

## 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  $^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR of compounds **7–12**

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

Figure S1. The details of the binding between EGFR and EGCG (**4**)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

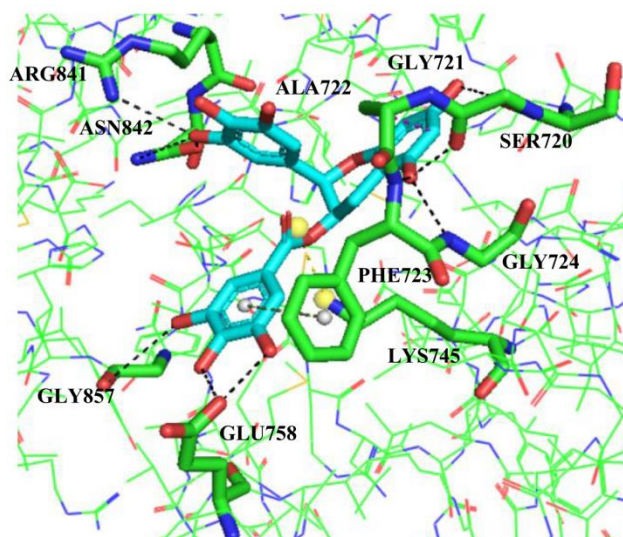
Figure S17.  $^{13}\text{C}$ -NMR spectra of compound **12**

**Table S1.** The characteristic <sup>1</sup>H-NMR and <sup>13</sup>C-NMR of compounds **7–12**.

Compounds	H-1'''		C-1''' $\delta$ (ppm)	H-1''''		C-1'''' $\delta$ (ppm)
	$\delta$ (ppm)	$J_{1'''-2'''}(\text{Hz})$		$\delta$ (ppm)	$J_{1''''-2''''}(\text{Hz})$	
<b>7</b>	—	—	—	4.9	9.0	102.7
<b>8</b>	4.7	9.5	107.0	4.5	9.5	107.3
<b>9</b>	—	—	—	4.7	9.0	108.2
<b>10</b>	4.7	9.5	107.0	4.5	9.5	107.8
<b>11</b>	—	—	—	4.9	9.0	102.7
<b>12</b>	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)
<b>4</b>	−7.7	−1.1	−3.8	−5.0	159.2
<b>11</b>	−8.1	−0.4	−10.9	2.4	1754.3
<b>12</b>	−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;  $\pi$ -stacking is shown as gray dotted lines; salt bridges were shown as yellow dotted lines.

