

Expanding benzoxazole based inosine 5'-monophosphate dehydrogenase (IMPDH) inhibitor structure-activity as potential anti-tuberculosis agents

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60439, USA

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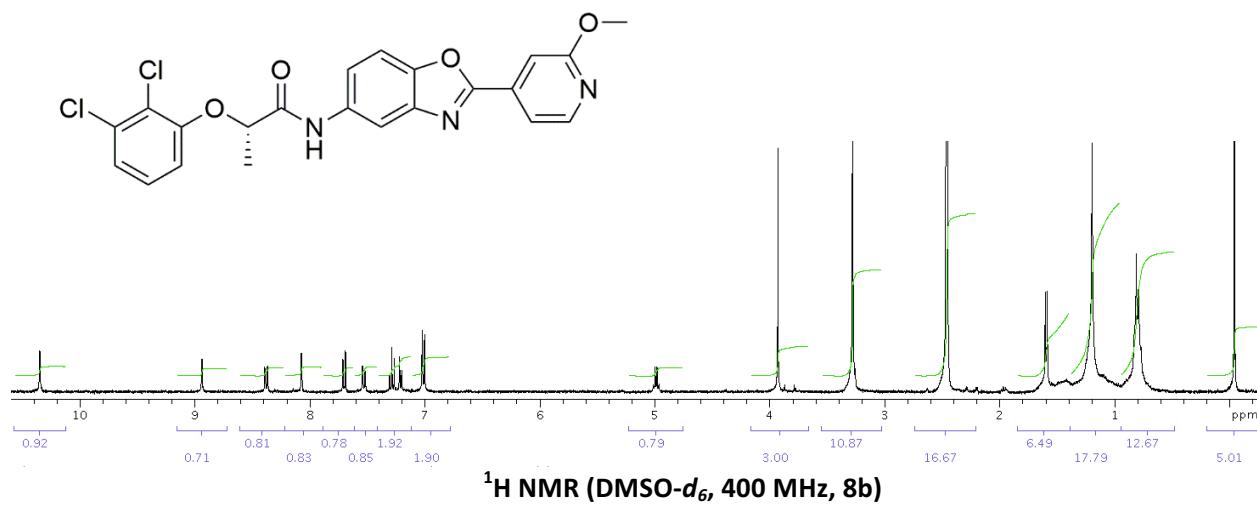
[‡]Department of Pharmacological and Pharmaceutical Sciences, College of Pharmacy, University of Houston, Health Building 2, 4849 Calhoun Rd., Houston, Texas 77204, United States

Supporting Information

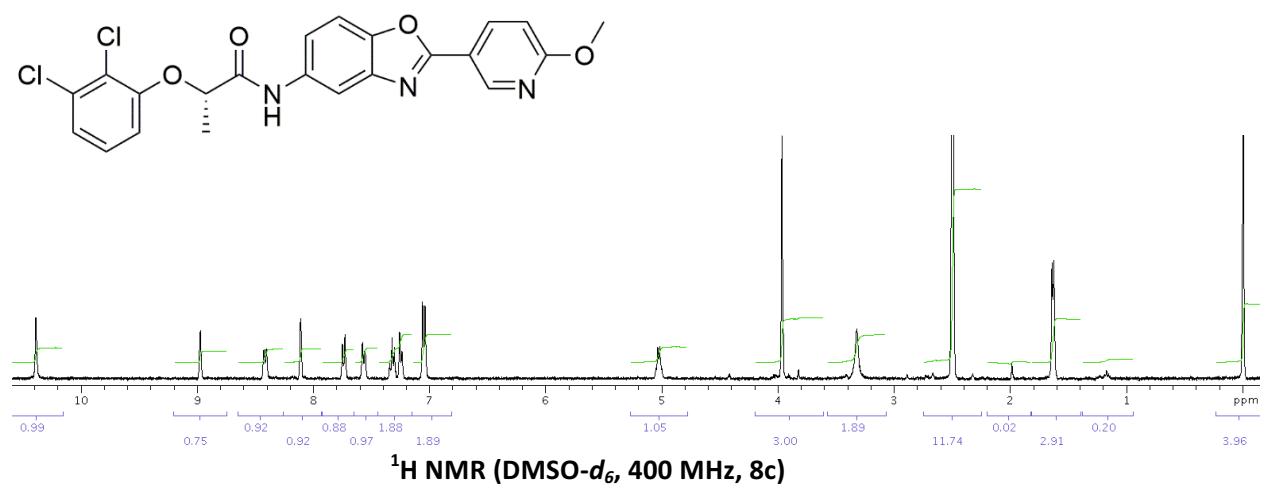
Contents

- 1) ^1H NMR S-2 – S-46

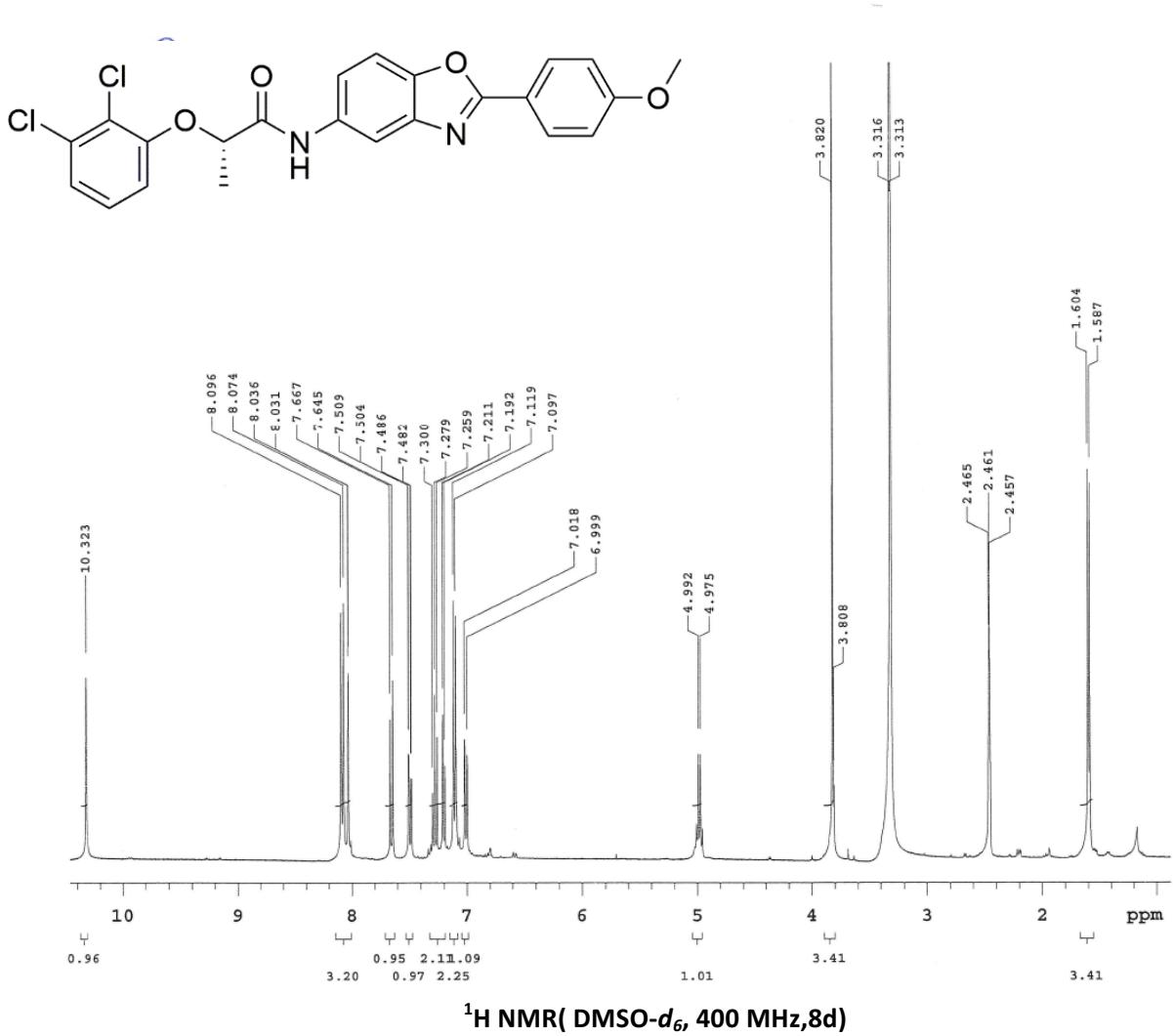
8b



8c

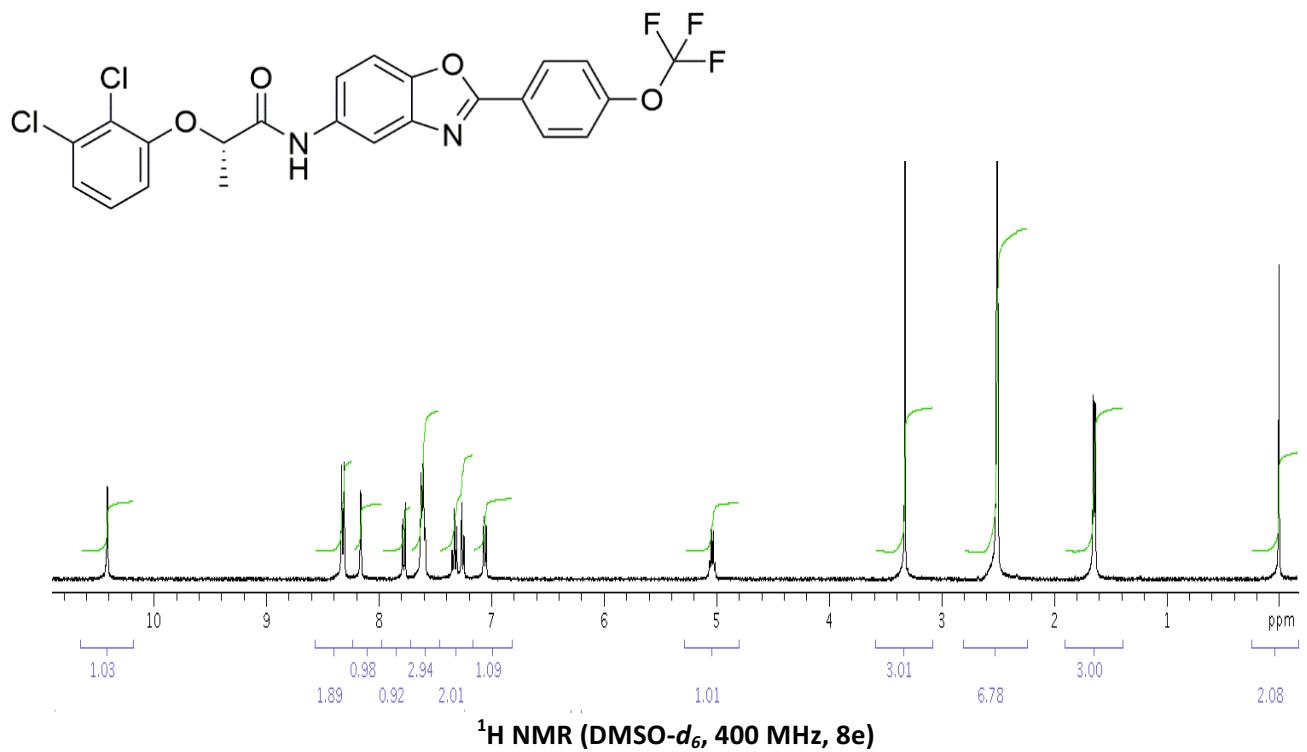


8d

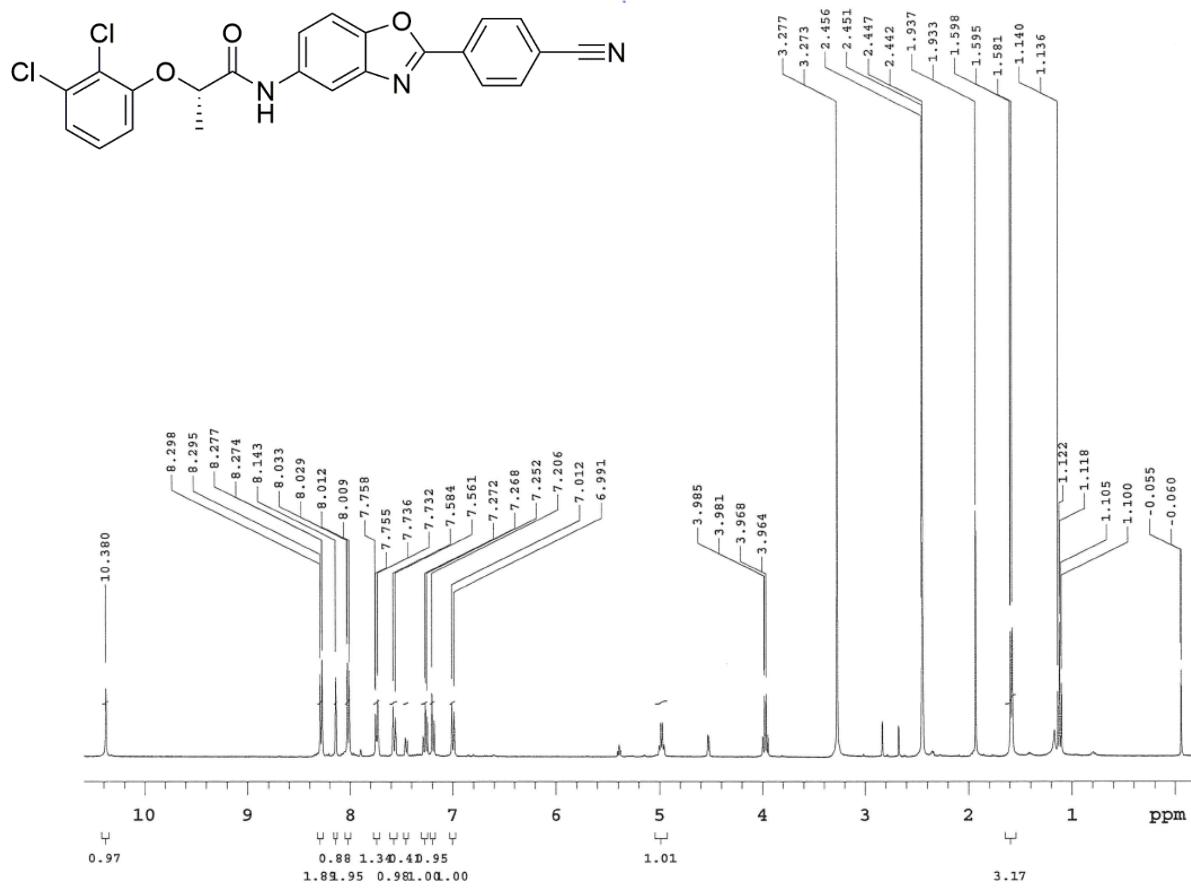


¹H NMR(DMSO-*d*₆, 400 MHz,8d)

