Supplementary Information

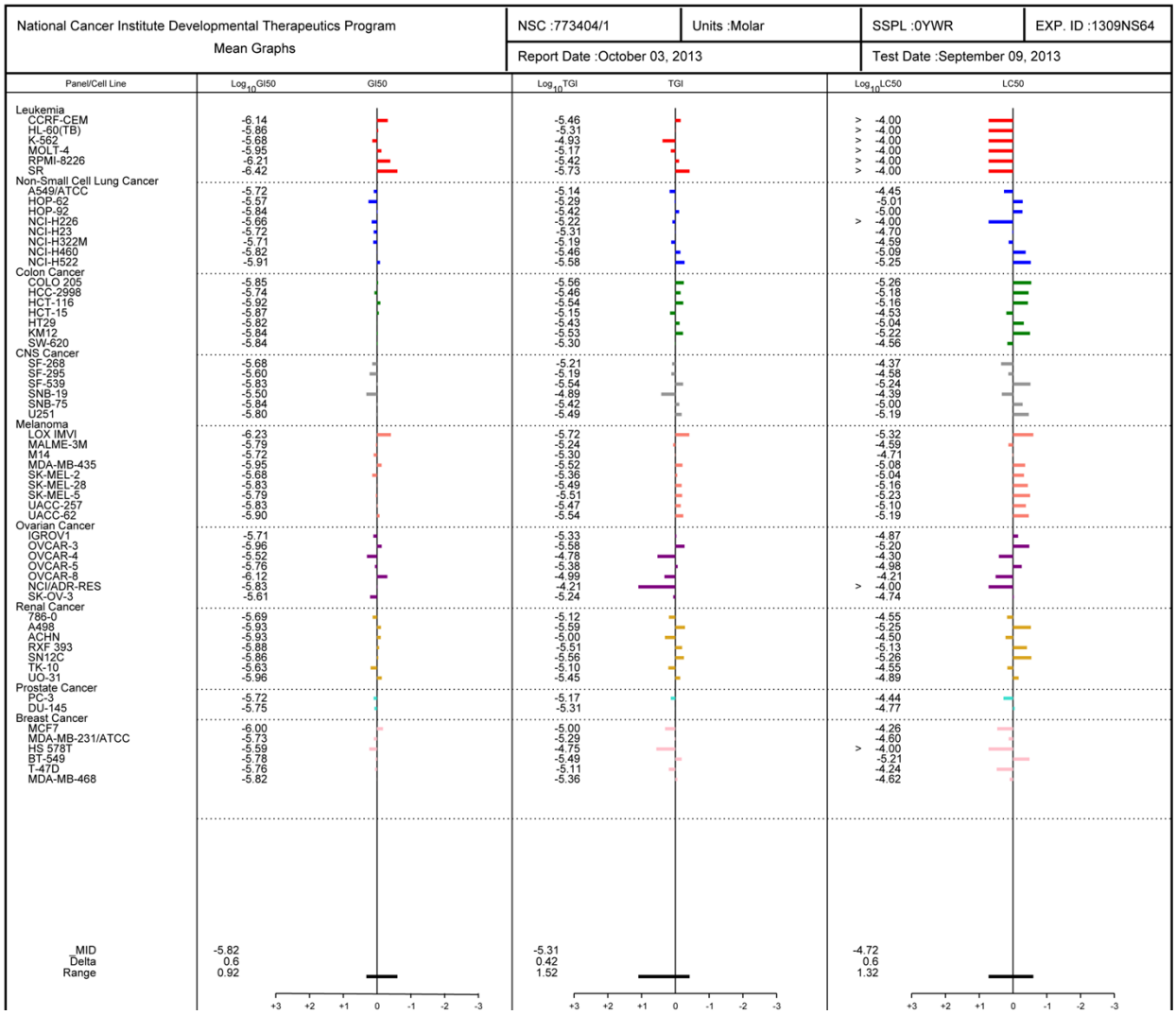
In-vitro five dose anticancer testing results of compound **3f**

