

Design, Synthesis and anti-proliferative evaluation of 1*H*-1,2,3-triazole grafted ferrocenyl/ organic tetrahydro- β -carboline-chalcone hybrids in Estrogen Responsive (ER+) and Triple Negative Breast Cancer (ER-) cells

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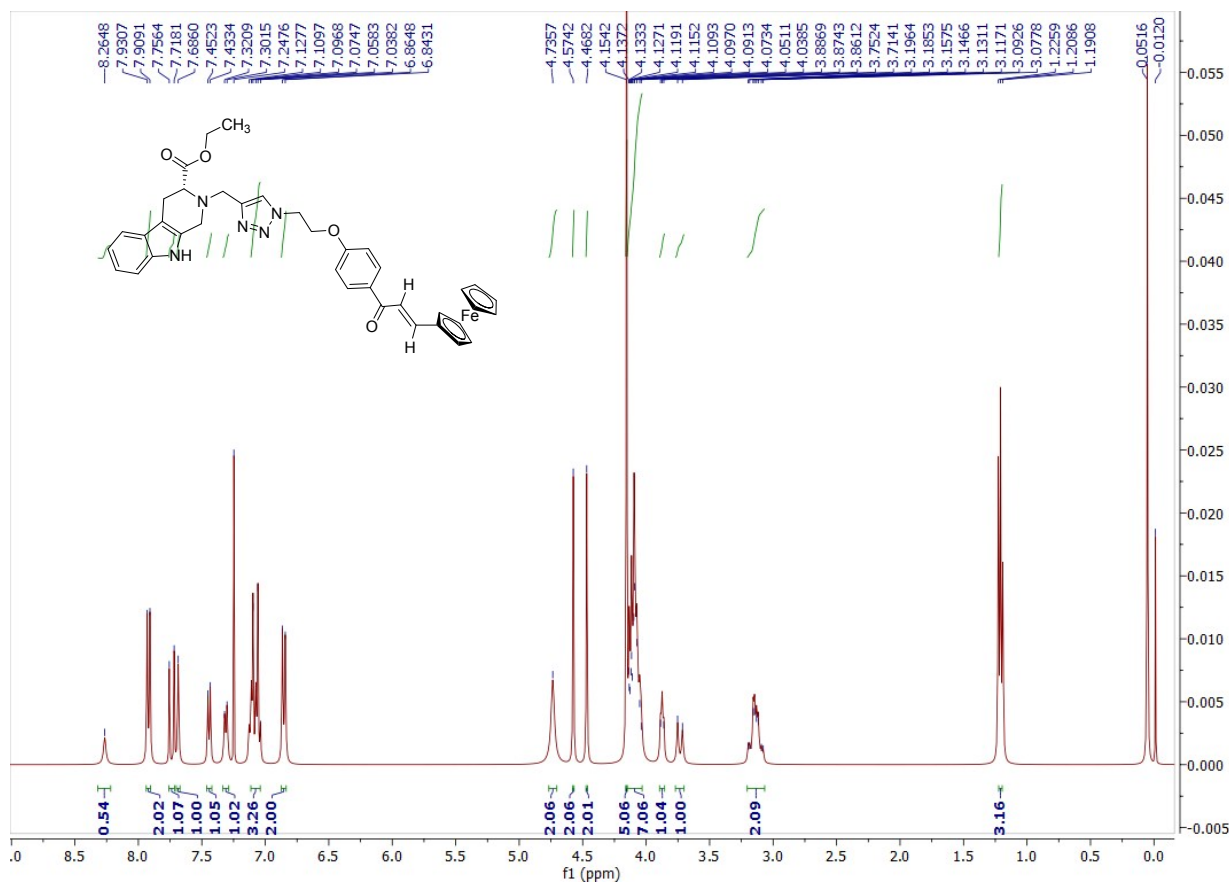
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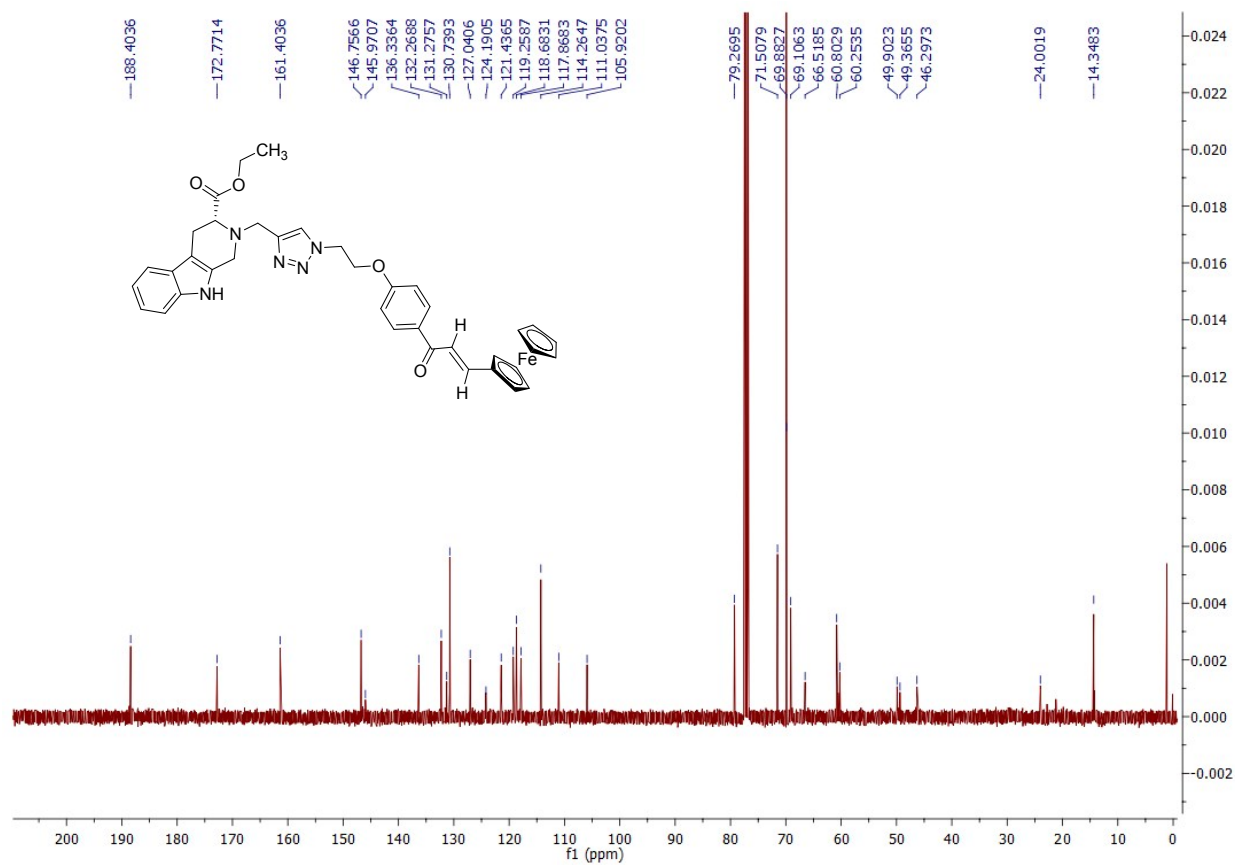
^cSchool of Chemistry and Physics, University of KwaZulu-Natal, P/Bag X54001, Westville, Durban, South Africa

Supporting information

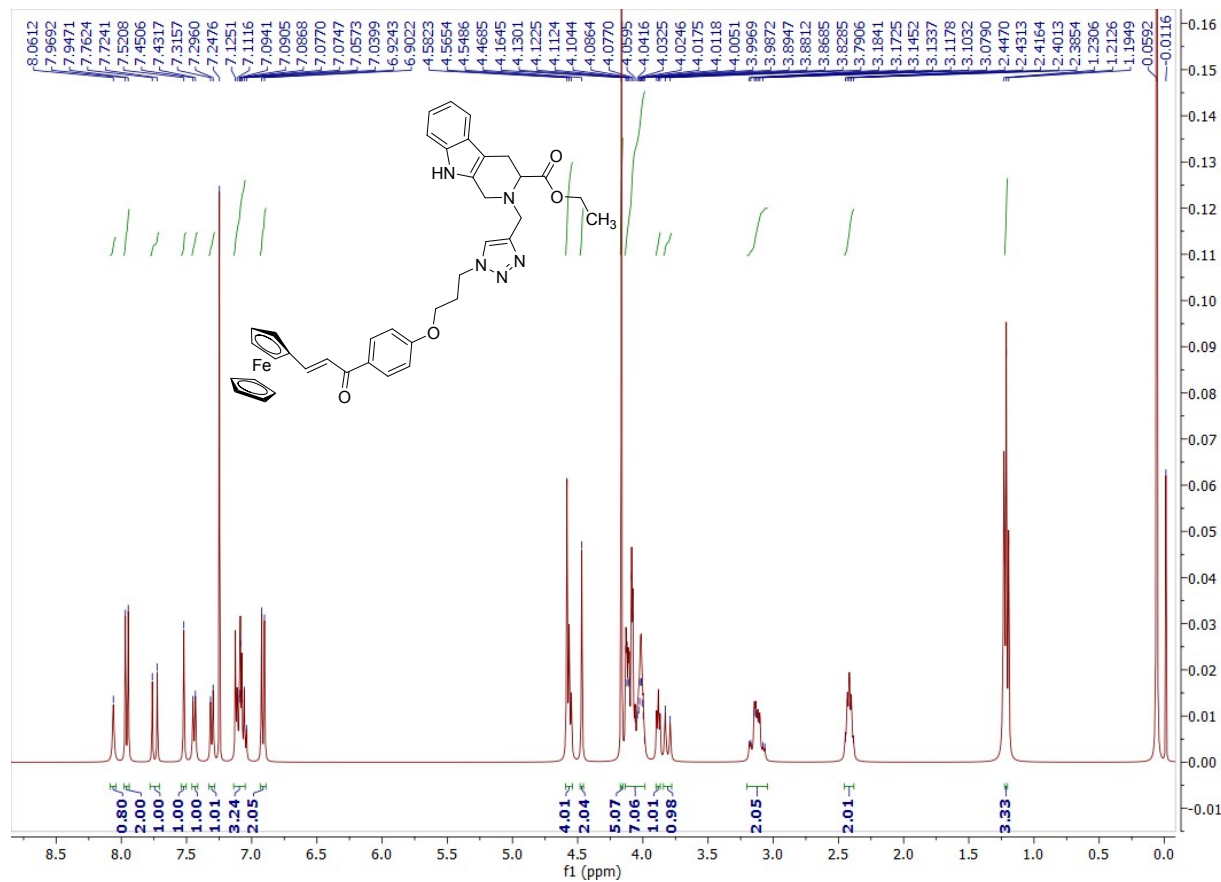
¹H NMR of 2-[1-(2-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-ethyl)-1*H*-[1,2,3]triazol-4-ylmethyl)-2,3,4,9-tetrahydro-1*H*- β -carboline-3-carboxylic acid ethyl ester (12a)