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

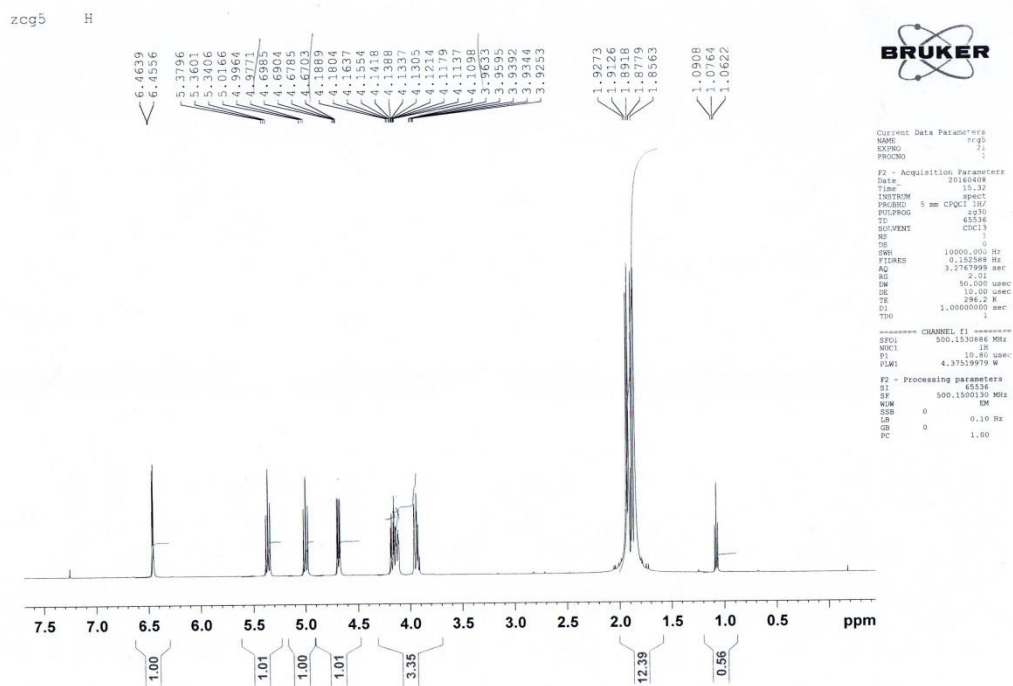
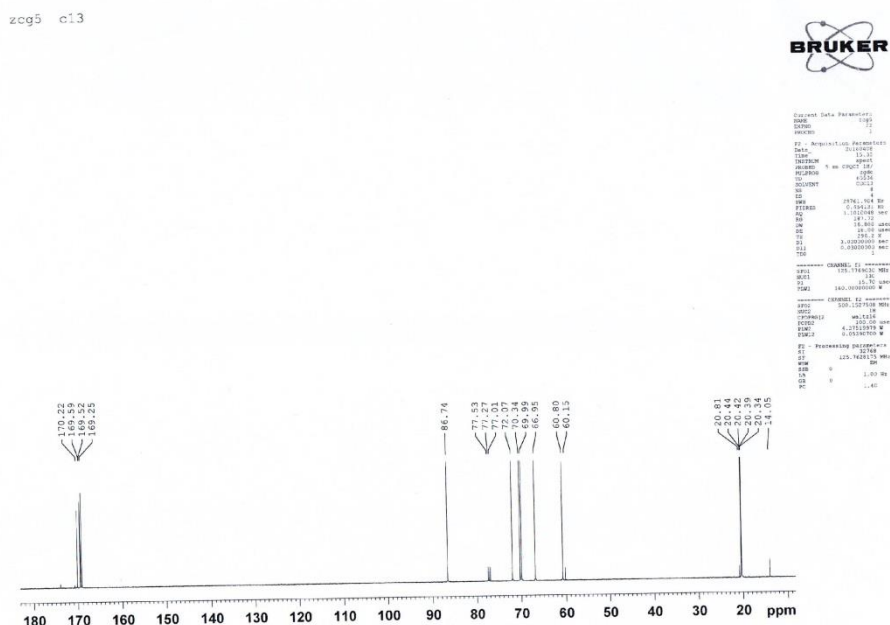


Figure S3.  $^{13}\text{C}$ -NMR spectra of compound **6**



zcg25 H

ppm — 7.90932

Peak (ppm)	Integration
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7.31192	1.0452
6.46115	0.9304
6.25371	0.4618
5.21163	2.0137
5.19462	
5.12657	
5.10228	
4.97475	
4.91273	
4.31139	0.6440
4.28550	
4.27414	1.2664
4.05870	
4.02802	
3.85802	
3.74628	
3.30670	
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3.00261	
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2.96000	
2.88932	1.3196
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Integrals

ppm 8 7 6 5 4 3 2

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PROCNO 1

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1D NMR plot parameters

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CY 12.00 cm  
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F1 331.70 Hz  
F2P 1.206 ppm  
F2 482.50 Hz  
NUC1 15N  
HSCN 129.56980 Hz/cm

c2 c13 and dept

13C NMR spectrum showing chemical shifts (ppm) and corresponding peak assignments:

Chemical Shift (ppm)
172.46
171.77
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157.64
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133.74
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Figure S6. HMBC spectra of compound 7

