Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and *in-vitro* anti-proliferative evaluation of naphthalimide-chalcone/pyrazoline conjugates as potential SERMs with computational validation

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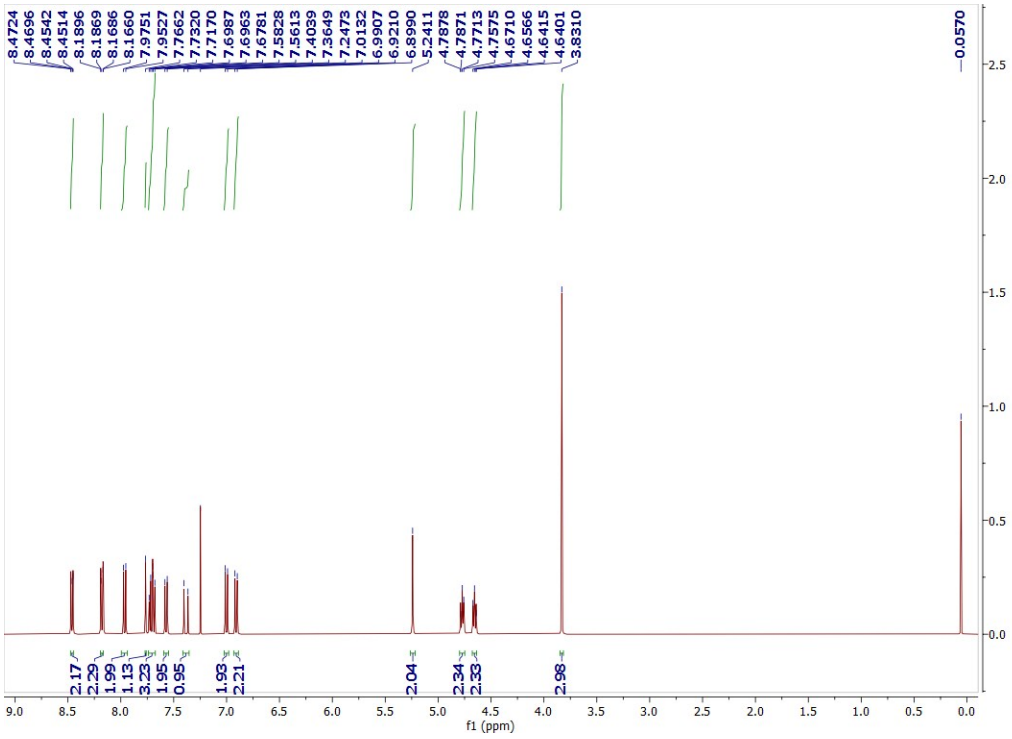
Table S1: Physicochemical and ADMET properties of compound **13f** and **13g .**

Properties	Predicted values		Properties	Predicted values	
	13f	**13g**		**13f**	**13g**
Absorption			**Distribution**		
Water solubility	-4.269	-4.148	VDss (human)	-0.768	-0.814
Caco2 permeability	0.590	0.558	BBB permeability	-1.615	-1.844
Intestinal absorption (human)	100	97.83	Fraction unbound (human)	0.311	0.32
P-glycoprotein I substrate	No	No	CNS permeability	-3.201	-3.345
P-glycoprotein II inhibitor	No	Yes	**Toxicity**		
Metabolism			Oral Rat Acute Toxicity	3.282	3.282
CYP2C19 inhibitor	Yes	Yes	Hepatotoxicity	Yes	Yes
CYP2C9 inhibitor	Yes	Yes	Skin Sensitisation	No	No
CYP2D6 substrate	Yes	Yes	*T.Pyriformis* toxicity	0.285	0.285
CYP1A2 inhibitor	No	Yes	Minnow toxicity	-2.349	-2.134
CYP3A4 substrate	Yes	Yes	**Log*P***	**4.96**	**4.98**
Excretion			**TPSA**	**120.91**	**130.14**
Total Clearance	**0.572**	0.602	**Num of HBA/HBD**	**8/0**	**9/0**
Renal OCT2 substrate	**No**	No	**Molar refractivity**	**186.47**	**192.96**

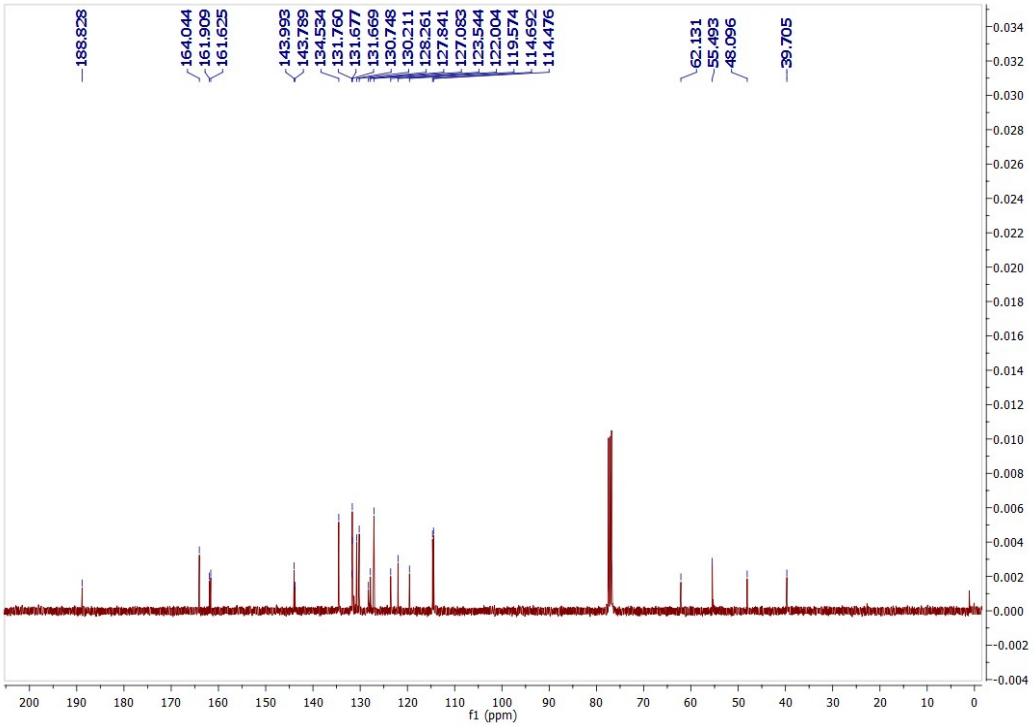
Scanned copies of ^{1}H and ^{13}C NMR spectra:

