Supporting Information

Novel per-butyrylated glucoses derivatives of (-)-epigallocatechin-3-gallate inhibit cancer cells proliferation by decreasing phosphorylation of the EGFR: Synthesis, cytotoxicity and molecular docking

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Table S1. The characteristic ^{1}H-NMR and ^{13}C-NMR of compounds **7**–**12**.

Compounds	H-1‴		C-1‴ δ (ppm)	H-1⁗		C-1⁗ δ (ppm)
	δ (ppm)	$J_{1'''\text{-}2'''}$(Hz)		δ (ppm)	$J_{1''''\text{-}2''''}$(Hz)	
7	—	—	—	4.9	9.0	102.7
8	4.7	9.5	107.0	4.5	9.5	107.3
9	—	—	—	4.7	9.0	108.2
10	4.7	9.5	107.0	4.5	9.5	107.8
11	—	—	—	4.9	9.0	102.7
12	4.7	9.5	107.1	4.6	9.5	107.8

Table S2. The energies of the binding between EGFR and compounds **4**, **11** and **12**.

Compd.	(vdW+Hbond+desolv)energy(kcal/mol)	Electrostatic energy (kcal/mol)	Total internal energy (kcal/mol)	The best docking energy (kcal/mol)	Inhibition constant (nM)
4	–7.7	–1.1	–3.8	–5.0	159.2
11	–8.1	–0.4	–10.9	2.4	1754.3
12	–8.4	–0.09	–10.4	1.91	455.5

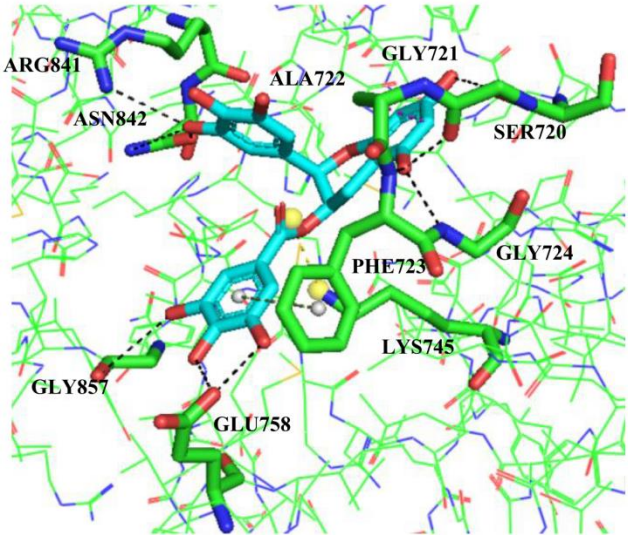

Figure S1. The details of the binding between EGFR and EGCG (**4**): the protein is shown as lines; ligand and the key residues are shown as sticks (ligand color: C cyan, N blue, O red and polar hydrogen); hydrogen bonds are shown as black dotted lines; hydrophobic interactions are shown as red dotted lines; π-stacking is shown as gray dotted lines; salt bridges were shown as yellow dotted lines.