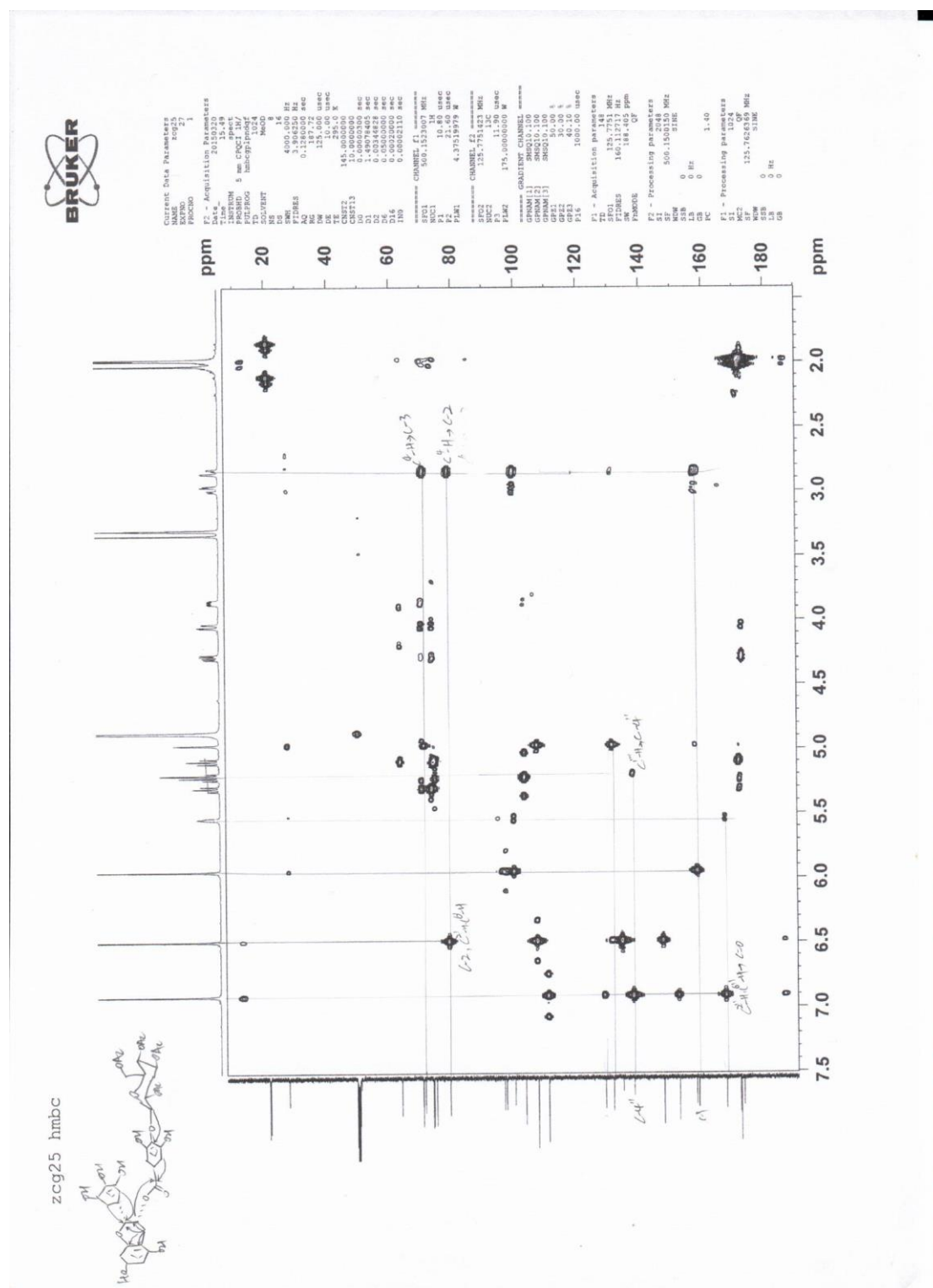


Figure S7.  $^1\text{H}$ -NMR spectra of compound **8**

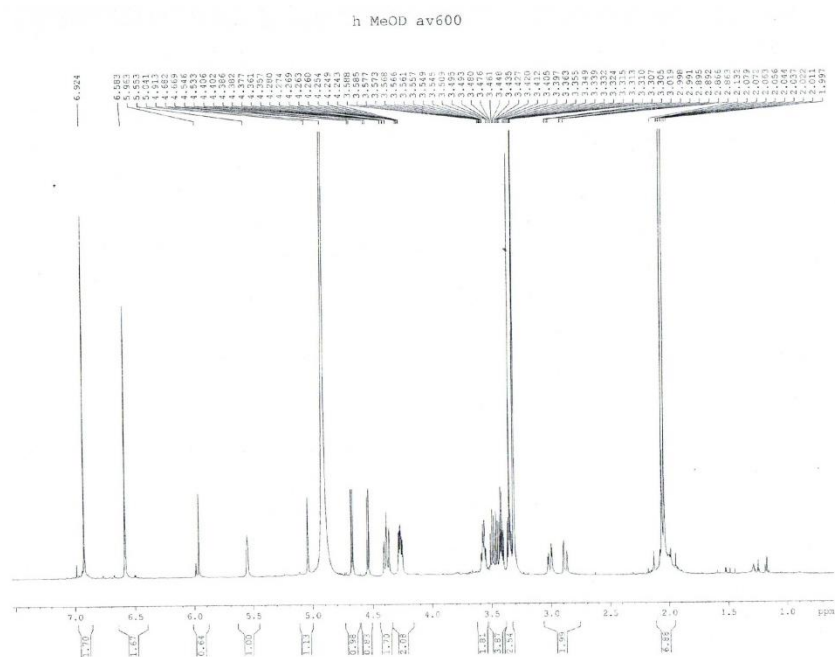


