molecules

MDPI

Supplementary Materials

Bioguided Fractionation of Local Plants against Matrix Metalloproteinase9 and Its Cytotoxicity against Breast Cancer Cell Models: *In Silico* and *In Vitro* Study (II)

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Figure S1: The mass spectrum of OTC.

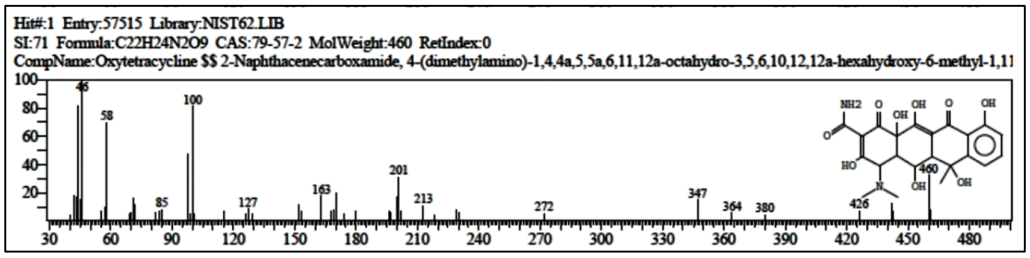


Figure S2: The ^{1}H-NMR spectrum of OTC.

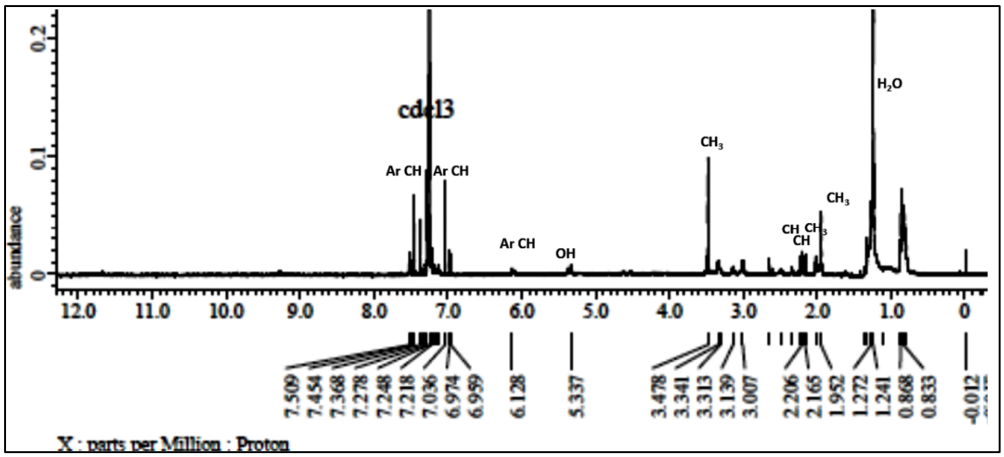


Figure S3: The FTIR spectrum of OTC.

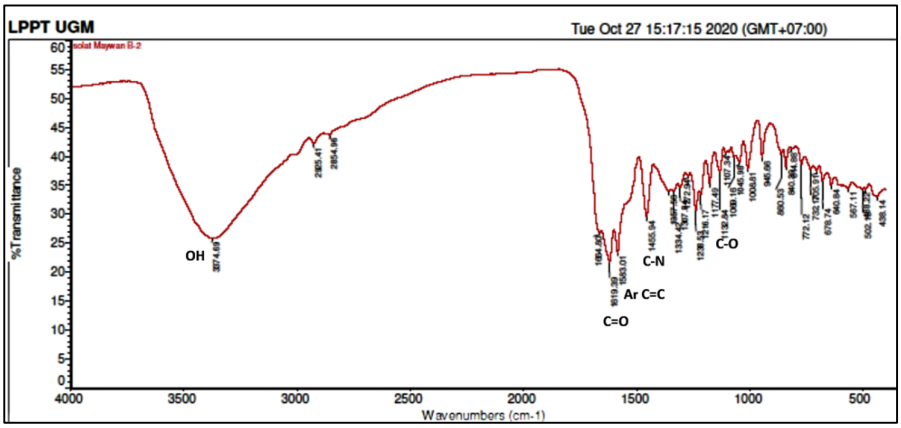


Figure S4: The ^{1}H-NMR spectrum of DOP.

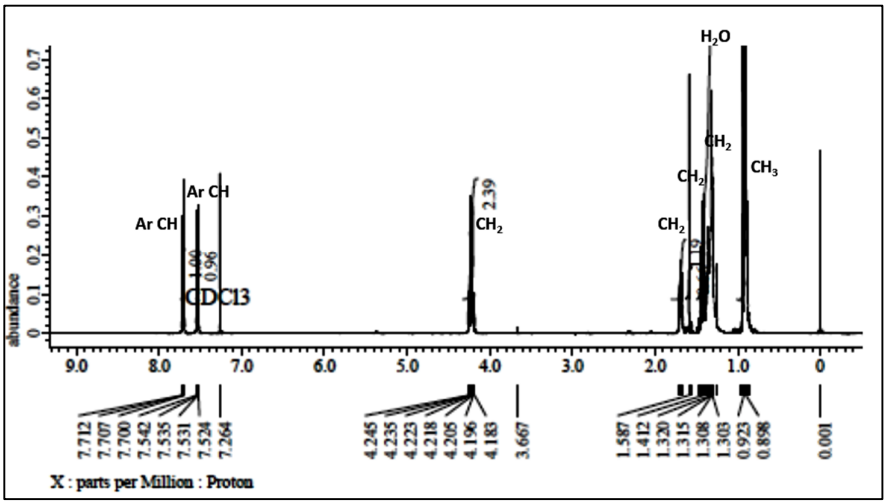


Figure S5: The ^{13}C-NMR spectrum of DOP.

