Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of Novel 10,11-Methylenedioxy-camptothecin Glycoside Derivatives and Investigation of Their Anti-tumor Effects *in Vivo*

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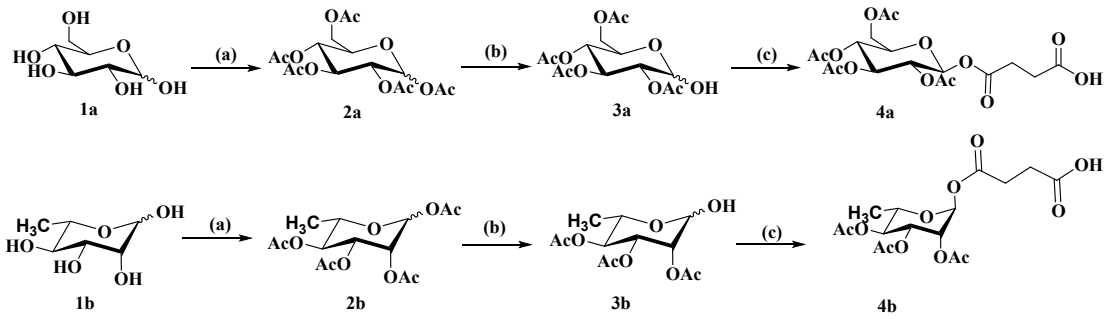
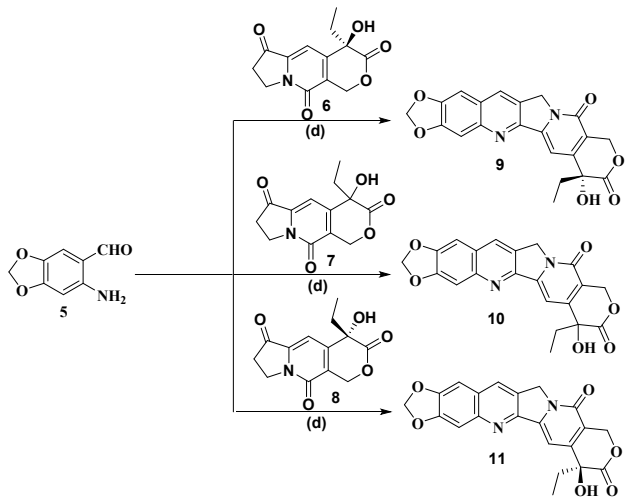
Table S1 Ligand binding free energy for topotecan and FL118 in Top1/DNA complex (PDB code 1K4T) (kcal/mol)

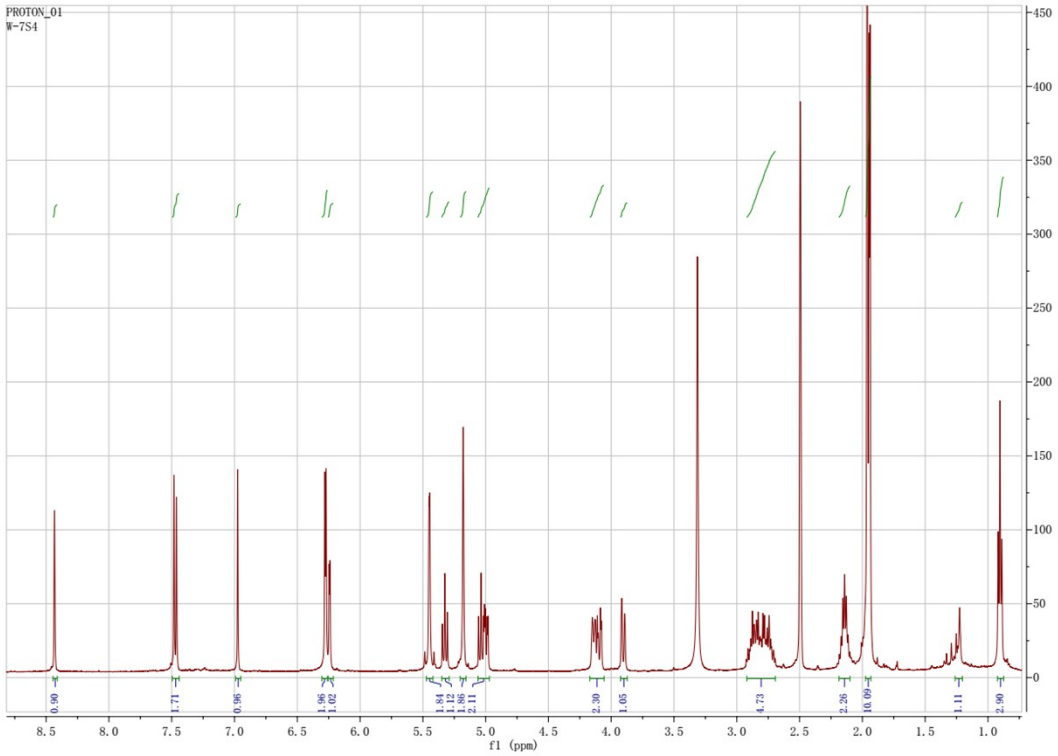
Compound	Top five scored conformation	Ligand binding free energy of 1K4T (kcal/mol)
Topotecan	1	-10.85
	2	-10.01
	3	-9.71
	4	-9.64
	5	-9.59
FL118	1	-9.57
	2	-9.34
	3	-9.17
	4	-9.14
	5	-8.51