Scanned copies of ^{1}H and ^{13}C NMR spectra of representative compounds *viz.* **12b**, **12g**, **13b**, **13d**, **13g**, **14b**, **15b.**

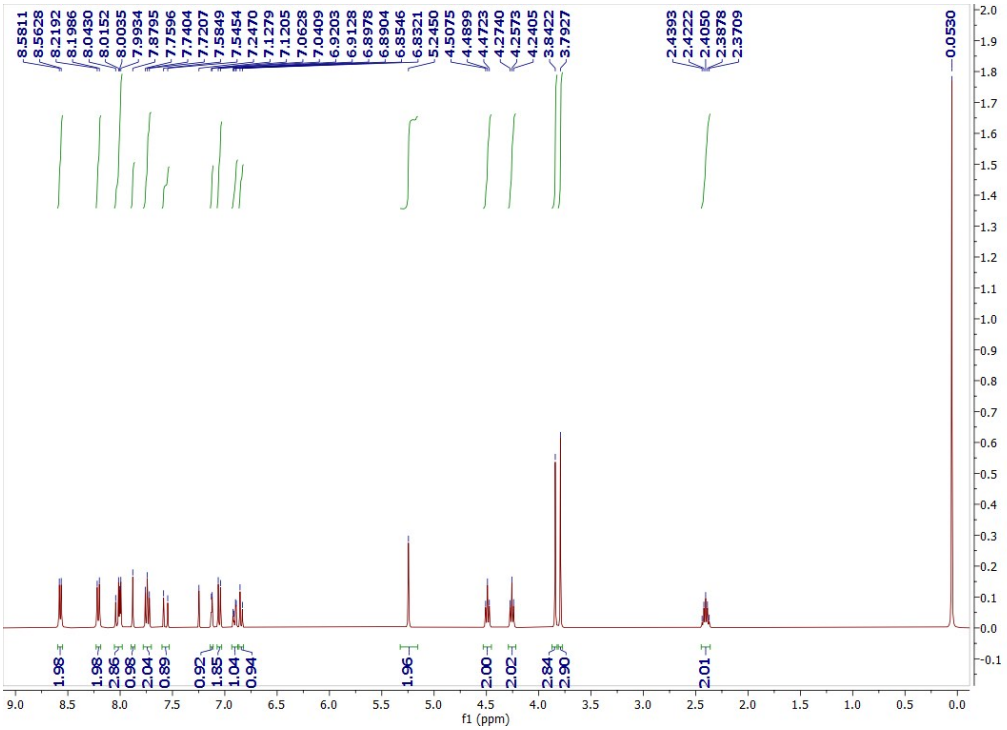
^{1}H NMR of (E)-2-(2-(4-((4-(3-(4-methoxyphenyl)acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (12b):



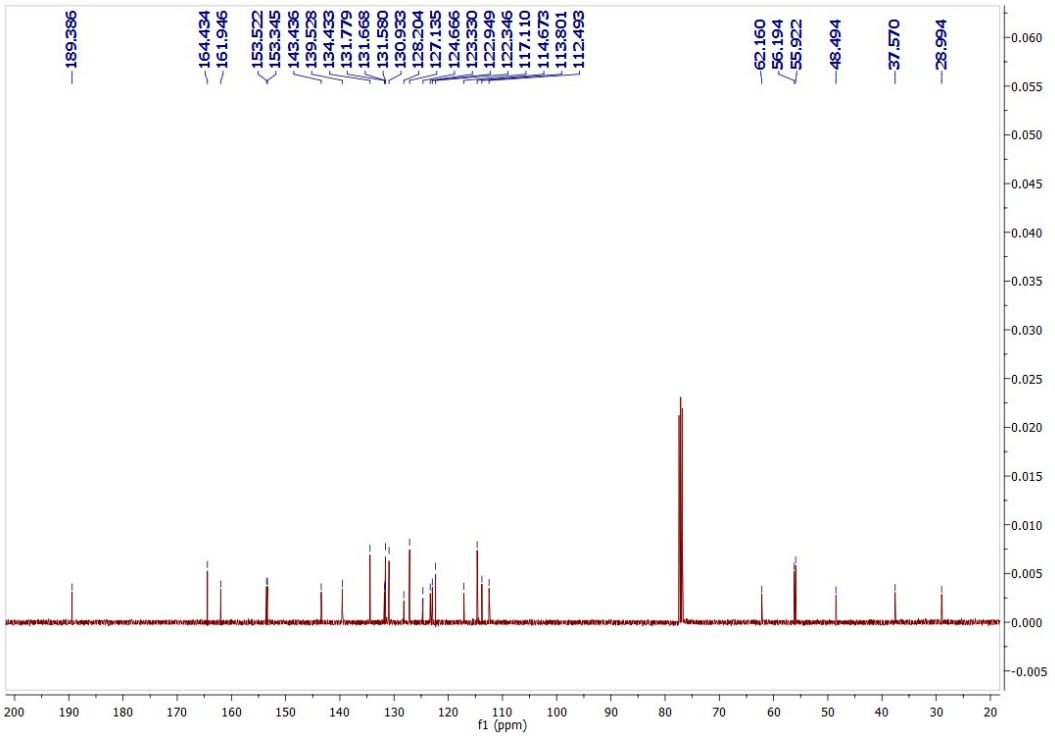
^{13}C NMR of (E)-2-(2-(4-((4-(3-(4-methoxyphenyl)acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (12b):



