



Supplementary materials

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

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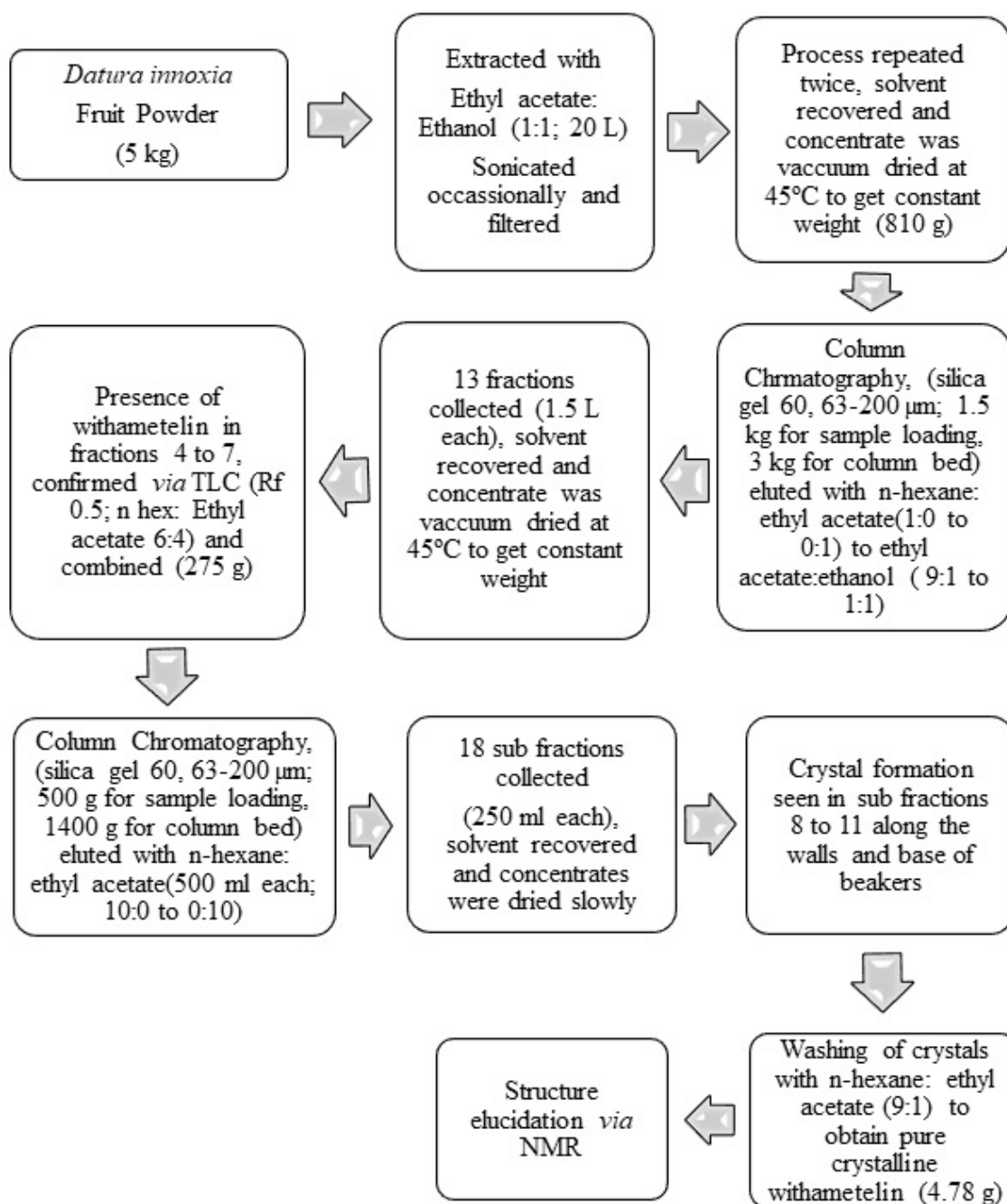


Figure S1.a. Isolation scheme of daturaolone.

