Concise Synthesis and Biological Evaluation of a Phorbazole Analogue-B1 Identifies a Multi-Kinase Inhibitor with Anti-AML Activity

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Table S1. Kinase selectivity profile of B1

Kinase	B1 (1μM)	B1(1μM)	STDEV	B1 (%inhibition)@1μM
PDGFRα	99.39	99.72	0.24	99.55
MNK2	97.58	99.15	1.11	98.37
TRKB	98.01	98.09	0.05	98.05
GAK	95.74	100.27	3.21	98.00
MNK1	96.15	92.76	2.40	94.46
MLK1	94.76	93.57	0.84	94.16
QIK	91.59	89.42	1.54	90.50
HGK	90.98	88.50	1.76	89.74
CLK1	87.21	84.72	1.76	85.97
LCK	83.42	82.12	0.92	82.77
FGFR1	83.23	81.59	1.16	82.41
ITK	78.52	83.93	3.83	81.22
AurB	81.64	78.89	1.95	80.26
KDR	81.33	78.17	2.23	79.75
ABL1	79.00	77.02	1.40	78.01
RSK1	74.86	75.60	0.52	75.23
CK1γ2	78.39	70.99	5.23	74.69
IRAK4	68.14	72.41	3.02	70.28
SRC	70.88	69.42	1.04	70.15
NEK1	60.42	59.05	0.97	59.74
AMPKα1/β1/γ1	58.17	54.24	2.78	56.21
HIPK1	51.21	58.38	5.07	54.79
MAP3K19	55.13	51.57	2.52	53.35
DYRK1B	51.12	52.90	1.26	52.01

CK1γ3	45.71	53.88	5.77	49.80
CK2α1/β	57.05	39.90	12.13	48.48
EPHB4	55.28	41.34	9.86	48.31
p70S6K	52.53	43.86	6.13	48.20
TGFβR2	46.34	45.52	0.58	45.93
IRAK1	34.70	48.68	9.89	41.69
CHK2	37.60	44.58	4.94	41.09
CK1α	45.53	36.04	6.71	40.78
NEK2	38.51	41.51	2.12	40.01
BMX	40.20	35.58	3.27	37.89
MARK4	42.23	32.58	6.83	37.41
Erk7	35.09	36.05	0.68	35.57
TIE2	31.42	31.04	0.27	31.23
BRSK2	30.43	29.51	0.65	29.97
PLK2	25.94	31.81	4.15	28.87
CDK2/CycE1	26.09	27.41	0.93	26.75
AXL	26.75	25.90	0.60	26.33
HPK1	26.94	24.49	1.74	25.71
CDK5/p35NCK	27.98	19.86	5.74	23.92
WEE1	29.64	14.90	10.42	22.27
DAPK1	22.58	21.22	0.96	21.90
SGK	20.66	14.14	4.60	17.40
EPHA2	14.99	14.86	0.10	14.93
MARK1	16.54	11.81	3.34	14.18
MET	19.40	6.74	8.95	13.07
PEK	6.49	19.35	9.09	12.92

CaMK1α	7.49	18.11	7.51	12.80
MRCKβ	19.47	5.45	9.92	12.46
IKKα	12.59	11.36	0.87	11.97
CDK18/CycY	12.78	10.91	1.33	11.84
JAK3	13.78	7.92	4.14	10.85
JNK1	13.10	7.90	3.67	10.50
TSSK1	16.17	2.38	9.76	9.28
PKD2	5.76	12.14	4.51	8.95
ULK2	13.38	4.41	6.34	8.90
TGFβR1	10.66	6.83	2.71	8.75
MAP2K1	-0.11	17.54	12.48	8.71
PKCα	18.42	-1.86	14.34	8.28
PIM1	4.12	3.88	0.17	4.00
PKACα	8.65	-1.33	7.06	3.66
AKT1	17.17	-10.50	19.56	3.34
CDK1/CycE1	3.50	2.32	0.84	2.91
SYK	3.94	1.44	1.77	2.69
ROCK1	2.62	2.21	0.29	2.41
MAPKAPK2	-0.11	4.77	3.45	2.33
TAOK1	7.76	-4.53	8.69	1.62
P38α	2.65	0.13	1.78	1.39
PAK2	0.09	0.86	0.55	0.47
DCAMKL2	2.22	-2.13	3.08	0.04
EGFR	1.12	-1.16	1.61	-0.02
IGF1R	0.08	-1.07	0.81	-0.49
PIK3CA	2.71	-6.20	6.30	-1.75