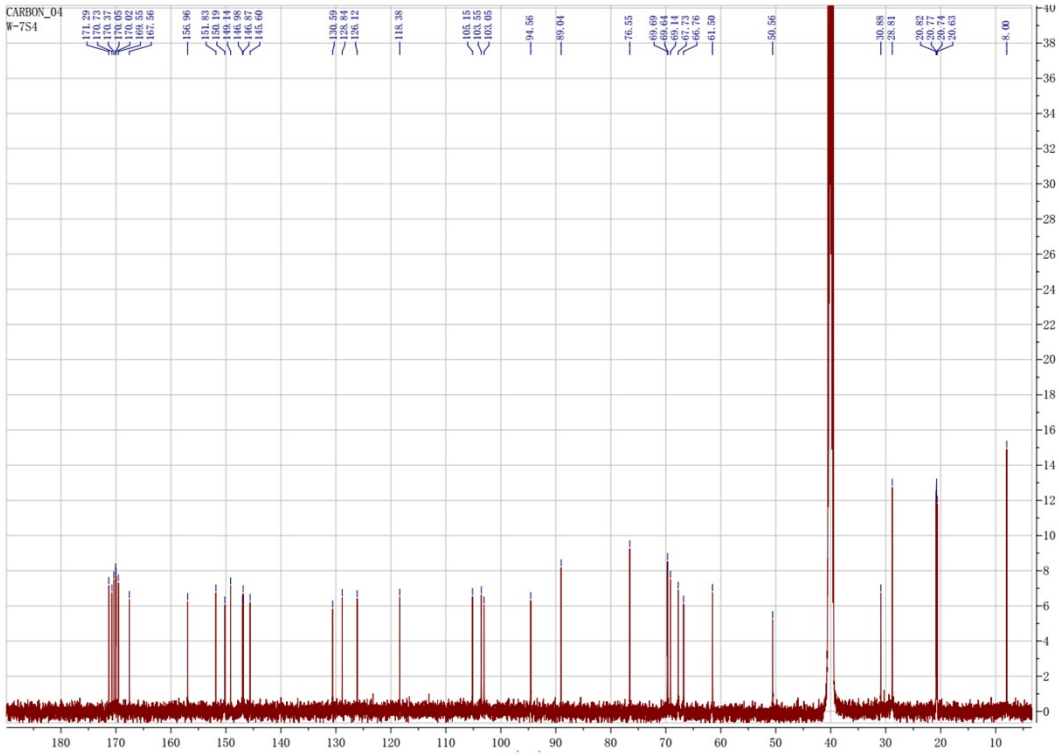
Scheme S1 Synthesis of glycosyl donors. Reagents and conditions: (a) pyridine/Ac_2O, r.t., 12 h; (b) benzylamine, THF, r.t. 12h.



Scheme S2 Synthesis of compounds 9-11. Reagents and conditions: (d) p-TsOH, toluene, reflux, 12h.

