Supplementary Information

Synthesis, Characterization and Preliminary Study on Acetylpyrazine N(4)Butylthiosemicarbazone as a Potential CDK2 Inhibitor Combined with DFT Calculations

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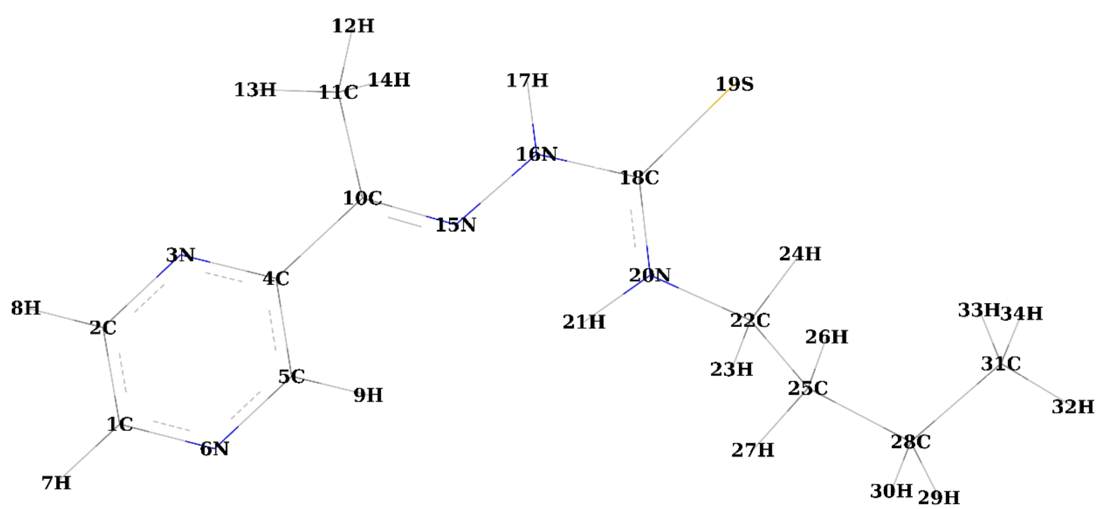

Figure S1. Numbering used for assignment of ^{1}H and ^{13}C NMR chemical shift signals for APBT.

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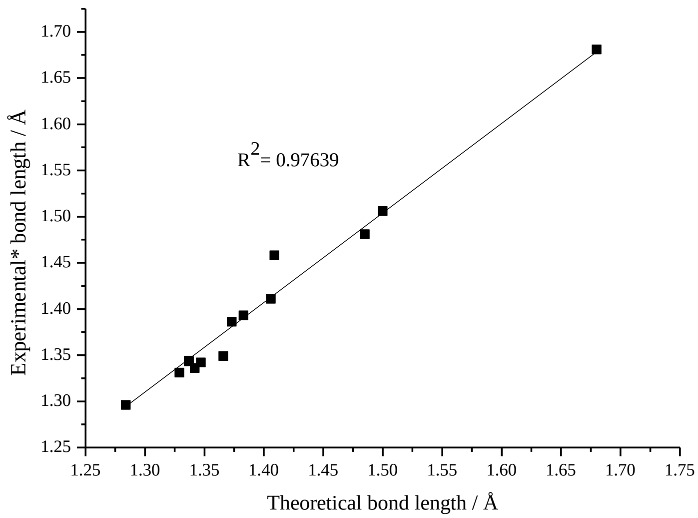

Figure S2. Bond length correlation coefficient of APBT.