Erk2	-0.76	-3.06	1.62	-1.91
GSK3β	-3.37	-1.55	1.29	-2.46
BRAF	-7.43	0.85	5.85	-3.29
CHK1	-8.69	-3.01	4.02	-5.85
ALK4	0.14	-19.86	14.14	-9.86
PLK1	-8.96	-14.40	3.85	-11.68

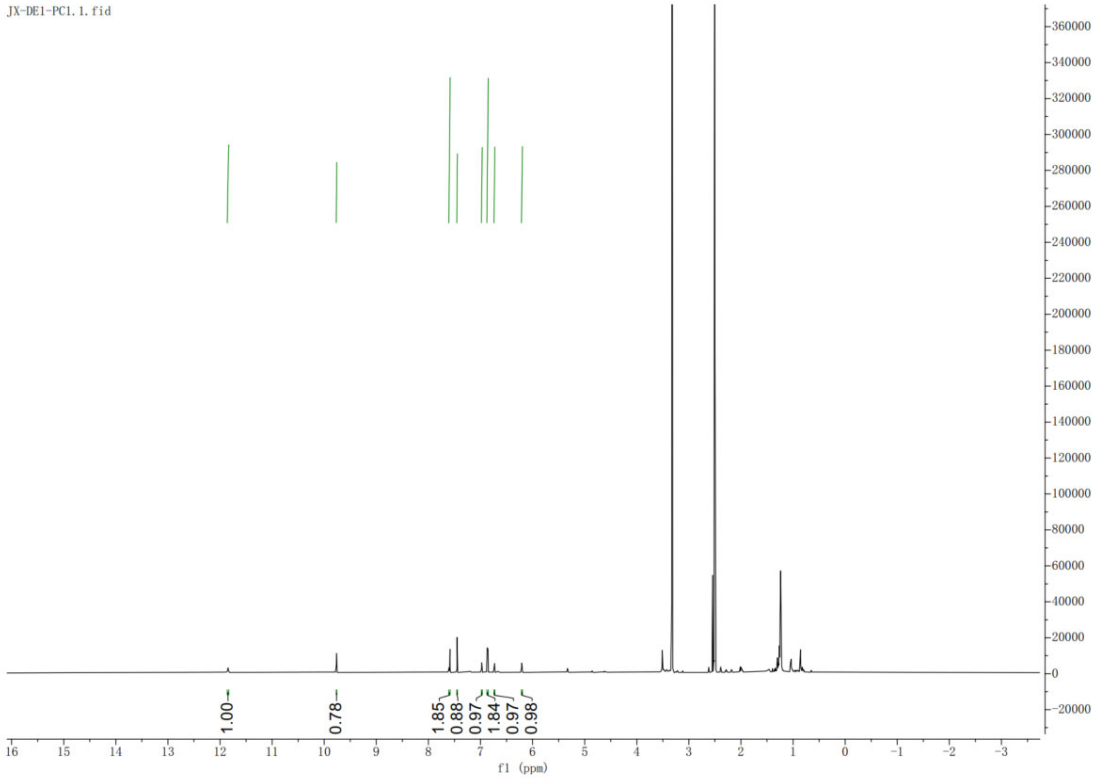


Figure S1. ^{1}H NMR Spectrum of deschloro-phorbazole (600 MHz, DMSO-d_6)