8e

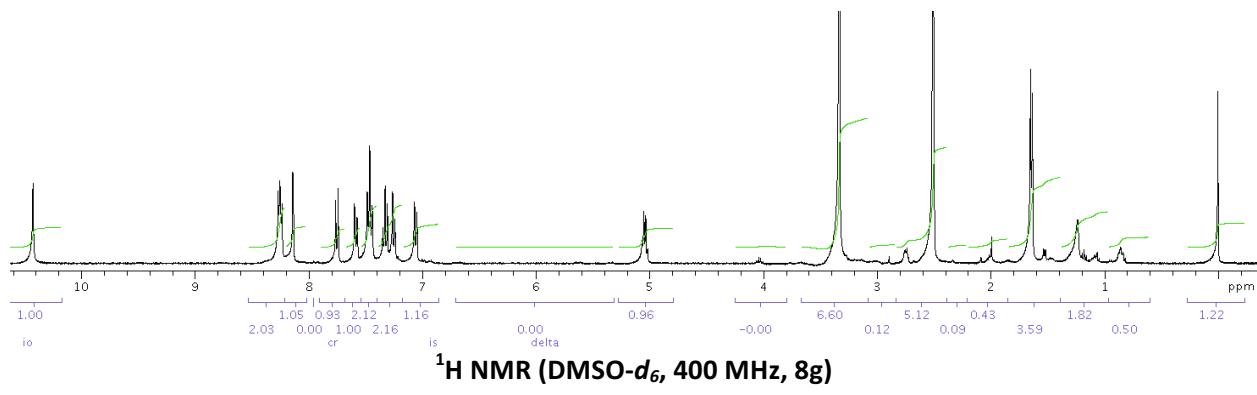
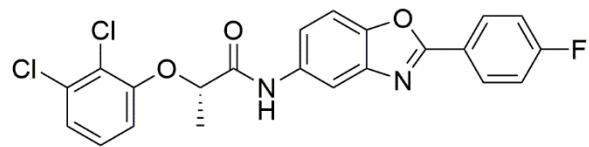


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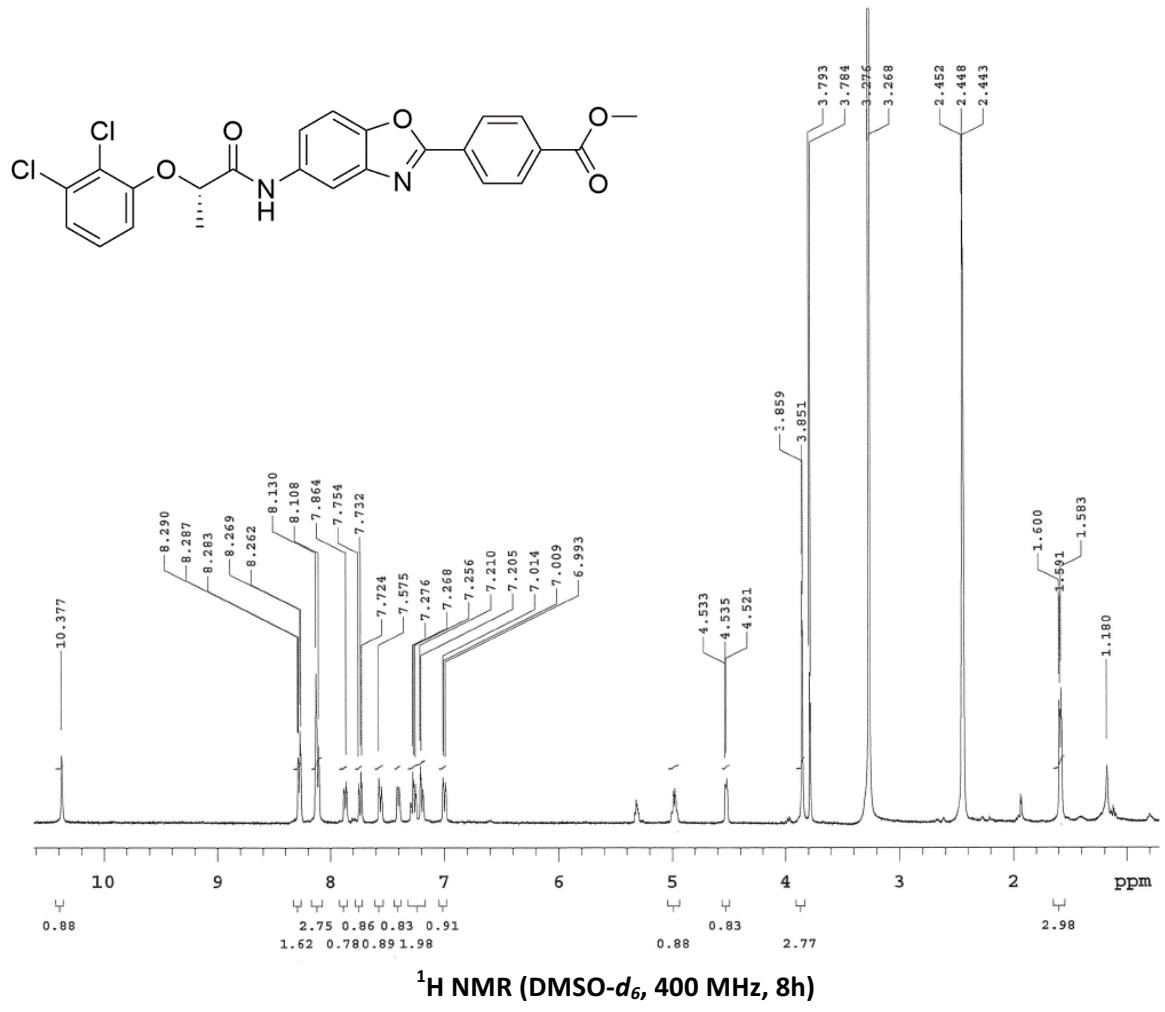
¹H NMR (DMSO-*d*₆, 400 MHz, 8f)

8g

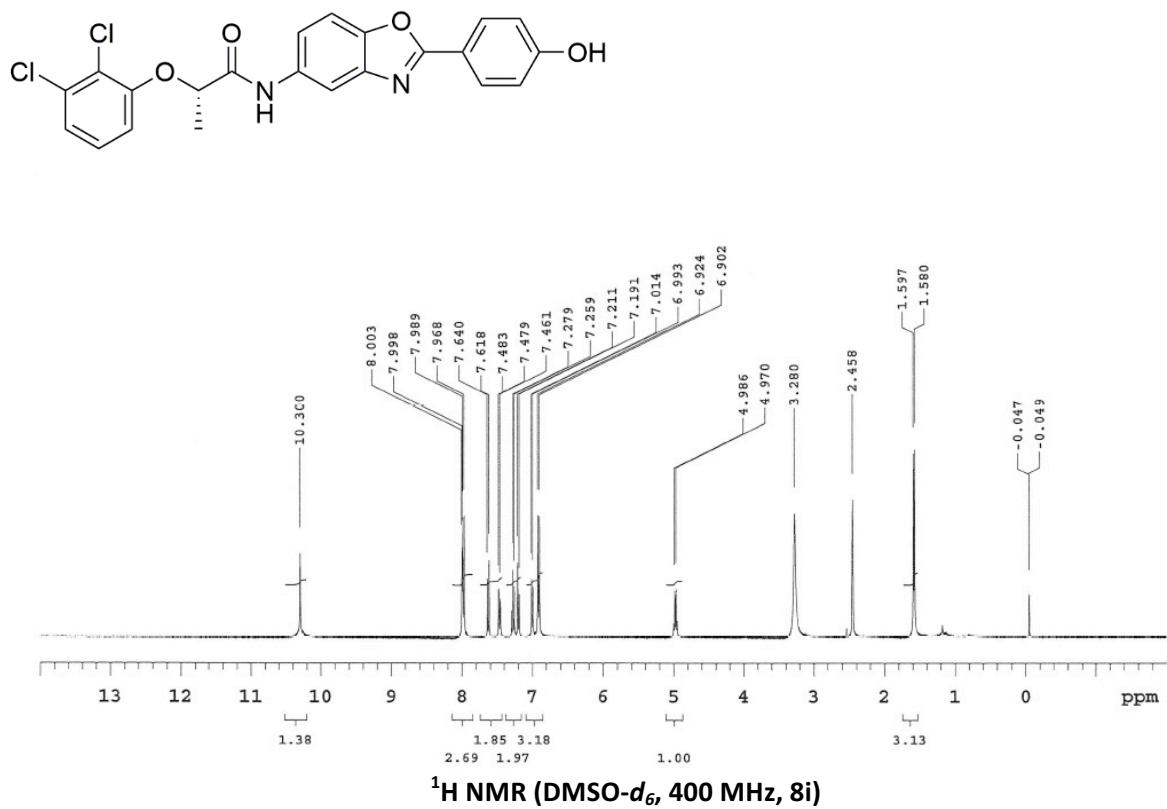


¹H NMR (DMSO-*d*₆, 400 MHz, 8g)

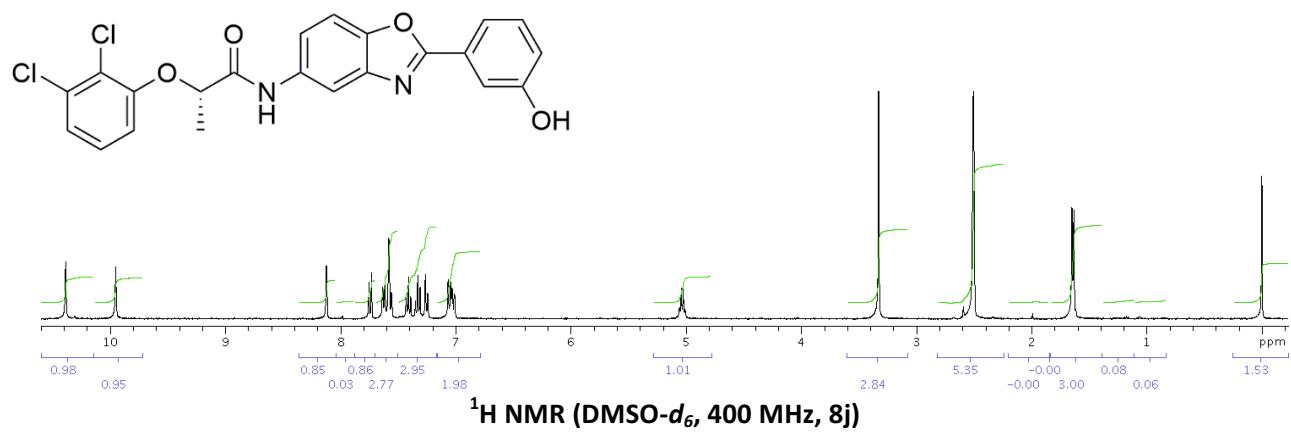
8h



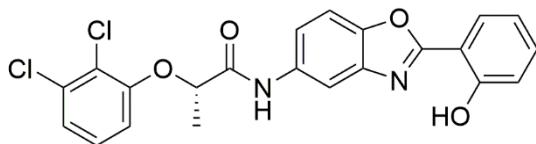
8i



8j



8k



Gradient Shimming

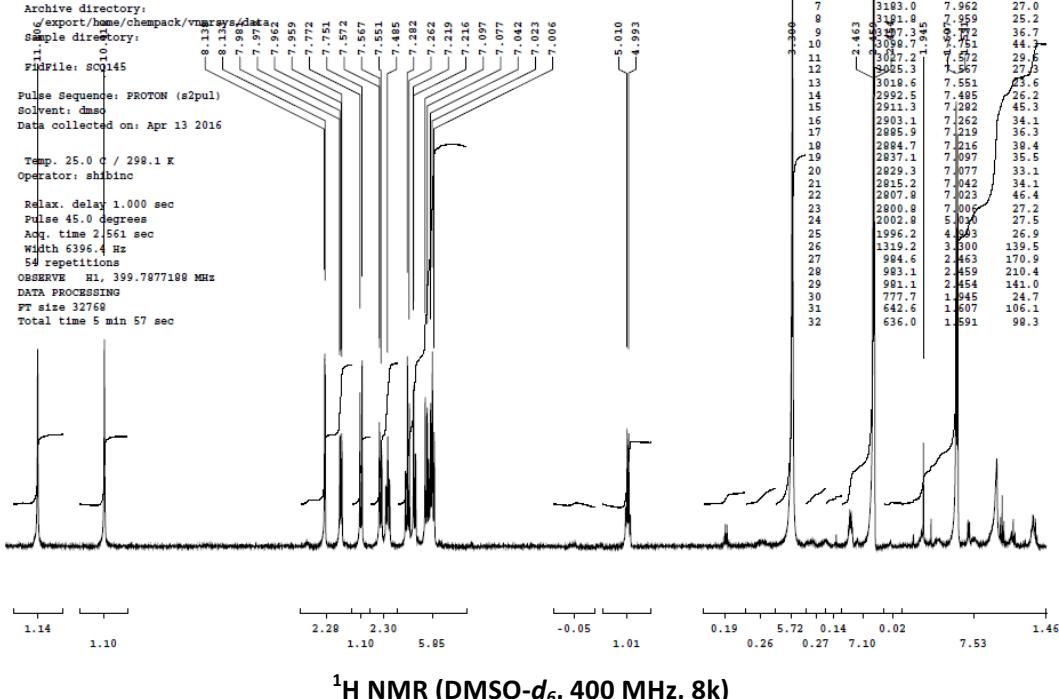
Sample Name:
SC_1_Q135
Data Collected on:
echoj-inova400
Archive directory:
/export/home/chempack/vnmarsys/data/
Sample directory:
SC_1_Q135
Fidfile: SC_1_Q145

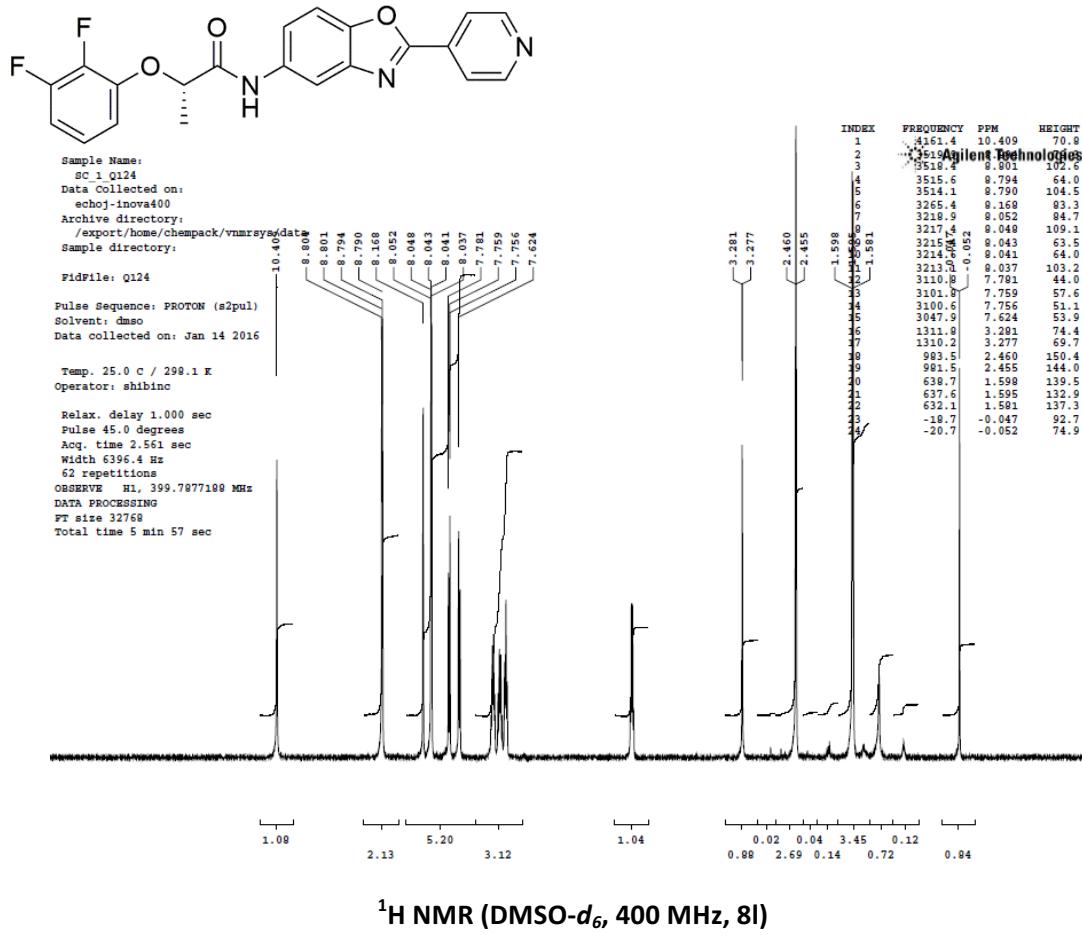
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Apr 13 2016

