Supplementary Material

Novel Piperidone Hydrazine Carbodithioate Derivative: Synthesis, *In Silico* Drug-Likeness Analysis and Anticancer Properties

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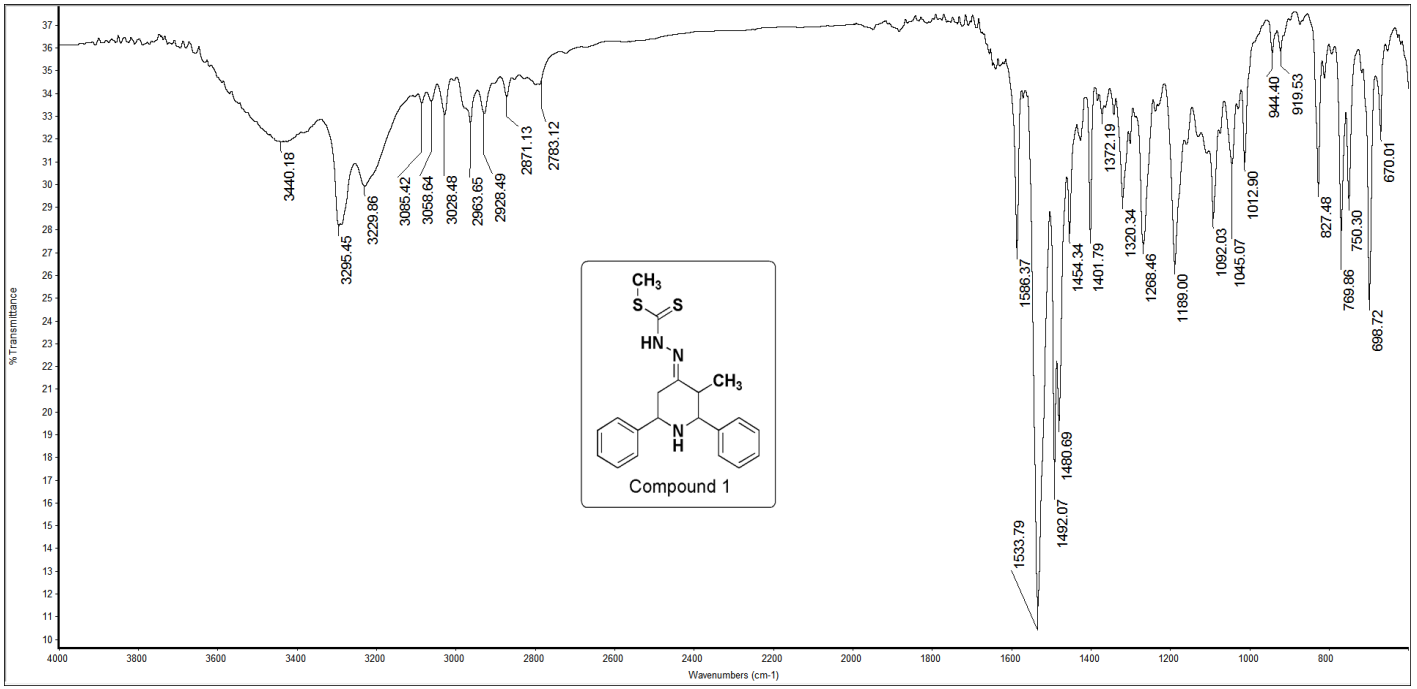