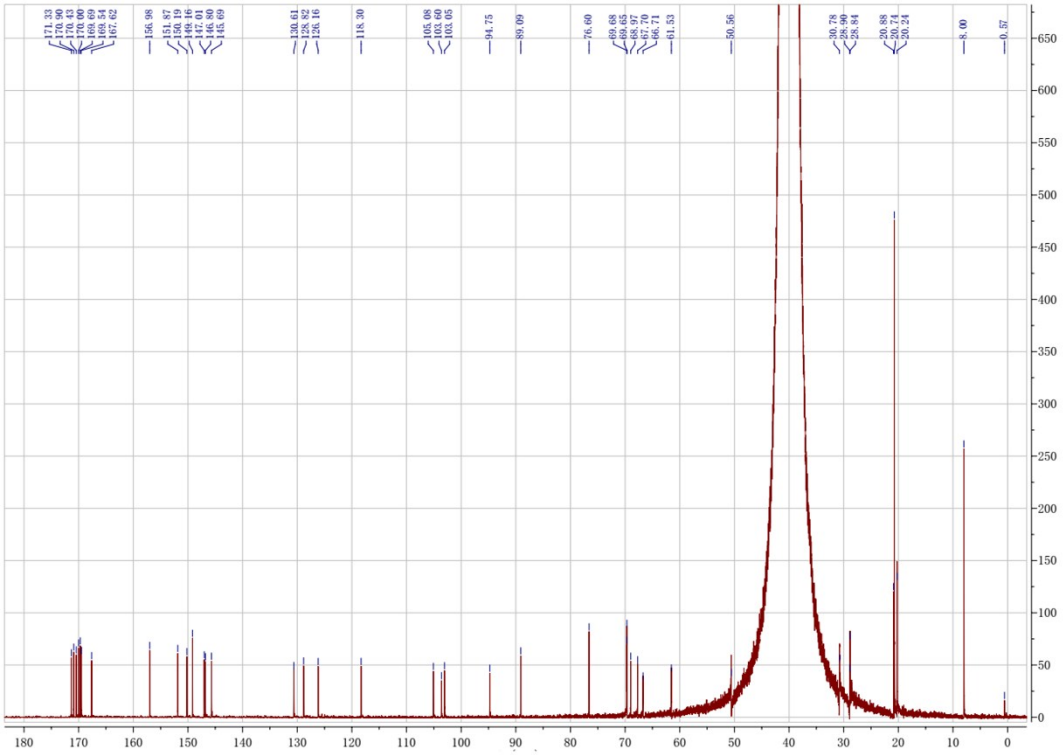


^{1}H NMR of compound **9a**

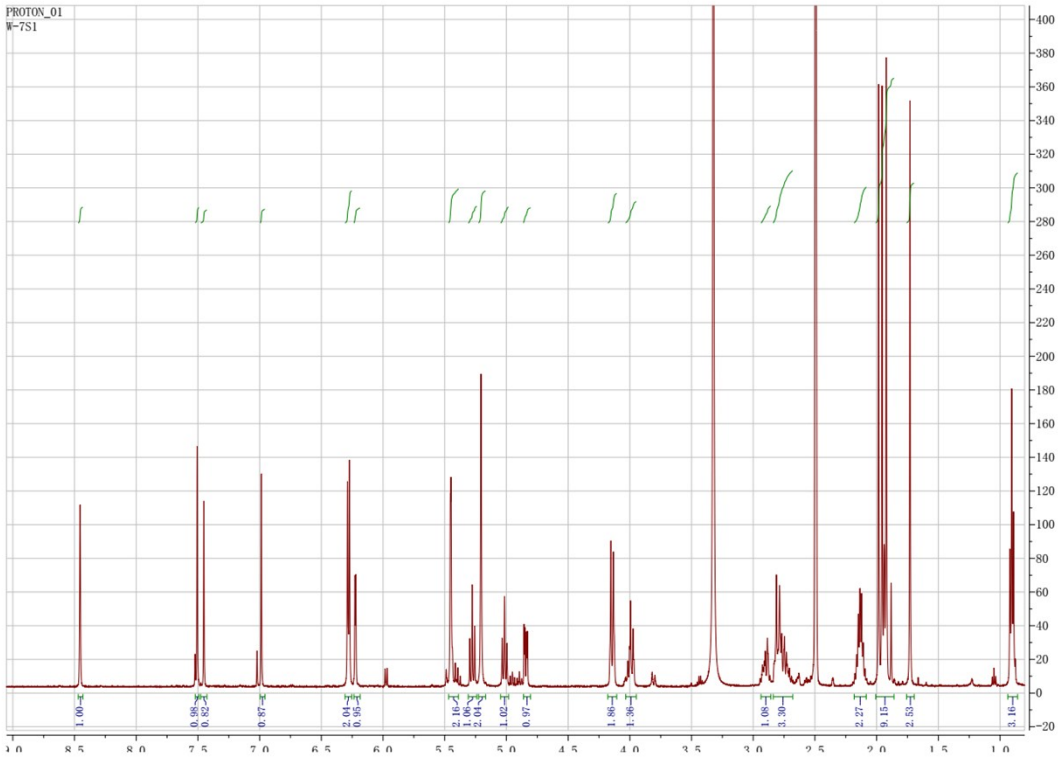


^{13}C NMR of compound **9a**

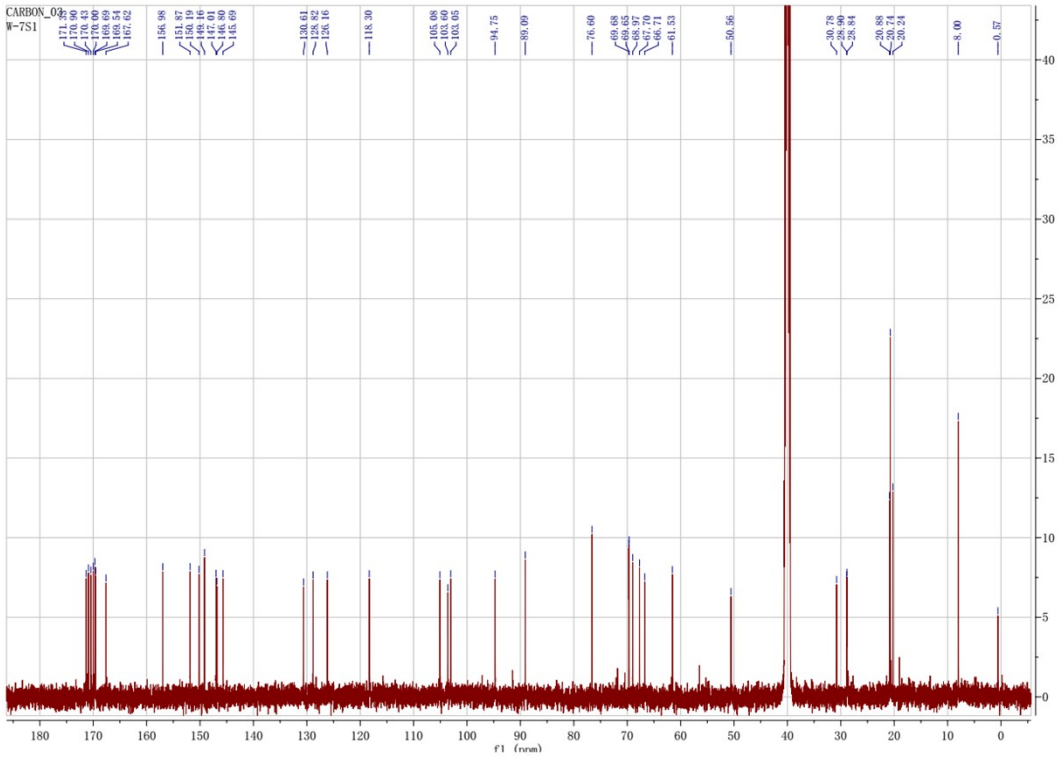
^{1}H NMR of compound **10a**



