

Correction

# Correction: Griffith, D.M., et al. Novel Improved Synthesis of HSP70 Inhibitor, Pifithrin- $\mu$ . In Vitro Synergy Quantification of Pifithrin- $\mu$ Combined with Pt Drugs in Prostate and Colorectal Cancer Cells. *Molecules* 2016, 21, 949

Aoife M. McKeon <sup>1</sup>, Alan Egan <sup>2</sup>, Jay Chandanshive <sup>1</sup>, Helena McMahon <sup>2</sup> and Darren M. Griffith <sup>1,\*</sup>

<sup>1</sup> Centre for Synthesis and Chemical Biology, Department of Pharmaceutical and Medicinal Chemistry, Royal College of Surgeons in Ireland, 123 St. Stephens Green, Dublin 2 D02 YN77, Ireland; aoifemckeon@rcsi.ie (A.M.M.); jaychandanshive@rcsi.ie (J.C.)

<sup>2</sup> Shannon ABC, South Campus, IT Tralee, Clash, Tralee, Co., Kerry V92 CX88, Ireland; ae12@hw.ac.uk (A.E.); helena.mcmahon@staff.ittralee.ie (H.M.)

\* Correspondence: dgriffith@rcsi.ie; Tel.: +353-1-4022246

Received: 27 October 2016; Accepted: 8 November 2016; Published: 17 November 2016

The authors are sorry to report that some of the <sup>1</sup>H- and <sup>13</sup>C-NMR data reported in their recently published paper [1] were incorrect. While this manuscript was in preparation the <sup>1</sup>H- and <sup>13</sup>C-NMR data and HPLC data for 2-chloro-2-phenylethene-1-sulfonamide were used as a placeholder. Consequently, the authors wish to make, at this time, the following corrections to the paper:

## 1. Change in Main Body Paragraphs

In the Section 2.1. *Syntheses of Pifithrin- $\mu$ , PES*, this paragraph “In the <sup>1</sup>H-NMR spectrum of pifithrin- $\mu$  (DMSO-*d*<sub>6</sub>) the two resonances, a multiplet at 7.47 integrating for three and a doublet integrating for two at 7.36 ppm, correspond to the five protons of the aromatic ring. The resonance observed at 7.29 ppm is attributed to the two protons of the sulfonamide NH<sub>2</sub>. In The <sup>13</sup>C-NMR spectrum signals at 147.2 and 145.1 ppm are assigned to the two alkyne carbons and 139.5, 130.3, 128.7 and 128.5 ppm are associated with the six aromatic carbons. ESI-MS in the negative mode assisted in identifying pifithrin- $\mu$  with a mass peak at 180.2 a.m.u. Elemental analysis correlated with required analysis for pifithrin- $\mu$ .” was incorrectly reported.

It should be “In the <sup>1</sup>H-NMR spectrum of pifithrin- $\mu$  (DMSO-*d*<sub>6</sub>), three resonances—a doublet at 7.61 integrating for two, a triplet integrating for one at 7.56 and a triplet integrating for two at 7.48 ppm—correspond to the five protons of the aromatic ring. The resonance observed at 8.24 ppm is attributed to the two protons of the sulfonamide NH<sub>2</sub>. In The <sup>13</sup>C-NMR spectrum, signals at 132.2 (2 × C), 131.2 (1 × C), 129.2 (2 × C) and 117.9 (1 × C) ppm are associated with the six aromatic carbons and signals at 87.5 and 84.3 ppm are assigned to the two alkyne carbons.”

In the section 3.2. *Syntheses of Pifithrin- $\mu$* , this paragraph “ $\delta$ <sub>H</sub> (400 MHz, DMSO-*d*<sub>6</sub>) 7.44 (3H, m, aromatic H), 7.36 (2H, d, <sup>3</sup>J 8 Hz, aromatic H), 7.33 (2H, br s, NH<sub>2</sub>).  $\delta$ <sub>C</sub> (100 MHz, DMSO-*d*<sub>6</sub>) 146.1 (alkyne C), 144.9 (alkyne C), 138.4 (aromatic C), 129.2 (aromatic C), 127.6 (aromatic C), 127.4 (aromatic C). (C<sub>8</sub>H<sub>7</sub>NO<sub>2</sub>S ·  $\frac{1}{2}$  H<sub>2</sub>O requires C, 50.52; H, 4.24; N, 7.36%. Found: C, 50.86; H, 4.67; N, 6.99%); HPLC: C18 column, isocratic 60% acetonitrile/40% water as an eluent, retention time: 8.63 min. Purity > 96%. MS (ESI-) *m/z*: 180.2.” was incorrectly reported.

