Supplementary Information

Antiproliferative activity of triterpenoids of *Nelumbo nucifera* Gaetrn. rhizomes and their derivatives: *In vitro* and *in silico* studies

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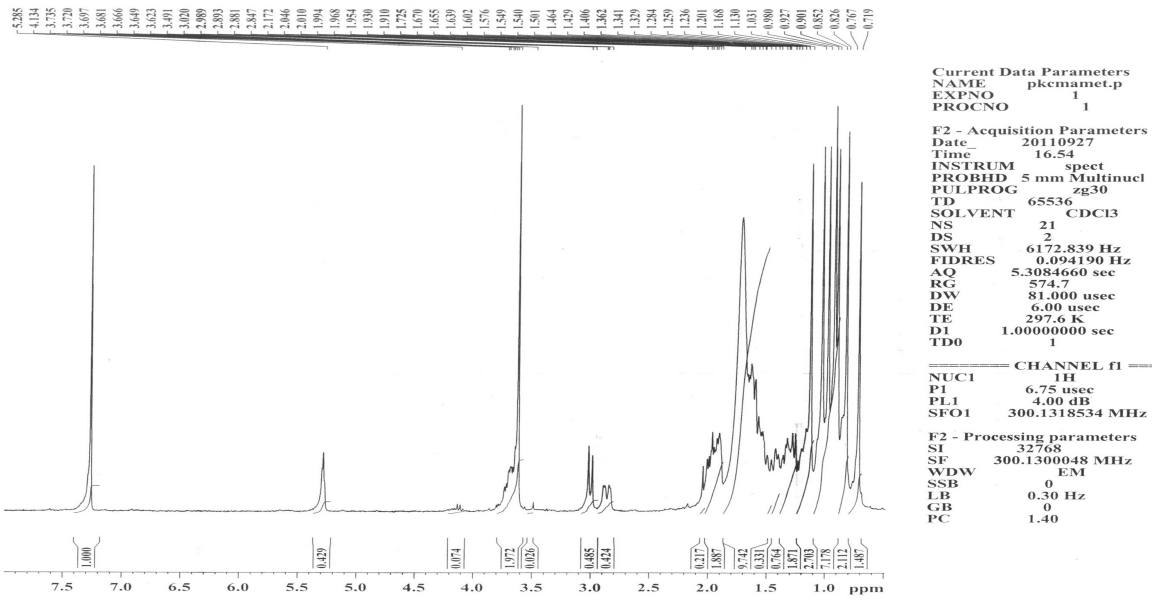
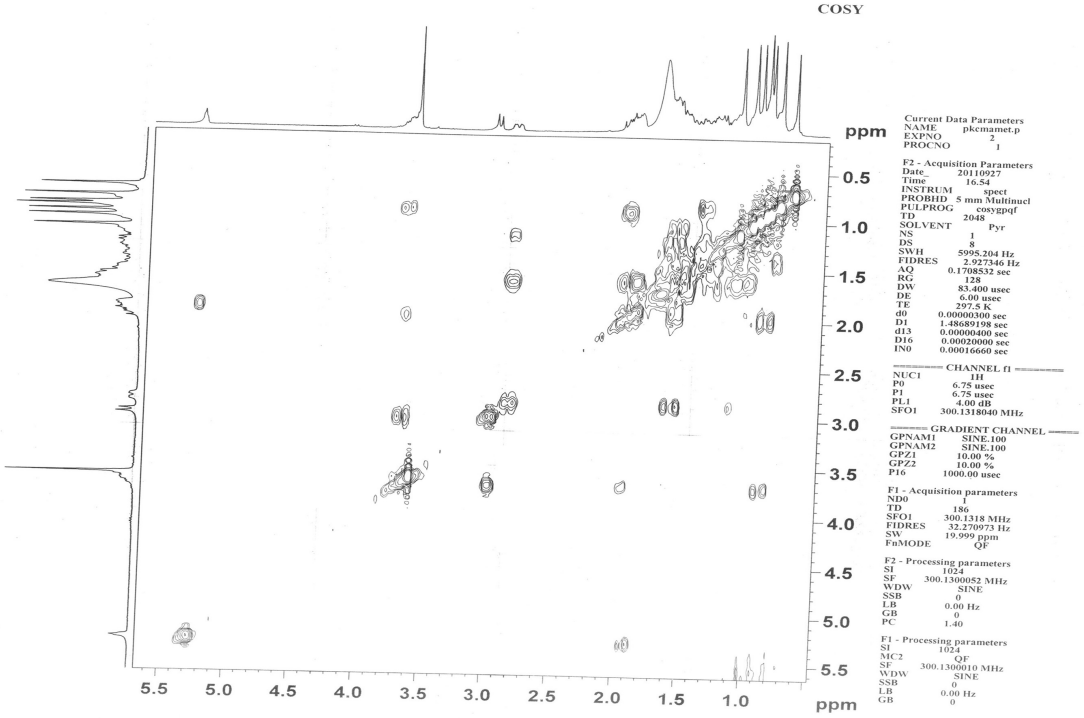
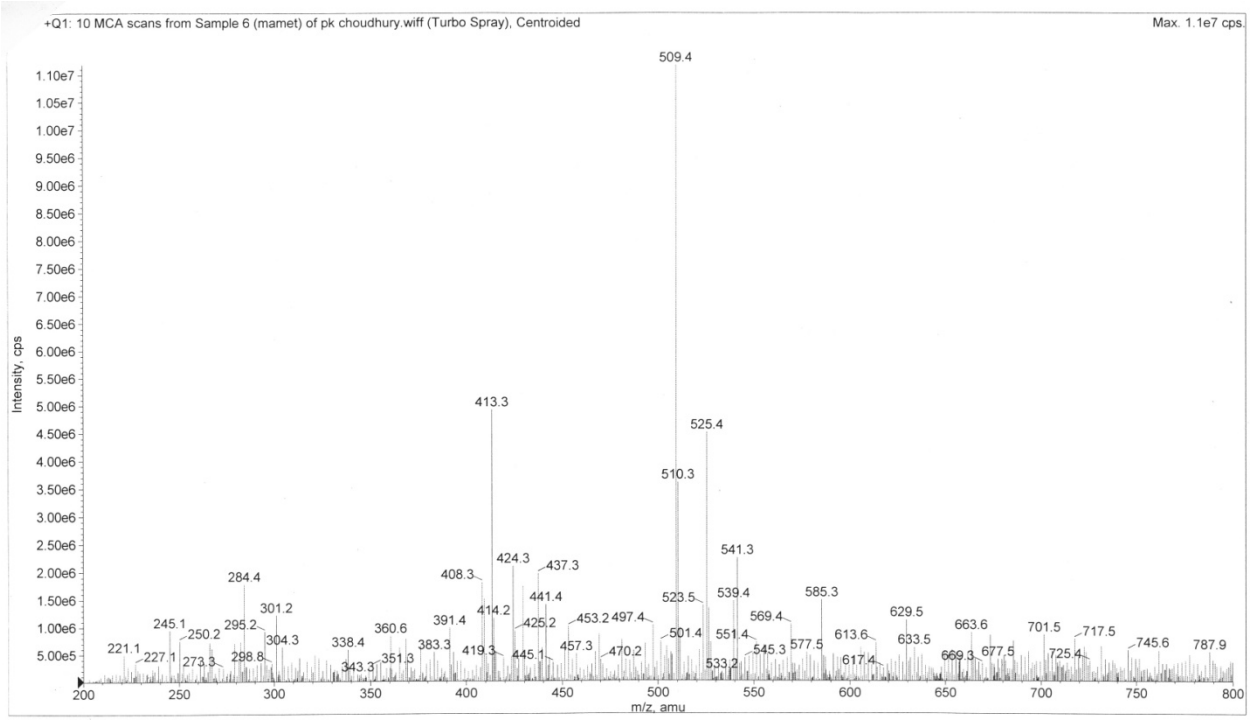


