Supporting Information

Synthesis and *in vitro* evaluation of naphthalimide-benzimidazole conjugates as potential antitumor agents

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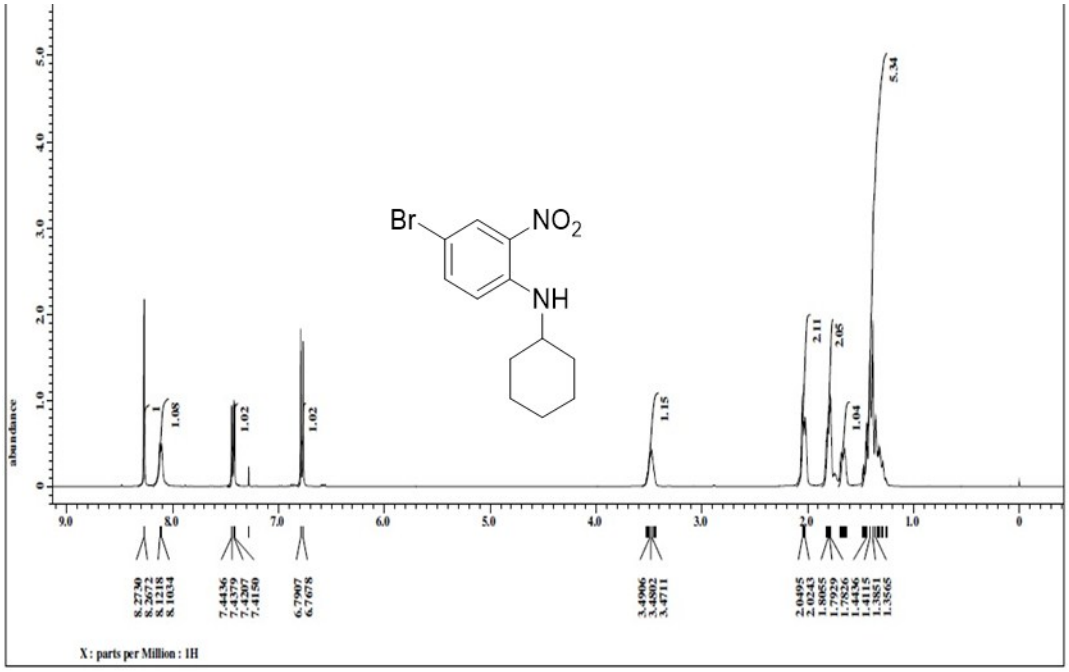

Figure S1: ^{1}H NMR spectrum of 4-bromo-*N*-cyclohexyl-2-nitroaniline (**3a**).

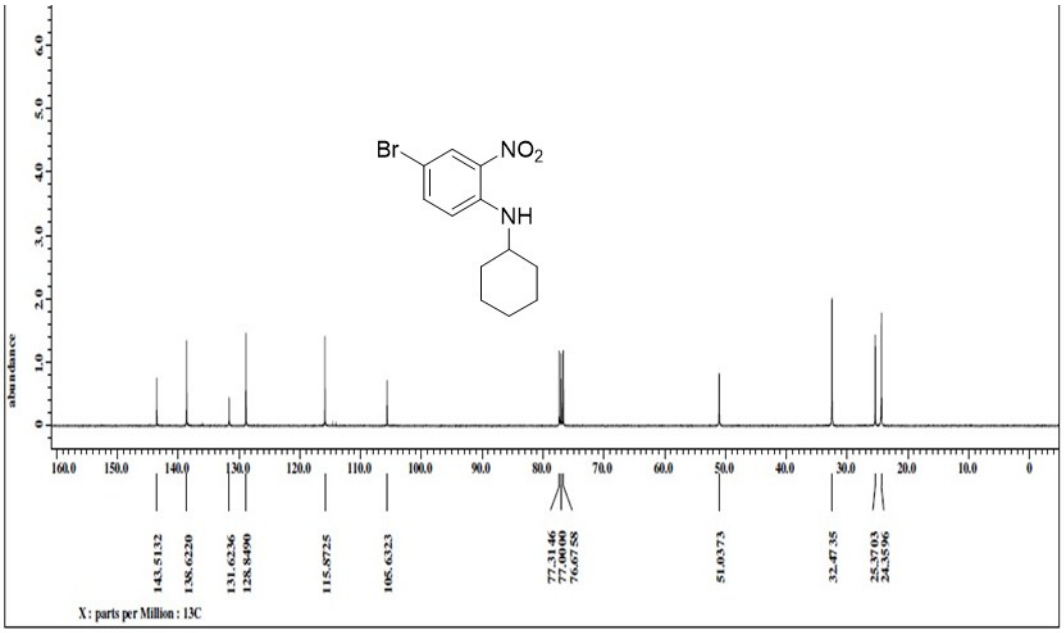

Figure S2: ^{13}C NMR spectrum of 4-bromo-*N*-cyclohexyl-2-nitroaniline (**3a**).

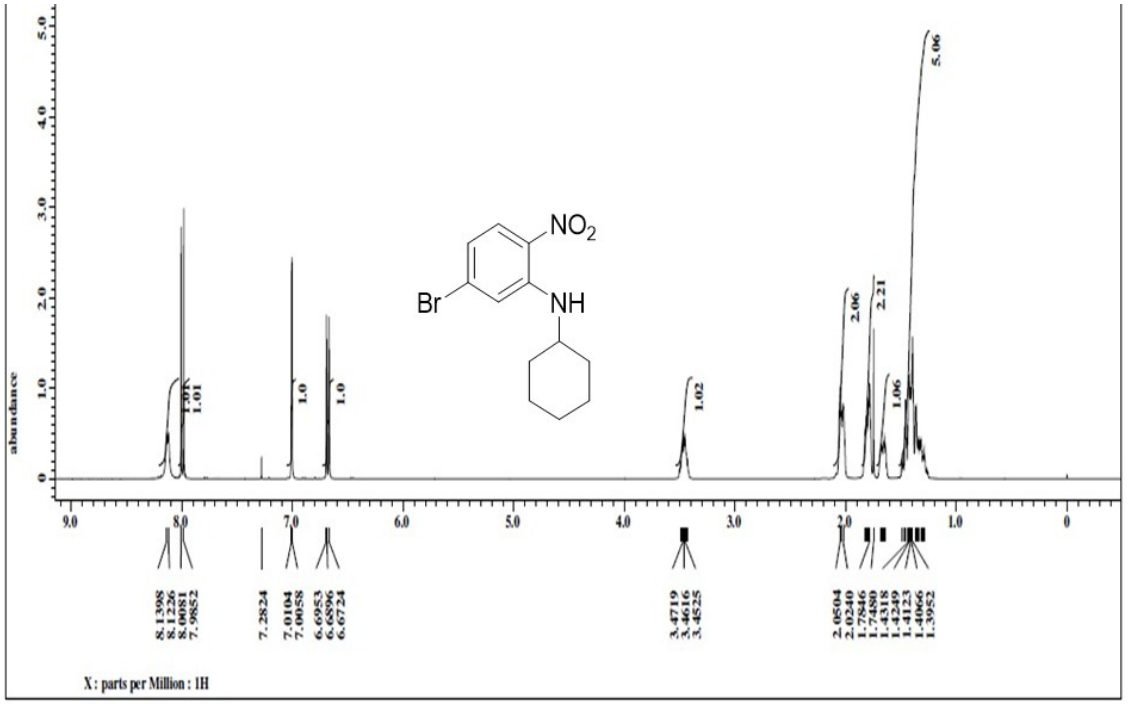

Figure S3: ^{1}H NMR spectrum of 5-bromo-*N*-cyclohexyl-2-nitroaniline (**3b**).

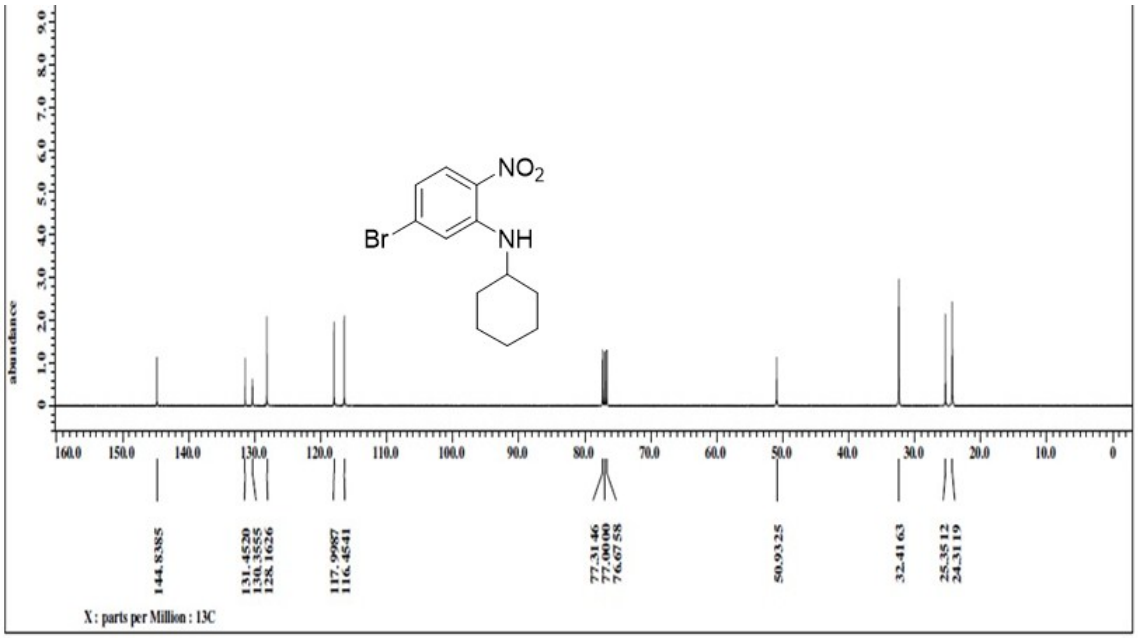

Figure S4: ^{13}C NMR spectrum of 5-bromo-*N*-cyclohexyl-2-nitroaniline (**3b**).

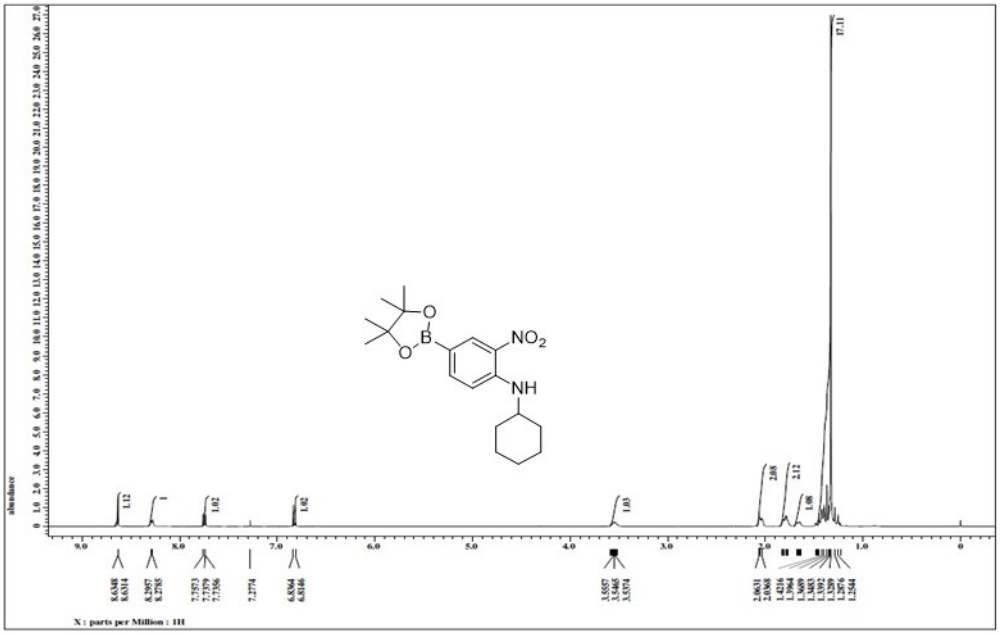

Figure S5: ^{1}H NMR spectrum of *N*-cyclohexyl-2-nitro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**4a**).

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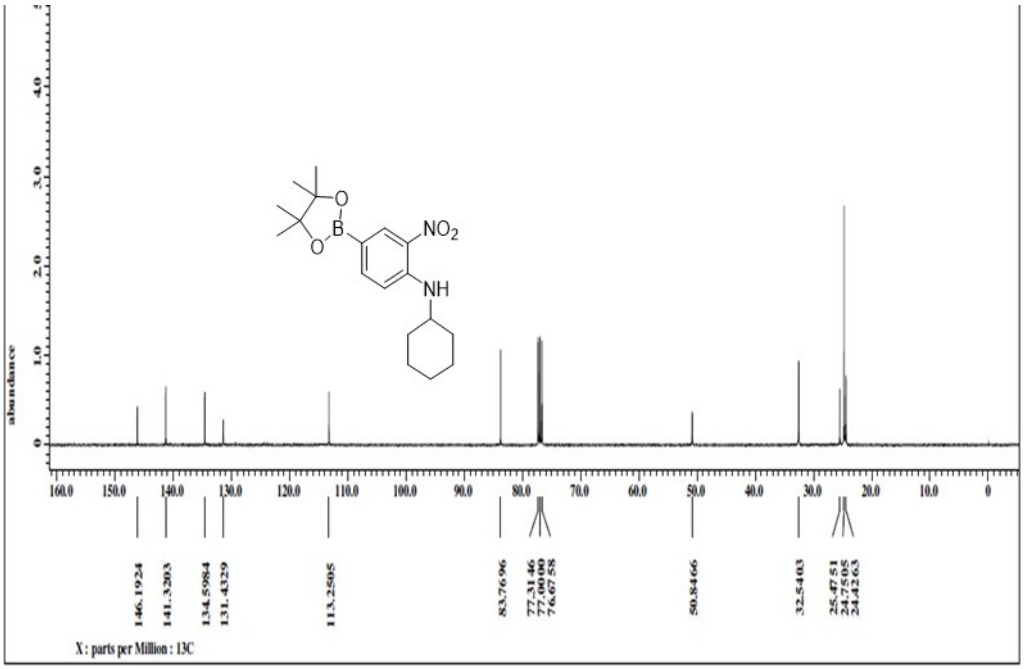


Figure S6: ^{13}C NMR spectrum of *N*-cyclohexyl-2-nitro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**4a**).

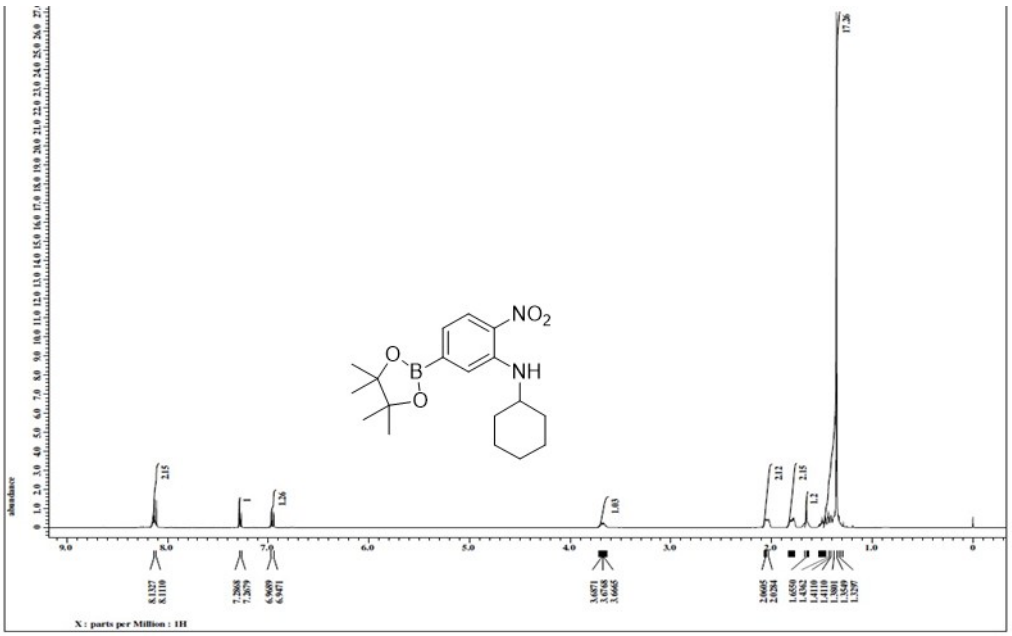


Figure S7: ^{1}H NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**4b**).

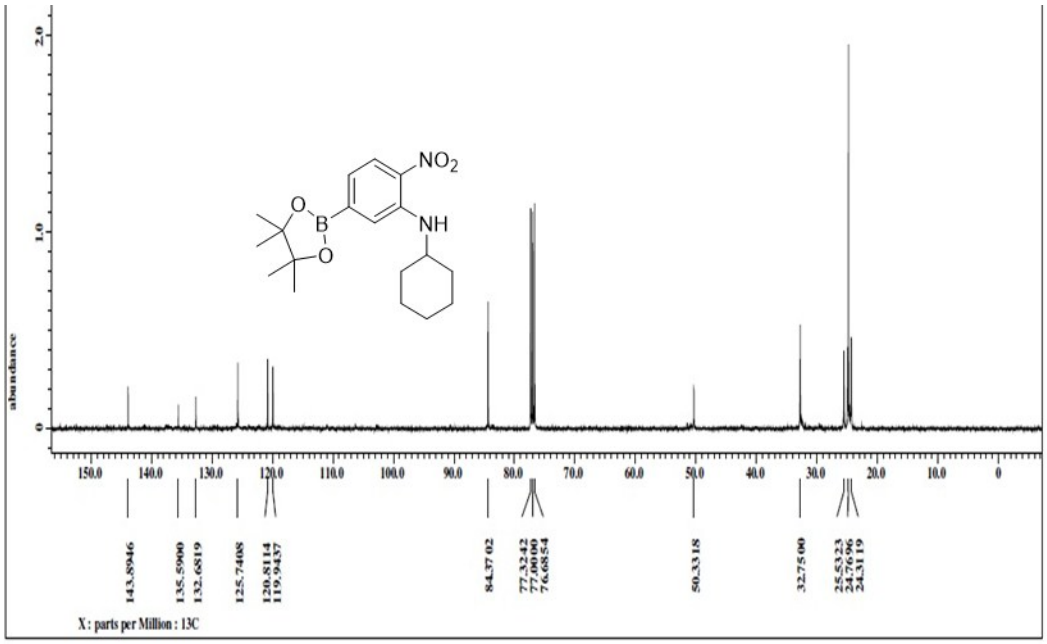


Figure S8: ^{13}C NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**4b**).

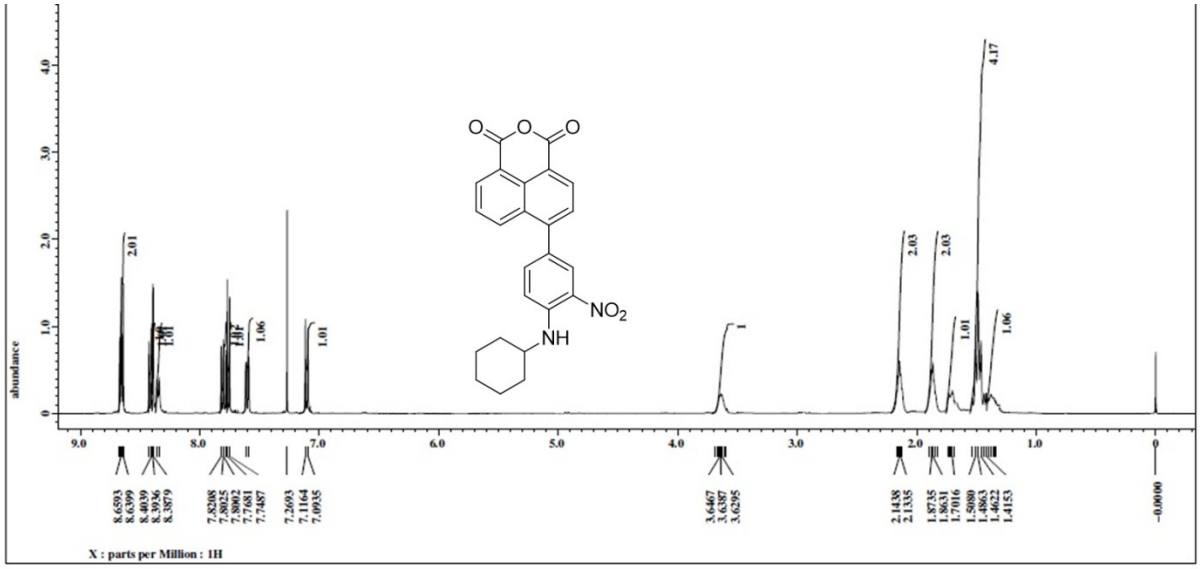


Figure S9: ^{1}H NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**6a**).

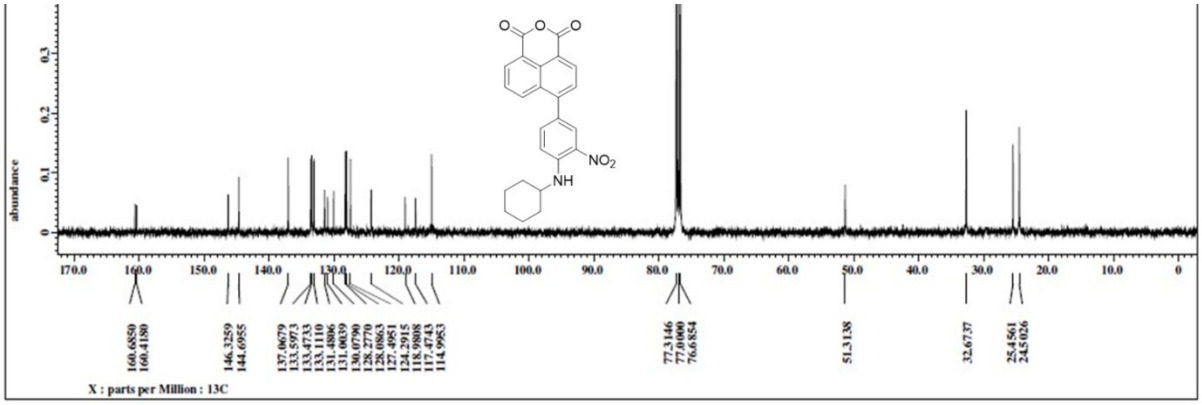


Figure S10: ^{13}C NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**6a**).

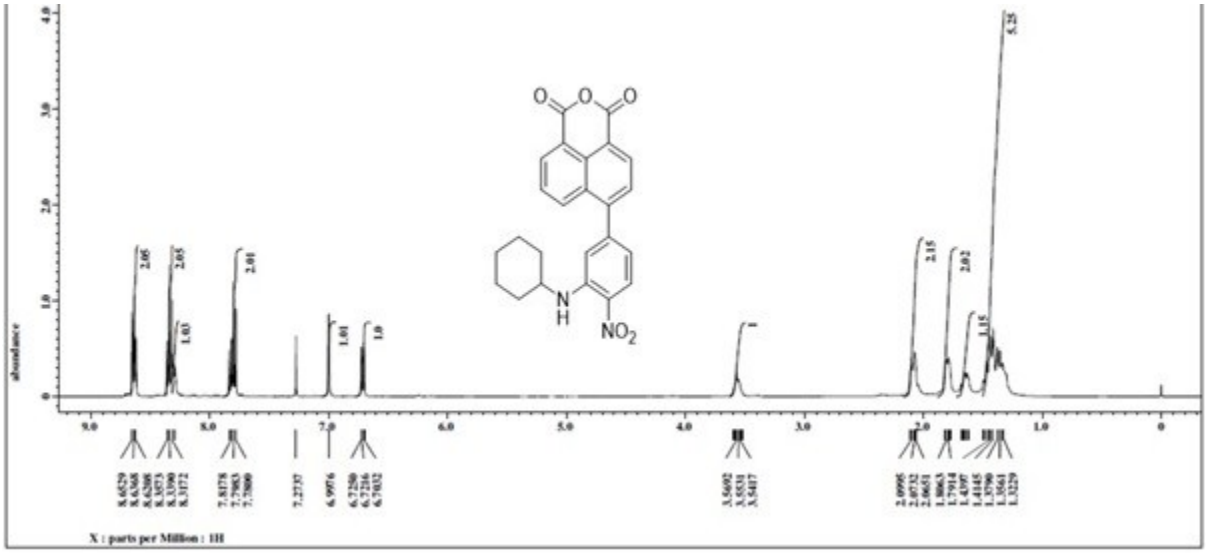


Figure S11: ^{1}H NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**6b**).

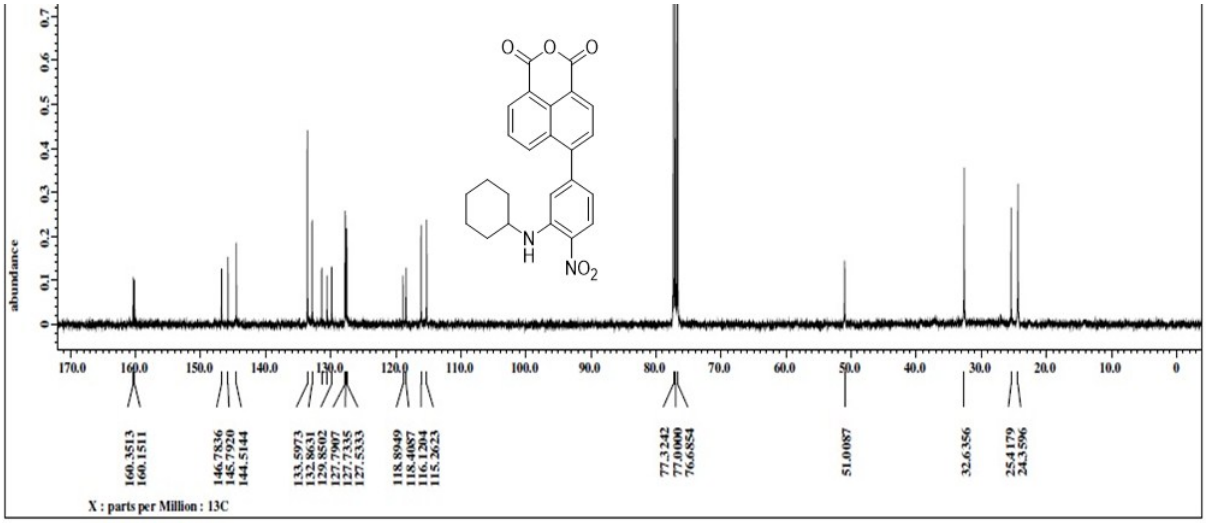


Figure S12: ^{1}H NMR spectrum of *N*-cyclohexyl-2-nitro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**6b**).

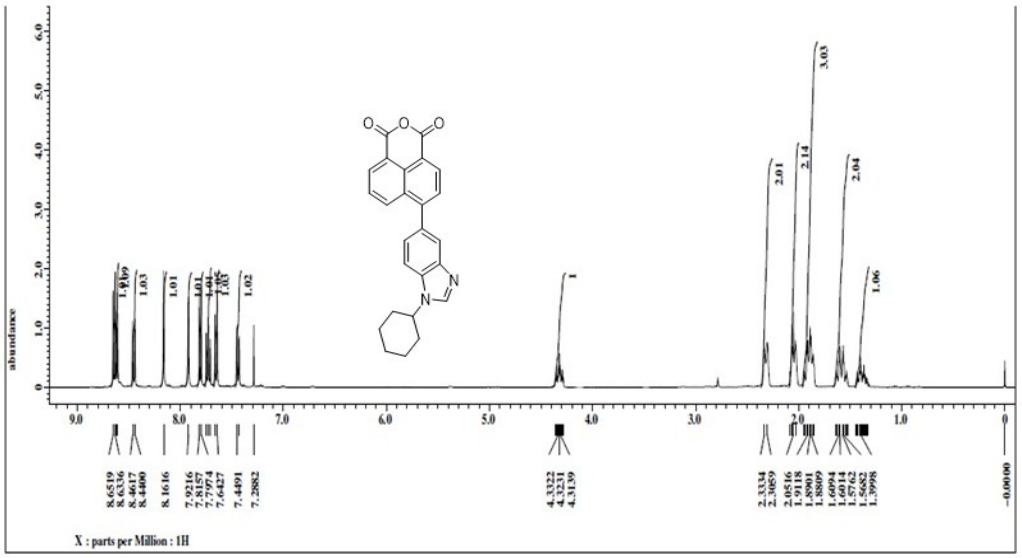


Figure S13: ^{1}H NMR spectrum of spectral data of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9a**).