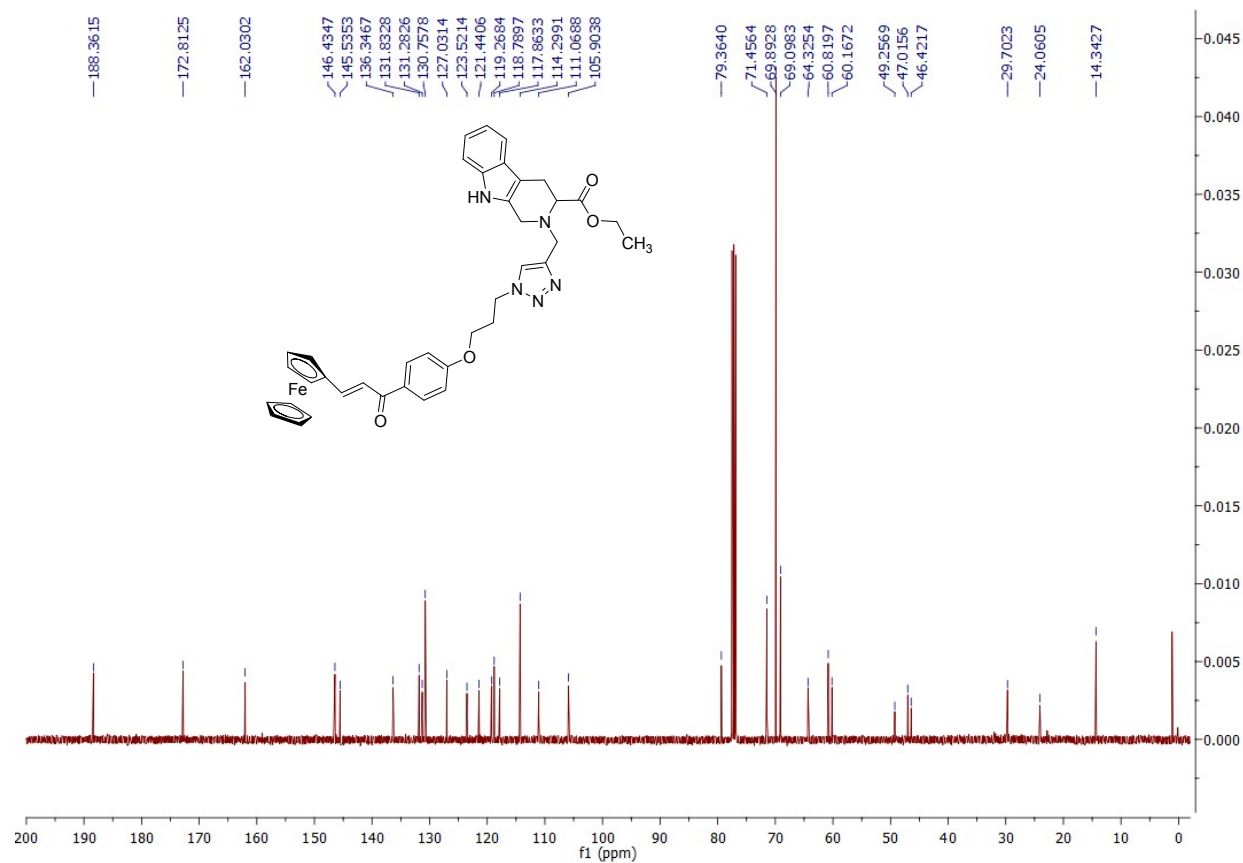
^{13}C NMR of 2-[1-(2-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12a)



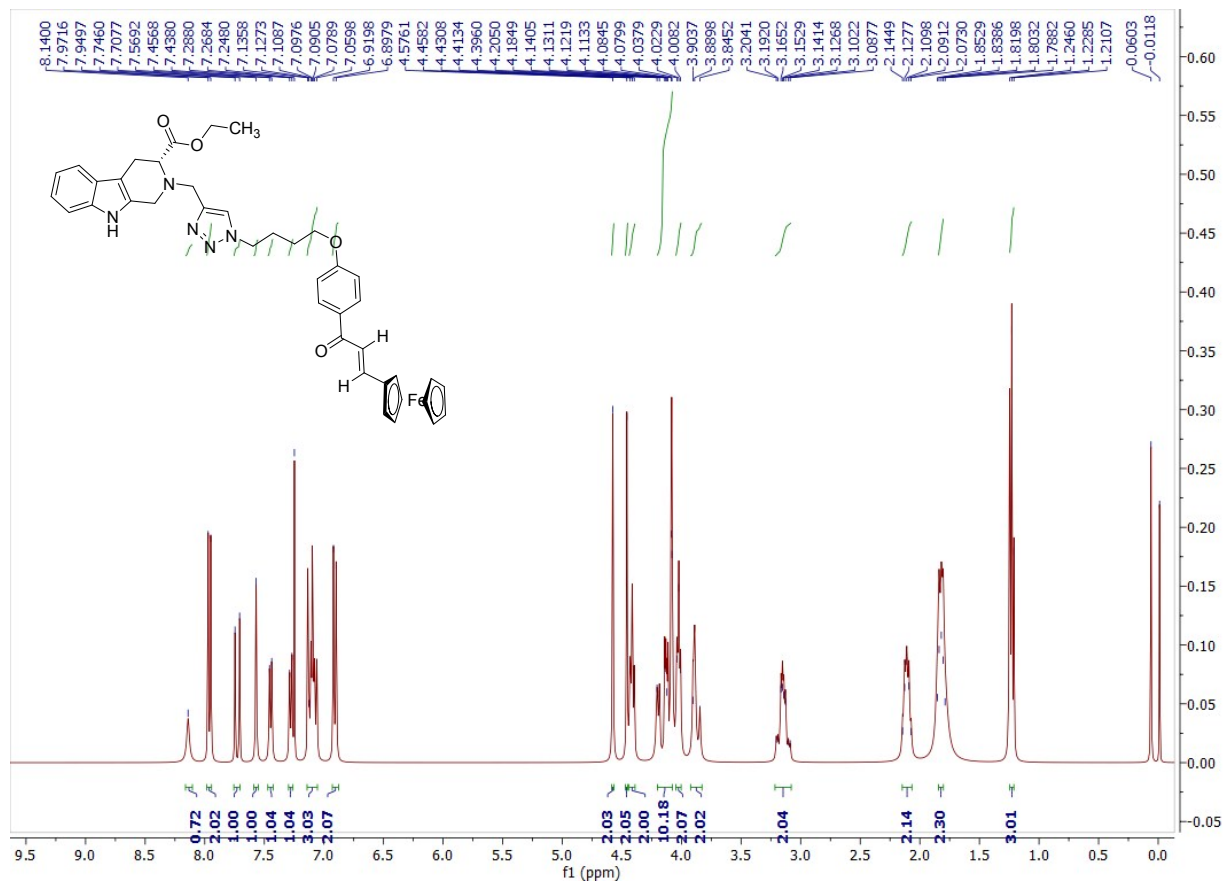
^1H NMR of 2-[1-(3-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-propyl)-1H-[1,2,3]triazol-4-ylmethyl)-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12b)