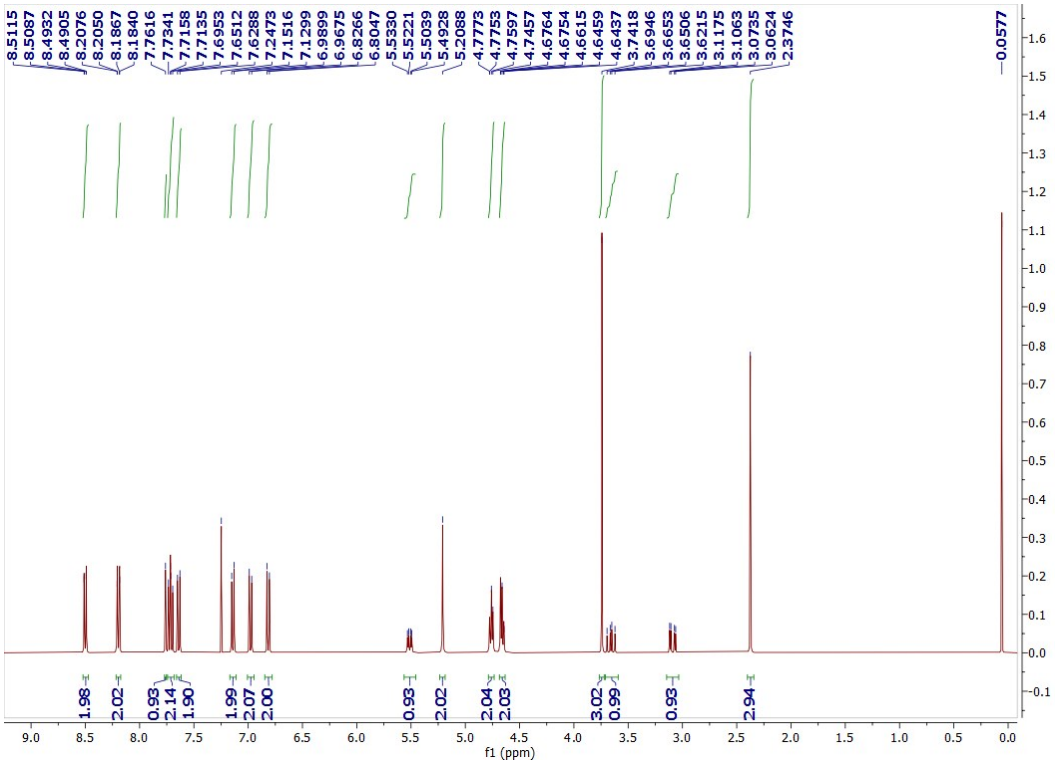
^{1}H NMR of (E)-2-(3-(4-((4-(3-(2,5-dimethoxyphenyl)acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (12g):



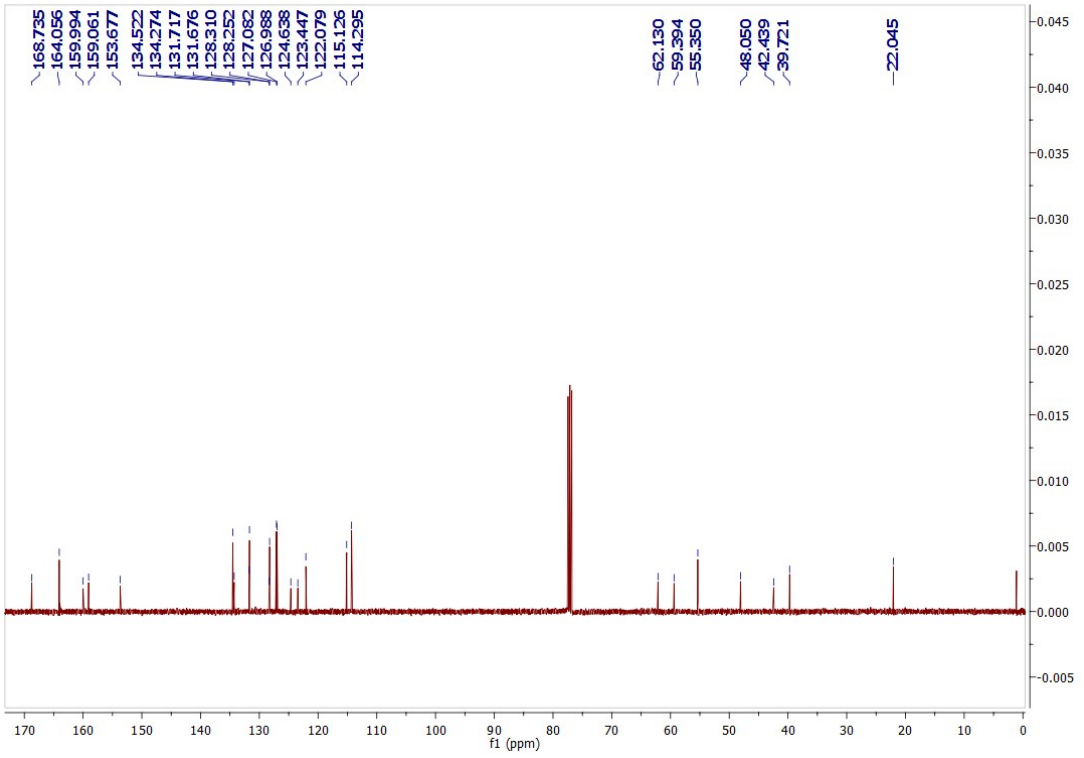
^{13}C NMR of (E)-2-(3-(4-((4-(3-(2,5-dimethoxyphenyl)acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (12g):



