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Supplementary materials

Anti-Inflammatory Potential of Daturaolone from *Datura innoxia* Mill.: In Silico, In Vitro and In Vivo Studies

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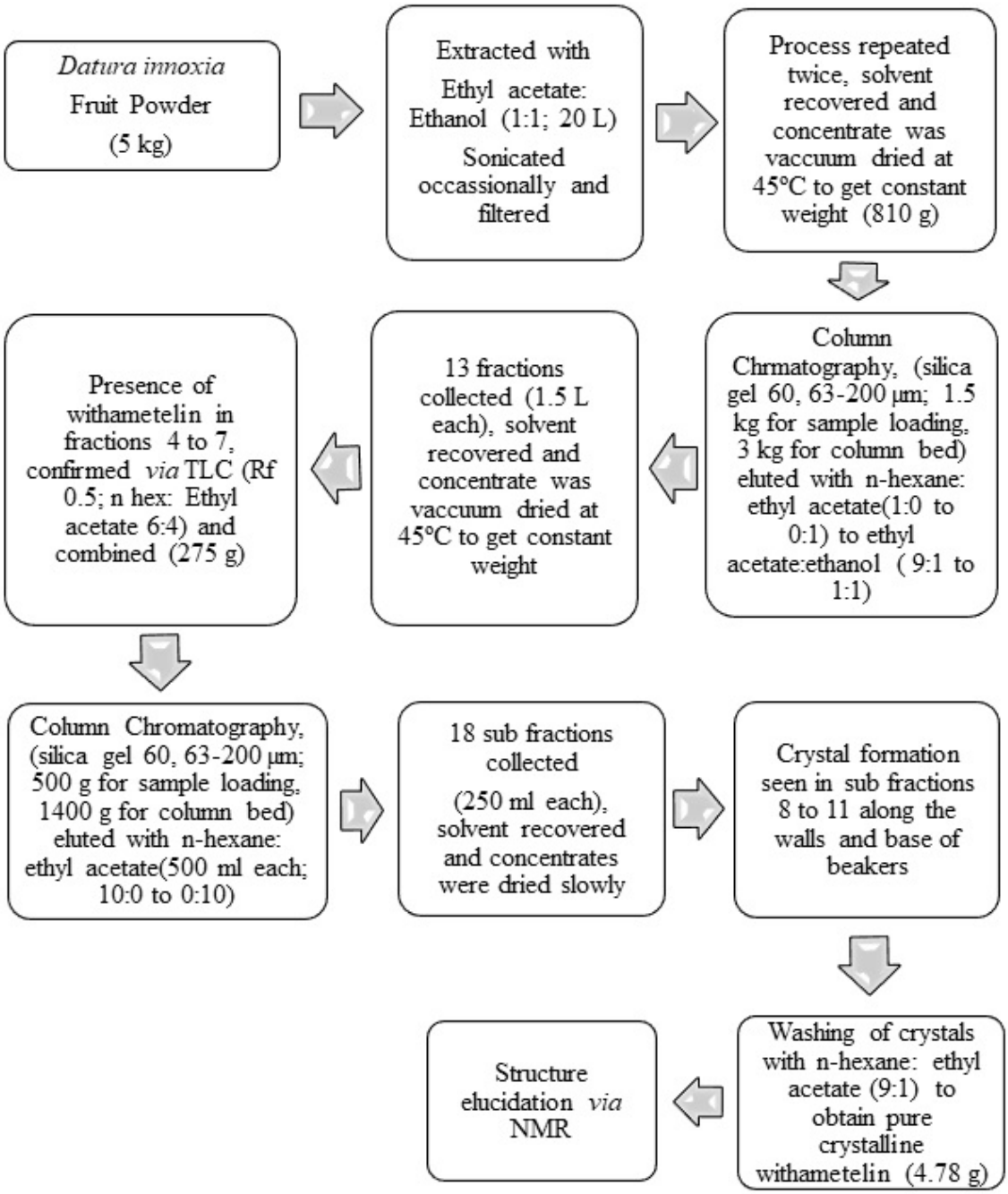