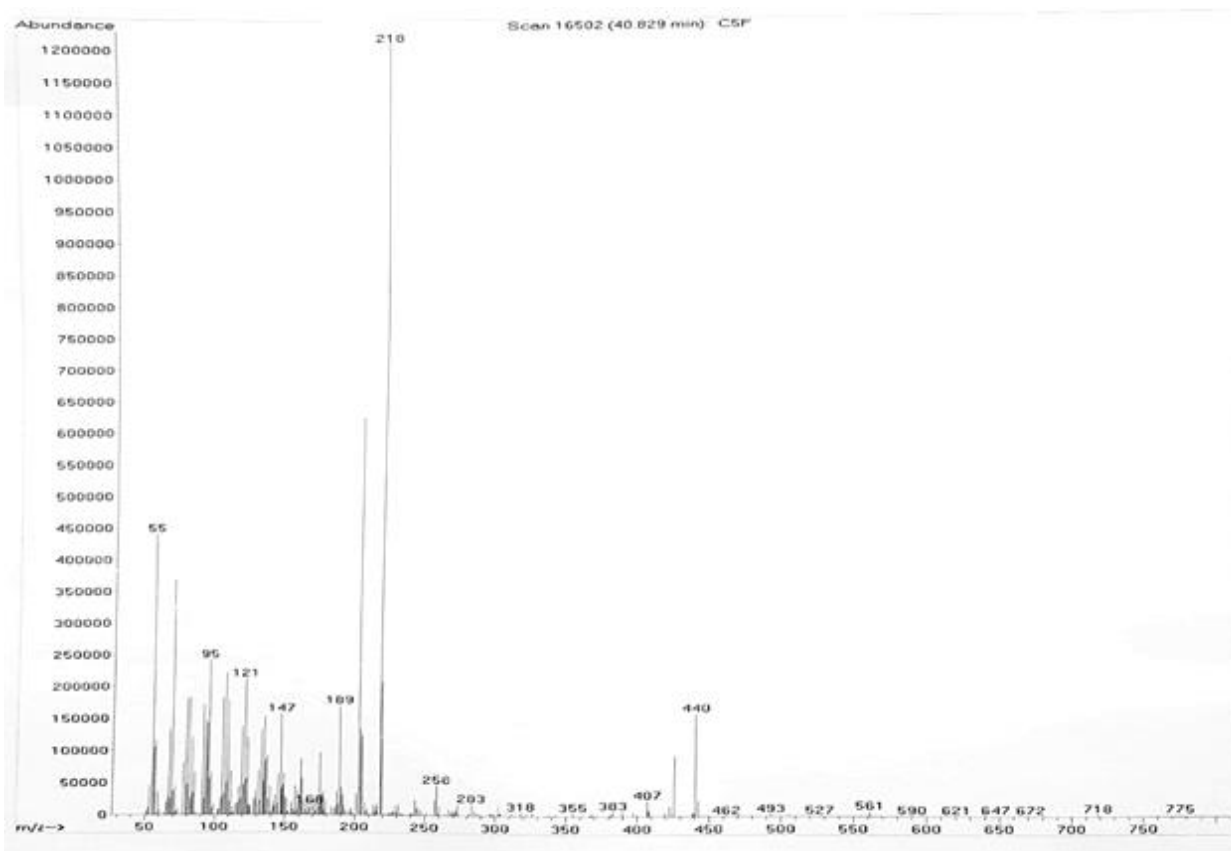


Figure S1b. GC-MS spectra of daturaolone

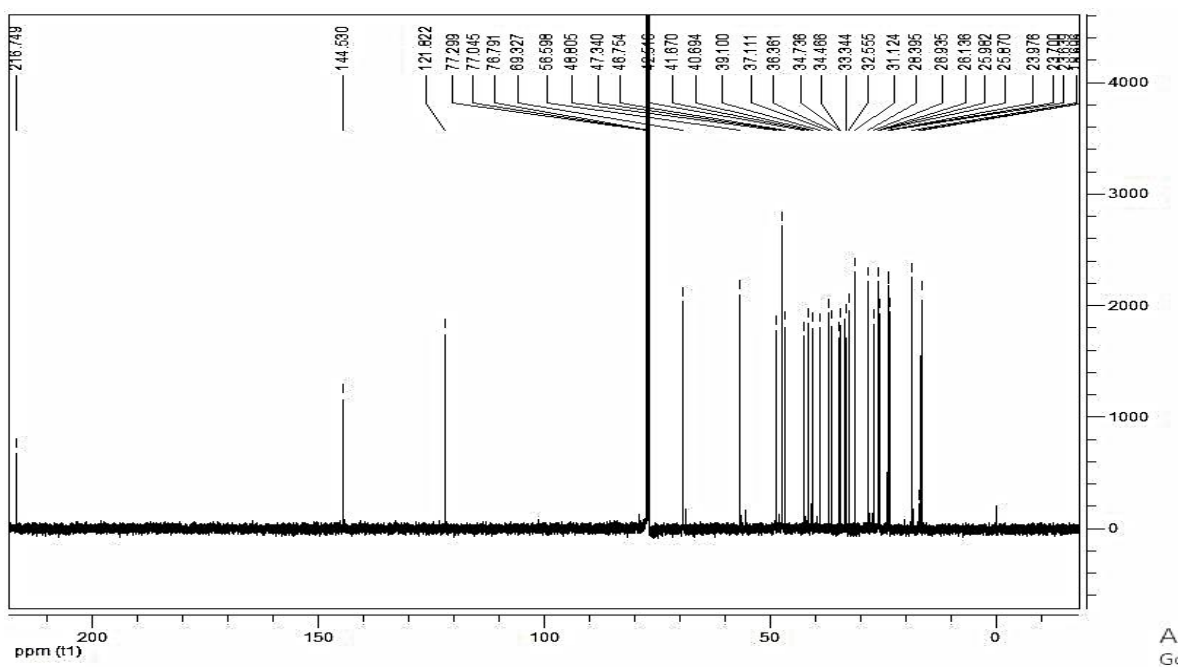


Figure S1c. ^{13}C -NMR

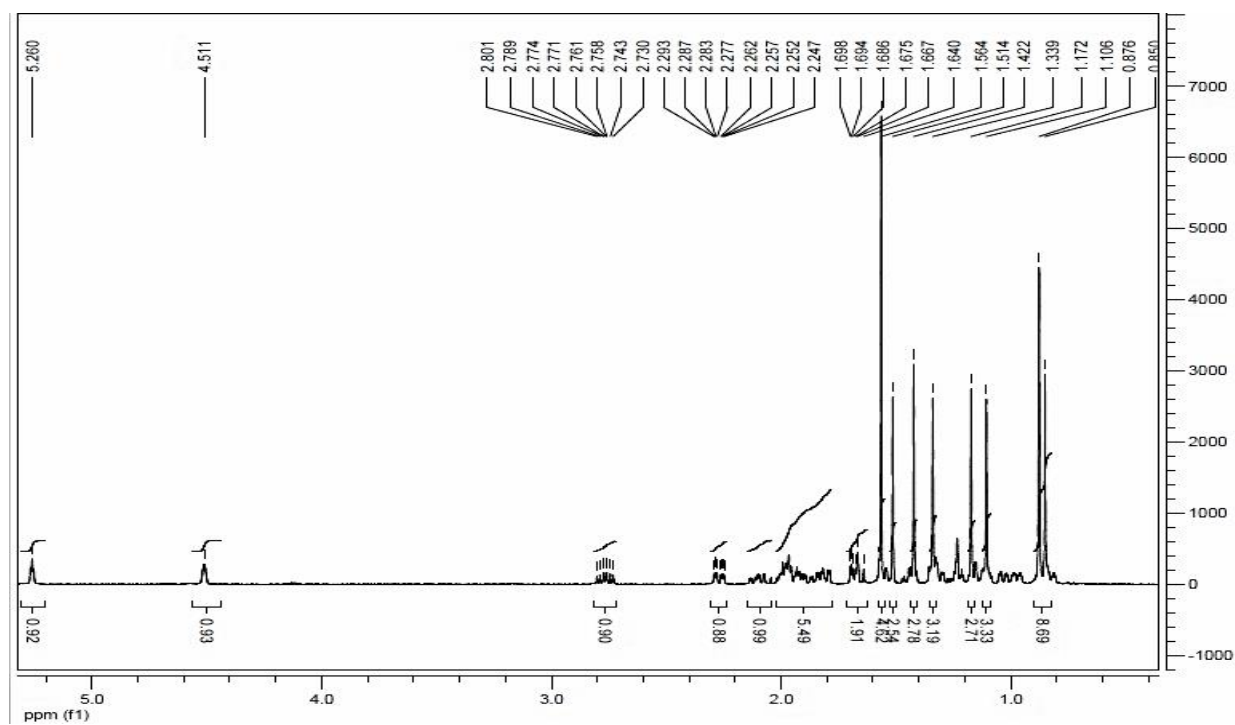


Figure S1d. ¹H-NMR

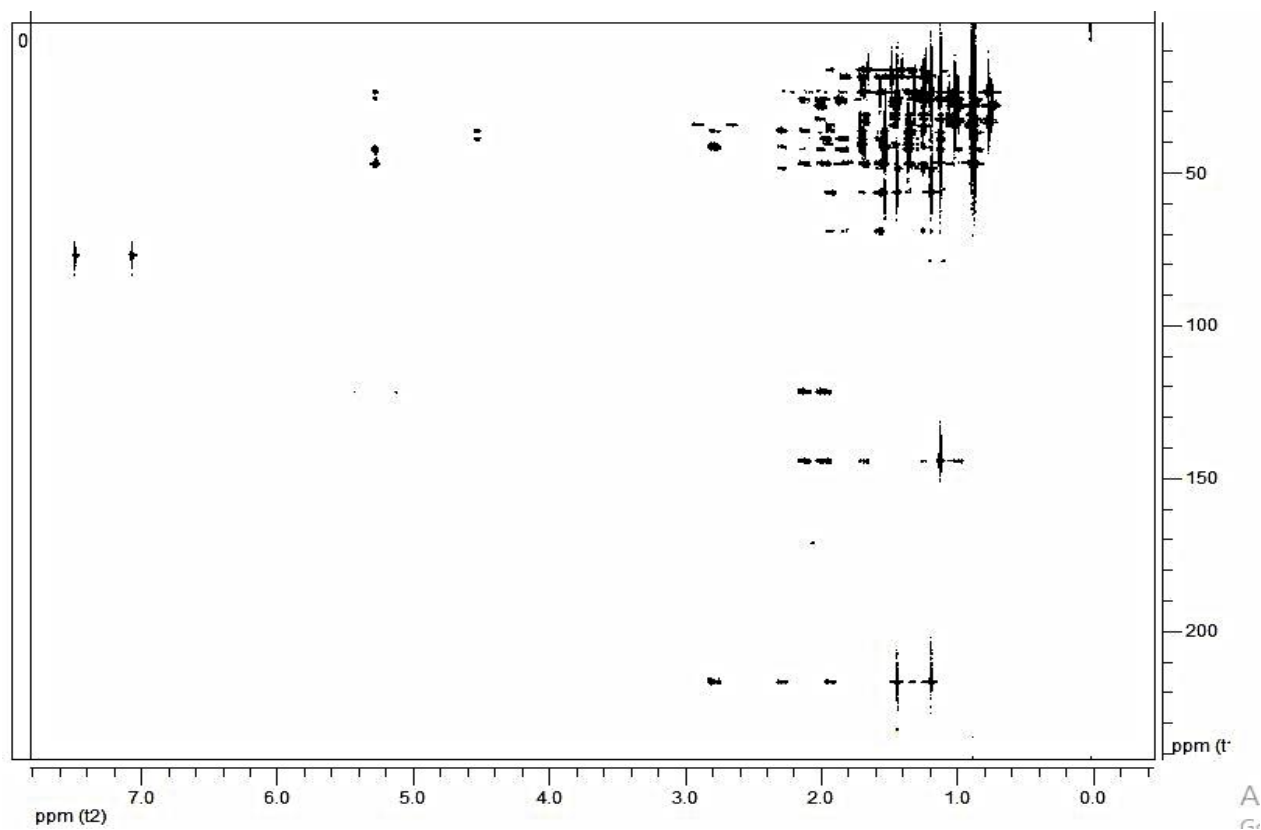


Figure S1e. HSQC NMR

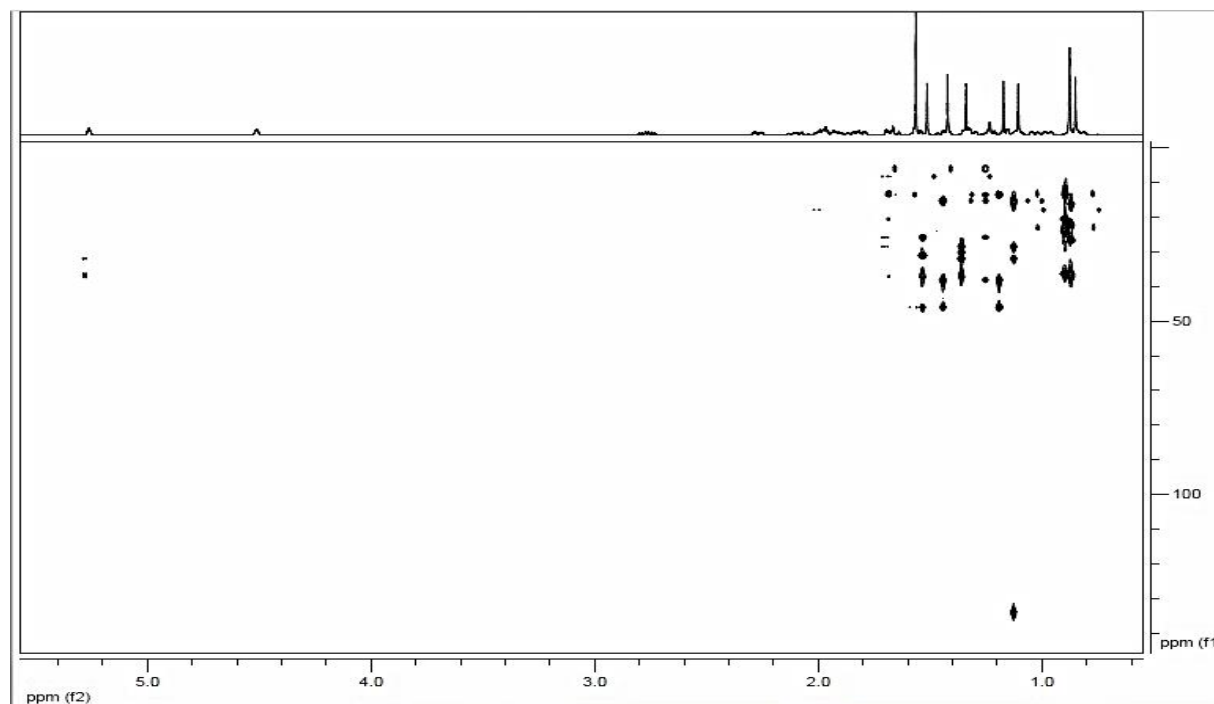


Figure S1f. HMBC NMR

