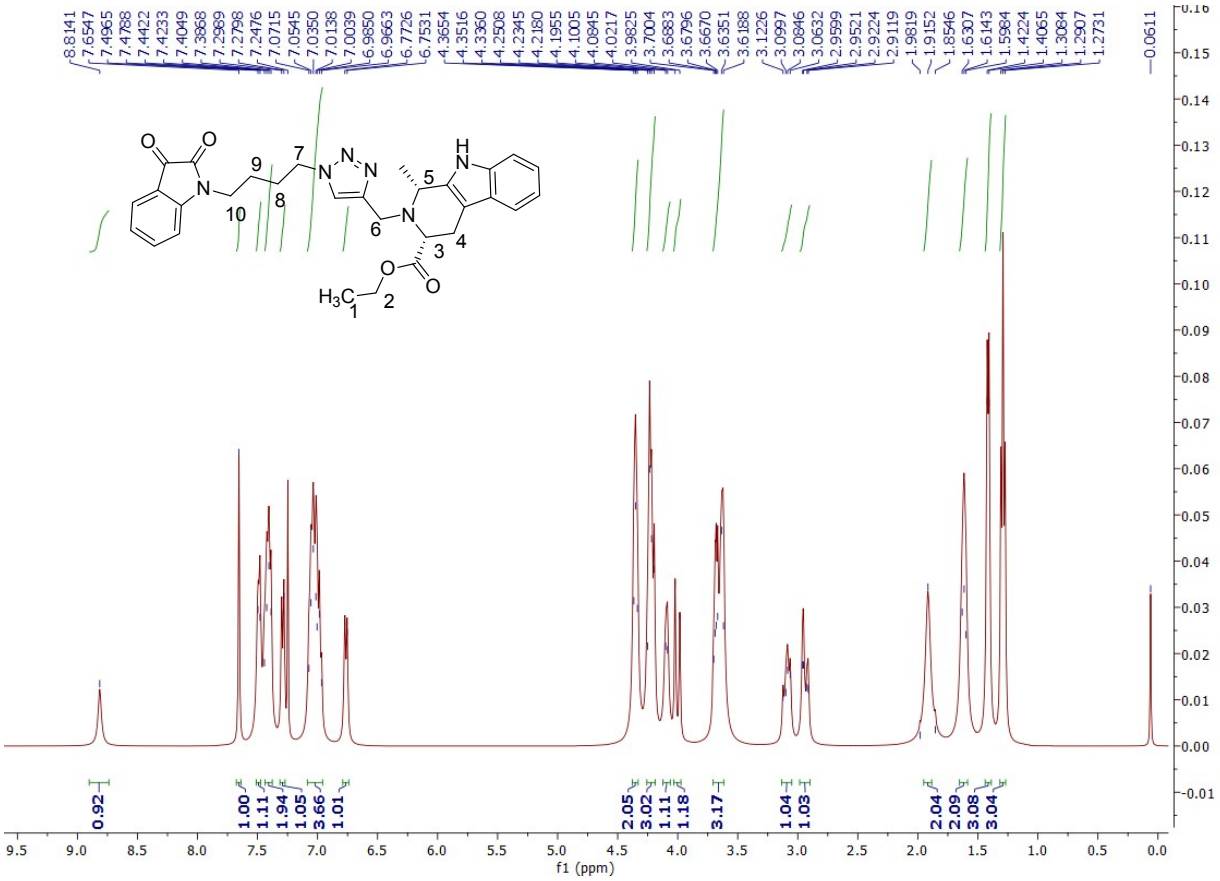
^{1}H NMR of2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H–β–carboline-3-carboxylic acid ethyl ester (**8c**)