Figure S1.a. Isolation scheme of daturaolone**.**

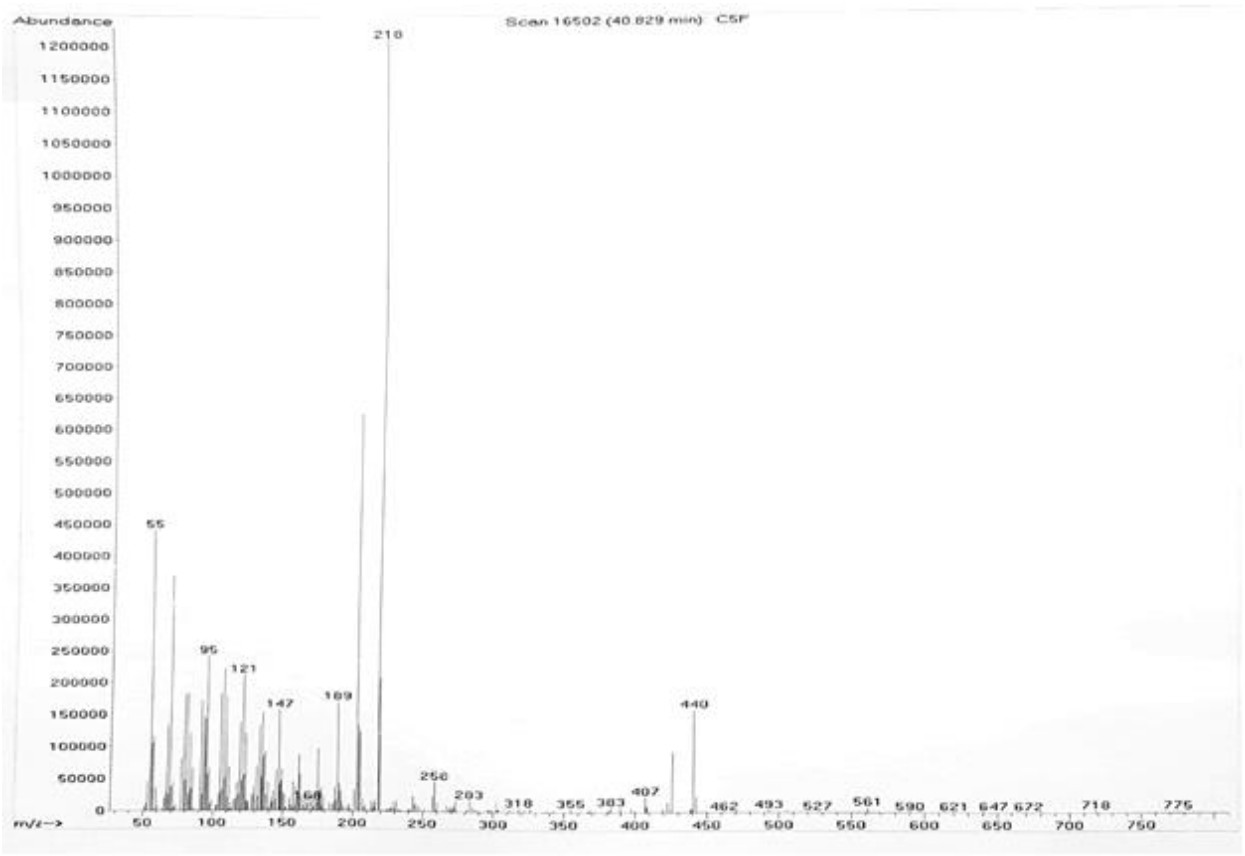

Figure S1b. GC-MS spectra of daturaolone

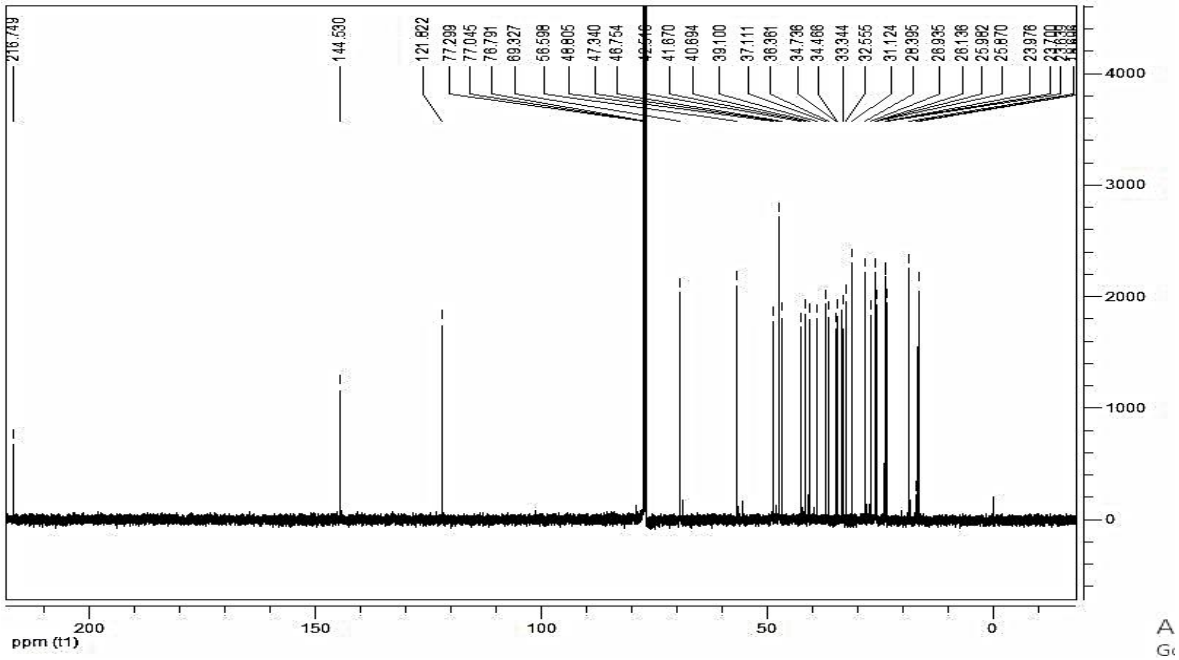

Figure S1c. ^{13}C-NMR

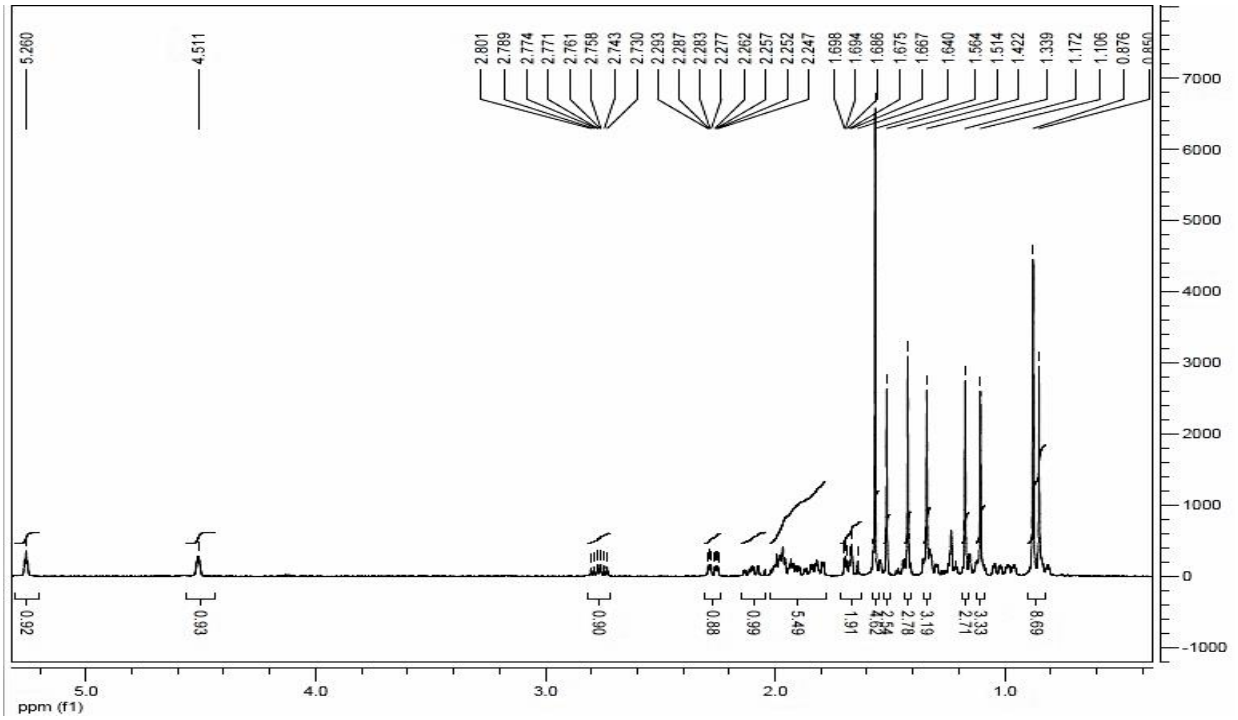

Figure S1d. 1H-NMR

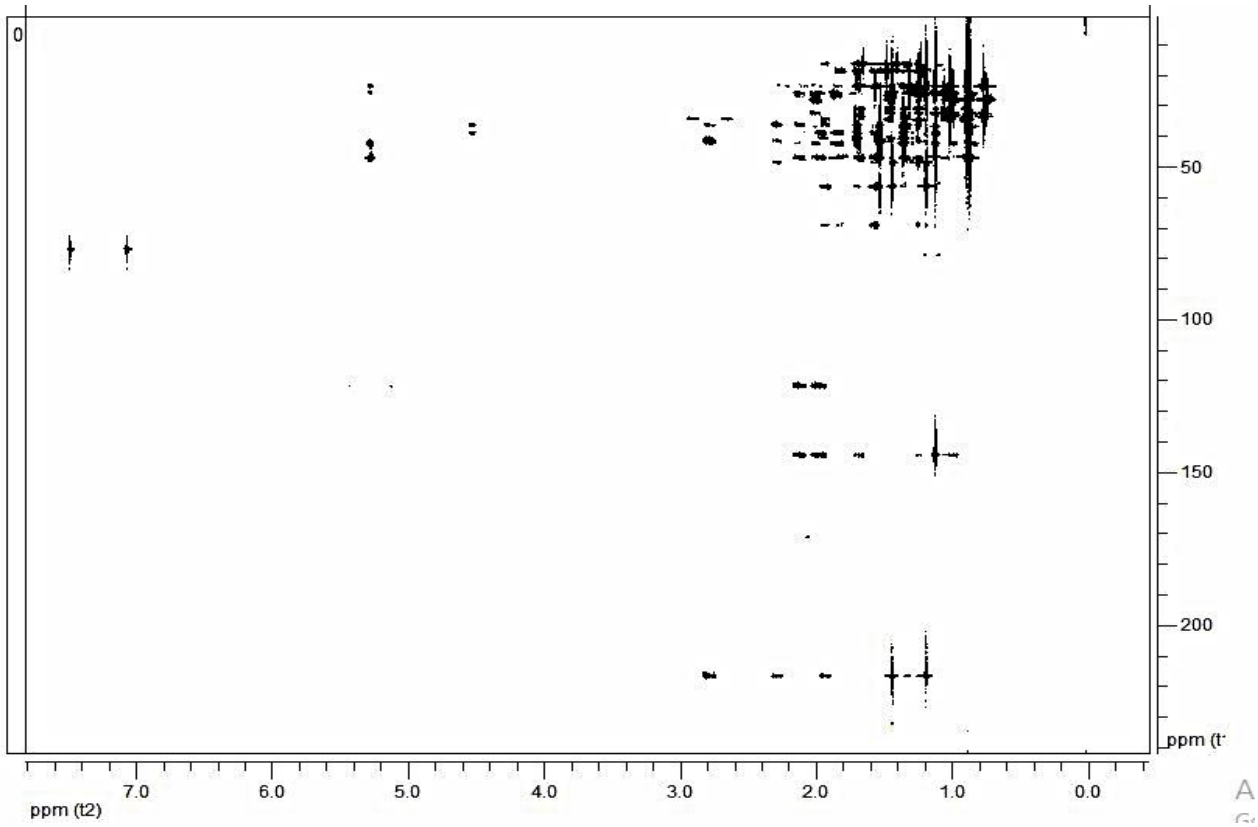

Figure S1e. HSQC NMR

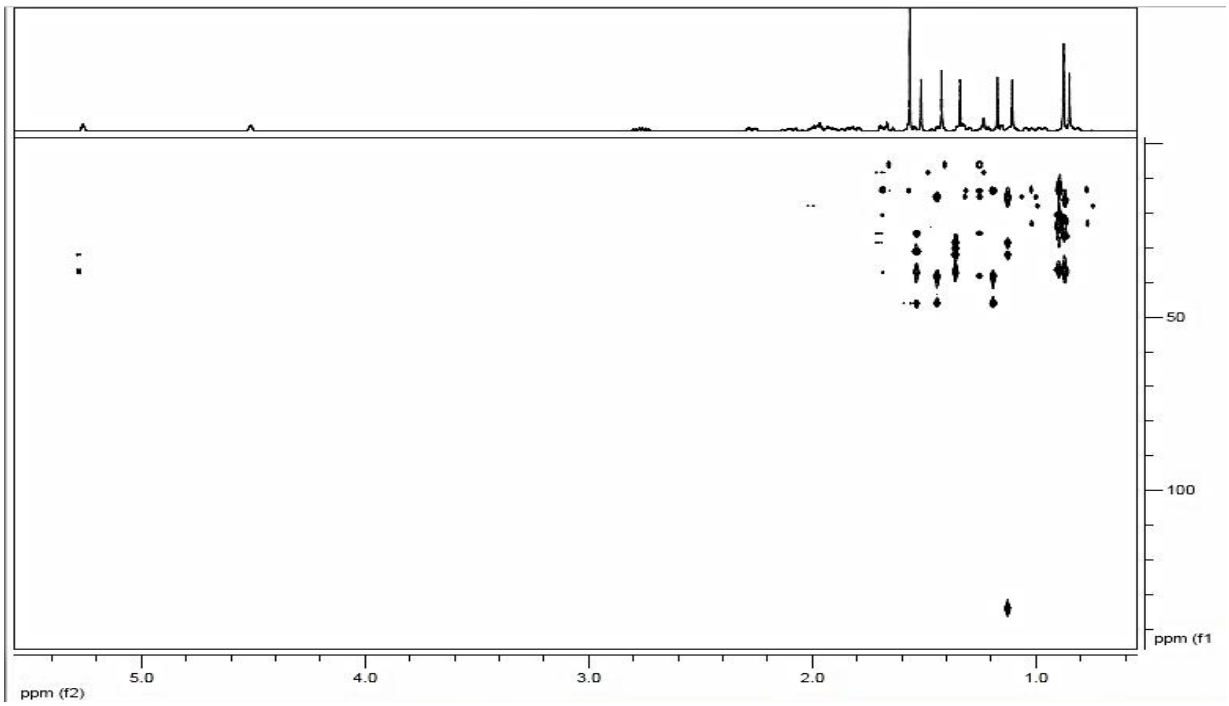

Figure S1f. HMBC NMR

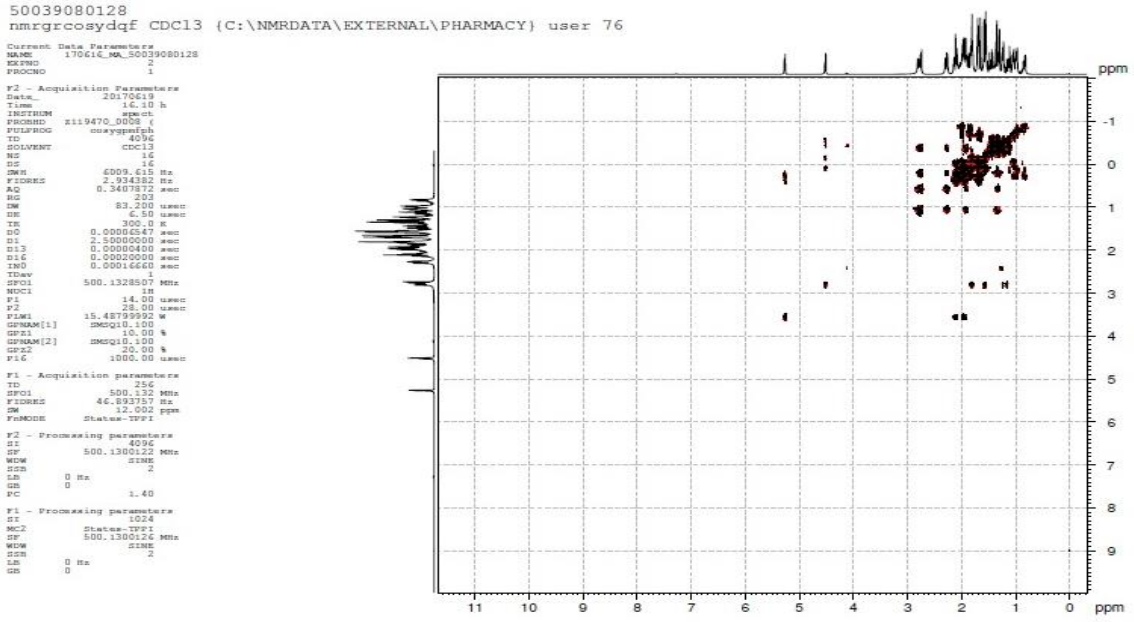

Figure S1g. COSY NMR

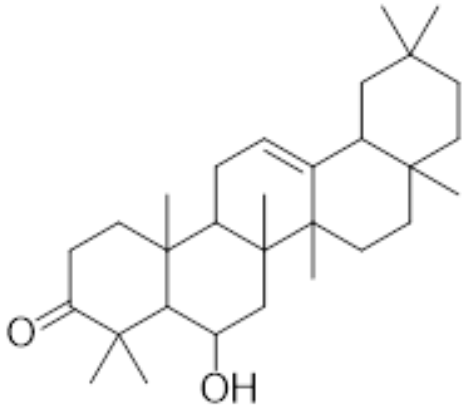

Figure S1h. Elucidated structure of daturaolone

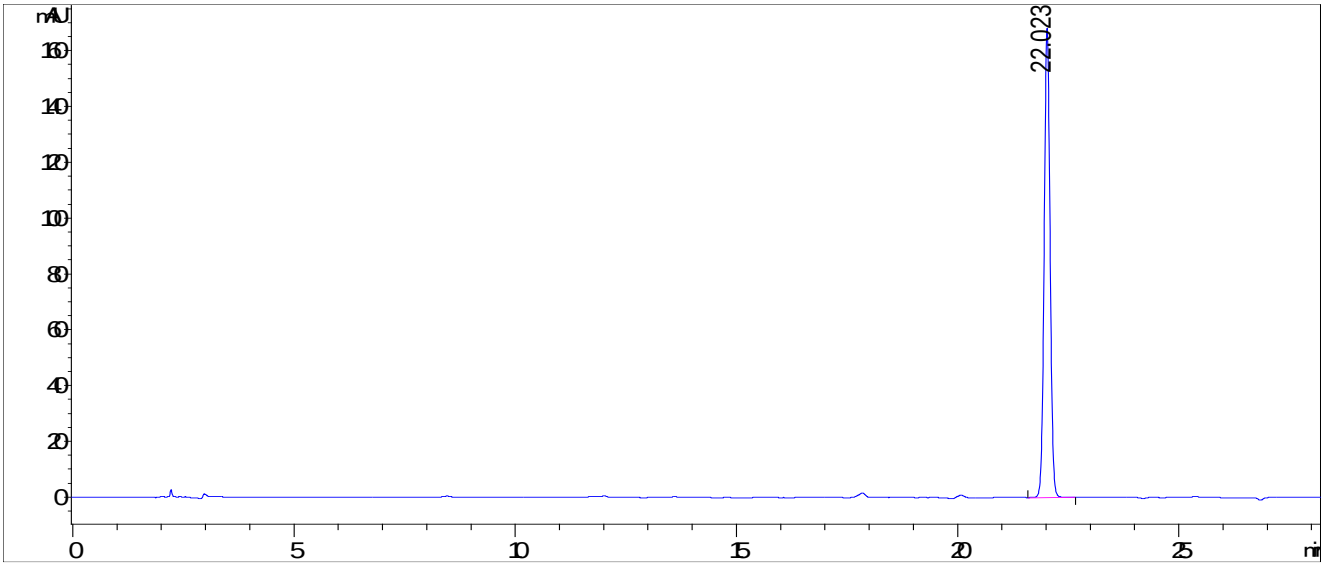

Figure S1i. HPLC DAD Chromatogram of daturaolone.

