Supporting information

PEGylated graphene oxide as nano drug delivery vehicle for podophyllotoxin (GO/PEG/PTOX) and in vitro α-amylase/α-glucosidase inhibition activities

Fawad Islam[1], Farman Ali Khan[1]*, Nasir Mehmood Khan[2], Shujaat Ahmad[3], Ahad Amer Alsaiari[4], Mazen Almehmadi[4], Nadeem Ahmad[5] and Zaheer Ul-Haq[5,6]. Abdul Khaliq Jan[1], Mamdouh Allahyani[4], Abdulaziz Alsharif [4] and Ebenezer Ola Falade [7]

[1] Department of Chemistry, Shaheed Benazir Bhutto University, Sheringal Dir Upper (18000), Khyber Pakhtunkhwa, Pakistan.

[2] Department of Agriculture, Shaheed Benazir Bhutto University, Sheringal Dir Upper (18000), Khyber Pakhtunkhwa, Pakistan.

[3] Department of Pharmacy, Shaheed Benazir Bhutto University, Sheringal Dir Upper (18000), Khyber Pakhtunkhwa, Pakistan.

[4] Department of Clinical Laboratory Sciences, College of Applied Medical Sciences, Taif University, P.O. Box , 11099, Taif 21944, Saudi Arabia,

[5] H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan.

[6] Dr. Panjwani Center for Molecular medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

[7] Institute of food science and technology, Chinese Academy of Agriculture Sciences, Beijing China.

Correspondence: **Dr. Farman Ali Khan**

Assistant Professor

Email: farmanali@gmail.com; Tel.: (+92-944855408)

Table S1: FT-IR analysis for various functionalities in GO-COOH, GO-COOH-PEG and GO-PEG-PTOX.

Characteristic peaks	**F1**	**F2**	**F3**
υ (O-H)	3200-3450 (s, br)	3300 (w)	3300 (w)
υ (C-H)	--	2900 (s) CH_3 1400 CH_2	3000 CH_3, 2800 CH 2900 CH_2
υ (C=O)	1633 (s)	1650	1573
υ (C-O)	1000 (s, br)	1100	1000 (acidic), 1100 (alcoholic)
υ (C=C) aromatic	--	1477	1436
υ (C-H) rocking	1301 (CH_2 of cyclohexane) however lower OOP	1332	1400
υ (C=C) OOP	--	1223	1111

Table S2: α-Amylase inhibition activities of Acarbose (standard drug)

concentration (µg/mL)	**log ε_{max} at 540 nm (λ_{max})**	**%age Inhibition**
1000	0.134	63.78378
500	0.168	54.59459
250	0.179	51.62162
125	0.22	40.54054
62.5	0.231	37.56757
31.25	0.252	31.89189
15.62	0.252	31.89189
7.81	0.263	28.91892
3.9	0.263	28.91892
1.95	0.293	20.81081
0.97	0.3	18.91892
IC_{50} = 300 µg/mL		

Note: The absorption of control (Enzyme + Starch + DNS) was obtained as 0.379.

Table S3: ^{13}C- and ^{1}H-NMR ($CDCl_3$, 100 & 400 MHz) chemical shifts and multiplicities of PTOX.

C. No	Multipilicity	^{13}C- NMR (δ_C)	^{1}H-NMR (δ_H)
1	CH	44.9	4.4 to 4.7 (1H, m)
2	CH	43.8	2.8 (1H, d, *J*= 2 Hz)
3	CH	41.5	2.6 (1H, d, *J*= 2 Hz)
4	CH	70.1	4.4 to 4.7 (1H, m)
4′	-C-	130.9	--
5	CH	106.5	7.1-7.5 (1H, m)
6	-C-	144.1	--
7	-C-	145.0	--
8	CH	109.7	7.1-7.5 (1H, m)
8′	-C-	131.7	--
2′ (carbonyl of lactone)	-C-	178.6	--
3′ (Methylene of lactone)	CH_2	69.2	4.13 (2H, m)
Acetal	CH_2	101.5	5.9 (2H, s)
1″	-C-	138.3	--
2″	CH	106.6	6.7 (1H, s)
3″	-C-	153.4	--
4″	-C-	139.5	--
5″	-C-	153.4	--
6″	CH	106.6	6.7 (1H, s)
3″-Methoxy	CH_3	55.7	4.13 (1H,s)
4″-Methoxy	CH_3	60.8	4.13 (1H,s)
5″-Methoxy	CH_3	55.7	4.13 (1H,s)
4-OH	--	--	3.65 (s)