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 773404 / 1	Experiment ID : 1309NS64	Test Type : 08	Units : Molar
Report Date : October 03, 2013	Test Date : September 09, 2013	QNS :	MC :
COMI : B2-35-3j (128346)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0YWR	

			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	0.719	3.201	3.195	3.092	1.782	0.454	0.463	100	96	43	-37	-36	7.31E-7	3.45E-6	> 1.00E-4
HL-60(TB)	0.687	2.905	2.809	2.824	2.091	0.491	0.430	96	96	63	-29	-37	1.40E-6	4.88E-6	> 1.00E-4
K-562	0.270	2.015	2.170	2.140	1.523	0.333	0.147	109	107	72	4	-46	2.09E-6	1.18E-5	> 1.00E-4
MOLT-4	0.800	3.014	3.078	3.040	1.981	0.712	0.574	103	101	53	-11	-28	1.13E-6	6.73E-6	> 1.00E-4
RPMI-8226	0.897	2.796	2.735	2.800	1.590	0.662	0.543	97	100	36	-26	-39	6.14E-7	3.82E-6	> 1.00E-4
SR	0.363	1.585	1.520	1.569	0.541	0.223	0.204	95	99	15	-39	-44	3.79E-7	1.88E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.429	2.197	2.128	1.996	1.729	0.379	0.078	96	89	74	-12	-82	1.89E-6	7.30E-6	3.51E-5
HOP-62	0.530	1.097	1.106	1.173	1.256	0.257	0.013	102	113	128	-52	-98	2.72E-6	5.17E-6	9.81E-6
HOP-92	1.034	1.646	1.556	1.529	1.461	0.517	0.090	85	81	70	-50	-91	1.46E-6	3.82E-6	1.00E-5
NCI-H226	1.344	2.907	2.876	2.797	2.722	1.006	0.825	98	93	88	-25	-39	2.17E-6	6.00E-6	> 1.00E-4
NCI-H23	0.703	2.097	2.086	2.102	1.877	0.436	0.155	99	100	84	-38	-78	1.91E-6	4.89E-6	2.00E-5
NCI-H322M	0.872	2.121	1.960	2.004	1.848	0.717	0.028	87	91	78	-18	-97	1.96E-6	6.52E-6	2.55E-5
NCI-H460	0.156	1.993	2.011	1.934	1.543	0.058	0.015	101	97	75	-63	-90	1.53E-6	3.50E-6	8.04E-6
NCI-H522	1.015	2.216	2.276	2.350	1.782	0.127	0.012	105	111	64	-88	-99	1.23E-6	2.64E-6	5.65E-6
Colon Cancer															
COLO 205	0.422	1.523	1.516	1.628	1.248	0.026	0.014	99	110	75	-94	-97	1.41E-6	2.78E-6	5.49E-6
HCC-2998	0.380	1.354	1.434	1.436	1.310	0.069	0.047	108	108	95	-82	-88	1.80E-6	3.45E-6	6.61E-6
HCT-116	0.223	2.260	2.300	2.368	1.460	0.064	-0.003	102	105	61	-71	-100	1.21E-6	2.88E-6	6.90E-6
HCT-15	0.252	1.449	1.443	1.429	0.957	0.226	0.016	99	98	59	-11	-94	1.34E-6	7.05E-6	2.98E-5
HT29	0.298	1.626	1.743	1.750	1.263	0.135	0.041	109	109	73	-55	-86	1.51E-6	3.71E-6	9.16E-6
KM12	0.339	1.784	1.804	1.823	1.433	0.047	0.017	101	103	76	-86	-95	1.44E-6	2.93E-6	5.97E-6
SW-620	0.208	1.662	1.631	1.627	1.152	0.151	0.046	98	98	65	-28	-78	1.45E-6	5.03E-6	2.79E-5
CNS Cancer															
SF-268	0.630	1.930	1.941	1.953	1.727	0.487	0.214	101	102	84	-23	-66	2.10E-6	6.14E-6	4.25E-5
SF-295	1.089	2.828	2.815	2.895	2.800	0.839	0.132	99	104	98	-23	-88	2.50E-6	6.46E-6	2.61E-5
SF-539	0.874	2.513	2.397	2.408	2.152	0.090	-0.011	93	94	78	-90	-100	1.47E-6	2.92E-6	5.79E-6
SNB-19	0.803	2.202	2.253	2.247	2.040	0.956	0.086	104	103	88	11	-89	3.13E-6	1.28E-5	4.05E-5
SNB-75	0.673	1.389	1.396	1.293	1.166	0.334	0.020	101	87	69	-50	-97	1.44E-6	3.77E-6	9.91E-6
U251	0.766	2.717	2.676	2.494	2.394	0.148	0.012	98	89	83	-81	-98	1.60E-6	3.22E-6	6.50E-6
Melanoma															