Figure S8.  $^{13}\text{C}$ -NMR spectra of compound **8**

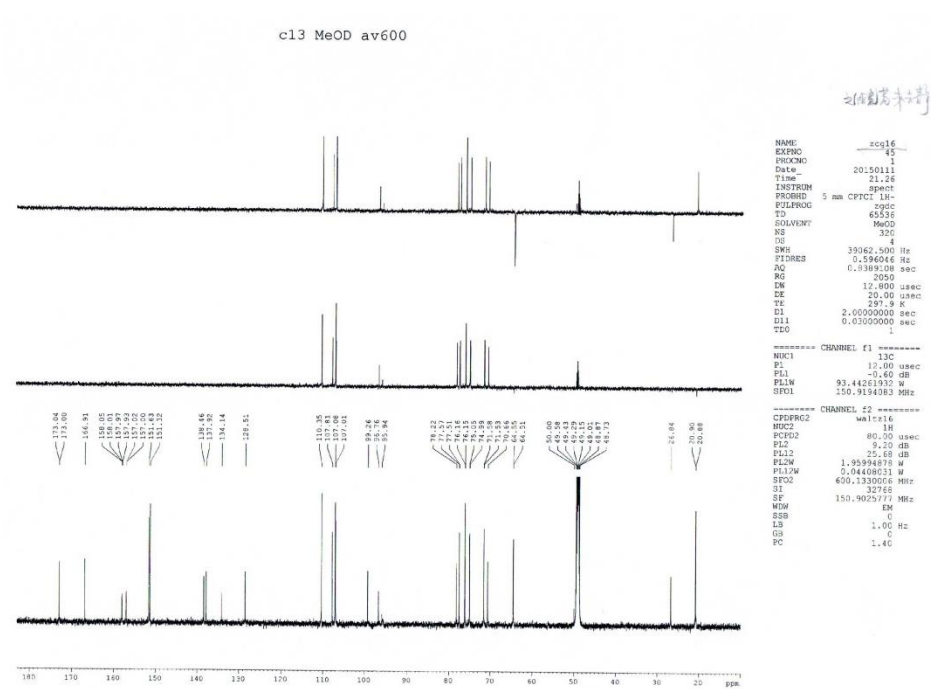


Figure S9. HMBC spectra of compound **8**

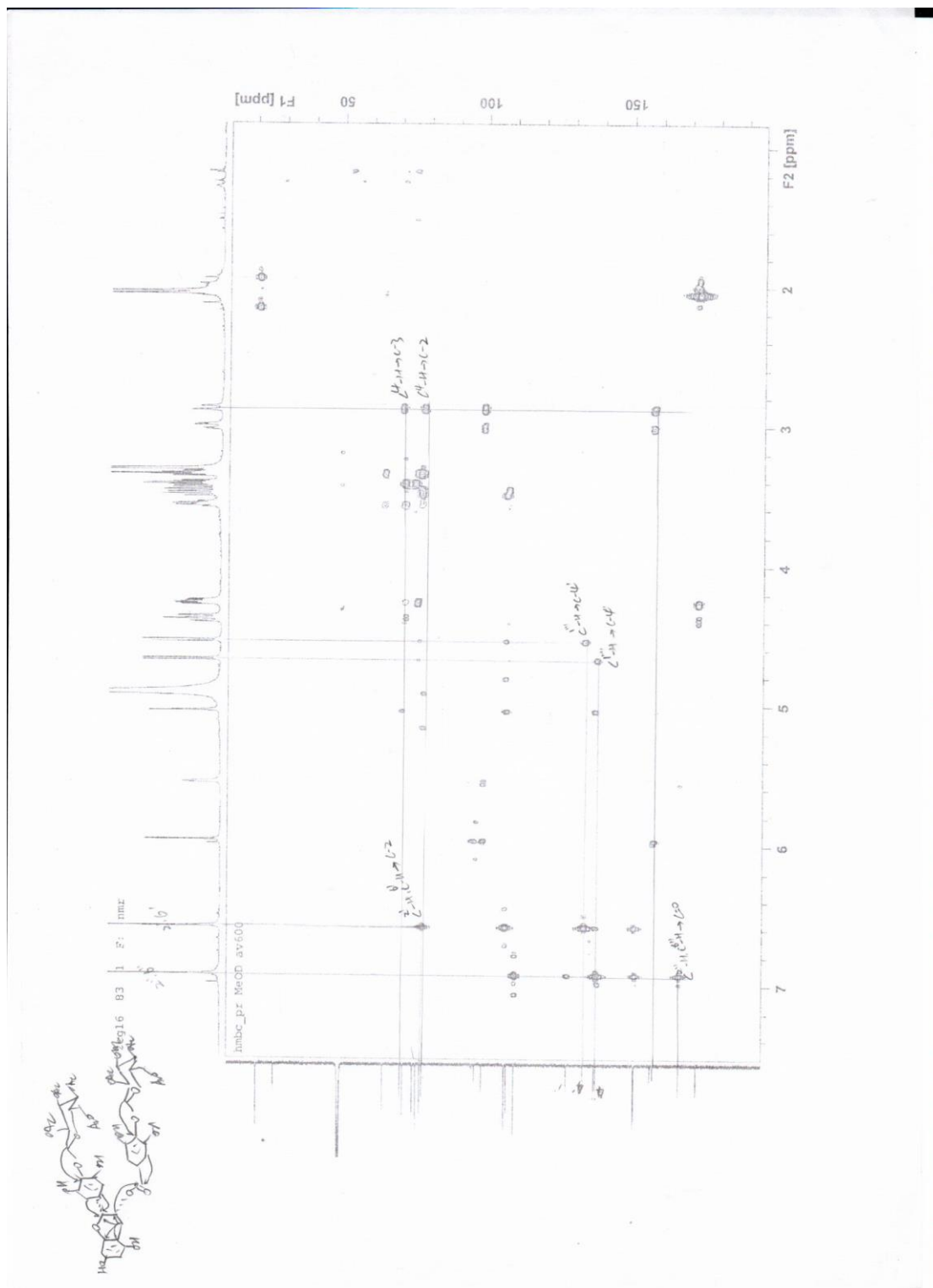


