

## Supplementary Information

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

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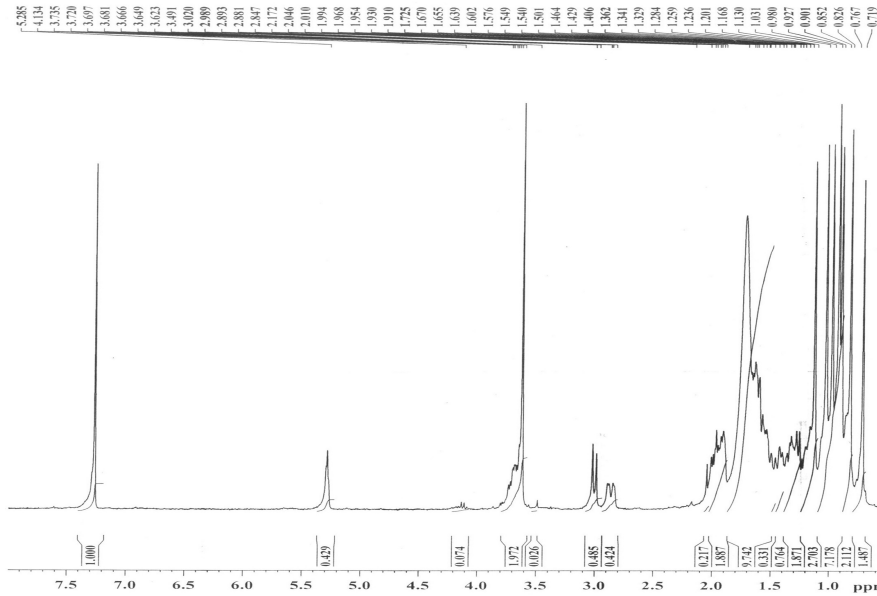
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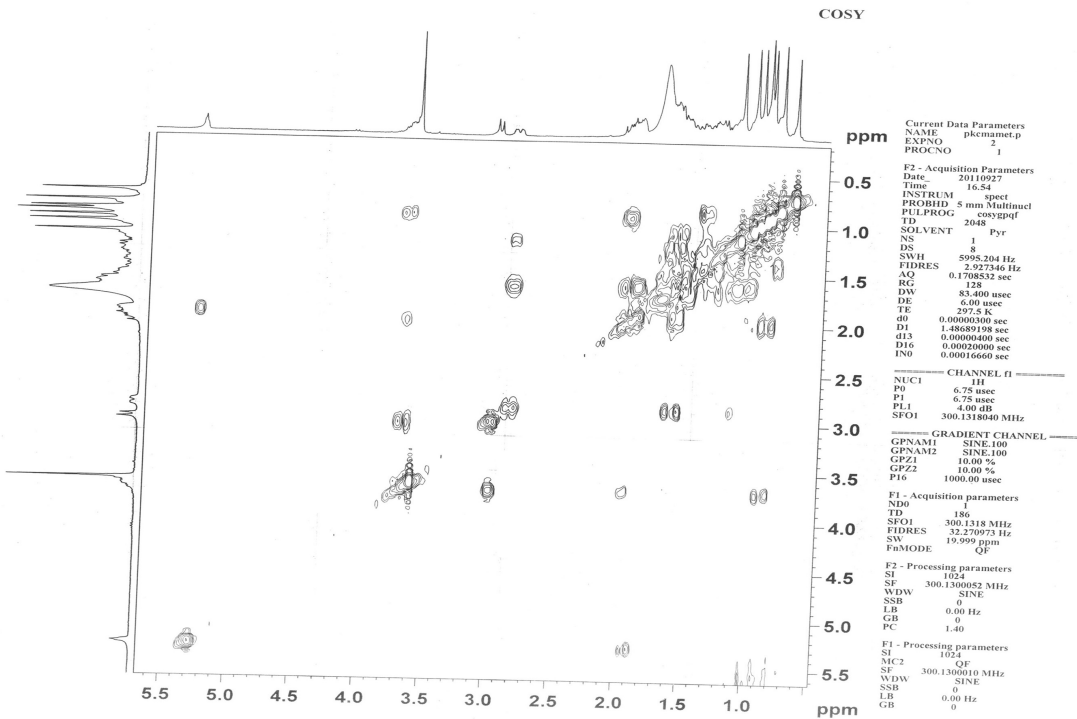
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 FIDRES 0.094190 Hz  
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 RG 574.7  
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<sup>1</sup>H NMR of compound **2a** at 300 MHz (CDCl<sub>3</sub>)



