

New 2-oxoindolin phosphonates As Novel Agents to Treat Cancer: A Green Synthesis and Molecular Modeling.

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2. Results

2.1. Chemistry

The mechanism of synthesis is as shown in Figure S1

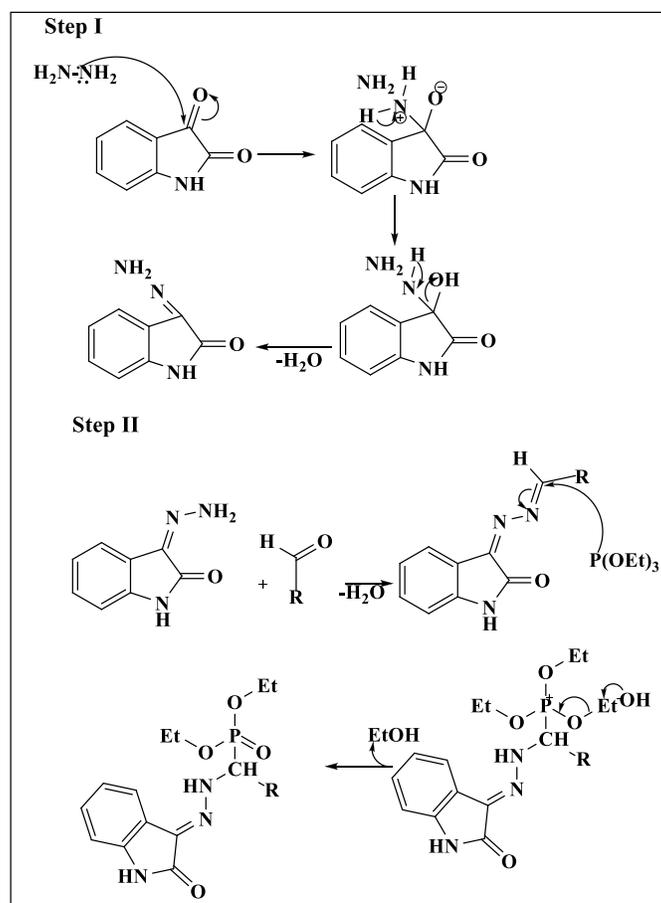


Figure S1. The proposed mechanism for the synthesis of **4(a-n)** derivatives.

***In Vitro* Anticancer evaluation**

In vitro anticancer activity images which were captured under the Eclipse Ti-S Inverted Research Microscope-Nikon and the images were processed using NIS-Elements software. The images of the *in vitro* anticancer activity of all the synthesized compounds **4(a-n)** on the MCF-7, IMR-32, SK-MEL-2, MG-63, HT-29 and Hep-G2 cancer cell lines are as shown in Figure S2, Figure S3, Figure S4, Figure S5, Figure S6 and Figure S7, respectively.