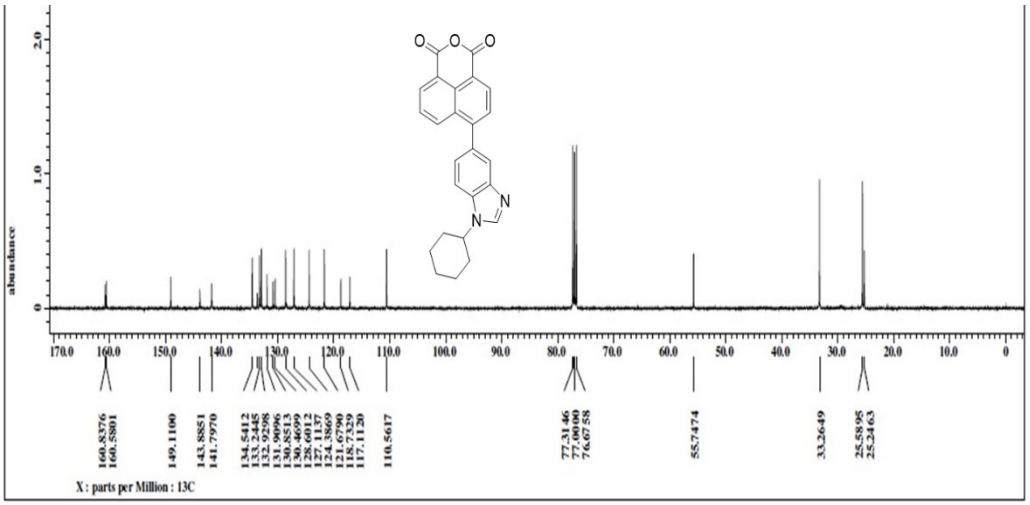


Figure S14: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9a**).

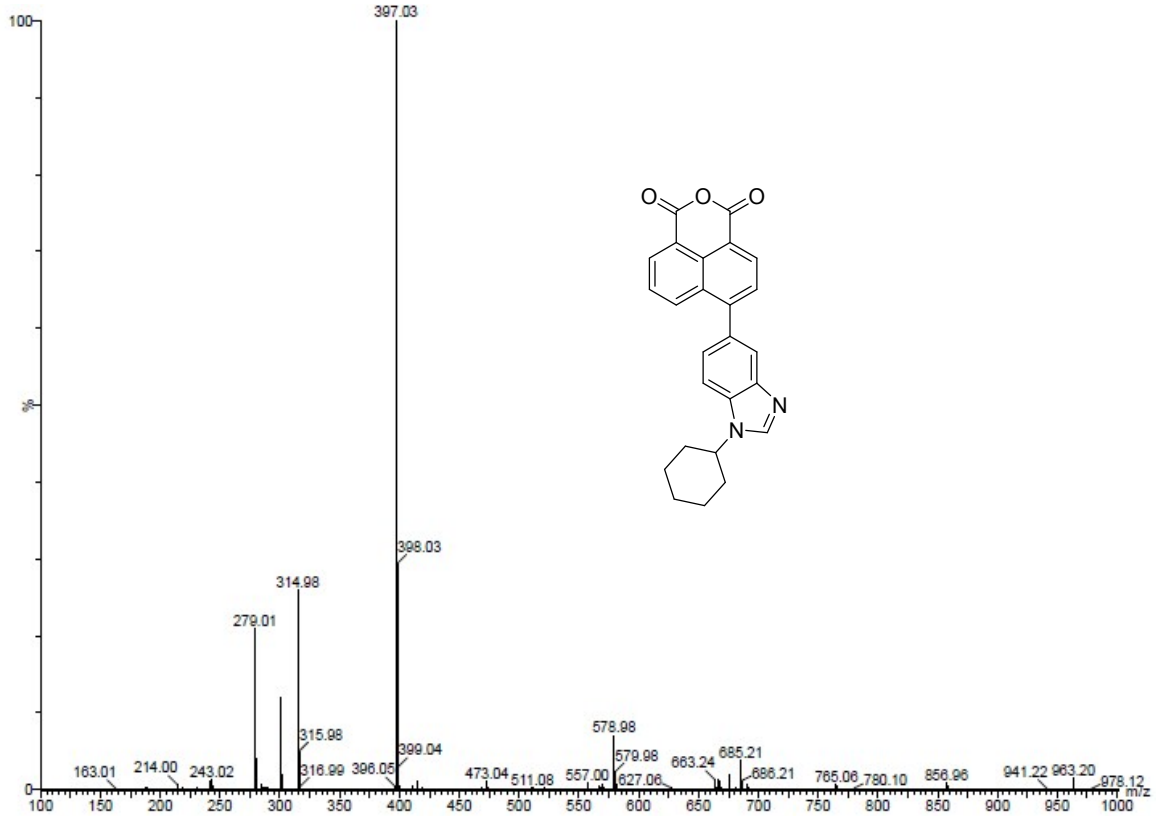


Figure S15: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9a**).

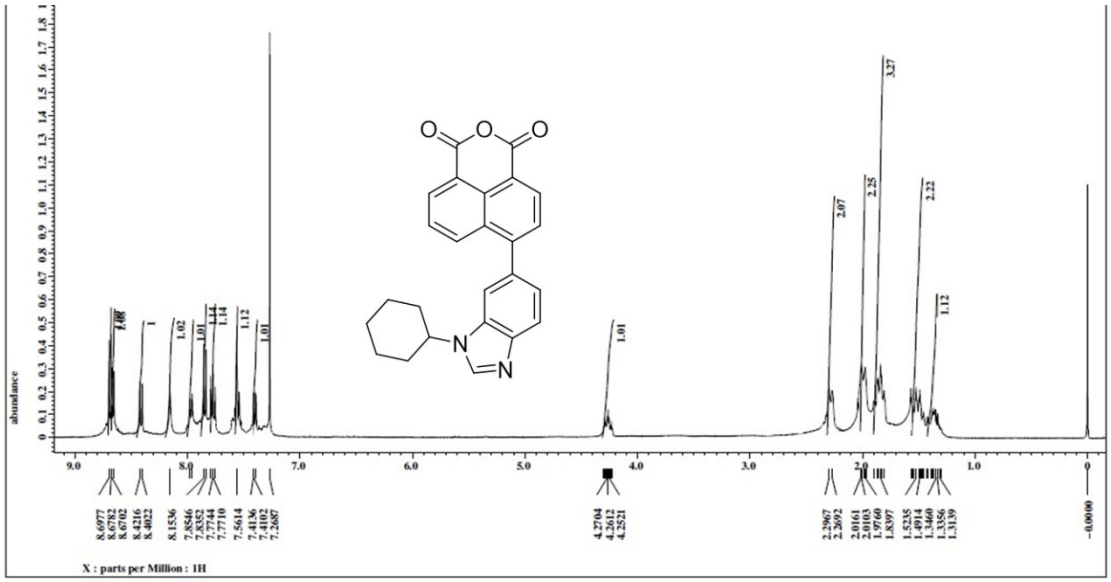


Figure S16: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9b**).

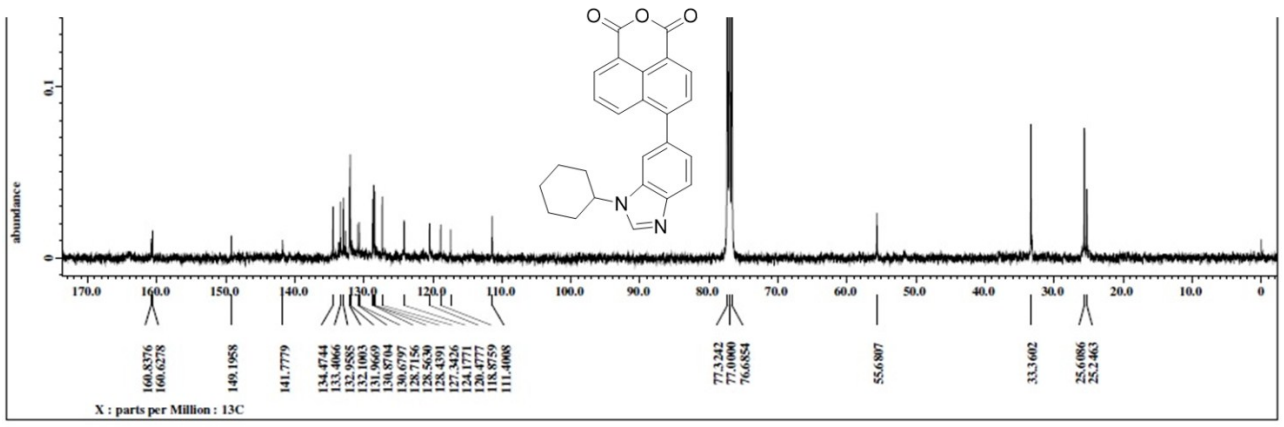


Figure S17: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9b**).

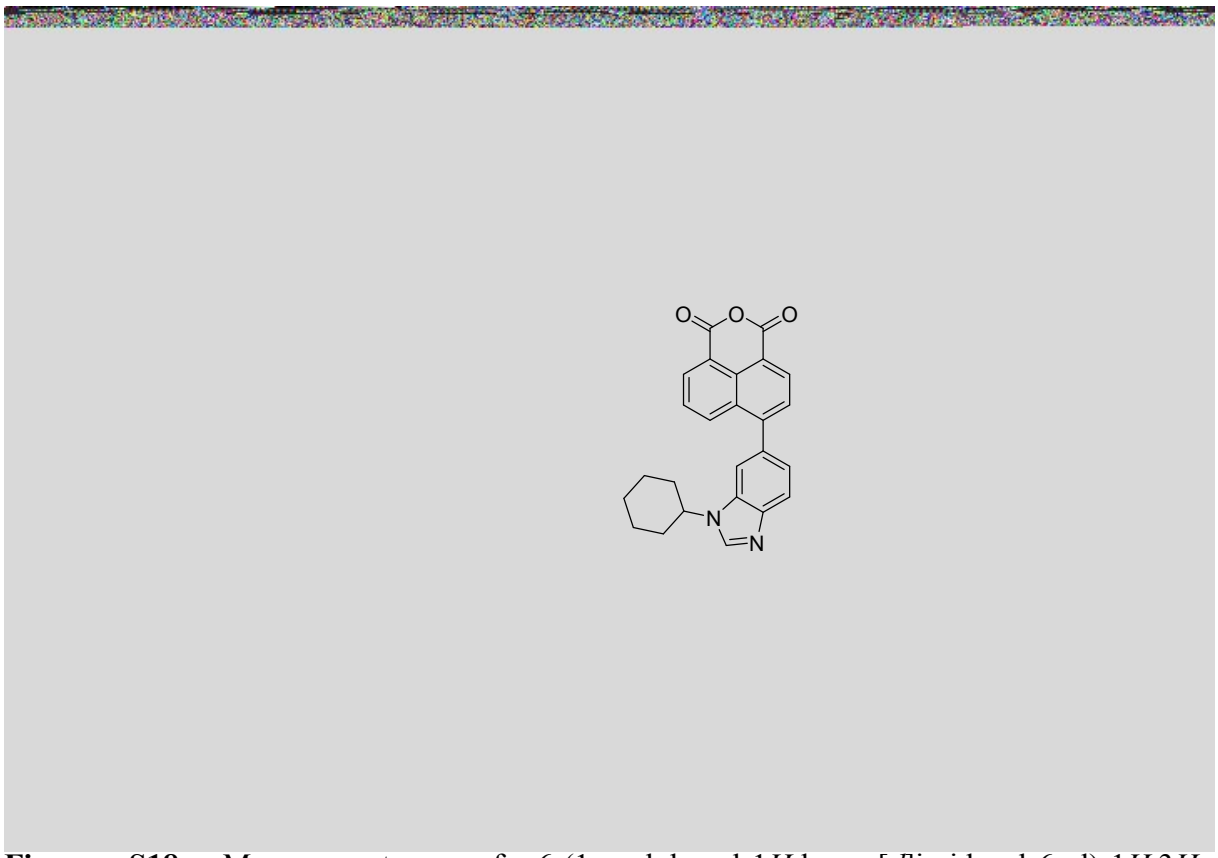


Figure S18: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**9b**).

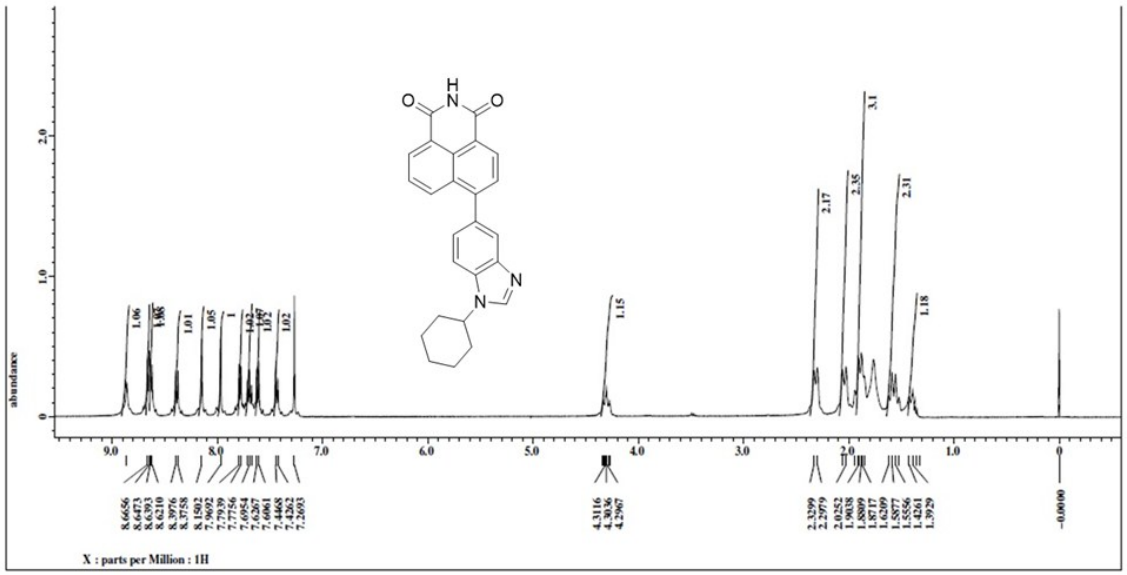


Figure S19: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**10a**).

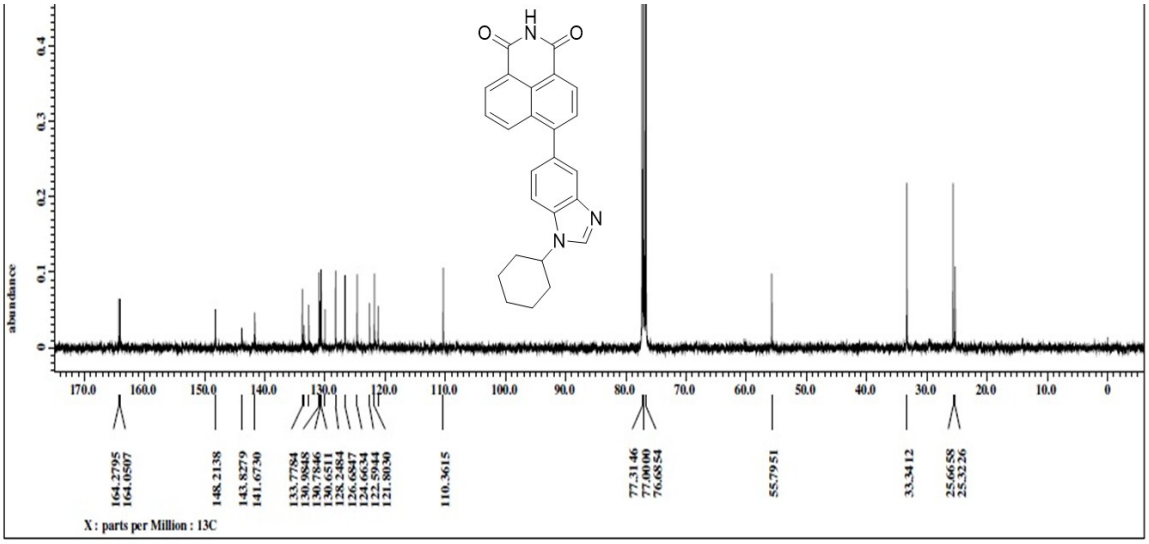


Figure S20: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**10a**).

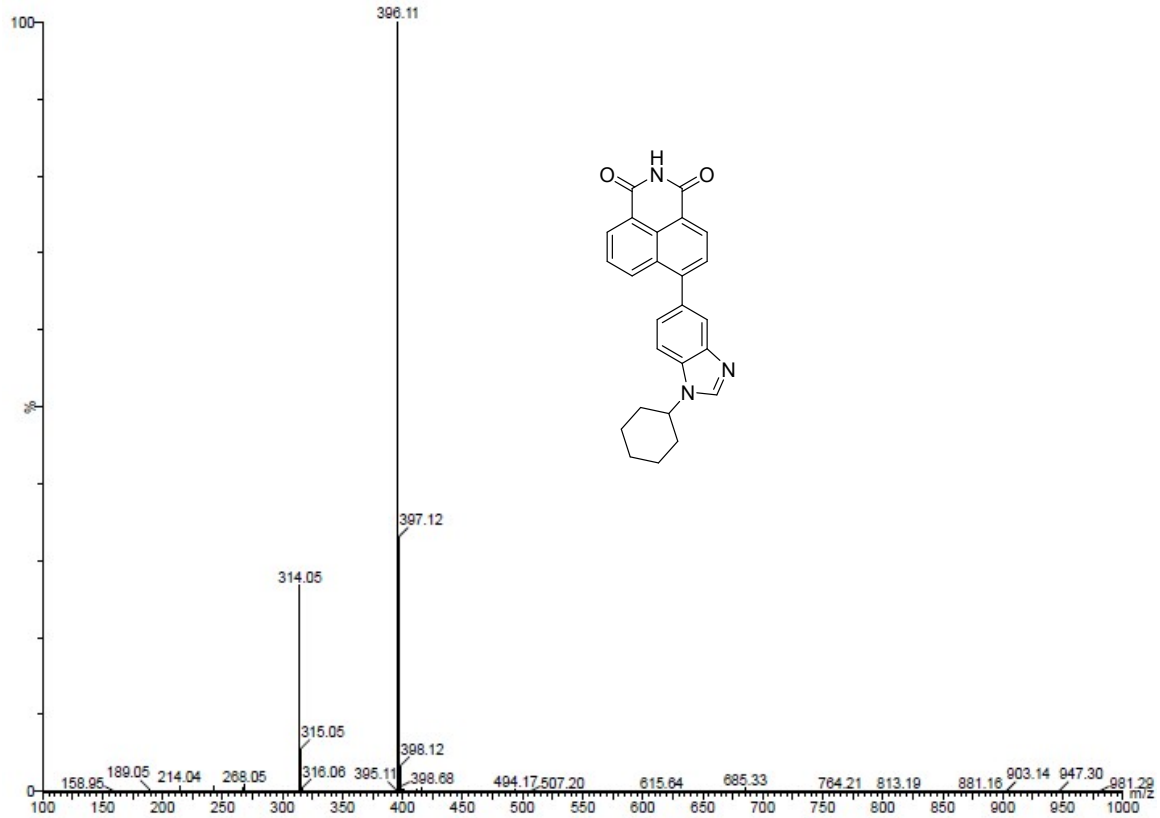


Figure S21: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de]*isoquinoline-1,3(2*H*)-dione (**10a**).

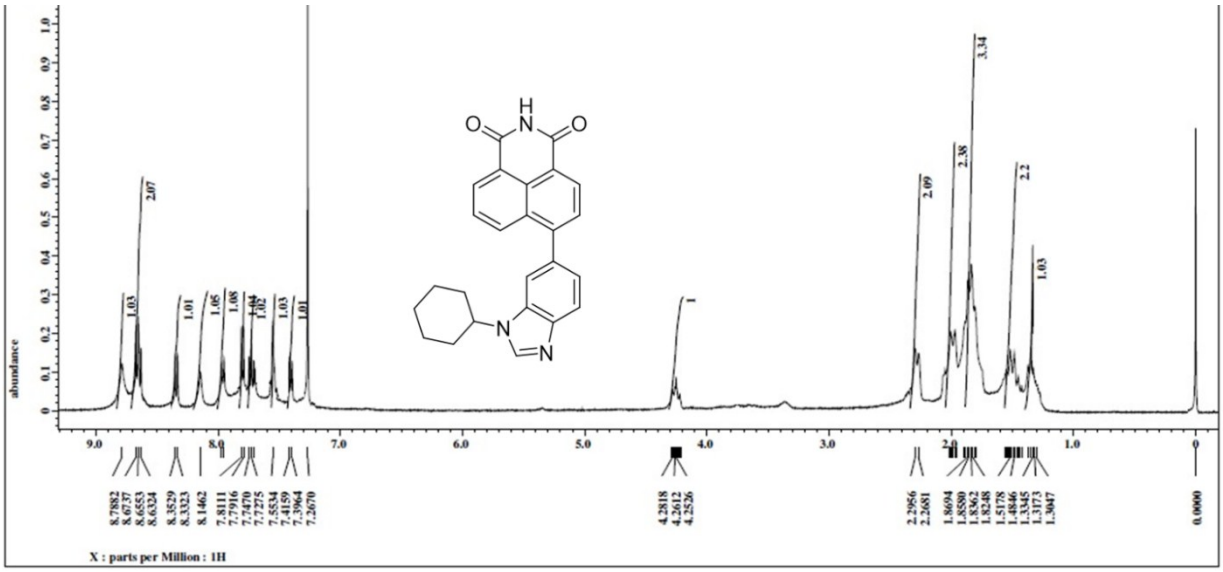


Figure S22: [1]H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(10b)**.

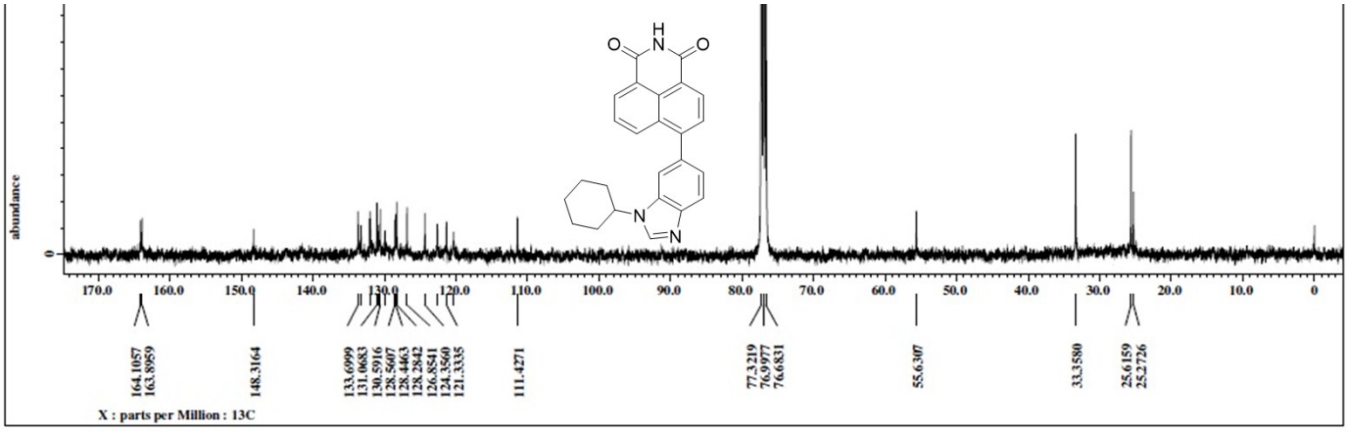


Figure S23: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(10b)**.

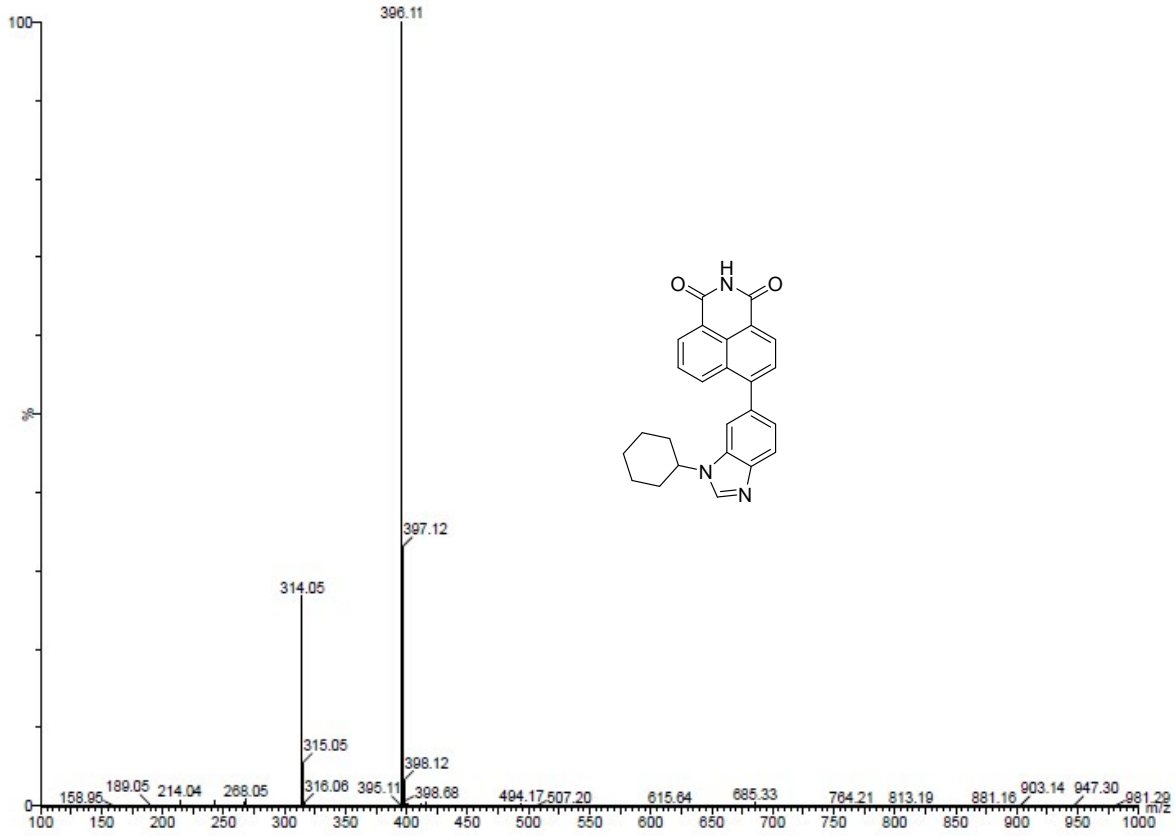


Figure S24: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(10b)**.

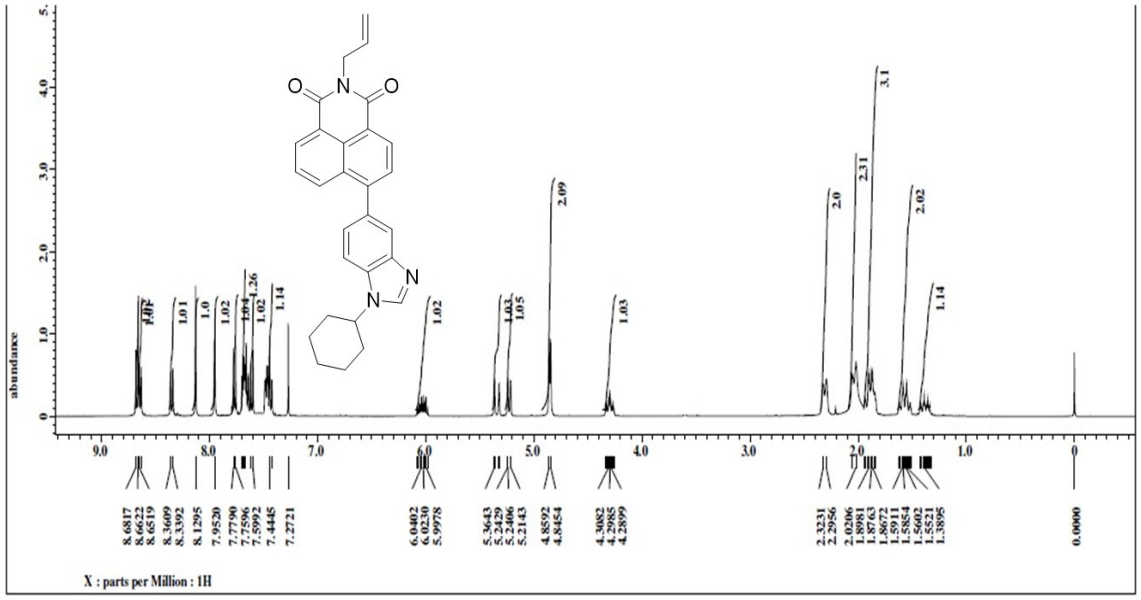


Figure S25: ^{1}H NMR spectrum of 2-allyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**11**).