Temp. 25.0 °C / 298.1 K
Operator: shibinc

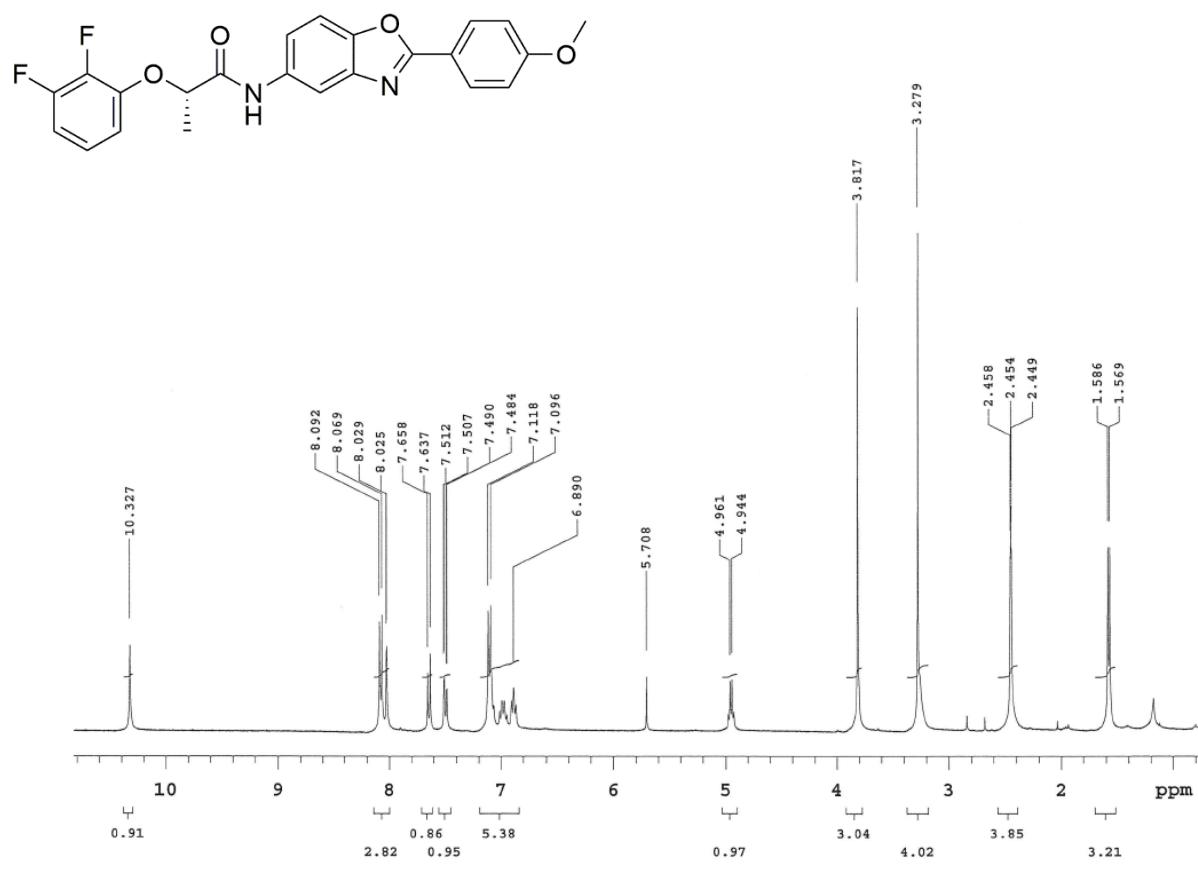
Relax. delay 1.000 sec
Pulse 45.0 degrees
Aq. time 2.551 sec
Width 6396.4 Hz
54 repetitions
OBSERVE: H1, 399.7877100 MHz
DATA PROCESSING
FT size 32768
Total time 5 min 57 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	4440.1	11.106	47.0
2	3156.4	9.338	45.9
3	3252.6	9.338	45.9
4	3151.3	8.133	43.4
5	3180.3	7.991	25.5
6	3189.6	7.979	26.6
7	3183.0	7.962	27.0
8	3181.9	7.959	25.2
9	3037.3	7.772	36.7
10	3039.7	7.751	44.7
11	3027.2	7.572	29.6
12	3045.3	7.567	27.1
13	3092.6	7.551	21.6
14	2992.7	7.359	45.2
15	2911.3	7.192	45.3
16	2903.1	7.126	34.1
17	2885.9	7.1219	36.3
18	2884.7	7.1216	38.4
19	2837.1	7.097	35.5
20	2829.3	7.077	33.1
21	2815.2	7.042	34.1
22	2800.8	7.023	46.4
23	2800.8	7.004	27.2
24	2002.8	5.036	27.5
25	1996.2	4.943	26.9
26	1319.2	3.300	139.5
27	984.6	2.463	170.9
28	983.1	2.459	210.4
29	981.1	2.454	141.0
30	777.7	1.945	24.7
31	642.6	1.607	106.1
32	636.0	1.591	98.3

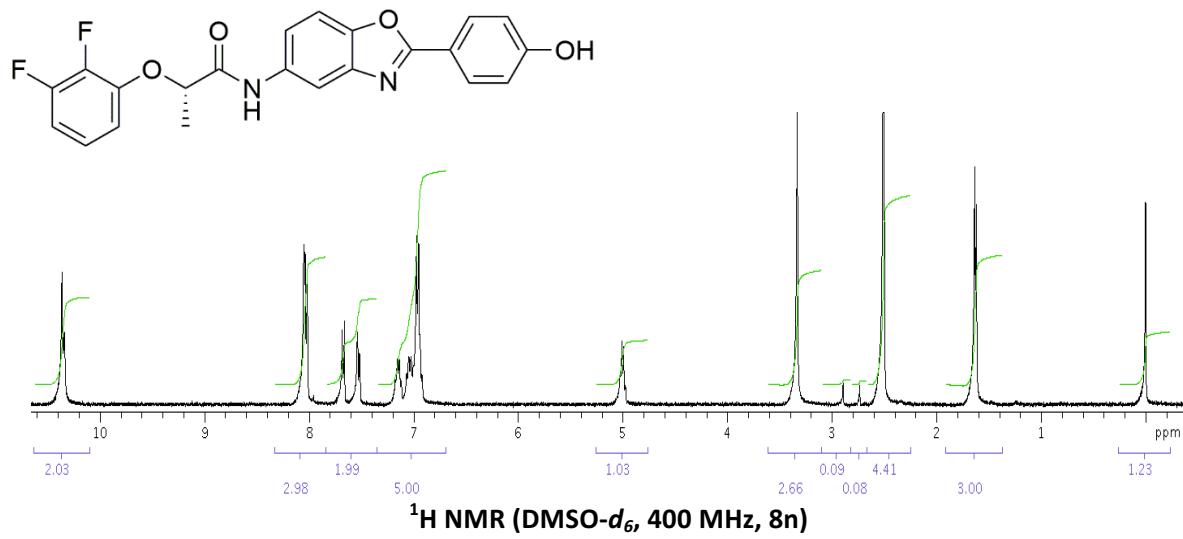




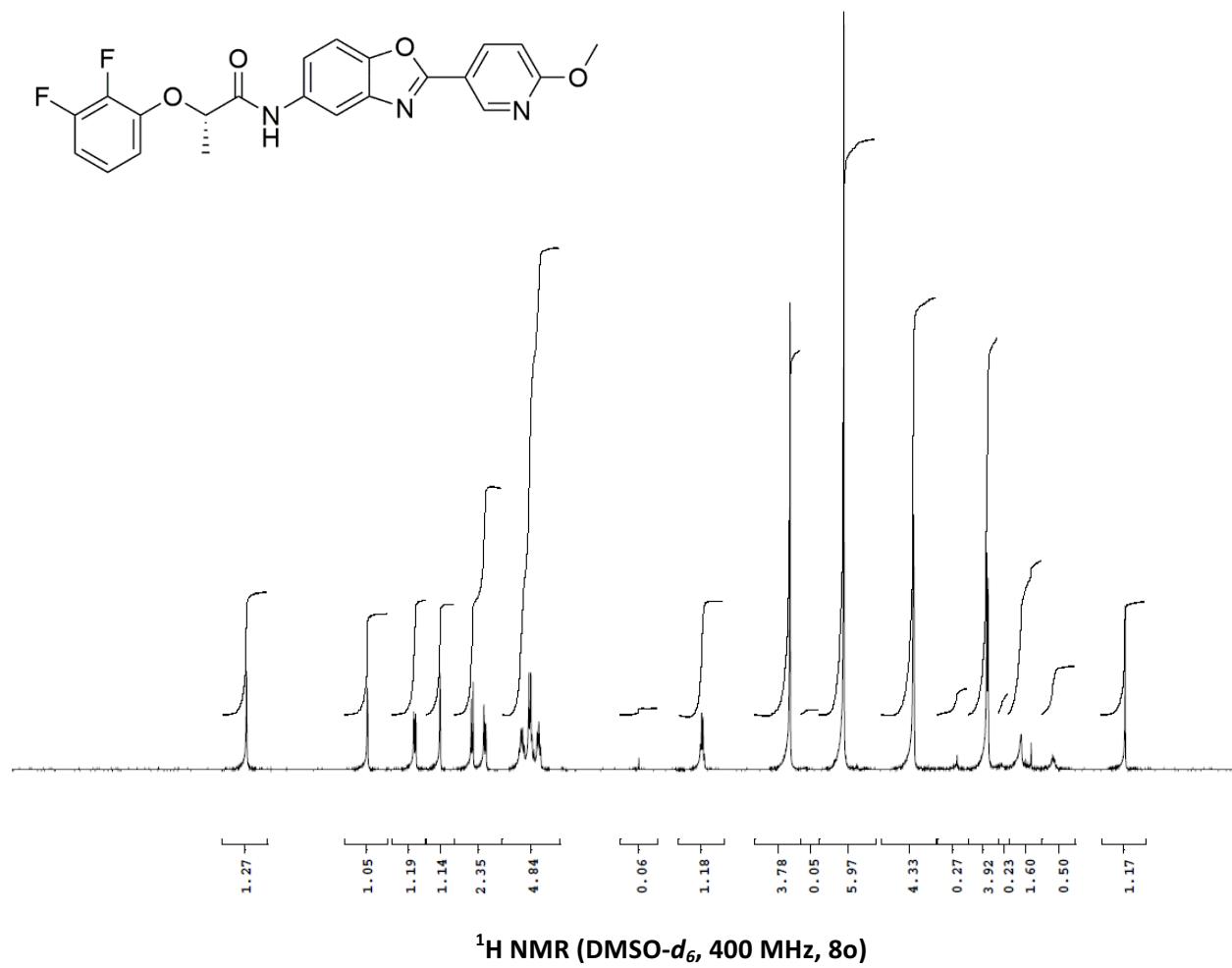
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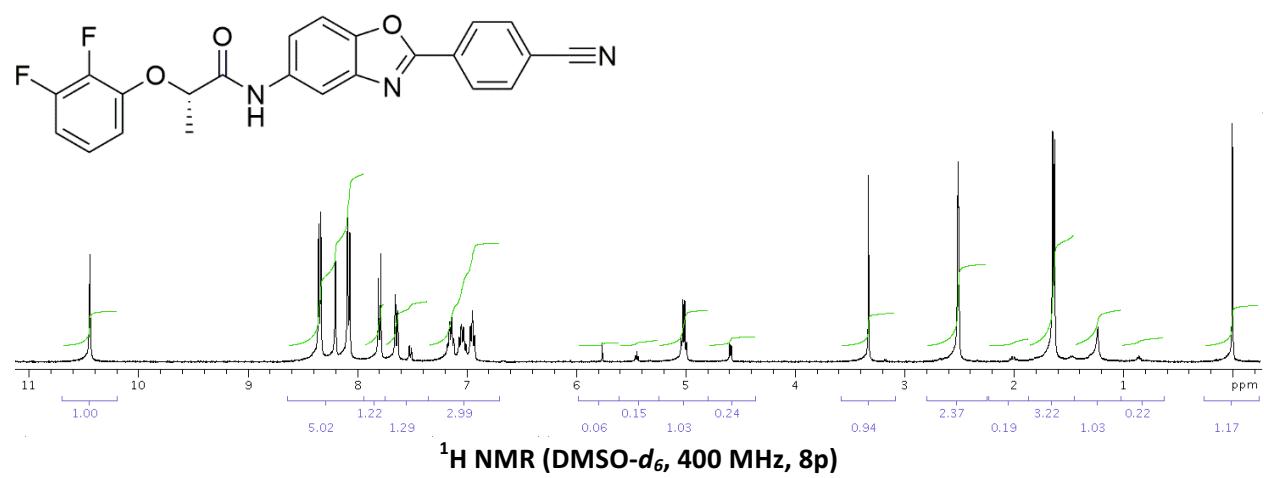
8n