LOX IMVI	0.427	2.787	2.796	2.759	1.262	0.041	0.054	100	99	35	-91	-87	5.88E-7	1.91E-6	4.77E-6
MALME-3M	0.698	1.244	1.169	1.167	1.078	0.544	0.074	86	86	70	-22	-89	1.63E-6	5.74E-6	2.60E-5
M14	0.524	2.253	2.258	2.232	1.960	0.340	0.074	100	99	83	-35	-86	1.90E-6	5.05E-6	1.96E-5
MDA-MB-435	0.503	2.243	2.115	2.089	1.466	0.206	0.037	93	91	55	-59	-93	1.11E-6	3.04E-6	8.32E-6
SK-MEL-2	1.302	2.368	2.392	2.443	2.376	0.559	0.244	102	107	101	-57	-81	2.10E-6	4.35E-6	9.02E-6
SK-MEL-28	0.643	1.855	1.840	1.824	1.567	0.167	0.035	99	97	76	-74	-95	1.49E-6	3.22E-6	6.92E-6
SK-MEL-5	1.012	3.145	3.079	2.992	2.895	0.095	0.043	97	93	88	-91	-96	1.64E-6	3.12E-6	5.93E-6
UACC-257	0.873	2.014	1.958	1.909	1.706	0.316	0.035	95	91	73	-64	-96	1.47E-6	3.42E-6	7.93E-6
UACC-62	0.789	2.464	2.429	2.393	1.874	0.189	0.034	98	96	65	-76	-96	1.27E-6	2.88E-6	6.53E-6
Ovarian Cancer															
IGROV1	0.738	2.431	2.388	2.408	2.241	0.409	0.097	97	99	89	-45	-87	1.95E-6	4.63E-6	1.34E-5
OVCAR-3	0.547	1.733	1.788	1.832	1.210	0.128	-0.008	105	108	56	-77	-100	1.11E-6	2.64E-6	6.29E-6
OVCAR-4	0.704	1.426	1.397	1.361	1.241	0.873	0.127	96	91	74	23	-82	3.01E-6	1.67E-5	4.97E-5
OVCAR-5	0.585	1.708	1.716	1.623	1.501	0.298	0.066	101	92	82	-49	-89	1.74E-6	4.21E-6	1.05E-5
OVCAR-8	0.562	2.333	2.238	2.215	1.339	0.578	0.207	95	93	44	1	-63	7.52E-7	1.03E-5	6.21E-5
NCI/ADR-RES	0.595	1.937	2.044	1.980	1.382	0.716	0.581	108	103	59	9	-2	1.49E-6	6.13E-5	> 1.00E-4
SK-OV-3	0.550	1.184	1.202	1.205	1.197	0.370	-0.019	103	103	102	-33	-100	2.43E-6	5.71E-6	1.80E-5
Renal Cancer															
786-0	0.453	1.938	1.914	1.888	1.600	0.407	0.009	98	97	77	-10	-98	2.05E-6	7.63E-6	2.84E-5
A498	1.817	2.580	2.376	2.254	2.273	0.244	0.117	73	57	60	-87	-94	1.17E-6	2.56E-6	5.62E-6
ACHN	0.389	1.909	1.890	1.864	1.207	0.391	-0.011	99	97	54	.	-100	1.18E-6	1.00E-5	3.17E-5
RXF 393	0.937	2.079	2.056	2.020	1.692	0.303	0.117	98	95	66	-68	-88	1.32E-6	3.12E-6	7.37E-6
SN12C	0.639	2.253	2.260	2.198	1.836	0.037	-0.001	100	97	74	-94	-100	1.39E-6	2.76E-6	5.46E-6
TK-10	0.884	1.589	1.602	1.582	1.484	0.800	-0.006	102	99	85	-10	-100	2.35E-6	7.93E-6	2.80E-5
UO-31	0.668	2.085	1.857	1.955	1.436	0.372	0.033	84	91	54	-44	-95	1.10E-6	3.55E-6	1.29E-5
Prostate Cancer															
PC-3	0.538	2.172	2.110	2.053	1.774	0.454	0.124	96	93	76	-16	-77	1.91E-6	6.73E-6	3.63E-5
DU-145	0.350	1.385	1.468	1.438	1.168	0.228	-0.009	108	105	79	-35	-100	1.80E-6	4.93E-6	1.70E-5
Breast Cancer															
MCF7	0.578	2.360	2.267	2.179	1.473	0.577	0.190	95	90	50	.	-67	1.01E-6	9.92E-6	5.55E-5
MDA-MB-231/ATCC	0.584	1.420	1.470	1.445	1.263	0.394	0.142	106	103	81	-33	-76	1.88E-6	5.18E-6	2.54E-5
HS 578T	0.614	1.524	1.459	1.460	1.341	0.679	0.486	93	93	80	7	-21	2.57E-6	1.79E-5	> 1.00E-4
BT-549	1.051	2.020	2.026	2.087	1.916	0.140	0.028	101	107	89	-87	-97	1.67E-6	3.22E-6	6.18E-6
T-47D	0.480	0.914	0.922	0.912	0.777	0.438	0.178	102	100	68	-9	-63	1.73E-6	7.68E-6	5.75E-5
MDA-MB-468	0.805	1.775	1.679	1.708	1.483	0.483	0.270	90	93	70	-40	-67	1.52E-6	4.32E-6	2.37E-5