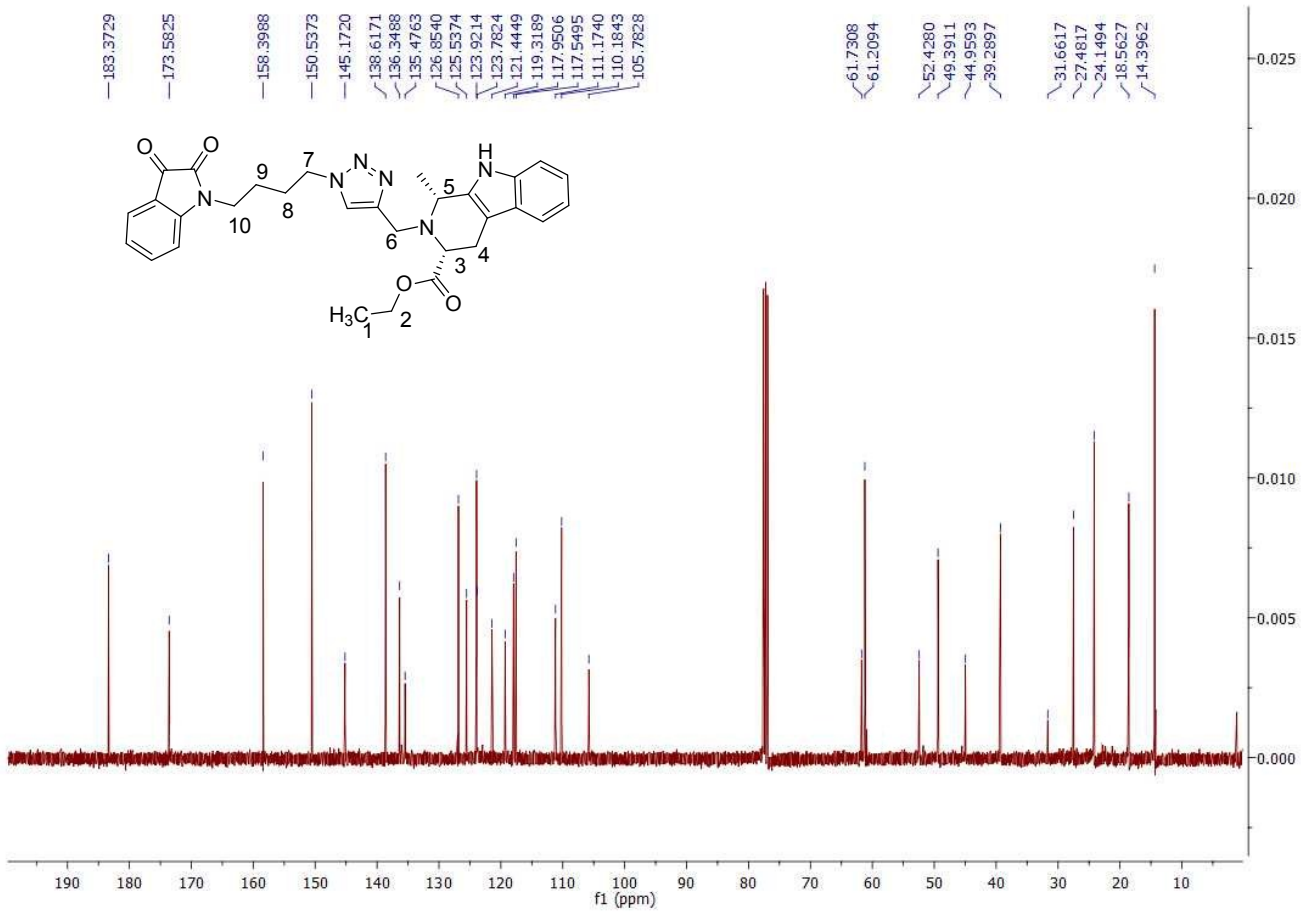
^{13}C NMR of2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8c**)