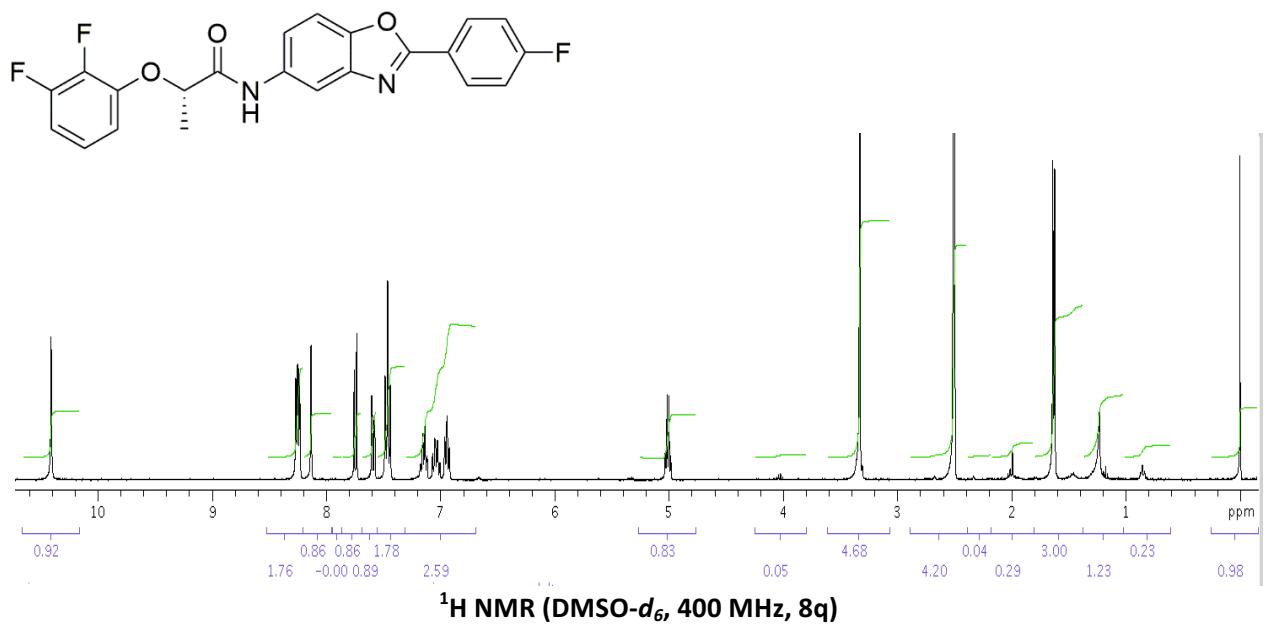
8o



8p

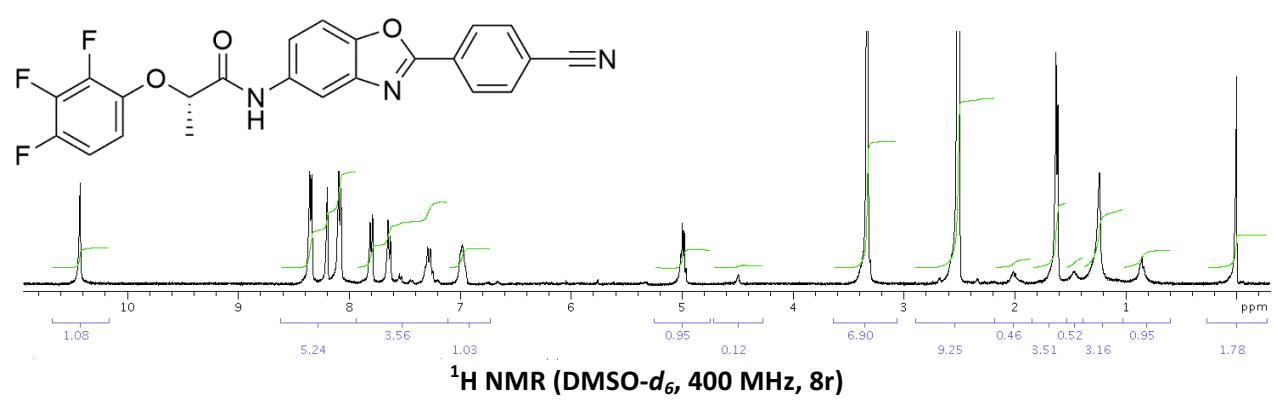


8q



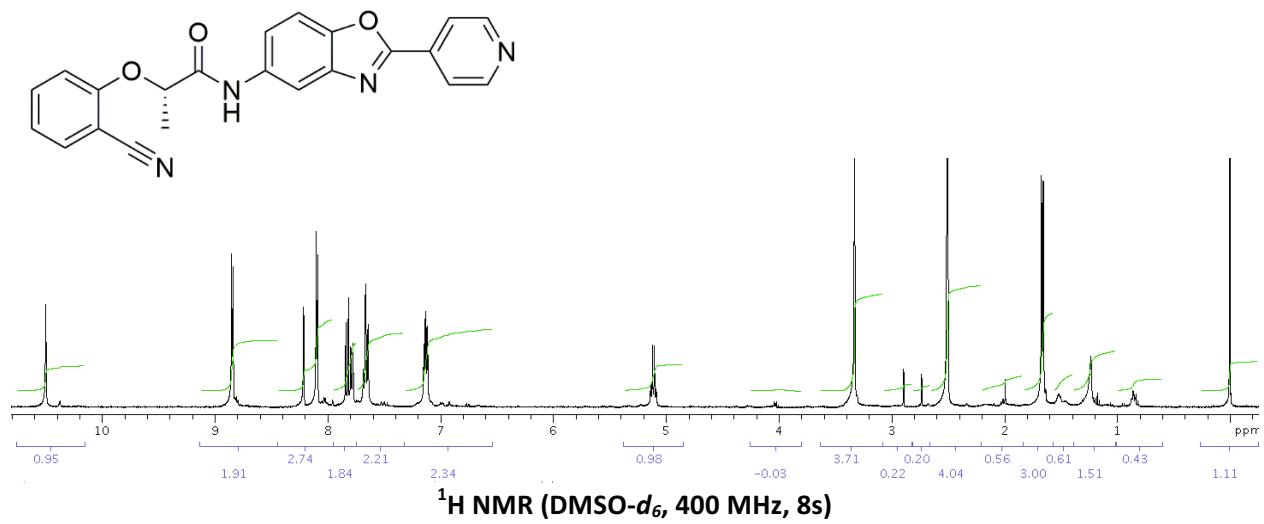
¹H NMR (DMSO-*d*₆, 400 MHz, 8q)

8r

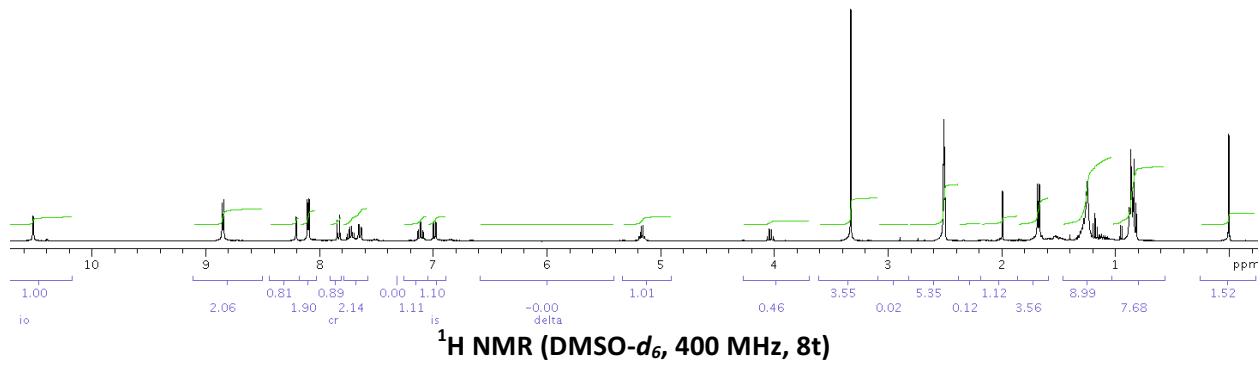
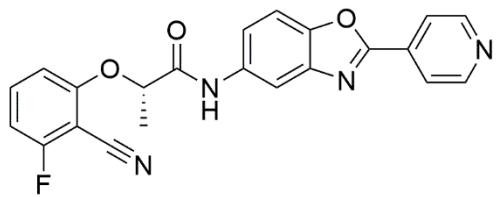


¹H NMR (DMSO-d₆, 400 MHz, 8r)