Fig. S1. FTIR spectrum of compound **1**

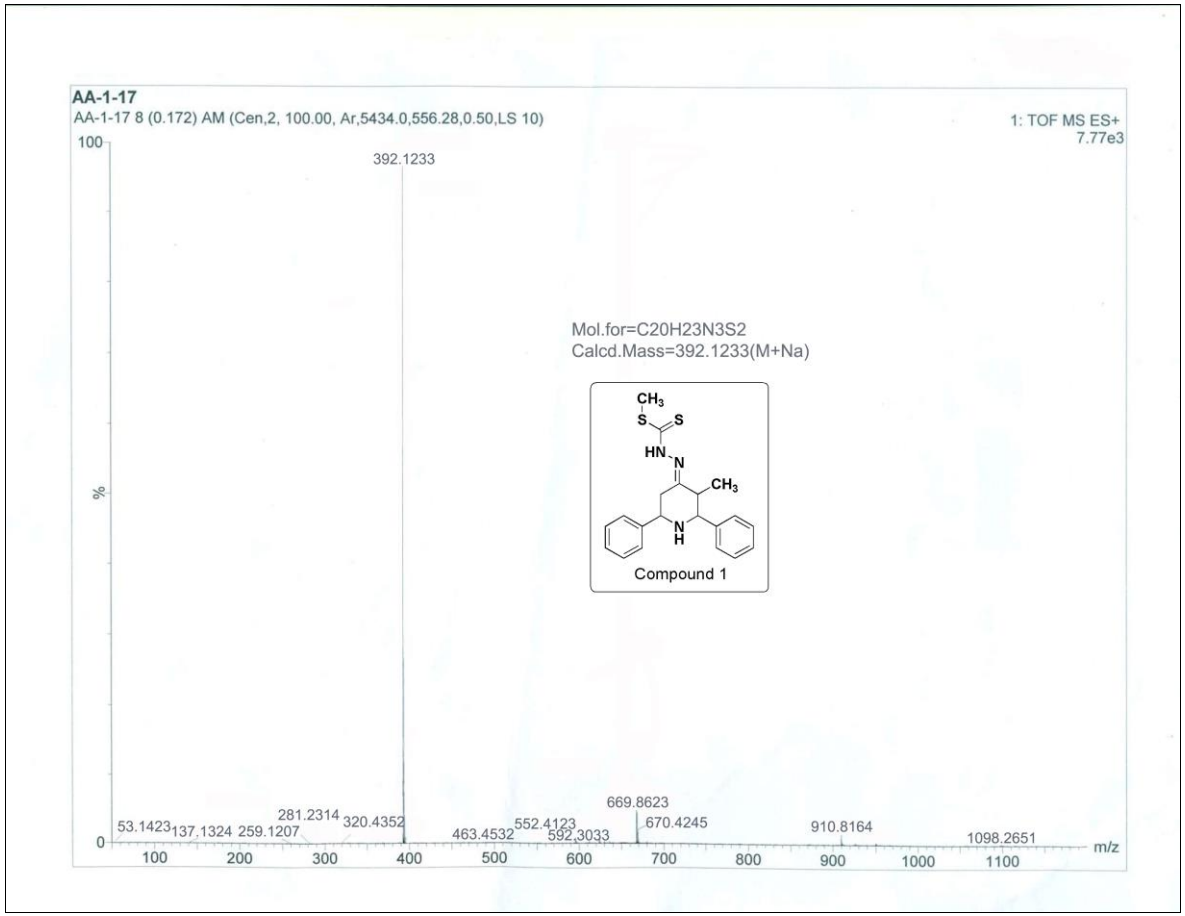

Fig. S2. Mass spectrum of compound **1**

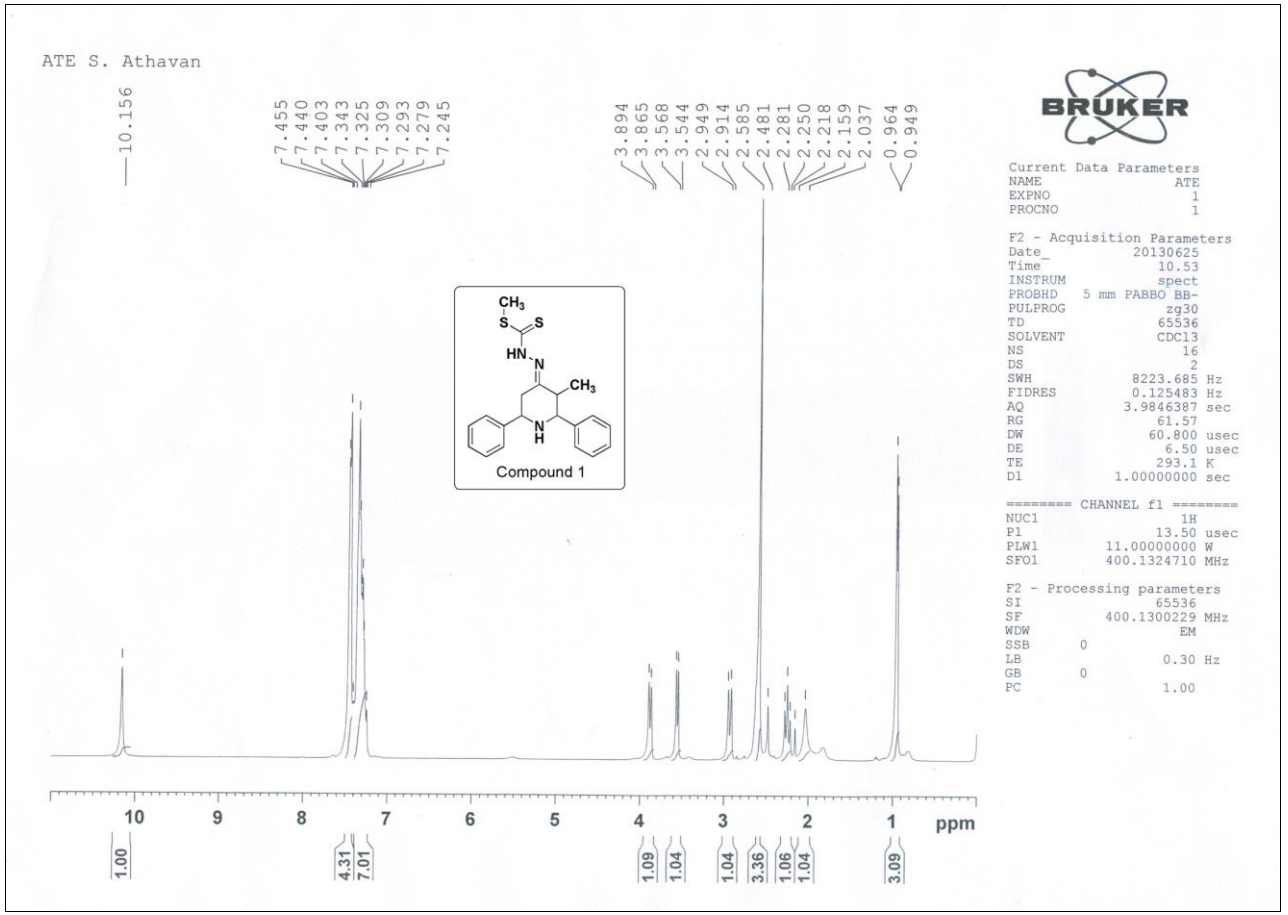

Fig. S3. ^{1}H NMR spectrum of compound **1**

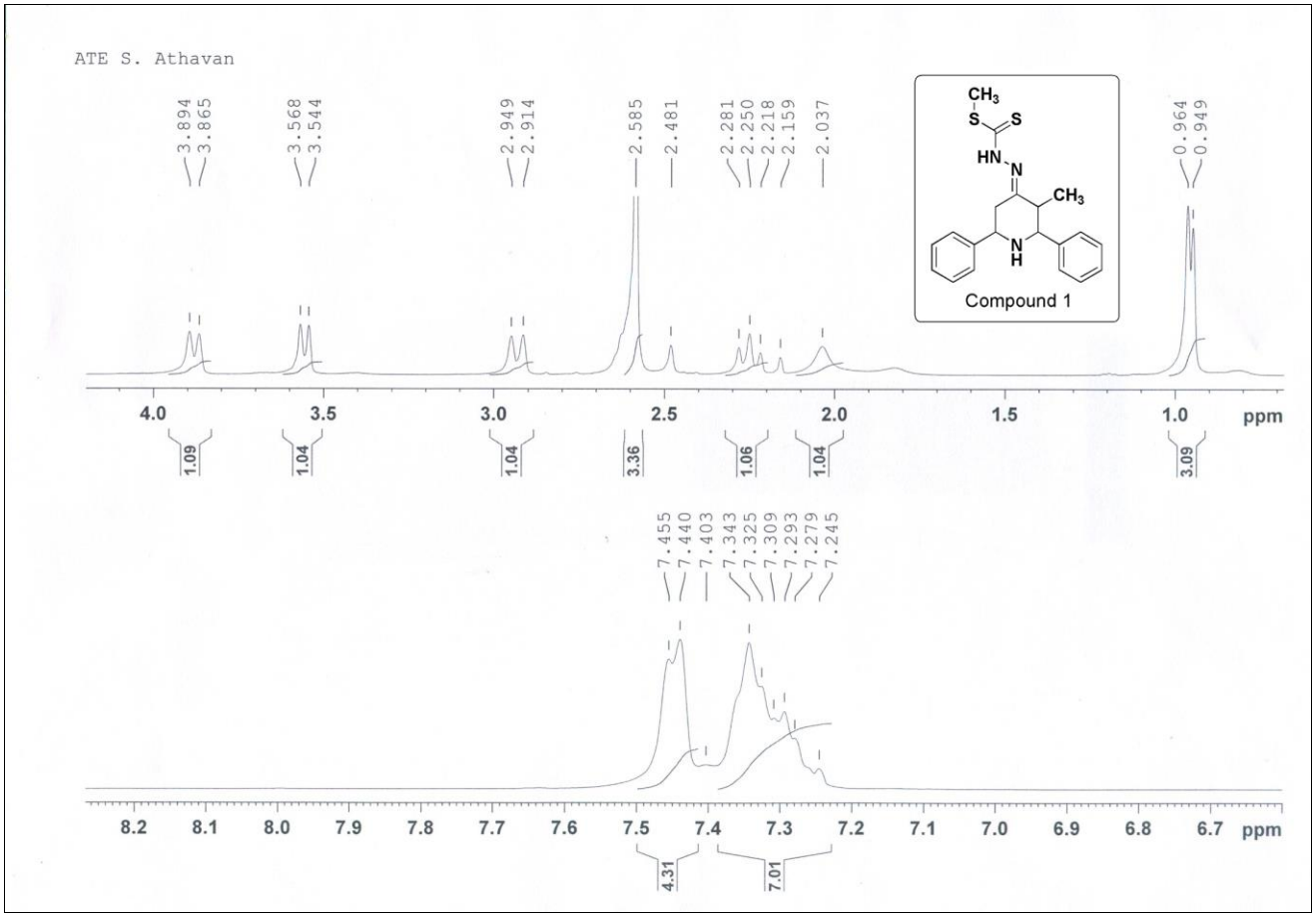

Fig. S4. Expansion of ^{1}H NMR spectrum of compound **1**

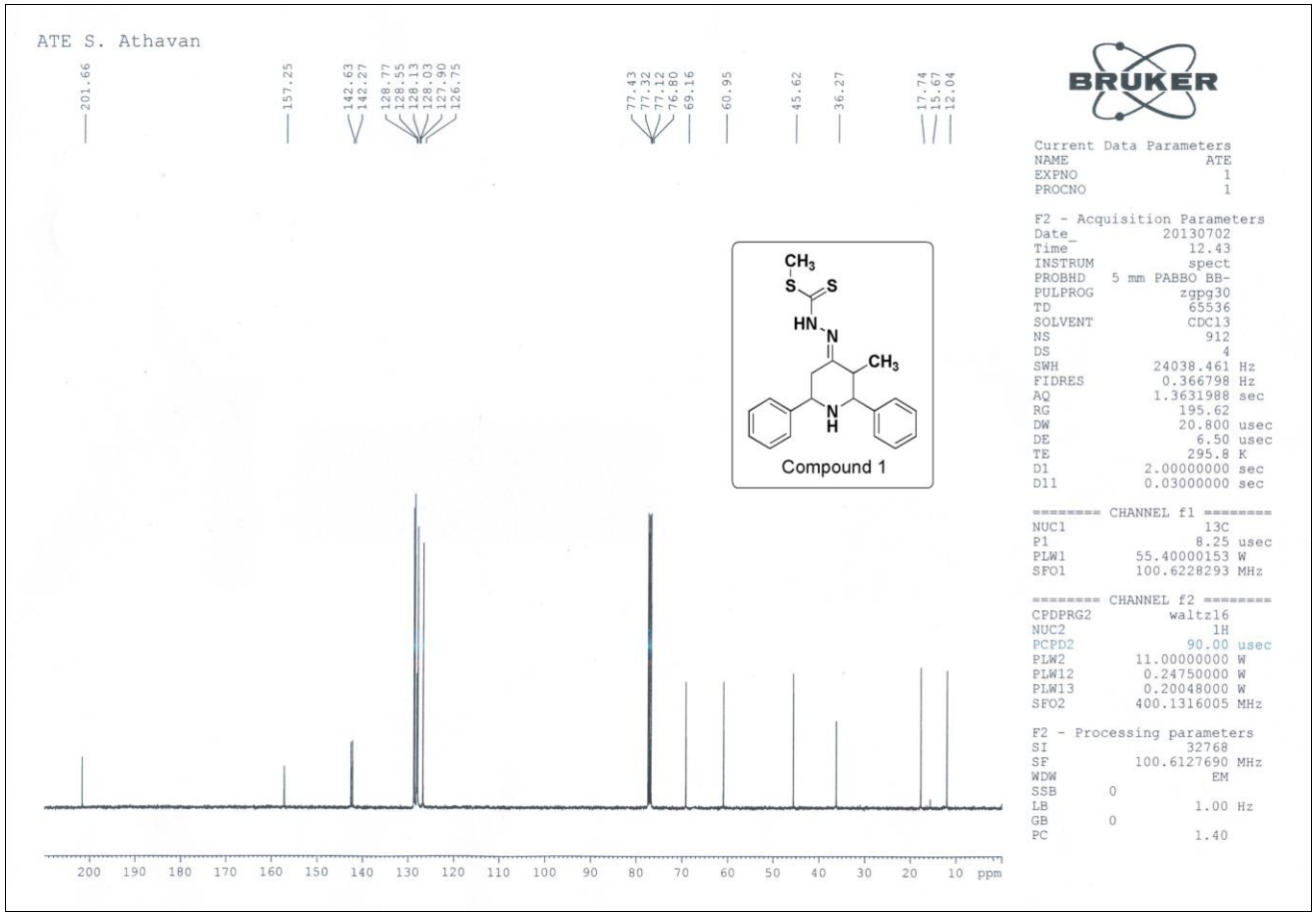

Fig. S5. ^{13}C NMR spectrum of compound **1**

Table S1: The *in silico* ADME (Absorption, Distribution, Metabolism and Excretion) prediction results for compound **1** using SwissADME web tool

