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1. Sequences

Coding sequences for NanoLuc

ATGAGAGGATCGCATCACCATCACCATCACGGATCCATGGTCTTCACACTCGAAGAT
TTCGTTGGGACTGGCGACAGACAGACGCCGGCTACAACCTGGACCAAGTCCTGAACAGGGAG
GTGTGTCAGTTGTTCAAGAACATCTCGGGGTCTCGTAACCTCCGATCCAAGGATTGTCCTGA
GCGGTGAAAATGGGCTGAAGATCGACATCCATGTCATCATCCGTATGAAGGTCTGAGCGG
CGACCAAATGGGCCAGATCGAAAAAAATTTAAGGTGGTGTACCCGTGGATGATCATCACT
TTAAGGTGATCCTGCACTATGGCACACTGGTAATCGACGGGTTACGCCAACATGATCGAC
TATTCGGACGGCGTATGAAGGCATGCCGTTCGACGGCAAAAGATCACTGTAACAG
GGACCCCTGTGGAACGGCAACAAAATTATCGACGAGCGCCTGATCAACCCGACGGCTCCCT
GCTGTTCCGAGTAACCATCAACGGAGTGACCGGCTGGCGGCTGTGCGAACGCATTCTGGCGT
AA

NanoLuc protein sequence

MRGSHHHHHGSMVFTLEDFVGDWRQTAGYNLDQVLEQGGVSSLFQNLGVSVTPIQRI
VLSGENGLKIDIHVIIPYEGLSGDQMGIKEKIFKVVYPVDDHHFKVILHYGTLVIDGVTPNMIDYF
GRPYEGIAVFDGKKITVTGTLWNGNKIIDERLINPDGSLLFRVTINGVTGWRLCERILA

2. Expression and purification of NanoLuc

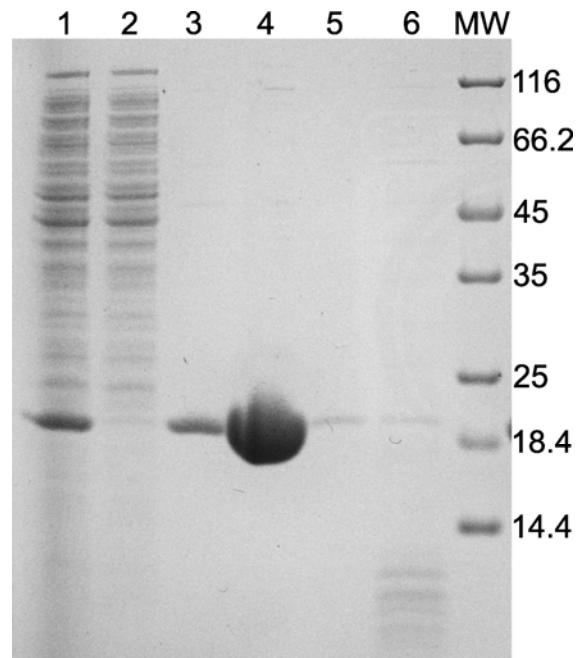
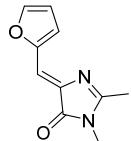
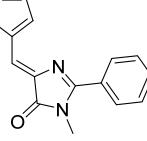
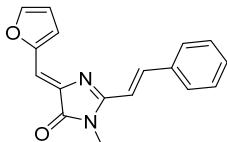
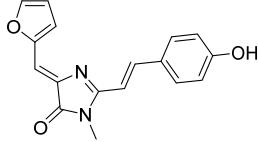
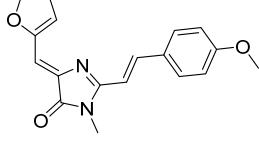
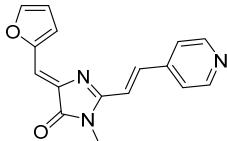
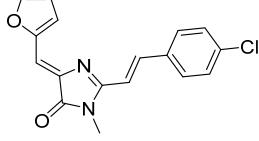
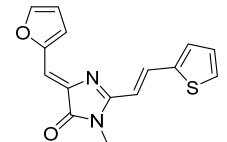
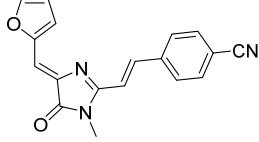
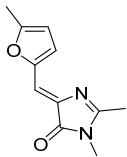
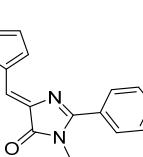
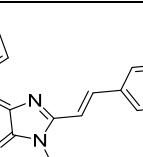
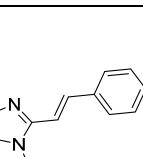
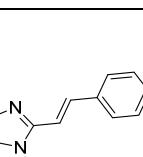
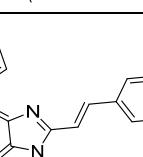
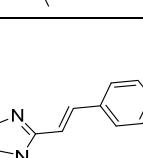
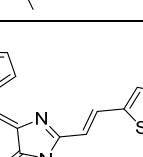
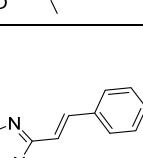


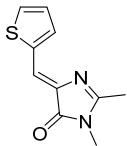
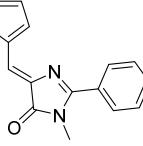
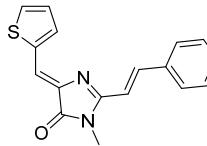
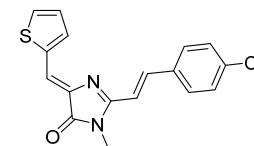
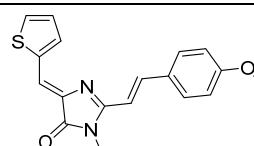
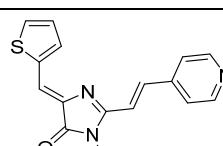
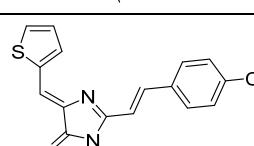
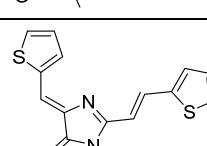
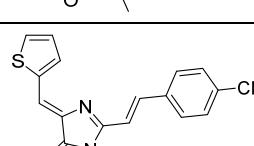
Figure S2.1. Purification of NanoLuc by immobilized metal affinity chromatography. (1) cell lysate, (2) flow-through, (3-5) elution fractions at 50 mM Imidazole, (6) elution at 500 mM Imidazole, MW - protein marker.

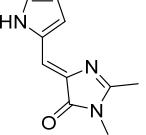
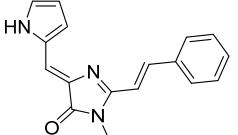
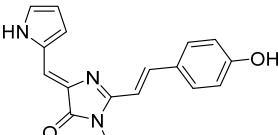
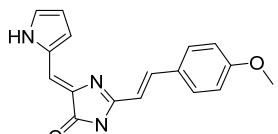
3. Screening *in vitro*

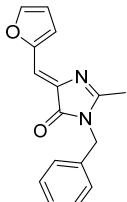
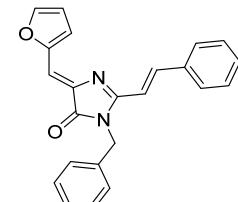
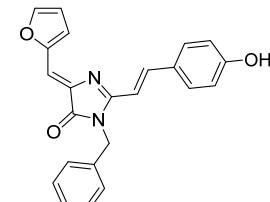
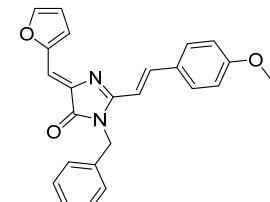
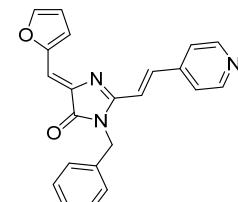
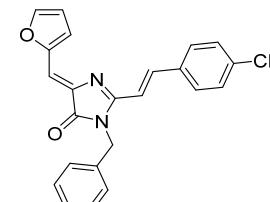
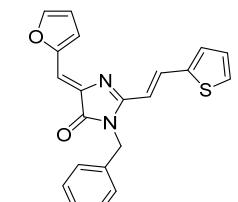
Table S3.1. Optical properties of chromophores and the results of interaction with Nanoluc

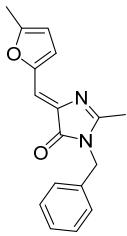
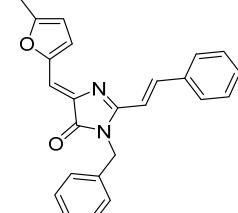
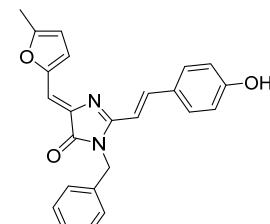
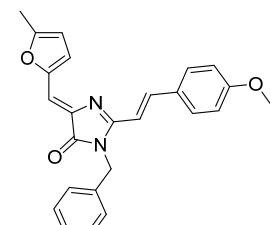
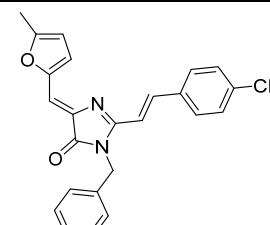
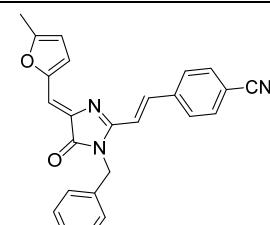
Cmpd	Structure	Abs ^a	Enhancement					
			380	430	480	530	580	630
1aa		372	1.6	1.2	1.1	1.1	1.3	1.0
1ab		394	1.3	1.2	1.1	1.1	1.2	1.1
1ac		429	1.5	1.6	1.6	1.1	1.1	0.9
1ad		432	1.5	1.7	1.9	1.4	1.1	0.9
1ae		433	1.4	1.5	1.5	1.1	1.0	1.7
1af		432	1.3	1.3	1.3	1.1	0.9	1.0
1ag		433	1.4	1.4	1.4	1.1	0.9	0.9
1ah		436	1.4	1.3	1.3	1.2	1.0	1.8
1ai		438	1.4	1.2	1.3	1.2	0.9	1.2

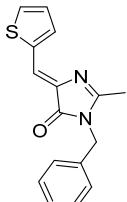
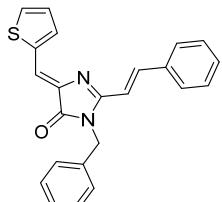
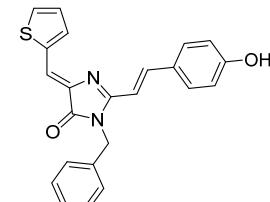
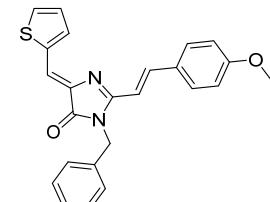
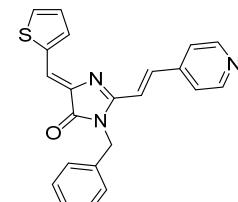
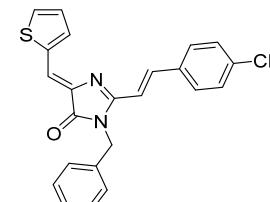
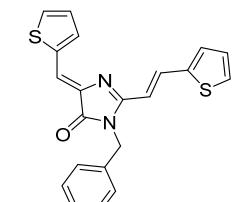
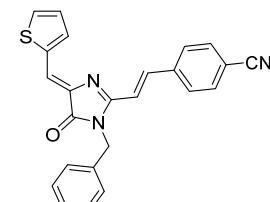
2aa		381	1.3	1.2	1.1	1.1	1.0	0.6
2ab		407	1.4	1.2	1.1	1.0	1.0	0.9
2ac		442	1.5	1.8	1.9	1.2	1.0	1.0
2ad		445	1.4	1.3	1.3	1.2	1.0	1.2
2ae		445	1.4	1.6	1.6	1.2	0.9	1.3
2af		446	1.4	1.3	1.3	1.1	1.1	1.3
2ag		445	1.5	1.6	1.6	1.1	0.9	1.1
2ah		452	1.4	1.3	1.5	1.3	1.1	0.9
2ai		451	1.4	1.4	1.4	1.2	1.1	1.1

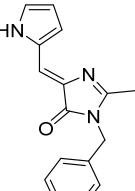
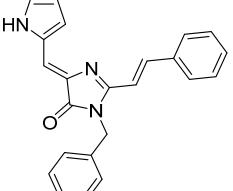
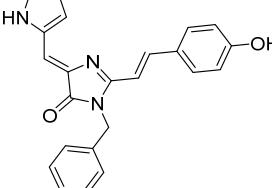
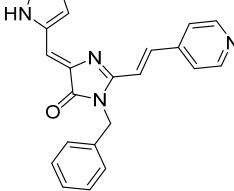
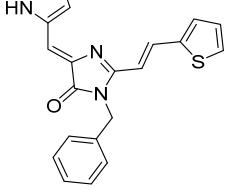
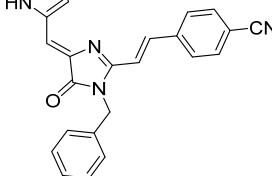
3aa		381	1.3	1.2	1.1	1.0	1.1	1.0
3ab		395	1.4	1.2	1.1	1.0	1.0	0.9
3ac		429	1.9	2.7	2.5	1.1	1.0	1.0
3ad		435	1.5	2.1	2.8	2.1	1.0	1.1
3ae		434	1.5	1.8	1.7	1.1	1.0	2.2
3af		432	1.4	1.7	1.7	1.1	1.2	1.7
3ag		432	1.5	1.6	1.6	1.1	1.0	0.9
3ah		437	1.4	1.5	1.8	1.3	1.1	1.1
3ai		437	1.4	1.7	1.7	1.1	1.1	1.2

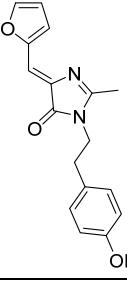
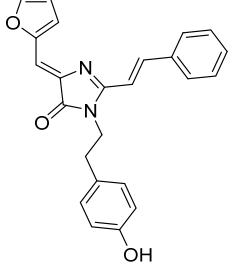
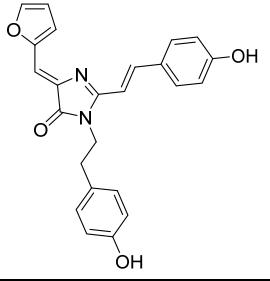
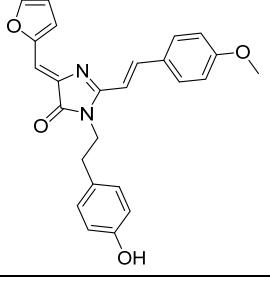
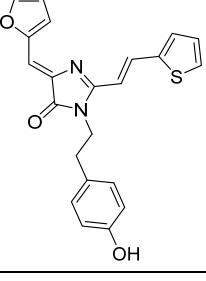
4aa		386	1.3	1.1	1.1	1.0	1.0	1.9
4ac		452	1.6	3.4	3.6	1.3	1.1	1.0
4ad		452	2.1	8.1	10.2	2.8	1.3	0.9
4ae		454	2.3	9.3	9.1	1.5	1.1	1.4

1ba		372	1.4	1.2	1.1	1.1	0.9	1.0
1bc		430	1.7	2.8	3.0	1.1	1.2	1.0
1bd		438	1.9	3.1	4.9	4.1	1.2	1.3
1be		434	1.4	1.5	1.3	1.1	1.0	1.0
1bf		433	1.7	2.7	2.6	1.1	1.0	0.7
1bg		433	1.4	1.5	1.3	1.0	1.0	1.0
1bh		439	1.2	1.8	2.8	1.8	1.2	0.9

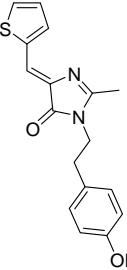
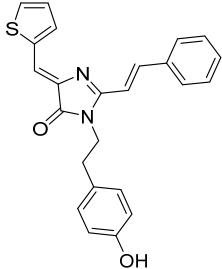
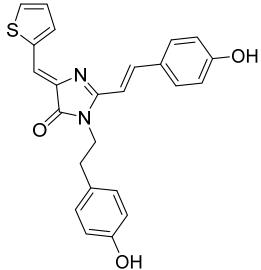
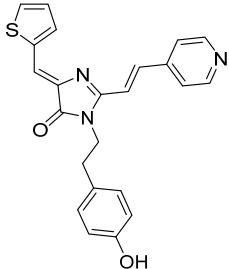
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2bc		443	1.5	2.6	2.8	1.1	1.0	0.9
2bd		448	1.9	3.0	4.7	3.4	1.0	1.3
2be		446	1.5	1.5	1.4	1.0	1.0	1.0
2bg		446	1.3	1.4	1.2	1.0	1.0	1.1
2bi		453	1.7	2.8	2.5	1.2	0.9	1.2

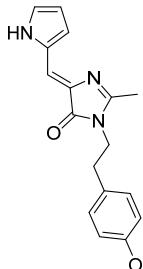
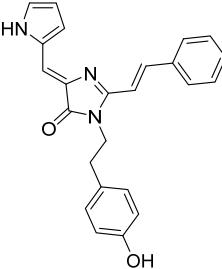
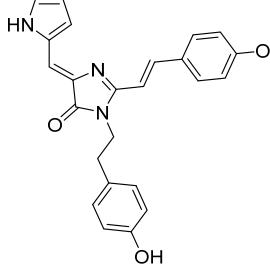
3ba		372	1.4	1.2	1.1	1.2	0.9	1.2
3bc		430	1.4	1.6	1.5	1.0	1.0	1.8
3bd		437	1.6	2.4	3.5	2.5	1.2	2.8
3be		437	1.3	1.4	1.3	1.1	1.0	1.2
3bf		433	2.3	4.3	3.0	1.2	1.0	1.0
3bg		433	1.4	1.7	1.4	1.1	1.3	1.8
3bh		441	1.4	1.9	3.0	1.4	1.4	1.1
3bi		438	1.6	2.8	2.4	1.2	1.8	1.3

4ba		390	1.4	1.2	1.1	1.2	1.2	1.0
4bc		453	1.8	4.6	5.8	1.7	1.5	1.2
4bd		456	1.9	3.7	5.7	5.0	2.0	1.3
4bf		461	1.8	4.6	5.8	2.7	1.7	1.0
4bh		461	2.0	4.5	7.9	6.7	1.0	1.2
4bi		464	2.0	3.5	4.8	3.3	2.5	0.9

1ca		373	1.4	1.2	1.1	1.1	1.1	1.1
1cc		430	2.0	3.1	2.6	1.1	1.3	1.5
1cd		437	1.5	1.8	2.3	1.2	0.9	1.0
1ce		436	1.6	2.1	2.6	1.2	1.3	1.1
1ch		439	1.4	1.6	1.7	1.2	1.0	0.9

2ca		383	1.4	1.2	1.1	1.1	1.4	1.1
2cc		443	2.1	4.1	2.9	1.2	1.1	1.0
2ce		446	1.7	2.5	3.0	1.2	1.0	1.1
2ch		452	1.4	1.5	1.7	1.2	1.0	0.9

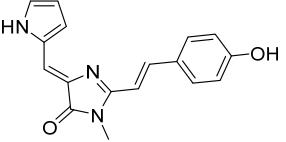
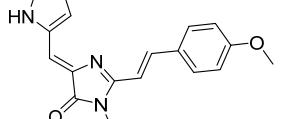
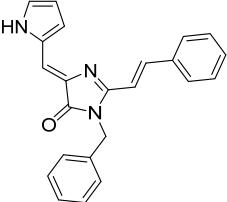
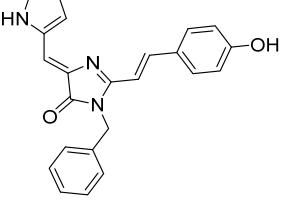
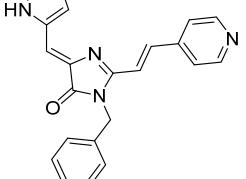
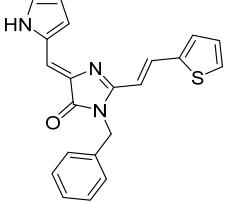
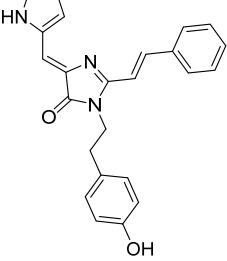
3ca		374	1.4	1.2	1.2	1.1	1.0	1.1
3cc		430	1.9	2.6	1.6	1.2	1.4	0.9
3cd		436	1.4	1.7	1.9	1.4	1.4	1.3
3cf		433	1.5	2.1	2.0	1.3	1.5	0.9

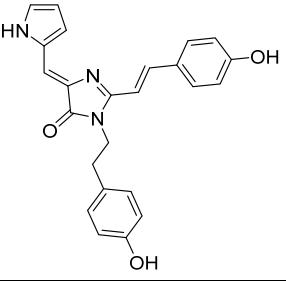
4ca		397	1.4	1.2	1.1	1.1	1.2	1.3
4cc		452	1.7	3.7	5.7	2.0	1.1	1.4
4cd		454	1.6	3.4	6.8	3.7	1.4	0.9

a – maxima position in nm;

4. Determination of affinity constants

Table S4.1. Dissociation constants values of complexes [Nanoluc-chromophore]

Chromophore	Structure	K _D , μM
4ad		>5
4ae		1.81±0.07
4bc		0.59±0.04
4bd		0.50±0.03
4bf		>5
4bh		0.32±0.02
4cc		0.55±0.04

4cd		0.48±0.02
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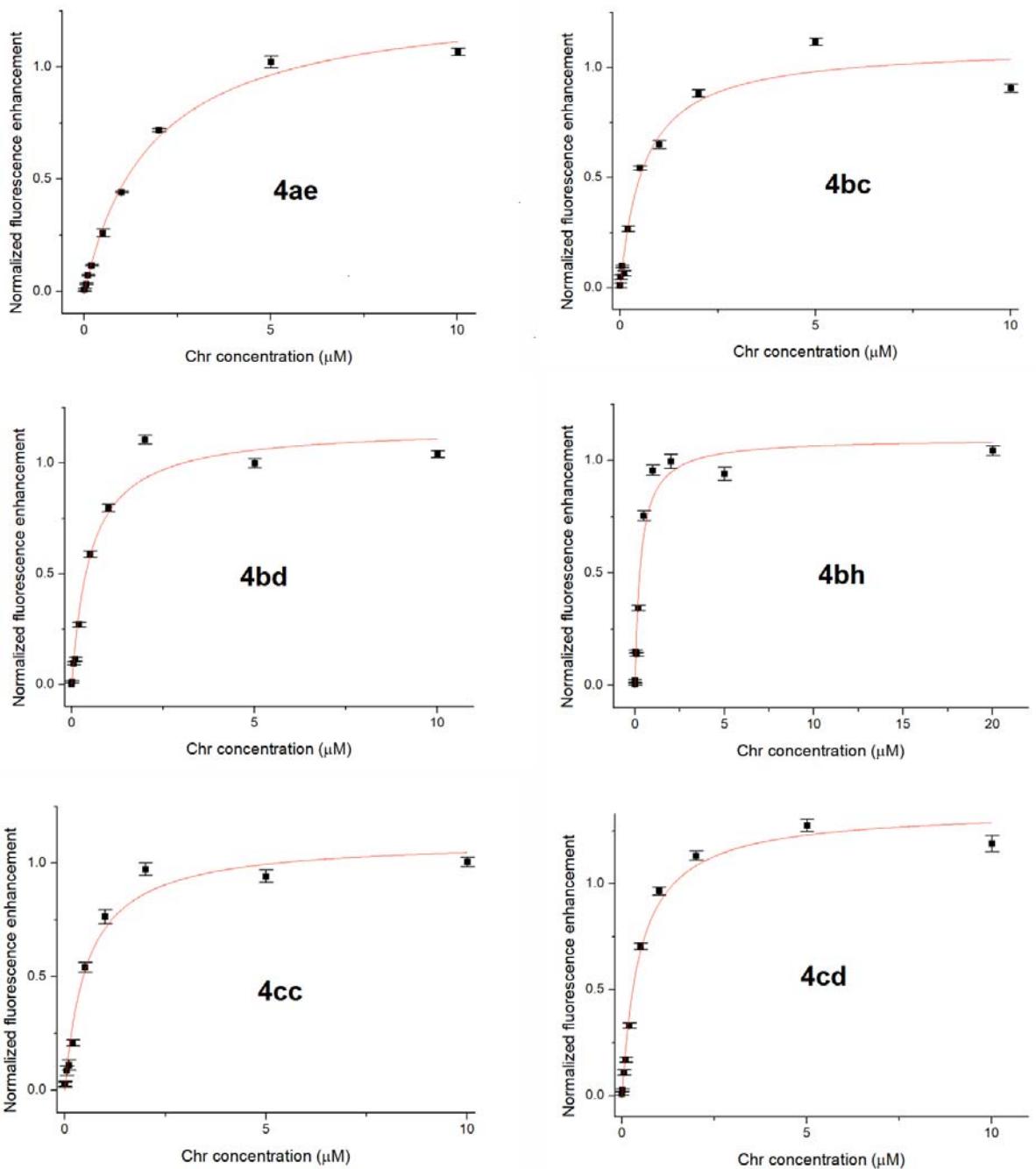


Fig S4.1. Titration curves.

5. Fluorescent microscopy

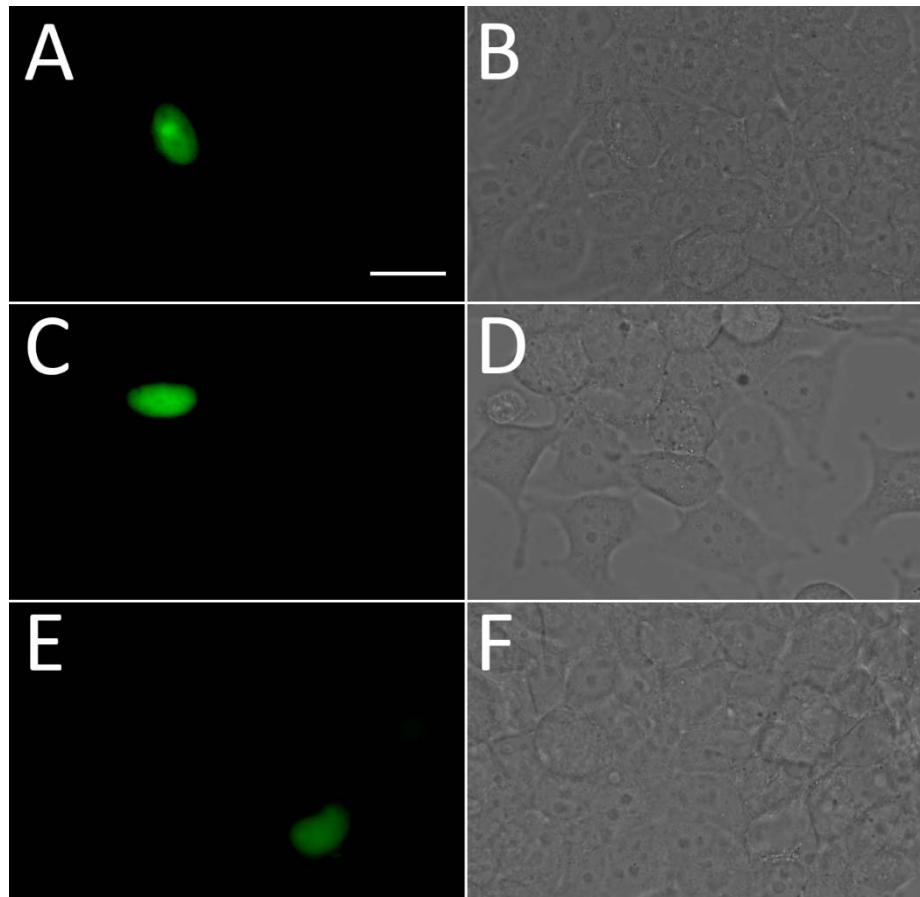


Fig. S 5.1. Live-cell imaging of sparsely expressing NanoLuc HEK293 cells with **4cc**, **4cd**, and **4bh** fluorogens at 1 μ M concentration. HEK293 cells were transiently transfected with NanoLuc-H2B and were imaged using GFP filter and bright field microscopy (B, D, F respectively) in the presence of fluorogens (A, C, E). Only NanoLuc expressing cells show fluorescent signal in the nuclei. Scale bar is 20 μ m.

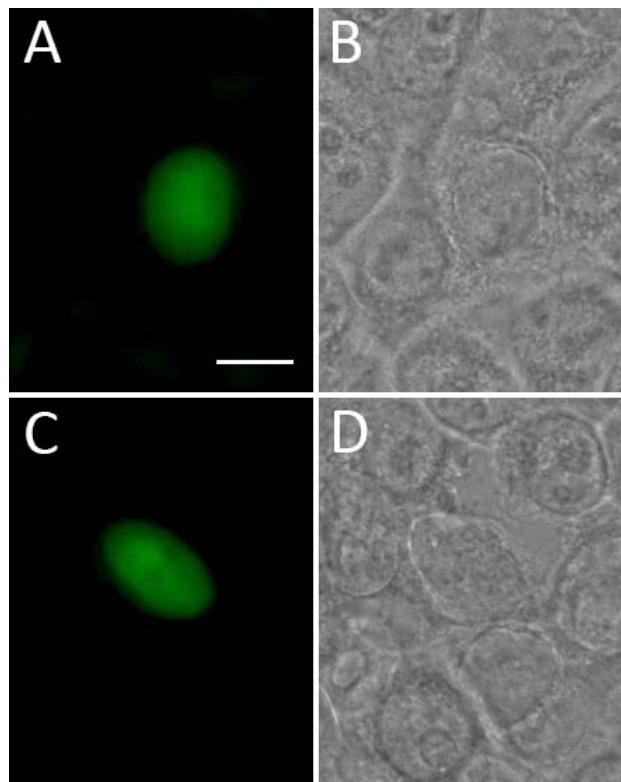
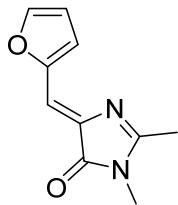


Fig. S 5.2. Imaging of fixated with methanol NanoLuc-H2B expressing HEK293 cells with **4cc** (A, B), **4cd** (C, D) fluorogens at 1 μ M concentration. Widefield fluorescent microscopy with GFP filter (A, C) and bright field microscopy (B, D) were used. Scale bar is 10 μ m.

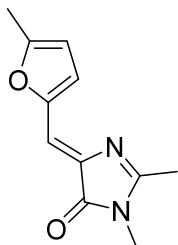
6. Spectral characteristics

5.1 5-(Z)-arylidene-2-methyl/phenyl-3-R-3,5-dihydro-4H-imidazol-4-ones



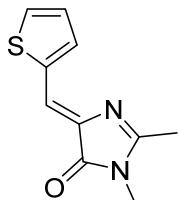
(Z)-5-(furan-2-ylmethylene)-2,3-dimethyl-3,5-dihydro-4H-imidazol-4-one (1aa)

Dark-yellow solid (0.95 g, 50%); mp 119-121 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.92 (d, *J*=1.1 Hz, 1 H), 7.32 (d, *J*=3.4 Hz, 1 H), 6.81 (s, 1 H), 6.70 (dd, *J*=3.0, 1.6 Hz, 1 H), 3.07 (s, 3 H), 2.33 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 163.8, 150.3, 146.2, 136.4, 117.8, 113.5, 111.9, 26.3, 15.4; HRMS (ESI) m/z: 191.0815 found (calcd for C₁₀H₁₁N₂O₂⁺, [M+H]⁺ 191.0815).



(Z)-5-((5-methylfuran-2-yl)methylene)-2,3-dimethyl-3,5-dihydro-4H-imidazol-4-one (2aa)

Orange solid (1.29 g, 63%); mp 132-134 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.26 (d, *J*=3.3 Hz, 1 H), 6.73 (s, 1 H), 6.36 (d, *J*=3.3 Hz, 1 H), 3.07 (s, 3 H), 2.35 (s, 3 H), 2.31 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 162.9, 155.9, 149.1, 135.2, 119.6, 112.1, 110.4, 26.3, 15.3, 13.7; HRMS (ESI) m/z: 205.0972 found (calcd for C₁₁H₁₃N₂O₂⁺, [M+H]⁺ 205.0972).



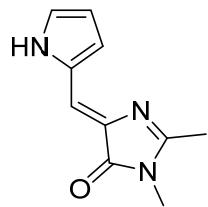
(Z)-5-(thiophen-2-ylmethylene)-2,3-dimethyl-3,5-dihydro-4H-imidazol-4-one (3aa)

Yellow solid (1.50 g, 73%); ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.85 (d, *J*=5.1 Hz, 1 H), 7.66 (d, *J*=3.4 Hz, 1 H), 7.32 (s, 1 H), 7.14 (dd, *J*=5.0, 3.6 Hz, 1 H), 3.08 (s, 3 H), 2.33 (s, 3 H).¹

¹ Zaitseva S.O., Golodukhina S.V., Baleeva N.S., Levina E.A., Smirnov A.Yu., Zagudaylova M.B., Baranov M.S. Chem. Select, **2018**, 3 (30), 8593-8596.

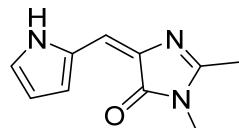
5-((1*H*-pyrrol-2-yl)methylene)-2,3-dimethyl-3,5-dihydro-4*H*-imidazol-4-one (4aa)

It was obtained as a mixture of two isomers. The mixture was successfully separated by column chromatography:



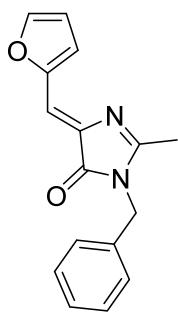
(Z)-5-((1*H*-pyrrol-2-yl)methylene)-2,3-dimethyl-3,5-dihydro-4*H*-imidazol-4-one (4aa-Z)

Yellow solid (1.05 g, 56%); mp 150-152 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.23 (br. s., 1 H), 7.15 (d, *J*=1.2 Hz, 1 H), 6.88 (s, 1 H), 6.81 (br. s., 1 H), 6.22 (ddd, *J*=3.5, 2.3, 2.2 Hz, 1 H), 3.08 (s, 3 H), 2.33 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.9, 160.0, 133.0, 128.1, 125.4, 117.9, 115.9, 110.5, 26.1, 15.1; HRMS (ESI) m/z: 190.0975 found (calcd for C₁₀H₁₂N₃O⁺, [M+H]⁺ 190.0975).



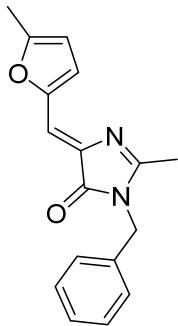
(E)-5-((1*H*-pyrrol-2-yl)methylene)-2,3-dimethyl-3,5-dihydro-4*H*-imidazol-4-one (4aa-E)

Yellow solid (0.76 g, 40%); mp 141-143 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.89 (br. s., 1 H), 7.30 (d, *J*=1.1 Hz, 1 H), 7.17 (s, 1 H), 6.82 (br. s., 1 H), 6.32 (ddd, *J*=3.6, 2.3, 2.1 Hz, 1 H), 3.16 (s, 3 H), 2.26 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.2, 155.9, 132.7, 128.3, 125.2, 124.7, 119.9, 111.4, 26.5, 14.6; HRMS (ESI) m/z: 190.0975 found (calcd for C₁₀H₁₂N₃O⁺, [M+H]⁺ 190.0975).



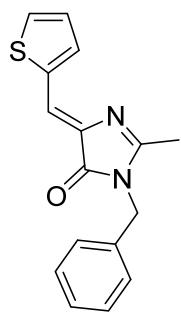
(Z)-5-(furan-2-ylmethylene)-3-benzyl-2-methyl-3,5-dihydro-4H-imidazol-4-one (1ba)

Yellow solid (1.31 g, 49%); mp 96-98 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.94 (d, *J*=1.3 Hz, 1 H), 7.34 - 7.38 (m, 3 H), 7.29 (t, *J*=7.4 Hz, 1 H), 7.24 (d, *J*=7.2 Hz, 2 H), 6.90 (s, 1 H), 6.72 (dd, *J*=3.2, 1.5 Hz, 1 H), 4.82 (s, 2 H), 2.25 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 162.9, 150.3, 146.5, 136.7, 135.7, 128.8, 127.5, 126.9, 118.3, 113.5, 112.8, 43.0, 15.6; HRMS (ESI) m/z: 267.1126 found (calcd for C₁₆H₁₅N₂O₂⁺, [M+H]⁺ 267.1128).



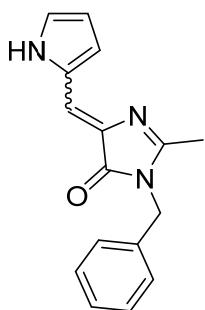
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-methyl-3,5-dihydro-4H-imidazol-4-one (2ba)

Dark-yellow solid (1.99 g, 71%); mp 98-100 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.36 (t, *J*=7.6 Hz, 2 H), 7.27 - 7.31 (m, 2 H), 7.23 (d, *J*=7.2 Hz, 2 H), 6.82 (s, 1 H), 6.37 (d, *J*=3.4 Hz, 1 H), 4.81 (s, 2 H), 2.37 (s, 3 H), 2.23 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 161.9, 156.3, 149.1, 136.8, 134.5, 128.8, 127.5, 126.9, 120.1, 112.9, 110.5, 43.0, 15.6, 13.7; HRMS (ESI) m/z: 281.1282 found (calcd for C₁₇H₁₇N₂O₂⁺, [M+H]⁺ 281.1285).



(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-methyl-3,5-dihydro-4H-imidazol-4-one (3ba)

Yellow solid (2.03 g, 72%); mp 101-103 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.87 (d, *J*=5.1 Hz, 1 H), 7.70 (d, *J*=3.4 Hz, 1 H), 7.41 (s, 1 H), 7.36 (t, *J*=7.5 Hz, 2 H), 7.29 (t, *J*=7.5 Hz, 1 H), 7.24 (d, *J*=7.2 Hz, 2 H), 7.16 (dd, *J*=5.1, 3.7 Hz, 1 H), 4.82 (s, 2 H), 2.25 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.1, 162.0, 137.2, 136.8, 135.8, 135.1, 134.5, 128.8, 127.6, 127.5, 126.9, 119.9, 43.0, 15.7; HRMS (ESI) m/z: 283.0897 found (calcd for C₁₆H₁₅N₂OS⁺, [M+H]⁺ 283.0900).



5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-methyl-3,5-dihydro-4*H*-imidazol-4-one (4ba)

Yellow solid (2.15 g, 81%); mp 127-129 °C.

It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(E)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-methyl-3,5-dihydro-4*H*-imidazol-4-one

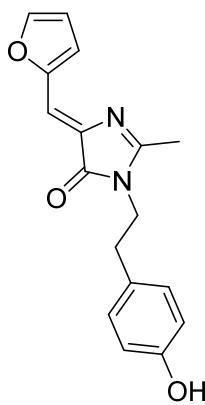
¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.84 (br. s., 1 H), 7.35 - 7.38 (m, 2 H), 7.32 (d, *J*=1.1 Hz, 1 H), 7.27 - 7.31 (m, 1 H), 7.24 - 7.27 (m, 3 H), 6.88 (br. s., 1 H), 6.35 (ddd, *J*=3.6, 2.5, 2.3 Hz, 1 H), 4.89 (s, 2 H), 2.19 (s, 3 H).

(Z)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-methyl-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.28 (br. s., 1 H), 7.34 - 7.37 (m, 2 H), 7.27 - 7.31 (m, 1 H), 7.23 (d, *J*=7.1 Hz, 2 H), 7.17 (d, *J*=1.1 Hz, 1 H), 6.97 (s, 1 H), 6.86 (br. s., 1 H), 6.24 (ddd, *J*=3.5, 2.4, 2.2 Hz, 1 H), 4.81 (s, 2 H), 2.24 (s, 3 H).

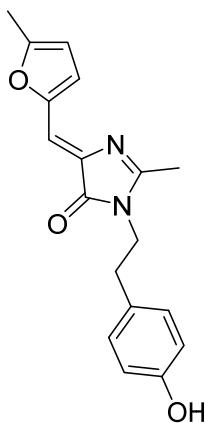
¹³C and HRMS data presented as is for a mixture:

¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.9, 168.2, 159.1, 155.1, 137.0, 136.8, 132.4, 132.1, 128.8 (2 C), 128.3, 128.0, 127.5 (2 C), 126.9, 126.8, 125.8 (2 C), 125.6, 120.6, 118.4, 116.8, 111.7, 110.7, 43.3, 42.8, 15.4, 15.0; HRMS (ESI) m/z: 266.1286 found (calcd for C₁₆H₁₆N₃O⁺, [M+H]⁺ 266.1288).



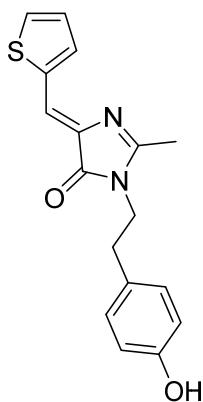
(Z)-5-(furan-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-methyl-3,5-dihydro-4H-imidazol-4-one (1ca)

Brown solid (1.99 g, 67%); mp 149-151 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.22 (s, 1 H), 7.91 (d, *J*=1.0 Hz, 1 H), 7.31 (d, *J*=3.2 Hz, 1 H), 6.96 (d, *J*=8.4 Hz, 2 H), 6.80 (s, 1 H), 6.70 (dd, *J*=3.0, 1.6 Hz, 1 H), 6.67 (d, *J*=8.4 Hz, 2 H), 3.70 (t, *J*=7.0 Hz, 2 H), 2.73 (t, *J*=7.1 Hz, 2 H), 2.03 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 163.3, 156.0, 150.3, 146.3, 136.0, 129.8, 128.2, 117.9, 115.3, 113.4, 112.0, 42.1, 33.4, 15.0; HRMS (ESI) m/z: 297.1231 found (calcd for C₁₇H₁₇N₂O₃⁺, [M+H]⁺ 297.1234).



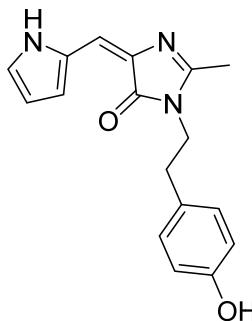
(Z)-5-((5-methylfuran-2-yl)methylene)-3-(4-hydroxyphenethyl)-2-methyl-3,5-dihydro-4H-imidazol-4-one (2ca)

Orange solid (1.71 g, 55%); mp 192-194 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.22 (s, 1 H), 7.24 (d, *J*=2.9 Hz, 1 H), 6.95 (d, *J*=8.4 Hz, 2 H), 6.72 (s, 1 H), 6.67 (d, *J*=8.2 Hz, 2 H), 6.35 (d, *J*=2.5 Hz, 1 H), 3.69 (t, *J*=7.0 Hz, 2 H), 2.72 (t, *J*=7.1 Hz, 2 H), 2.36 (s, 3 H), 2.01 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 162.3, 156.0, 156.0, 149.1, 134.8, 129.8, 128.3, 119.7, 115.3, 112.1, 110.4, 42.1, 33.5, 15.0, 13.7; HRMS (ESI) m/z: 311.1388 found (calcd for C₁₈H₁₉N₂O₃⁺, [M+H]⁺ 311.1390).



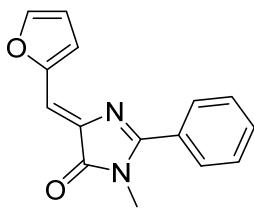
(Z)-5-(thiophen-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-methyl-3,5-dihydro-4H-imidazol-4-one (3ca)

Yellow solid (2.22 g, 71%); mp 135-137 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.22 (s, 1 H), 7.84 (d, *J*=5.0 Hz, 1 H), 7.66 (d, *J*=3.4 Hz, 1 H), 7.29 (s, 1 H), 7.15 (dd, *J*=5.1, 3.7 Hz, 1 H), 6.97 (d, *J*=8.4 Hz, 2 H), 6.67 (d, *J*=8.4 Hz, 2 H), 3.70 (t, *J*=7.1 Hz, 2 H), 2.74 (t, *J*=7.1 Hz, 2 H), 2.05 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.0, 162.3, 156.0, 137.3, 136.1, 134.7, 134.2, 129.8, 128.2, 127.6, 119.0, 115.3, 42.1, 33.5, 15.1; HRMS (ESI) m/z: 313.1003 found (calcd for C₁₇H₁₇N₂O₂S⁺, [M+H]⁺ 313.1005).



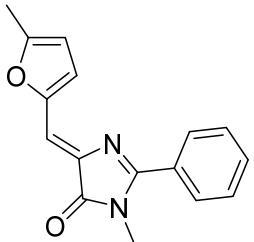
(E)-5-((1*H*-pyrrol-2-yl)methylene)-3-(4-hydroxyphenethyl)-2-methyl-3,5-dihydro-4*H*-imidazol-4-one (4ca)

Dark-yellow solid (2.07 g, 70%); mp ~230 °C with decomposition; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.88 (br. s., 1 H), 9.24 (br. s., 1 H), 7.31 (br. s., 1 H), 7.16 (s, 1 H), 6.96 (d, *J*=8.0 Hz, 2 H), 6.83 (br. s., 1 H), 6.68 (d, *J*=8.2 Hz, 2 H), 6.33 (br. s., 1 H), 3.76 (t, *J*=7.1 Hz, 2 H), 2.78 (t, *J*=7.1 Hz, 2 H), 1.97 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.1, 156.0, 155.5, 132.4, 129.8, 128.4, 128.2, 125.4, 124.9, 120.1, 115.3, 111.5, 42.4, 33.4, 14.4; HRMS (ESI) m/z: 296.1391 found (calcd for C₁₇H₁₈N₃O₂⁺, [M+H]⁺ 296.1394).



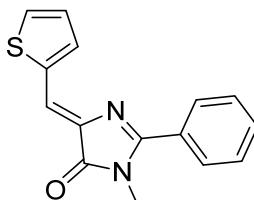
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-phenyl-3,5-dihydro-4H-imidazol-4-one (1ab)

Yellow solid (0.60 g, 31%); mp 153-155 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.99 (d, *J*=1.6 Hz, 1 H), 7.94 (dd, *J*=7.8, 1.6 Hz, 2 H), 7.56 - 7.67 (m, 3 H), 7.48 (d, *J*=3.5 Hz, 1 H), 7.02 (s, 1 H), 6.76 (dd, *J*=3.4, 1.8 Hz, 1 H), 3.27 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 170.1, 162.1, 150.5, 146.8, 136.2, 131.6, 128.9, 128.8, 128.7, 119.0, 113.8 (2 C), 28.8; HRMS (ESI) m/z: 253.0971 found (calcd for C₁₅H₁₃N₂O₂⁺, [M+H]⁺ 253.0972).



(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-phenyl-3,5-dihydro-4H-imidazol-4-one (2ab)

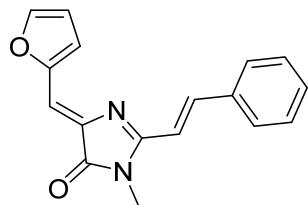
Orange solid (0.40 g, 15%); mp 164-166 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.92 (dd, *J*=7.9, 1.6 Hz, 2 H), 7.54 - 7.66 (m, 3 H), 7.42 (d, *J*=3.4 Hz, 1 H), 6.93 (s, 1 H), 6.42 (d, *J*=3.3 Hz, 1 H), 3.25 (s, 3 H), 2.38 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 170.0, 161.1, 156.6, 149.4, 135.1, 131.4, 129.0, 128.8, 128.6, 120.8, 113.9, 110.8, 28.7, 13.8; HRMS (ESI) m/z: 267.1126 found (calcd for C₁₆H₁₅N₂O₂⁺, [M+H]⁺ 267.1128).



(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-phenyl-3,5-dihydro-4H-imidazol-4-one (3ab)

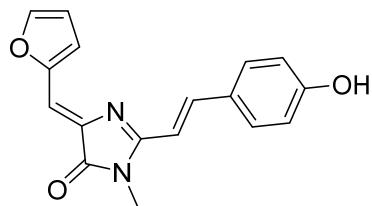
Yellow solid (0.56 g, 21%); mp 142-144 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.88 - 8.03 (m, 3 H), 7.75 (d, *J*=3.4 Hz, 1 H), 7.52 - 7.69 (m, 4 H), 7.19 (dd, *J*=5.1, 3.7 Hz, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.8, 161.1, 137.6, 136.4, 135.4, 135.1, 131.5, 129.0, 128.8, 128.7, 127.7, 121.2, 28.8; HRMS (ESI) m/z: 269.0740 found (calcd for C₁₅H₁₃N₂OS⁺, [M+H]⁺ 269.0743).

5.2 5-(Z)-arylidene-2-(E)-arylvinylic-3-methyl-3,5-dihydro-4H-imidazol-4-ones



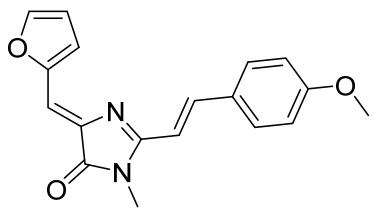
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (1ac)

Brown solid (178 mg, 64%); mp 143-145 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 8.04 (d, *J*=15.8 Hz, 1 H), 7.96 (d, *J*=1.3 Hz, 1 H), 7.87 (d, *J*=7.1 Hz, 2 H), 7.57 (d, *J*=3.4 Hz, 1 H), 7.43 - 7.49 (m, 3 H), 7.24 (d, *J*=15.8 Hz, 1 H), 6.88 (s, 1 H), 6.78 (dd, *J*=3.2, 1.5 Hz, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.5, 160.0, 150.9, 146.4, 140.4, 137.1, 135.1, 130.2, 129.0, 128.4, 118.5, 113.9 (2 C), 111.9, 26.5; HRMS (ESI) m/z: 279.1125 found (calcd for C₁₇H₁₅N₂O₂⁺, [M+H]⁺ 279.1128).



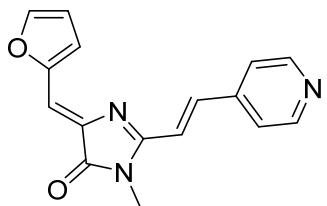
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (1ad)

Brown solid (270 mg, 92%); mp ~250 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 10.07 (s, 1 H), 7.90 - 8.02 (m, 2 H), 7.72 (d, *J*=8.3 Hz, 2 H), 7.52 (d, *J*=3.3 Hz, 1 H), 6.99 (d, *J*=15.6 Hz, 1 H), 6.85 (d, *J*=8.5 Hz, 2 H), 6.80 (s, 1 H), 6.76 (br. s., 1 H), 3.25 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.5, 160.4, 159.9, 151.0, 146.1, 141.0, 137.3, 130.5, 126.4, 117.9, 115.9, 113.8, 110.7, 109.9, 26.4; HRMS (ESI) m/z: 295.1074 found (calcd for C₁₇H₁₅N₂O₃⁺, [M+H]⁺ 295.1077).



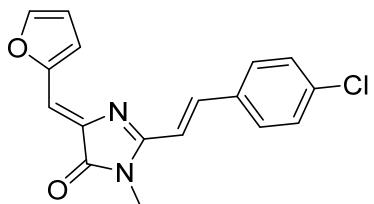
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (1ae)

Orange solid (123 mg, 40%); mp 142-144 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.01 (d, *J*=15.7 Hz, 1 H), 7.95 (d, *J*=1.3 Hz, 1 H), 7.84 (d, *J*=8.7 Hz, 2 H), 7.55 (d, *J*=3.4 Hz, 1 H), 7.00 - 7.12 (m, 3 H), 6.82 (s, 1 H), 6.77 (dd, *J*=4.3, 1.5 Hz, 1 H), 3.83 (s, 3 H), 3.26 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.5, 161.1, 160.3, 151.0, 146.2, 140.5, 137.3, 130.3, 127.9, 118.1, 114.5, 113.8, 111.1 (2 C), 55.4, 26.5; HRMS (ESI) m/z: 309.1231 found (calcd for C₁₈H₁₇N₂O₃⁺, [M+H]⁺ 309.1234).



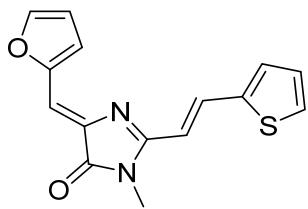
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-2-(pyridine-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (1af)

Brown solid (117 mg, 42%); mp 192-194 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.67 (d, *J*=5.6 Hz, 2 H), 7.93 - 8.04 (m, 2 H), 7.82 (d, *J*=5.9 Hz, 2 H), 7.60 (d, *J*=3.4 Hz, 1 H), 7.49 (d, *J*=15.9 Hz, 1 H), 6.95 (s, 1 H), 6.80 (dd, *J*=3.1, 1.4 Hz, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 159.3, 150.8, 150.4, 146.9, 142.1, 137.5, 136.8, 122.1, 119.2, 118.6, 114.0, 113.1, 26.6; HRMS (ESI) m/z: 280.1077 found (calcd for C₁₆H₁₄N₃O₂⁺, [M+H]⁺ 280.1081).



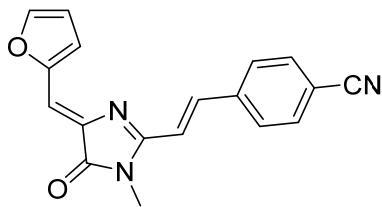
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (1ag)

Orange solid (168 mg, 54%); mp 189-191 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 8.03 (d, *J*=15.8 Hz, 1 H), 7.97 (d, *J*=1.1 Hz, 1 H), 7.91 (d, *J*=8.4 Hz, 2 H), 7.57 (d, *J*=3.4 Hz, 1 H), 7.54 (d, *J*=8.6 Hz, 2 H), 7.27 (d, *J*=15.8 Hz, 1 H), 6.89 (s, 1 H), 6.78 (dd, *J*=2.9, 1.5 Hz, 1 H), 3.27 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.3, 159.7, 150.8, 146.4, 138.9, 137.0, 134.6, 134.1, 130.0, 128.9, 118.5, 114.6, 113.8, 112.0, 26.4; HRMS (ESI) m/z: 313.0734 found (calcd for C₁₇H₁₄ClN₂O₂⁺, [M+H]⁺ 313.0738).



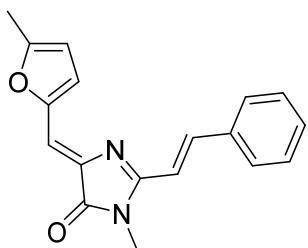
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (1ah)

Red solid (162 mg, 57%); mp 154-156 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.21 (d, *J*=15.5 Hz, 1 H), 7.96 (d, *J*=1.3 Hz, 1 H), 7.78 (d, *J*=4.9 Hz, 1 H), 7.67 (d, *J*=3.4 Hz, 1 H), 7.55 (d, *J*=3.4 Hz, 1 H), 7.20 (dd, *J*=5.0, 3.7 Hz, 1 H), 6.81 - 6.90 (m, 2 H), 6.77 (dd, *J*=3.3, 1.7 Hz, 1 H), 3.24 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.3, 159.6, 150.9, 146.2, 140.3, 137.1, 133.1, 131.6, 129.9, 128.7, 118.2, 113.7, 112.1, 111.4, 26.3; HRMS (ESI) m/z: 285.0694 found (calcd for C₁₅H₁₃N₂O₂S⁺, [M+H]⁺ 285.0692).



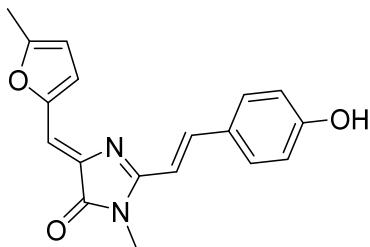
(Z)-5-(furan-2-ylmethylene)-3-methyl-2-((E)-4-cyanostyryl)-3,5-dihydro-4H-imidazol-4-one (1ai)

Orange solid (58 mg, 19%); mp 240-242 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.03 - 8.13 (m, 3 H), 7.99 (d, *J*=1.1 Hz, 1 H), 7.94 (d, *J*=8.3 Hz, 2 H), 7.60 (d, *J*=3.4 Hz, 1 H), 7.43 (d, *J*=16.0 Hz, 1 H), 6.93 (s, 1 H), 6.79 (dd, *J*=3.0, 1.5 Hz, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 159.4, 150.8, 146.8, 139.6, 138.1, 136.9, 132.7, 129.0, 119.0, 118.7, 117.5, 113.9, 112.8, 111.8, 26.5; HRMS (ESI) m/z: 304.1079 found (calcd for C₁₈H₁₄N₃O₂⁺, [M+H]⁺ 304.1081).



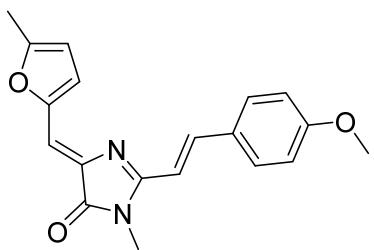
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (2ac)

Orange solid (184 mg, 63%); mp 145-147 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.01 (d, *J*=15.8 Hz, 1 H), 7.86 (d, *J*=6.1 Hz, 2 H), 7.39 - 7.56 (m, 4 H), 7.22 (d, *J*=15.9 Hz, 1 H), 6.80 (s, 1 H), 6.45 (br. s., 1 H), 3.27 (s, 3 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 159.0, 156.2, 149.7, 140.0, 136.0, 135.2, 130.1, 128.9, 128.4, 120.3, 113.9, 112.0, 110.9, 26.4, 13.8; HRMS (ESI) m/z: 293.1282 found (calcd for C₁₈H₁₇N₂O₂⁺, [M+H]⁺ 293.1285).



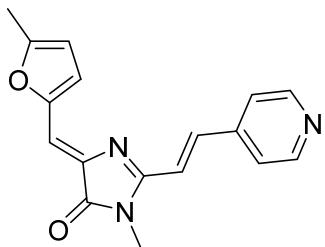
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (2ad)

Red solid (253 mg, 82%); mp ~250 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 10.05 (br. s, 1 H), 7.94 (d, *J*=15.7 Hz, 1 H), 7.70 (d, *J*=8.5 Hz, 2 H), 7.47 (d, *J*=3.4 Hz, 1 H), 6.97 (d, *J*=15.7 Hz, 1 H), 6.84 (d, *J*=8.5 Hz, 2 H), 6.73 (s, 1 H), 6.42 (d, *J*=2.9 Hz, 1 H), 3.24 (s, 3 H), 2.38 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 159.8, 159.5, 155.8, 149.8, 140.5, 136.2, 130.4, 126.5, 119.7, 115.9, 110.9, 110.7, 110.0, 26.4, 13.8; HRMS (ESI) m/z: 309.1231 found (calcd for C₁₈H₁₇N₂O₃⁺, [M+H]⁺ 309.1234).



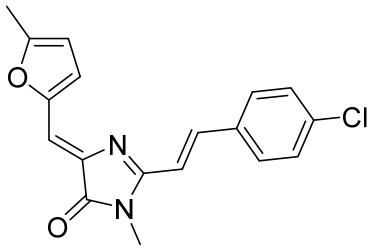
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (2ae)

Red solid (132 mg, 41%); mp 133-135 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.98 (d, *J*=15.6 Hz, 1 H), 7.82 (d, *J*=8.8 Hz, 2 H), 7.49 (d, *J*=3.2 Hz, 1 H), 7.01 - 7.07 (m, 3 H), 6.75 (s, 1 H), 6.43 (d, *J*=3.2 Hz, 1 H), 3.83 (s, 3 H), 3.25 (s, 3 H), 2.39 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 161.0, 159.4, 155.9, 149.8, 140.0, 136.2, 130.2, 128.0, 119.8, 114.5, 111.2, 111.1, 110.8, 55.4, 26.4, 13.8; HRMS (ESI) m/z: 323.1387 found (calcd for C₁₉H₁₉N₂O₃⁺, [M+H]⁺ 323.1390).



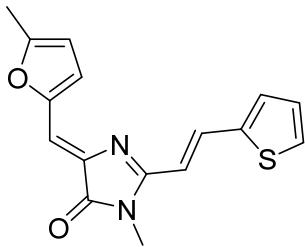
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-2-(pyridin-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (2af)

Red solid (182 mg, 62%); mp 174-176 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.66 (br. s., 2 H), 7.95 (d, *J*=15.9 Hz, 1 H), 7.81 (d, *J*=4.8 Hz, 2 H), 7.55 (d, *J*=3.0 Hz, 1 H), 7.47 (d, *J*=15.7 Hz, 1 H), 6.87 (s, 1 H), 6.46 (d, *J*=2.2 Hz, 1 H), 3.27 (s, 3 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.3, 156.8, 150.3, 149.6, 142.2, 137.0, 135.7, 122.1, 121.0, 118.6, 113.2, 111.1, 26.5, 13.8; HRMS (ESI) m/z: 294.1237 found (calcd for C₁₇H₁₆N₃O₂⁺, [M+H]⁺ 294.1237).



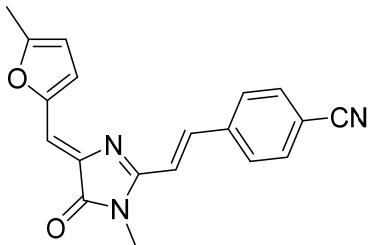
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (2ag)

Orange solid (241 mg, 74%); mp 177-179 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.00 (d, *J*=15.7 Hz, 1 H), 7.90 (d, *J*=8.4 Hz, 2 H), 7.48 - 7.58 (m, 3 H), 7.25 (d, *J*=15.9 Hz, 1 H), 6.81 (s, 1 H), 6.45 (d, *J*=3.3 Hz, 1 H), 3.26 (s, 3 H), 2.40 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.2, 158.8, 156.2, 149.6, 138.4, 135.9, 134.4, 134.1, 129.9, 128.9, 120.3, 114.6, 112.2, 110.8, 26.4, 13.7; HRMS (ESI) m/z: 327.0891 found (calcd for C₁₈H₁₆ClN₂O₂⁺, [M+H]⁺ 327.0895).



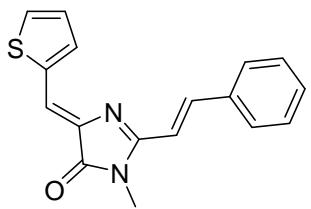
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (2ah)

Red solid (197 mg, 66%); mp 171-173 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 8.17 (d, *J*=15.4 Hz, 1 H), 7.76 (d, *J*=5.1 Hz, 1 H), 7.65 (d, *J*=3.6 Hz, 1 H), 7.50 (d, *J*=3.4 Hz, 1 H), 7.19 (dd, *J*=5.0, 3.6 Hz, 1 H), 6.83 (d, *J*=15.6 Hz, 1 H), 6.77 (s, 1 H), 6.43 (d, *J*=3.4 Hz, 1 H), 3.23 (s, 3 H), 2.39 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.8, 156.1, 149.7, 140.4, 136.0, 132.8, 131.5, 129.8, 128.7, 120.1, 112.2, 111.6, 110.8, 26.3, 13.8; HRMS (ESI) m/z: 299.0845 found (calcd for C₁₆H₁₅N₂O₂S⁺, [M+H]⁺ 299.0849).



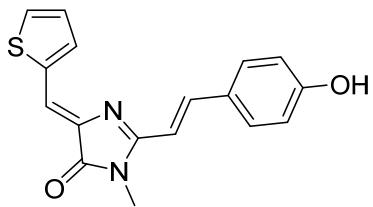
(Z)-5-((5-methylfuran-2-yl)methylene)-3-methyl-2-((E)-4-cyanostyryl)-3,5-dihydro-4H-imidazol-4-one (2ai)

Orange solid (117 mg, 37%); mp 222-224 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.01 - 8.09 (m, 3 H), 7.93 (d, *J*=8.4 Hz, 2 H), 7.55 (d, *J*=3.2 Hz, 1 H), 7.41 (d, *J*=15.9 Hz, 1 H), 6.85 (s, 1 H), 6.46 (d, *J*=3.1 Hz, 1 H), 3.27 (s, 3 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.5, 156.7, 149.7, 139.7, 137.7, 135.8, 132.7, 128.9, 120.9, 118.7, 117.5, 112.9, 111.7, 111.1, 26.5, 13.8; HRMS (ESI) m/z: 318.1228 found (calcd for C₁₉H₁₆N₃O₂⁺, [M+H]⁺ 318.1237).



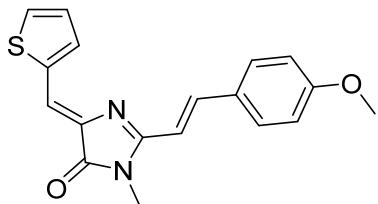
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (3ac)

Orange solid (91 mg, 31%); mp 172-174 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.97 (d, *J*=15.8 Hz, 1 H), 7.92 (d, *J*=5.0 Hz, 1 H), 7.85 (d, *J*=7.2 Hz, 2 H), 7.73 (d, *J*=3.6 Hz, 1 H), 7.44 - 7.49 (m, 3 H), 7.40 (s, 1 H), 7.24 (d, *J*=15.8 Hz, 1 H), 7.19 (dd, *J*=5.0, 3.6 Hz, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 159.2, 140.1, 138.1, 137.2, 135.1, 134.9, 134.7, 130.2, 129.0, 128.4, 127.8, 119.3, 114.1, 26.5; HRMS (ESI) m/z: 295.0897 found (calcd for C₁₇H₁₅N₂OS⁺, [M+H]⁺ 295.0900).



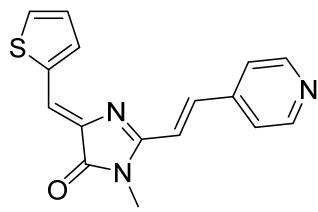
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (3ad)

Orange solid (180 mg, 58%); mp ~250 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 10.07 (br. s., 1 H), 7.85 - 7.96 (m, 2 H), 7.64 - 7.74 (m, 3 H), 7.32 (s, 1 H), 7.17 (dd, *J*=4.7, 3.7 Hz, 1 H), 6.99 (d, *J*=15.6 Hz, 1 H), 6.85 (d, *J*=8.6 Hz, 2 H), 3.25 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 159.8, 159.6, 140.6, 138.2, 137.4, 134.3, 134.1, 130.5, 127.7, 126.3, 118.0, 115.9, 110.1, 26.4; HRMS (ESI) m/z: 311.0846 found (calcd for C₁₇H₁₅N₂O₂S⁺, [M+H]⁺ 311.0849).



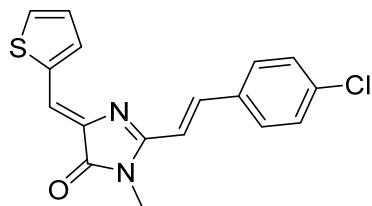
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (3ae)

Orange solid (143 mg, 44%); mp 169-171 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.94 (d, *J*=15.7 Hz, 1 H), 7.89 (d, *J*=5.1 Hz, 1 H), 7.82 (d, *J*=8.8 Hz, 2 H), 7.71 (d, *J*=3.4 Hz, 1 H), 7.34 (s, 1 H), 7.18 (dd, *J*=4.8, 3.9 Hz, 1 H), 7.00 - 7.12 (m, 3 H), 3.83 (s, 3 H), 3.26 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 161.1, 159.5, 140.1, 138.2, 137.4, 134.5, 134.3, 130.2, 127.8, 127.7, 118.4, 114.5, 111.3, 55.4, 26.4; HRMS (ESI) m/z: 325.1002 found (calcd for C₁₈H₁₇N₂O₂S⁺, [M+H]⁺ 325.1005).



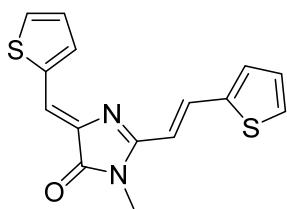
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-2-(pyridine-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (3af)

Red-orange solid (150 mg, 51%); mp 203-205 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.67 (d, *J*=5.1 Hz, 2 H), 7.96 (d, *J*=4.9 Hz, 1 H), 7.89 (d, *J*=15.8 Hz, 1 H), 7.81 (d, *J*=5.7 Hz, 2 H), 7.77 (d, *J*=3.4 Hz, 1 H), 7.44 - 7.55 (m, 2 H), 7.20 (dd, *J*=4.6, 4.1 Hz, 1 H), 3.29 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.1, 158.5, 150.4, 142.1, 137.9, 137.1, 137.0, 135.5, 135.3, 127.9, 122.1, 120.6, 118.8, 26.6; HRMS (ESI) m/z: 296.0851 found (calcd for C₁₆H₁₄N₃OS⁺, [M+H]⁺ 296.0852).



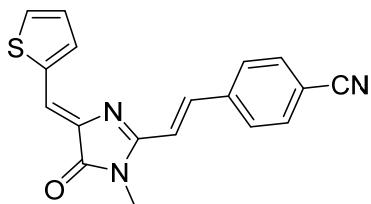
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (3ag)

Orange solid (190 mg, 58%); mp 204-206 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.94 (d, *J*=15.8 Hz, 1 H), 7.92 (d, *J*=5.1 Hz, 1 H), 7.89 (d, *J*=8.6 Hz, 2 H), 7.74 (d, *J*=3.6 Hz, 1 H), 7.54 (d, *J*=8.4 Hz, 2 H), 7.40 (s, 1 H), 7.27 (d, *J*=15.6 Hz, 1 H), 7.19 (dd, *J*=5.0, 3.8 Hz, 1 H), 3.27 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.1, 158.9, 138.5, 138.0, 137.1, 134.8, 134.6 (2 C), 134.0, 129.9, 128.9, 127.7, 119.4, 114.8, 26.4; HRMS (ESI) m/z: 329.0511 found (calcd for C₁₇H₁₄ClN₂OS⁺, [M+H]⁺ 329.0510).



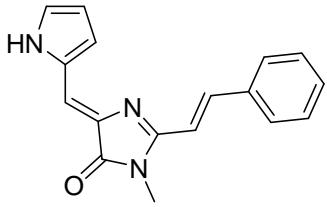
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (3ah)

Orange solid (171 mg, 57%); mp 131-133 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.11 (d, *J*=15.6 Hz, 1 H), 7.91 (d, *J*=5.1 Hz, 1 H), 7.78 (d, *J*=5.0 Hz, 1 H), 7.72 (d, *J*=3.6 Hz, 1 H), 7.67 (d, *J*=3.4 Hz, 1 H), 7.37 (s, 1 H), 7.17 – 7.19 (m, 2 H), 6.87 (d, *J*=15.5 Hz, 1 H), 3.24 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.0, 158.8, 140.2, 138.0, 137.2, 134.6, 134.4, 132.7, 131.4, 129.8, 128.7, 127.7, 118.7, 112.3, 26.3; HRMS (ESI) m/z: 301.0463 found (calcd for C₁₅H₁₃N₂OS₂⁺, [M+H]⁺ 301.0464).



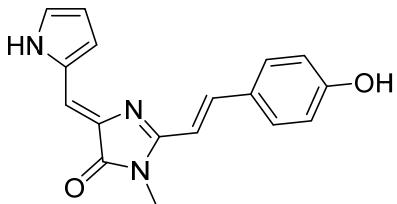
(Z)-5-(thiophen-2-ylmethylene)-3-methyl-2-((E)-4-cyanostyryl)-3,5-dihydro-4H-imidazol-4-one (3ai)

Red solid (124 mg, 39%); mp 231-233 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.06 (d, *J*=8.4 Hz, 2 H), 7.91 - 8.02 (m, 4 H), 7.76 (d, *J*=3.4 Hz, 1 H), 7.38 - 7.49 (m, 2 H), 7.17 - 7.23 (m, 1 H), 3.28 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.1, 158.6, 139.6, 138.0, 137.8, 137.1, 135.3, 135.1, 132.8, 128.9, 127.9, 120.3, 118.7, 117.7, 111.8, 26.5; HRMS (ESI) m/z: 320.0853 found (calcd for C₁₈H₁₄N₃OS⁺, [M+H]⁺ 320.0852).



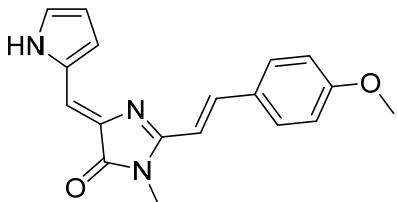
**(Z)-5-((1*H*-pyrrol-2-yl)methylene)-3-methyl-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one
(4ac)**

Orange solid (150 mg, 54%); mp 191-193 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 11.42 (br. s., 1 H), 8.18 (d, *J*=15.9 Hz, 1 H), 7.83 (d, *J*=6.9 Hz, 2 H), 7.42 - 7.51 (m, 3 H), 7.25 (br. s., 1 H), 7.19 (d, *J*=15.8 Hz, 1 H), 6.96 (s, 1 H), 6.89 (br. s., 1 H), 6.24 - 6.34 (m, 1 H), 3.27 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.9, 156.5, 139.2, 135.5, 133.8, 129.7, 128.9, 128.8, 128.0, 126.3, 118.8, 116.0, 113.8, 110.9, 26.2; HRMS (ESI) m/z: 278.1285 found (calcd for C₁₇H₁₆N₃O⁺, [M+H]⁺ 278.1288).



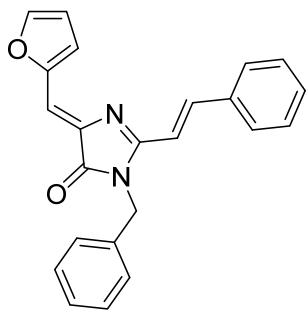
(Z)-5-((1*H*-pyrrol-2-yl)methylene)-3-methyl-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (4ad)

Dark-red solid (149 mg, 51%); mp ~190 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 11.39 (br. s., 1 H), 10.00 (br. s., 1 H), 8.09 (d, *J*=15.8 Hz, 1 H), 7.68 (d, *J*=8.7 Hz, 2 H), 7.22 (br. s., 1 H), 6.94 (d, *J*=15.7 Hz, 1 H), 6.82 - 6.90 (m, 4 H), 6.22 - 6.31 (m, 1 H), 3.24 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.0, 159.4, 157.0, 139.7, 134.0, 130.0, 128.9, 126.7, 125.8, 118.2, 115.8, 114.9, 110.7, 109.9, 26.2; HRMS (ESI) m/z: 294.1235 found (calcd for C₁₇H₁₆N₃O₂⁺, [M+H]⁺ 294.1237).



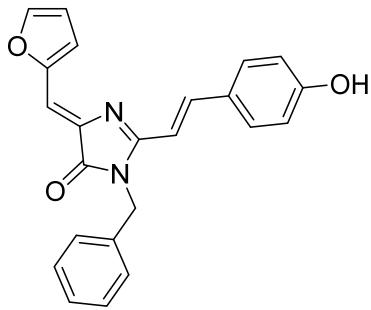
(Z)-5-((1*H*-pyrrol-2-yl)methylene)-3-methyl-2-((*E*)-4-methoxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (4ae)

Orange solid (144 mg, 47%); mp 182-184 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 11.40 (br. s., 1 H), 8.14 (d, *J*=15.8 Hz, 1 H), 7.79 (d, *J*=8.7 Hz, 2 H), 7.23 (br. s., 1 H), 6.99 - 7.07 (m, 3 H), 6.91 (s, 1 H), 6.86 (br. s., 1 H), 6.23 - 6.30 (m, 1 H), 3.83 (s, 3 H), 3.25 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.9, 160.7, 156.9, 139.1, 133.9, 129.8, 128.9, 128.2, 125.9, 118.4, 115.2, 114.4, 111.1, 110.7, 55.3, 26.2; HRMS (ESI) m/z: 308.1391 found (calcd for C₁₈H₁₈N₃O₂⁺, [M+H]⁺ 308.1394).



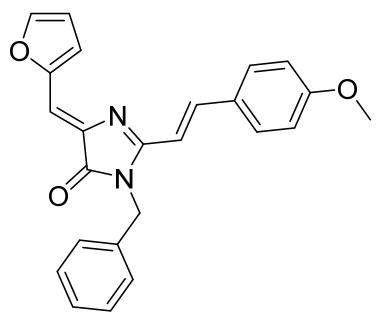
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (1bc)

Dark-red solid (198 mg, 56%); mp 157-159 °C; ^1H NMR (700 MHz, DMSO- d_6) δ ppm 8.02 (d, $J=15.6$ Hz, 1 H), 7.99 (d, $J=1.5$ Hz, 1 H), 7.77 (d, $J=7.1$ Hz, 2 H), 7.61 (d, $J=3.4$ Hz, 1 H), 7.40 - 7.47 (m, 3 H), 7.35 (t, $J=7.5$ Hz, 2 H), 7.30 (d, $J=7.4$ Hz, 2 H), 7.26 (t, $J=7.2$ Hz, 1 H), 7.20 (d, $J=15.8$ Hz, 1 H), 6.96 (s, 1 H), 6.79 (dd, $J=3.1, 1.4$ Hz, 1 H), 5.07 (s, 2 H); ^{13}C NMR (75 MHz, DMSO- d_6) δ ppm 169.4, 159.3, 150.8, 146.7, 140.6, 137.3, 136.6, 135.0, 130.3, 129.0, 128.8, 128.4, 127.5, 126.9, 118.9, 114.0, 113.6, 112.6, 42.6; HRMS (ESI) m/z: 355.1436 found (calcd for $\text{C}_{23}\text{H}_{19}\text{N}_2\text{O}_2^+$, $[\text{M}+\text{H}]^+$ 355.1441).



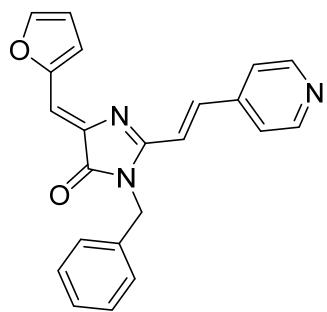
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (1bd)

Dark-red solid (155 mg, 42%); mp 174-176 °C; ^1H NMR (700 MHz, DMSO- d_6) δ ppm 10.06 (s, 1 H), 7.91 - 7.98 (m, 2 H), 7.62 (d, $J=8.4$ Hz, 2 H), 7.56 (d, $J=3.4$ Hz, 1 H), 7.34 (t, $J=7.5$ Hz, 2 H), 7.25 - 7.30 (m, 3 H), 6.94 (d, $J=15.6$ Hz, 1 H), 6.88 (s, 1 H), 6.82 (d, $J=8.4$ Hz, 2 H), 6.77 (d, $J=1.7$ Hz, 1 H), 5.03 (s, 2 H); ^{13}C NMR (75 MHz, DMSO- d_6) δ ppm 169.5, 159.9, 159.7, 151.0, 146.3, 141.1, 137.3, 136.8, 130.5, 128.8, 127.5, 126.9, 126.2, 118.3, 115.9, 113.8, 111.3, 109.7, 42.5; HRMS (ESI) m/z: 371.1384 found (calcd for $\text{C}_{23}\text{H}_{19}\text{N}_2\text{O}_3^+$, $[\text{M}+\text{H}]^+$ 371.1390).