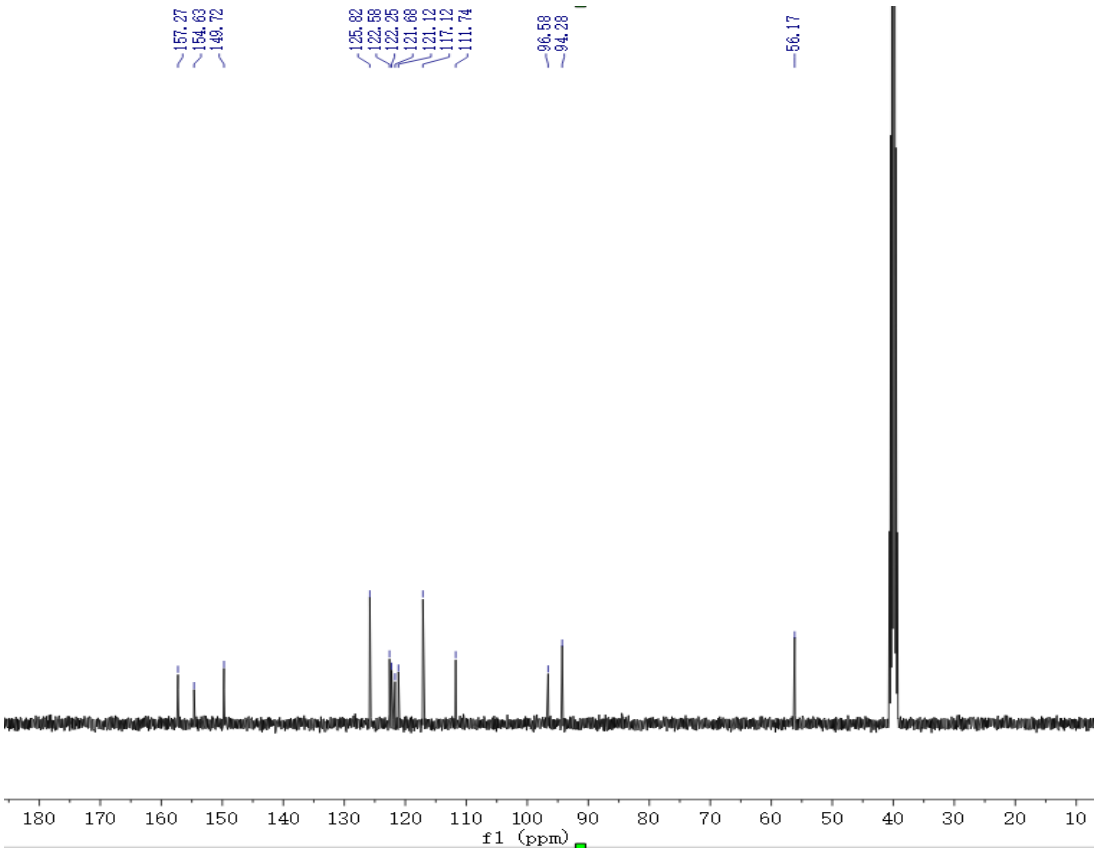


Figure S2. ^{13}C NMR Spectrum of Deschloro-Phorbazoles (125 MHz, DMSO-d_6)