50039080128
nmrgcossydcf CDC13 (C:\NMRDATA\EXTERNAL\PHARMACY) user 76

Current Data Parameters
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EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
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Time: 16.10 h
INSTRUM: spect
PROBHD: zll9470_0008 (4096
PULPROG: zgpg30
TD: 65536
SOLVENT: cdcl3
NS: 16
DS: 4
SWH: 6009.615 Hz
FIDRES: 2.934382 Hz
AQ: 0.3407872 sec
RG: 203
SW: 83.200 ussec
DE: 6.50 ussec
TE: 300.2 K
D0: 0.0000647 sec
D1: 2.30000000 sec
D13: 0.00000400 sec
D16: 0.00000000 sec
IN0: 0.00016660 sec
TD0: 1
SFO1: 500.1328507 MHz
NUC1: 1H
P1: 14.00 ussec
P2: 28.00 ussec
PL1: 15.48799992 W
SFO2: 500.132 MHz
F2RES: 46.893757 Hz
SW: 12.002 ppm
F2WDW: Shaped-TF2
SI: 4096
SF: 500.1300123 MHz
WDW: EM
SSB: 0 Hz
GB: 0
PC: 1.40

F1 - Acquisition parameters
TD: 256
SFO1: 500.132 MHz
FIDRES: 46.893757 Hz
SW: 12.002 ppm
F2WDW: Shaped-TF2
SI: 4096
SF: 500.1300123 MHz
WDW: EM
SSB: 0 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
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PC: 1.40