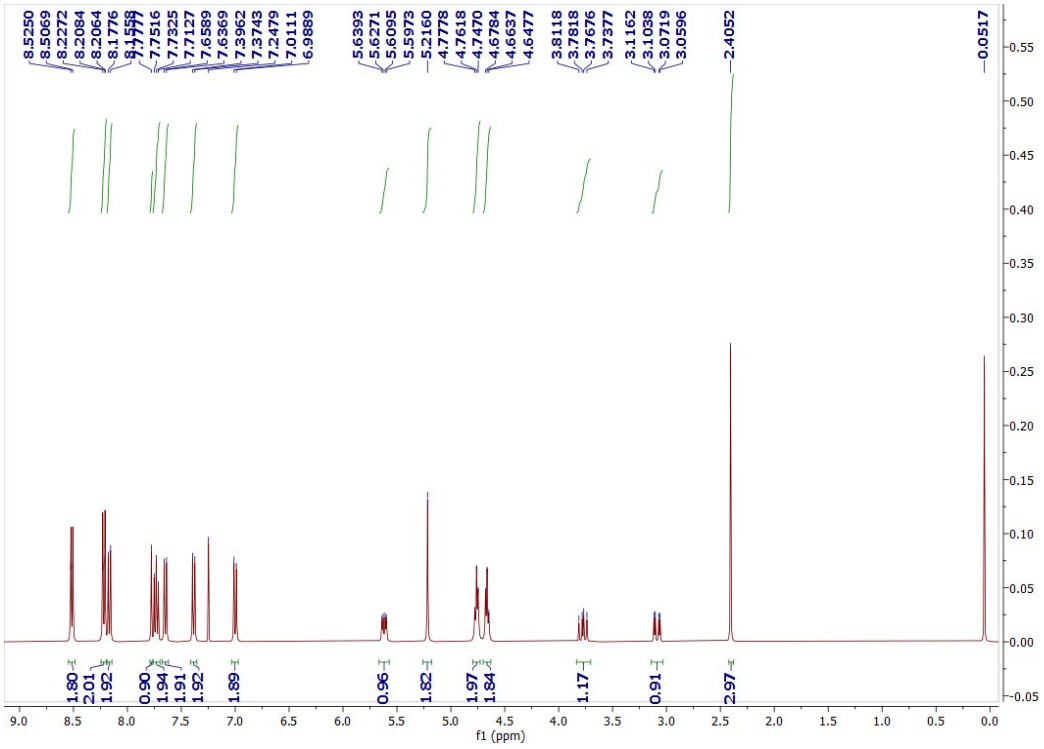
^{1}H NMR of 2-(2-(4-((4-(1-acetyl-5-(4-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13b):



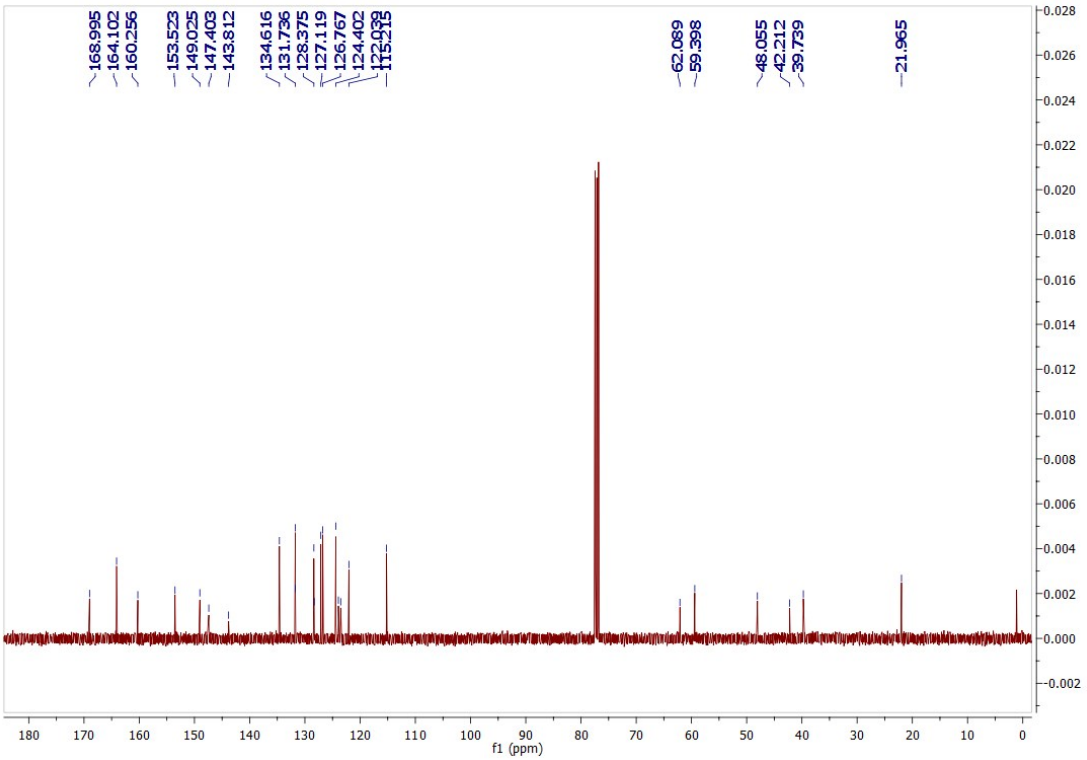
^{13}C NMR of 2-(2-(4-((4-(1-acetyl-5-(4-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13b):