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 FIDRES 2.927346 Hz  
 AQ 0.1708532 sec  
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 DE 6.00 usec  
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 D0 0.00000300 sec  
 D1 1.48689198 sec  
 d13 0.00000400 sec  
 D16 0.00020000 sec  
 D30 0.00016660 sec

CHANNEL f1  
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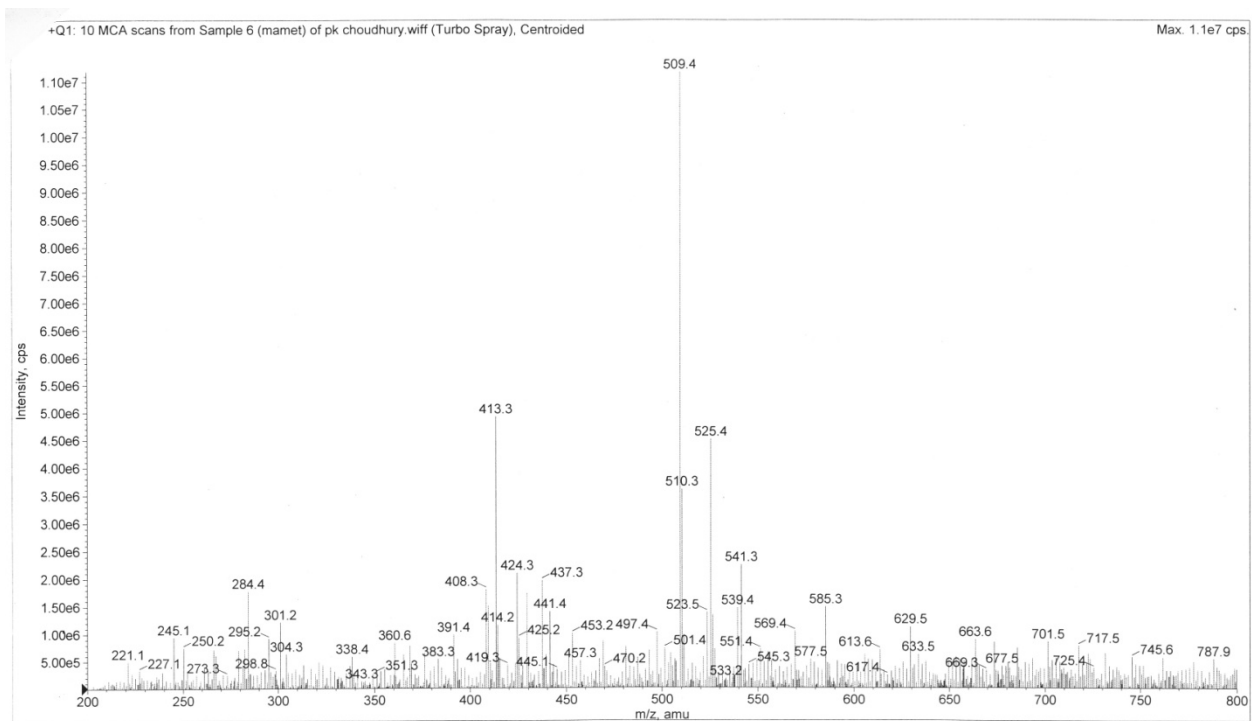
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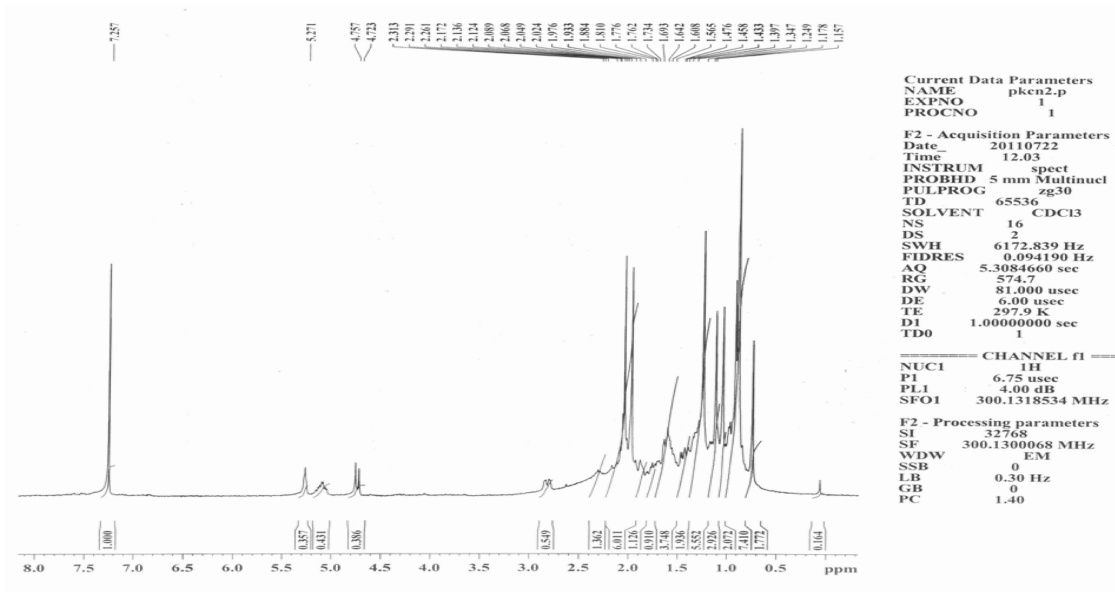
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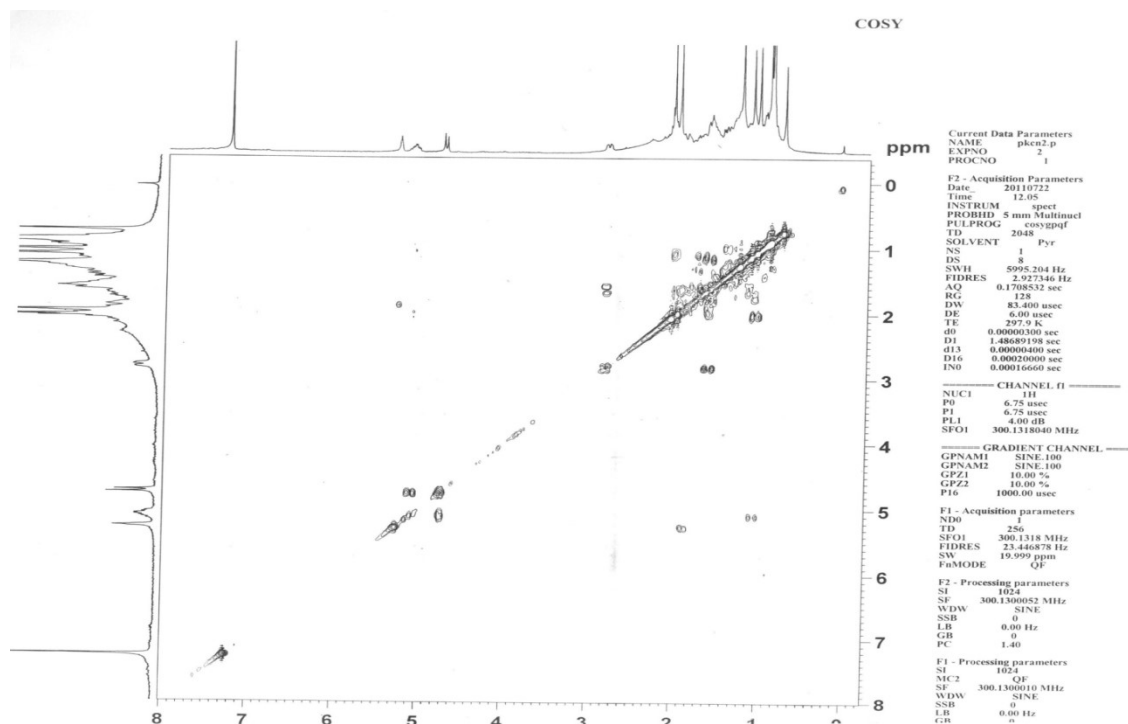
<sup>1</sup>H-<sup>1</sup>H COSY of compound **2a** at 300 MHz (CDCl<sub>3</sub>)