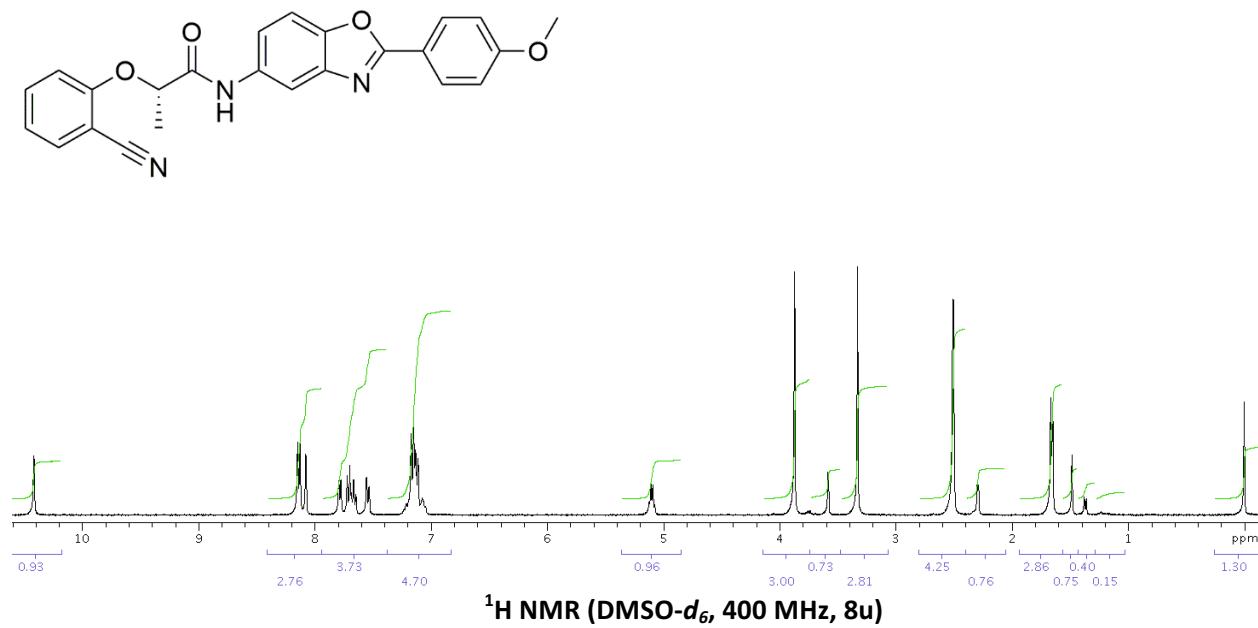
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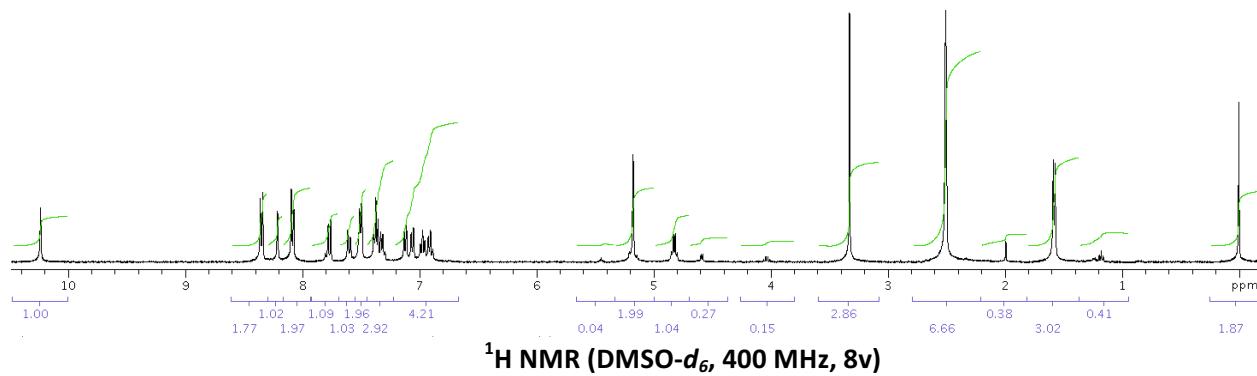
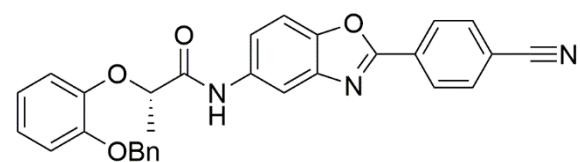
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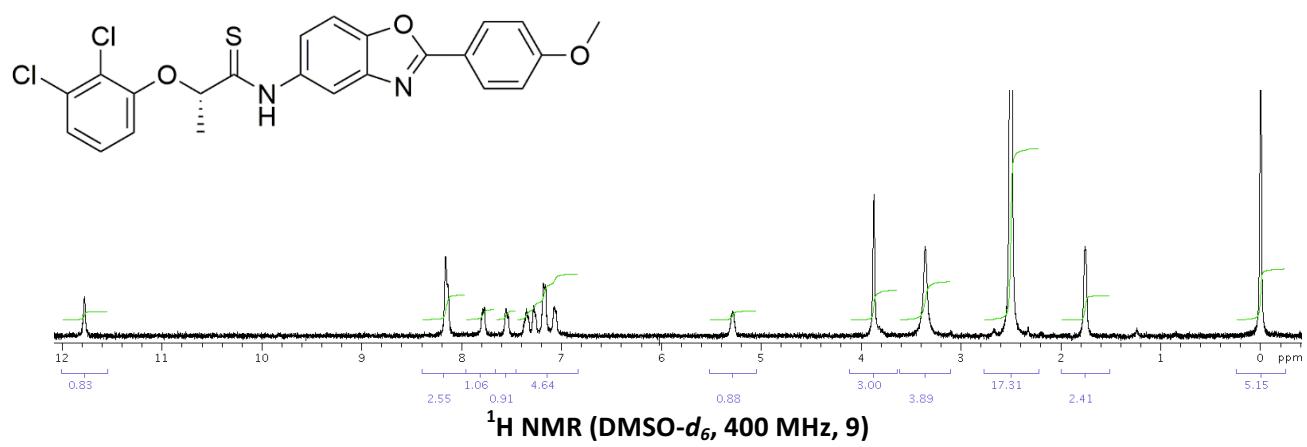
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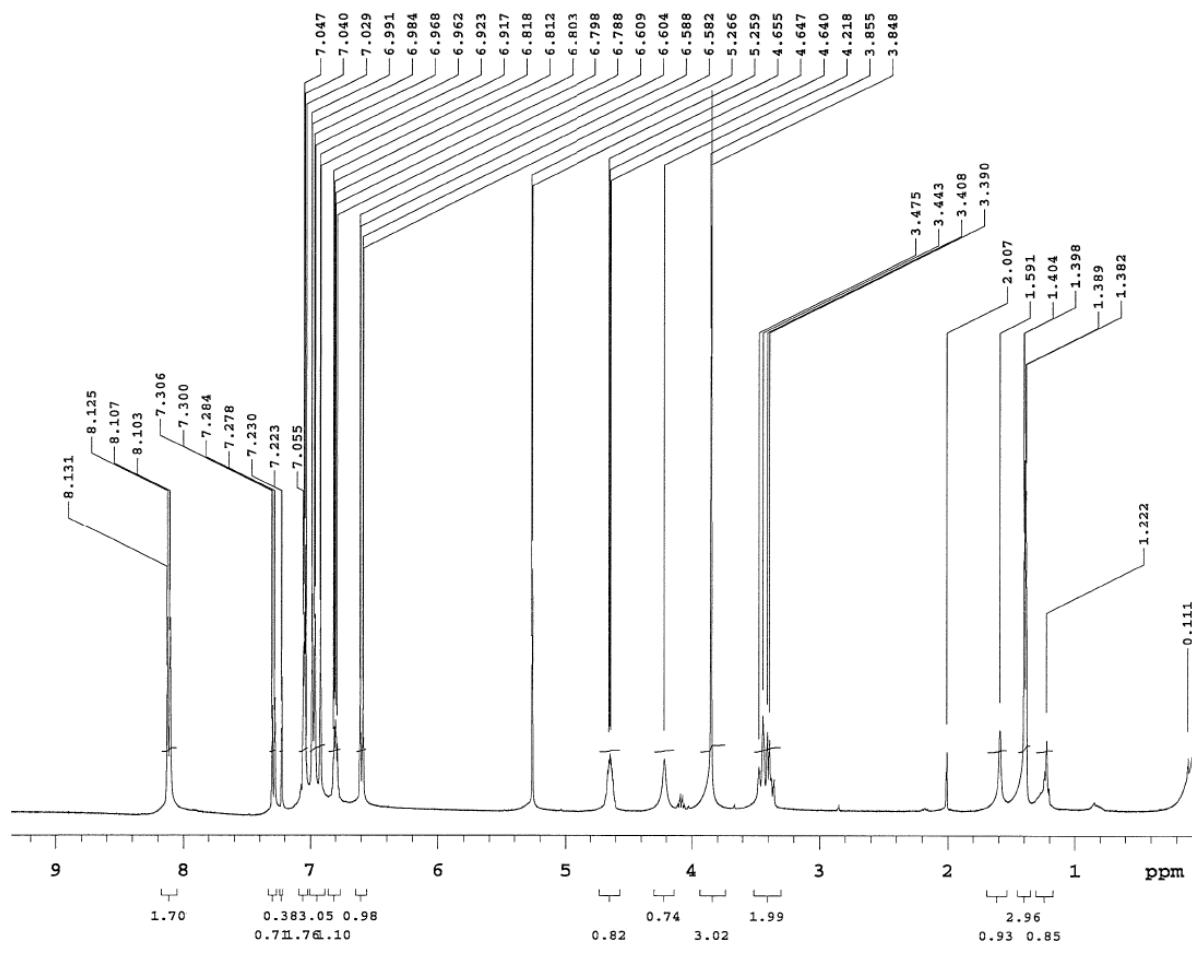
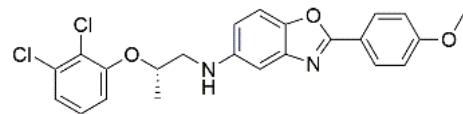
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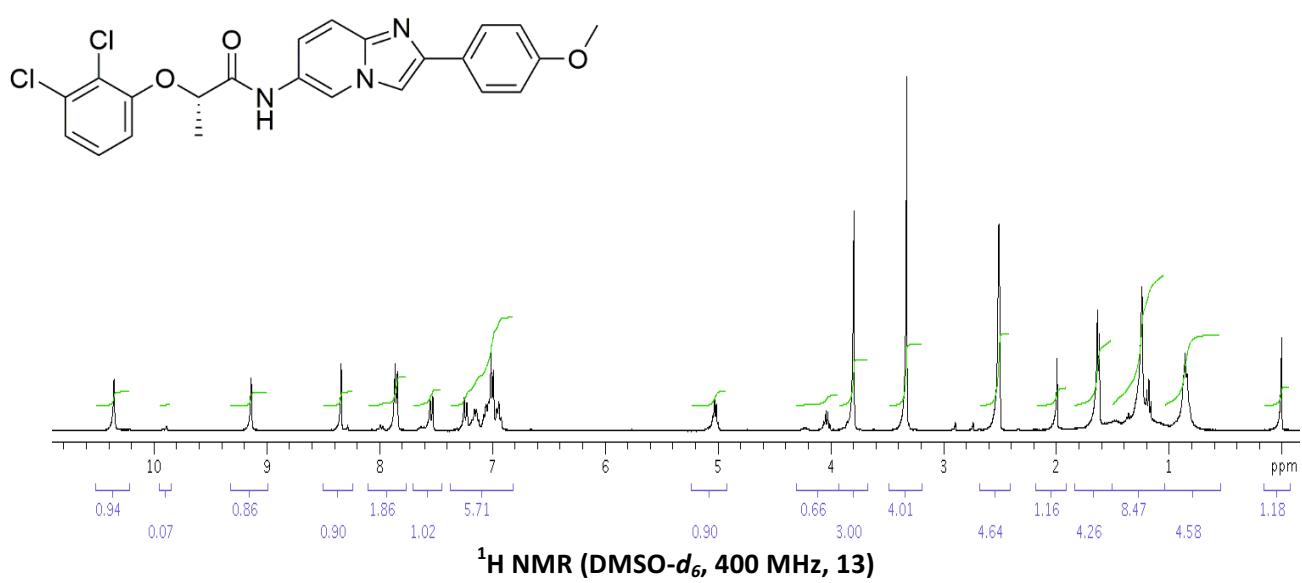
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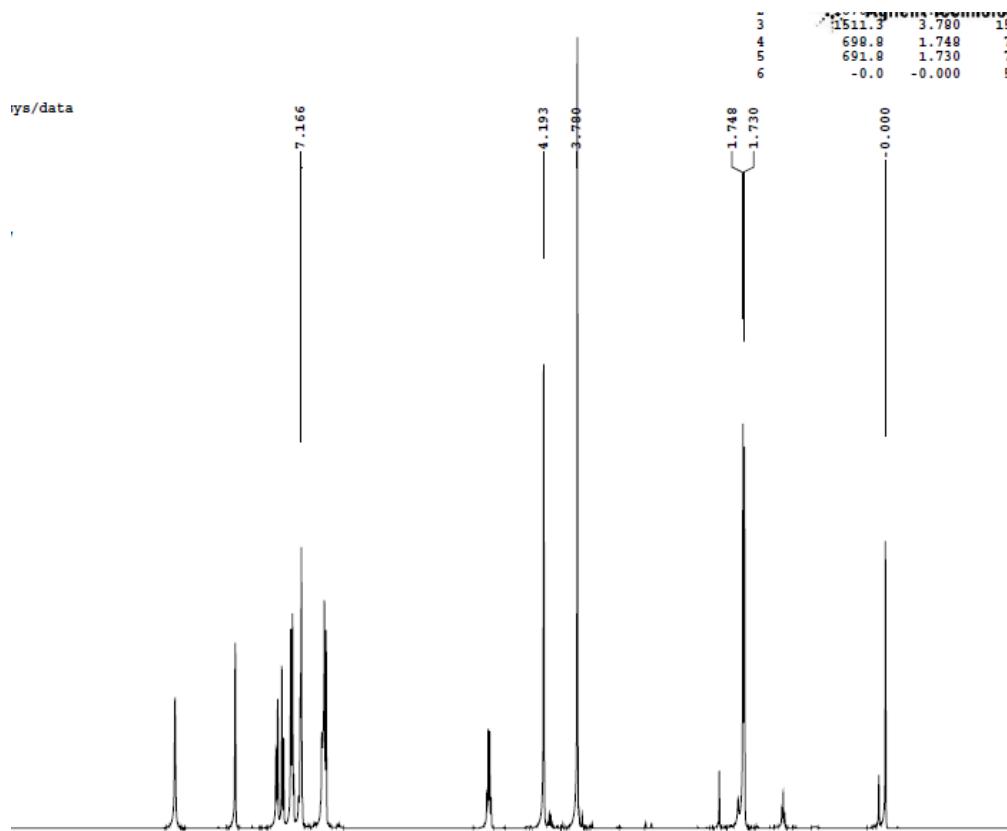
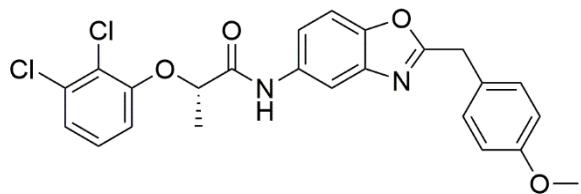
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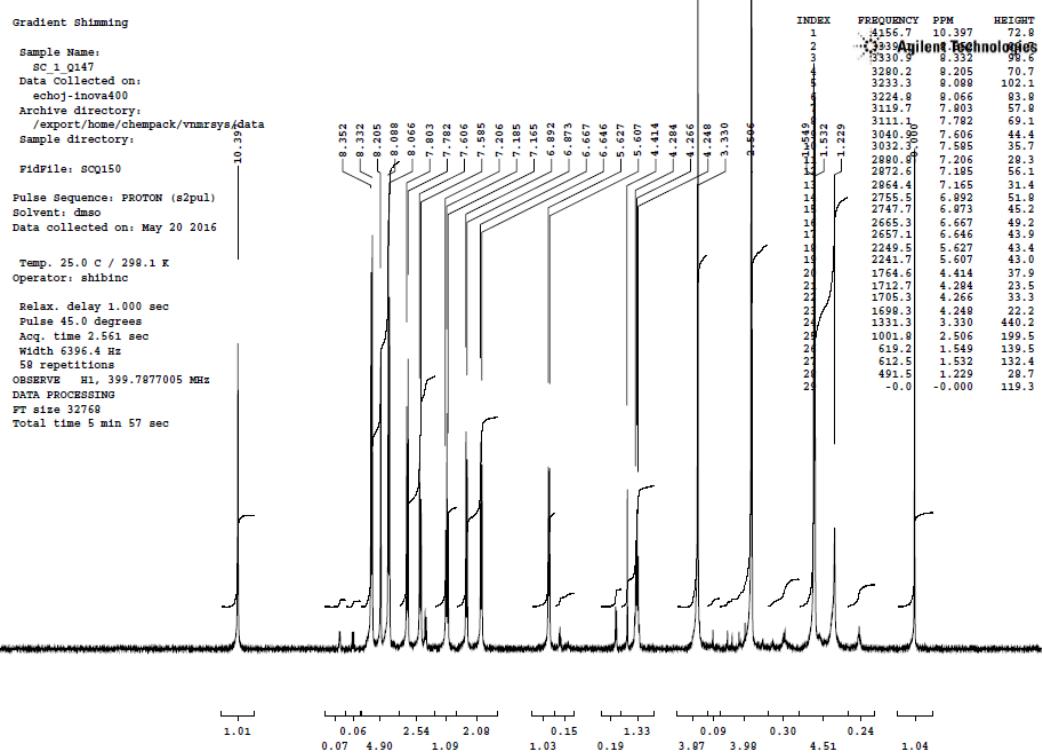
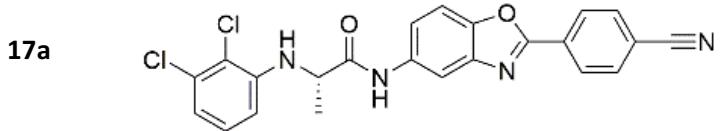
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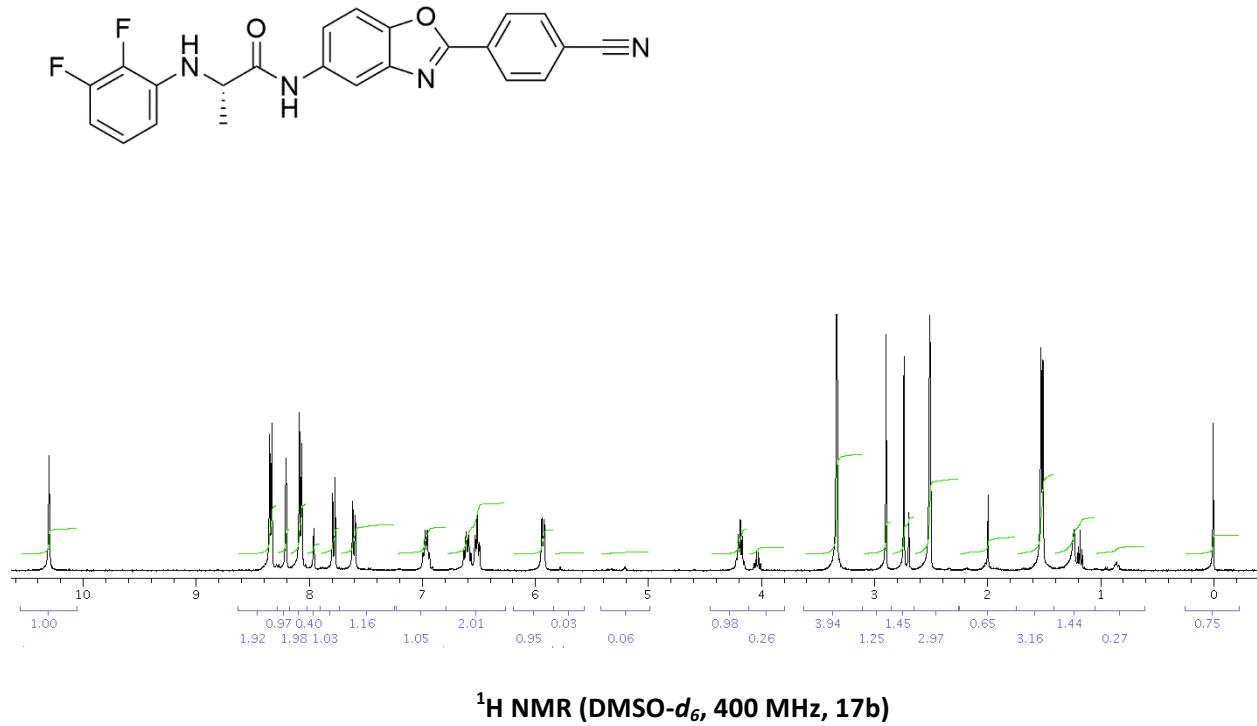


¹H NMR (DMSO-*d*₆, 400 MHz, 15)



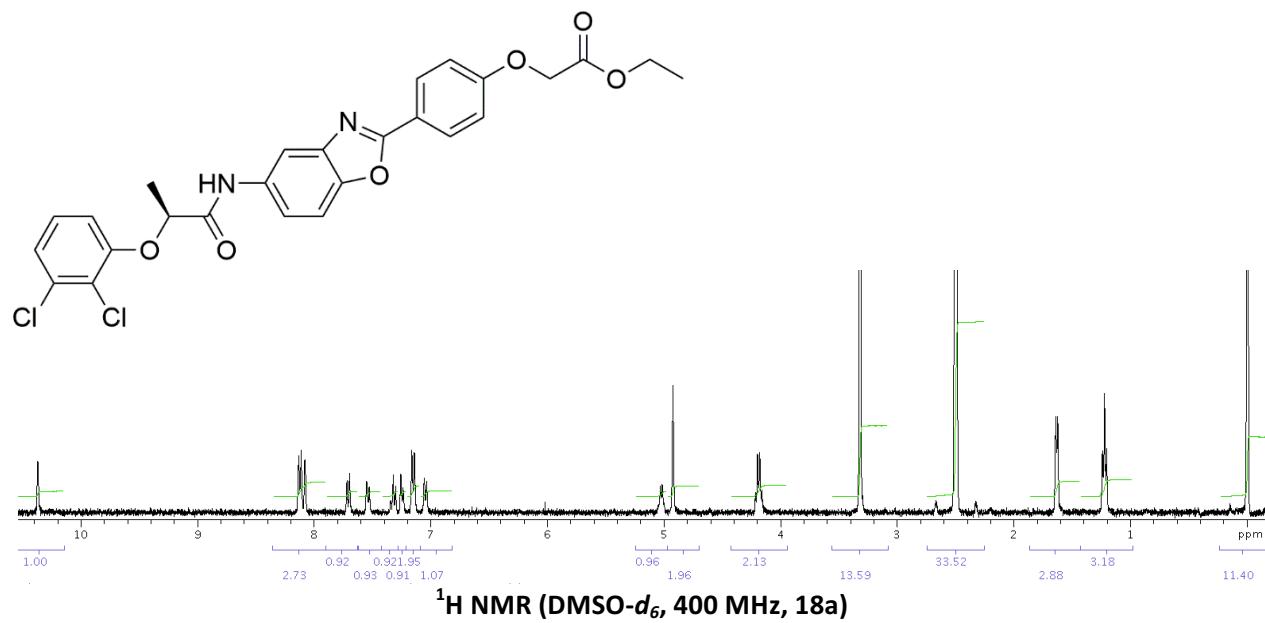
¹H NMR (DMSO-*d*₆, 400 MHz, 17a)

17b



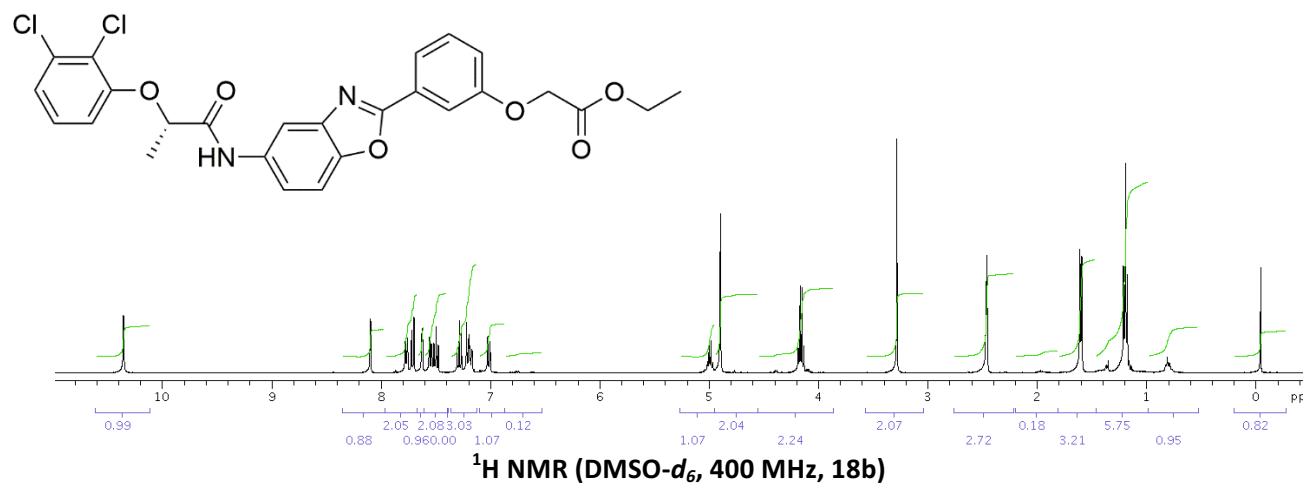
¹H NMR (DMSO-*d*₆, 400 MHz, 17b)