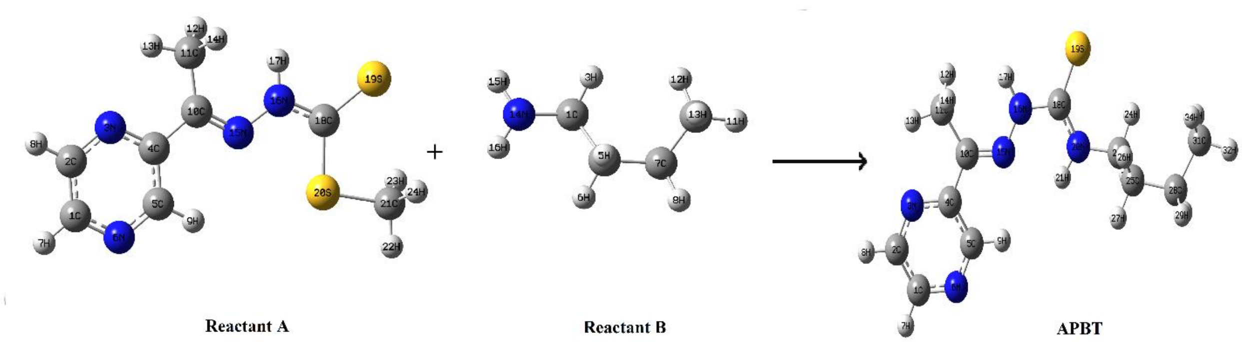

Figure S3. Optimized geometries of the reactants and product involved in the chemical reaction calculated at the B3LYP/6-311++G(d,p).

Table S1. The experimental and calculated geometric parameters of APBT

Geometric parameter	Experimental[1]	Calculated B3LYP/6-311++G(d,p)
Bond length / Å		
S19–C18	1.680	1.681
N6–C5	1.329	1.331
N1–C6	1.347	1.342
N3–C2	1.342	1.336
N3–C4	1.337	1.344
N15–N16	1.366	1.349
N15–C10	1.284	1.296
N16–C18	1.373	1.386
N20–C18	1.337	1.343
N20–C22	1.409	1.458
C4–C5	1.406	1.411
C1–C2	1.383	1.393
C4–C10	1.485	1.481
C10–C11	1.500	1.506
Bond angle / degree		
C5–N6–C1	116.5	116.5
C2–N3–C4	116.5	117.1
N16–N15–C10	120.4	118.6
N15–N16–C18	117.9	121.9
C18–N20–C22	133.3	125.1
N15–C10–C4	122.1	122.6
N6–C1–C2	121.4	121.6
N3–C2–C1	122.4	122.0
N3–C4–C10	121.1	120.2
C10–C4–C5	121.8	122.4
N15–C10–C4	114.0	116.5
N15–C10–C11	126.6	123.9
C4–C10–C11	119.4	119.6
S19–C18–N16	119.1	118.3
S19–C18–N20	127.4	127.0
N16–C18–N20	113.4	114.7

Table S2. Observed and calculated vibrational frequencies of APBT with B3LYP/6-311++ G(d,p)

Mode No.	Experimental frequency / cm^{-1}	Calculated frequency / cm^{-1}		Intensity	Vibrational assignment (PED ≥ 10 / %)
		Unscaled	Scaled		
1	3363	3587	3453	53.59	ν[(N20H21)] (99)
2	3219	3571	3438	35.78	ν[(N16H17)] (99)
3	3096	3210	3090	4.30	ν[(C5H9)] (96)
4	3080	3192	3073	48.20	ν[(C1H7)] (93)
5	–	3182	3063	1.94	ν[(C11H13)] (93)
6	–	3172	3054	10.96	ν[(C1H7)] (95)
7	3004	3139	3022	4.76	ν[(C22H24)] (86)
8	2995	3117	3001	45.24	ν[(C31H33)] (84)
9	–	3115	2999	45.35	ν[(C31H32)] (93)
10	–	3084	2969	25.46	ν[(C25H26)] (80)
11	–	3083	2968	11.05	ν[(C11H12)] (97)
12	–	3064	2950	25.24	ν[(C28H29)] (78)
13	2929	3049	2935	40.63	ν[(C22H23)] (85)
14	–	3046	2932	15.59	ν[(C31H32)] (94)
15	–	3033	2920	24.87	ν[(C25H27)] (85)
16	–	3031	2918	6.97	ν[(C11H12)] (93)
17	2867	3024	2911	25.51	ν[(C28H29)] (13)
18	1630	1660	1598	63.95	ν[(N15C11)] (63)
19	1599	1612	1552	29.64	ν[(N15C10)] (52) + δ[(H8C2N3)] (21)
20	–	1588	1529	278.74	ν[(N20C18)] (53) + δ[(H21N20C22)] (30)
21	1504	1582	1523	139.60	ν[(N6C5)] (69)
22	1470	1541	1484	264.09	δ[(H17N16N1)5] (53)
23	1464	1522	1465	3.67	δ[(H32C31H33)] (68) + τ[(H29C28C31H33)] (10)
24	–	1518	1461	6.14	δ[(H26C25H27)] (70) + τ[(H29C28N25C22)] (12)
25	–	1514	1458	8.68	δ[(H13C11H14)] (81) + τ[(C11H12C10H13)] (13)
26	–	1508	1452	60.63	δ[(H26C25H27)] (57)