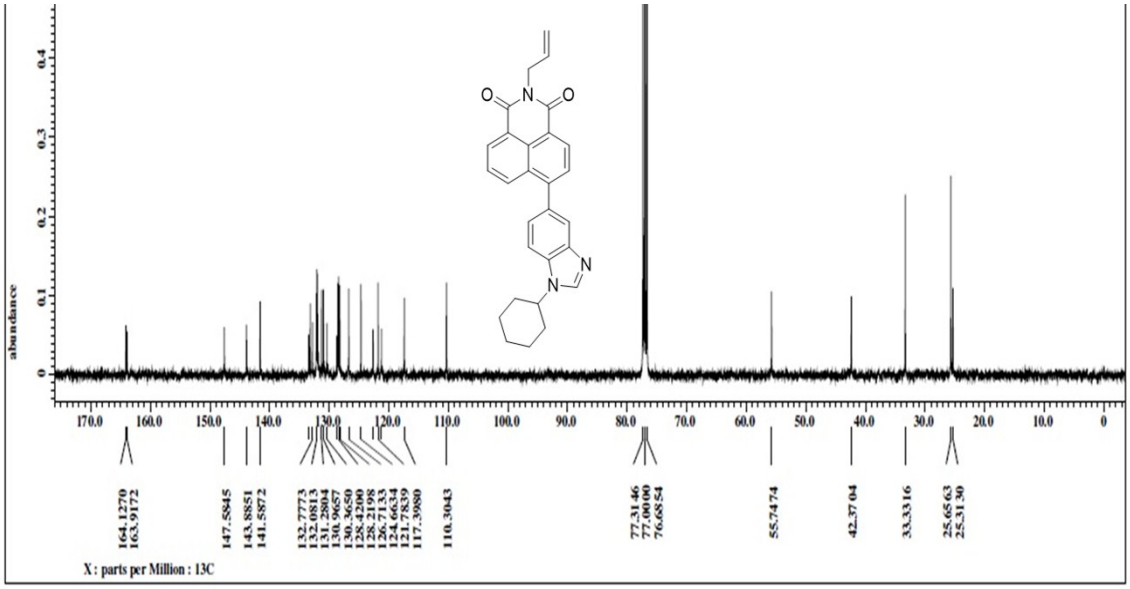


Figure S26: ^{13}C NMR spectrum of 2-allyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**11**).

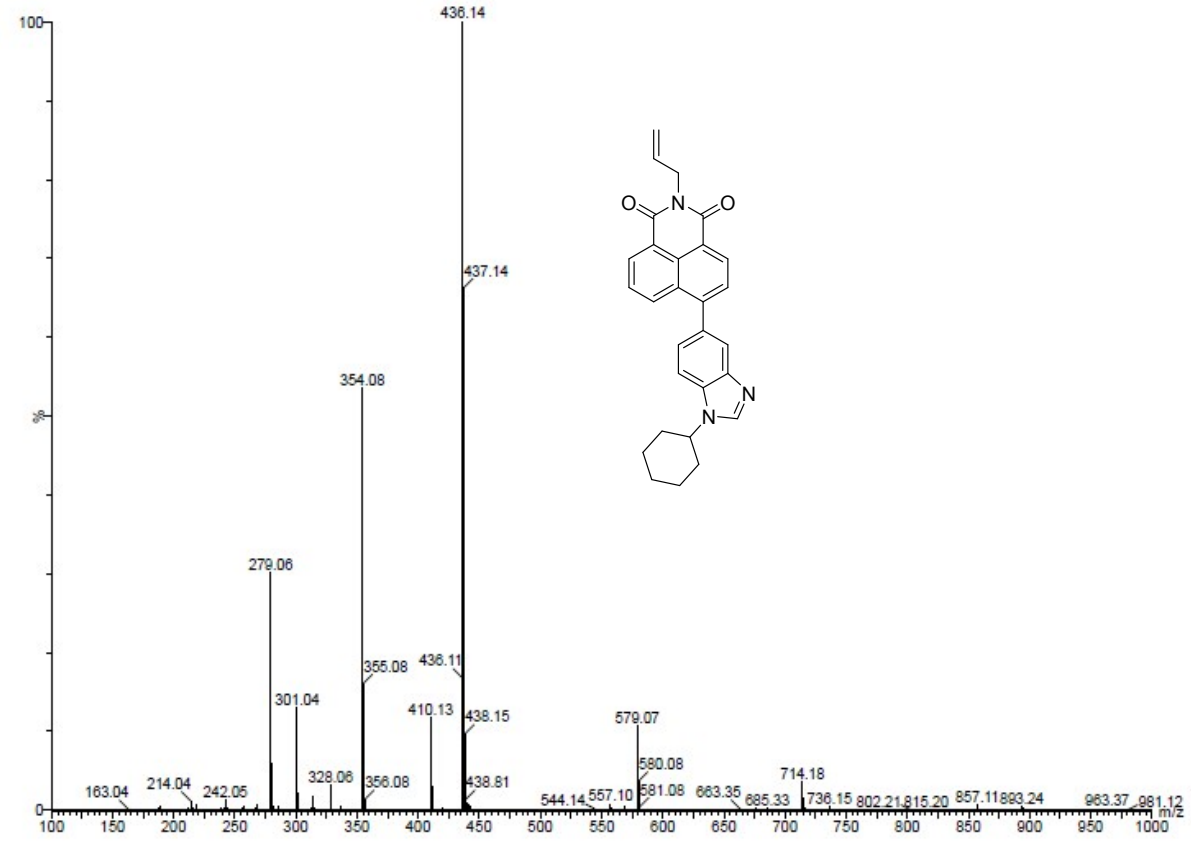


Figure S27: Mass spectrum of 2-allyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**11**).

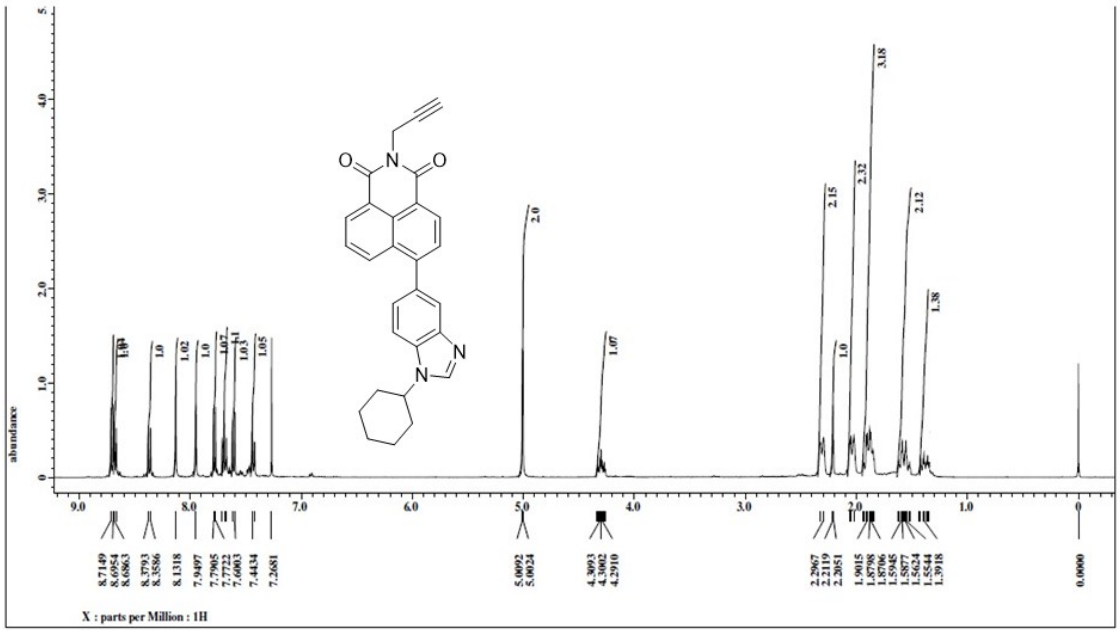


Figure S28: [1]H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(prop-2-yn-1-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**12**).

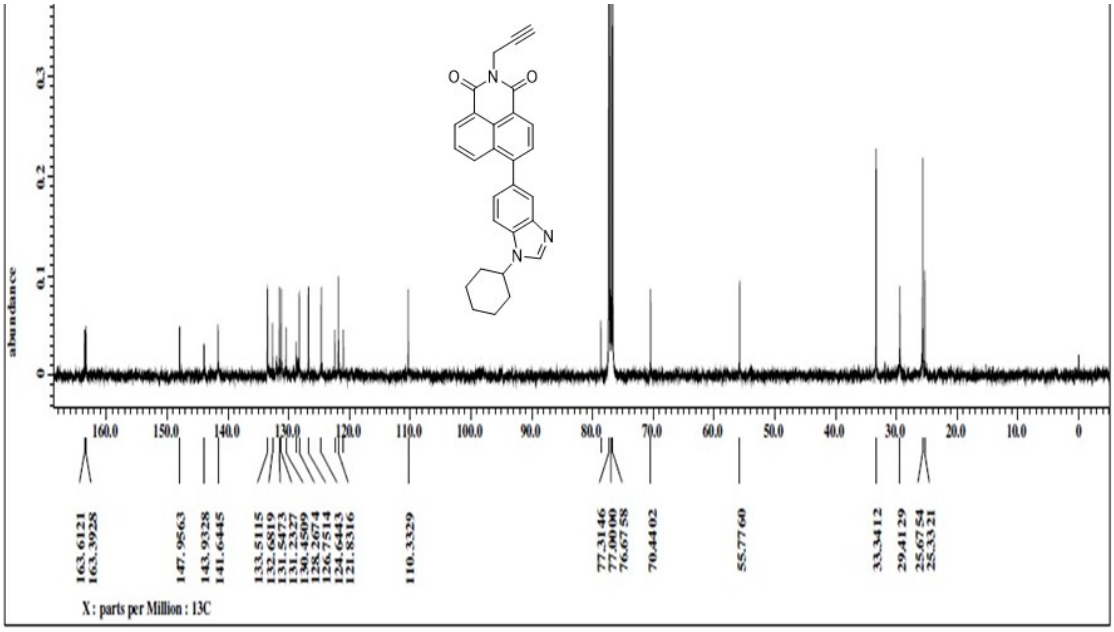


Figure S29: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(prop-2-yn-1-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**12**).

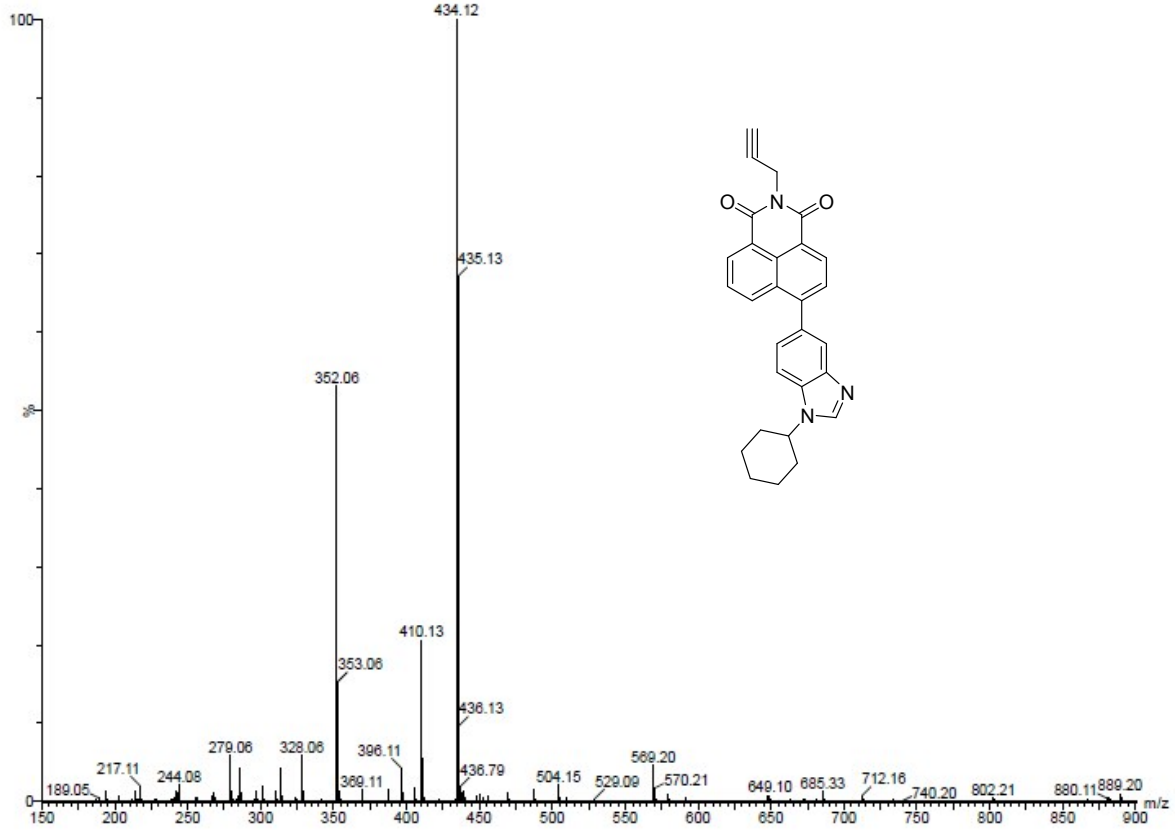


Figure S30: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(prop-2-yn-1-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**12**).

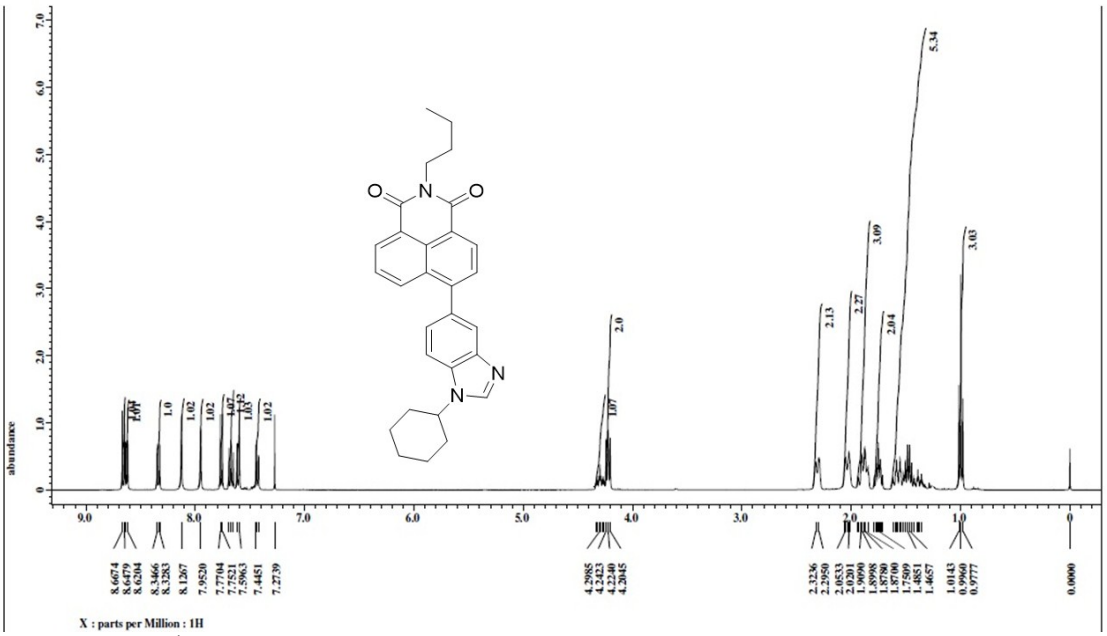


Figure S31: ^{1}H NMR spectrum of 2-butyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**13**).

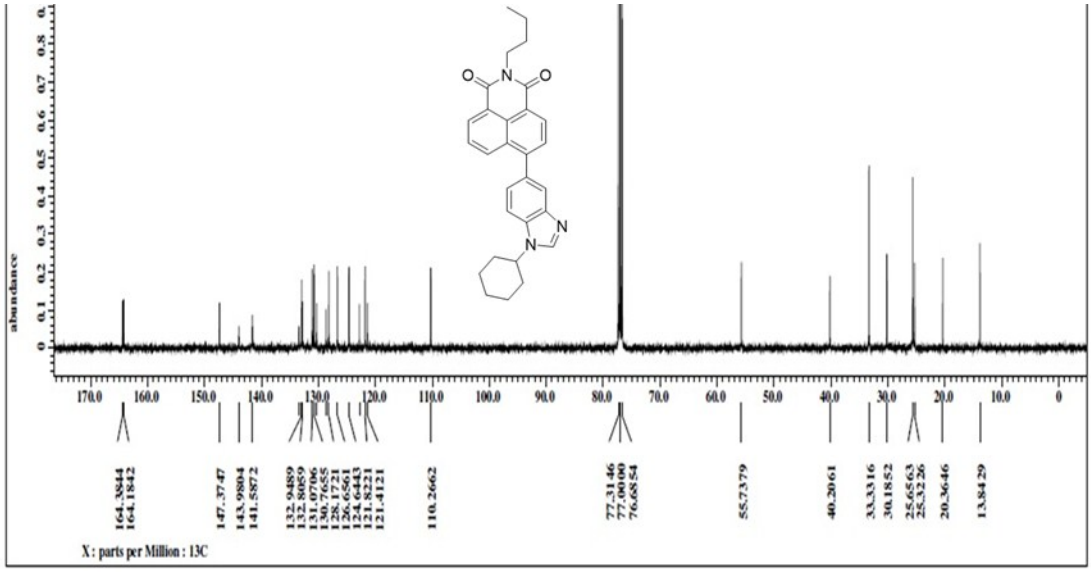


Figure S32: ^{13}C NMR spectrum of 2-butyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**13**).

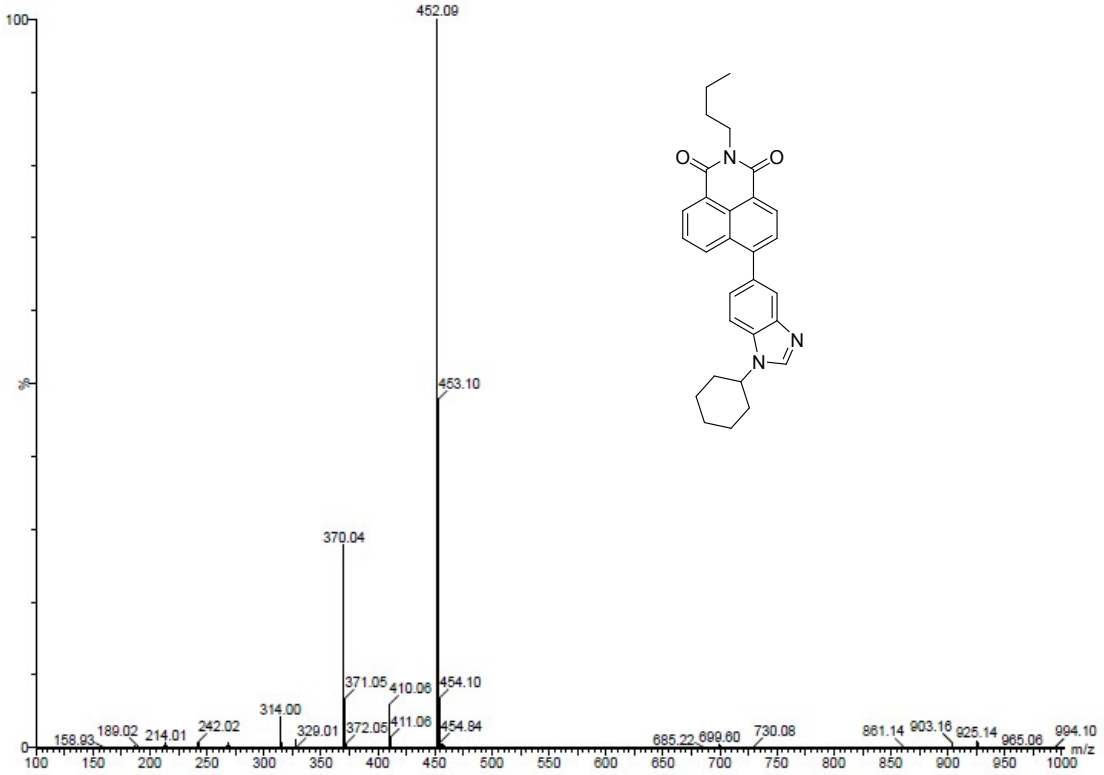


Figure S33: Mass spectrum of 2-butyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**13**).

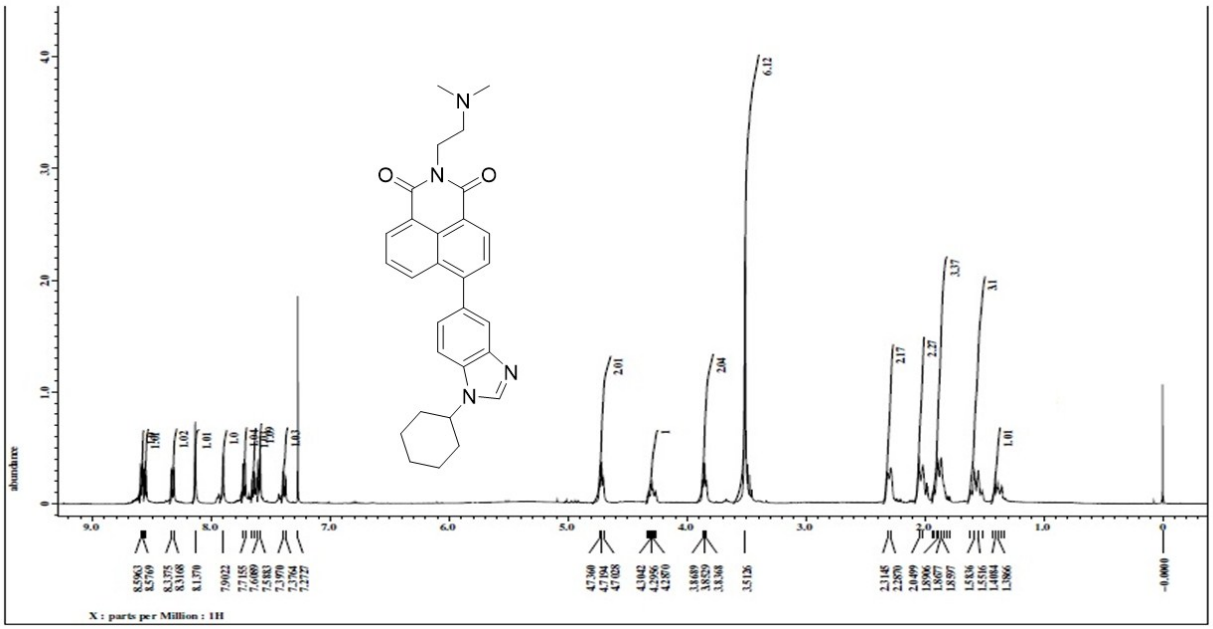


Figure S34: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**14**).

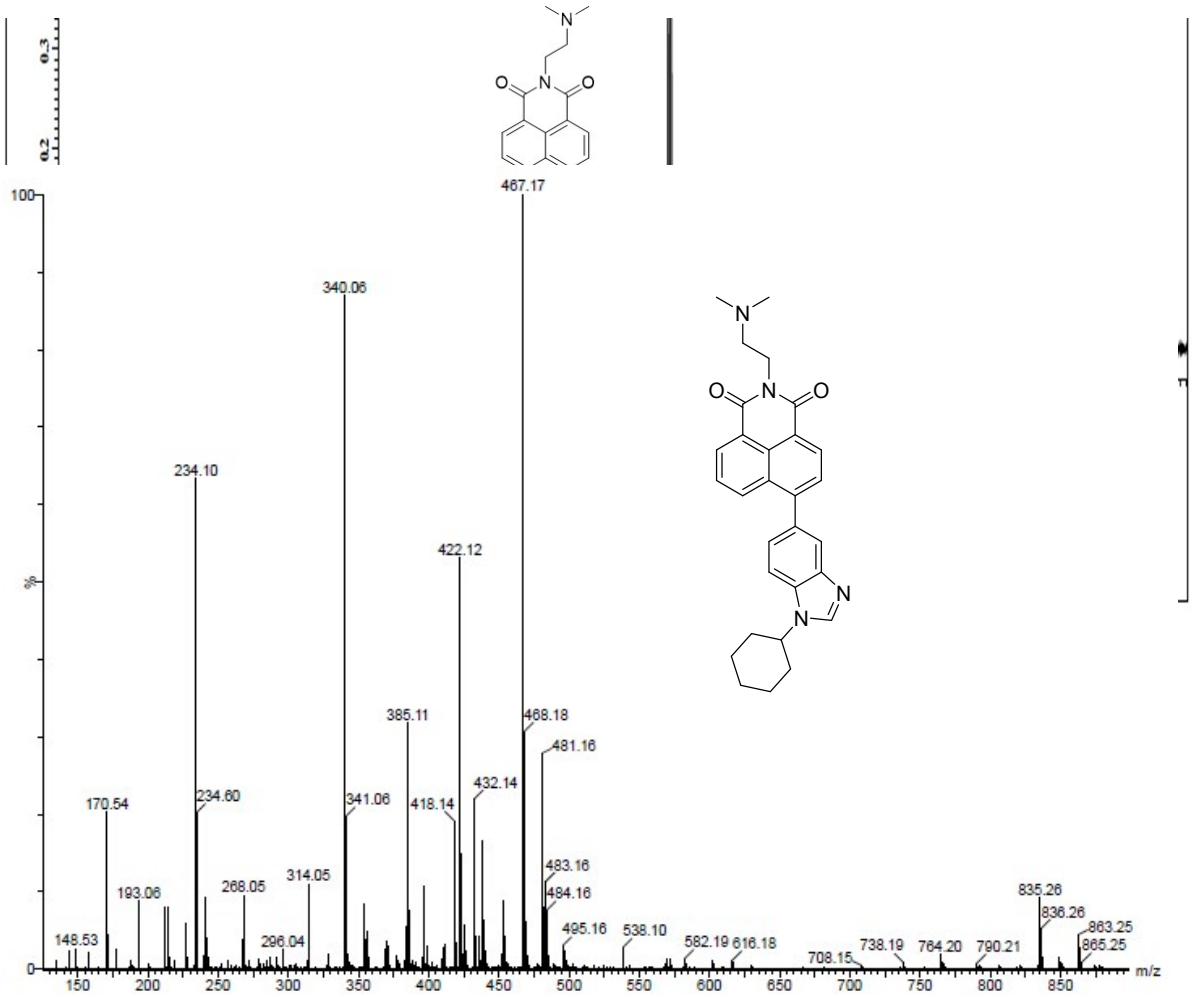


Figure S35: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**14**).

Figure S36: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**14**).