Figure S2. ^{1}H-NMR spectra of compound **6**

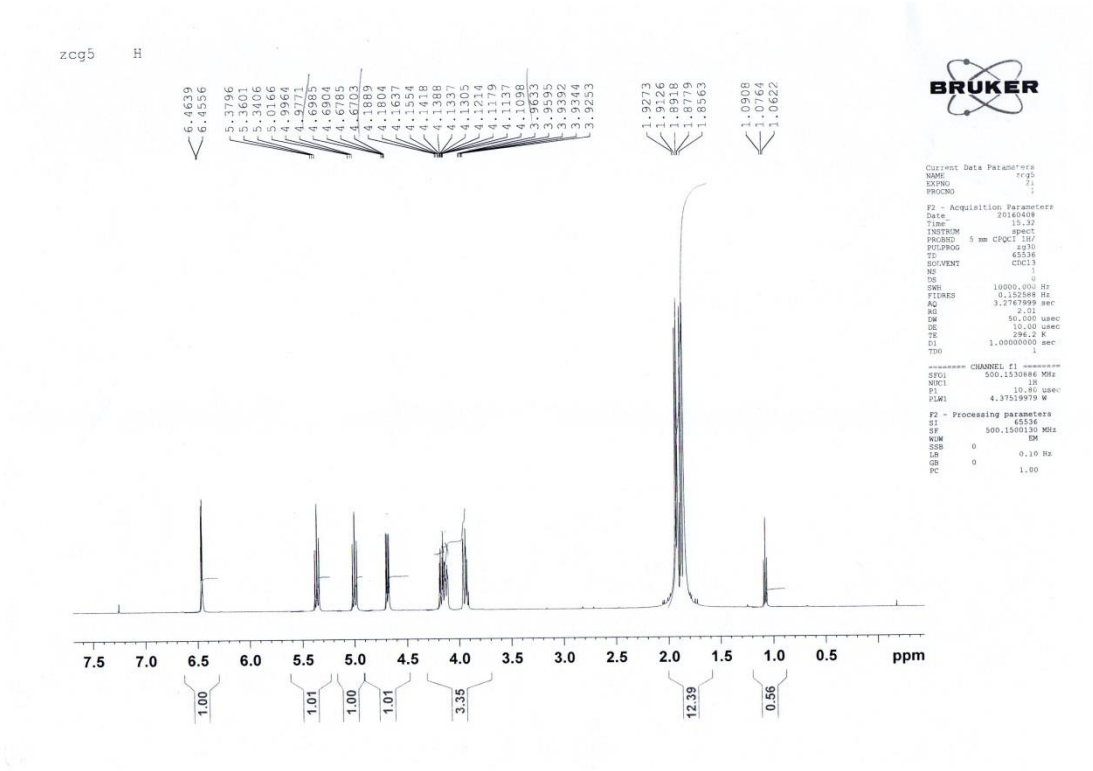

Figure S3. ^{13}C-NMR spectra of compound **6**

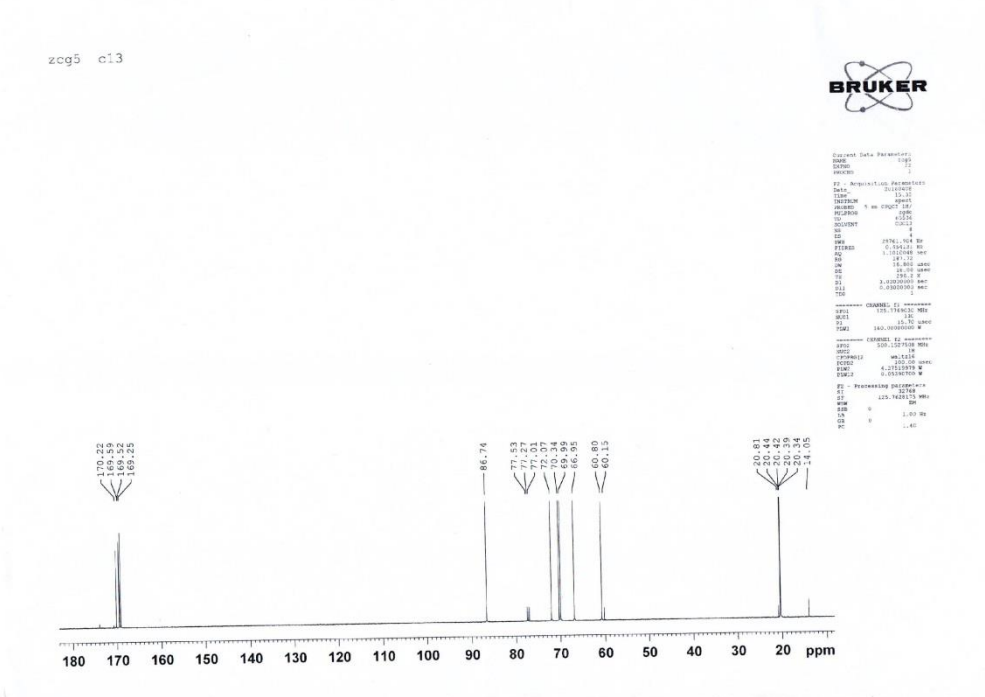