18a

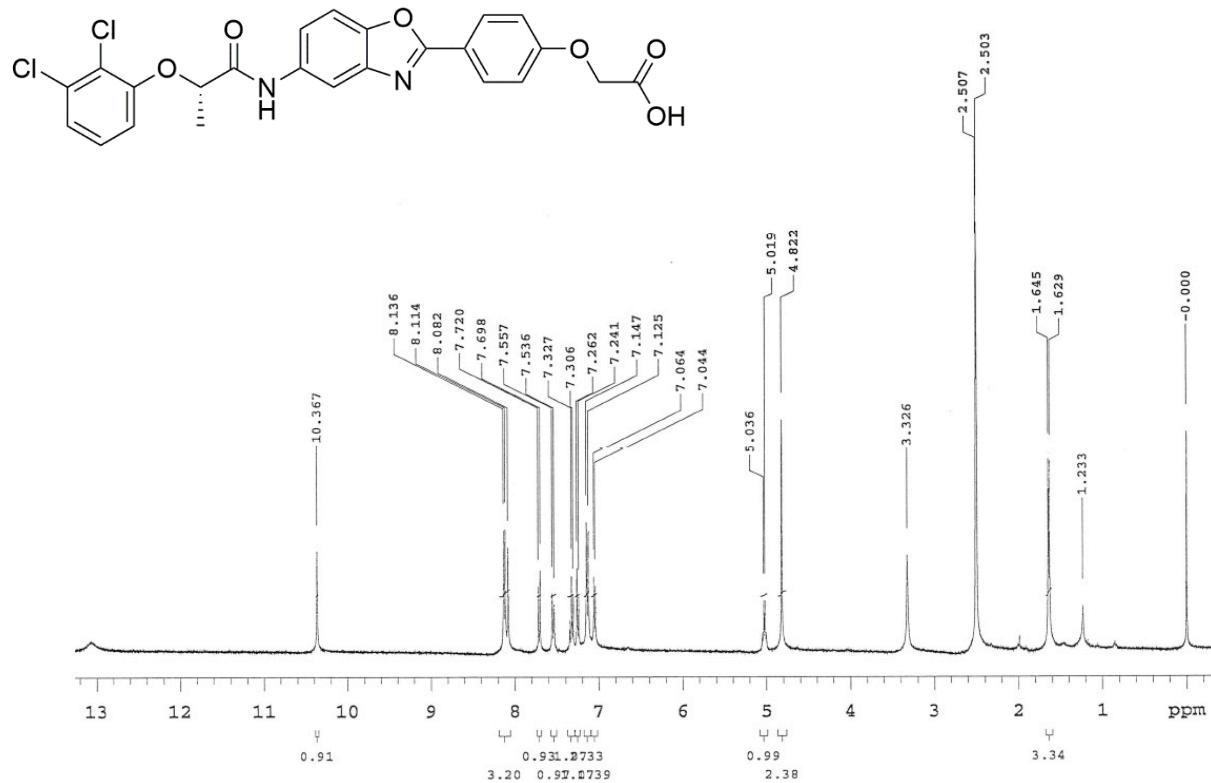


¹H NMR (DMSO-d₆, 400 MHz, 18a)

18b

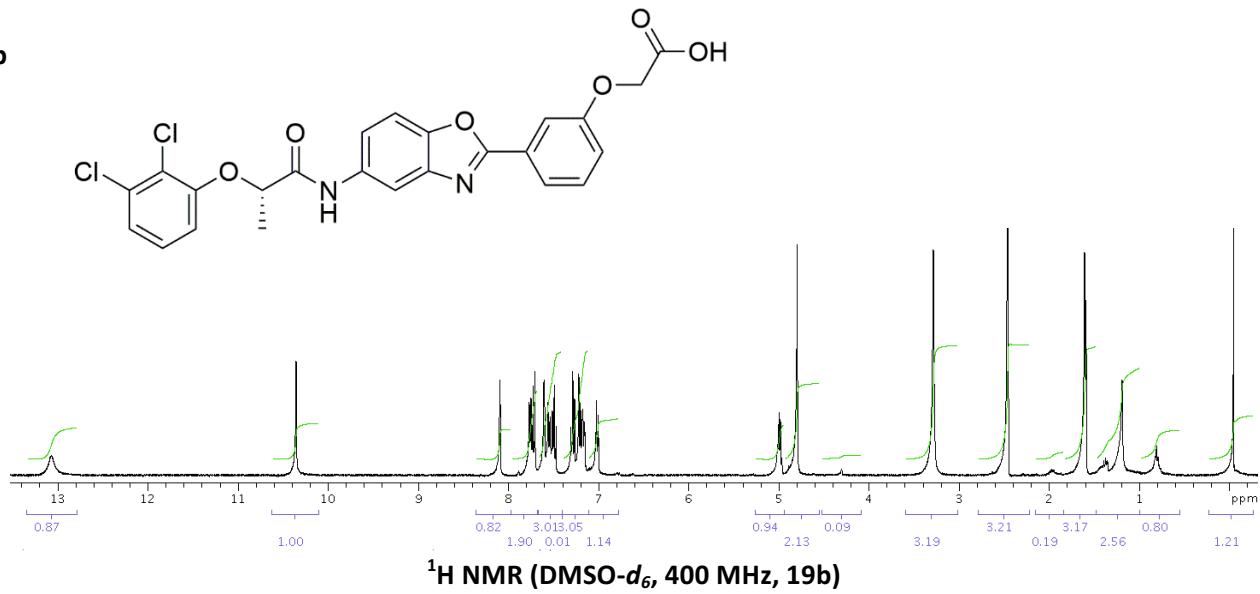


19a

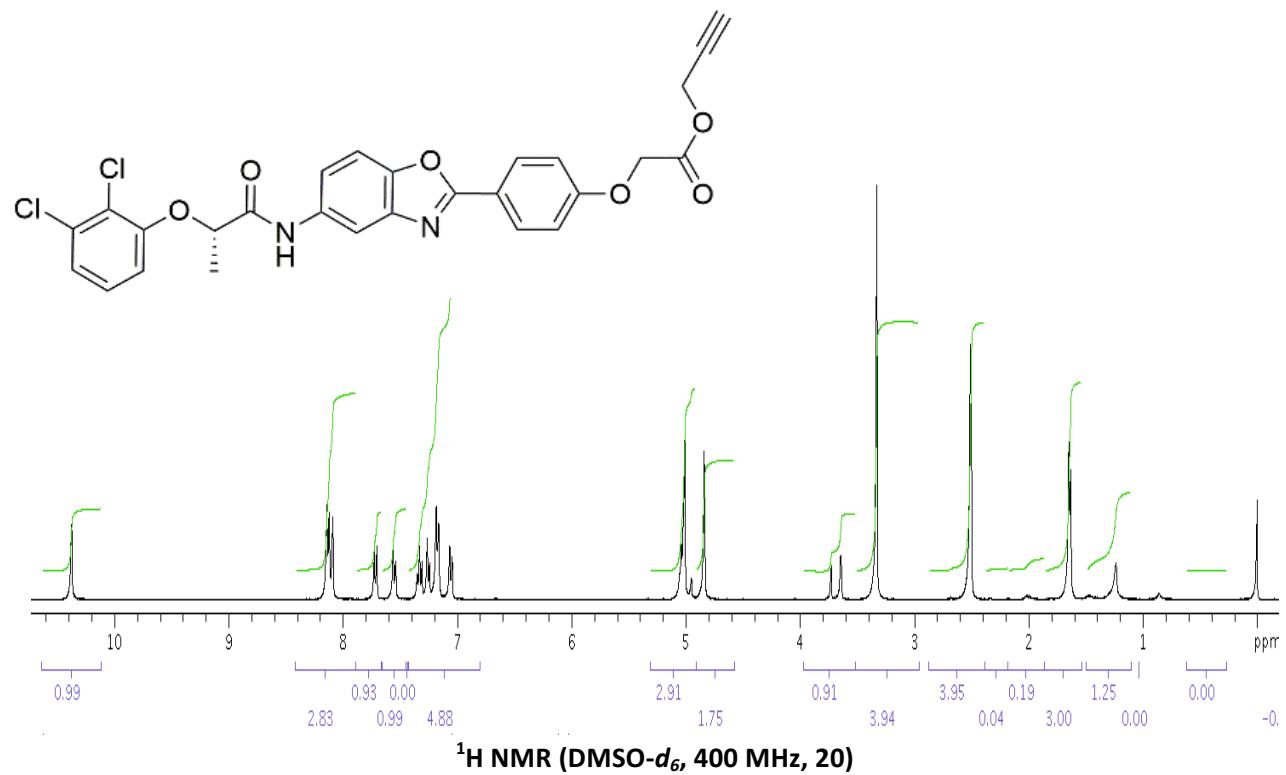


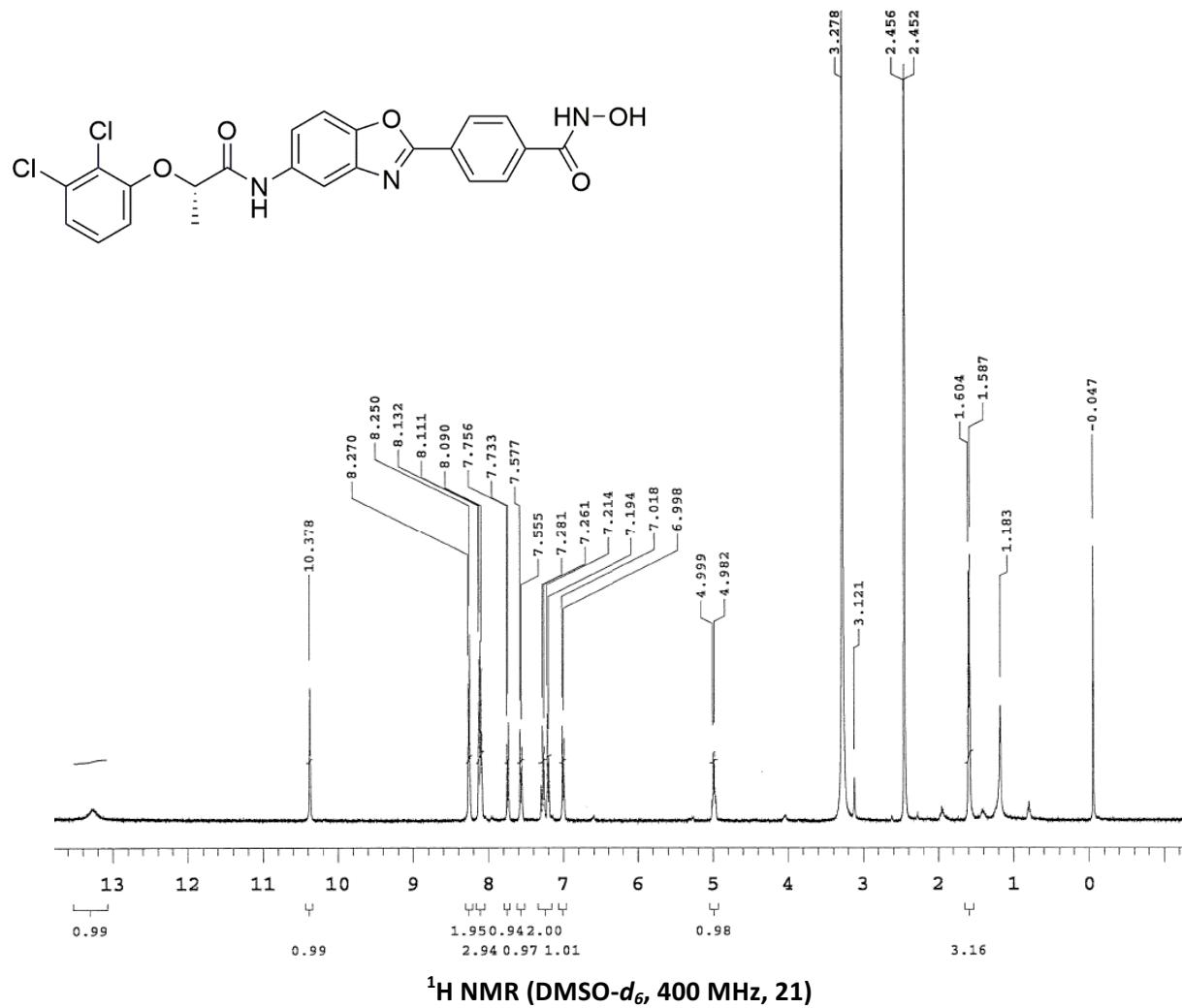
¹H NMR (DMSO-*d*₆, 400 MHz, 19a)