Canonical SMILES: CSC(=S)N/N=C/1\CC(NC(C1C)c1ccccc1)c1ccccc1		
(i) Physiochemical Properties		
1	Formula	$C_{20}H_{23}N_3S_2$
2	Molecular Weight	369.55
3	Number of heavy atoms	25
4	Number of aromatic heavy atoms	12
5	Fraction Csp3	0.3
6	Number of rotatable bonds	5
7	Number of H-bond acceptors	2
8	Number of H-bond donors	2
9	Molar refractivity	116.02
10	Topological polar surface area (TPSA)	93.81
(ii) Lipophilicity		
1	Log $P_{o/w}$ (iLOGP)	3.56
2	Log $P_{o/w}$ (XLOGP3)	4.21
3	Log $P_{o/w}$ (WLOGP)	3.66
4	Log $P_{o/w}$ (MLOGP)	3.24
5	Log $P_{o/w}$ (SILICOS.IT)	4.94
6	Consensus Log $P_{o/w}$	3.92
(iii)Water Solubility		
1	ESOL Log S	-4.81
2	ESOL Solubility (mg/ml)	5.74E-03
3	ESOL Solubility (mol/l)	1.55E-05
4	ESOL Class	Moderately soluble
5	Ali Log S	-5.89
6	Ali Solubility (mg/ml)	4.76E-04
7	Ali Solubility (mol/l)	1.29E-06
8	Ali Class	Moderately soluble
9	Silicos-IT LogSw	-6.73

10	Silicos-IT Solubility (mg/ml)	6.87E-05
11	Silicos-IT Solubility (mol/l)	1.86E-07
12	Silicos-IT class	Poorly soluble
(iv)Pharmacokinetics		
1	GI absorption	High
2	BBB permeant	No
3	P-gp substrate	Yes
4	CYP1A2 inhibitor	Yes
5	CYP2C19 inhibitor	Yes
6	CYP2C9 inhibitor	Yes
7	CYP2D6 inhibitor	No
8	CYP3A4 inhibitor	Yes
9	Log K_p (skin permeation, cm/s)	-5.57
(v) Druglikeness		
1	Lipinski number of violations	0
2	Ghose number of violations	0
3	Veber number of violations	0
4	Egan number of violations	0
5	Muegge number of violations	0
6	Bioavailability Score	0.55
(vi)Medicinal Chemistry		
1	PAINS number of alerts	0
2	Brenk number of alerts	2
3	Leadlikeness number of violations	2
4	Synthetic accessibility	3.99