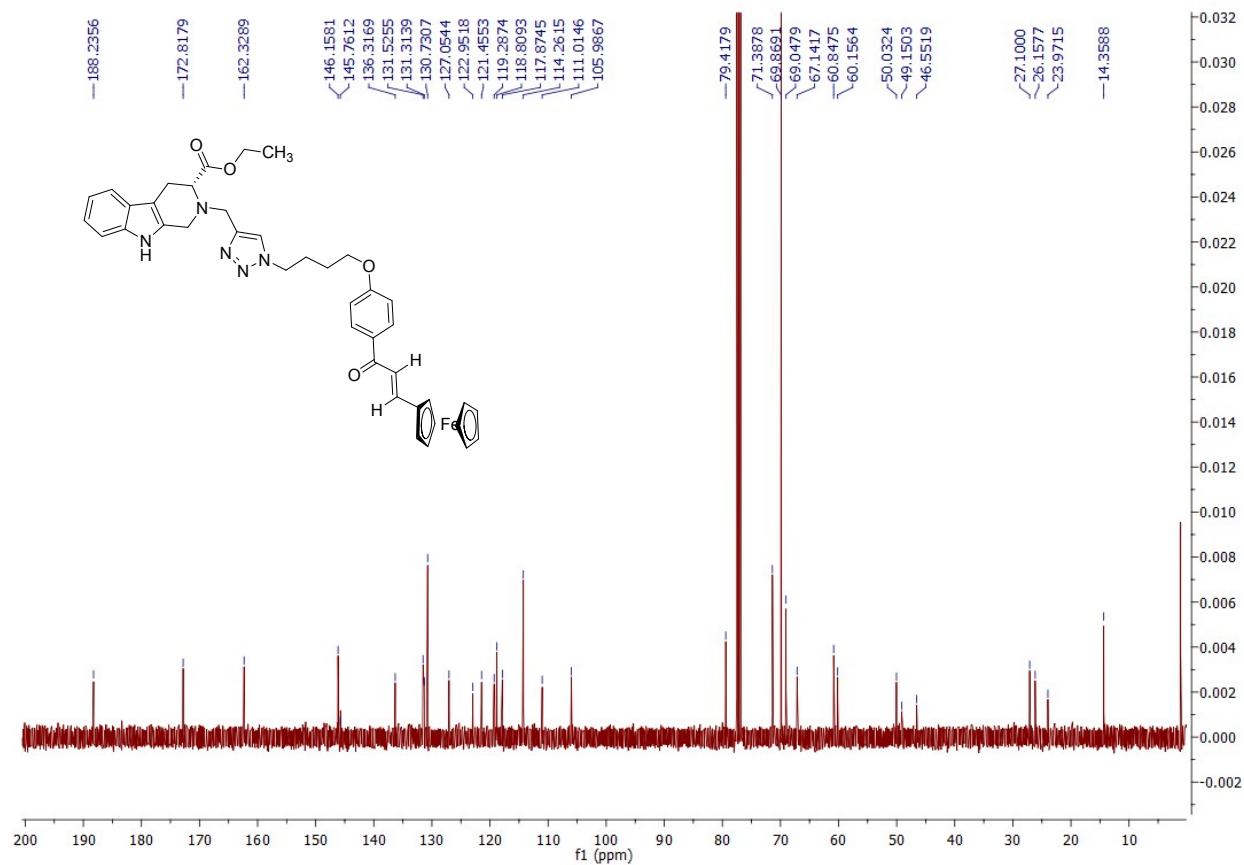
¹³C NMR of 2-[1-(3-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-propyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12b)



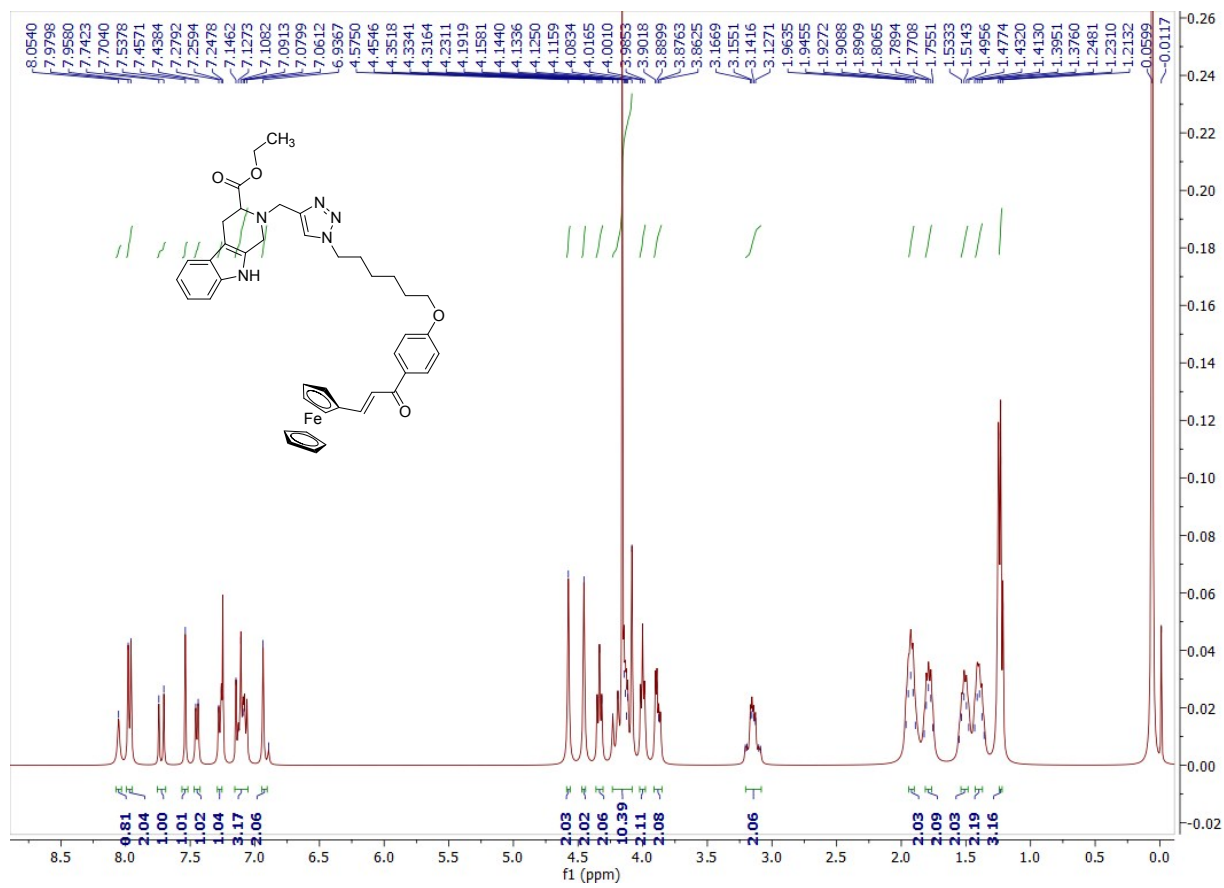
^1H NMR of 2-[1-(4-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-butyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12c)



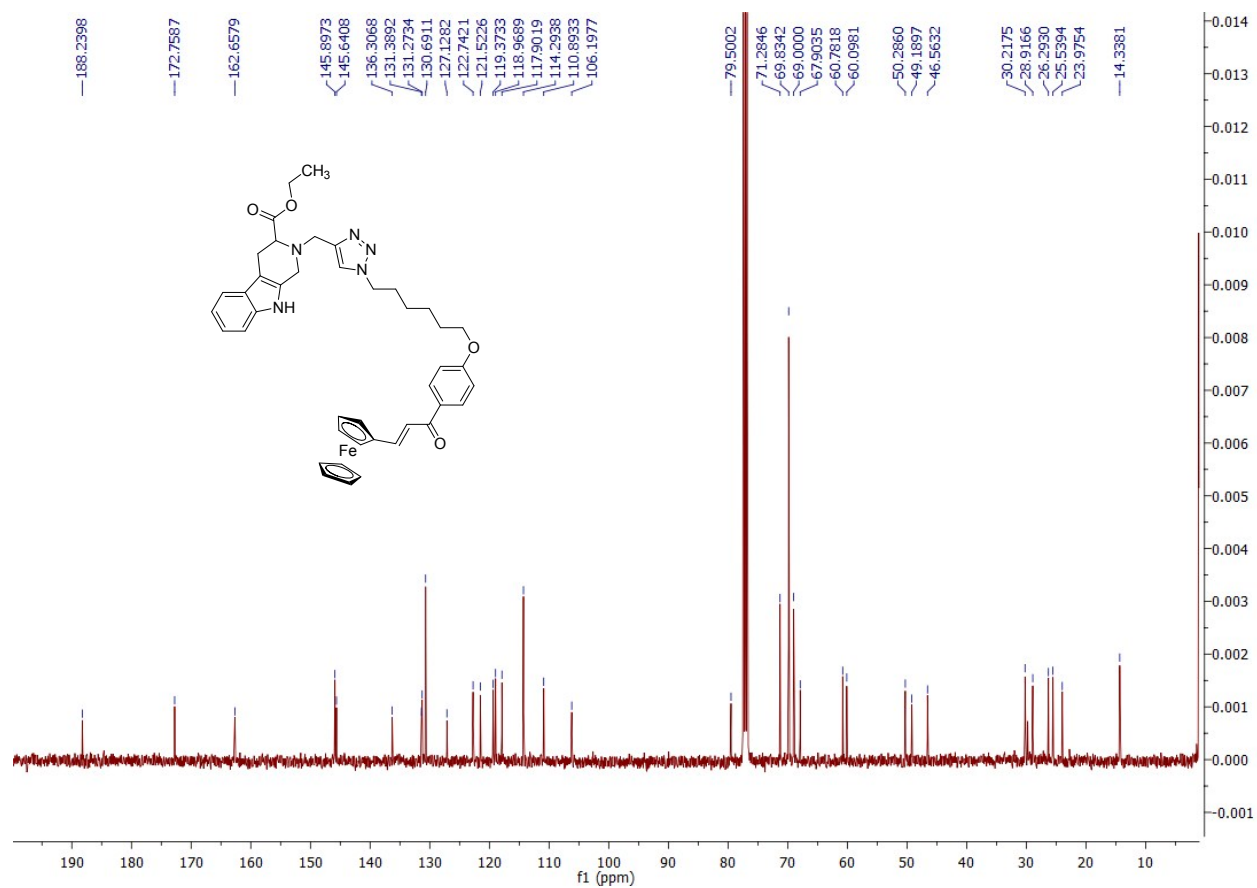
^{13}C NMR of 2-[1-(4-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-butyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12c)



¹H NMR of 2-[1-(6-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12e)



^{13}C NMR of 2-[1-(6-{4-[3-(ferrocenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (12e)