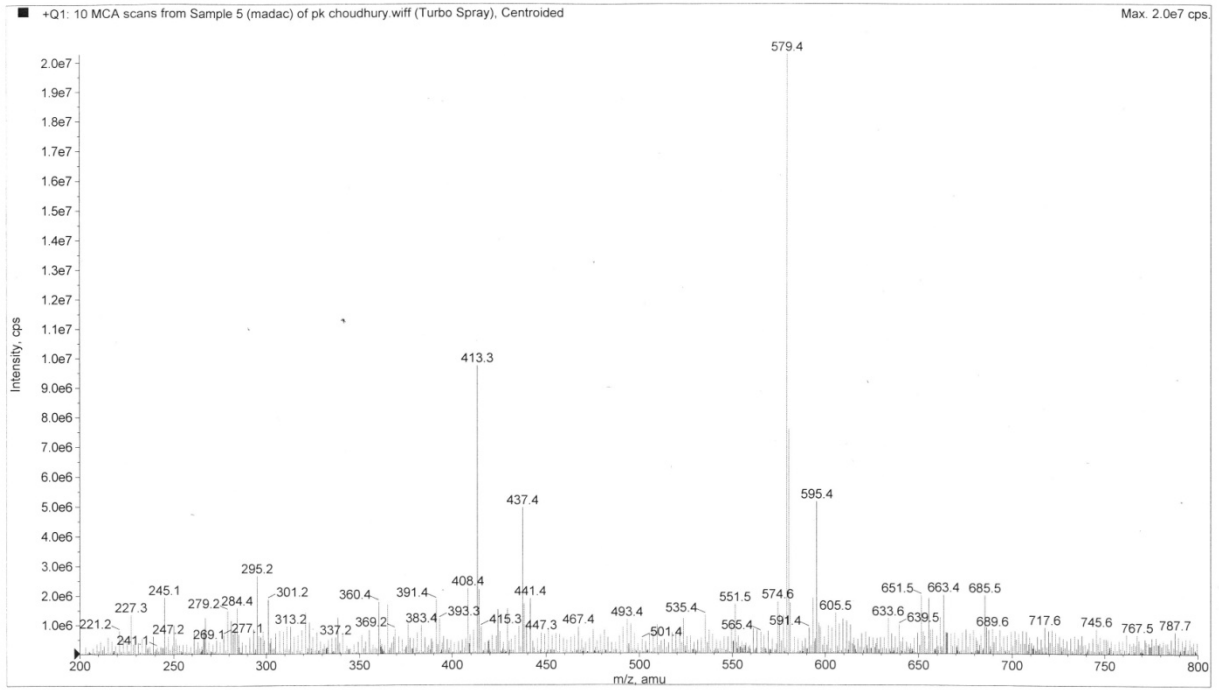
ESI-MS of compound **2a**

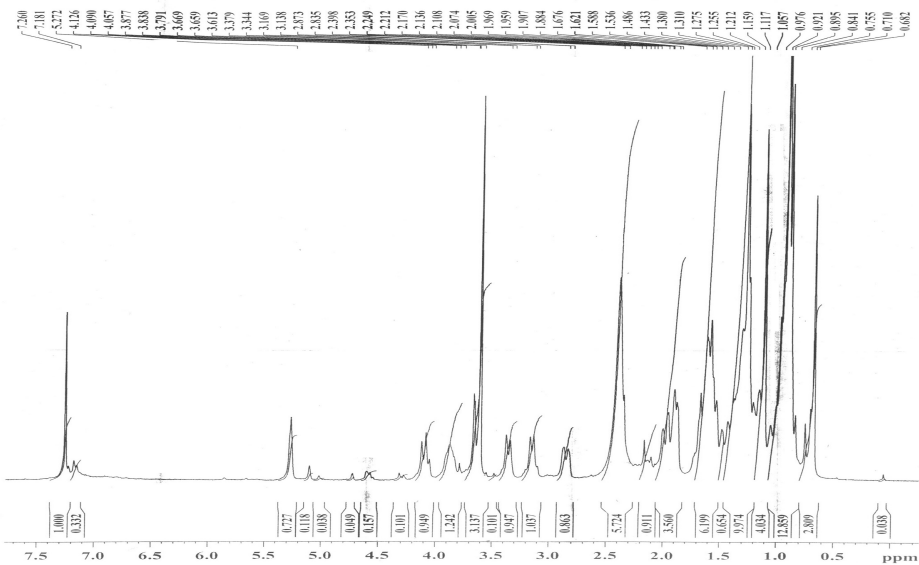


$^1\text{H}$  NMR of compound **2b** at 300 MHz ( $\text{CDCl}_3$ )



$^1\text{H}$ - $^1\text{H}$  COSY of compound **2b** at 300 MHz ( $\text{CDCl}_3$ )