Figure S4. ^{1}H-NMR spectra of compound **7**

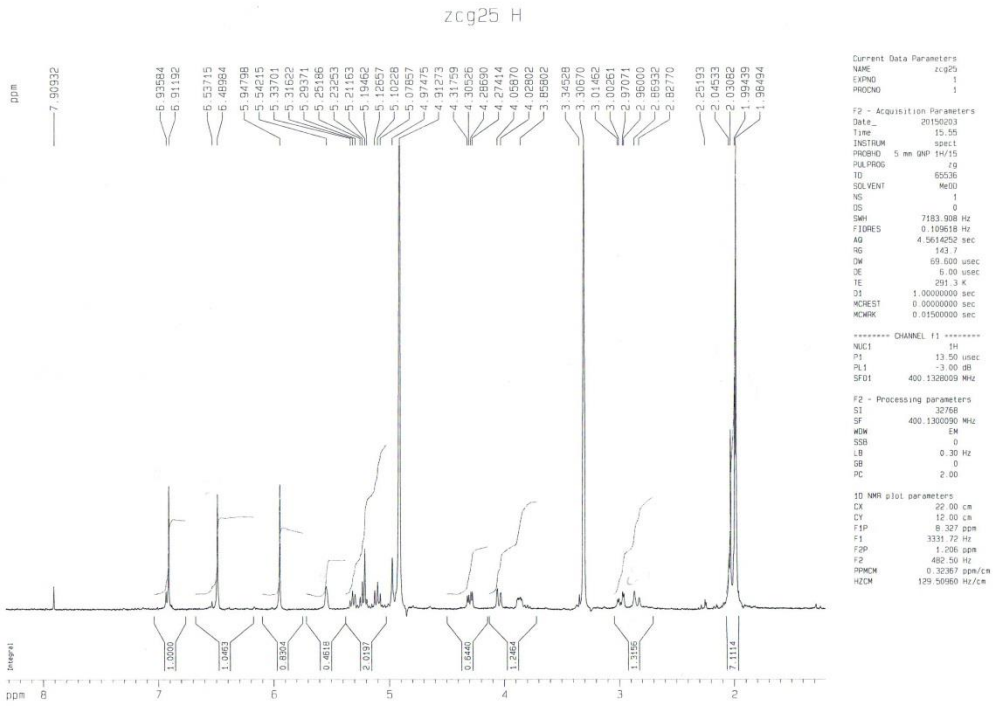

Figure S5. ^{13}C-NMR spectra of compound **7**

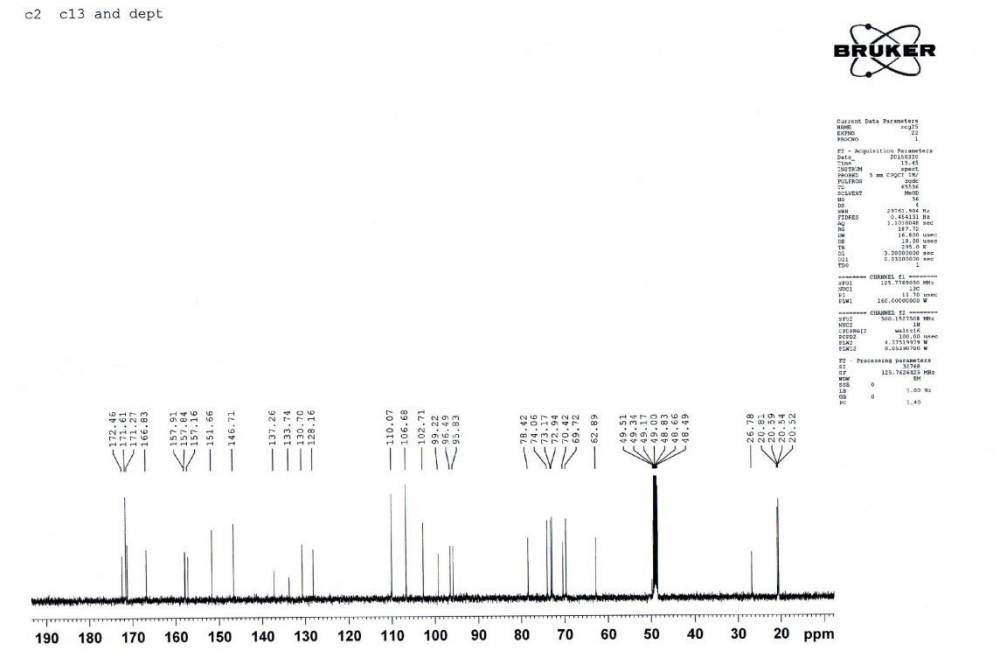

Figure S6. HMBC spectra of compound **7**