Five dose testing Mean Graph of compound **3f**



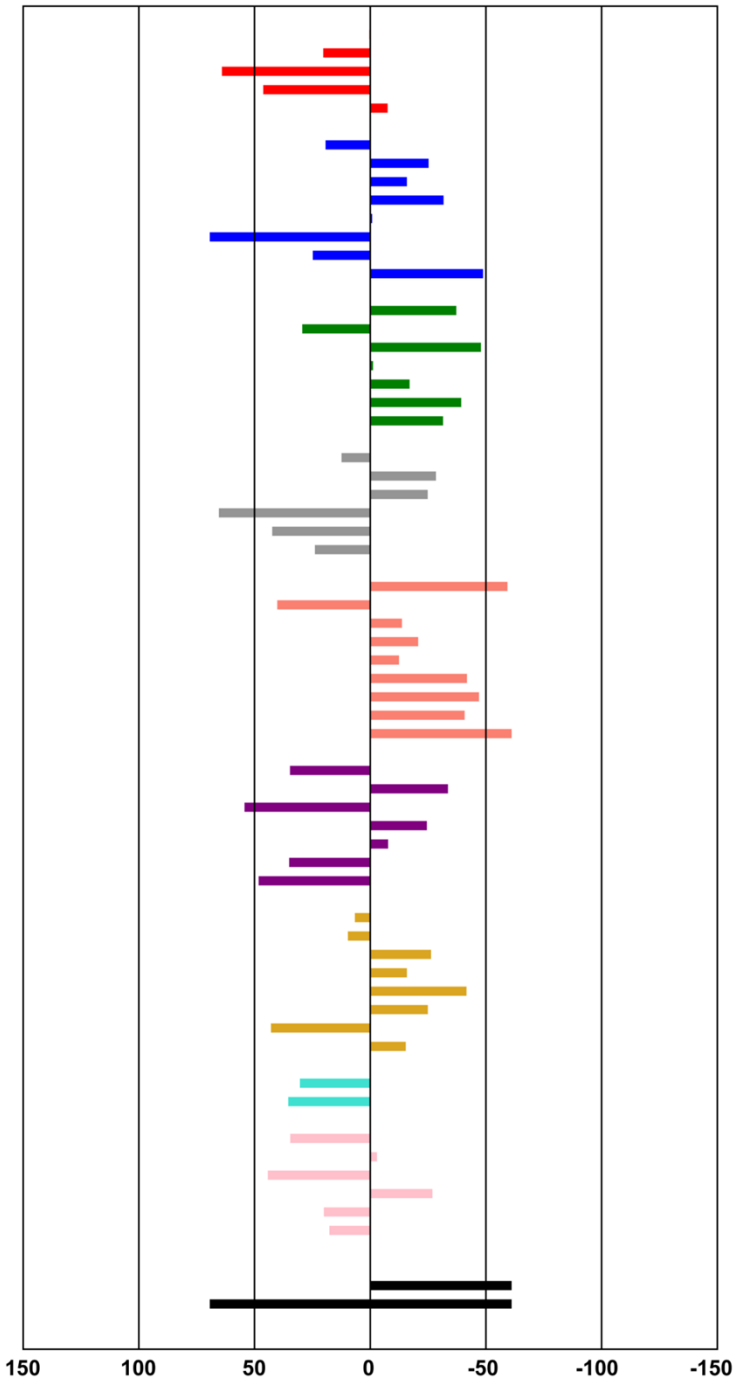
Single dose testing Mean Graph of compound **3f**