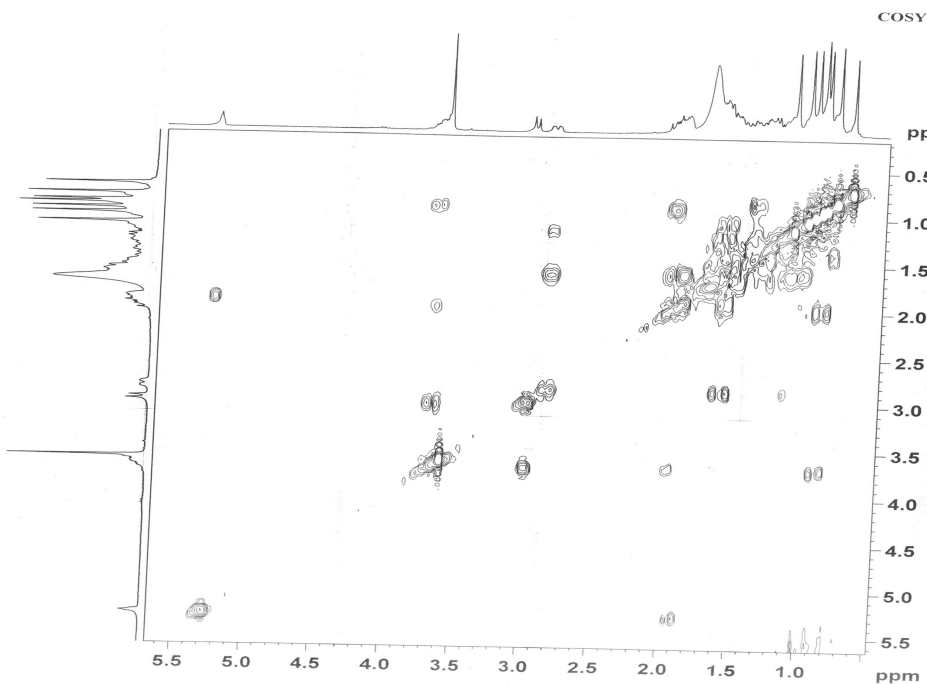
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 SOLVENT CDCl3  
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 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 362  
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 DE 6.00 usec  
 TE 296.3 K  
 D1 1.0000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 6.75 usec  
 PL1 4.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
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 PC 1.40

$^1\text{H}$  NMR of compound **3a** at 300 MHz ( $\text{CDCl}_3$ )



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 SOLVENT Pyr  
 NS 1  
 DS 8  
 SWH 5995.204 Hz  
 FIDRES 2.927346 Hz  
 AQ 0.1708532 sec  
 RG 128  
 DW 83.400 usec  
 DE 6.00 usec  
 TE 297.5 K  
 D1 0.00000300 sec  
 D11 1.48689198 sec  
 D16 0.00000400 sec  
 D10 0.00020000 sec  
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CHANNEL f1  
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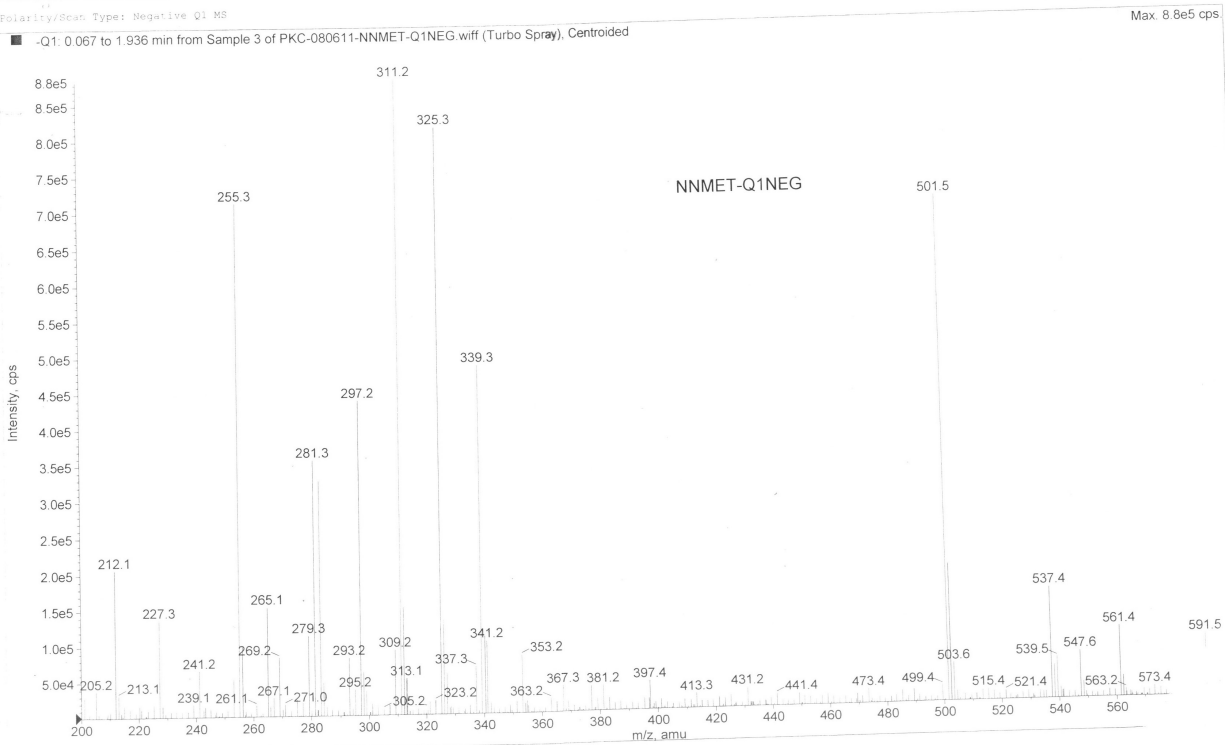
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 GPNAM2 SINE.100  
 GPZ1 10.00 %  
 GPZ2 10.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
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 TD 186  
 SFO1 300.1318 MHz  
 FIDRES 32.370973 Hz  
 SW 19.999 ppm  
 FhMODE QF