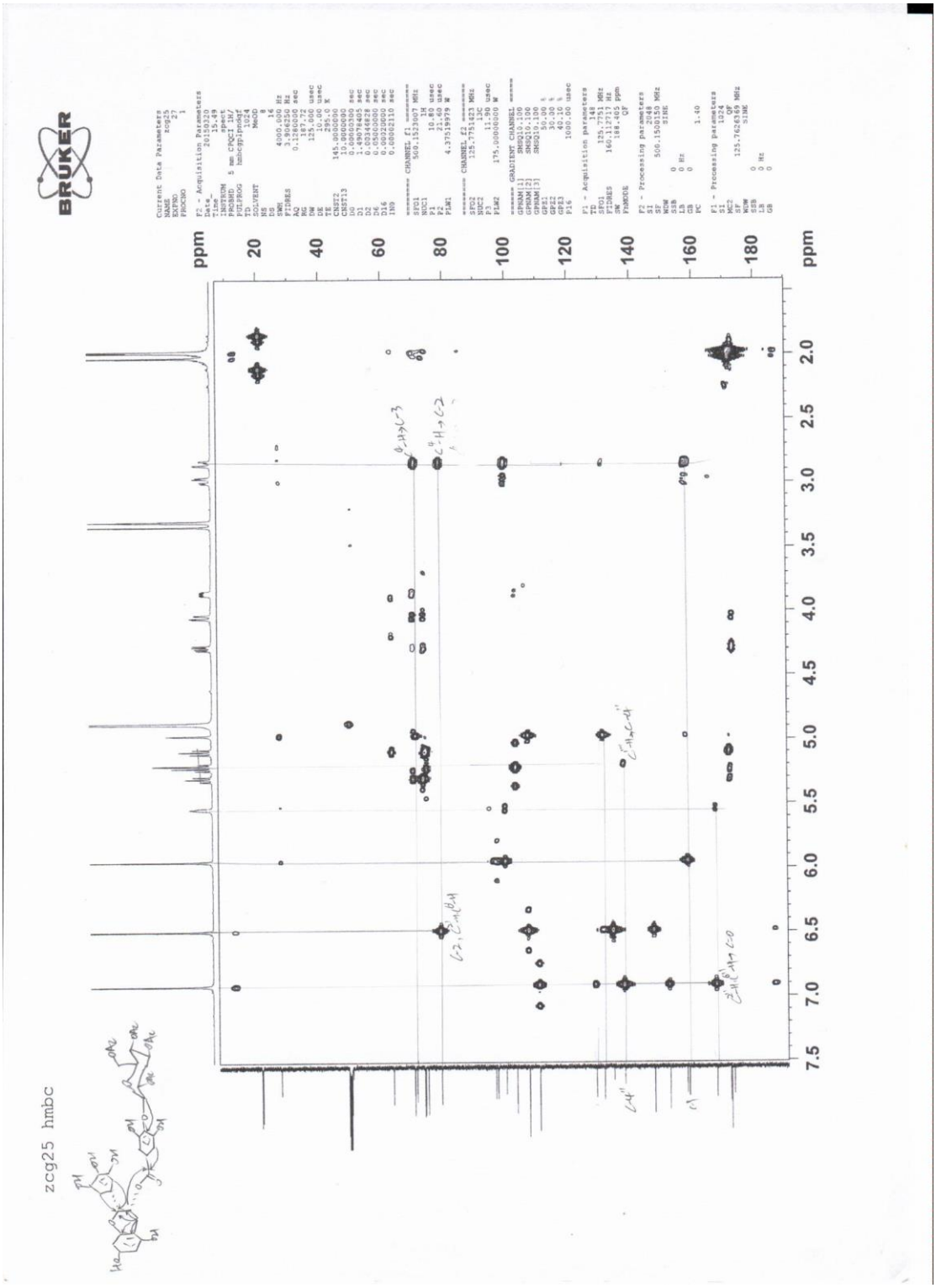

Figure S7. ^{1}H-NMR spectra of compound **8**

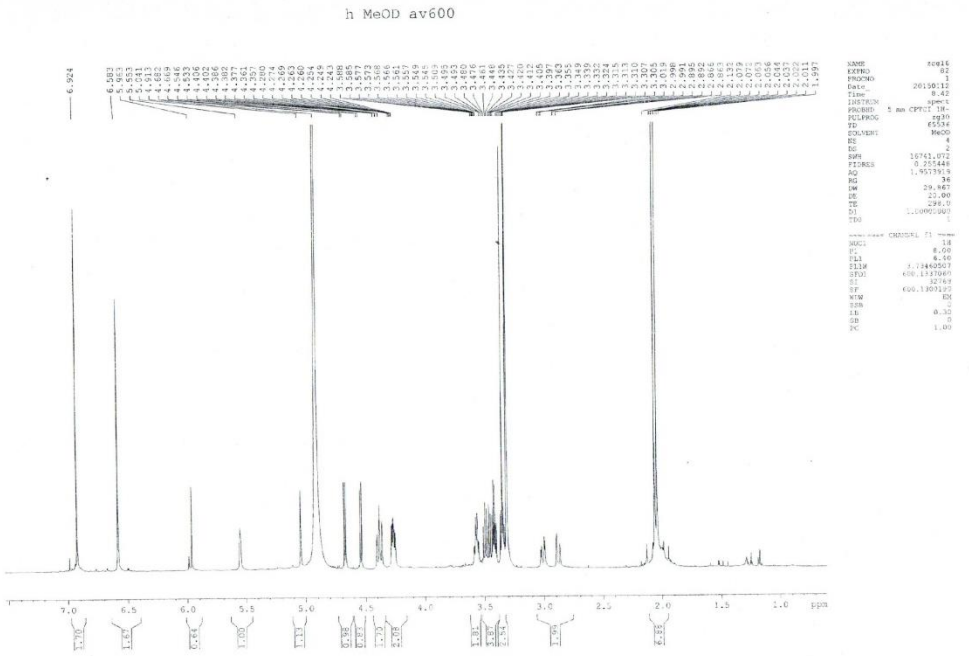

Figure S8. ^{13}C-NMR spectra of compound **8**