19b

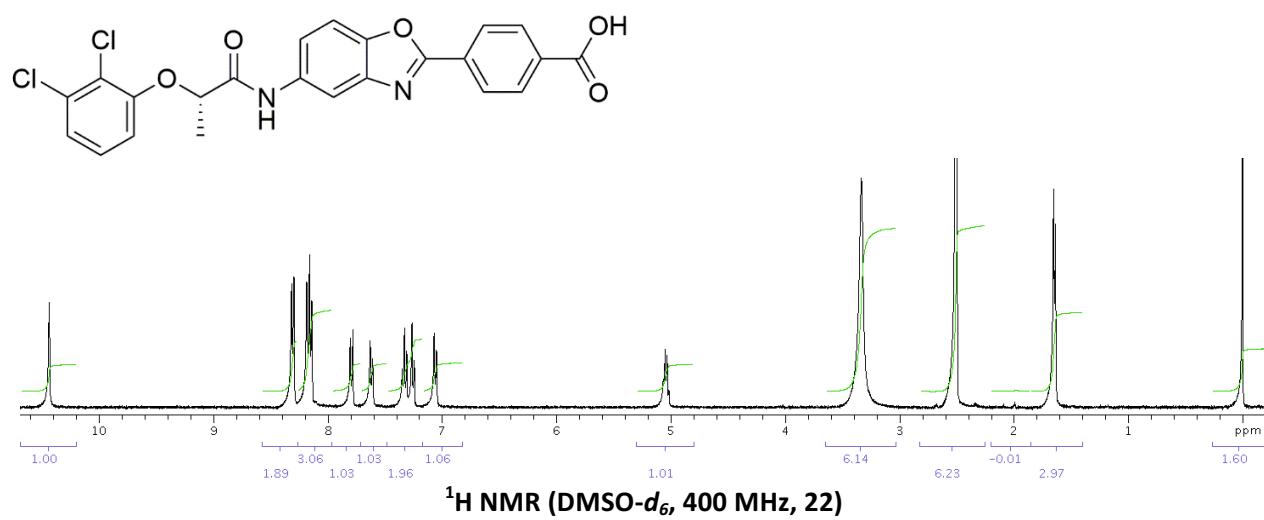


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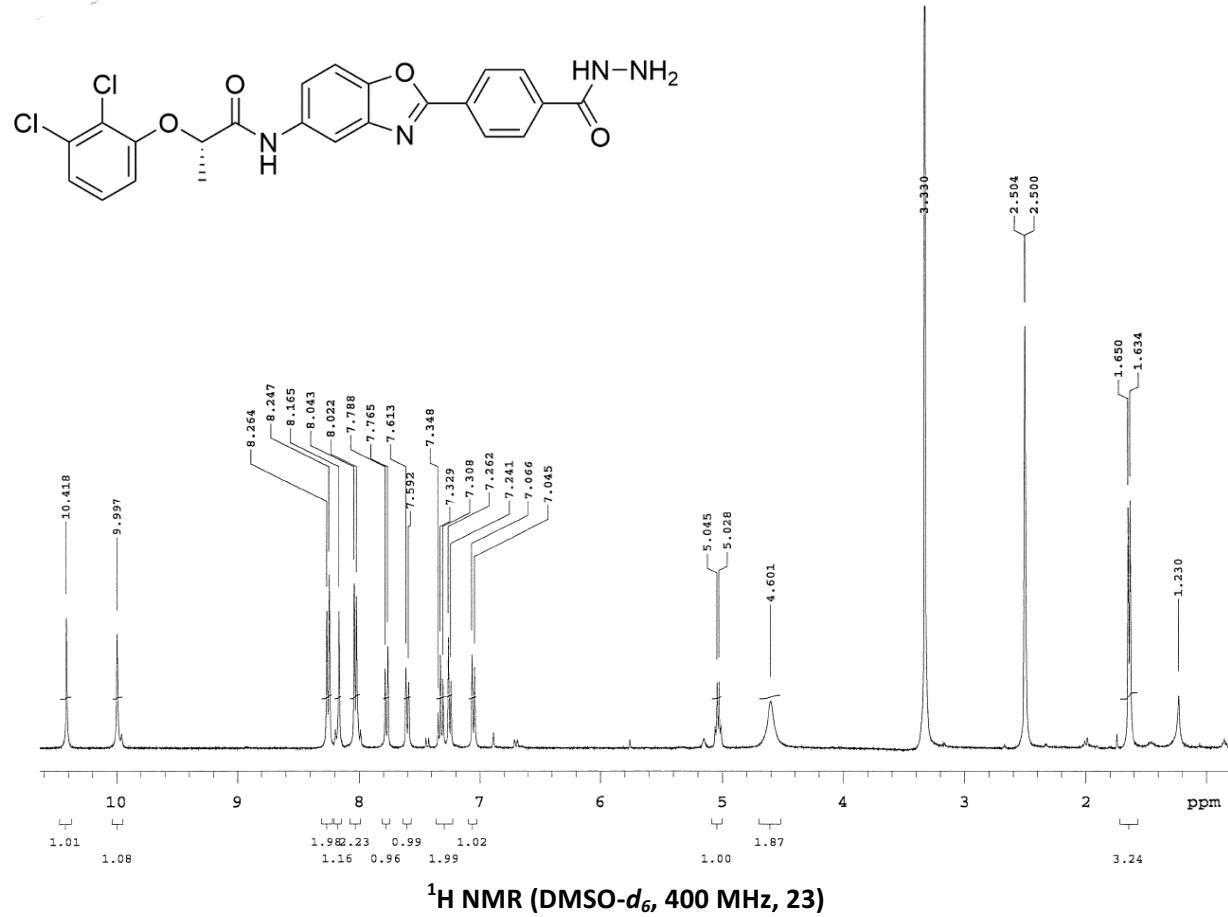




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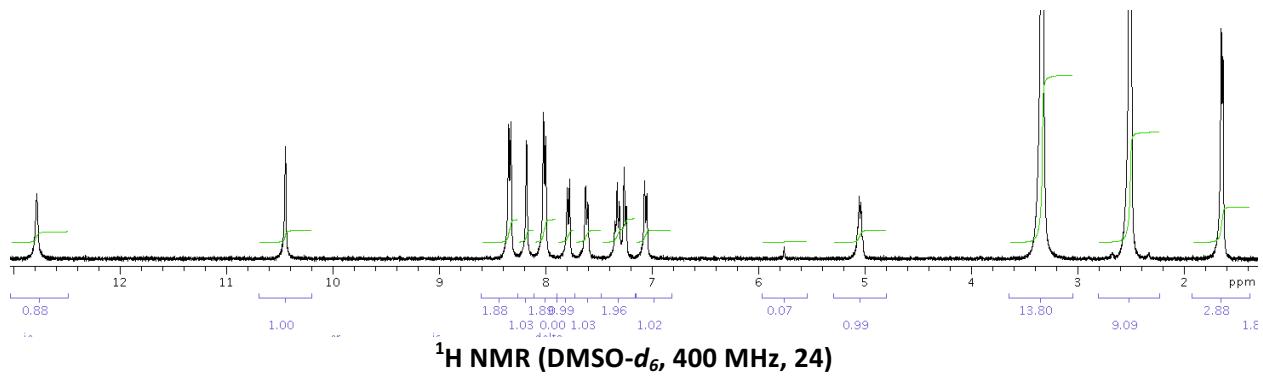
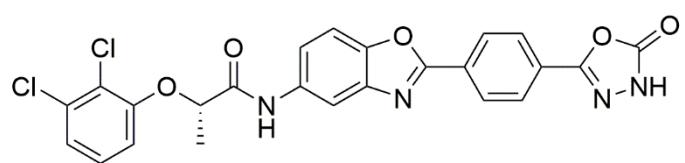


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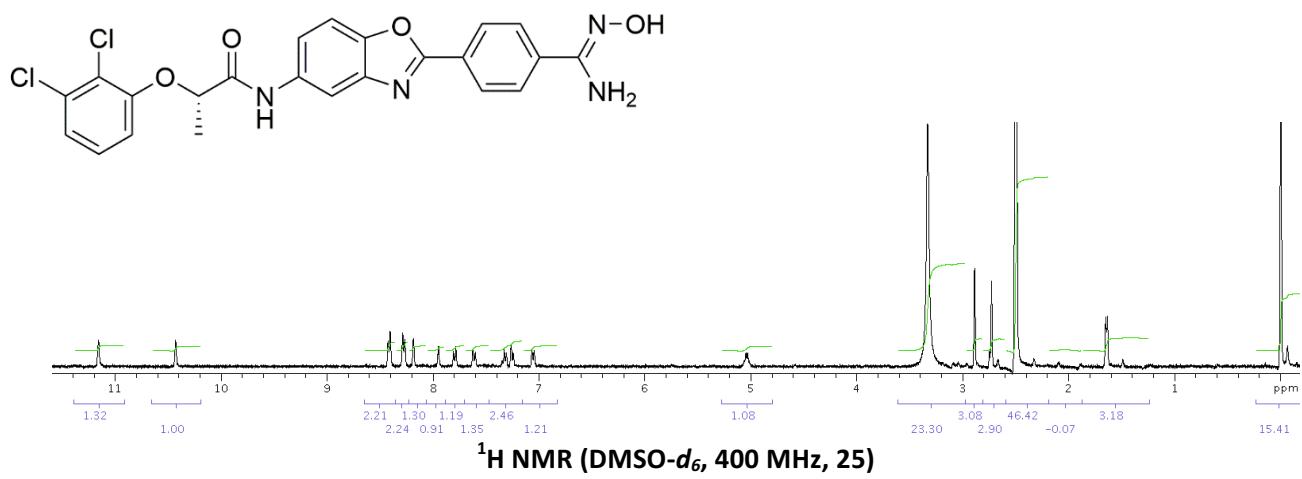
¹H NMR (DMSO-*d*₆, 400 MHz, 23)

24

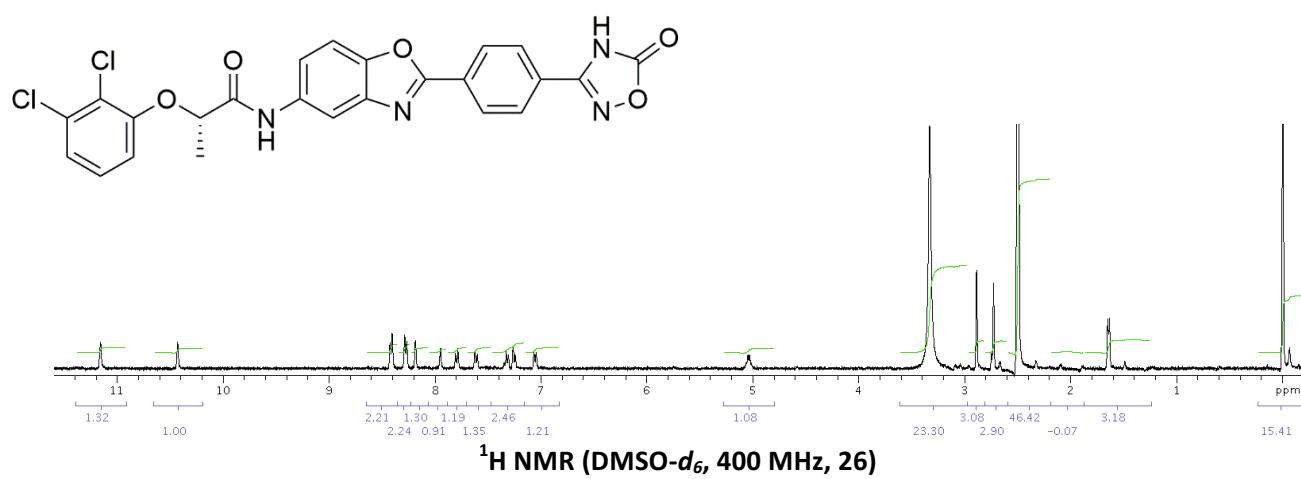


^1H NMR ($\text{DMSO}-d_6$, 400 MHz, 24)

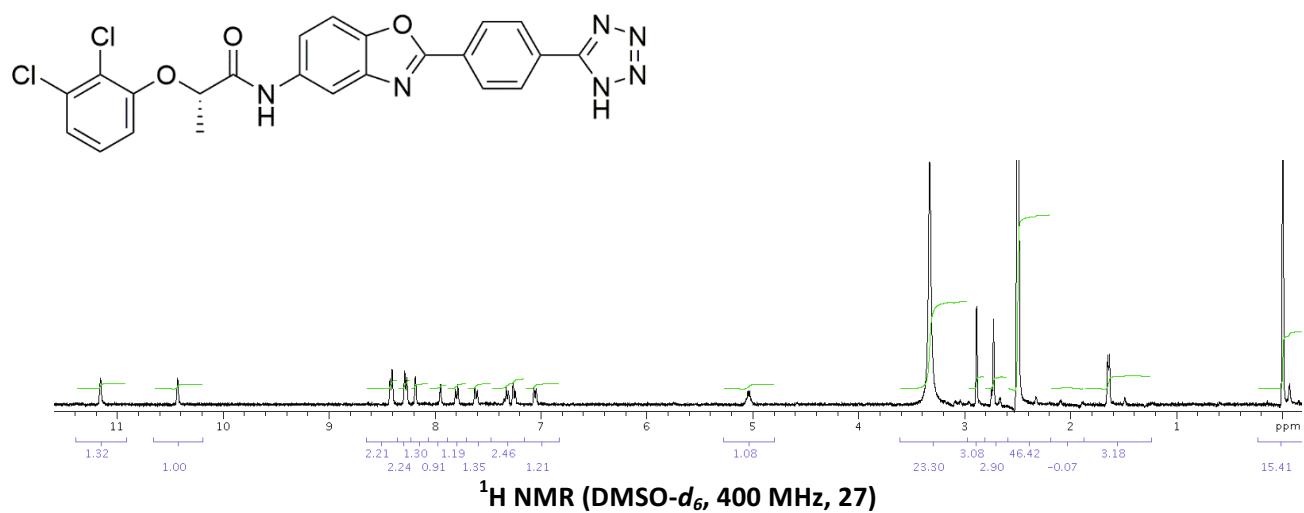
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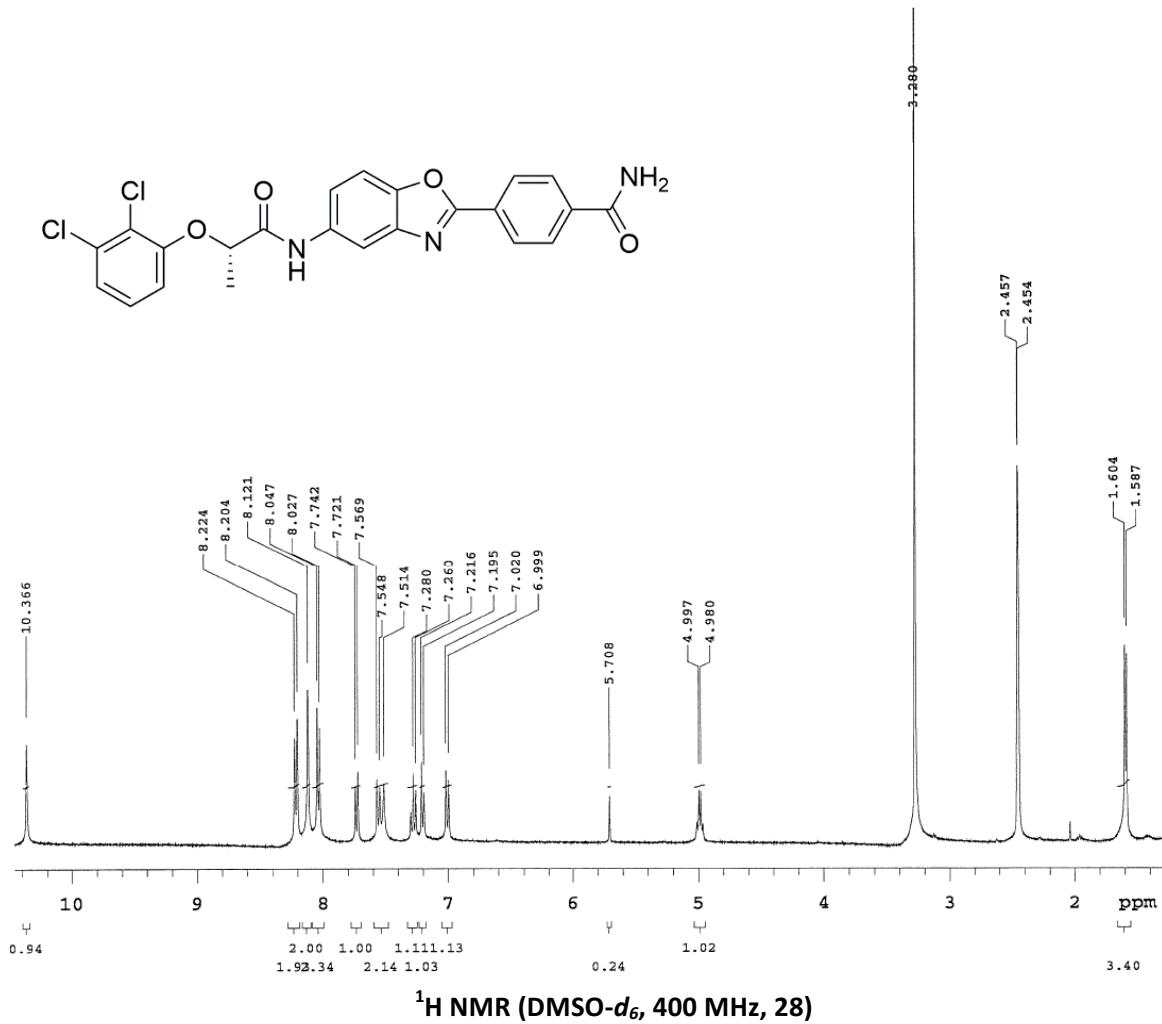