27	–	1506	1450	55.80	δ[(H26C25H27)] (56)
28	–	1503	1447	0.97	γ[(H26C25H28)] (65)
29	–	1495	1439	48.60	δ[(H23C22H24)] (63) + τ[(C11H12C10H14)] (14)
30	1421	1482	1427	104.67	δ[(H13C11C10)] (41) + τ[(C11H12C10H14)] (23)
31	1403	1446	1392	52.93	δ[(H7C1N6)] (38)
32	–	1436	1382	3.78	γ[(H32C31H33)] (84)
33	–	1428	1375	24.58	τ[(H24C22N20C18)] (53)
34	–	1409	1356	7.95	γ[(H12C11H14)] (78)
35	–	1393	1341	43.04	δ[(H21N20C22)] (21)
36	1318	1387	1335	36.12	τ[(H29C28C31H33)] (46)
37	1297	1355	1304	2.83	δ[(H26C25C28)] (42) + τ[(H34C31C28C25)] (10)
38	1255	1349	1299	25.77	γ[(H23C22N20)] (53) + δ[(H23C22N20)] (12)
39	–	1329	1279	94.59	ν[(C4C10)] (17) + δ[(H21N20N22)] (12)
40	–	1323	1274	11.05	ν[(C4C5)] (28) + δ[(H8C2N3)] (51)
41	–	1300	1252	17.36	γ[(H26C25C28)] (24) + τ[(H23C22N20C18)] (43)
42	1224	1276	1228	113.42	δ[(H23C22C20)] (39)
43	–	1263	1216	72.73	ν[(N3C2)] (70)
44	1176	1217	1172	359.38	ν[(N16C18)] (41) + τ[(H29C28C25C22)] (10)
45	–	1207	1162	13.16	ν[(C1C6)] (18) + δ[(H9C5N6)] (13)
46	1113	1180	1136	33.01	ν[(N15N160)] (17) + τ[(H29C28C25C22)] (26)
47	1104	1171	1127	60.45	ν[(N15N16)] (38)
48	–	1137	1095	16.91	[(C22C25)] (30) + δ[(C25C22N20)] (12) + τ[(H34C31C28C25)] (31)
49	–	1124	1082	14.80	δ[(H13N11N10)] (10) + δ[(C2C1N6)] (14) + τ[(C11H12C10H14)] (11)
50	1064	1096	1055	55.20	ν[(C22C25)] (30) + ν [(S19C18)] (30) + τ[(H33C31C28C25)] (10)
51	–	1076	1036	10.99	ν[(C1C2)] (62)
52	–	1073	1033	16.58	ν[(C28C31)] (73)
53	1008	1055	1016	0.26	γ[(H13C11H14)] (14) + τ[(C11H12C10H13)] (72)
54	–	1030	992	33.21	δ[(C10N15N16)] (21) + δ[(C2N3C4)] (19) + δ[(C1C2N3)] (41)
55	960	992	955	3.40	ν[(C10C11)](38) + γ[(H23C22H24)] (10)

