

# Supplementary Materials: Development of Parvifloron D-loaded Smart Nanoparticles to Target Pancreatic Cancer

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**Table S1.** NMR data of PvD, (CDCl<sub>3</sub>, 1H 400 MHz, 13C 100 MHz;  $\delta$  in ppm, J in Hz).

Position	$\delta_H$	$J_{H,H}$	$\delta_C$	HSQC
1 $\alpha$	1.74 dd	(1 $\alpha$ , 1 $\beta$ ) 13.0	38.37	t
1 $\beta$	3.76 ddd	(1 $\alpha$ , 2 $\beta$ ) 11.4		
2 $\beta$	5.59 tt			
3 $\alpha$	1.56 dd			
3 $\beta$	2.15 ddd		67.87	d
4	---		45.06	t
5	---		38.58	s
6	6.41 d		164.84	s
7	---		118.69	d
8	6.79 d		139.13	d
9	---		127.45	s
10	---		127.17	s
11	---	(1 $\beta$ , 2 $\beta$ ) 4.4	43.91	s
12	---	(2 $\beta$ , 3 $\alpha$ ) 11.4	146.40	s
13	---	(2 $\beta$ , 3 $\beta$ ) 4.4	178.24	s
14	---	(3 $\alpha$ , 3 $\beta$ ) 12.5	141.61	s
15	6.96 d	(6, 7) 6.9	133.57	d
Me-16*	3.15 sept of d	(15,16(17)) 6.8	26.52	d
Me-17*	1.18 d	(14,15) 0.8	21.84	q
Me-18	1.16 d	(1 $\beta$ ,3 $\beta$ ) 2.4	21.63	q
Me-19	1.29 s	(2',3';5',6') 8.9	33.03	q
Me-20	1.42 s		30.58	q
1'	1.64 s		25.52	q
2', 6'	---		122.43	s
3',5'	7.93 d		131.89	d
4'	6.88 d		115.23	d
7'	---		160.58	s
4'-OH	---		166.18	s
11-OH	~7.70 br			
	~7.20 br			

**Table S2.** Significant assignments observed on HMBC experiment for PvD.

<b>Position</b>	<b>HMBC</b>
H-2',6'	C-7', C-4'
H-14	C-7, C-8, C-9, C-12, C-15
H-3',5'	C-1', C-4'
H-7	C-5, C-6, C-8, C-9, C-14
H-6	C-4, C-5, C-7, C-8, C-10
H-2 $\beta$	CO-(Ph)
H-1 $\beta$	C-2, C-3, C-5, C-20
H-15	C-12, C-13, C-14, C-16(17)
H-3 $\beta$	C-1, C-2, C-4, C-5, C-18, C-19
H-1 $\alpha$	C-2, C-3, C-5, C-9, C-20
H-3 $\alpha$	C-1, C-2, C-4, C-5, C-18, C-19
Me-20	C-1, C-5, C-9, C-10
Me-19	C-3, C-4, C-5, C-18
Me-18	C-3, C-4, C-5, C-19
Me-16(17)	C-13, C-15

**Table S3.** IC<sub>50</sub> ( $\mu$ M) values in different time points, 24h and 48h, of different cell lines-cytotoxicity assays.

	<b>Ins1-E</b>	<b>MCF7</b>	<b>Caco-2</b>
<b>24 h</b>	21.6	35.1	32.1
<b>48 h</b>	20.9	34.7	31.9