Supporting Information

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An Efficient Method for the Synthesis of Benzofused Five-Membered Cyclic Sulfamates

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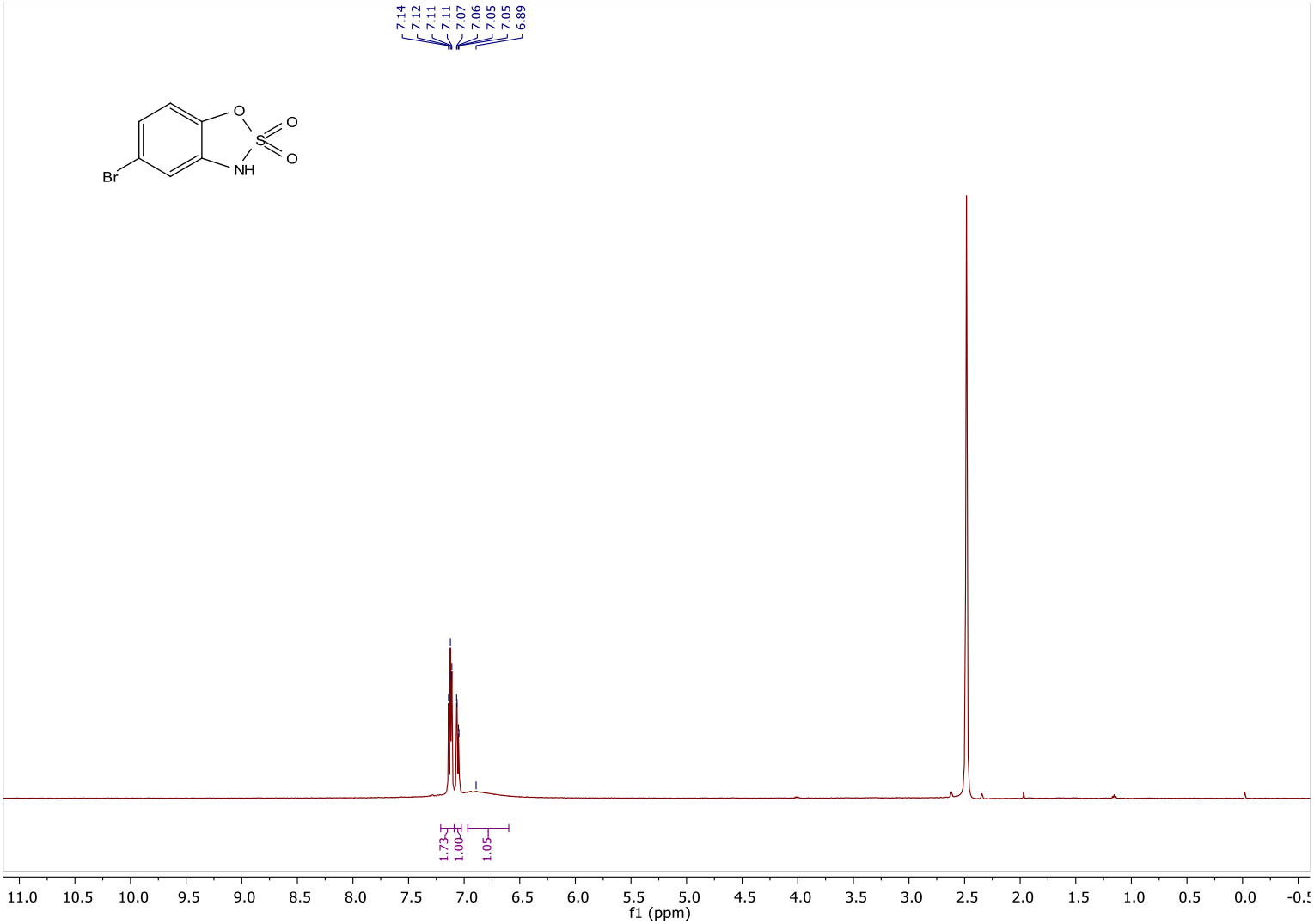
Virtual library

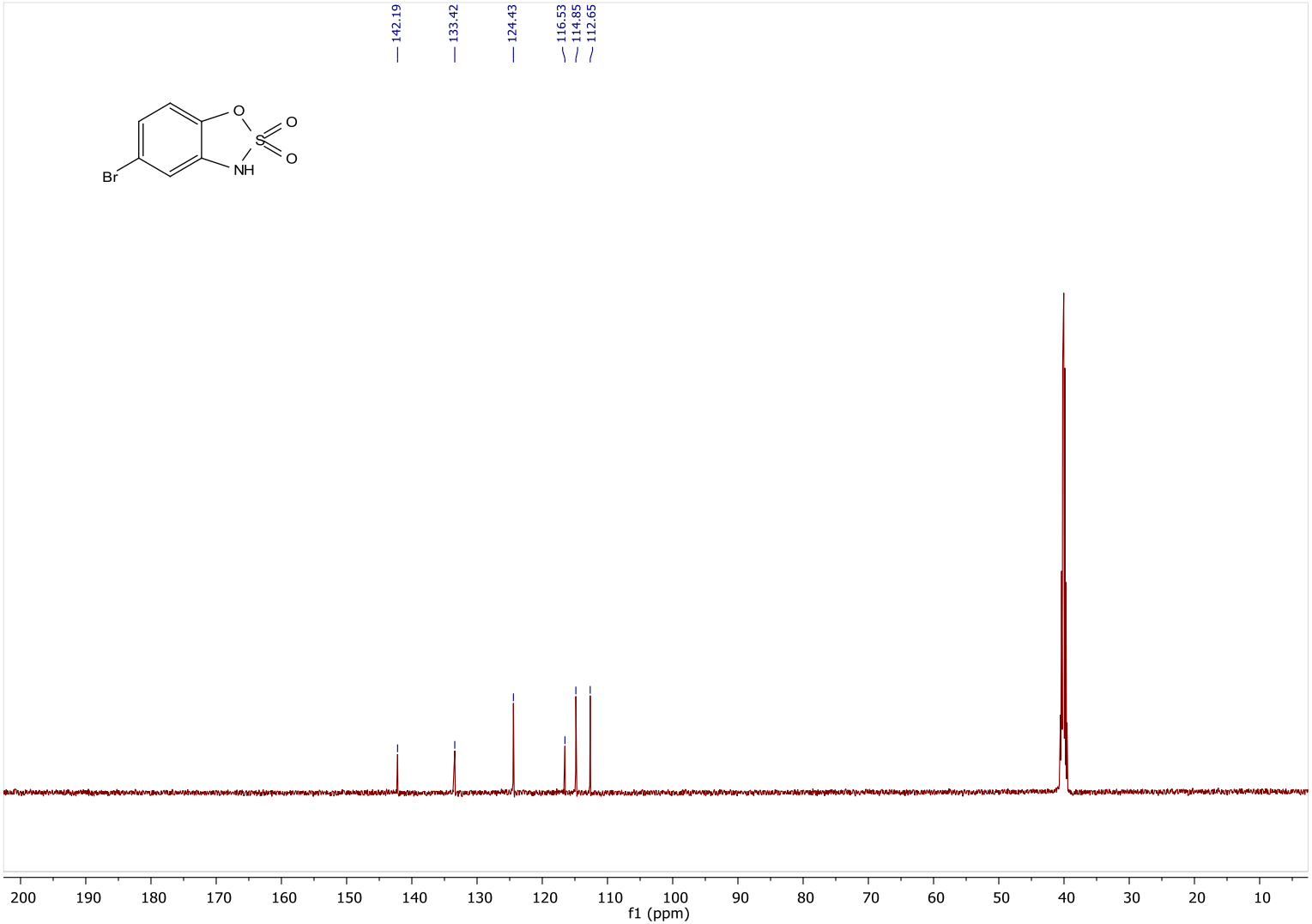
Table S1. Virtual library data table.

Entry No.	Smiles	MW	Log*P*	TPSA
1	O=C(Nc1ccc2NS(=O)(=O)Oc2c1)c1cccnc1	291.28	-0.13	97.39
2	COCC(=O)Nc1ccc2NS(=O)(=O)Oc2c1	258.25	-0.41	93.73
3	Cc1cc(no1)C(=O)Nc1ccc2NS(=O)(=O)Oc2c1	295.27	0.57	110.53
4	CC(C)C(=O)Nc1ccc2NS(=O)(=O)Oc2c1	256.28	1.01	84.50
5	O=C(Cc1c[nH]c2ccccc12)Nc1ccc2NS(=O)(=O)Oc2c1	343.36	1.70	100.29
6	Fc1ccccc1CC(=O)Nc1ccc2NS(=O)(=O)Oc2c1	322.31	1.74	84.50
7	COc1ccc(cc1)N1c2cc(ccc2OS1(=O)=O)C(O)=O	321.30	1.91	93.14
8	Cc1ccc(nc1)N1c2cc(ccc2OS1(=O)=O)C(O)=O	306.29	1.96	96.80
9	OC(=O)c1ccc2OS(=O)(=O)N(Cc3cnoc3)c2c1	296.25	0.50	109.94
10	CC(C)N1c2cc(ccc2OS1(=O)=O)C(O)=O	257.26	1.18	83.91
11	OC(=O)c1ccc2OS(=O)(=O)N(Cc3ccc(cc3)C#N)c2c1	330.31	1.99	107.70
12	Cc1ncsc1CN1c2cc(ccc2OS1(=O)=O)C(O)=O	326.34	0.87	96.80
13	OC(=O)c1ccc2OS(=O)(=O)N(c3cn[nH]c3)c2c1	281.24	0.37	112.59
14	OC(=O)c1ccc2OS(=O)(=O)N(c2c1)c1cncnc1	293.25	0.14	109.69
15	COc1ccc(Nc2ccc3NS(=O)(=O)Oc3c2)cc1	292.31	1.81	76.66
16	Cc1ccc(Nc2ccc3NS(=O)(=O)Oc3c2)nc1	277.30	0.00	80.32
17	O=S1(=O)Nc2ccc(NCc3cnoc3)cc2O1	267.26	-0.32	93.46
18	CC(C)Nc1ccc2NS(=O)(=O)Oc2c1	228.27	0.18	67.43
19	O=S1(=O)Nc2ccc(NCc3ccc(cc3)C#N)cc2O1	301.32	1.16	91.22
20	Cc1ncsc1CNc1ccc2NS(=O)(=O)Oc2c1	297.35	0.24	80.32
21	O=S1(=O)Nc2ccc(Nc3cn[nH]c3)cc2O1	252.25	-0.42	96.11
22	O=S1(=O)Nc2ccc(Nc3cncnc3)cc2O1	264.26	0.04	93.21
23	COCCS(=O)(=O)Nc1ccc2NS(=O)(=O)Oc2c1	308.32	-0.99	110.80

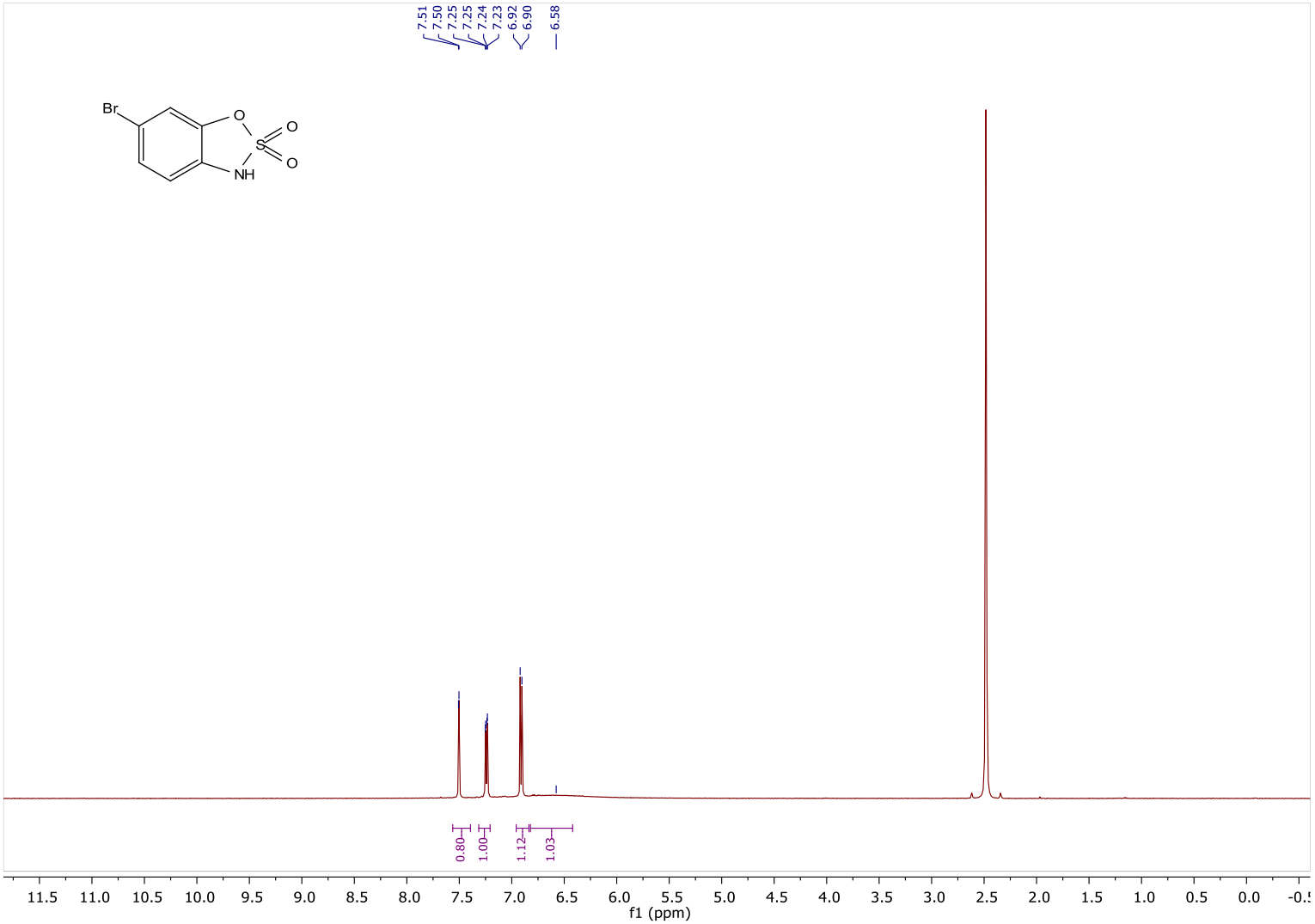
24	CC(C)S(=O)(=O)Nc1ccc2NS(=O)(=O)Oc2c1	292.32	-0.02	101.57
25	O=S(=O)(Nc1ccc2NS(=O)(=O)Oc2c1)c1cccnc1	327.33	-0.20	114.46
26	FC(F)(F)S(=O)(=O)Nc1ccc2NS(=O)(=O)Oc2c1	318.24	1.01	101.57
27	Cc1cc(no1)S(=O)(=O)Nc1ccc2NS(=O)(=O)Oc2c1	331.32	0.17	127.60
28	CN1CCC(CC1)Nc1ccc2NS(=O)(=O)Oc2c1	283.35	-1.31	70.67
29	Fc1ccc(CNc2ccc3NS(=O)(=O)Oc3c2)cc1	294.30	1.45	67.43
30	O=S1(=O)Nc2ccc(NC3COC3)cc2O1	242.25	-0.61	76.66
31	O=S1(=O)Nc2ccc(NCc3ccncc3)cc2O1	277.30	-0.25	80.32
32	O=S1(=O)Nc2ccc(NCc3c[nH]cn3)cc2O1	266.28	-1.85	96.11
33	FC(F)(F)CCNc1ccc2NS(=O)(=O)Oc2c1	282.24	0.49	67.43
34	O=S1(=O)Nc2ccc(NCCc3ccccc3)cc2O1	290.34	1.29	67.43
35	Fc1ccc(CNc2ccc3NS(=O)(=O)Oc3c2)cc1	294.30	1.45	67.43
36	Fc1cccc(CNC(=O)Nc2ccc3NS(=O)(=O)Oc3c2)c1	337.33	1.52	96.53
37	Cc1noc(C)c1NC(=O)Nc1ccc2NS(=O)(=O)Oc2c1	324.31	0.37	122.56
38	O=C(NC1CCCC1)Nc1ccc2NS(=O)(=O)Oc2c1	297.33	1.01	96.53
39	O=C(Nc1ccncc1)Nc1ccc2NS(=O)(=O)Oc2c1	306.30	-0.59	109.42
40	O=C(Nc1ccc2NS(=O)(=O)Oc2c1)Nc1cccc(c1)C#N	330.32	1.53	120.32
41	O=C(N1CCOCC1)c1ccc2OS(=O)(=O)Nc2c1	284.29	-0.39	84.94
42	O=C(Nc1ncccn1)c1ccc2OS(=O)(=O)Nc2c1	292.27	0.38	110.28
43	CN(C)C(=O)c1ccc2OS(=O)(=O)Nc2c1	242.25	-0.17	75.71
44	O=C(NCC1CC1)c1ccc2OS(=O)(=O)Nc2c1	268.29	0.38	84.50
45	O=C(Nc1cc[nH]n1)c1ccc2OS(=O)(=O)Nc2c1	280.26	0.34	113.18
46	O=C(Nc1cccc2[nH]ccc12)c1ccc2OS(=O)(=O)Nc2c1	329.33	1.72	100.29
47	O=S1(=O)Nc2ccc(Nc3cc[nH]n3)cc2O1	252.25	0.20	96.11
48	O=S1(=O)Nc2ccc(Nc3cncnc3)cc2O1	264.26	0.04	93.21
49	O=S1(=O)Nc2ccc(Nc3ccncc3)cc2O1	263.27	-1.10	80.32



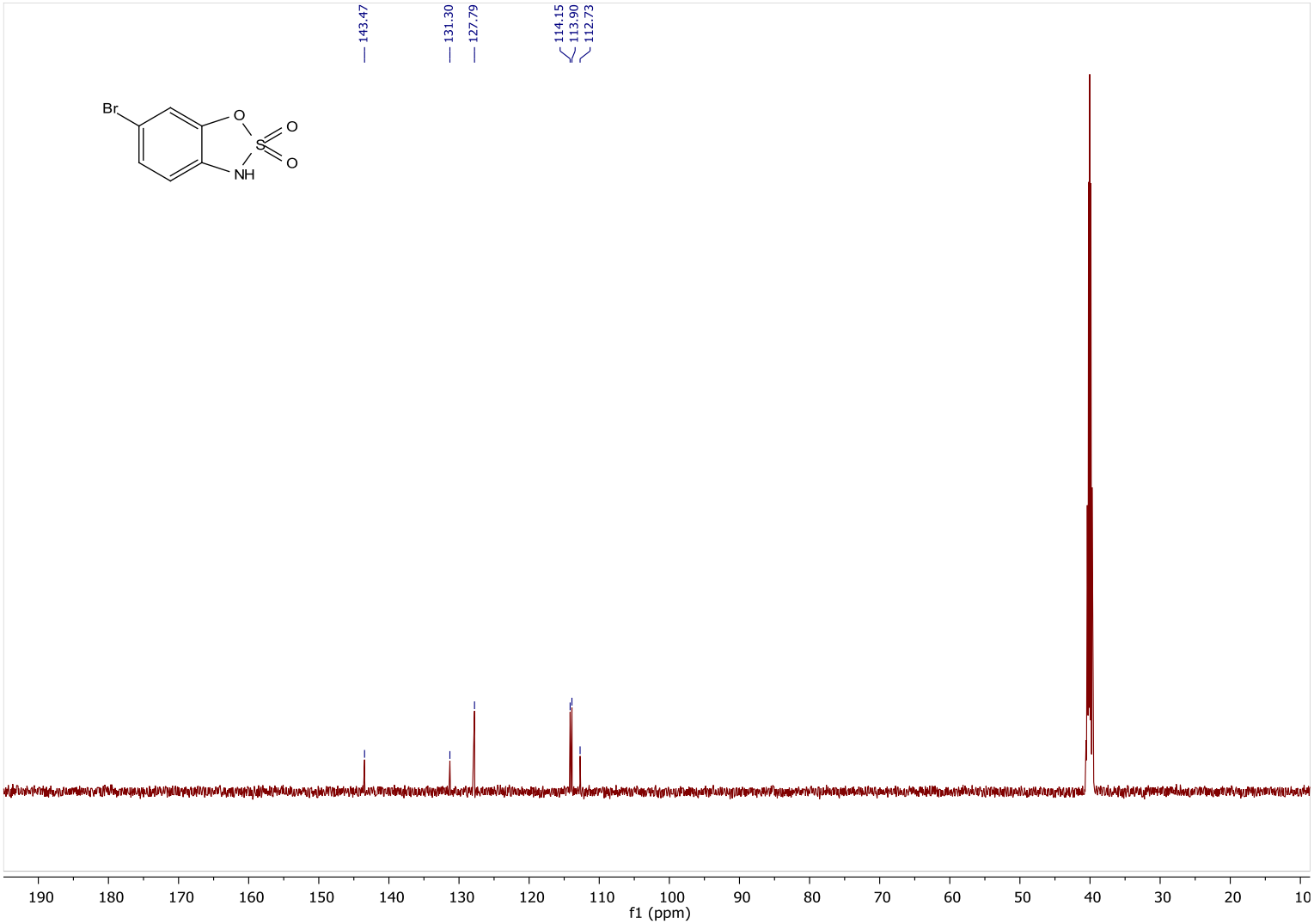
5-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3a) ^{1}H NMR (500 MHz, DMSO-d_6)



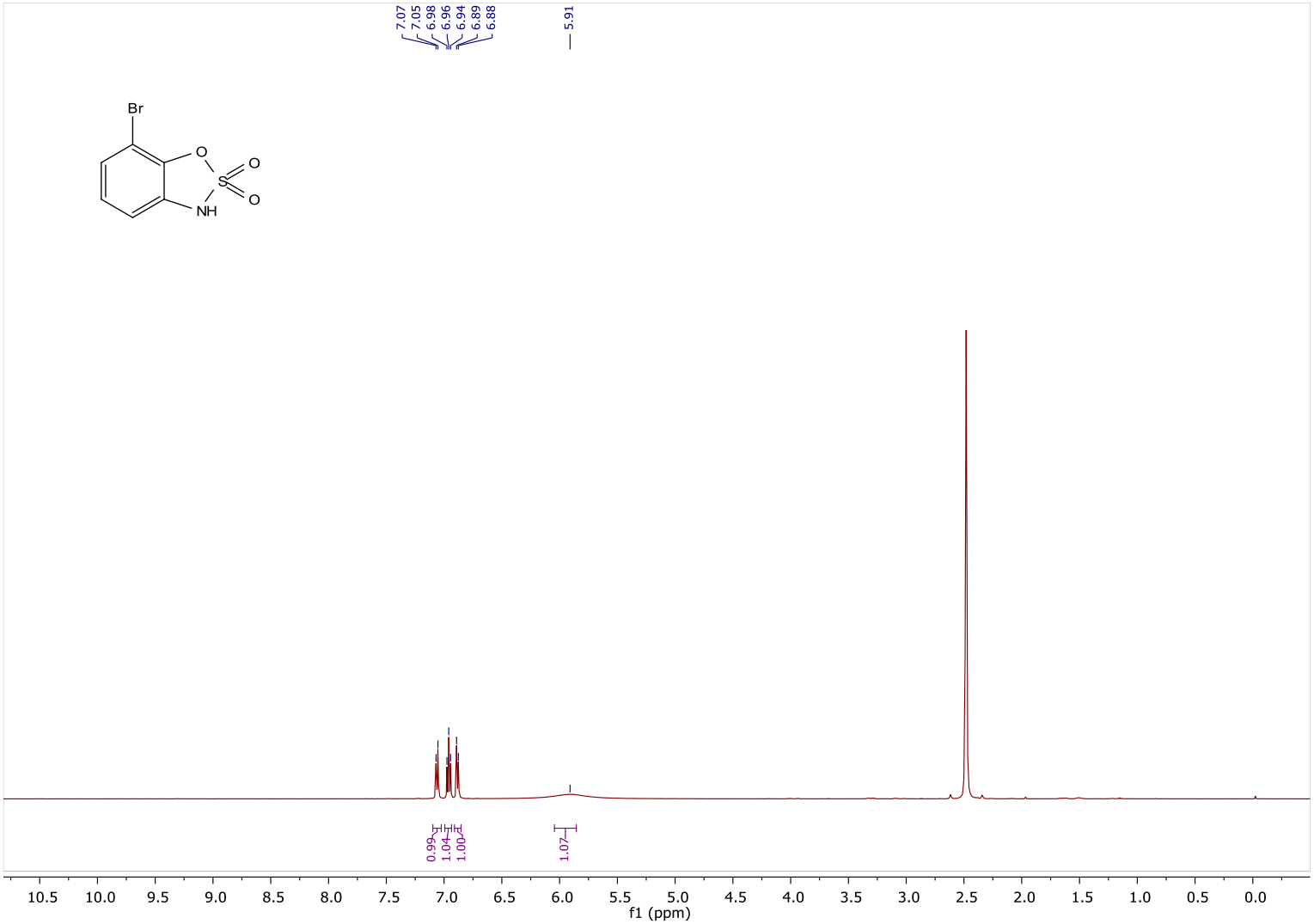
5-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3a) ^{13}C NMR (126 MHz, DMSO-d_6)



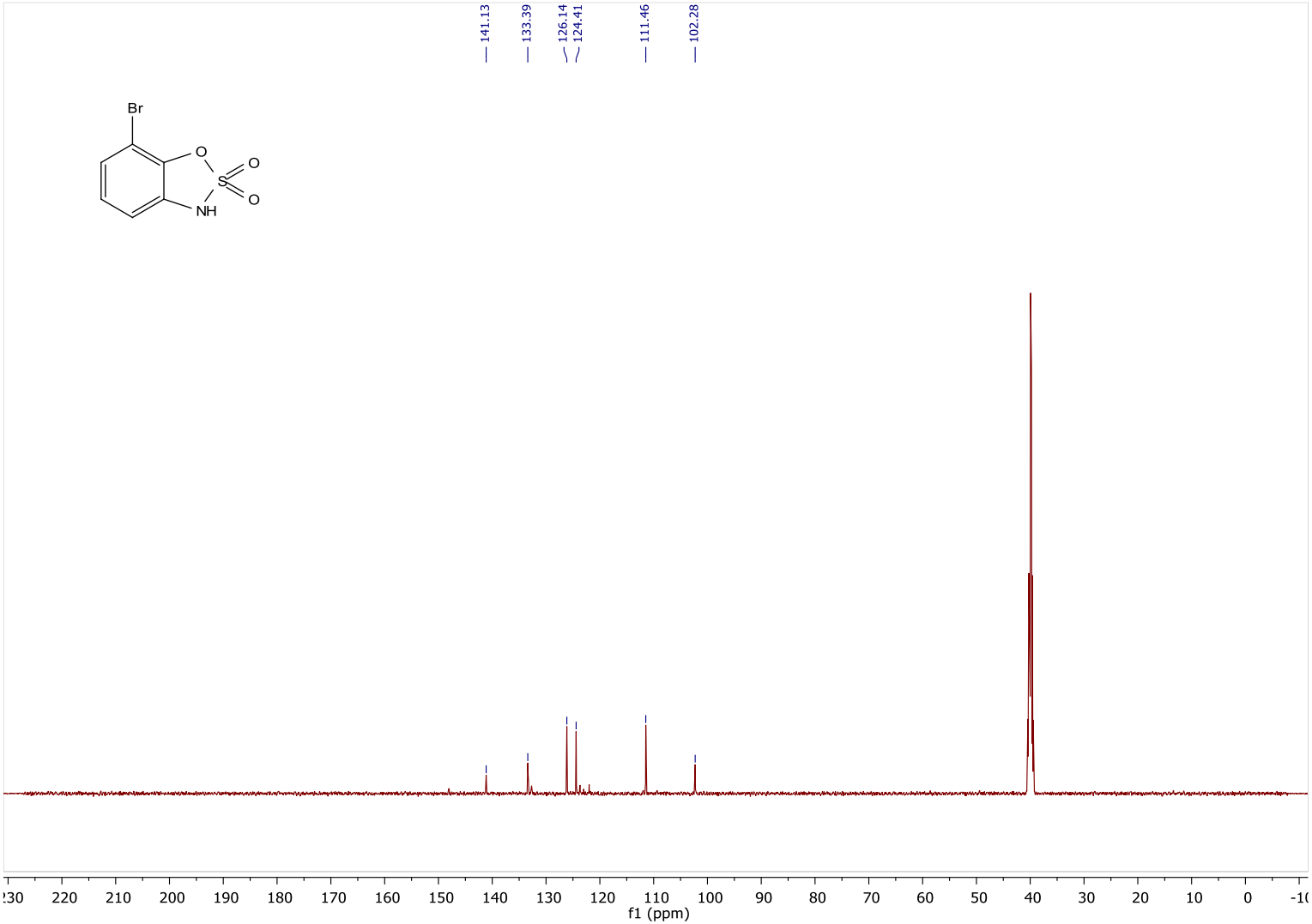
6-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3b) ^{1}H NMR (500 MHz, DMSO-d_6)



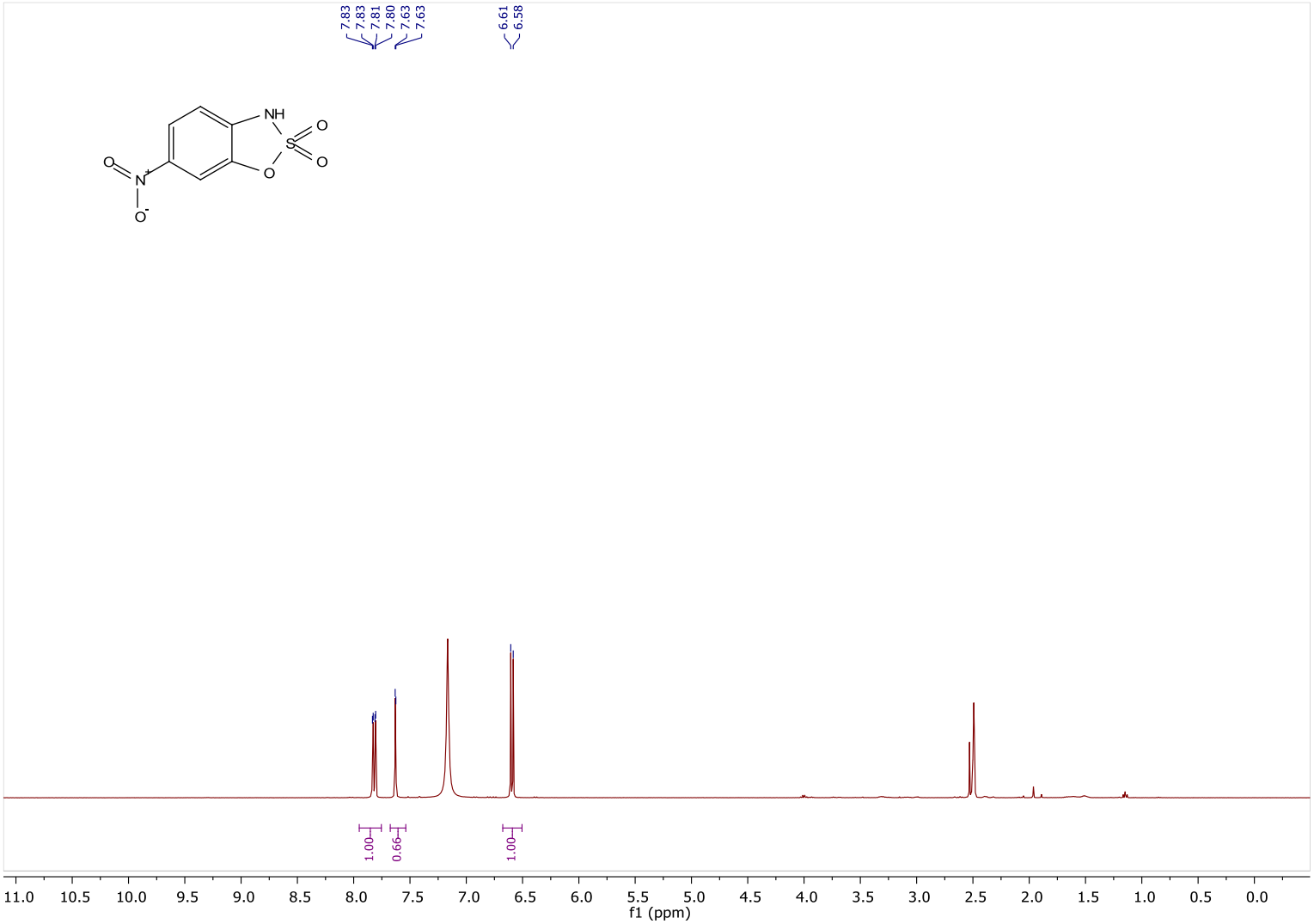
6-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3b) ^{13}C NMR (126 MHz, DMSO-d_6)



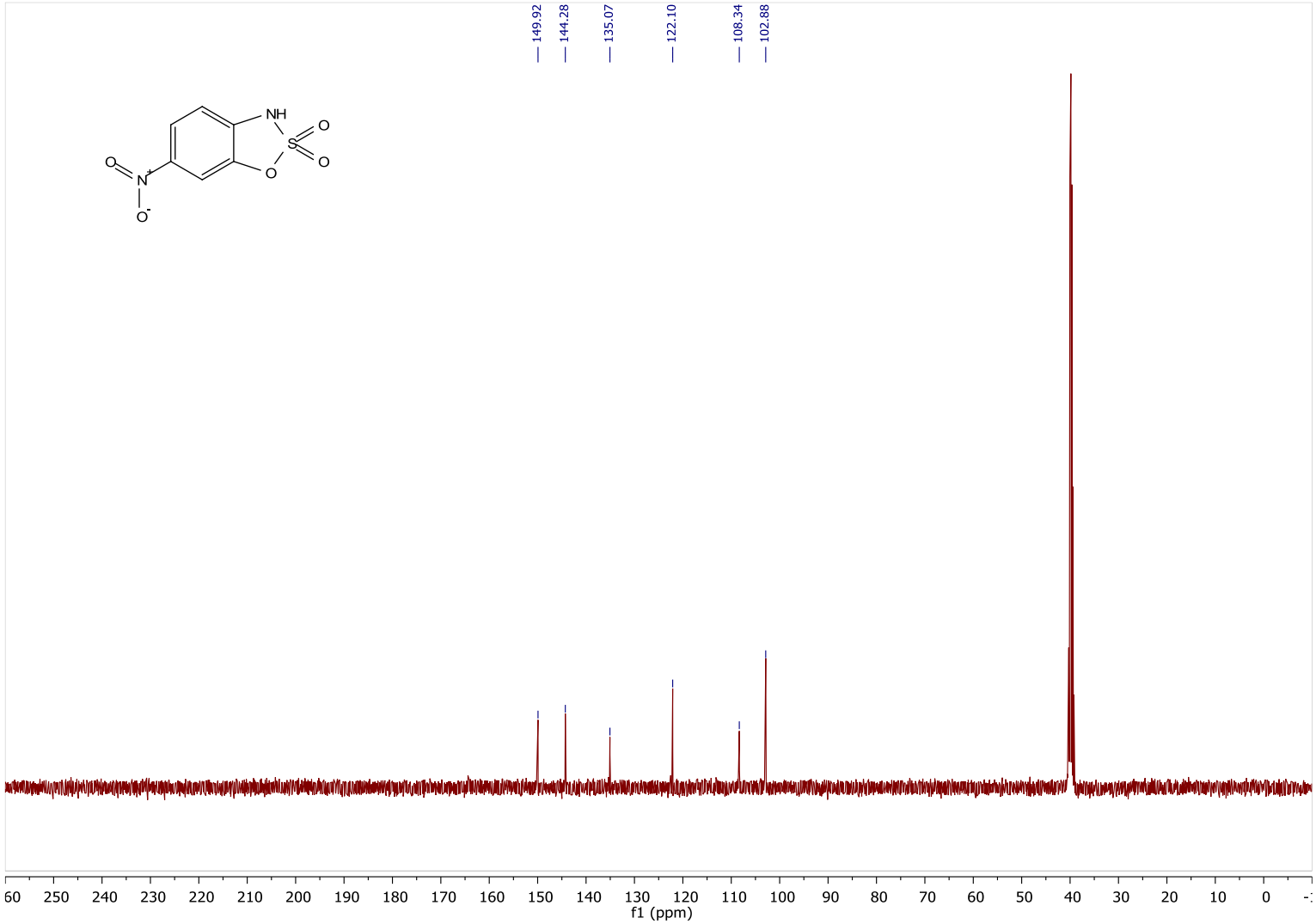
7-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3c) ^{1}H NMR (500 MHz, DMSO-d_6)



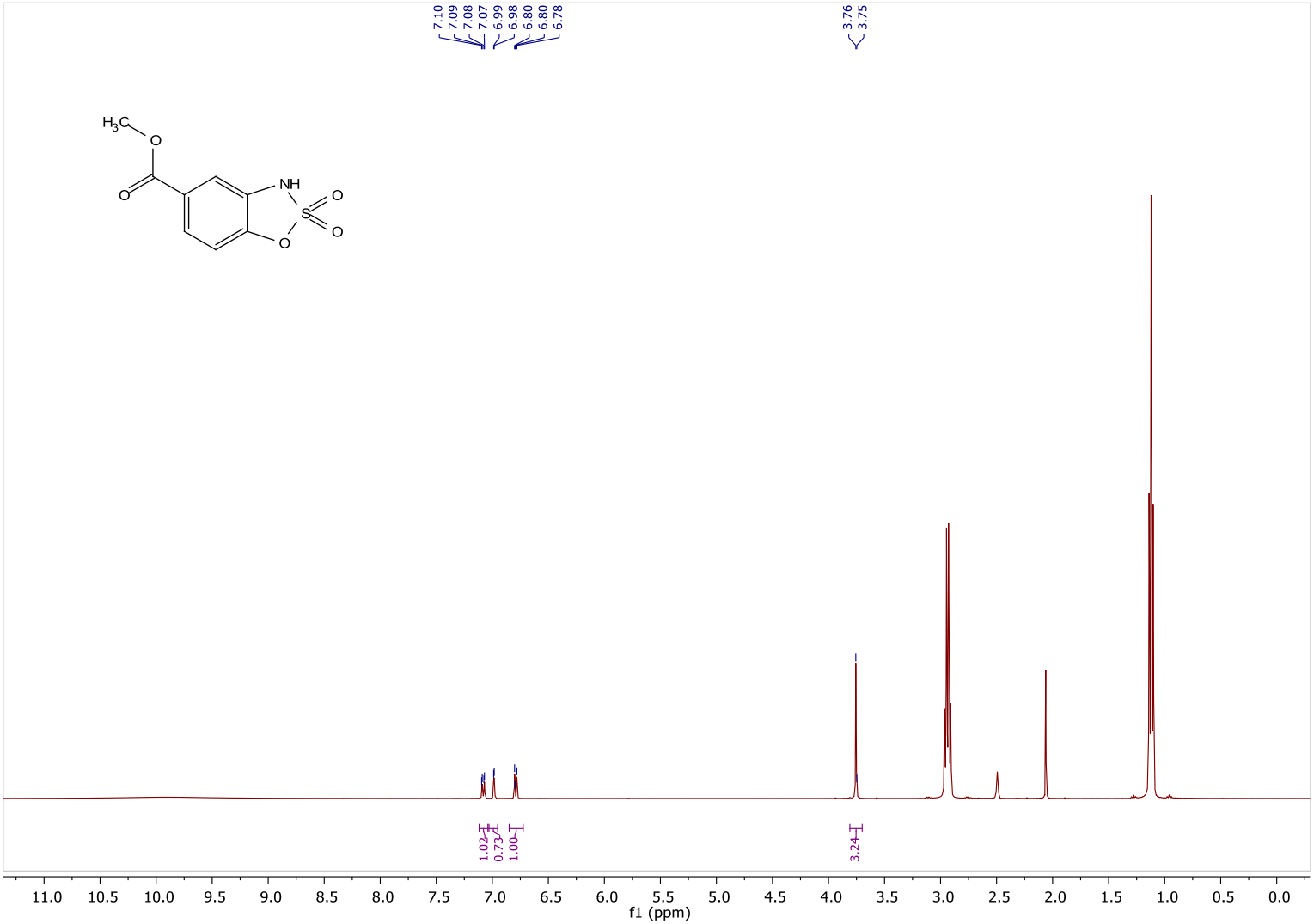
7-Bromo-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3c) ^{13}C NMR (126 MHz, DMSO-d_6)



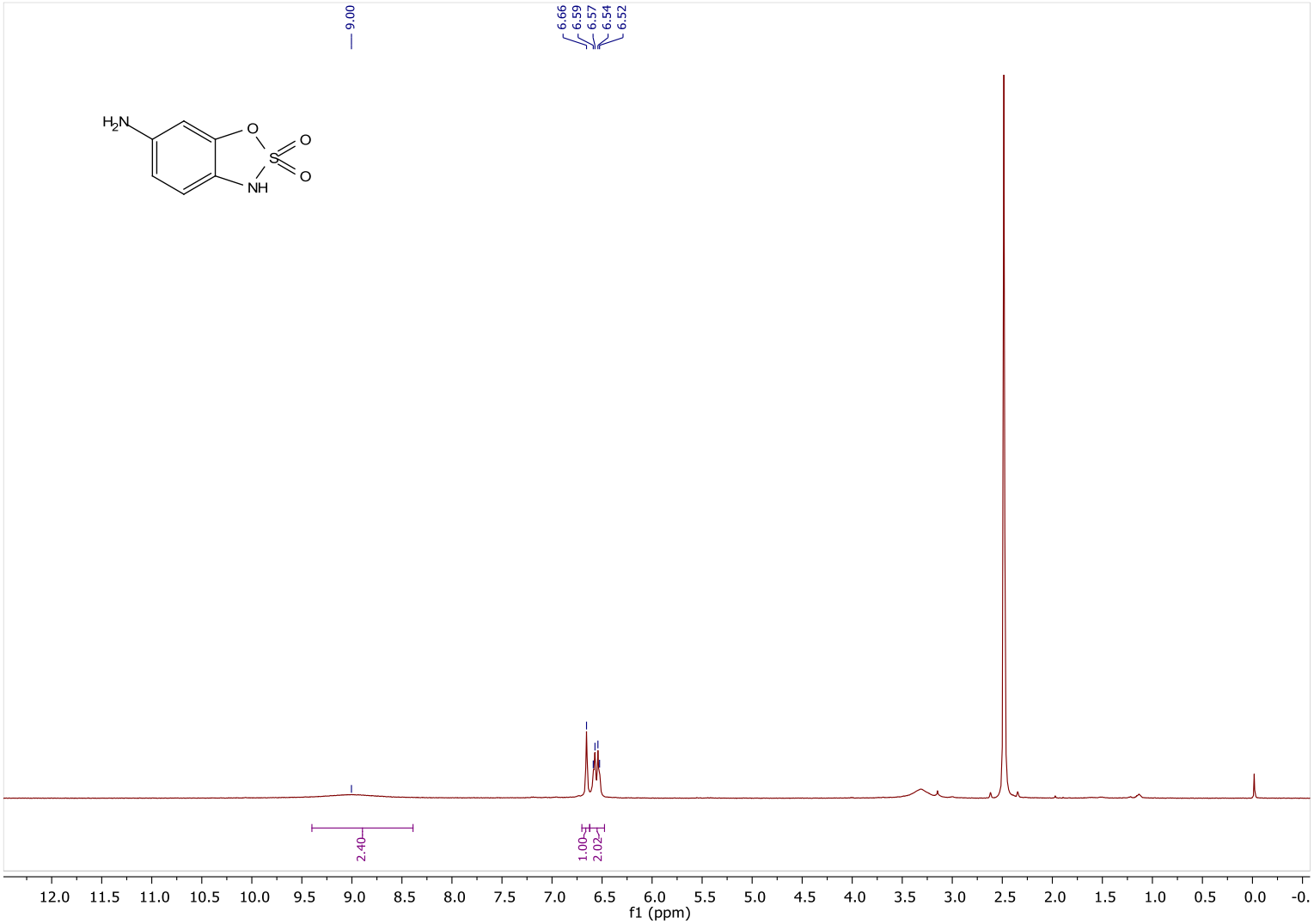
6-Nitro-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3d) ^{1}H NMR (400 MHz, DMSO-d_6)



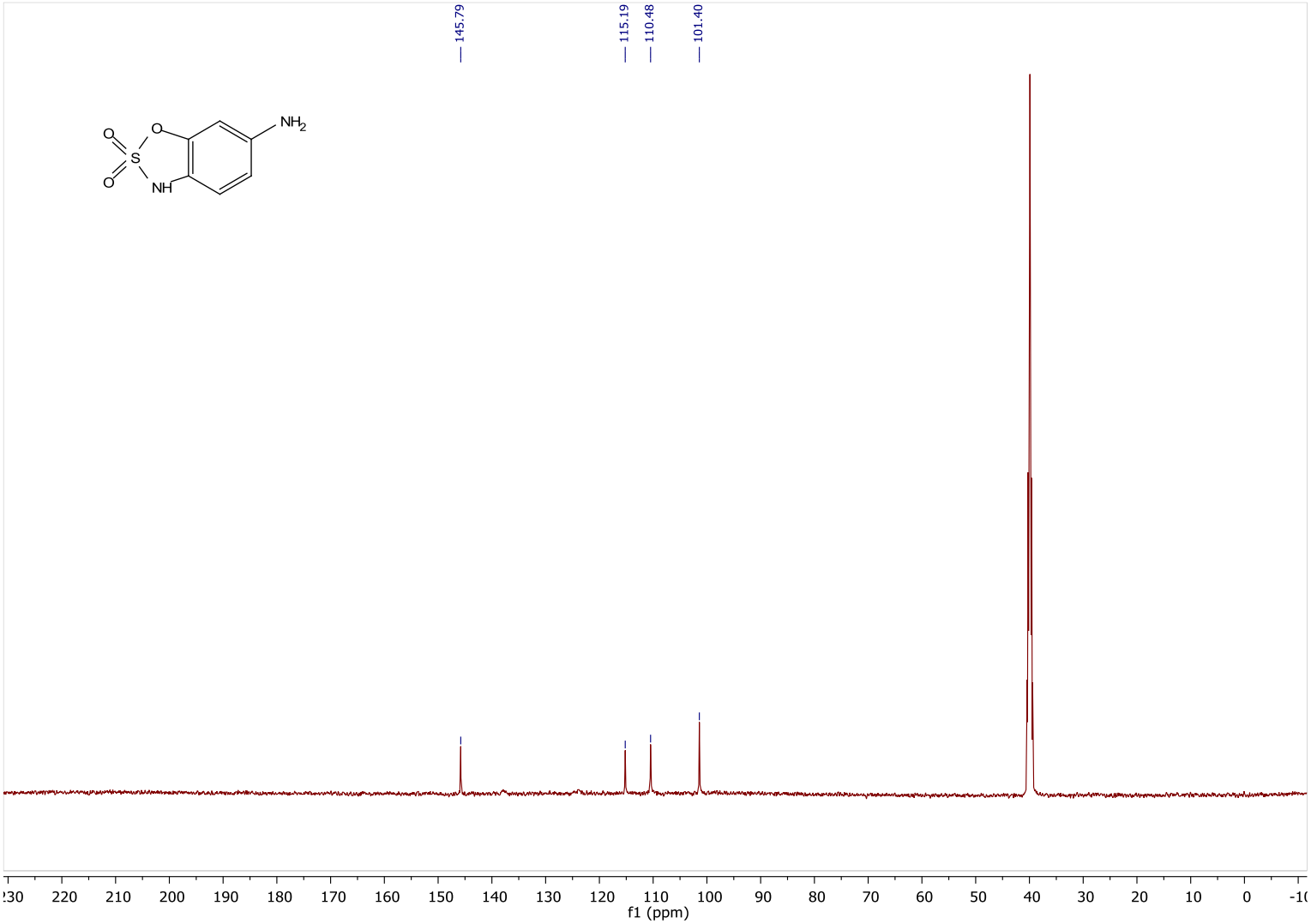
6-Nitro-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3d) ^{13}C NMR (101 MHz, DMSO-d_6)



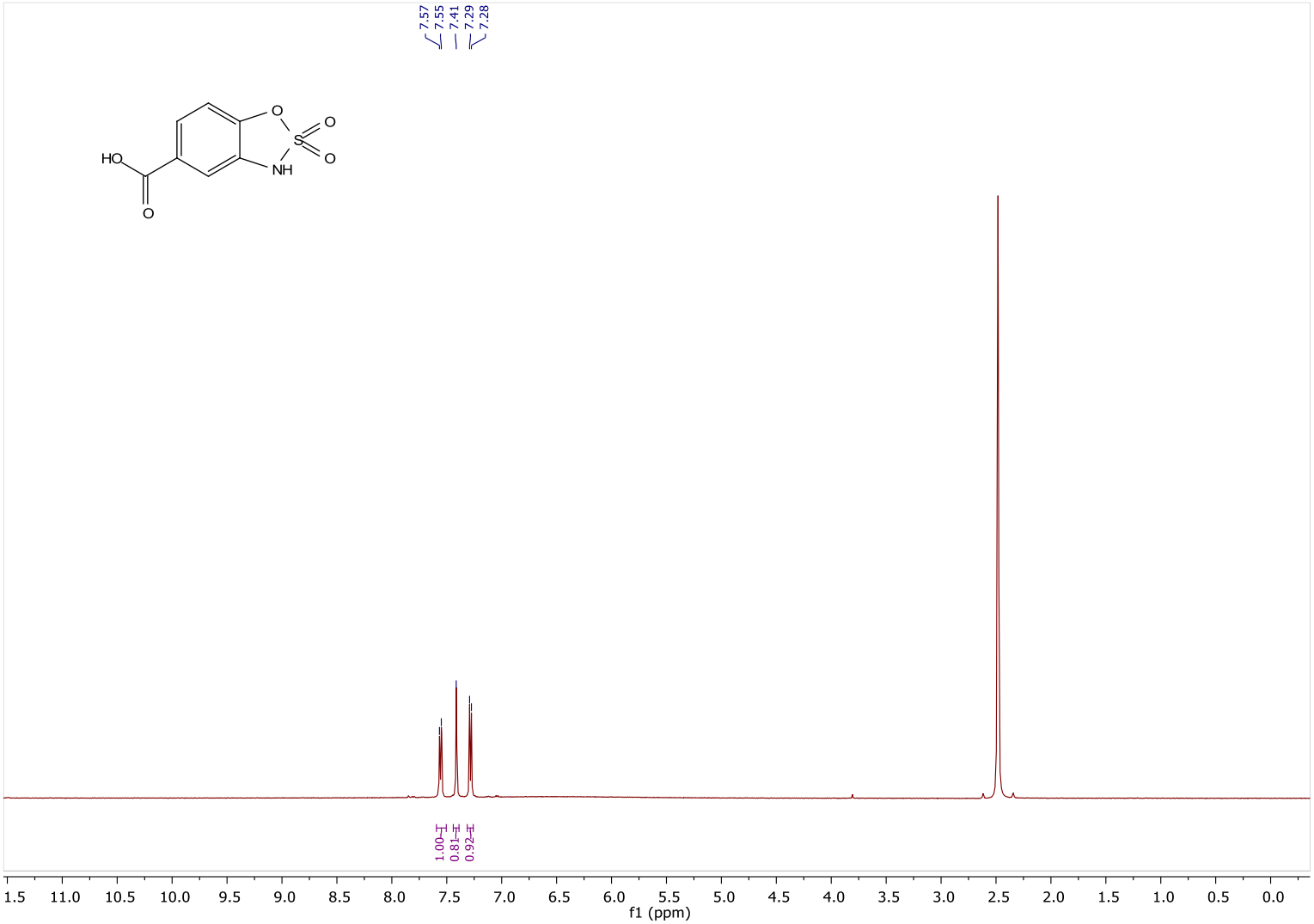
Methyl 3*H*-benzo[*d*][1,2,3]oxathiazole-5-carboxylate 2,2-dioxide (3e) ^{1}H NMR (400 MHz, DMSO-d_6)



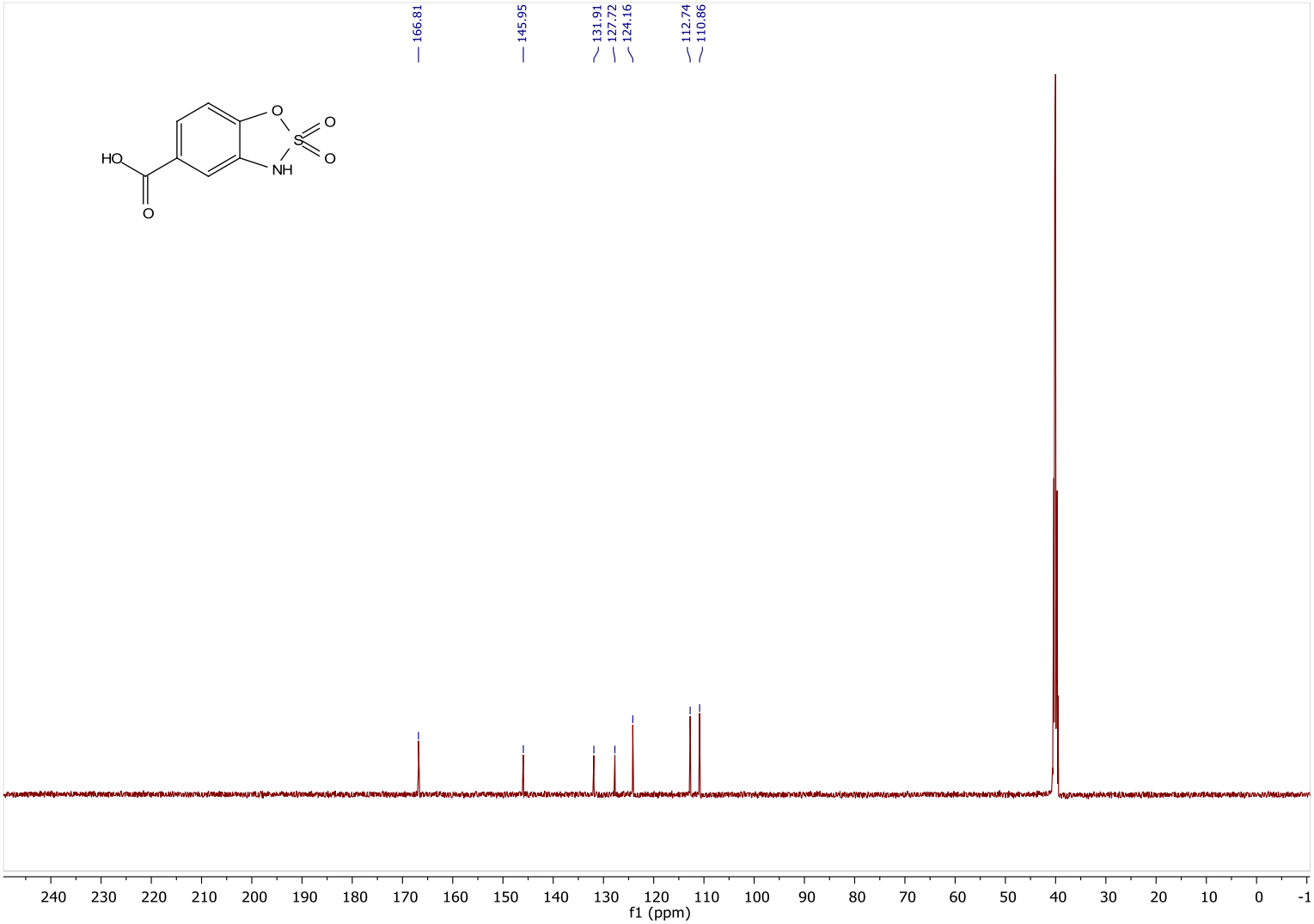
6-Amino-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3f) ^{1}H NMR (500 MHz, DMSO-d_6)



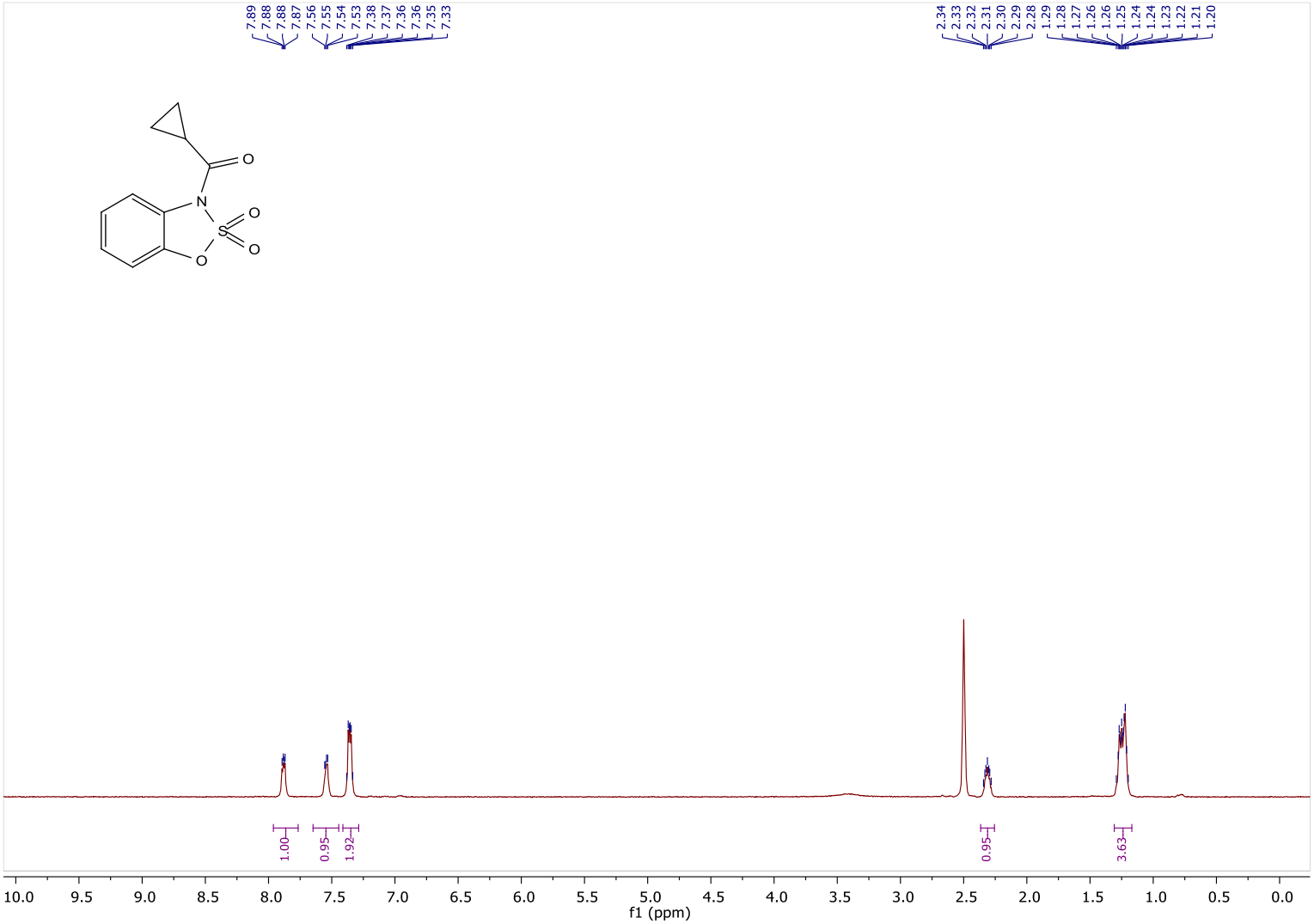
6-Amino-3*H*-benzo[*d*][1,2,3]oxathiazole 2,2-dioxide (3f) ^{13}C NMR (126 MHz, DMSO-d_6)



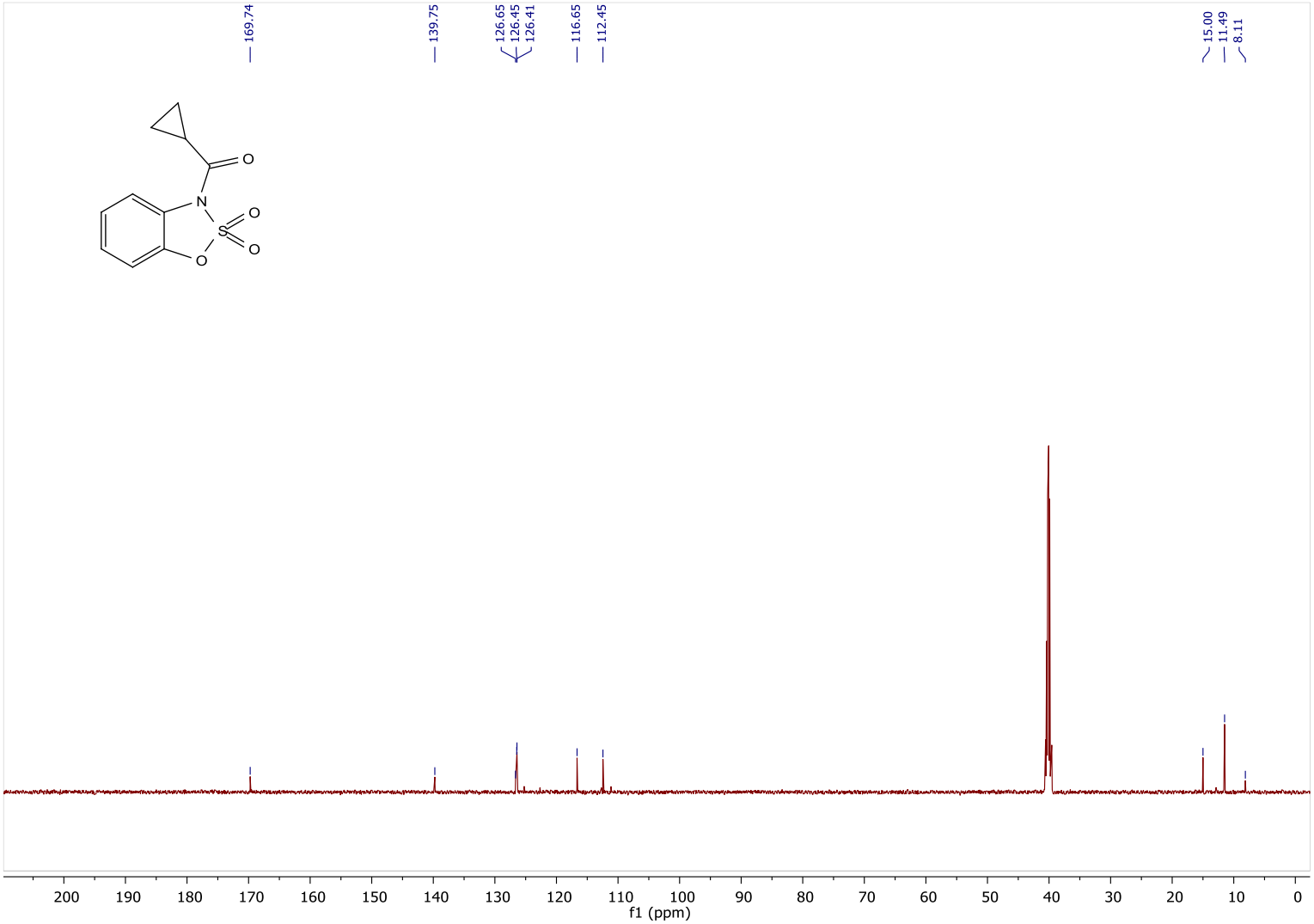
3*H*-Benzo[*d*][1,2,3]oxathiazole-5-carboxylic acid 2,2-dioxide (3g) ^{1}H NMR (500 MHz, DMSO-d_6)