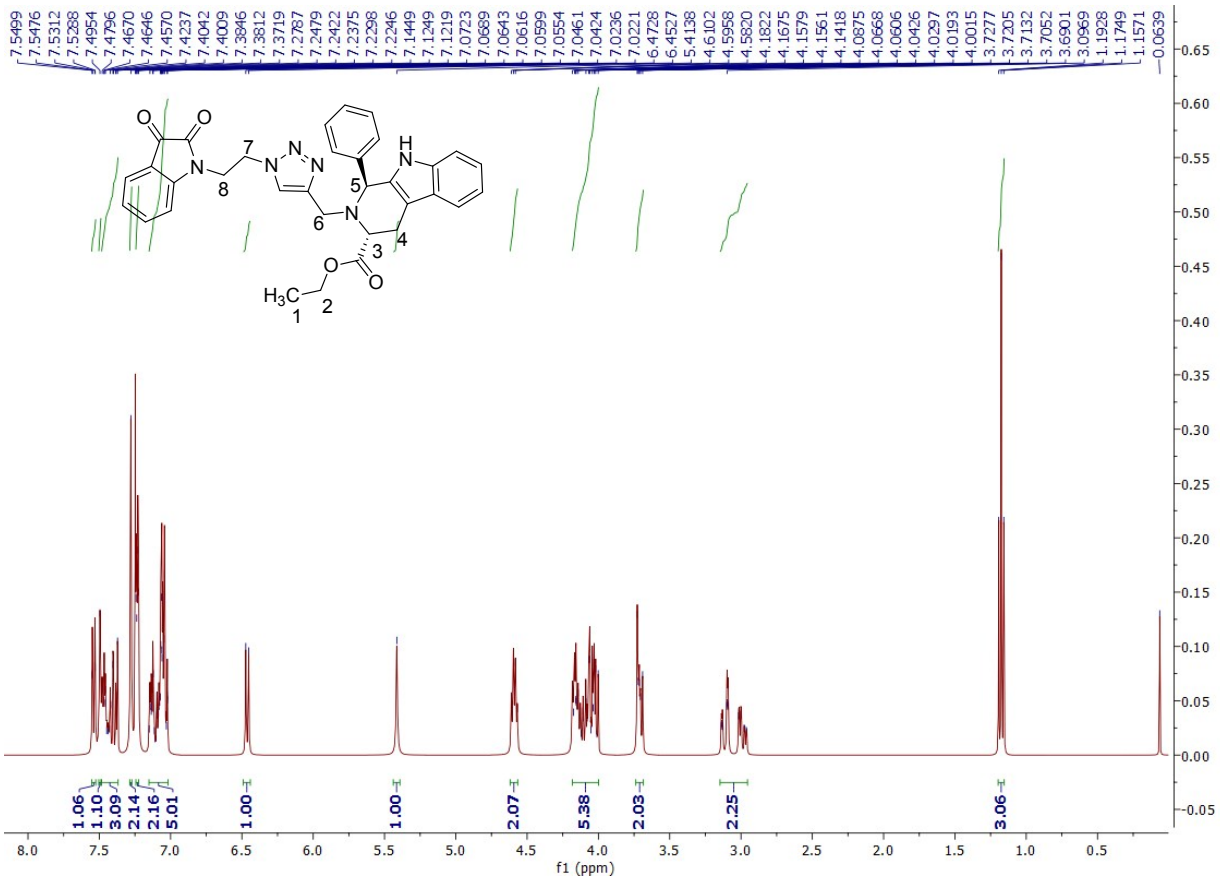
^{1}H NMR of 2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-methyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8f)**



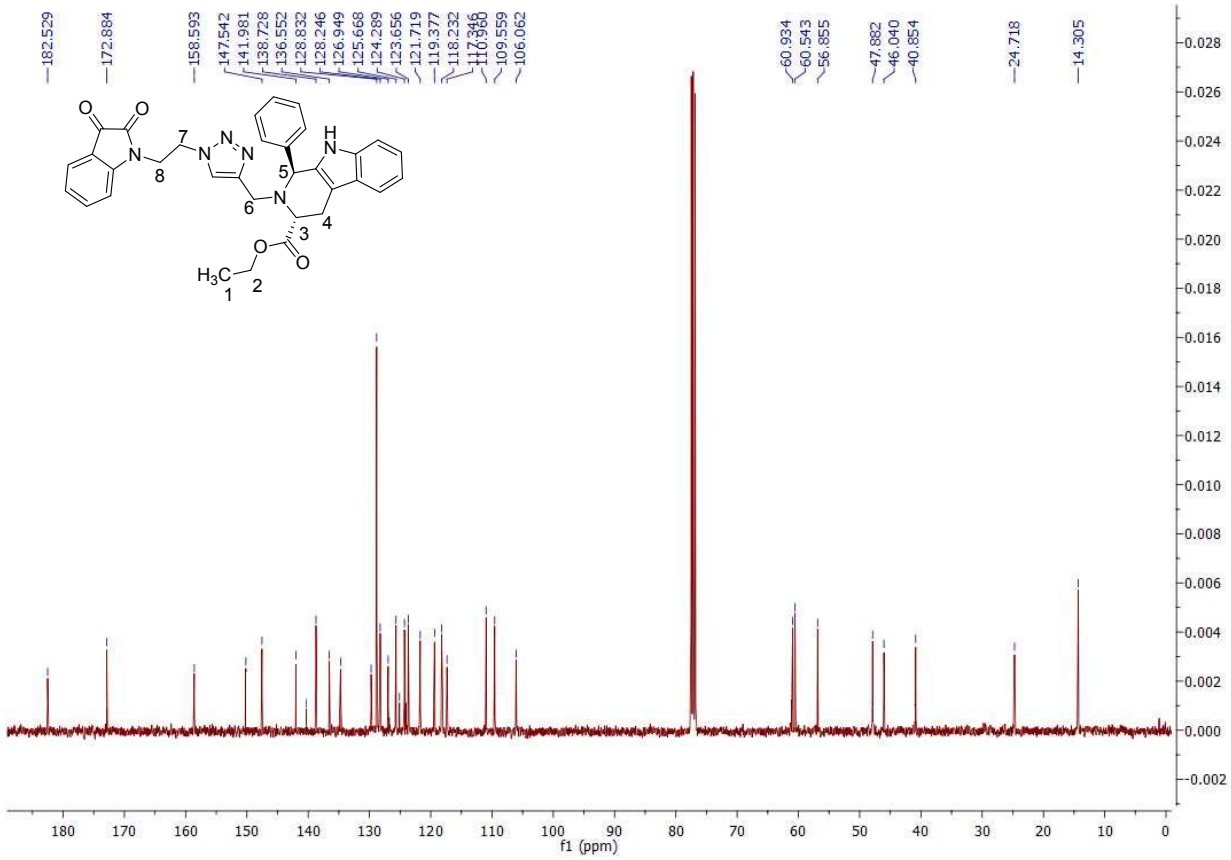
^{13}C NMR of 2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-methyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8f)**