It should be “ $\delta$ <sub>H</sub> (400 MHz, DMSO-*d*<sub>6</sub>) 8.24 (2H, br s, NH<sub>2</sub>), 7.61 (2H, d, <sup>3</sup>J = 8 Hz, aromatic H), 7.56 (1H, t, <sup>3</sup>J = 8 Hz, aromatic H), 7.48 (2H, t, <sup>3</sup>J = 8 Hz, aromatic H).  $\delta$ <sub>C</sub> (100 MHz, DMSO-*d*<sub>6</sub>) 132.2 (aromatic C × 2), 131.2 (aromatic C × 1), 129.2 (aromatic C × 2), 117.9 (aromatic C × 1), 87.5 (alkyne C), 84.3 (alkyne C). (C<sub>8</sub>H<sub>7</sub>NO<sub>2</sub>S ·  $\frac{1}{2}$  H<sub>2</sub>O requires C, 50.52; H, 4.24; N, 7.36%. Found: C, 50.86; H, 4.67;

N, 6.99%); HPLC: C18 column, isocratic 60% acetonitrile/40% water as an eluent, retention time: 4.19 min. Purity >99%. MS (ESI-)  $m/z$ : 180.2."

## 2. Change in Figures in the Supplementary Material

The correct spectroscopic data ( $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ ) and correct HPLC data (chromatogram and report) for pifithrin- $\mu$  are as follows (Figures S1–S4, S6 and S7):

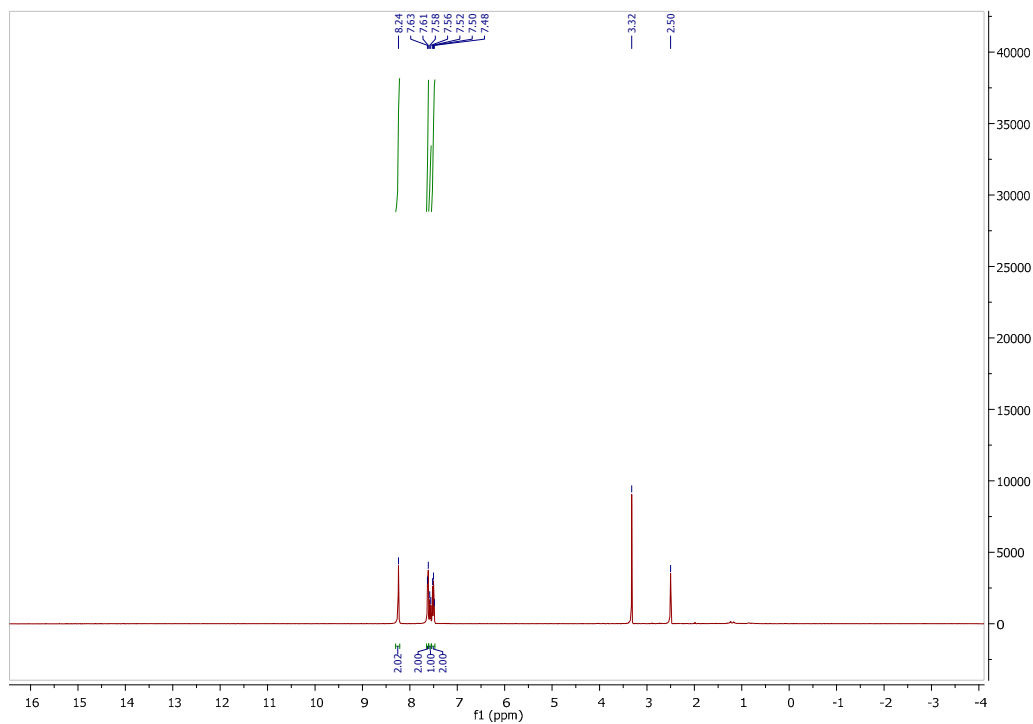


Figure S1.  $^1\text{H-NMR}$  spectrum of pifithrin  $\mu$  in  $\text{DMSO-}d_6$ .

