Synthesis of novel Phthalazine-based derivatives with potent cytotoxicity against HCT-116 cells through apoptosis and VEGFR2 inhibition.

Table of contents

Figure S1 The ¹ H-NMR spectrum of compound 3
Figure S2 The ¹³ C-NMR spectrum of compound 3
Figure S3 The IR spectrum of compound 3
Figure S4 The ¹ H-NMR spectrum of compound 45
Figure S5 The ¹ H-NMR spectrum of compound 56
Figure S6 The ¹³ C-NMR spectrum of compound 56
Figure S7 The D2O spectrum of compound 57
Figure S8 The IR spectrum of compound 57
Figure S9 The ¹ H-NMR spectrum of compound 7a
Figure S10 The ¹³ C-NMR spectrum of compound 7a
Figure S11 The D2O spectrum of compound 7a9
Figure S12 The IR spectrum of compound 7a9
Figure S13 The ¹ H-NMR spectrum of compound 7b10
Figure S14 The ¹³ C-NMR spectrum of compound 7b10
Figure S15 The IR spectrum of compound 7b11
Figure S16 The ¹ H-NMR spectrum of compound 7c11
Figure S17 The ¹³ C-NMR spectrum of compound 7c12
Figure S18 The D2O spectrum of compound 7c12
Figure S19 The IR spectrum of compound 7c
Figure S20 The ¹ H-NMR spectrum of compound 7d13
Figure S21 The ¹³ C-NMR spectrum of compound 7d14
Figure S22 The IR spectrum of compound 7d
Figure S23 The ¹ H-NMR spectrum of compound 7e15
Figure S24 The ¹³ C-NMR spectrum of compound 7e15
Figure S25 The D2O spectrum of compound 7e16
Figure S26 The IR spectrum of compound 7e
Figure S27 The ¹ H-NMR spectrum of compound 7f
Figure S28 The ¹³ C-NMR spectrum of compound 7f
Figure S29 The D2O spectrum of compound 7f
Figure S30 The IR spectrum of compound 7f
Figure S31 The ¹ H-NMR spectrum of compound 7g
Figure S32 The ¹³ C-NMR spectrum of compound 7g
Figure S33 The IR spectrum of compound 7g
Figure S34 The ¹ H-NMR spectrum of compound 8a. 20
Figure S35 The ¹³ C-NMR spectrum of compound 8a
Figure S36 The D2O spectrum of compound 8a
Figure S37 The IR spectrum of compound 8a 22

Figure S38 The ¹ H-NMR spectrum of compound 8b	22
Figure S39 The ¹³ C-NMR spectrum of compound 8b	23
Figure S40 The D2O spectrum of compound 8b	23
Figure S41 The IR spectrum of compound 8b	24
Figure S42 The ¹ H-NMR spectrum of compound 8c	24
Figure S43 The ¹³ C-NMR spectrum of compound 8c	25
Figure S44 The D2O spectrum of compound 8c	25
Figure S45 The IR spectrum of compound 8c	26
Figure S46 The ¹ H-NMR spectrum of compound 9a	26
Figure S47 The ¹³ C-NMR spectrum of compound 9a	27
Figure S48 The D2O spectrum of compound 9a	27
Figure S49 The IR spectrum of compound 9a	28
Figure S50 The ¹ H-NMR spectrum of compound 9b	28
Figure S51 The ¹³ C-NMR spectrum of compound 9b	29
Figure S52 The D2O spectrum of compound 9b	29
Figure S53 The IR spectrum of compound 9b	30
Figure S54 The ¹ H-NMR spectrum of compound 9c	30
Figure S55 The ¹³ C-NMR spectrum of compound 9c	31
Figure S56 The D2O spectrum of compound 9c	31
Figure S57: The IR spectrum of compound 9c	32
Figure S58: The ¹ H-NMR spectrum of compound 11a	32
Figure S59: The ¹³ C-NMR spectrum of compound 11a	33
Figure S60: The D2O spectrum of compound 11a	33
Figure S61: The IR spectrum of compound 11a	34
Figure 62: The ¹ H-NMR spectrum of compound 11b	34
Figure 63: The ¹³ C-NMR spectrum of compound 11b	35
Figure S64: The D2O spectrum of compound 11b	35
Figure S65: The IR spectrum of compound 11b	36
Figure S66: The ¹ H-NMR spectrum of compound 11c	37
Figure S67: The ¹³ C-NMR spectrum of compound 11c	37
Figure S68: The D2O spectrum of compound 11c	38
Figure S69: The IR spectrum of compound 11c	38
Figure S70 : The ¹ H-NMR spectrum of compound 11d	39
Figure S71: The ¹³ C-NMR spectrum of compound 11d	39
Figure S72: The D2O spectrum of compound 11d	40
Figure S73: The IR spectrum of compound 11d	40
Figure S74: The ¹ H-NMR spectrum of compound 12a	41
Figure S75: The ¹³ C-NMR spectrum of compound 12a	41
Figure S76: The D2O spectrum of compound 12a	42
Figure S77: The IR spectrum of compound 12a	42
Figure S78: The ¹ H-NMR spectrum of compound 12b	43
Figure S79: The ¹³ C-NMR spectrum of compound 12b	43
Figure S80: The D2O spectrum of compound 12b	44
Figure S81: The IR spectrum of compound 12b.	44

Figure S82: The dept135 spectrum of compound 12b	45
Figure S83: The ¹ H-NMR spectrum of compound 12c	45
Figure S84: The ¹³ C-NMR spectrum of compound 12c	46
Figure S85: The D2O spectrum of compound 12c	46
Figure S86: The IR spectrum of compound 12c	47
Figure S87: The ¹ H-NMR spectrum of compound 13a	47
Figure S88: The D2O spectrum of compound 13a	48
Figure S89: The IR spectrum of compound 13a	48
Figure S90: The ¹ H-NMR spectrum of compound 13b	49
Figure S91: The D2O spectrum of compound 13b	49
Figure S92: The IR spectrum of compound 13b	50
Figure S93: The ¹ H-NMR spectrum of compound 13c	50
Figure S94: The D2O spectrum of compound 13c	51
Figure S95: The ¹ H-NMR spectrum of compound 13d	51
Figure S96: The D2O spectrum of compound 13d	52
Figure S97: The IR spectrum of compound 13d	52

Electronic supporting information (ESI)



Figure S2 The ¹³C-NMR spectrum of compound 3.







