

Supplementary Information

Synthesis, Structure and Stereochemistry of Dispirocompounds Based on Imidazothiazolotriazine and Pyrrolidineoxindole

Alexei N. Izmes't'ev ¹, Valentina A. Karnoukhova ², Alexander A. Larin ¹, Angelina N. Kravchenko ¹, Leonid L. Fershtat ¹ and Galina A. Gazieva ^{1,*}

¹ N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prosp., Moscow 119991, Russia

² A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilova Street, Moscow 119991, Russia

* Correspondence: gaz@ioc.ac.ru

Table of Contents

1. Column chromatography	S2
2. Crystallographic data for 3a , 4e and 7c	S3
3. Spectra ¹ H and ¹³ C NMR of compounds 3a-e and { ¹ H- ¹ H} NOESY NMR of 3a,b	S4
4. Spectra ¹ H and ¹³ C NMR of compounds 4a-e	S16
5. Spectra ¹ H and ¹³ C NMR of compounds 6a-e and { ¹ H- ¹ H} NOESY NMR of 6a	S26
6. Spectra ¹ H and ¹³ C NMR of compounds 7a-e and { ¹ H- ¹ H} NOESY NMR of 7b	S37

Column chromatography

Column chromatography was carried out with silica gel (Acros Silica gel, for column chromatography, 60 Angstrom pore size, 0.040–0.063 mm) and to monitor the preparative separations, analytical thin layer chromatography (TLC) was performed at room temperature on pre-coated 0.25 mm thick silica gel 60 F₂₅₄ aluminum plates 20 × 20 cm Merck, Darmstadt, Germany. Propanol-2 was used as eluent without preliminary purification.

Example of preparative separation of a mixture of diastereomers **3a** and **4a** using column chromatography. Chromatograms of the collected fractions of diastereomers **3a** ($R_f = 0.21$) and **4a** ($R_f = 0.53$).