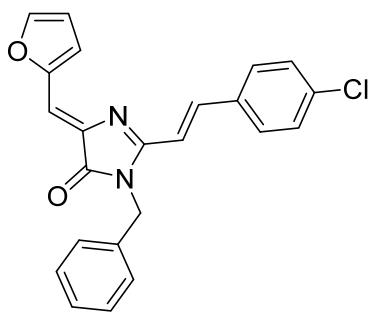
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (1be)

Dark-red solid (173 mg, 45%); mp 168-170 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.94 - 8.04 (m, 2 H), 7.74 (d, *J*=8.7 Hz, 2 H), 7.59 (d, *J*=3.4 Hz, 1 H), 7.23 - 7.39 (m, 5 H), 6.97 - 7.09 (m, 3 H), 6.90 (s, 1 H), 6.78 (br. s., 1 H), 5.05 (s, 2 H), 3.81 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 161.2, 159.6, 150.9, 146.4, 140.6, 137.3, 136.8, 130.3, 128.8, 127.7, 127.5, 126.9, 118.4, 114.5, 113.9, 111.7, 110.9, 42.5, 29.0; HRMS (ESI) m/z: 385.1542 found (calcd for C₂₄H₂₁N₂O₃⁺, [M+H]⁺ 385.1547).



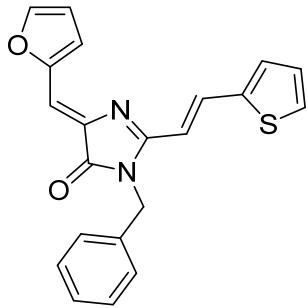
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-(pyridin-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (1bf)

Brown solid (85 mg, 24%); mp 184-186 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 8.64 (d, *J*=5.9 Hz, 2 H), 8.02 (d, *J*=1.1 Hz, 1 H), 7.97 (d, *J*=15.8 Hz, 1 H), 7.72 (d, *J*=6.1 Hz, 2 H), 7.64 (d, *J*=3.6 Hz, 1 H), 7.47 (d, *J*=15.8 Hz, 1 H), 7.35 (t, *J*=7.5 Hz, 2 H), 7.28 - 7.32 (m, 2 H), 7.26 (t, *J*=7.2 Hz, 1 H), 7.03 (s, 1 H), 6.81 (dd, *J*=2.9, 1.7 Hz, 1 H), 5.08 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.6, 150.7, 150.4, 147.2, 141.9, 137.7, 137.2, 136.3, 128.8, 127.6, 126.9, 122.0, 119.6, 118.2, 114.1, 113.8, 42.6; HRMS (ESI) m/z: 356.1389 found (calcd for C₂₂H₁₈N₃O₂⁺, [M+H]⁺ 356.1394).



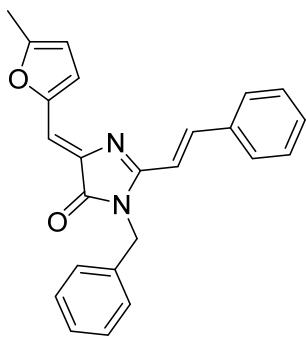
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (1bg)

Orange solid (58 mg, 15%); mp 189-191 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 8.01 (d, *J*=15.8 Hz, 1 H), 7.99 (d, *J*=1.1 Hz, 1 H), 7.82 (d, *J*=8.4 Hz, 2 H), 7.61 (d, *J*=3.4 Hz, 1 H), 7.51 (d, *J*=8.6 Hz, 2 H), 7.34 (t, *J*=7.6 Hz, 2 H), 7.28 (d, *J*=7.4 Hz, 2 H), 7.22 - 7.27 (m, 2 H), 6.96 (s, 1 H), 6.79 (d, *J*=1.3 Hz, 1 H), 5.06 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 159.1, 150.8, 146.8, 139.2, 137.2, 136.5, 134.8, 134.0, 130.1, 129.0, 128.8, 127.5, 126.9, 119.1, 114.4, 114.0, 112.8, 42.6; HRMS (ESI) m/z: 389.1047 found (calcd for C₂₃H₁₈ClN₂O₂⁺, [M+H]⁺ 389.1051).



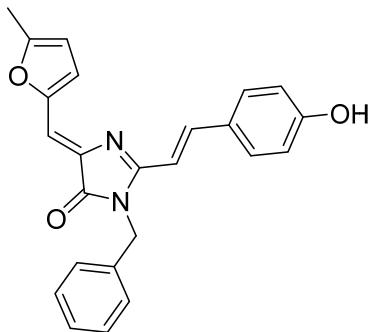
(Z)-5-((furan-2-ylmethylene)-3-benzyl-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (1bh)

Red solid (133 mg, 37%); mp 145-147 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.16 (d, *J*=15.6 Hz, 1 H), 7.98 (br. s, 1 H), 7.73 (d, *J*=5.3 Hz, 1 H), 7.56 - 7.62 (m, 2 H), 7.32 - 7.39 (m, 2 H), 7.24 - 7.30 (m, 3 H), 7.17 (dd, *J*=4.5, 3.8 Hz, 1 H), 6.93 (s, 1 H), 6.73 - 6.84 (m, 2 H), 5.02 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 159.0, 150.9, 146.6, 140.3, 137.2, 136.7, 133.3 (2 C), 131.8, 130.2, 128.8, 127.6, 126.9, 118.8, 113.9, 112.1 (2 C), 42.5; HRMS (ESI) m/z: 361.1001 found (calcd for C₂₁H₁₇N₂O₂S⁺, [M+H]⁺ 361.1005).



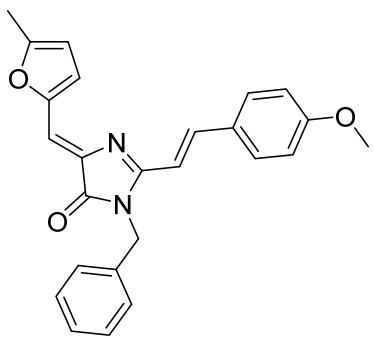
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (2bc)

Dark-red solid (224 mg, 61%); mp 105-107 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.99 (d, *J*=15.8 Hz, 1 H), 7.76 (d, *J*=7.1 Hz, 2 H), 7.56 (d, *J*=3.2 Hz, 1 H), 7.40 – 7.46 (m, 3 H), 7.34 (t, *J*=7.6 Hz, 2 H), 7.29 (d, *J*=7.2 Hz, 2 H), 7.26 (t, *J*=7.2 Hz, 1 H), 7.18 (d, *J*=15.8 Hz, 1 H), 6.88 (s, 1 H), 6.46 (d, *J*=3.2 Hz, 1 H), 5.05 (s, 2 H), 2.41 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 158.3, 156.5, 149.7, 140.1, 137.3, 135.5, 135.1, 130.2, 129.0, 128.8, 128.3, 127.5, 126.9, 120.7, 113.7, 112.7, 111.0, 42.5, 13.8; HRMS (ESI) m/z: 369.1592 found (calcd for C₂₄H₂₁N₂O₂⁺, [M+H]⁺ 369.1598).



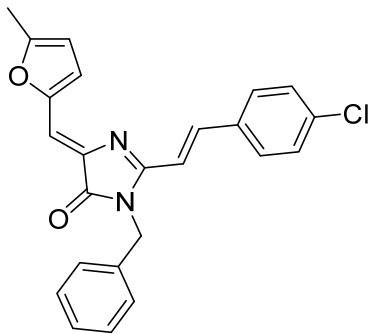
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (2bd)

Dark-red solid (242 mg, 63%); mp ~220 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 10.05 (s, 1 H), 7.91 (d, *J*=15.7 Hz, 1 H), 7.61 (d, *J*=8.4 Hz, 2 H), 7.51 (d, *J*=3.4 Hz, 1 H), 7.24 - 7.37 (m, 5 H), 6.93 (d, *J*=15.5 Hz, 1 H), 6.76 - 6.85 (m, 3 H), 6.44 (d, *J*=3.0 Hz, 1 H), 5.02 (s, 2 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.4, 159.8, 158.8, 156.1, 149.8, 140.6, 137.4, 135.8, 130.4, 128.7, 127.5, 126.9, 126.3, 120.1, 115.9, 111.5, 110.9, 109.8, 42.5, 13.8; HRMS (ESI) m/z: 385.1541 found (calcd for C₂₄H₂₁N₂O₃⁺, [M+H]⁺ 385.1547).



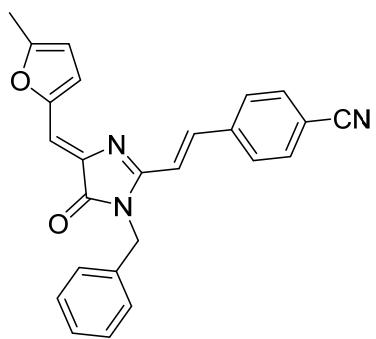
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (2be)

Dark-red solid (107 mg, 27%); mp 146-148 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.96 (d, *J*=15.6 Hz, 1 H), 7.73 (d, *J*=8.7 Hz, 2 H), 7.54 (d, *J*=3.3 Hz, 1 H), 7.24 - 7.37 (m, 5 H), 6.97 - 7.06 (m, 3 H), 6.83 (s, 1 H), 6.45 (d, *J*=3.1 Hz, 1 H), 5.03 (s, 2 H), 3.81 (s, 3 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 161.1, 158.7, 156.2, 149.8, 140.1, 137.4, 135.7, 130.1, 128.7, 127.8, 127.5, 126.9, 120.3, 114.5, 113.4, 111.8, 110.9, 55.4, 42.5, 13.8; HRMS (ESI) m/z: 399.1699 found (calcd for C₂₅H₂₃N₂O₃⁺, [M+H]⁺ 399.1703).



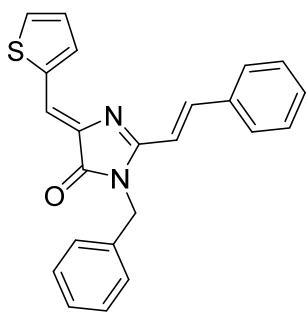
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (2bg)

Red solid (180 mg, 45%); mp 168-170 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.98 (d, *J*=15.8 Hz, 1 H), 7.81 (d, *J*=8.5 Hz, 2 H), 7.57 (d, *J*=3.2 Hz, 1 H), 7.51 (d, *J*=8.4 Hz, 2 H), 7.18 - 7.38 (m, 6 H), 6.88 (s, 1 H), 6.46 (d, *J*=3.1 Hz, 1 H), 5.05 (s, 2 H), 2.40 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.2, 156.7, 149.7, 138.7, 137.3, 135.4, 134.6, 134.0, 130.0, 129.0, 128.8, 127.5, 126.9, 120.9, 114.4, 112.9, 111.1, 42.5, 13.8; HRMS (ESI) m/z: 403.1204 found (calcd for C₂₄H₂₀ClN₂O₂⁺, [M+H]⁺ 403.1208).



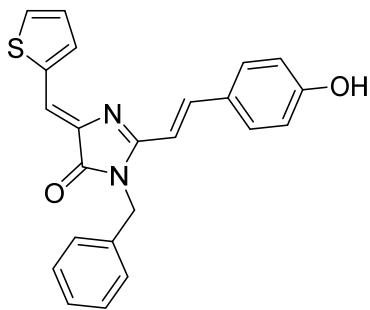
(Z)-5-((5-methylfuran-2-yl)methylene)-3-benzyl-2-((E)-4-cyanostyryl)-3,5-dihydro-4*H*-imidazol-4-one (2bi)

Red solid (189 mg, 48%); mp 167-169 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.03 (d, *J*=15.8 Hz, 1 H), 7.97 (d, *J*=8.4 Hz, 2 H), 7.90 (d, *J*=8.4 Hz, 2 H), 7.60 (d, *J*=3.4 Hz, 1 H), 7.39 (d, *J*=15.6 Hz, 1 H), 7.23 - 7.23 (m, 5 H), 6.93 (s, 1 H), 6.48 (d, *J*=3.2 Hz, 1 H), 5.06 (s, 2 H), 2.41 (s, 3 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.1, 157.7, 156.9, 149.6, 139.5, 137.8, 137.2, 135.3, 132.6, 128.7 (2 C), 127.4, 126.8, 121.3, 118.6, 117.1, 113.5, 111.7, 111.1, 42.5, 13.7; HRMS (ESI) m/z: 394.1557 found (calcd for C₂₅H₂₀N₃O₂⁺, [M+H]⁺ 394.1550).



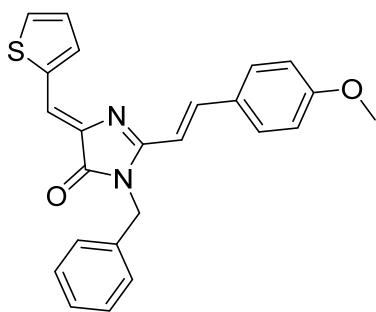
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (3bc)

Orange solid (222 mg, 60%); mp 185-187 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.92 – 7.96 (m, 2 H), 7.77 (d, *J*=3.6 Hz, 1 H), 7.75 (d, *J*=6.8 Hz, 2 H), 7.48 (s, 1 H), 7.42 - 7.47 (m, 3 H), 7.35 (t, *J*=7.6 Hz, 2 H), 7.30 (d, *J*=7.3 Hz, 2 H), 7.26 (t, *J*=7.3 Hz, 1 H), 7.18 - 7.23 (m, 2 H), 5.07 (s, 2 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 169.1, 158.5, 140.2, 138.0, 137.3, 136.7, 135.3, 135.1, 134.9, 130.3, 129.0, 128.8, 128.3, 127.9, 127.5, 126.9, 120.0, 113.8, 42.5; HRMS (ESI) m/z: 371.1207 found (calcd for C₂₃H₁₉N₂OS⁺, [M+H]⁺ 371.1213).



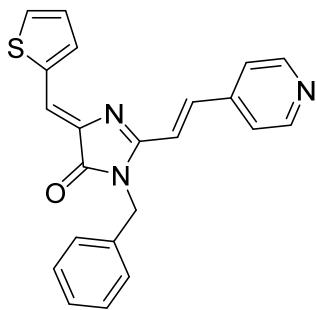
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (3bd)

Orange solid (154 mg, 40%); mp ~250 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 10.08 (br. s., 1 H), 7.83 - 7.93 (m, 2 H), 7.73 (d, *J*=3.5 Hz, 1 H), 7.60 (d, *J*=8.6 Hz, 2 H), 7.40 (s, 1 H), 7.23 - 7.38 (m, 5 H), 7.19 (dd, *J*=5.1, 3.8 Hz, 1 H), 6.96 (d, *J*=15.7 Hz, 1 H), 6.82 (d, *J*=8.6 Hz, 2 H), 5.04 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 159.9, 158.9, 140.7, 138.1, 137.4, 136.9, 134.7, 134.5, 130.4, 128.8, 127.8, 127.5, 126.9, 126.1, 118.7, 116.0, 109.9, 42.5; HRMS (ESI) m/z: 387.1156 found (calcd for C₂₃H₁₉N₂O₂S⁺, [M+H]⁺ 387.1162).



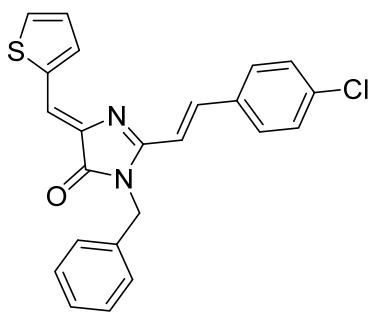
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-4-methoxystyryl)-3,5-dihydro-4H-imidazol-4-one (3be)

Red solid (200 mg, 49%); mp 204-206 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.86 - 7.97 (m, 2 H), 7.67 - 7.77 (m, 3 H), 7.42 (s, 1 H), 7.24 - 7.38 (m, 5 H), 7.20 (dd, *J*=5.0, 3.8 Hz, 1 H), 6.96 - 7.09 (m, 3 H), 5.05 (s, 2 H), 3.82 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 161.1, 158.8, 140.2, 138.1, 137.4, 136.9, 134.8, 134.7, 130.2, 128.8, 127.8, 127.6, 127.5, 126.9, 119.1, 114.6, 111.1, 55.4, 42.5; HRMS (ESI) m/z: 401.1314 found (calcd for C₂₄H₂₁N₂O₂S⁺, [M+H]⁺ 401.1318).



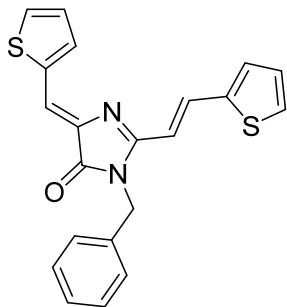
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-2-(pyridine-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (3bf)

Orange solid (156 mg, 42%); mp 173-175 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.65 (d, *J*=5.3 Hz, 2 H), 7.99 (d, *J*=5.0 Hz, 1 H), 7.88 (d, *J*=15.7 Hz, 1 H), 7.81 (d, *J*=3.6 Hz, 1 H), 7.72 (d, *J*=5.9 Hz, 2 H), 7.56 (s, 1 H), 7.48 (d, *J*=15.7 Hz, 1 H), 7.26 - 7.38 (m, 5 H), 7.22 (dd, *J*=4.9, 3.9 Hz, 1 H), 5.08 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.9, 157.8, 150.4, 141.8, 137.8, 137.3, 137.2, 136.5, 135.9, 135.7, 128.8, 128.0, 127.6, 126.9, 122.0, 121.4, 118.4, 42.6; HRMS (ESI) m/z: 372.1160 found (calcd for C₂₂H₁₈N₃OS⁺, [M+H]⁺ 372.1165).



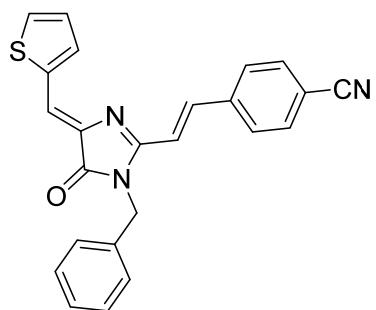
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-4-chlorostyryl)-3,5-dihydro-4H-imidazol-4-one (3bg)

Orange solid (141 mg, 35%); mp 210-212 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 7.95 (d, *J*=5.0 Hz, 1 H), 7.92 (d, *J*=15.8 Hz, 1 H), 7.80 (d, *J*=8.4 Hz, 2 H), 7.78 (d, *J*=3.6 Hz, 1 H), 7.51 (d, *J*=8.6 Hz, 2 H), 7.48 (s, 1 H), 7.34 (t, *J*=7.5 Hz, 2 H), 7.29 (d, *J*=7.4 Hz, 2 H), 7.23 - 7.28 (m, 2 H), 7.21 (dd, *J*=4.9, 3.9 Hz, 1 H), 5.06 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.1, 158.3, 138.8, 138.0, 137.3, 136.7, 135.4, 135.2, 134.7, 133.9, 130.0, 129.0, 128.8, 127.9, 127.5, 126.9, 120.3, 114.6, 42.5; HRMS (ESI) m/z: 405.0819 found (calcd for C₂₃H₁₈ClN₂OS⁺, [M+H]⁺ 405.0823).



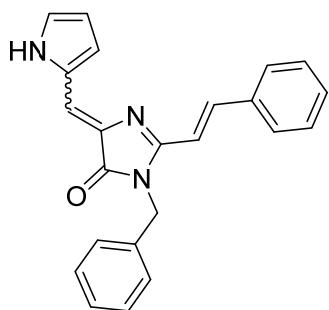
(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (3bh)

Orange solid (165 mg, 44%); mp 182-184 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 8.06 (d, *J*=15.5 Hz, 1 H), 7.93 (d, *J*=5.1 Hz, 1 H), 7.70 - 7.79 (m, 2 H), 7.59 (d, *J*=3.4 Hz, 1 H), 7.46 (s, 1 H), 7.24 - 7.40 (m, 5 H), 7.13 - 7.23 (m, 2 H), 6.80 (d, *J*=15.4 Hz, 1 H), 5.02 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.0, 158.2, 140.1, 138.0, 137.2, 136.8, 135.1, 134.9, 132.8, 131.7, 130.1, 128.8 (3 C), 127.9, 127.6, 126.9, 119.6, 112.2, 42.5; HRMS (ESI) m/z: 377.0772 found (calcd for C₂₁H₁₇N₂OS₂⁺, [M+H]⁺ 377.0777).



(Z)-5-(thiophen-2-ylmethylene)-3-benzyl-2-((E)-4-cyanostyryl)-3,5-dihydro-4*H*-imidazol-4-one (3bi)

Orange solid (40 mg, 10%); mp 193-195 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 7.88 - 8.01 (m, 6 H), 7.80 (d, *J*=3.8 Hz, 1 H), 7.54 (s, 1 H), 7.42 (d, *J*=16.0 Hz, 1 H), 7.25 - 7.37 (m, 5 H), 7.22 (dd, *J*=4.5, 4.1 Hz, 1 H), 5.08 (s, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.0, 157.9, 139.4, 138.0, 137.9, 137.2, 136.6, 135.8, 135.6, 132.8, 128.9, 128.8, 128.0, 127.5, 126.9, 121.1, 118.7, 117.4, 111.9, 42.6; HRMS (ESI) m/z: 396.1154 found (calcd for C₂₄H₁₈N₃OS⁺, [M+H]⁺ 396.1165).



5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one (4bc)

Dark-red solid (243 mg, 69%); mp 120-122 °C.

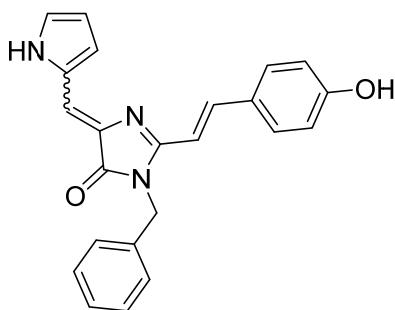
It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(*E*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.97 (br. s., 1 H), 7.71 - 7.77 (m, 1 H), 7.70 (d, *J*=7.3 Hz, 2 H), 7.23 - 7.46 (m, 9 H), 7.14 (d, *J*=15.8 Hz, 1 H), 6.94 (br. s., 1 H), 6.39 (d, *J*=3.5 Hz, 1 H), 5.15 (s, 2 H).

(*Z*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.45 (br. s., 1 H), 8.15 (d, *J*=15.8 Hz, 1 H), 7.71 - 7.77 (m, 2 H), 7.23 - 7.46 (m, 8 H), 7.14 (d, *J*=15.8 Hz, 1 H), 7.03 (s, 1 H), 6.94 (br. s., 1 H), 6.31 (d, *J*=3.3 Hz, 1 H), 5.05 (s, 2 H).

¹³C and HRMS data presented as is for a mixture:

¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.8, 168.0, 155.8, 152.6, 139.2, 137.5, 137.3, 137.2, 135.4, 135.3, 133.3, 133.1, 129.8, 129.6, 129.2, 128.9, 128.8 (2 C), 128.7 (2 C), 128.0, 127.8, 127.5, 127.4, 126.9, 126.8, 126.7, 126.6, 125.8, 121.3, 119.3, 116.7, 113.8, 113.6, 112.1, 111.1, 42.8, 42.4; HRMS (ESI) m/z: 354.1597 found (calcd for C₂₃H₂₀N₃O⁺, [M+H]⁺ 354.1601).



5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (4bd)

Red solid (79 mg, 22%); mp ~240 °C with decomposition.

It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(*E*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one

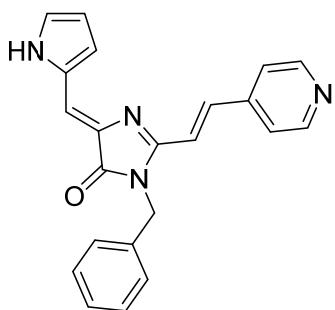
¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.93 (br. s., 1 H), 9.91 (br. s., 1 H), 7.66 (d, *J*=15.8 Hz, 1 H), 7.54 (d, *J*=8.6 Hz, 2 H), 7.23 - 7.36 (m, 7 H), 6.85 - 6.92 (m, 2 H), 6.79 (d, *J*=8.6 Hz, 2 H), 6.35 - 6.39 (m, 1 H), 5.11 (s, 2 H).

(*Z*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.41 (br. s., 1 H), 9.98 (br. s., 1 H), 8.07 (d, *J*=15.6 Hz, 1 H), 7.58 (d, *J*=8.6 Hz, 4 H), 7.23 - 7.36 (m, 6 H), 6.97 (s, 1 H), 6.85 - 6.92 (m, 2 H), 6.82 (d, *J*=8.6 Hz, 2 H), 6.27 - 6.30 (m, 1 H), 5.02 (s, 2 H).

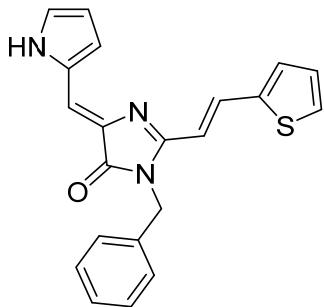
¹³C and HRMS data presented as is for a mixture:

¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 168.9, 168.1, 159.5, 159.2, 156.4, 153.2, 139.7, 137.6 (2 C), 137.3, 133.5, 133.3, 130.0, 129.7, 129.2, 128.9, 128.7 (2 C), 127.4 (2 C), 126.9, 126.8, 126.6, 126.5, 126.2, 126.1, 124.8, 120.7, 118.7, 115.9, 115.8, 115.5, 111.9, 110.9, 110.1, 109.8, 42.8, 42.3; HRMS (ESI) m/z: 370.1544 found (calcd for C₂₃H₂₀N₃O₂⁺, [M+H]⁺ 370.1550).



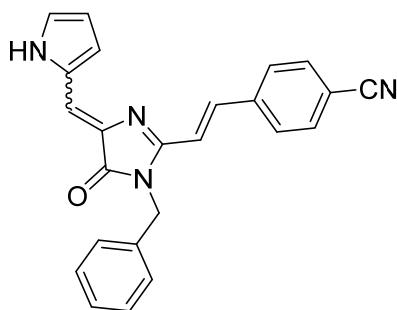
(Z)-5-((1H-pyrrol-2-yl)methylene)-3-benzyl-2-((E)-2-(pyridine-4-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (4bf)

Brown solid (193 mg, 55%); mp 196-198 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.48 (br. s., 1 H), 8.64 (dd, *J*=4.5, 1.4 Hz, 2 H), 8.09 (d, *J*=15.8 Hz, 1 H), 7.66 (dd, *J*=4.6, 1.3 Hz, 2 H), 7.41 (d, *J*=15.8 Hz, 1 H), 7.34 (t, *J*=7.5 Hz, 2 H), 7.28 - 7.31 (m, 3 H), 7.26 (t, *J*=7.2 Hz, 1 H), 7.10 (s, 1 H), 6.99 (br. s., 1 H), 6.33 (dt, *J*=3.7, 2.3 Hz, 1 H), 5.07 (s, 2 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.6, 154.9, 150.3, 142.3, 137.4, 136.2, 133.1, 128.8, 128.7 (2 C), 127.4, 126.8, 121.6, 120.0, 118.1, 117.8, 111.3, 42.4; HRMS (ESI) m/z: 355.1548 found (calcd for C₂₂H₁₉N₄O⁺, [M+H]⁺ 355.1553).



(Z)-5-((1H-pyrrol-2-yl)methylene)-3-benzyl-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (4bh)

Red solid (180 mg, 50%); mp 152-154 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.44 (br. s., 1 H), 8.28 (d, *J*=15.4 Hz, 1 H), 7.69 (d, *J*=5.0 Hz, 1 H), 7.50 (d, *J*=3.4 Hz, 1 H), 7.34 - 7.36 (m, 2 H), 7.26 - 7.28 (m, 4 H), 7.16 (dd, *J*=5.0, 3.8 Hz, 1 H), 7.01 (s, 1 H), 6.77 (d, *J*=15.4 Hz, 1 H), 6.30 (d, *J*=3.4 Hz, 1 H), 5.01 (s, 2 H); ¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.7, 155.4, 140.6, 137.4, 133.3, 131.9, 130.2, 129.2, 128.9, 128.7, 128.6, 127.4, 126.8, (2 C), 119.2, 116.3, 112.3, 111.0, 42.3; HRMS (ESI) m/z: 360.1155 found (calcd for C₂₁H₁₈N₃OS⁺, [M+H]⁺ 360.1165).



5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-cyanostyryl)-3,5-dihydro-4*H*-imidazol-4-one (4bi**)**

Red solid (210 mg, 56%); mp 201-203 °C.

It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(*E*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-cyanostyryl)-3,5-dihydro-4*H*-imidazol-4-one

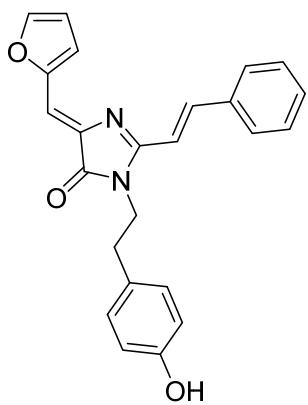
¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 13.00 (br. s., 1 H), 7.90 - 7.94 (m, 2 H), 7.86 - 7.88 (m, 2 H), 7.79 (d, *J*=15.8 Hz, 1 H), 7.41 - 7.43 (m, 2 H), 7.25 - 7.37 (m, 6 H), 6.99 (br. s., 1 H), 6.41 (ddd, *J*=3.8, 2.4, 2.2 Hz, 1 H), 5.16 (s, 2 H).

(*Z*)-5-((1*H*-pyrrol-2-yl)methylene)-3-benzyl-2-((*E*)-4-cyanostyryl)-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.47 (br. s., 1 H), 8.18 (d, *J*=15.8 Hz, 1 H), 7.90 - 7.94 (m, 4 H), 7.25 - 7.37 (m, 7 H), 7.08 (s, 1 H), 6.99 (br. s., 1 H), 6.33 (ddd, *J*=3.7, 2.3, 2.1 Hz, 1 H), 5.06 (s, 2 H).

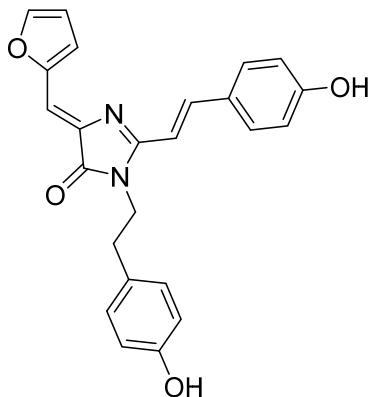
¹³C and HRMS data presented as is for a mixture:

¹³C NMR (176 MHz, DMSO-*d*₆) δ ppm 168.6, 167.8, 155.1, 151.9, 139.8, 137.4, 137.1, 137.0, 135.0, 133.2, 132.9, 132.7 (2 C), 132.6, 129.2, 128.9, 128.7, 128.6, 128.4 (2 C), 128.3, 127.4 (2 C), 127.1, 126.9, 126.8, 126.5, 121.8, 119.9, 118.6, 117.5, 117.3, 117.1, 112.4, 111.4, 111.3, 111.2, 42.9, 42.4; HRMS (ESI) m/z: 379.1545 found (calcd for C₂₄H₁₉N₄O⁺, [M+H]⁺ 379.1553).



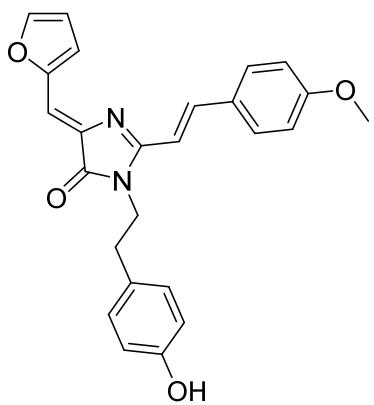
(Z)-5-(furan-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (1cc)

Brown solid (316 mg, 82%); mp 193–195 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.13 (s, 1 H), 7.96 (d, *J*=1.1 Hz, 1 H), 7.92 (d, *J*=15.6 Hz, 1 H), 7.75 (d, *J*=7.2 Hz, 2 H), 7.55 (d, *J*=3.4 Hz, 1 H), 7.46 (t, *J*=7.2 Hz, 2 H), 7.41 – 7.44 (m, 1 H), 7.00 (d, *J*=8.4 Hz, 2 H), 6.89 (d, *J*=15.6 Hz, 1 H), 6.85 (s, 1 H), 6.77 (dd, *J*=3.1, 1.5 Hz, 1 H), 6.63 (d, *J*=8.4 Hz, 2 H), 3.97 (t, *J*=7.0 Hz, 2 H), 2.76 (t, *J*=7.0 Hz, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 159.6, 156.0, 150.9, 146.5, 140.1, 136.8, 135.1, 130.1, 129.9, 128.9, 128.4, 128.0, 118.5, 115.2, 113.9, 113.6, 111.8, 41.3, 34.1; HRMS (ESI) m/z: 385.1542 found (calcd for C₂₄H₂₁N₂O₃⁺, [M+H]⁺ 385.1547).



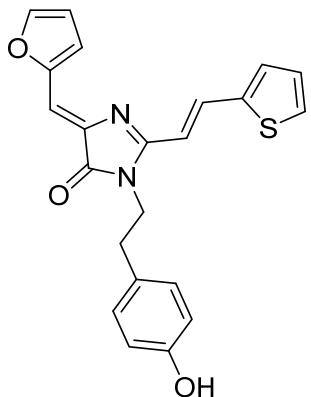
(Z)-5-(furan-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (1cd)

Red solid (133 mg, 33%); mp ~220 °C with decomposition; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 10.03 (s, 1 H), 9.13 (s, 1 H), 7.93 (d, *J*=1.1 Hz, 1 H), 7.87 (d, *J*=15.4 Hz, 1 H), 7.61 (d, *J*=8.6 Hz, 2 H), 7.50 (d, *J*=3.4 Hz, 1 H), 7.00 (d, *J*=8.4 Hz, 2 H), 6.84 (d, *J*=8.6 Hz, 2 H), 6.76 (s, 1 H), 6.74 – 6.76 (m, 1 H), 6.68 (d, *J*=15.6 Hz, 1 H), 6.63 (d, *J*=8.4 Hz, 2 H), 3.93 (t, *J*=7.0 Hz, 2 H), 2.75 (t, *J*=7.0 Hz, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 160.0, 159.7, 155.9, 151.0, 146.0, 140.6, 137.0, 130.4, 129.8, 128.1, 126.3, 117.8, 115.8, 115.2, 113.7, 110.6, 109.7, 41.2, 34.1; HRMS (ESI) m/z: 401.1491 found (calcd for C₂₄H₂₁N₂O₄⁺, [M+H]⁺ 401.1496).



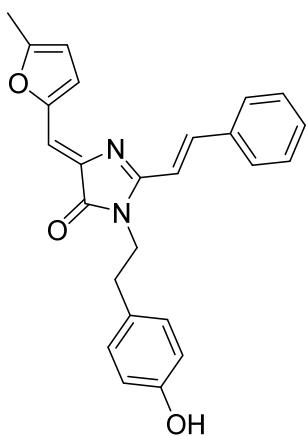
(Z)-5-(furan-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-4-methoxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (1ce)

Brown solid (213 mg, 51%); mp 201-203 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.12 (s, 1 H), 7.93 (br. s, 1 H), 7.90 (d, *J*=15.6 Hz, 1 H), 7.72 (d, *J*=8.6 Hz, 2 H), 7.52 (d, *J*=3.2 Hz, 1 H), 7.02 (d, *J*=8.8 Hz, 2 H), 7.00 (d, *J*=8.2 Hz, 2 H), 6.79 (s, 1 H), 6.72 - 6.78 (m, 2 H), 6.63 (d, *J*=8.4 Hz, 2 H), 3.95 (t, *J*=6.9 Hz, 2 H), 3.83 (s, 3 H), 2.75 (t, *J*=6.8 Hz, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.3, 161.0, 155.9, 151.0, 146.2, 133.0, 130.2, 129.9, 129.8, 128.1, 127.9, 118.1, 115.2 (2 C), 114.4, 113.8, 113.4, 110.9, 55.4, 41.2, 34.1; HRMS (ESI) m/z: 415.1648 found (calcd for C₂₅H₂₃N₂O₄⁺, [M+H]⁺ 415.1652).



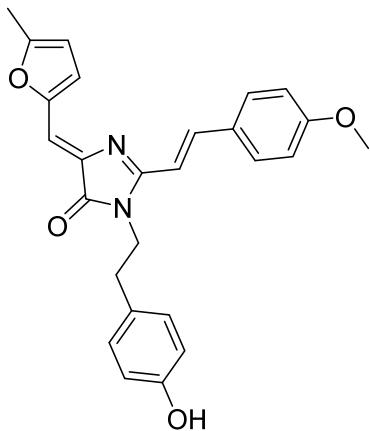
(Z)-5-(furan-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4*H*-imidazol-4-one (1ch)

Brown solid (334 mg, 86%); mp 169-171 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.12 (s, 1 H), 8.06 (d, *J*=15.4 Hz, 1 H), 7.95 (br. s., 1 H), 7.75 (d, *J*=4.6 Hz, 1 H), 7.58 (br. s., 1 H), 7.53 (d, *J*=2.9 Hz, 1 H), 7.16 - 7.19 (m, 1 H), 6.97 (d, *J*=8.2 Hz, 2 H), 6.82 (s, 1 H), 6.76 (br. s., 1 H), 6.63 (d, *J*=8.0 Hz, 2 H), 6.49 (d, *J*=15.3 Hz, 1 H), 3.91 (t, *J*=6.6 Hz, 2 H), 2.74 (t, *J*=6.6 Hz, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 159.3, 156.0, 150.9, 146.4, 140.4, 136.9, 132.9, 131.6, 129.9, 129.8, 128.6, 128.0, 118.4, 115.3, 113.8, 111.9, 111.4, 41.4, 34.0; HRMS (ESI) m/z: 391.1106 found (calcd for C₂₂H₁₉N₂O₃S⁺, [M+H]⁺ 391.1111).



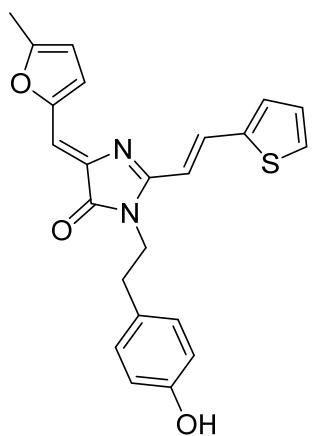
(Z)-5-((5-methylfuran-2-yl)methylene)-3-(4-hydroxyphenethyl)-2-((E)-styryl)-3,5-dihydro-4*H*-imidazol-4-one (2cc)

Red solid (212 mg, 53%); mp ~210 °C with decomposition; ¹H NMR (300 MHz, DMSO-*d*₆) δ ppm 9.14 (s, 1 H), 7.89 (d, *J*=15.7 Hz, 1 H), 7.74 (d, *J*=6.6 Hz, 2 H), 7.39 - 7.52 (m, 4 H), 7.00 (d, *J*=8.2 Hz, 2 H), 6.88 (d, *J*=15.7 Hz, 1 H), 6.77 (s, 1 H), 6.63 (d, *J*=8.3 Hz, 2 H), 6.43 (d, *J*=2.8 Hz, 1 H), 3.95 (t, *J*=6.5 Hz, 2 H), 2.75 (t, *J*=6.5 Hz, 2 H), 2.39 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 158.7, 156.3, 155.9, 149.7, 139.7, 135.7, 135.2, 130.0, 129.9, 128.9, 128.3, 128.1, 120.3, 115.2, 113.6, 111.9, 110.9, 41.2, 34.1, 13.8; HRMS (ESI) m/z: 399.1699 found (calcd for C₂₅H₂₃N₂O₃⁺, [M+H]⁺ 399.1703).



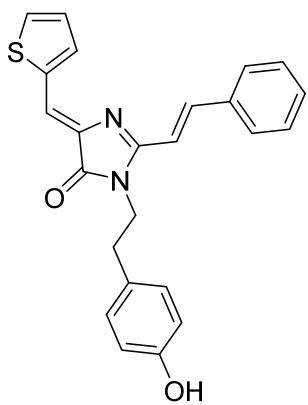
(Z)-5-((5-methylfuran-2-yl)methylene)-3-(4-hydroxyphenethyl)-2-((E)-4-methoxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (2ce)

Brown solid (146 mg, 34%); mp 192-194 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.12 (s, 1 H), 7.86 (d, *J*=15.4 Hz, 1 H), 7.71 (d, *J*=8.8 Hz, 2 H), 7.47 (d, *J*=3.1 Hz, 1 H), 6.99 - 7.03 (m, 4 H), 6.71 - 6.75 (m, 2 H), 6.63 (d, *J*=8.2 Hz, 2 H), 6.42 (br. s., 1 H), 3.94 (t, *J*=7.0 Hz, 2 H), 3.83 (s, 3 H), 2.75 (t, *J*=7.0 Hz, 2 H), 2.39 (s, 3 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.2, 160.9, 159.0, 155.9 (2 C), 149.8, 139.7, 135.9, 130.1, 129.9, 128.1, 127.9, 119.9, 115.2, 114.4, 111.1, 110.9, 110.8, 55.4, 41.2, 34.1, 13.8; HRMS (ESI) m/z: 429.1806 found (calcd for C₂₆H₂₅N₂O₄⁺, [M+H]⁺ 429.1809).



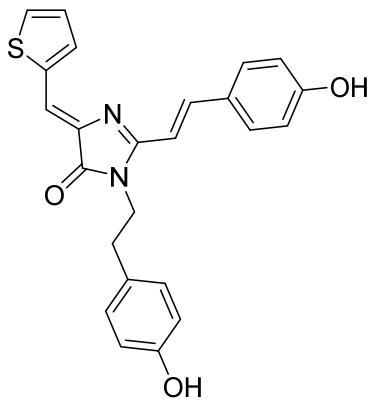
(Z)-5-((5-methylfuran-2-yl)methylene)-3-(4-hydroxyphenethyl)-2-((E)-2-(thiophen-2-yl)vinyl)-3,5-dihydro-4H-imidazol-4-one (2ch)

Dark-red solid (102 mg, 25%); mp 244-246 °C; ^1H NMR (700 MHz, DMSO- d_6) δ ppm 9.13 (s, 1 H), 8.02 (d, $J=15.4$ Hz, 1 H), 7.73 (d, $J=5.0$ Hz, 1 H), 7.56 (d, $J=3.2$ Hz, 1 H), 7.48 (d, $J=3.2$ Hz, 1 H), 7.17 (dd, $J=5.0$, 3.6 Hz, 1 H), 6.97 (d, $J=8.2$ Hz, 2 H), 6.74 (s, 1 H), 6.63 (d, $J=8.4$ Hz, 2 H), 6.48 (d, $J=15.4$ Hz, 1 H), 6.43 (d, $J=3.1$ Hz, 1 H), 3.90 (t, $J=6.9$ Hz, 2 H), 2.73 (t, $J=6.9$ Hz, 2 H), 2.39 (s, 3 H); ^{13}C NMR (176 MHz, DMSO- d_6) δ ppm 169.0, 158.3, 156.1, 155.9, 149.7, 140.4, 135.7, 132.3, 131.2, 129.7, 129.6, 128.5, 128.0, 120.1, 115.2, 112.0, 111.4, 110.8, 41.3, 34.0, 13.7; HRMS (ESI) m/z: 405.1263 found (calcd for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_3\text{S}^+$, $[\text{M}+\text{H}]^+$ 405.1267).



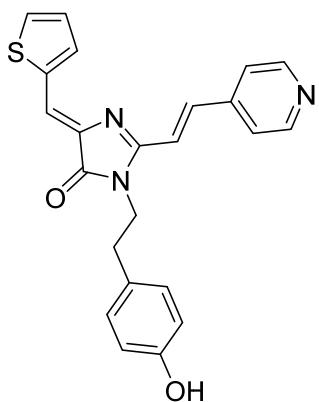
(Z)-5-(thiophen-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-styryl)-3,5-dihydro-4H-imidazol-4-one (3cc)

Orange solid (219 mg, 55%); mp 101-103 °C; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 9.13 (s, 1 H), 7.91 (d, *J*=5.0 Hz, 1 H), 7.86 (d, *J*=15.6 Hz, 1 H), 7.70 - 7.77 (m, 3 H), 7.47 (t, *J*=7.2 Hz, 2 H), 7.44 (t, *J*=6.7 Hz, 1 H), 7.36 (s, 1 H), 7.19 (dd, *J*=5.1, 3.7 Hz, 1 H), 7.01 (m, *J*=8.4 Hz, 2 H), 6.91 (d, *J*=15.6 Hz, 1 H), 6.63 (m, *J*=8.4 Hz, 2 H), 3.97 (t, *J*=7.0 Hz, 2 H), 2.77 (t, *J*=7.0 Hz, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.0, 158.8, 156.0, 139.8, 138.0, 136.9, 135.0, 134.9, 134.7, 130.1, 129.9, 129.0, 128.3, 128.1, 127.8, 119.2, 115.2, 113.8, 41.2, 34.1; HRMS (ESI) m/z: 401.1314 found (calcd for C₂₄H₂₁N₂O₂S⁺, [M+H]⁺ 401.1318).



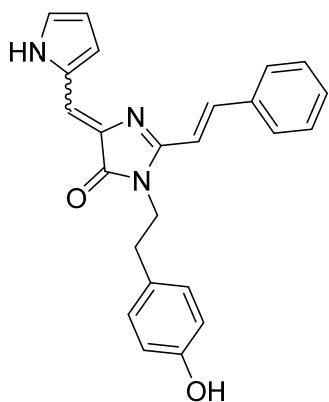
(Z)-5-(thiophen-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-4-hydroxystyryl)-3,5-dihydro-4H-imidazol-4-one (3cd)

Orange solid (200 mg, 48%); mp ~240 °C with decomposition; ¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 10.04 (br. s., 1 H), 9.13 (s, 1 H), 7.87 (d, *J*=5.0 Hz, 1 H), 7.81 (d, *J*=15.6 Hz, 1 H), 7.69 (d, *J*=2.9 Hz, 1 H), 7.59 (d, *J*=8.2 Hz, 2 H), 7.28 (s, 1 H), 7.16 - 7.18 (m, 1 H), 7.01 (d, *J*=7.8 Hz, 2 H), 6.85 (d, *J*=7.6 Hz, 2 H), 6.69 (d, *J*=15.4 Hz, 1 H), 6.64 (d, *J*=8.2 Hz, 2 H), 3.93 (t, *J*=6.9 Hz, 2 H), 2.76 (t, *J*=6.8 Hz, 2 H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ ppm 169.1, 159.7, 159.2, 155.9, 140.3, 138.2, 137.2, 134.3, 134.2, 130.4, 129.9, 128.1, 127.7, 126.3, 118.0, 115.9, 115.2, 109.9, 41.2, 34.2; HRMS (ESI) m/z: 417.1263 found (calcd for C₂₄H₂₁N₂O₃S⁺, [M+H]⁺ 417.1267).



(Z)-5-(thiophen-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((E)-2-(pyridine-4-yl)vinyl)-3,5-dihydro-4*H*-imidazol-4-one (3cf)

Brown solid (378 mg, 94%); mp ~230 °C with decomposition; ^1H NMR (300 MHz, DMSO-*d*₆) δ ppm 9.12 (s, 1 H), 8.65 (d, *J*=5.5 Hz, 2 H), 7.95 (d, *J*=4.9 Hz, 1 H), 7.69 - 7.78 (m, 2 H), 7.66 (d, *J*=5.5 Hz, 2 H), 7.44 (s, 1 H), 7.20 (dd, *J*=4.6, 4.1 Hz, 1 H), 7.10 (d, *J*=15.7 Hz, 1 H), 6.99 (d, *J*=8.1 Hz, 2 H), 6.60 (d, *J*=8.2 Hz, 2 H), 3.99 (t, *J*=6.2 Hz, 2 H), 2.76 (t, *J*=6.7 Hz, 2 H); ^{13}C NMR (201 MHz, DMSO-*d*₆) δ ppm 168.7, 158.0, 155.9, 150.1, 141.9, 137.8, 136.7, 136.4, 135.2, 135.0, 129.8, 127.9, 127.8, 121.8, 120.3, 118.2, 115.1, 41.2, 33.9; HRMS (ESI) m/z: 402.1267 found (calcd for C₂₃H₂₀N₃O₂S⁺, [M+H]⁺ 402.1271).



5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one (4cc)

Dark-red solid (249 mg, 65%); mp ~180 °C with decomposition.

It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(*E*)-5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one

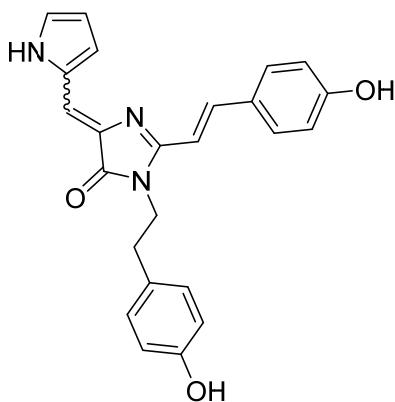
¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.99 (br. s., 1 H), 9.13 (s, 1 H), 7.69 (d, *J*=7.4 Hz, 2 H), 7.66 (d, *J*=15.6 Hz, 1 H), 7.42 - 7.47 (m, 3 H), 7.37 (br. s., 1 H), 7.29 (s, 1 H), 7.02 (d, *J*=8.4 Hz, 2 H), 6.89 (br. s., 1 H), 6.86 (d, *J*=15.8 Hz, 1 H), 6.60 - 6.66 (m, 2 H), 6.38 (ddd, *J*=3.6, 2.4, 2.2 Hz, 1 H), 4.04 (t, *J*=7.2 Hz, 2 H), 2.81 (t, *J*=7.1 Hz, 2 H).

(*Z*)-5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-styryl)-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.39 (br. s., 1 H), 9.11 (s, 1 H), 8.05 (d, *J*=16.0 Hz, 1 H), 7.72 (d, *J*=7.2 Hz, 2 H), 7.42 - 7.47 (m, 1 H), 7.39 (d, *J*=7.2 Hz, 2 H), 7.24 (br. s., 1 H), 7.00 (d, *J*=8.6 Hz, 2 H) 6.93 (s, 1 H), 6.89 (br. s., 1 H), 6.85 (d, *J*=15.8 Hz, 1 H), 6.60 - 6.66 (m, 2 H), 6.26 - 6.30 (m, 1 H), 3.95 (t, *J*=7.1 Hz, 2 H), 2.76 (t, *J*=6.9 Hz, 2 H).

¹³C and HRMS data presented as is for a mixture:

¹³C NMR (201 MHz, DMSO-*d*₆) δ ppm 168.6, 167.9, 156.1, 155.9, 155.8, 152.9, 138.8, 136.8, 135.4 (2 C), 133.5, 133.3, 129.7 (2 C), 129.5, 129.3, 129.1, 128.8, 128.7 (2 C), 128.2, 128.1, 127.9, 127.7, 126.4, 126.0, 125.1, 120.7, 118.7, 115.7, 115.1 (2 C), 113.7, 113.5, 111.8, 110.8, 41.5, 41.0, 34.1, 33.9; HRMS (ESI) m/z: 384.1701 found (calcd for C₂₄H₂₂N₃O₂⁺, [M+H]⁺ 384.1707).



5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one (4cd)

Dark-red solid (205 mg, 51%); mp ~250 °C with decomposition.

It was obtained as a mixture of two inseparable isomers. ¹H NMR signals were assigned to individual isomers:

(*E*)-5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 12.95 (br. s., 1 H), 9.89 (s, 1 H), 9.14 (s, 1 H), 7.56 - 7.61 (m, 1 H), 7.53 (d, *J*=8.6 Hz, 2 H), 7.33 (br. s., 1 H), 7.22 (s, 1 H), 7.02 (d, *J*=8.4 Hz, 2 H), 6.80 - 6.85 (m, 3 H), 6.62 - 6.66 (m, 3 H), 6.35 (ddd, *J*=3.6, 2.3, 2.1 Hz, 1 H), 4.00 (t, *J*=7.2 Hz, 2 H), 2.79 (t, *J*=7.2 Hz, 2 H).

(*Z*)-5-(1*H*-pyrrol-2-ylmethylene)-3-(4-hydroxyphenethyl)-2-((*E*)-4-hydroxystyryl)-3,5-dihydro-4*H*-imidazol-4-one

¹H NMR (700 MHz, DMSO-*d*₆) δ ppm 11.35 (br. s., 1 H), 9.95 (s, 1 H), 9.12 (s, 1 H), 7.99 (d, *J*=15.6 Hz, 1 H), 7.56 - 7.61 (m, 2 H), 7.21 (br. s., 1 H), 7.00 (d, *J*=8.6 Hz, 2 H), 6.86 (s, 1 H), 6.80 - 6.85 (m, 3 H), 6.62 - 6.66 (m, 3 H), 6.26 (ddd, *J*=3.5, 2.3, 2.1 Hz, 1 H), 3.92 (t, *J*=7.1 Hz, 2 H), 2.75 (t, *J*=7.0 Hz, 2 H).

¹³C and HRMS data presented as is for a mixture:

¹³C NMR (201 MHz, DMSO-*d*₆) δ ppm 168.7, 168.0, 159.2, 159.0, 156.6, 155.8 (2 C), 153.4, 139.3, 137.2, 133.7, 133.5, 129.8, 129.7, 129.5, 129.1, 128.8, 128.7, 128.1, 128.0, 126.6, 125.7, 125.5, 124.1, 120.1, 118.1, 115.7, 115.6, 115.5, 115.1 (2 C), 114.7, 111.6, 110.6, 110.0, 109.7, 41.4, 40.9, 34.1, 33.9; HRMS (ESI) m/z: 400.1651 found (calcd for C₂₄H₂₂N₃O₃⁺, [M+H]⁺ 400.1656).

7. Structure confirmation

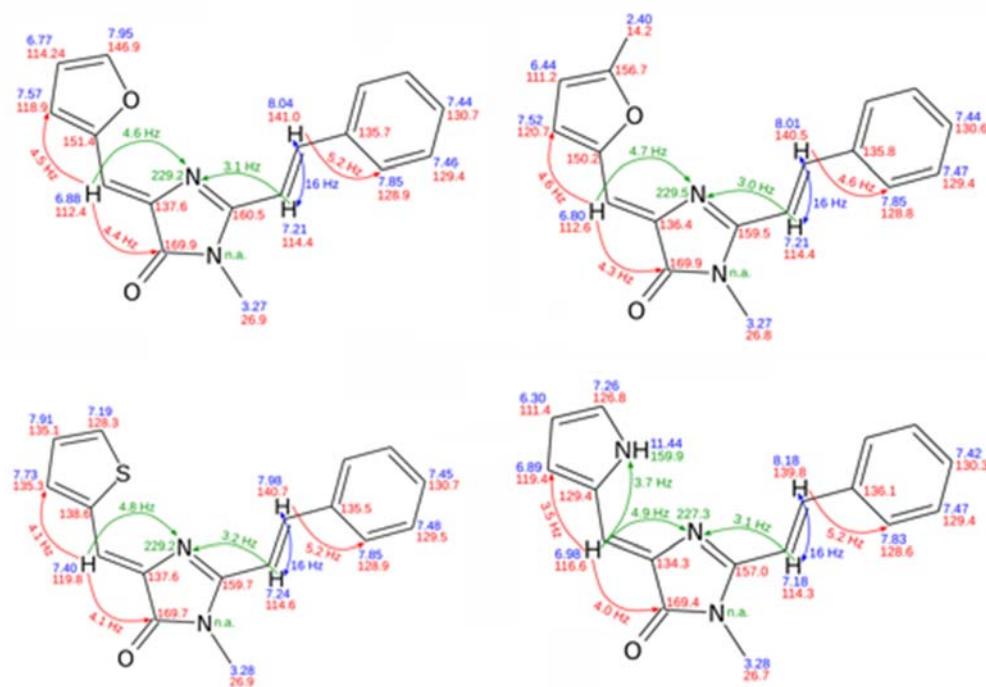
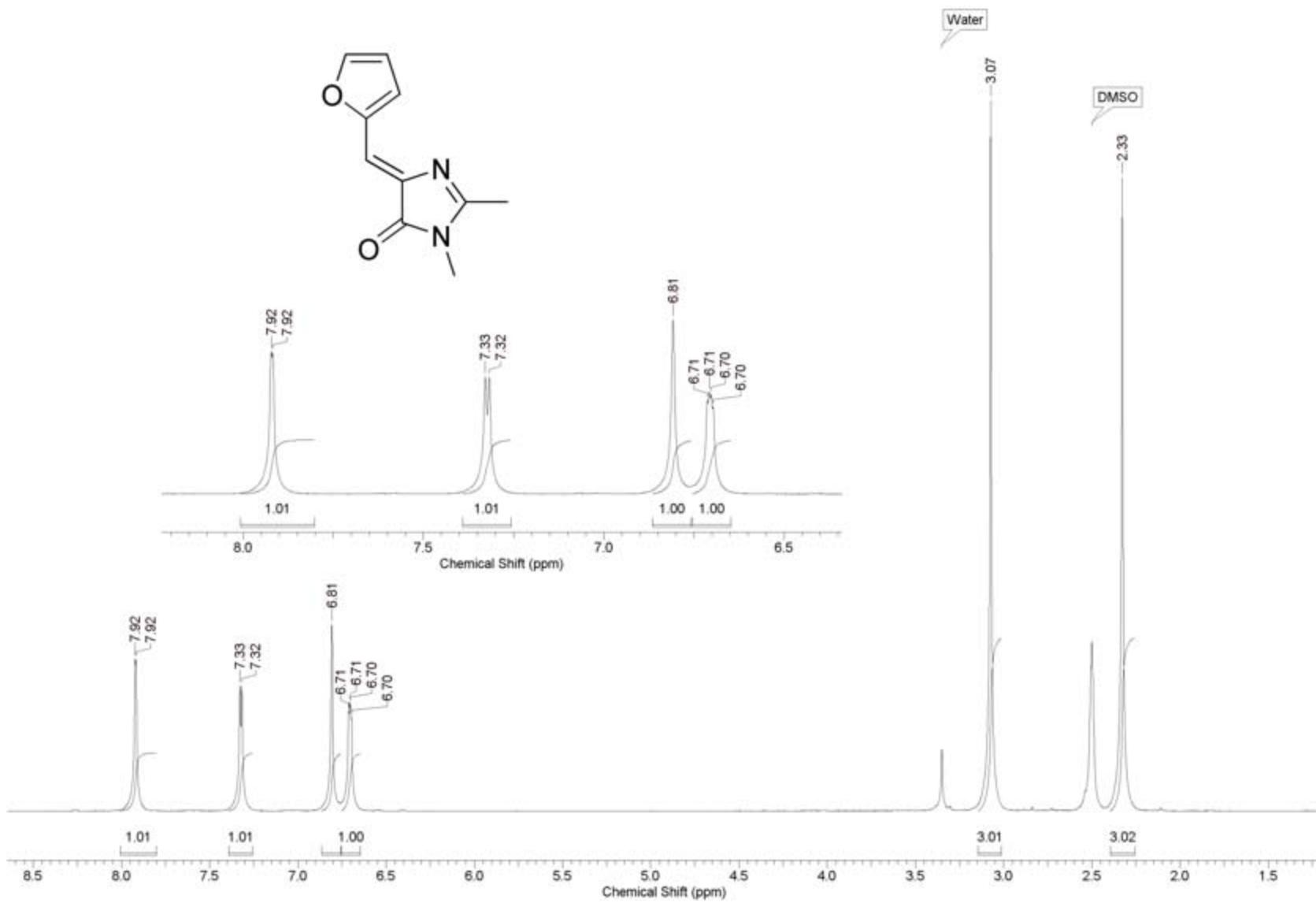
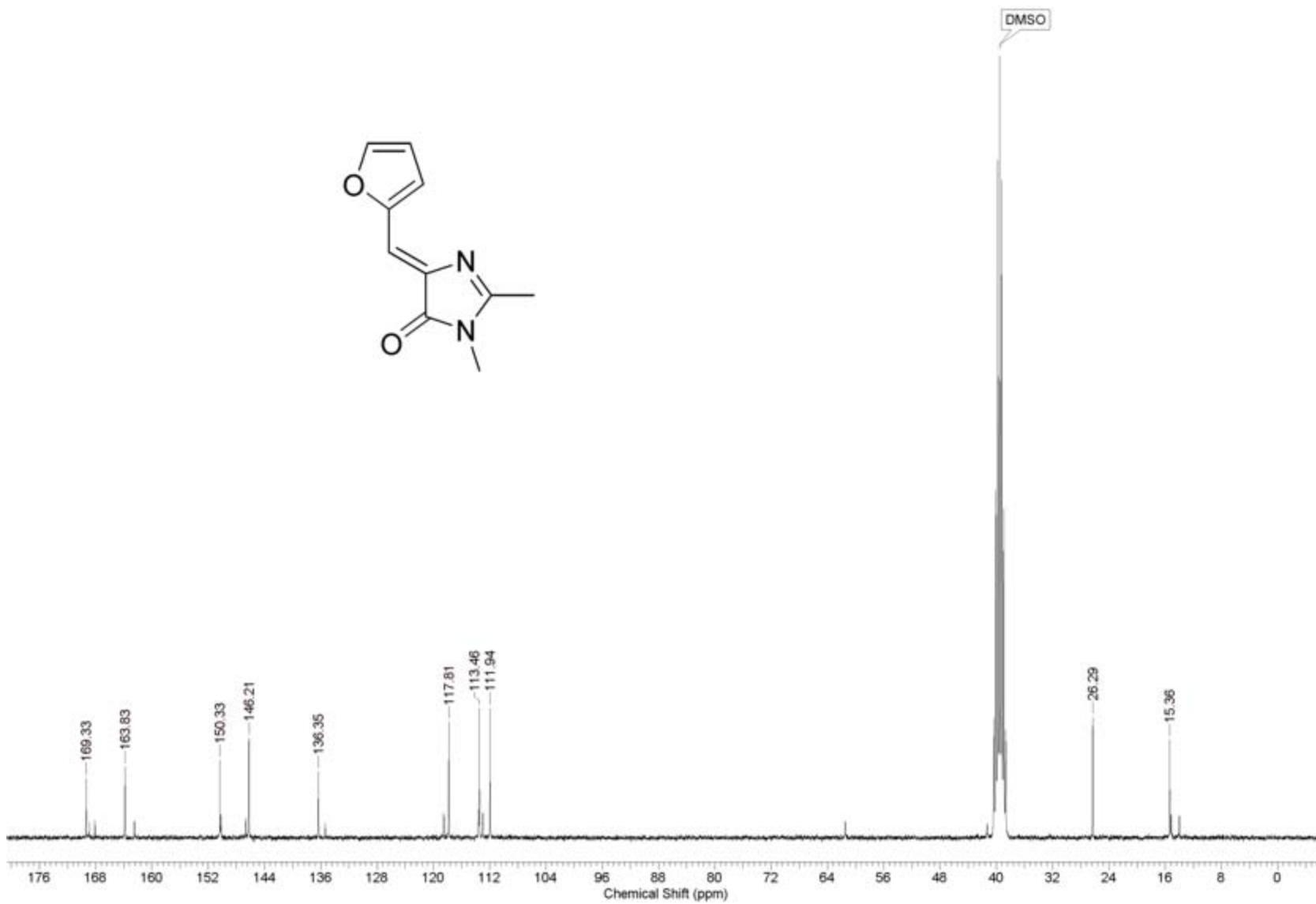
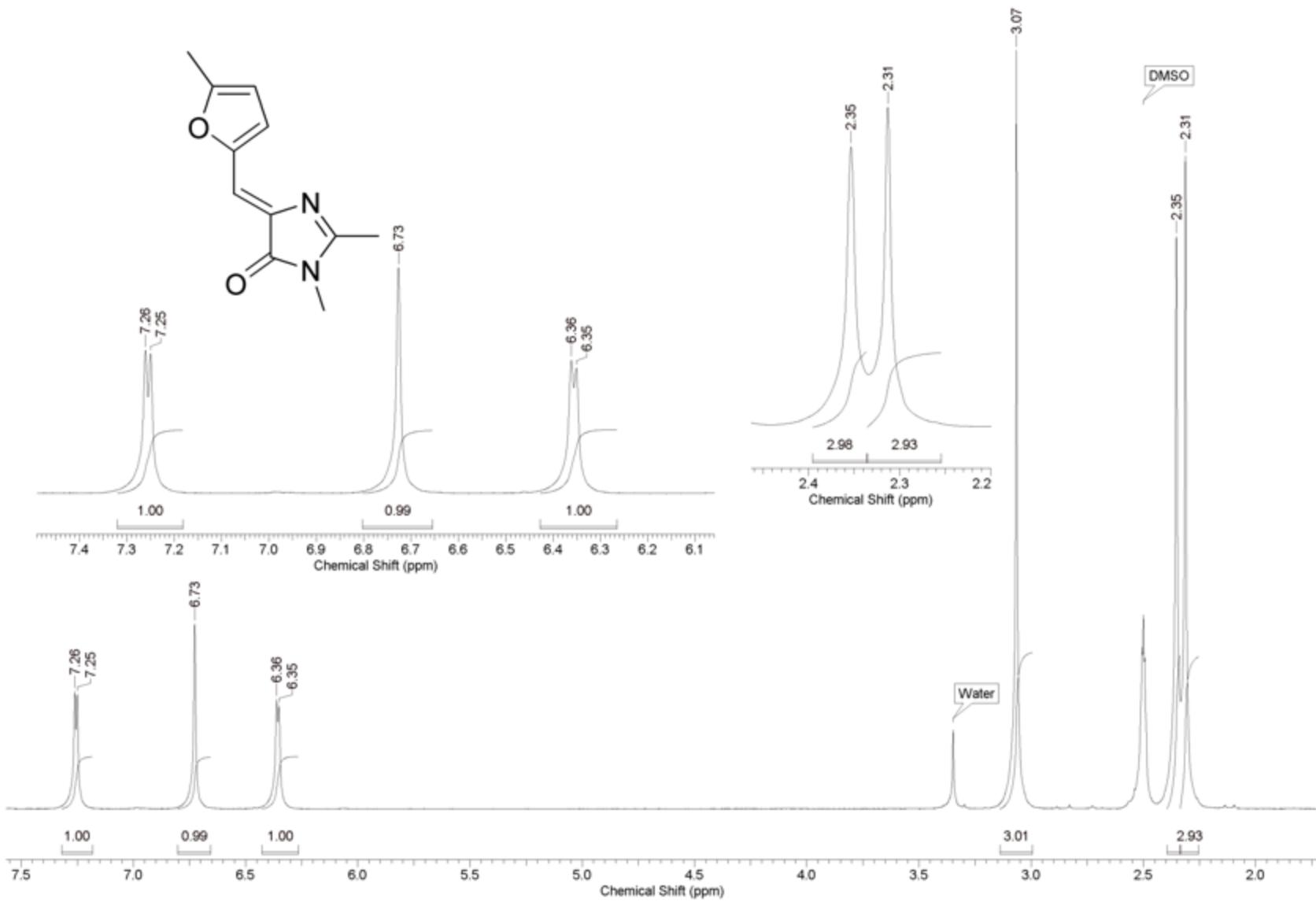


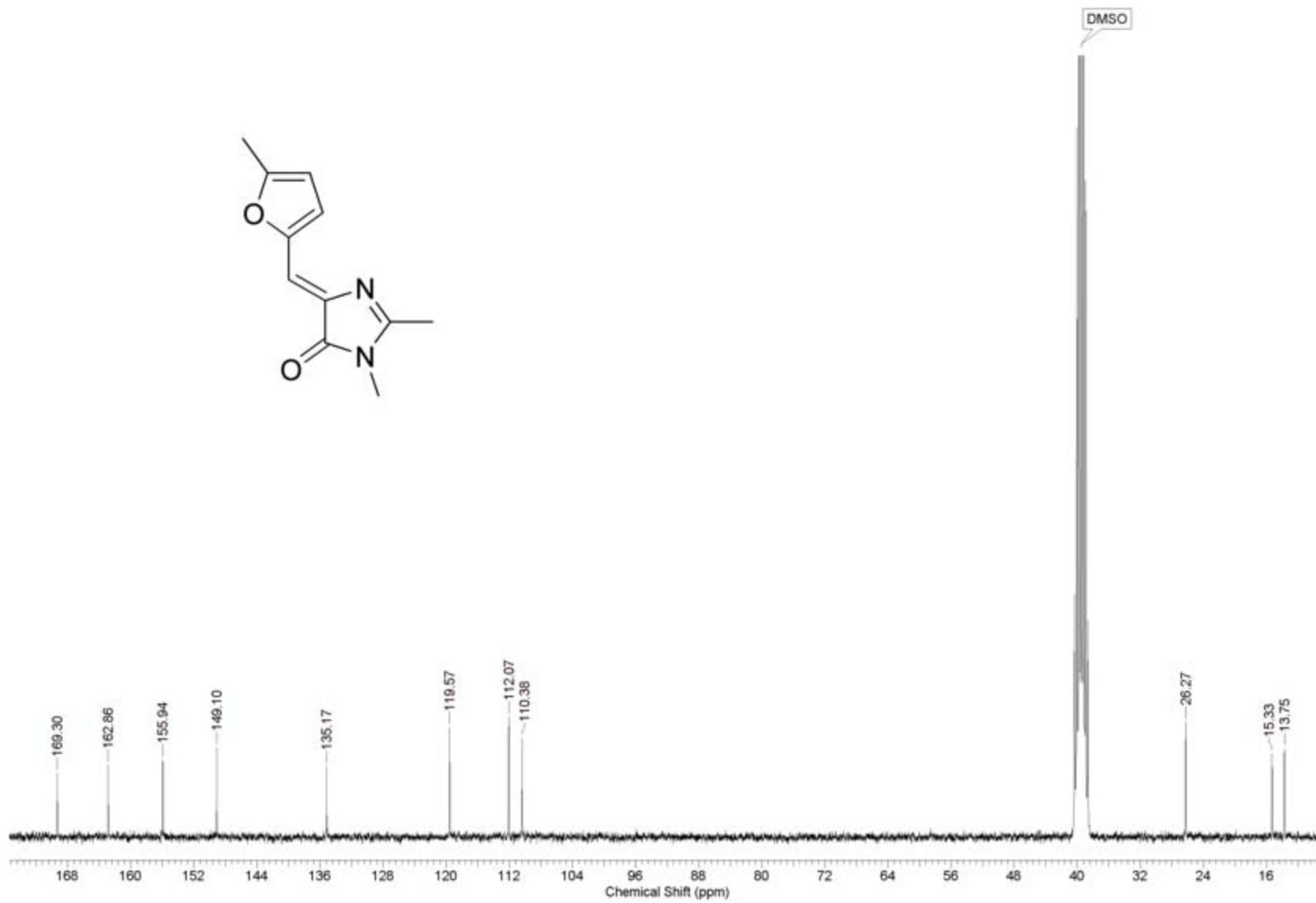
Fig S7.1. Results of the investigation of the structure of compounds **1ac**, **2ac**, **3ac**, and **4ac** by heteronuclear NMR spectroscopy. Chemical shifts of ^1H (in blue), ^{13}C (in red), and ^{15}N (in green) are shown. Key spin-spin coupling interactions are denoted with arrows.