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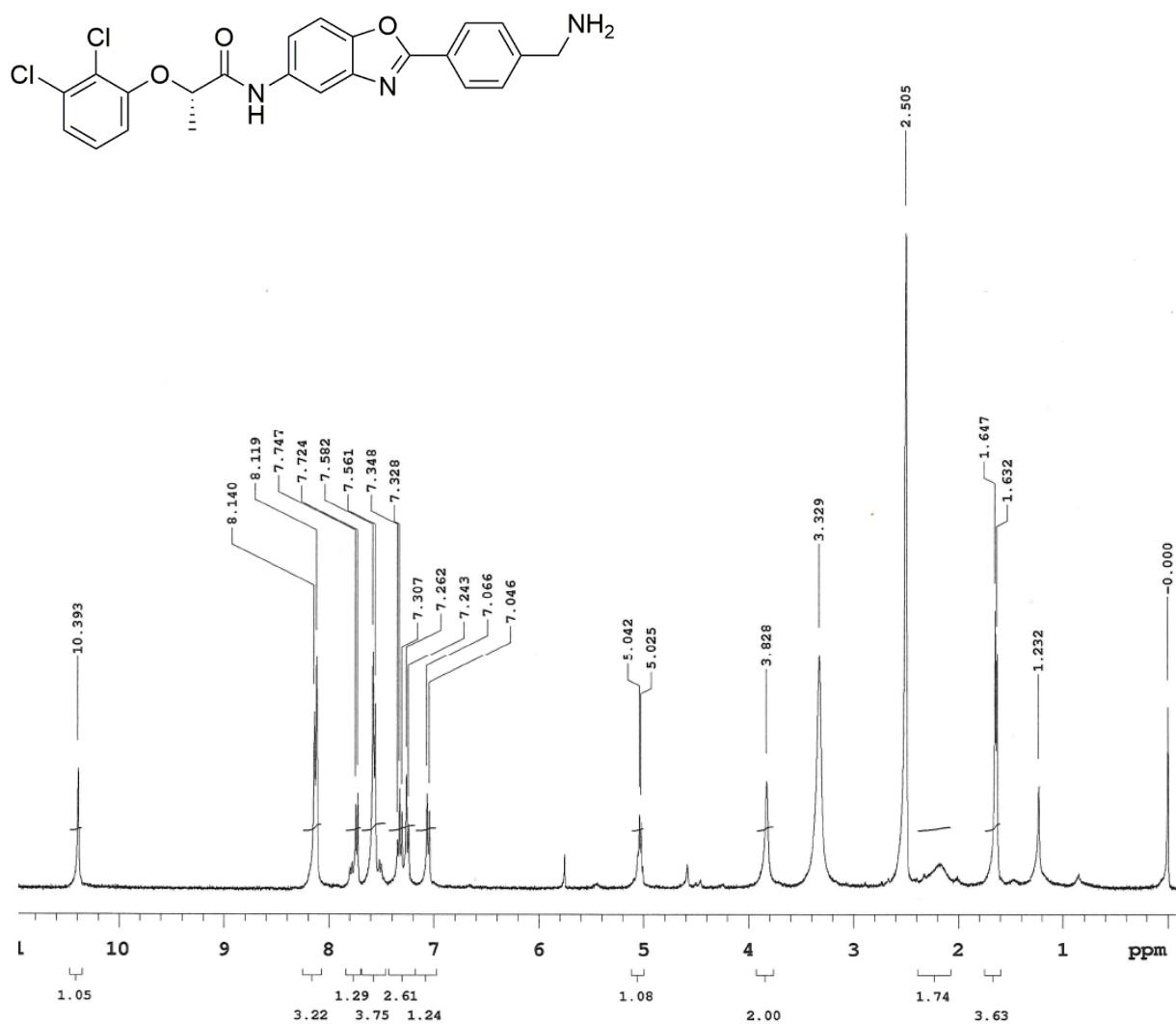


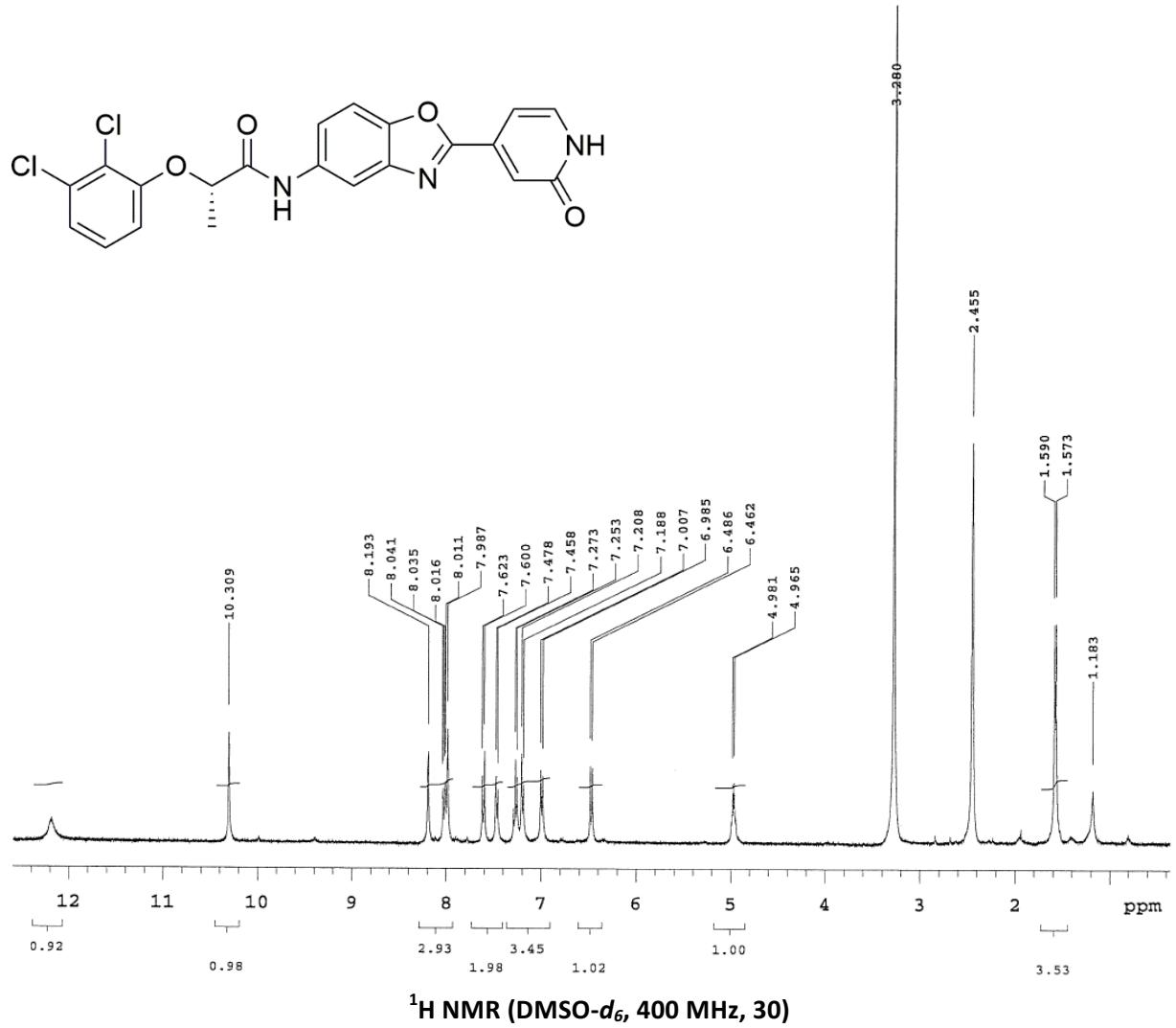
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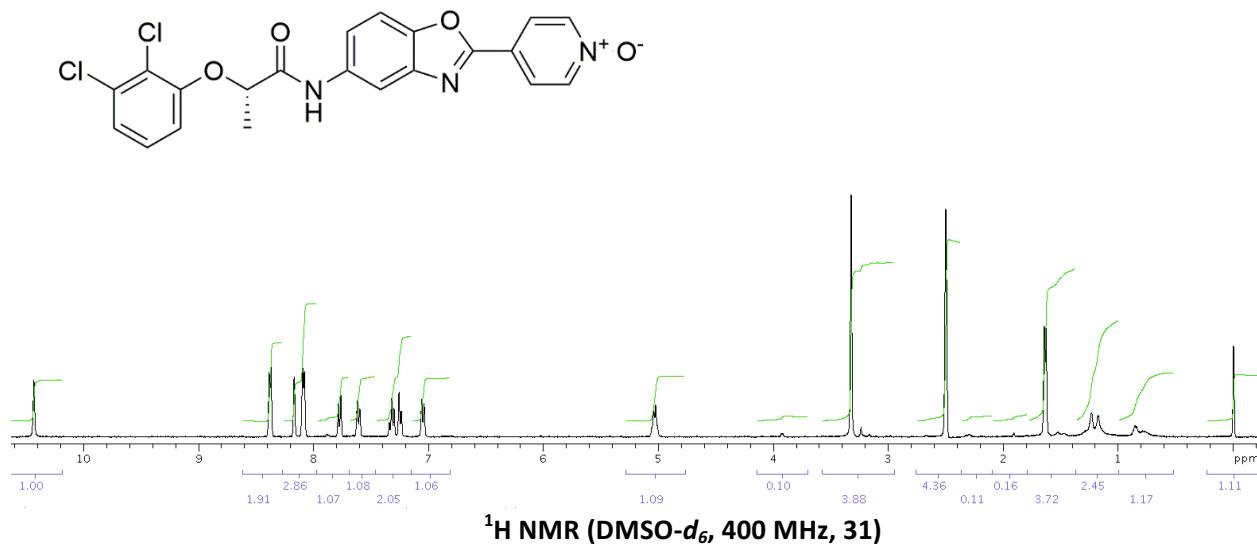


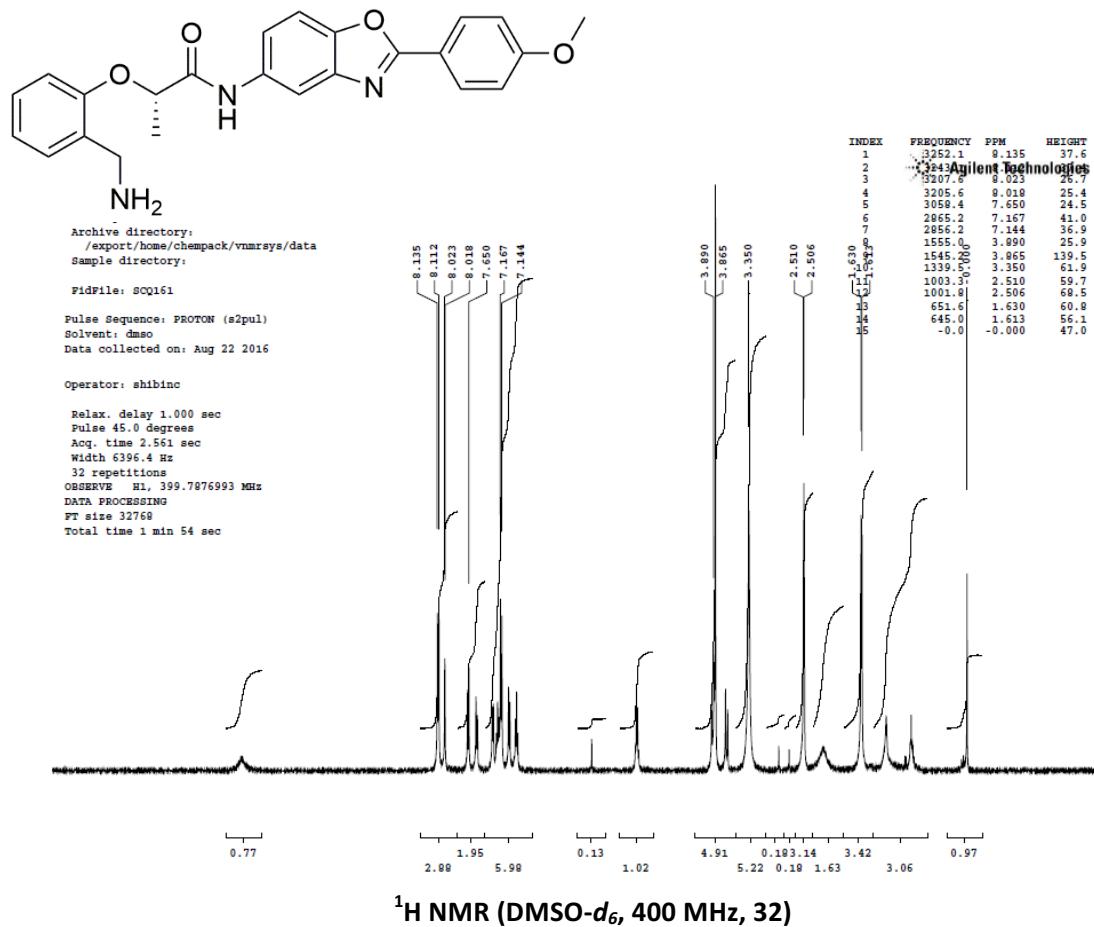
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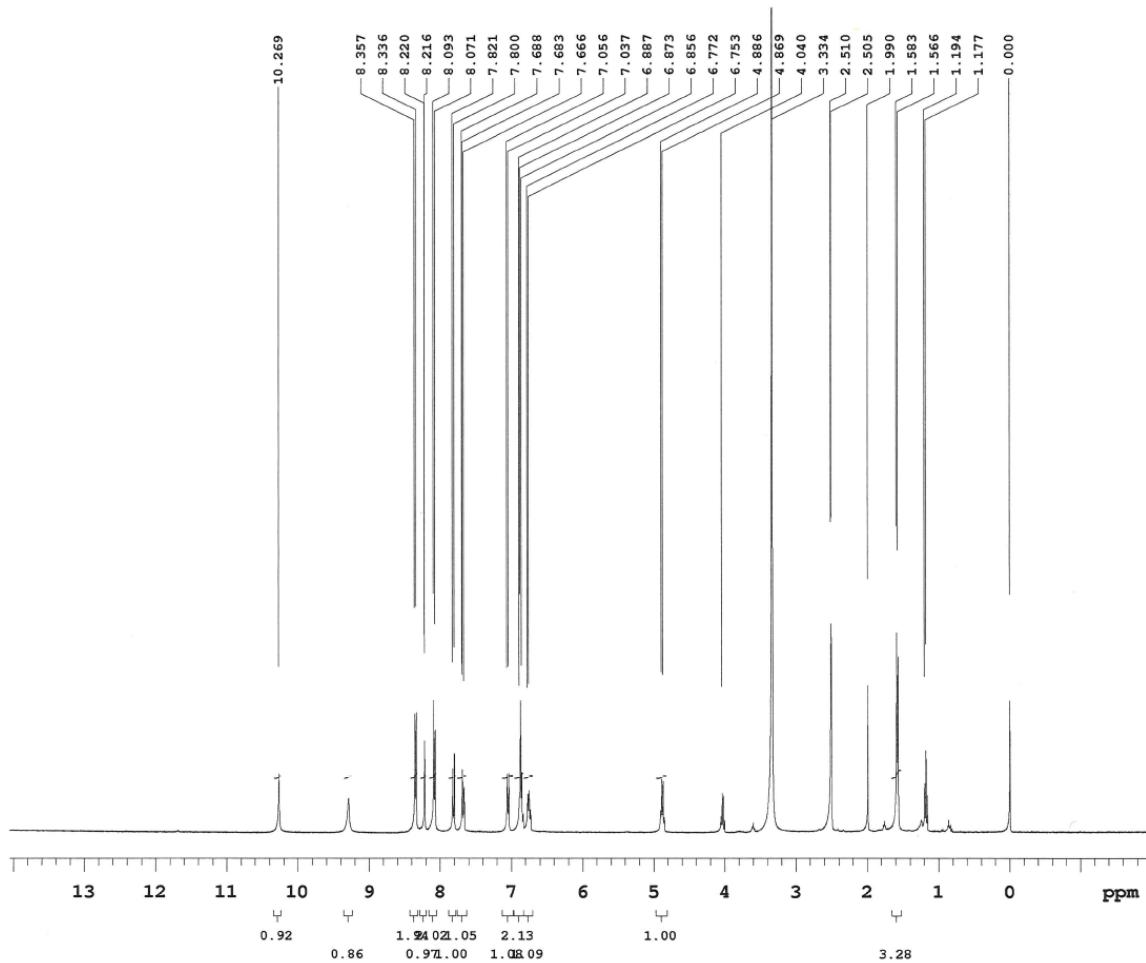
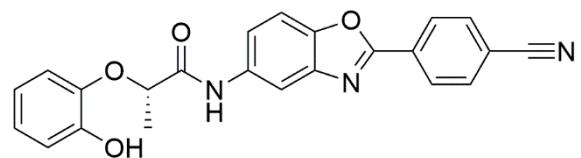


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¹H NMR (DMSO-*d*₆, 400 MHz, 33)