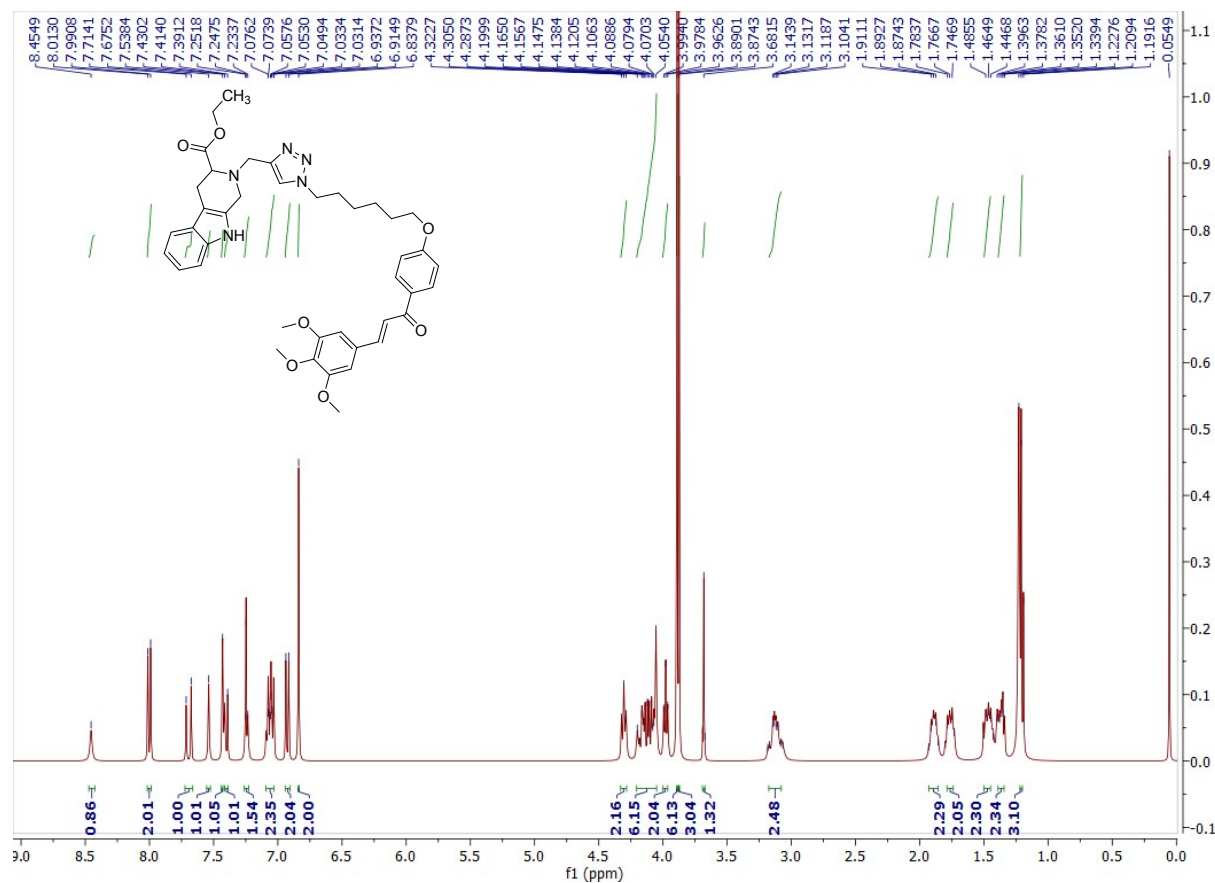
Chemical structure of compound 10:

COc1ccc(cc1C(=O)C=Cc2ccc(OC)c(OC)c2)N3Cc4c[nH]c5ccccc45C3N(Cc6nn[nH]6)C(=O)OCC

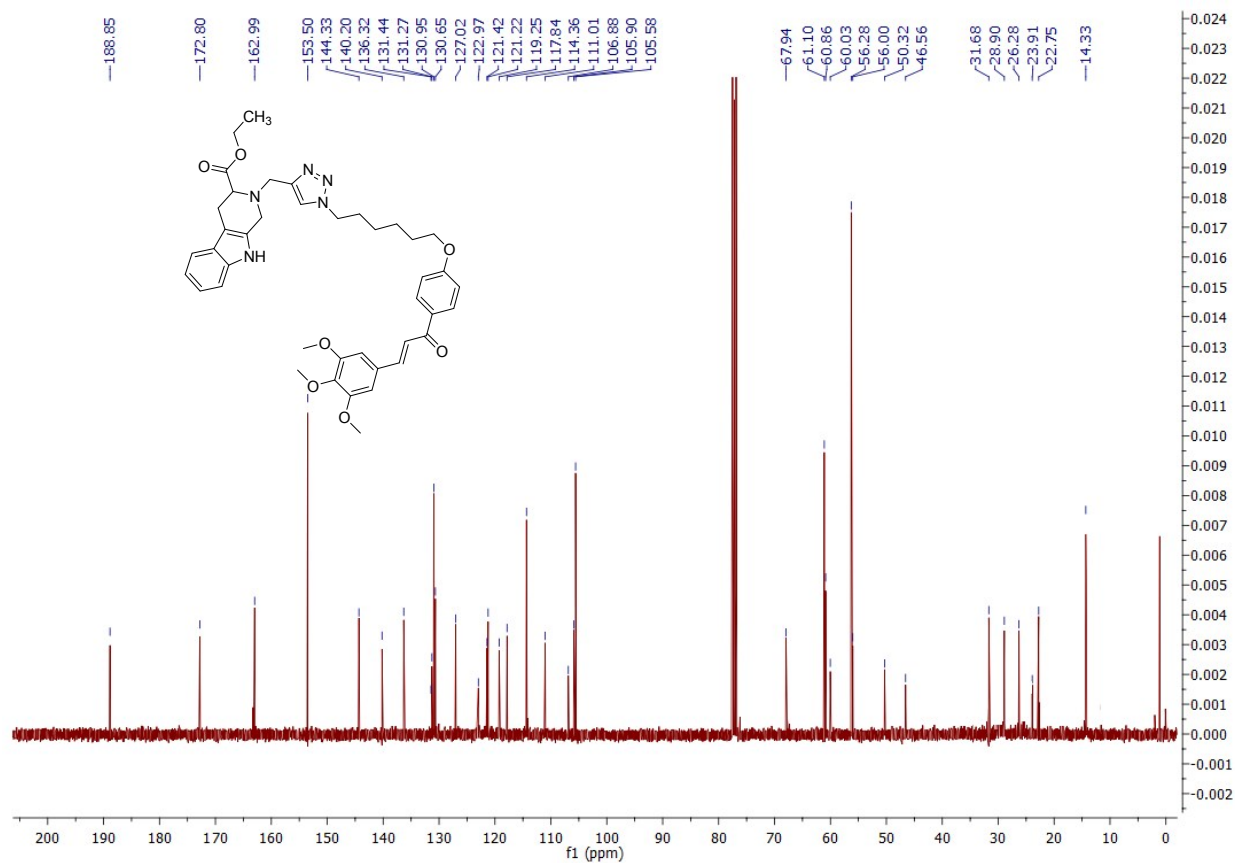
¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
8.5981	0.78
7.9968	2.05
7.9748	1.00
7.7077	1.06
7.6689	1.01
7.5524	1.03
7.4195	1.40
7.3804	2.24
7.2471	2.01
7.2305	2.05
7.0782	
7.0782	
7.0606	
7.0401	
7.0204	
7.0029	
6.9074	
6.8856	
6.8331	
4.3868	
4.3702	
4.3537	
4.1705	
4.1523	
4.1339	
4.1260	
4.1080	
4.0920	
4.0748	
4.0479	
3.9923	
3.9785	
3.9645	
3.8823	
3.8684	
3.6745	
3.1769	
3.1648	
3.1379	
3.1263	
3.1112	
3.0971	
3.0724	
3.0582	
2.0755	
2.0579	
2.0399	
2.0231	
1.7913	
1.7743	
1.7577	
1.2148	
1.1968	
1.1790	
0.0551	
0.0285	

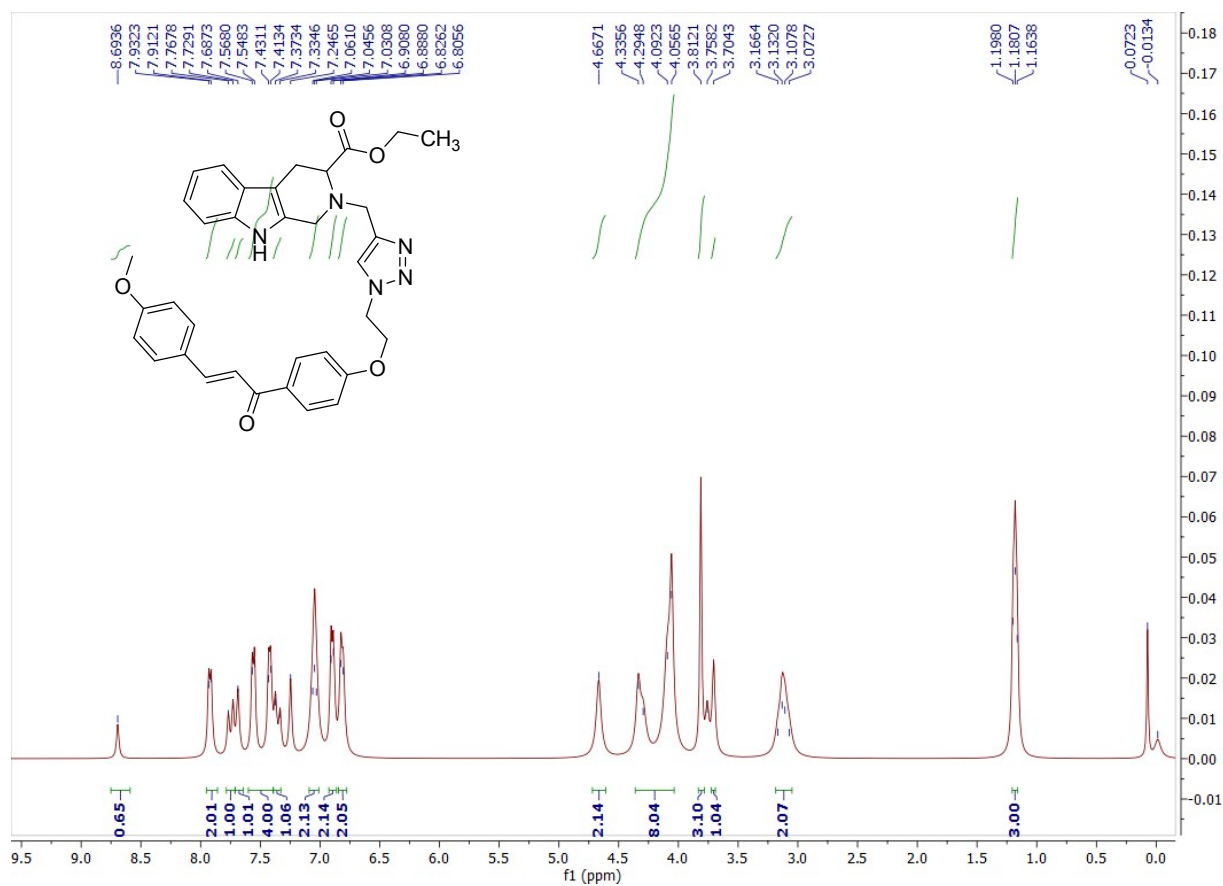
¹H NMR of 2-[1-(6-{4-[3-(3,4,5-Trimethoxy-phenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester (13e)