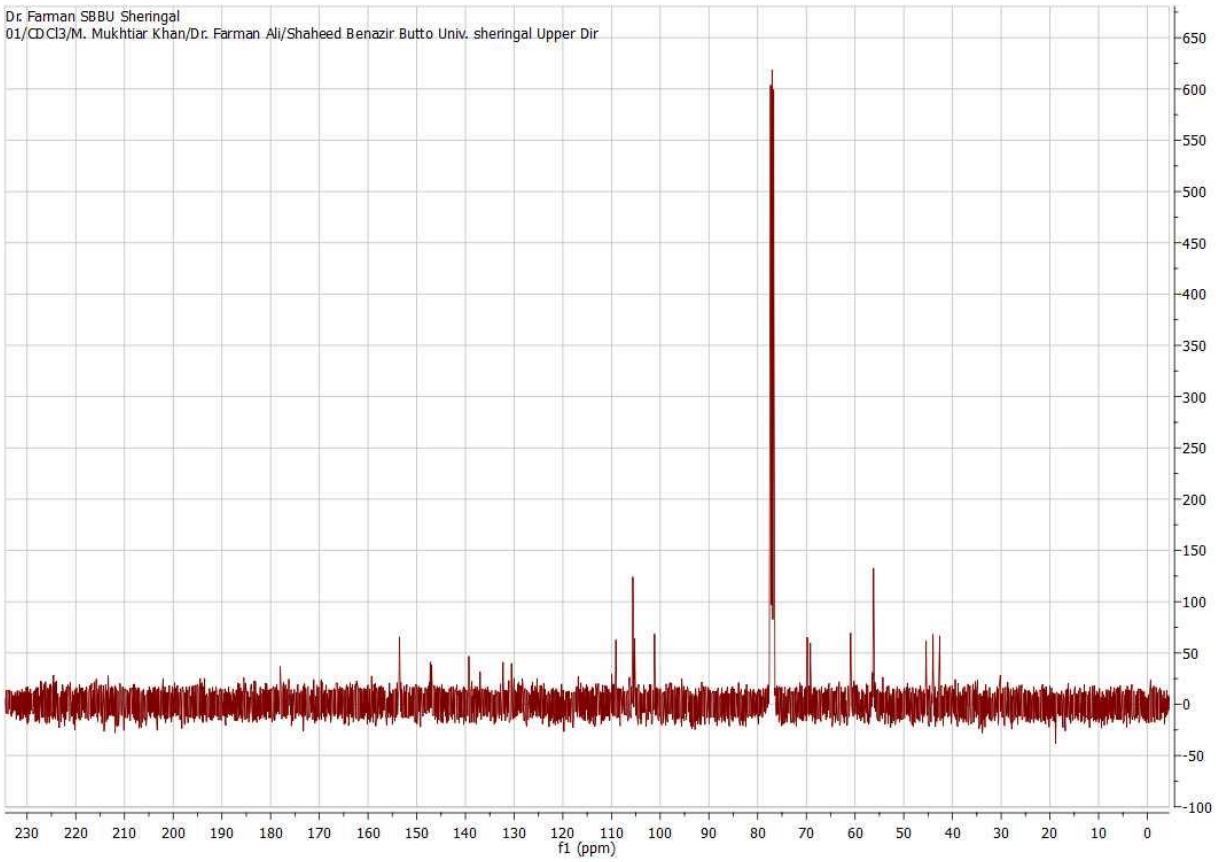

Figure S1: ^{13}C-NMR spectrum of podophyllotoxin in $CDCl_3$.

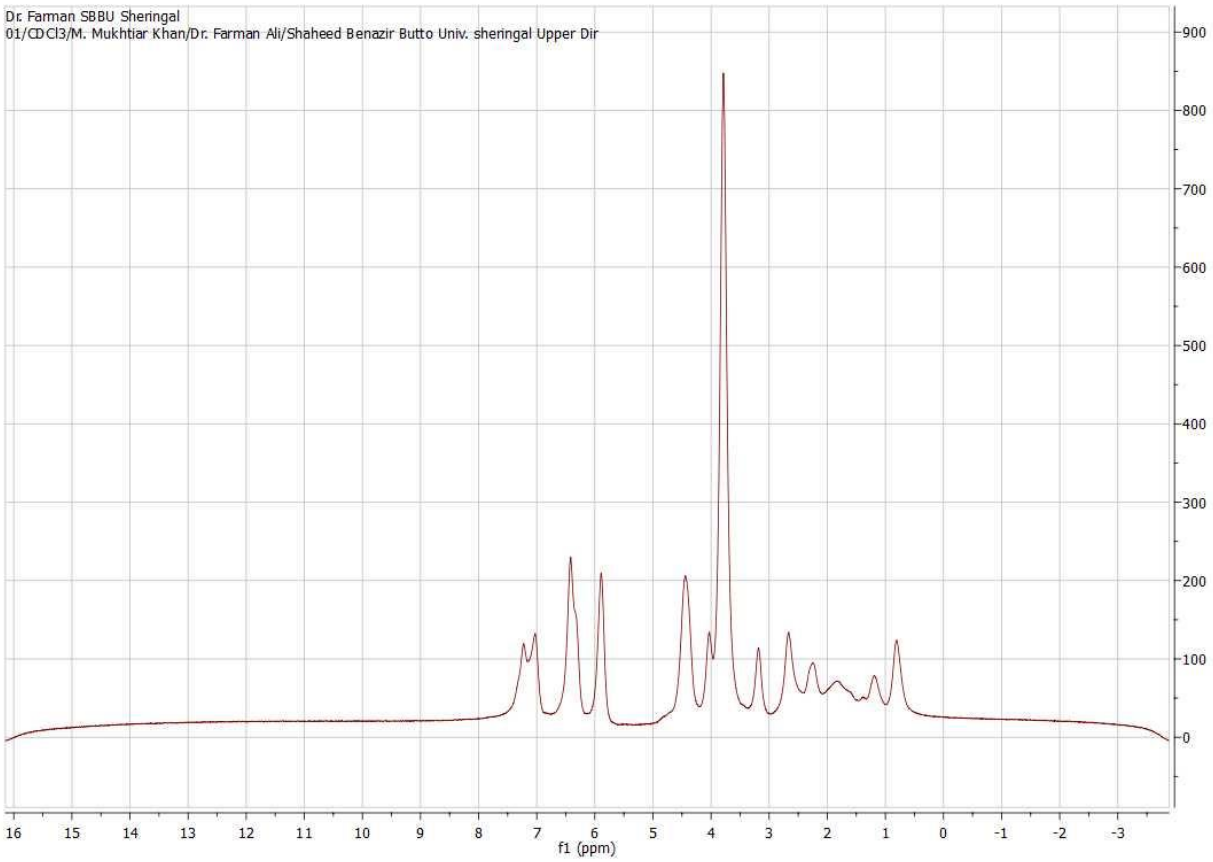

Figure S2: ^{1}H-NMR spectrum of podophyllotoxin in $CDCl_3$.

SI	RSI	Compound Name	Library	Probability	RT
586	607	Podofilox	replib	68.18	27.40
527	543	Cholestan-26-oic acid, 3,7,12-trihydroxy-, (3ä,5á,7ä,12ä)-	MAINLIB	12.32	27.40
503	578	1,1'-Biazulene, 3,3',8,8'-tetramethyl-5,5'-bis(1-methylethyl)-	MAINLIB	4.13	27.40

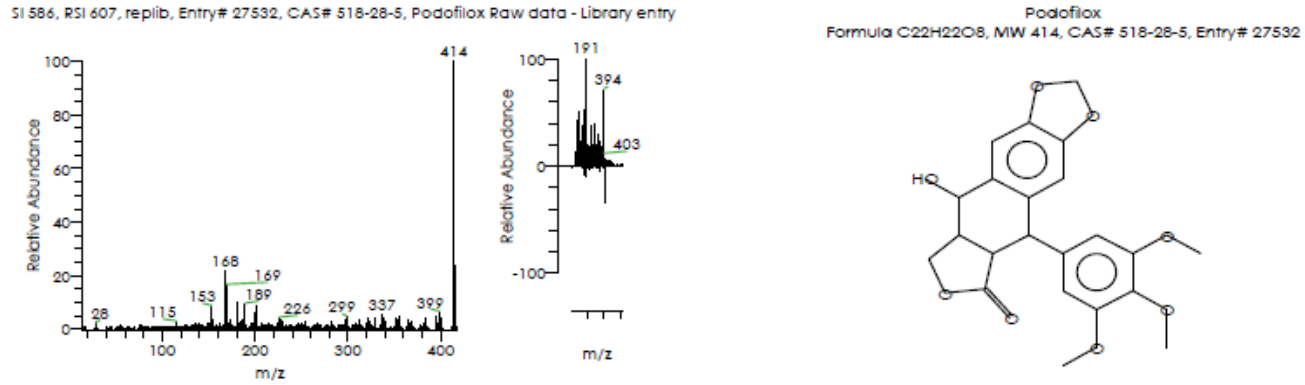

Figure S3: EI-MS spectrum and identification information of PTOX in RIPLAB data base.