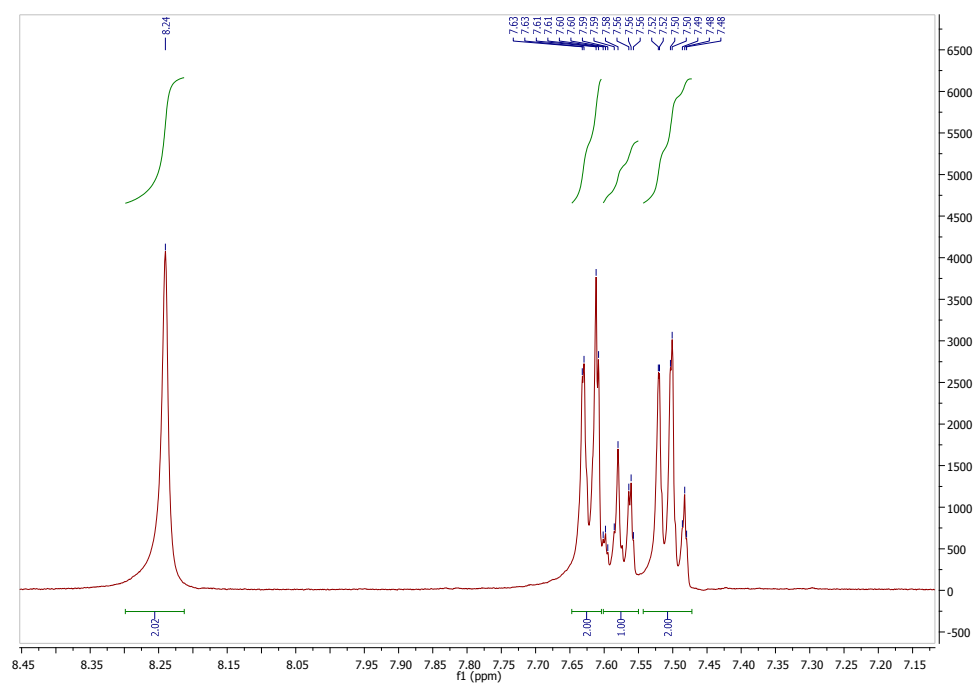


Figure S2.  $^1\text{H-NMR}$  spectrum of pifithrin- $\mu$  in  $\text{DMSO-}d_6$ .