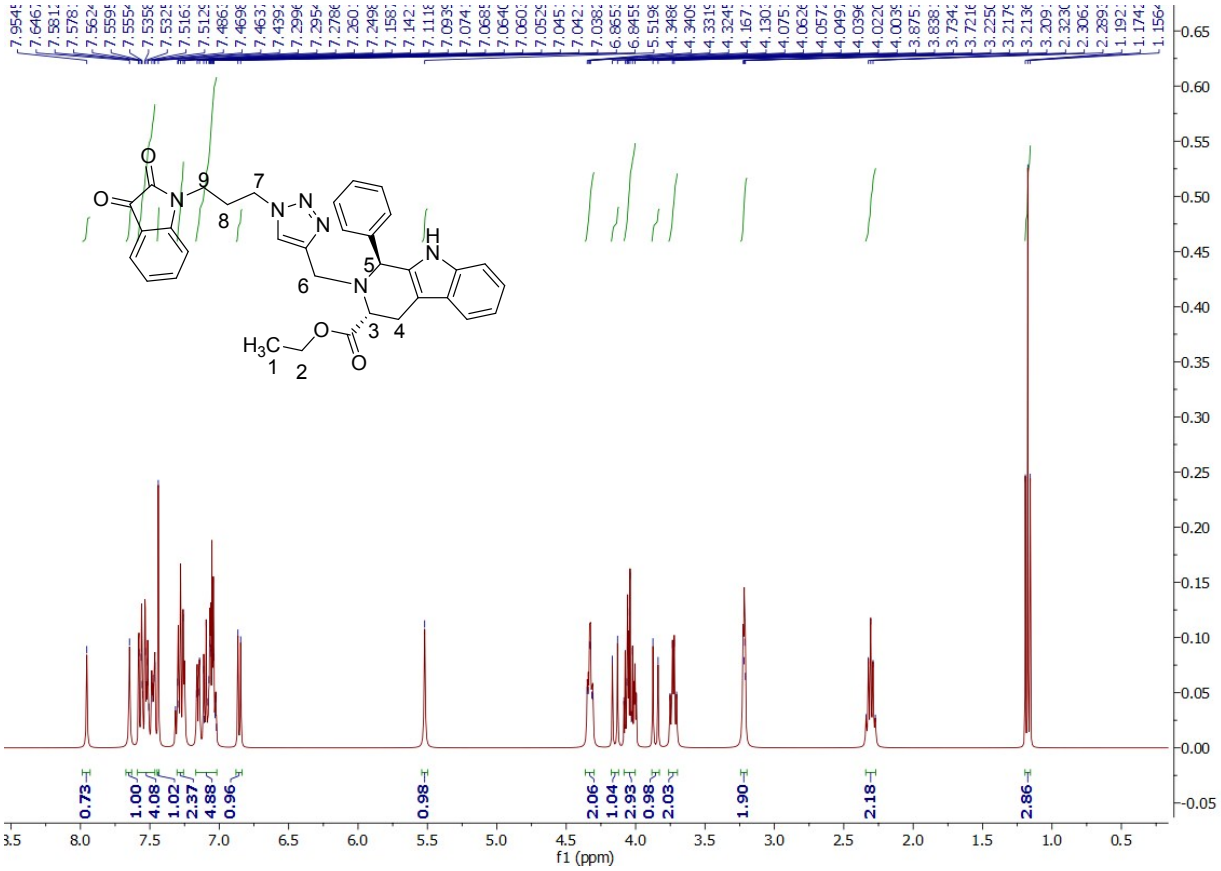
^{1}H NMR of2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8g)**