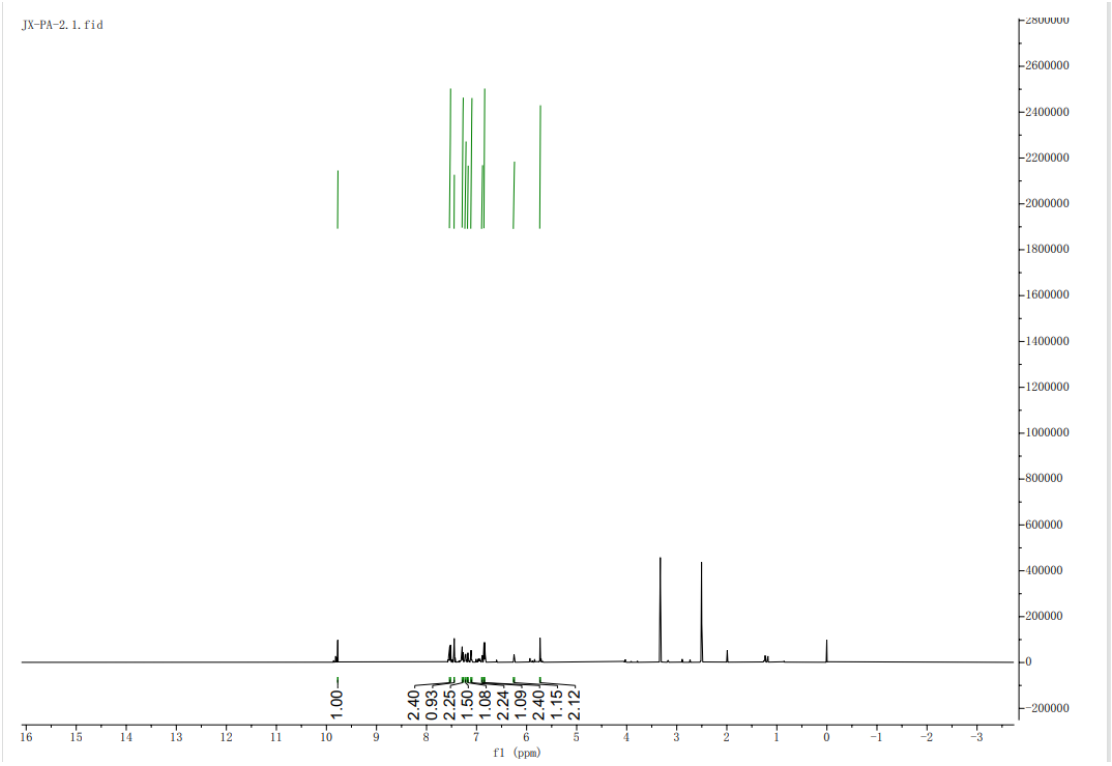


Figure S3.[1]H NMR Spectrum of **compound 3** (600 MHz, DMSO-d_6)

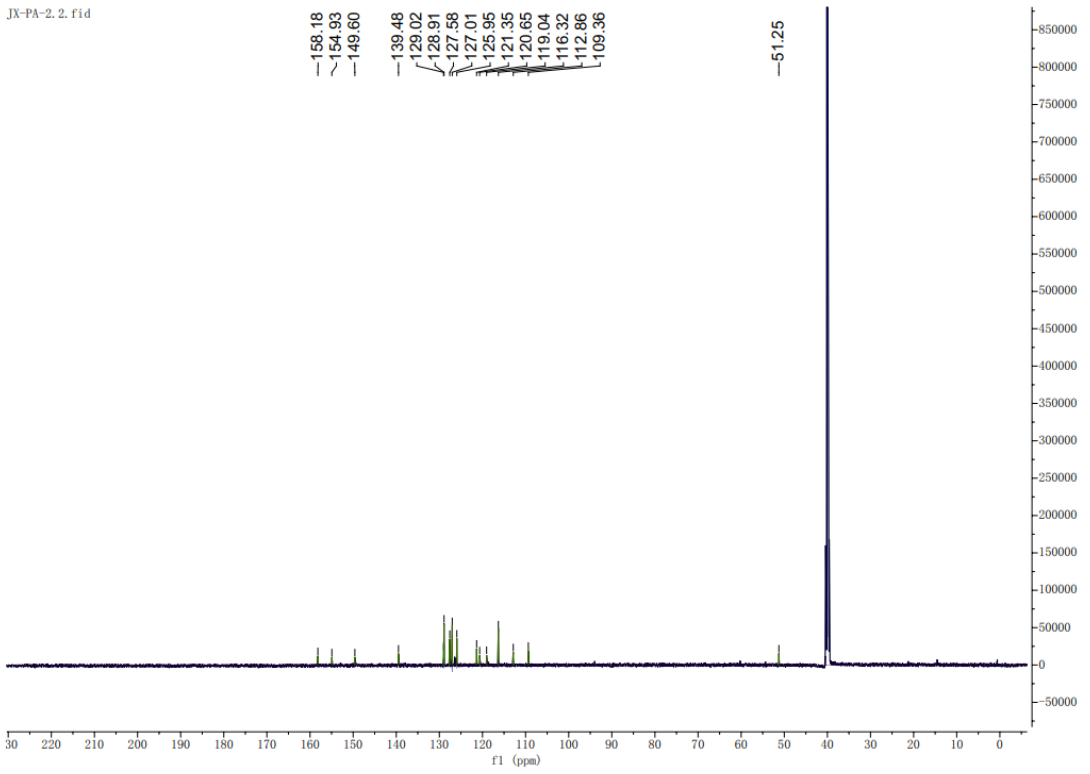


Figure S4.[13]C NMR Spectrum of **compound 3** (150 MHz, DMSO-d_6)