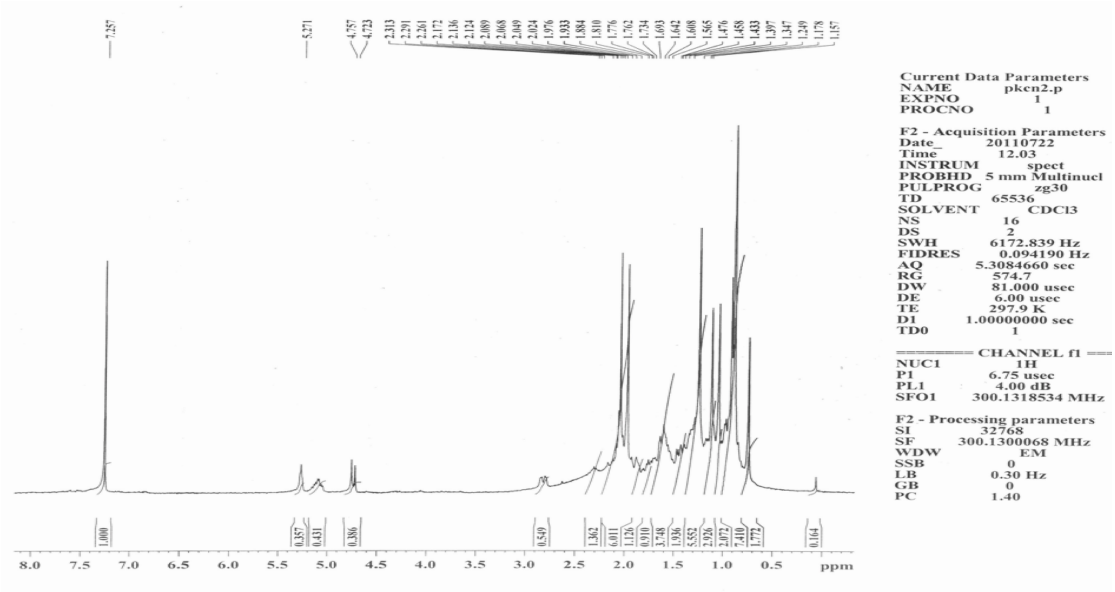
^{1}H NMR of compound **2a** at 300 MHz ($CDCl_3$)