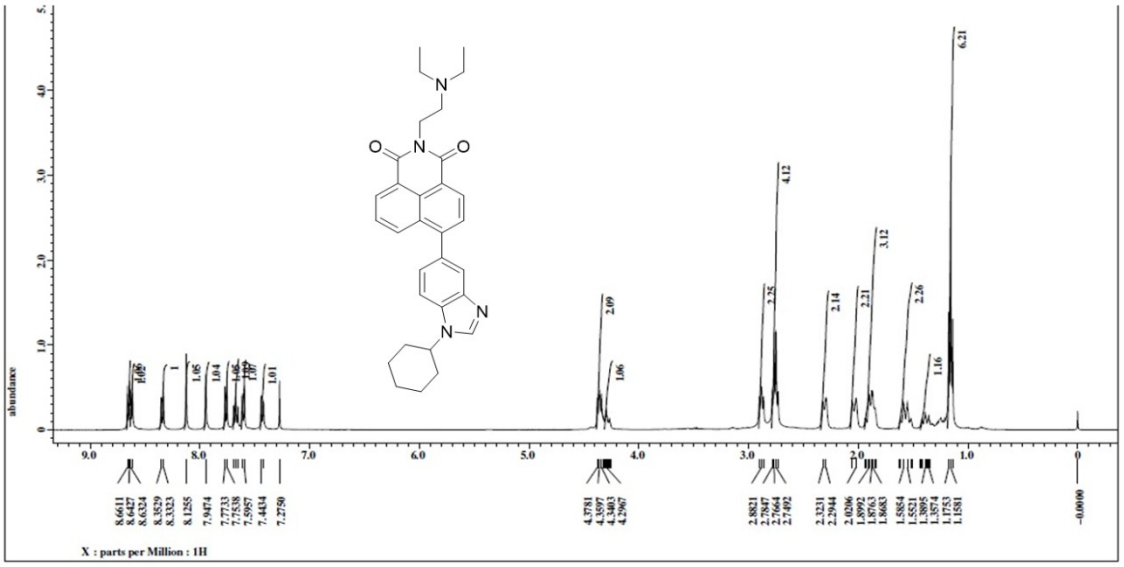


Figure S37: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(diethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**15**).

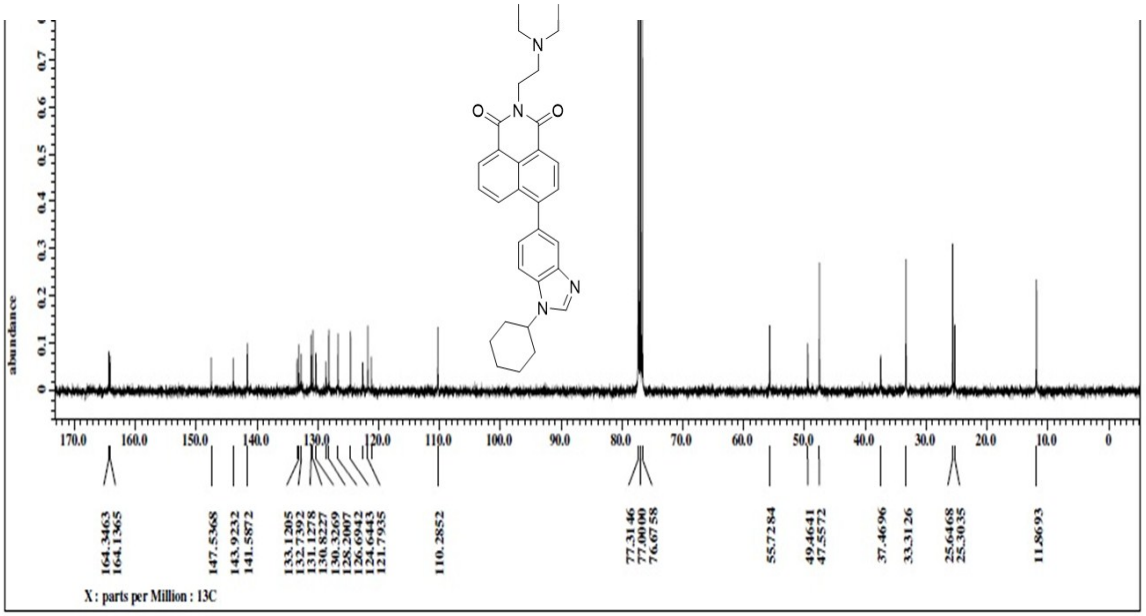


Figure S38: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(diethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**15**).

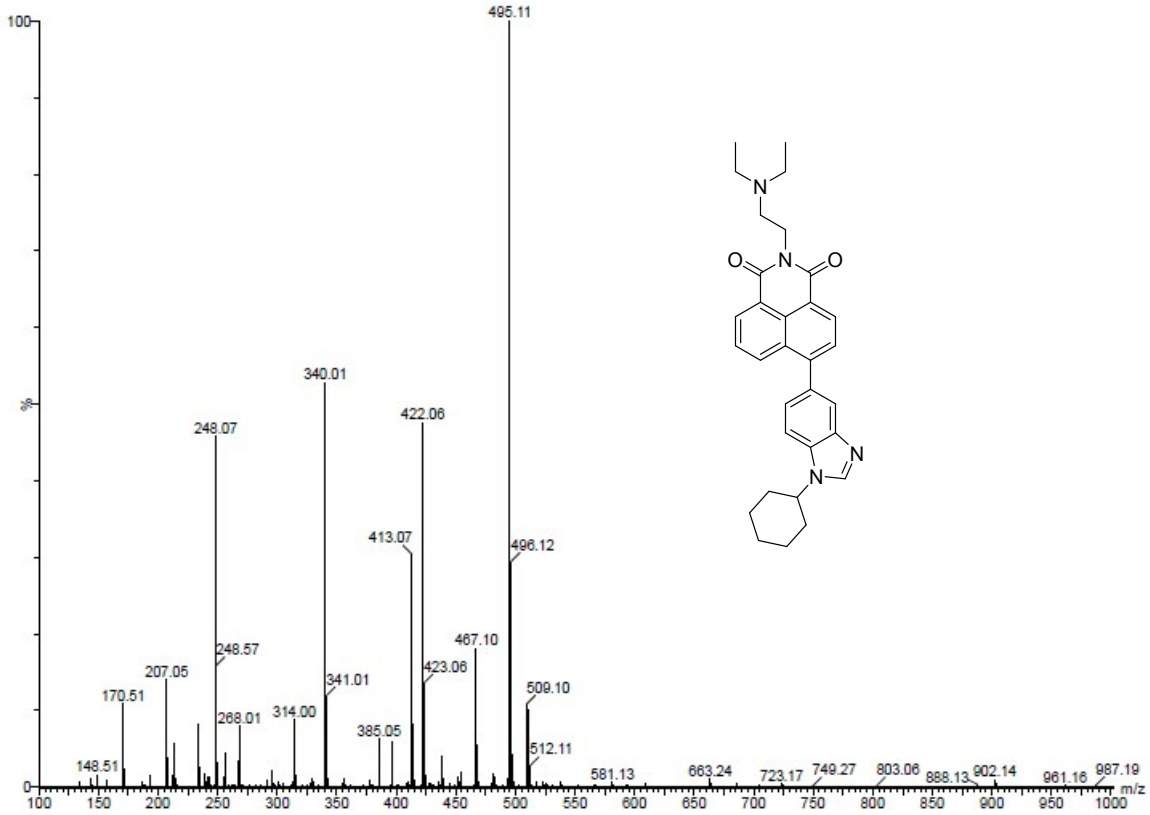


Figure S39: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-(diethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**15**).

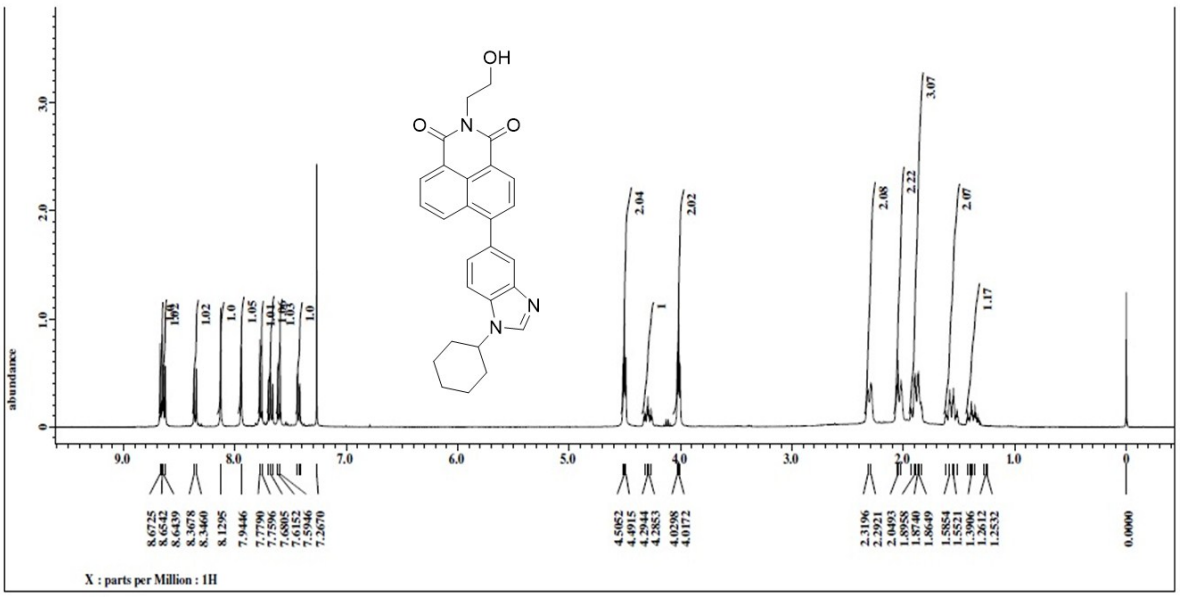


Figure S40: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**16**).

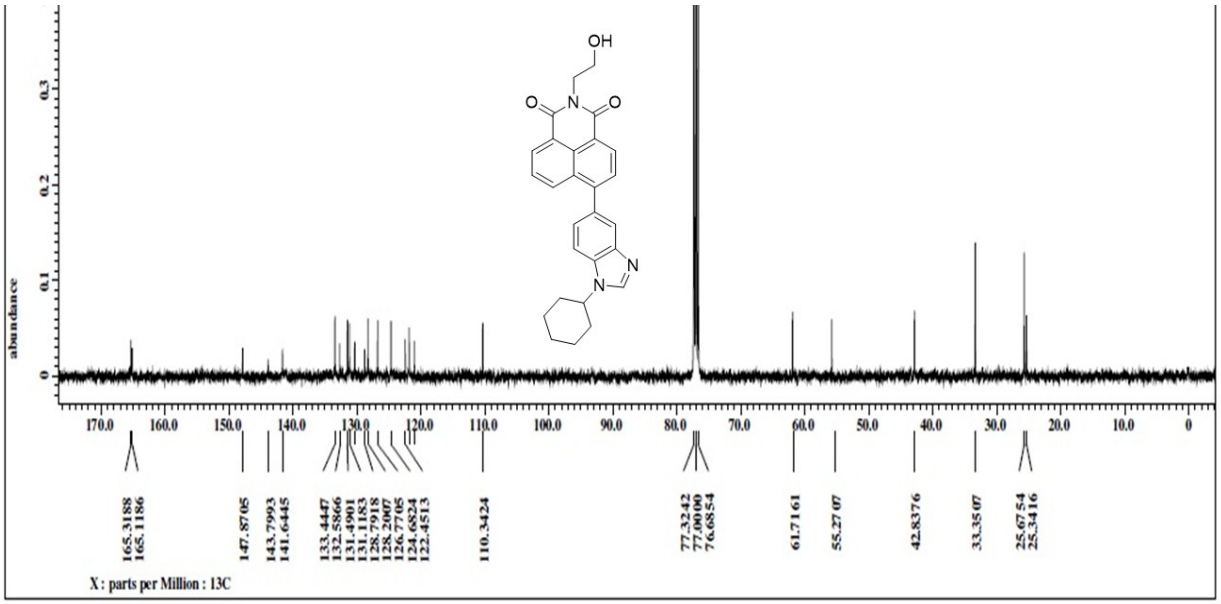


Figure S41: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**16**).

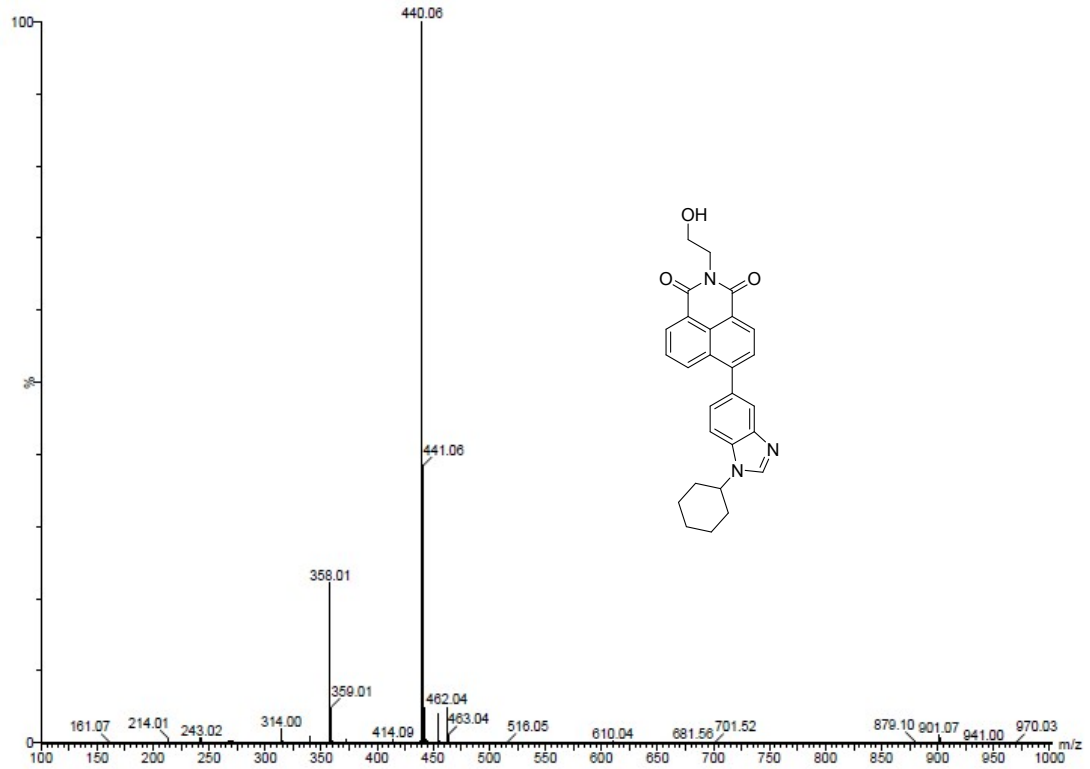


Figure S42: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**16**).

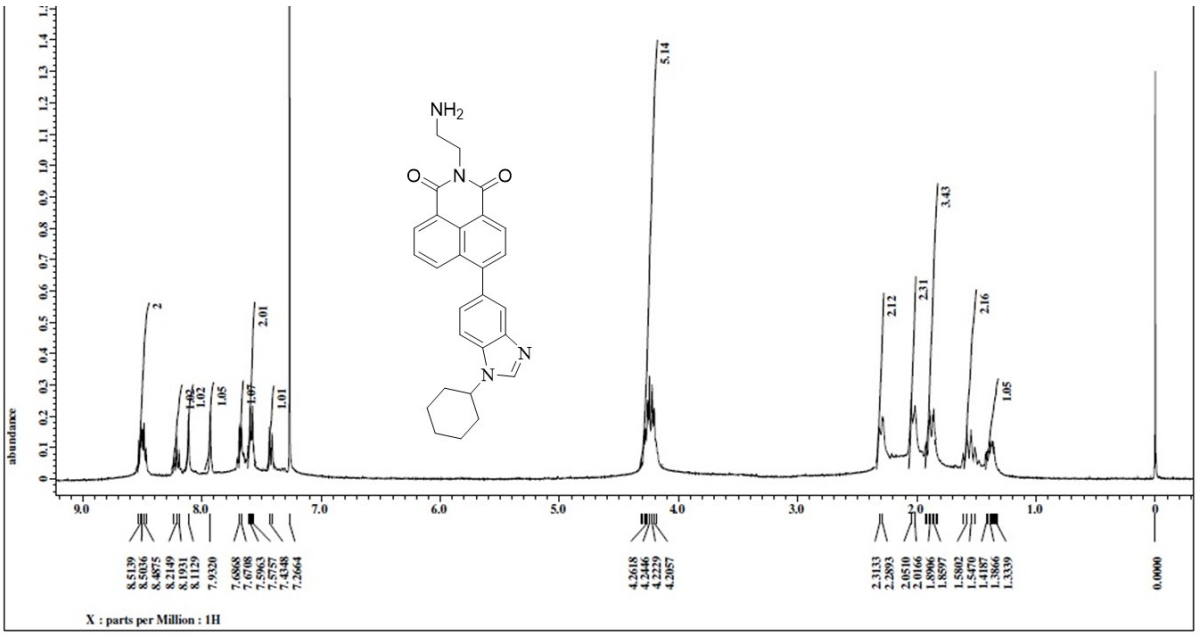


Figure S43: ^{1}H NMR spectrum of 2-(2-aminoethyl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**17**).

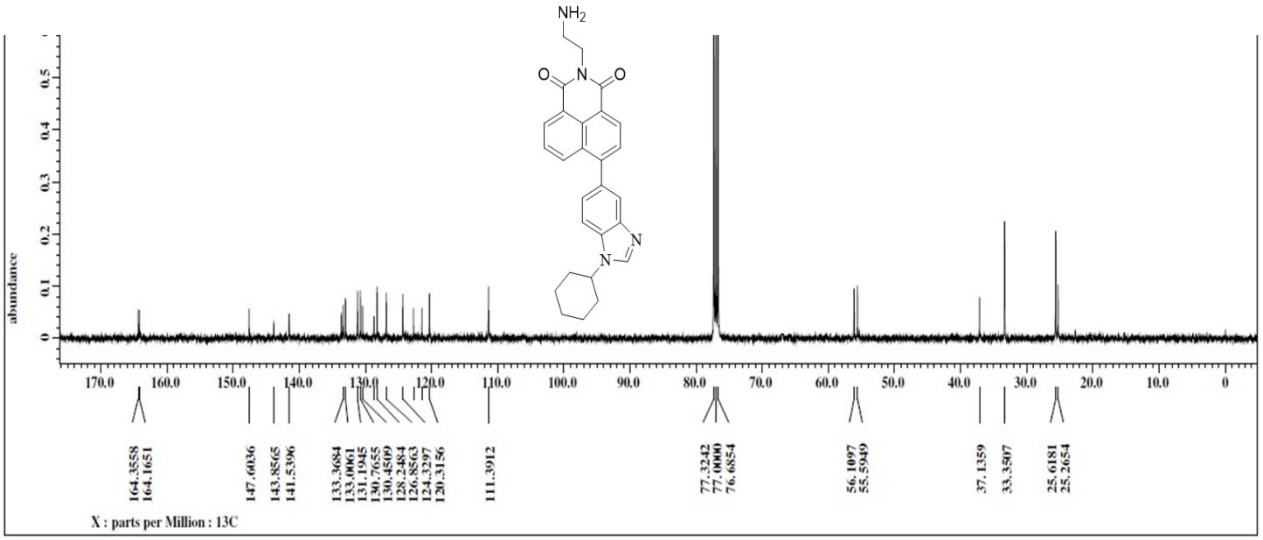


Figure S44: ^{13}C NMR spectrum of 2-(2-aminoethyl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**17**).

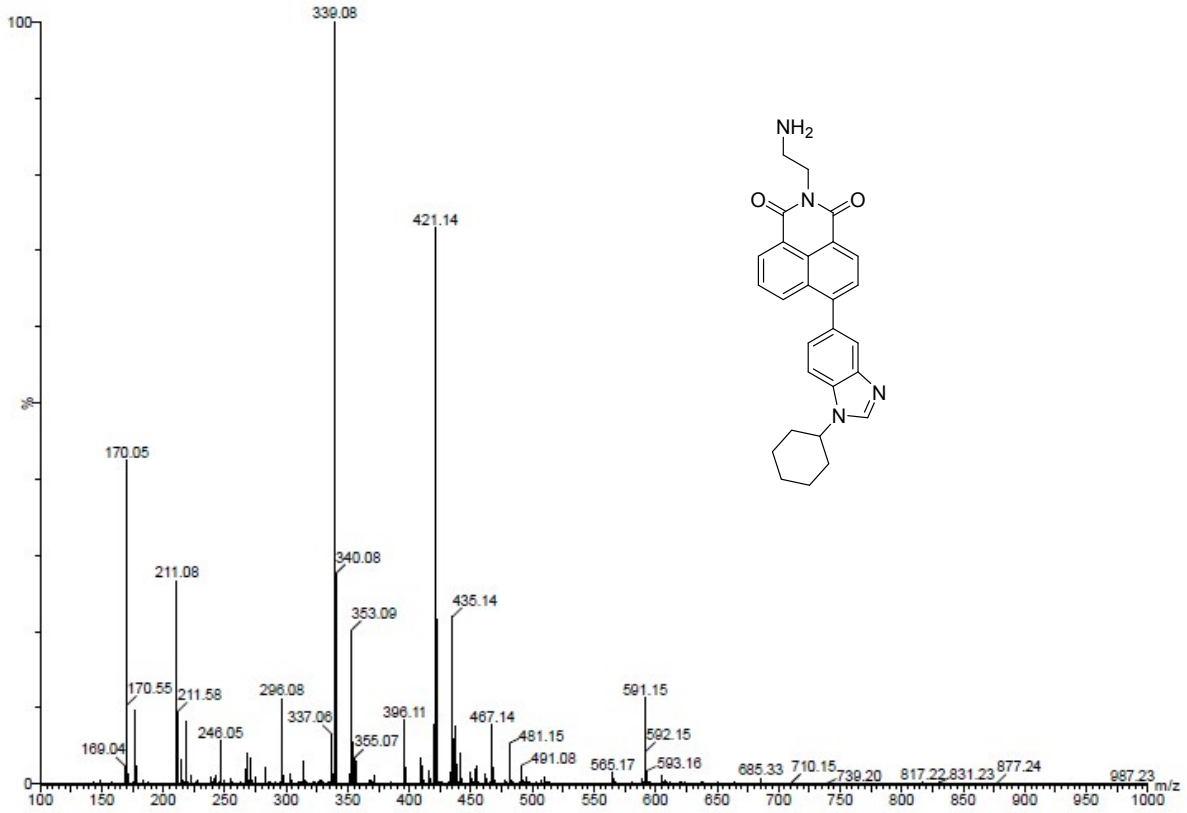


Figure S45: Mass spectrum of 2-(2-aminoethyl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**17**).

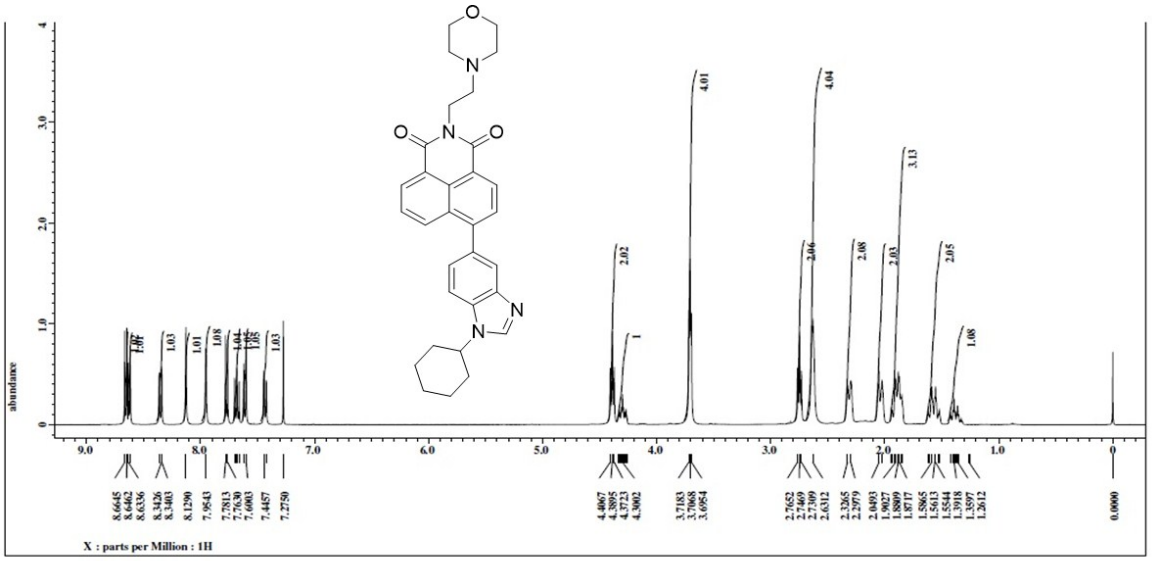


Figure S46: [1]H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**18**).

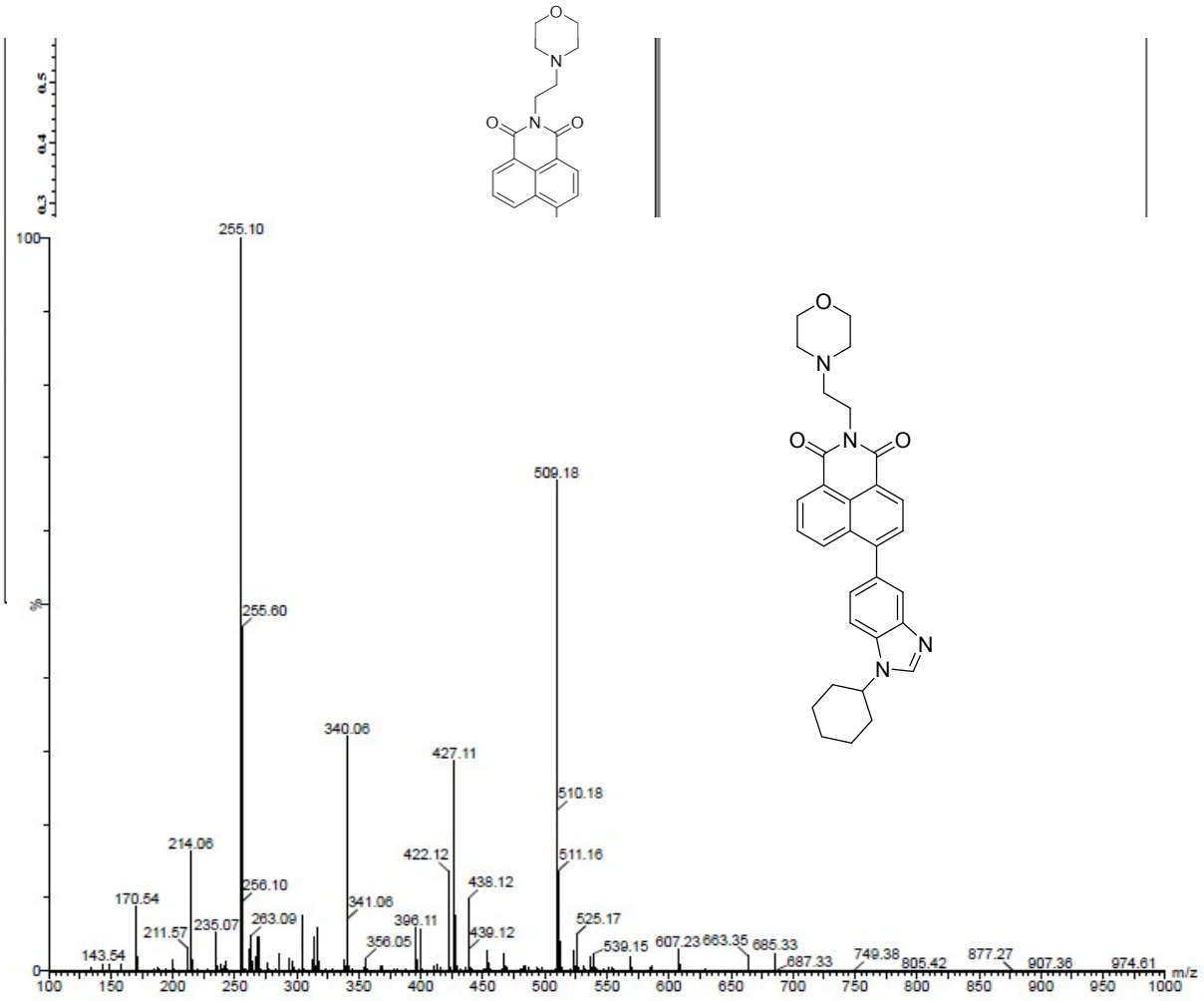


Figure S47: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**18**).

Figure S48: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**18**).