Developmental Therapeutics Program

One Dose Mean Graph

NSC: 773404 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Apr 22, 2013
Experiment ID: 1304OS71		**Report Date:** Jun 12, 2013

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-23.88
HL-60(TB)	-3.97
K-562	39.78
MOLT-4	21.93
RPMI-8226	-31.13
Non-Small Cell Lung Cancer	
A549/ATCC	-4.99
HOP-62	-48.81
HOP-92	-39.42
NCI-H226	-55.28
NCI-H23	-24.46
NCI-H322M	45.05
NCI-H460	0.54
NCI-H522	-72.37
Colon Cancer	
COLO 205	-60.78
HCC-2998	5.08
HCT-116	-71.46
HCT-15	-24.78
HT29	-40.61
KM12	-62.91
SW-620	-55.08
CNS Cancer	
SF-268	-11.85
SF-295	-51.99
SF-539	-48.44
SNB-19	41.12
SNB-75	18.07
U251	-0.39
Melanoma	
LOX IMVI	-82.92
MALME-3M	15.88
M14	-37.34
MDA-MB-435	-44.30
SK-MEL-2	-36.05
SK-MEL-28	-65.41
SK-MEL-5	-70.59
UACC-257	-64.42
UACC-62	-84.68
Ovarian Cancer	
IGROV1	10.38
OVCAR-3	-57.18
OVCAR-4	30.04
OVCAR-5	-48.09
OVCAR-8	-31.30
NCI/ADR-RES	10.78
SK-OV-3	23.95
Renal Cancer	
786-0	-17.65
A498	-14.61
ACHN	-49.87
CAKI-1	-39.45
RXF 393	-65.21
SN12C	-48.49
TK-10	18.58
UO-31	-38.98
Prostate Cancer	
PC-3	6.09
DU-145	11.13
Breast Cancer	
MCF7	10.29
MDA-MB-231/ATCC	-26.52
HS 578T	19.97
BT-549	-50.47
T-47D	-4.25
MDA-MB-468	-6.61
Mean	-23.94
Delta	60.74
Range	129.73