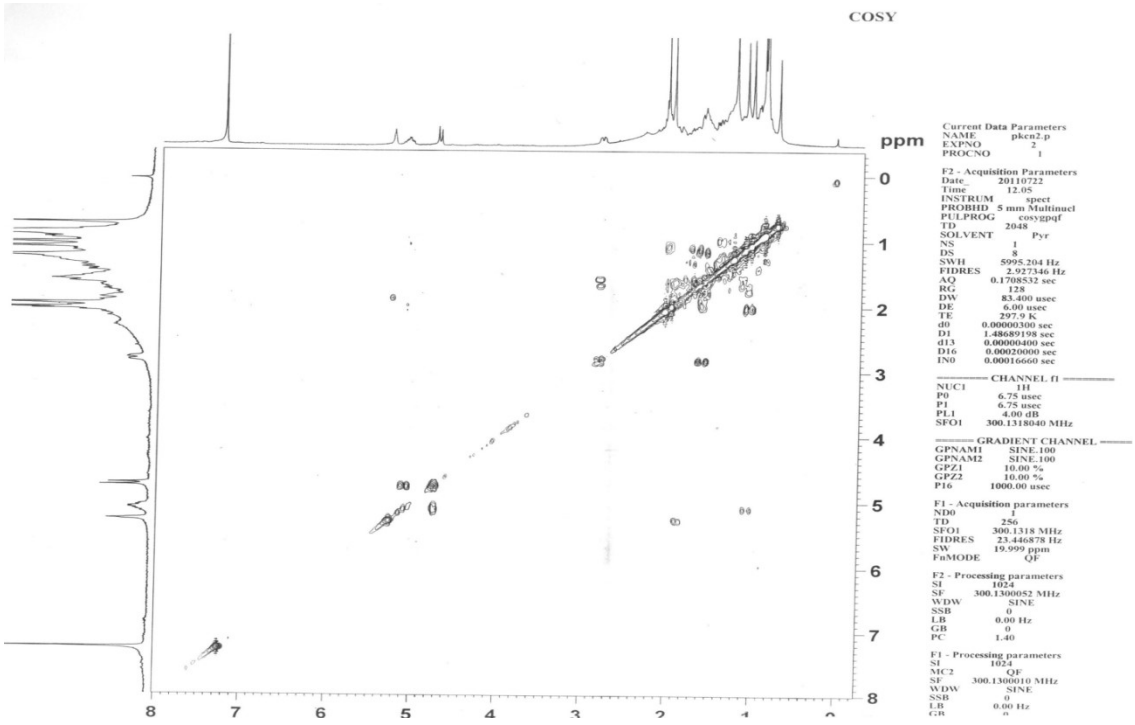
^{1}H-^{1}H COSY of compound **2a** at 300 MHz ($CDCl_3$)



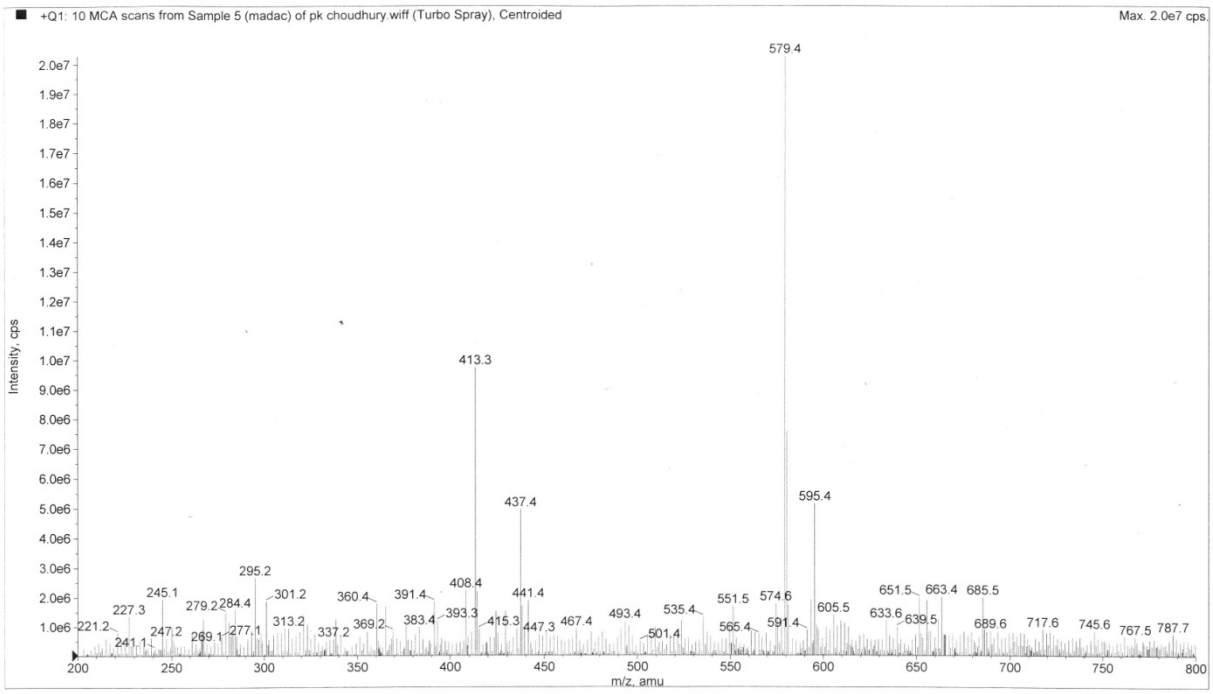
ESI-MS of compound **2a**



^{1}H NMR of compound **2b** at 300 MHz ($CDCl_3$)



^{1}H-^{1}H COSY of compound **2b** at 300 MHz ($CDCl_3$)