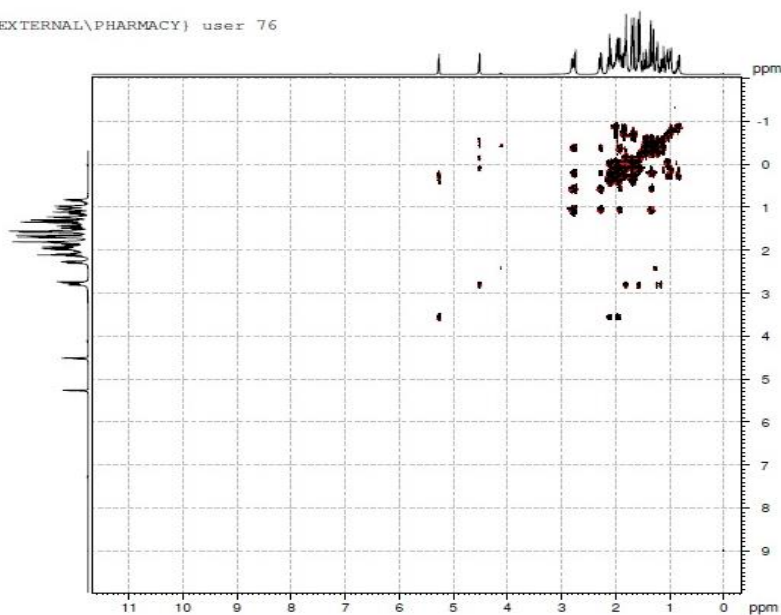


Figure S1g. COSY NMR

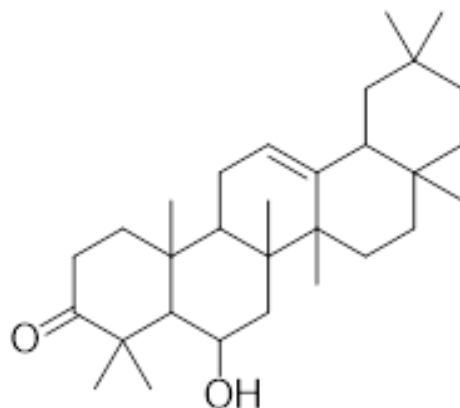


Figure S1h. Elucidated structure of daturaolone

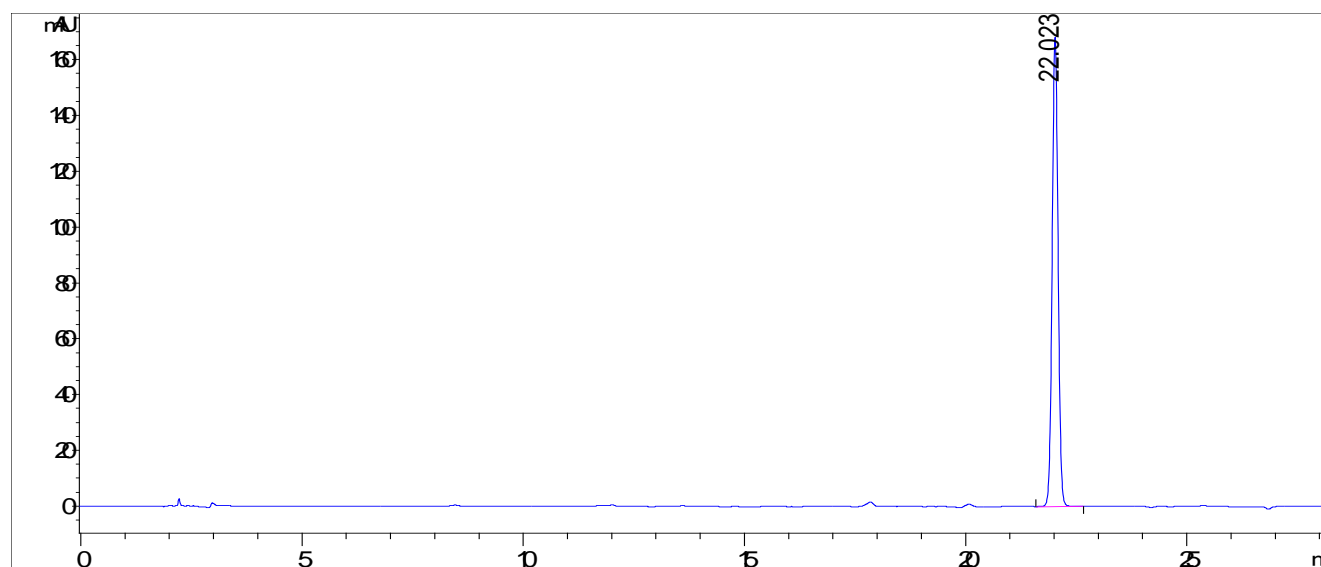


Figure S1i. HPLC DAD Chromatogram of daturaolone.

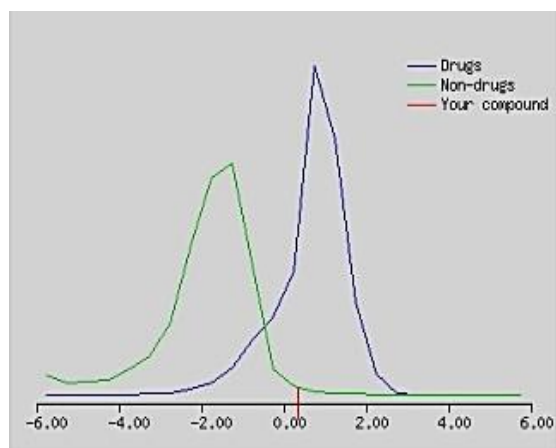


Figure S2. Drug likeliness prediction by molsoft with score of 0.33

Table S1. ADME data table of Daturaolone from SWISS ADME

Molecule	Daturaolone