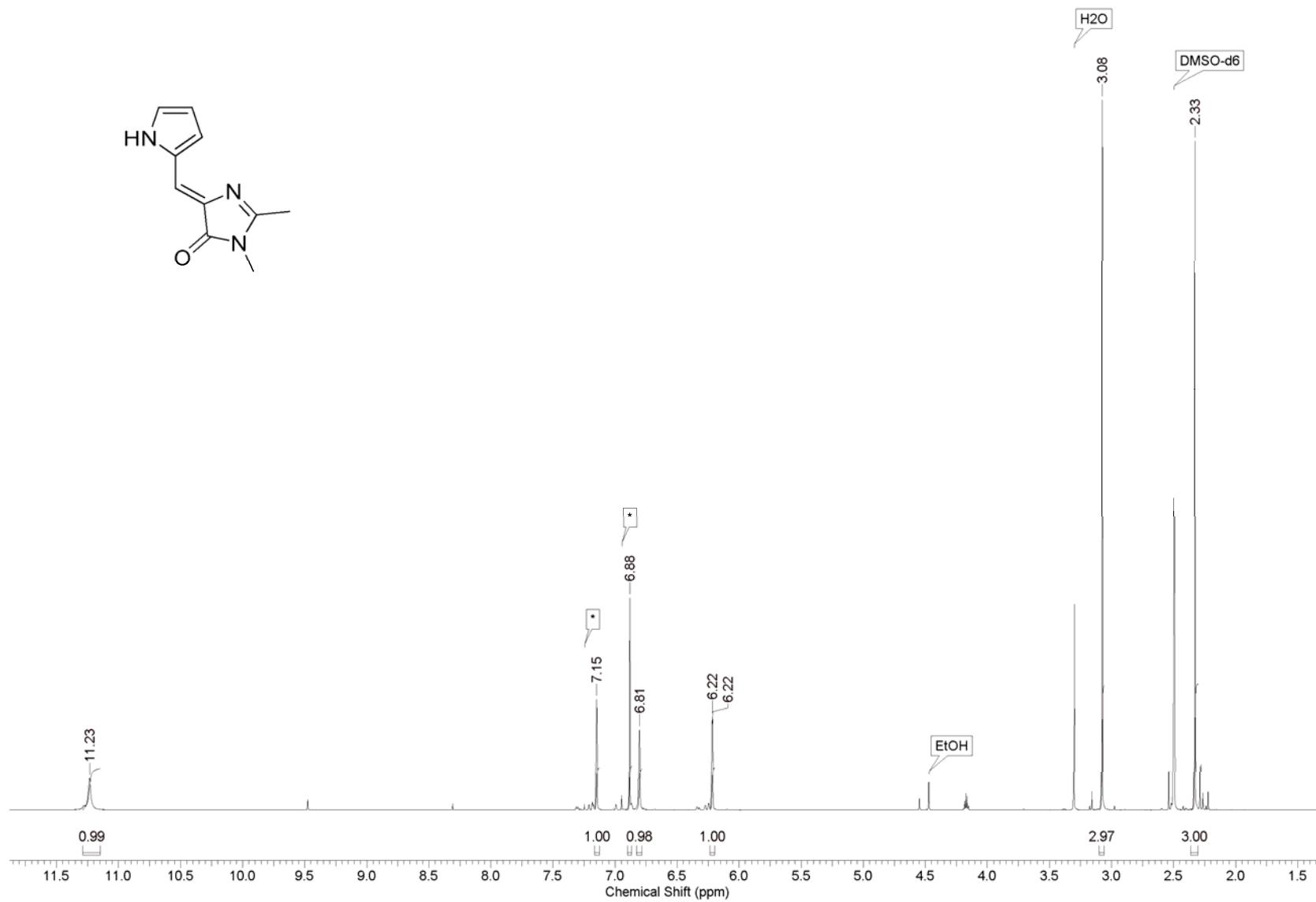
8. Copies of ^1H and ^{13}C NMR spectra

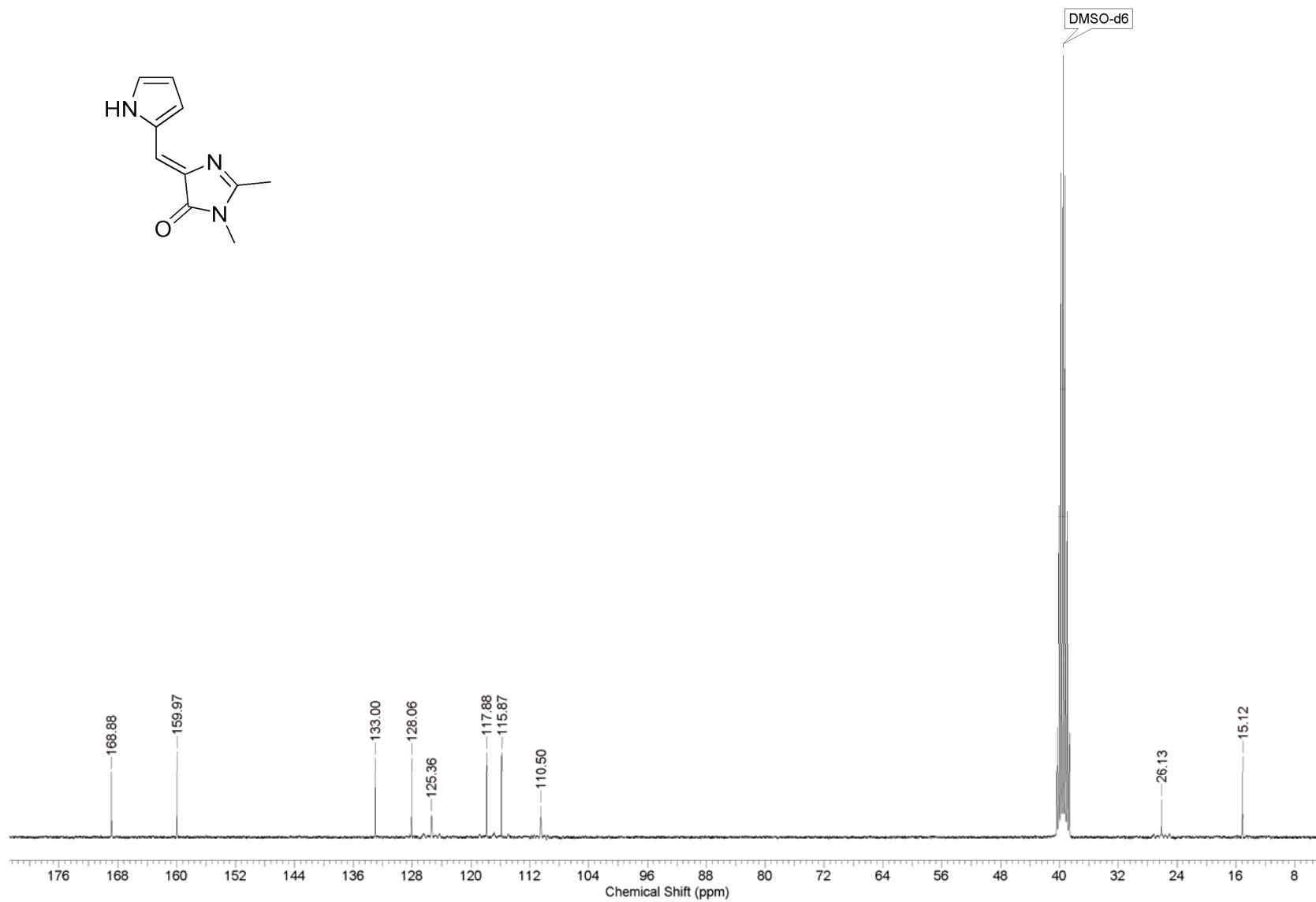


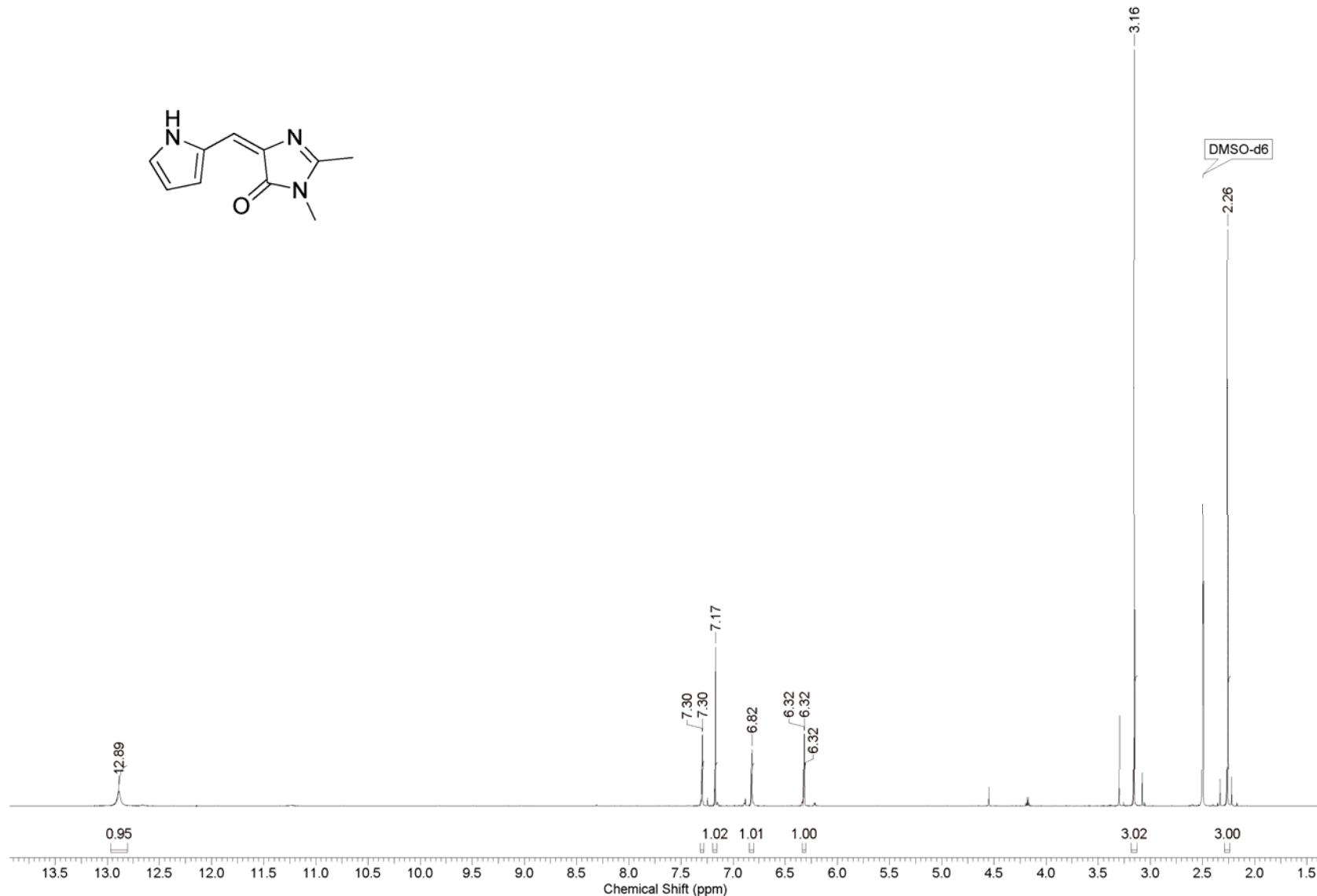


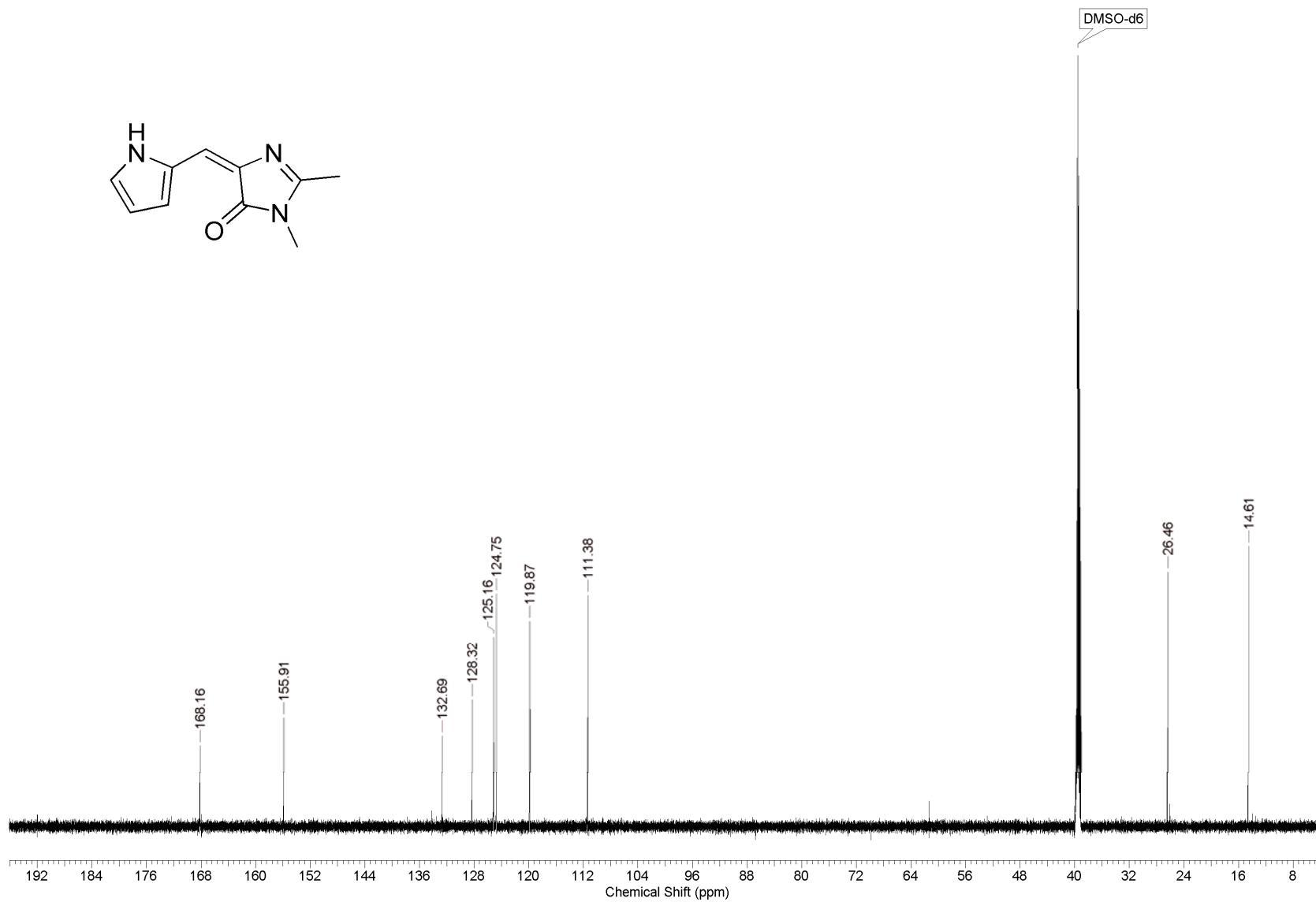


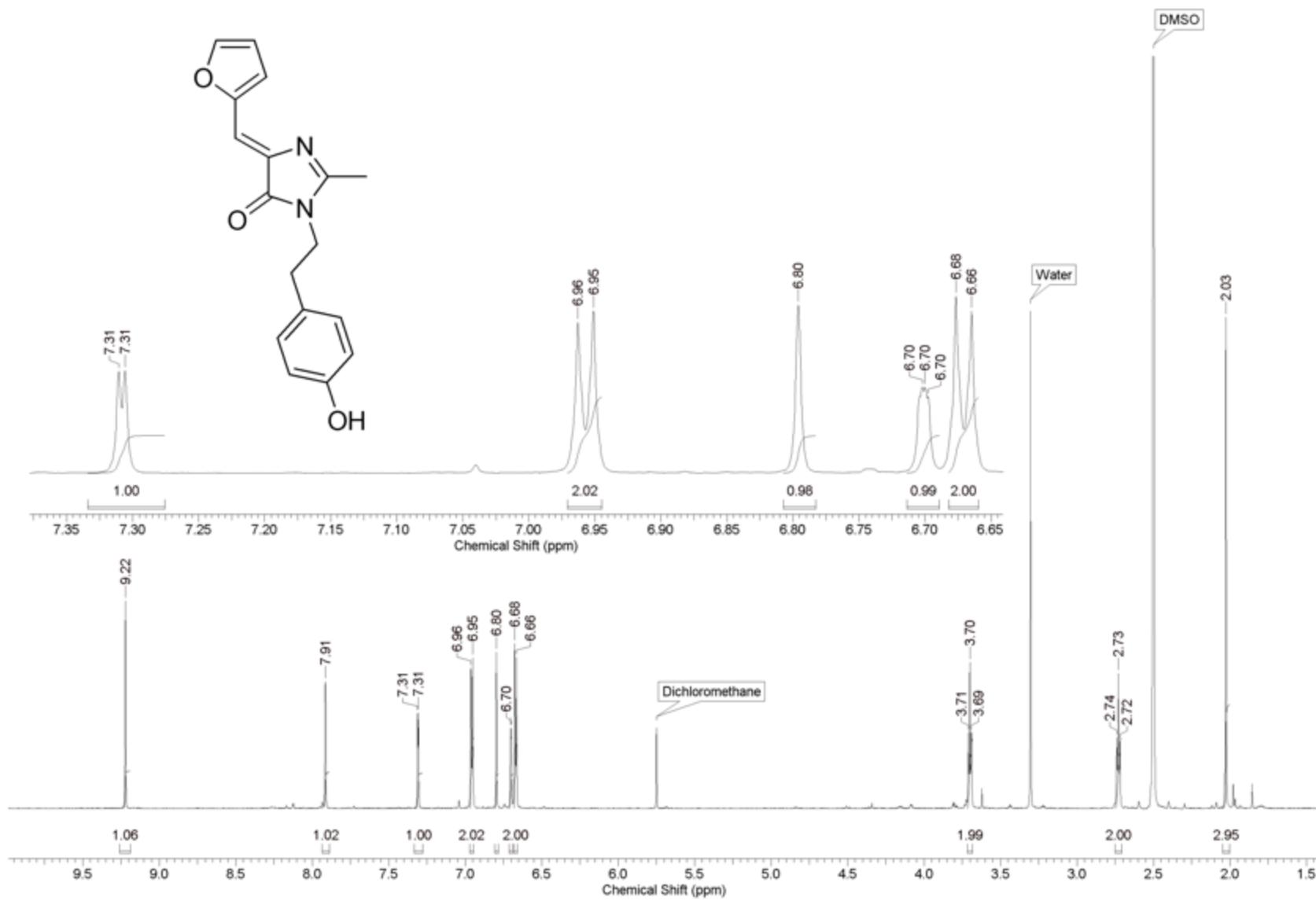


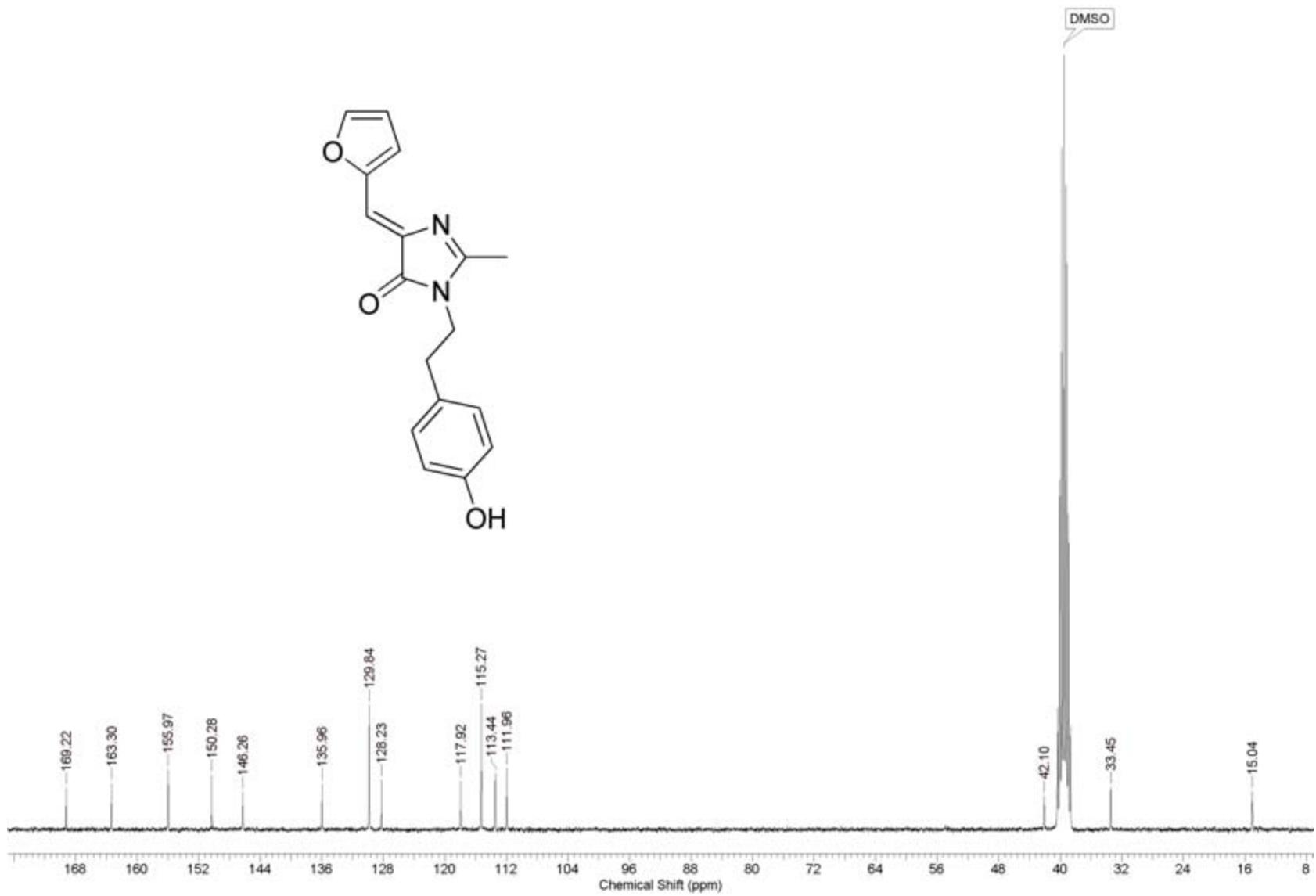


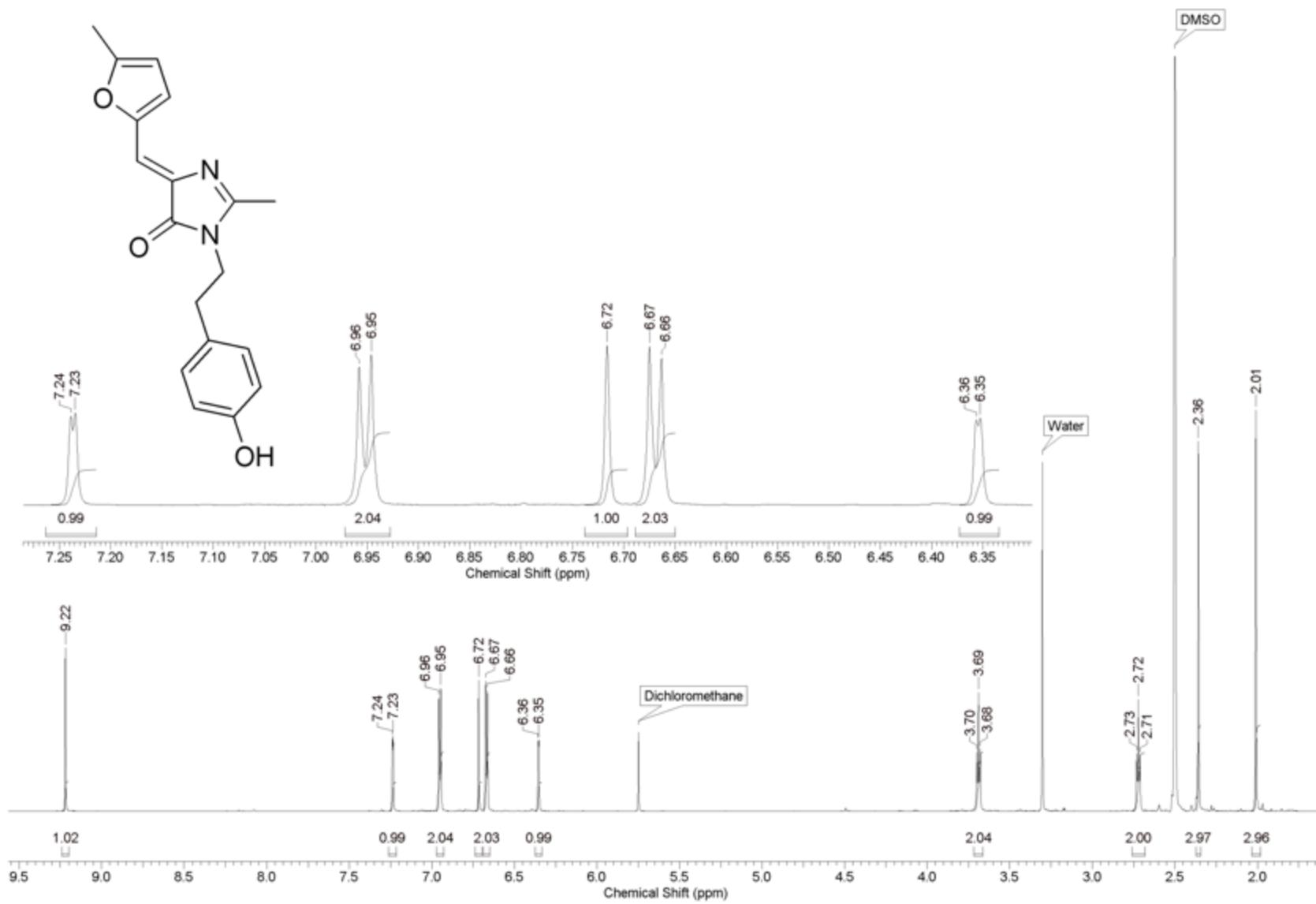


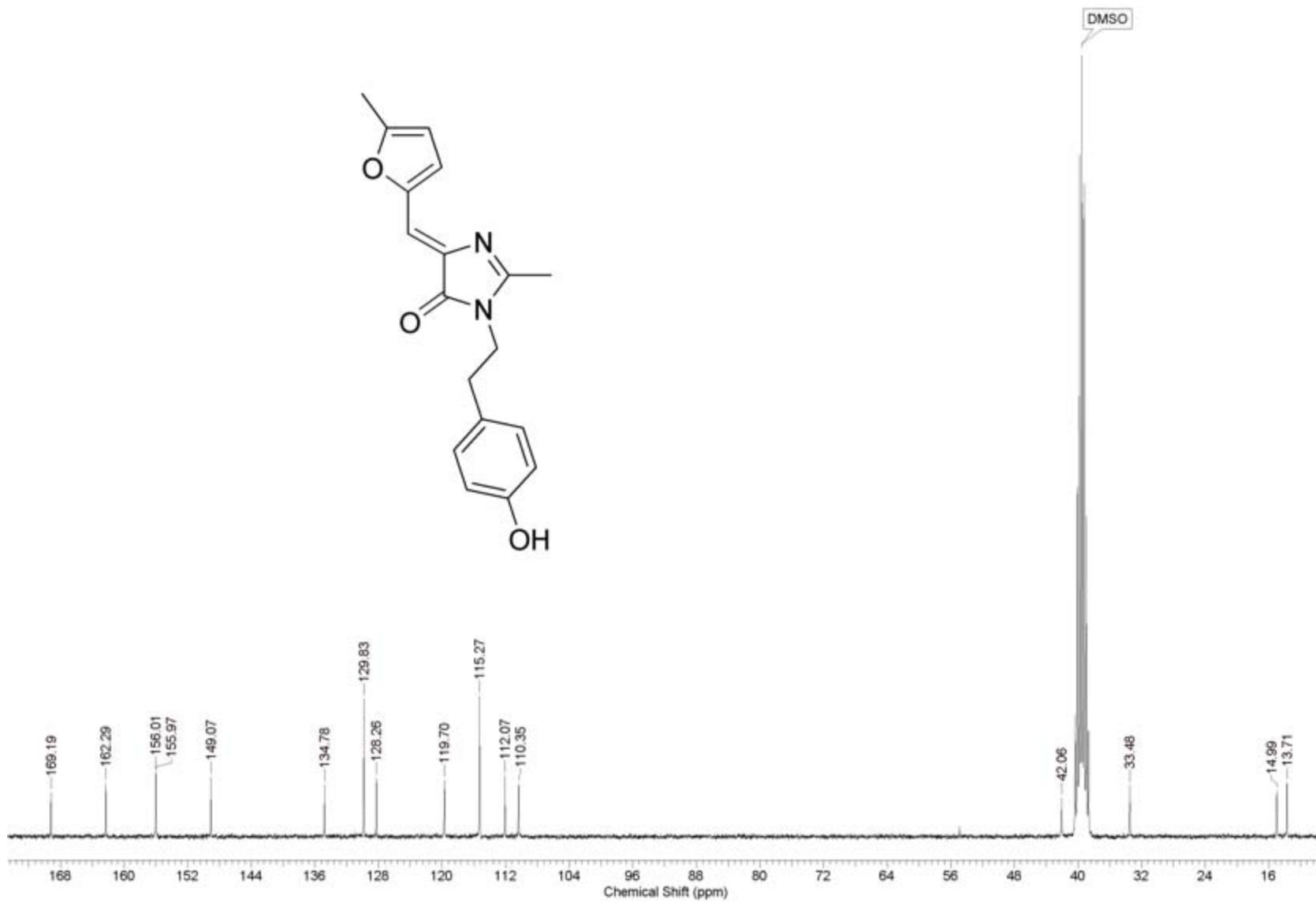


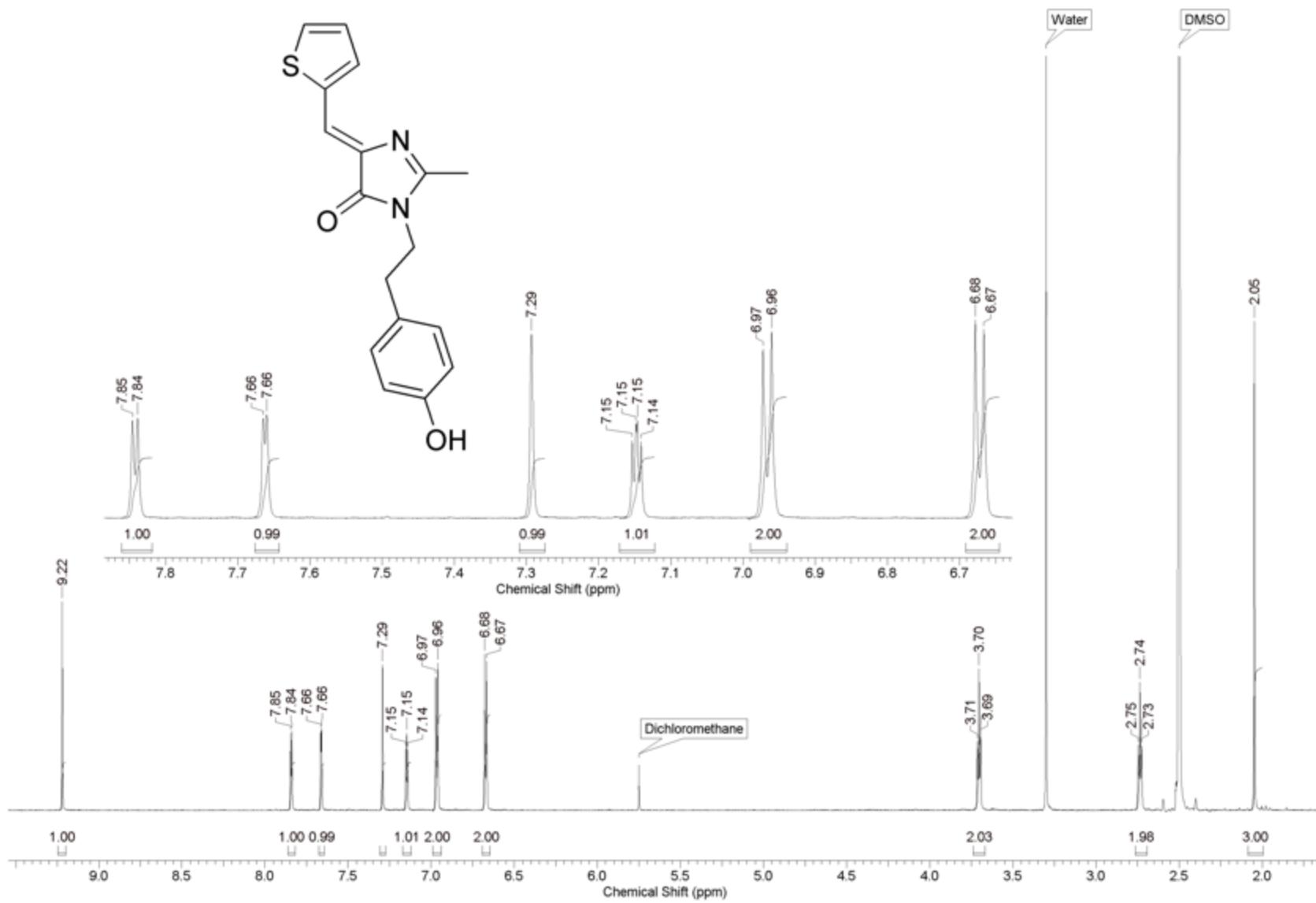


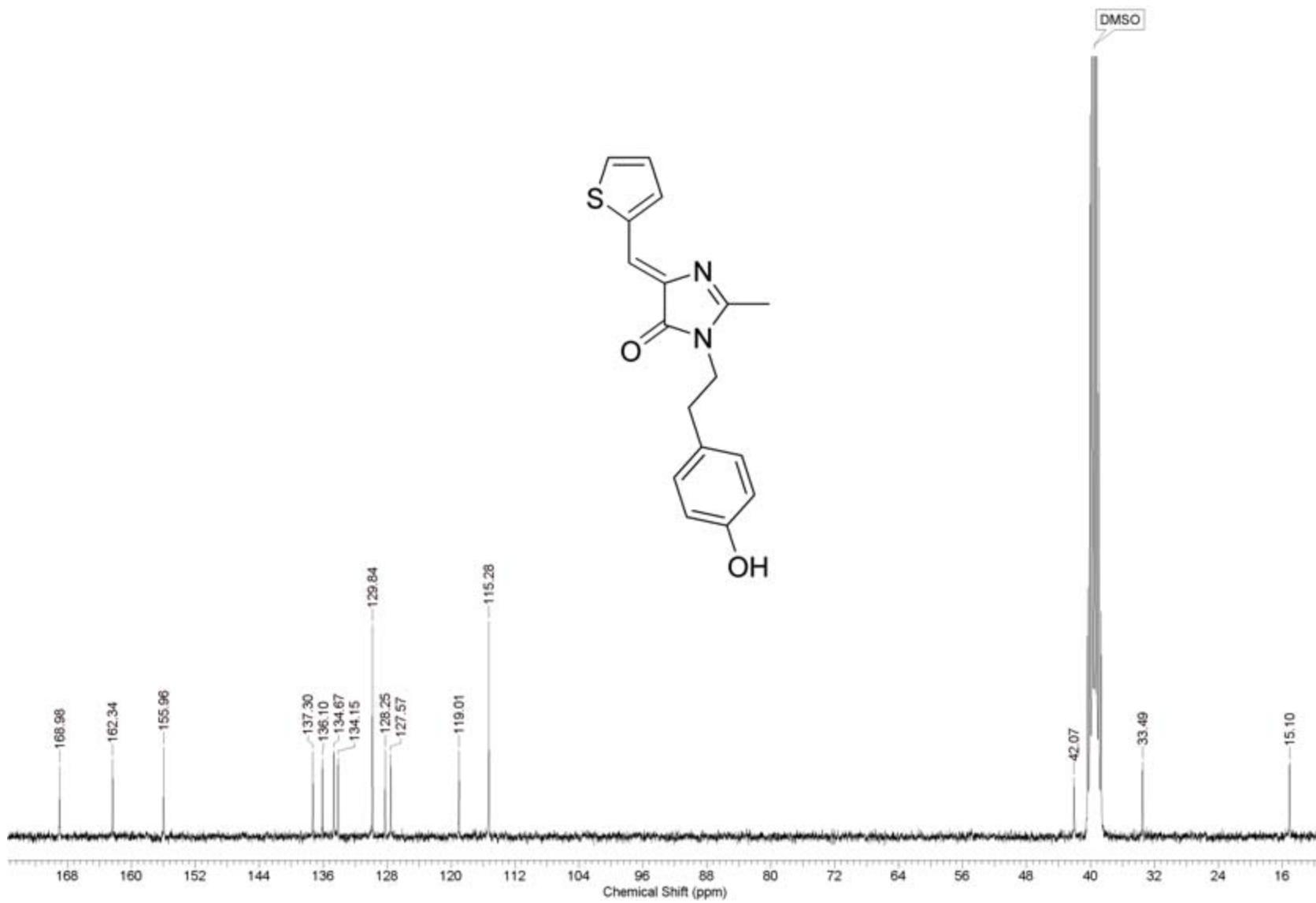


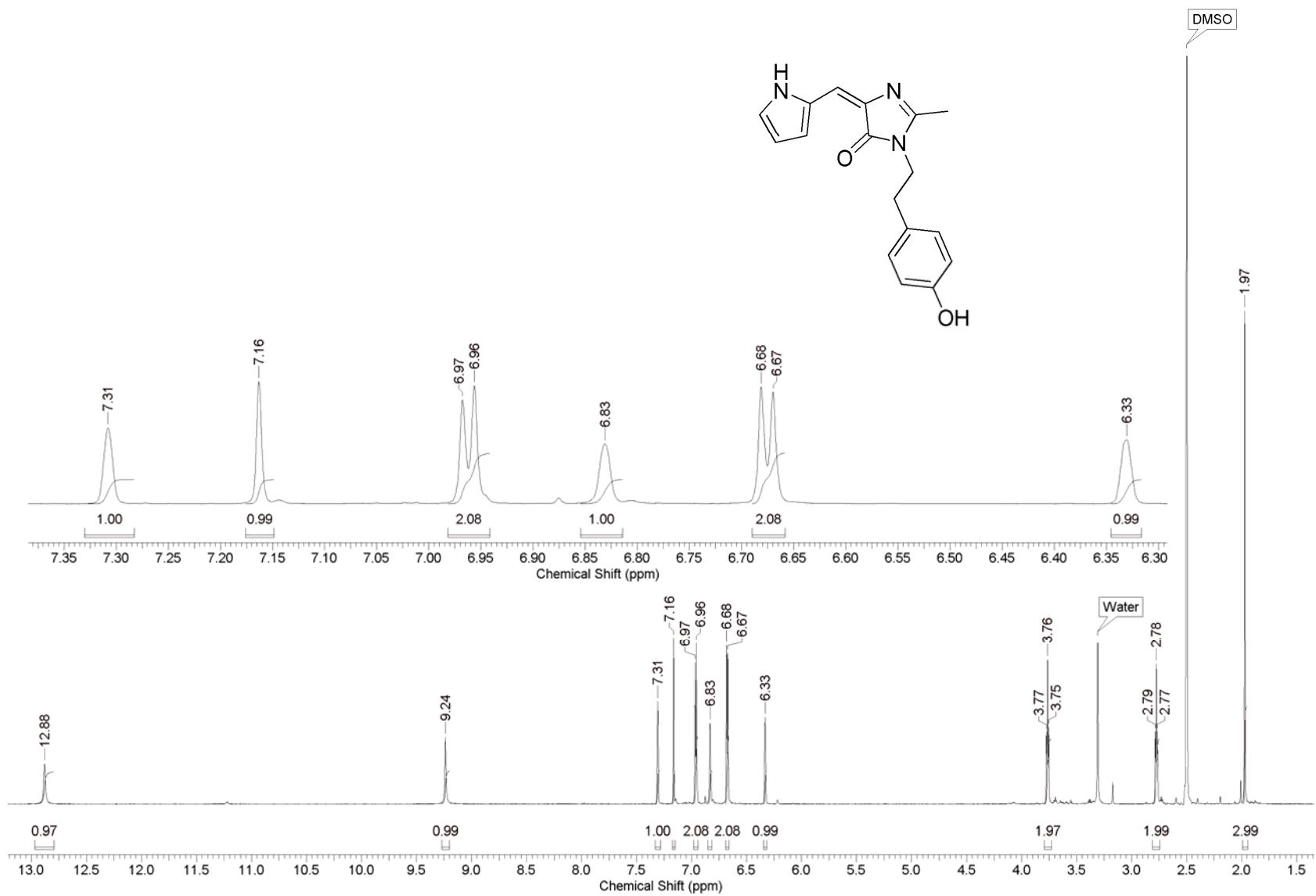


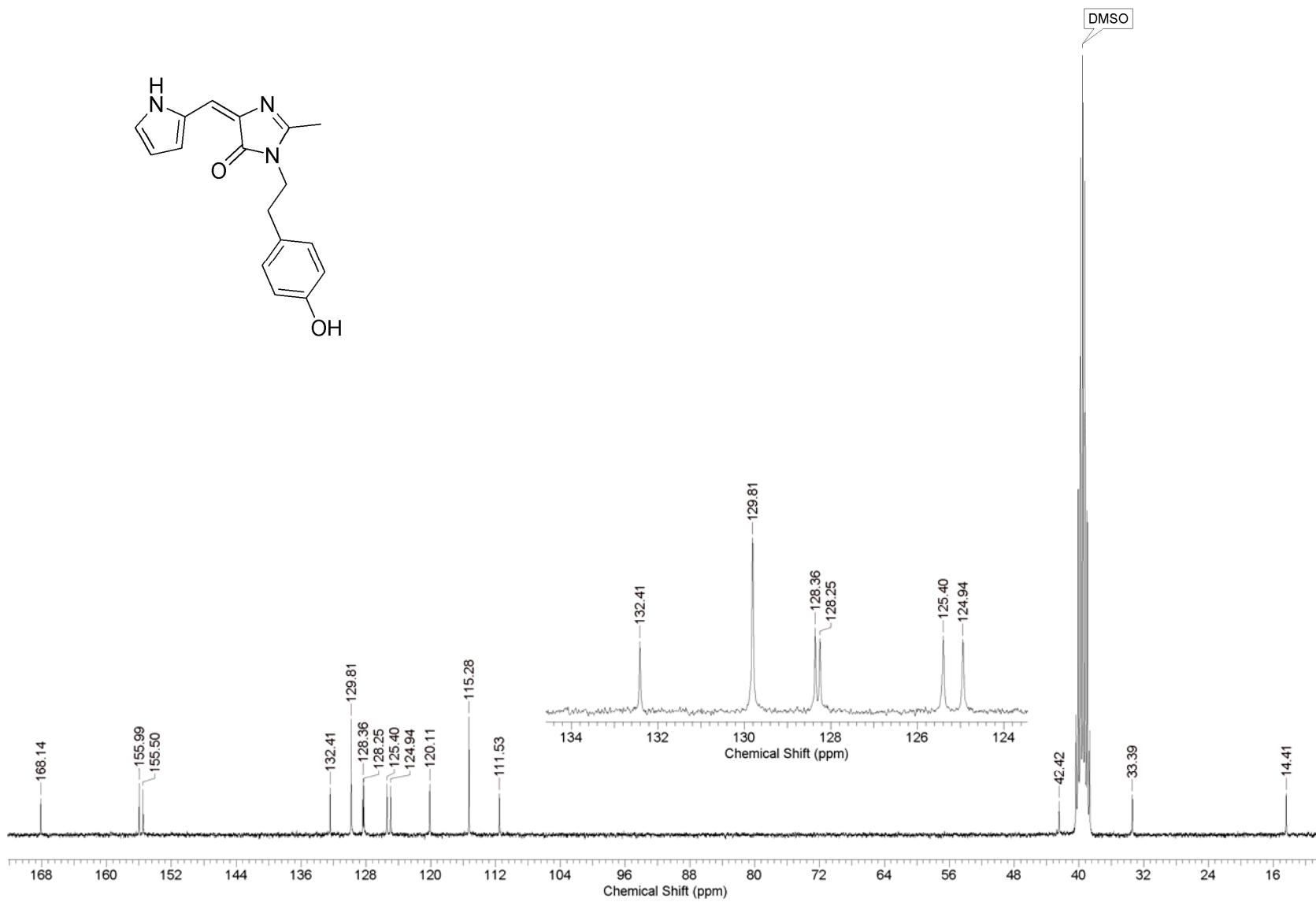


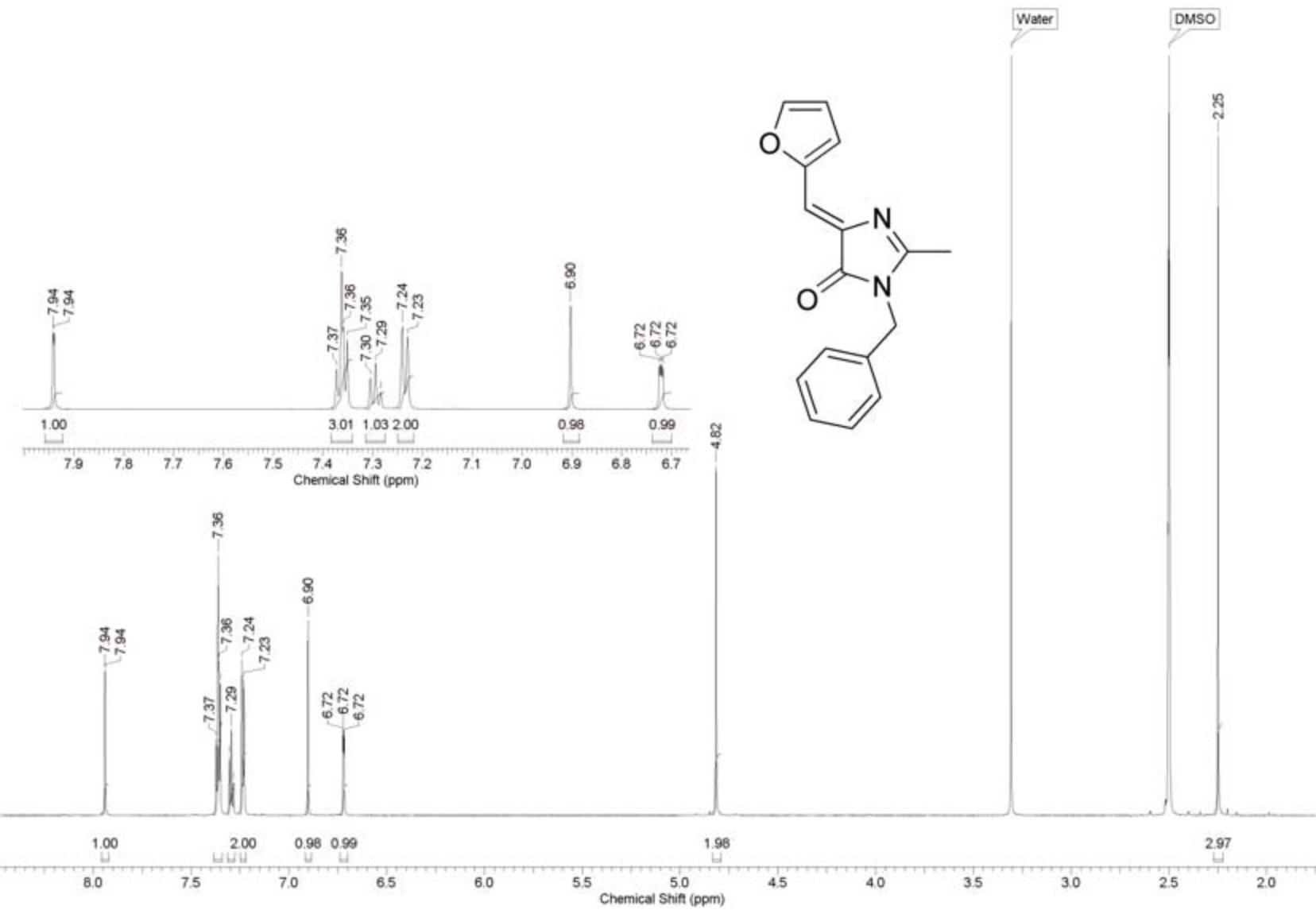


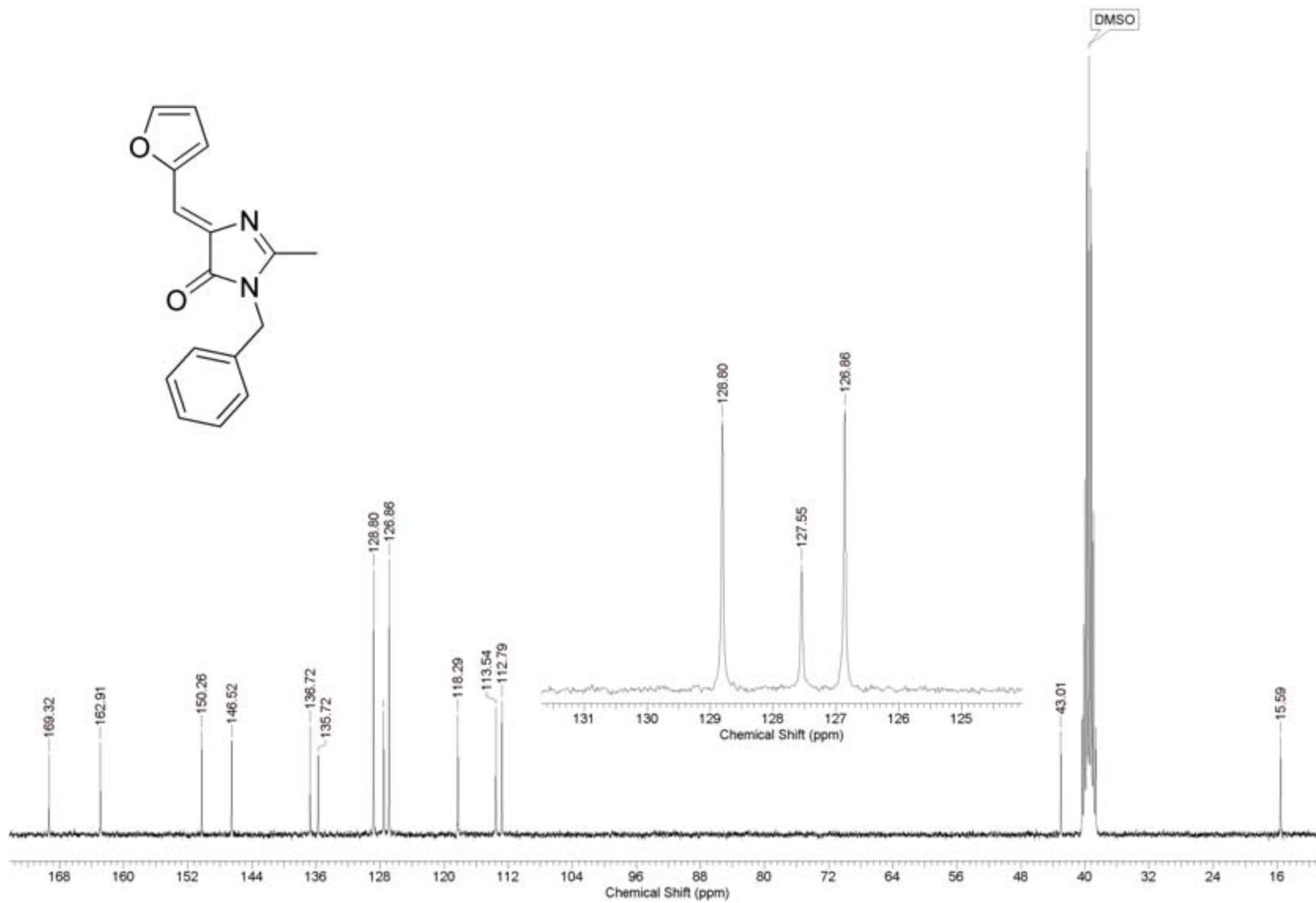


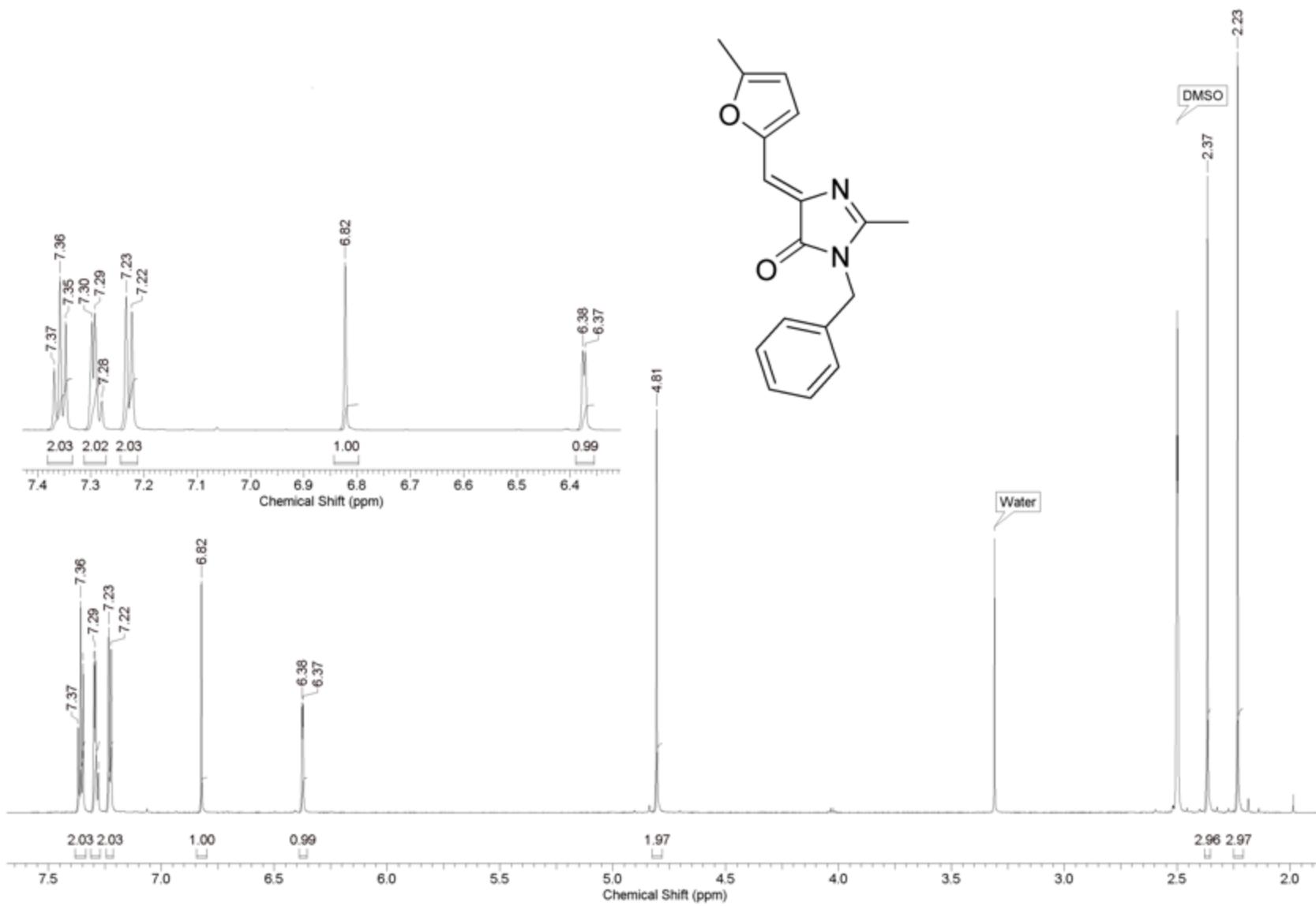


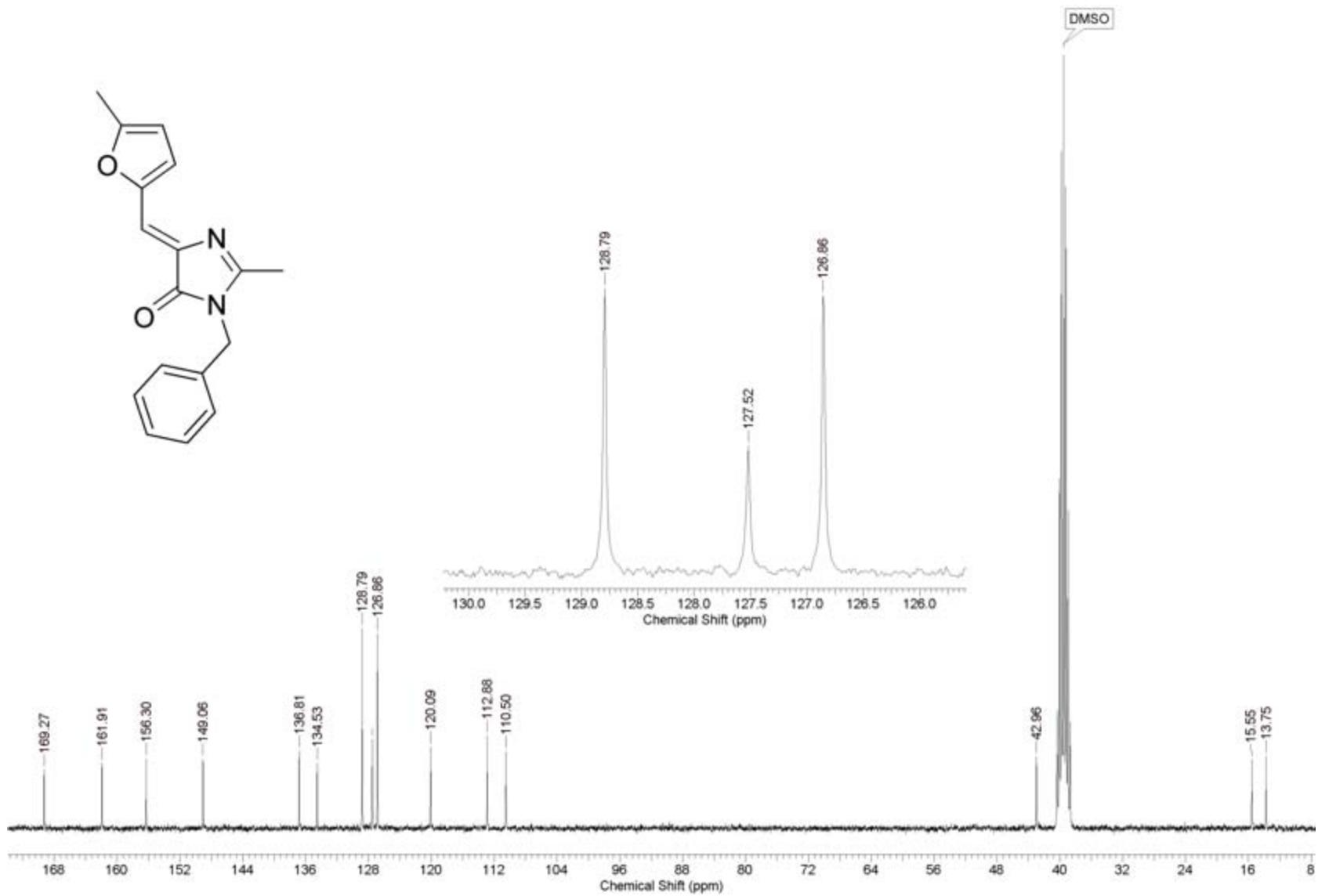


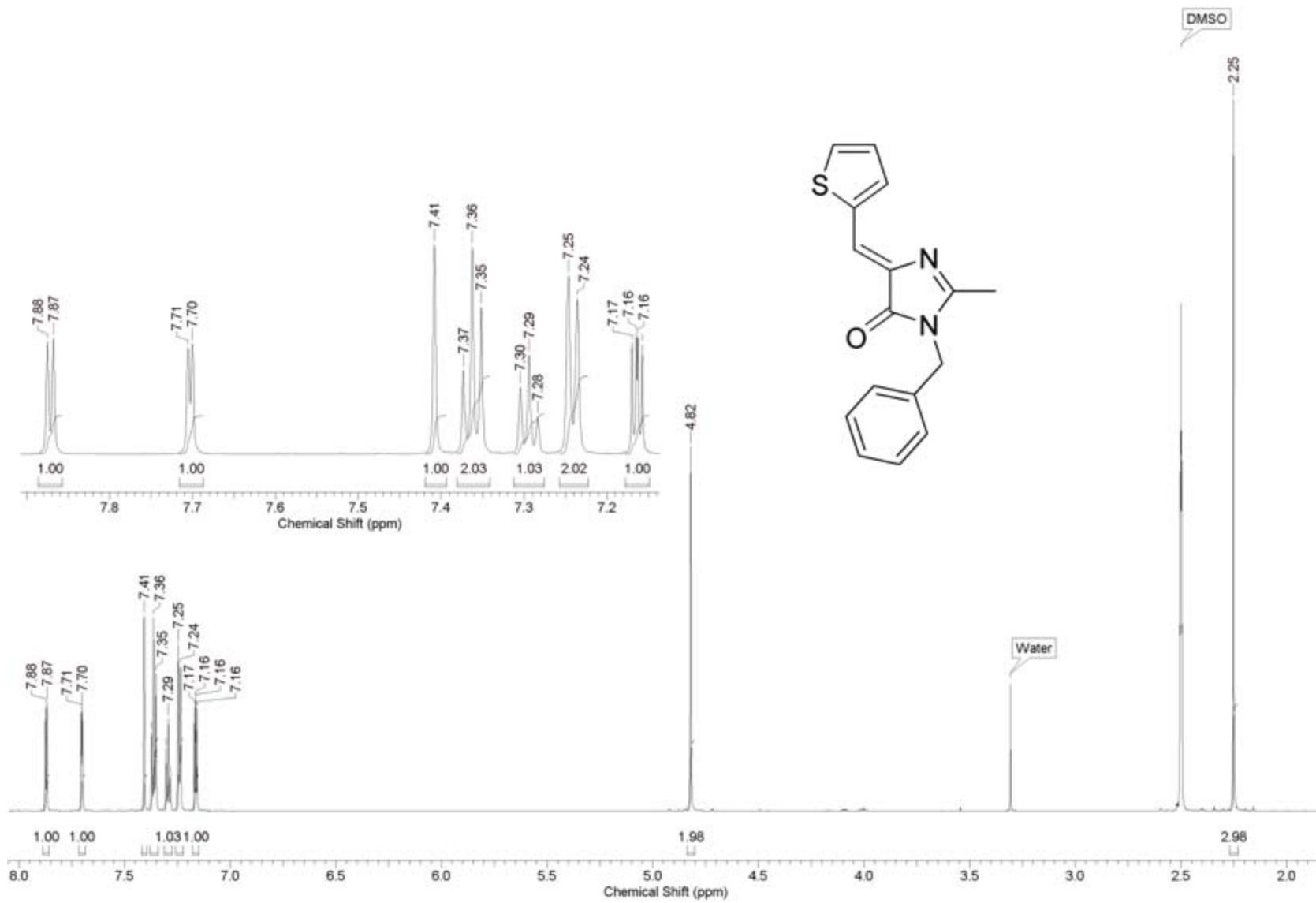


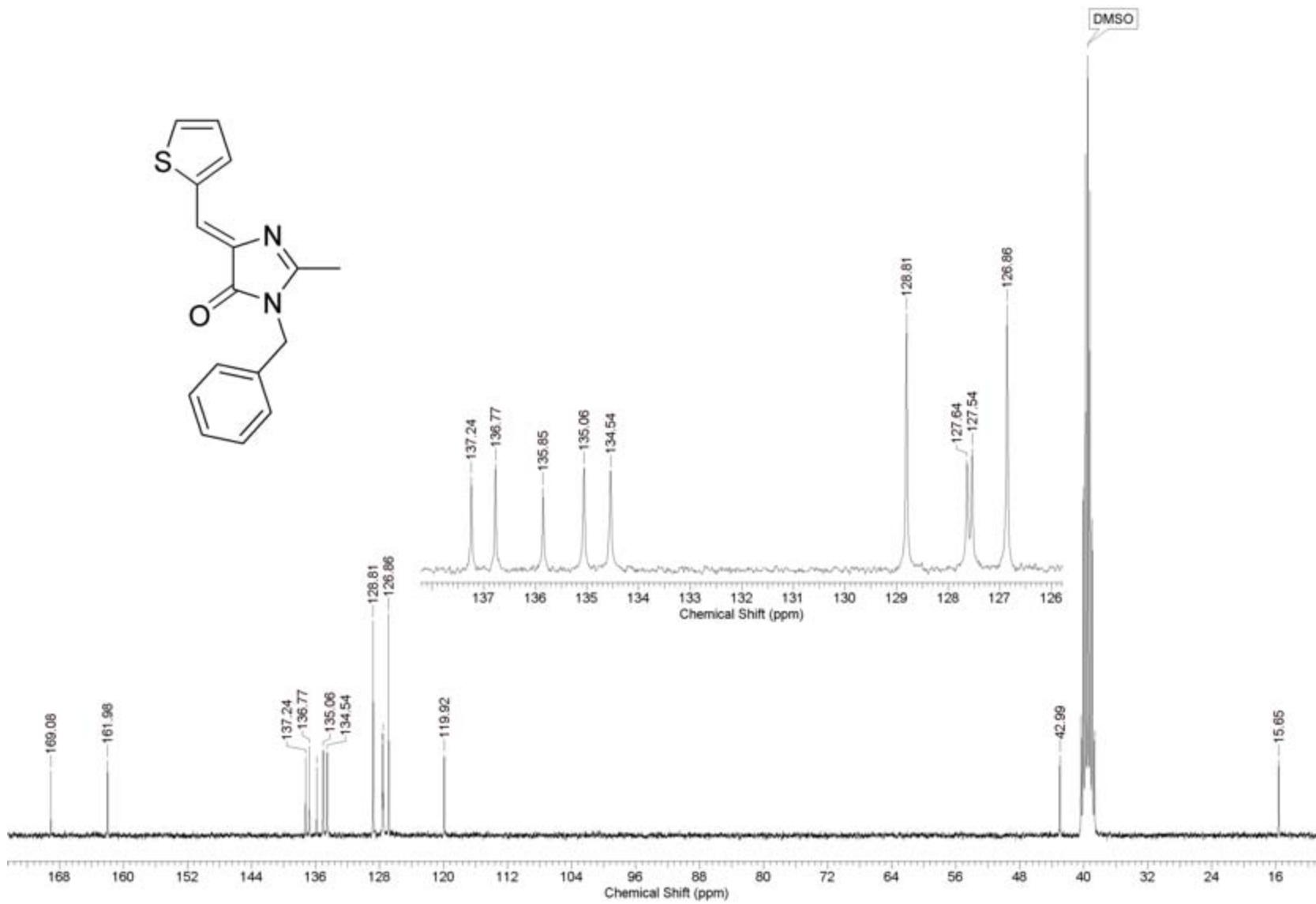


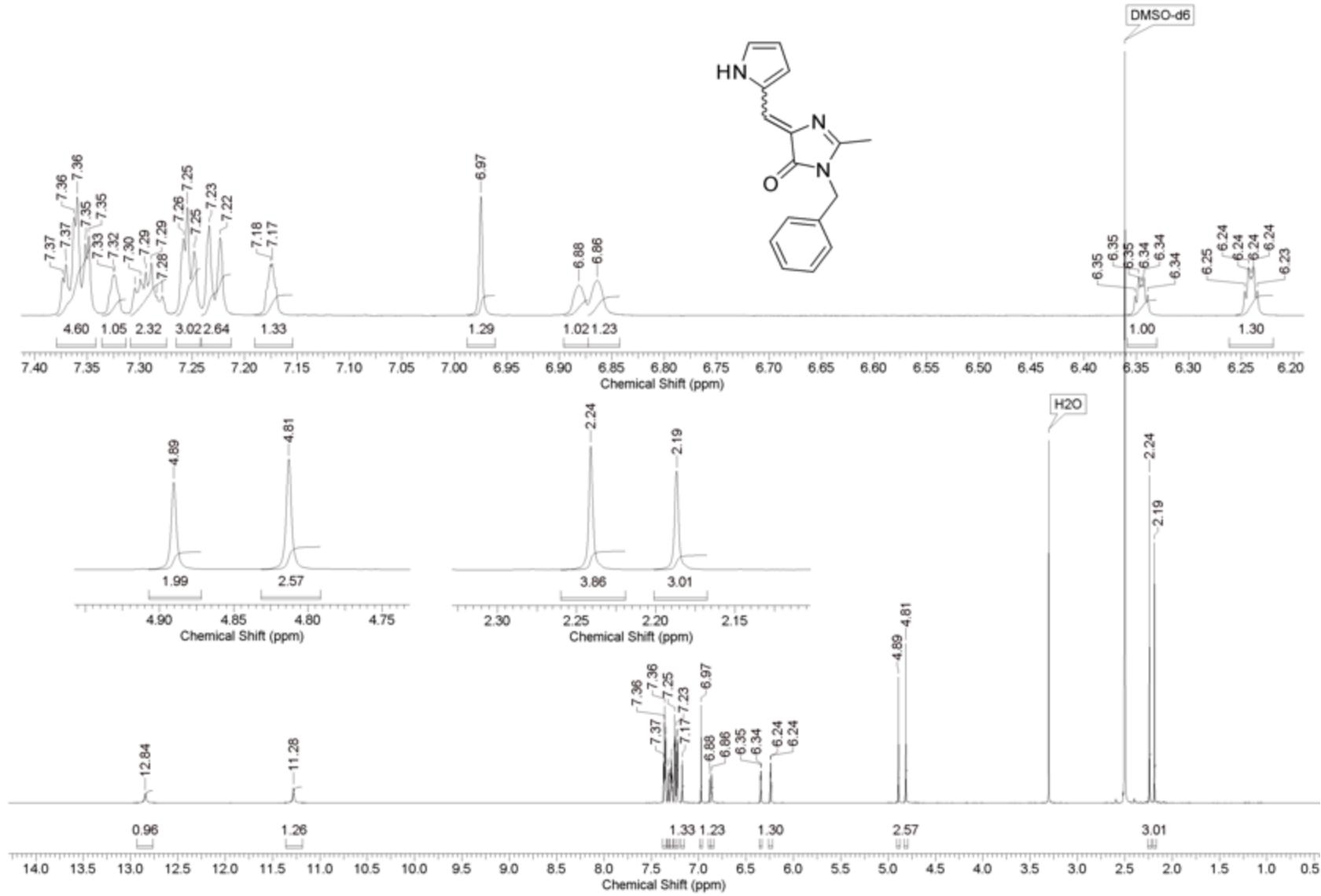


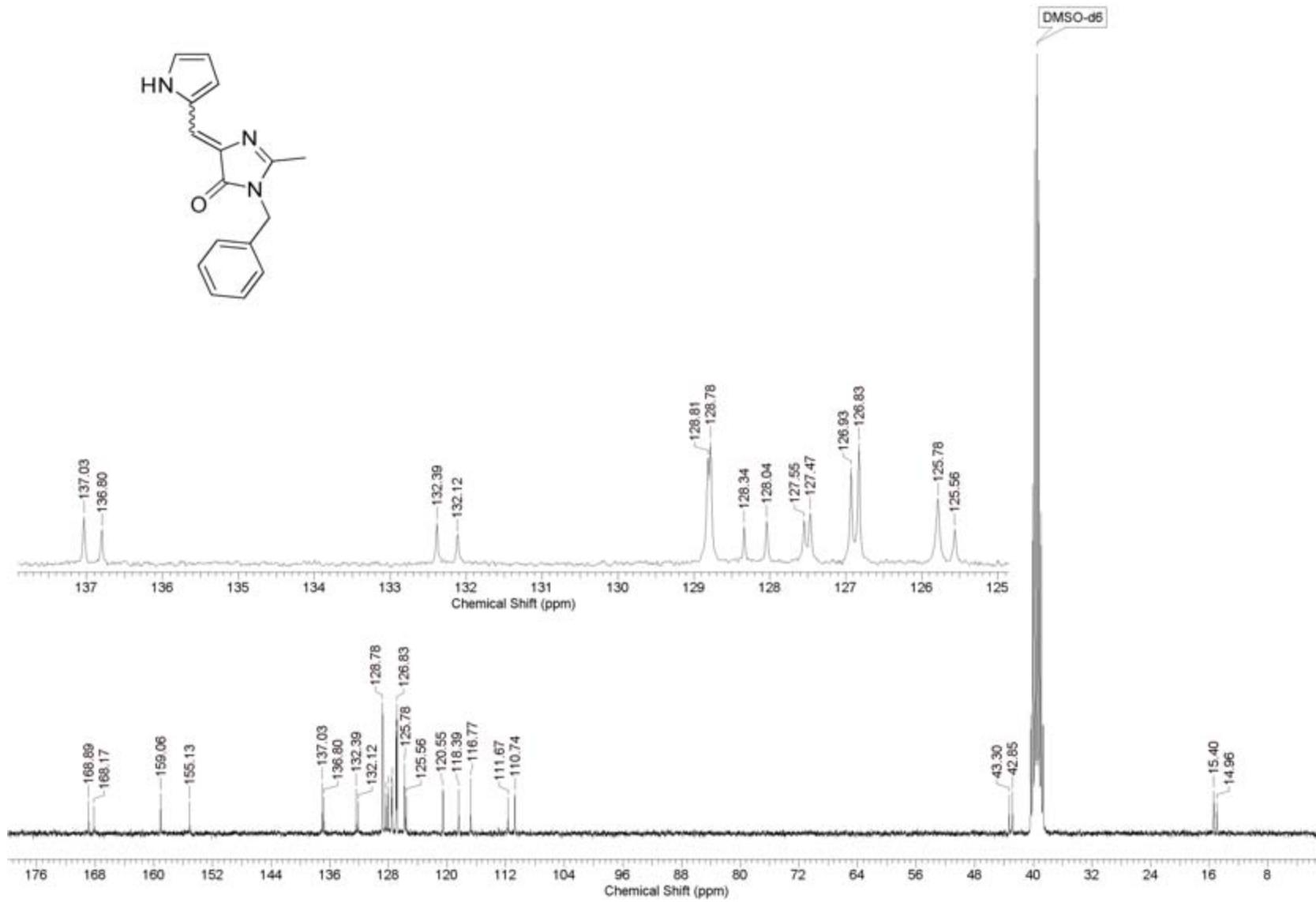


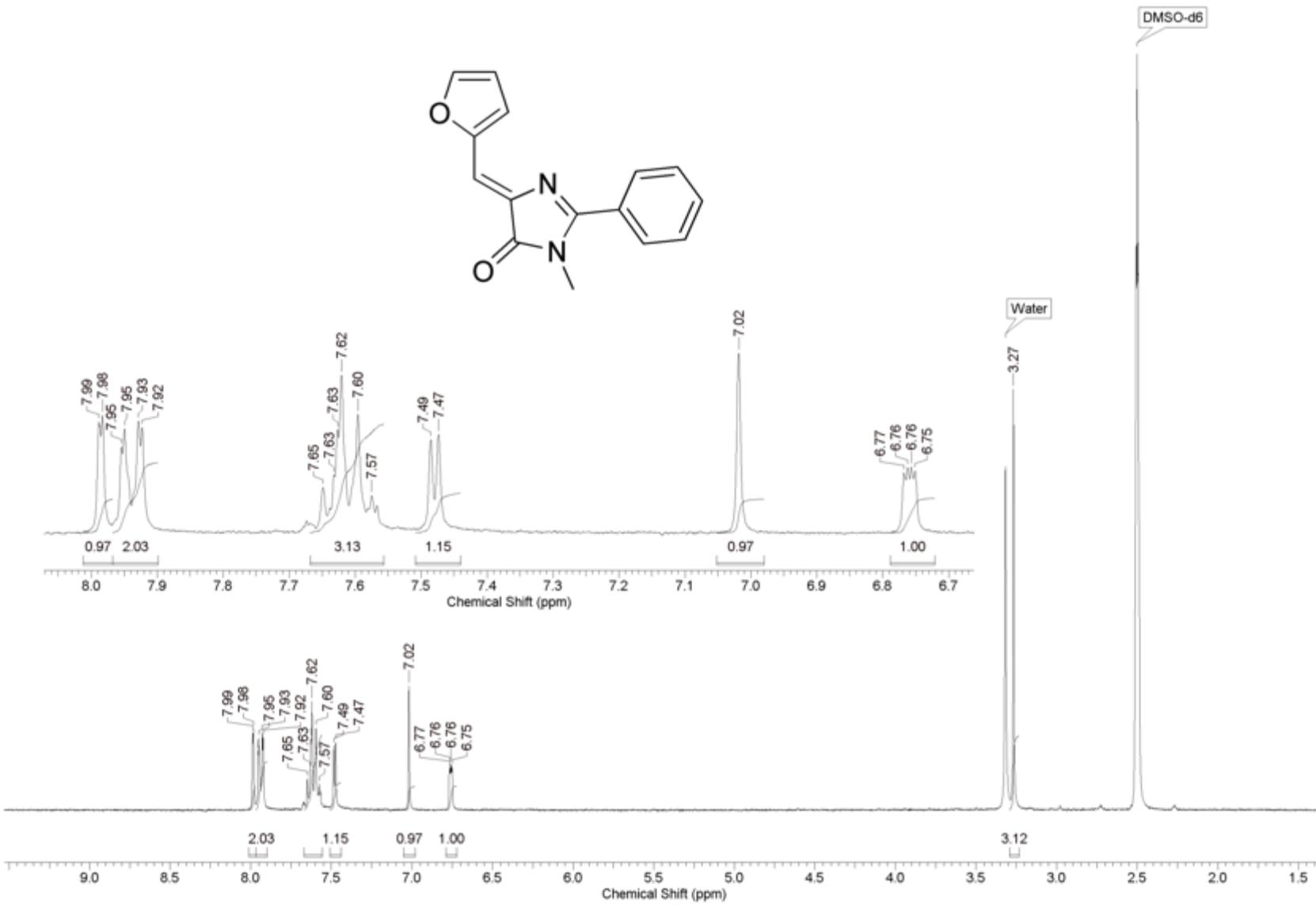


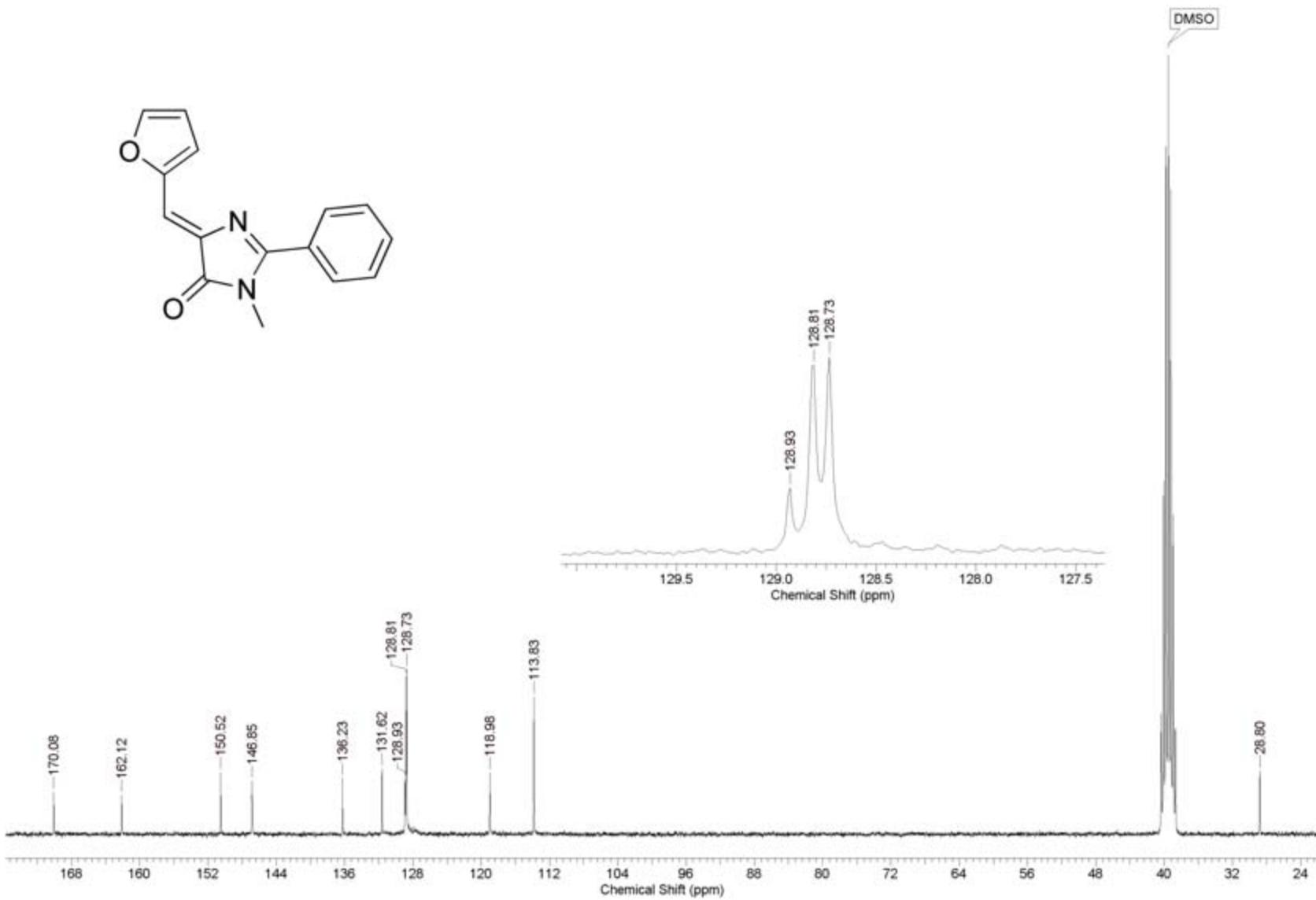


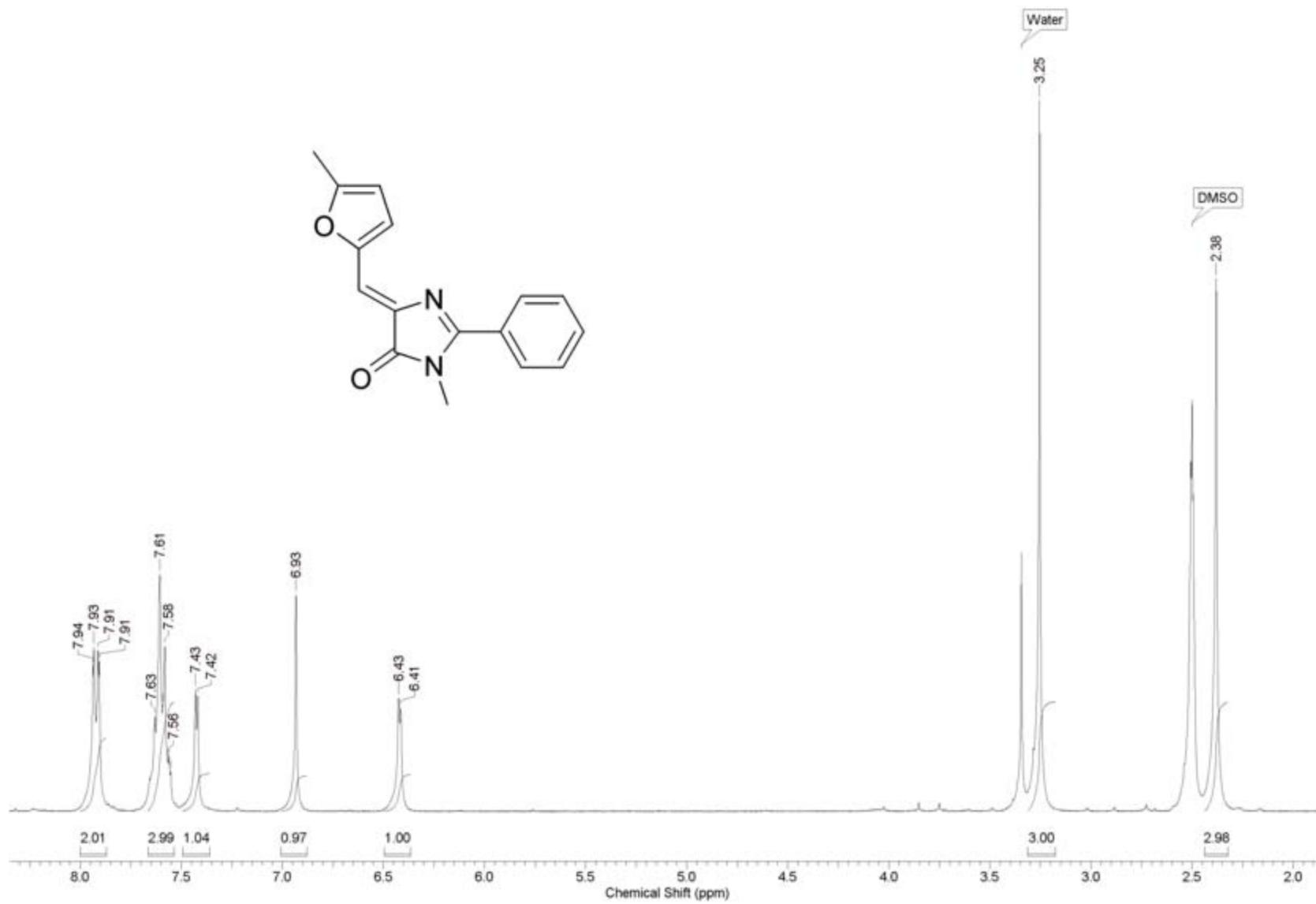


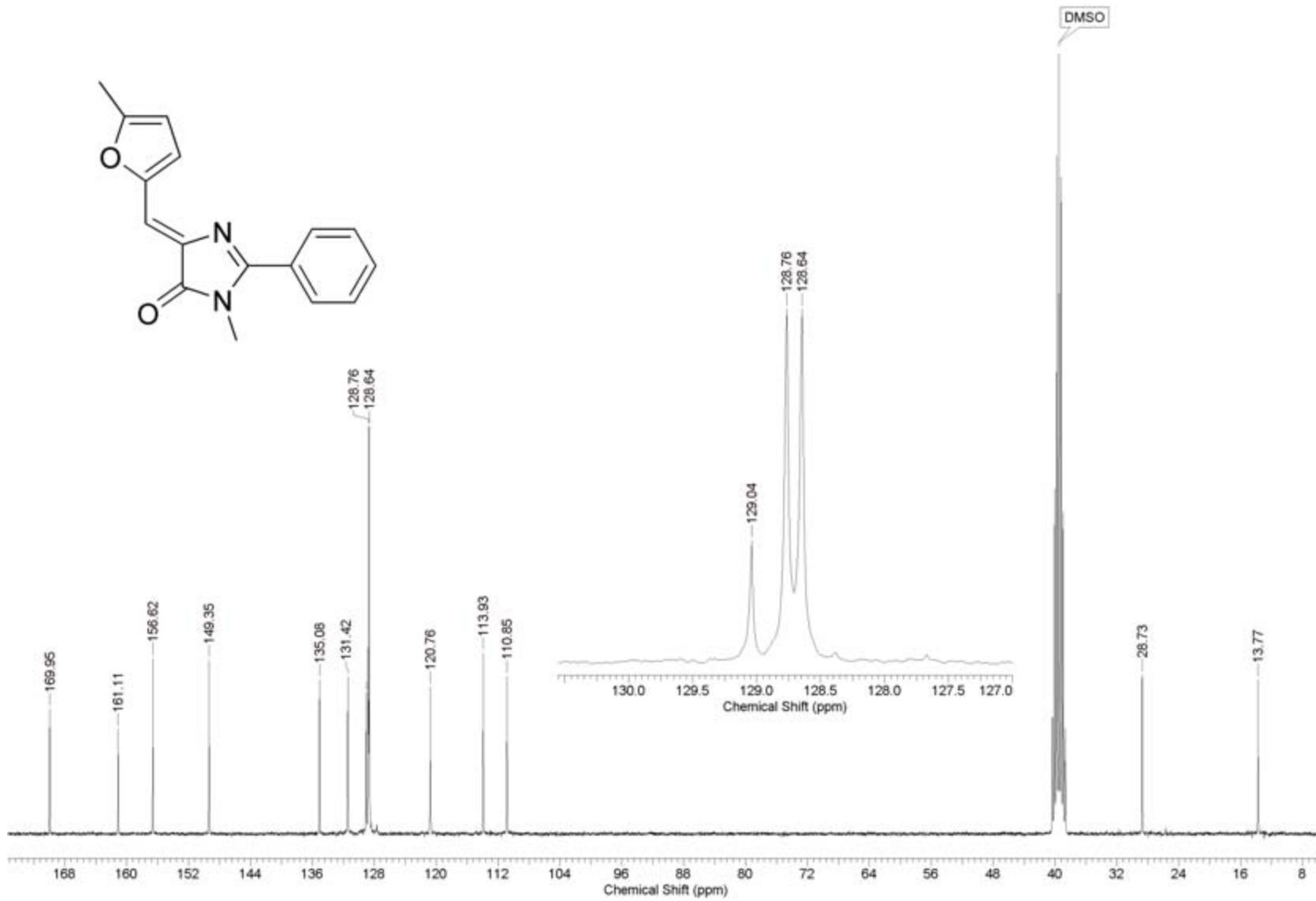


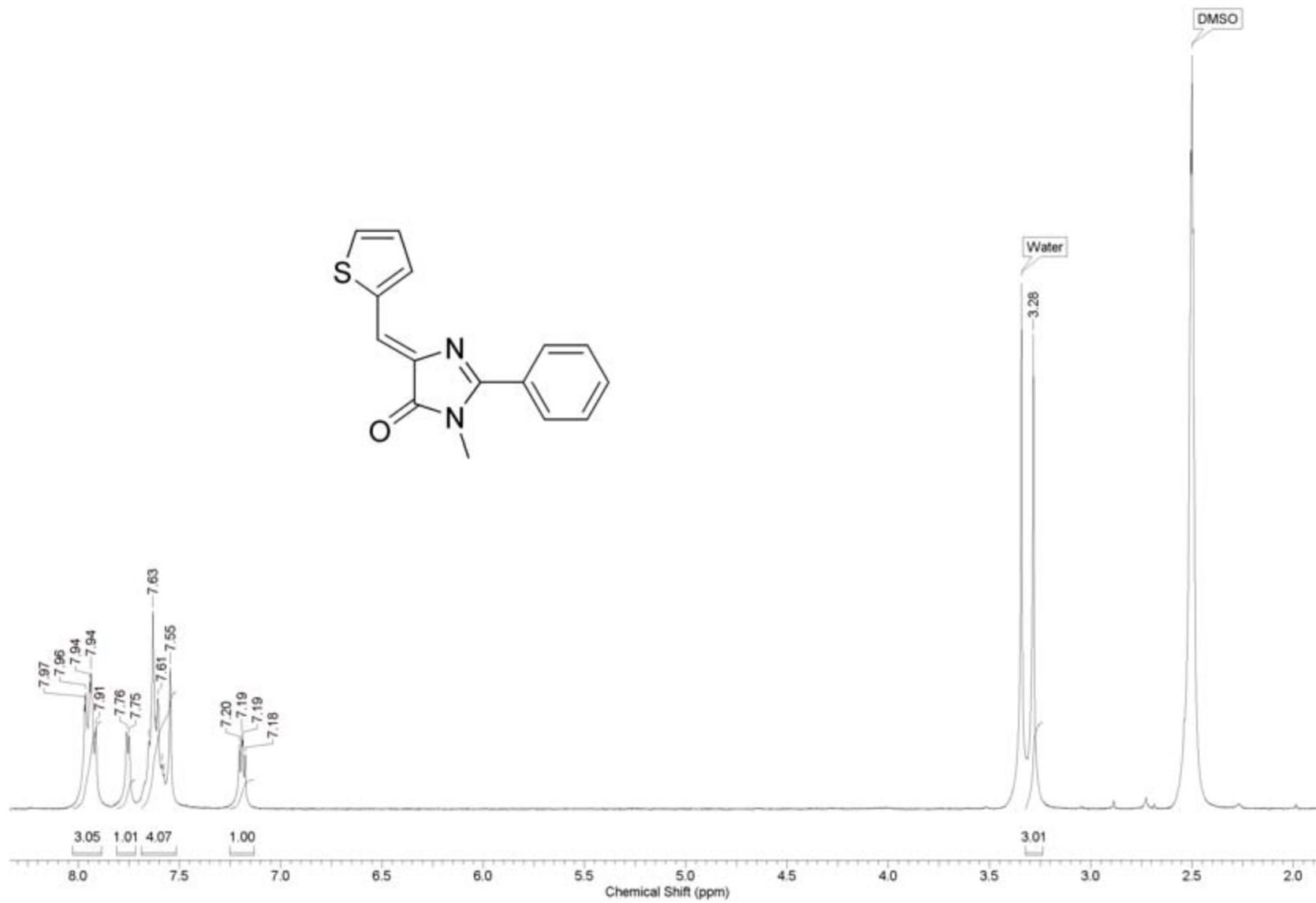


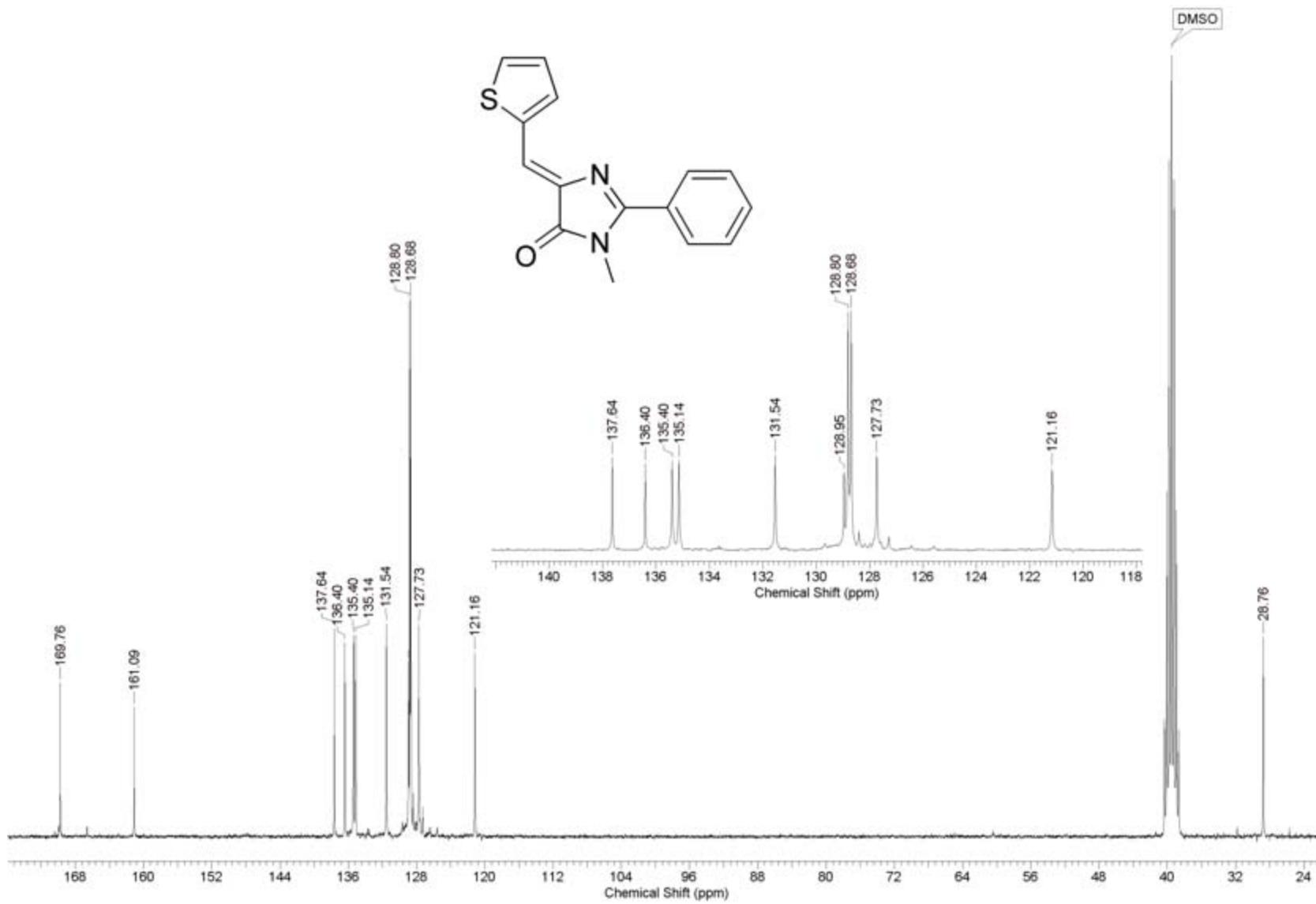


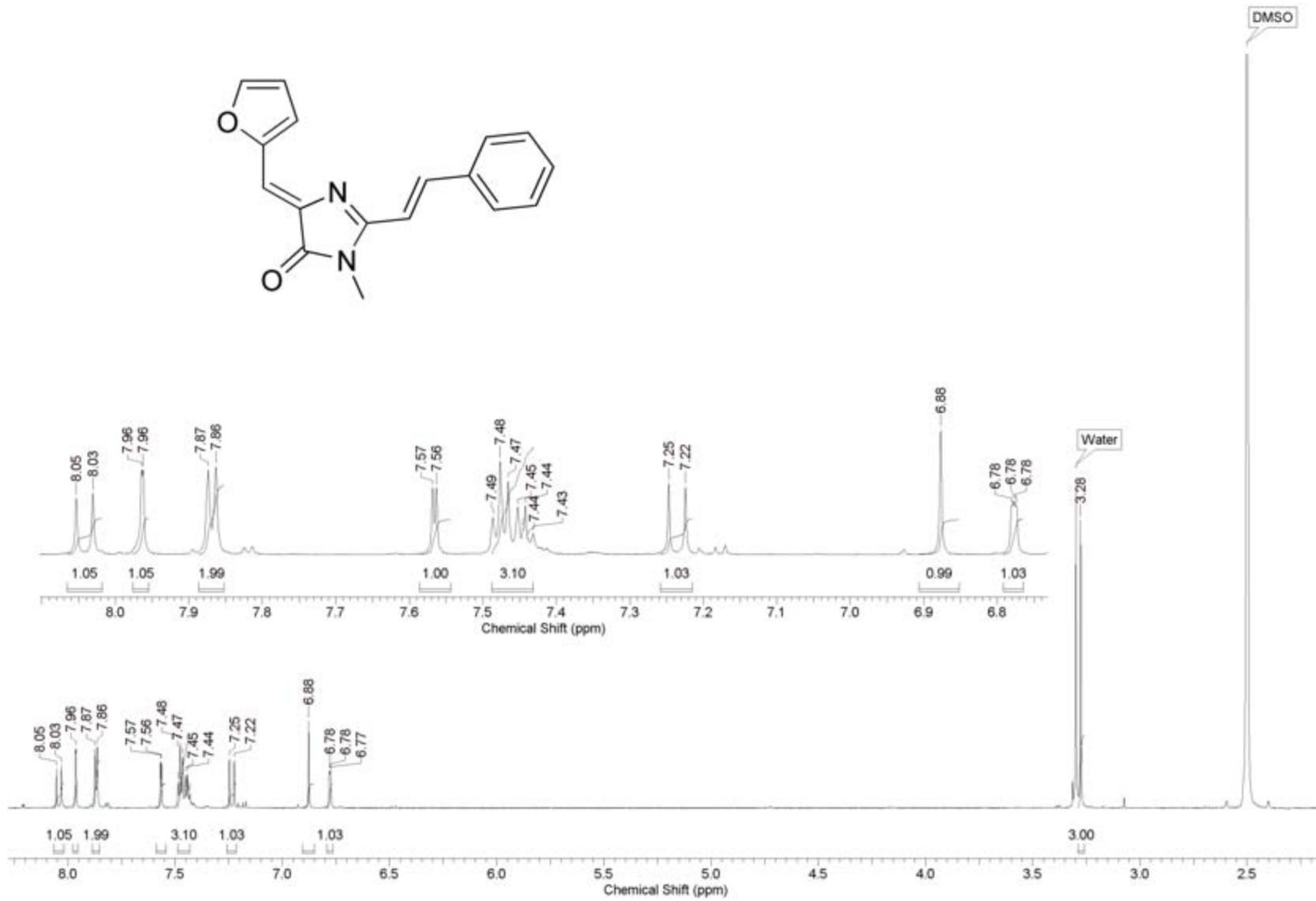


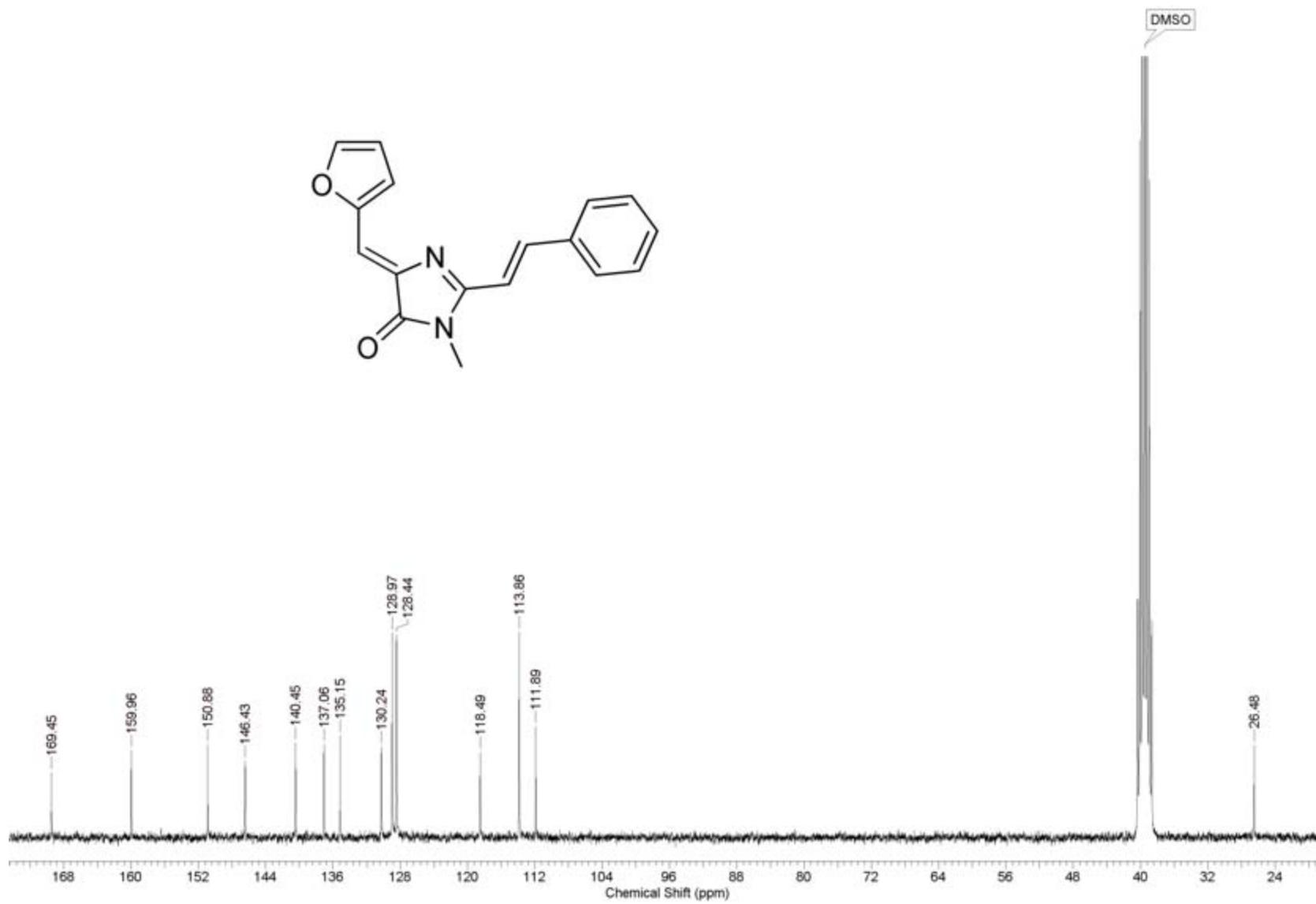


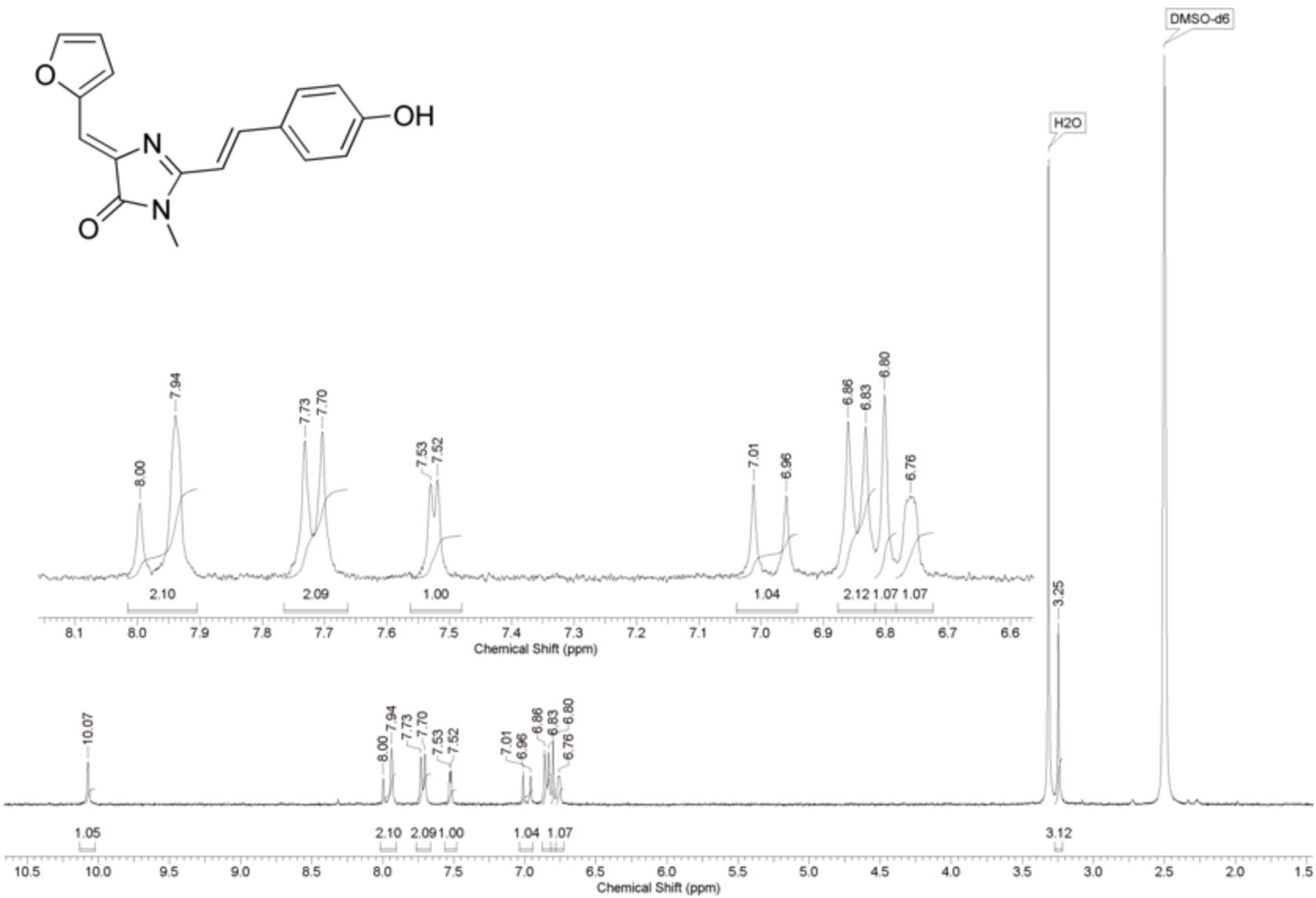
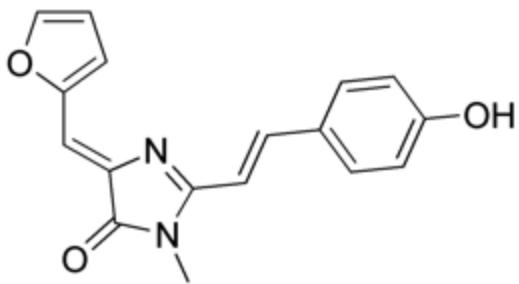


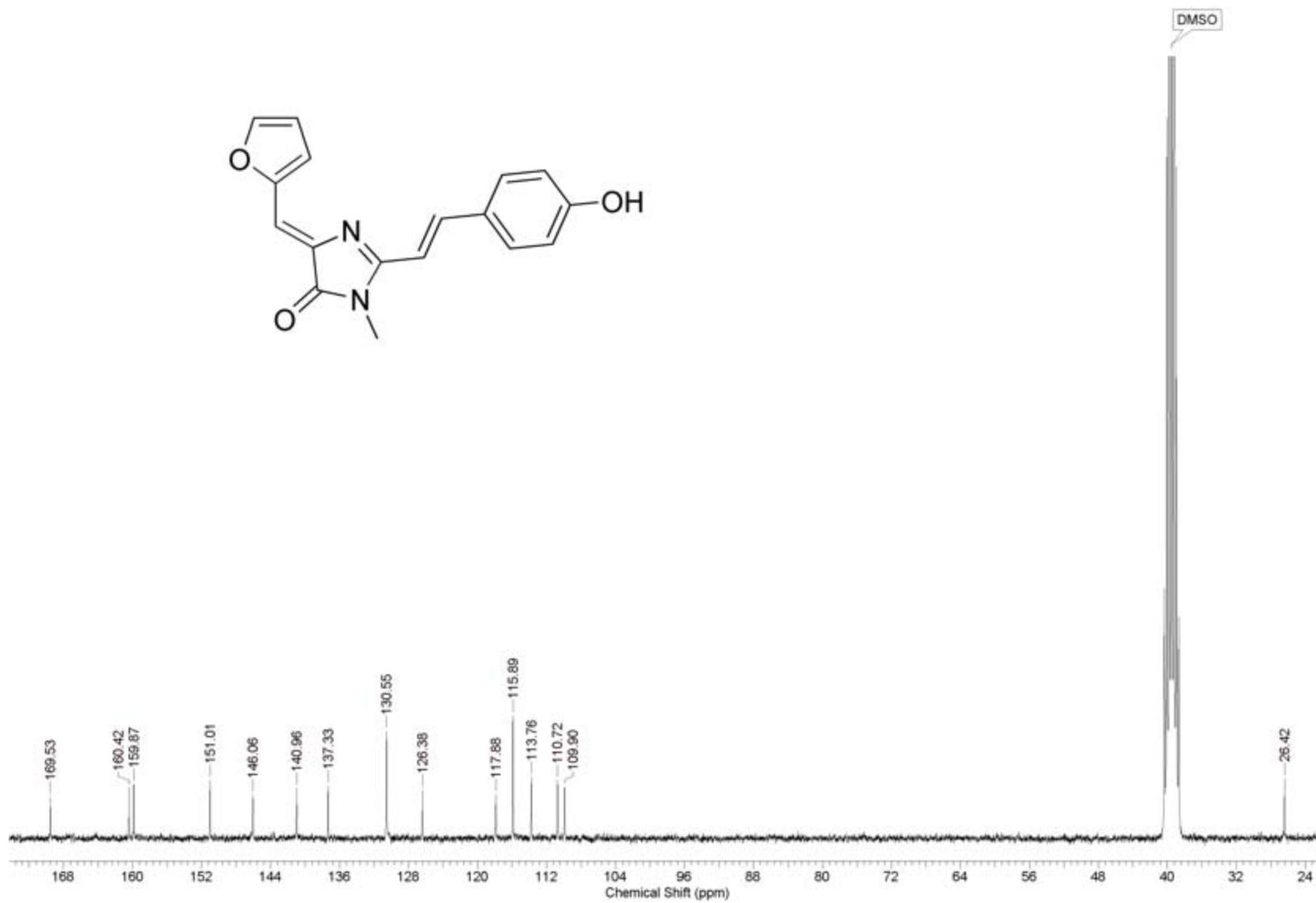


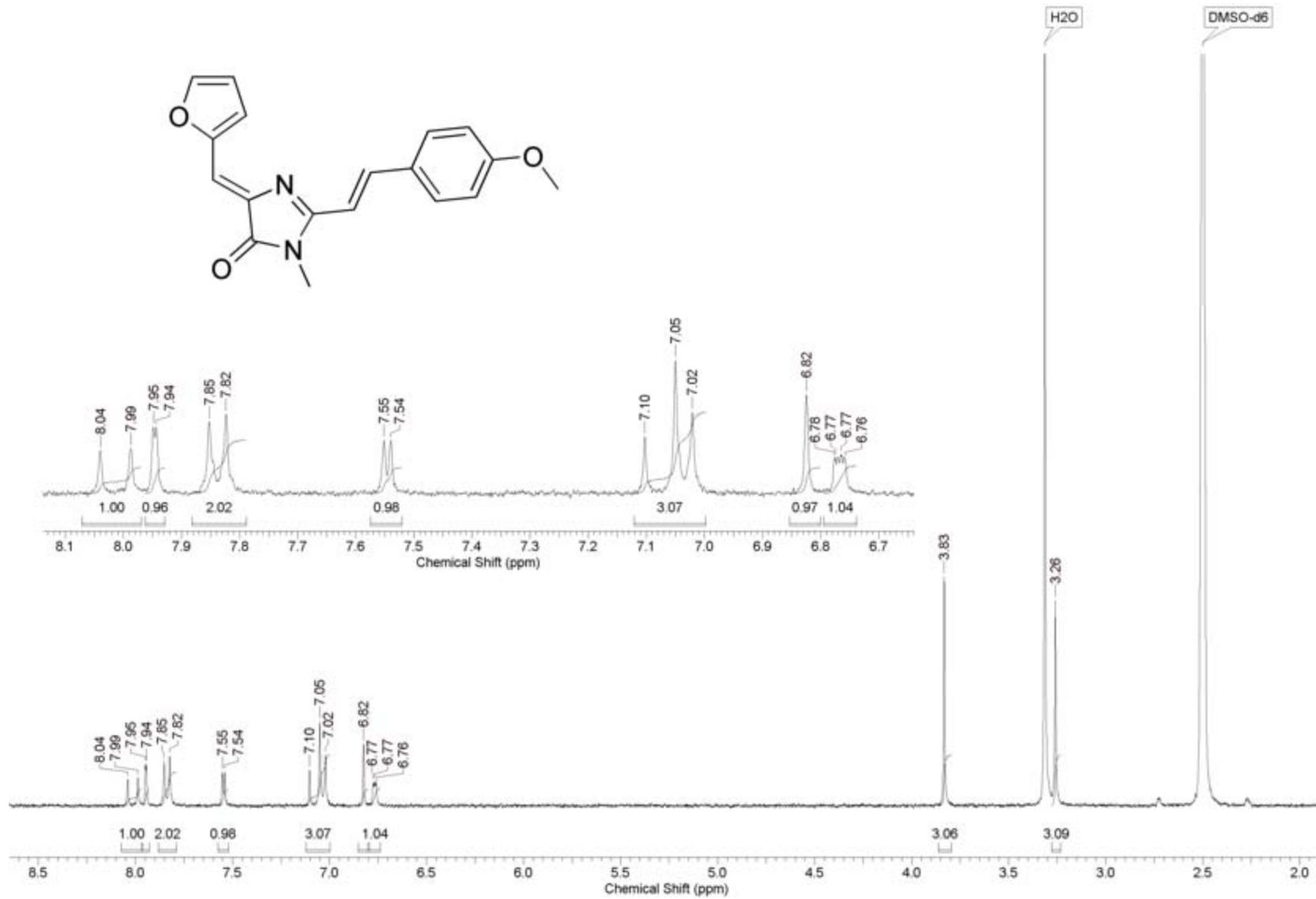
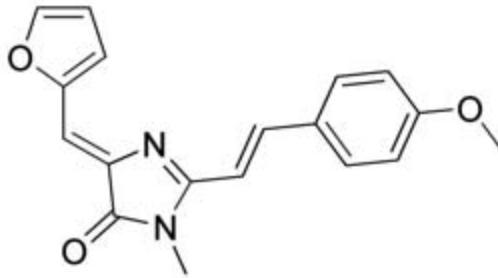


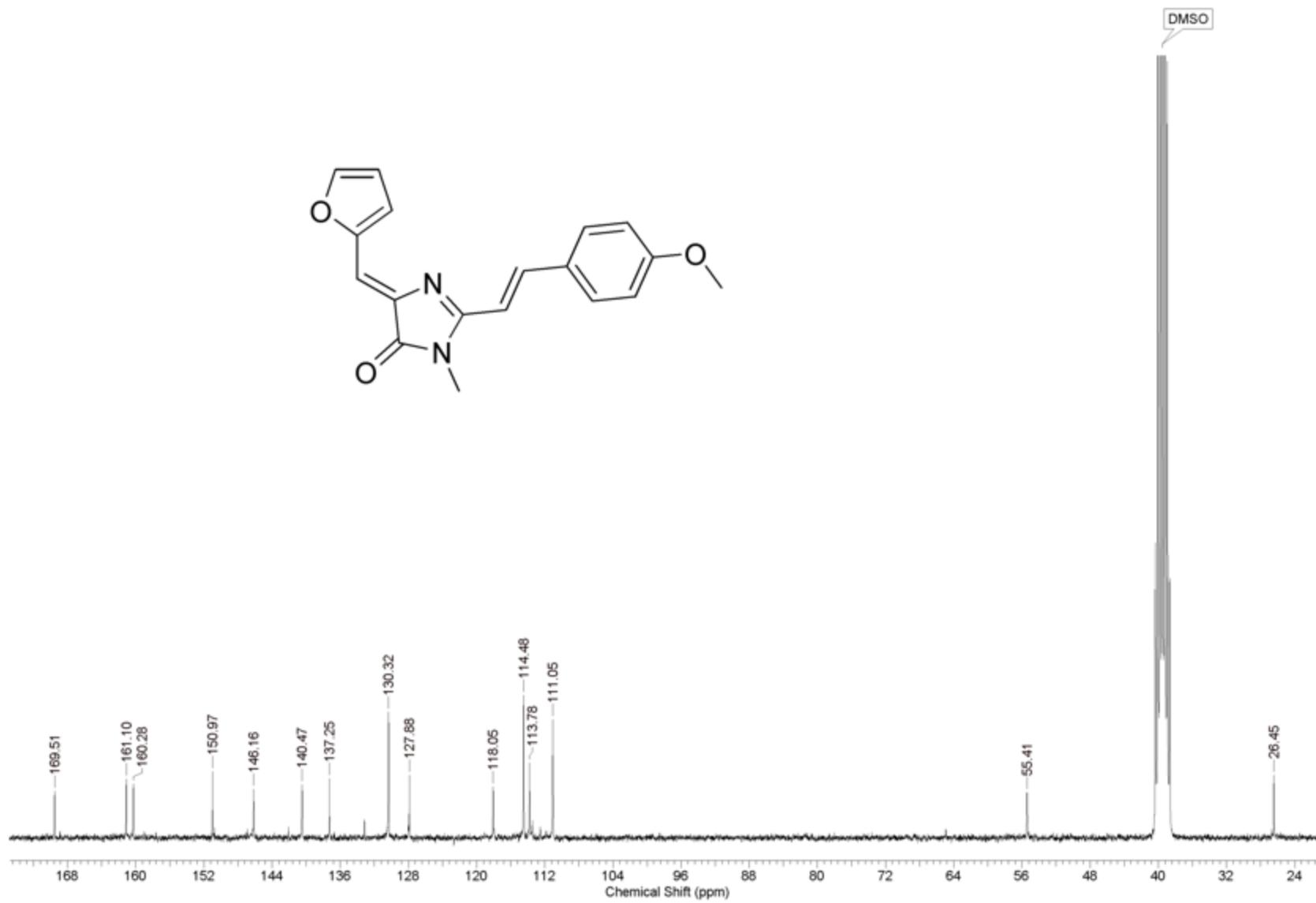


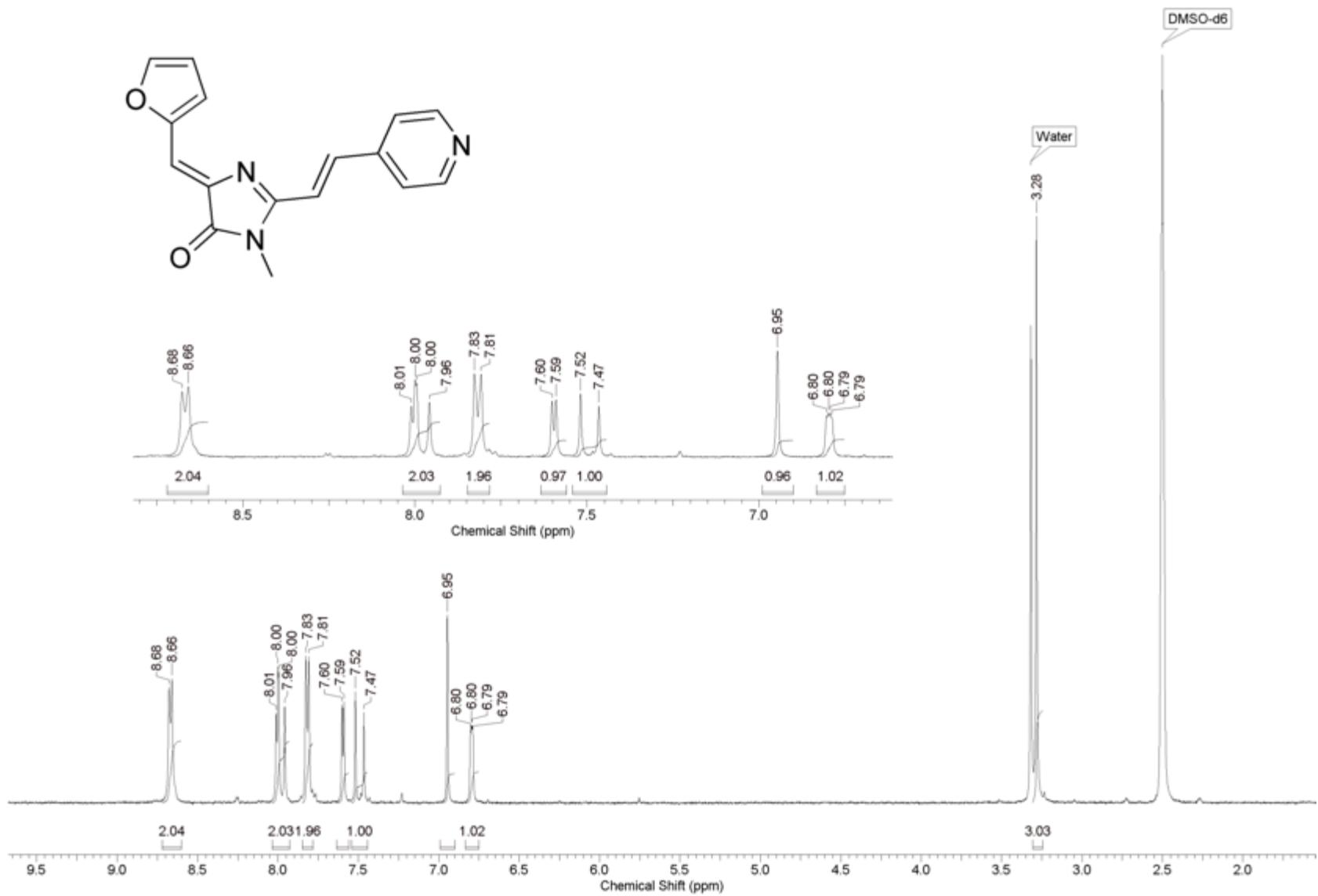


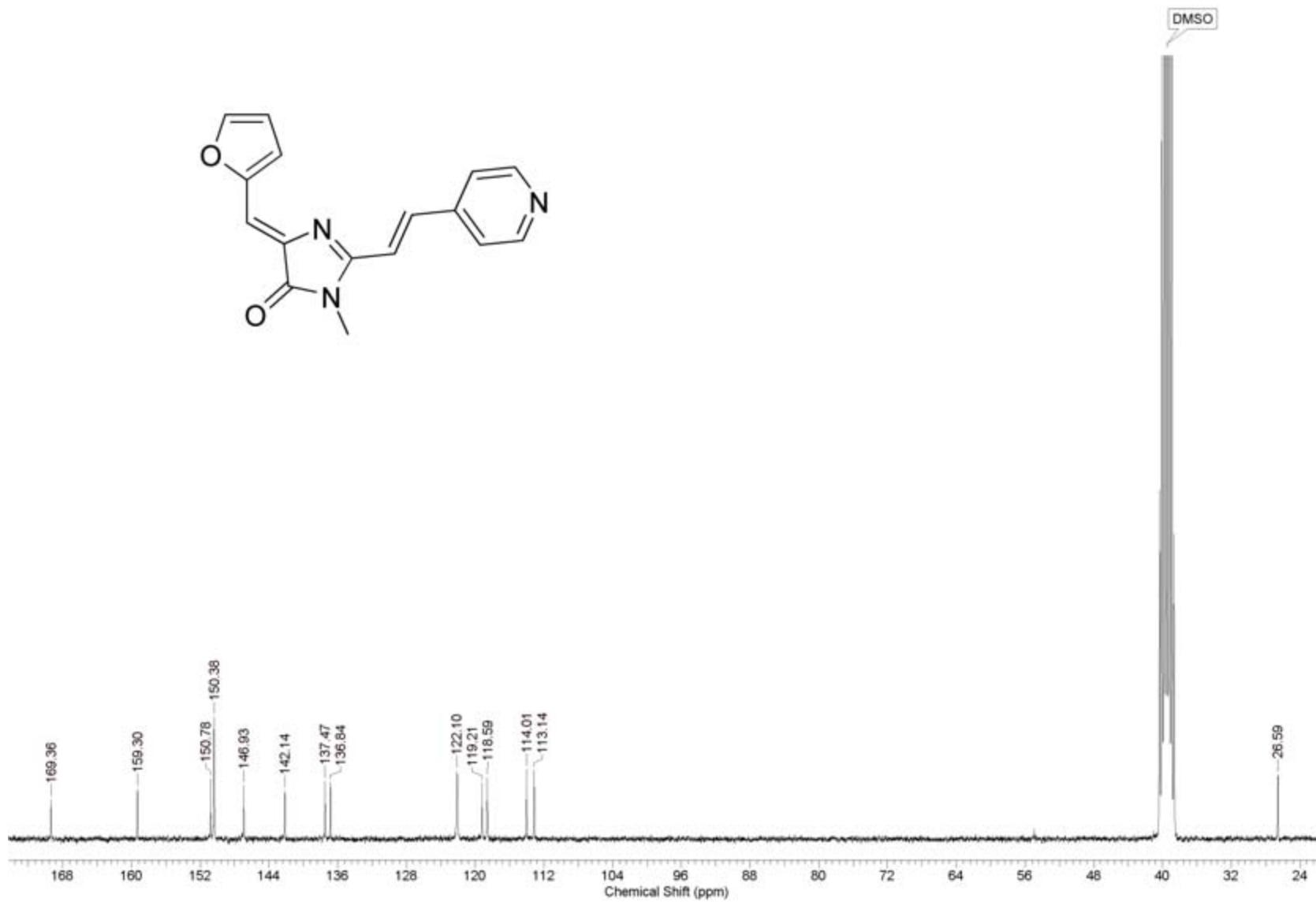


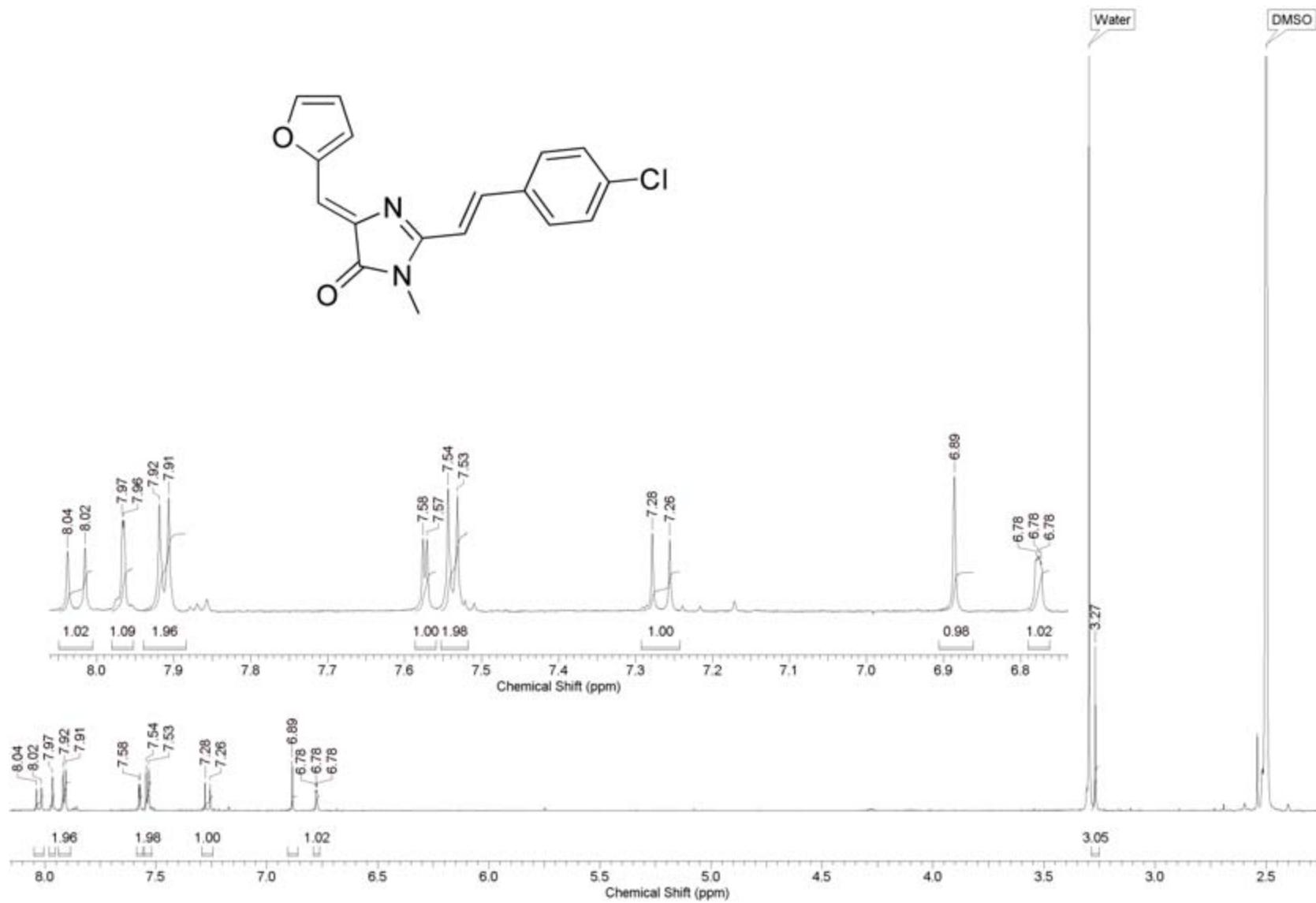


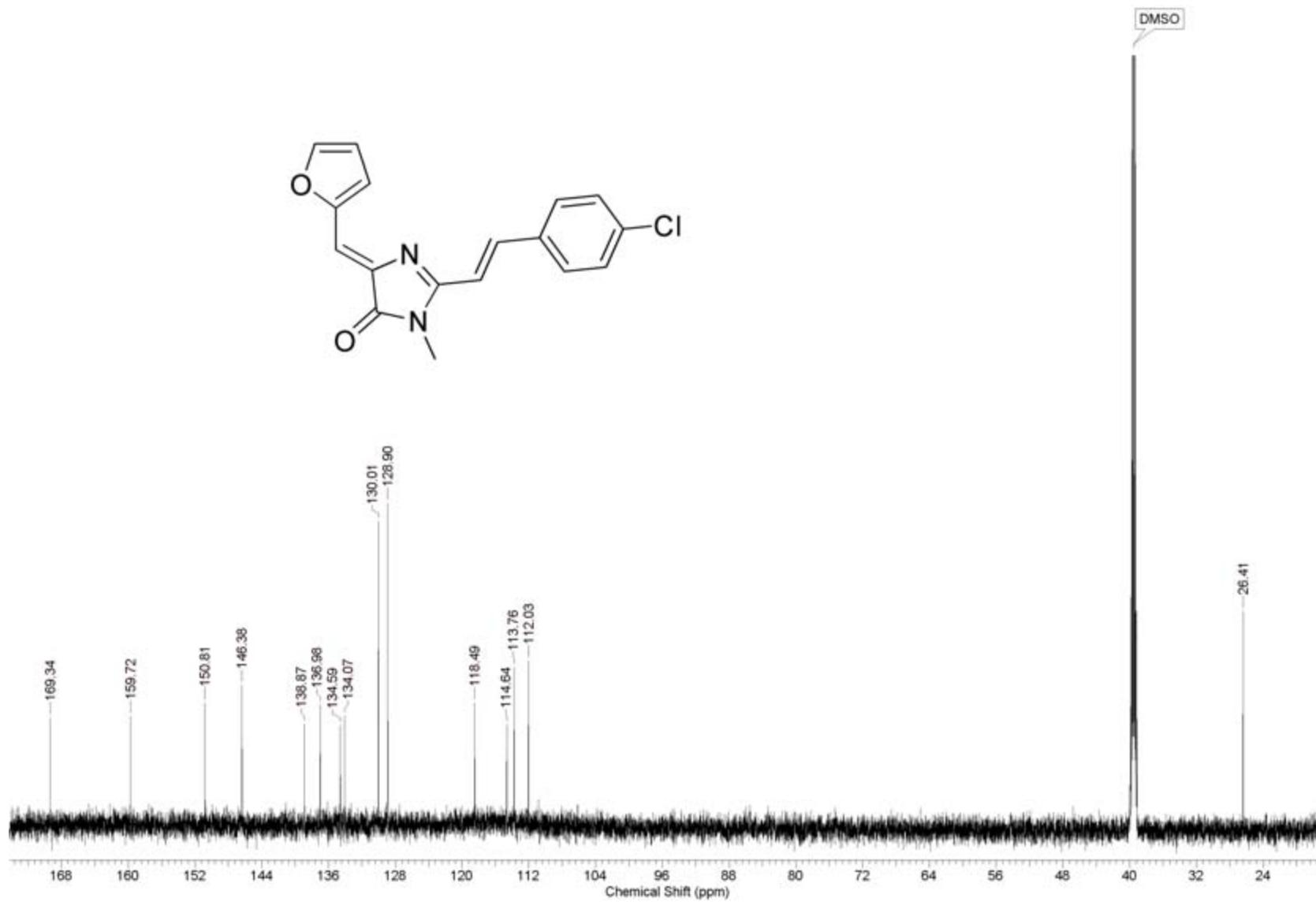


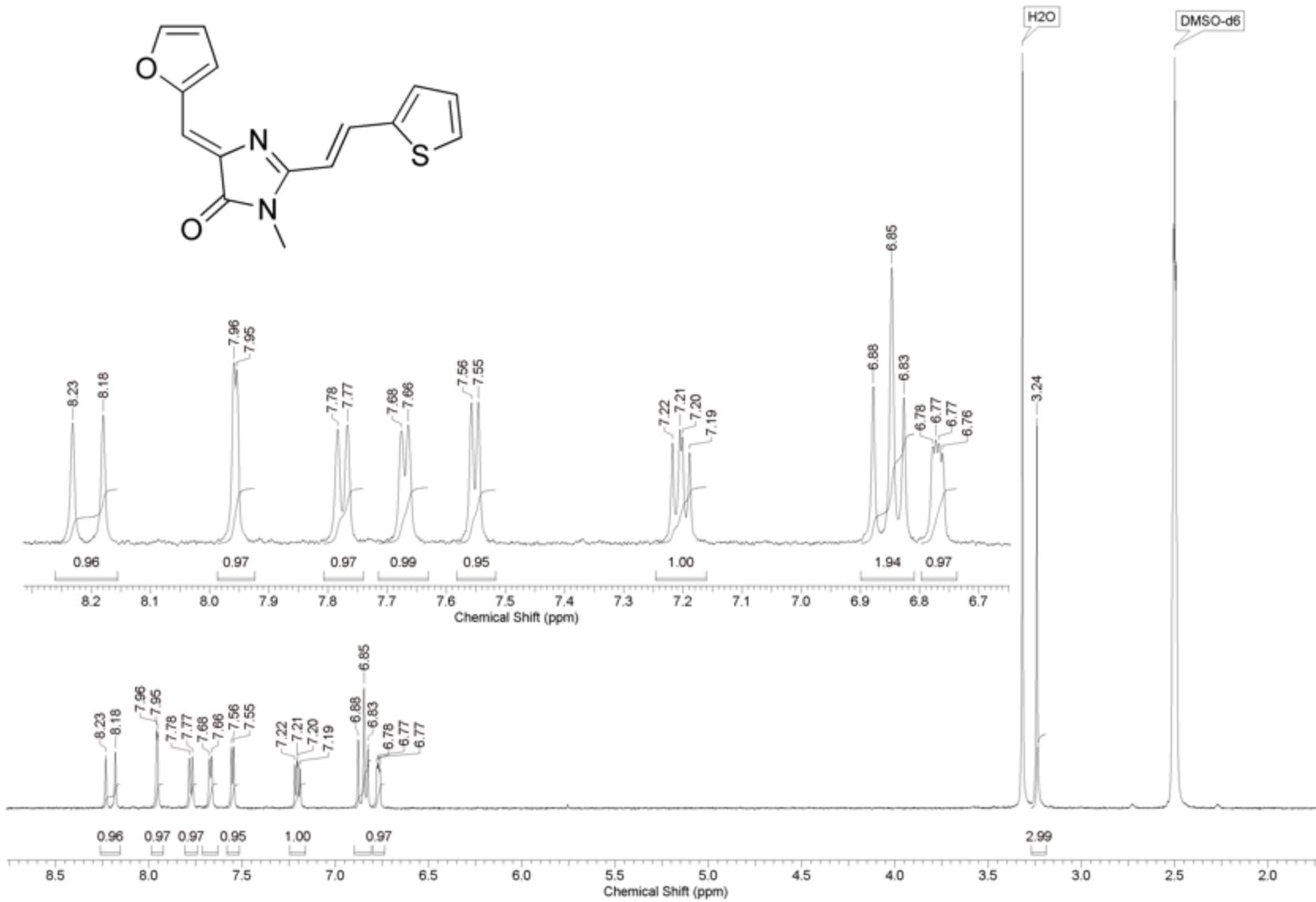
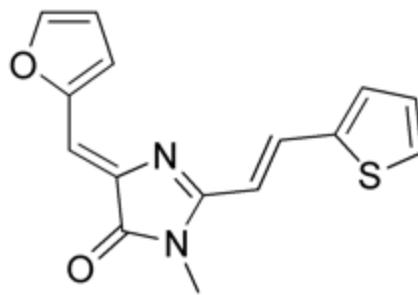


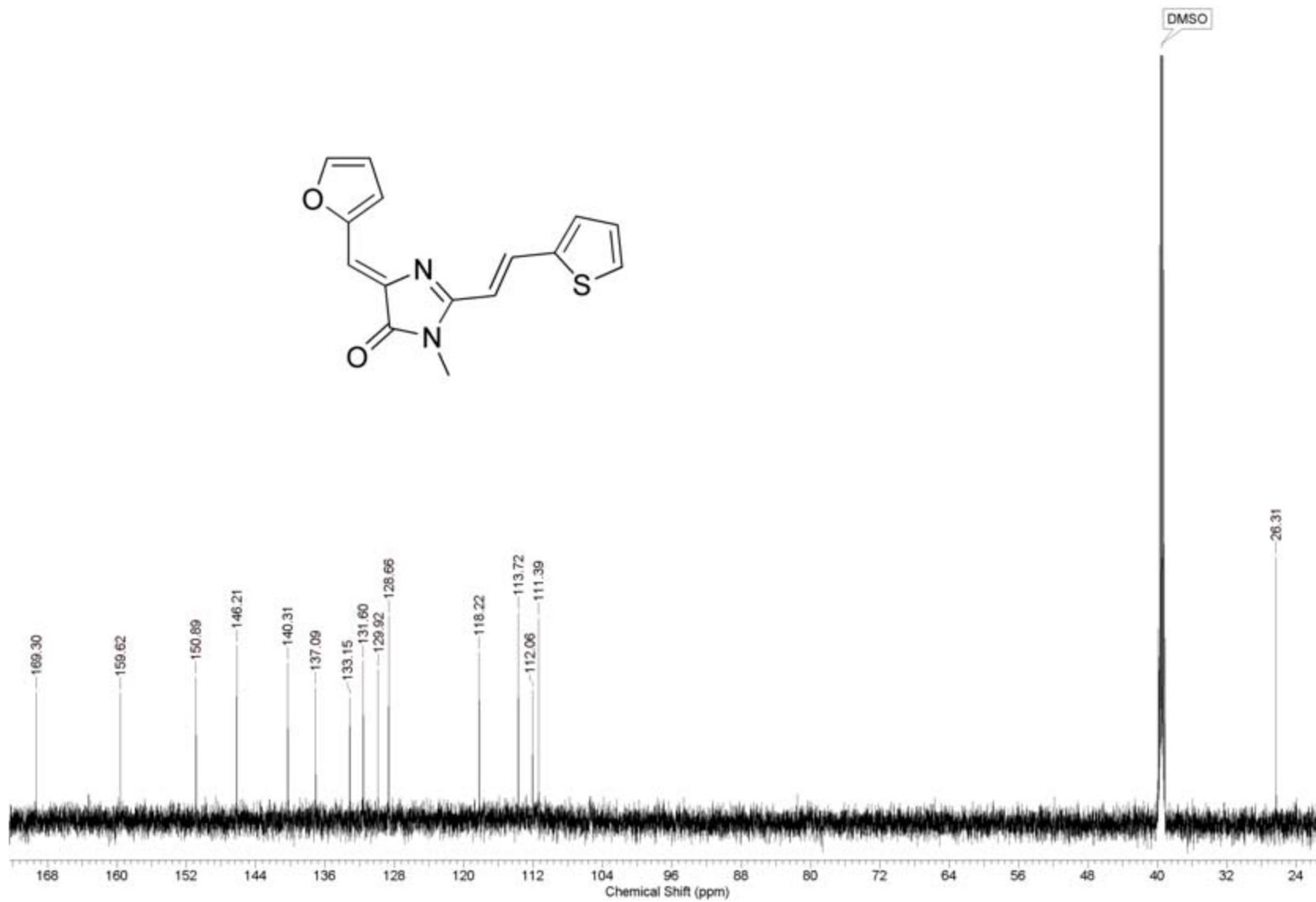


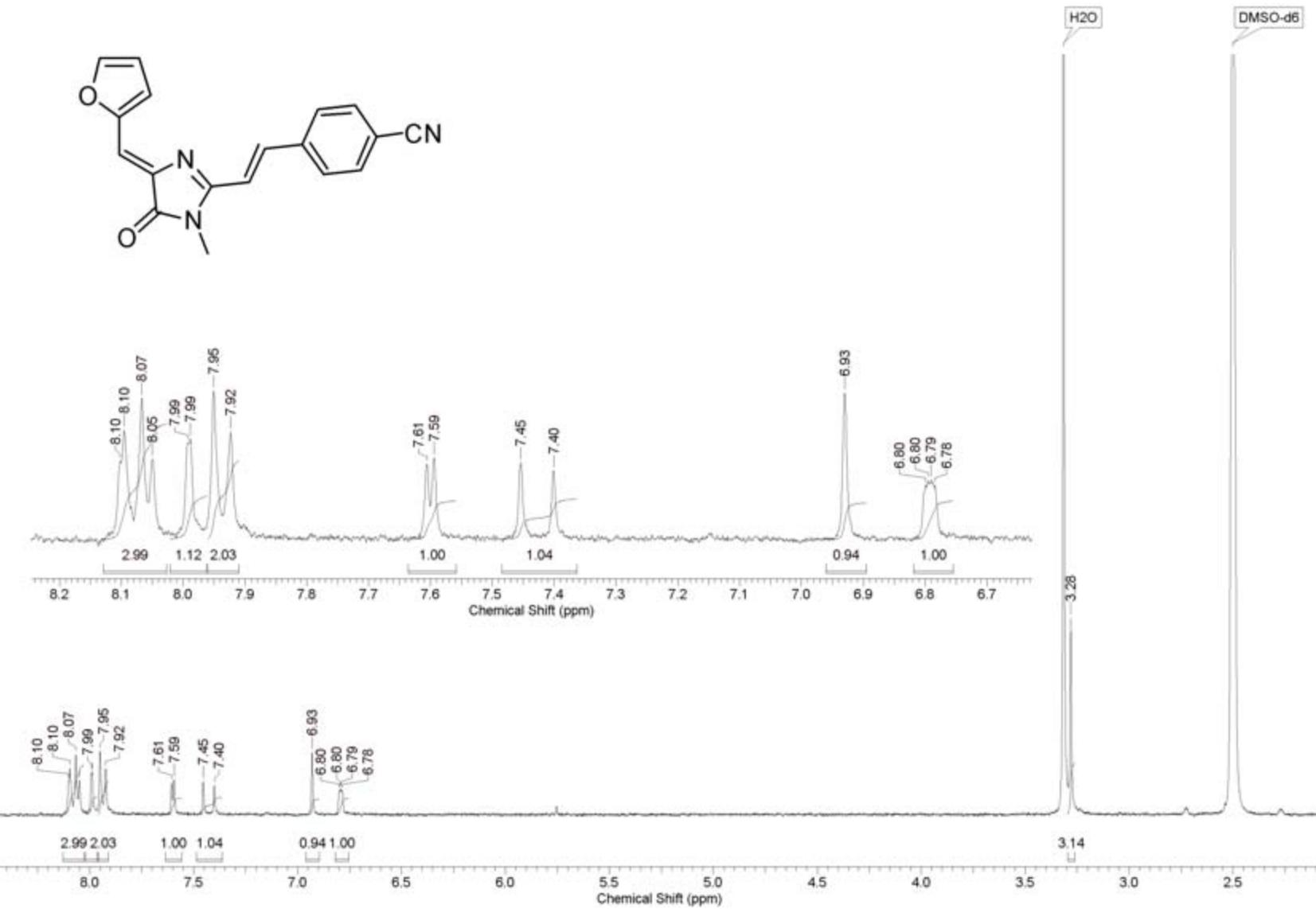
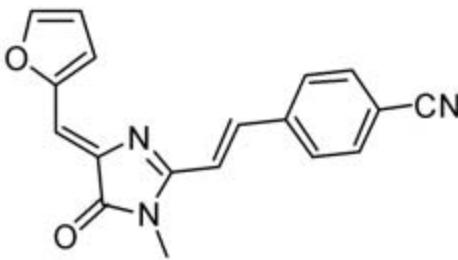


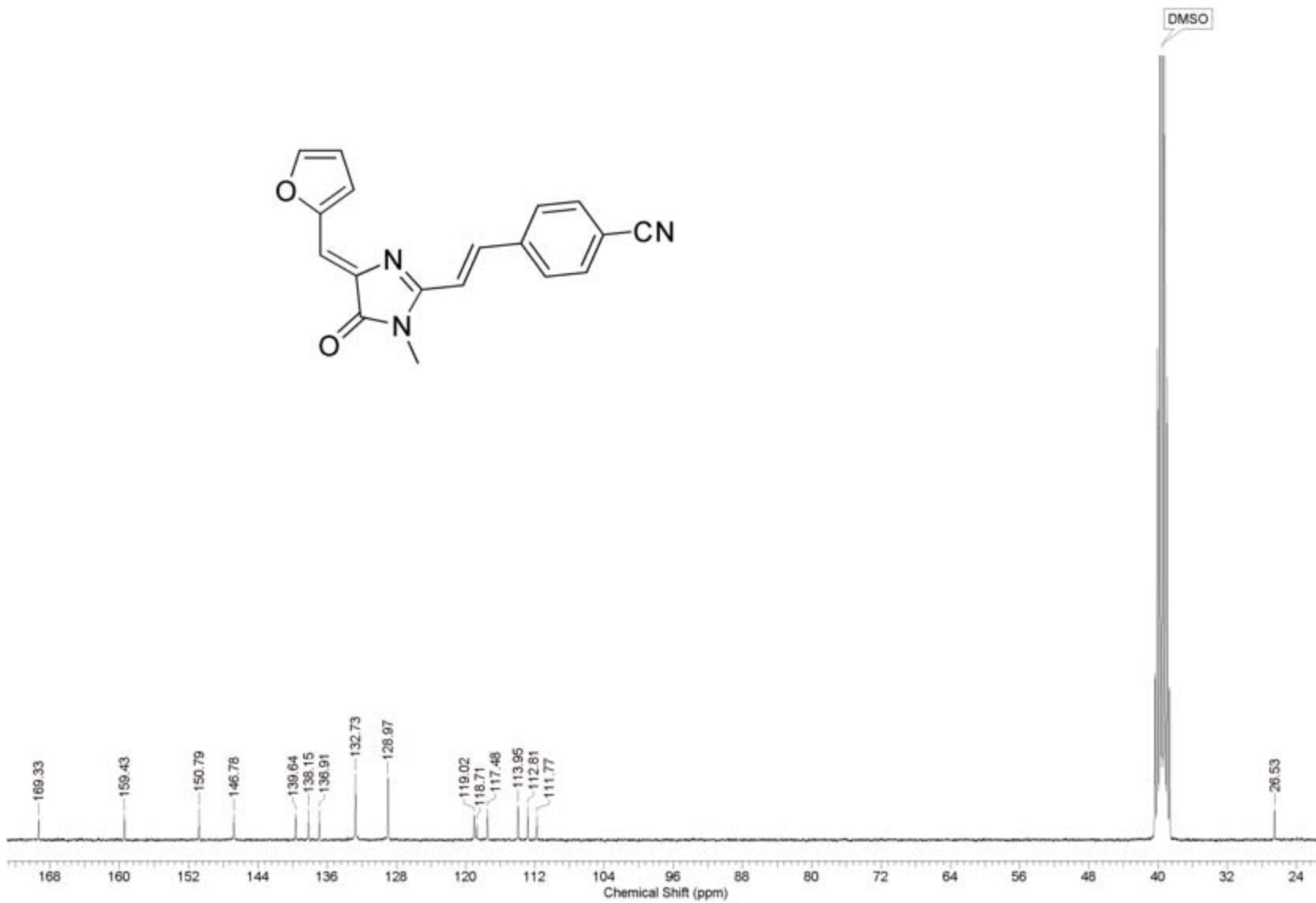
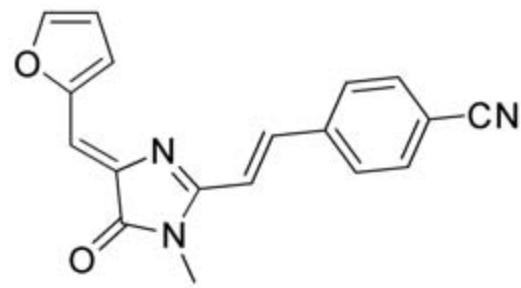


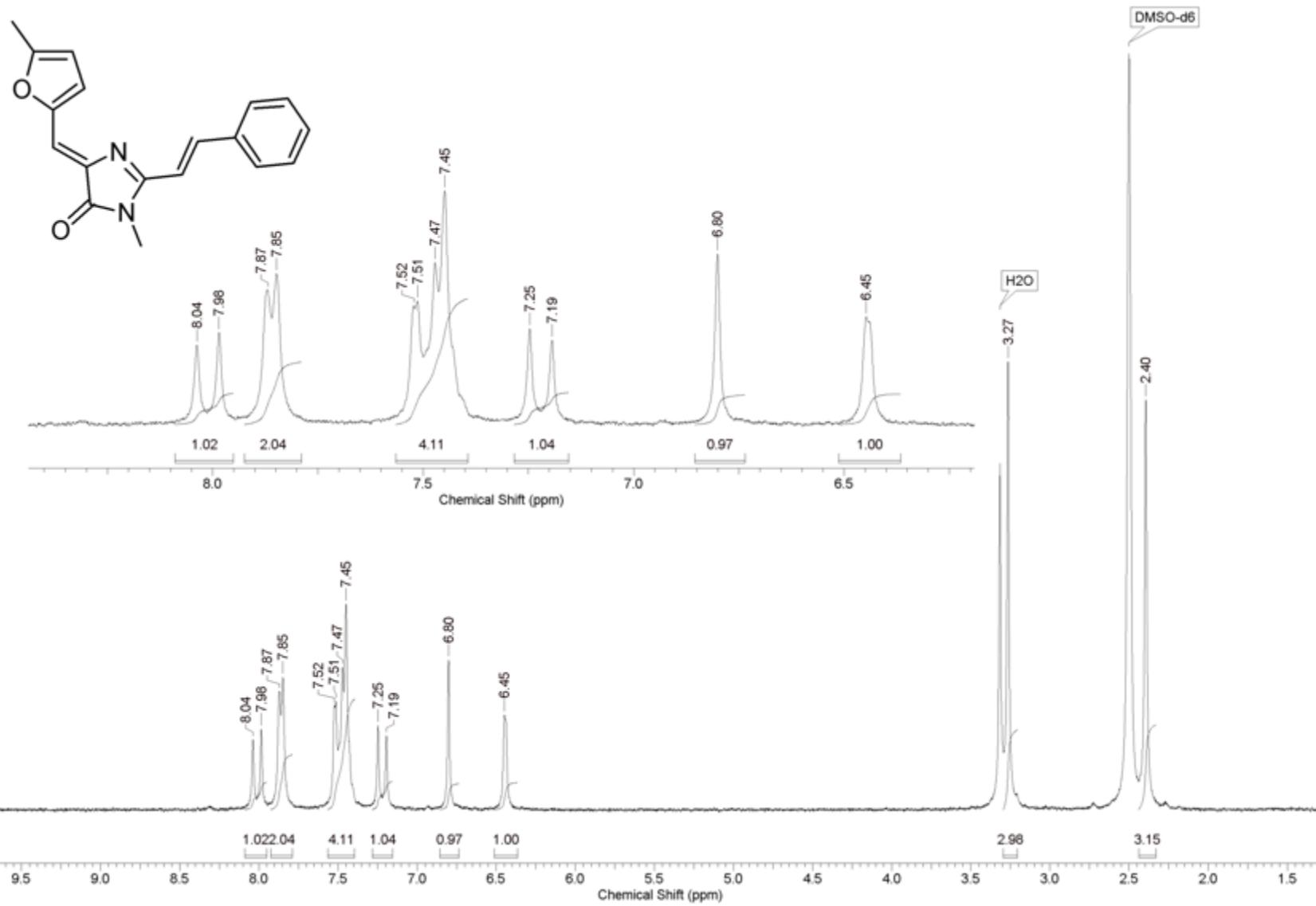


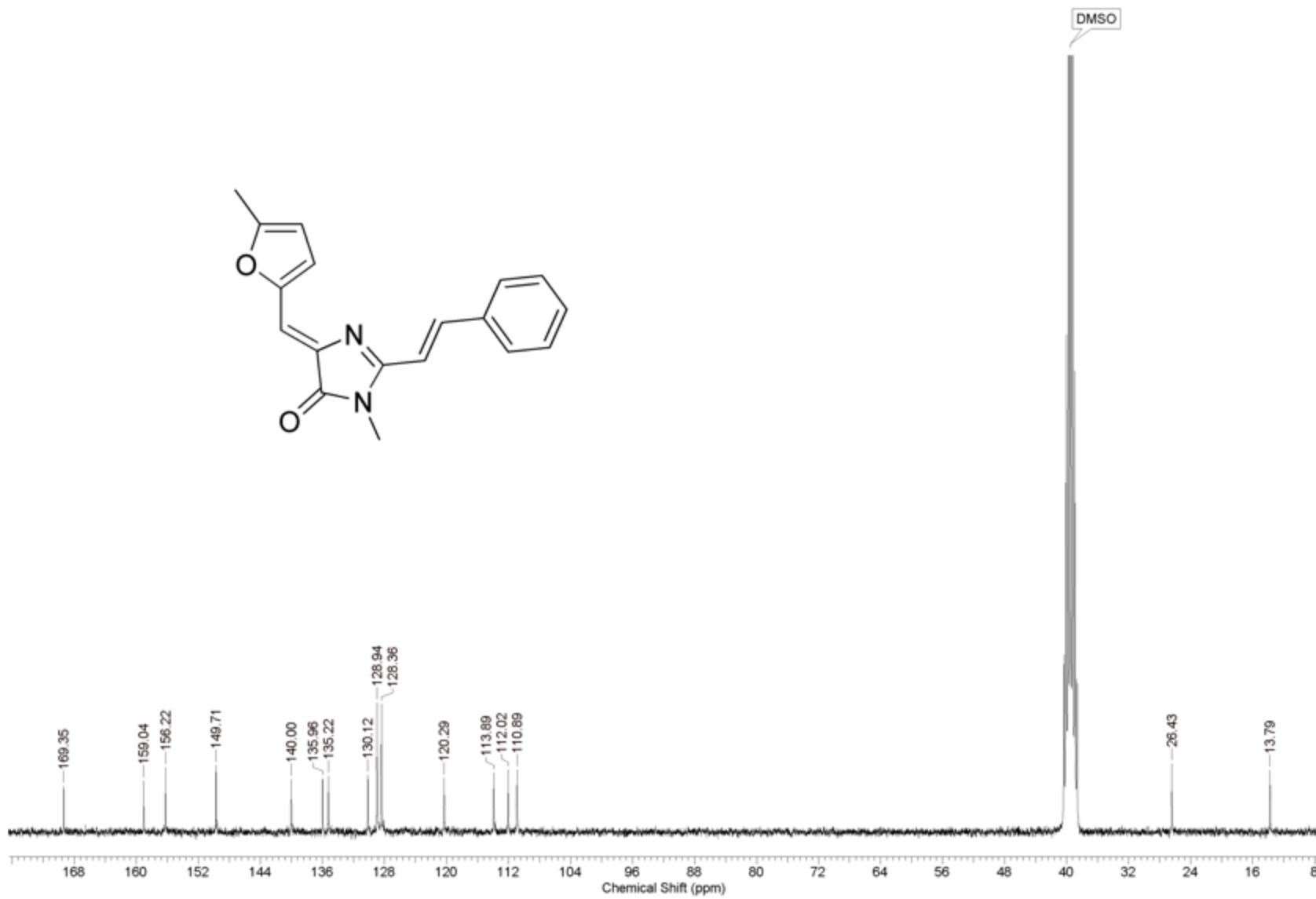


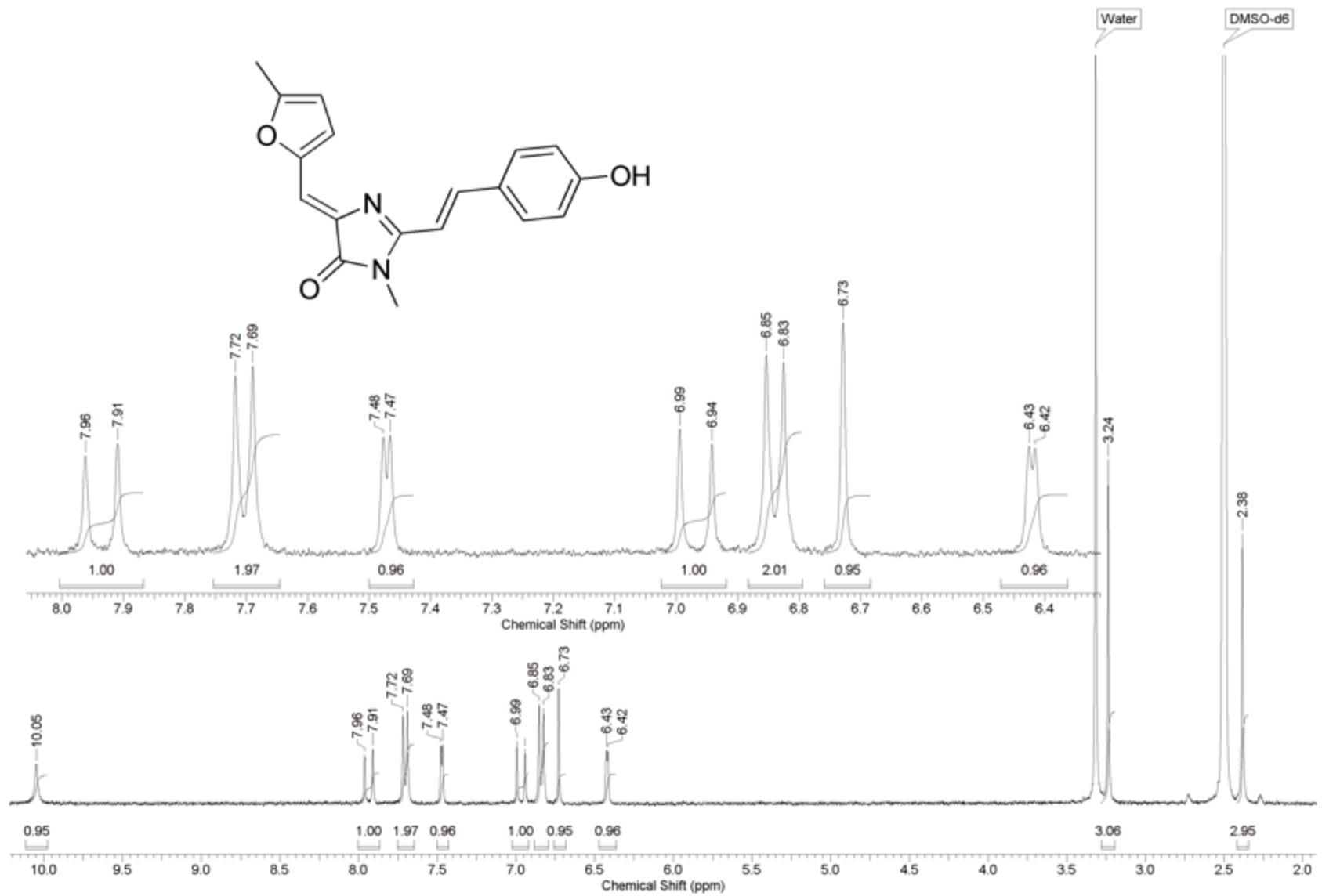


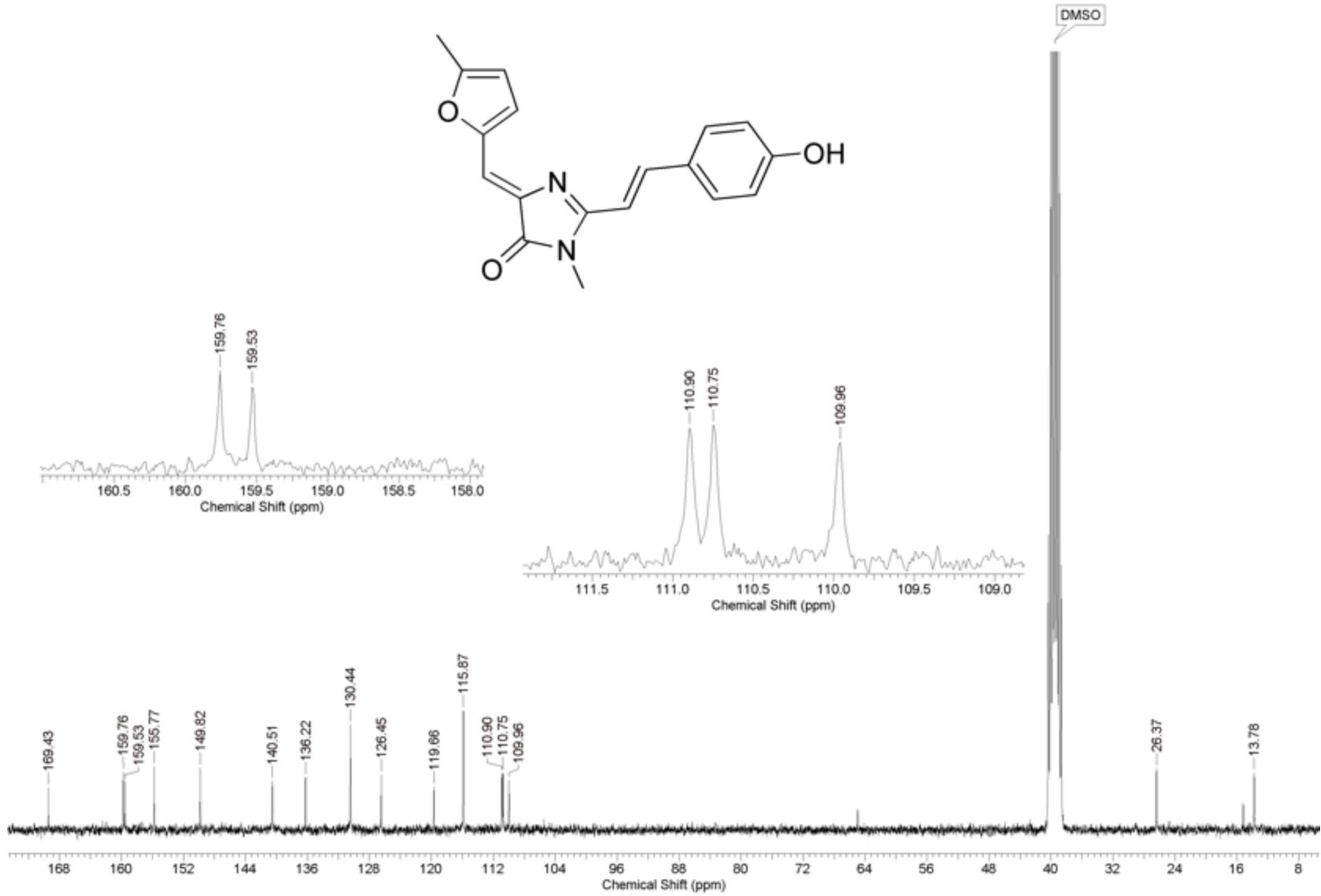


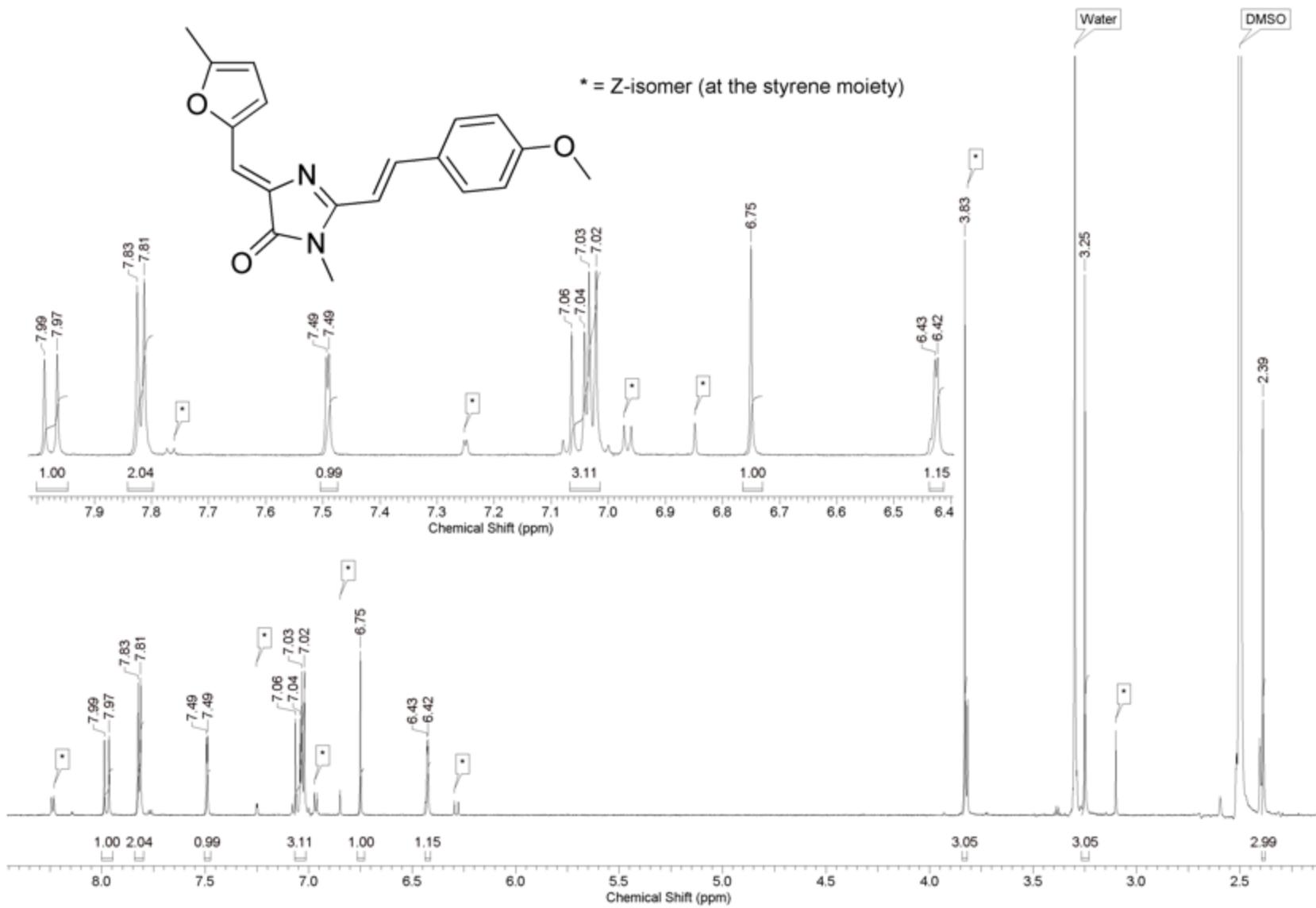


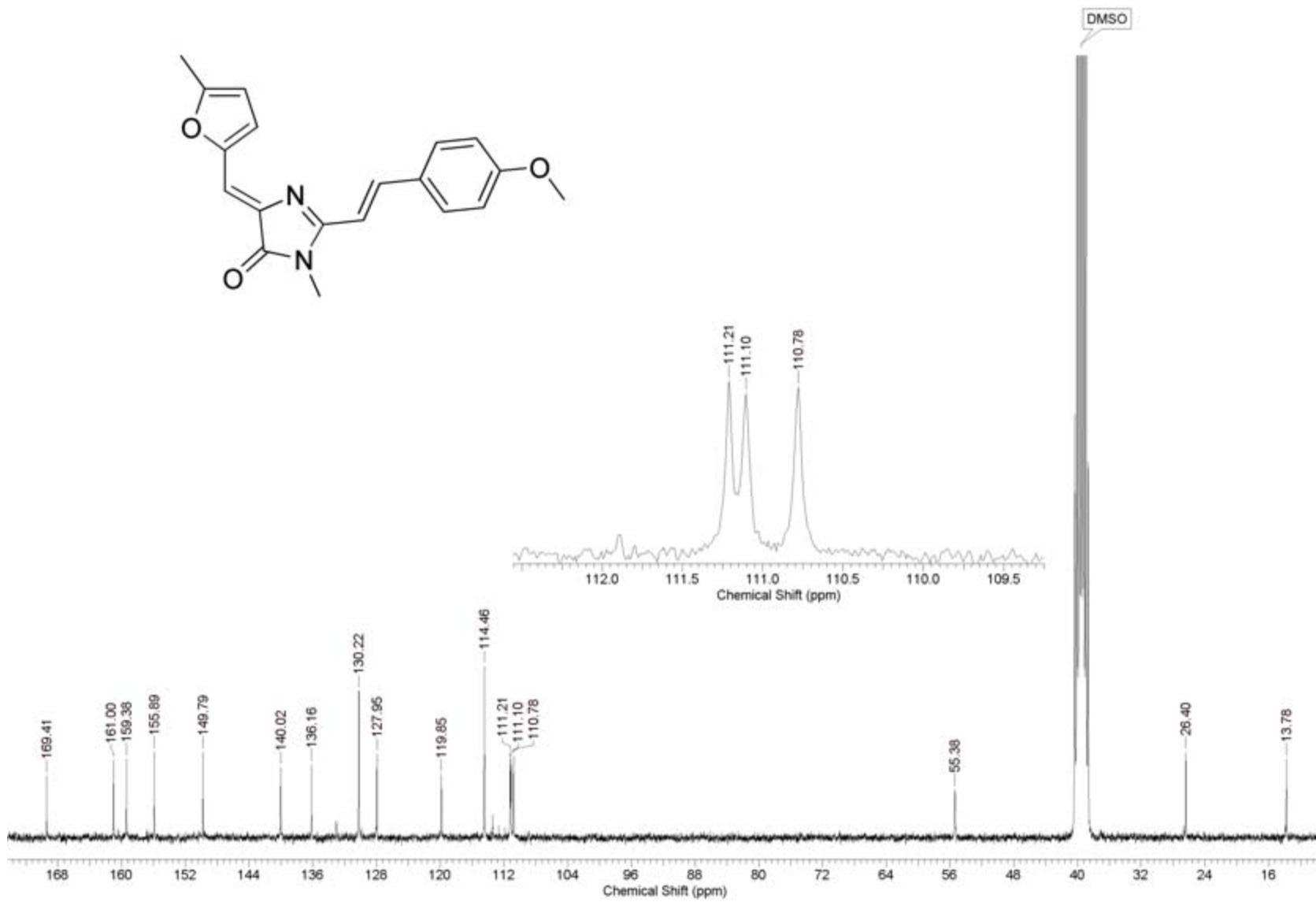


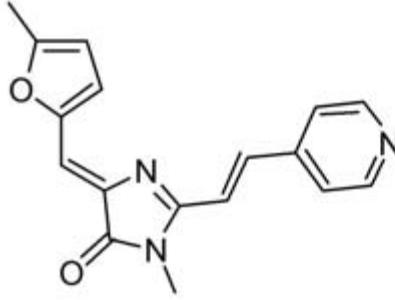




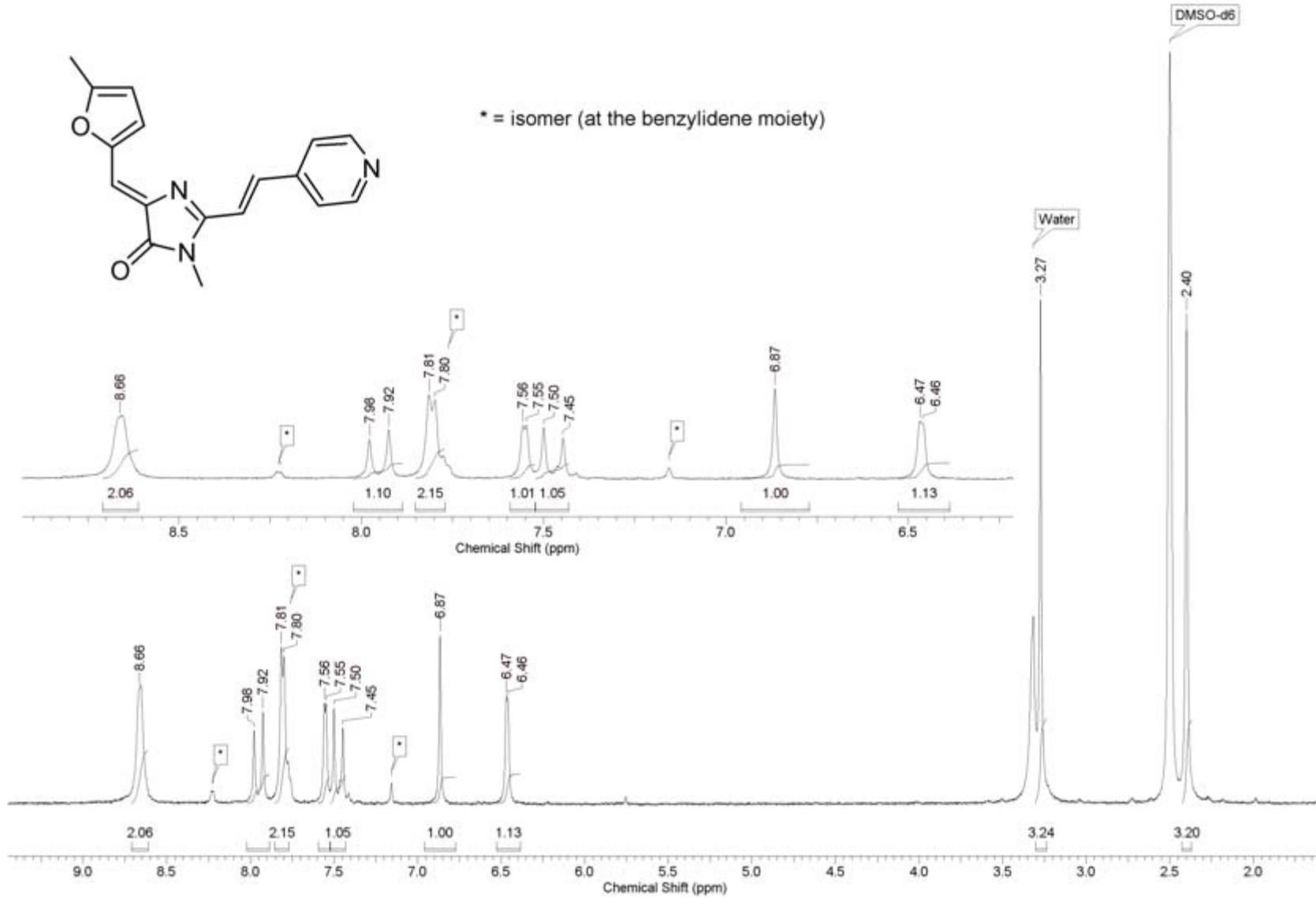


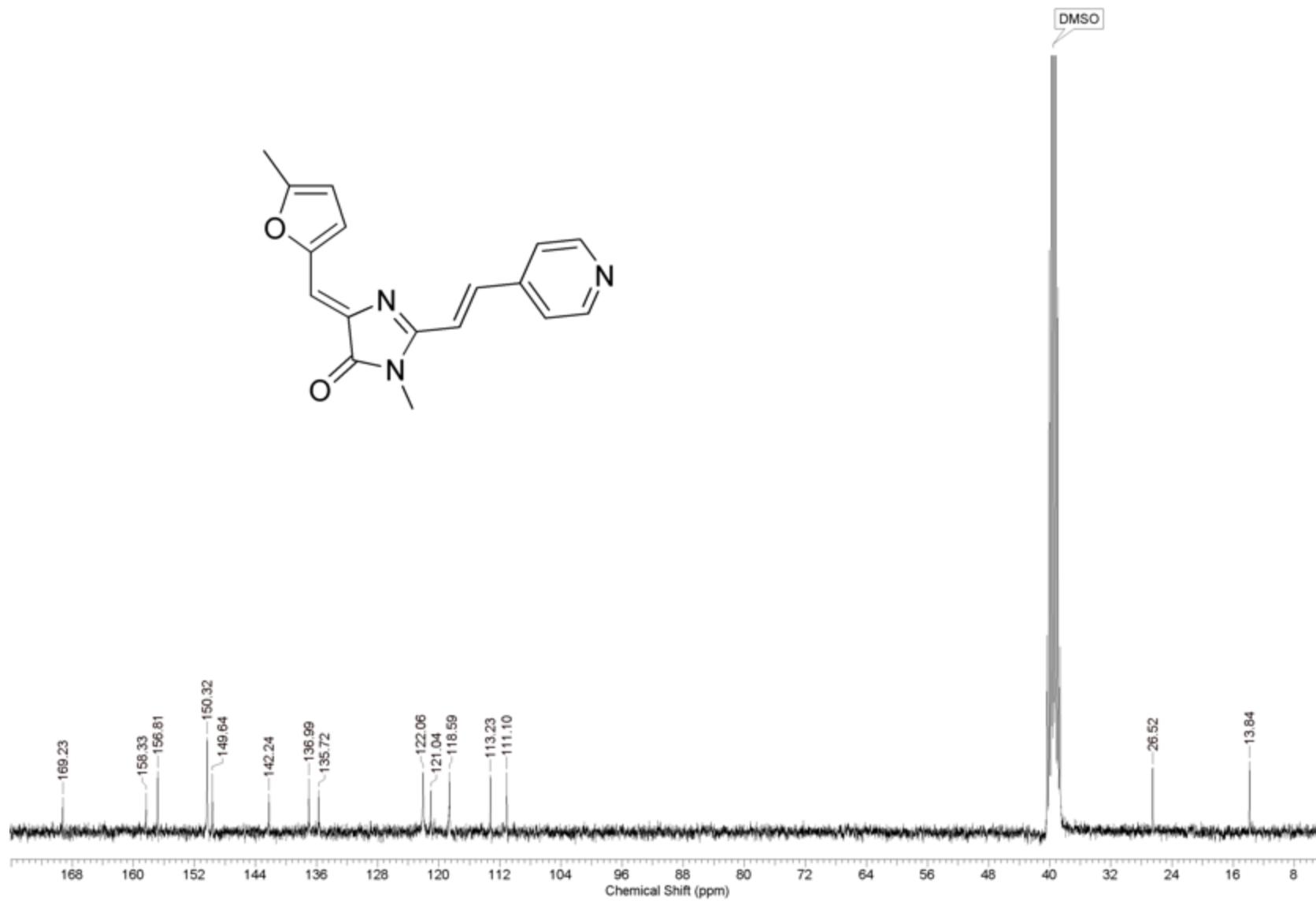


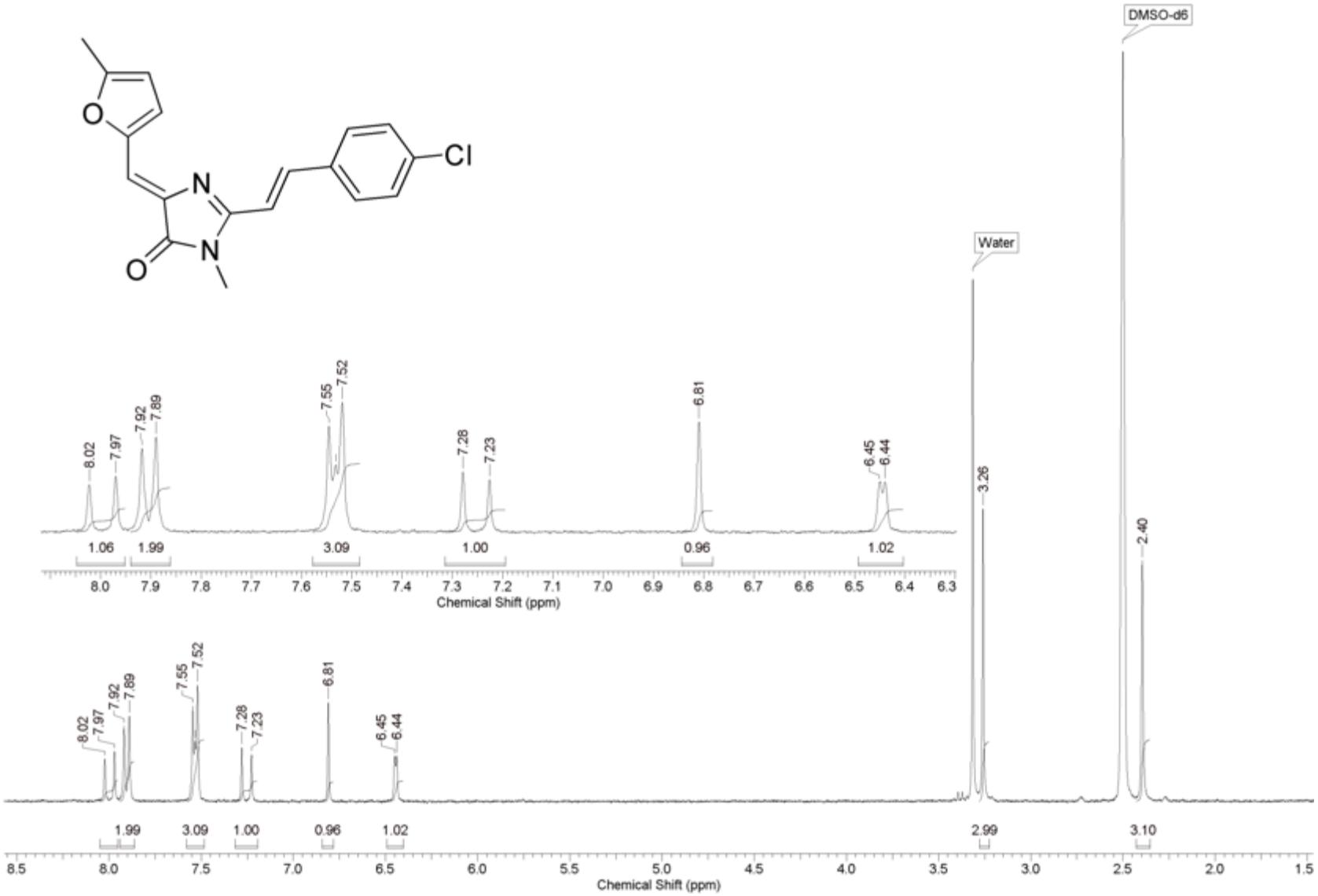
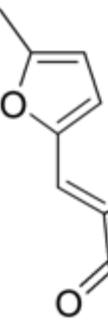


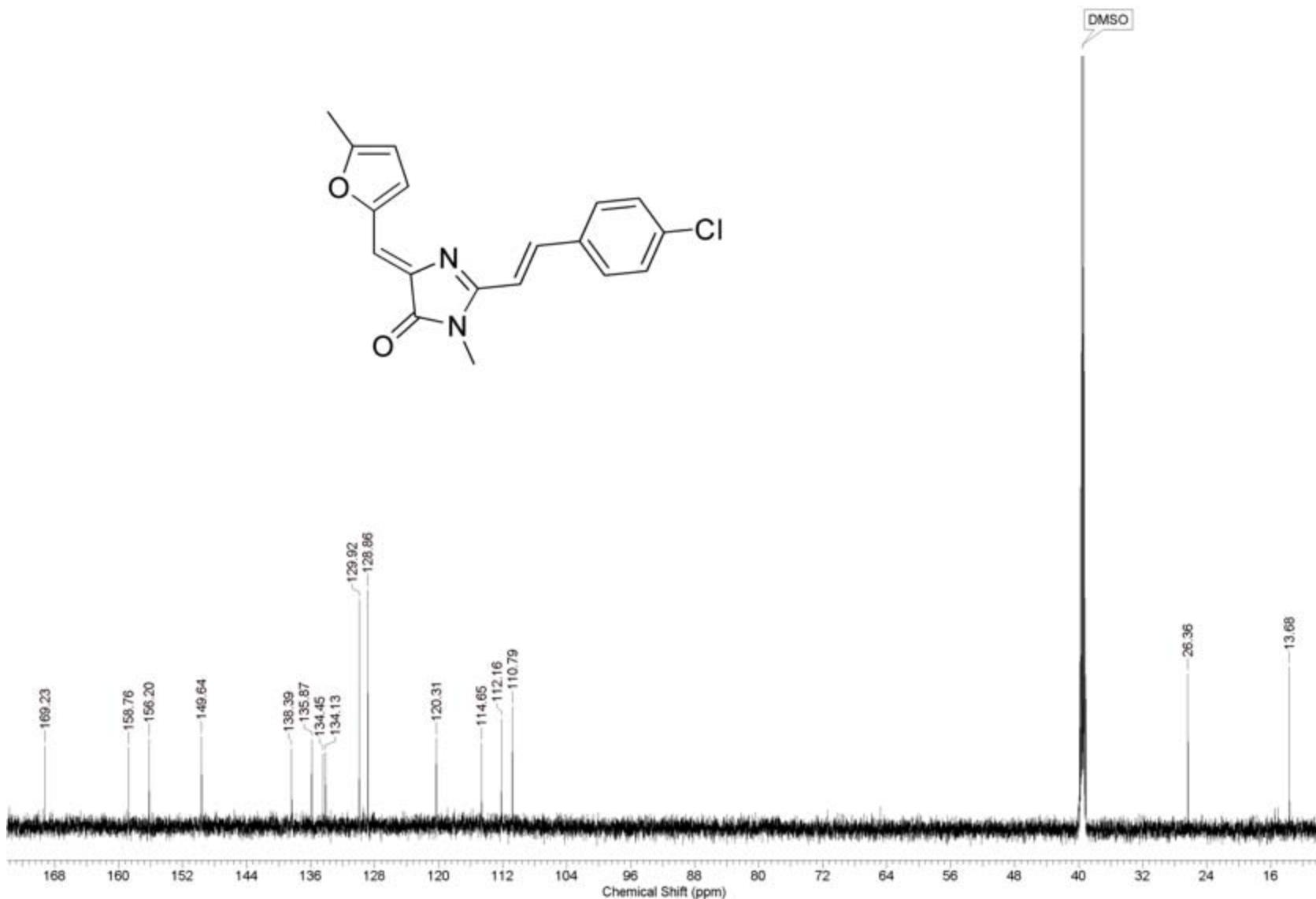


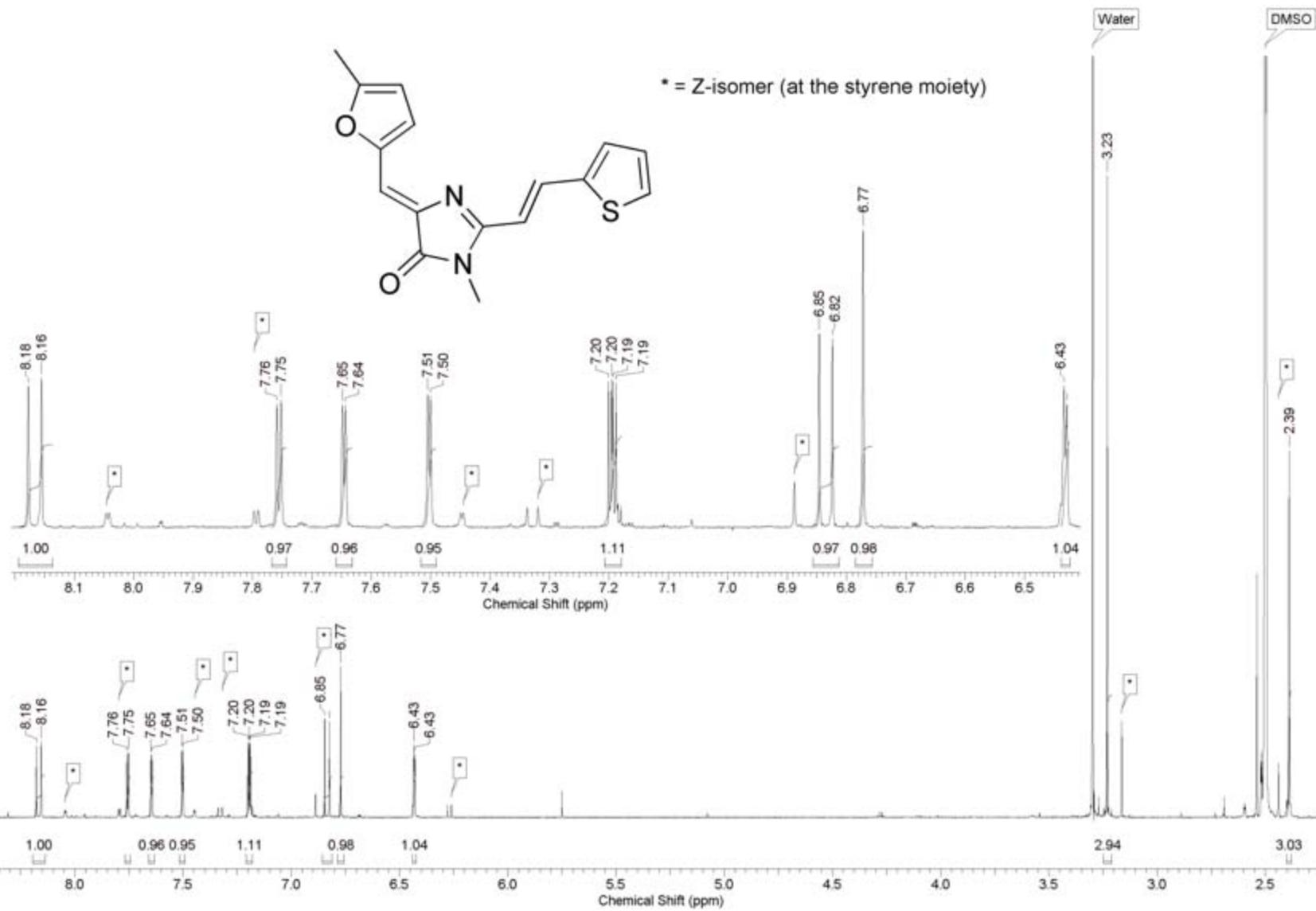
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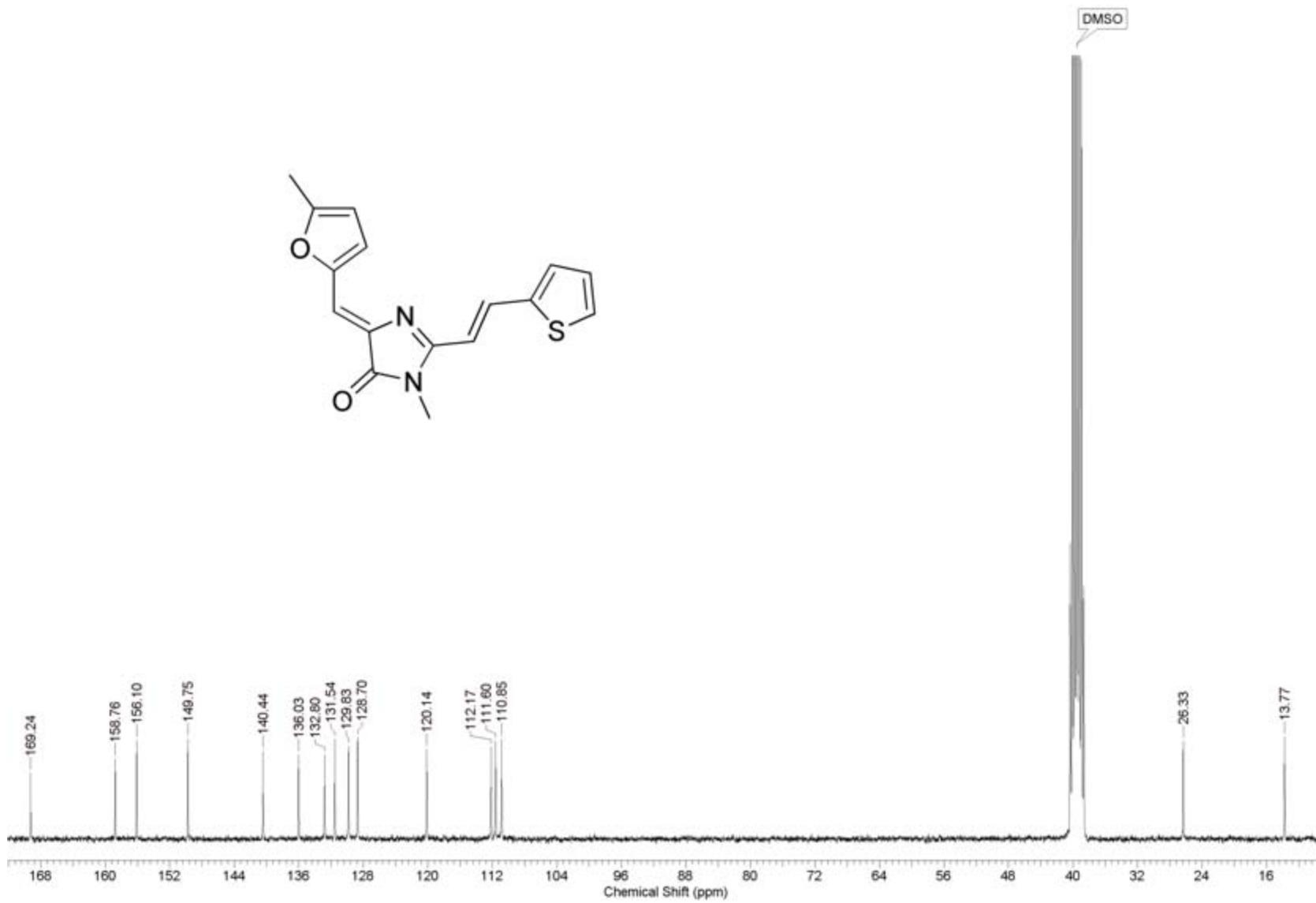


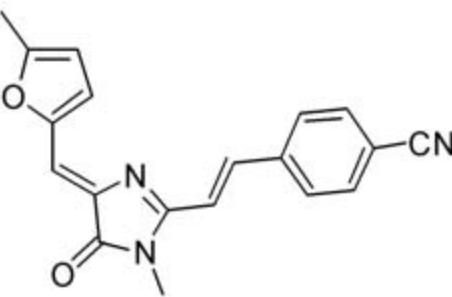




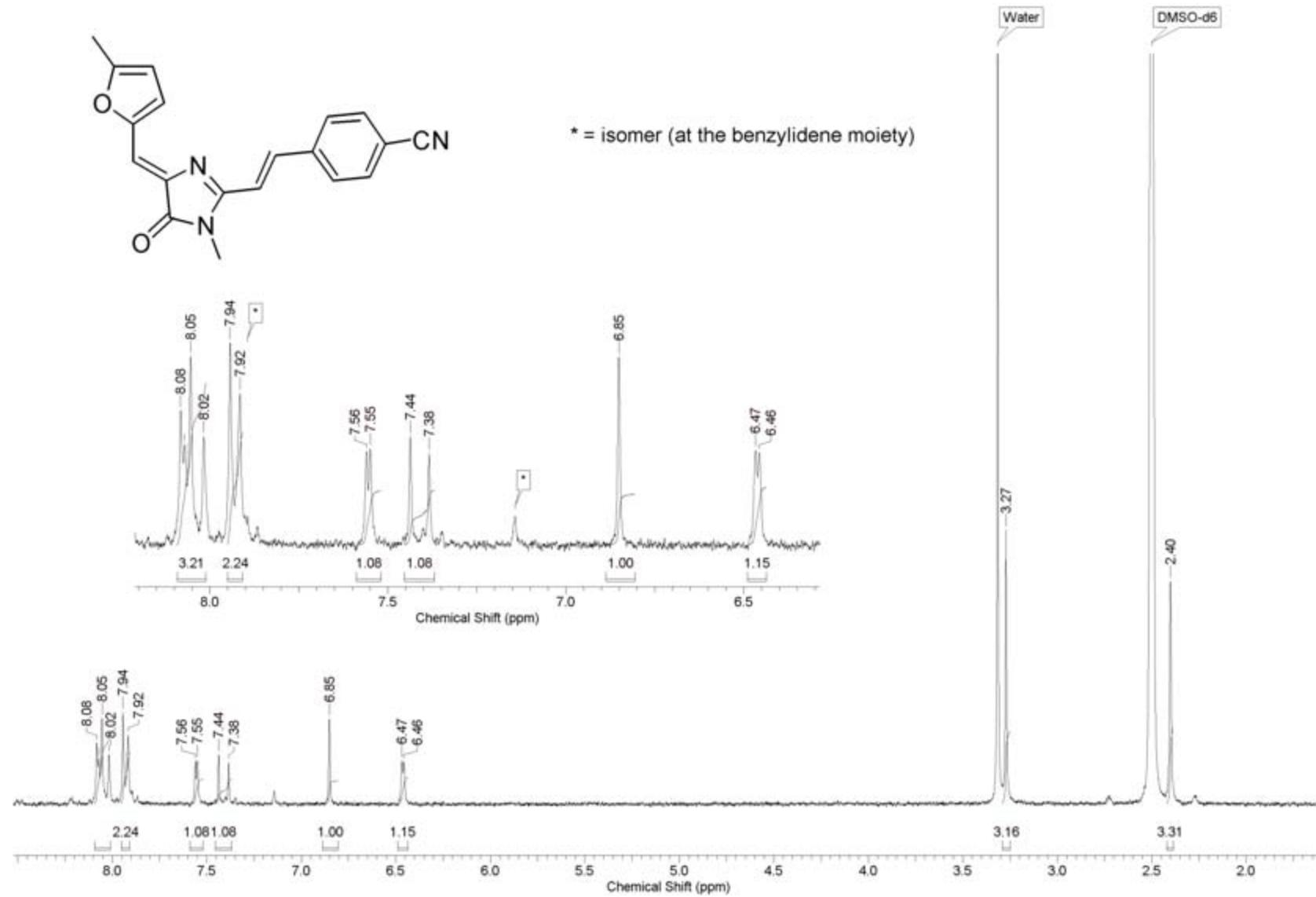


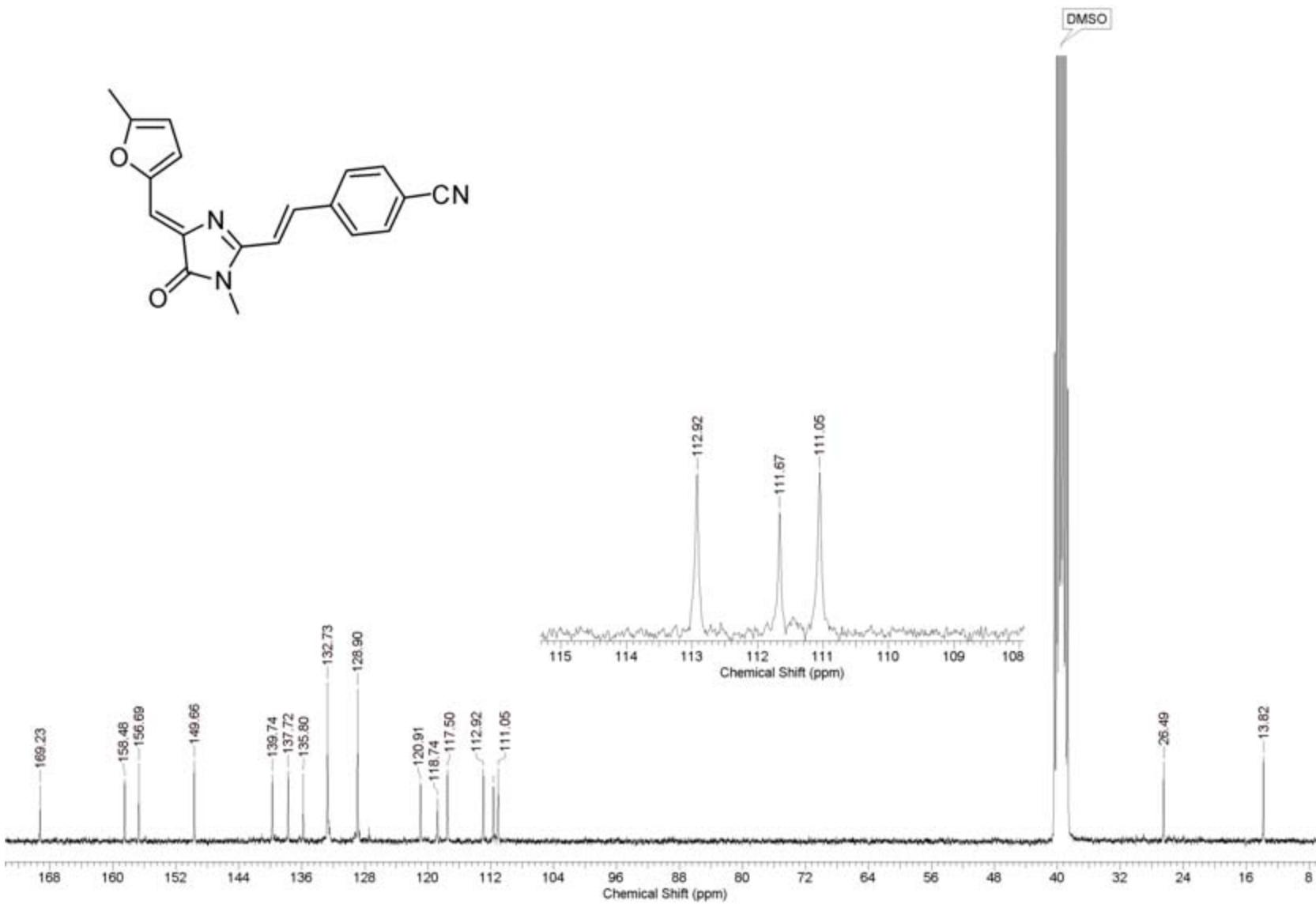


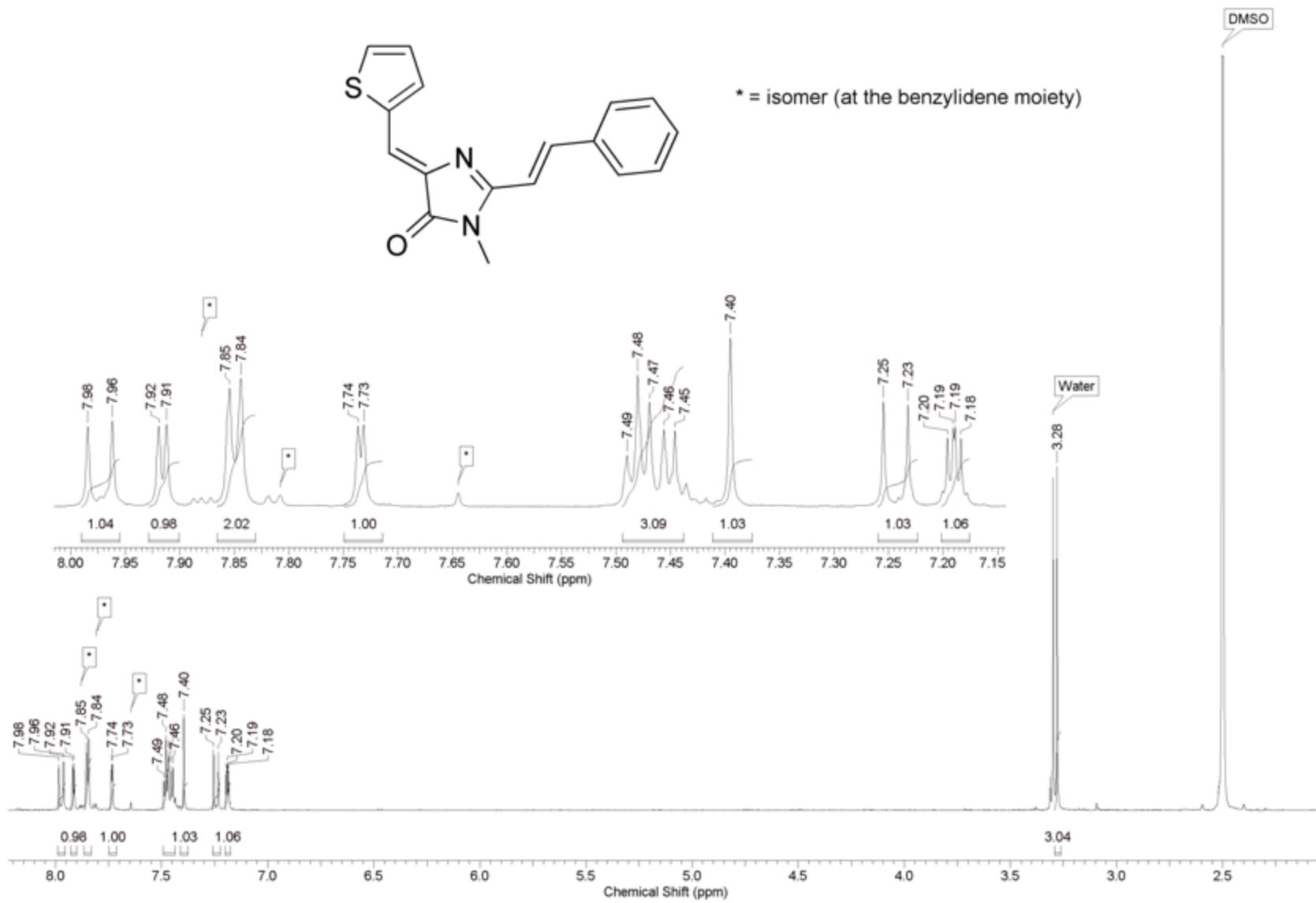


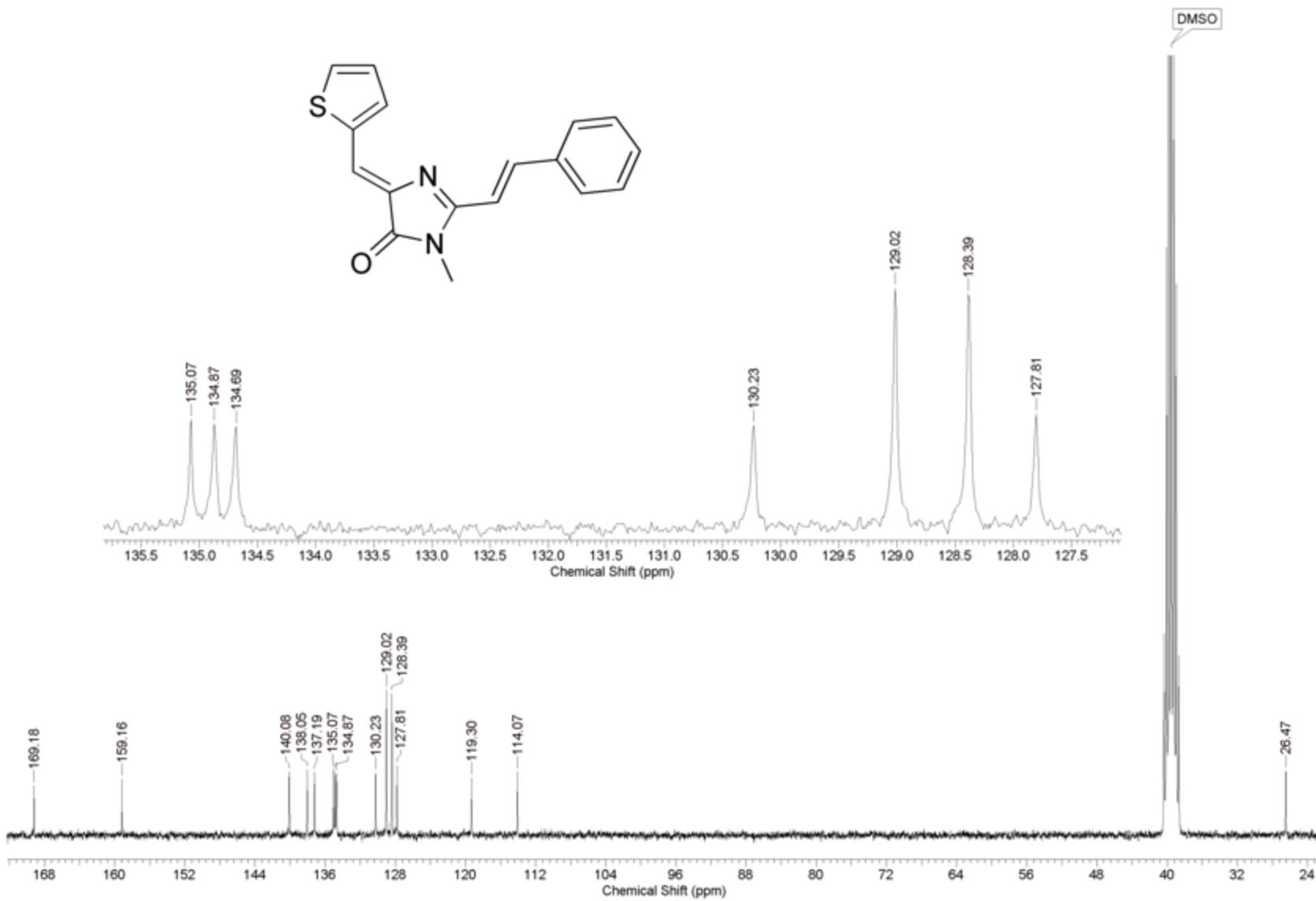
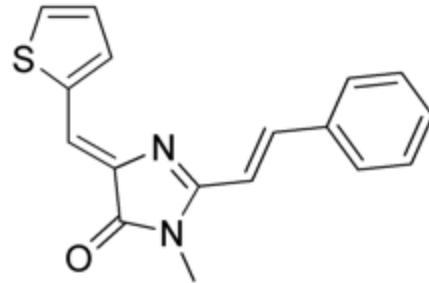


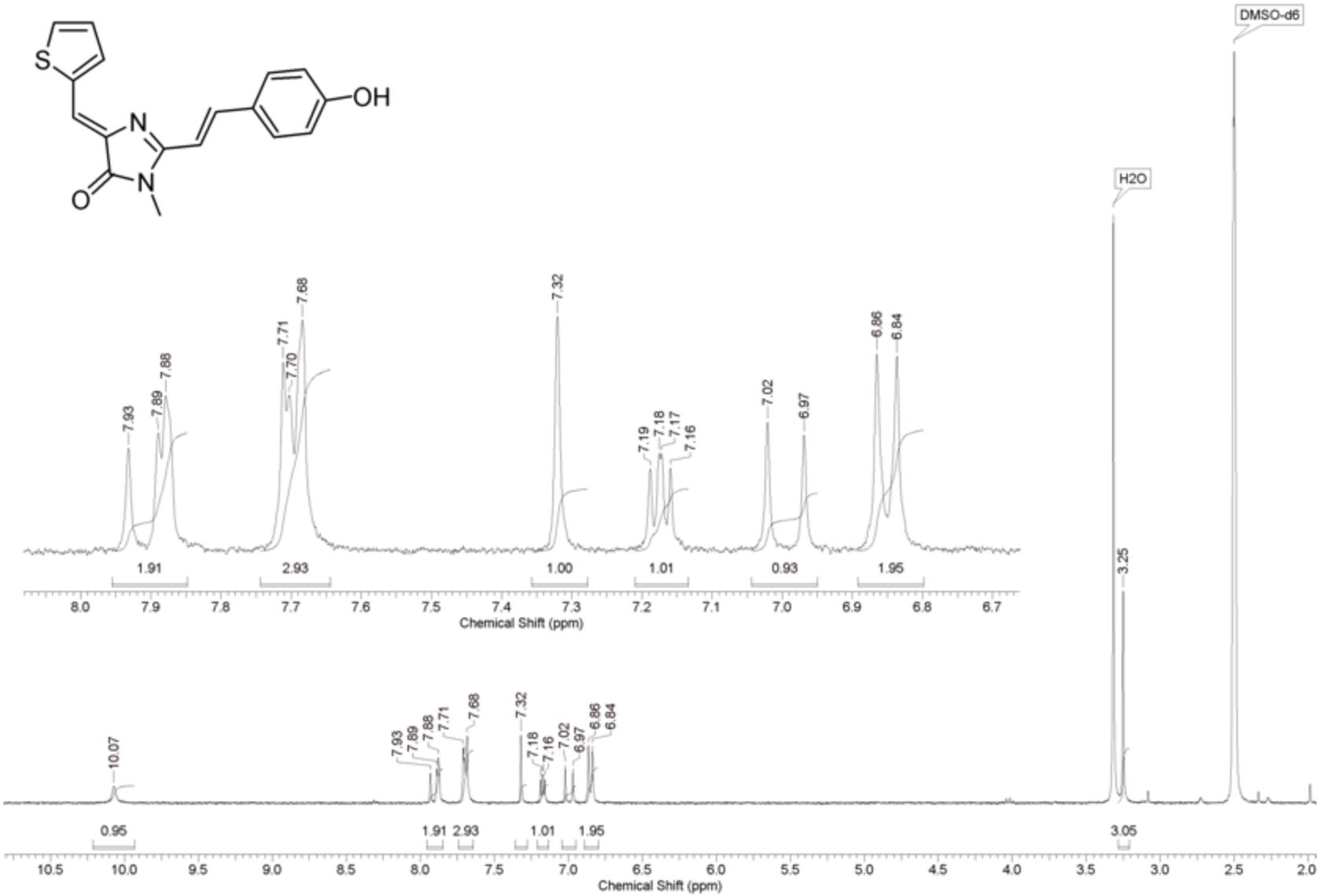
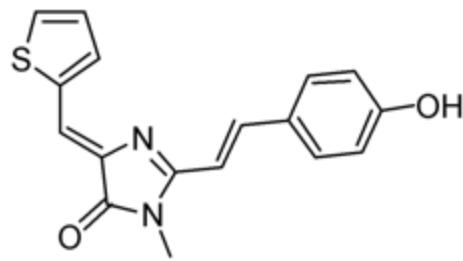
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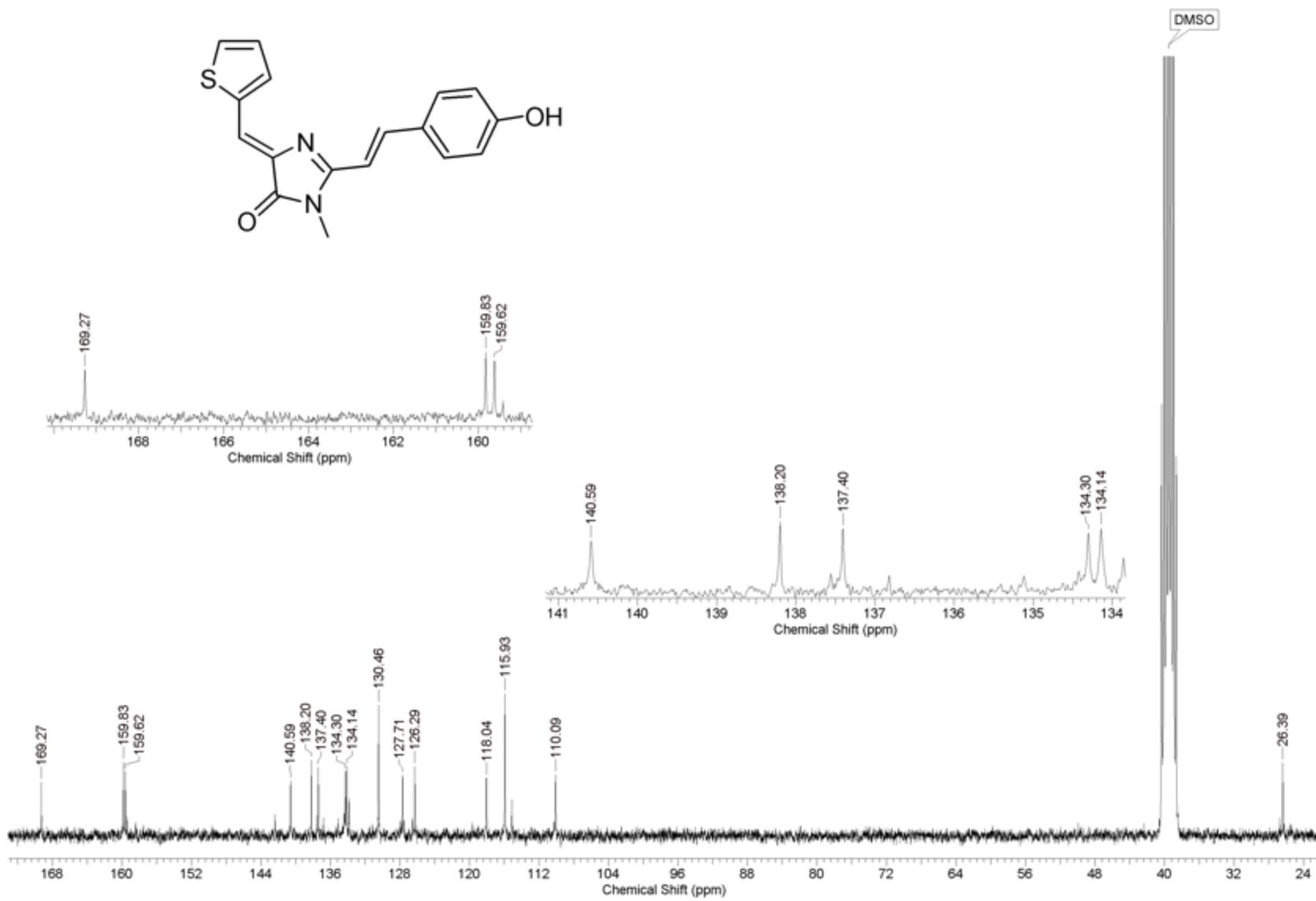


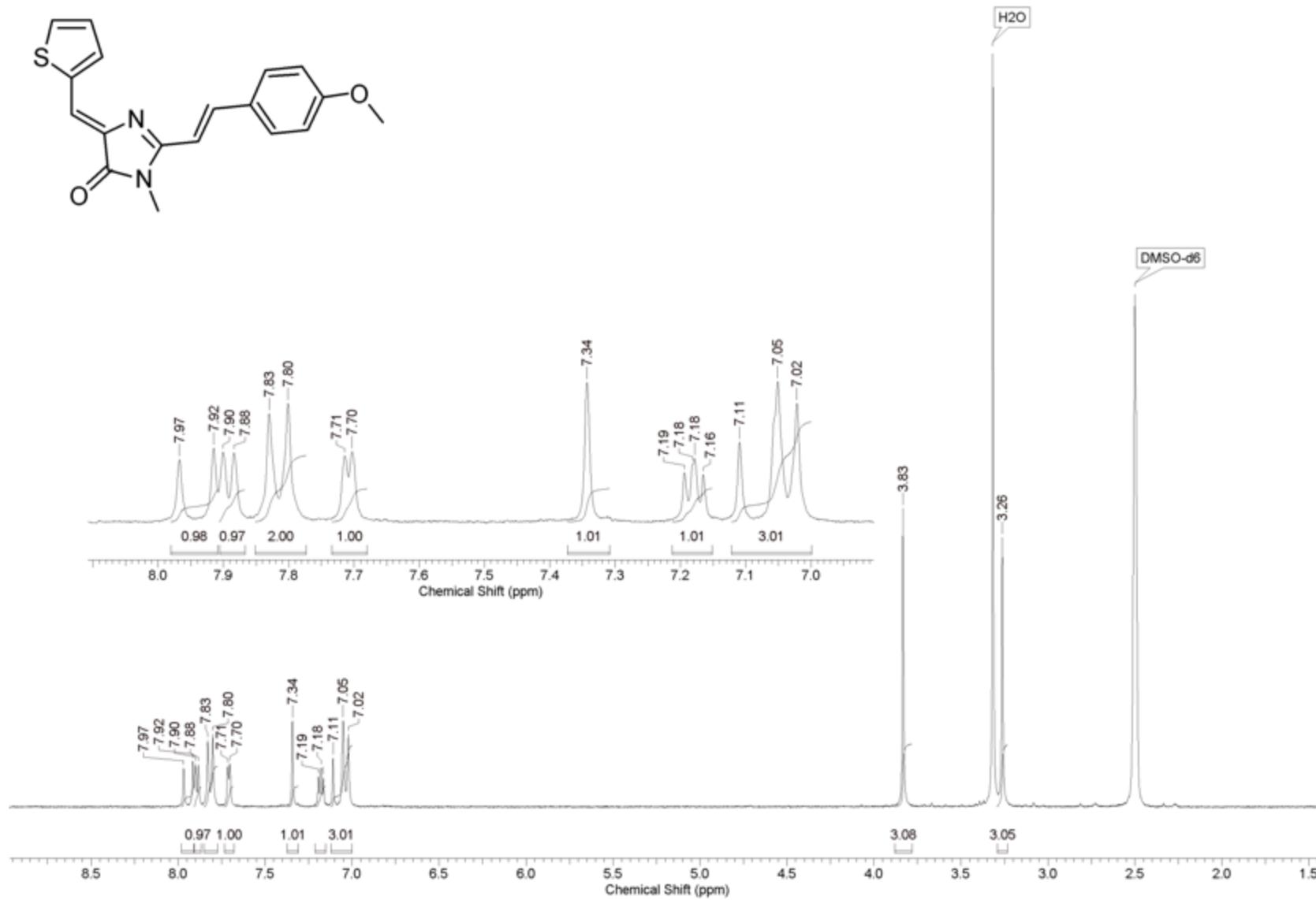
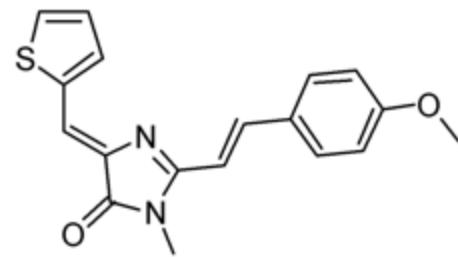


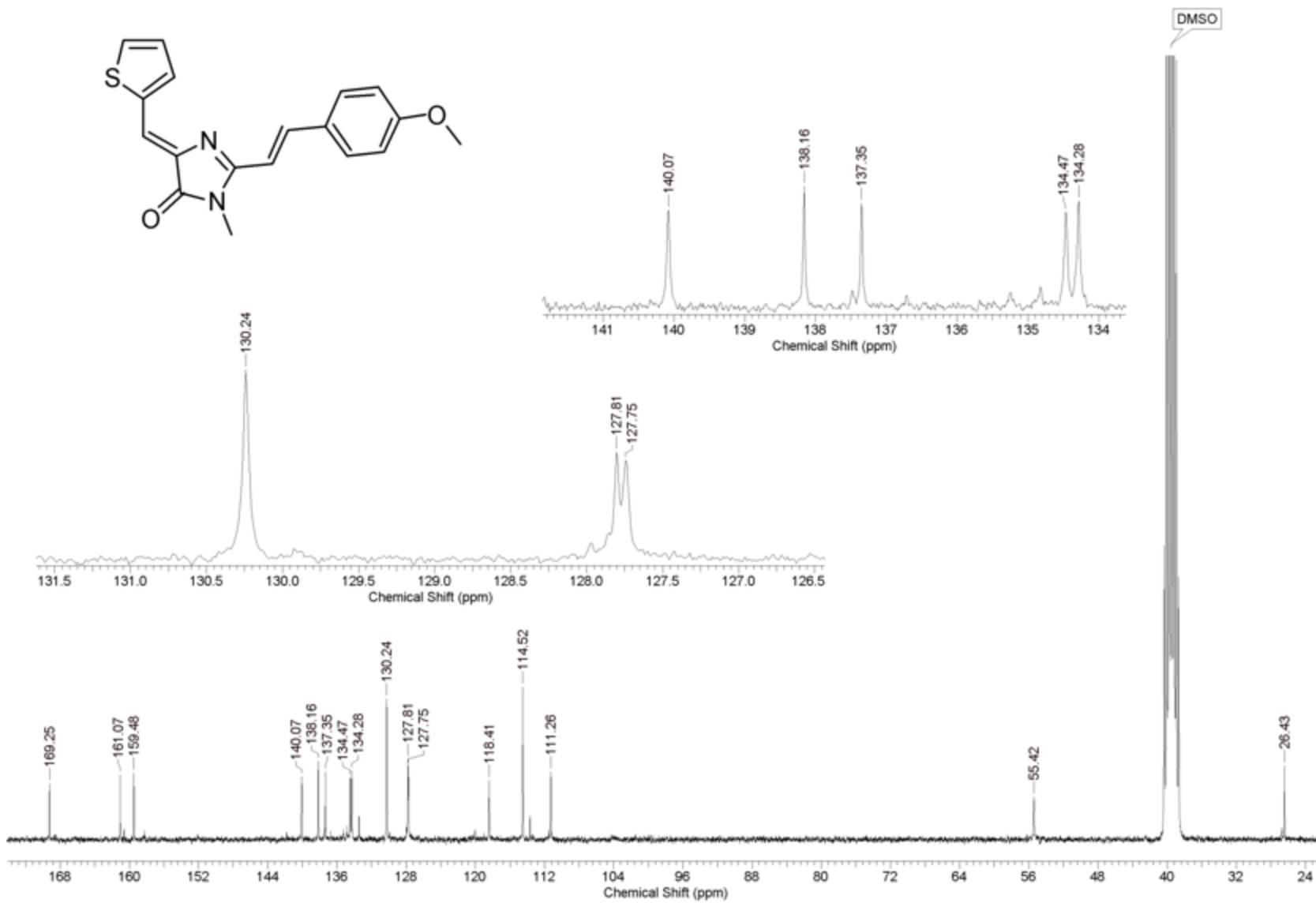


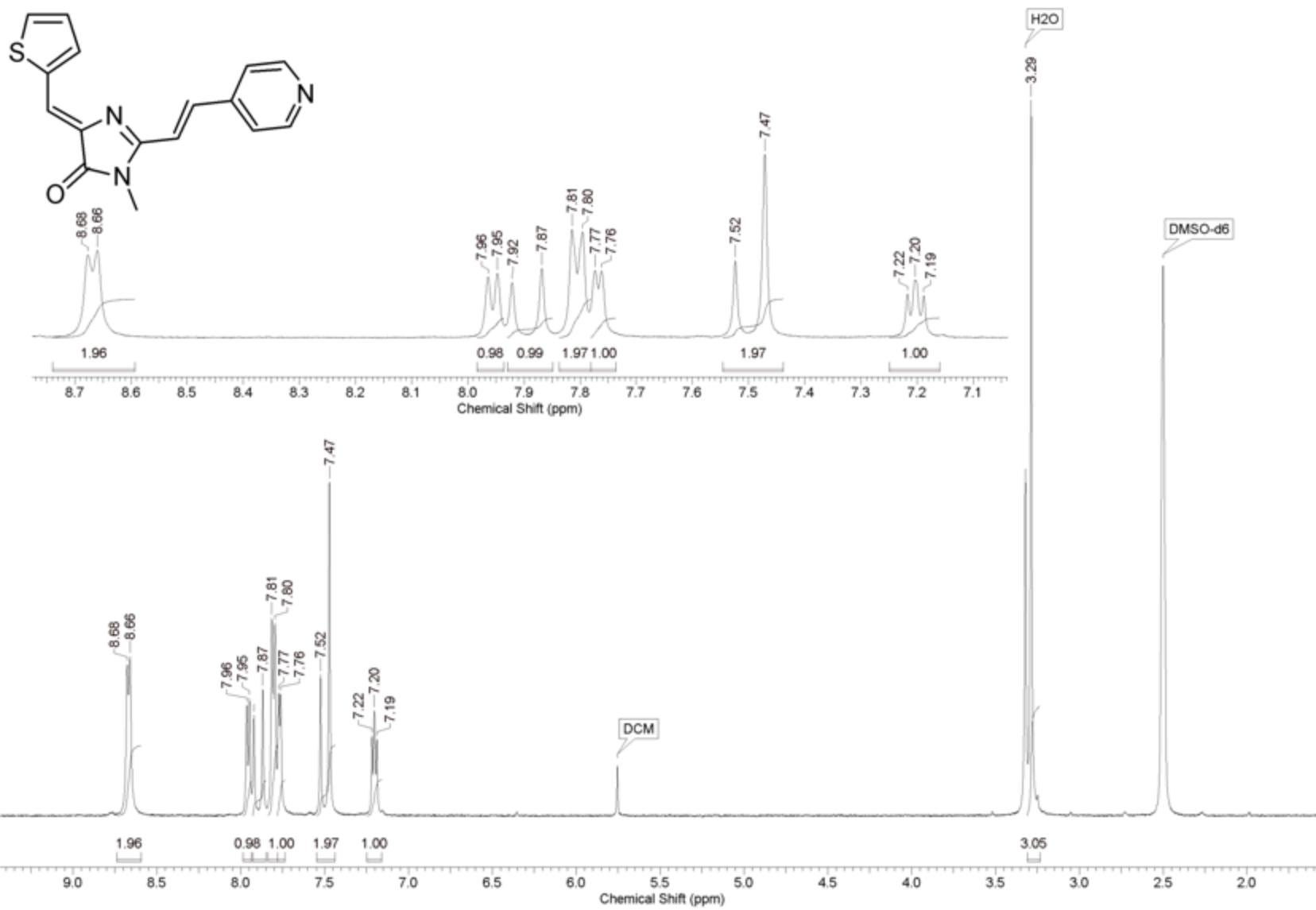


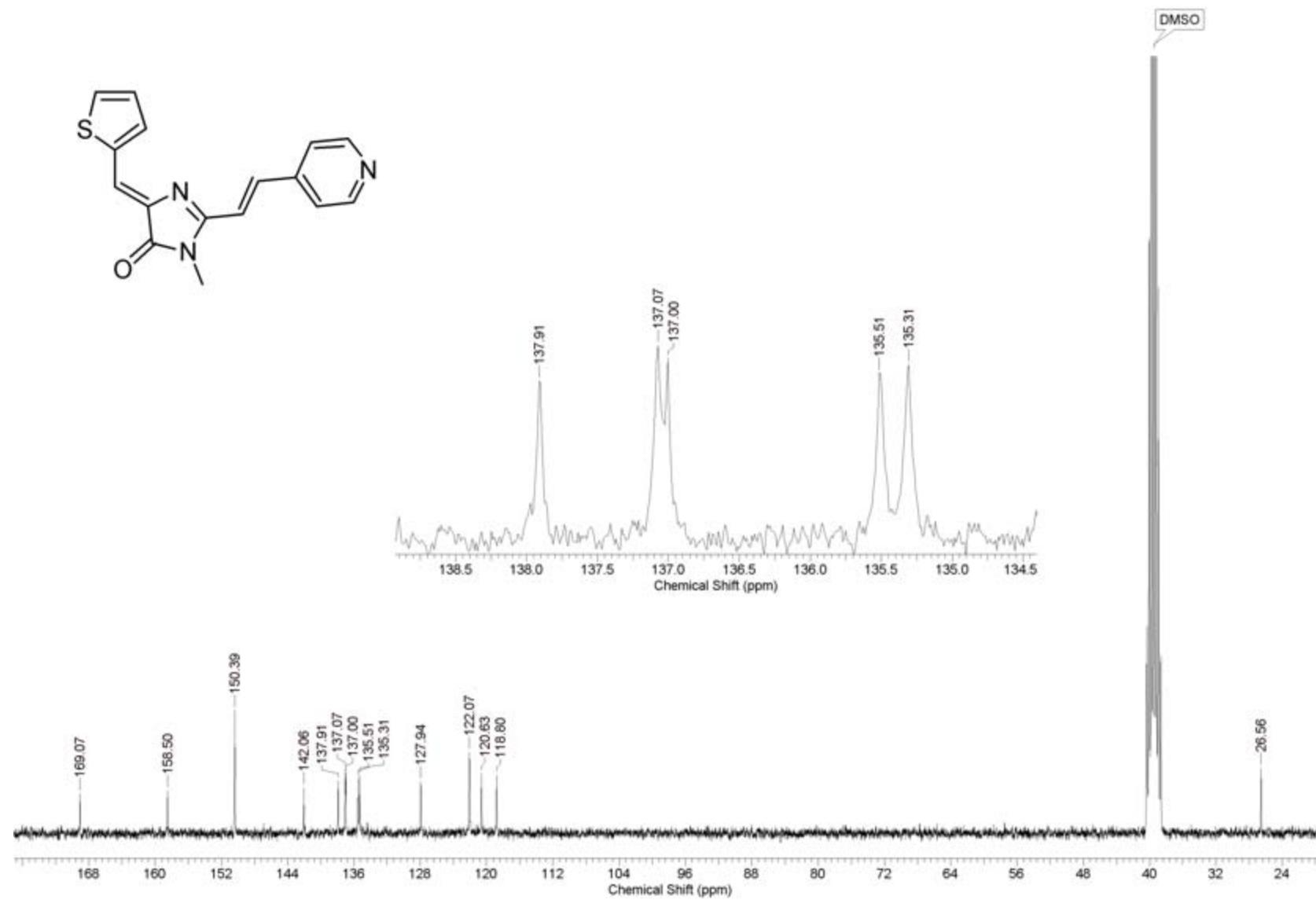
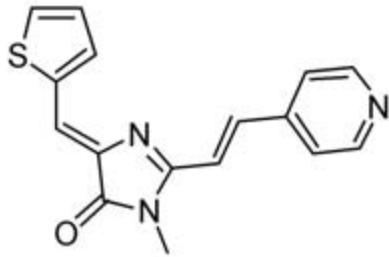


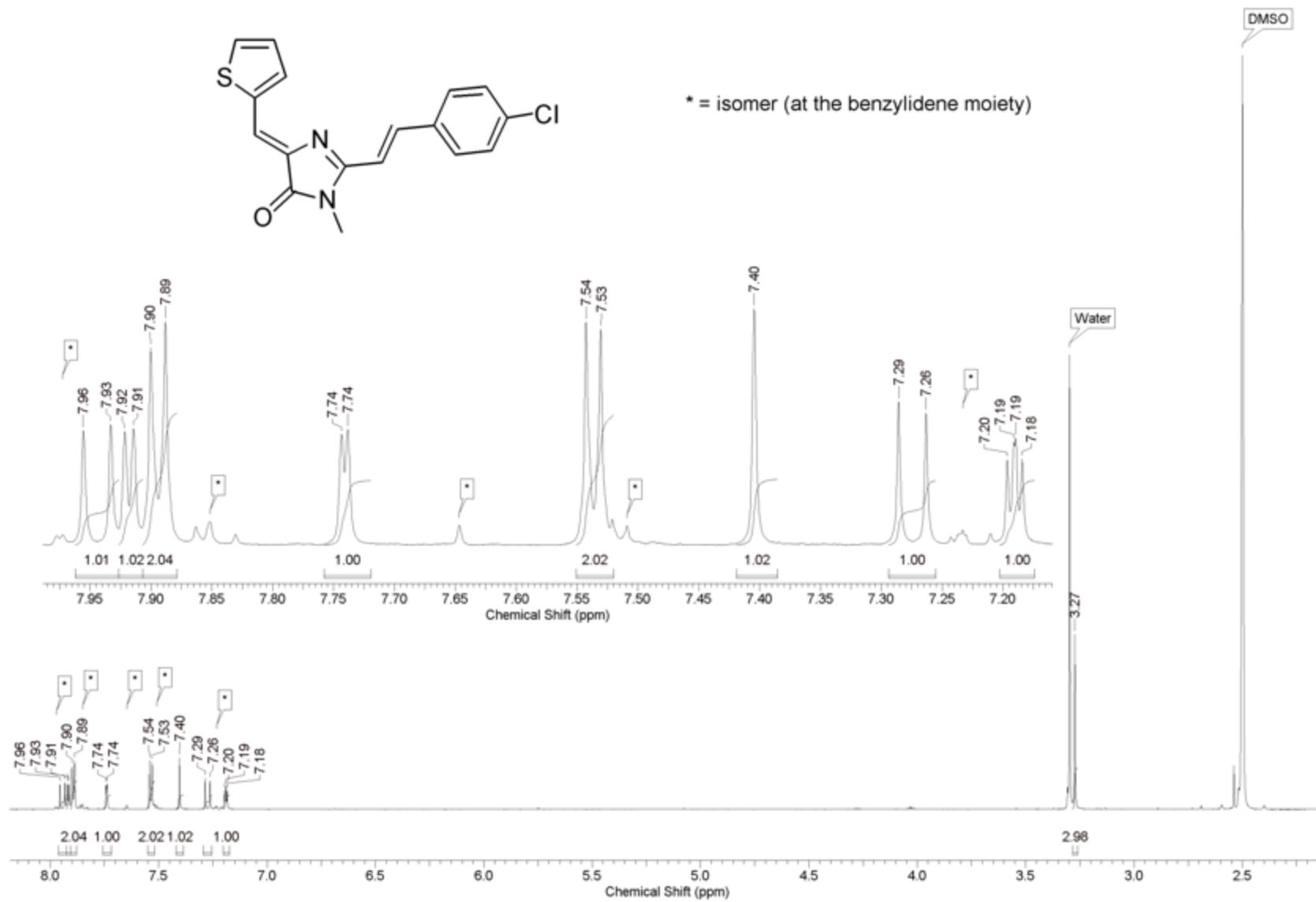


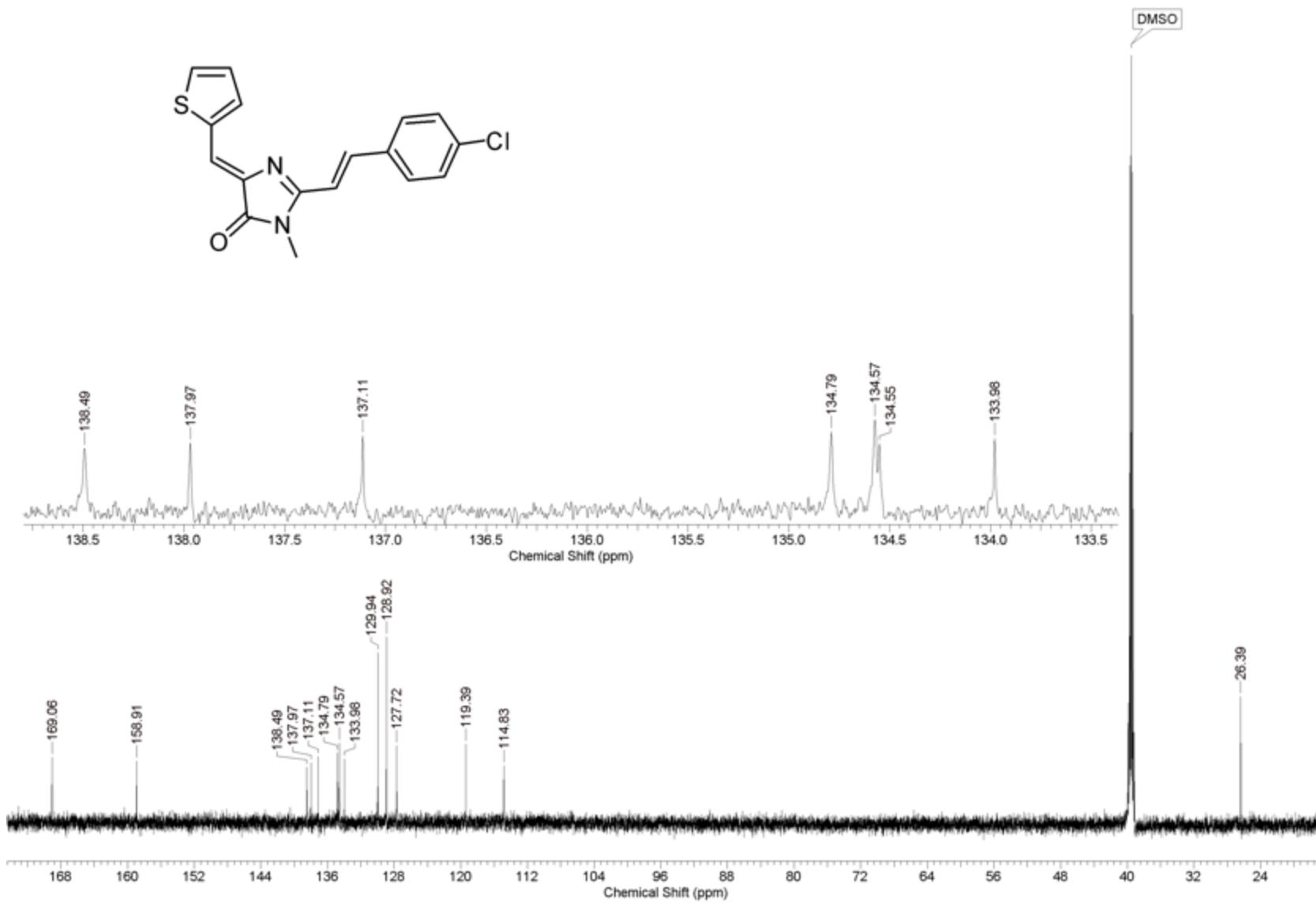


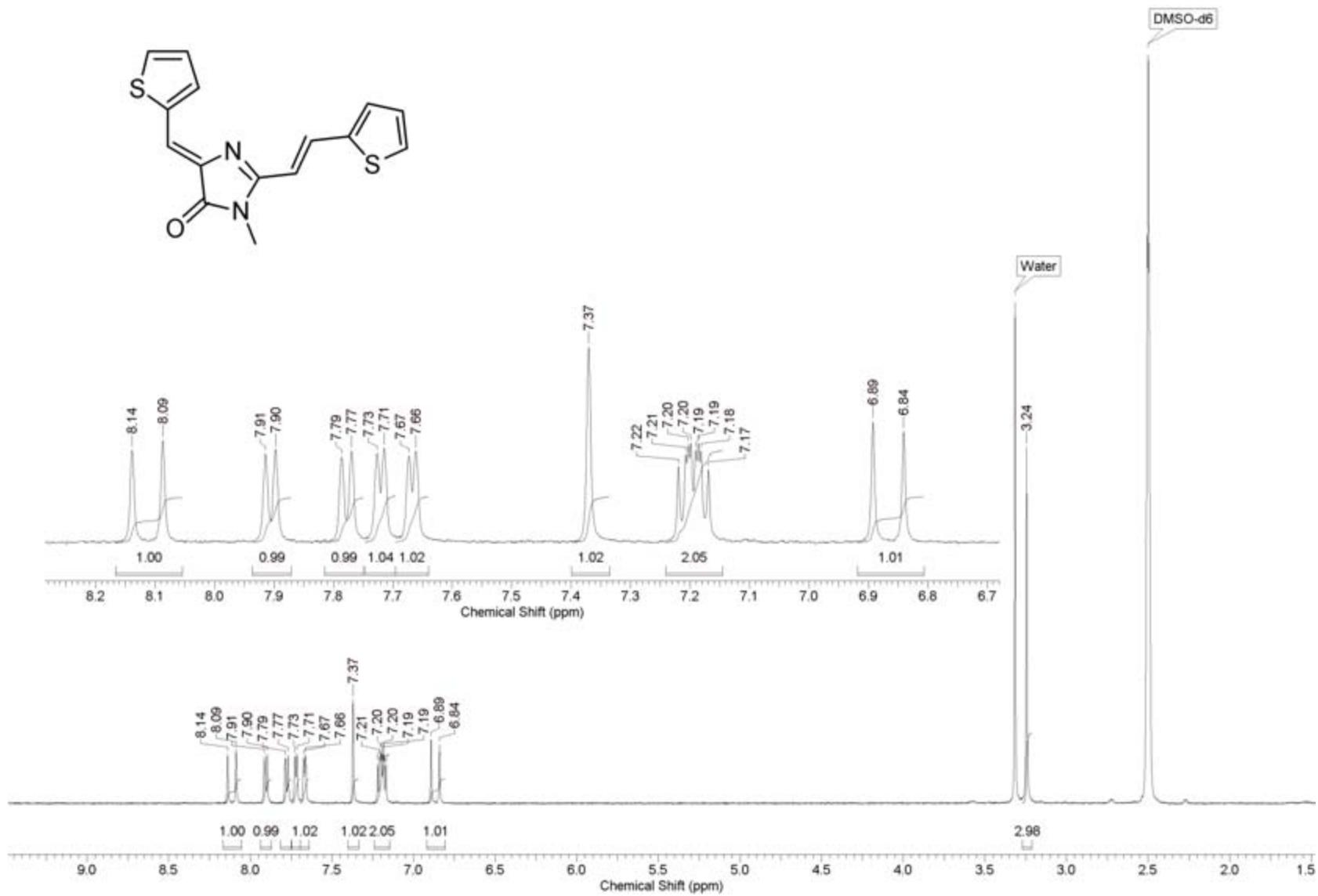


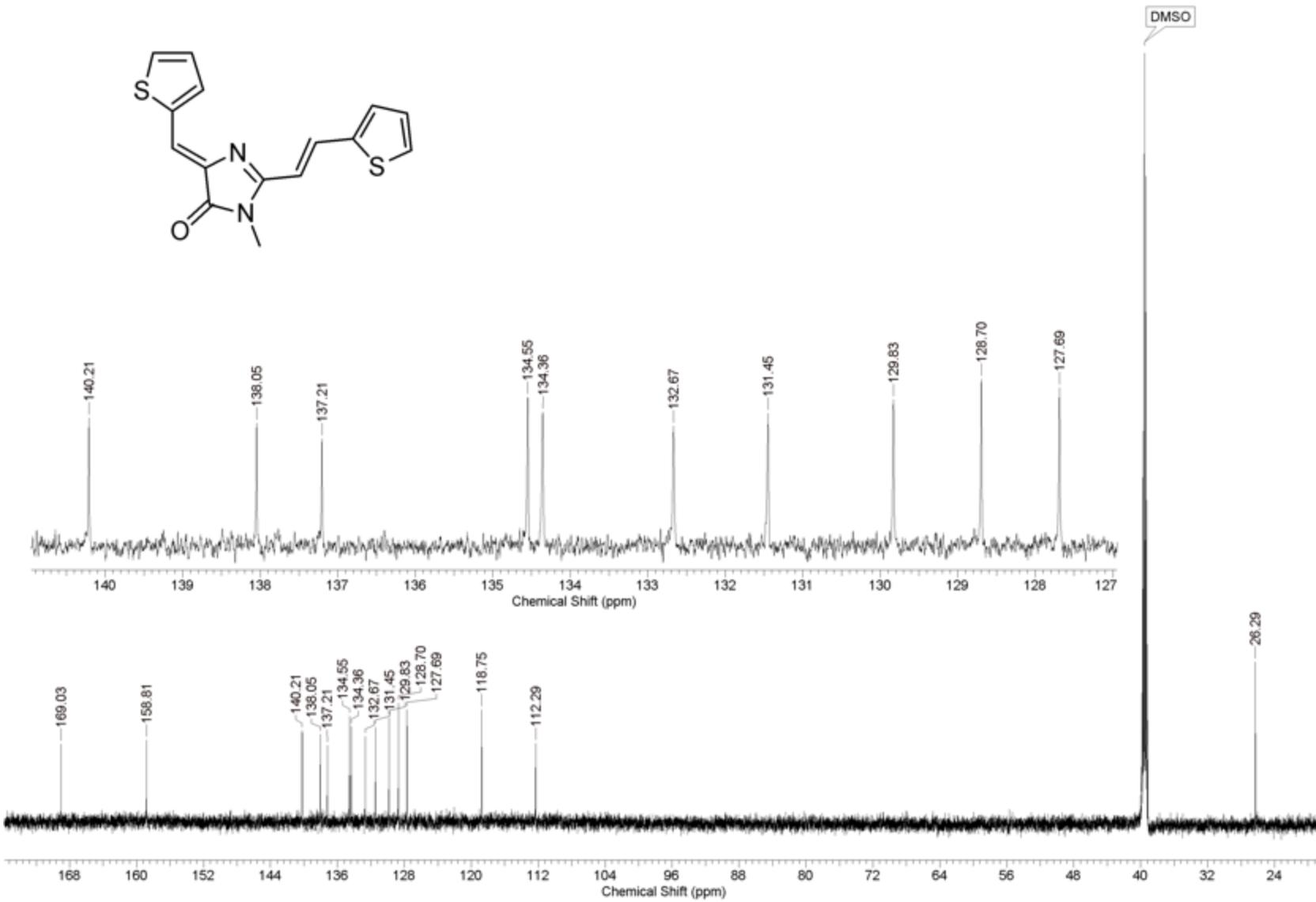
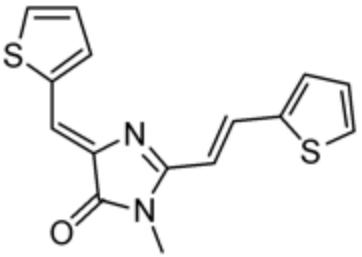


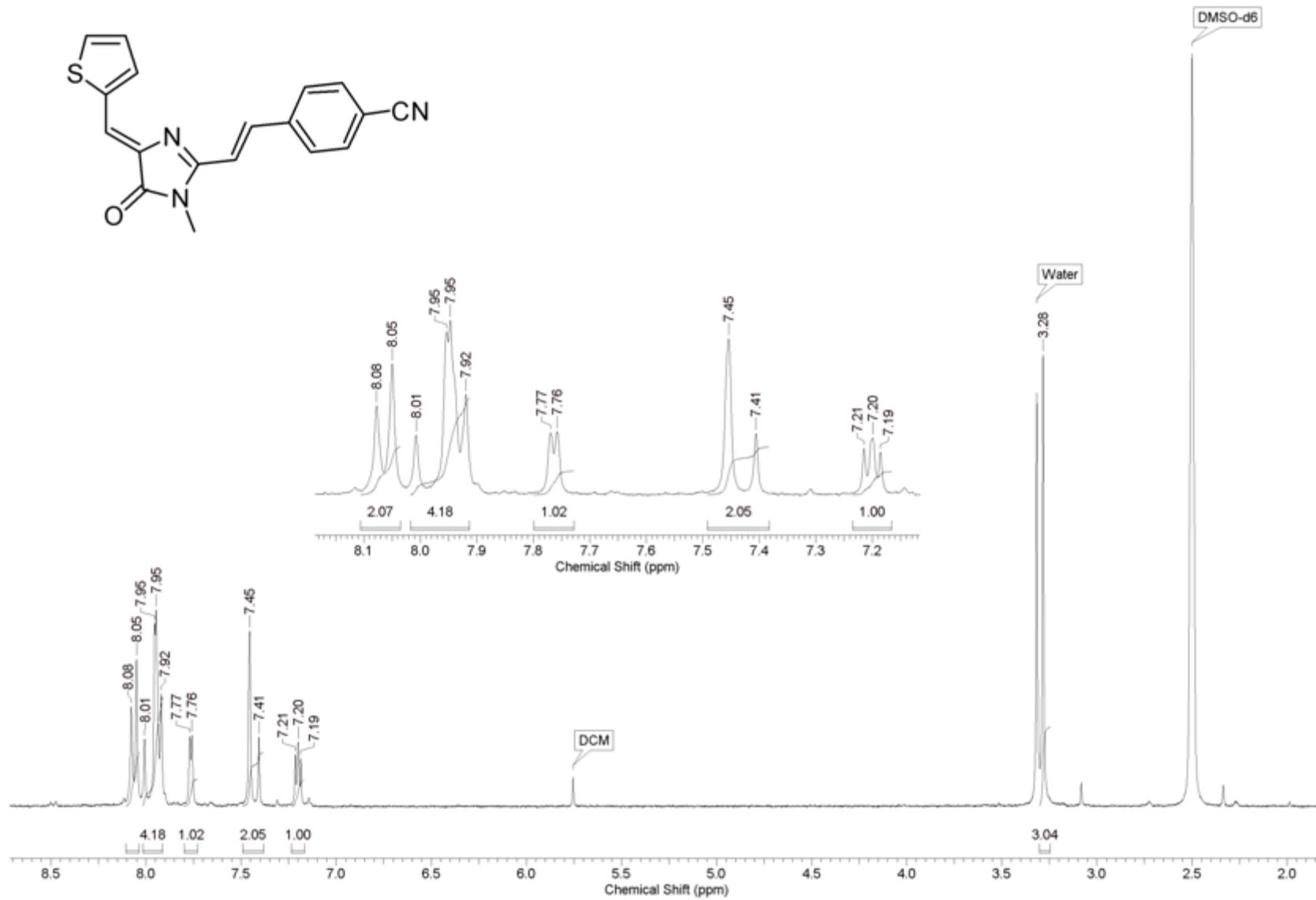


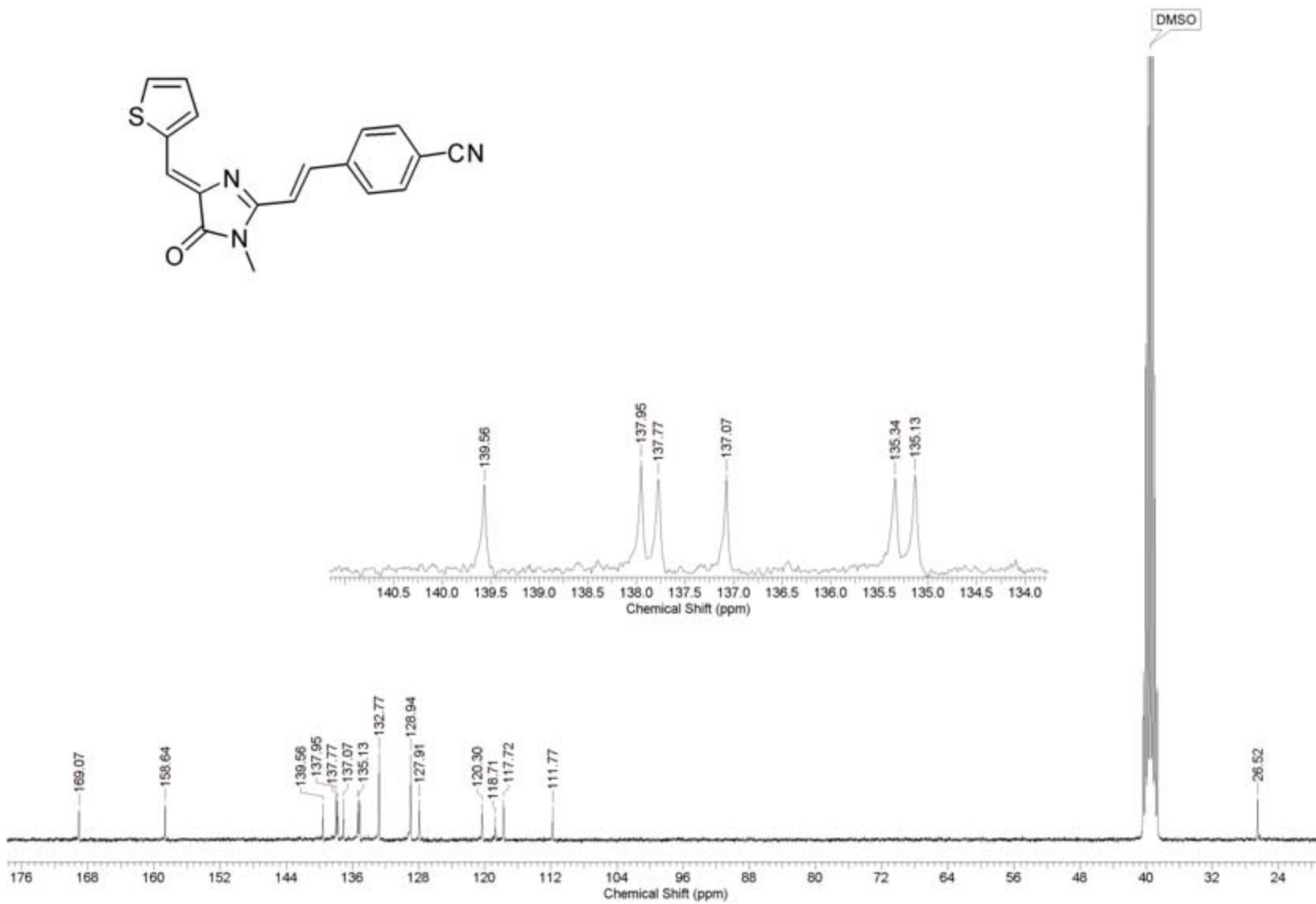


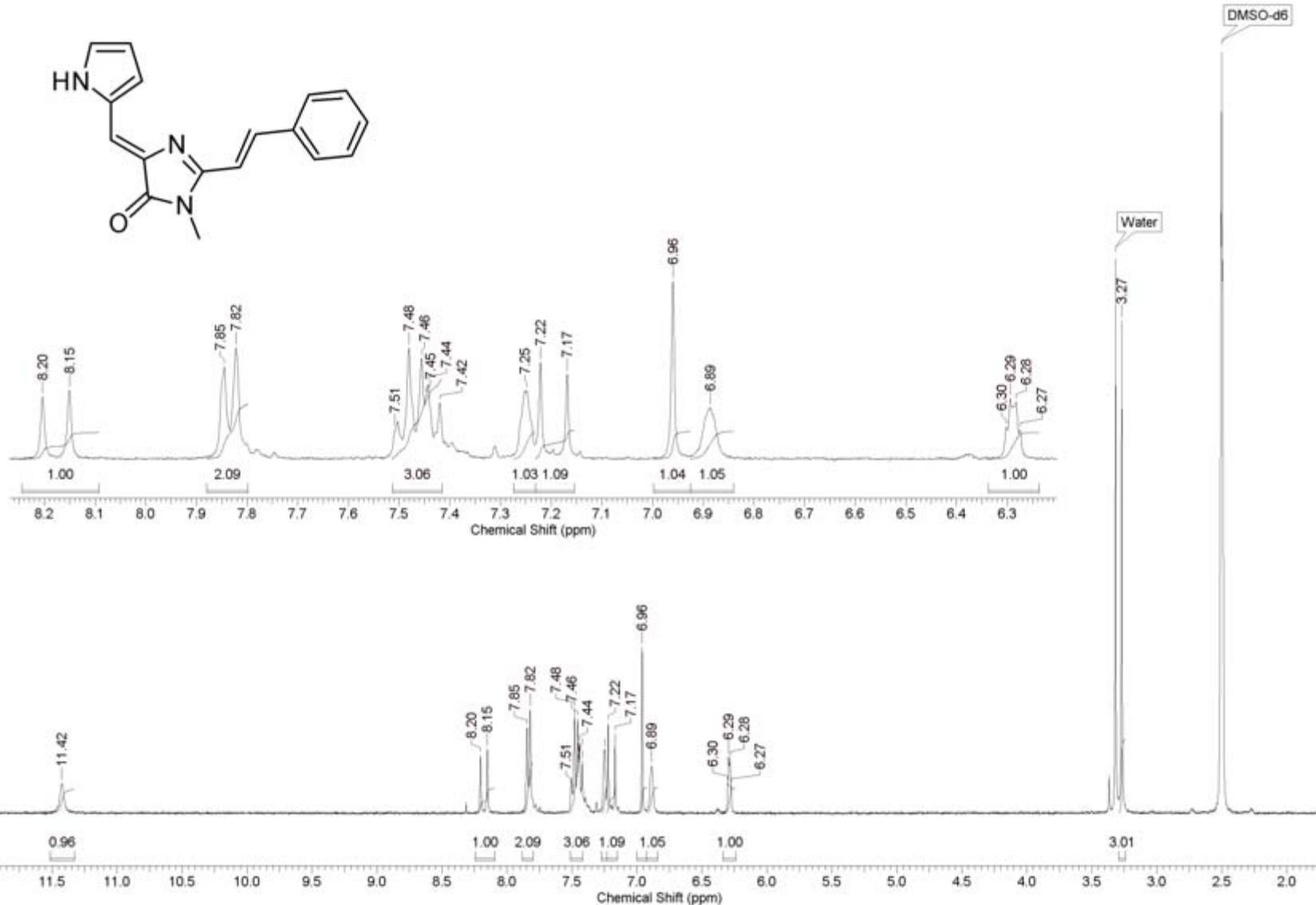
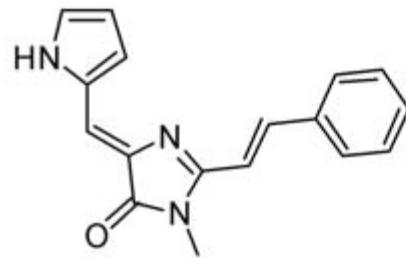


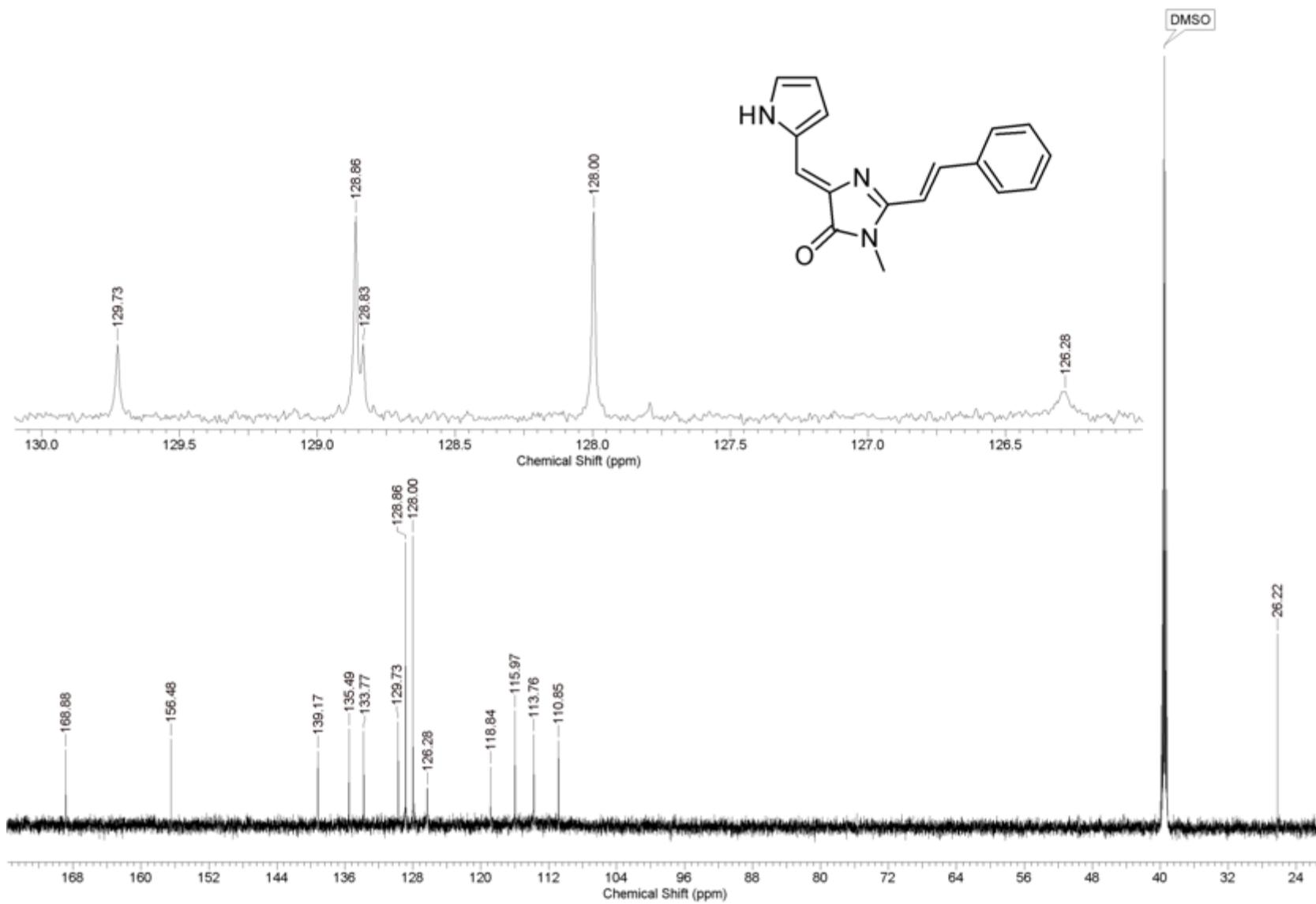


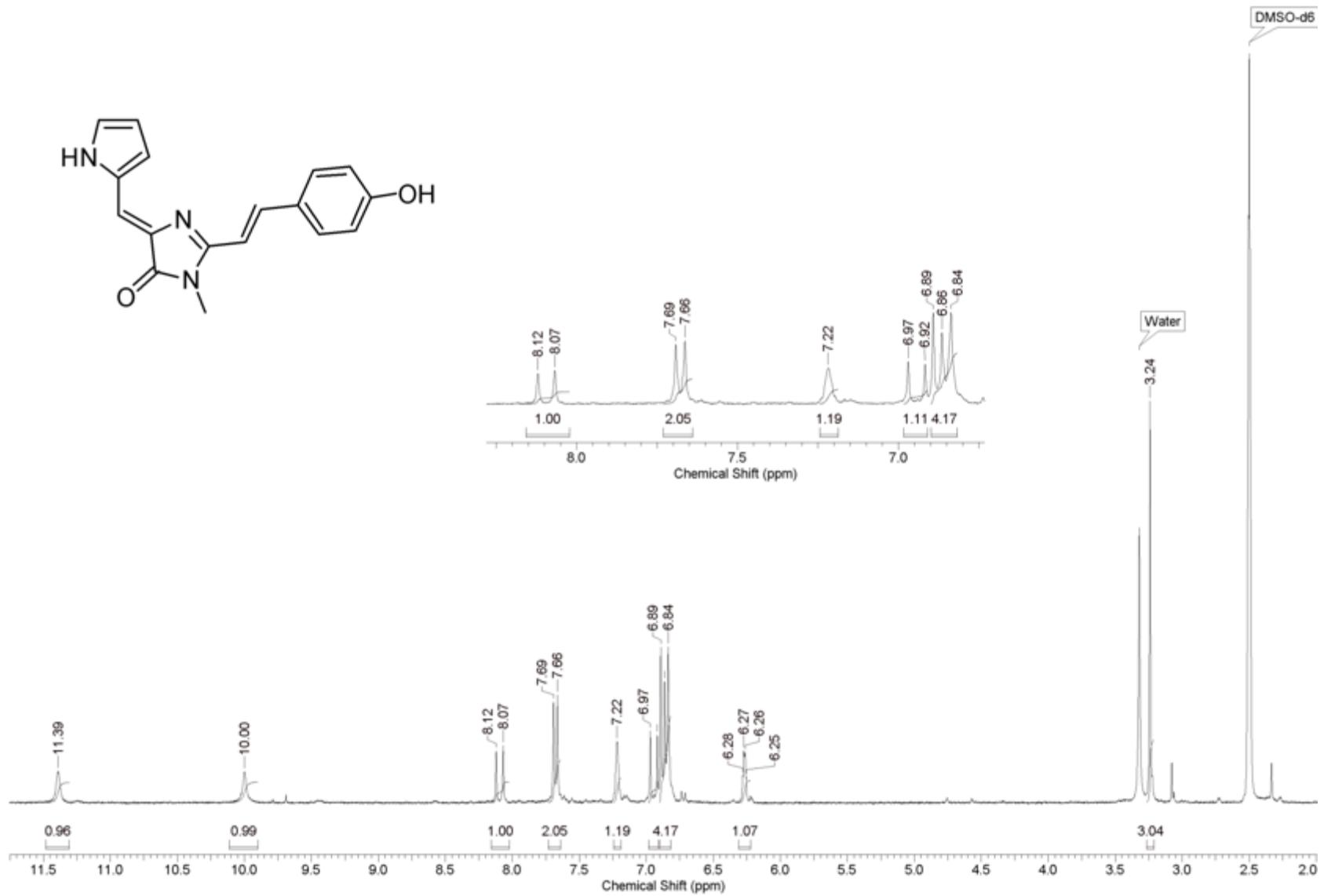


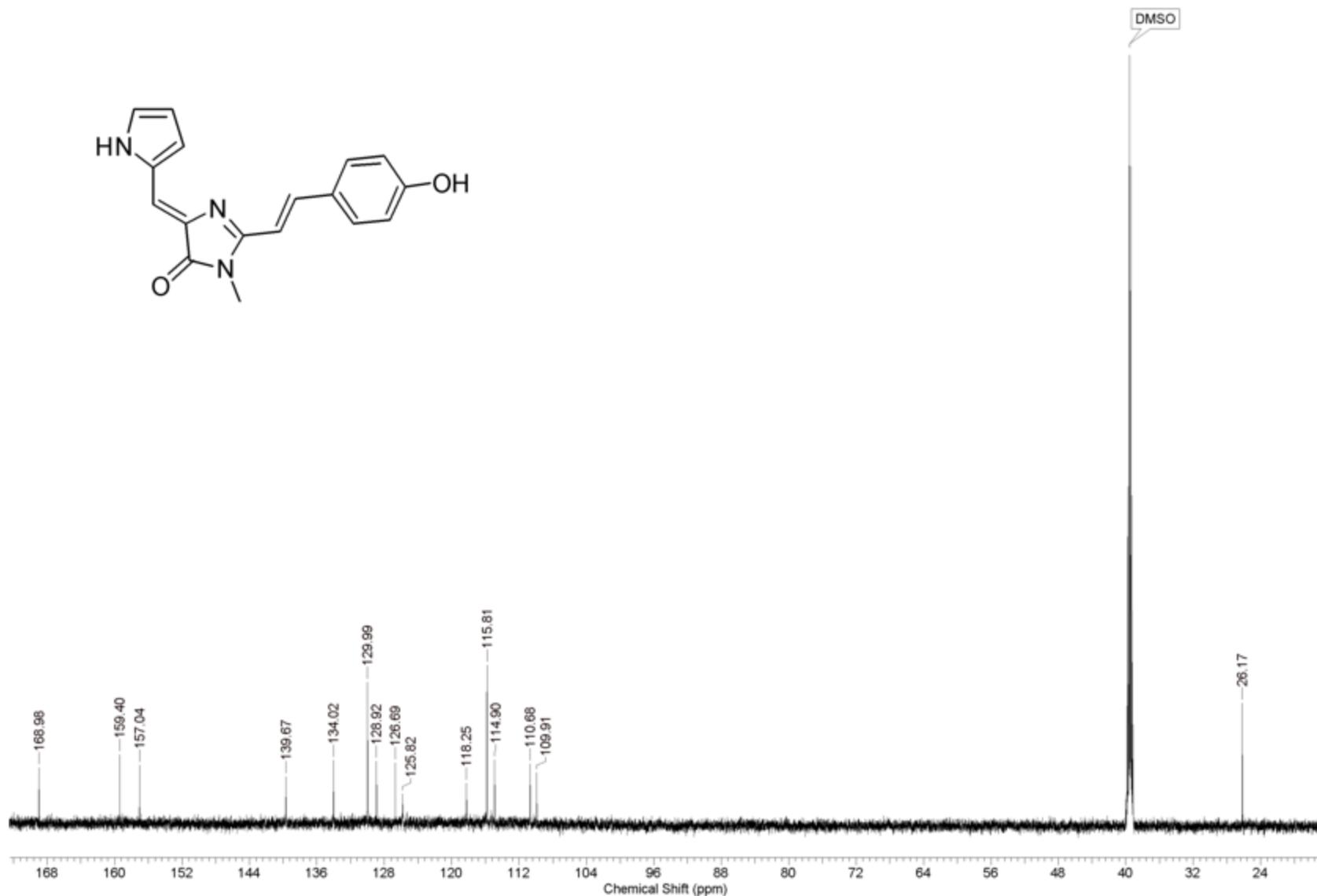


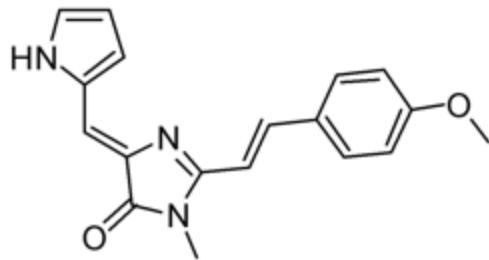




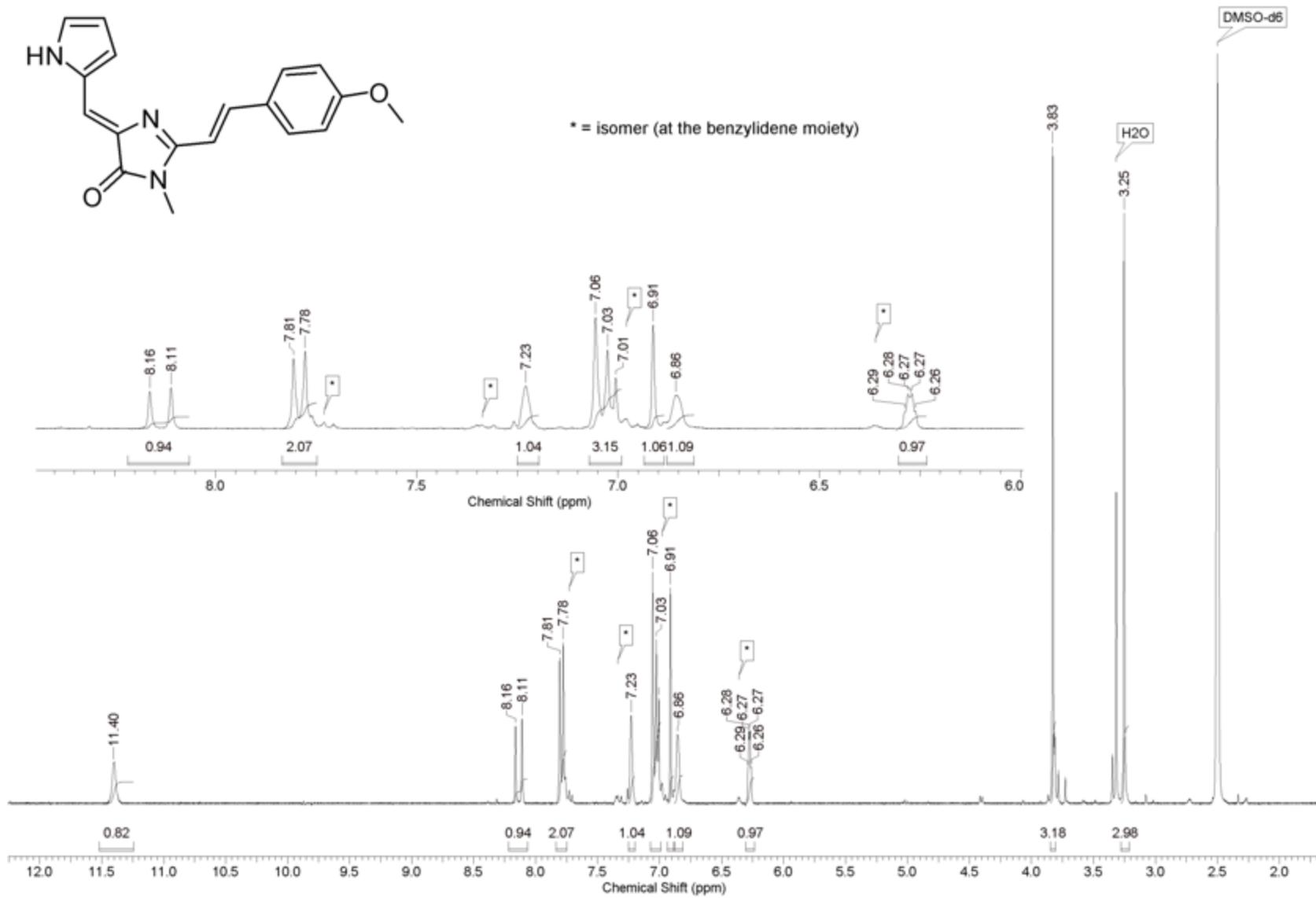


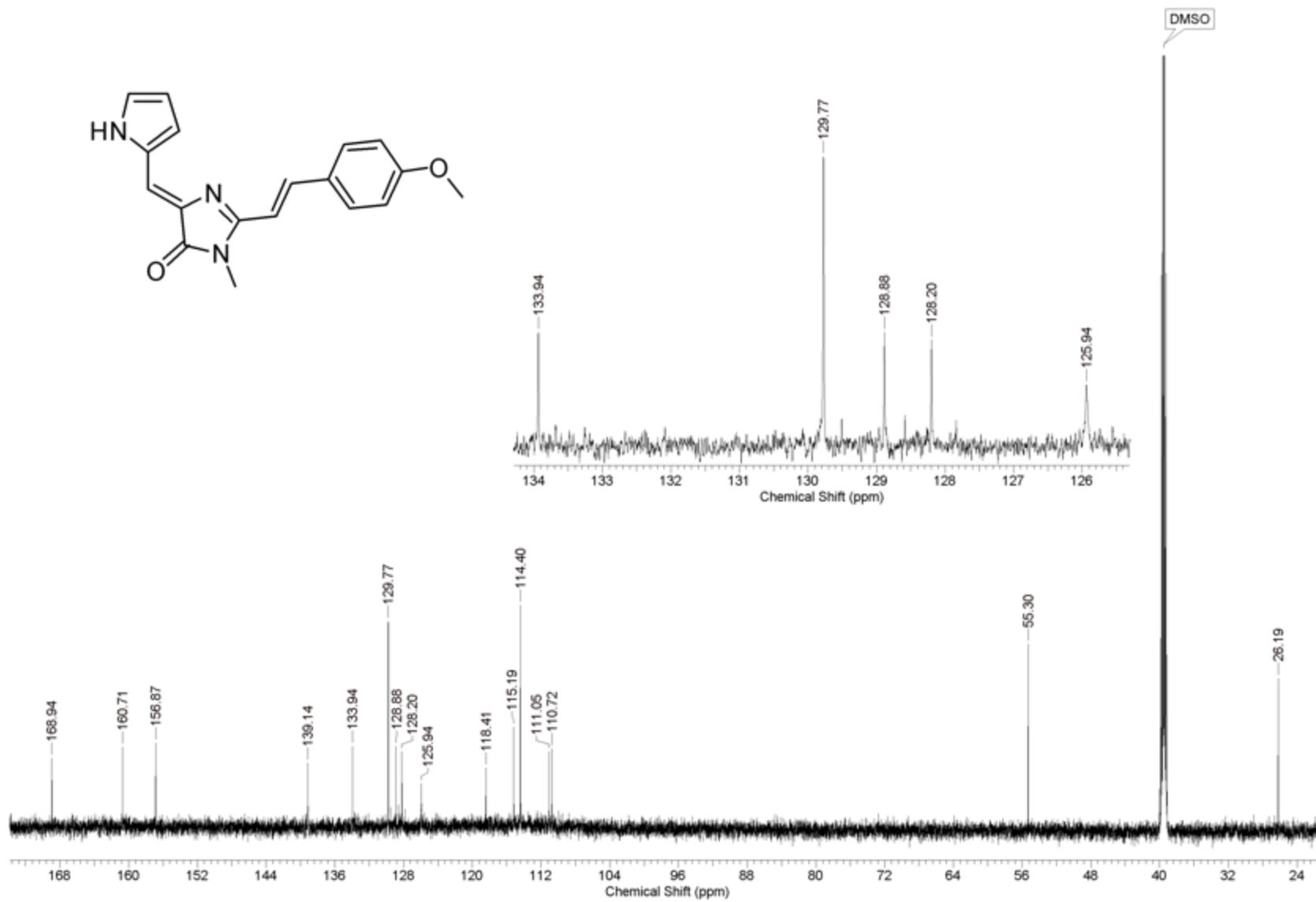


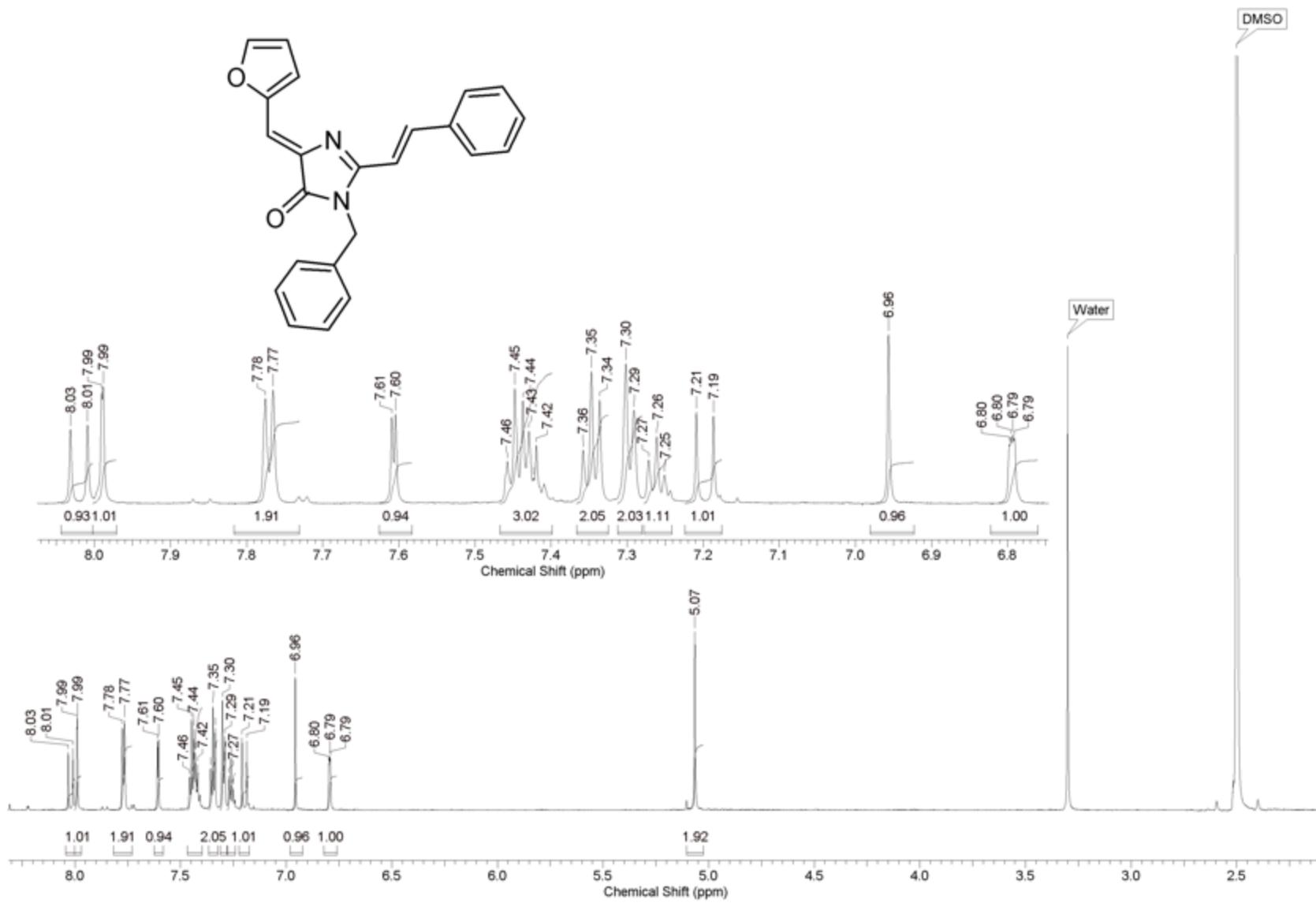


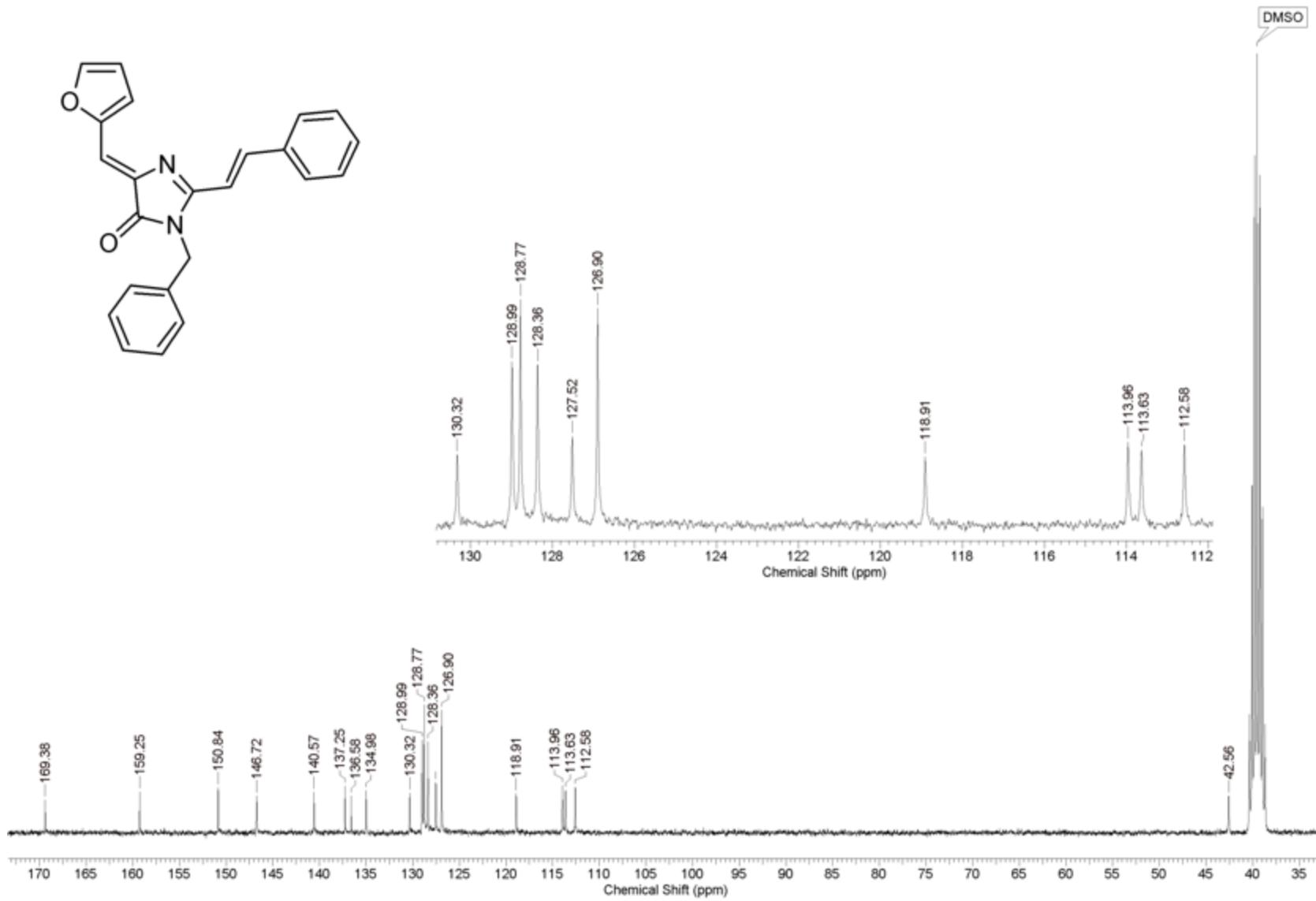


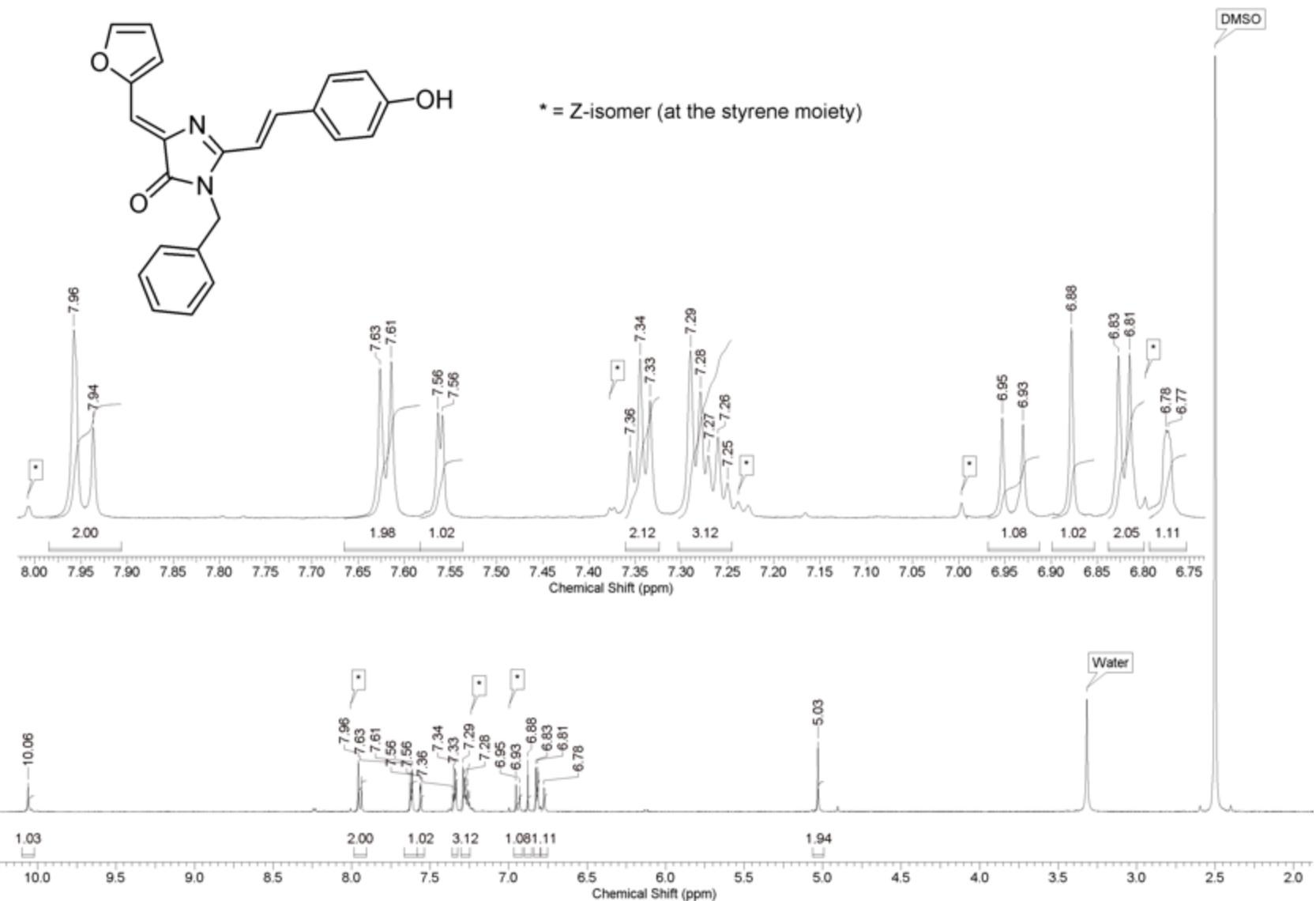
* = isomer (at the benzylidene moiety)

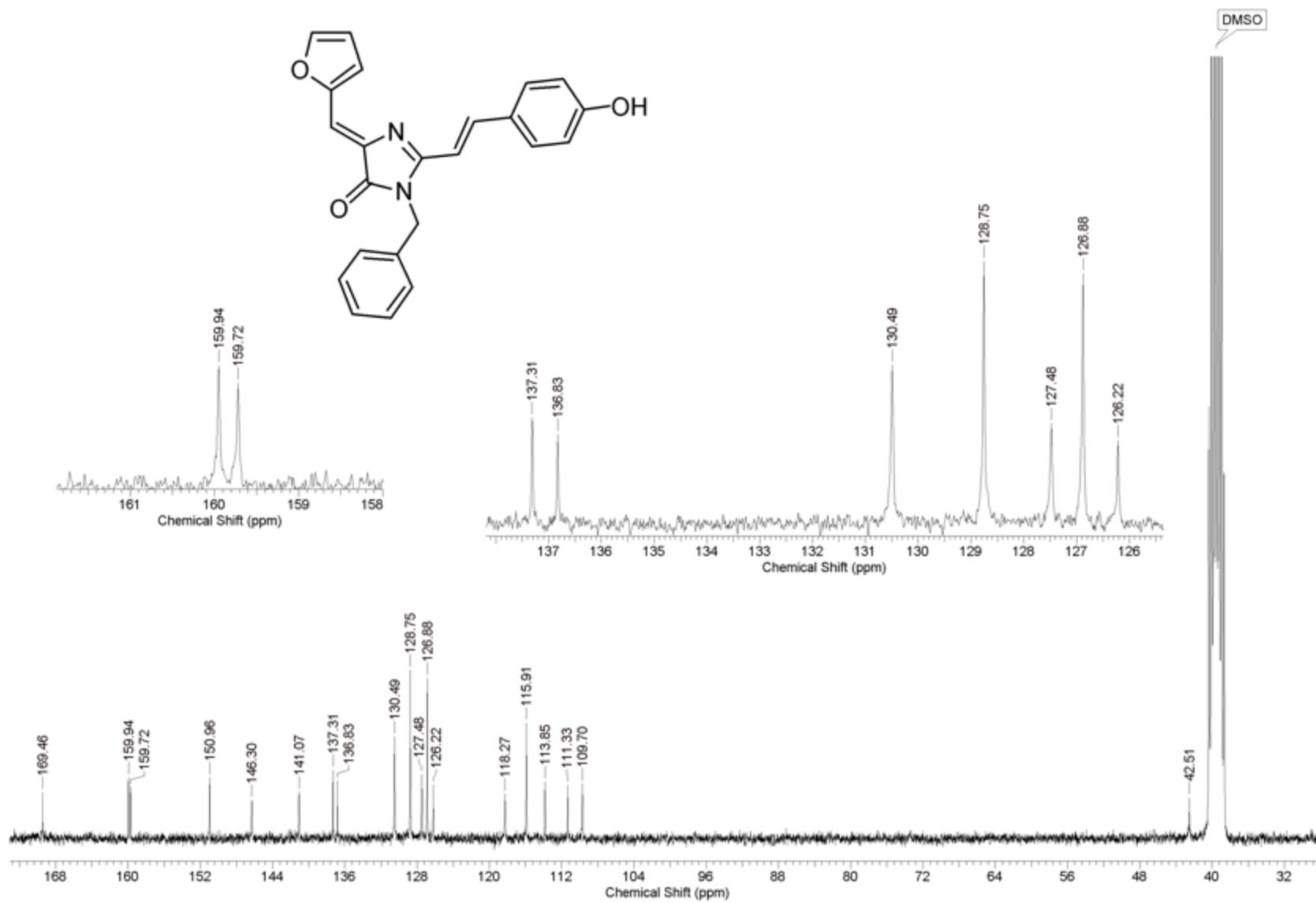


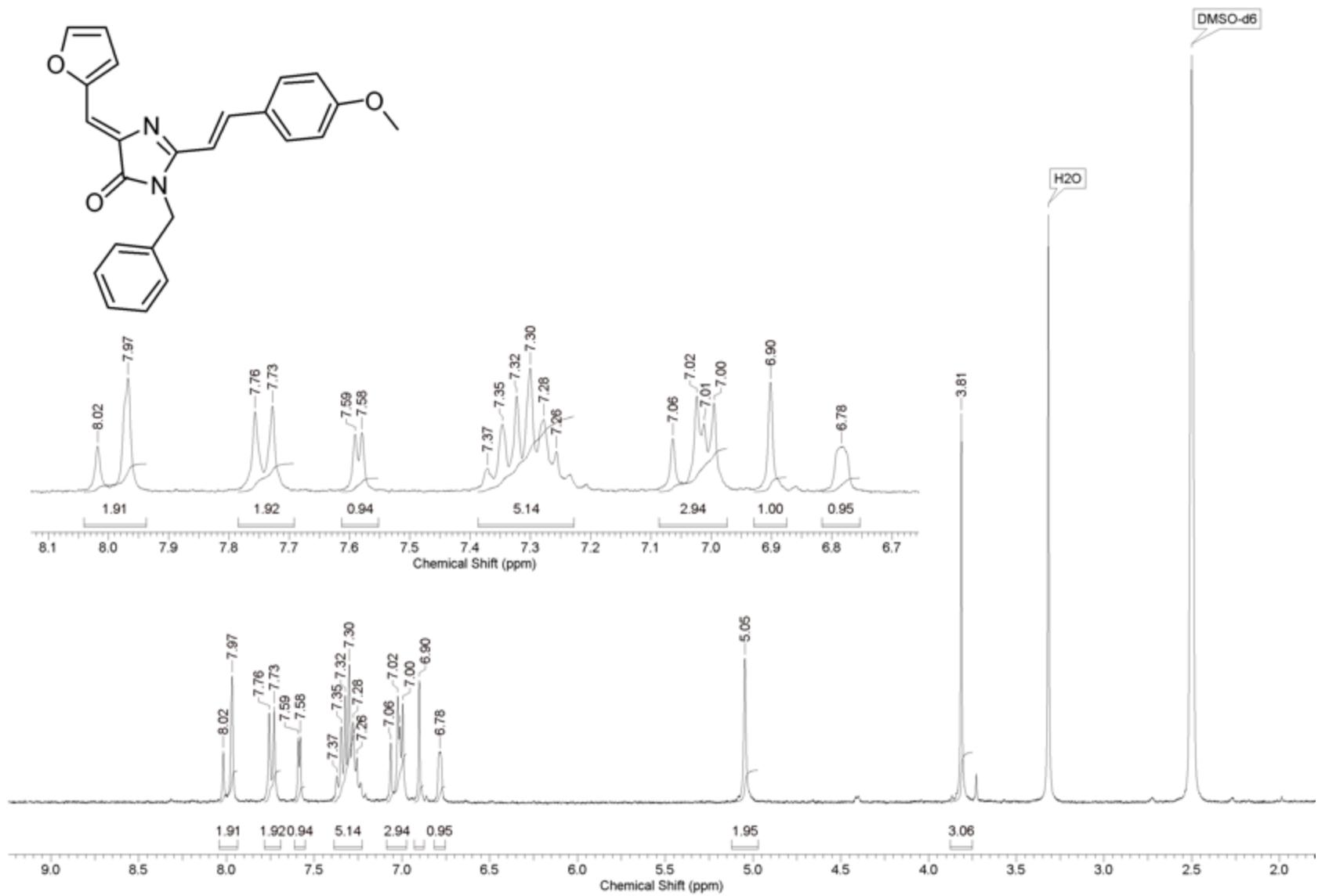


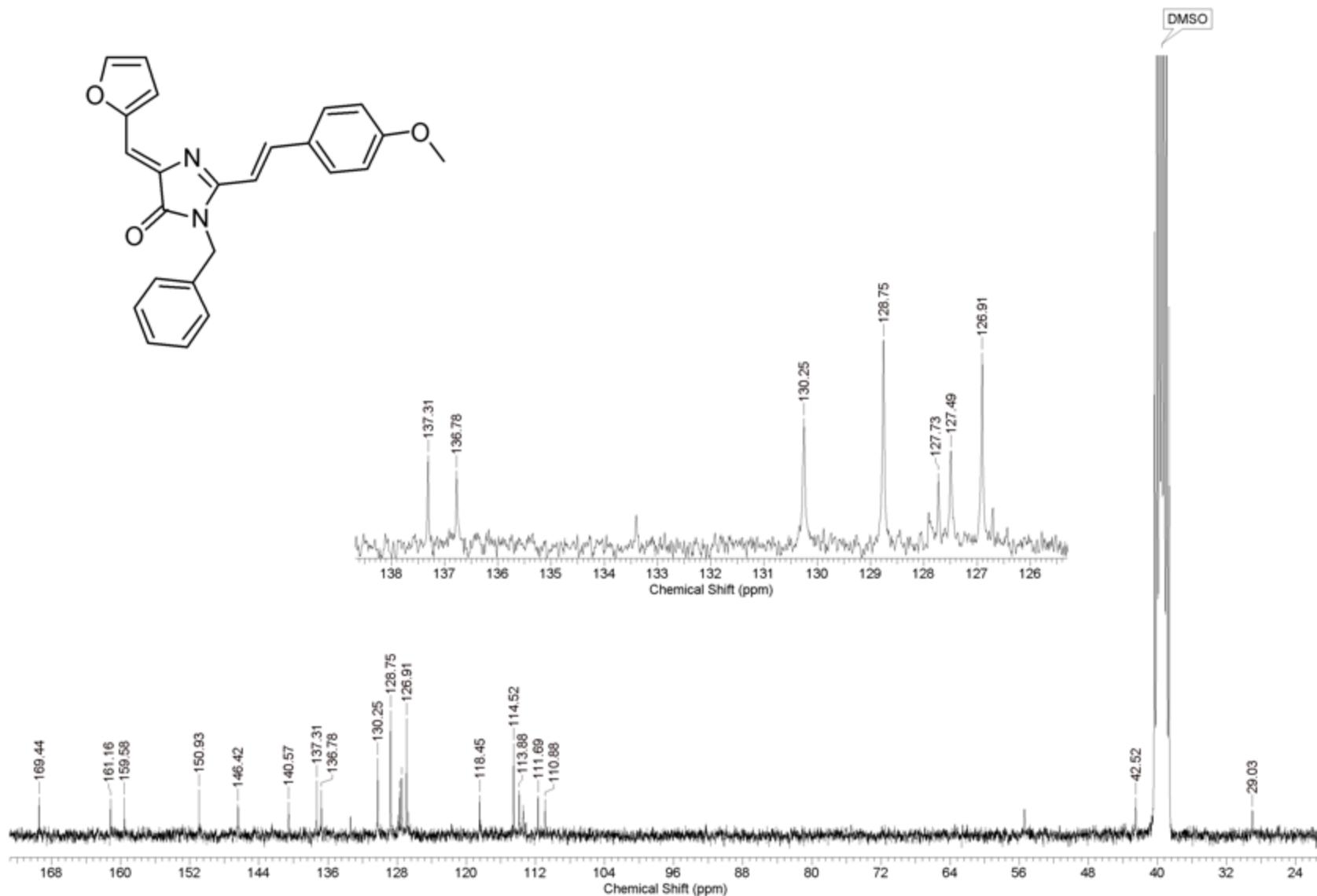


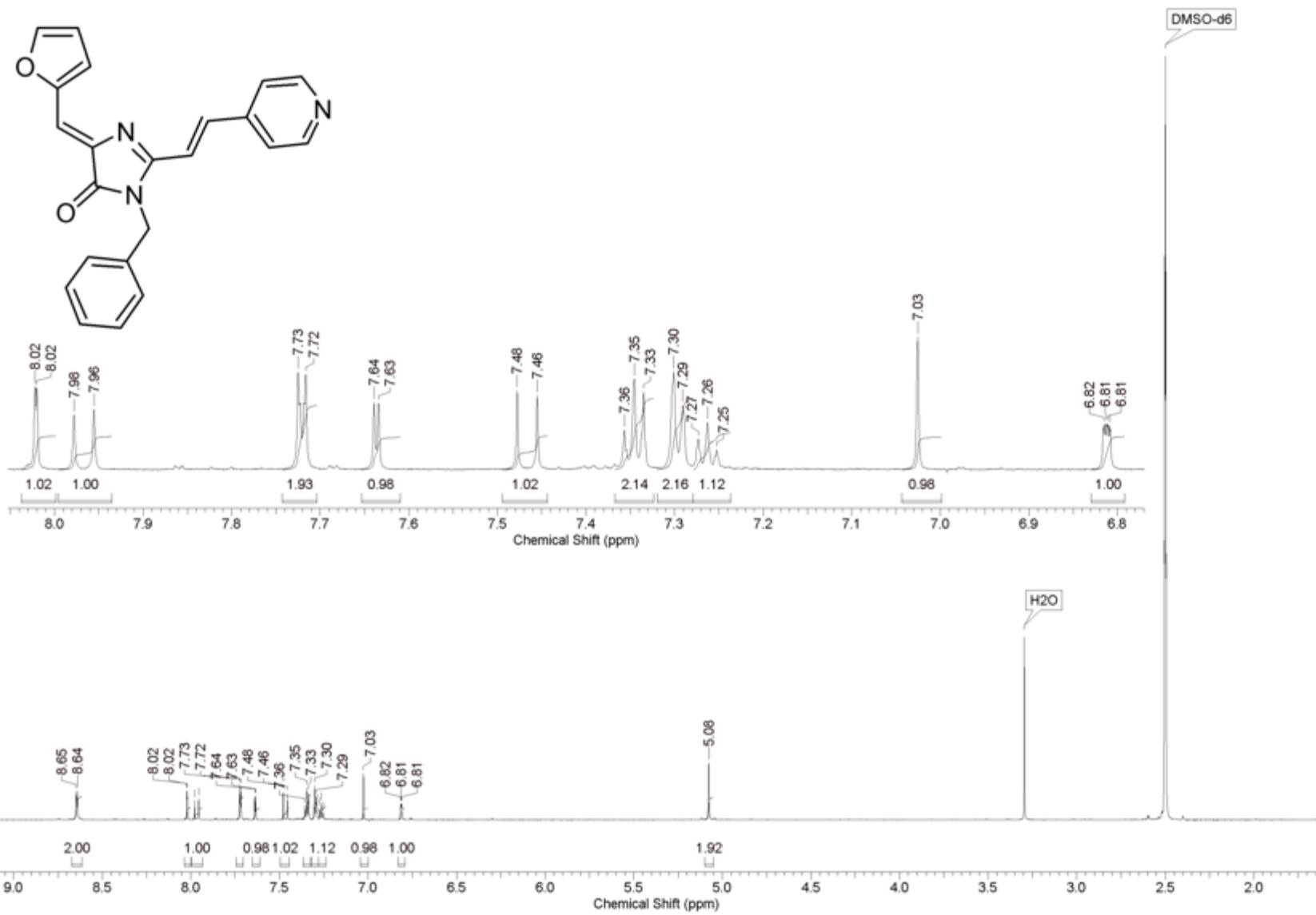


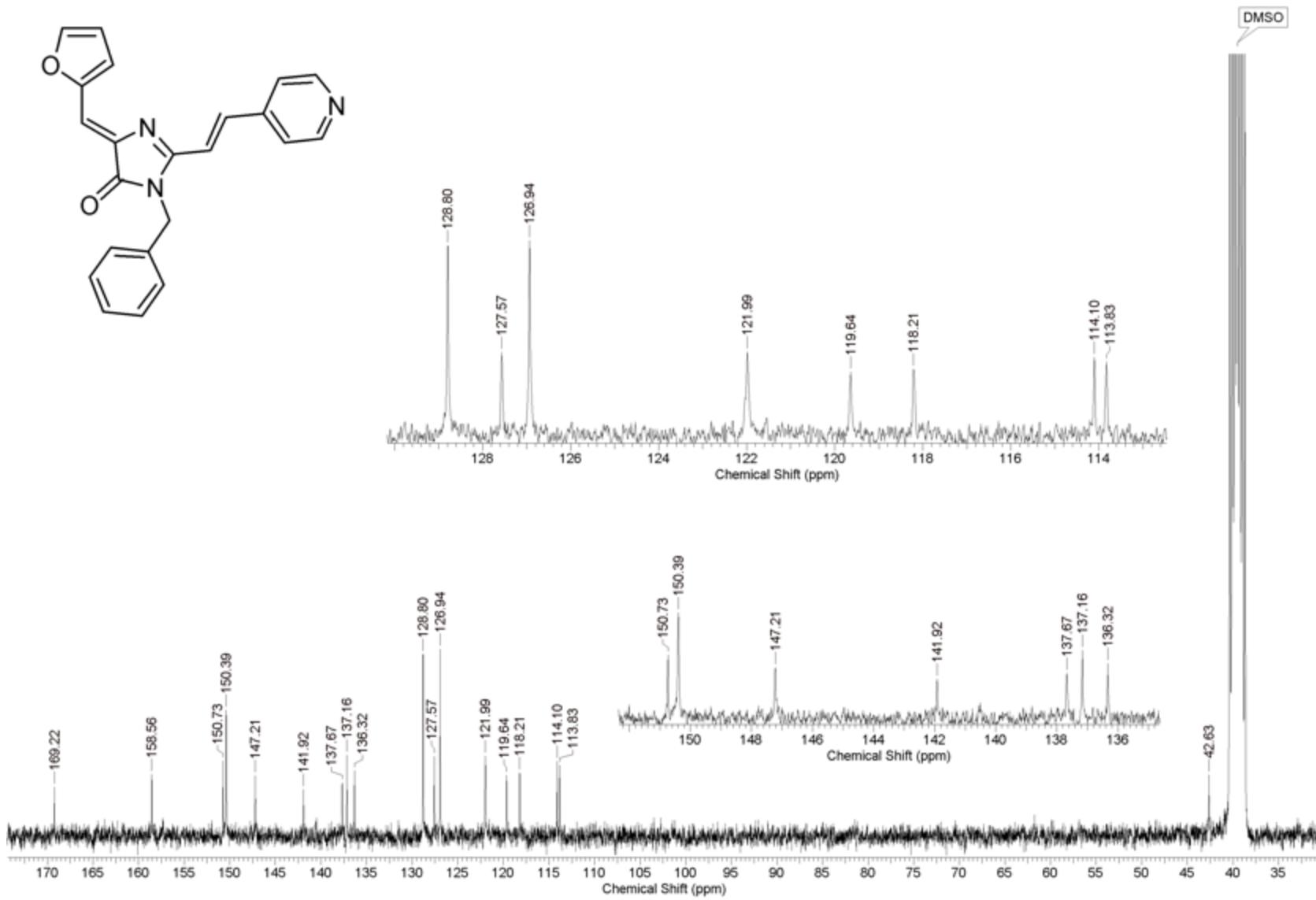
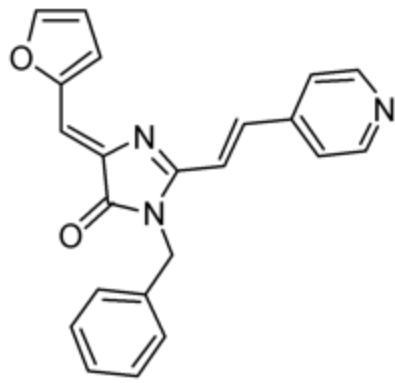


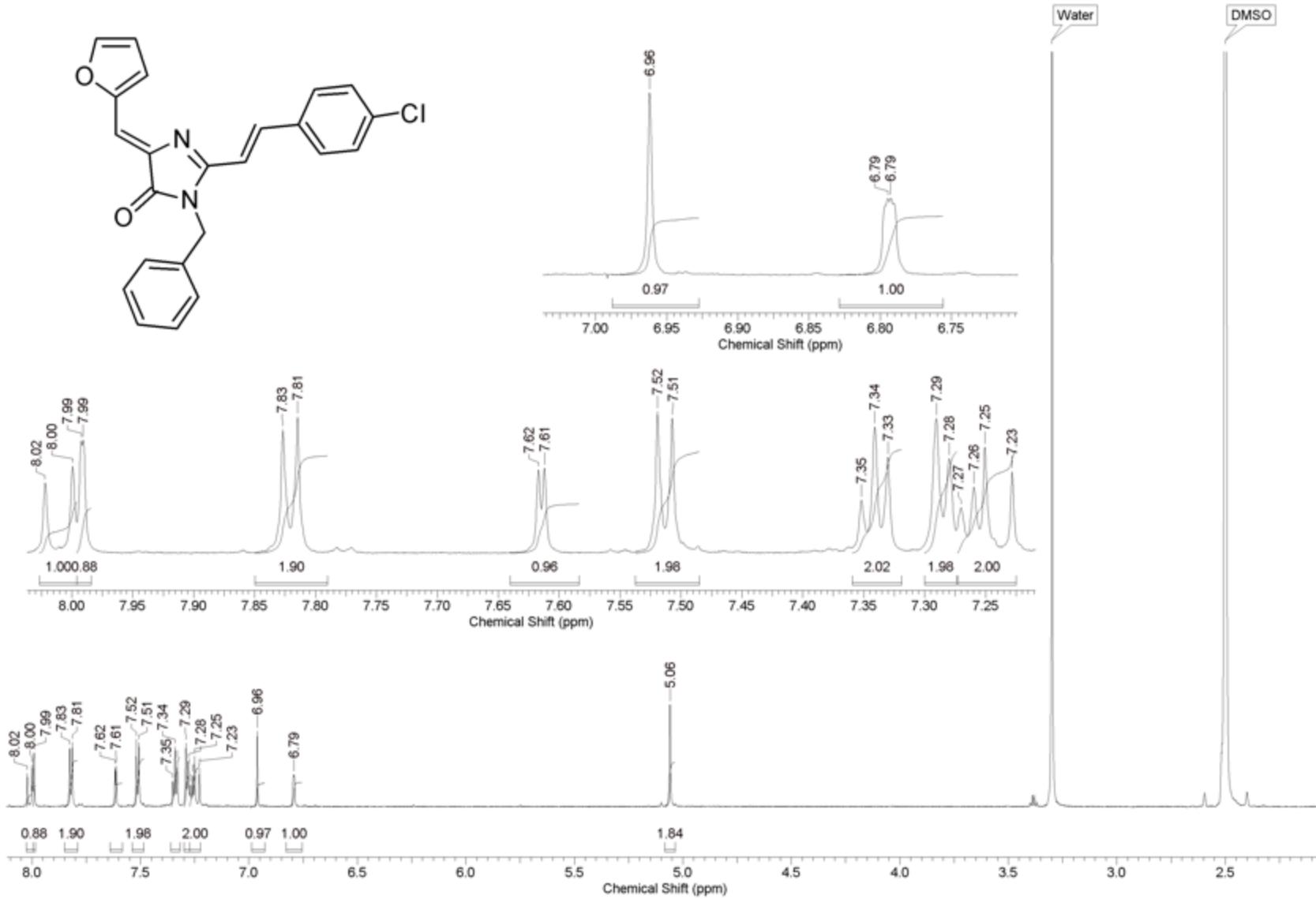
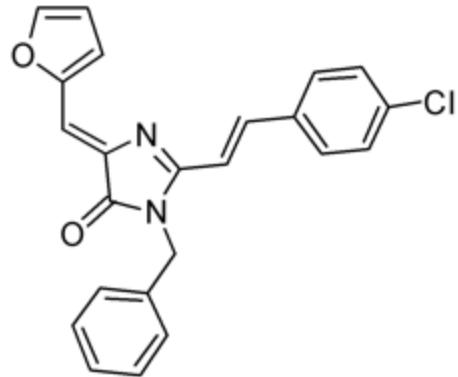


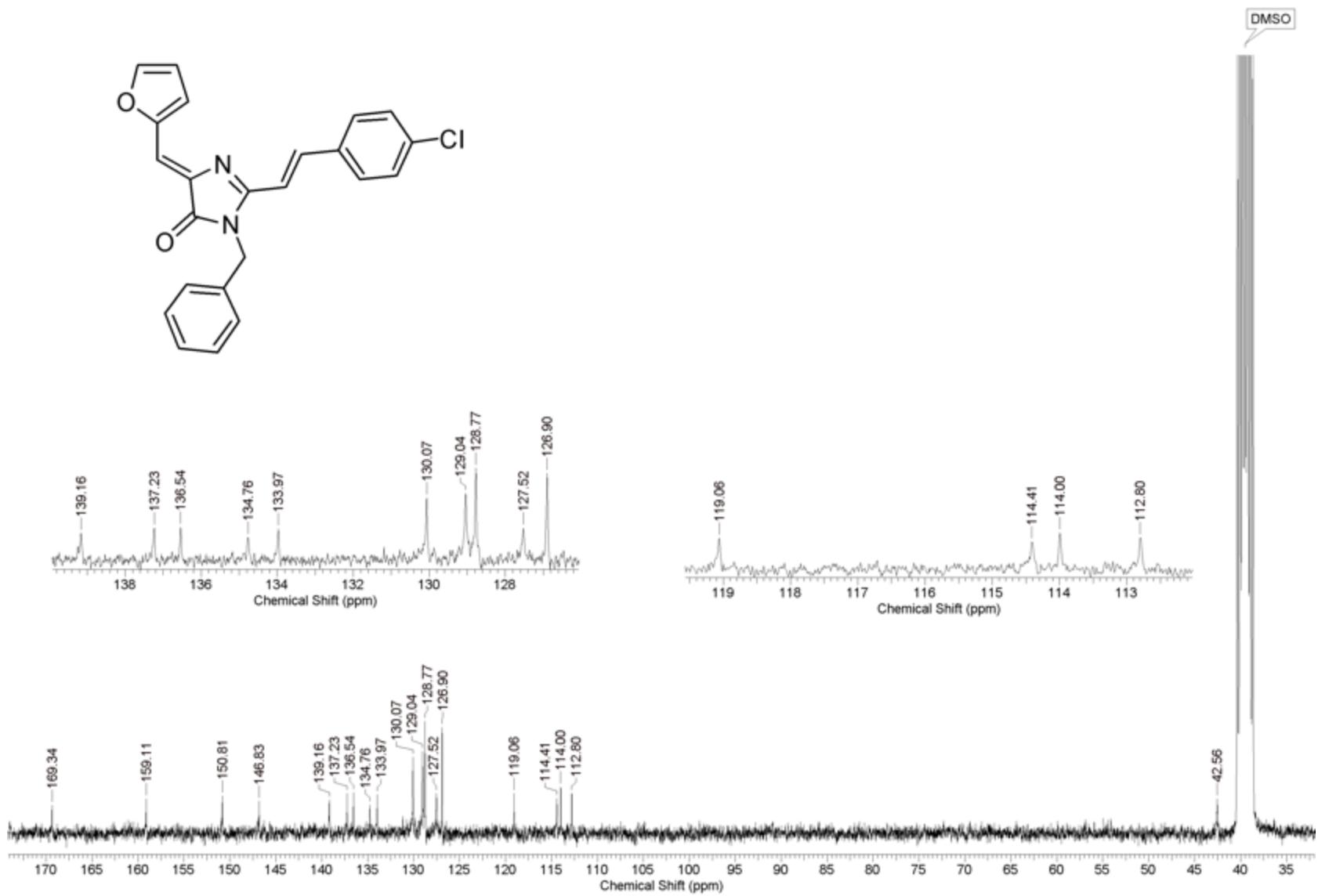


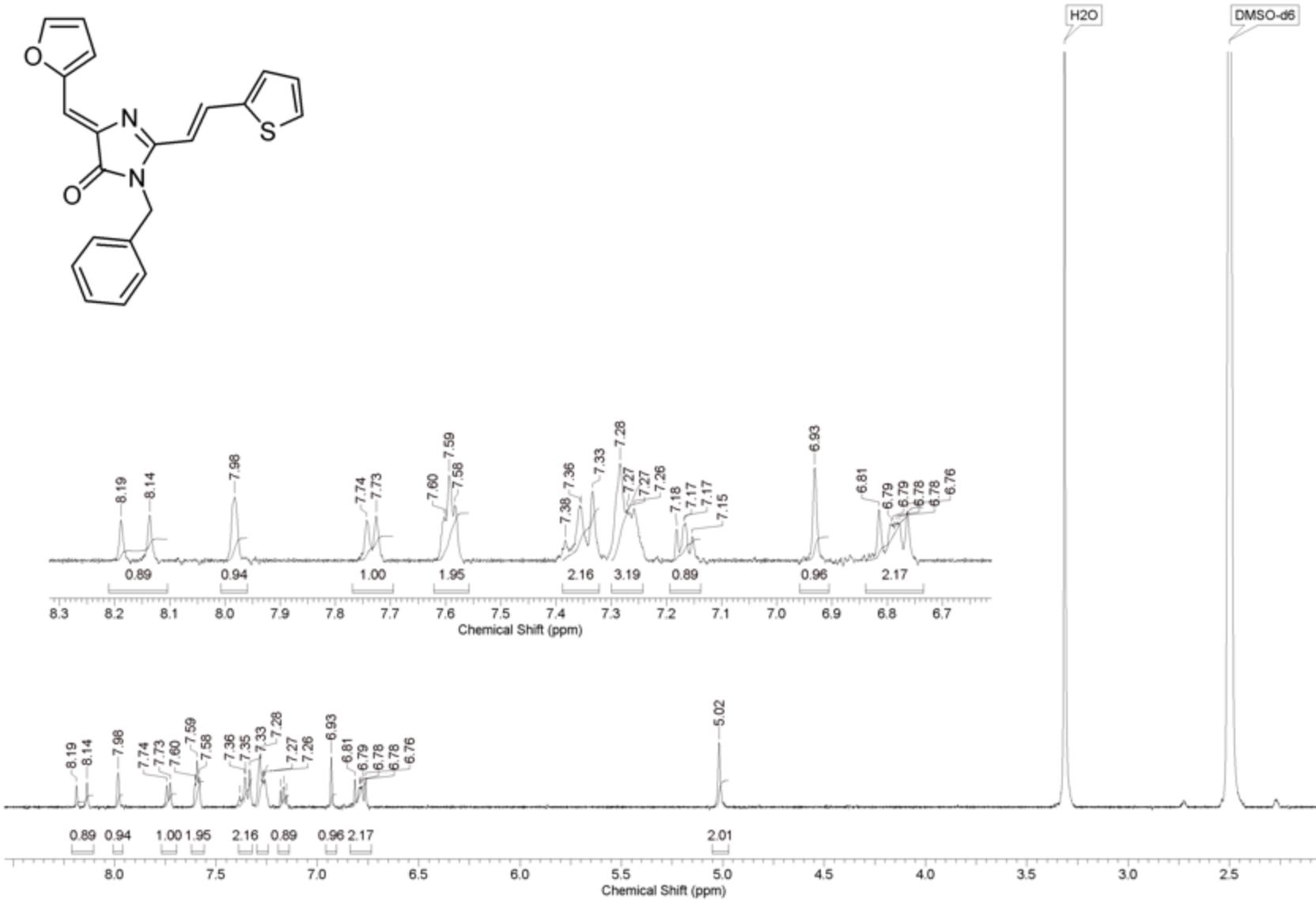
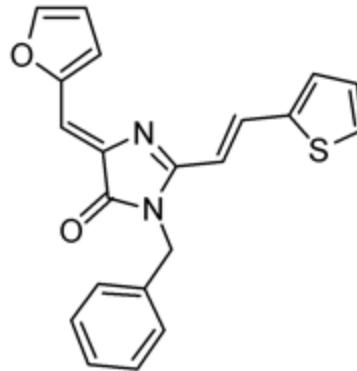


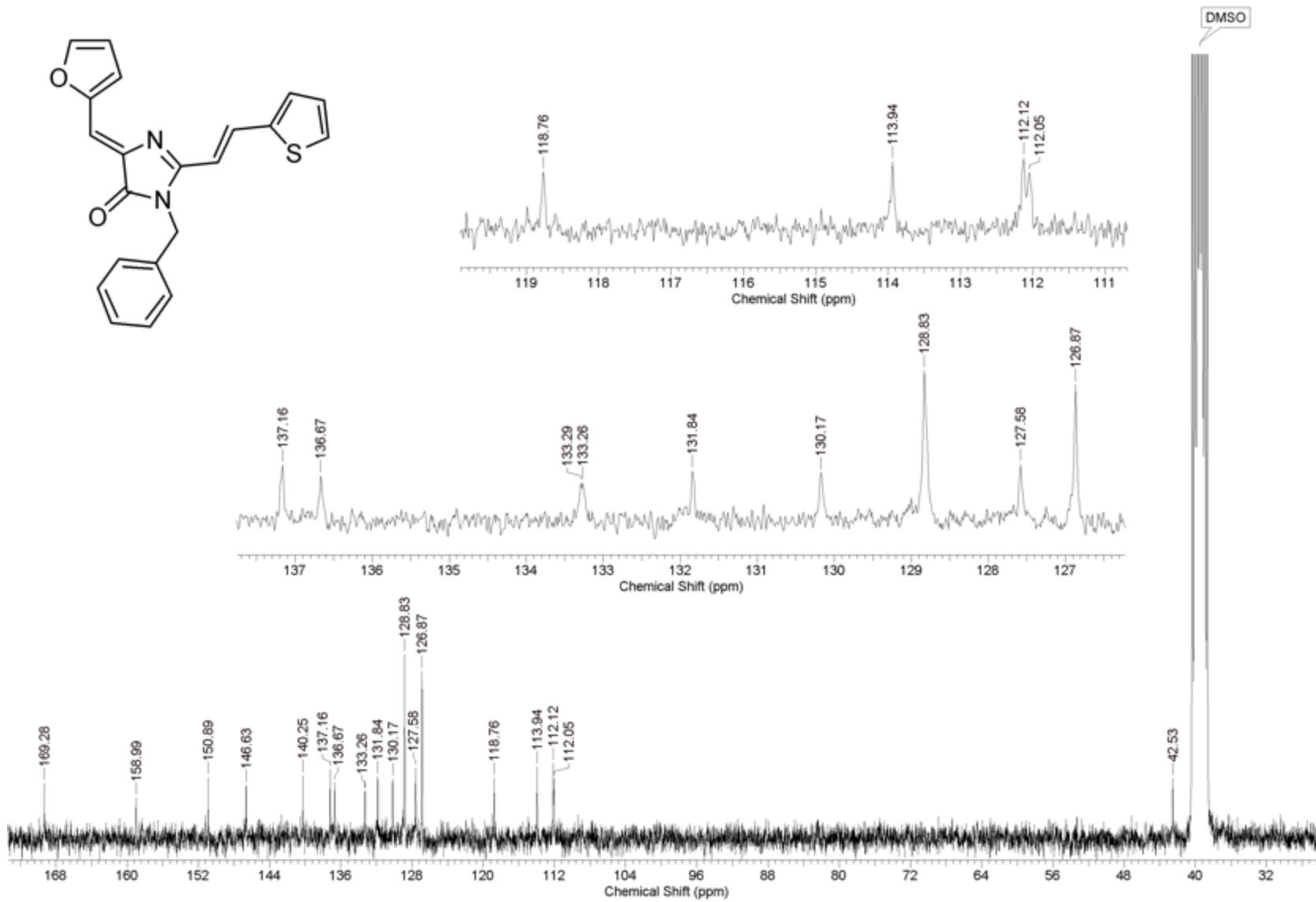
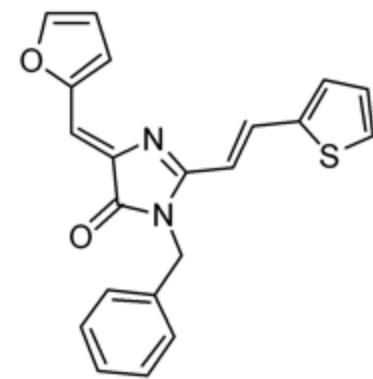


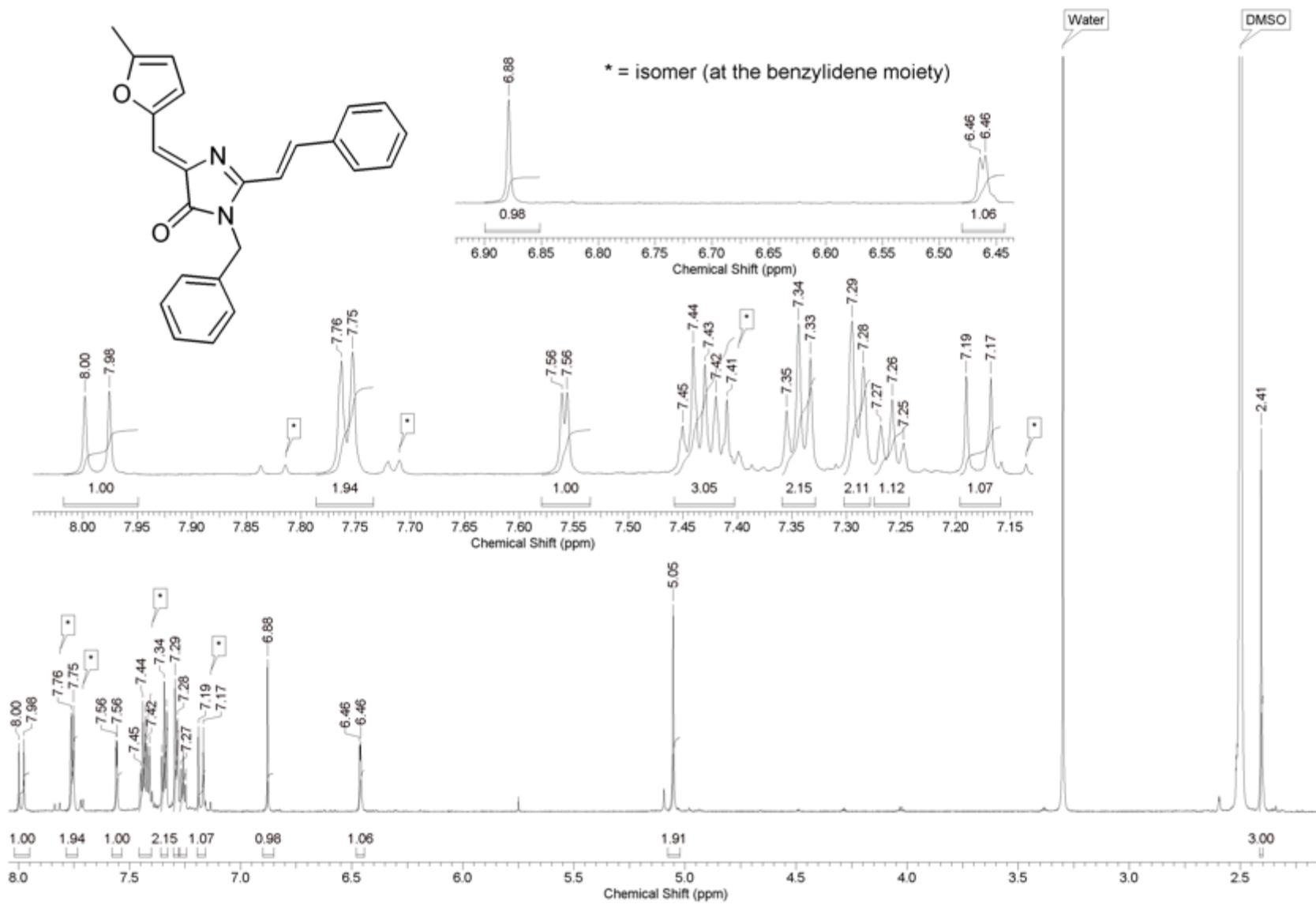


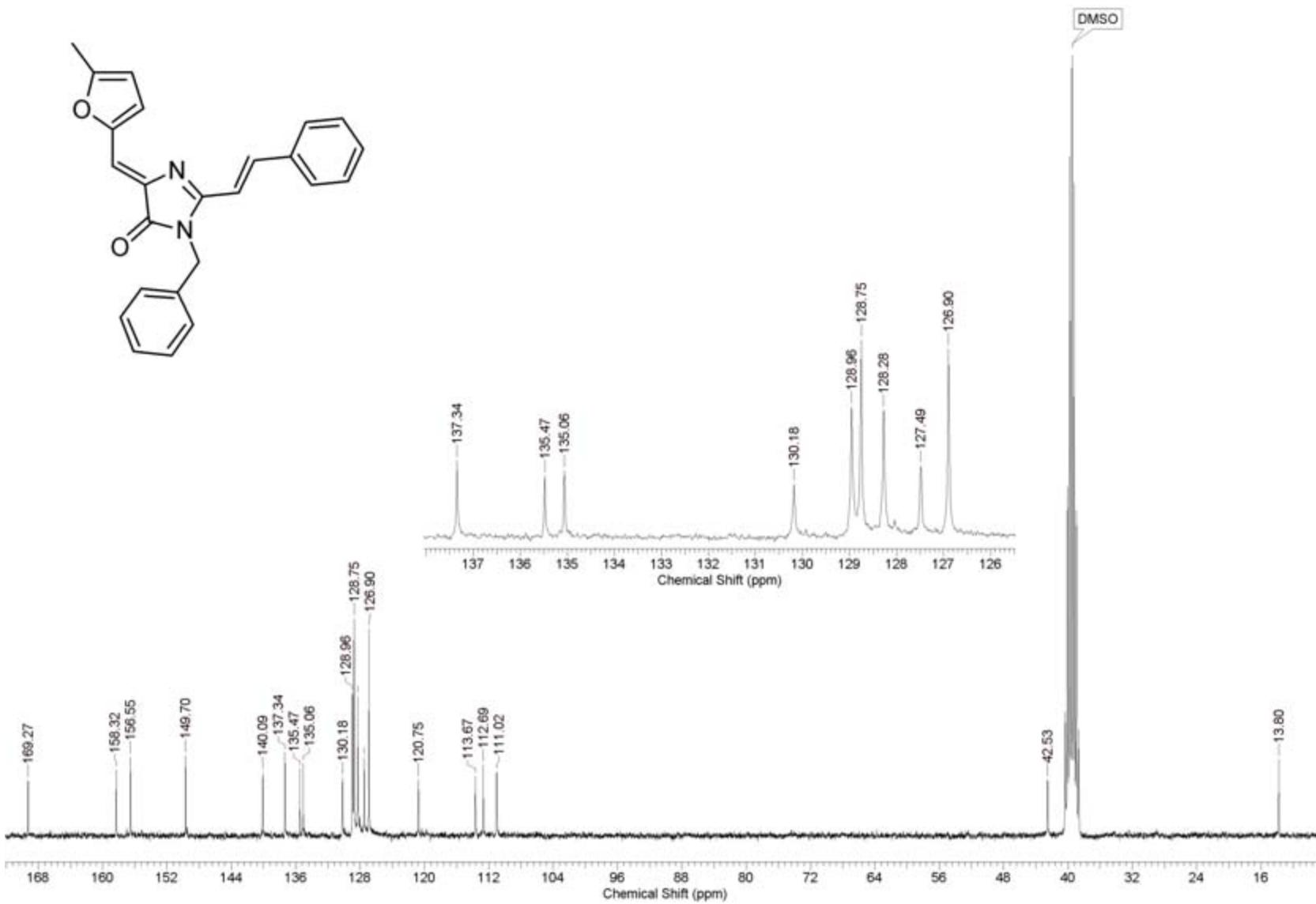


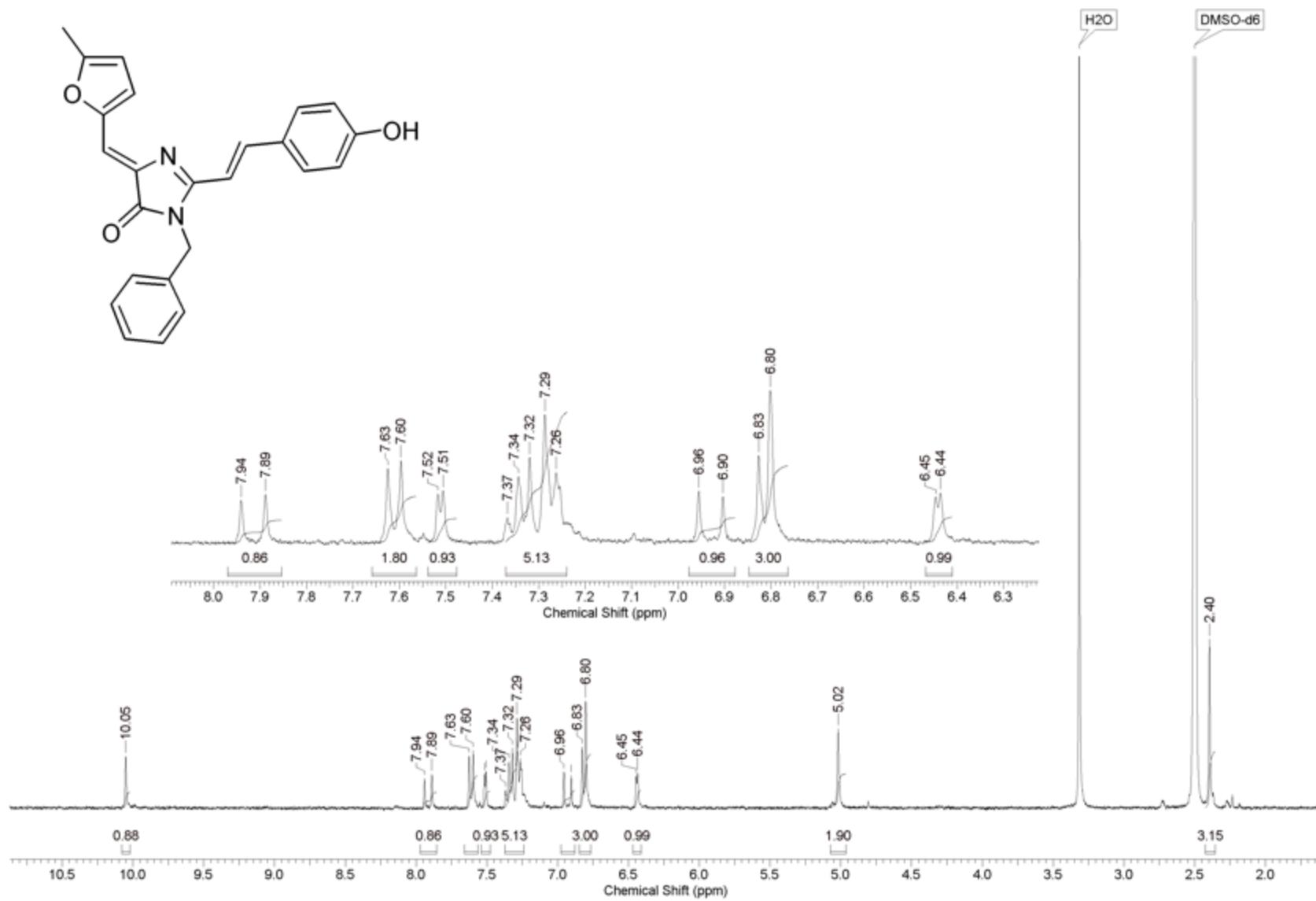


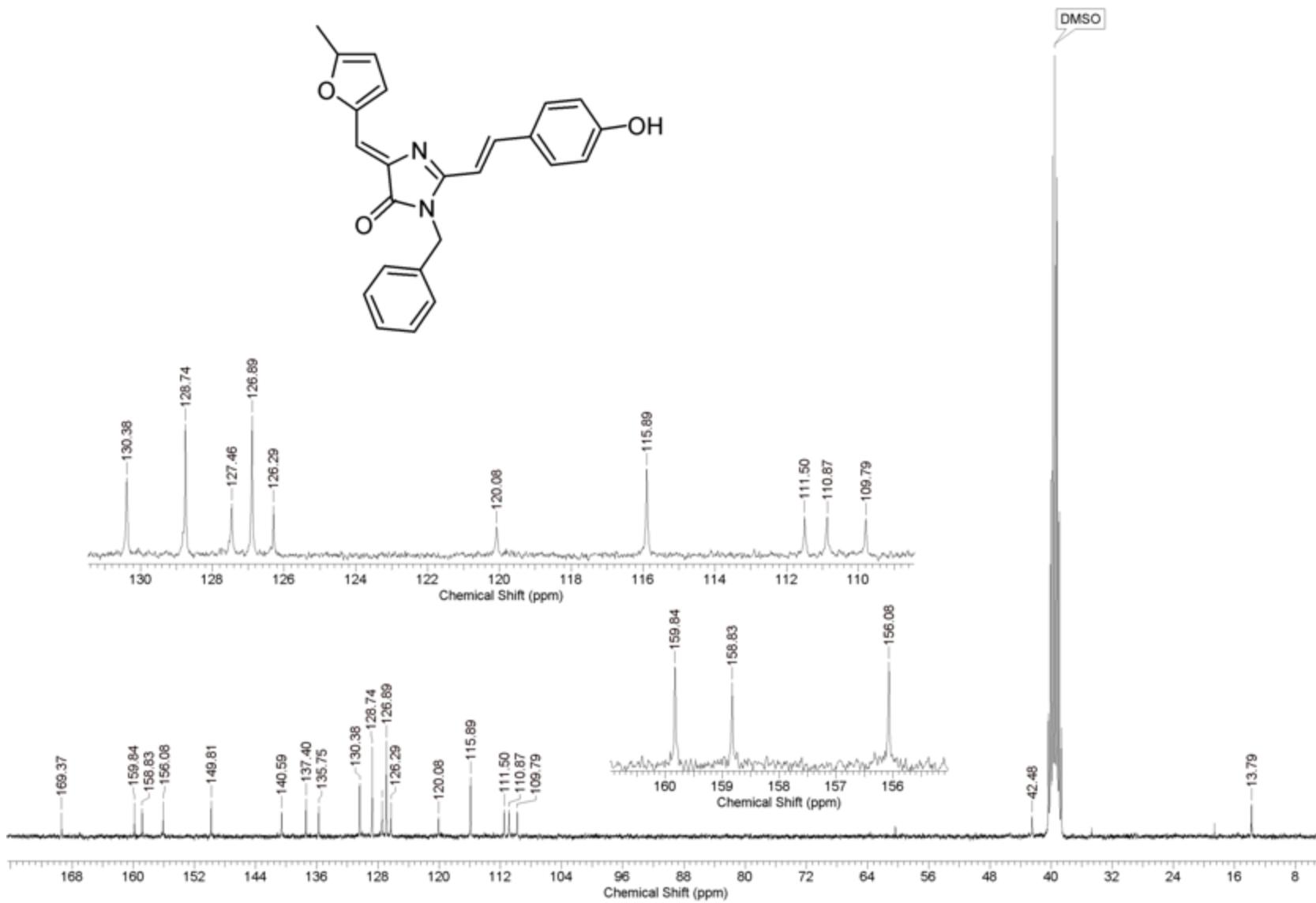


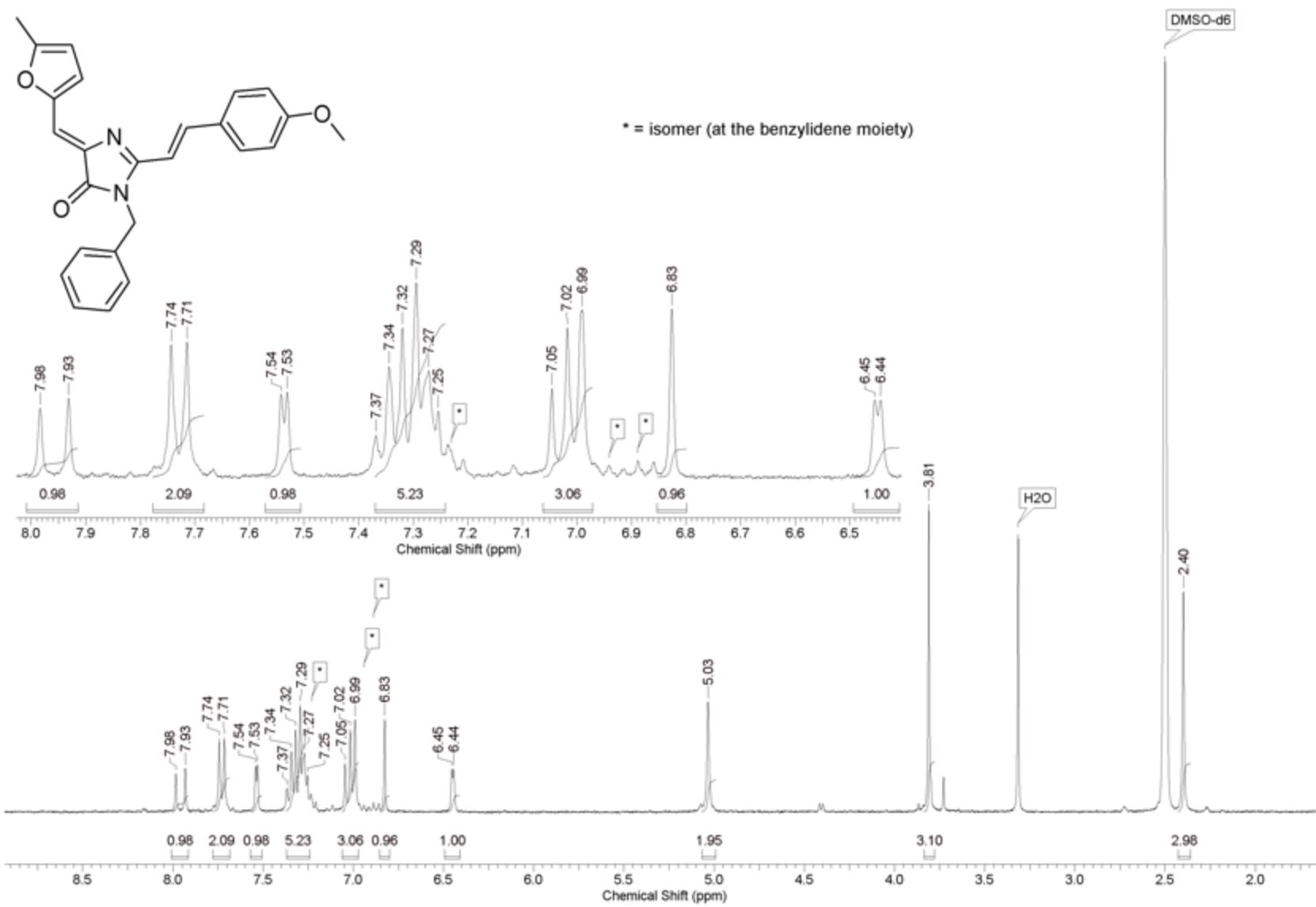


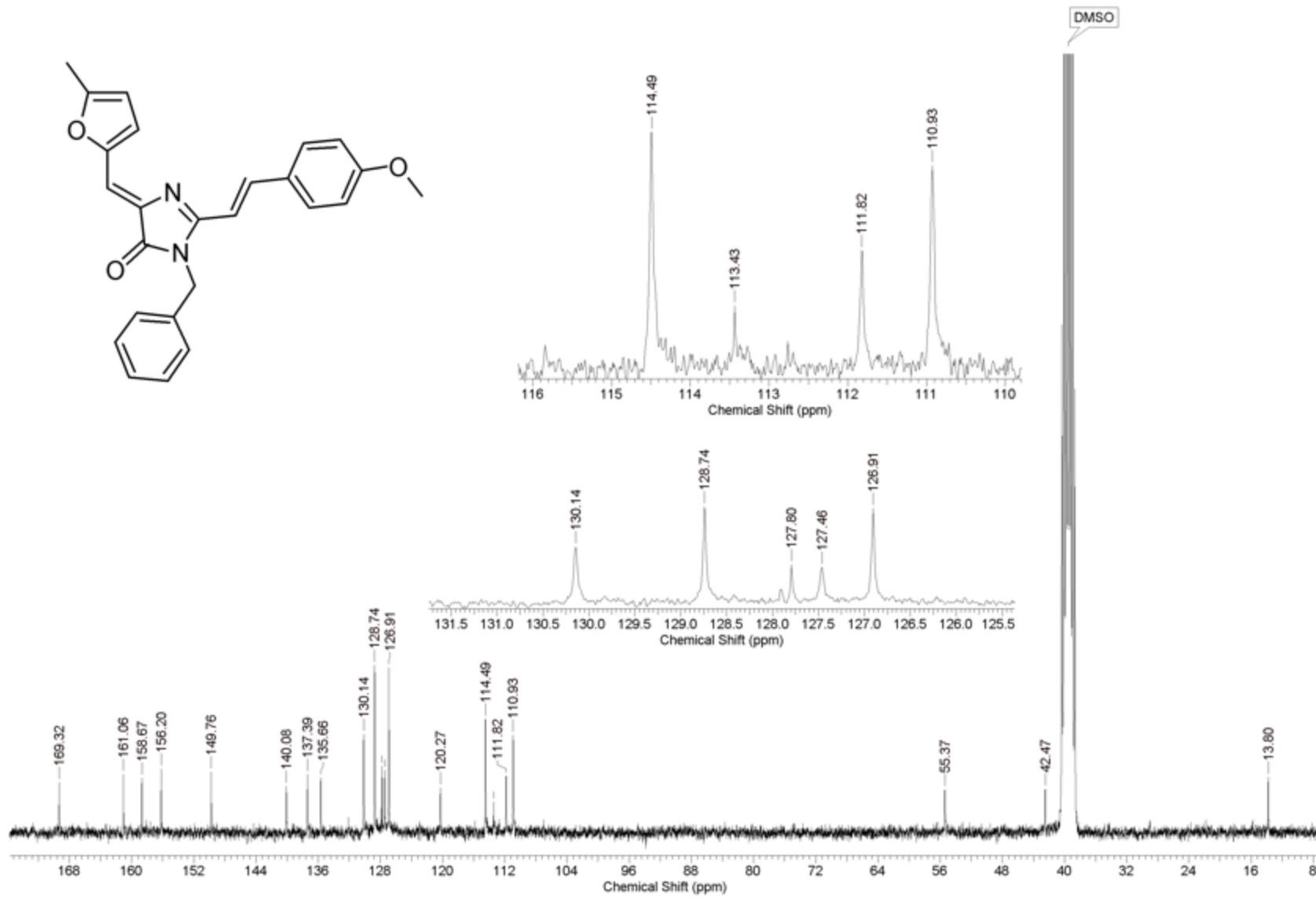


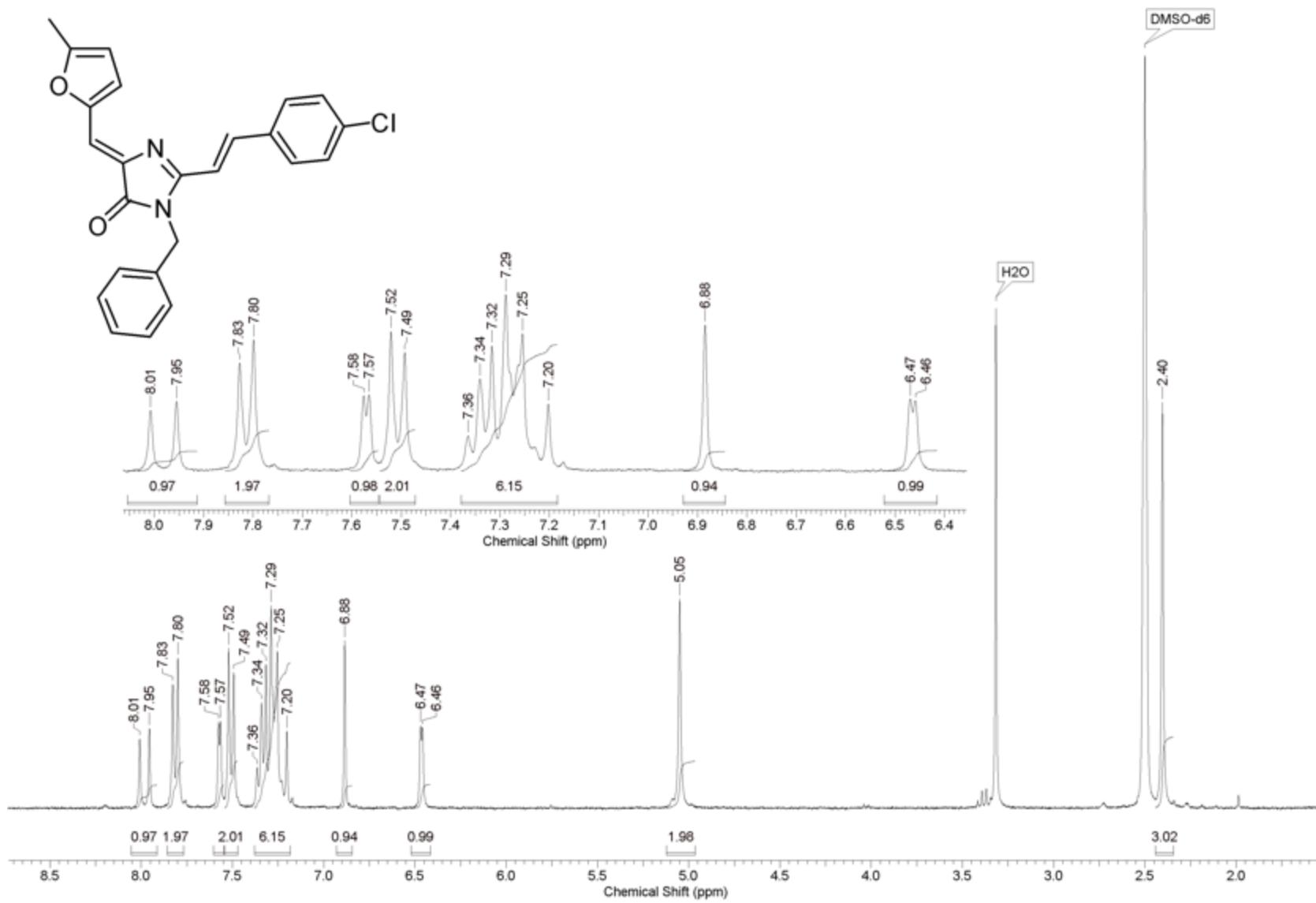


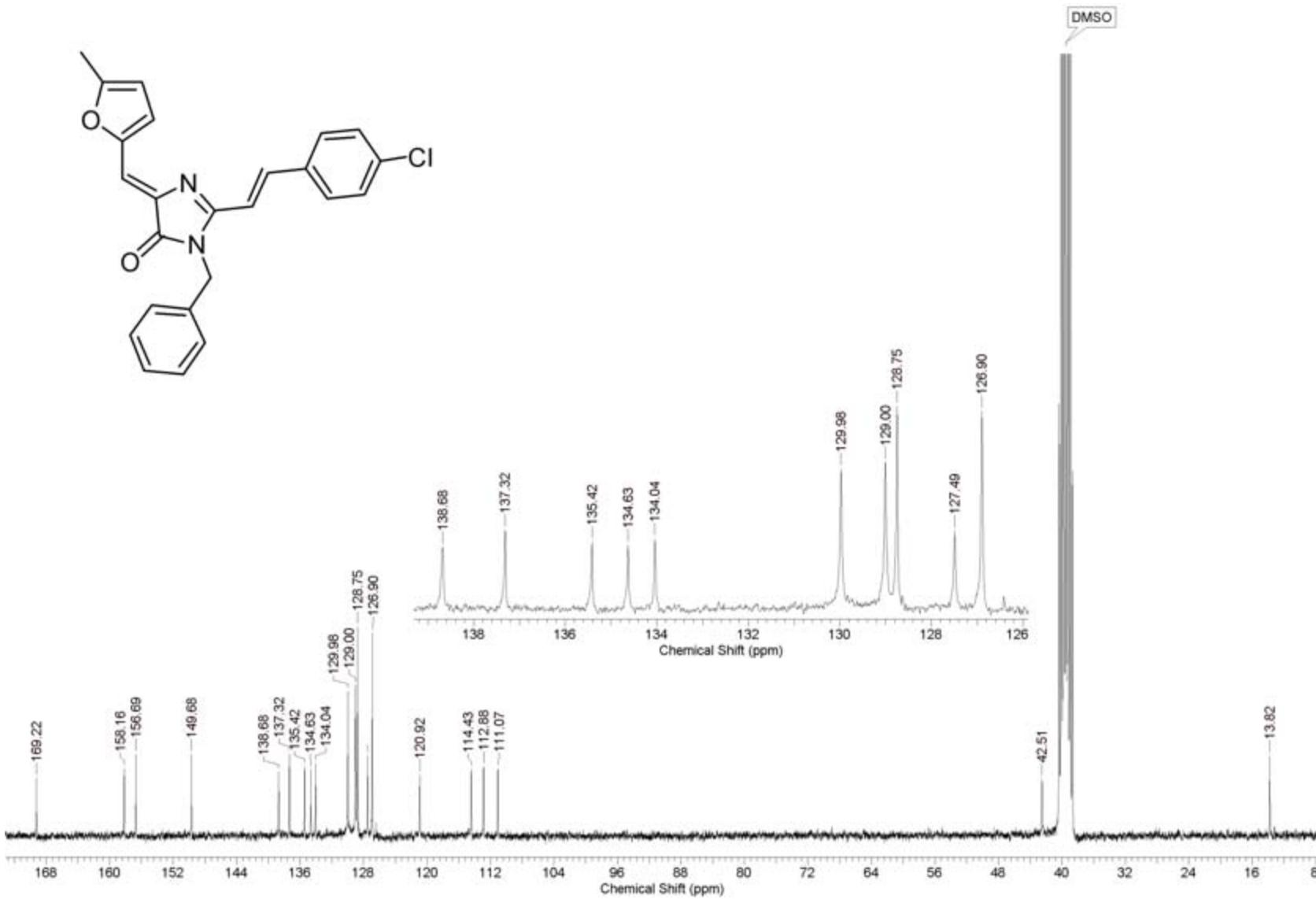


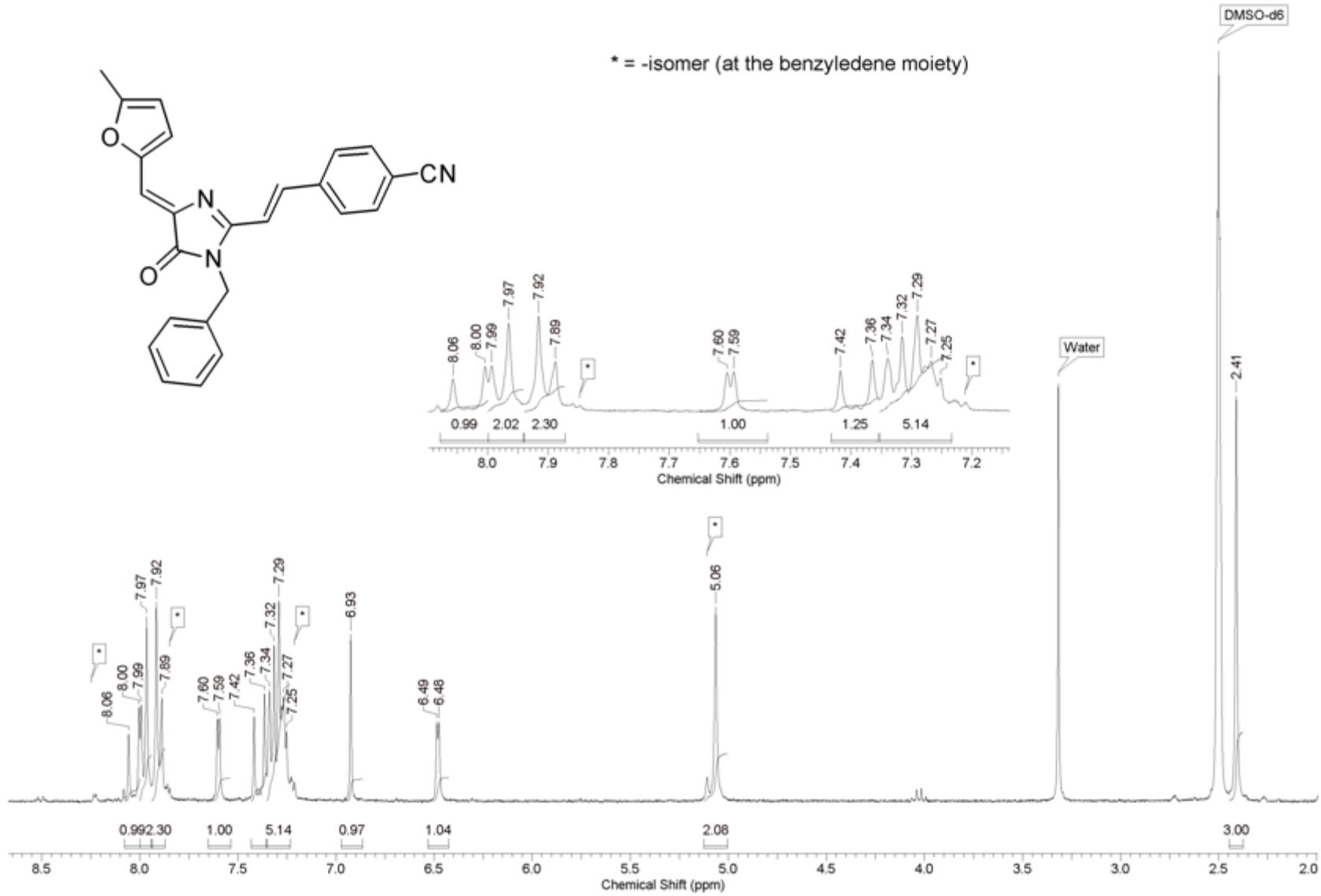


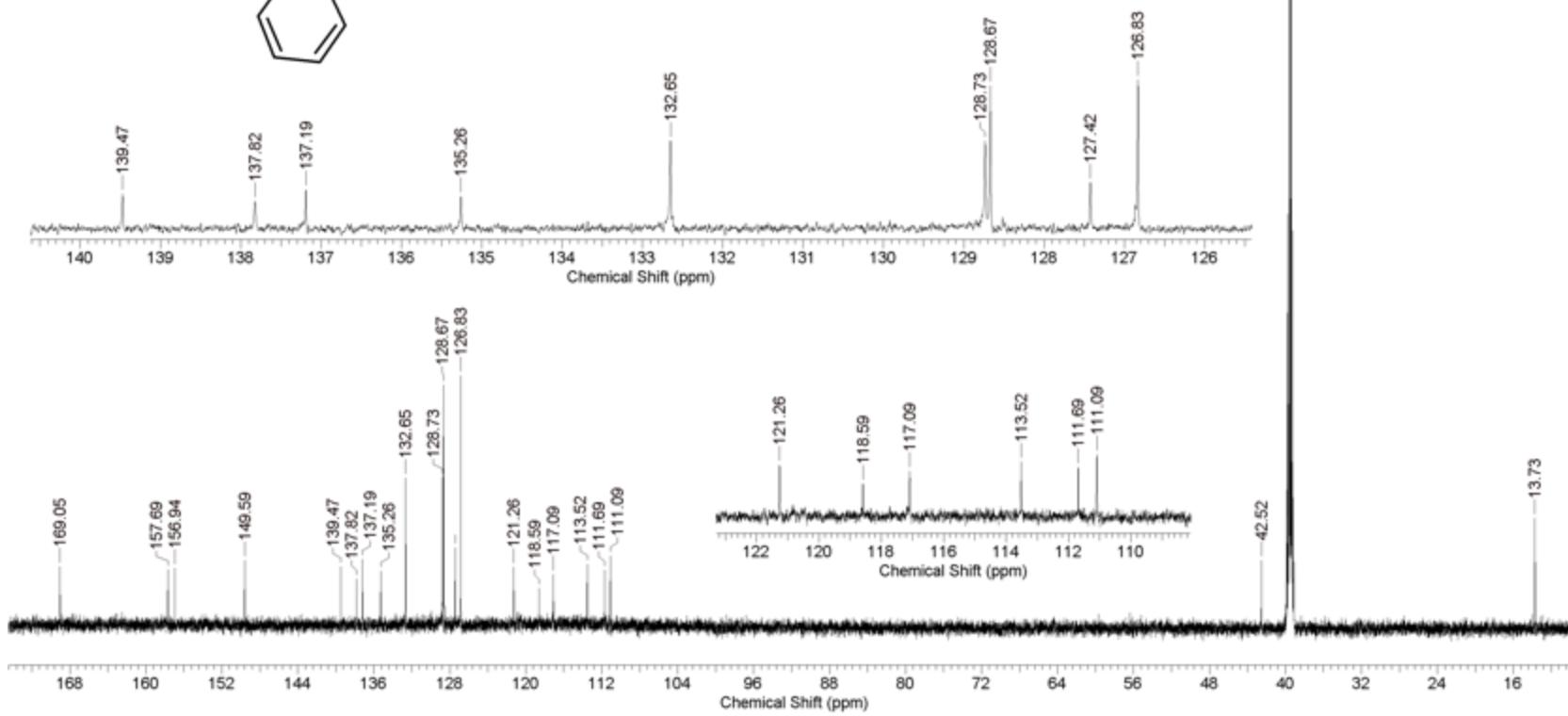
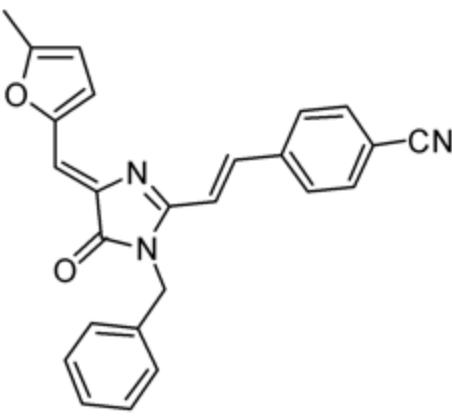


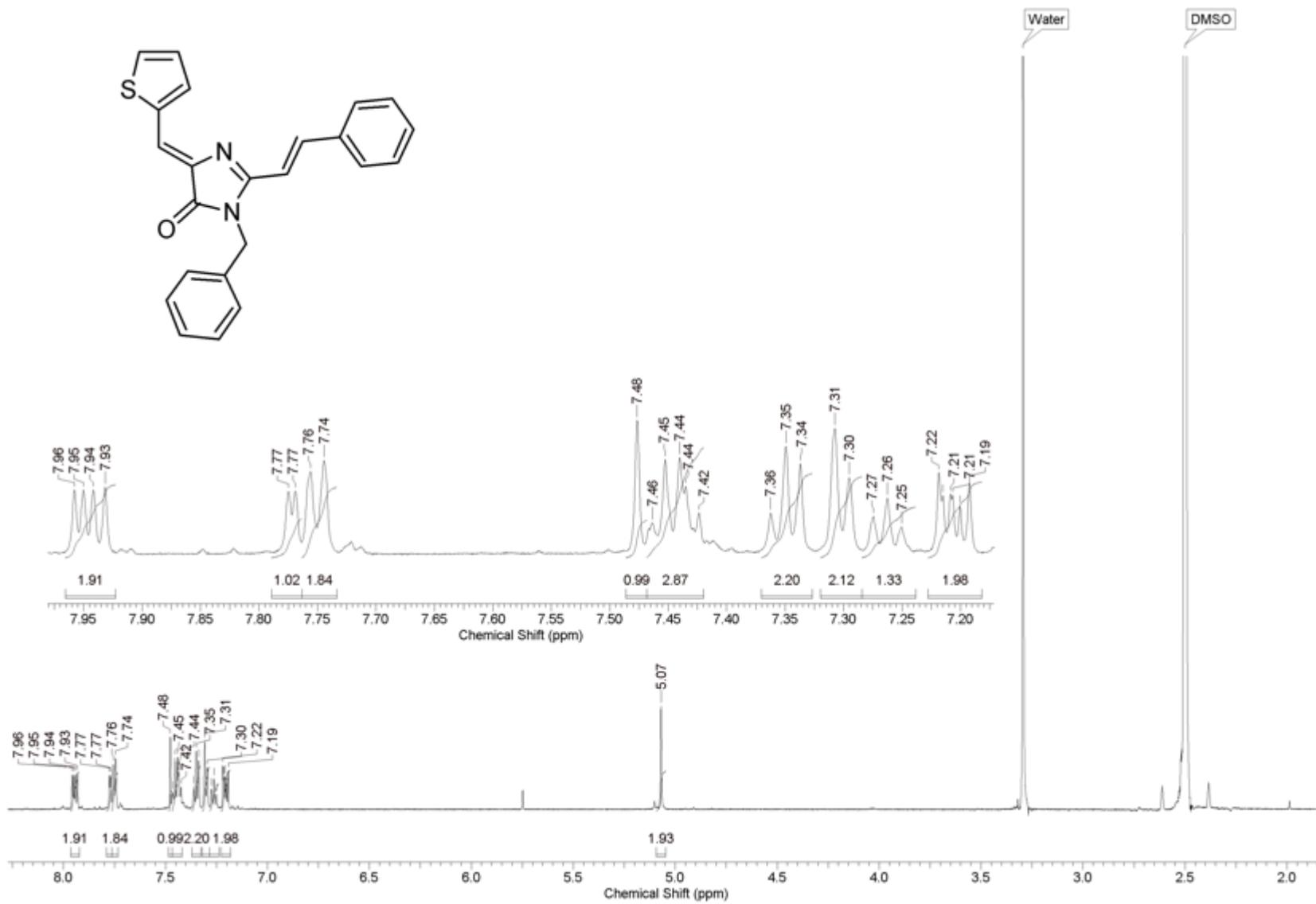


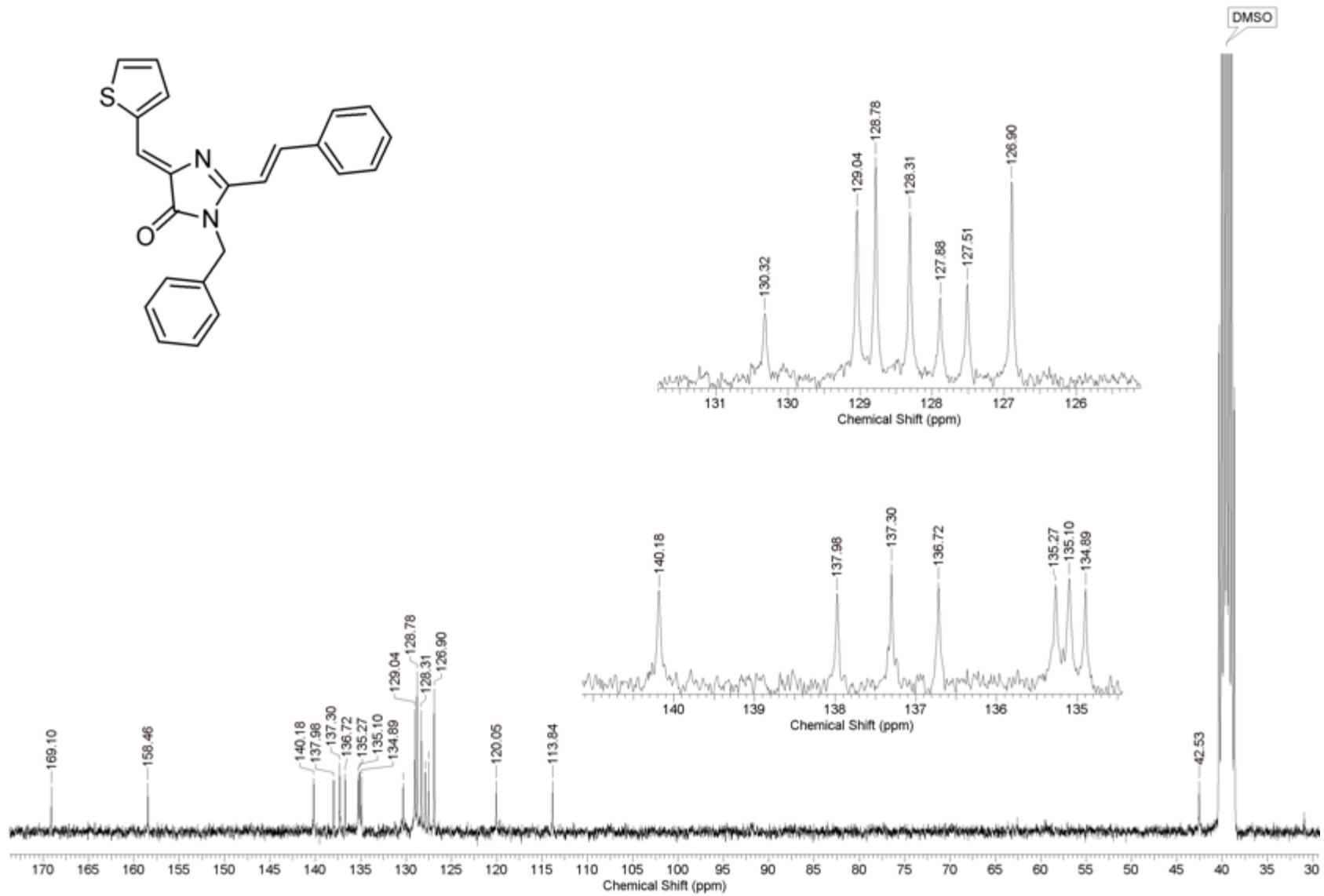


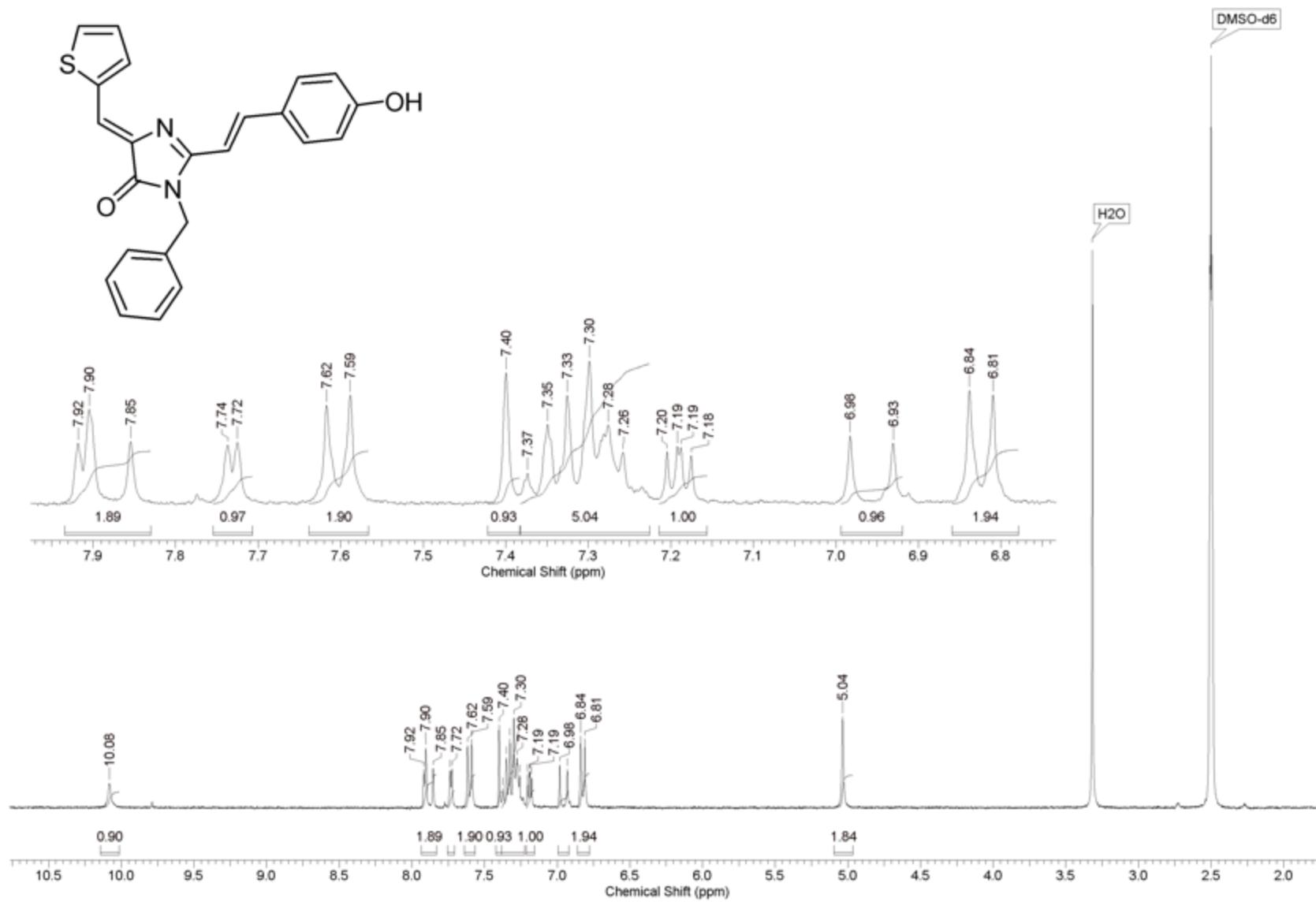


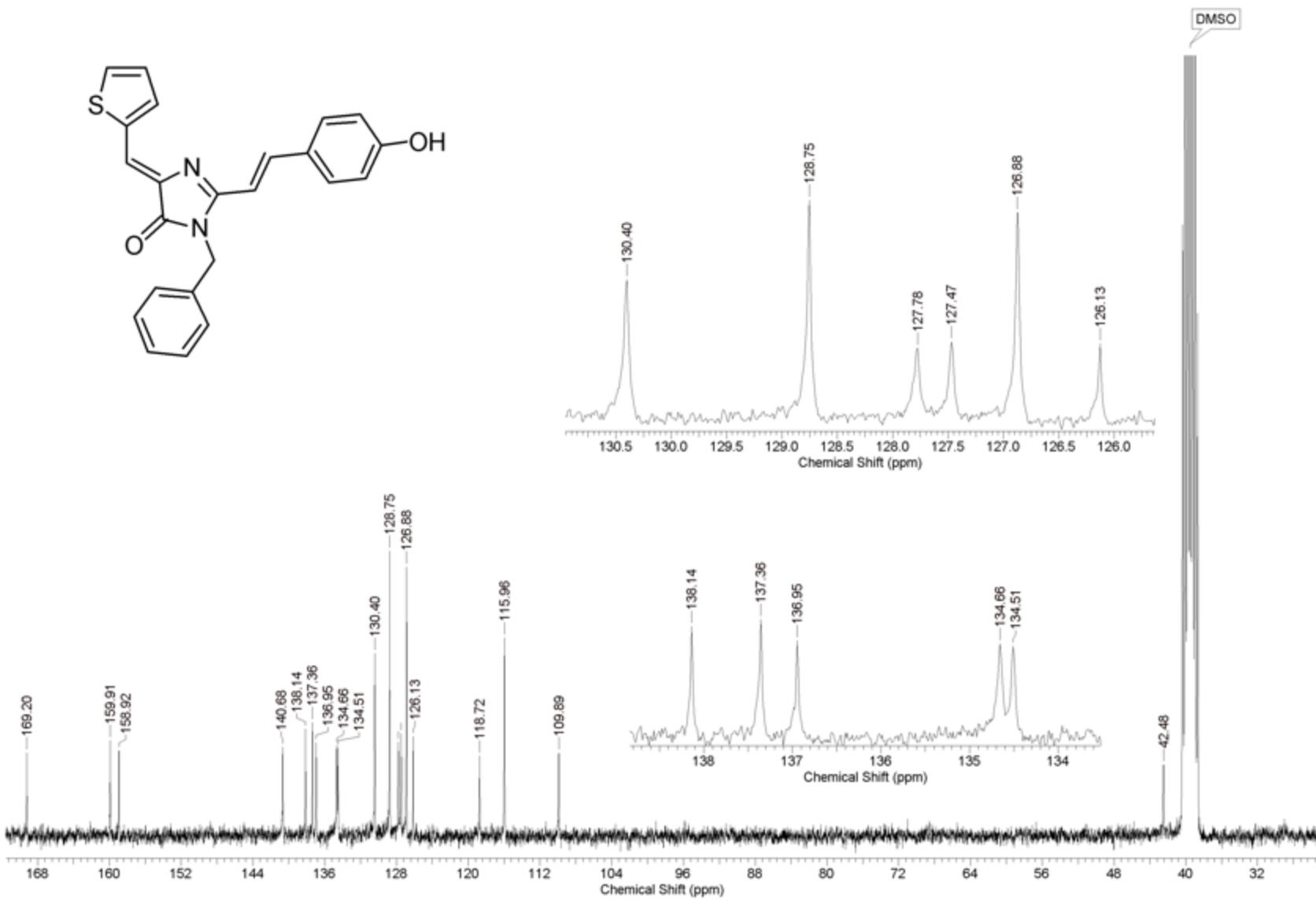


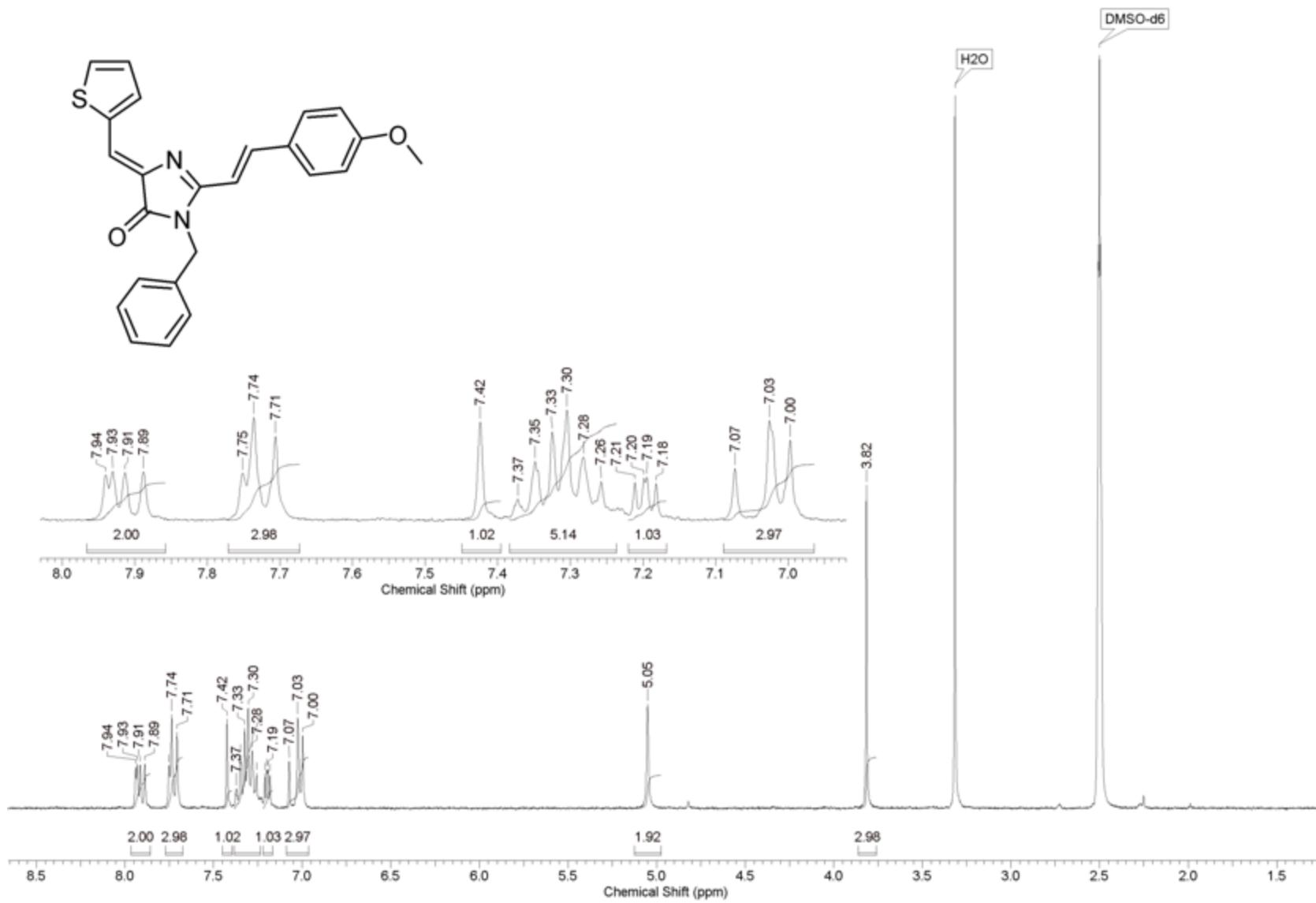


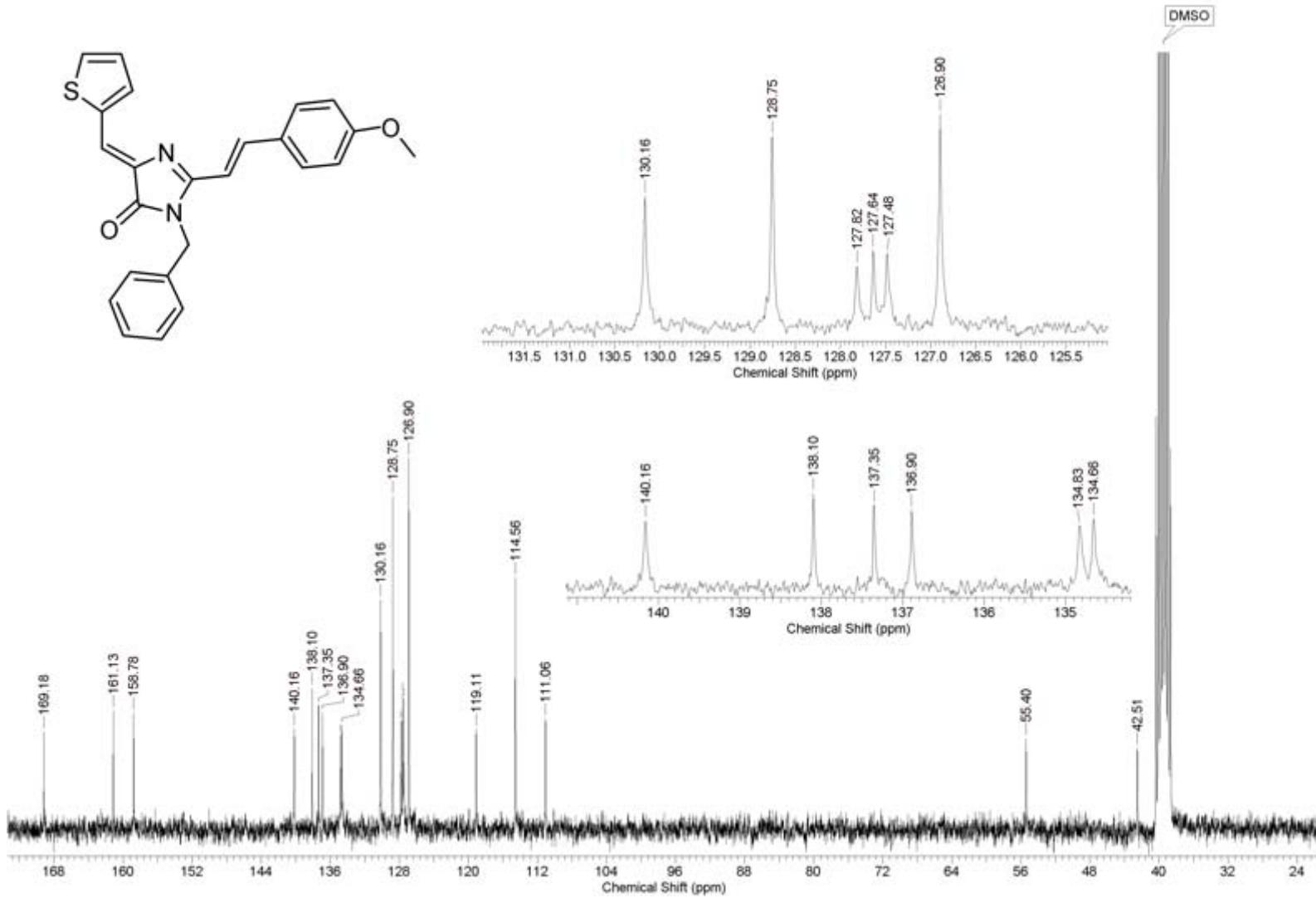


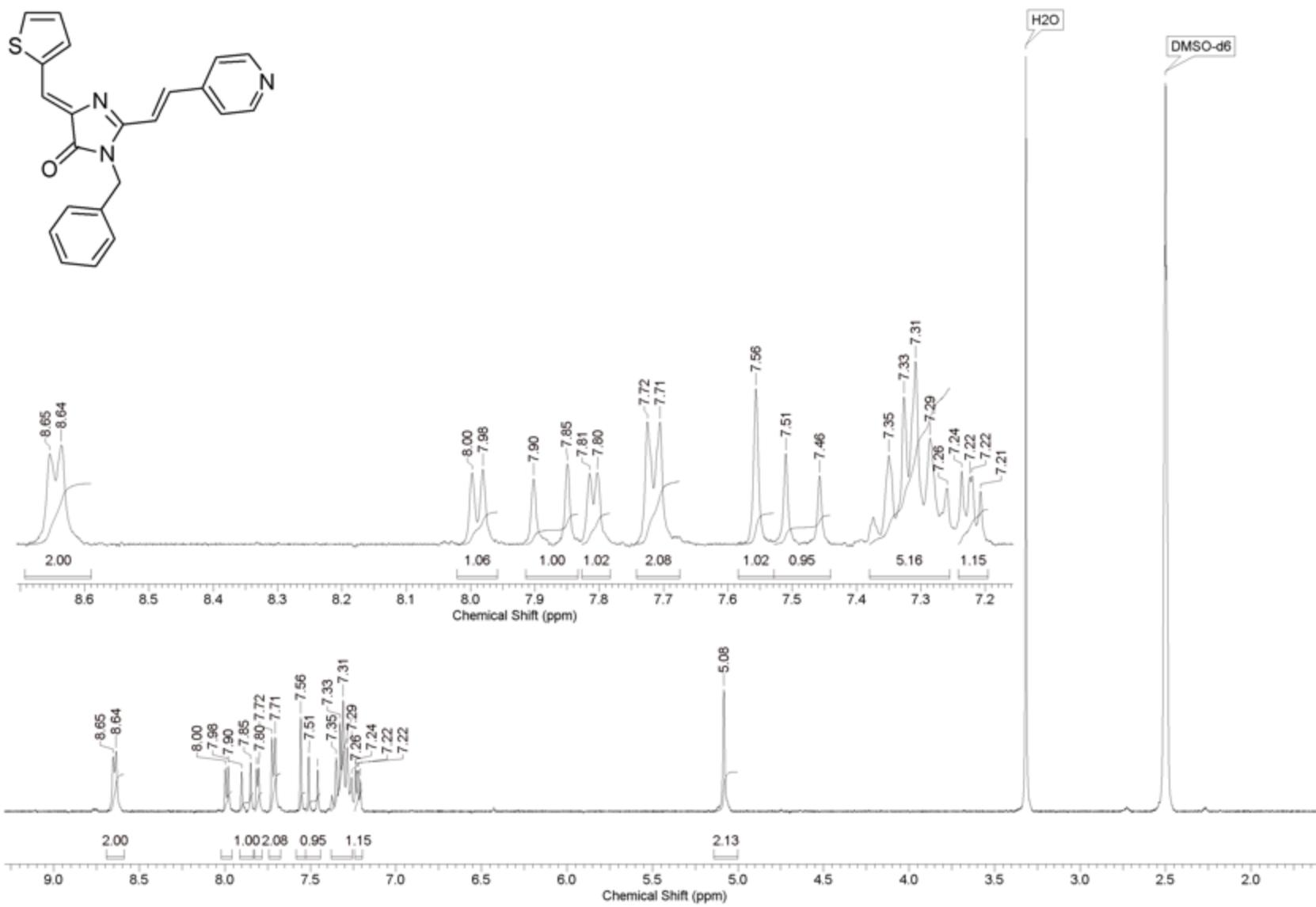


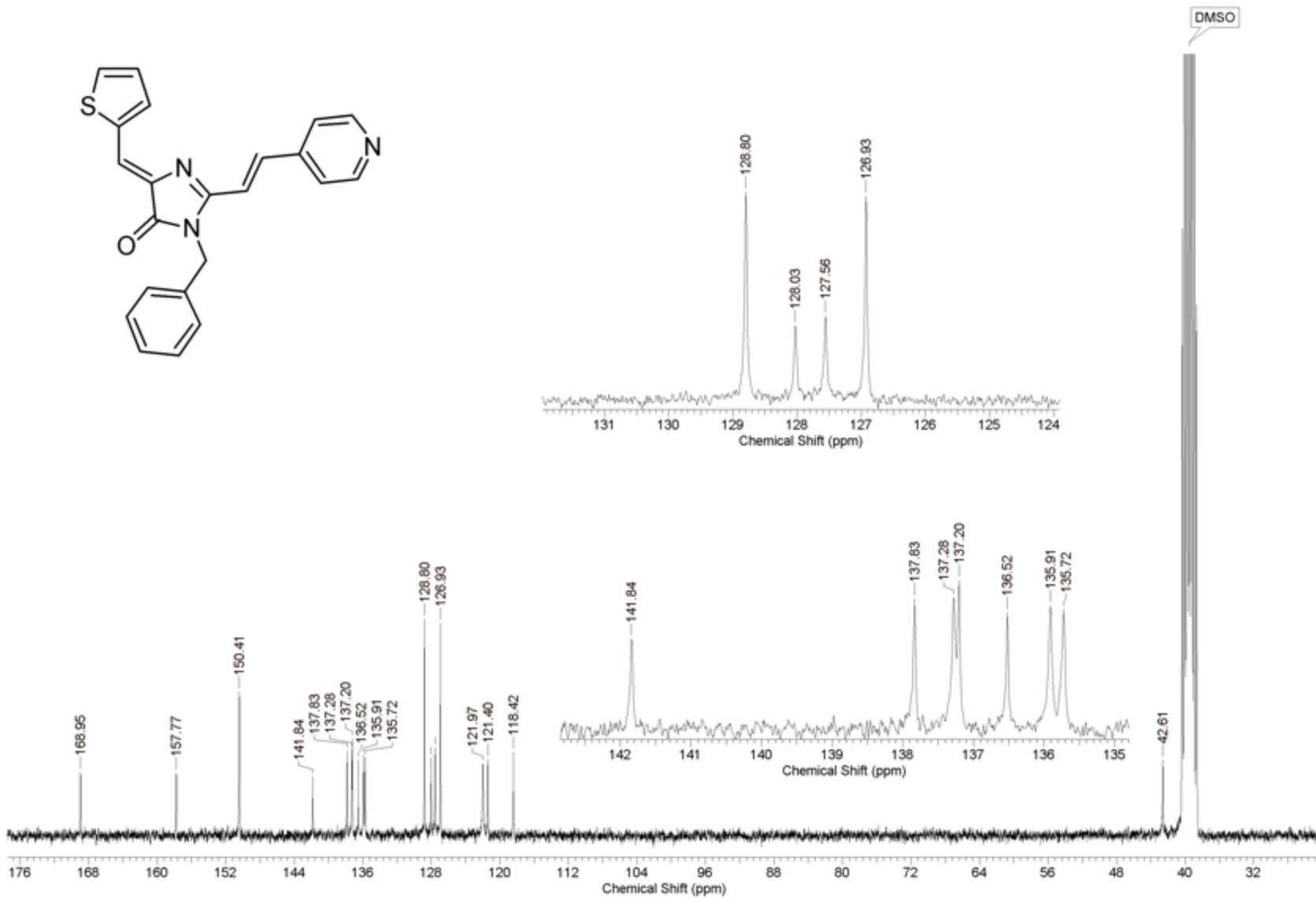
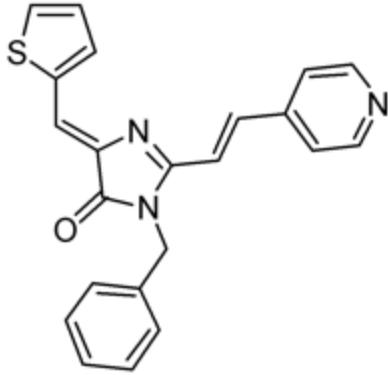


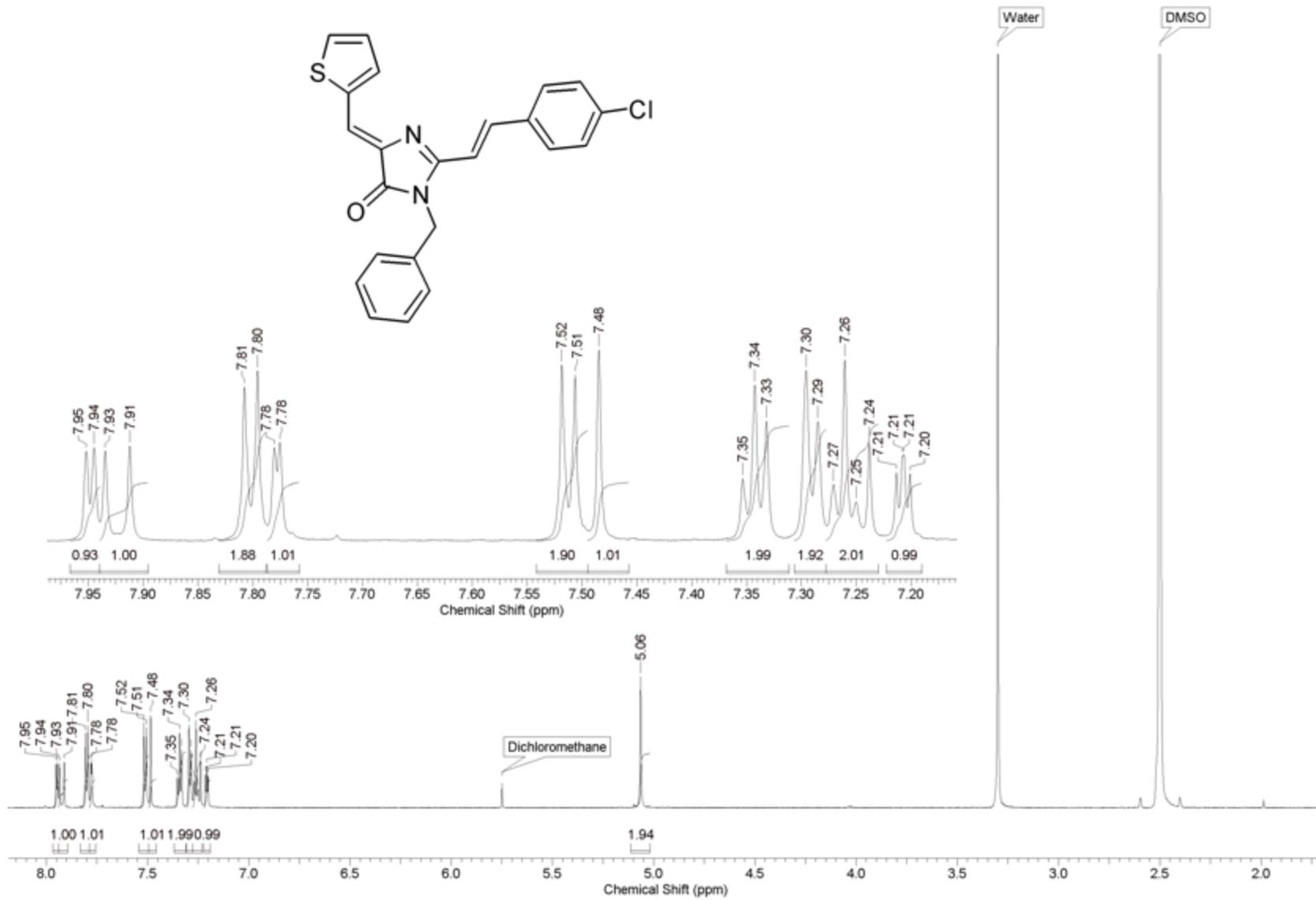
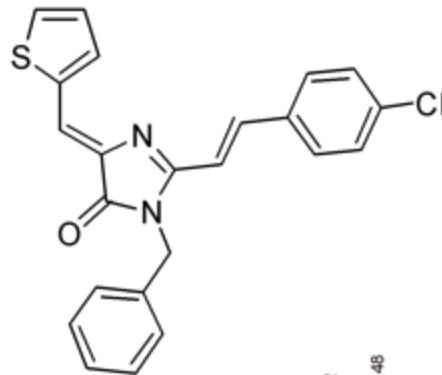