+Q1: 10 MCA scans from Sample 5 (madac) of pk choudhury.wiff (Turbo Spray), Centroided
Max. 2.0e7 cps.
Intensity, cps
m/z, amu
579.4
413.3
437.4
595.4
295.2
408.4
245.1
301.2
360.4
391.4
441.4
227.3
279.2
284.4
393.3
551.5
574.6
605.5
651.5
663.4
685.5
221.2
247.2
269.1
277.1
313.2
337.2
369.2
383.4
415.3
447.3
467.4
493.4
535.4
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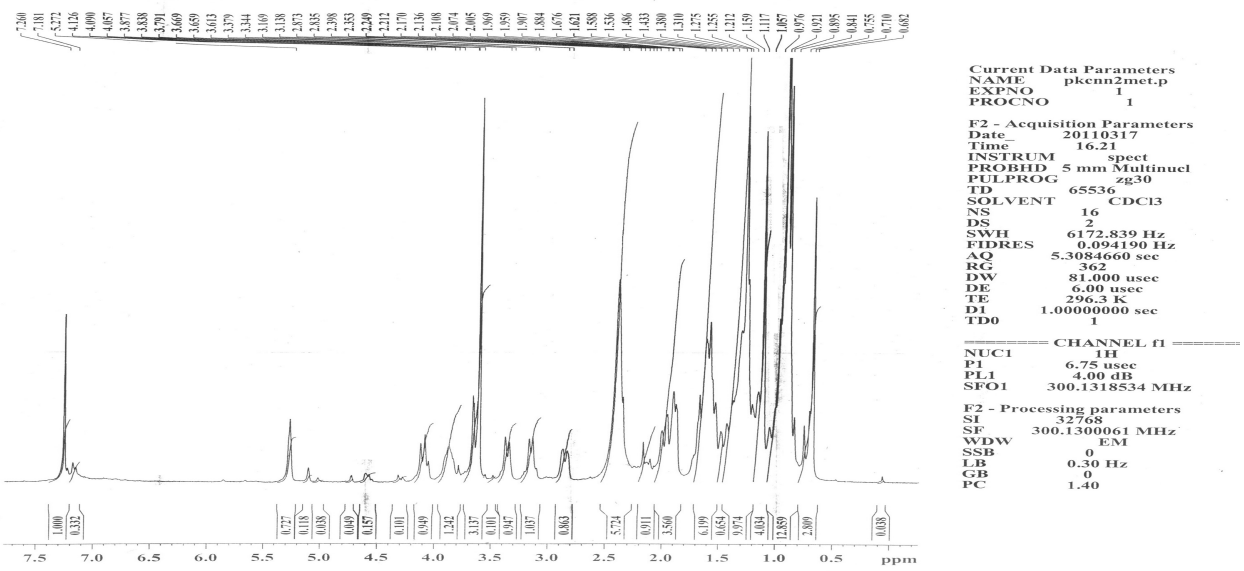
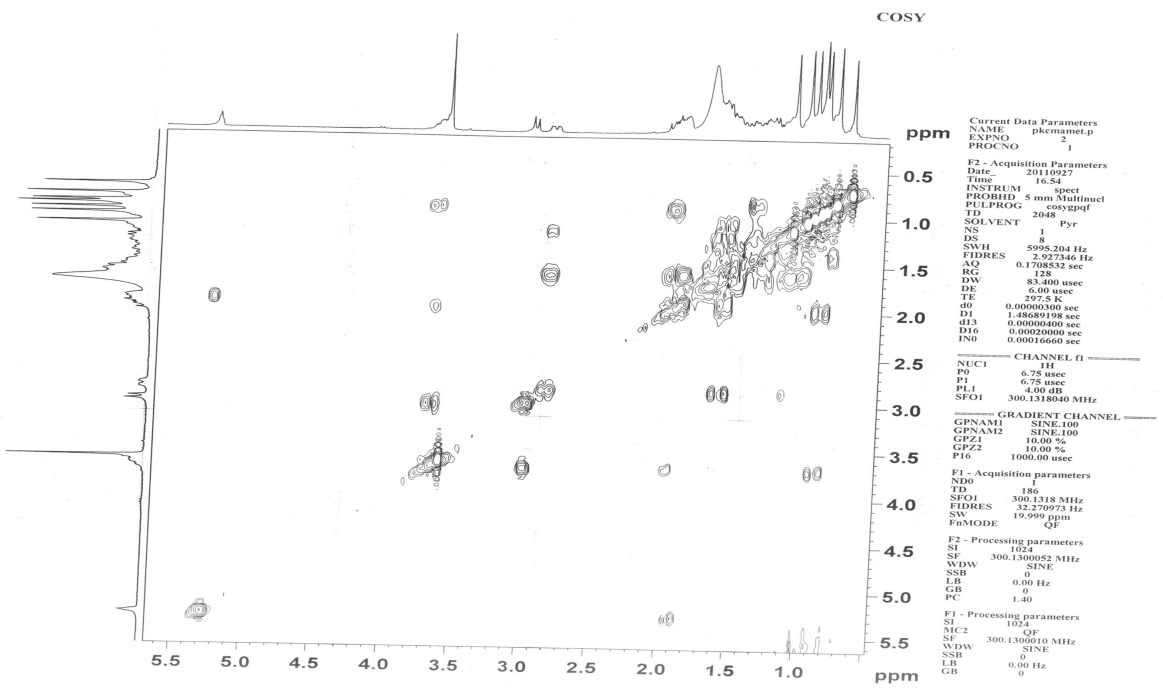
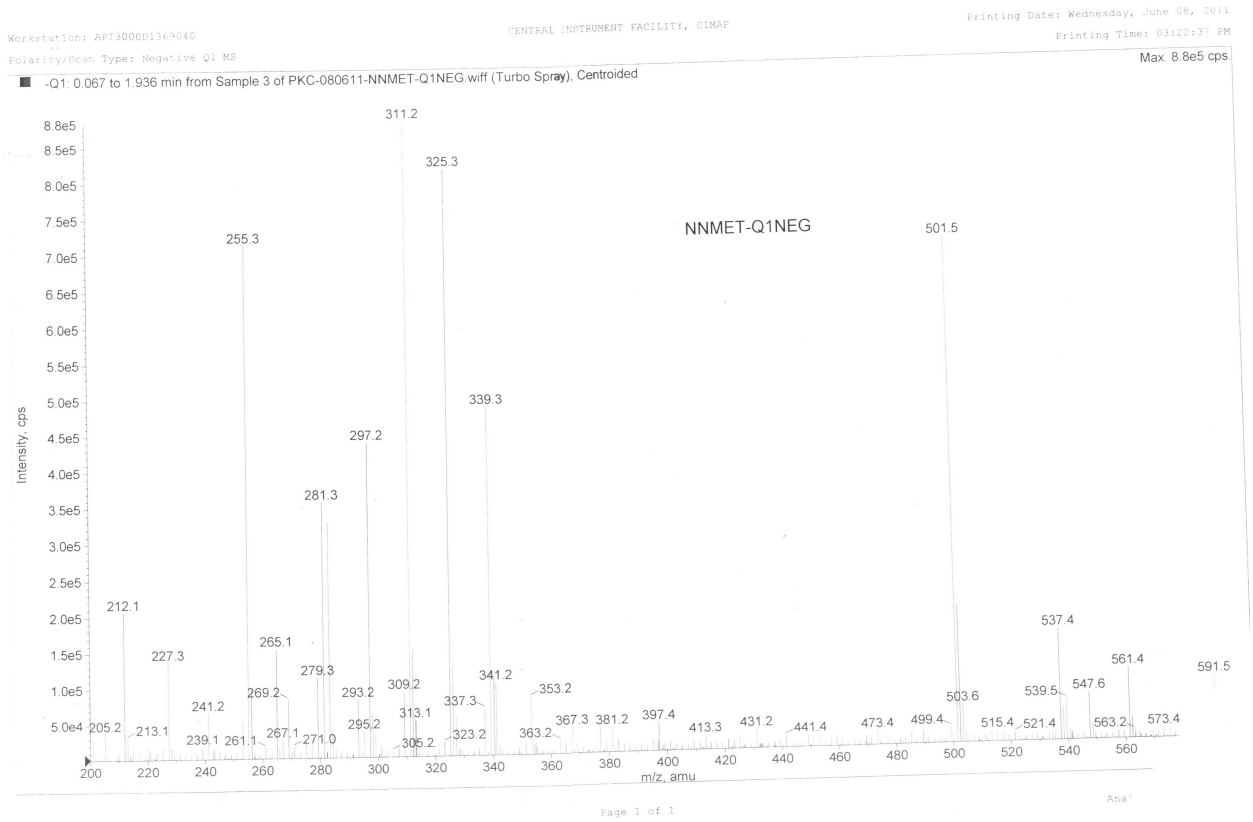
591.4
633.6
639.5
689.6
717.6
745.6
767.5
787.7
241.1
501.4