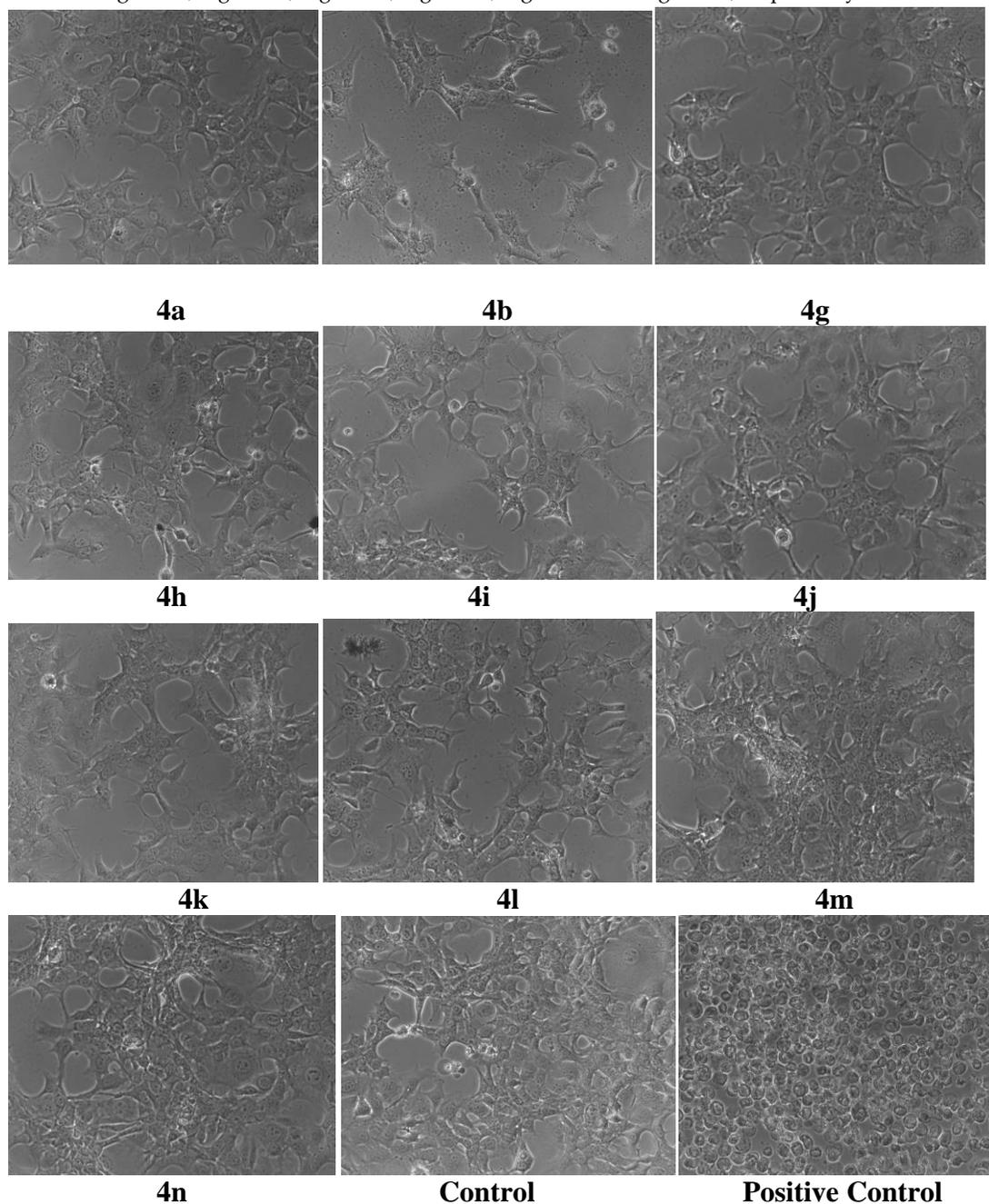


Figure S2. Images for *in-vitro* anticancer activity against MCF-7 cell line of the synthesized compounds **4 (a-n)**, control and positive control.