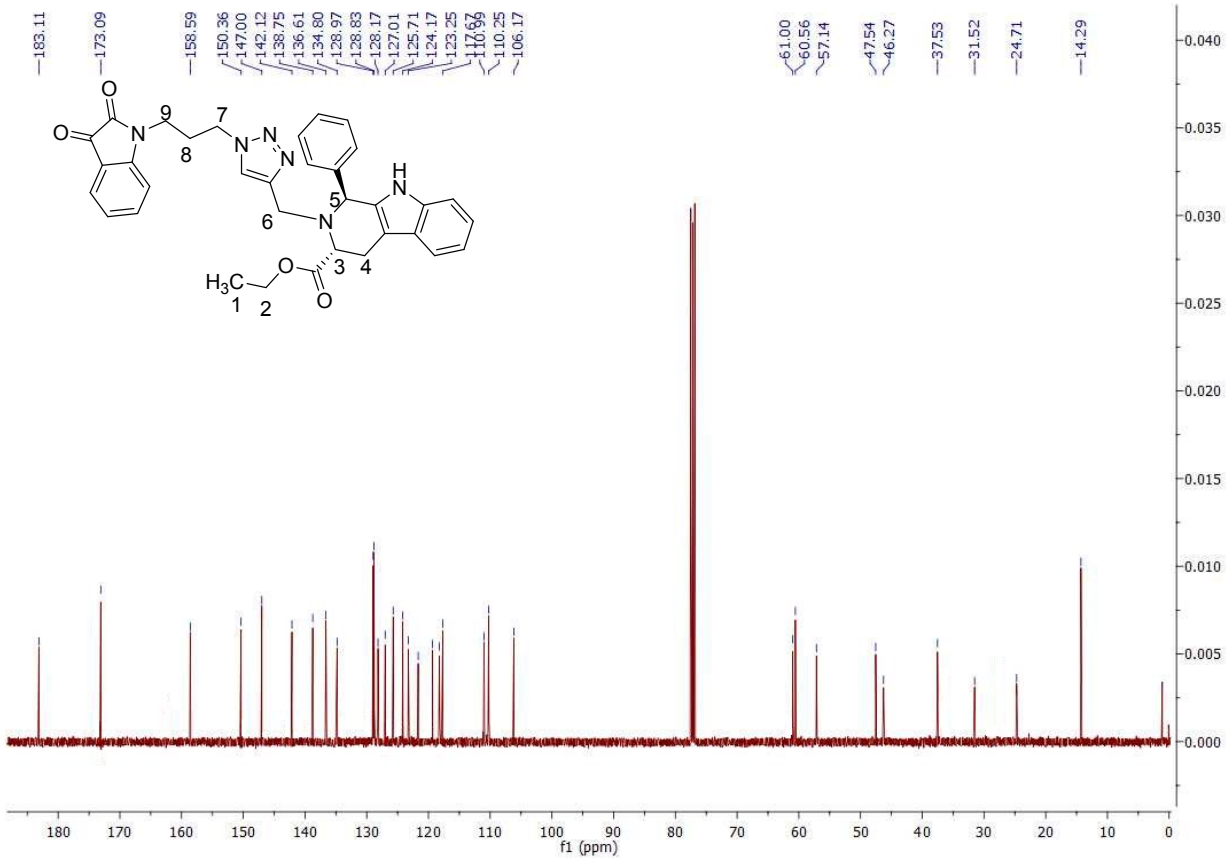
^{13}C NMR of2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8g)**