Figure S10.  $^1\text{H}$ -NMR spectra of compound **9**

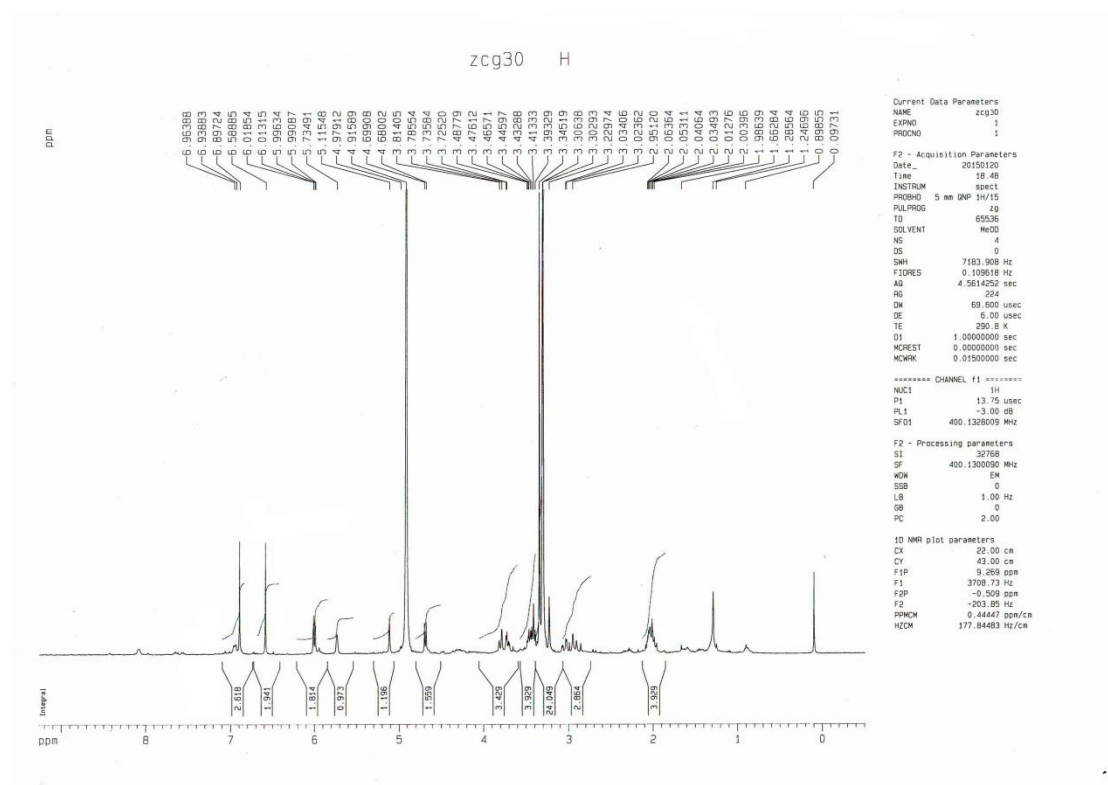


Figure S11.  $^{13}\text{C}$ -NMR spectra of compound **9**