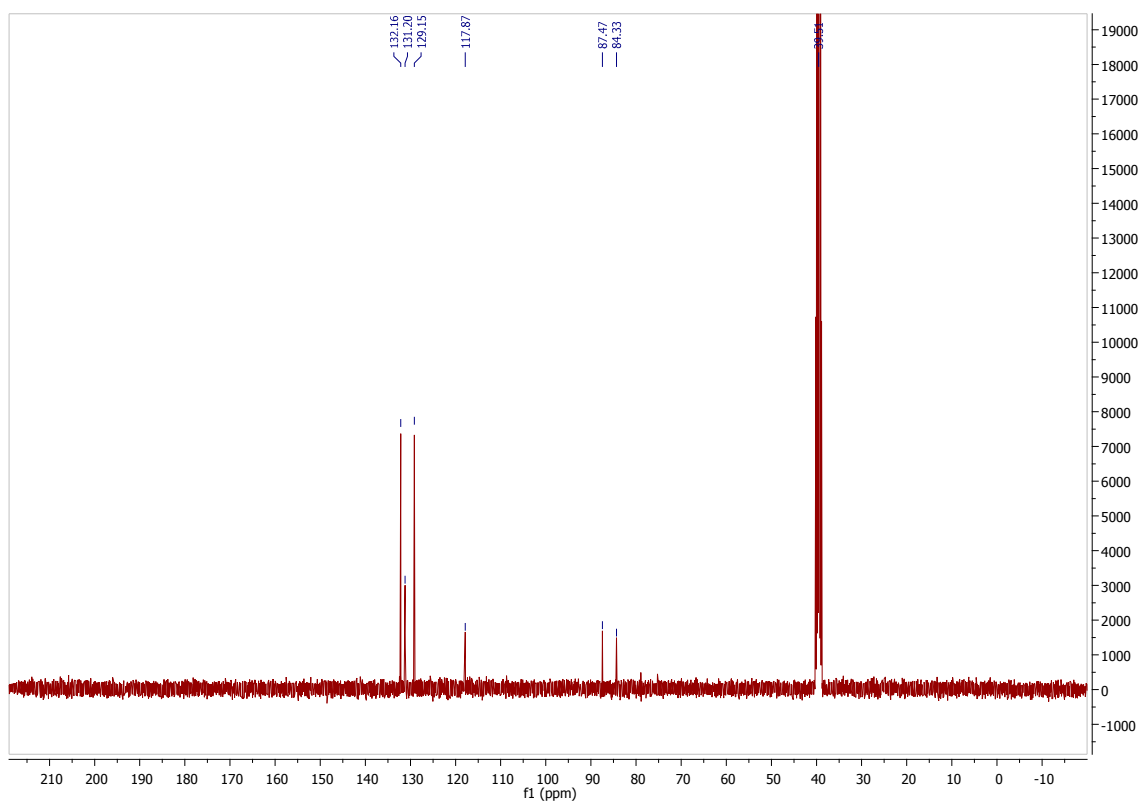


Figure S3.  $^{13}\text{C}$ -NMR spectrum of pifithrin- $\mu$  in  $\text{DMSO-}d_6$ .

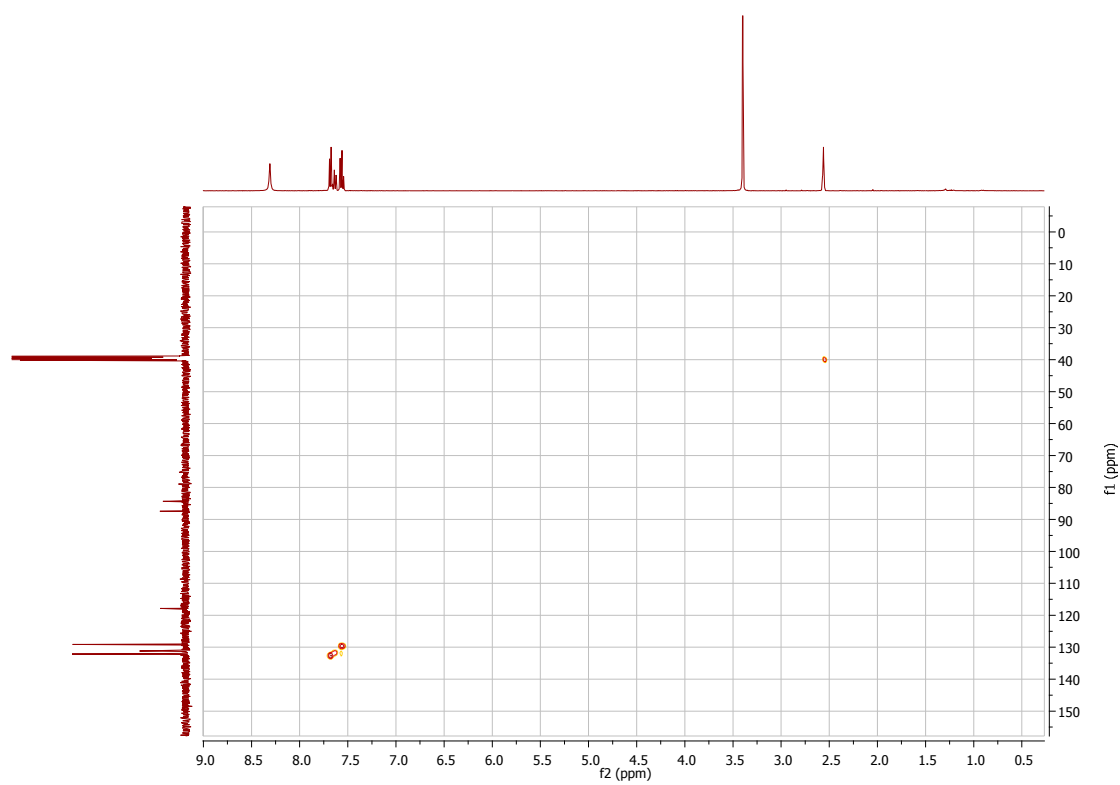


Figure S4. HSQC spectrum of pifithrin- $\mu$  in  $\text{DMSO-}d_6$ .