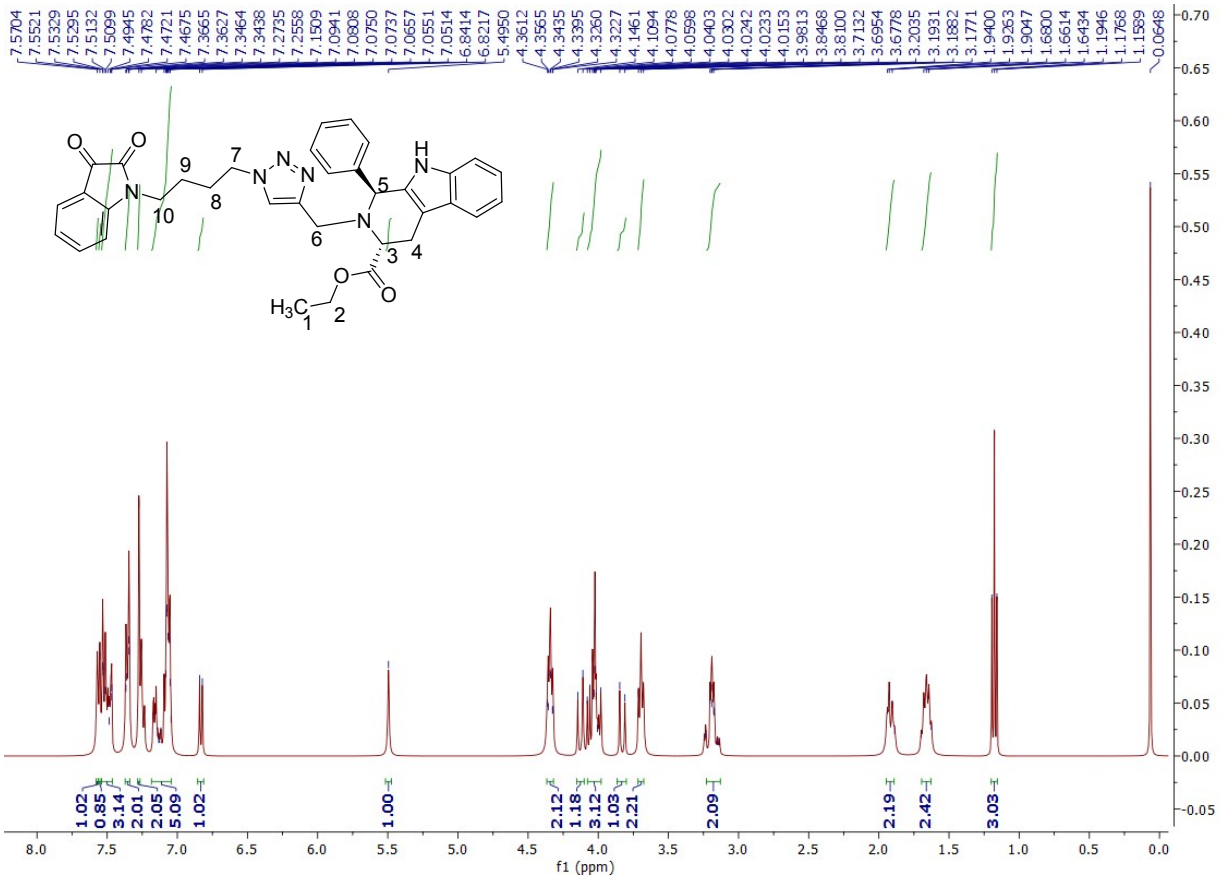
^{1}H NMR of 2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8h)**



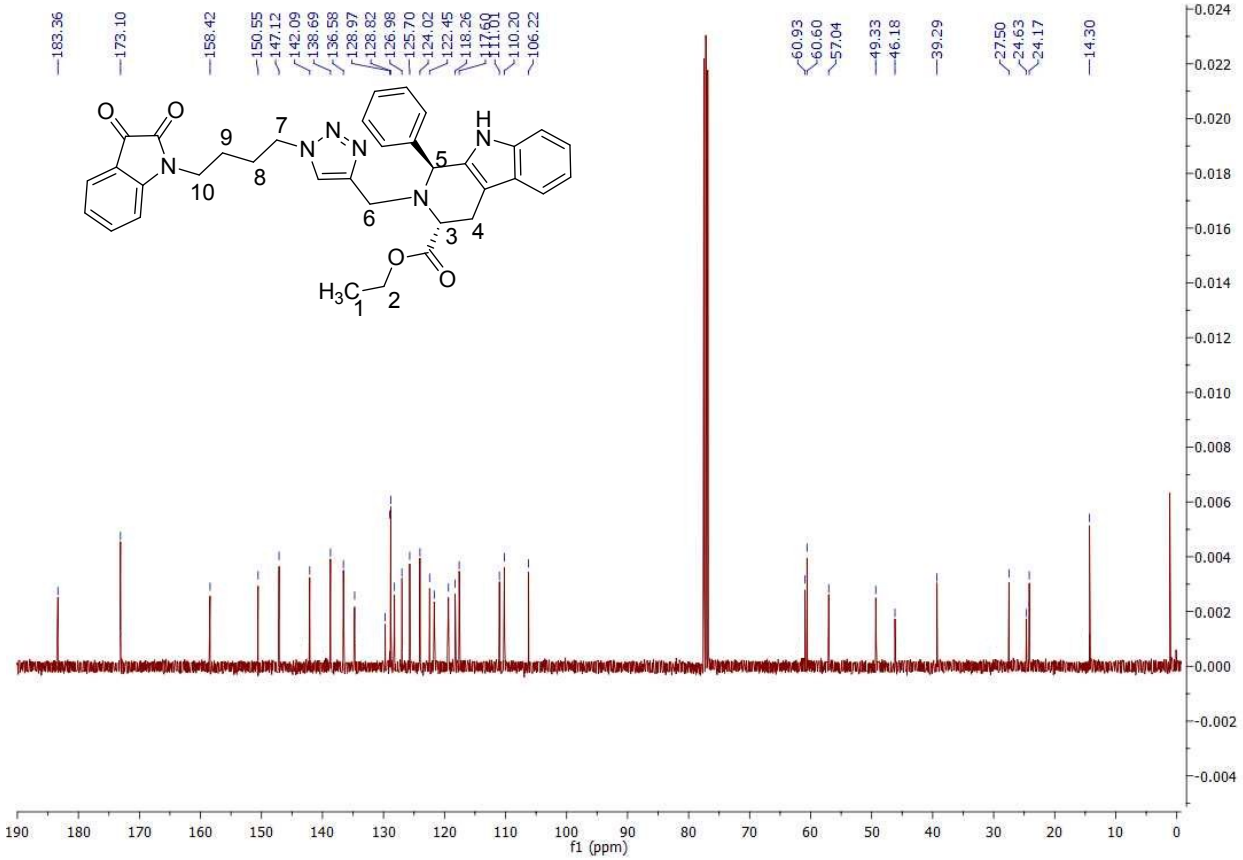
^{13}C NMR of 2-{1-[3-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-propyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8h)**