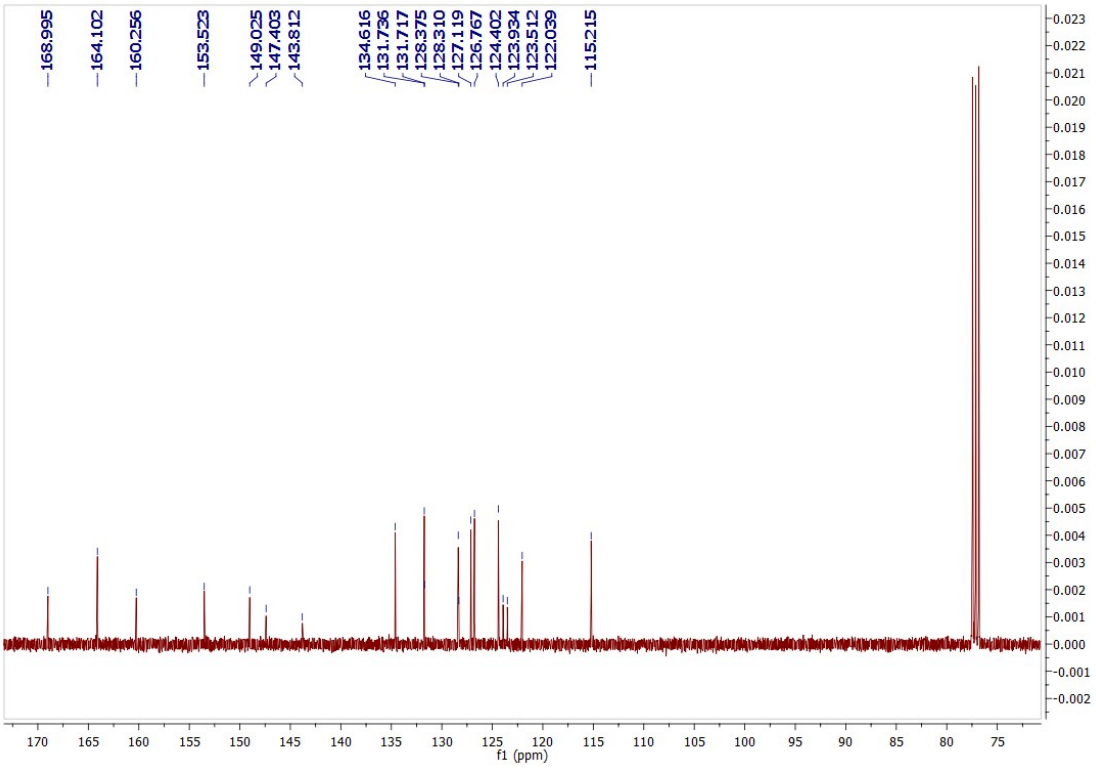
^{1}H NMR of 2-(2-(4-((4-(1-acetyl-5-(4-nitrophenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13d):



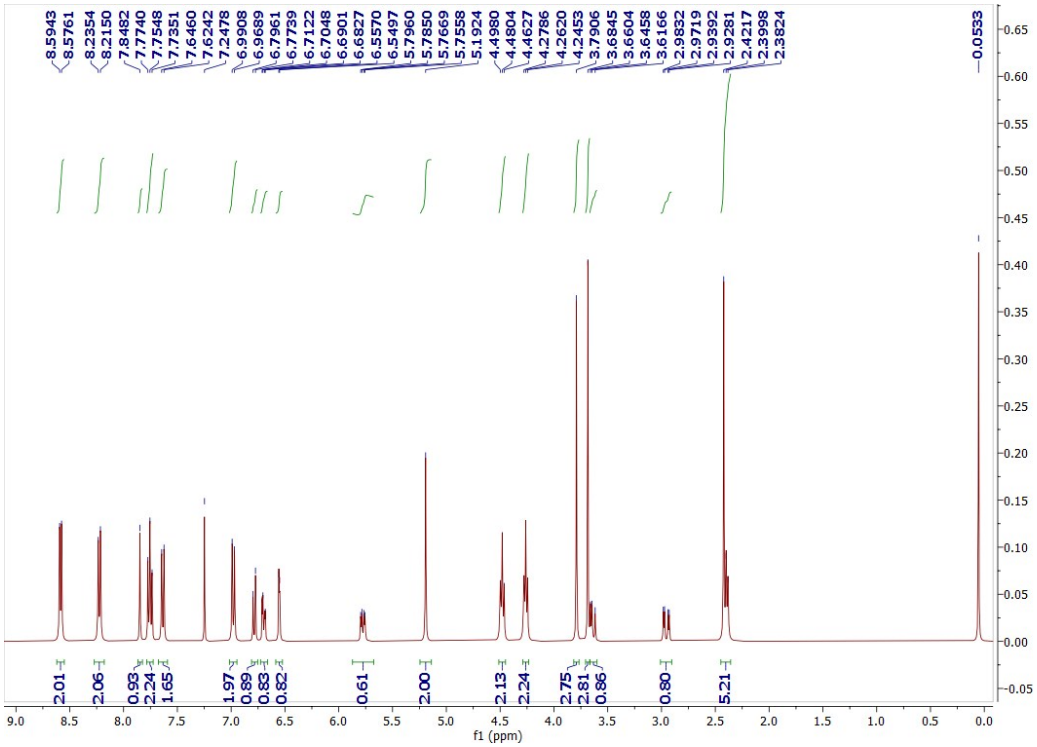
^{13}C NMR of 2-(2-(4-((4-(1-acetyl-5-(4-nitrophenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13d):