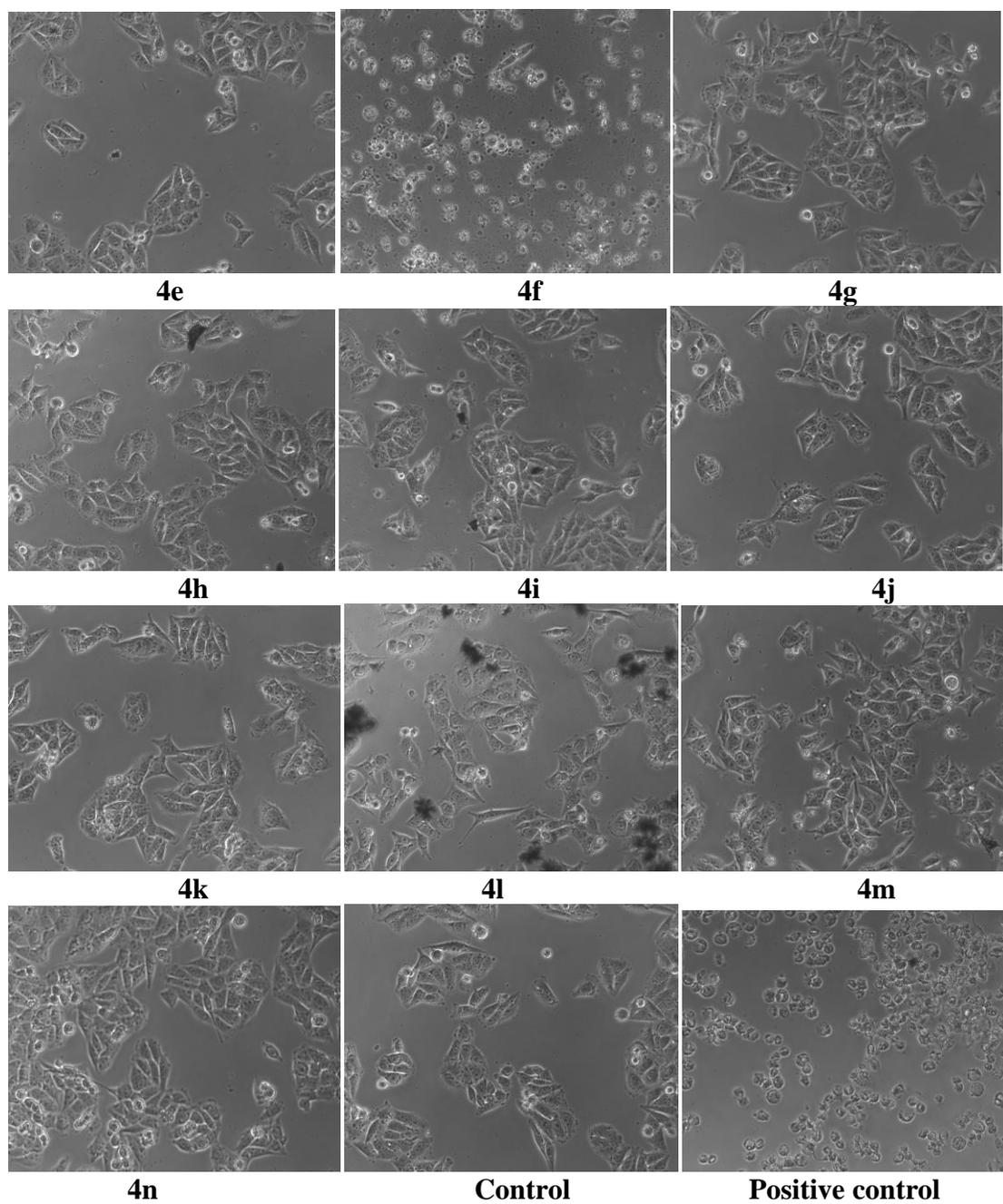


Figure S3. Images for *in-vitro* anticancer activity against IMR-32 cell line of the synthesized compounds **4(a-n)**, control and positive control.

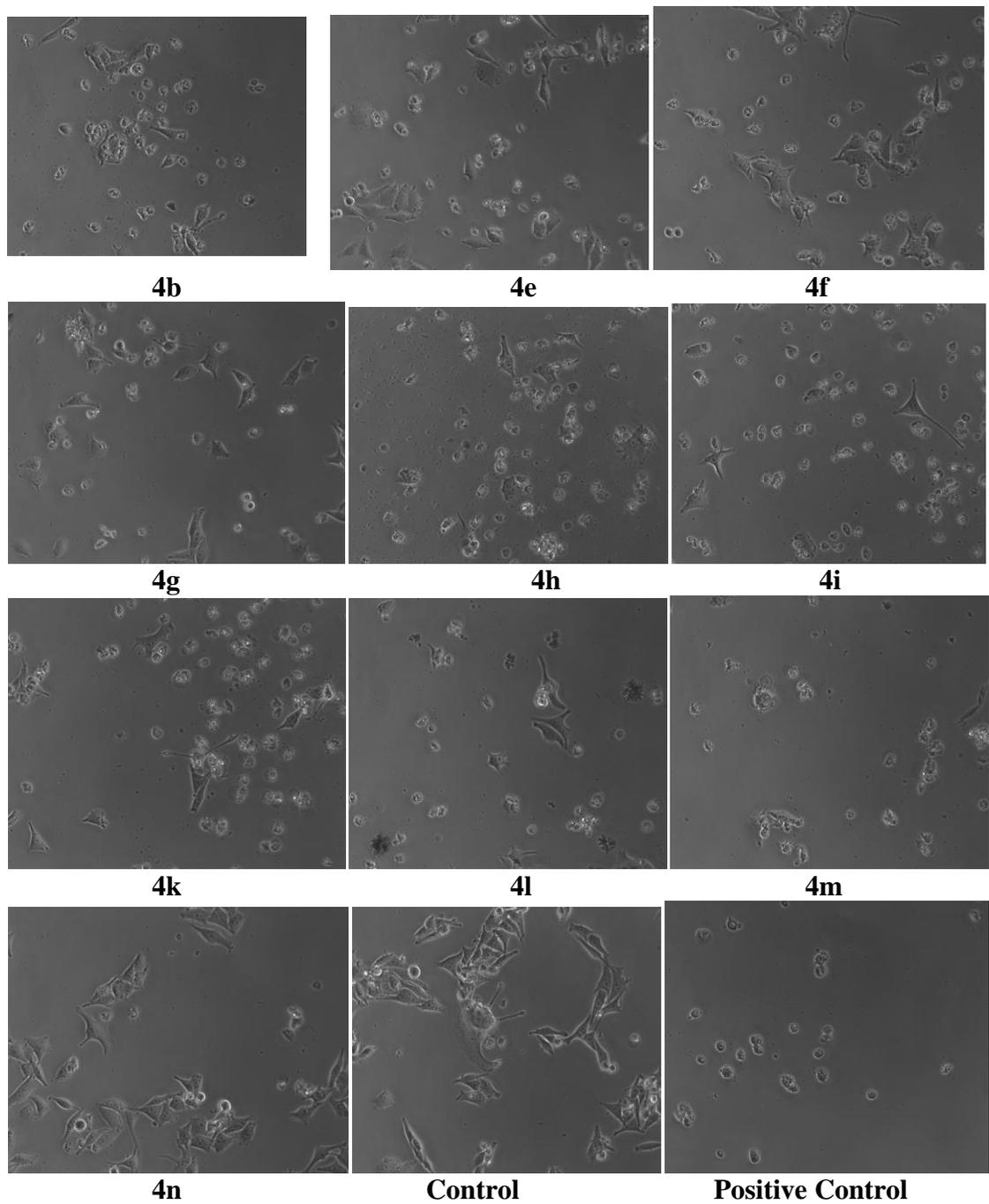


Figure S4. Images for *in-vitro* anticancer activity against SK-MEL-2 cell line of the synthesized compounds **4(a-n)**, control and positive control.