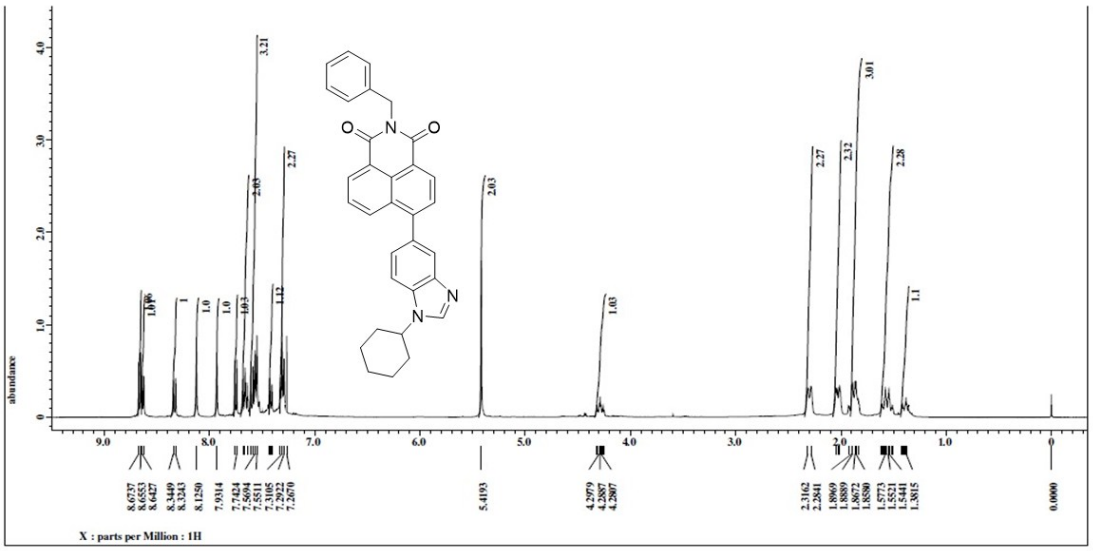


Figure S49: [1]H NMR spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**19**).

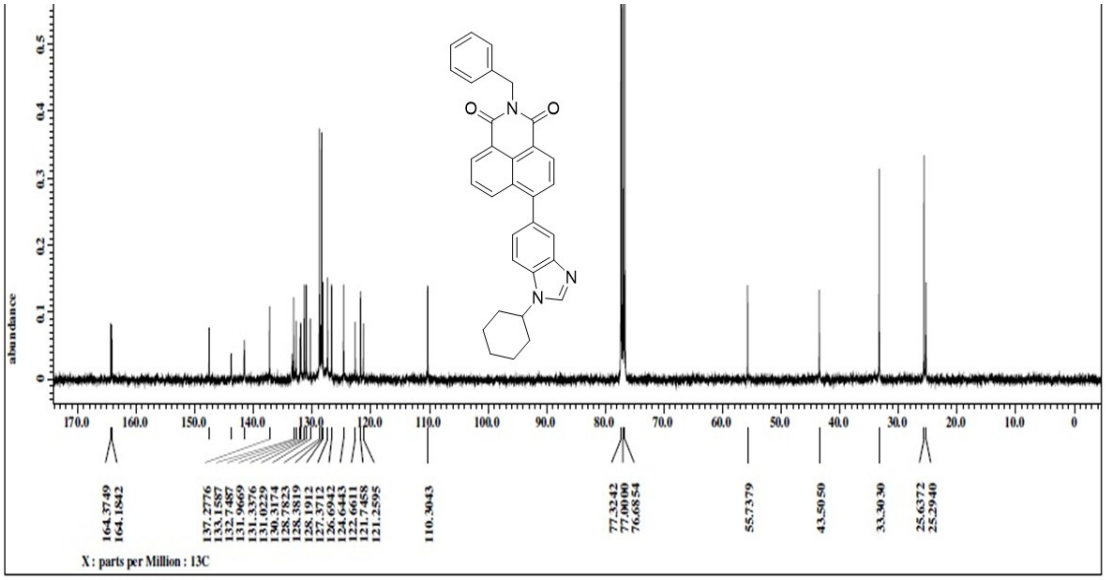


Figure S50: [13]C NMR spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**19**).

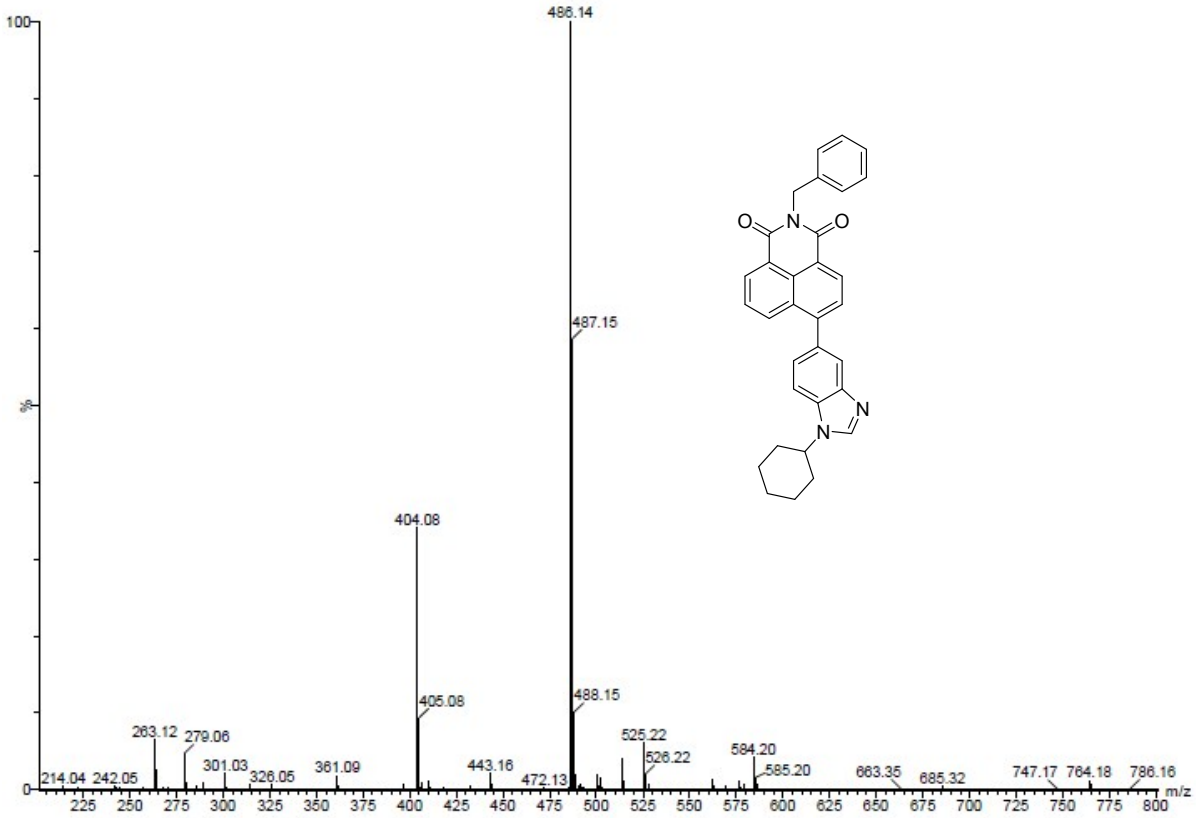


Figure S51: Mass spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**19**).

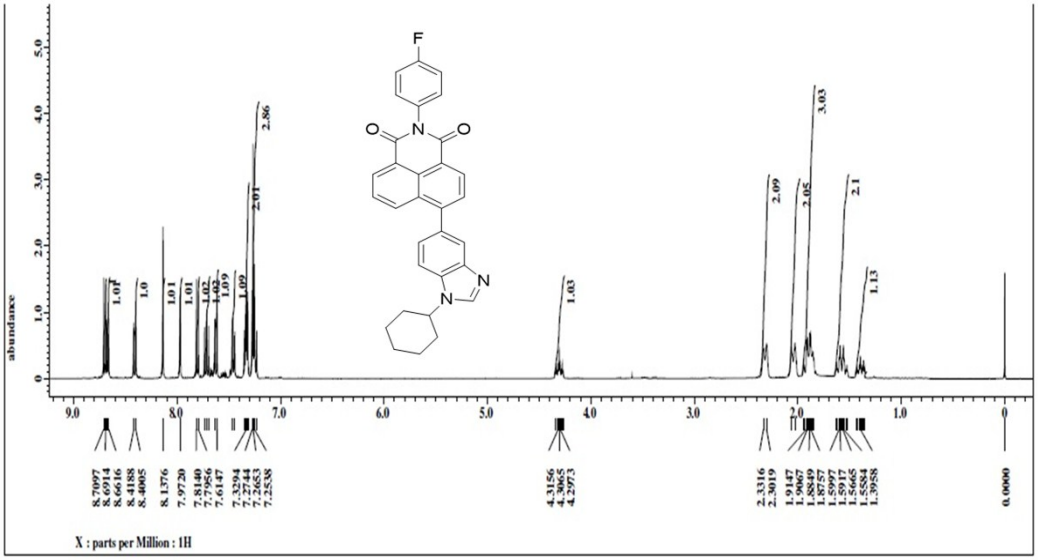


Figure S52: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(4-fluorophenyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**20**).

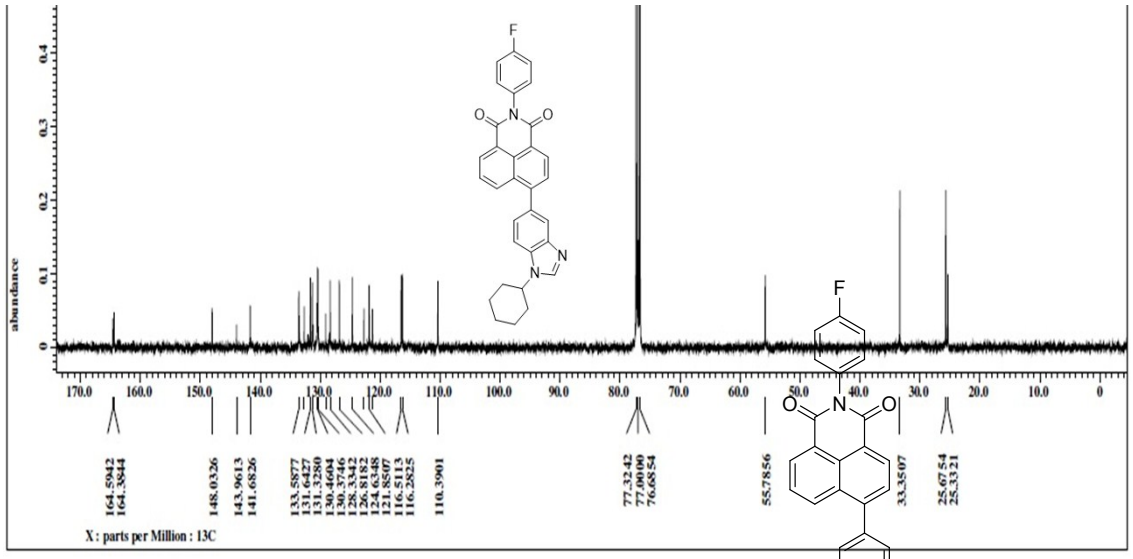


Figure S53: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(4-fluorophenyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**20**).

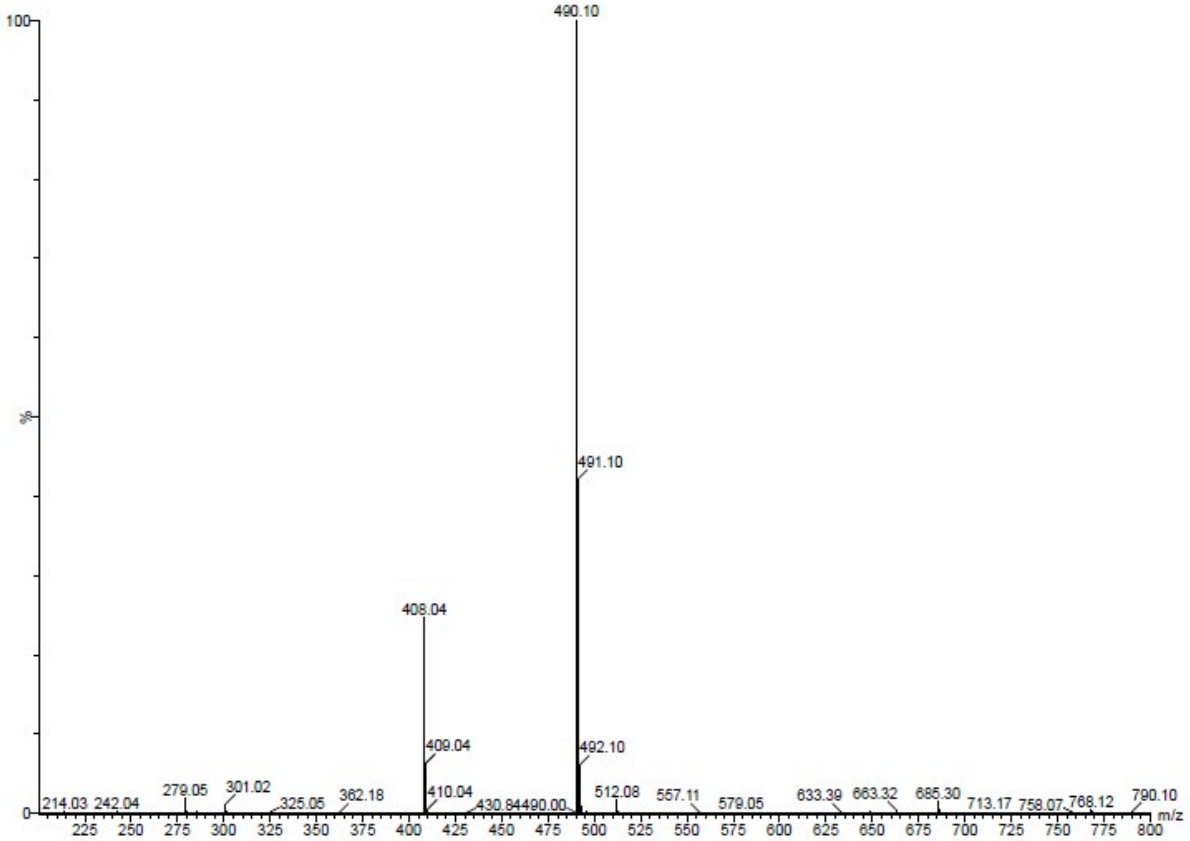


Figure S54: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-2-(4-fluorophenyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**20**).

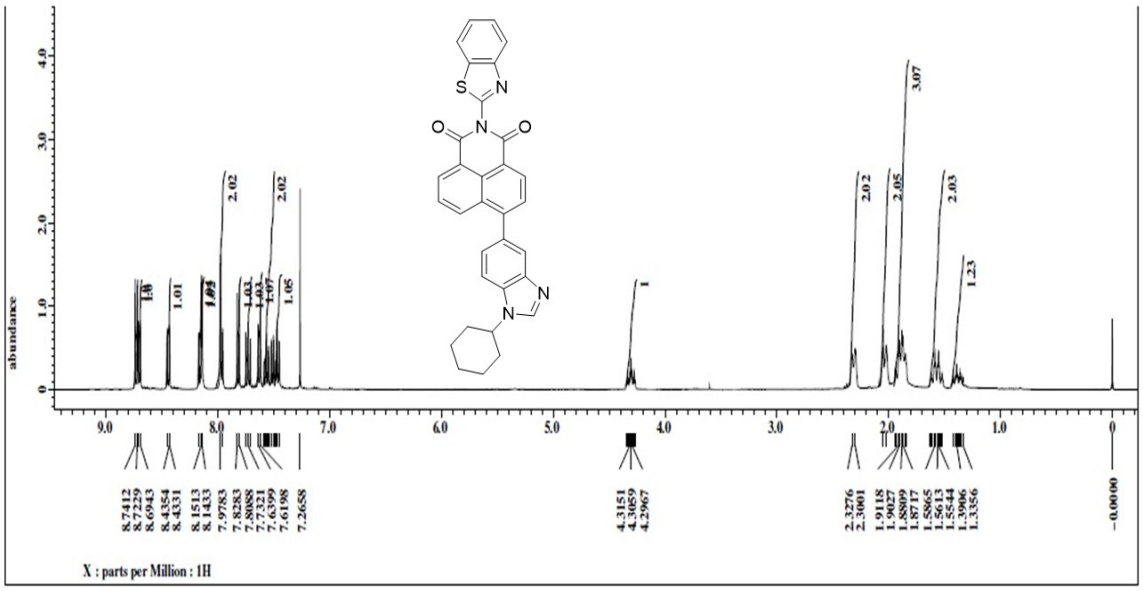


Figure S55: ^{1}H NMR spectrum of 2-(benzo[*d*]thiazol-2-yl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**21**).

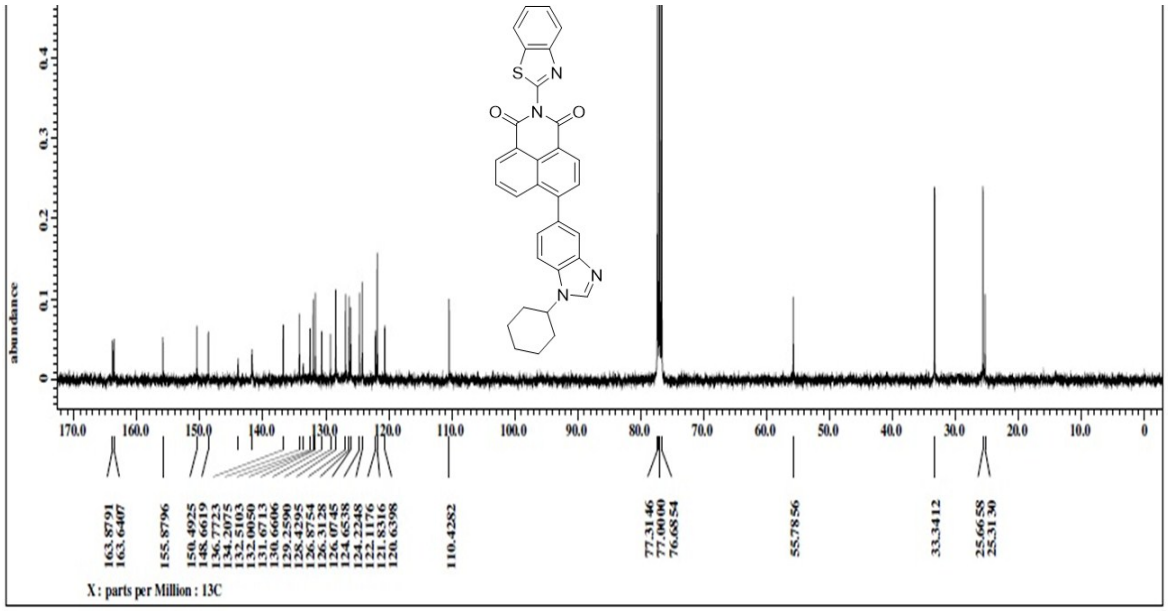


Figure S56: ^{13}C NMR spectrum of 2-(benzo[*d*]thiazol-2-yl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**21**).

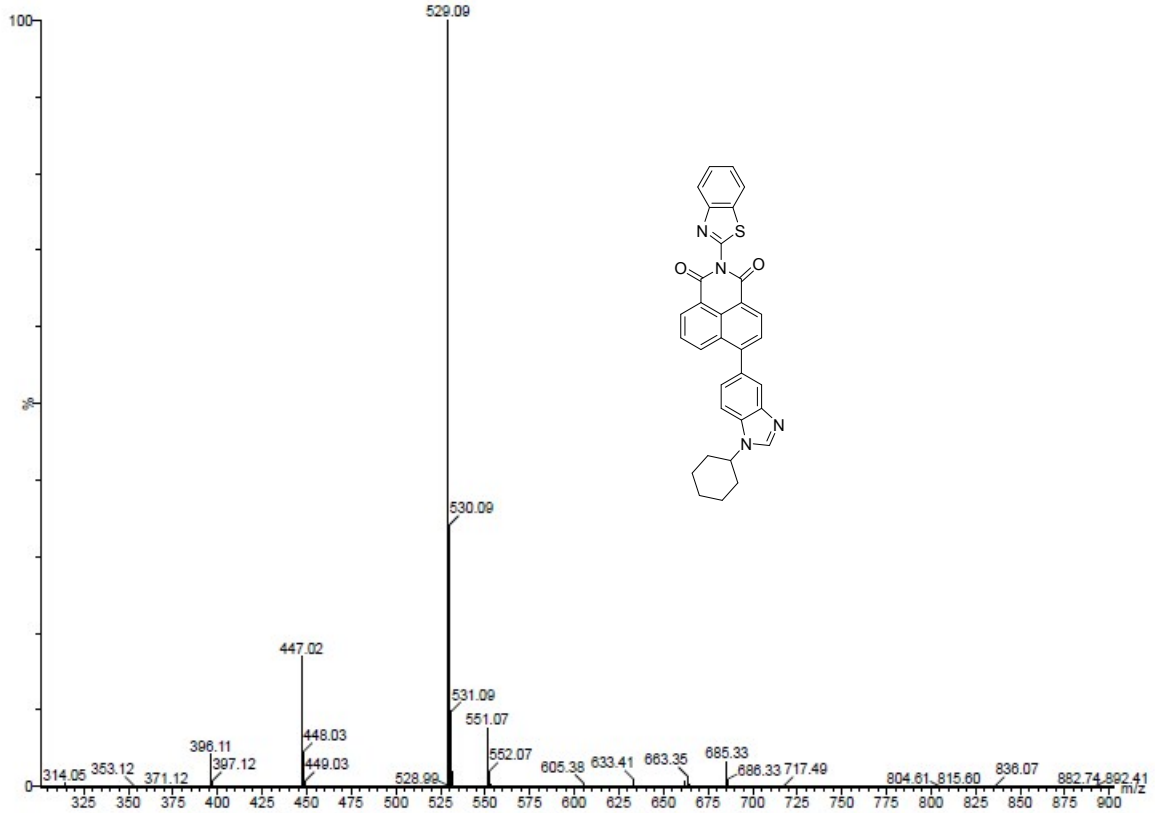


Figure S57: Mass spectrum of 2-(benzo[*d*]thiazol-2-yl)-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**21**).

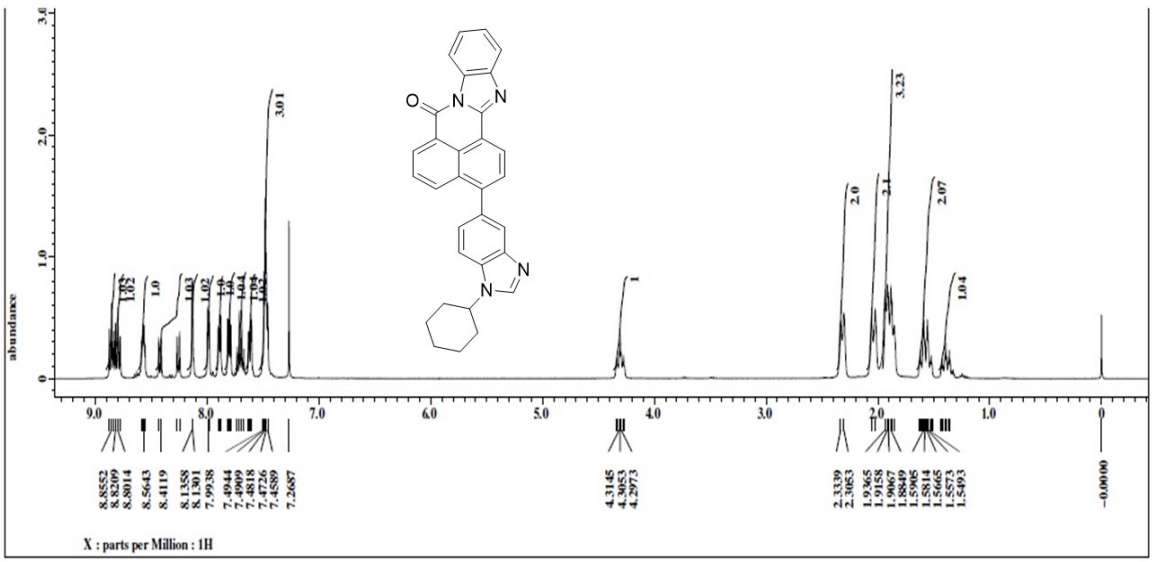


Figure S58: ^{1}H NMR spectrum of 3-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-7*H*-benzo[*de*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-7-one (**22**).

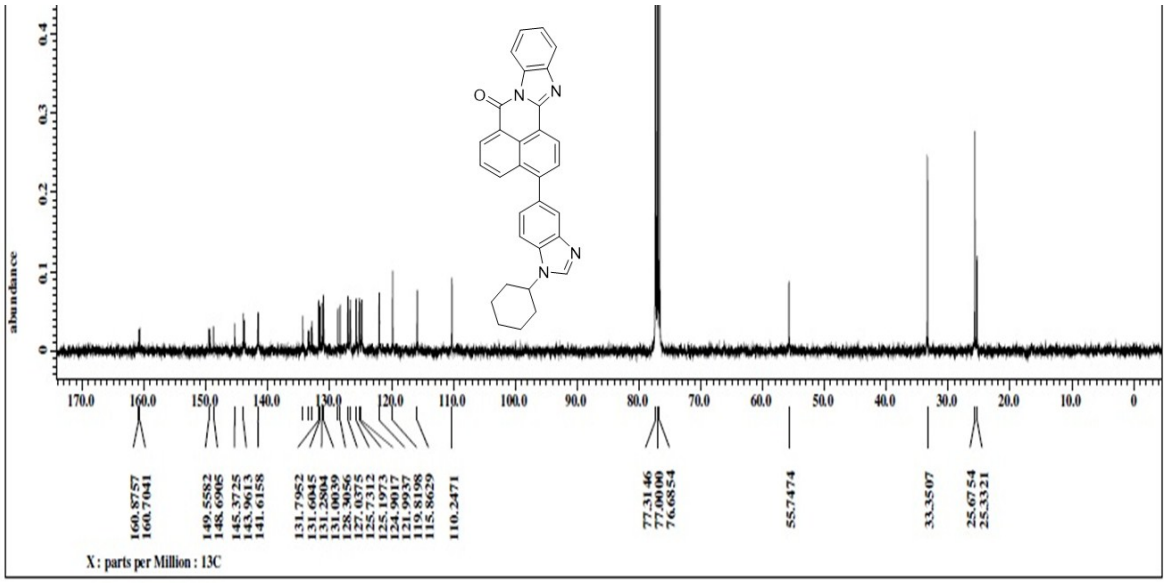


Figure S59: ^{13}C NMR spectrum of 3-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-5-yl)-7*H*-benzo[*de*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-7-one (**22**).

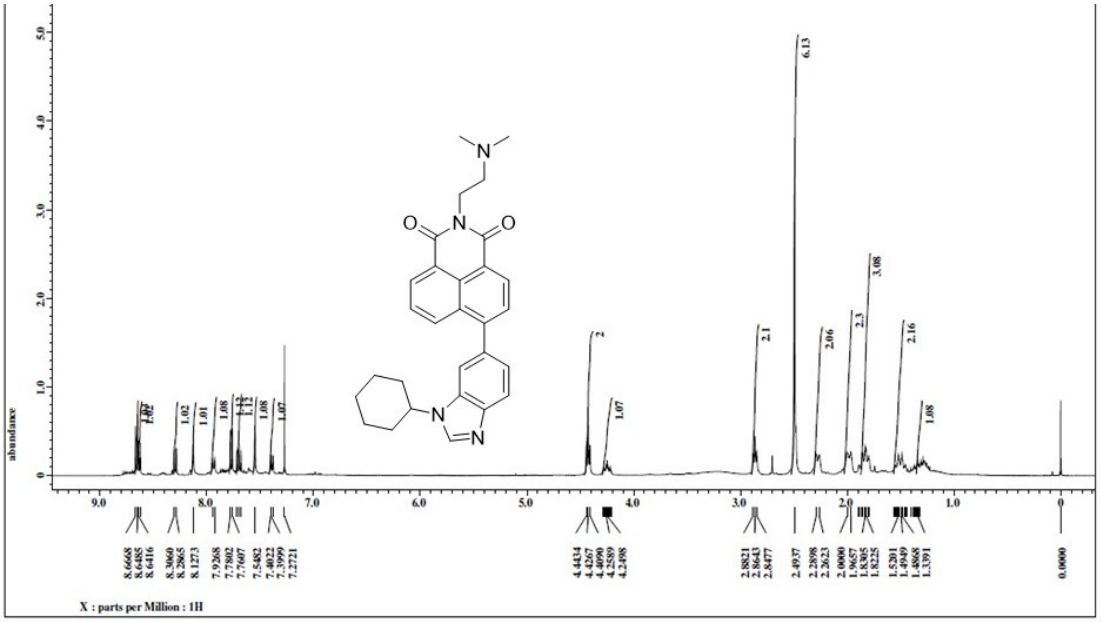


Figure S60: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(23)**.