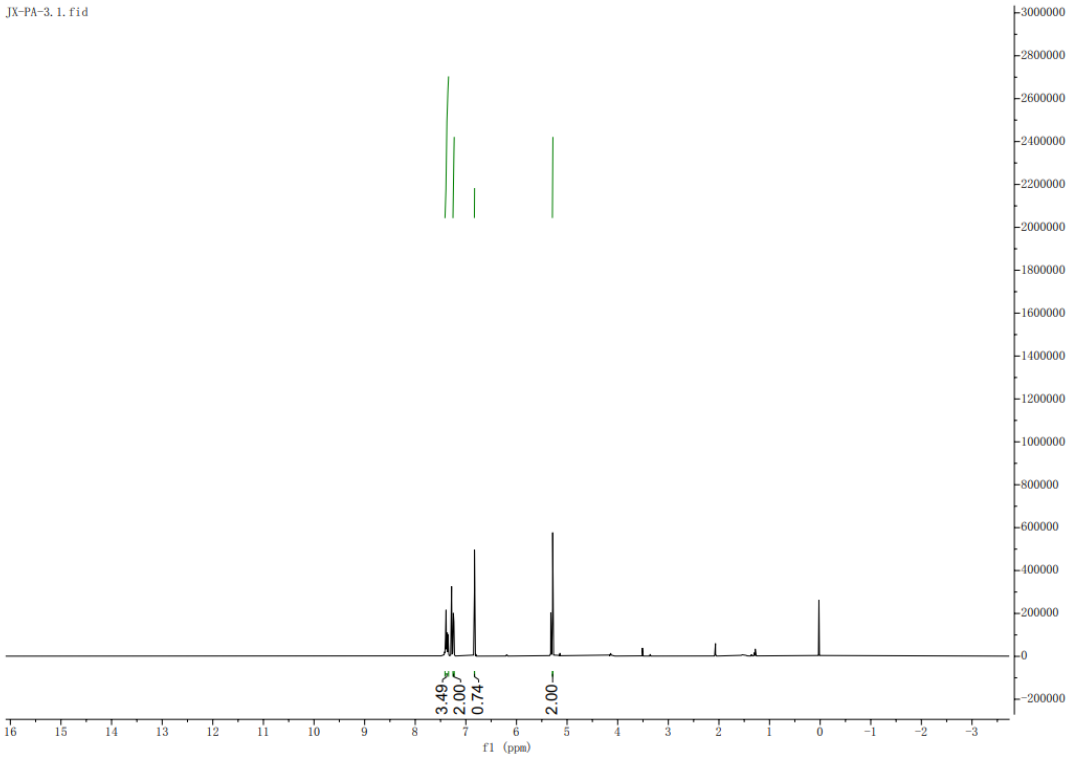


Figure S5.^{1}H NMR Spectrum of **compound 4** (600 MHz, $CDCl_3$)