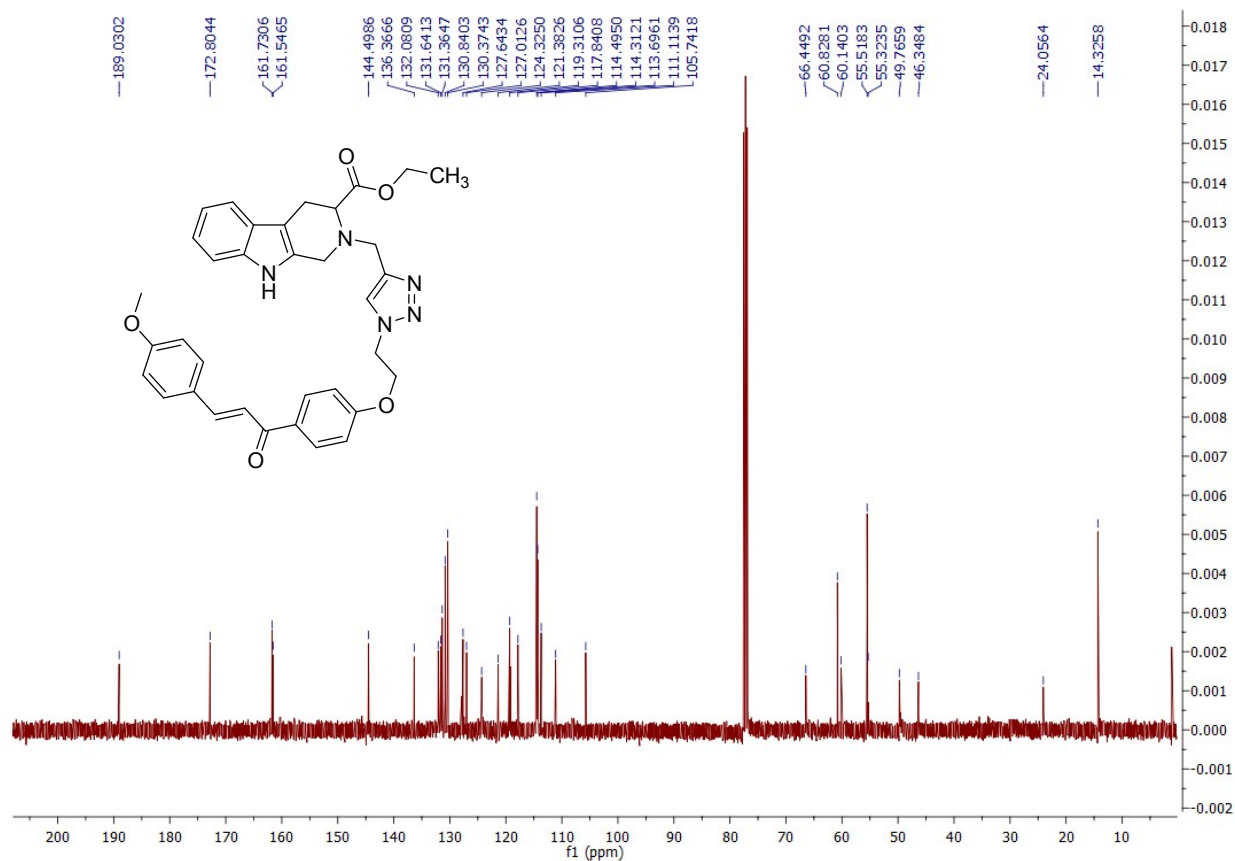
¹³C NMR of 2-[1-(6-{4-[3-(3,4,5-Trimethoxy-phenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester (13e)



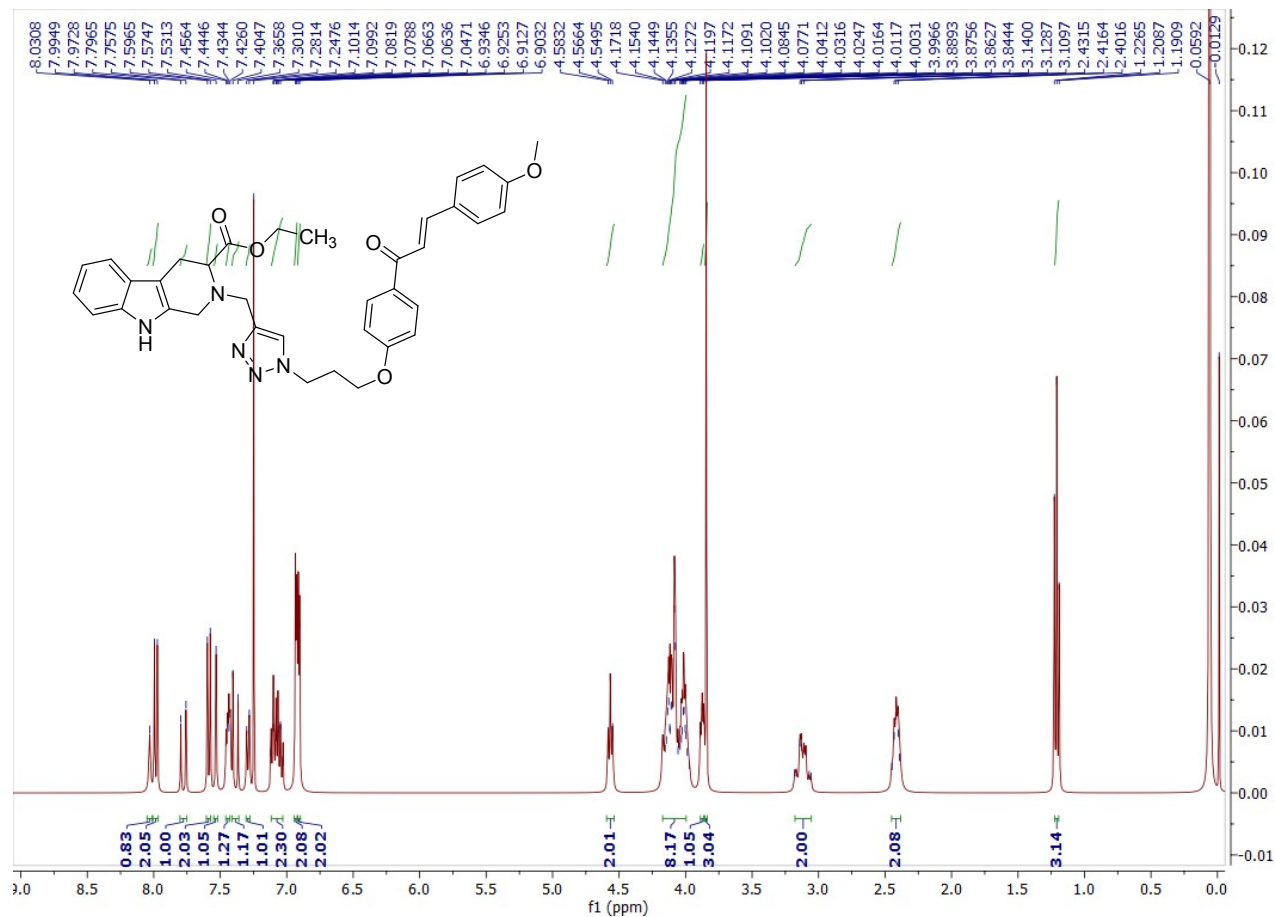
¹H NMR of 2-[1-(2-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13f)



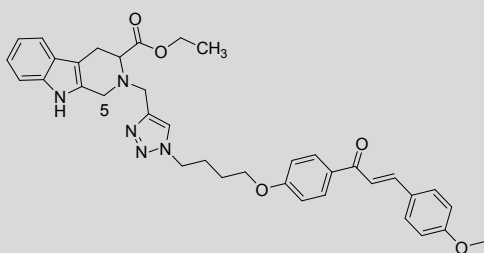
^{13}C NMR of 2-[1-(2-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13f)



¹H NMR of 2-[1-(3-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-propyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H-β-carboline-3-carboxylic acid ethyl ester (13g)

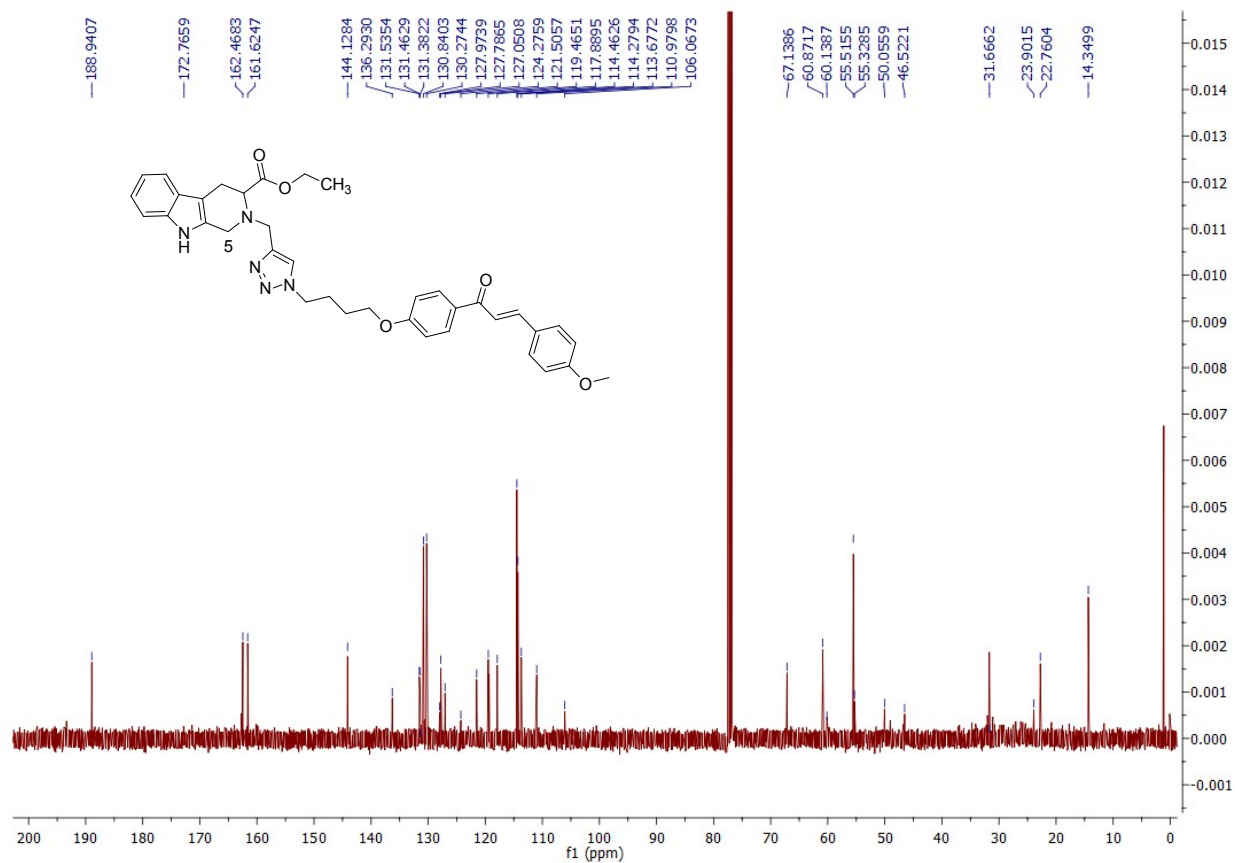


¹H NMR of 2-[1-(4-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-butyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13h)

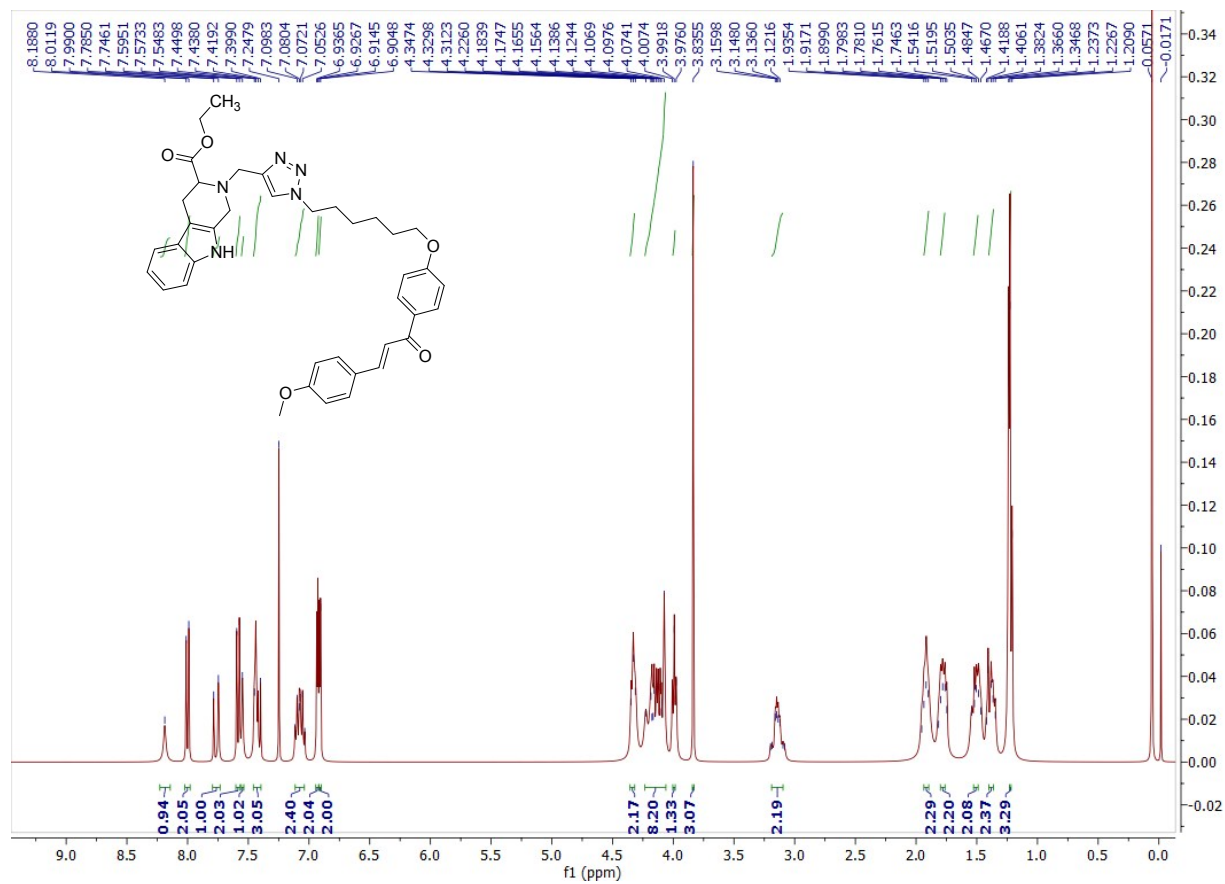


^{13}C NMR of 2-[1-(4-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-butyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13h)

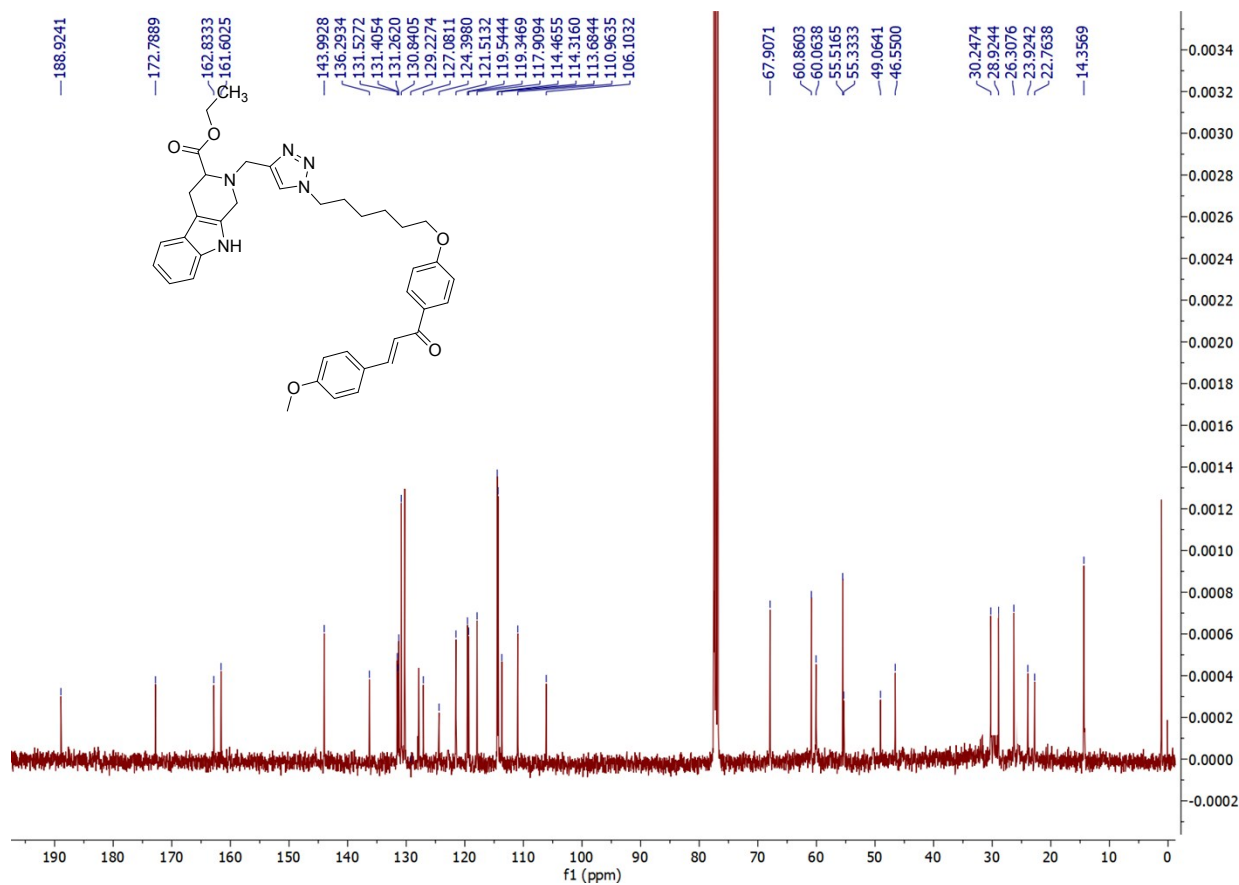
v



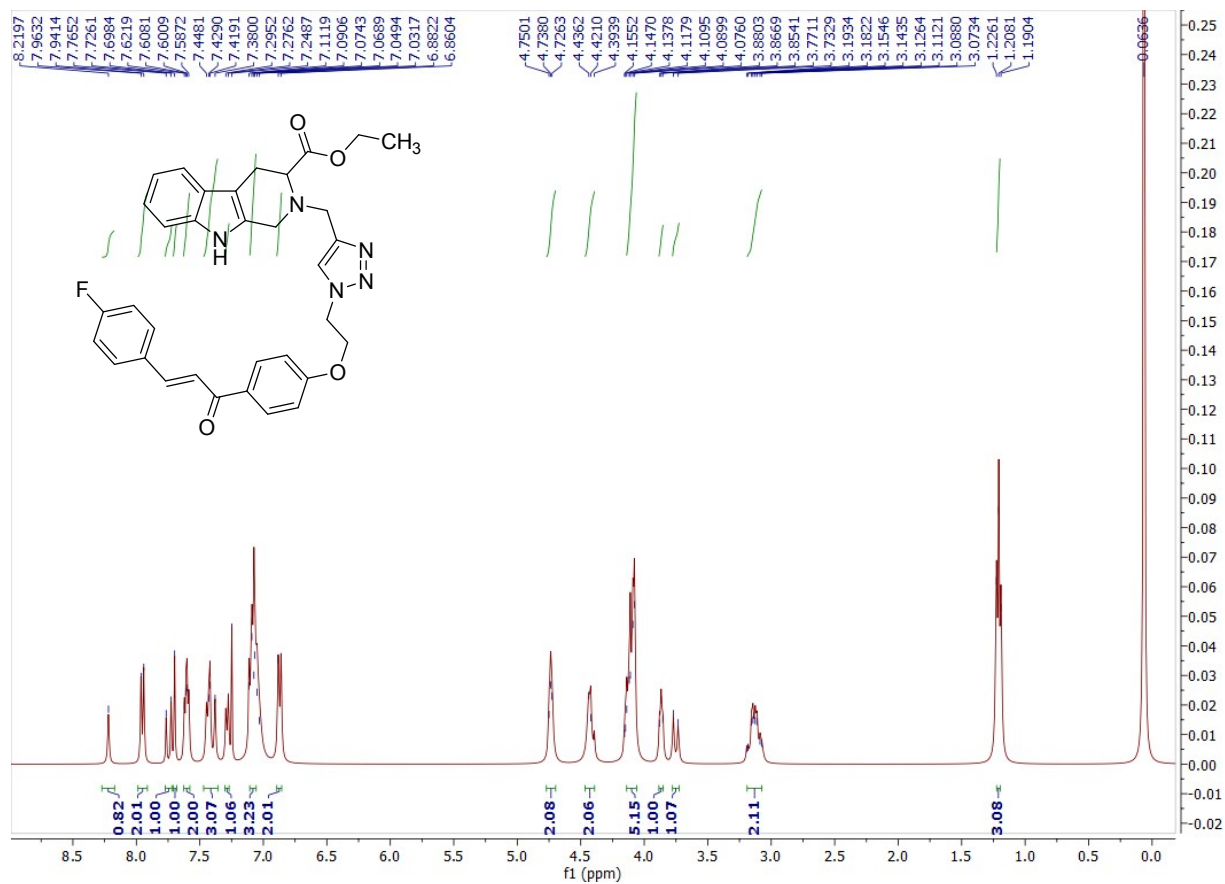
¹H NMR of 2-[1-(6-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13j)



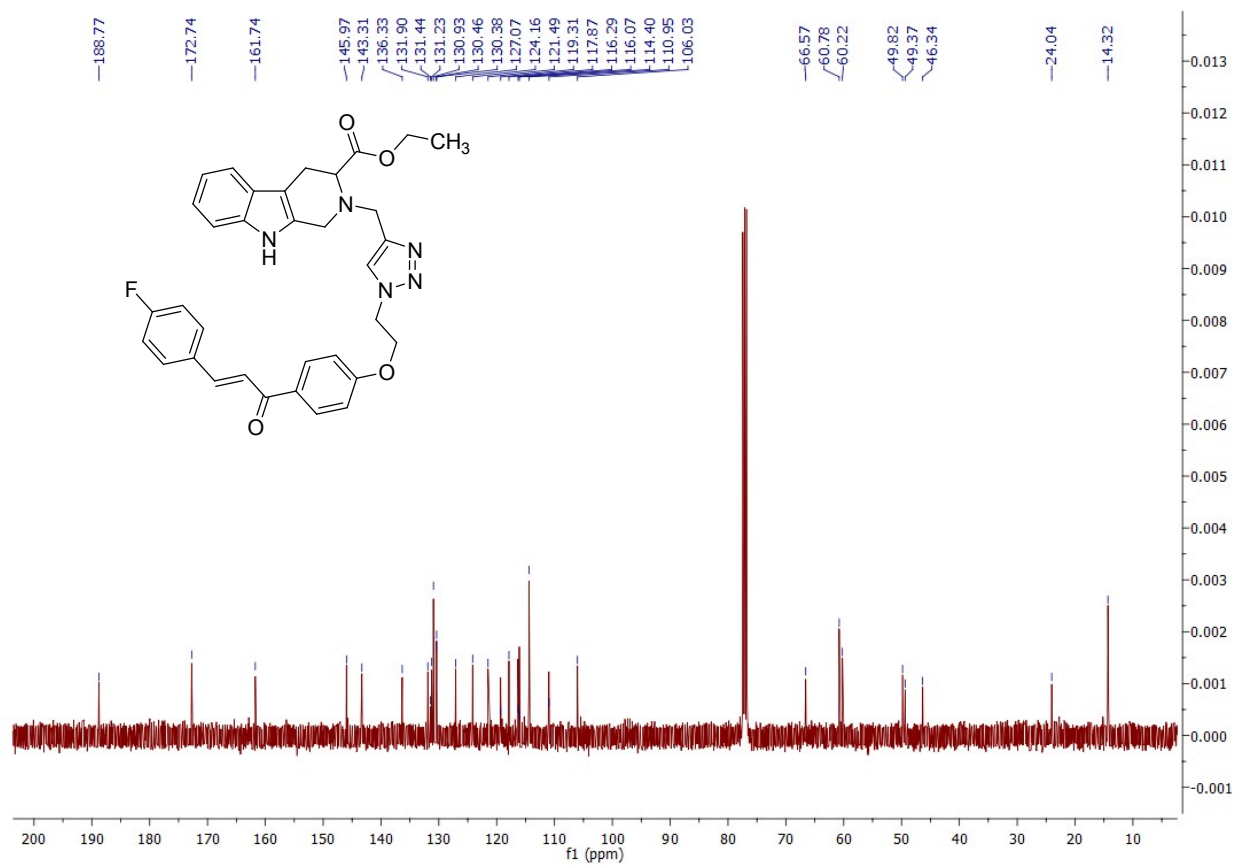
^{13}C NMR of 2-[1-(6-{4-[3-(4-Methoxy-phenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13j)



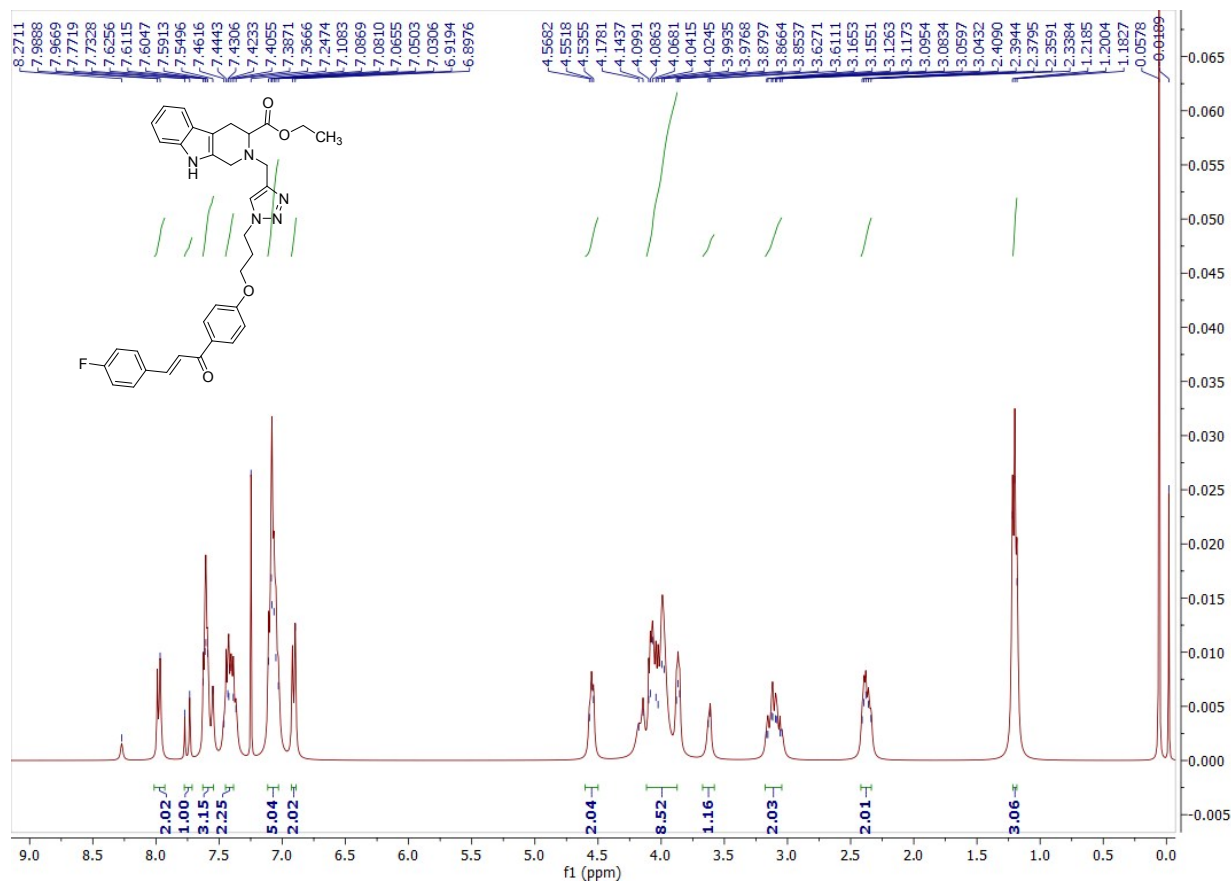
¹H NMR of 2-[1-(2-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13k)