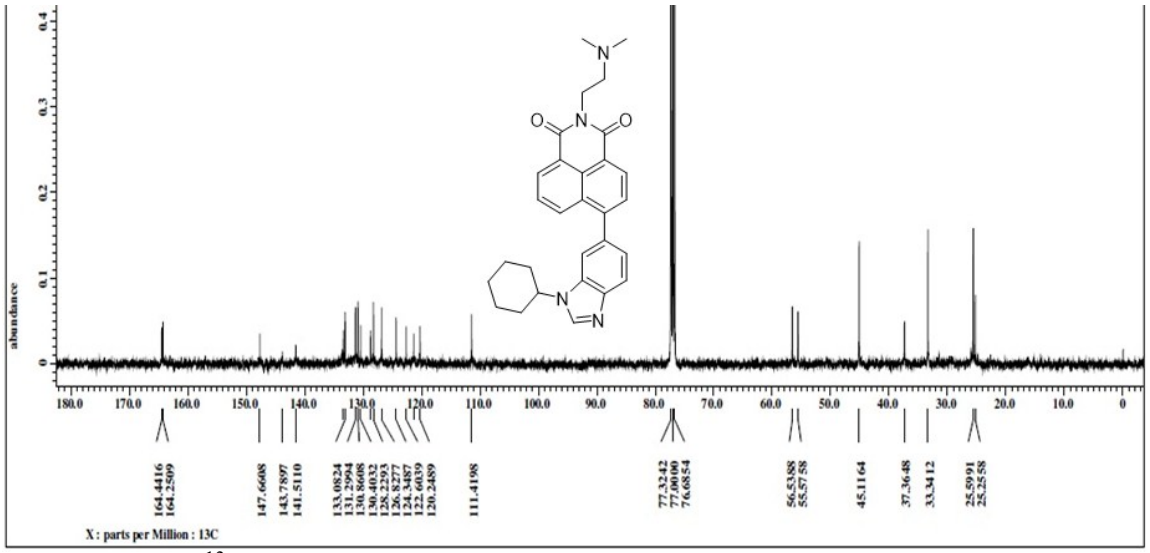


Figure S61: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(23)**.

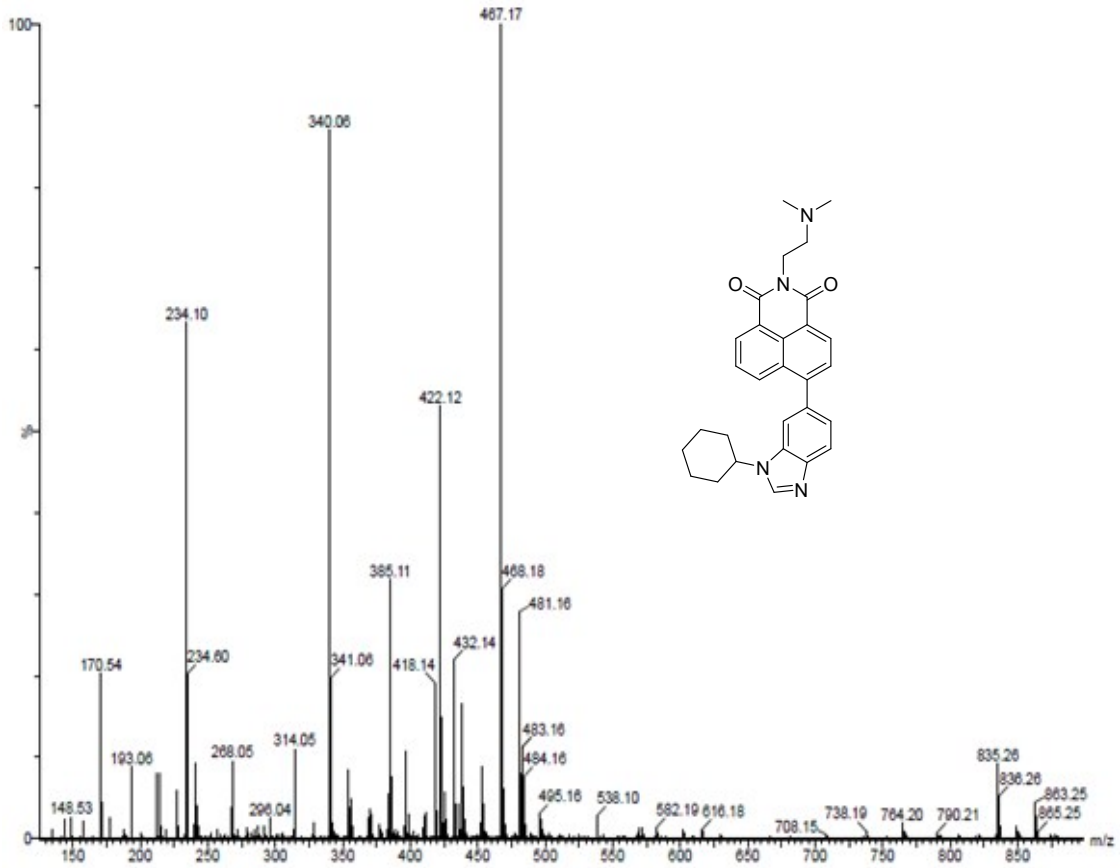


Figure S62: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-(dimethylamino)ethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(23)**.

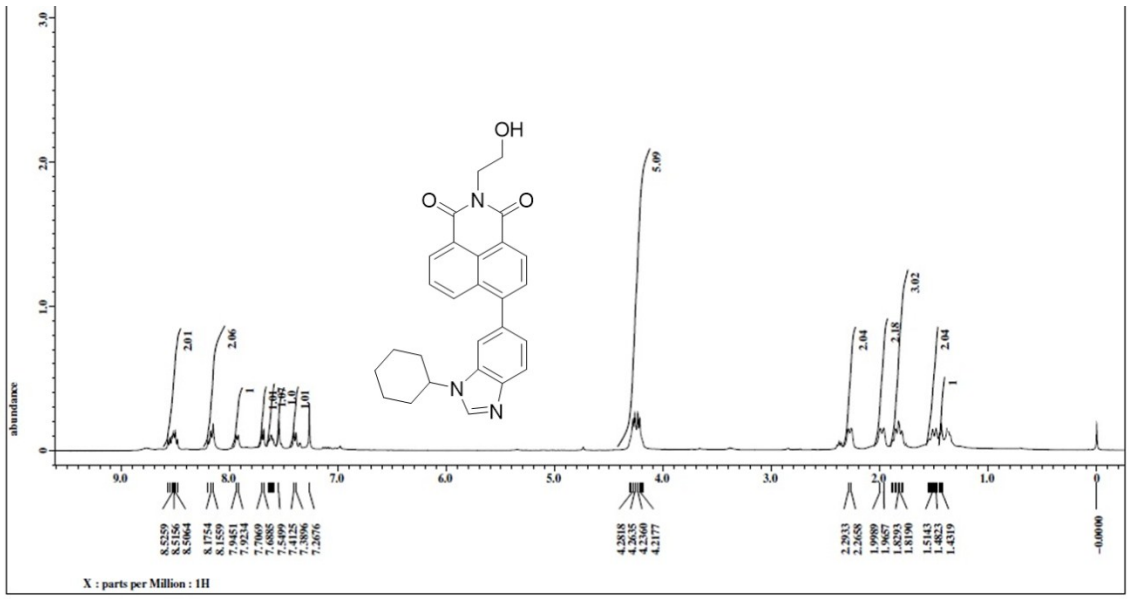


Figure S63: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(24)**.

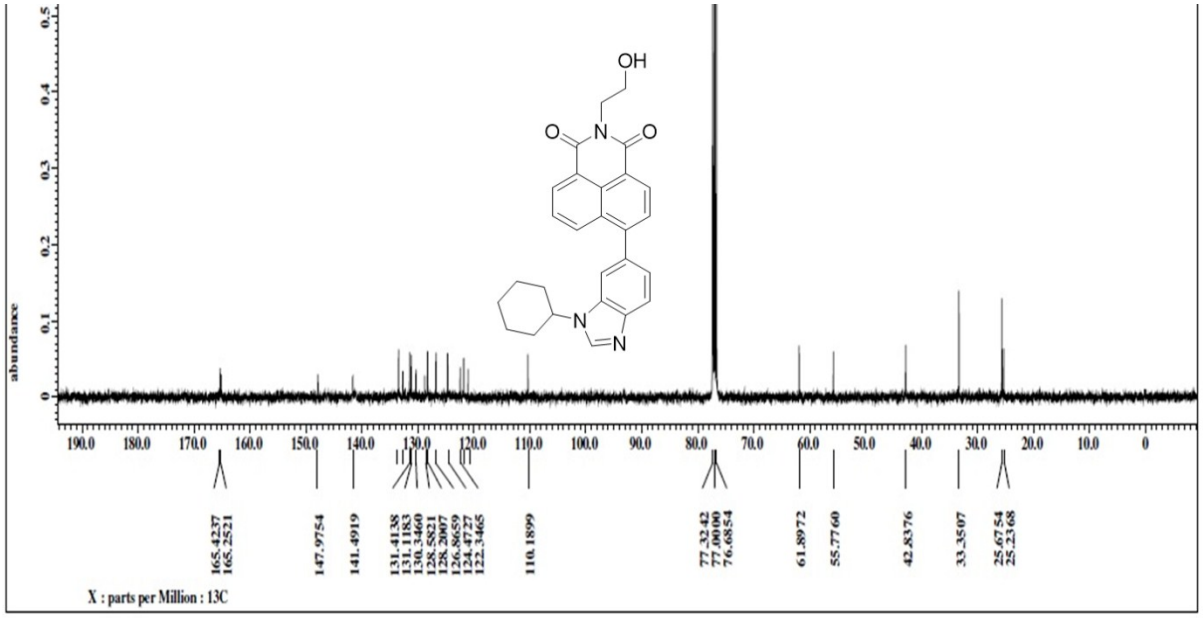


Figure S64: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(24)**.

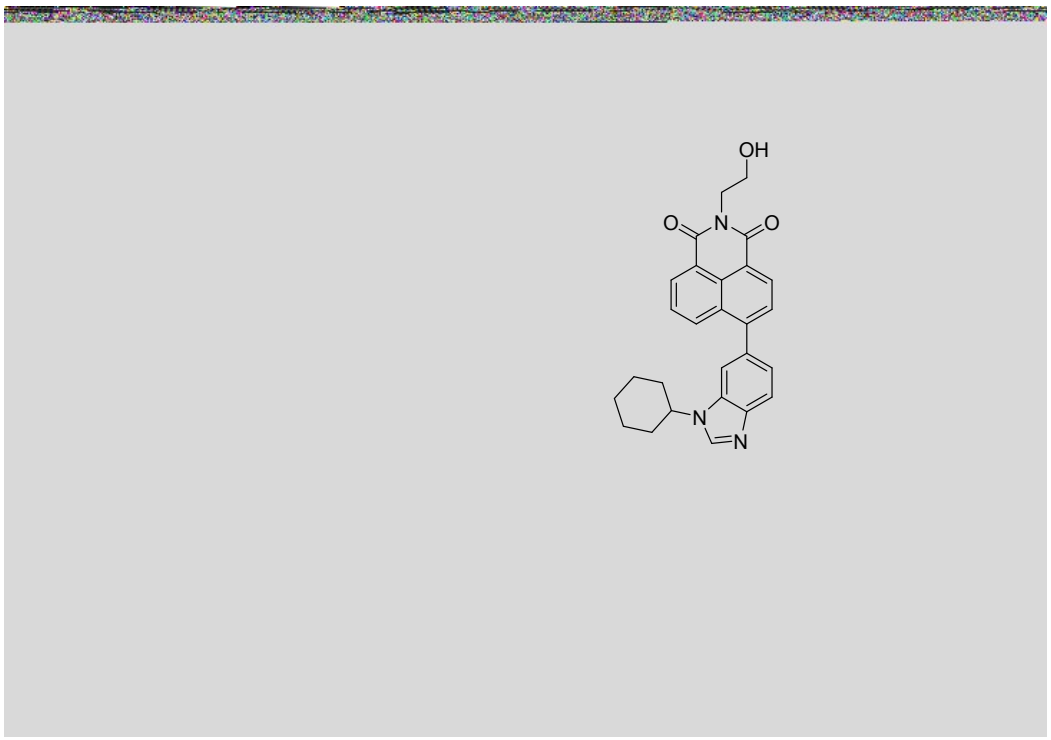


Figure S65: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-hydroxyethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(24)**.

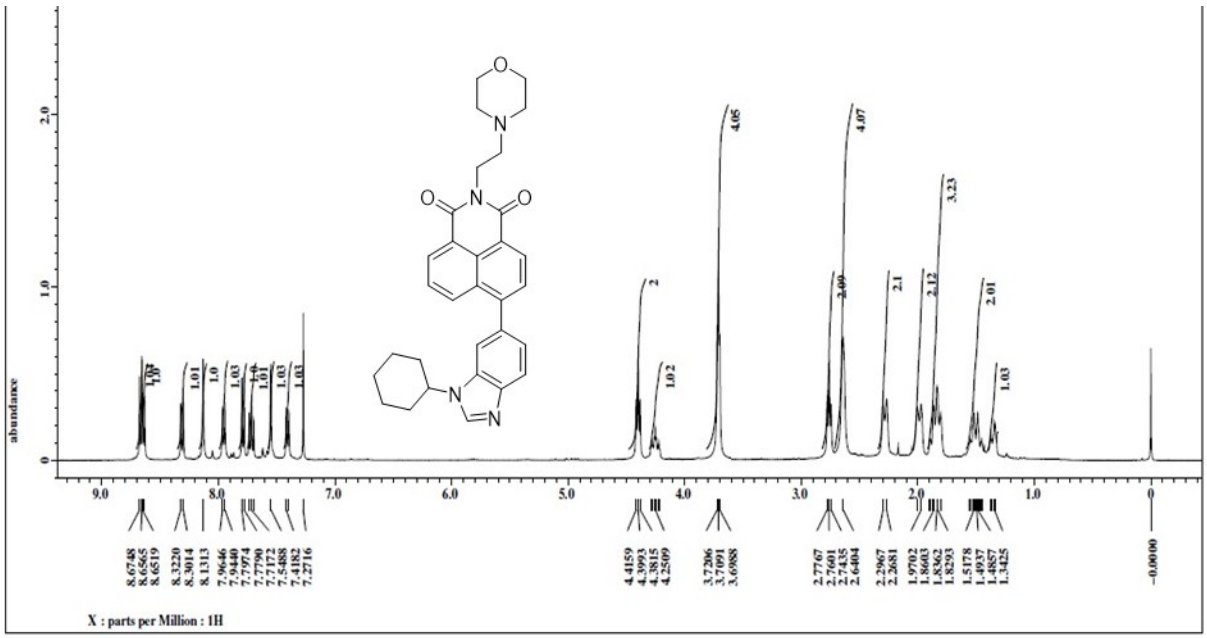


Figure S66: ^{1}H NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(25)**.

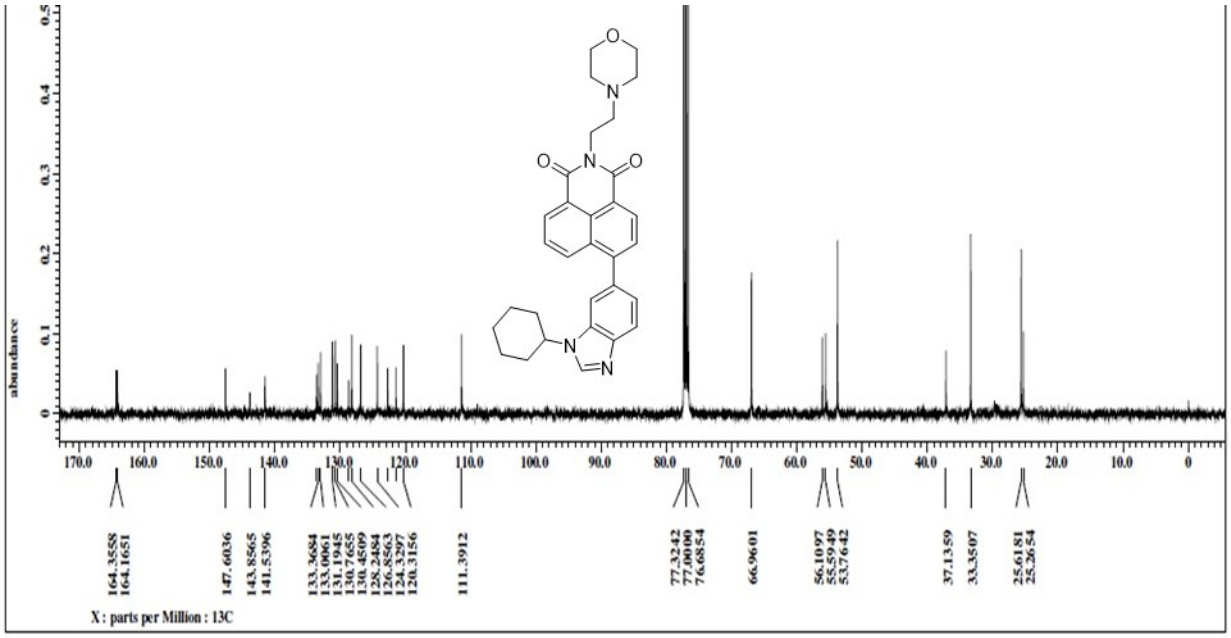


Figure S67: ^{13}C NMR spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(25)**.

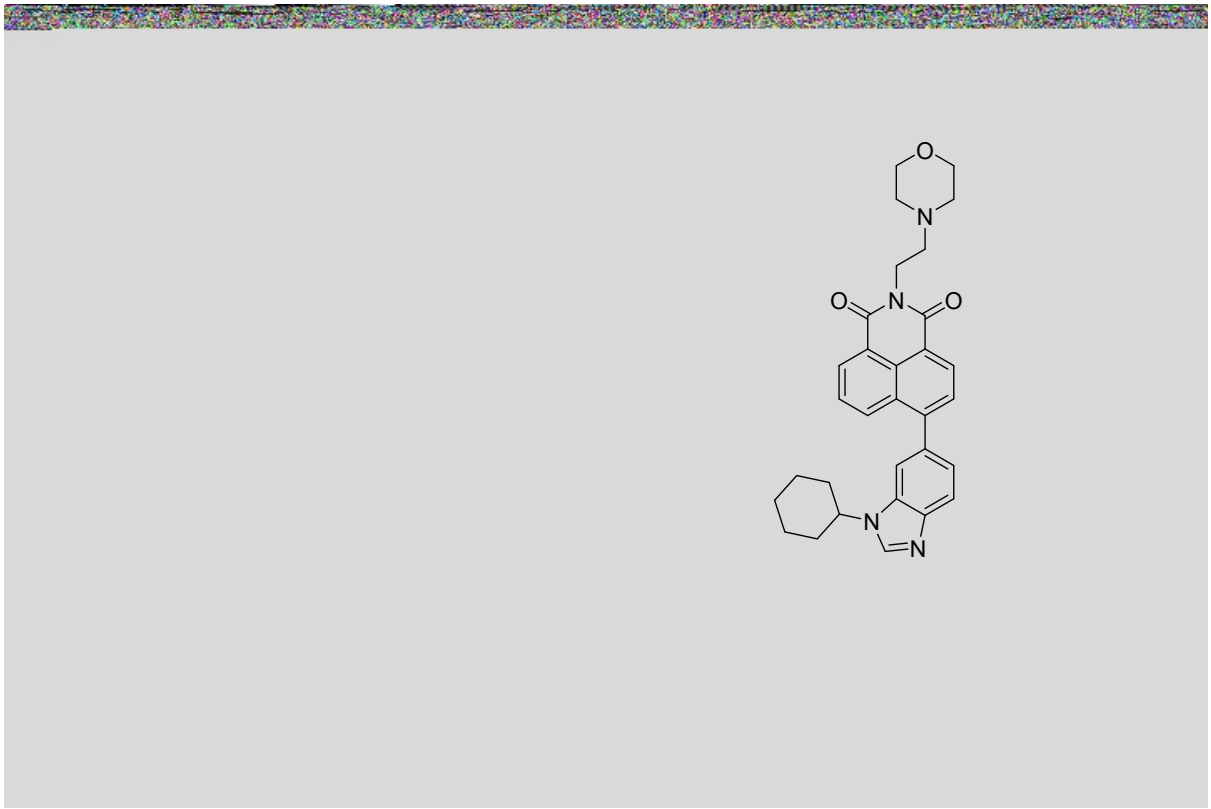


Figure S68: Mass spectrum of 6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-2-(2-morpholinoethyl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(25)**.

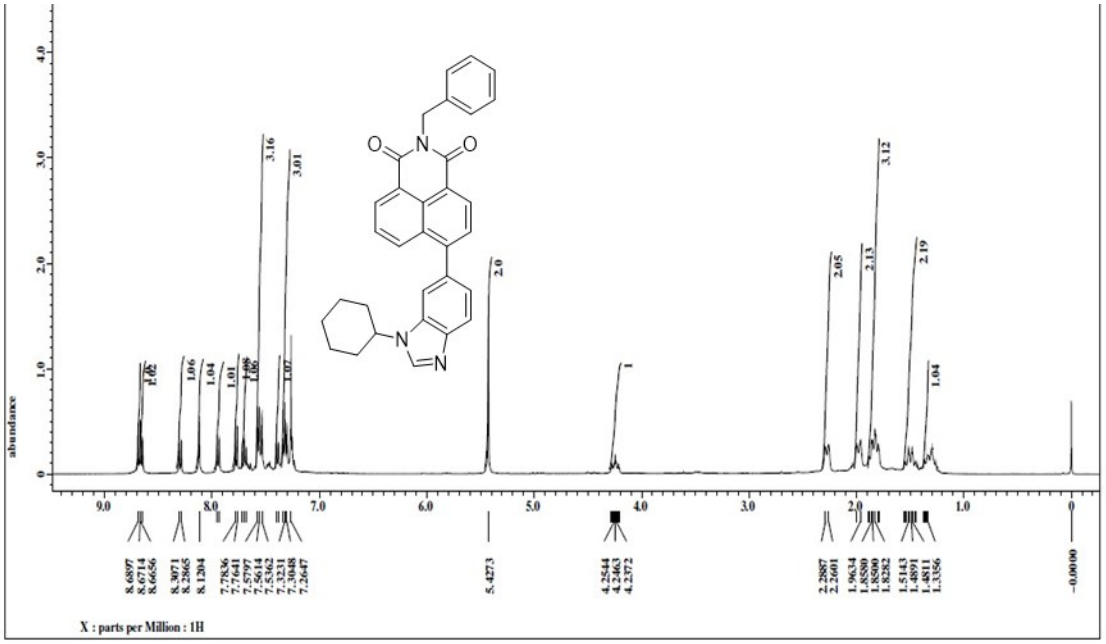


Figure S69: ^{1}H NMR spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(26)**.

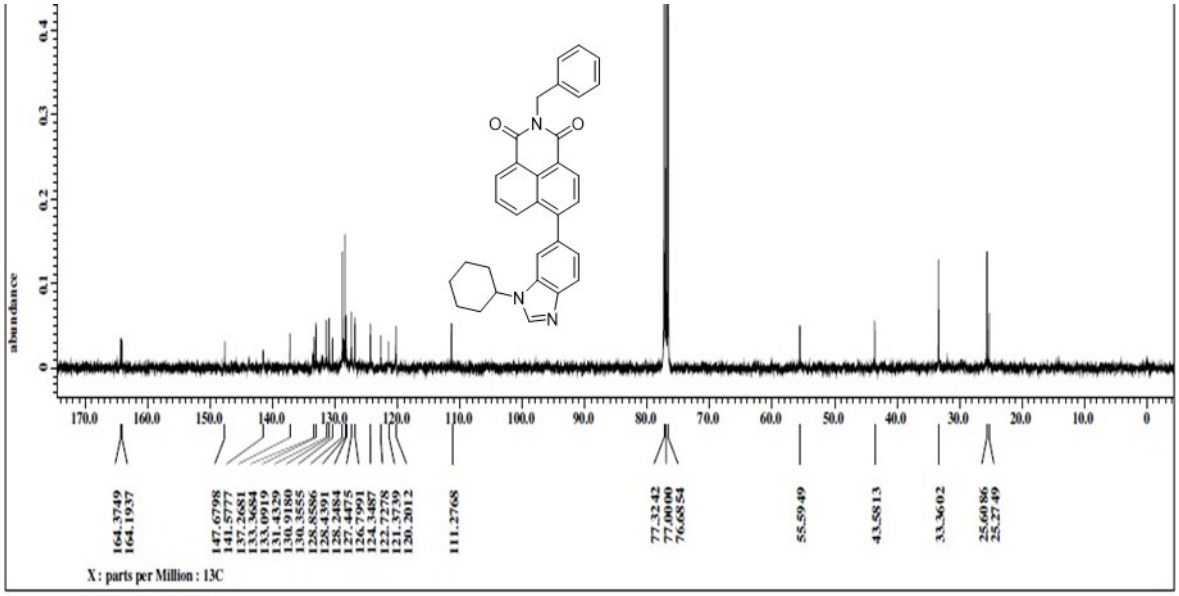
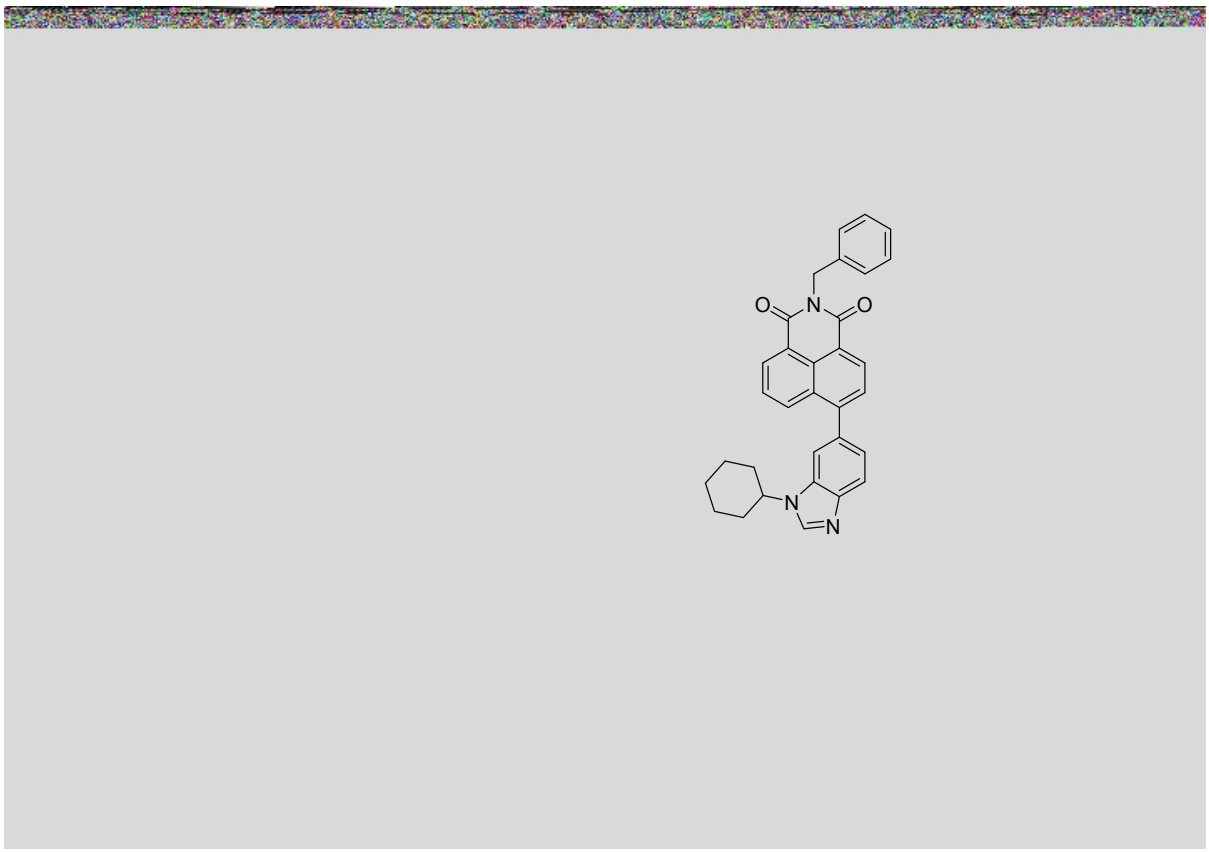


Figure S70: ^{13}C NMR spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(26)**.