Characterization

*(E)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**a**)*

Yield: 80%; m.p: 96-98 ºC; IR (KBr,): 2928 (CH_3), 1677 (C=O), 1632 (C=C) cm^{-1}; ^1H NMR (DMSO-d6, 300 MHz, δ ppm): 2.64 (s, 3H, C2-CH_3), 6.50 (d, 1H, J = 15.9 Hz, H-α), 6.99 (t, 2H, J = 7.2 Hz C5,C6-H), 7.29 (t, 1H, J = 7.4 Hz, C4'-H), 7.38 (t, 2H, J = 7.4 Hz, C3',C5'-H), 7.41-7.49 (m, 4H, C4,C7,C2', C6'-H), 7.57 (d, 1H, J = 15.9 Hz, H-β); ^{13}C NMR (DMSO-d6, 75 MHz, δ ppm): 14.94, 114.69, 118.93, 124.50, 127.07, 128.63, 129.18, 130.70, 131.79, 134.69, 139.15, 144.39, 147.55, 168.14; MS (*m/z*): 263 [$(M+H)^+$, a], 262 (M^+), 147, 131, 117, 103, 90, 77; Anal. Calcd. for $C_{17}H_{14}N_2O$ (262.11): C, 77.84%; H, 5.38%; N, 10.68%; Found: C, 77.79%; H, 5.35%; N, 10.62%; HPLC purity: 98.67%, t_R-14.2 min.

*(E)-1-(5,6-dimethyl-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**b**)*

Yield: 85%; m.p: 218-220 ºC; IR (KBr): 2911 and 2885 (CH_3), 1655 (C=O), 1623 (C=C) cm^{-1}; ^1H NMR (DMSO-d6, 300 MHz, δ ppm): 2.48 (s, 6H, C5,C6-CH_3), 6.90 (d, 1H, J = 15 Hz, H-α), 7.39-7.47 (m, 3H, C4,C7,C4'-H), 7.53 (t, 2H, J = 7.8 Hz, C3',C5'-H), 7.59 (t, 2H, J = 7.8 Hz, C2',C6'-H), 7.79 (d, 1H, J = 15 Hz, H-β), 8.07 (s, 1H, C2-H); ^{13}C NMR (DMSO-d6, 75 MHz, δ ppm): 19.59, 116.29, 128.24, 128.60, 129.48, 129.64, 130.22, 130.46, 134.63, 135.26, 142.97, 147. 61, 164.39; MS (*m/z*): 277 [$(M+H)^+$, a], 276 (M^+), 146, 131, 116, 103, 77; Anal. Calcd. for $C_{18}H_{16}N_2O$ (276.33): C, 78.24%; H, 5.84%; N, 10.14%; Found: C, 77.85%; H, 5.85%; N, 10.25%; HPLC purity: 99.26%, t_R-14.8 min.

*(E)-1-(6-methyl-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**c**)*

Yield: 82%; m.p: 218-220 ºC (Dec); IR (KBr): 2920 (CH_3), 1695 (C=O), 1622 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz, δ ppm): 2.50 (s, 3H, C6-CH_3), 7.20 (d, 1H, *J* = 15.5 Hz, H-α), 7.25-7.32 (m, 2H, C4,C4'-H), 7.46-7.52 (m, 3H,C7,C3',C5'-H), 8.05 (d, 1H, *J* = 15.5 Hz, H-β), 8.14-8.18 (m, 3H, C5,C2'C6'-H), 8.50 (s, 1H, C2-H); ^{13}C NMR ($CDCl_3$, 125 MHz, δ ppm): 21.56, 115.82, 115.94, 126.49, 128.60, 129.15, 129.87, 131.35, 133.90, 134.95, 140.01, 140.54, 148.51, 162.52; MS (*m/z*): 262/263 (M^+, a), 146, 131, 103, 77; Anal. Calcd. for $C_{17}H_{14}N_2O$ (262.31): C, 77.84%; H, 5.38%; N, 10.68%; Found: C, 77.80%; H, 5.31%; N, 10.65%; HPLC purity: 98.17% t_R-15.5 min.