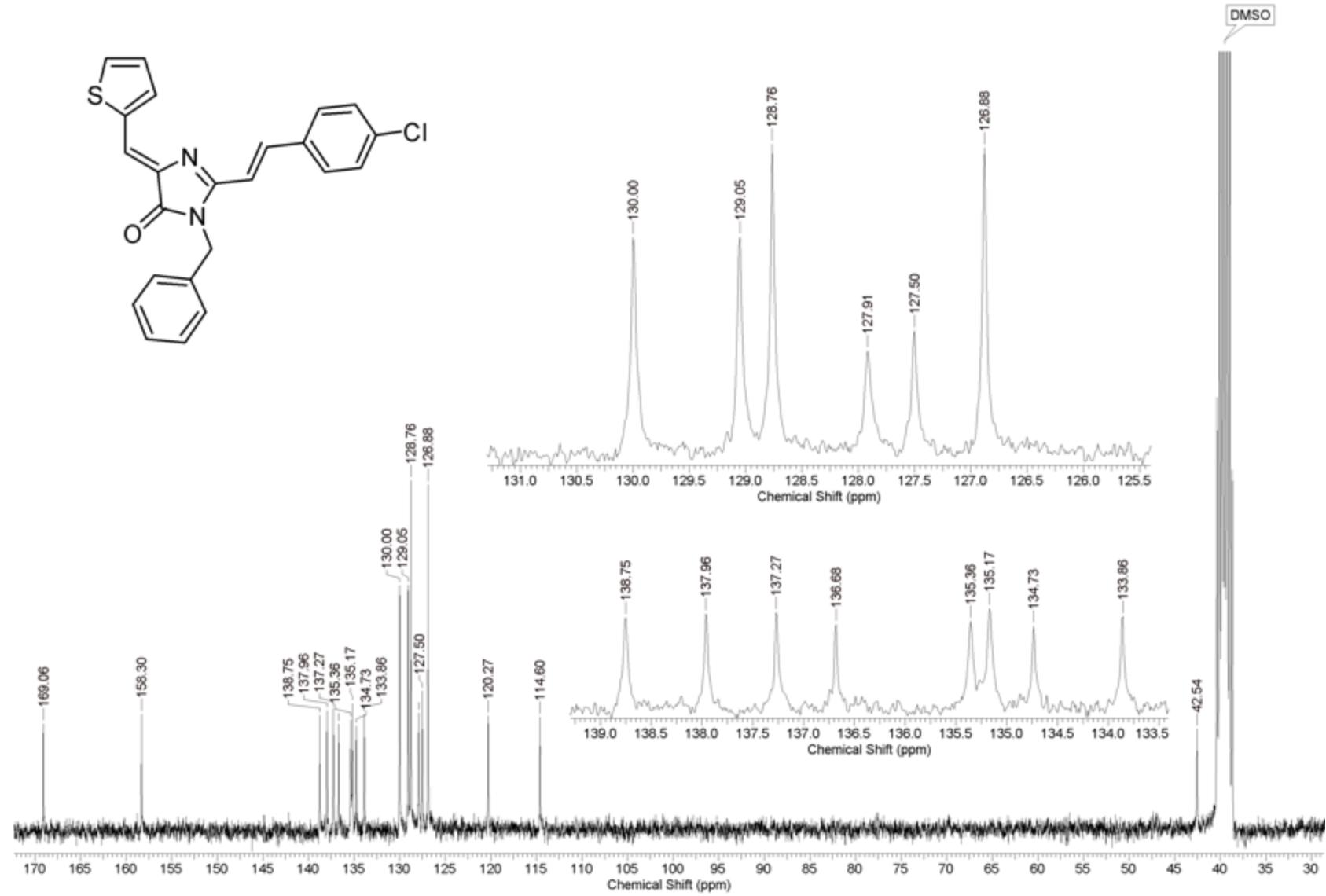


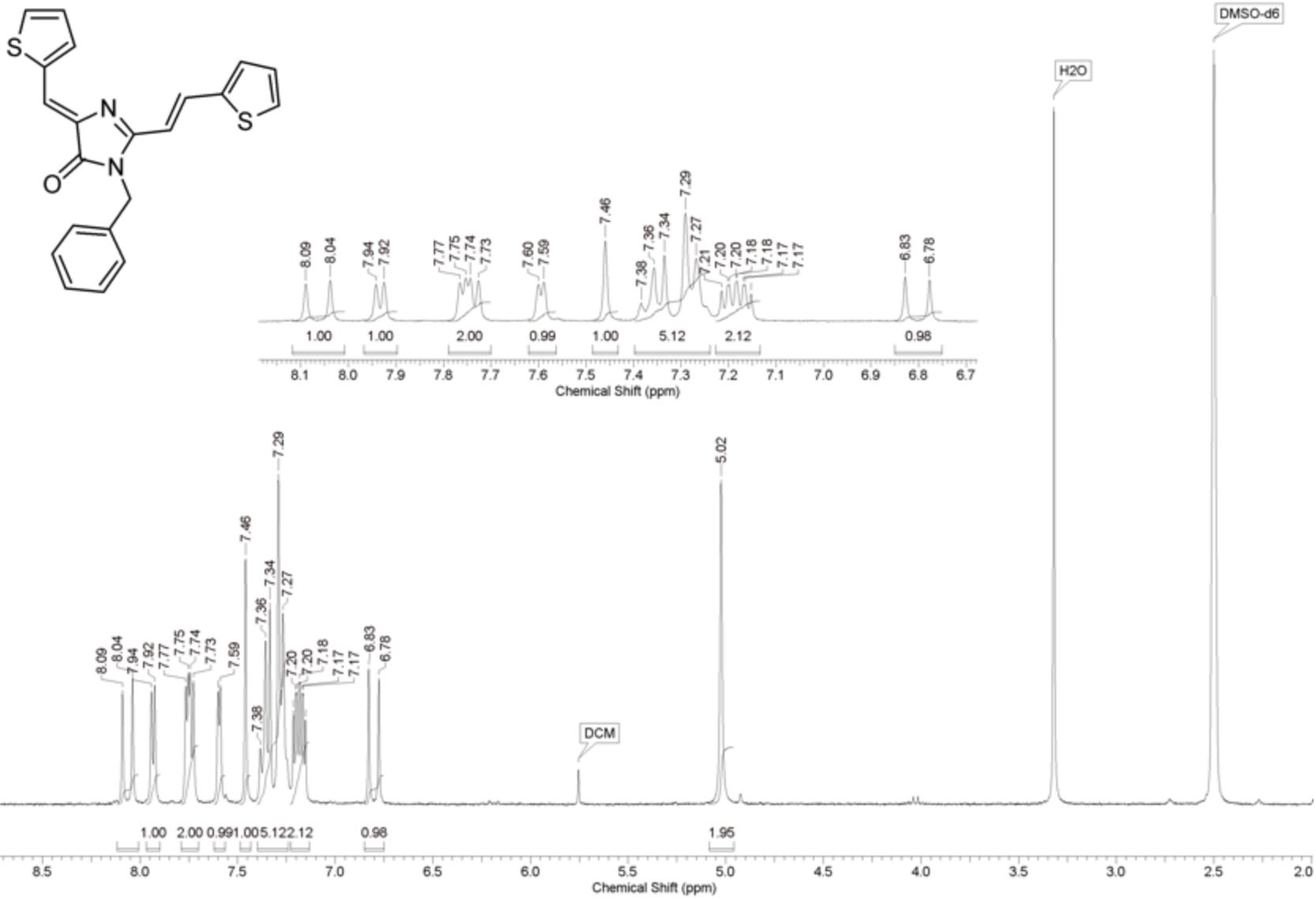


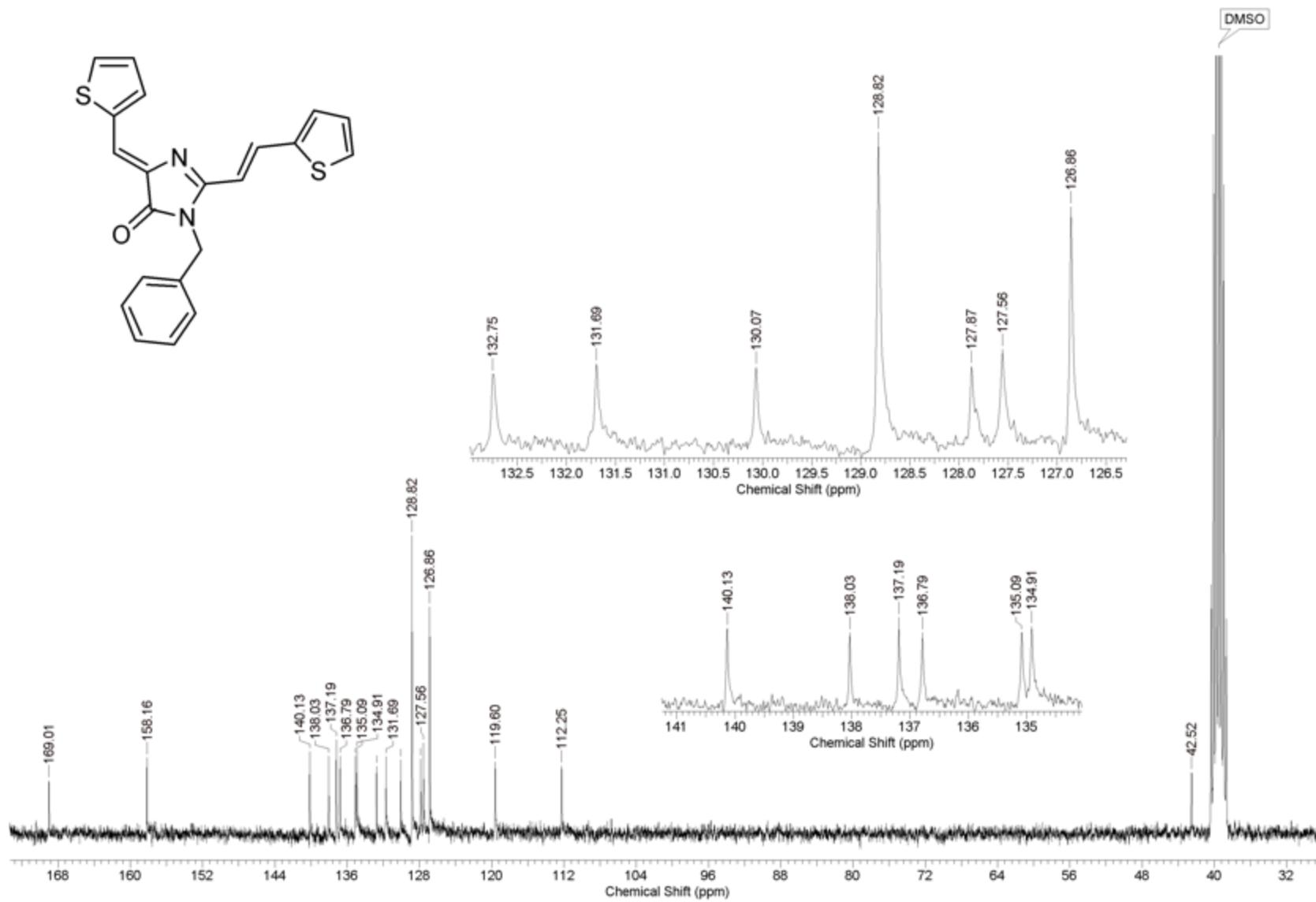


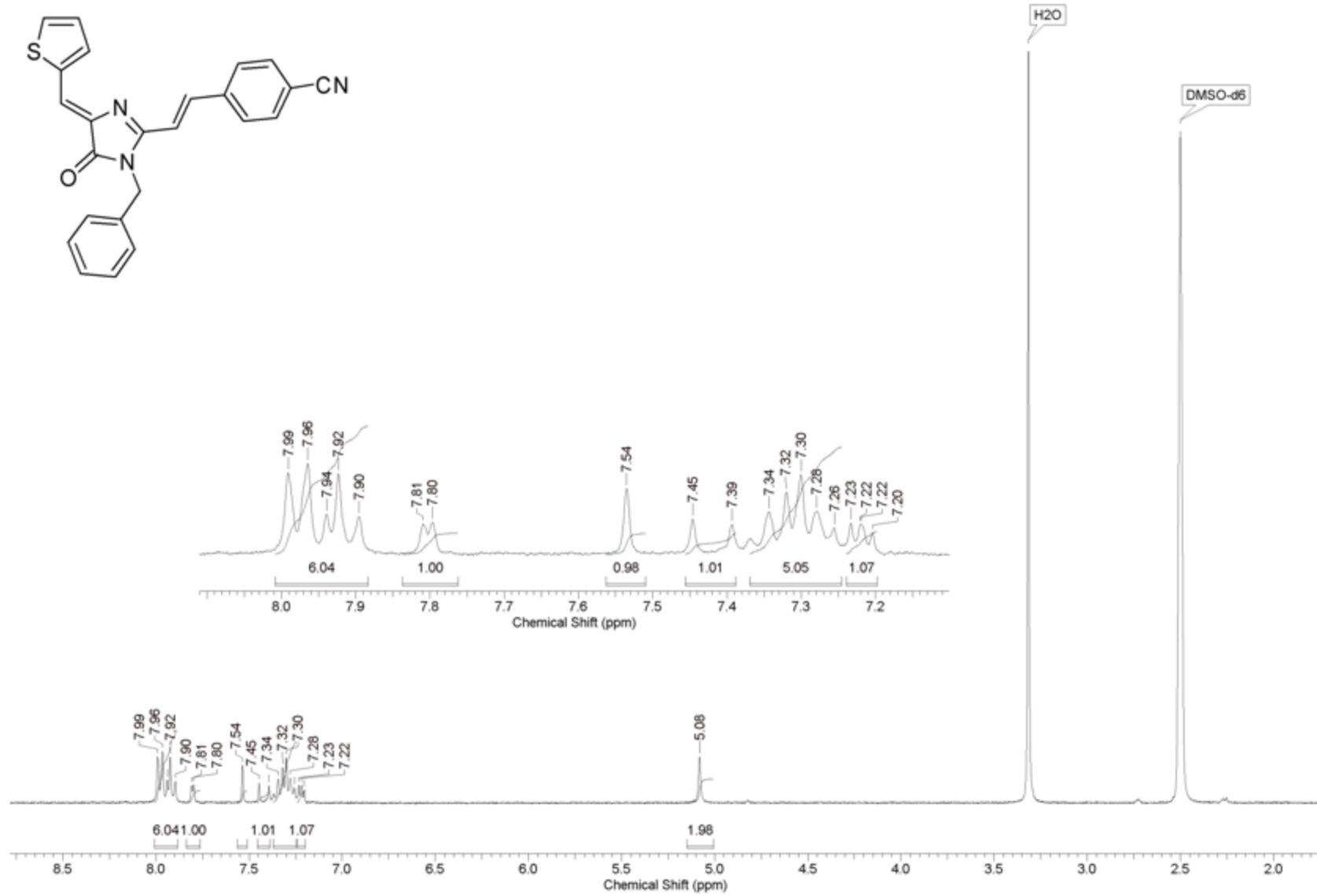
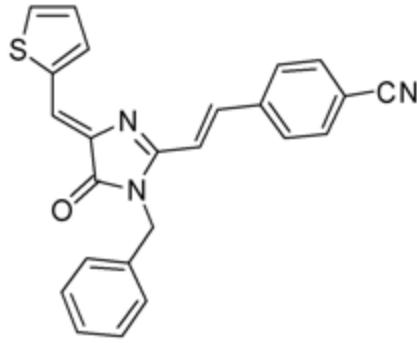


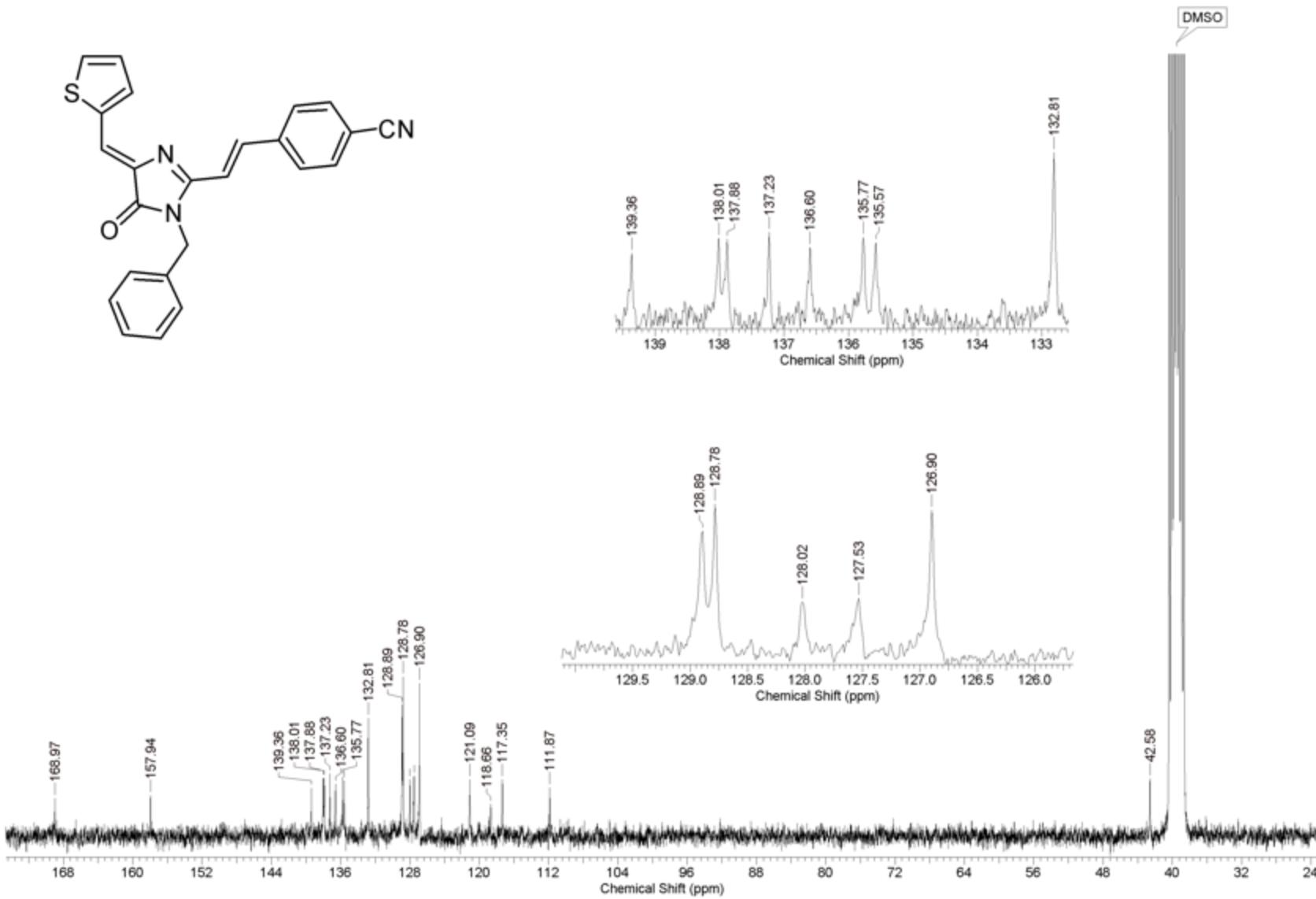


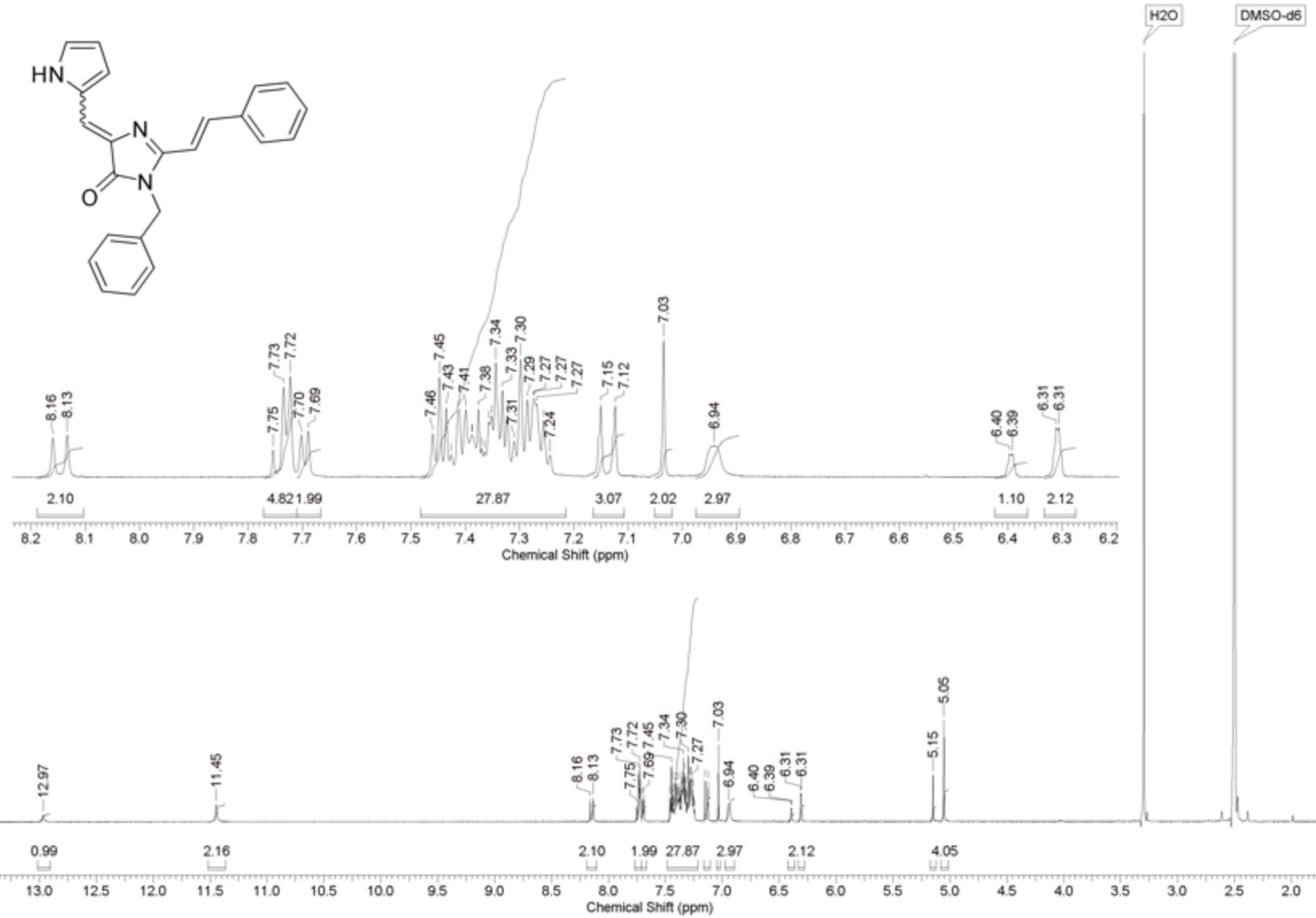
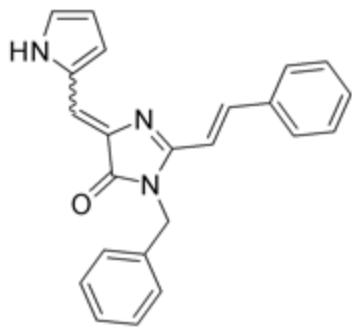


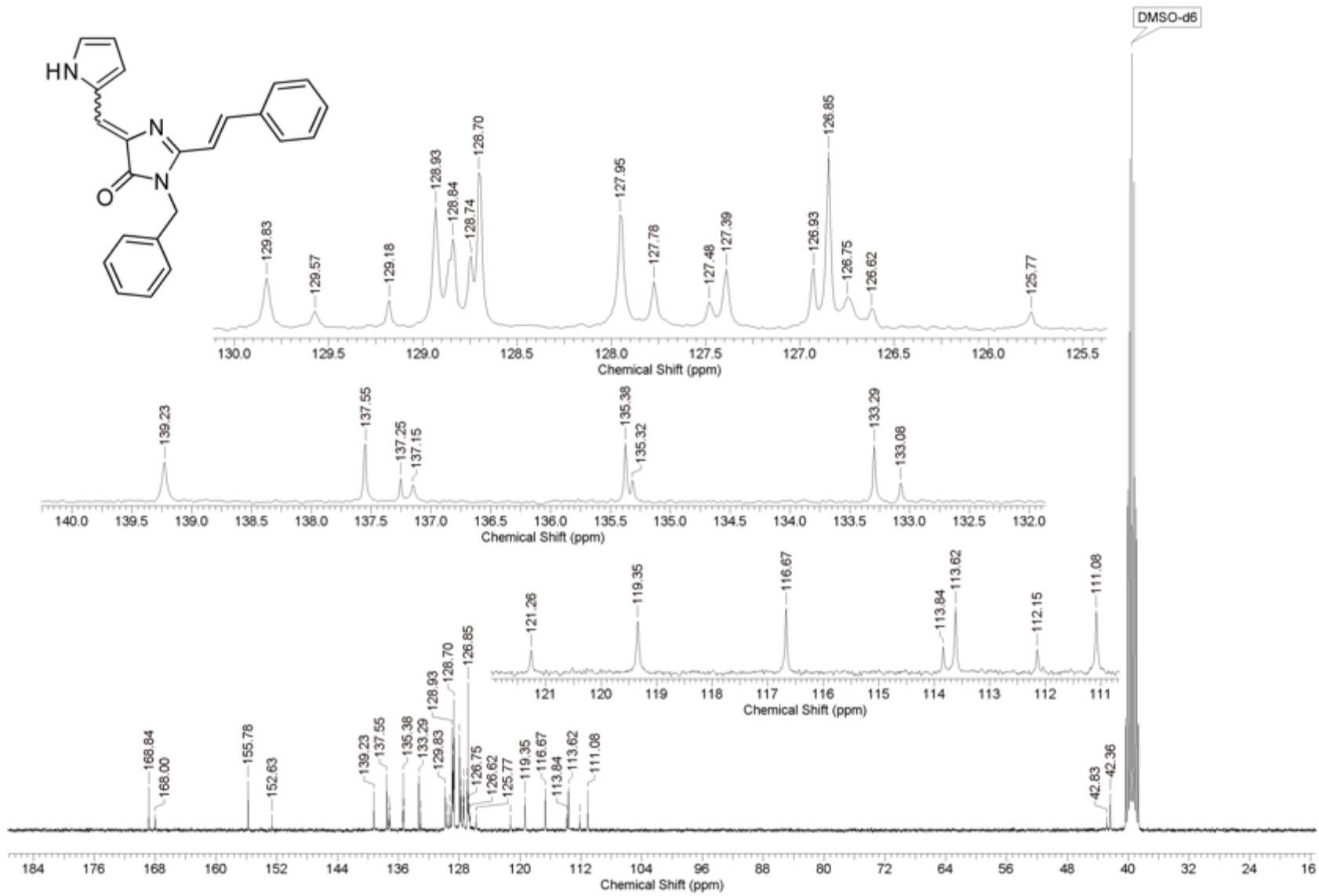


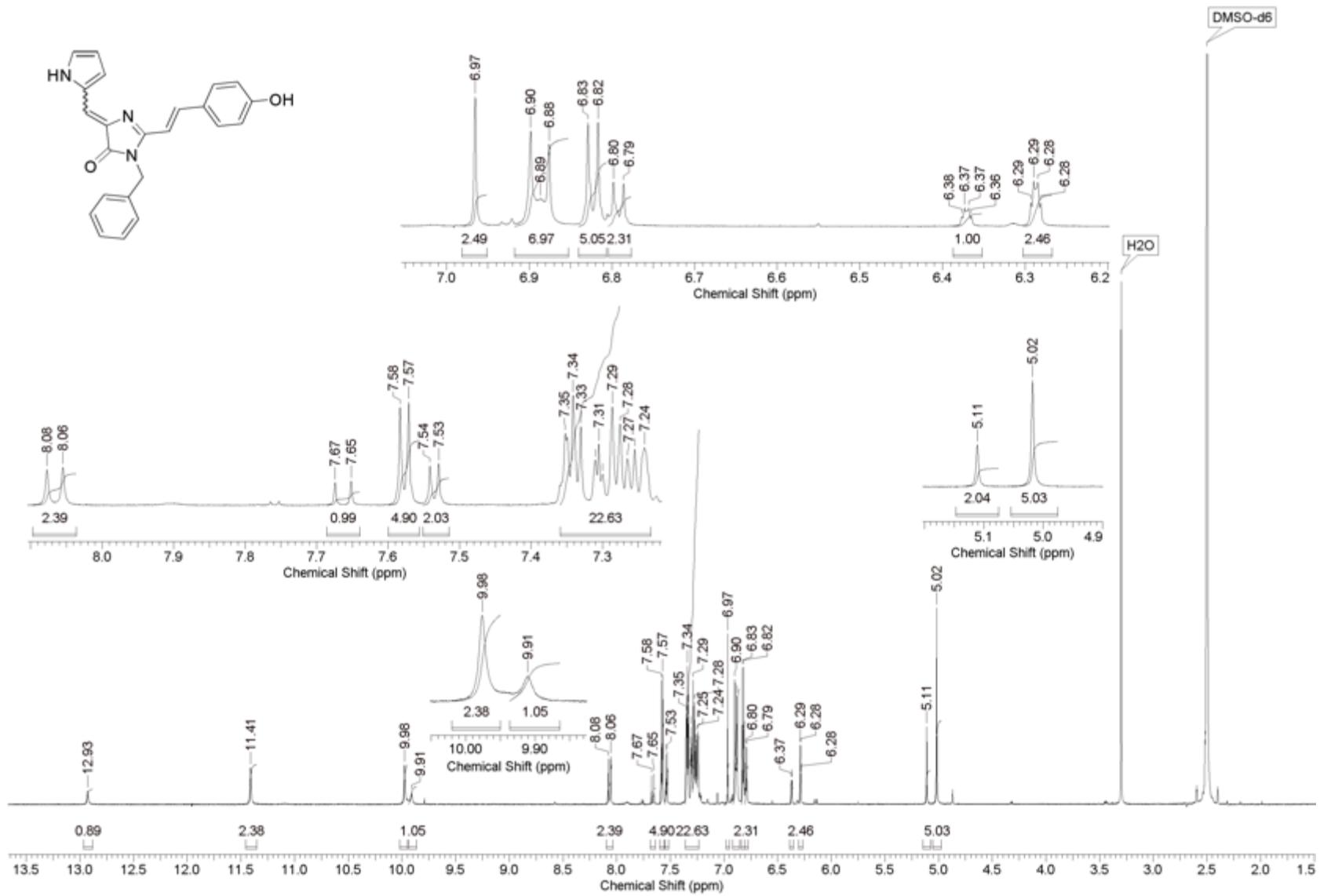


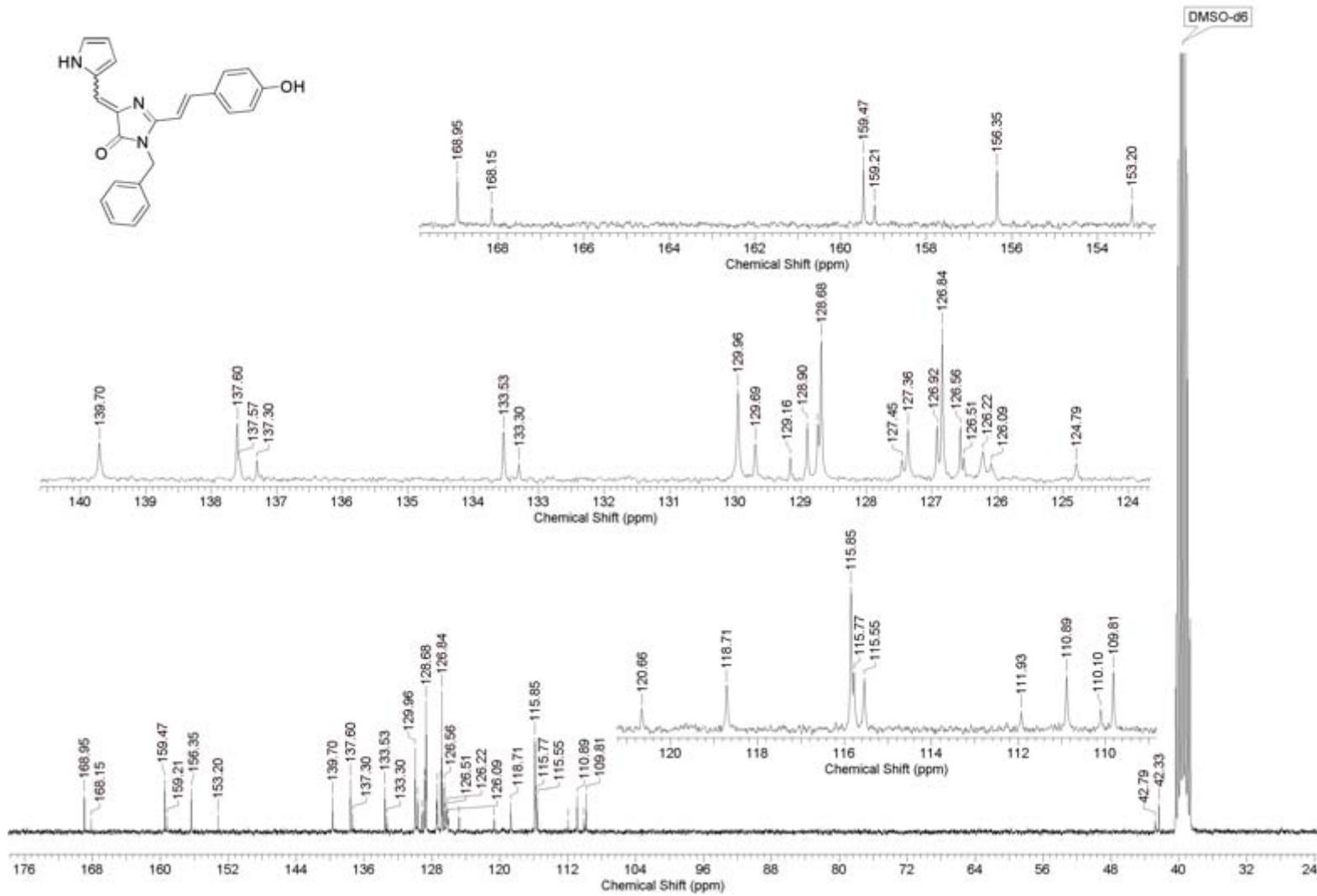


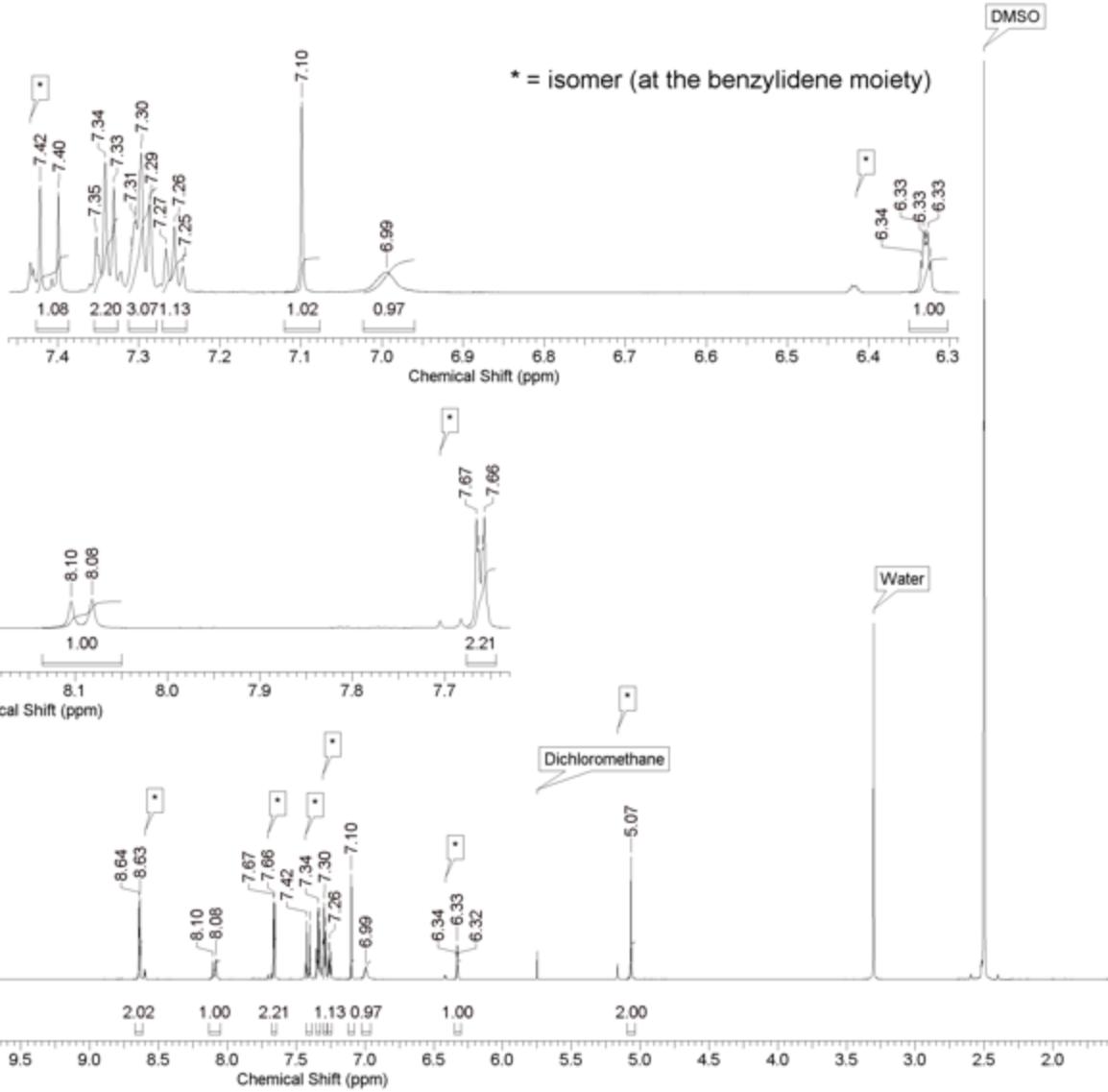
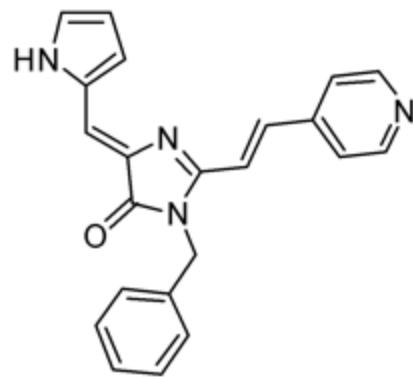


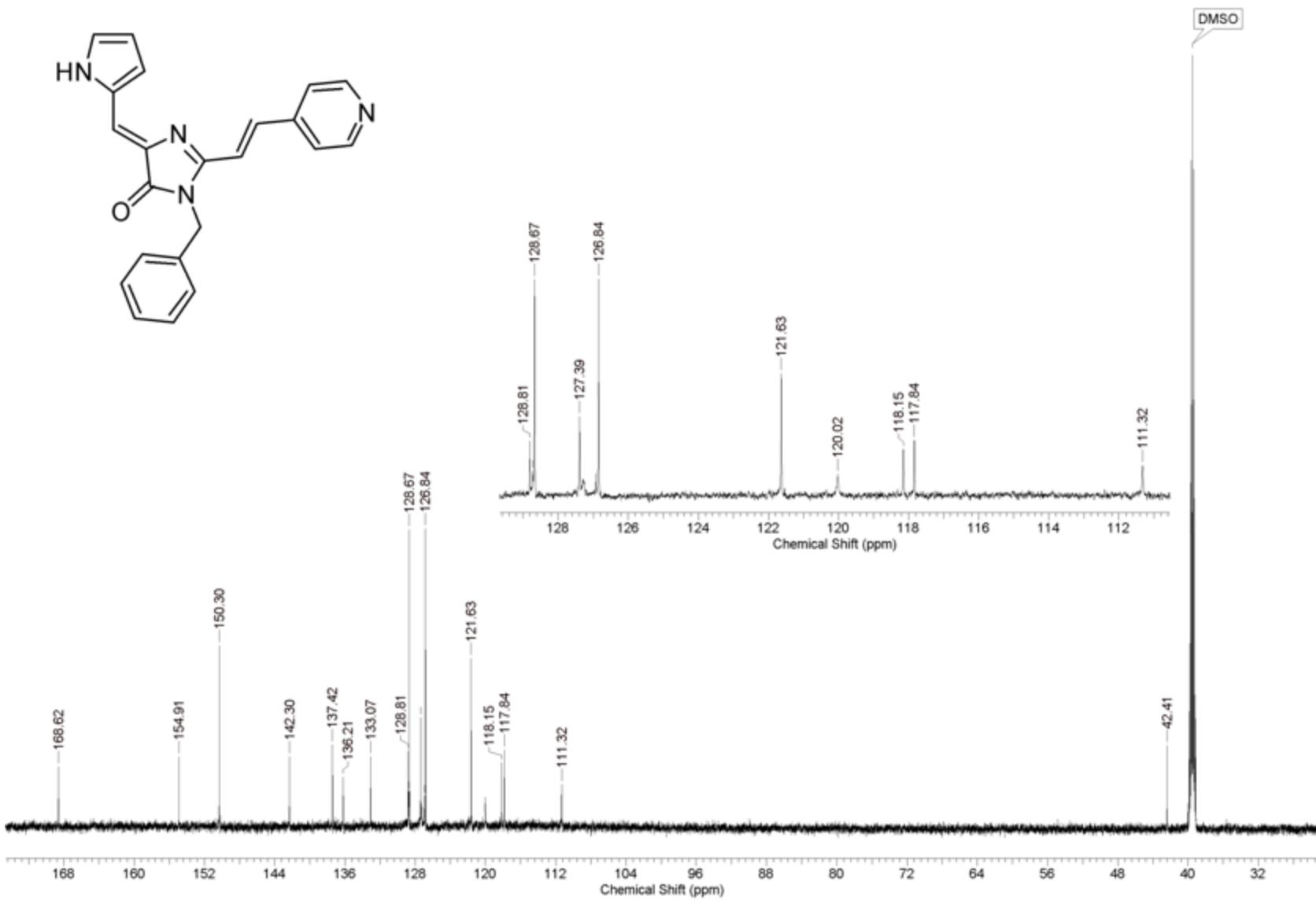


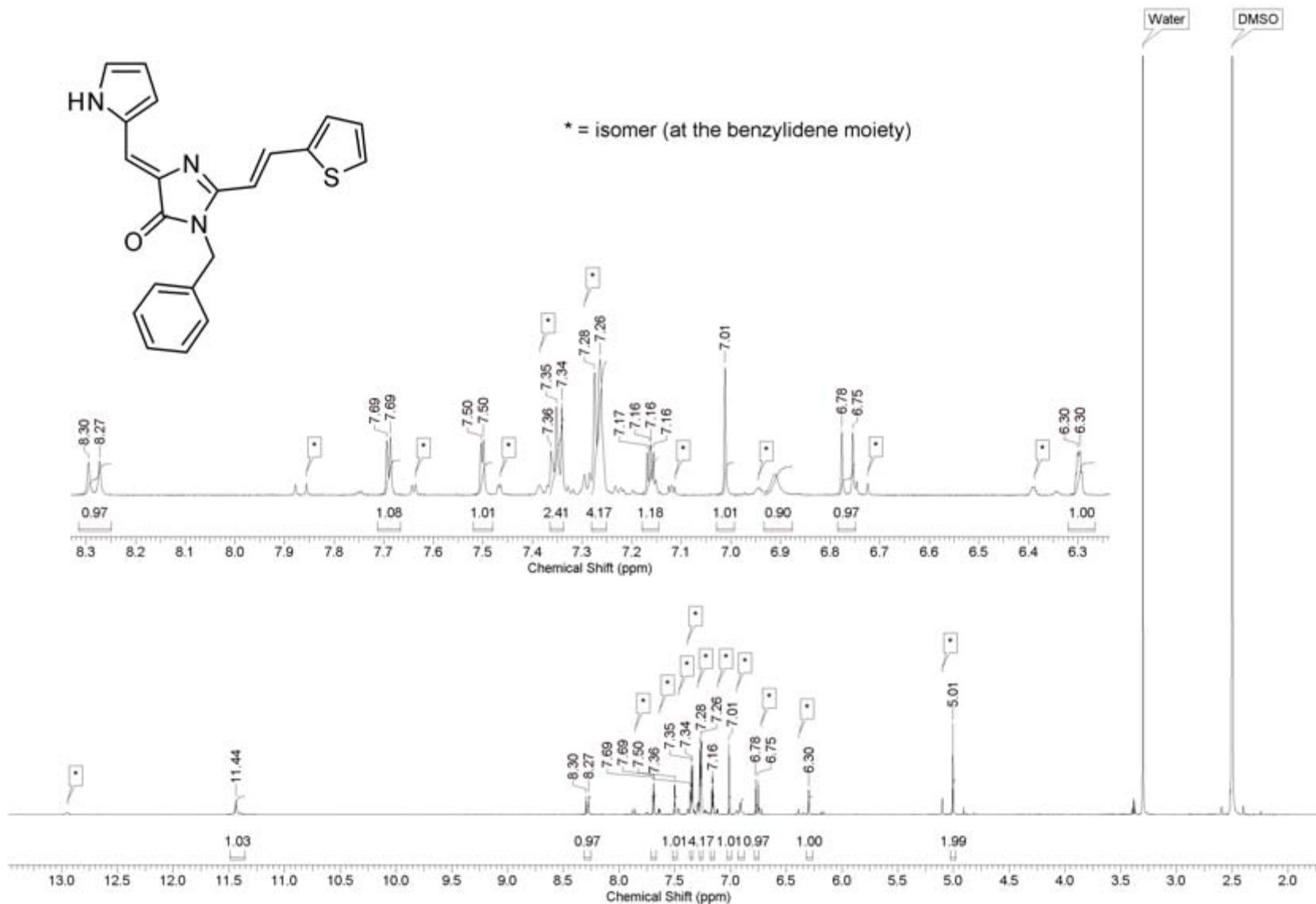


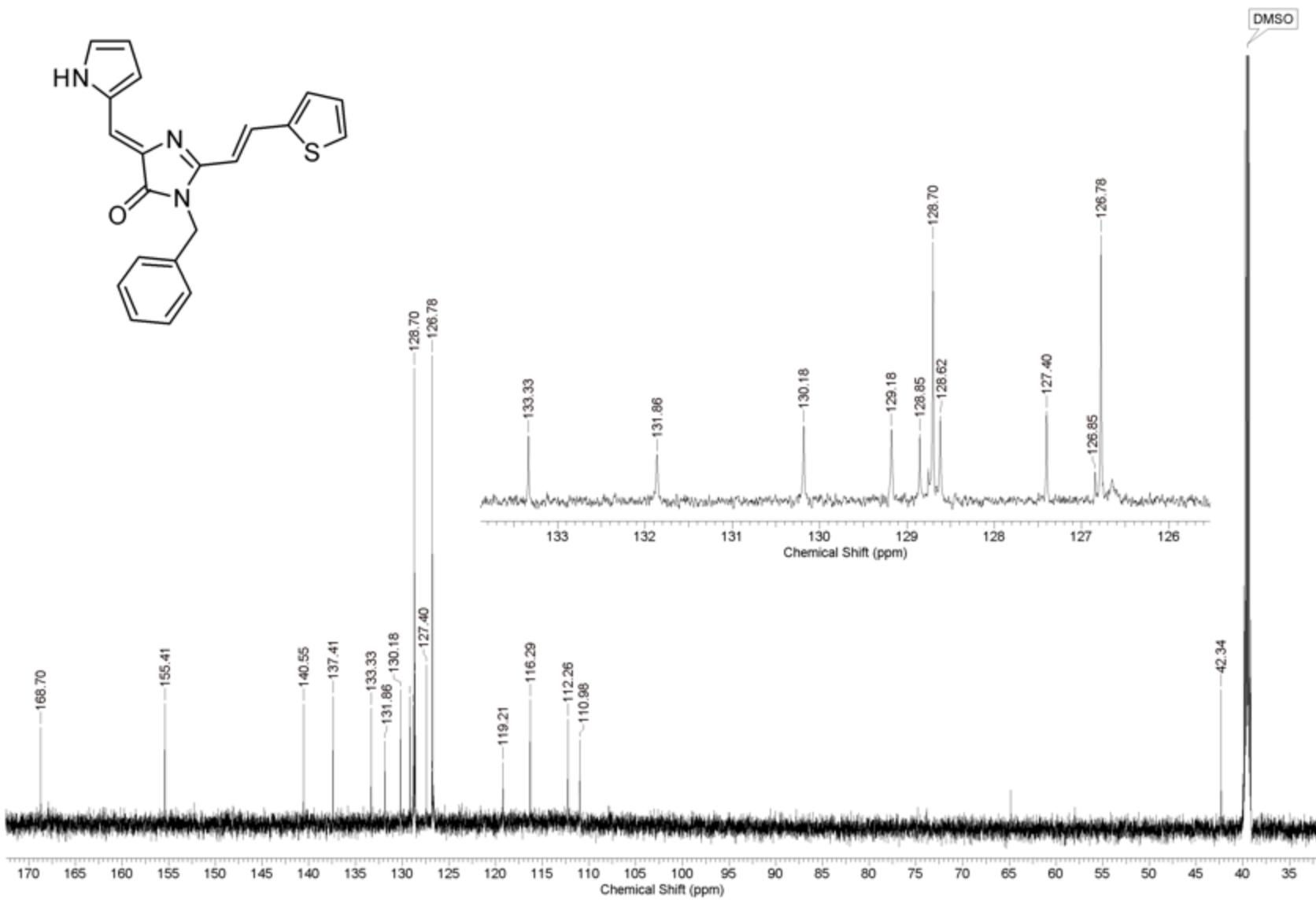


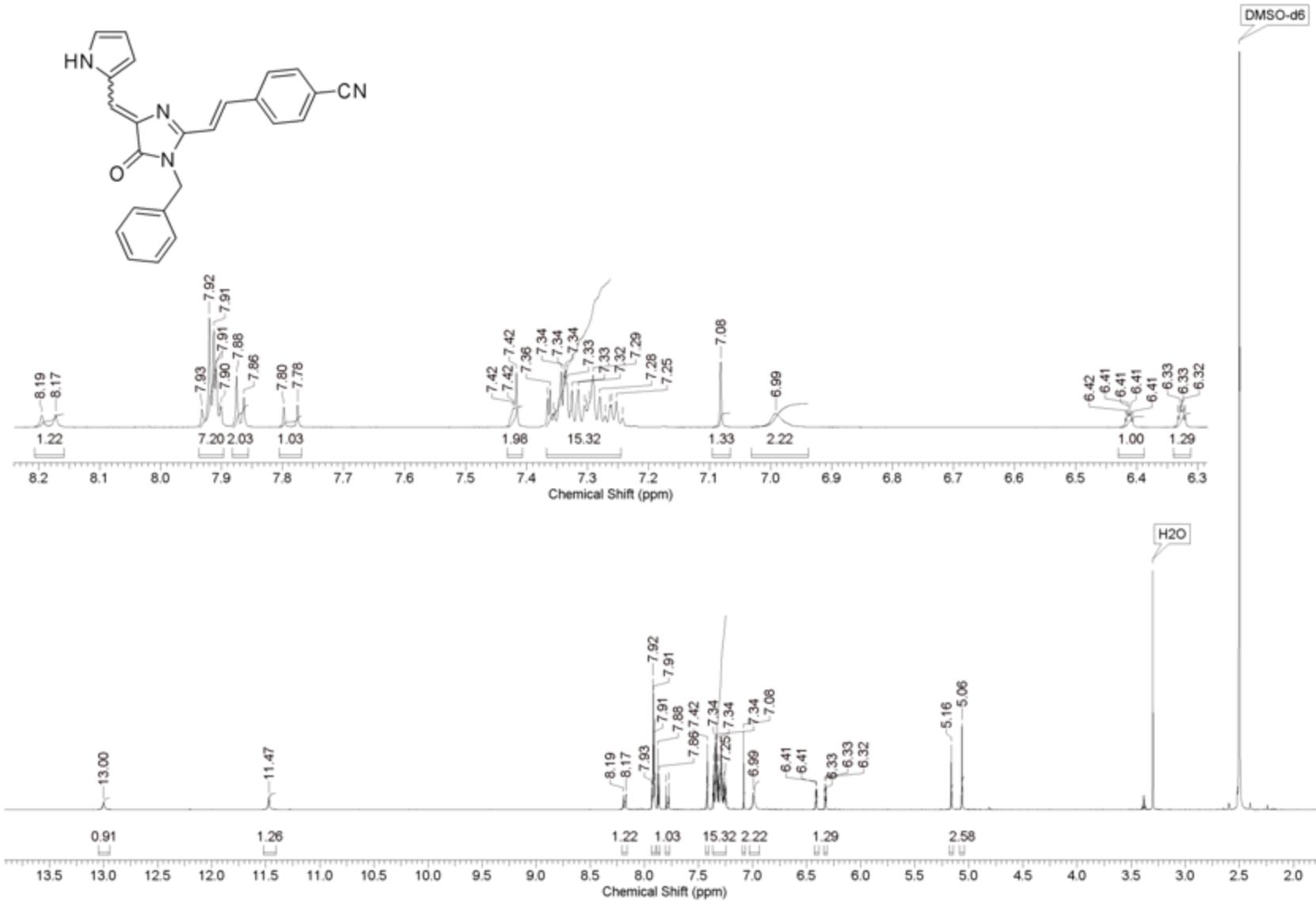


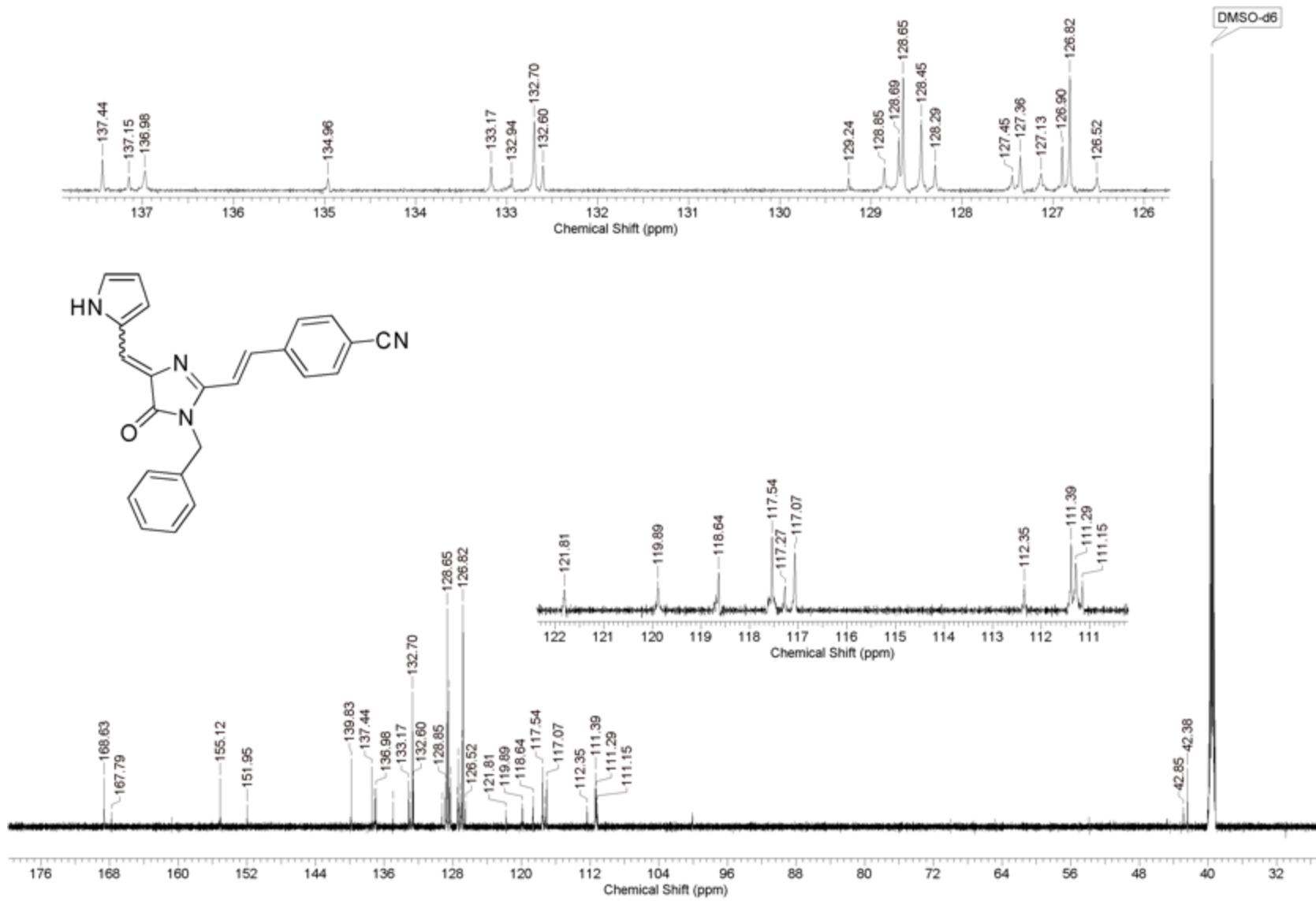


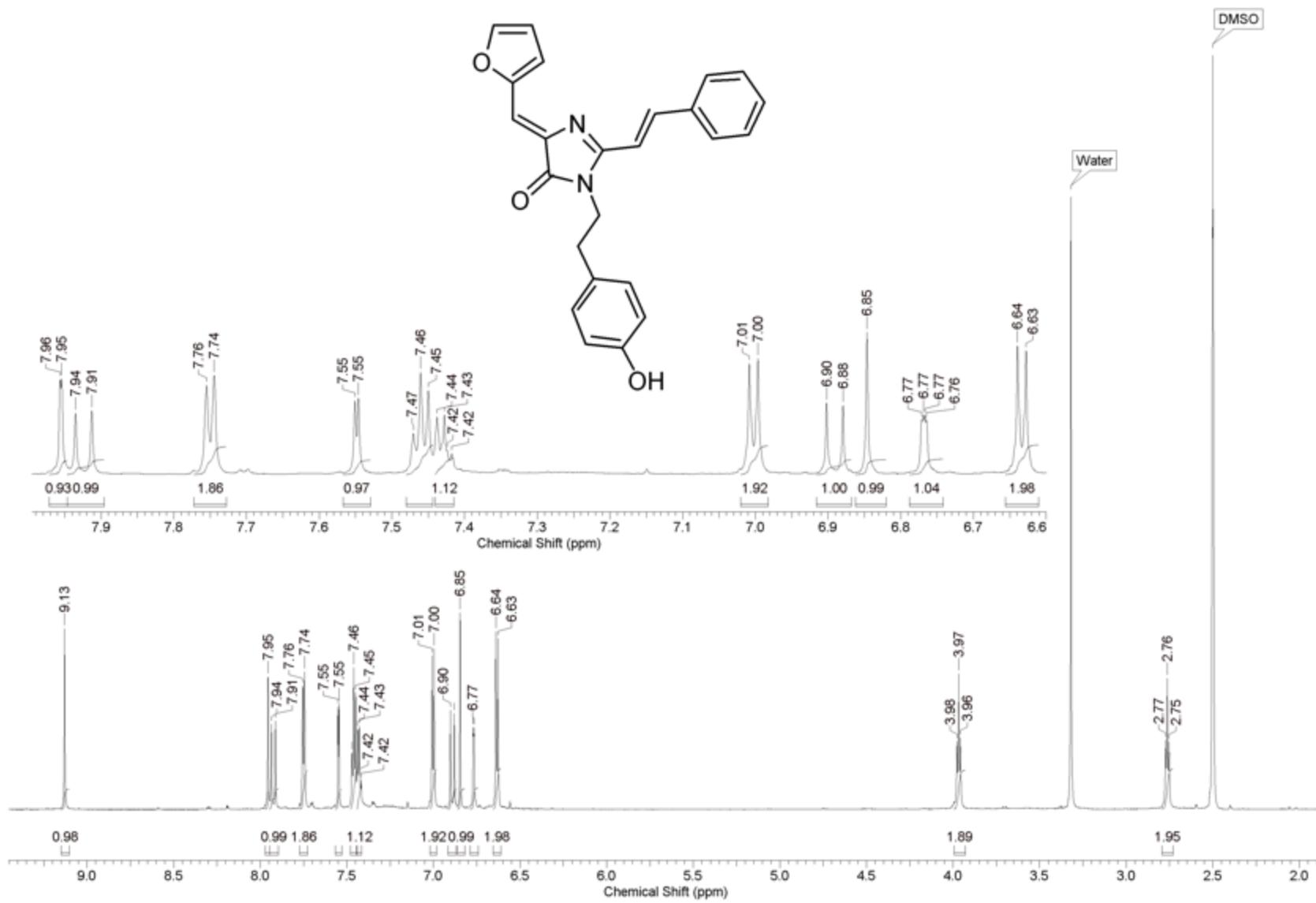


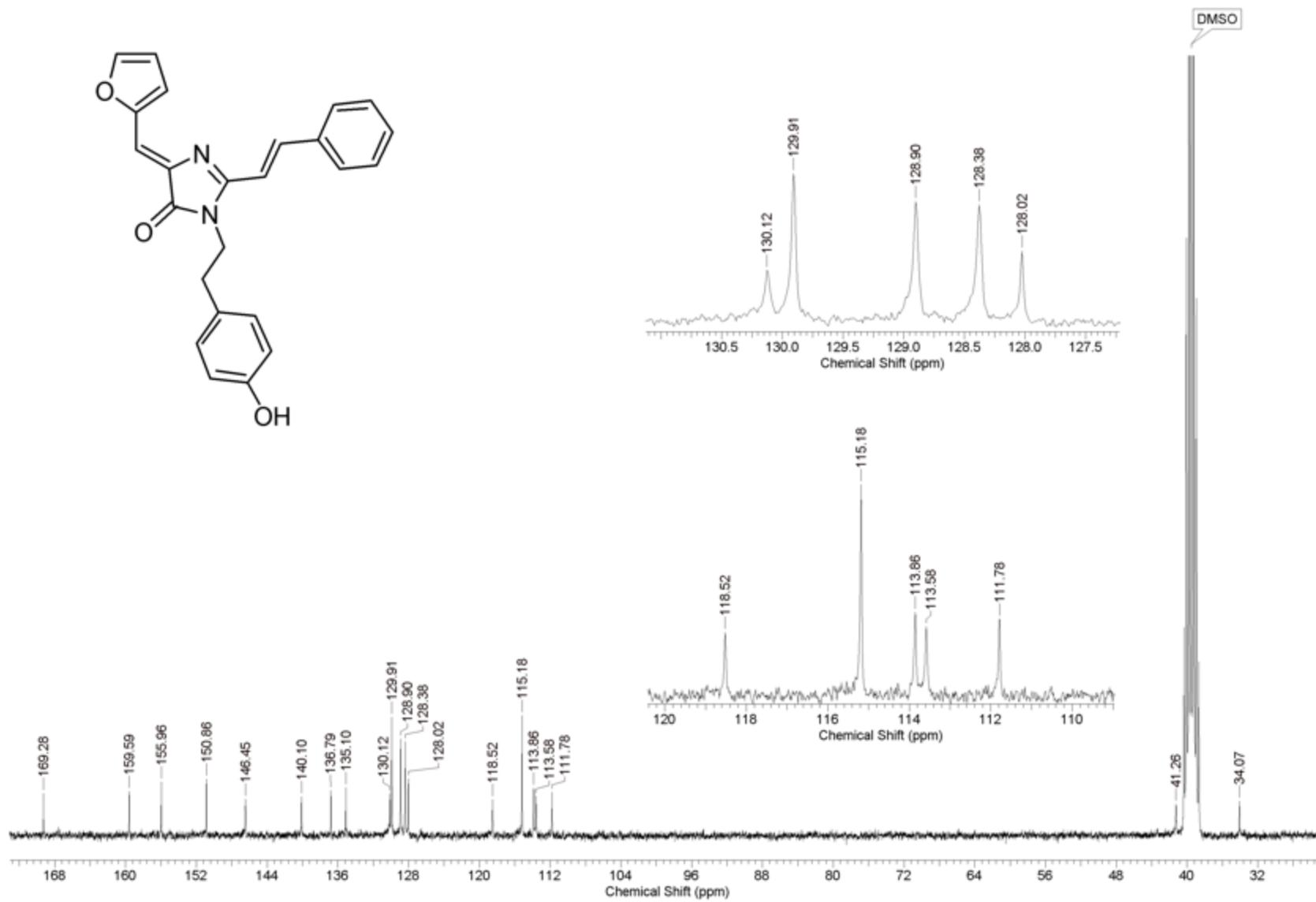


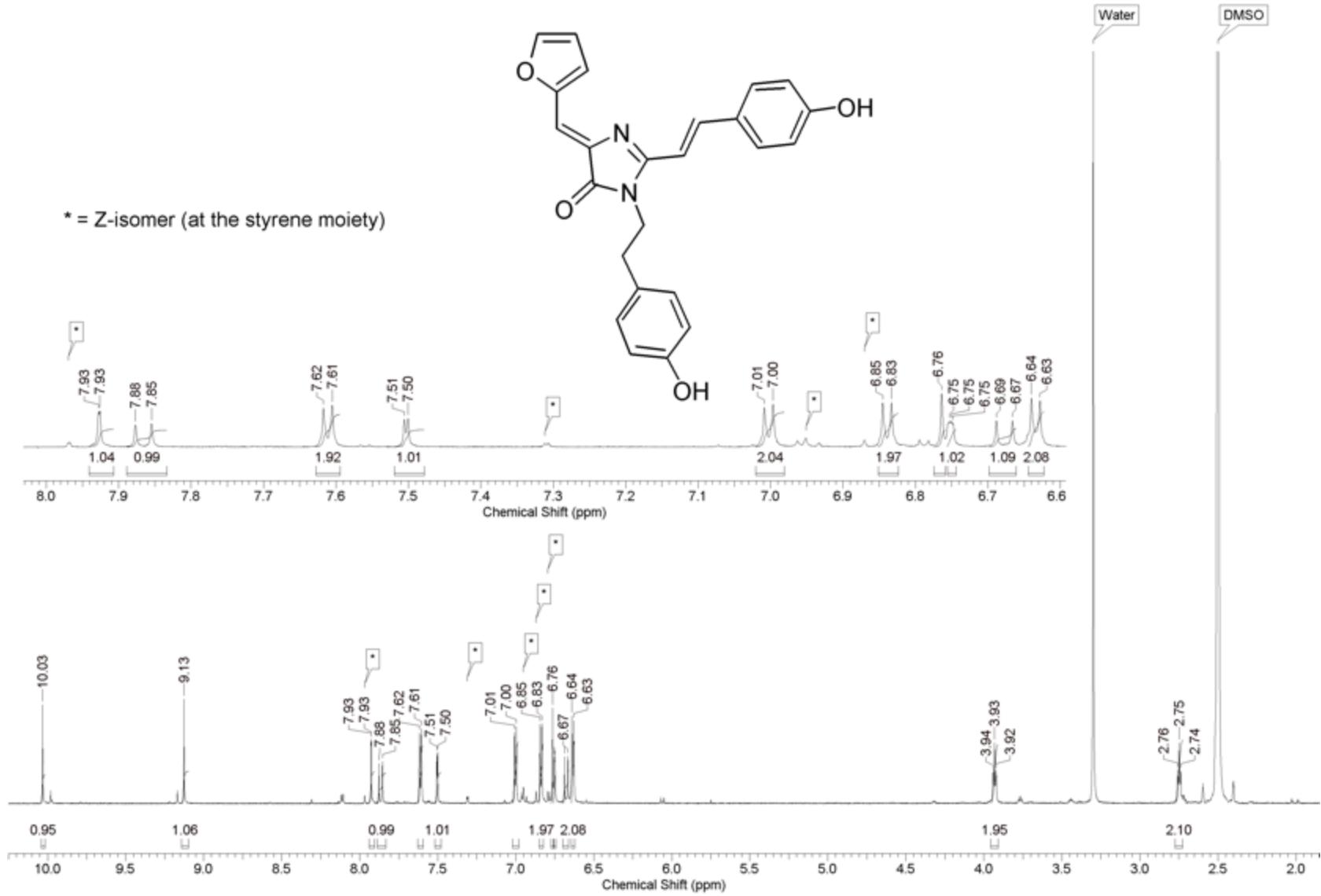


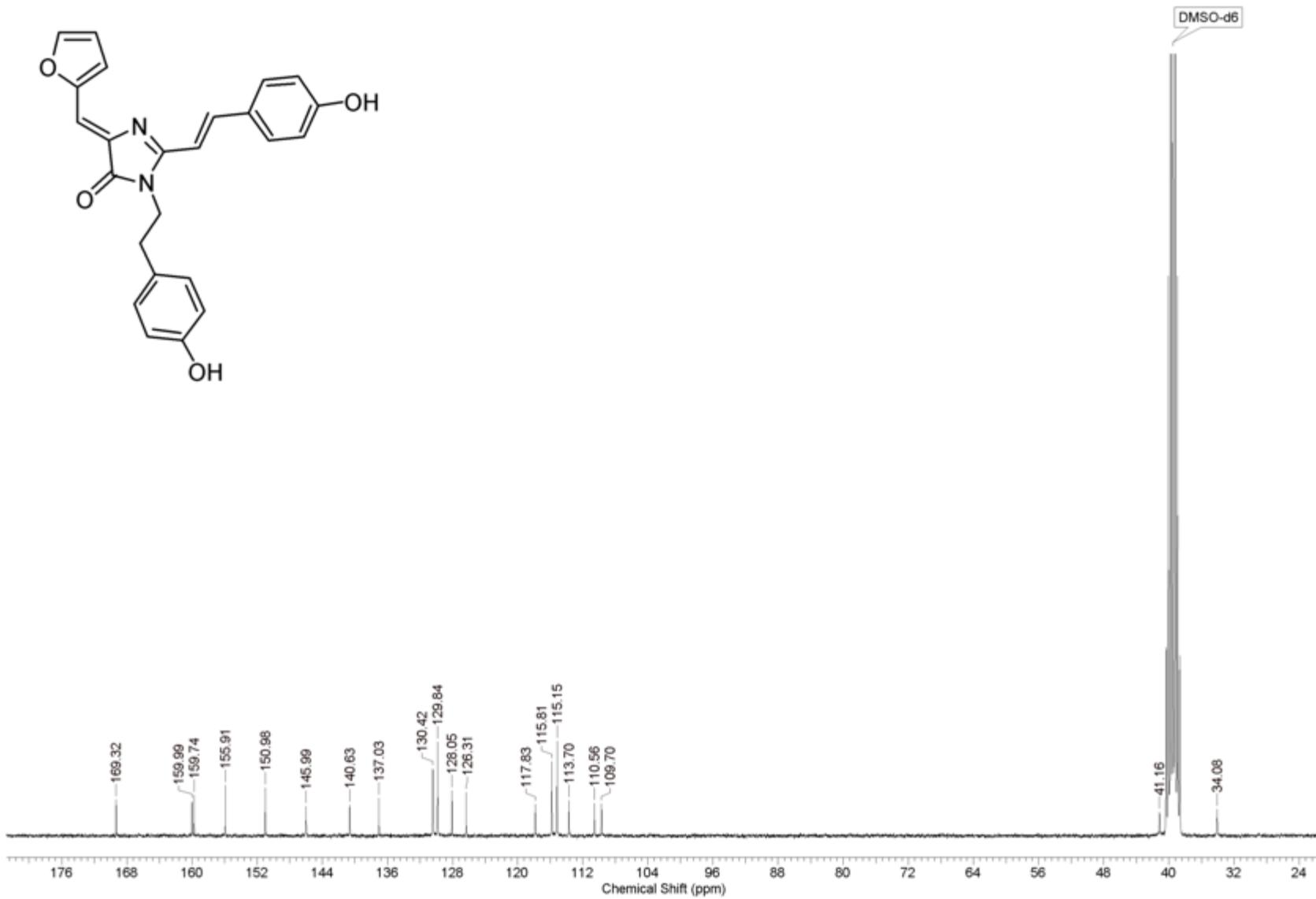
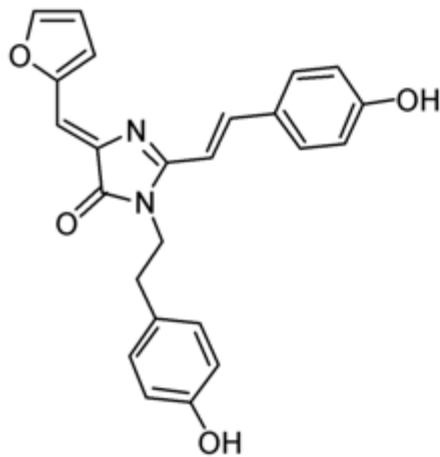


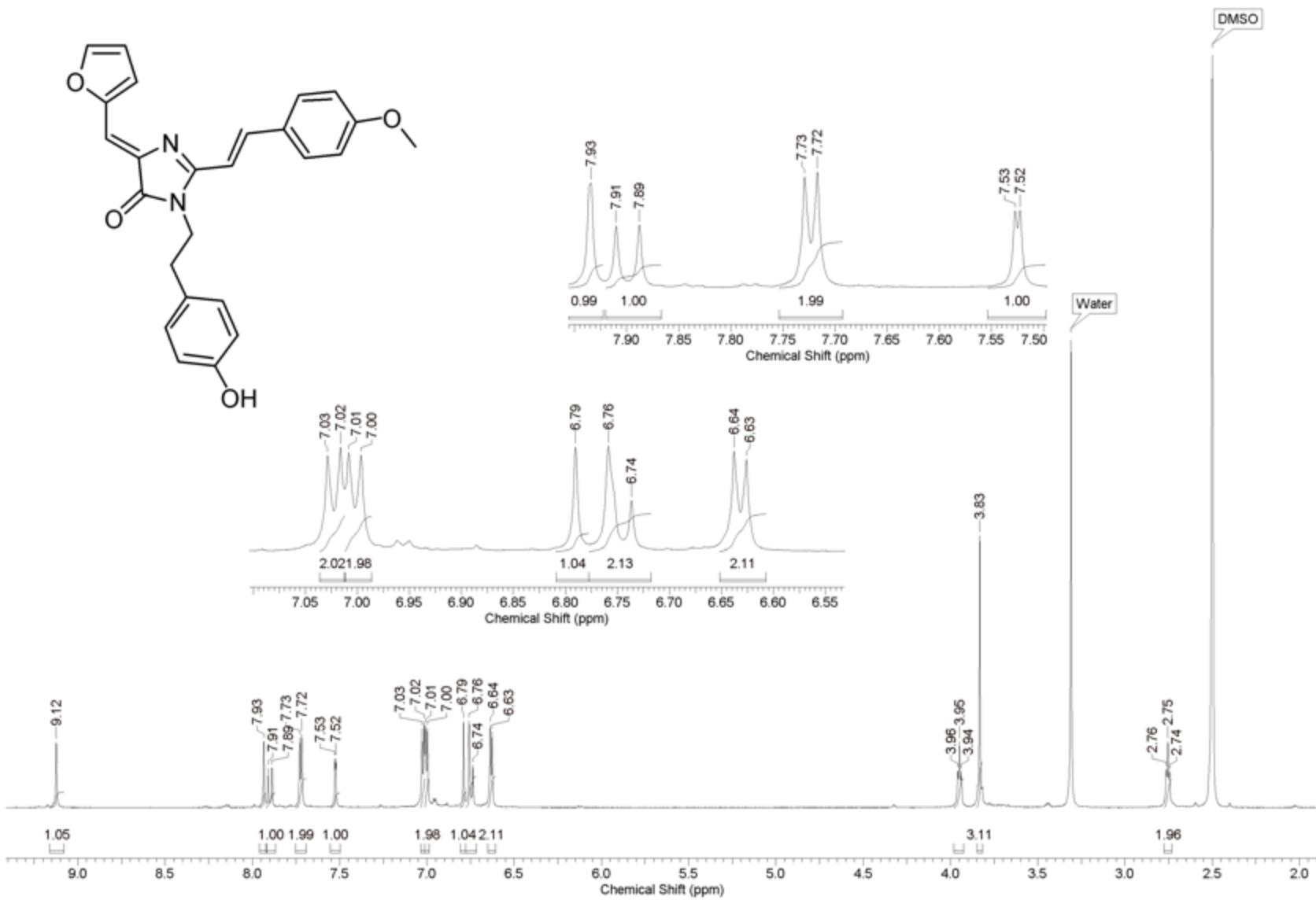


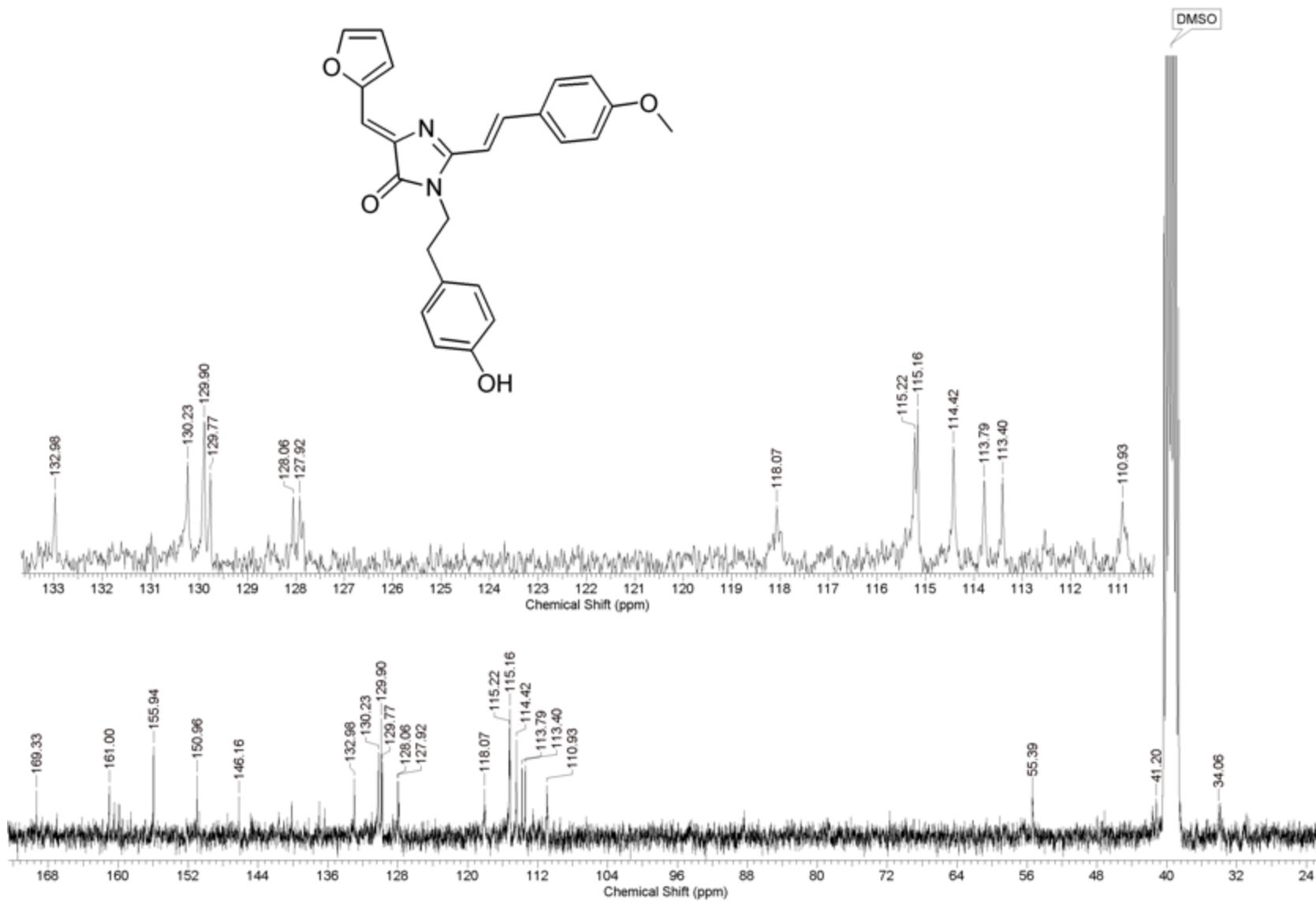


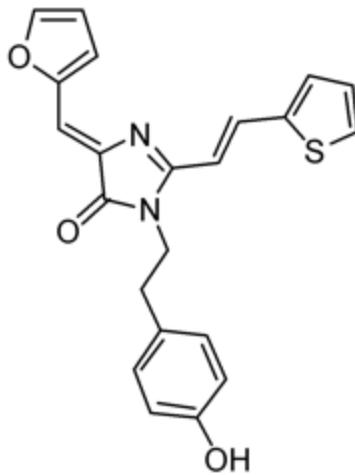












* = Z-isomer (at the styrene moiety)