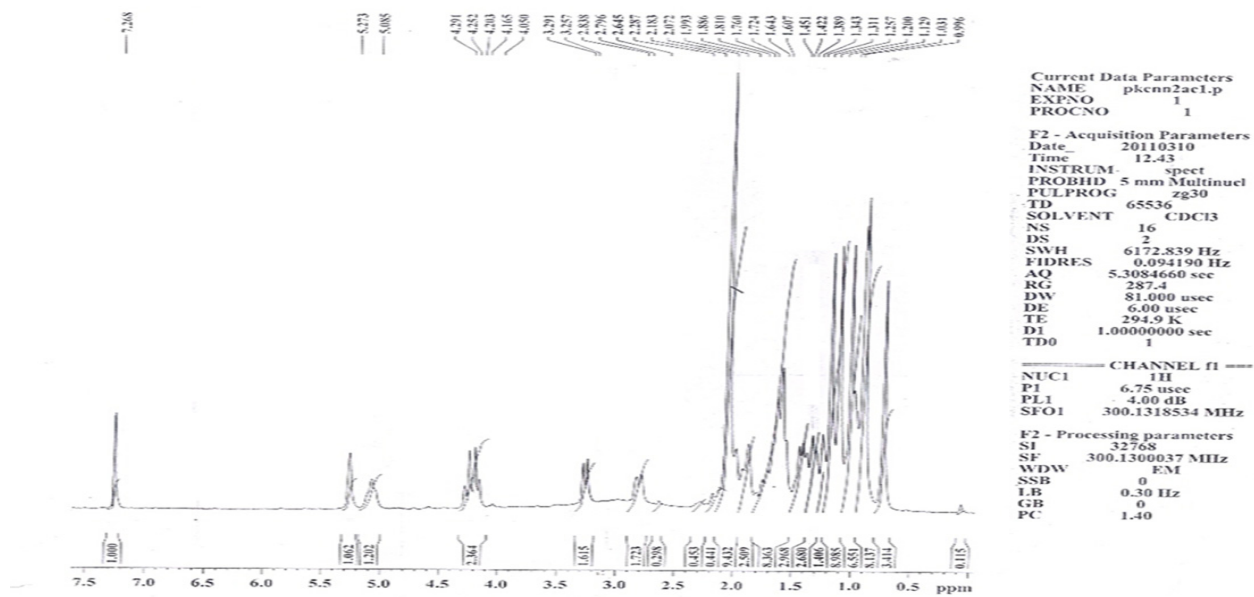
F2 - Processing parameters  
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F1 - Processing parameters  
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 SSB 0  
 LB 0.00 Hz  
 GB 0

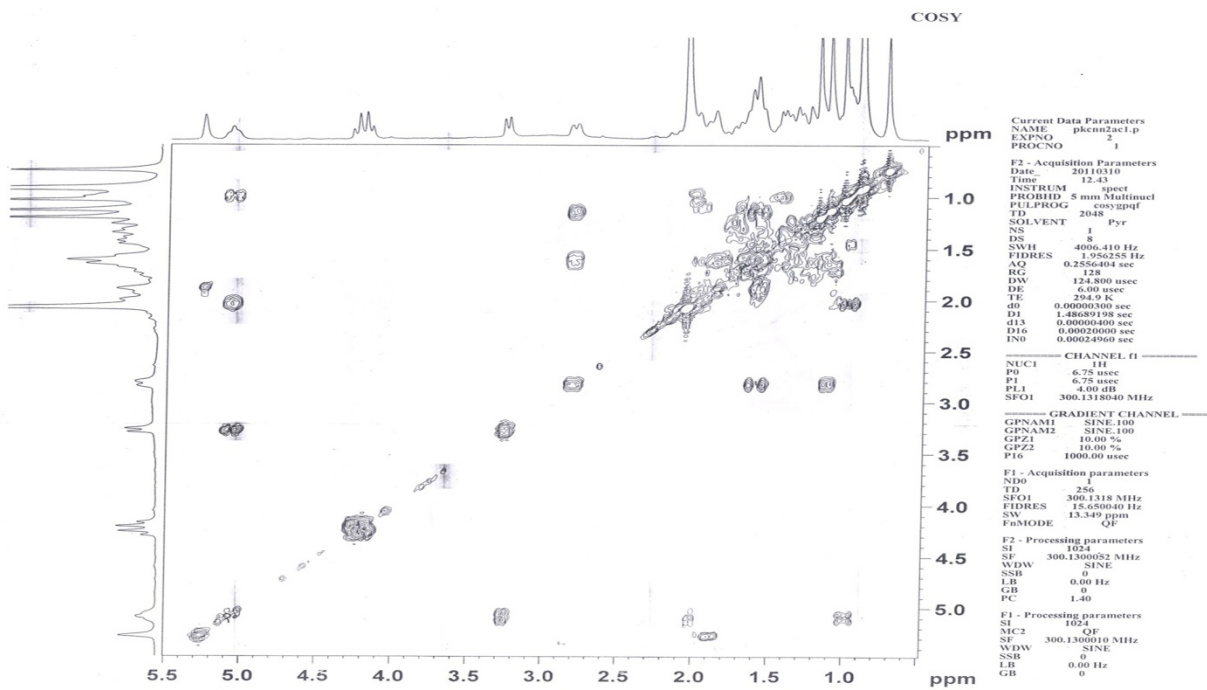
$^1\text{H}$ - $^1\text{H}$  COSY of compound **3a** at 300 MHz ( $\text{CDCl}_3$ )