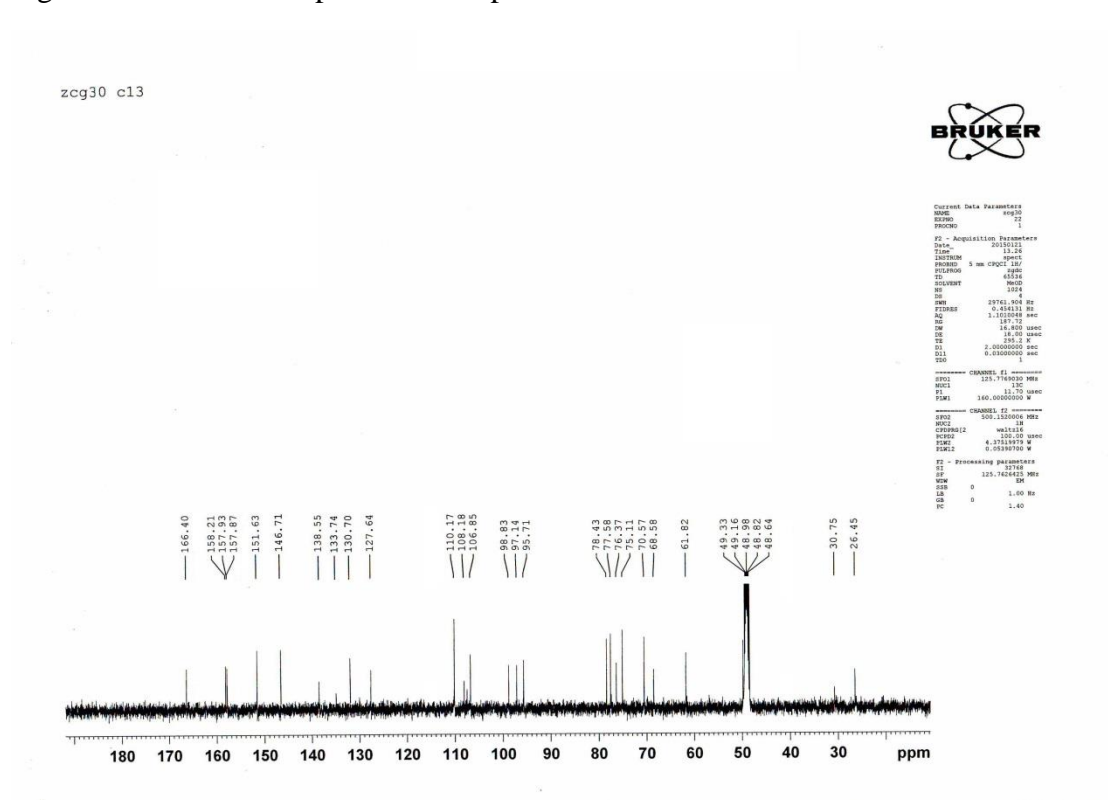


Figure S12.  $^1\text{H}$ -NMR spectra of compound **10**

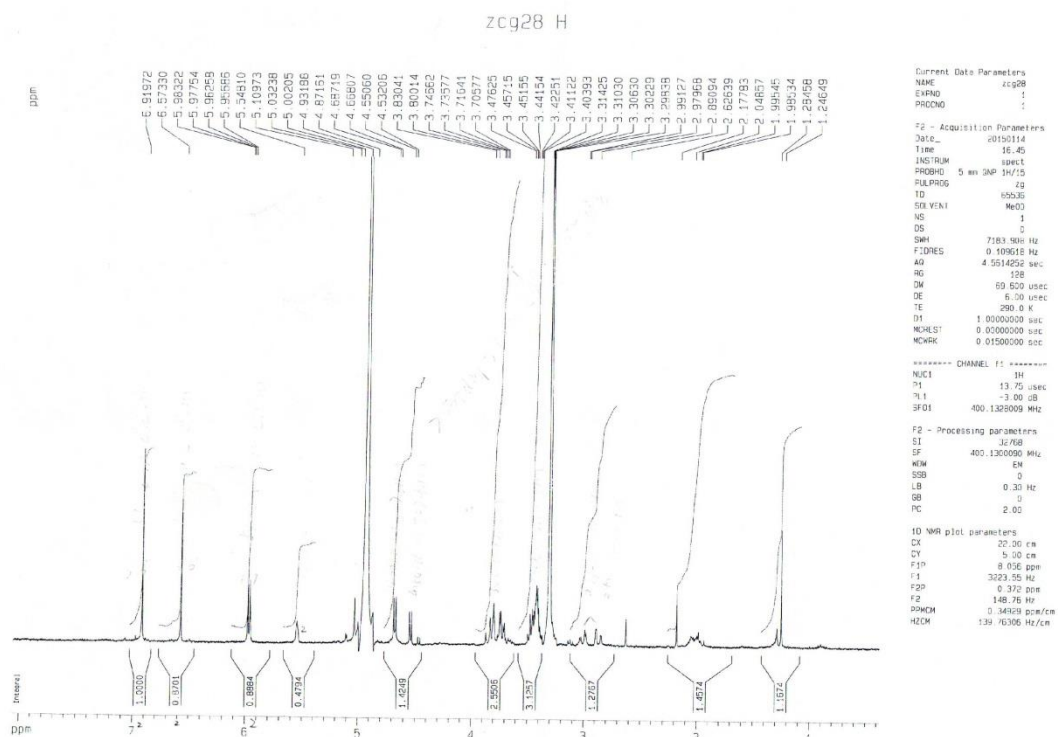