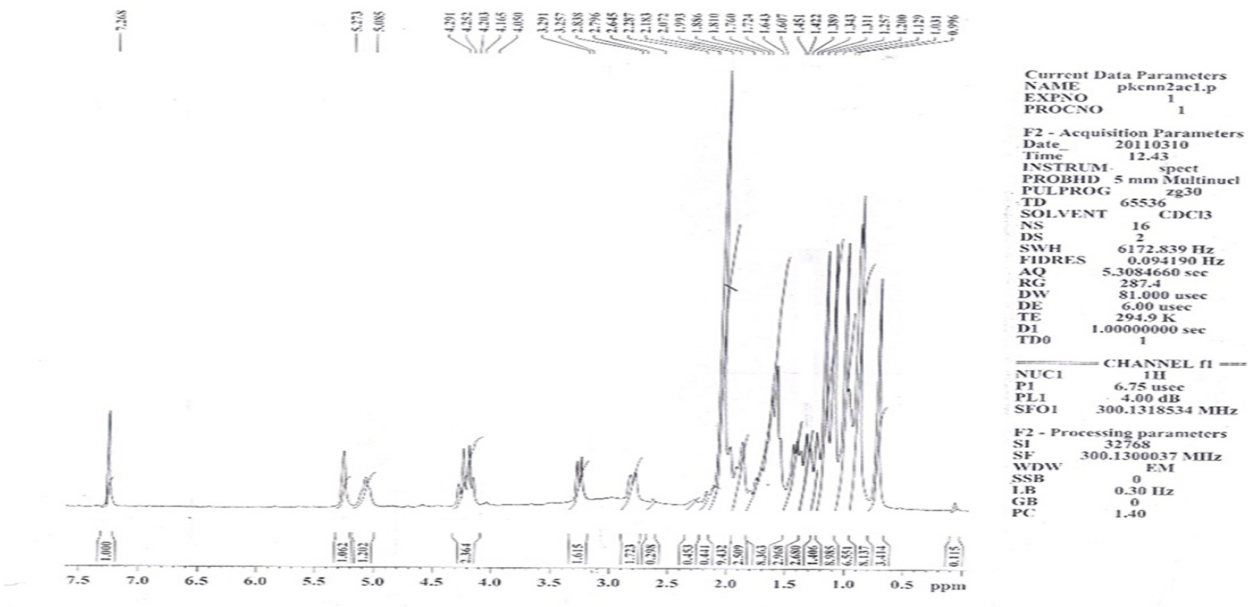
^{1}H NMR of compound **3a** at 300 MHz ($CDCl_3$)