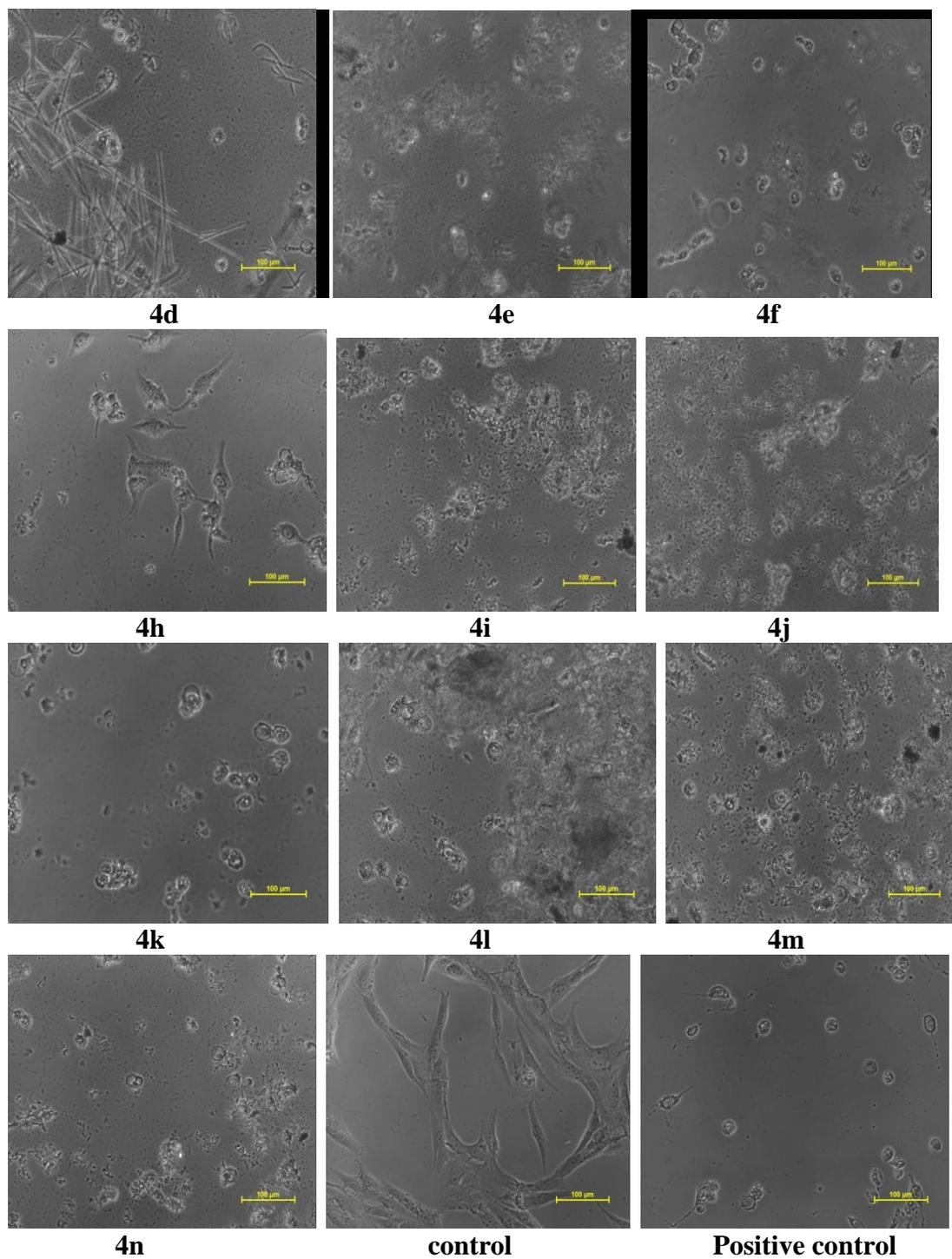
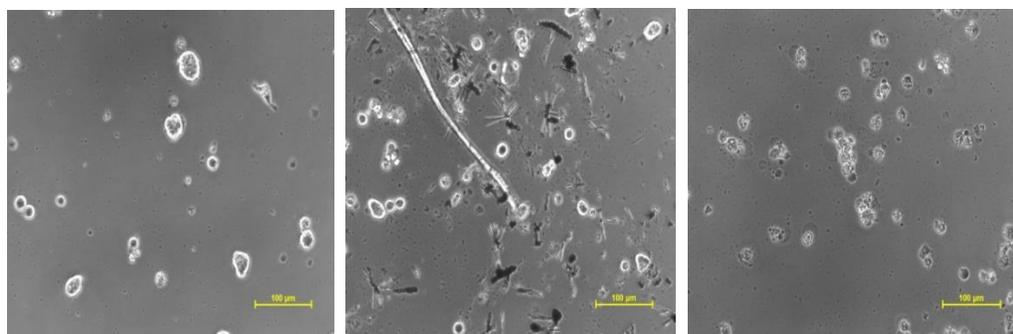