Figure S4 The ¹H-NMR spectrum of compound 4.



Figure S5 The ¹H-NMR spectrum of compound 5.



Figure S6 The ¹³C-NMR spectrum of compound 5.



Figure S8 The IR spectrum of compound 5







Figure S10 The ¹³C-NMR spectrum of compound 7a



Figure S11 The D2O spectrum of compound 7a



Figure S12 The IR spectrum of compound 7a



Figure S13 The ¹H-NMR spectrum of compound 7b



Figure S14 The ¹³C-NMR spectrum of compound 7b







Figure S16 The ¹H-NMR spectrum of compound 7c



Figure S17 The ¹³C-NMR spectrum of compound 7c



Figure S18 The D2O spectrum of compound 7c



Figure S19 The IR spectrum of compound 7c



Figure S20 The ¹H-NMR spectrum of compound 7d



Figure S22 The IR spectrum of compound 7d



Figure S23 The ¹H-NMR spectrum of compound 7e



Figure S24 The ¹³C-NMR spectrum of compound 7e



Figure S25 The D2O spectrum of compound 7e



Figure S26 The IR spectrum of compound 7e



Figure S28 The ¹³C-NMR spectrum of compound 7f



Figure S29 The D2O spectrum of compound 7f



Figure S30 The IR spectrum of compound 7f



Figure S32 The ¹³C-NMR spectrum of compound 7g



Figure S33 The IR spectrum of compound 7g



Figure S34 The ¹H-NMR spectrum of compound 8a



Figure S35 The ¹³C-NMR spectrum of compound 8a



Figure S36 The D2O spectrum of compound 8a







Figure S38 The ¹H-NMR spectrum of compound 8b



Figure S39 The ¹³C-NMR spectrum of compound 8b



Figure S40 The D2O spectrum of compound 8b







Figure S42 The ¹H-NMR spectrum of compound 8c







Figure S44 The D2O spectrum of compound 8c







Figure S46 The ¹H-NMR spectrum of compound 9a



Figure S47 The ¹³C-NMR spectrum of compound 9a



Figure S48 The D2O spectrum of compound 9a



Figure S49 The IR spectrum of compound 9a



Figure S50 The ¹H-NMR spectrum of compound 9b



Figure S52 The D2O spectrum of compound 9b



Figure S53 The IR spectrum of compound 9b



Figure S54 The ¹H-NMR spectrum of compound 9c



Figure S55 The ¹³C-NMR spectrum of compound 9c



Figure S56 The D2O spectrum of compound 9c



Nov15-2023.120.fid DH-21 14000 proton_su CDCl3 {D:\NMR Data} Student 1 7.38 8.37 7.67 7.67 7.65 7.64 7.28 7.19 7.18 5.06 5.04 4.60 4.58 3.96 3.86 3.85 3.83 2.90 2.88 2.87 7.70 7.22 5.13 4.28 3.95 3.84 8.37 .26 7.21 7.20 4.57 3.97 2 13000 8.3 5.1 12000 11000 10000 9000 - 8000 N H II O 0 7000 11 a - 6000 - 5000 4000 3000 2000 1000 0 6.37 J 1.88 12.50 -פוש ы ۲ 2.00 ₫ t1 (ppm) 2.03 4.06 2.01 -1000 8.5 8.0 7.0 6.5 6.0 5.5 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 Figure S58: The ¹H-NMR spectrum of compound 11a



Figure S60: The D2O spectrum of compound 11a



Figure S61: The IR spectrum of compound 11a



Figure 62: The ¹H-NMR spectrum of compound 11b







Figure S64: The D2O spectrum of compound 11b



Figure S65: The IR spectrum of compound 11b







Figure S68: The D2O spectrum of compound 11c



Figure S69: The IR spectrum of compound 11c



Figure S70 : The ¹H-NMR spectrum of compound 11d



Figure S71:The ¹³C-NMR spectrum of compound 11d



Figure S72: The D2O spectrum of compound 11d



Figure S73: The IR spectrum of compound 11d



Figure S75: The ¹³C-NMR spectrum of compound 12a



Figure S76: The D2O spectrum of compound 12a



Figure S77: The IR spectrum of compound 12a



Figure S78: The ¹H-NMR spectrum of compound 12b



Figure S79: The ¹³C-NMR spectrum of compound 12b



Figure S80: The D2O spectrum of compound 12b



Figure S81: The IR spectrum of compound 12b



Figure S82: The dept135 spectrum of compound 12b



Figure S83: The ¹H-NMR spectrum of compound 12c



Figure S84: The ¹³C-NMR spectrum of compound 12c



Figure S85: The D2O spectrum of compound 12c



Figure S87: The ¹H-NMR spectrum of compound 13a



Figure S88: The D2O spectrum of compound 13a



Figure S89: The IR spectrum of compound 13a





Figure S91: The D2O spectrum of compound 13b







Figure S93: The ¹H-NMR spectrum of compound 13c







Figure S95:The ¹H-NMR spectrum of compound 13d



Figure S96: The D2O spectrum of compound 13d



Figure S97: The IR spectrum of compound 13d