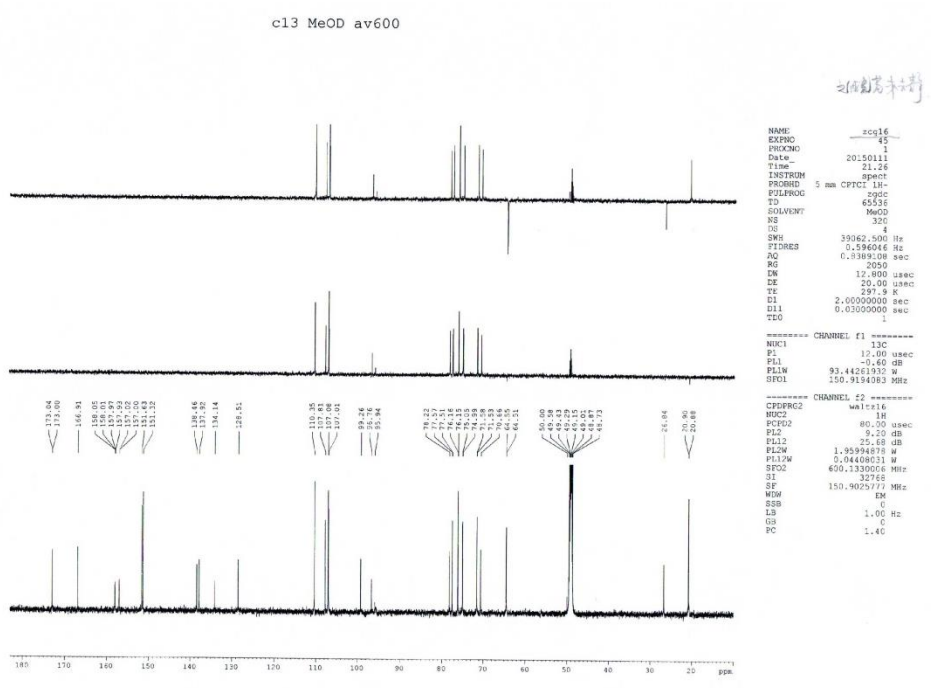

Figure S9. HMBC spectra of compound **8**

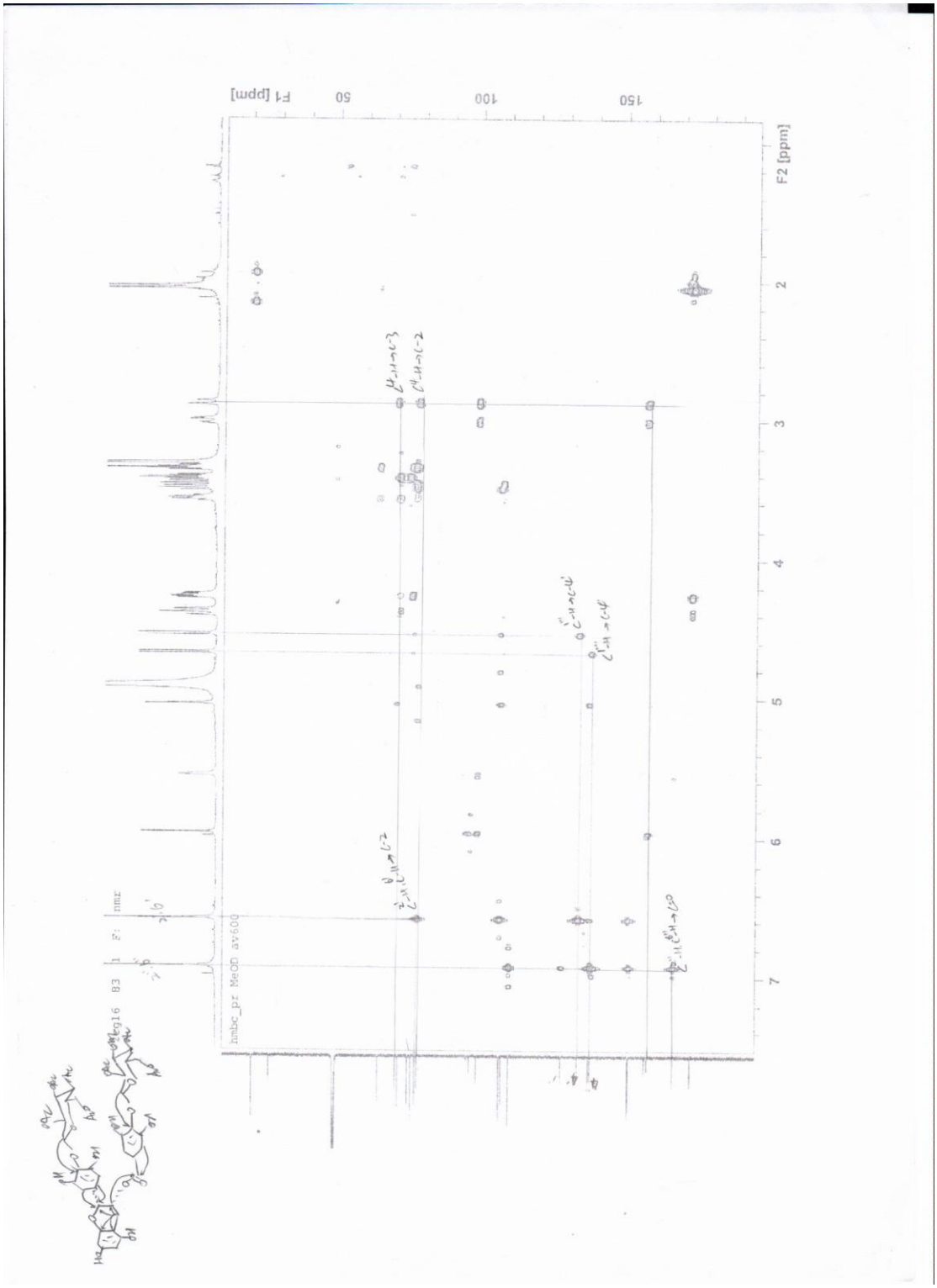

Figure S10. ^{1}H-NMR spectra of compound **9**

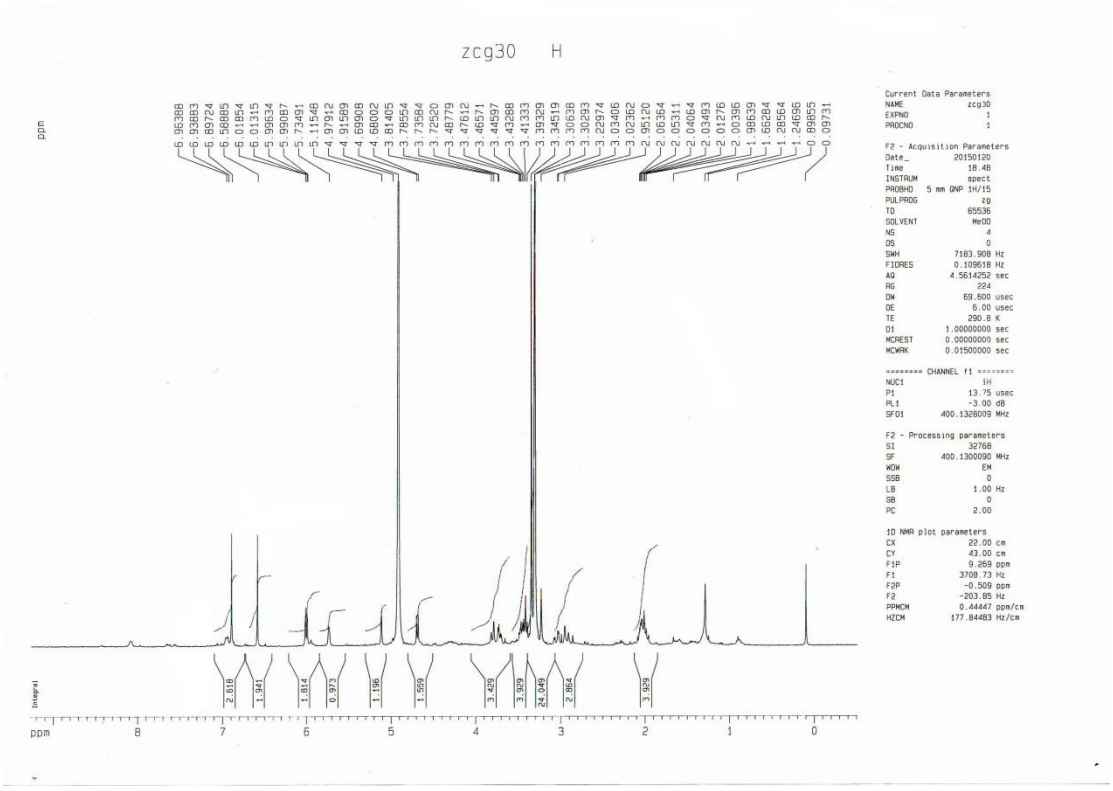