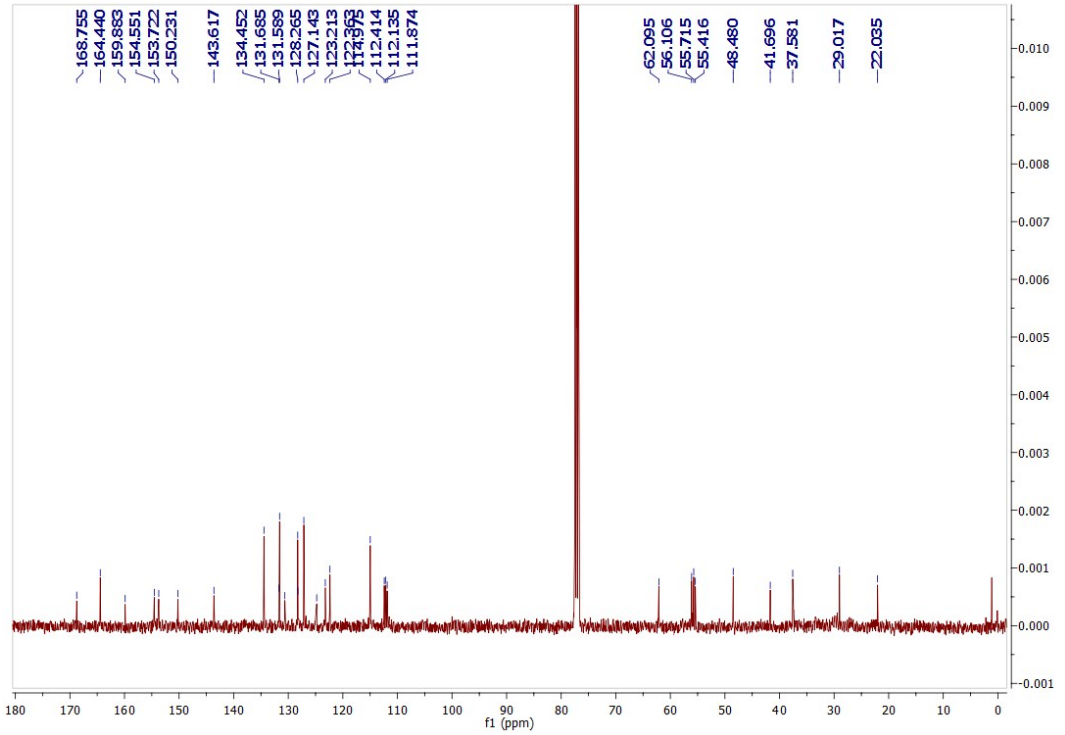
Expanded ^{13}C NMR of 13d:



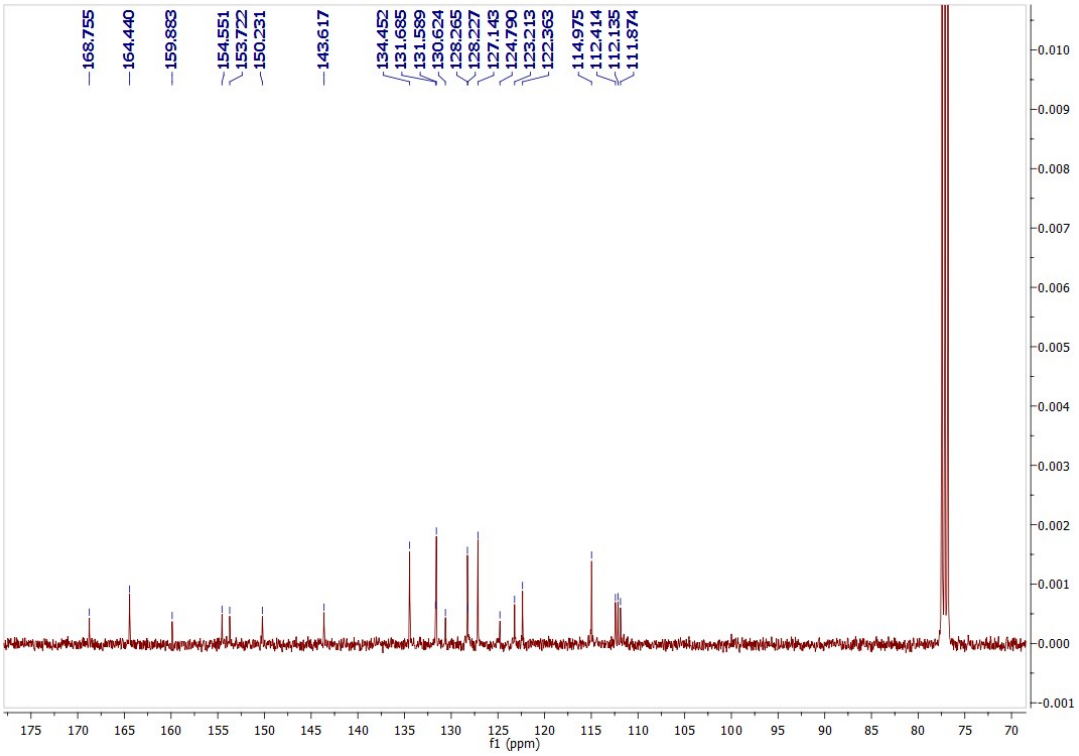
^{1}H NMR of 2-(3-(4-((4-(1-acetyl-5-(2,5-dimethoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13g):