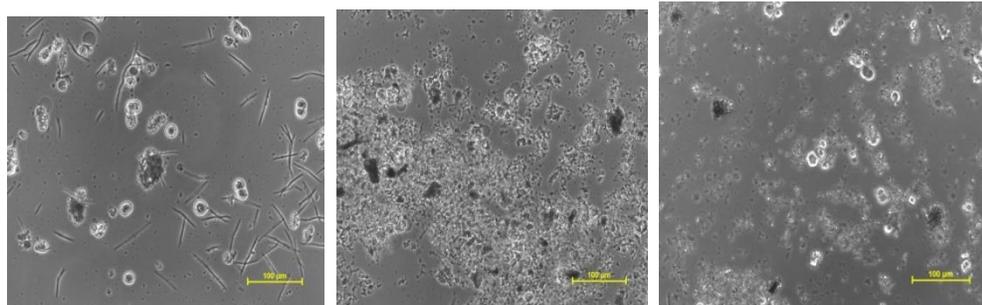
Figure S5. Images for *in-vitro* anticancer activity against MG-63 cell line of the synthesized compounds **4 (a-n)**, control and positive control.



4d

4e

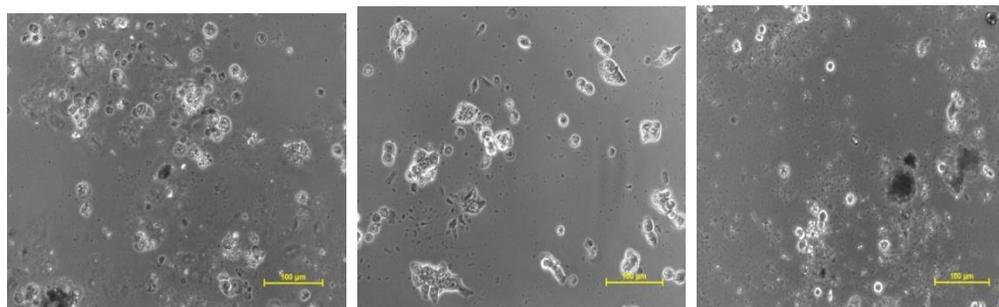
4f



4h

4i

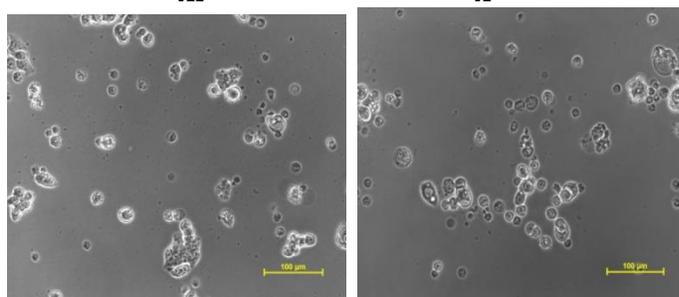
4j



4k

4l

4m



Control

positive control

Figure S6. Images for *in-vitro* anticancer activity against HT-29 cell line of the synthesized compounds **4(a-n)**, control and positive control.

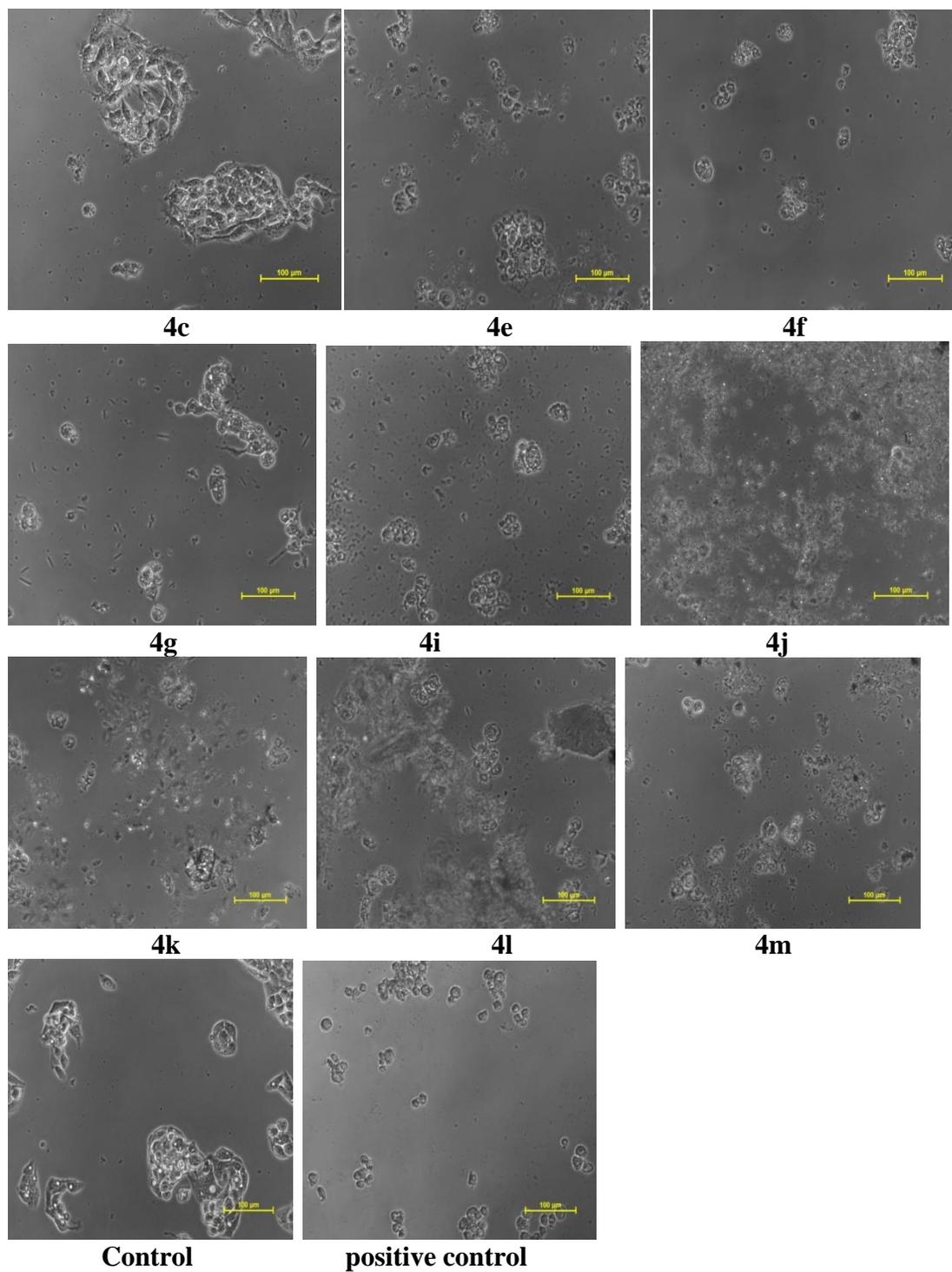
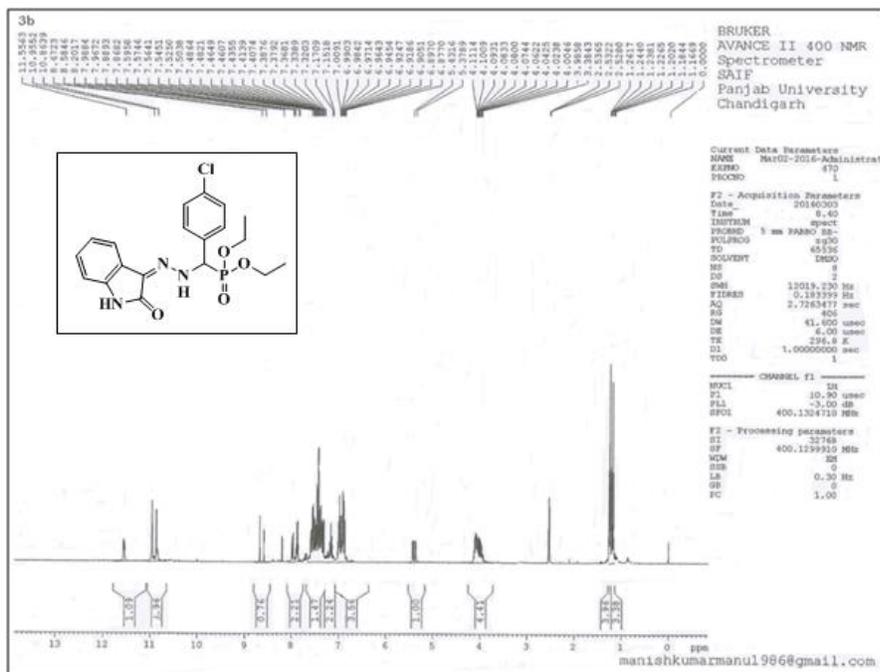
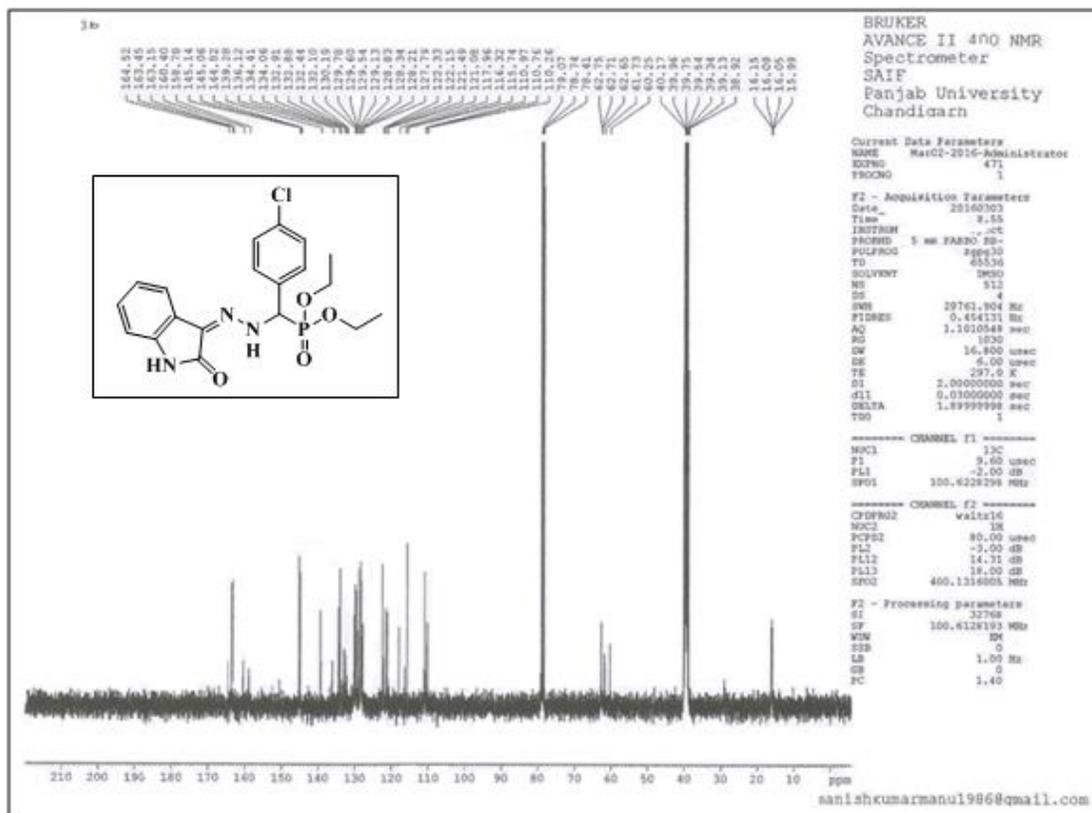


Figure S7. Images for *in-vitro* anticancer activity against Hep-G2 cell line of the synthesized compounds **4(a-n)**, control and positive control.

¹H NMR spectrum of compound 4b

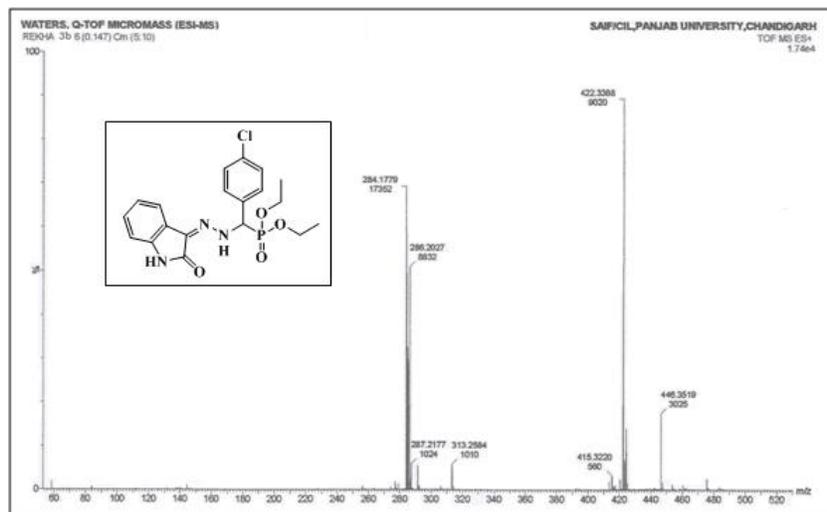


¹³C NMR spectrum of compound 4b

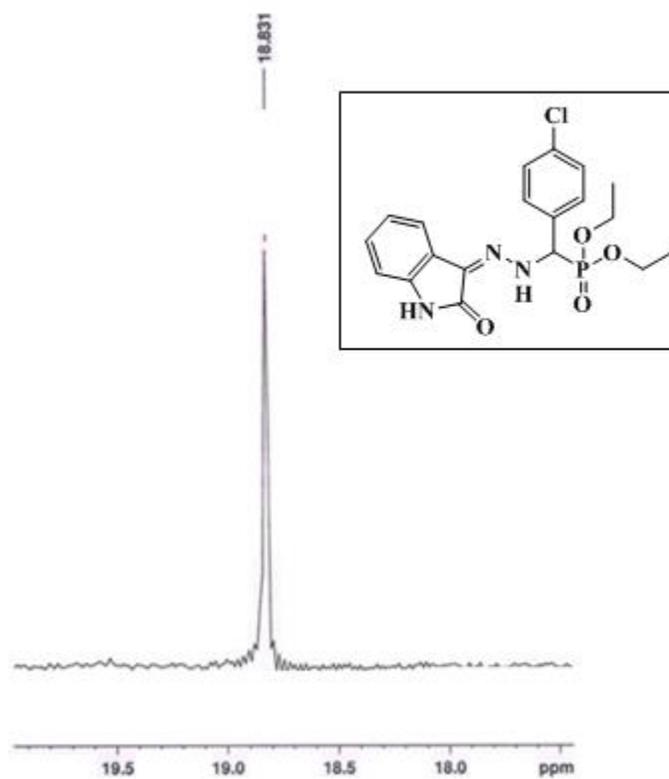


Mass spectra of compound 4b

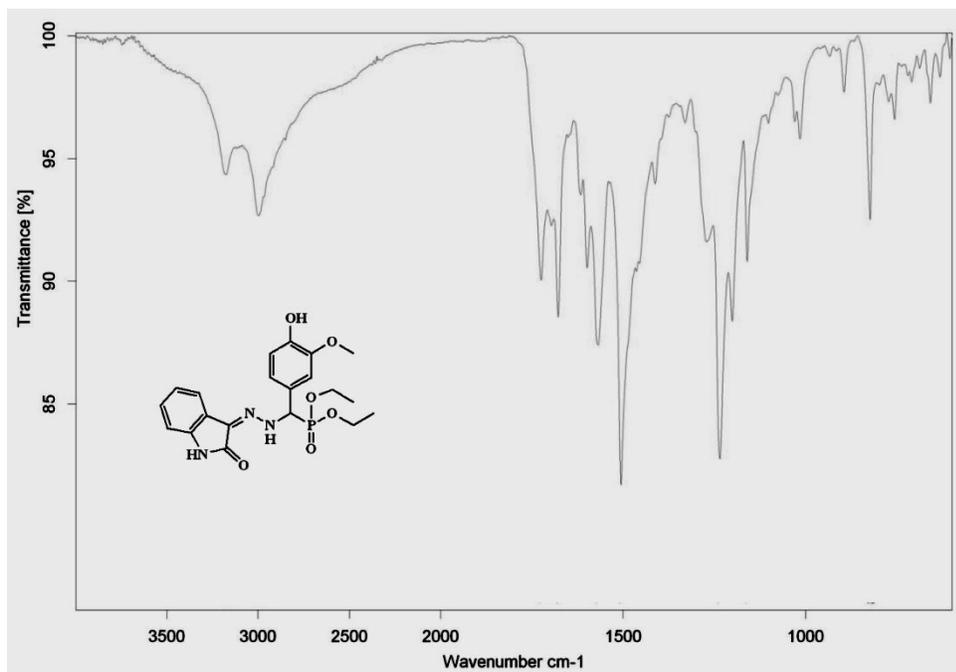
Molecular Weight: 421.81, Molecular ion peak: 422.33



³¹P NMR spectrum of compound 4b

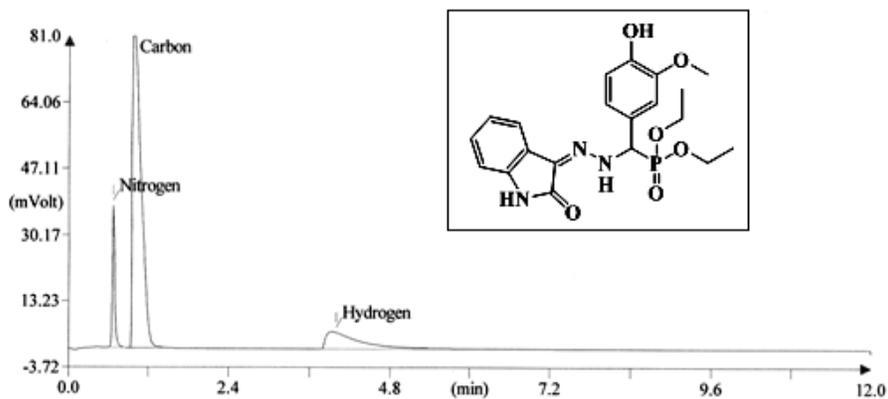


IR spectra of 4g



Elemental analysis of compound 4g

Method name: CHNS
 Analysed: 05/18/2017 13:00
 Printed: 05-18-2017 17:10
 Sample ID: 18May17016
 Analysis type: UnkNown
 Chromatogram filename: C:\[redacted]18May17R1.DAT



Component Name	Retention Time (min)	Area (.1* μ V*sec)	Element %
Nitrogen	0.658	1048085	9.758
Carbon	0.975	6991914	55.490
Hydrogen	3.942	1499294	5.512
		9539293	70.760