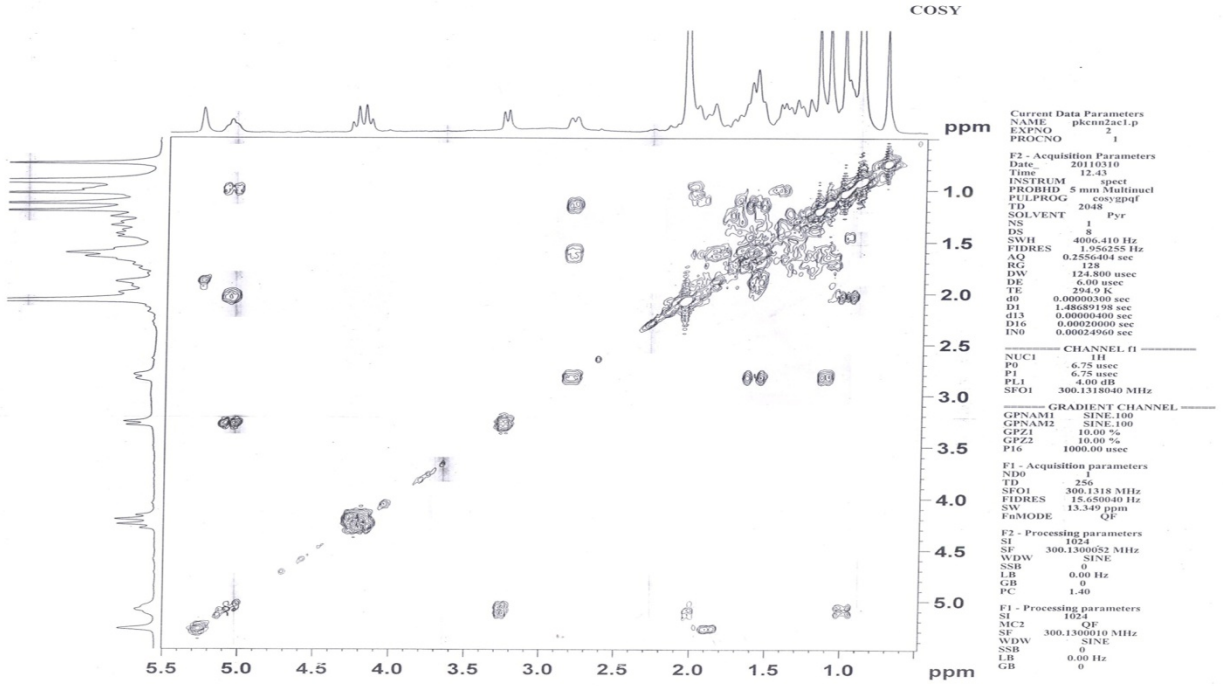
^{1}H-^{1}H COSY of compound **3a** at 300 MHz ($CDCl_3$)