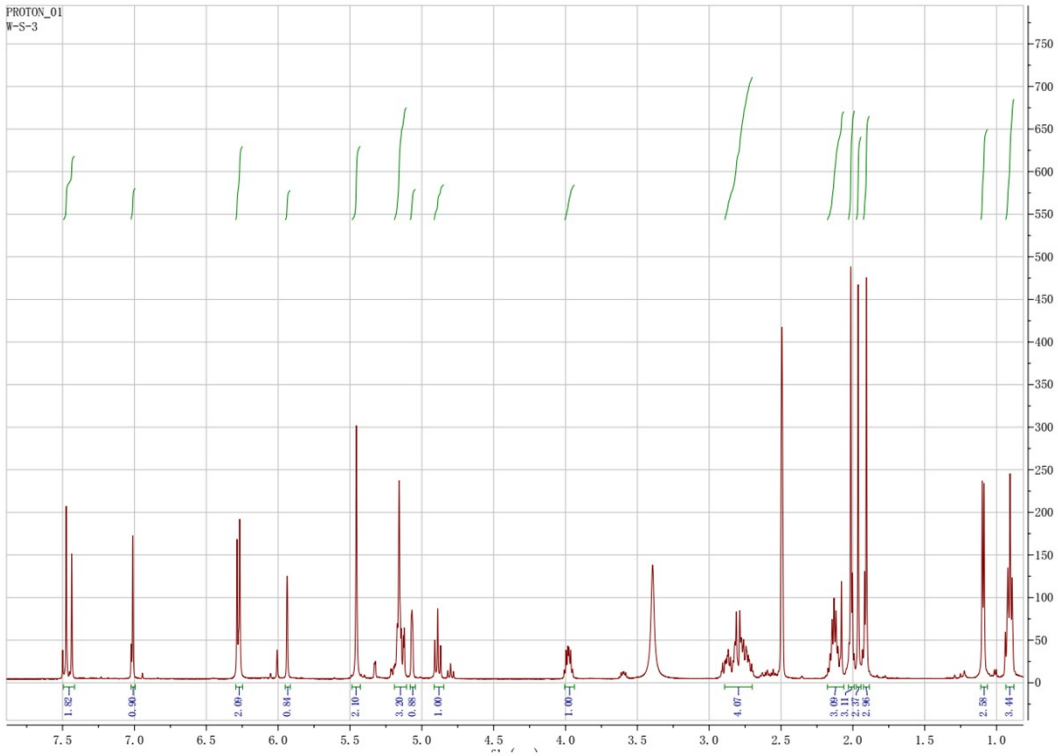
^{13}C NMR of compound **10a**



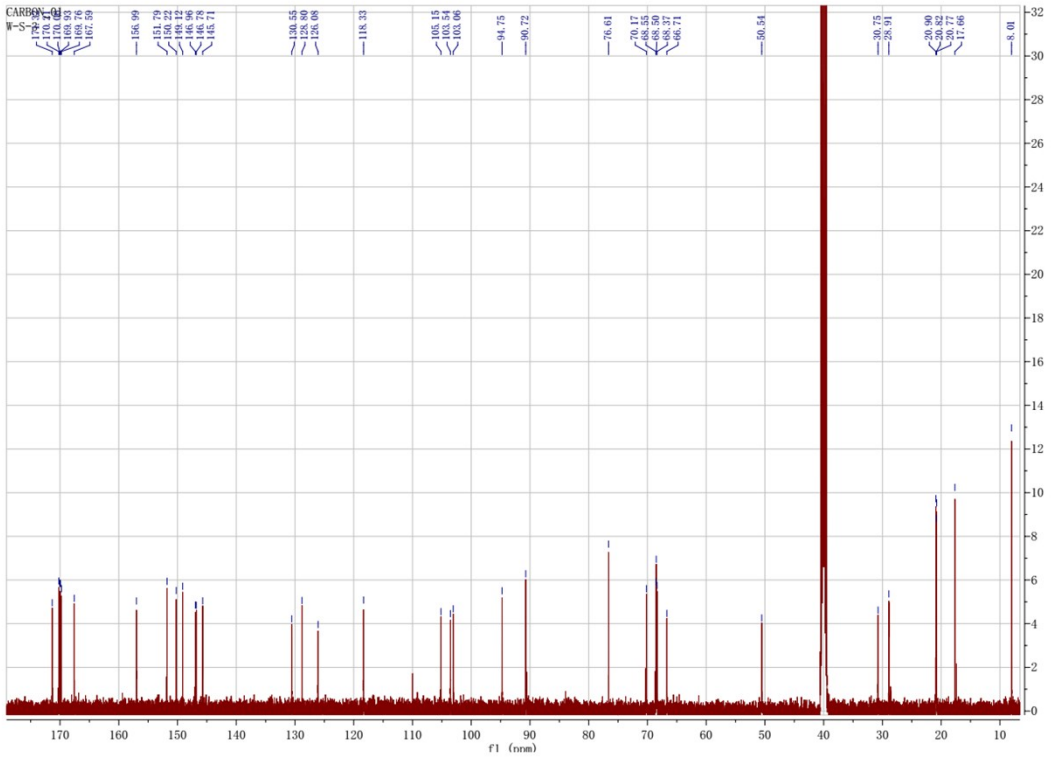
^{1}H NMR of compound **11a**



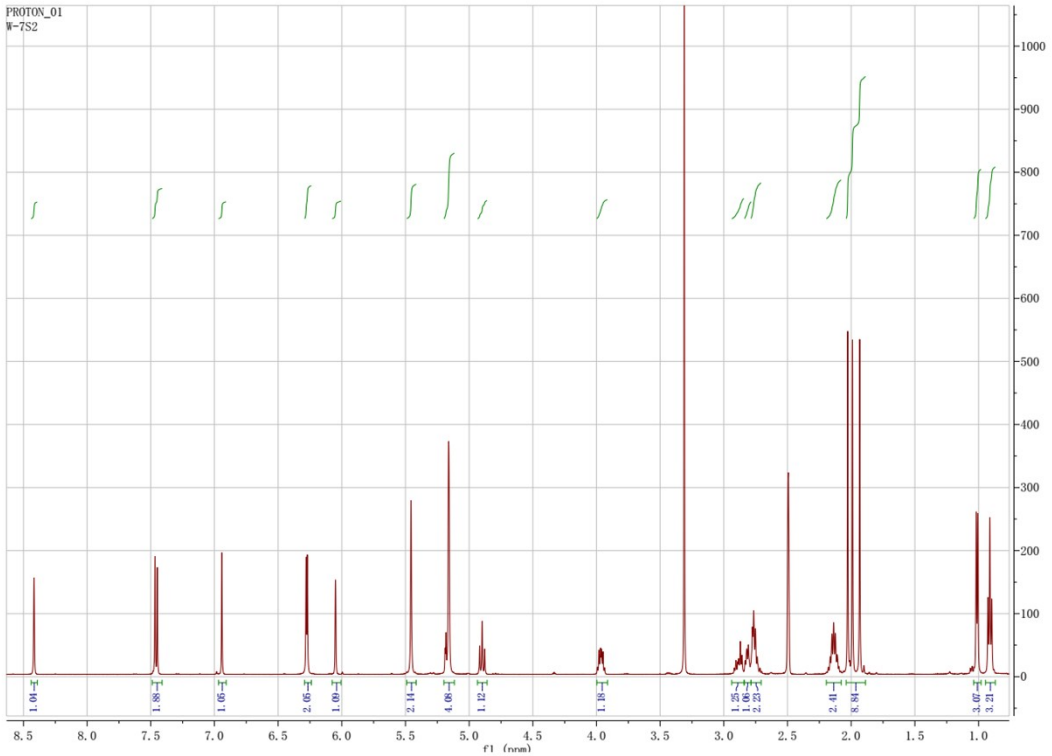
^{13}C NMR of compound **11a**



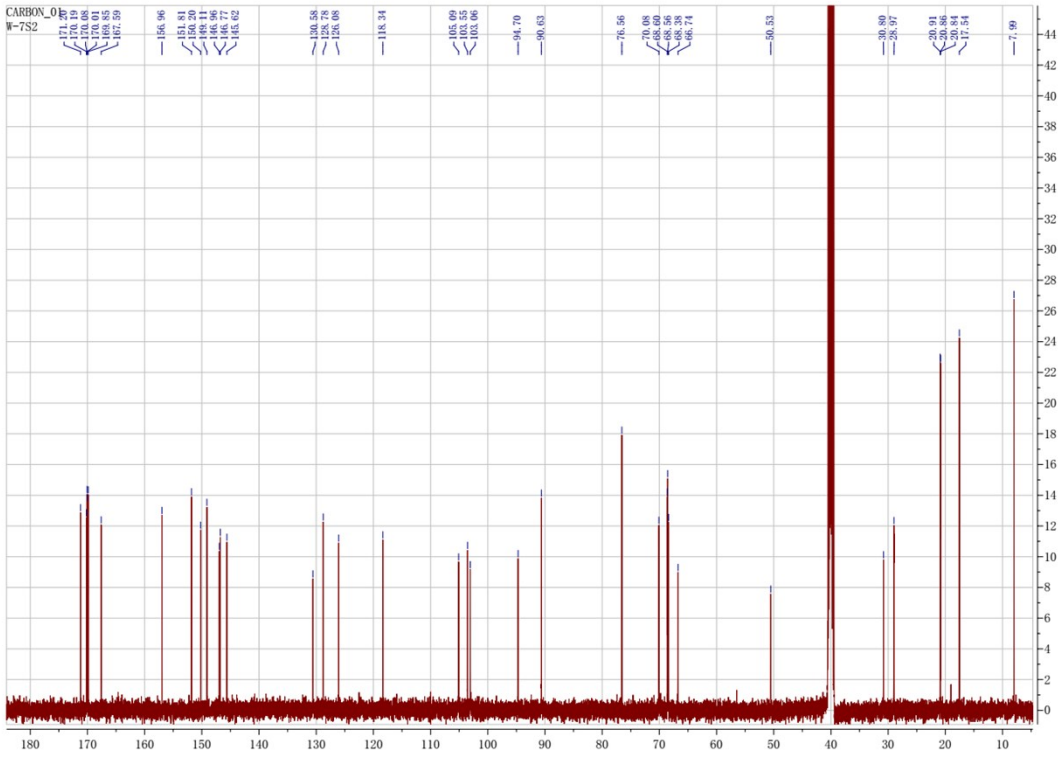