56	–	984	947	0.09	ν[(C22C25)] (30) + τ[(H7C1C2H8)] (86)
57	–	983	946	3.21	τ[(H34C31C28C25)] (15)
58	928	963	927	0.33	τ[(H8C2C1N6)] (86)
59	–	956	920	5.13	τ[(H33C31C28C25)] (48)
60	848	888	855	2.81	ν[(C28C25)] (61) + τ[(H22C25C20C23)] (10)
61	–	868	836	13.51	τ[(H7C1N6C5)] (91)
62	800	856	824	29.52	ν[(S19C18)] (25) + δ[(C1C2N3)] (14)
63	761	798	768	7.33	τ[(H29C28C31H33)] (37)
64	–	788	759	1.30	τ[(H32C31C28C25)] (20)
65	–	777	748	1.43	τ[(C2N3C4C5)] (77)
66	704	756	728	8.20	τ[(C22C25N20H23)] (58)
67	641	672	647	7.31	ν[(S19C18)] (11) + δ[(C11C10N15)] (46)
68	–	644	620	8.39	τ[(C18N16N20S19)] (80)
69	–	626	603	0.52	δ[(C1N6C5)] (80)
70	585	599	577	12.59	δ[(C18N20C22)] (23)+ τ[(C2C1N6C5)] (25)
71	–	596	574	27.96	γ[(N20C18S19)] (12) + τ[(C11C4N15C10)] (41)
72	537	565	544	41.93	τ[(H21N20C18S19)] (80)
73	529	542	522	2.57	δ[(C18N16N15)] (45)
74	497	521	502	47.10	τ[(H17N16C18S19)] (76)
75	481	480	462	36.55	τ[(N3C2C1N6)] (83)
76	–	468	451	9.68	γ[(C22C25C28)] (45)
77	417	423	407	12.83	τ[(C2C1N6C5)] (84)
78	–	418	402	10.69	δ[(C5C4C10)] (56)
79	–	361	348	1.38	δ[(C25C28C31)] (57)
80	–	313	301	0.80	δ[(C11C10N15)] (62)
81	–	310	298	4.31	γ[(C22C25C28)] (41) + τ[(H33C31C28C25)] (12)
82	–	292	281	0.10	τ[(C4C10N15N16)] (53)
83	–	279	269	2.87	δ[(N20C18S19)] (28) + τ[(H33C31C28C25)] (31)
84	–	232	223	0.50	γ[(C18N20C22)] (45) + τ[(H29C28C25C22)] (14)

85	–	211	203	4.09	δ[(C2C1N6)] (10) + γ[(C18C20C22)] (18) + τ[(H29C28C25C22)] (24)
86	–	177	170	9.55	δ[(C5C4C10)] (64)
87	–	169	163	1.12	τ[(H12C11C10C4)] (79)
88	–	139	134	1.78	τ[(H12C11C10C4)] (13) + τ[(C10C4C5N6)] (67)
89	–	116	112	0.30	τ[(C28C25C22N20)] (57)
90	–	108	104	0.45	τ[(C10N15N16C18)] (56) + τ[(N4N10C15N16)] (10)
91	–	72	69	1.33	γ[(C10N15N16)] (59)
92	–	59	57	0.45	τ[(C18N20C22C25)] (63)
93	–	48	46	1.89	τ[(N3C4C10N15)] (16) + τ[(C4C10N15N16)] (66)
94	–	42	40	0.26	τ[(C31C28C25C22)] (10) + τ[(C28C25C22N20)] (57)
95	–	27	26	0.12	τ[(C22N20C18N16)] (65)
96	–	18	17	0.65	τ[(N3C4C10N15)] (84)

PED: potential energy distribution; ν: stretching; δ: in-plane bending; γ: out-of-plane bending; τ: torsion.[2] Scaling factor = 0.9627.

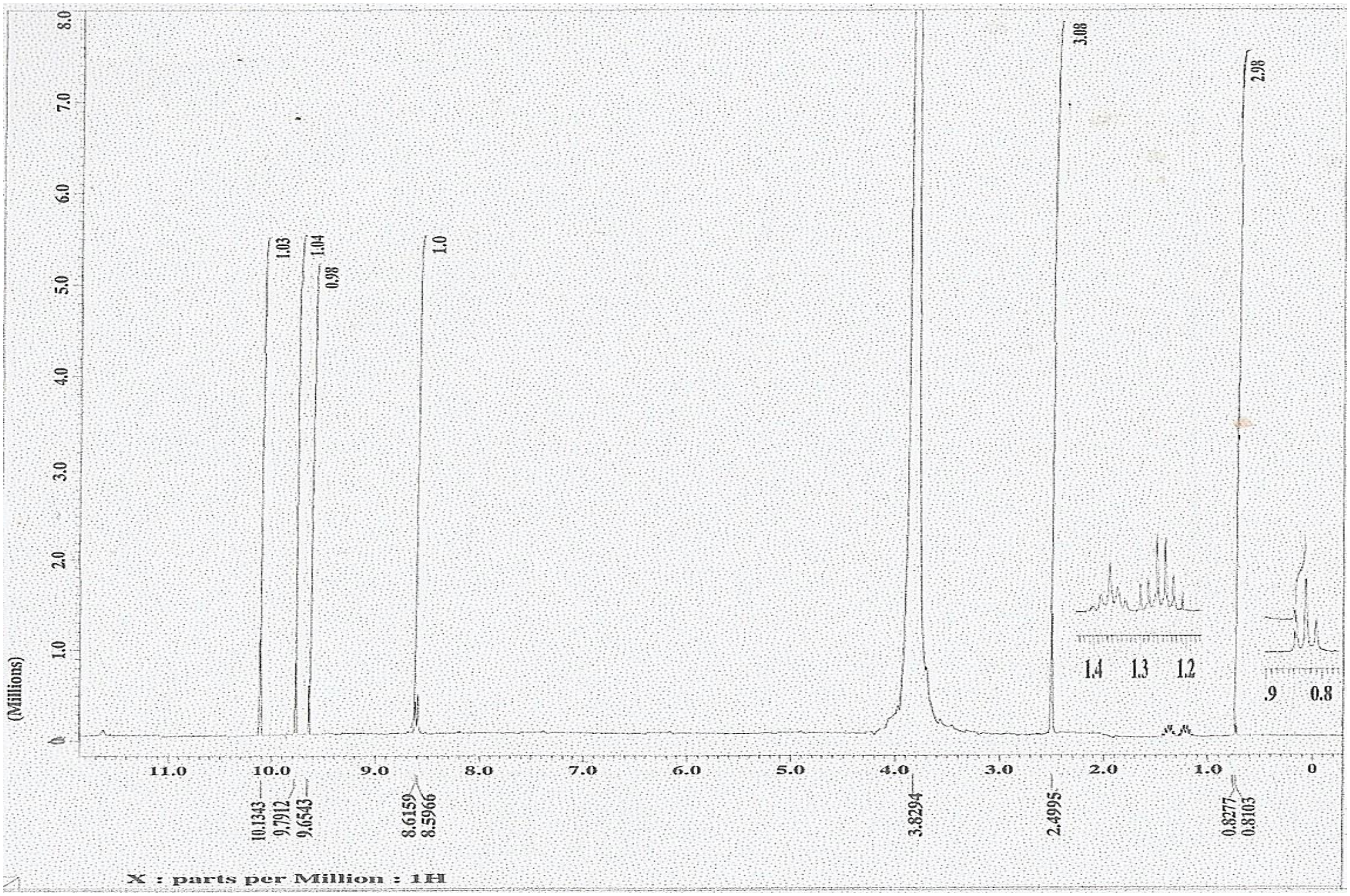

Figure S4. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of APBT.