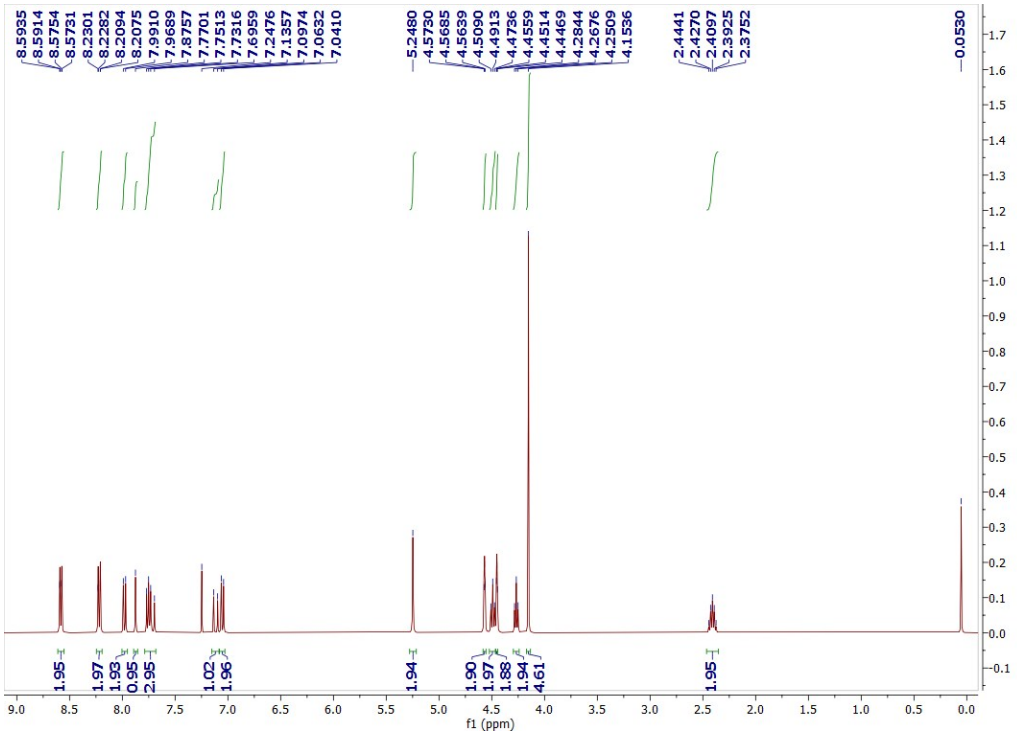
^{13}C NMR of 2-(3-(4-((4-(1-acetyl-5-(2,5-dimethoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (13g):



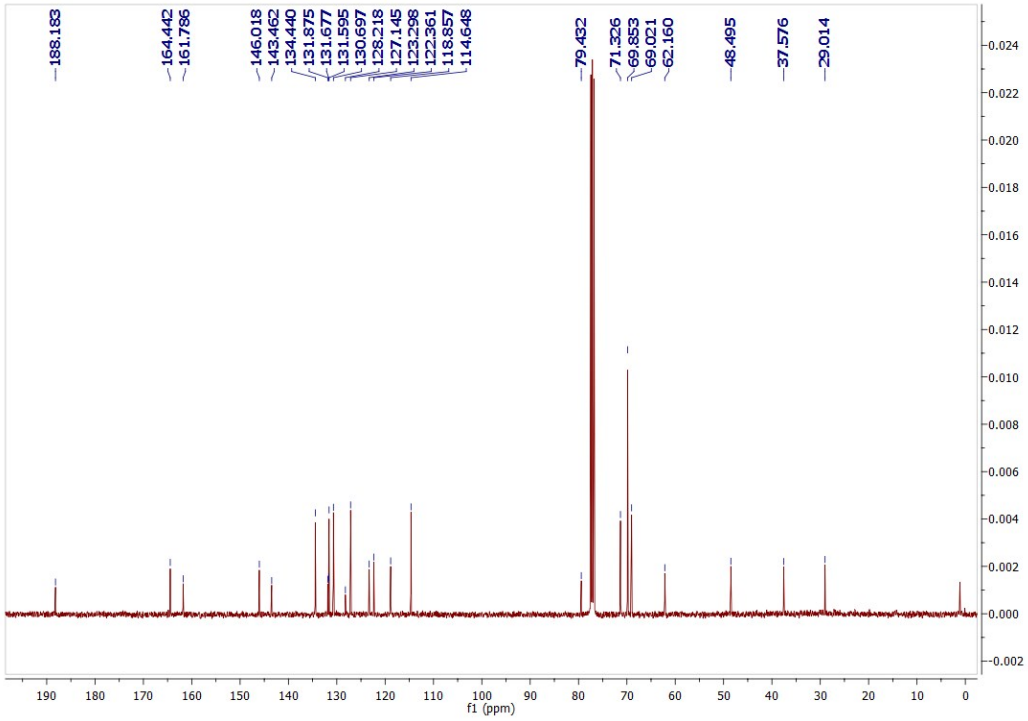
Expanded ^{13}C NMR of 13g:



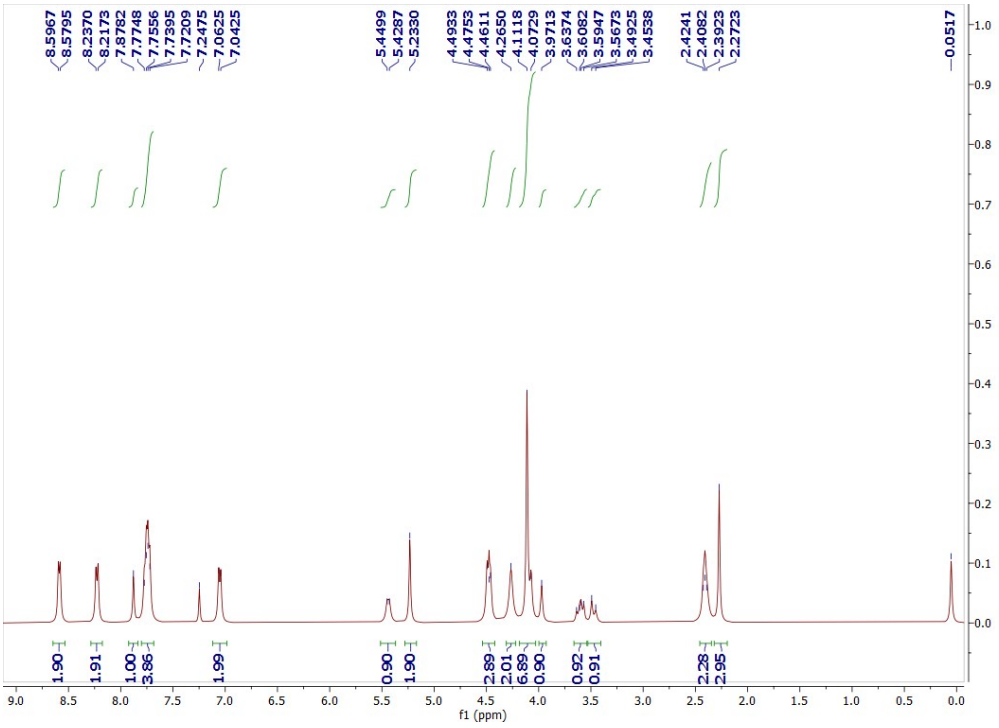
^{1}H NMR of (E)-2-(2-(4-((4-(3-ferrocenyl-acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (14b):



^{13}C NMR of (E)-2-(2-(4-((4-(3-ferrocenyl-acryloyl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (14b):



^{1}H NMR of 2-(2-(4-((4-(1-acetyl-5-ferrocenyl-4,5-dihydro-1H-pyrazol-3-yl)phenoxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (15b):



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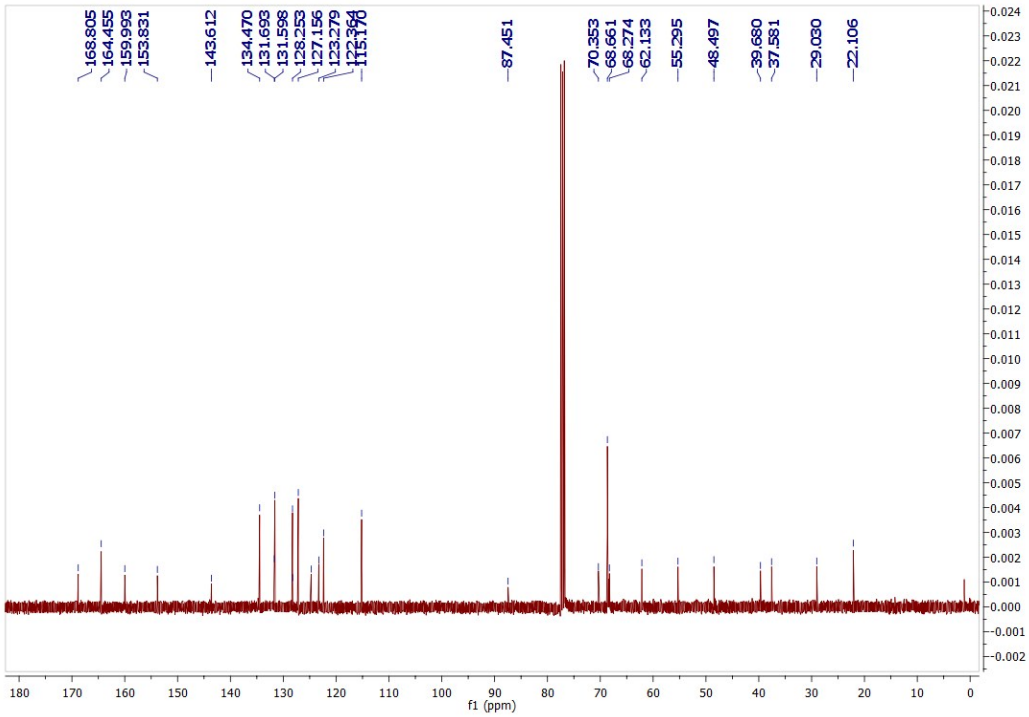

Expanded ^{13}C NMR of 15b: