Supplementary Materials: Novel Improved Synthesis of HSP70 Inhibitor, Pifithrin μ. in vitro Synergy Quantification of Pifithrin μ Combined with Pt Drugs in Prostate and Colorectal Cancer Cells

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Table S1. Table representing the CI index and Fa calculated for oxaliplatin and pifithrin-μ at varying combined concentrations against HT29 colorectal cancer cells.

Oxaliplatin (μM)	PES (μM)	CI (*n* = 3)	SEM	Fa (*n* = 3)	SEM
40	20	0.771	0.205	0.888	0.027
40	10	0.372	0.097	0.857	0.079
40	5	0.315	0.161	0.872	0.033
20	20	0.312	0.135	0.942	0.063
20	10	0.595	0.089	0.643	0.075
20	5	0.315	0.161	0.821	0.044
10	20	0.381	0.142	0.931	0.049
10	10	0.244	0.050	0.916	0.022
10	5	1.048	0.339	0.631	0.079
5	20	0.512	0.040	0.890	0.015
5	10	0.496	0.166	0.745	0.062
5	5	0.355	0.095	0.732	0.006
2.5	20	0.704	0.157	0.795	0.082
2.5	10	0.372	0.158	0.833	0.076
2.5	5	0.390	0.135	0.579	0.190

Table S2. Table representing the CI index and Fa calculated for cisplatin and pifithrin-μ at varying combined concentrations against PC-3 prostate cancer cells.

Cisplatin (μM)	PES (μM)	CI (*n* = 3)	SEM	Fa (*n* = 3)	SEM
20	15	0.665	0.114	0.855	0.026
20	10	0.627	0.164	0.814	0.013
20	5	0.549	0.072	0.758	0.027
10	15	0.689	0.073	0.829	0.027
10	10	0.767	0.065	0.729	0.009
10	5	0.799	0.126	0.583	0.032
5	15	0.927	0.097	0.755	0.036
5	10	1.164	0.064	0.577	0.020
5	5	1.232	0.190	0.262	0.116
2.5	15	0.940	0.080	0.743	0.030
2.5	10	1.333	0.275	0.531	0.030
2.5	5	1.668	0.262	0.268	0.092
1	15	1.058	0.118	0.705	0.027
1	10	1.401	0.234	0.484	0.011
1	5	1.721	0.108	0.224	0.011

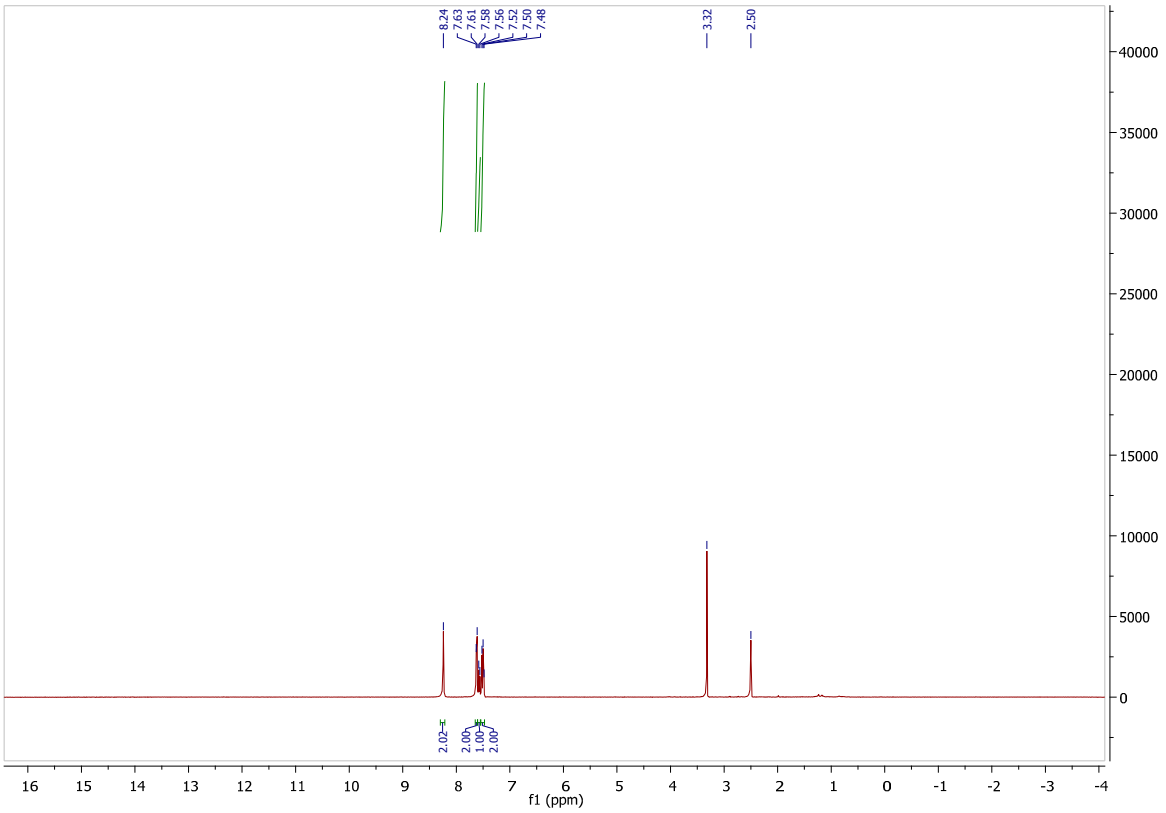

Figure S1 [1]H-NMR spectrum of pifithrin-μ in DMSO-d_6.

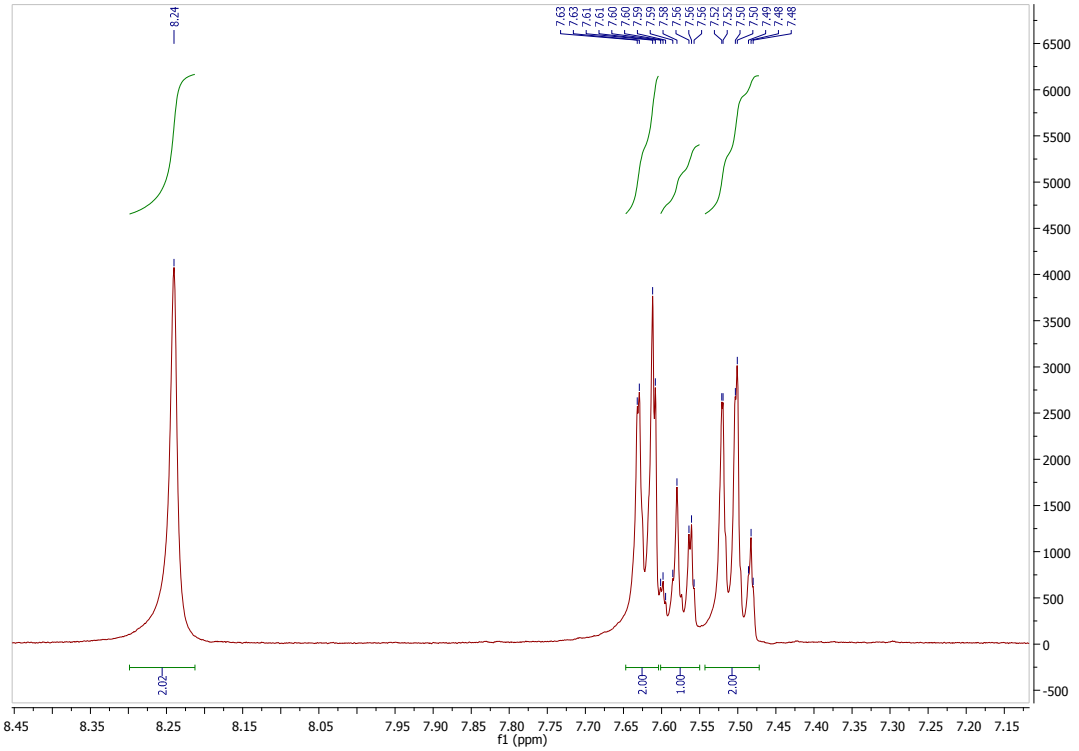

Figure S2. [1]H-NMR spectrum of pifithrin-μ in DMSO-d_6.