Figure S11. ^{13}C-NMR spectra of compound **9**

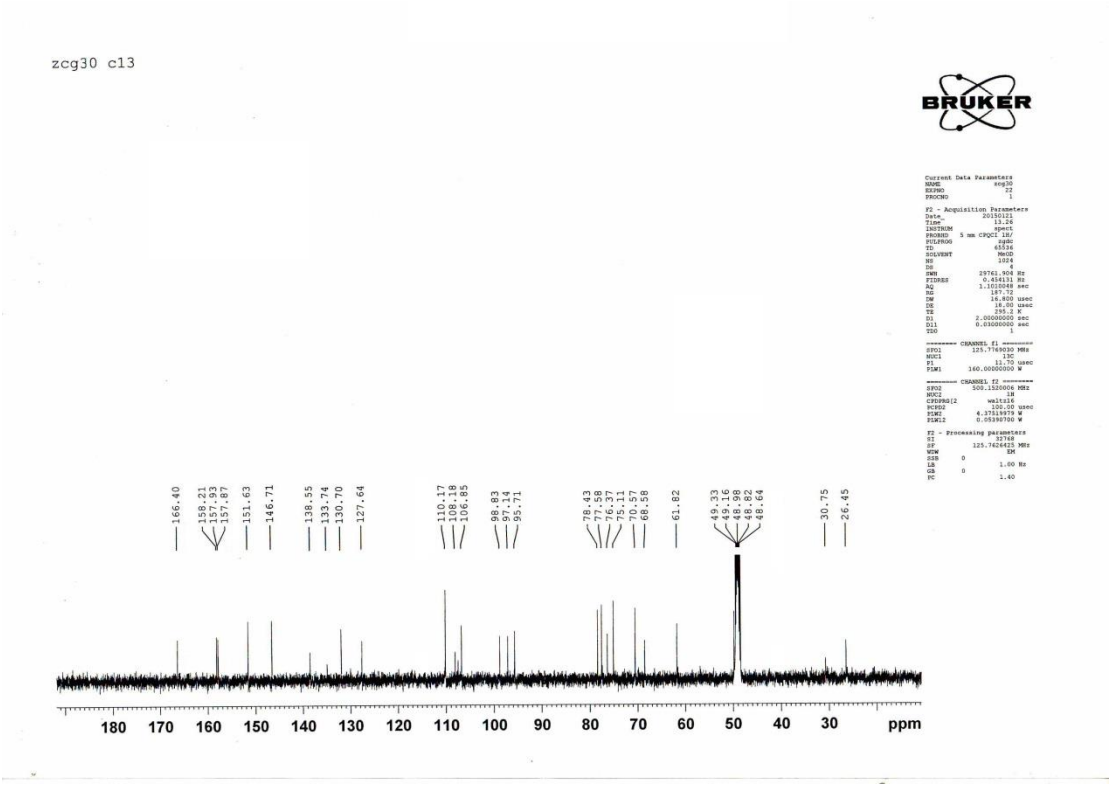

Figure S12. ^{1}H-NMR spectra of compound **10**

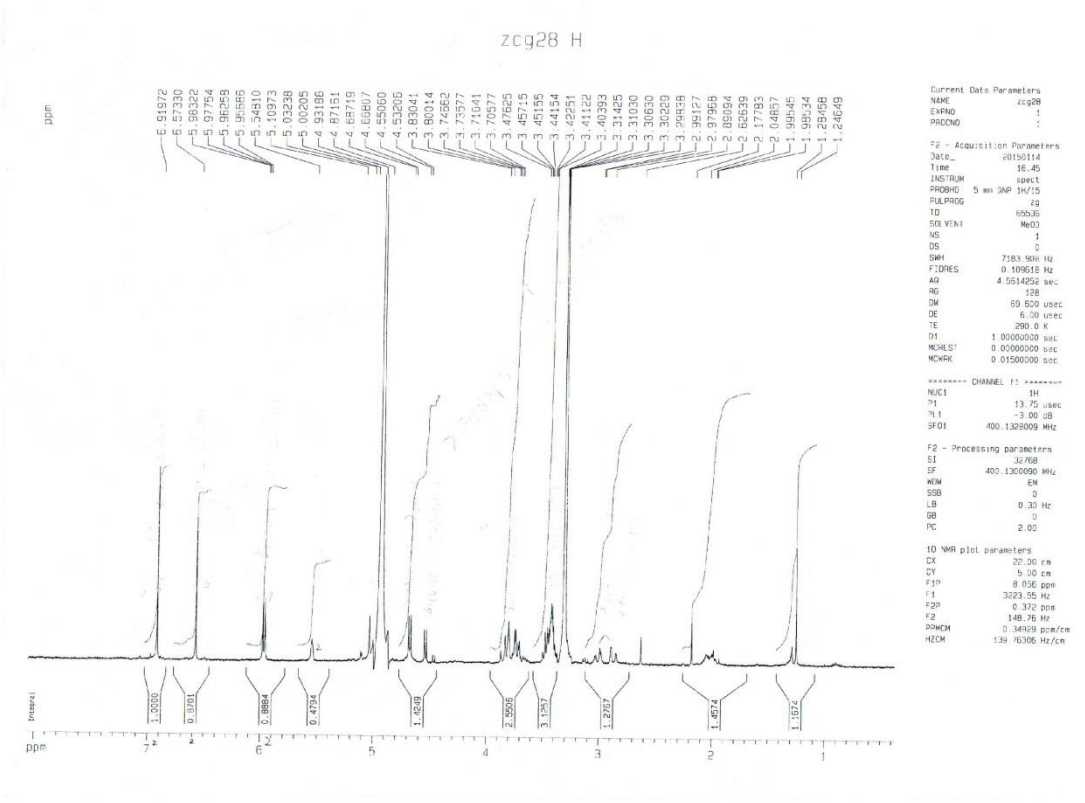

Figure S13. ^{13}C-NMR spectra of compound **10**

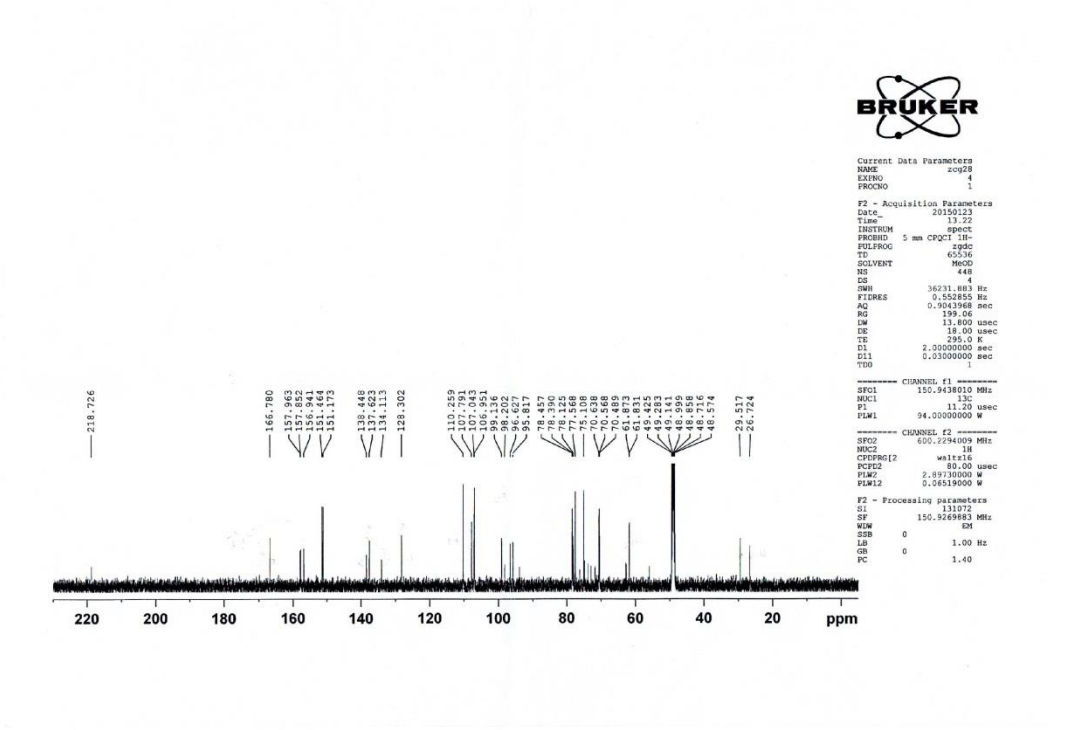

Figure S14. ^{1}H-NMR spectra of compound **11**

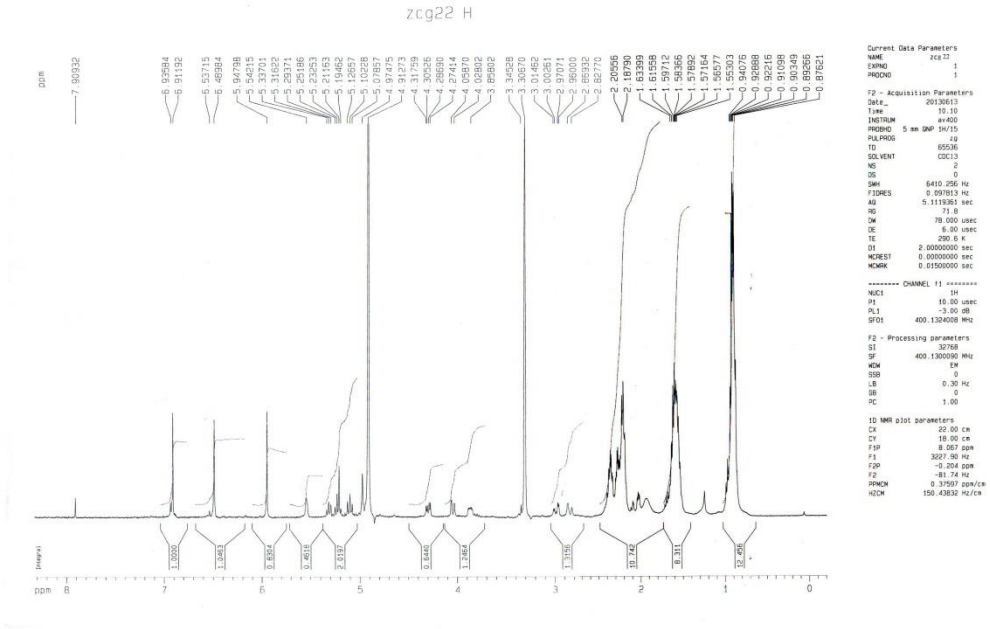

Figure S15. ^{13}C-NMR spectra of compound **11**