Fgure S71: Mass spectrum of 2-benzyl-6-(1-cyclohexyl-1*H*-benzo[*d*]imidazol-6-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(26)**.

Table S1. Percent growth inhibition of compounds **9a-b, 10b** and **11-16** at one dose concentration level (10^{-5} M)

Cell Panel	**Cell Line**	**9a**	**9b**	**10b**	**11**	**12**	**13**	**14**	**15**	**16**
Leukemia	CCRF-CEM	13.46	0.74	27.58	67.01	30.87	--	63.33	88.63	20.98
	HL-60(TB)	20.74	5.71	27.38	74.51	14.08	0.33	33.55	-15.20	--
	K-562	24.85	17.17	43.49	73.82	NT	14.04	NT	-14.20	NT
	MOLT-4	11.56	8.40	65.32	94.60	27.66	5.30	82.74	-9.62	28.12
	RPMI-8226	24.63	9.04	42.76	70.46	48.67	--	73.24	-32.97	33.73
	SR	22.34	20.64	56.83	60.25	15.27	8.94	61.09	-13.96	15.28
Non-Small	A549/ATCC	--	--	38.72	41.74	2.94	9.19	53.16	81.16	4.44
Cell Lung	EXVX	2.02	2.93	14.96	47.08	21.36	0.22	33.42	84.37	23.65
Cancer	HOP-62	--	4.65	30.45	32.86	10.23	14.77	46.10	91.28	18.08
	HOP-92	15.76	8.35	NT	67.59	63.12	5.42	75.13	-7.68	48.94
	NCI-H226	--	--	19.55	55.15	6.56	--	28.42	-29.93	23.01

	NCI-H23	5.81	11.12	12.04	49.48	8.94	4.03	45.36	79.81	21.39
	NCI-H322M	2.37	12.29	8.91	6.15	--	--	36.99	56.83	8.19
	NCI-H460	13.35	--	39.55	41.76	1.02	--	79.49	-30.87	5.90
	NCI-H522	--	20.09	51.23	48.04	15.71	30.43	43.63	78.66	26.26
Colon	COLO 205	--	--	27.32	52.98	--	5.97	50.74	-20.39	--
Cancer	HCC-2998	12.39	3.46	9.15	24.83	6.52	--	29.51	63.35	6.80
	HCT-116	6.03	5.54	25.47	68.04	23.21	8.30	75.47	-66.14	19.98
	HCT-15	--	--	15.42	55.05	11.33	--	64.12	91.39	1.55
	HT29	11.02	1.93	30.65	76.57	18.58	15.90	68.61	99.26	16.43
	KM12	2.53	3.75	19.23	50.64	12.87	7.86	38.54	75.70	13.32
	SW-620	--	--	25.85	13.74	--	--	65.74	88.83	--
CNS	SF-268	7.89	0.48	16.42	27.64	9.39	--	42.96	60.14	6.06
Cancer	SF-295	--	0.39	12.41	55.45	11.32	3.27	50.25	-41.68	18.07
	SF-539	0.31	--	--	28.57	1.95	--	33.84	-76.24	0.98
	SNB-19	--	--	11.93	23.87	4.39	--	48.12	67.38	1.88
	SNB-75	11.09	12.43	9.95	49.76	14.48	7.72	33.11	95.59	13.35
	U251	--	--	25.94	47.98	8.97	1.68	51.30	85.35	6.83
Melanoma	LOX IMVI	3.26	9.55	22.08	49.71	6.91	--	52.55	-81.64	12.63
	MALME-3M	6.75	5.34	--	44.04	1.20	4.63	23.30	-74.50	--
	M14	--	6.74	--	49.98	3.94	7.88	25.18	-62.81	--
	MDA-MB-435	--	--	--	60.60	--	--	28.79	83.04	--
	SK-MEL-2	--	--	5.34	NT	6.16	NT	11.94	NT	10.51
	SK-MEL-28	--	--	--	23.26	--	--	27.18	-38.21	--
	SK-MEL-5	--	--	19.41	-27.80	36.14	--	41.73	-96.57	37.98
	UACC-257	--	--	38.09	55.43	--	--	--	-14.97	5.54
	UACC-62	11.21	7.70	29.90	56.02	30.72	7.19	40.38	77.99	25.56
Ovarian	IGROV1	10.75	11.58	14.21	32.91	8.28	--	49.80	71.62	3.80
Cancer	OVCAR-3	--	--	1.67	37.57	3.33	--	27.84	55.22	11.09
	OVCAR-4	1.33	--	7.55	67.68	28.49	2.36	45.32	67.05	14.04
	OVCAR-5	4.90	--	--	24.67	--	1.74	38.57	63.60	--
	OVCAR-8	0.40	--	38.43	50.50	10.35	10.08	54.20	74.08	16.77
	NCI/ADR-RES	--	0.57	16.94	60.37	10.84	7.54	58.13	78.15	10.94

	SK-OV-3	--	--	4.00	25.59	--	7.69	11.90	78.81	--
Renal	786-0	0.33	--	12.94	41.20	5.74	--	69.97	-46.10	4.59
Cancer	A498	--	--	22.15	23.10	--	--	41.38	-11.58	--
	ACHN	--	1.50	5.29	44.66	9.66	--	72.71	89.96	5.27
	CAKI-1	NT	NT	36.73	47.85	29.41	6.27	45.99	80.28	22.49
	RXF 393	--	--	5.26	--	--	--	34.74	-11.35	--
	SN12C	--	--	18.07	38.55	10.17	--	59.49	76.17	6.24
	TK-10	--	--	6.54	30.14	--	--	22.67	67.89	--
	UO-31	21.04	25.37	43.11	65.55	37.72	17.88	69.74	-23.74	37.88
Prostate	PC-3	17.63	17.42	42.77	77.16	34.66	5.66	58.13	94.79	14.97
Cancer	DU-145	--	--	10.35	27.43	6.17	--	42.37	71.56	--
Breast	MCF7	8.89	6.45	25.45	62.37	23.38	3.29	53.51	-7.00	2.17
Cancer	MDA-MB-231/ATCC	2.53	--	24.16	42.94	22.90	--	31.86	88.24	28.85
	HS 578T	--	--	12.96	NT	2.02	NT	21.36	NT	5.27
	BT-549	--	--	21.34	83.04	12.45	0.56	19.89	95.43	4.82
	T-47D	17.72	18.92	28.65	88.83	33.06	18.13	46.25	-9.17	32.03
	MDA-MB-468	--	--	14.16	65.41	3.90	--	33.30	-6.34	21.10

Table S2. Percent growth inhibition of compounds **17-23** and **25-26** at one dose concentration level (10^{-5} M)

Cell Panel	**Cell Line**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**25**	**26**
Leukemia	CCRF-CEM	4.95	0.16	7.54	14.97	17.00	25.61	84.59	39.35	20.26
	HL-60(TB)	2.08	2.72	--	3.82	24.00	16.39	85.19	53.60	70.50
	K-562	NT	NT	NT	NT	NT	26.95	93.24	56.10	46.18
	MOLT-4	10.81	8.05	7.97	25.94	18.93	30.74	-18.71	88.92	48.79
	RPMI-8226	3.37	16.33	26.70	32.02	24.37	38.69	92.49	59.15	45.09
	SR	0.35	--	--	20.80	19.01	28.69	96.41	54.67	20.35
Non-Small	A549/ATCC	0.79	--	0.79	3.03	--	12.18	96.66	60.79	40.00
Cell Lung	EXVX	12.28	3.35	25.74	29.75	23.59	20.80	70.20	29.70	34.19
Cancer	HOP-62	13.18	8.80	18.24	12.10	18.05	2.81	76.57	37.54	29.29
	HOP-92	11.28	28.53	33.20	47.45	23.98	49.90	NT	NT	NT

	NCI-H226	10.57	--	11.23	19.94	15.86	35.19	74.94	16.59	9.16
	NCI-H23	4.89	--	15.72	18.36	13.65	32.79	69.52	22.11	15.06
	NCI-H322M	10.07	0.05	0.04	--	8.31	26.40	74.71	11.88	9.47
	NCI-H460	--	--	2.54	4.16	5.19	19.27	98.60	59.47	11.87
	NCI-H522	16.09	20.04	16.67	11.80	21.82	30.99	95.35	35.20	48.90
Colon	COLO 205	--	--	--	6.10	10.20	13.91	91.31	33.74	13.58
Cancer	HCC-2998	--	2.74	5.93	9.09	7.02	6.60	60.24	10.99	2.02
	HCT-116	8.12	20.52	25.22	29.74	15.57	28.27	91.40	50.80	28.27
	HCT-15	--	5.32	7.48	22.38	40.46	24.24	87.51	32.20	21.70
	HT29	2.49	16.40	21.18	29.13	16.01	40.51	92.55	39.29	26.71
	KM12	6.65	--	8.80	16.84	16.22	24.64	75.15	29.92	19.54
	SW-620	2.01	--	--	--	--	14.38	78.58	39.61	12.41
CNS	SF-268	6.67	5.51	0.97	7.67	5.91	10.90	64.20	32.93	14.82
Cancer	SF-295	--	--	9.46	5.39	9.55	28.87	76.86	15.42	10.26
	SF-539	--	5.38	--	13.73	4.28	10.32	68.11	17.63	2.35
	SNB-19	--	0.62	--	6.20	5.35	8.67	76.65	30.38	11.24
	SNB-75	15.74	12.54	20.27	23.56	24.80	40.66	59.87	32.80	23.21
	U251	--	--	11.97	17.60	23.07	11.26	87.37	33.09	30.89
Melanoma	LOX IMVI	7.66	0.57	5.17	11.88	15.16	17.80	86.23	26.02	10.30
	MALME-3M	1.08	--	5.46	13.45	7.00	20.24	69.23	5.57	--
	M14	--	8.52	6.35	0.14	6.15	19.80	69.77	11.67	7.08
	MDA-MB-435	--	--	--	--	--	1.57	60.14	14.93	8.51
	SK-MEL-2	8.37	4.67	4.33	--	18.61	NT	NT	--	23.47
	SK-MEL-28	--	--	--	--	3.36	6.11	52.80	1.91	6.80
	SK-MEL-5	3.30	10.70	14.08	27.26	25.42	44.59	78.60	43.79	22.19
	UACC-257	--	--	--	0.03	--	17.42	76.93	49.57	43.09
	UACC-62	10.55	8.33	22.08	20.64	26.99	39.73	75.39	39..94	42.30
Ovarian	IGROV1	9.35	--	4.77	--	7.70	45.49	79.57	21.19	8.52
Cancer	OVCAR-3	--	--	6.44	13.25	10.25	20.70	62.40	15.26	16.18
	OVCAR-4	--	9.68	22.68	27.73	20.93	46.72	69.18	33.78	24.16
	OVCAR-5	--	--	--	1.84	--	29.11	64.20	10.42	5.45
	OVCAR-8	5.02	0.25	7.74	8.27	2.04	14.56	85.33	43.00	26.69
	NCI/ADR-RES	0.96	--	3.58	8.26	8.69	14.23	79.91	32.51	12.43

	SK-OV-3	--	--	--	--	5.01	--	76.95	17.48	11.79
Renal	786-0	0.23	4.92	7.31	12.09	7.03	4.72	80.95	26.75	8.67
Cancer	A498	--	0.98	--	--	--	--	95.31	36.51	9.45
	ACHN	0.04	1.52	12.26	3.26	15.33	24.82	86.22	48.22	11.18
	CAKI-1	22.50	8.36	32.50	20.67	27.23	28.99	74.97	46.36	38.54
	RXF 393	--	--	--	0.92	--	--	73.74	19.02	0.83
	SN12C	3.47	3.11	5.55	11.12	16.29	24.28	80.73	36.84	18.41
	TK-10	--	--	--	4.81	0.38	0.34	73.27	19.03	4.27
	UO-31	35.03	25.88	37.47	48.32	43.79	48.52	97.58	62.22	40.14
Prostate	PC-3	9.46	3.52	25.57	30.73	28.79	41.58	77.91	50.70	47.92
Cancer	DU-145	--	--	1.05	2.42	--	7.85	73.01	10.96	2.12
Breast	MCF7	1.69	10.51	3.49	24.10	31.03	60.66	87.91	23.87	22.20
Cancer	MDA-MB-231/ATCC	14.52	9.39	7.73	21.89	26.04	44.24	66.43	27.06	36.94
	HS 578T	8.01	--	5.70	6.06	7.08	NT	59.18	15.26	13.41
	BT-549	--	15.15	12.58	13.81	4.18	24.15	43.49	22.61	11.11
	T-47D	18.55	11.03	33.98	36.81	27.38	62.90	72.21	41.44	35.45
	MDA-MB-468	7.66	--	12.11	10.22	7.98	55.14	95.67	15.89	8.68

Table S3 Overview of the preliminary anticancer assay at single dose concentration of 10^{-5} M

Compd	Mean growth percent	Range of growth inhibition	The most sensitive cell lines	Positive cytostatic effect	Positive cytotoxic effect	No. of sensitive cell lines
11	49.68	-27.80 to 94.60	SK-MEL-5 (Melanoma)	26/58	1/58	27/58
14	46.00	50.25 to 83.74	MOLT-4 (Leukemia)	23/59	0/59	23/59
15	78.83	-96.57 to 99.26	SK-MEL-5 (Melanoma)	33/58	25/58	58/58
23	77.95	-18.71 to 98.60	MOLT-4 (Leukemia)	57/58	1/58	58/58
25	32.52	50.70 to 88.92	MOLT-4 (Leukemia)	9/59	0/59	9/59

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 800757 / 1	Experiment ID : 1710NS90	Test Type : 08	Units : Molar
Report Date : July 25, 2018	Test Date : October 30, 2017	QNS :	MC :
COMI : IS-80-F-5	Stain Reagent : SRB Dual-Pass Related	SSPL : 0YFW	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.310	1.595	1.577	1.597	1.070	0.319	0.278	99	100	59	1	-10	1.43E-6	1.16E-5	> 1.00E-4
HL-60(TB)	0.899	3.046	2.788	2.914	2.805	0.495	0.565	88	94	89	-45	-37	1.95E-6	4.61E-6	> 1.00E-4
K-562	0.161	1.601	1.427	1.358	0.655	0.124	0.119	88	83	34	-23	-26	4.76E-7	3.97E-6	> 1.00E-4
MOLT-4	0.590	1.965	2.038	2.007	1.330	0.368	0.337	105	103	54	-38	-43	1.10E-6	3.88E-6	> 1.00E-4
RPMI-8226	0.796	2.819	2.889	2.812	1.950	0.421	0.670	103	100	57	-47	-16	1.17E-6	3.53E-6	> 1.00E-4
SR	0.364	1.423	1.343	1.407	0.576	0.206	0.293	92	98	20	-44	-20	4.14E-7	2.06E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.416	1.635	1.759	1.952	1.795	0.109	0.219	110	126	113	-74	-47	2.18E-6	4.03E-6	.
EKVX	0.826	2.879	2.627	2.908	2.173	0.288	0.409	88	101	66	-65	-51	1.32E-6	3.18E-6	7.66E-6
HOP-62	0.524	1.627	1.527	1.670	1.361	0.101	0.218	91	104	76	-81	-58	1.46E-6	3.05E-6	6.36E-6
HOP-92	1.249	1.787	1.688	1.704	1.378	0.171	0.460	82	85	24	-86	-63	3.72E-7	1.65E-6	4.69E-6
NCI-H226	0.825	2.276	2.177	2.250	1.939	0.198	0.662	93	98	77	-76	-20	1.50E-6	3.18E-6	.
NCI-H23	0.716	2.086	2.085	2.085	1.508	0.166	0.379	100	100	58	-77	-47	1.14E-6	2.69E-6	.
NCI-H322M	0.742	1.858	1.778	1.757	1.659	0.522	0.137	93	91	82	-30	-82	1.94E-6	5.42E-6	2.46E-5
NCI-H460	0.226	2.580	2.729	2.842	2.162	0.048	0.136	106	111	82	-79	-40	1.58E-6	3.24E-6	.
NCI-H522	0.823	1.695	1.650	1.676	1.738	0.277	0.636	95	98	105	-66	-23	2.09E-6	4.10E-6	.
Colon Cancer															
COLO 205	0.439	1.791	1.721	1.746	1.353	0.107	0.242	95	97	68	-76	-45	1.33E-6	2.96E-6	.
HCC-2998	0.714	2.080	1.917	1.998	1.980	0.064	0.375	88	94	93	-91	-47	1.71E-6	3.19E-6	.
HCT-116	0.235	1.935	1.833	1.671	0.701	0.014	0.410	94	84	27	-94	10	4.02E-7	.	.
HCT-15	0.324	2.609	2.532	2.539	1.747	0.139	0.218	97	97	62	-57	-33	1.27E-6	3.32E-6	.
HT29	0.230	1.288	1.247	1.252	0.583	0.096	0.189	96	97	33	-58	-18	5.46E-7	2.31E-6	.
KM12	0.428	2.494	2.534	2.472	2.043	0.101	0.133	102	99	78	-77	-69	1.52E-6	3.20E-6	6.74E-6
SW-620	0.206	1.788	1.895	1.912	1.410	0.075	0.117	107	108	76	-64	-43	1.54E-6	3.50E-6	.
CNS Cancer															
SF-268	0.484	1.759	1.778	1.803	1.485	0.119	0.256	101	103	78	-75	-47	1.53E-6	3.24E-6	.
SF-295	0.724	2.674	2.417	2.577	1.896	0.148	0.306	87	95	60	-80	-58	1.18E-6	2.69E-6	6.14E-6
SF-539	0.810	2.585	2.531	2.664	2.098	0.062	0.243	97	104	73	-92	-70	1.37E-6	2.75E-6	5.54E-6
SNB-19	0.572	1.872	1.880	1.880	1.608	0.161	0.296	101	101	80	-72	-48	1.57E-6	3.36E-6	.
SNB-75	0.937	1.680	1.493	1.575	1.329	0.130	0.015	75	86	53	-86	-98	1.05E-6	2.40E-6	5.49E-6
U251	0.402	1.804	1.824	1.890	1.479	0.051	0.319	101	106	77	-87	-21	1.46E-6	2.94E-6	.
Melanoma															
LOX IMVI	0.618	2.989	3.030	2.986	2.549	0.029	0.383	102	100	81	-95	-38	1.51E-6	2.89E-6	.
MALME-3M	0.578	1.546	1.545	1.498	1.279	0.066	0.255	100	95	72	-89	-56	1.38E-6	2.81E-6	5.75E-6
M14	0.440	1.773	1.683	1.739	1.529	0.062	0.323	93	97	82	-86	-27	1.55E-6	3.07E-6	.
MDA-MB-435	0.486	2.497	2.391	2.493	2.295	0.064	0.066	95	100	90	-87	-87	1.68E-6	3.23E-6	6.18E-6
SK-MEL-2	1.237	2.229	2.283	2.250	2.393	0.260	0.728	105	102	117	-79	-41	2.19E-6	3.94E-6	.
SK-MEL-28	0.684	2.009	1.957	1.995	1.854	0.059	0.245	96	99	88	-91	-64	1.63E-6	3.10E-6	5.88E-6
SK-MEL-5	0.838	3.189	3.202	3.286	2.496	0.011	0.261	101	104	71	-99	-69	1.32E-6	2.61E-6	5.15E-6
UACC-257	1.089	2.014	2.146	2.236	2.272	0.052	0.416	114	124	128	-95	-62	2.23E-6	3.74E-6	6.27E-6
UACC-62	0.888	2.786	2.849	2.893	2.477	0.090	0.220	103	106	84	-90	-75	1.56E-6	3.03E-6	5.89E-6
Ovarian Cancer															
IGROV1	0.501	1.962	1.997	1.963	1.669	0.199	0.391	102	100	80	-60	-22	1.64E-6	3.72E-6	.
OVCAR-3	0.397	1.329	1.374	1.333	1.209	0.127	0.044	105	100	87	-68	-89	1.73E-6	3.64E-6	7.64E-6
OVCAR-4	0.725	1.613	1.543	1.553	1.190	0.529	0.173	92	93	52	-27	-76	1.07E-6	4.56E-6	2.93E-5
OVCAR-5	0.595	1.813	1.674	1.876	1.590	0.280	0.280	89	105	82	-53	-53	1.72E-6	4.04E-6	9.50E-6
OVCAR-8	0.441	1.812	1.924	2.006	1.521	0.266	0.305	108	114	79	-40	-31	1.75E-6	4.62E-6	> 1.00E-4
NCI/ADR-RES	0.496	1.751	1.716	1.777	1.339	0.300	0.399	97	102	67	-40	-20	1.45E-6	4.25E-6	> 1.00E-4
SK-OV-3	0.828	1.776	1.716	1.824	1.727	0.350	0.010	94	105	95	-58	-99	1.97E-6	4.18E-6	8.89E-6
Renal Cancer															
786-0	0.613	2.242	2.026	2.138	1.542	0.044	0.721	87	94	57	-93	7	1.11E-6	.	.
A498	1.109	2.133	2.165	2.174	2.003	0.170	0.272	103	104	87	-85	-76	1.65E-6	3.22E-6	6.28E-6
ACHN	0.370	1.635	1.729	1.703	1.104	0.130	0.164	107	105	58	-65	-56	1.16E-6	2.96E-6	7.57E-6
CAKI-1	0.452	1.740	1.658	1.702	1.394	0.334	0.026	94	97	73	-26	-94	1.71E-6	5.45E-6	2.23E-5
RXF 393	0.688	1.459	1.474	1.584	1.225	0.039	0.395	102	116	70	-94	-43	1.32E-6	2.66E-6	.
SN12C	0.563	2.187	2.059	2.134	1.619	0.104	0.261	92	97	65	-82	-54	1.27E-6	2.78E-6	6.09E-6
TK-10	0.713	2.135	2.099	2.155	1.865	0.391	0.264	97	101	81	-45	-63	1.76E-6	4.39E-6	1.87E-5
UO-31	0.625	1.757	1.631	1.582	1.071	0.184	0.166	89	85	39	-71	-73	5.83E-7	2.28E-6	6.50E-6
Prostate Cancer															
PC-3	0.493	1.248	1.232	1.247	1.051	0.313	0.460	98	100	74	-37	-7	1.64E-6	4.66E-6	> 1.00E-4
DU-145	0.276	1.428	1.367	1.401	1.232	0.051	0.014	95	98	83	-82	-95	1.59E-6	3.20E-6	6.43E-6
Breast Cancer															
MCF7	0.361	2.314	2.229	2.324	1.885	0.221	0.217	96	100	78	-39	-40	1.74E-6	4.66E-6	> 1.00E-4
MDA-MB-231/ATCC	0.556	1.280	1.340	1.335	1.180	0.085	0.209	108	108	86	-85	-63	1.63E-6	3.19E-6	6.26E-6
HS 578T	1.026	2.187	2.236	2.240	1.974	0.548	1.028	104	105	82	-47	.	1.77E-6	.	> 1.00E-4
BT-549	1.014	2.072	1.943	2.020	1.526	0.148	0.403	88	95	48	-85	-60	9.22E-7	2.30E-6	5.43E-6
T-47D	0.666	1.488	1.390	1.481	1.232	0.547	0.556	88	99	69	-18	-17	1.65E-6	6.22E-6	> 1.00E-4
MDA-MB-468	0.749	1.286	1.278	1.434	1.195	0.229	0.405	99	128	83	-69	-46	1.65E-6	3.51E-6	.