*(E)-3-phenyl-1-(2-phenyl-1H-benzo[d]imidazol-1-yl)prop-2-en-1-one (**3d**)*

Yield: 72%; m.p: 130-132 ºC; IR (KBr): 1697 (C=O), 1630 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz, δ ppm): 6.85 (d, 1H, *J* = 16 Hz, H-α), 7.28 (t, 2H, *J* = 7.4 Hz, C5,C6-H of Benzimidazole), 7.39 (t, 1H, *J* = 7.2 Hz, C4'-H)7.46-7.51 (m, 3H, C3',C5',C4 of Ph), 7.56-7.72 (m, 6H, Ar-H), 7.93 (d, 1H, *J* = 16 Hz, H-β), 8.36 (d, 2H, *J* = 8.4 Hz, C2,C6-H of Ph); ^{13}C NMR ($CDCl_3$, 125 MHz, δ ppm): 114.23, 115.46, 124.41, 127.68, 127.98, 128.63, 128.82, 129.45, 130.43, 130.82, 130.96, 131.29, 135.43, 139.43, 142.01, 147.85, 167.94; MS (*m/z*): 324/325 (M^+, a), 193, 147, 131, 103, 77; Anal. Calcd. for $C_{22}H_{16}N_2O$ (324.38): C, 81.46%; H, 4.97%; N, 8.64%; Found: C, 81.41%; H, 4.99%; N, 8.61%; HPLC purity: 98.88%, t_R-18.2 min.

*(E)-1-(2-(4-methoxyphenyl)-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**e**)*

Yield: 78%; m.p: 98-100 ºC; IR (KBr): 2918 (CH_3), 1681 (C=O), 1621 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz, δ ppm): 3.60 (s, 3H, O-CH_3 of Ph), 6.12 (d, 1H, *J* = 15.2 Hz, H-α), 6.83 (d, 2H, *J* = 8.8 Hz, C3,C5-H of Ph), 7.09 (t, 2H, *J* = 7.4 Hz, C5,C6-H of Benzimidazole), 7.16 (t, 1H, *J* = 7.2 Hz, C4'-H), 7.43 (t, 2H, *J* = 7.2 Hz, C3',C5'-H), 7.44-7.52 (m, 4H, Ar-H), 7.75 (d, 1H, *J* = 15.2 Hz, H-β), 8.52 (d, 2H *J* = 8.0 Hz, C2,C6-H of Ph); ^{13}C NMR ($CDCl_3$, 100 MHz, δ ppm): 54.86, 114.11, 114.92, 115.31, 122.96, 123.12, 128.23, 128.64, 128.88, 130.46, 130.52, 130.86, 135.34, 138.93, 141.87, 147.63, 160.82, 165.63; MS (*m/z*): 357 (M^{+3}), 227, 147, 131, 121, 103, 91, 78; Anal. Calcd. for $C_{23}H_{18}N_2O_2$ (354.40): C, 77.95%; H, 5.12%; N, 7.90%; Found: C, 77.89%; H, 5.06%; N, 7.88%; HPLC purity: 98.76%, t_R-18.8 min.

*(E)-1-(2-(4-chlorophenyl)-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**f**)*

Yield: 84%; m.p: 116-118 ºC; IR (KBr): 1686 (C=O), 1614 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz, δ ppm): 6.41 (d, 1H, *J* = 16 Hz, H-α), 7.16 (t, 2H, *J* = 7.4 Hz, C5,C6-H of Benzimidazole), 7.37 (t, 1H, *J* = 7.2 Hz, C4'H), 7.44 (t, 2H, *J* = 7.2 Hz, C3',C5'-H), 7.60-7.70 (m, 6H, Ar-H), 7.83 (d, 1H, *J* = 16 Hz, H-β), 8.11 (d, 2H, *J* = 8.1 Hz, C2,C6-H of Ph); ^{13}C NMR ($CDCl_3$, 100 MHz, δ ppm): 114.53, 116.75, 125.02, 128.43, 128.60, 129.09, 129.12, 129.81, 130.99, 133.73, 134.29, 136.86, 142.68, 147.11, 165.32; MS (*m/z*): 358/360/359 (M^+, a), 228, 147, 131, 103, 90, 77; Anal. Calcd. for $C_{22}H_{15}ClN_2O$ (358.82): C, 73.64%; H, 4.21%; N, 7.81%; Found: C, 73.55%; H, 4.20%; N, 7.77%; HPLC purity: 99.41%, t_R-19.2 min.