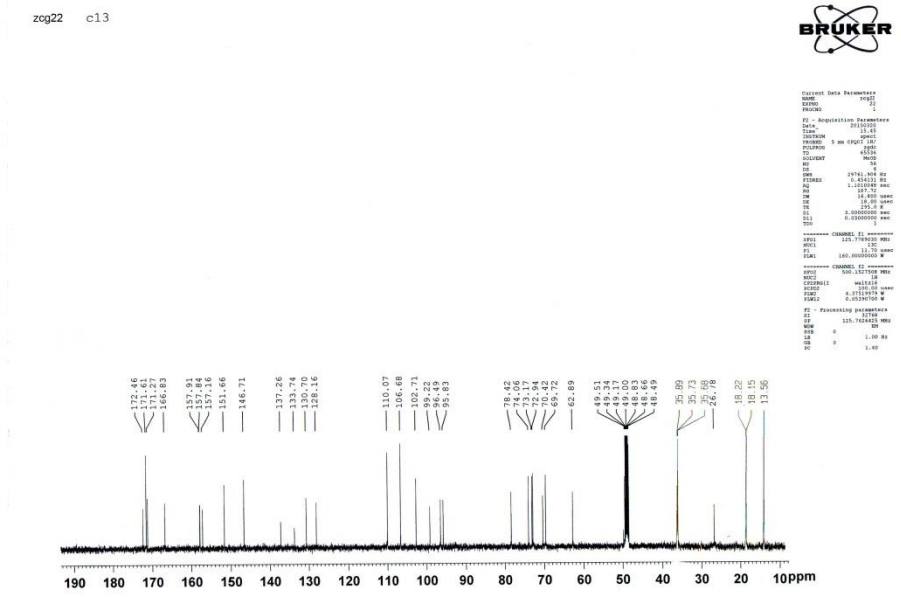

Figure S16. ^{1}H-NMR spectra of compound **12**

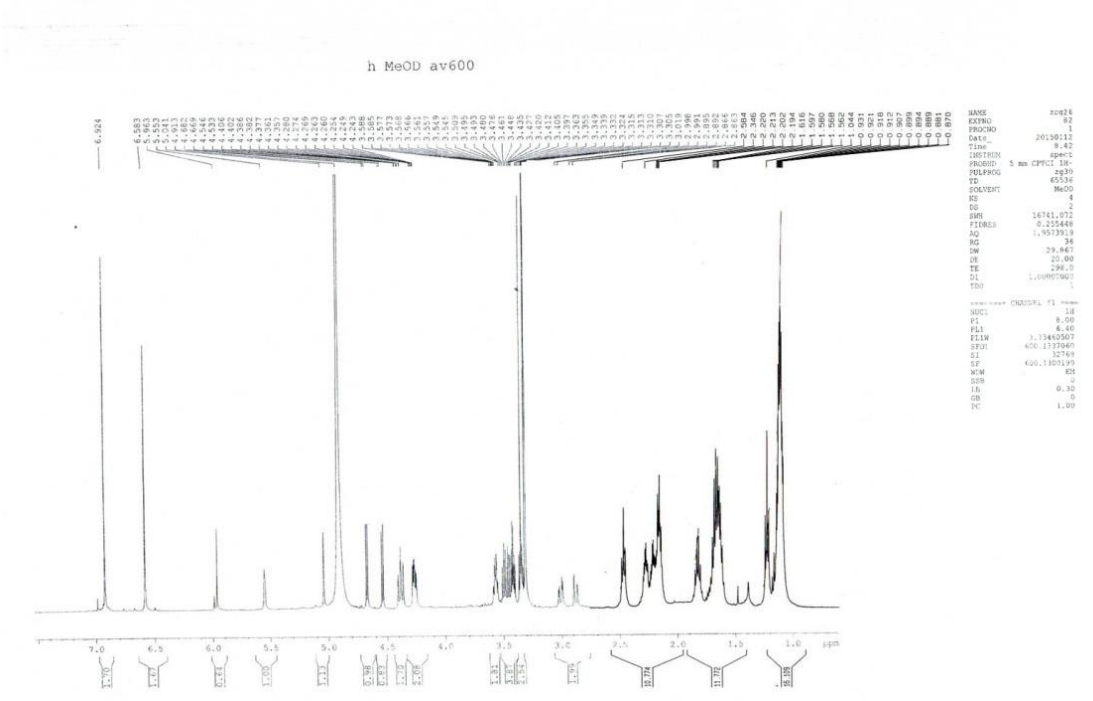

Figure S17. ^{13}C-NMR spectra of compound **12**