Figure S13.  $^{13}\text{C}$ -NMR spectra of compound **10**

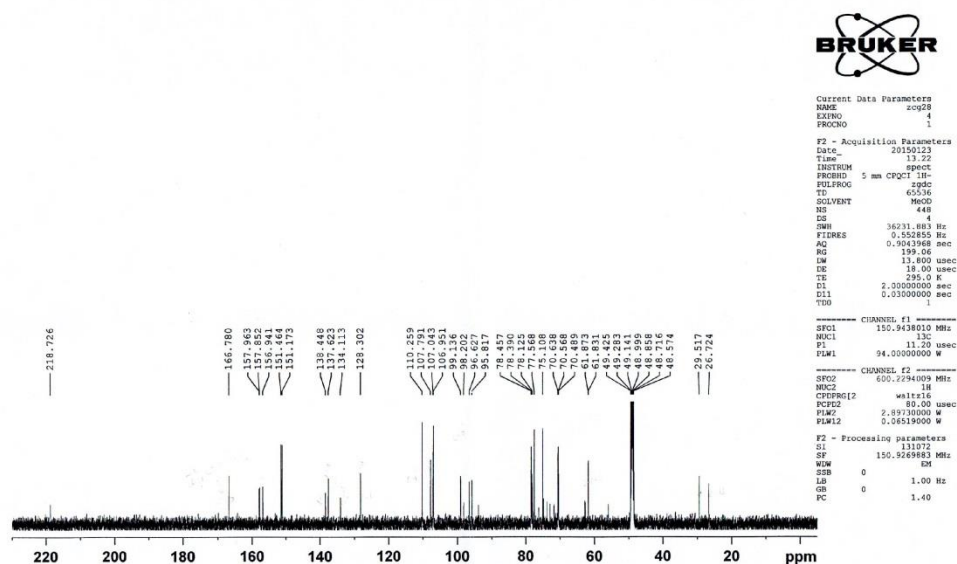


Figure S14.  $^1\text{H}$ -NMR spectra of compound **11**