Canonical SMILES	<chem>OC1CC2(C)C(C3(C1C(C)(C)C(=O)CC3)C)CC=C1C2(C)CCC2(C1CC(CC2)(C)C)C</chem>
Formula	C ₃₀ H ₄₈ O ₂
MW	440.7
#Heavy atoms	32
#Aromatic heavy atoms	0
Fraction Csp ³	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

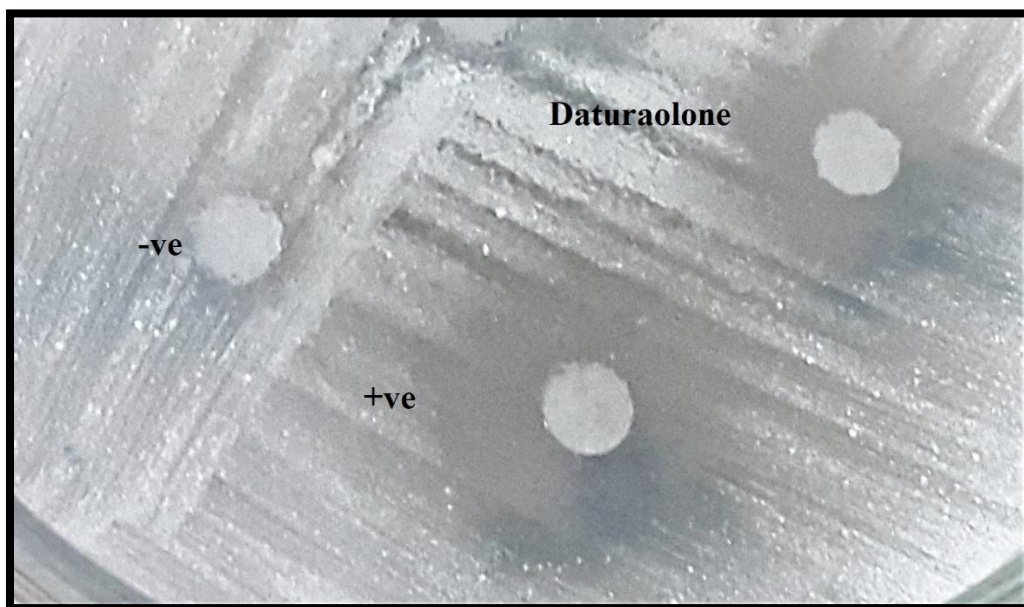


Figure S3. Protein kinase (PK) inhibitory potential of daturaolone (20 ug/disc). Surfactin infused disc was used as positive control and DMSO infused disc was used as negative control.