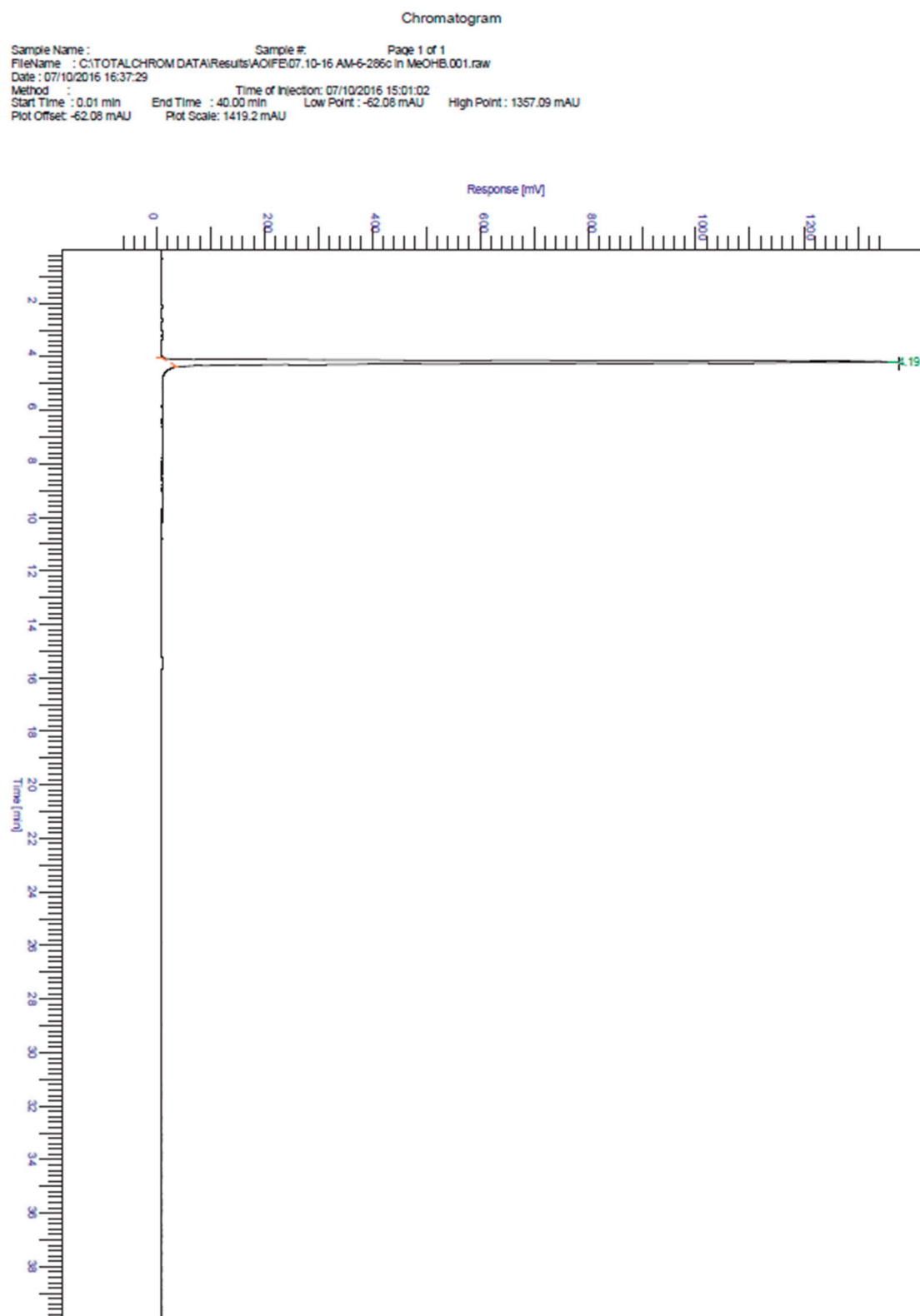


Figure S6. HPLC chromatogram of pifithrin- $\mu$ .

```

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

The authors would like to apologize for any inconvenience caused to the readers by these changes.

## Reference

- McKeon, A.M.; Egan, A.; Chandanshive, J.; McMahan, H.; Griffith, D.M. Novel Improved Synthesis of HSP70 Inhibitor, Pifithrin- $\mu$ . In Vitro Synergy Quantification of Pifithrin- $\mu$  Combined with Pt Drugs in Prostate and Colorectal Cancer Cells. *Molecules* **2016**, *21*, 949. [[CrossRef](#)] [[PubMed](#)]



© 2016 by the authors; licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC-BY) license (<http://creativecommons.org/licenses/by/4.0/>).