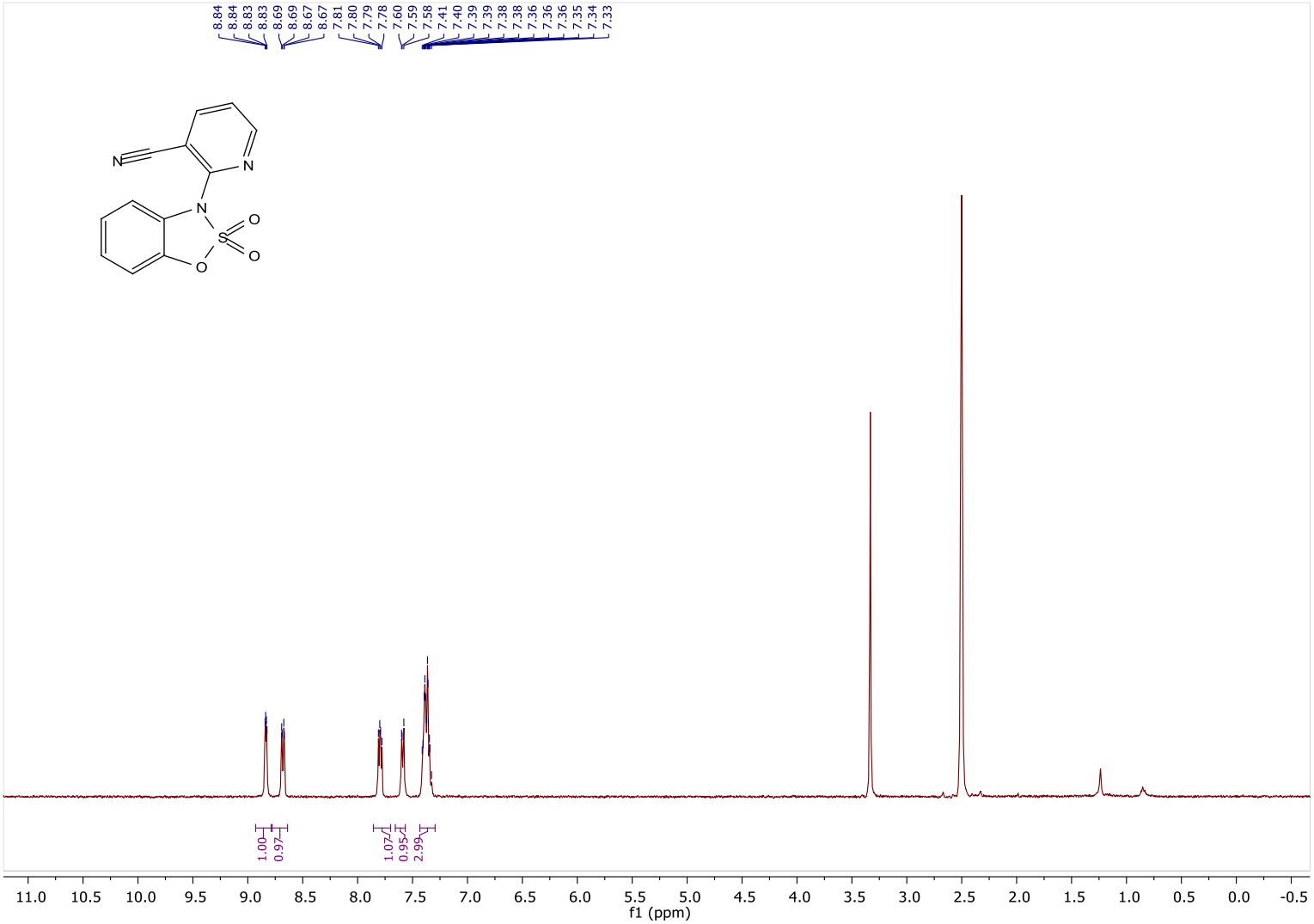
3*H*-Benzo[*d*][1,2,3]oxathiazole-5-carboxylic acid 2,2-dioxide (3g) ^{13}C NMR (126 MHz, DMSO-d_6)



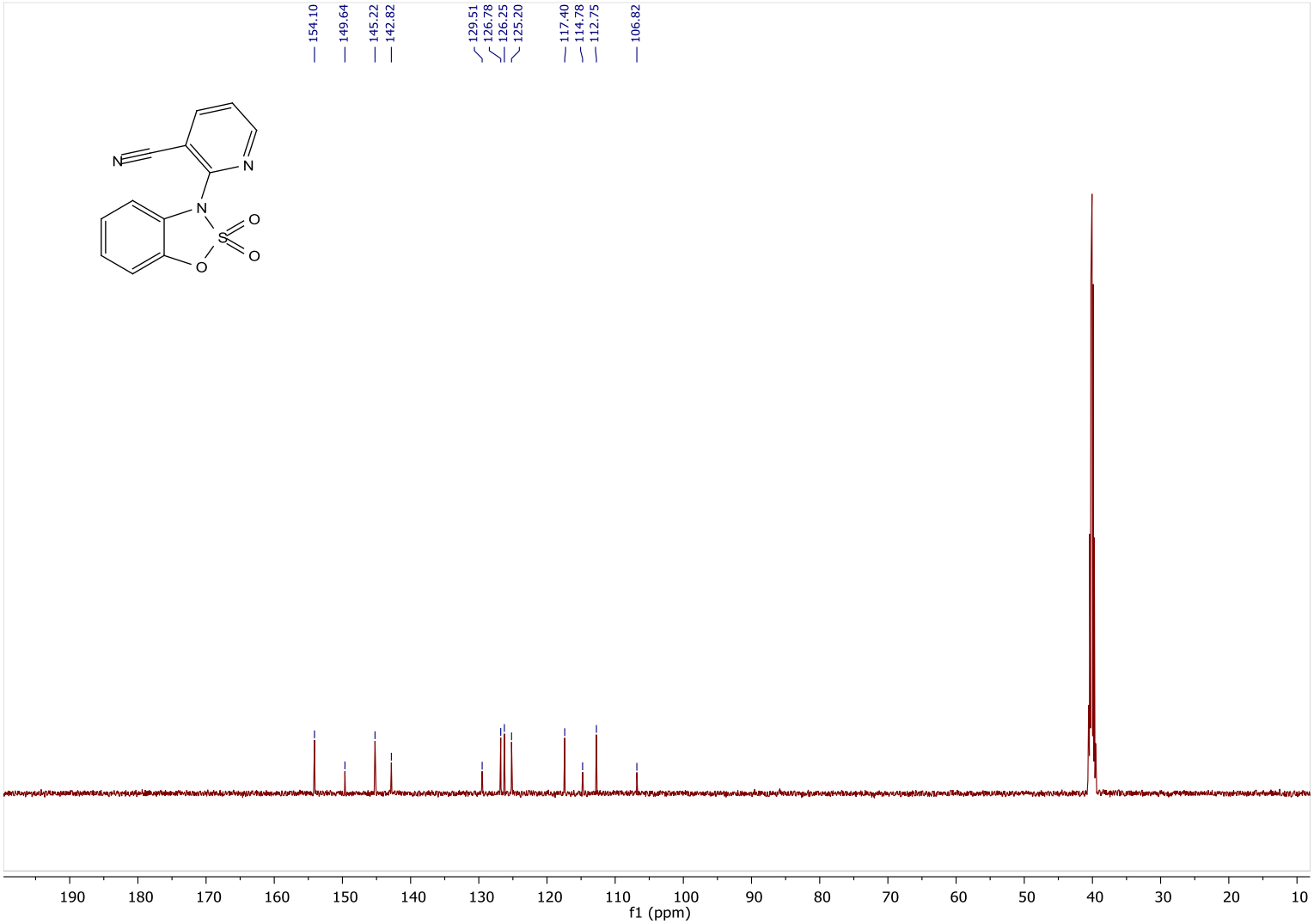
Cyclopropyl(2,2-dioxido-3*H*-benzo[*d*][1,2,3]oxathiazol-3-yl)methanone (5a) ^{1}H NMR (400 MHz, DMSO-d_6)



Cyclopropyl(2,2-dioxido-3*H*-benzo[*d*][1,2,3]oxathiazol-3-yl)methanone (5a) ^{13}C NMR (126 MHz, DMSO-d_6)



2-(2,2-Dioxido-3*H*-benzo[*d*][1,2,3]oxathiazol-3-yl)nicotinonitrile (5b) ^{1}H NMR (400 MHz, DMSO-d_6)



2-(2,2-Dioxido-3*H*-benzo[*d*][1,2,3]oxathiazol-3-yl)nicotinonitrile (5b) ^{13}C NMR (126 MHz, DMSO-d_6)