^{1}H NMR of compound **9b**



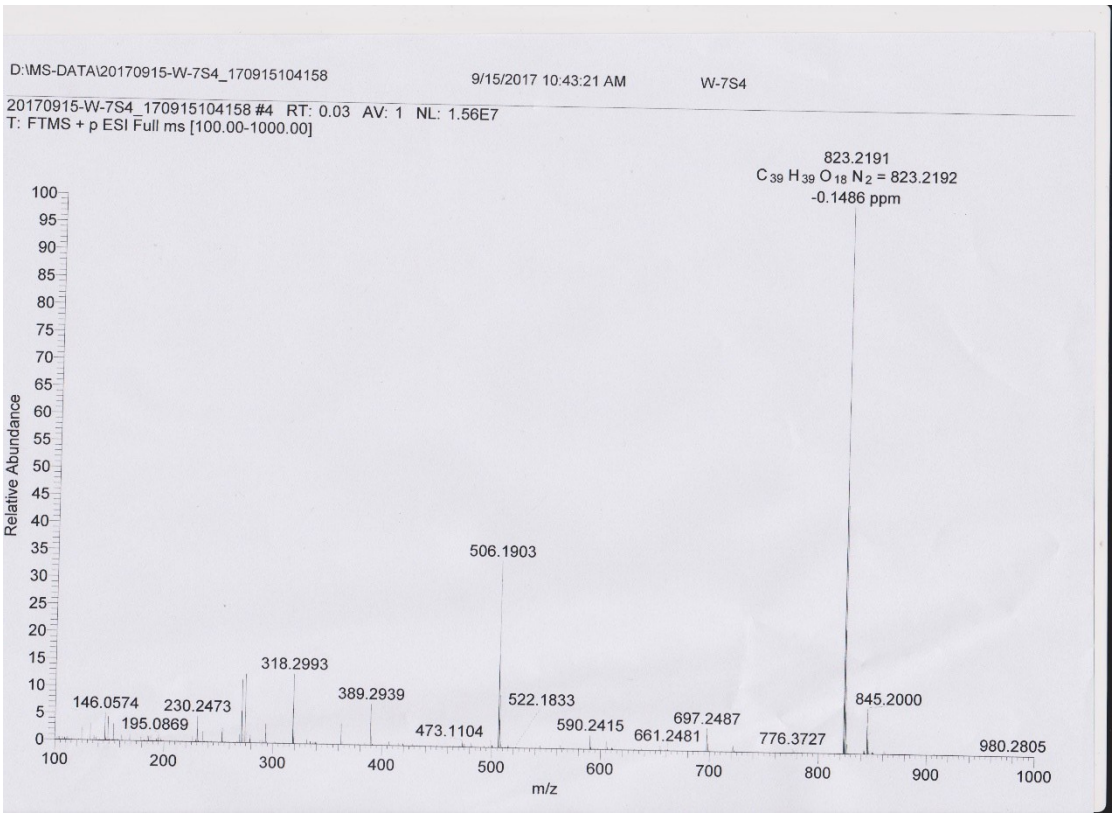
^{13}C NMR of compound **9b**



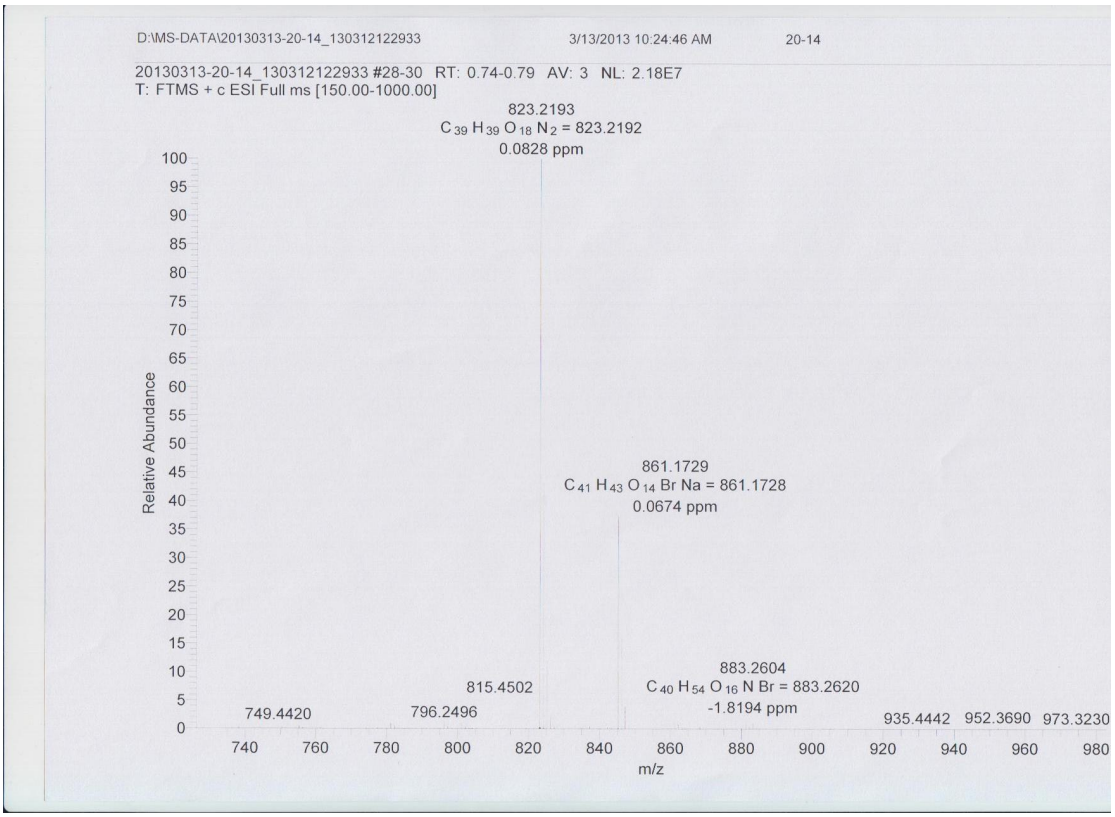
^{1}H NMR of compound **11b**



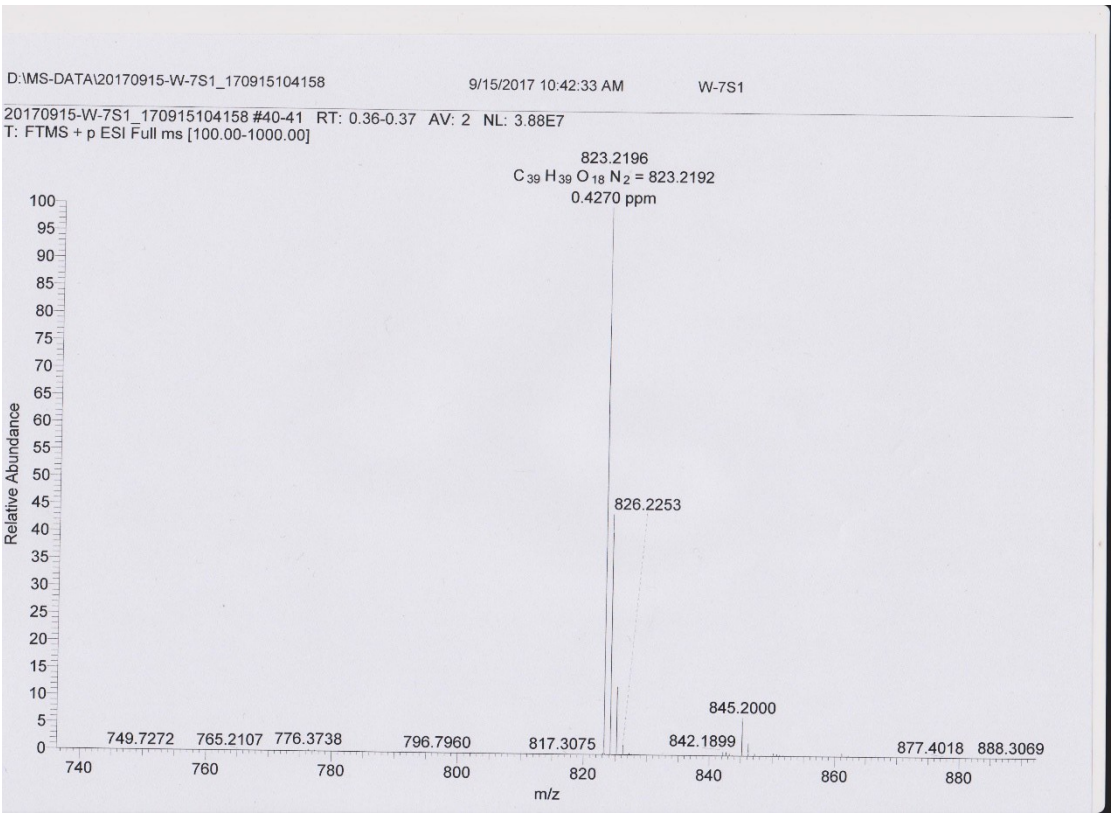