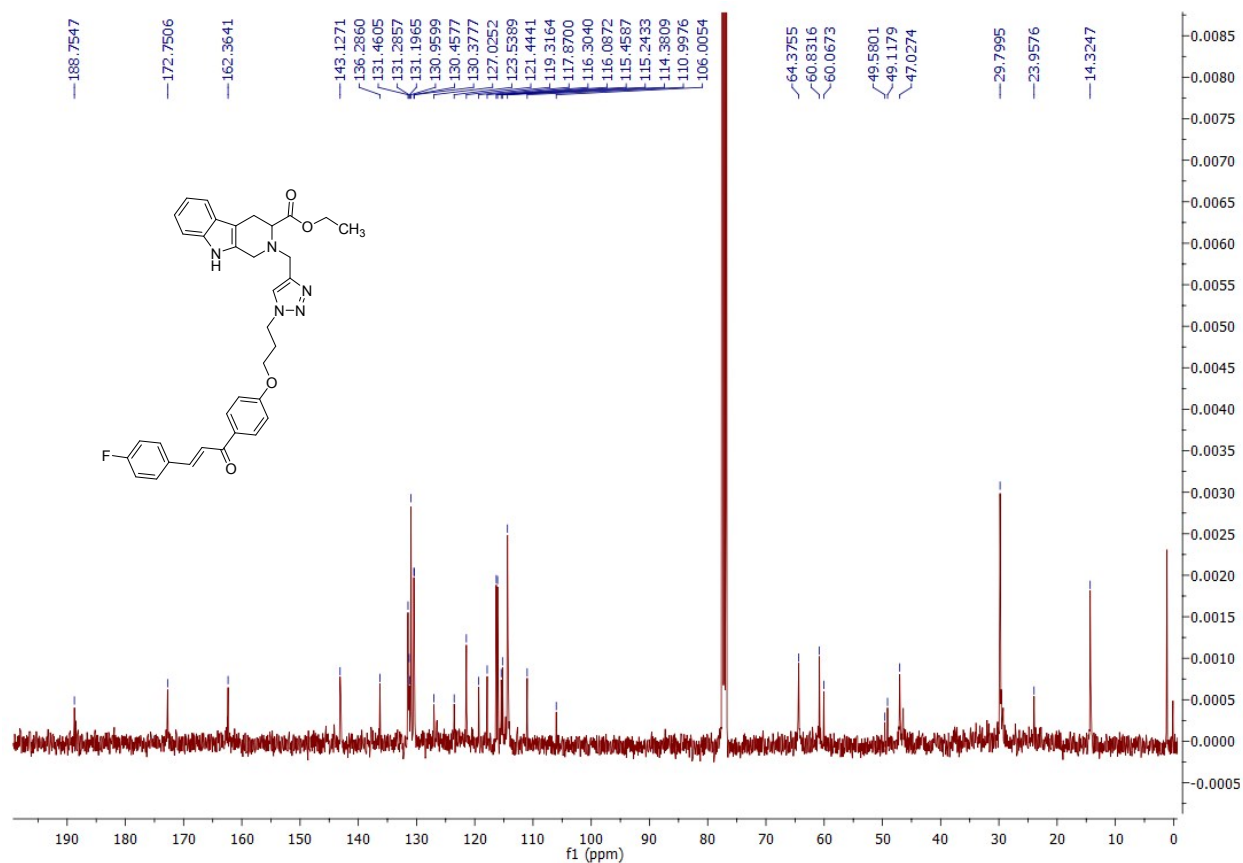
^{13}C NMR of 2-[1-(2-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13k)



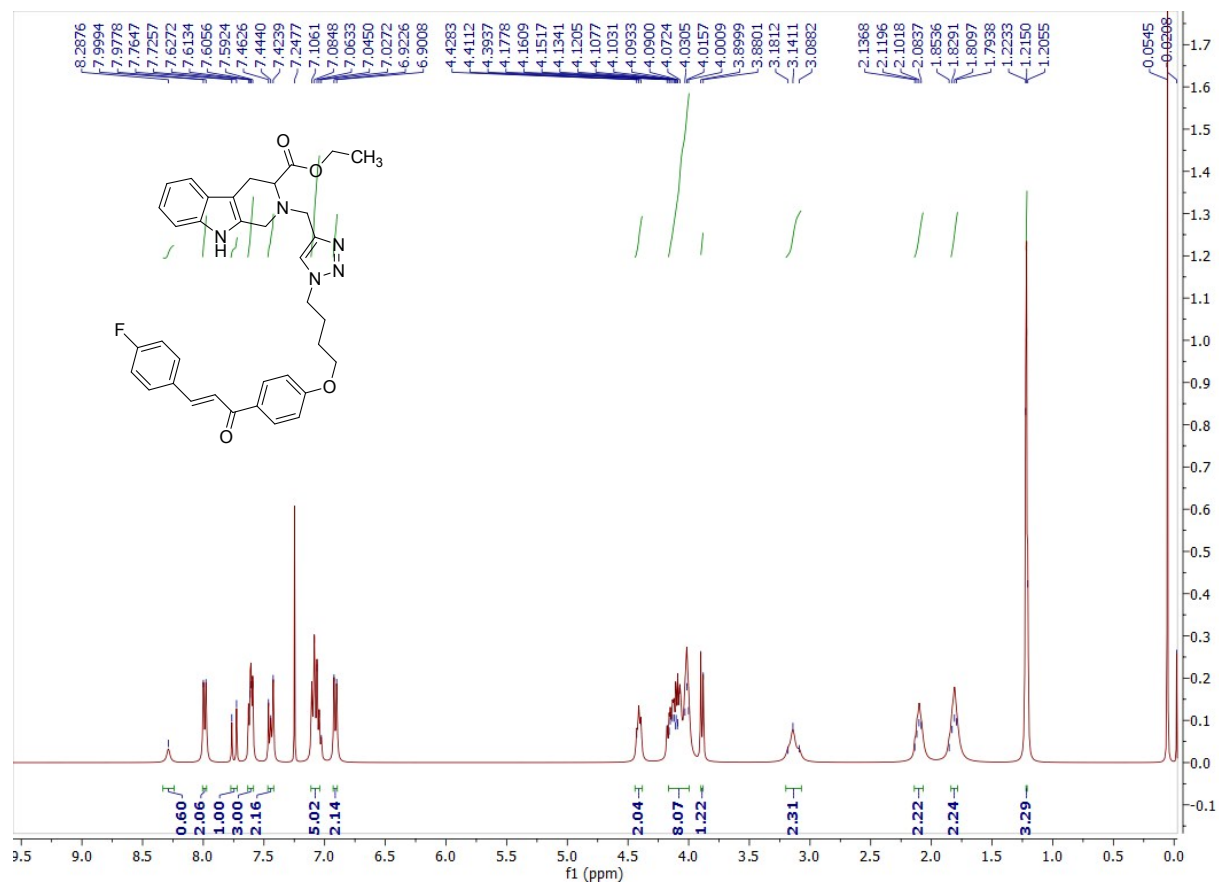
¹H NMR of 2-[1-(3-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-propyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13l)



^{13}C NMR of 2-[1-(3-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-propyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13l)



¹H NMR of 2-[1-(4-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-butyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13m)



Chemical structure of compound 10 is shown in the top left. The ^1H NMR spectrum (CDCl₃) is displayed below, with the x-axis representing the chemical shift in ppm (f1) from 9.0 to 0.0. The spectrum shows several multiplets and singlets, with integration values provided below the baseline. A list of peak chemical shifts (ppm) is provided on the right side of the spectrum.

Chemical structure of compound 10: CCOC(=O)N1Cc2c(c[nH]2)c3ccccc31CN(C#N)CCCCOc4ccc(cc4)C(=O)/C=C/c5ccc(F)cc5

Integration values (from left to right): 0.87, 2.03, 1.02, 2.13, 1.00, 2.02, 1.49, 4.07, 2.02, 6.02, 2.01, 1.00, 2.03, 2.19, 2.20, 2.06, 2.03, 3.19.

Peak chemical shifts (ppm) (from left to right): 8.3705, 8.0112, 7.9890, 7.7634, 7.7244, 7.6233, 7.6097, 7.6015, 7.5880, 7.5370, 7.4751, 7.4449, 7.4360, 7.4272, 7.3601, 7.2479, 7.2415, 7.1024, 7.0979, 7.0809, 7.0688, 7.0645, 7.0599, 7.0454, 7.0432, 6.9394, 6.9171, 4.3344, 4.3165, 4.2967, 4.1755, 4.1661, 4.1581, 4.1487, 4.1310, 4.1154, 4.0979, 4.0700, 4.0622, 4.0026, 3.9869, 3.9711, 3.8864, 3.8734, 3.8603, 3.1553, 3.1431, 1.9232, 1.9048, 1.8863, 1.7926, 1.7755, 1.7557, 1.5141, 1.4953, 1.4764, 1.3909, 1.3734, 1.3554, 1.2366, 1.2184, 1.2006, 0.0618, -0.0171.

^{13}C NMR of 2-[1-(6-{4-[3-(4-Fluoro-phenyl)-acryloyl]-phenoxy}-hexyl)-1H-[1,2,3]triazol-4-ylmethyl]-2,3,4,9-tetrahydro-1H- β -carboline-3-carboxylic acid ethyl ester (13o)