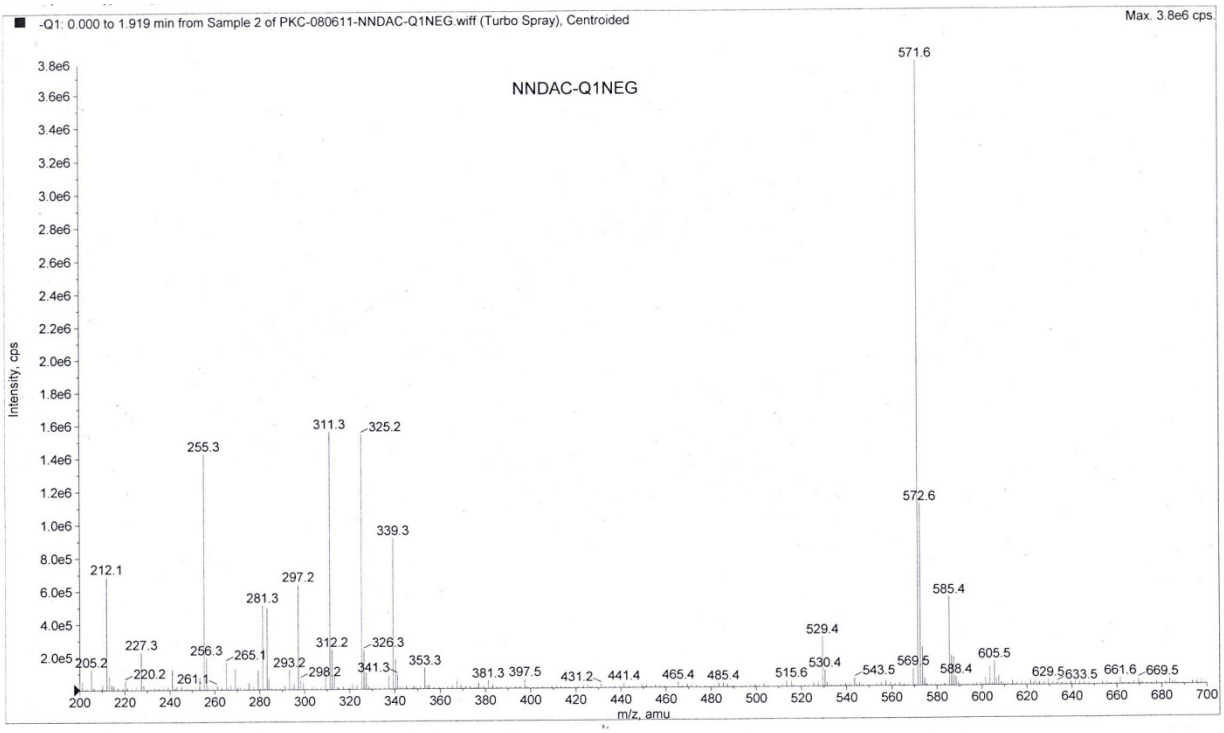
ESI-MS of compound **3a**



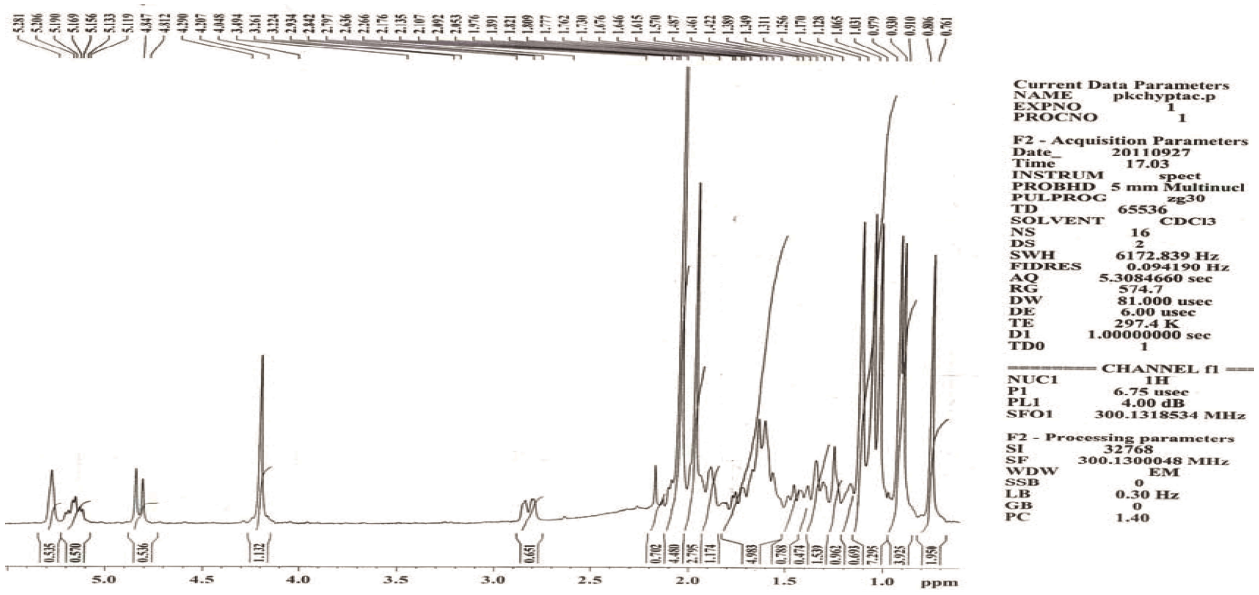
^{1}H NMR of compound **3b** at 300 MHz ($CDCl_3$)



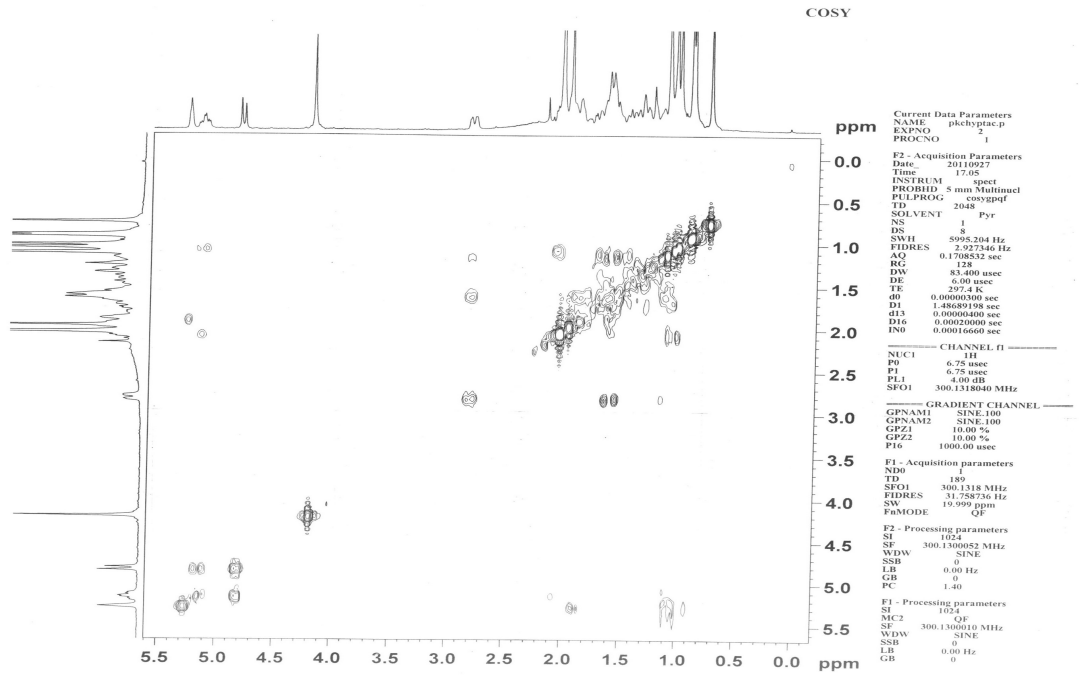
^{1}H-^{1}H COSYof compound **3b** at 300 MHz ($CDCl_3$)