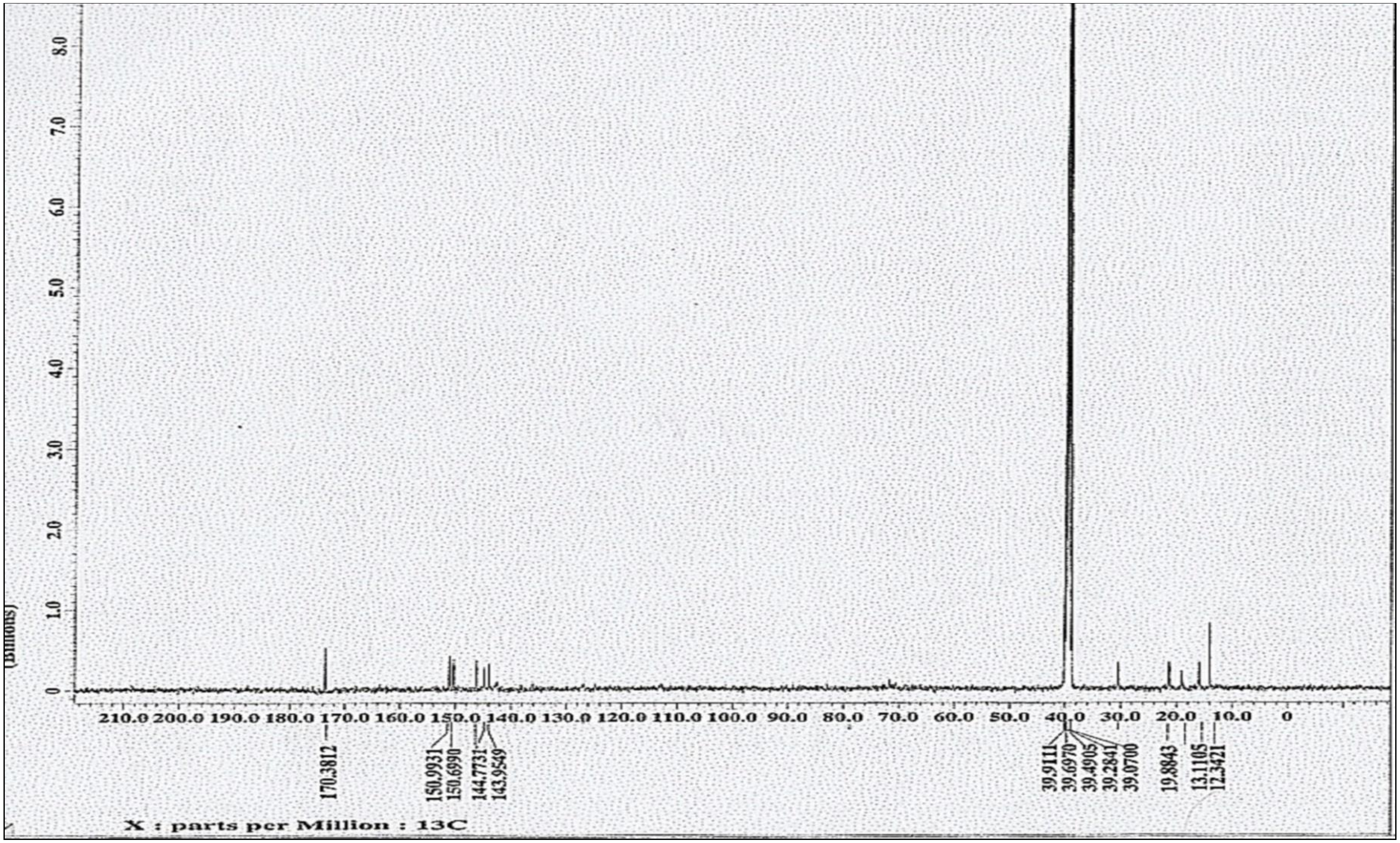

Figure S5. ^{13}C NMR (400 MHz, DMSO-d_6) spectrum of APBT.

References

1. Normaya, E.; Farina, Y.; Halim, S. N. A.; Tienkink, E. R. T.; *Acta Crystallogr.* **2011**, *E67*, o943.
2. Sert, Y.; Miroslaw, B.; Cirak, C.; Dogan, H.; Szulczyk, D.; Struga, M.; *Spectrochim. Acta, Part A* **2014**, *128*, 91.

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