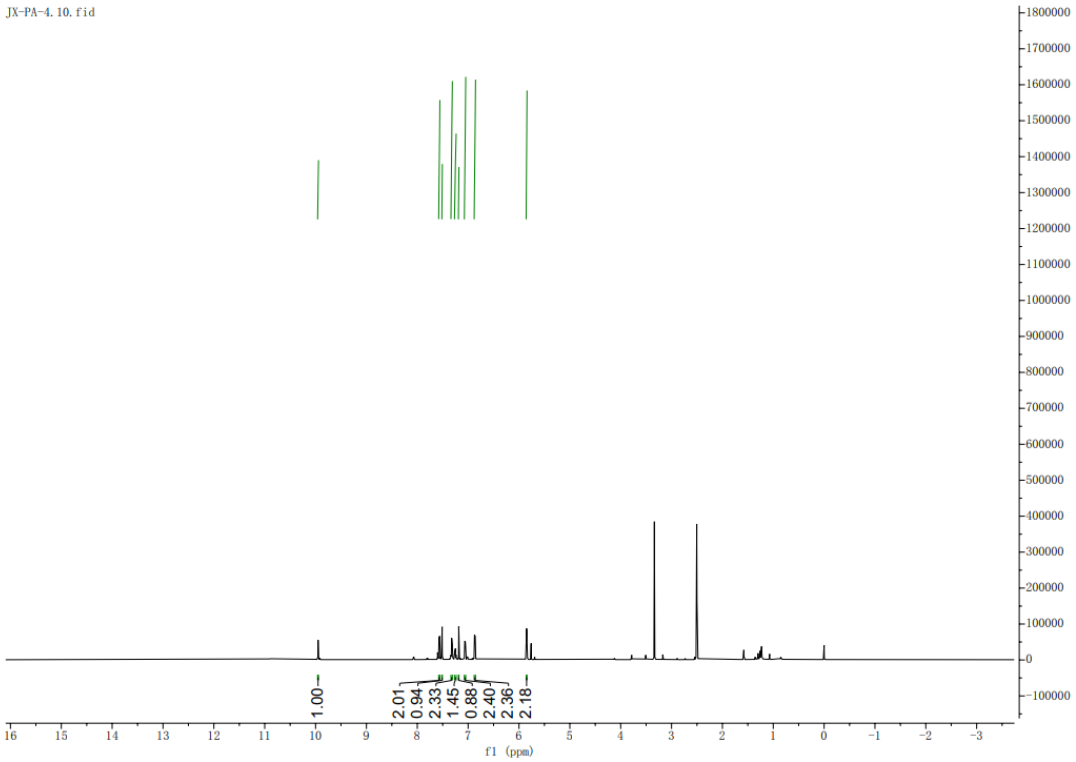


Figure S6.^{1}H NMR Spectrum of **compound 6** (600 MHz, DMSO-d_6)

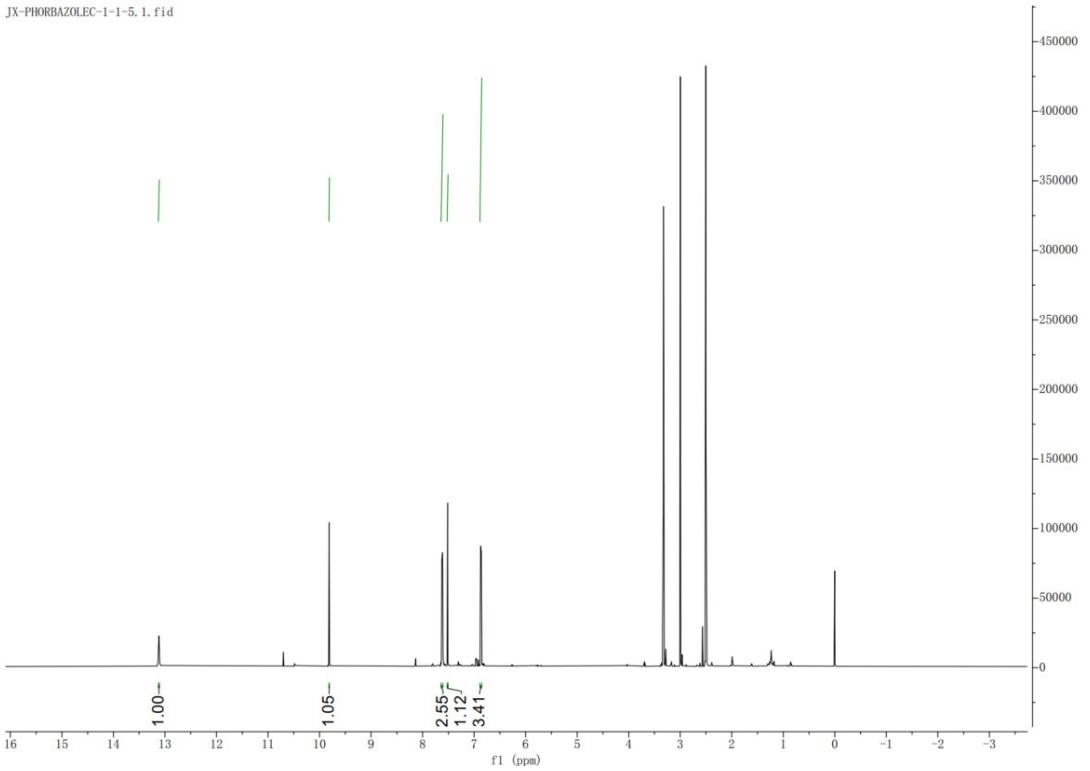


Figure S7.[1]H NMR Spectrum of **Phorbazole C** (600 MHz, DMSO-d_6)