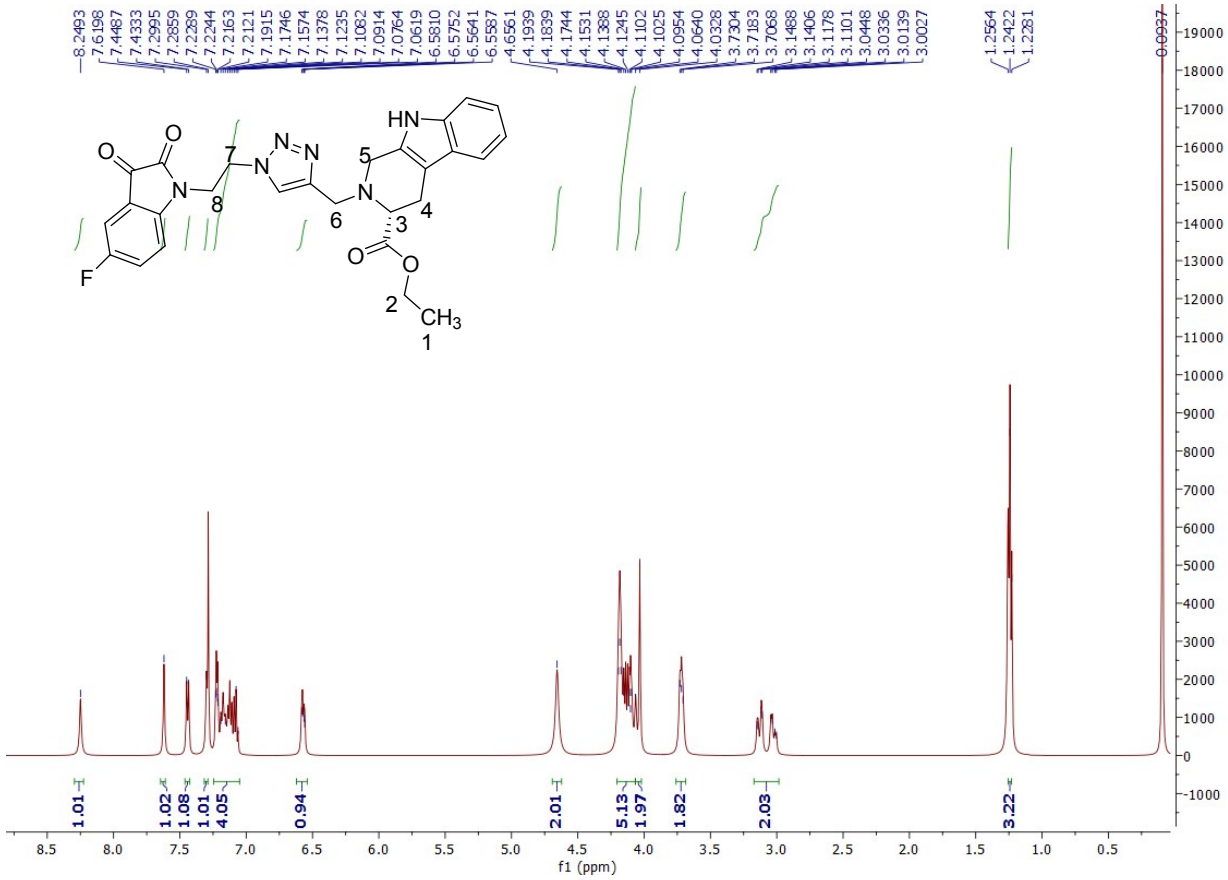
^{1}H NMR of 2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8i)**