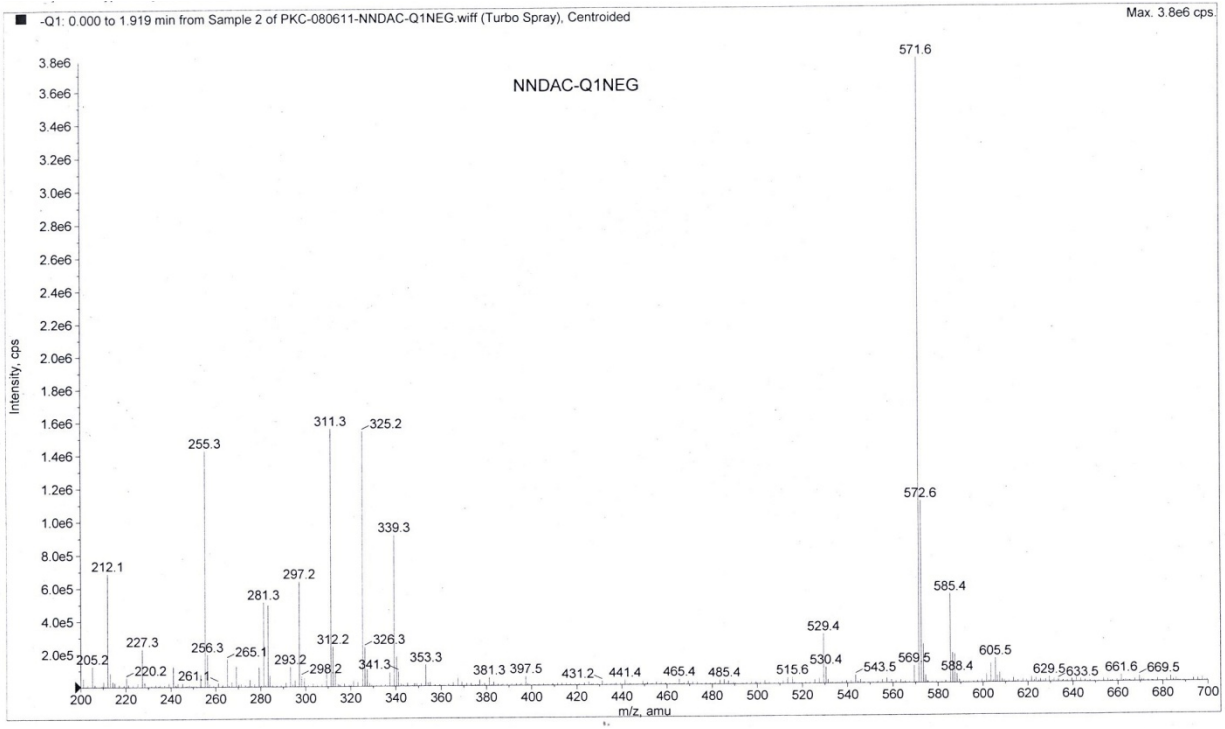
ESI-MS of compound 3a



$^1\text{H}$  NMR of compound **3b** at 300 MHz ( $\text{CDCl}_3$ )

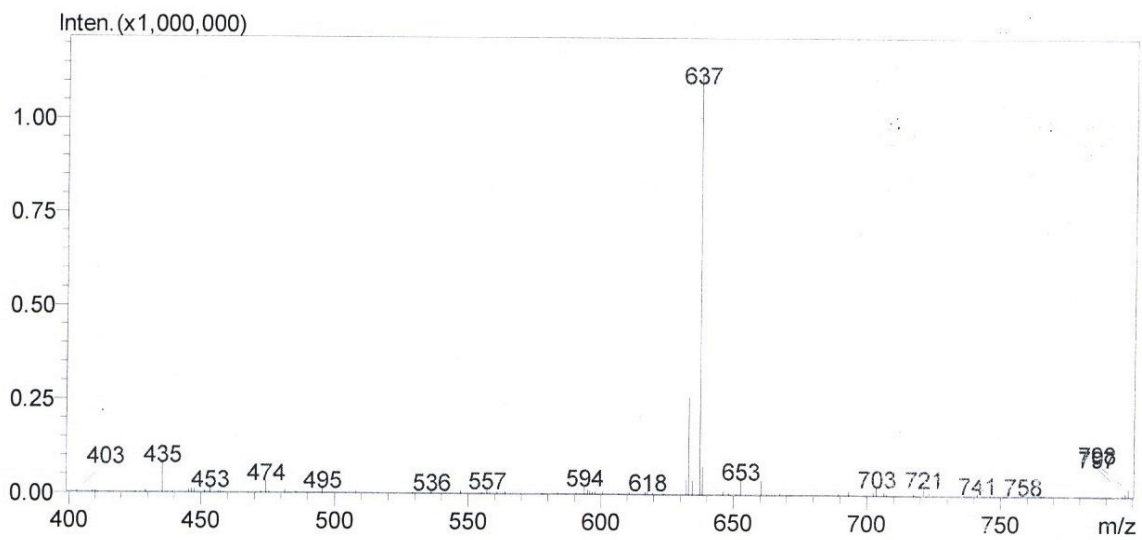


$^1\text{H}$ - $^1\text{H}$  COSY of compound **3b** at 300 MHz ( $\text{CDCl}_3$ )

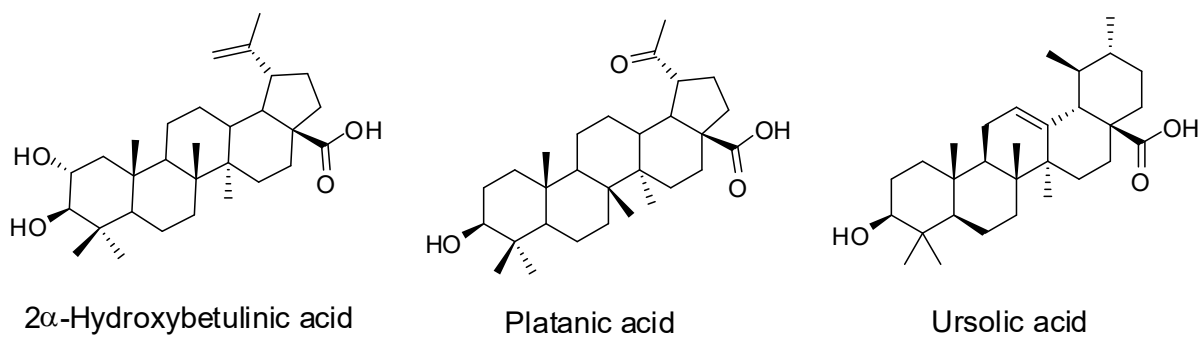


ESI-MS of compound **3b**





ESI-MS of compound 3c



**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.)	$R_{L20}^2$	$r^2$ (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