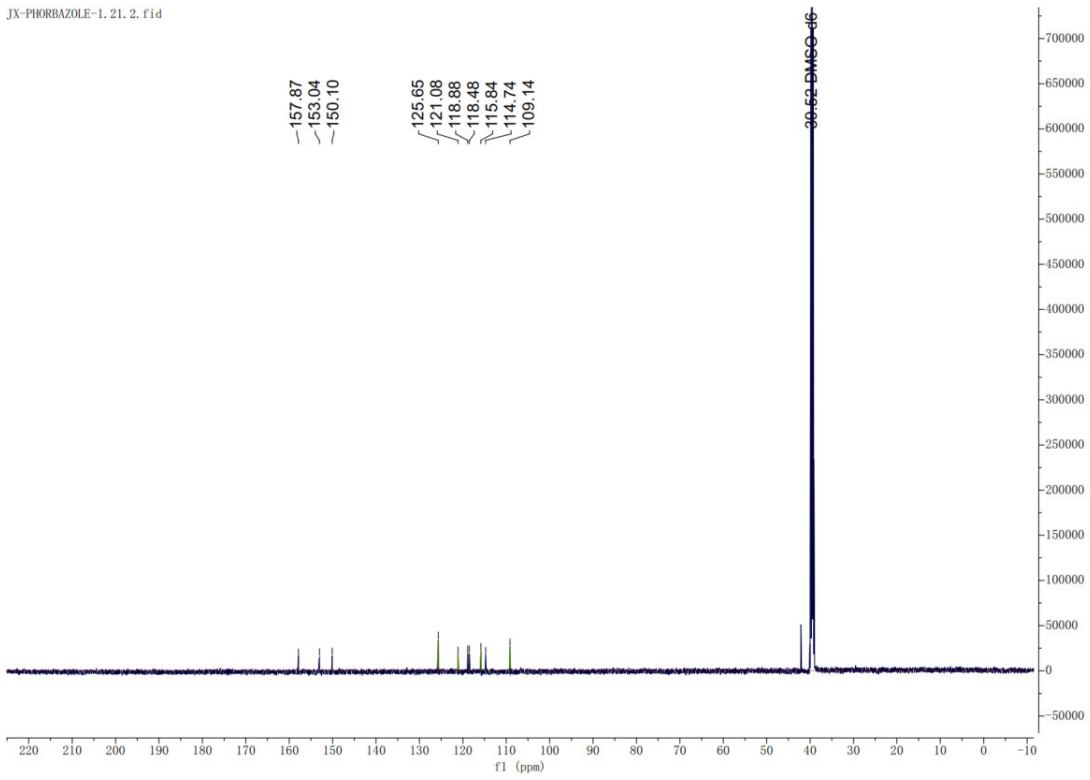


Figure S8.[13]C NMR Spectrum of **Phorbazole C** (125 MHz, DMSO-d_6)