Figure S72. *In vitro* anticancer activity of compound **15** at five dose concentration level (10^{-4} – 10^{-8} M)

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 799082 / 1	Experiment ID : 1708NS48	Test Type : 08	Units : Molar
Report Date : July 25, 2018	Test Date : August 07, 2017	QNS :	MC :
COMI : IS-50-F-4	Stain Reagent : SRB Dual-Pass Related	SSPL : 0Z9N	

			Log10 Concentration											
	Time		Mean Optical Densities					Percent Growth						
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.553	2.704	2.676	2.795	2.108	0.487	0.466	99	104	72	-12	-16	1.84E-6	7.22E-6	> 1.00E-4
HL-60(TB)	0.763	2.933	2.822	2.845	2.390	0.785	0.410	95	96	75	1	-46	2.18E-6	1.05E-5	> 1.00E-4
K-562	0.072	0.531	0.517	0.494	0.325	0.102	0.120	97	92	55	7	10	1.27E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.638	2.779	2.661	2.767	1.138	0.639	0.504	94	99	23	.	-21	4.46E-7	1.01E-5	> 1.00E-4
RPMI-8226	0.485	1.511	1.532	1.517	1.007	0.418	0.384	102	101	51	-14	-21	1.03E-6	6.10E-6	> 1.00E-4
SR	0.311	1.391	1.385	1.226	0.687	0.273	0.242	99	85	35	-12	-22	4.96E-7	5.47E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.431	1.813	1.743	1.752	1.213	0.078	0.158	95	96	57	-82	-63	1.12E-6	2.56E-6	5.88E-6
EKVX	0.616	1.944	1.770	1.831	1.641	0.556	0.448	87	91	77	-10	-27	2.05E-6	7.72E-6	> 1.00E-4
HOP-62	0.680	1.528	1.459	1.453	1.265	0.584	0.302	92	91	69	-14	-56	1.69E-6	6.75E-6	7.30E-5
HOP-92	0.950	1.492	1.455	1.502	1.344	0.788	0.375	93	102	73	-17	-61	1.79E-6	6.45E-6	5.72E-5
NCI-H226	0.744	1.369	1.344	1.348	1.273	0.667	0.306	96	97	85	-10	-59	2.32E-6	7.78E-6	6.55E-5
NCI-H23	0.504	1.713	1.635	1.607	1.282	0.271	0.185	94	91	64	-46	-63	1.35E-6	3.82E-6	1.66E-5
NCI-H322M	0.635	1.727	1.674	1.628	1.307	0.594	0.065	95	91	62	-6	-90	1.48E-6	8.04E-6	3.33E-5
NCI-H460	0.226	2.339	2.544	2.526	1.288	0.209	0.064	110	109	50	-8	-72	1.01E-6	7.41E-6	4.59E-5
NCI-H522	1.234	2.677	2.514	2.512	2.382	0.851	0.550	89	89	80	-31	-55	1.85E-6	5.24E-6	5.98E-5
Colon Cancer															
COLO 205	0.455	1.512	1.495	1.510	1.066	0.292	0.220	98	100	58	-36	-52	1.21E-6	4.14E-6	7.87E-5
HCC-2998	0.731	2.267	2.257	2.152	2.031	0.374	0.211	99	92	85	-49	-71	1.82E-6	4.30E-6	1.12E-5
HCT-116	0.216	1.921	1.805	1.875	0.585	0.247	0.111	93	97	22	2	-49	4.22E-7	1.09E-5	> 1.00E-4
HCT-15	0.338	2.489	2.288	2.403	1.566	0.367	0.157	91	96	57	1	-54	1.34E-6	1.06E-5	8.57E-5
HT29	0.286	1.652	1.594	1.564	0.952	0.272	0.194	96	94	49	-5	-32	9.38E-7	8.11E-6	> 1.00E-4
KM12	0.342	1.923	1.900	1.900	1.507	0.438	0.189	99	99	74	6	-45	2.24E-6	1.32E-5	> 1.00E-4
SW-620	0.243	1.912	1.947	1.933	1.099	0.280	0.126	102	101	51	2	-48	1.06E-6	1.10E-5	> 1.00E-4
CNS Cancer															
SF-268	0.661	2.406	2.294	2.289	2.098	0.804	0.204	94	93	82	8	-69	2.73E-6	1.28E-5	5.66E-5
SF-295	0.647	2.467	2.245	2.295	1.849	0.522	0.287	88	91	66	-19	-56	1.54E-6	5.93E-6	6.96E-5
SF-539	0.815	2.496	2.221	2.343	2.123	0.786	0.246	84	91	78	-4	-70	2.19E-6	9.03E-6	5.01E-5
SNB-19	0.490	1.845	1.817	1.867	1.365	0.646	0.361	98	102	65	12	-26	1.88E-6	2.01E-5	> 1.00E-4
SNB-75	1.089	2.056	1.802	1.844	1.724	1.119	0.169	74	78	66	3	-85	1.78E-6	1.08E-5	4.04E-5
U251	0.245	1.151	1.184	1.179	0.876	0.283	0.085	104	103	70	4	-65	2.00E-6	1.15E-5	6.02E-5
Melanoma															
LOX IMVI	0.330	2.072	1.942	1.932	1.135	0.109	0.202	93	92	46	-67	-39	8.26E-7	2.56E-6	.
MALME-3M	0.539	1.121	1.135	1.154	1.086	0.193	0.243	102	106	94	-64	-55	1.90E-6	3.93E-6	8.12E-6
M14	0.408	1.776	1.695	1.695	1.577	0.132	0.164	94	94	85	-68	-60	1.70E-6	3.61E-6	7.67E-6
MDA-MB-435	0.456	2.260	2.142	2.219	2.003	0.513	0.160	93	98	86	3	-65	2.71E-6	1.11E-5	6.04E-5
SK-MEL-2	1.037	2.335	2.347	2.258	2.106	0.903	0.372	101	94	82	-13	-64	2.19E-6	7.32E-6	5.29E-5
SK-MEL-28	0.619	1.975	1.869	1.876	1.849	0.435	0.230	92	93	91	-30	-63	2.18E-6	5.66E-6	4.09E-5
SK-MEL-5	0.637	3.007	2.858	3.068	2.447	0.054	0.156	94	103	76	-92	-76	1.44E-6	2.85E-6	5.65E-6
UACC-257	1.022	1.873	1.834	1.888	1.956	0.931	0.448	95	102	110	-9	-56	3.19E-6	8.41E-6	7.39E-5
UACC-62	0.831	2.945	2.857	2.819	2.578	0.323	0.482	96	94	83	-61	-42	1.69E-6	3.76E-6	.
Ovarian Cancer															
IGROV1	0.445	1.918	1.897	1.720	1.234	0.373	0.327	99	87	54	-16	-27	1.12E-6	5.86E-6	> 1.00E-4
OVCAR-3	0.458	1.648	1.674	1.635	1.416	0.436	0.208	102	99	80	-5	-55	2.28E-6	8.78E-6	8.09E-5
OVCAR-4	0.694	1.351	1.269	1.332	1.150	0.756	0.505	87	97	69	9	-27	2.11E-6	1.81E-5	> 1.00E-4
OVCAR-5	0.614	1.438	1.325	1.370	1.303	0.722	0.430	86	92	84	13	-30	2.99E-6	2.01E-5	> 1.00E-4
OVCAR-8	0.427	1.745	1.739	1.718	1.145	0.425	0.294	99	98	54	.	-31	1.21E-6	9.76E-6	> 1.00E-4
NCI/ADR-RES	0.460	1.610	1.612	1.534	1.068	0.507	0.330	100	93	53	4	-28	1.14E-6	1.34E-5	> 1.00E-4
SK-OV-3	0.849	1.465	1.429	1.478	1.401	0.798	0.286	94	102	90	-6	-66	2.59E-6	8.64E-6	5.36E-5
Renal Cancer															
786-0	0.555	2.268	2.055	2.109	1.597	0.680	0.135	88	91	61	7	-76	1.59E-6	1.22E-5	4.90E-5
A498	1.329	2.452	2.508	2.630	2.388	0.811	0.078	105	116	94	-39	-94	2.15E-6	5.10E-6	1.58E-5
ACHN	0.304	1.329	1.288	1.282	0.646	0.133	0.072	96	95	33	-56	-76	5.39E-7	2.36E-6	8.52E-6
CAKI-1	0.479	2.162	1.933	1.979	1.441	0.421	0.140	86	89	57	-12	-71	1.27E-6	6.67E-6	4.41E-5
RXF 393	0.738	1.378	1.366	1.360	1.181	0.164	0.207	98	97	69	-78	-72	1.35E-6	2.96E-6	6.47E-6
SN12C	0.402	1.705	1.725	1.705	1.062	0.481	0.131	102	100	51	6	-67	1.03E-6	1.21E-5	5.79E-5
TK-10	0.732	1.481	1.401	1.371	1.260	0.796	0.177	89	85	71	8	-76	2.14E-6	1.26E-5	4.94E-5
UO-31	0.666	1.986	1.807	1.740	1.373	0.084	0.151	86	81	54	-87	-77	1.06E-6	2.40E-6	5.42E-6
Prostate Cancer															
PC-3	0.410	1.621	1.557	1.588	1.250	0.320	0.301	95	97	69	-22	-27	1.63E-6	5.75E-6	> 1.00E-4
DU-145	0.286	1.328	1.447	1.403	1.209	0.399	0.077	111	107	89	11	-73	3.14E-6	1.35E-5	5.31E-5
Breast Cancer															
MCF7	0.313	1.840	1.700	1.701	1.252	0.351	0.149	91	91	61	2	-53	1.56E-6	1.11E-5	8.99E-5
MDA-MB-231/ATCC	0.620	1.515	1.529	1.518	1.299	0.616	0.245	102	100	76	.	-60	2.18E-6	9.78E-6	6.68E-5
HS 578T	0.738	1.665	1.722	1.744	1.616	0.856	0.536	106	109	95	13	-27	3.51E-6	2.08E-5	> 1.00E-4
BT-549	1.784	2.955	2.914	2.986	2.898	2.011	0.482	96	103	95	19	-73	3.95E-6	1.62E-5	5.64E-5
T-47D	0.877	1.821	1.676	1.785	1.719	0.980	0.715	85	96	89	11	-19	3.16E-6	2.34E-5	> 1.00E-4
MDA-MB-468	0.694	1.434	1.412	1.470	1.287	0.377	0.336	97	105	80	-46	-52	1.73E-6	4.33E-6	5.28E-5

Figure S73. *In vitro* anticancer activity of compound **23** at five dose concentration level (10^{-4} – 10^{-8} M)

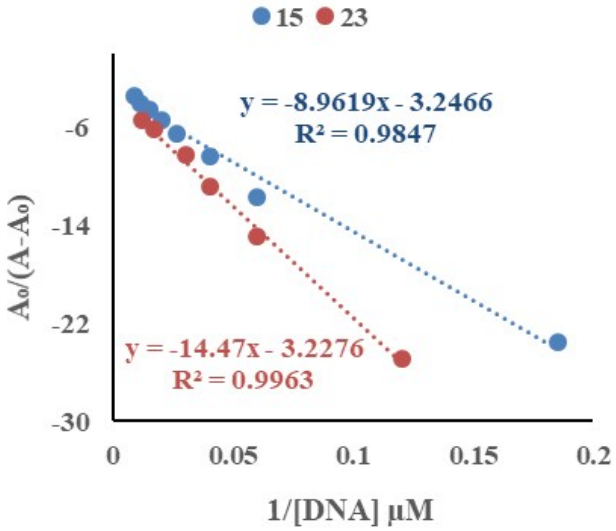


Figure S74. Benesi-Hildebrand plot of compounds **15** and **23** $\{A_0/(A- A_0)$ vs.1/[DNA]$\}$.

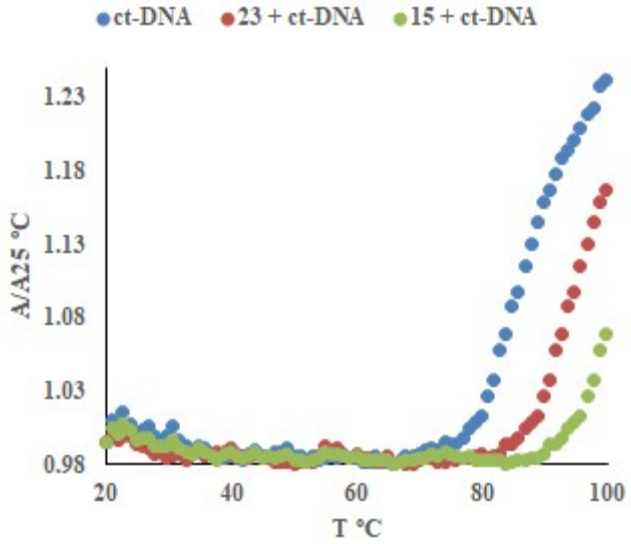


Figure S75. Thermal denaturation plots of ct–DNA in the absence and presence of compounds **15** and **23**.

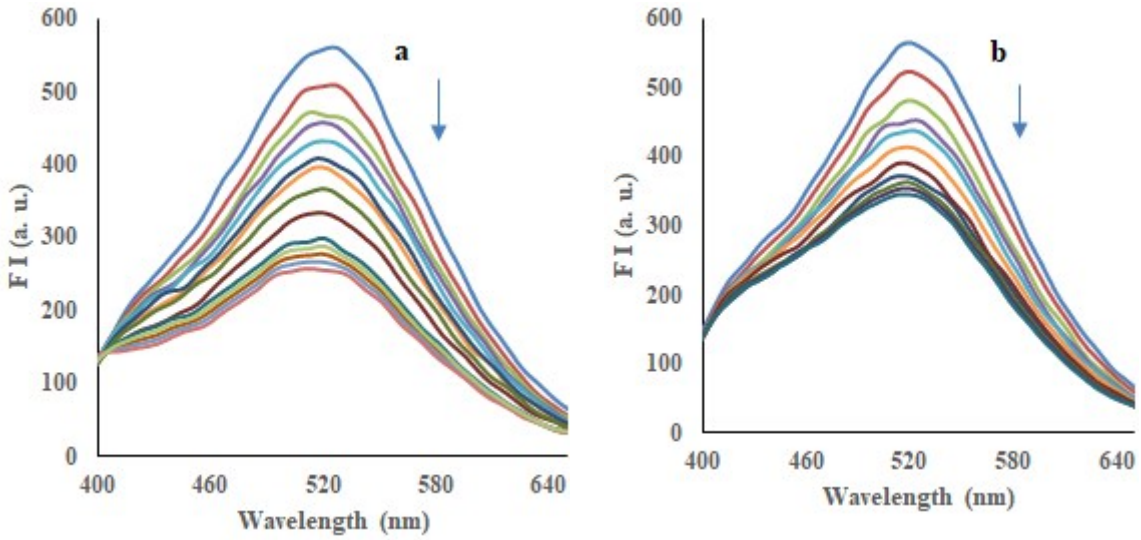


Figure S76. Emission spectra of compound **15** (5.0 μM) at different temperatures (a) 308 K and (b) 318 K in the presence of ct-DNA (308 K: 0-35 μM and 318 K: 0-35 μM) in phosphate buffer (*p*H 7.4)

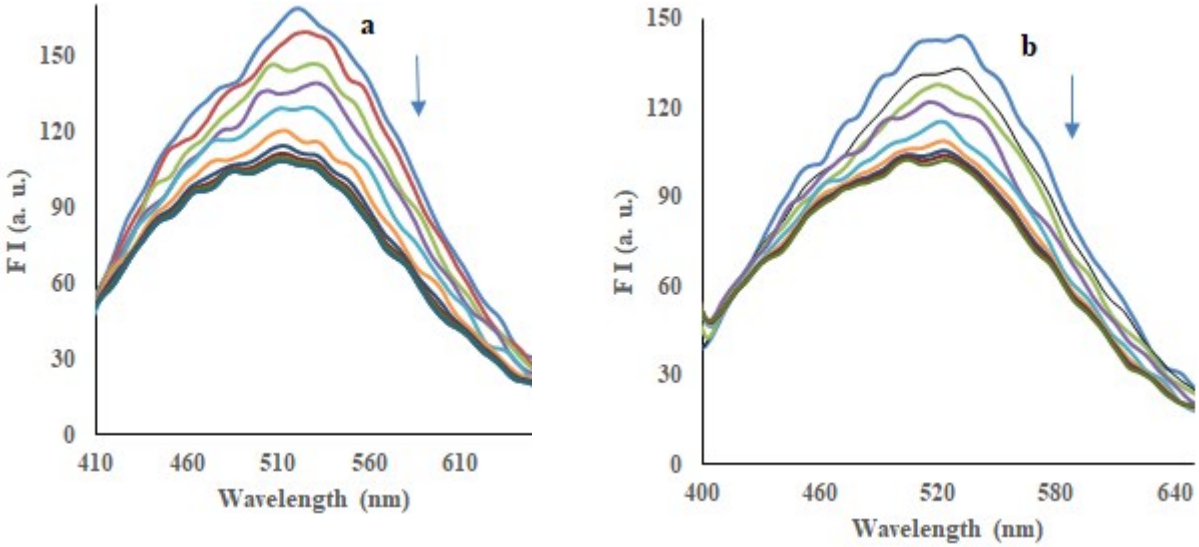


Figure S77 Emission spectra of compound **23** (5.0 μM) at different temperatures (a) 308 K and (b) 318 K in the presence of ct-DNA (308 K: 0-25 μM and 318 K: 0-30 μM) in phosphate buffer (*p*H 7.4).

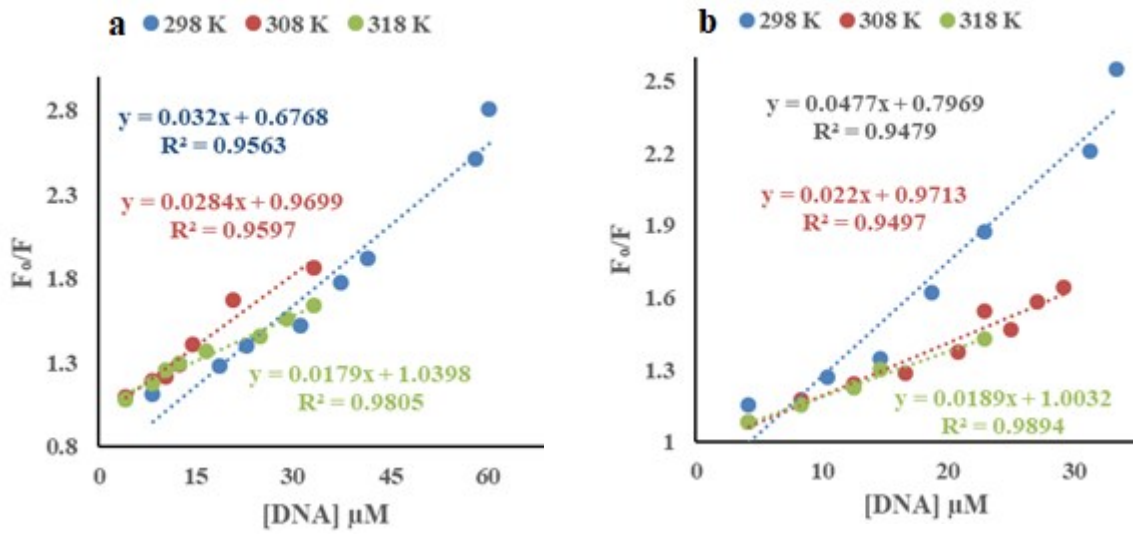


Figure S78 Stern-Volmer plot of compounds (a) **15** and (b) **23** at different temperatures {F_o/F vs. [DNA]}

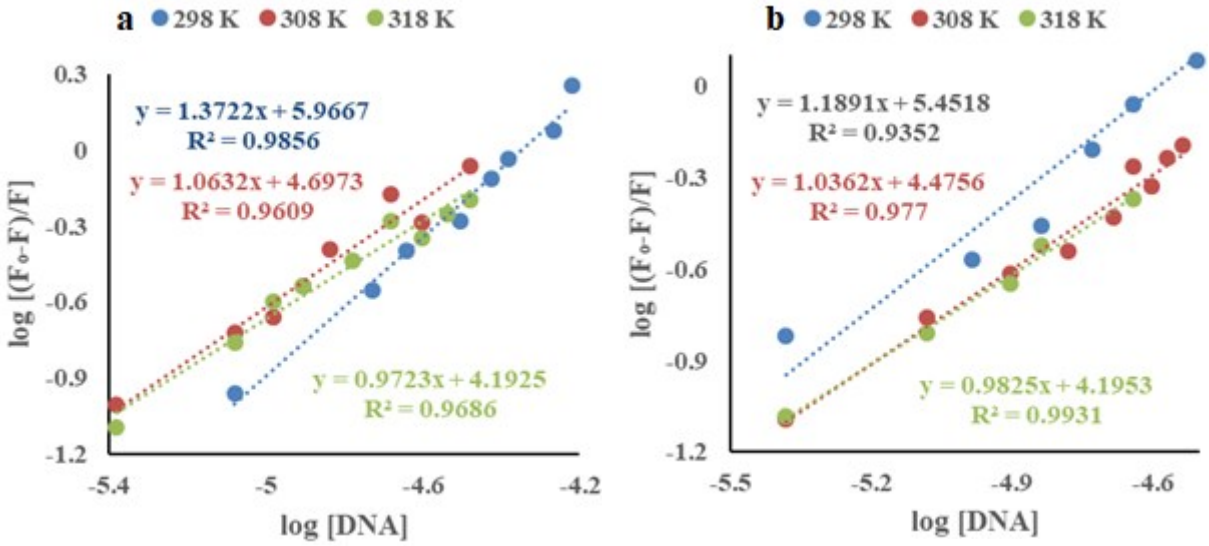


Figure S79 Modified Stern-Volmer plot of compounds (a) **15** and (b) **23** at different temperatures {$\log[(F_o-F)/F]$ vs. log[DNA]}

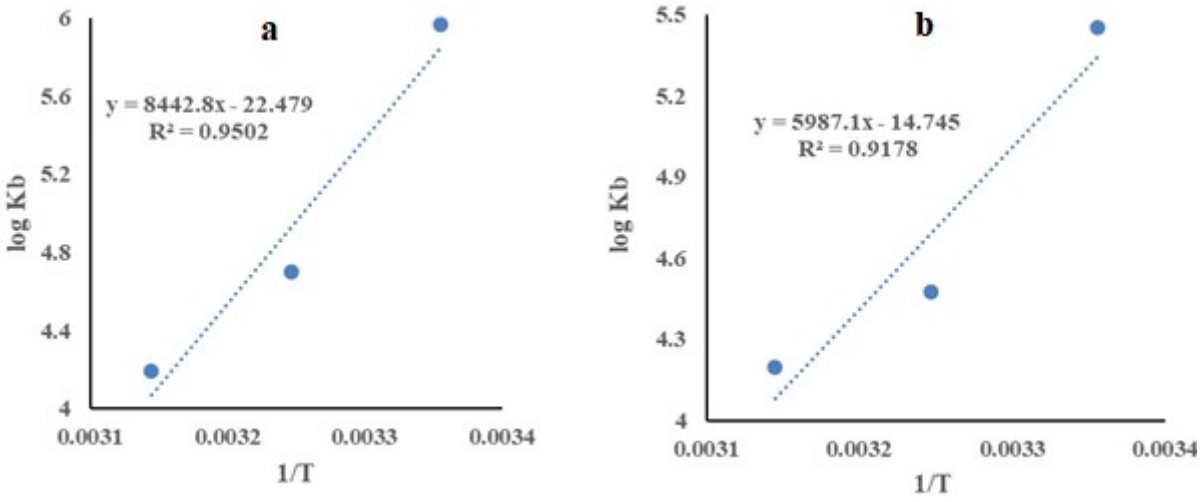


Figure S80 Von't Hoff plot of compounds (a) **15** and (b) **23** at different temperatures {logK_b vs. 1/T}

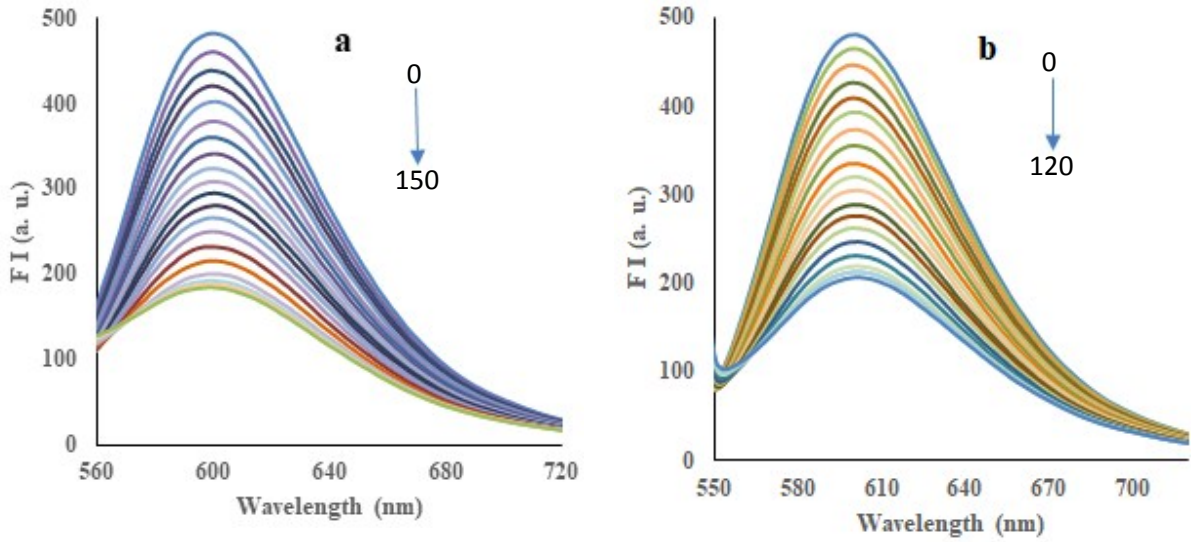
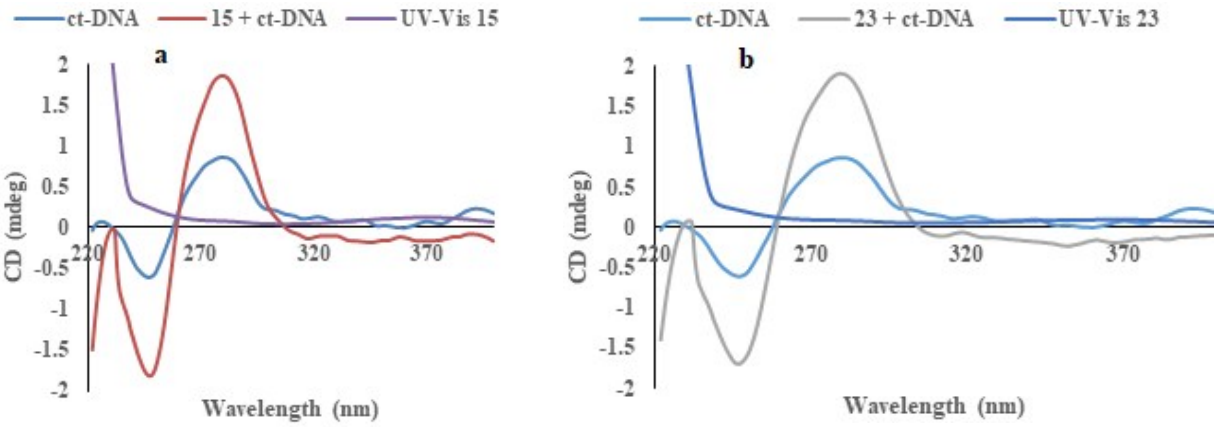


Figure S81 Emission spectra of EB-DNA complex in the absence and presence of the compounds (a) **15** and (b) **23** in phosphate buffer at *p*H 7.4.



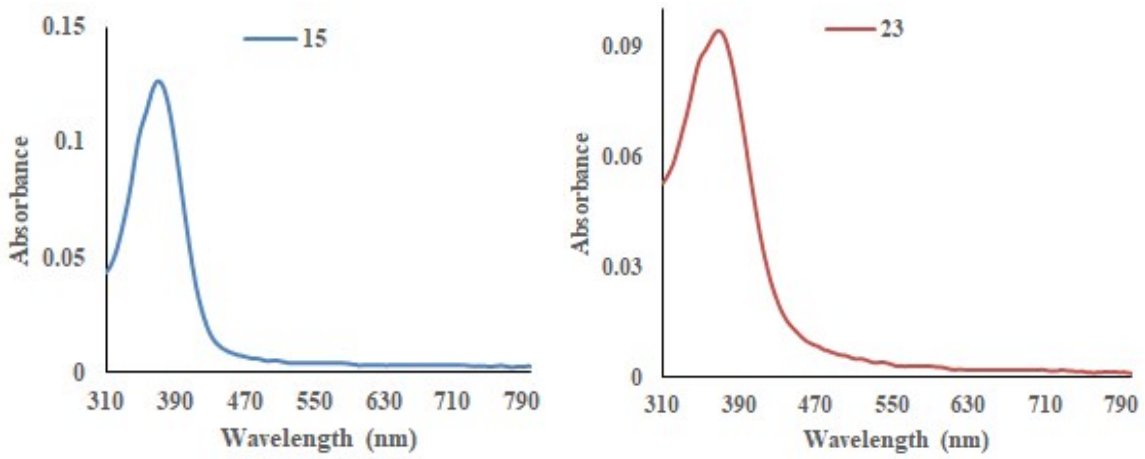


Figure S82. (a) CD spectra of free ct-DNA (blue line), **15**-DNA complex (red line) and UV-vis spectra of the compound **15** (violet line); (b) CD spectra of free ct-DNA (blue line), **15**-DNA complex (red line) and UV-vis spectra of the compound **15** (dark blue line); (c) UV-vis spectra of the compound **15**; (d) UV-vis spectra of the compound **23**

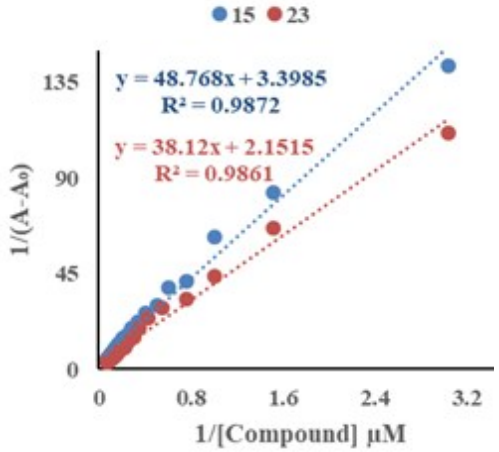


Figure S83 Benesi-Hildebrand plot of compounds **15** and **23** {1/(A- A_0) vs.1/[compound]}

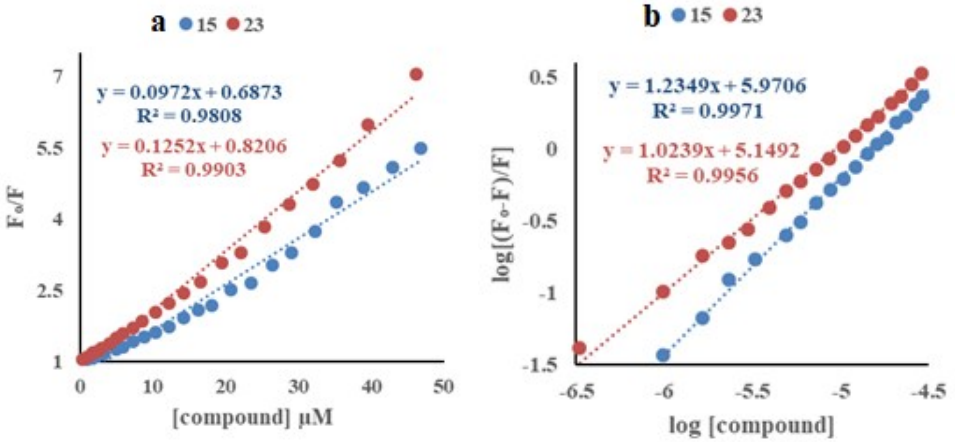


Figure S84 (a) Stern-Volmer plot of compounds **15** and **23** {F_0/F vs. [compound]}; (b) Modified Stern-Volmer Plot of compounds **15** and **23** {log[(F_0-F)/F] vs. log[compound]}.