*(E)-1-(2-(2-hydroxyphenyl)-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (3**g**)*

Yield: 56%; m.p: 198-200 ºC; IR (KBr): 3315 (OH), 1681 (C=O), 1633 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz, δ ppm): 6.73 (d, 1H, *J* = 16 Hz, H-α), 6.91 (d, 1H, *J* = 6.8 Hz, C3-H of Ph), 7.04 (t, 1H, *J* = 7.0 Hz, C5-H of Ph), 7.31(m, 3H, C4-H of Ph, C5,C6-H of Benzimidazole), 7.38 (t, 1H, *J* = 7.4 Hz, C4'-H) 7.48 (t, 2H, *J* = 7.4 Hz, C3',C5'-H), 7.61-7.69 (m, 5H, Ar-H), 7.78 (d, 1H, *J* = 16 Hz, H-β), 8.03 (s, 1H, -OH D_2O exchangeable); ^{13}C NMR ($CDCl_3$, 100 MHz, δ ppm): 13.50, 46.92, 114.51, 115.36, 123.10, 128.06, 128.61, 128.83, 128.92, 130.43, 130.58, 130.76, 135.36, 139.13, 141.93, 147.33, 165.88; MS (*m/z*): 340/341 (M^+, a), 209, 131, 103, 90, 77; Anal. Calcd. for $C_{22}H_{16}N_2O_2$ (340.37): C, 77.63%; H, 4.74%; N, 8.23%; Found: C, 77.56%; H, 4.76%; N, 8.21%; HPLC purity: 98.74%, t_R-17.7 min.

*(E)-1-(2-(4-hydroxyphenyl)-1H-benzo[d]imidazol-1-yl)-3-phenylprop-2-en-1-one (**3h**)*

Yield: 71%; m.p: 120-122 ºC; IR (KBr): 3280 (OH), 1680 (C=O), 1649 (C=C) cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz, δ ppm): 6.62 (d, 1H, *J* = 16 Hz, H-α), 6.84 (d, 2H, *J* = 8.4 Hz, C3,C5-H of Ph), 7.26 (t, 2H, *J* = 7.4 Hz, C5,C6-H of Benzimidazole), 7.39 (t, 1H, *J* = 7.6 Hz, C4'-H), 7.51 (t, 2H, *J* = 7.6, C3',C5'-H), 7.60-7.66 (m, 4H, Ar-H), 7.86 (d, 1H, *J* = 16 Hz, H-β), 7.92 (d, 2H, *J* = 7.8 Hz, C2,C6-H of Ph), 8.12 (s, 1H, -OH D_2O exchangeable); ^{13}C NMR ($CDCl_3$, 100 MHz, δ ppm): 114.15, 115.82, 116.93, 123.12, 123.23, 128.03, 128.42, 128.56, 130.61, 130.83, 135.23, 138.93, 142.62, 147.45, 158.82, 165.33; MS (*m/z*): 340/341 (M^+, a), 209, 131, 103, 90, 77; Anal. Calcd. for $C_{22}H_{16}N_2O_2$

(340.37): C, 77.63%; H, 4.74%; N, 8.23%; Found: C, 77.55%; H, 4.72%; N, 8.21%; HPLC purity: 98.55%, t_R-18.3 min.

X-ray diffraction analysis

The single crystals of the size of 0.30x0.20x0.20 mm were selected under a polarizing microscope and it was mounted on a glass fiber for x-ray diffraction data collection. The high resolution X-ray diffraction data sets for both complexes were collected on a Bruker SMART APEX2 CCD Diffractometer using Mo K_α radiation (λ = 0.71073 Å) at 296 K. The crystal-to-detector distance was fixed at 40 mm. The diffraction data have been scaled for absorption effect by the multi-scanning method. Data collection has been performed by applying the apex-II Software system. Structures were solved by direct methods and refined on F^2 by weighted full-matrix least-squares. Programs SHELXS97 and SHELXL97 integrated in the WinGX v. 1.70.01 software system were used to solve and refine structure. All non-hydrogen atoms were refined anisotropically. The ortep and packing diagrams are generated using the Mercury 3.3.