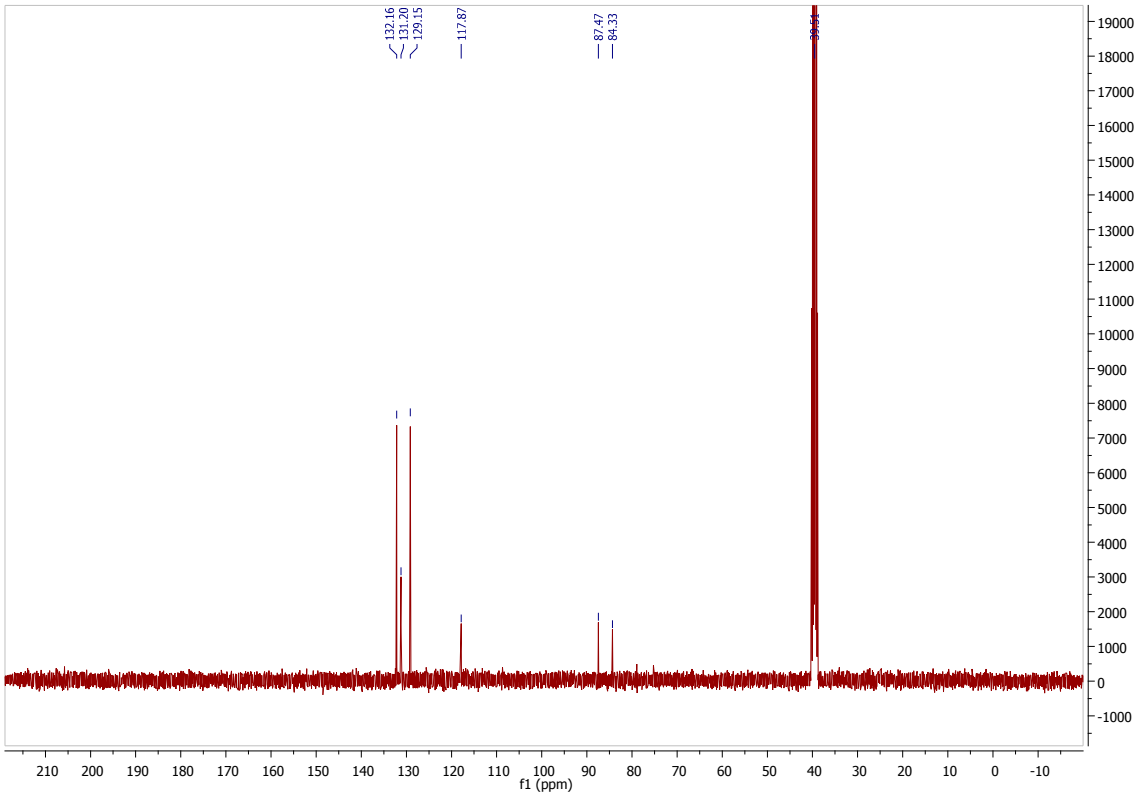

Figure S3. ^{13}C-NMR spectrum of pifithrin-μ in DMSO-*d*$_6$.

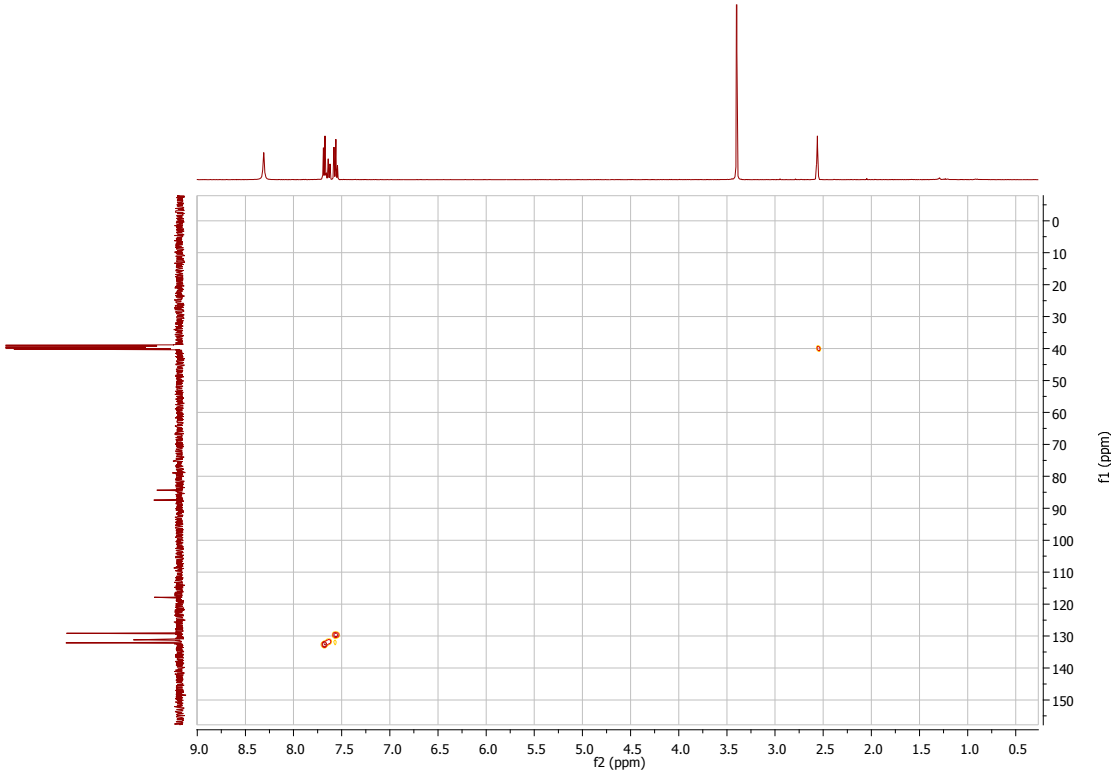

Figure S4. HSQC spectrum of pifithrin-μ in DMSO-*d*$_6$.

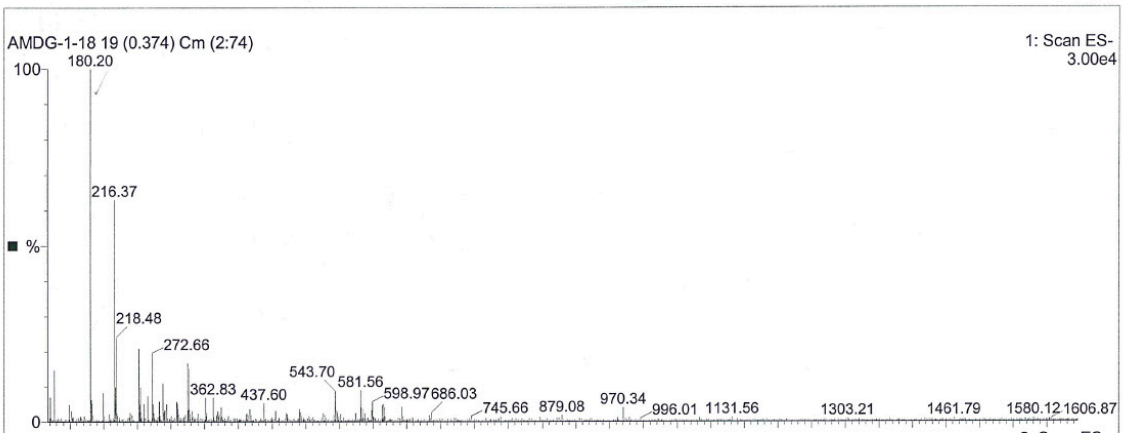

Figure S5. ESI mass spectrum of pifithrin-μ.