^{13}C NMR of compound **11b**



HRMS of compound **9a**



HRMS of compound **10a**



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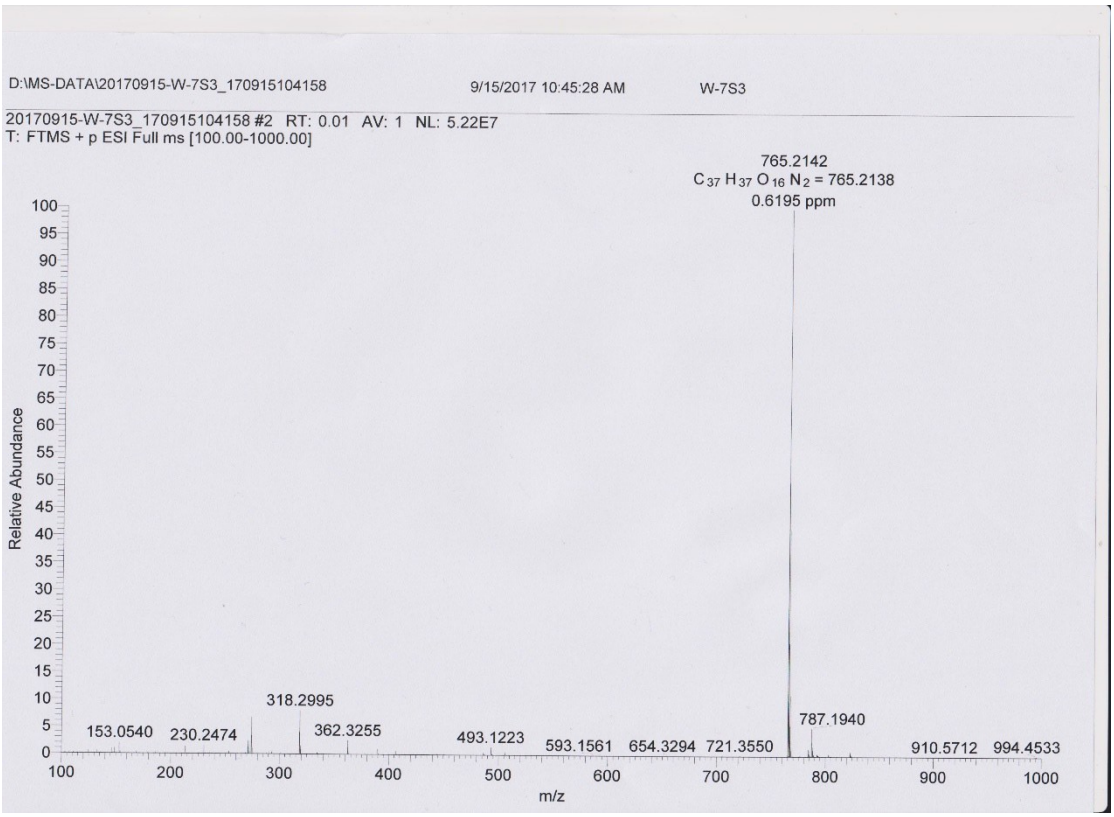
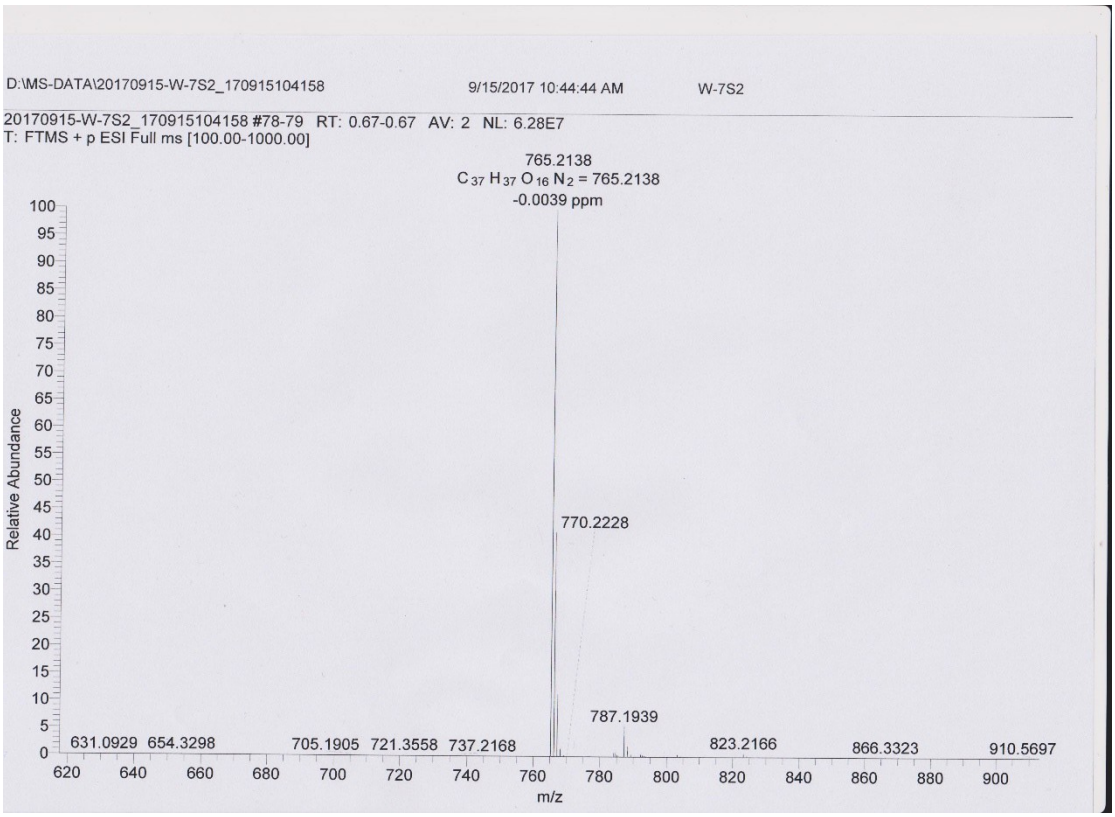
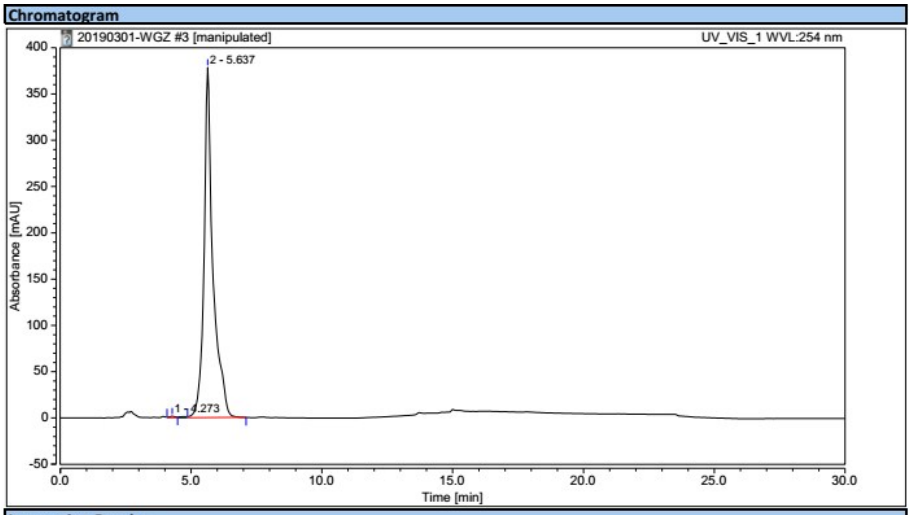


HRMS of compound **9b**



HRMS of compound **11b**

Method: MeOH, flow rate = 1 mL/min, Agilent Eclipse Plus-C18 4.6*250 mm, 5 μm, temp 25 deg, wavelength 254 nm.



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.273	0.452	1.684	0.30	0.44	n.a.
2		5.637	150.931	378.270	99.70	99.56	n.a.
Total:			**151.383**	**379.953**	**100.00**	**100.00**	

Fig. S1 HPLC analysis of compound **11b**

Compound **11b:** Ret time: 5.637 min, Purity 99.56%.