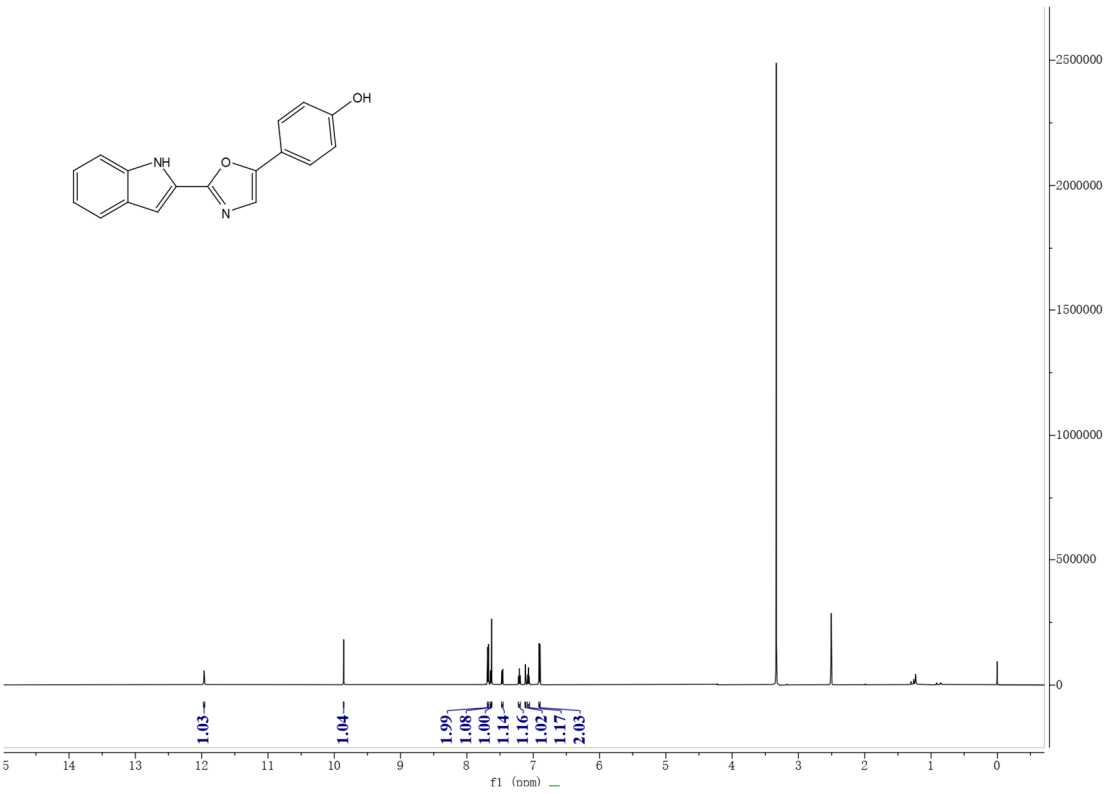


Figure S9.[1]H NMR Spectrum of **B1** (600 MHz, DMSO-*d*$_6$)

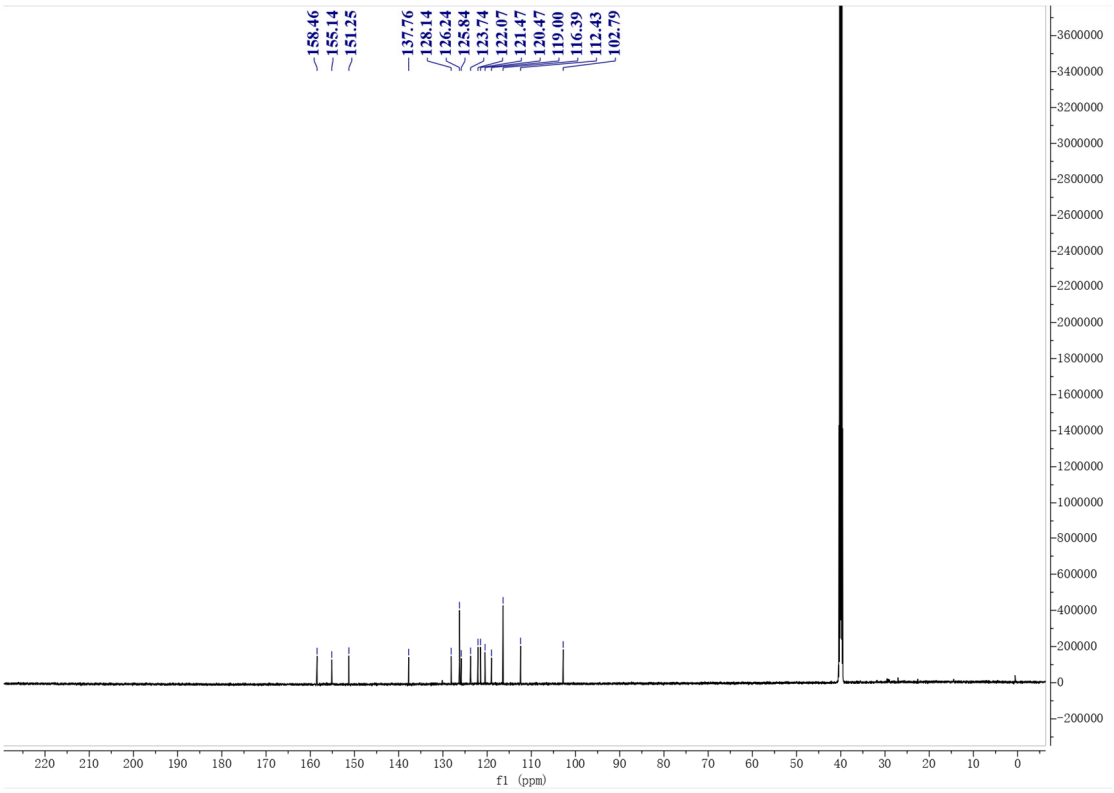


Figure S10.[13]C NMR Spectrum of **B1** (150 MHz, DMSO-*d6*)