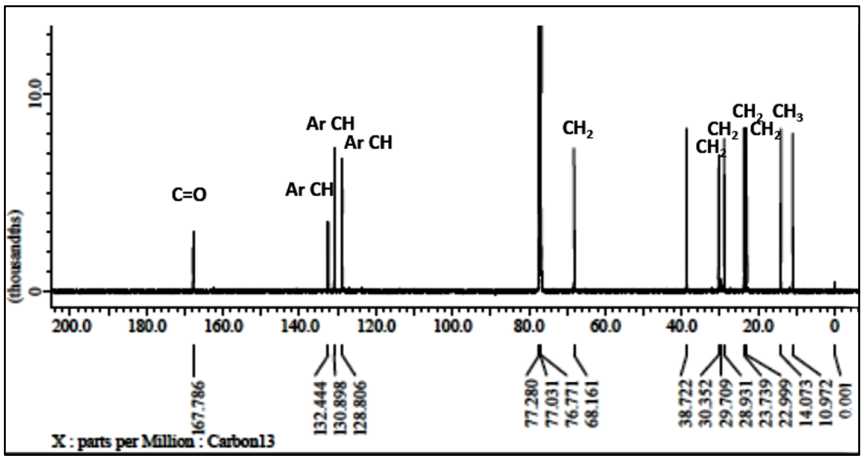


Figure S6. The mass spectrum of DOP.

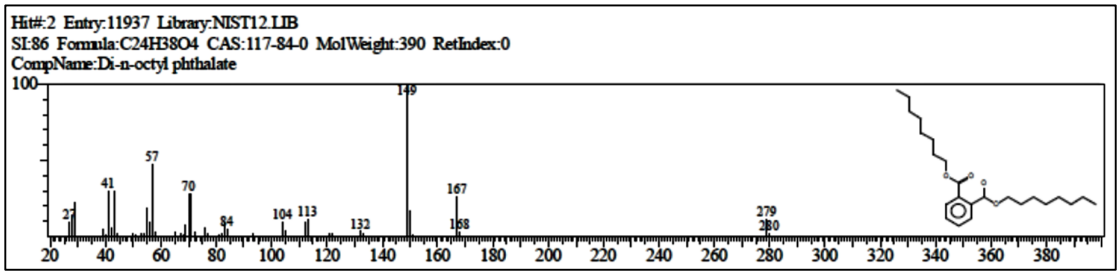
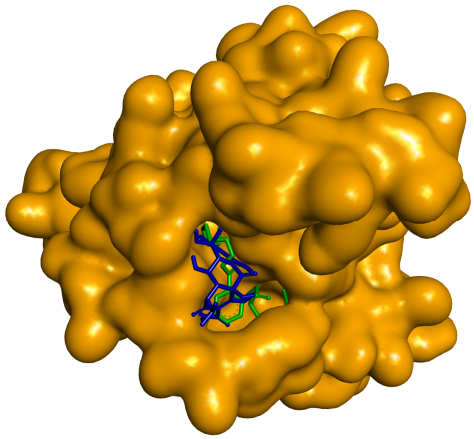


Figure S7. The overlapped pose of OTC and DOP into the GTP-binding site of Cdc42. The FEB of DOP = -6.73 kcal/mol whereas OTC = -5.64 kcal/mol. The protein is presented in surface model (orange), the ligands are presented in blue stick model (OTC) and green stick model (DOP).



GC-MS condition :

Sample : 5 mg / 1 mL of chloroform

Volume of injection : 0.5 µL

Column : Rtx 5 MS column (diphenyldiethylpolysiloxane)

Carrier gas : Helium

Ion source temperature : 250 °C

Table S1. The additional information of the GC-MS condition.

Samples	Initial Temperature	Final Temperature	Rate	Held Time	m/z range
AC *n*-hexane	-	50 °C	-	2 mins	50 - 550
	50 °C	130 °C	20 °C/min	5 mins	
	130 °C	180 °C	12 °C/min	10 mins	
IC *n*-hexane	-	50 °C	-	2 mins	50 - 550
	50 °C	130 °C	20 °C/min	5 mins	
	130 °C	180 °C	12 °C/min	10 mins	
IC ethylacetate	-	60 °C	-	3.40 mins	50 - 1000
	60 °C	240 °C	12 °C/min	5 mins	
	240 °C	290 °C	60 °C/min	2 mins	