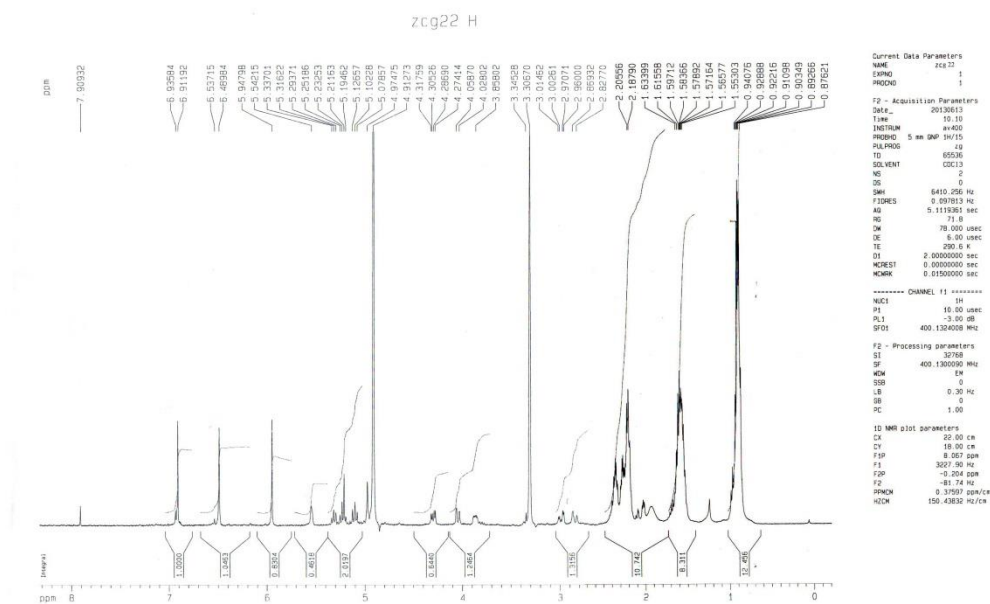
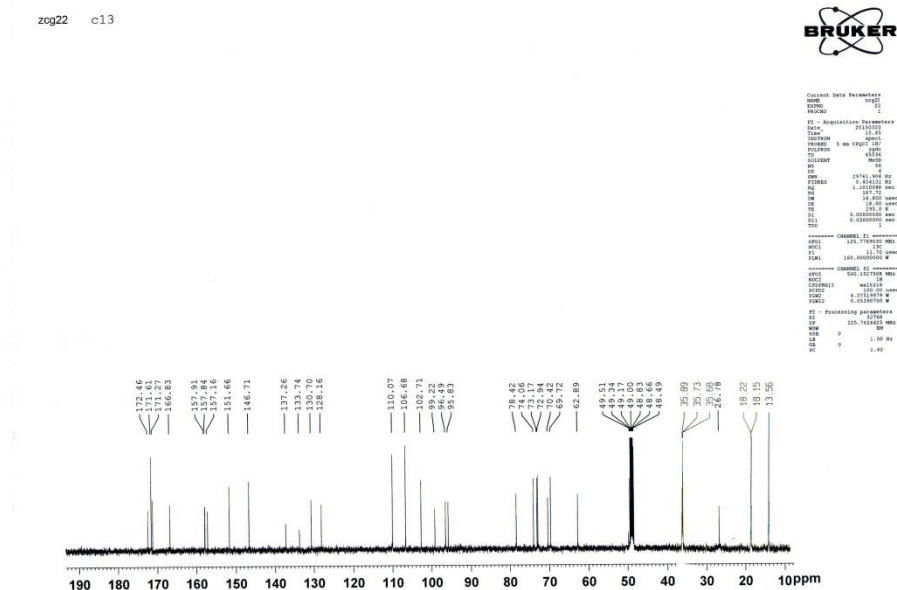


Figure S15.  $^{13}\text{C}$ -NMR spectra of compound **11**



[illegible]

zcg26 c13 MeOD av600