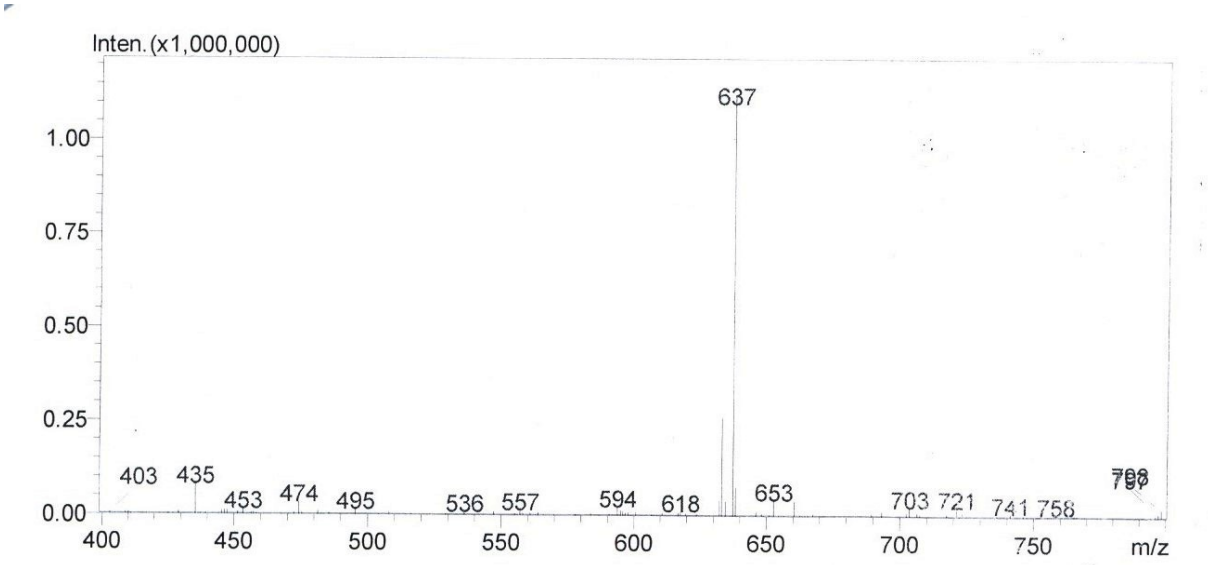
ESI-MS of compound **3b**



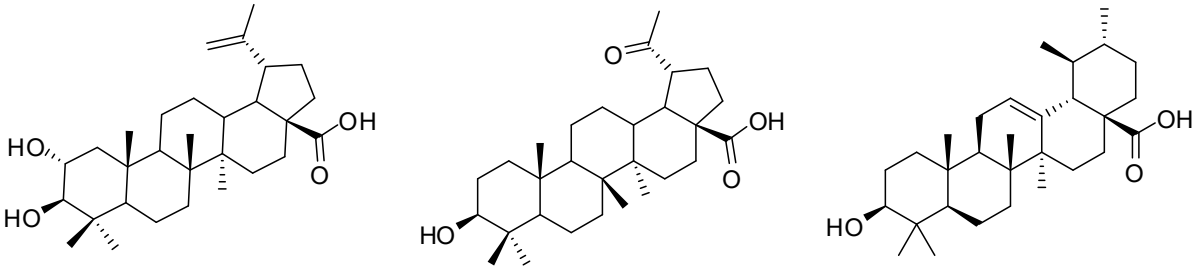
^{1}H NMR of compound **3c** at 300 MHz ($CDCl_3$)



^{1}H-^{1}H COSY of compound **3c** at 300 MHz ($CDCl_3$)



ESI-MS of compound **3c**



2α-Hydroxybetulinic acid Platanic acid Ursolic acid

Fig. S1. Structure of three external test set compound used in this study for QSAR modeling.

Table 1S QSAR models parameter for training set obtained from MLR, methodology.

QSAR models	R^2 (Training)	R_a^2 (adj.)	R_{L2O}^2	r^2 (Test)	S_{PRESS}	MAE	RMSE
MCF-7	0.96	0.90	0.83	0.87	0.135	0.07	0.08
PC3	0.91	0.75	0.68	0.84	0.234	0.12	0.12