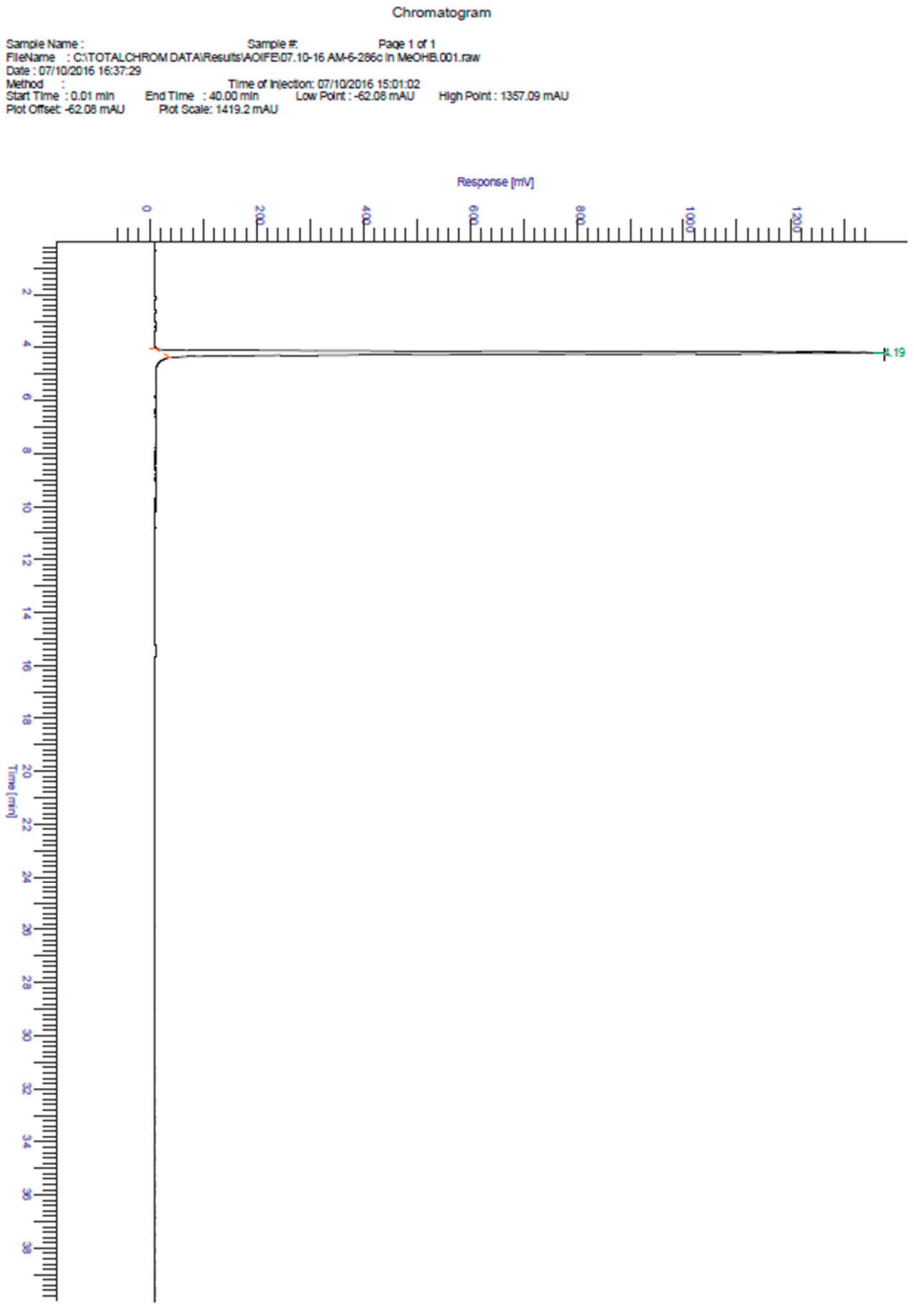

Figure S6. HPLC chromatogram of pifithrin-μ.

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Software Version	: 6.3.1.0504	Date	: 07/10/2016 16:37:27
Operator	: manager	Sample Name	:
Sample Number	:	Study	:
AutoSampler	: SER200	Rack/Vial	: 0/4
Instrument Name	: PerkinElmer LC	Channel	: B
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time	: 0.00 min	End Time	: 40.00 min
Sampling Rate	: 2.2727 pts/s		
Sample Volume	: 1.000000 ul		
Sample Amount	: 1.0000	Area Reject	: 0.000000
Data Acquisition Time	: 07/10/2016 15:01:02	Dilution Factor	: 1.00
		Cycle	: 1

Raw Data File : C:\TOTALCHROM DATA\Results\AOIFE\07.10-16 AM-6-286c in MeOHB.001.raw
Result File : C:\TOTALCHROM DATA\Results\AOIFE\07.10-16 AM-6-286c in MeOHB.001.rst [Editing in Progress]
Inst Method : C:\TOTALCHROM DATA\Methods\60-40_ACN-Water_1ml_40min from C:\TOTALCHROM DATA\Results\AOIFE\07.10-16 AM-6-286c in MeOHB.001.raw
Proc Method : C:\TOTALCHROM DATA\Methods\60-40_ACN-Water_1ml_40min from C:\TOTALCHROM DATA\Results\AOIFE\07.10-16 AM-6-286c in MeOHB.001.rst [Editing in Progress]
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Report Format File: C:\PenExe\TcWS\Ver6.3.1\Config\User\manager\Default.rpt
Sequence File : C:\TOTALCHROM DATA\Sequences\ff-.ad.B10%.1ml.-.-20161006-144053.seq

DEFAULT REPORT

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]	Cal. Range	Volt Range	BL	Raw Amount	Adjusted Amount
1		4.185	10584198.01	1.33e+06	100.00	100.00			BB	10.5842	10.5842
			10584198.01	1.33e+06	100.00	100.00				10.5842	10.5842

Missing Component Report

Component	Expected Retention (Calibration File)

All components were found

Figure S7. HPLC report for pifithrin-μ.