^{13}C NMR of 2-{1-[4-(2,3-Dioxo-2,3-dihydro-indol-1-yl)-butyl]-1H-[1,2,3]triazol-4-ylmethyl}-1-phenyl-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8i)**



^{1}H NMR of 2-{1-[2-(5-Fluoro-2,3-dioxo-2,3-dihydro-indol-1-yl)-ethyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8j)**



^{13}C NMR of 2-{1-[2-(5-Fluoro-2,3-dioxo-2,3-dihydro-indol-1-yl)-ethyl]-1H-[1,2,3]triazol-4-ylmethyl}-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester **(8j**)

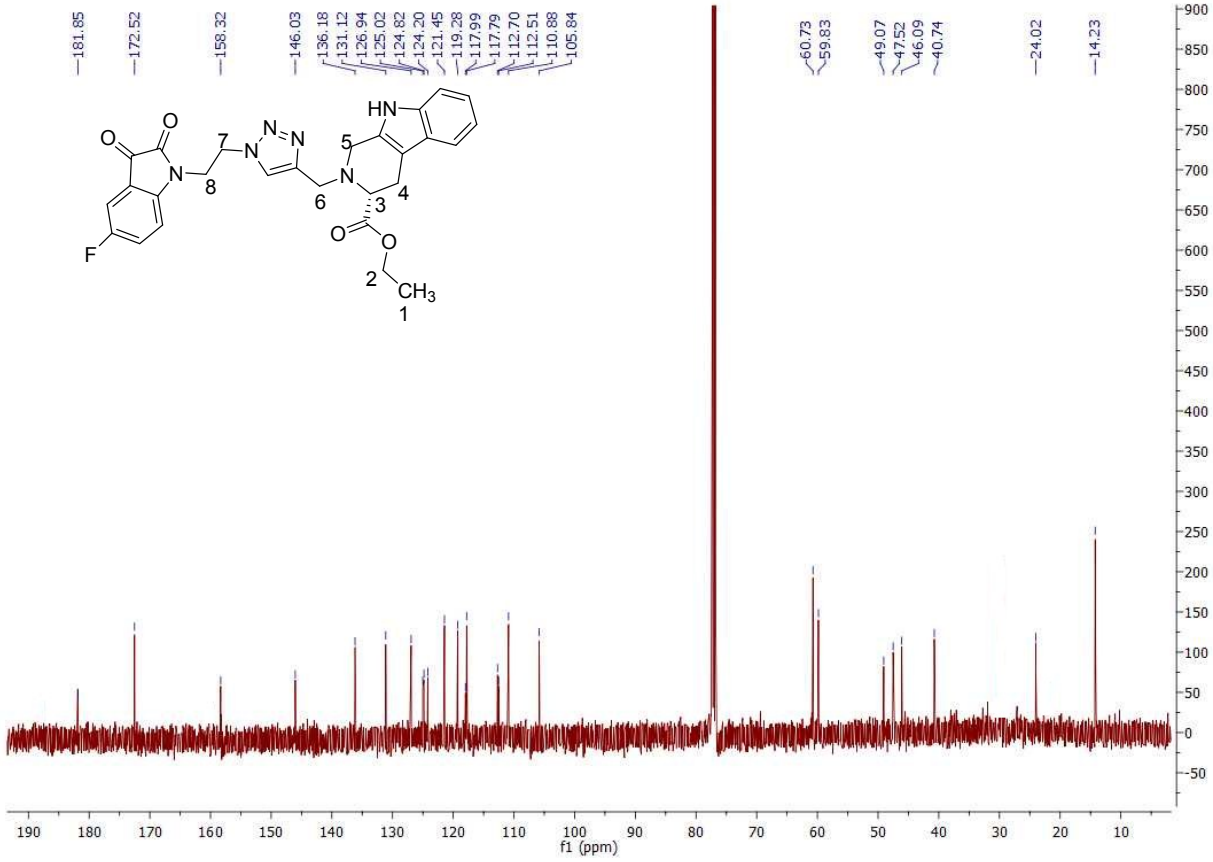


Table 3: Physical properties of the docked compounds

Compound ID	**logP**	**TPSA/ Å^2**	**Rotatable bonds**	**Molecular Weight/ g.mol^{-1}**	**Pharmacophore features**		
					Acceptors	**Donors**	**Ionisable groups/charge**
8b	2.27	110.01	9	514.58	6	3	1/-
8d	2.17	110.01	8	514.58	6	3	1/-
8e	2.43	110.01	9	528.60	6	3	1/+
8r	3.94	110.01	11	622.69	7	3	1/-

Table 4

Grid Point Parameters	
Grid center co-ordinates	**Grid size**
X = 30.173 Y = -1.997 Z = 24.207	X = 40 Y = 30 Z = 40