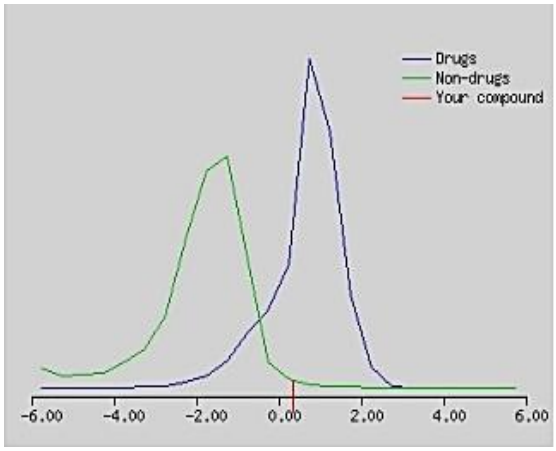

Figure S2. Drug likeliness prediction by molsoft with score of 0.33

Table S1. ADME data table of Daturaolone from SWISS ADME

Molecule	Daturaolone
Canonical SMILES	OC1CC2(C)C(C3(C1C(C)(C)C(=O)CC3)C)CC=C1C2(C)CCC2(C1CC(CC2)(C)C)C
Formula	$C_{30}H_{48}O_2$
MW	440.7
#Heavy atoms	32
#Aromatic heavy atoms	0
Fraction Csp3	0.9
#Rotatable bonds	0
#H-bond acceptors	2
#H-bond donors	1
MR	135.08
TPSA	37.3
iLOGP	4.37
XLOGP3	7.49
WLOGP	7.35
MLOGP	5.89
Silicos-IT Log P	6.61
Consensus Log P	6.34
ESOL Log S	-7.29
ESOL Solubility (mg/ml)	2.25E-05
ESOL Solubility (mol/l)	5.12E-08
ESOL Class	Poorly soluble
Ali Log S	-8.11
Ali Solubility (mg/ml)	3.45E-06

Ali Solubility (mol/l)	7.82E-09
Ali Class	Poorly soluble
Silicos-IT LogSw	-7.04
Silicos-IT Solubility (mg/ml)	4.02E-05
Silicos-IT Solubility (mol/l)	9.12E-08
Silicos-IT class	Poorly soluble
BBB permeant	No
Pgp substrate	No
Lipinski #violations	1
Bioavailability Score	0.55
PAINS #alerts	0
Brenk #alerts	1
Leadlikeness #violations	2
Synthetic Accessibility	5.95

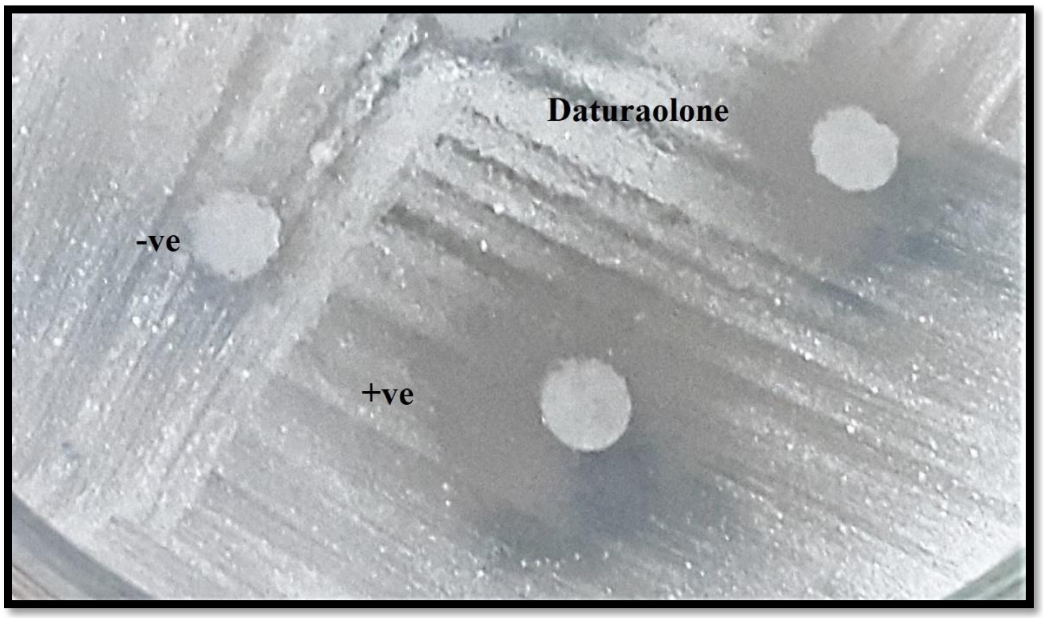

Figure S3. Protein kinase (PK) inhibitory potential of daturaolone (20 ug/disc). Surfactin infused disc was used as positive control and DMSO infused disc was used as negative control.