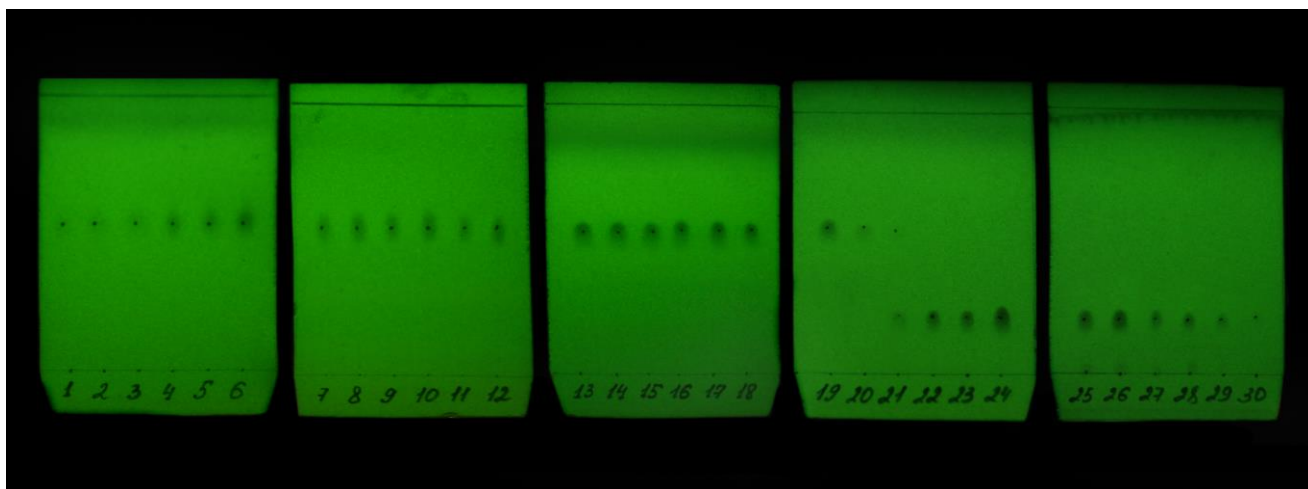


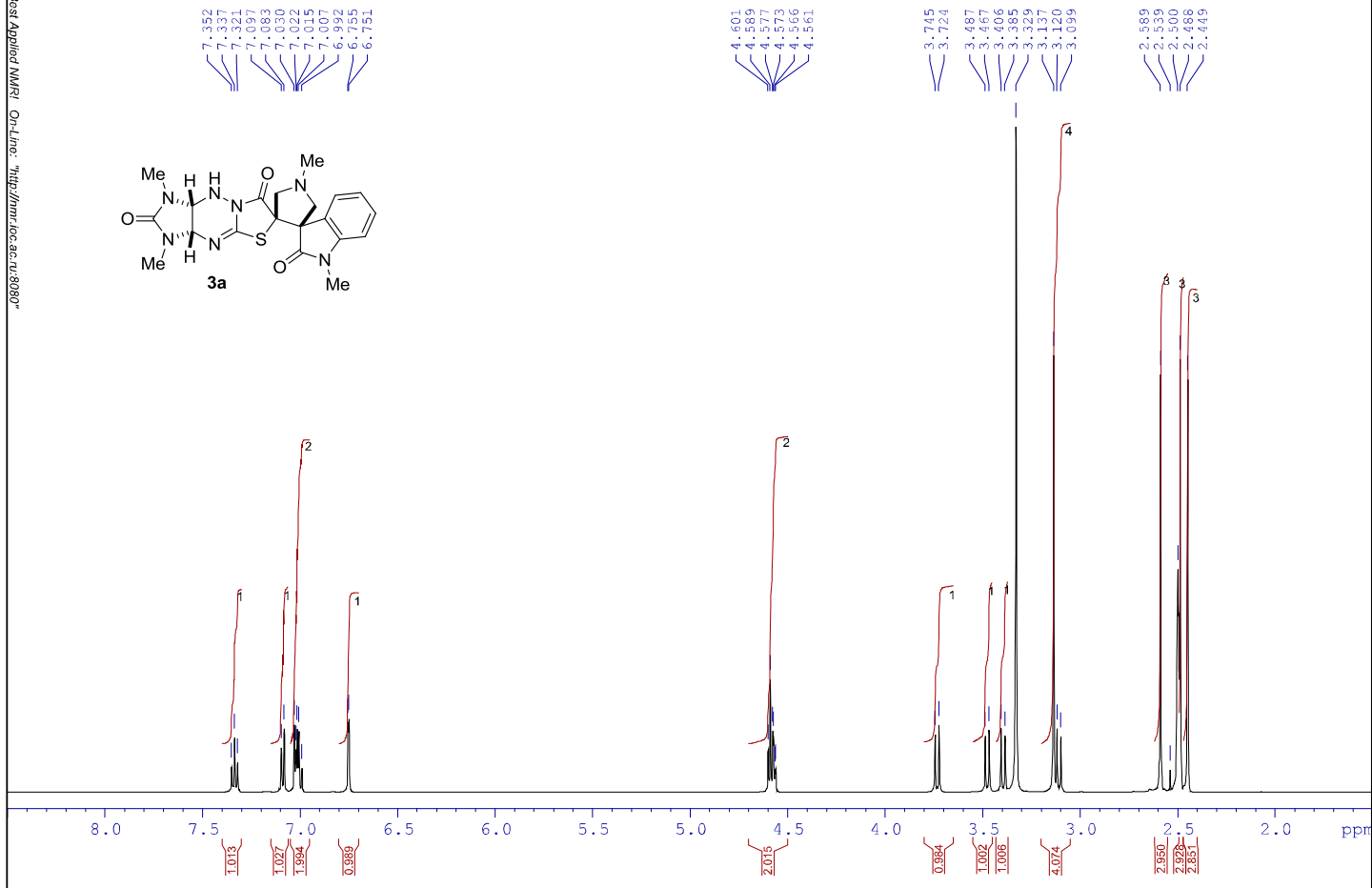
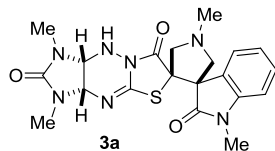
Table S1. Crystallographic data for **3a**, **4e** and **7c**

	3a	4e	7c
CCDC	2215817	2215818	2215819
Empirical formula	C ₂₀ H ₂₃ N ₇ O ₃ S	C ₂₇ H ₃₉ N ₇ O ₅ S	C ₂₀ H ₂₃ N ₇ O ₂ S ₂
Formula weight	441.51	573.71	457.57
T (K)	120	295	120
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	P2 ₁ /c	P2 ₁ 2 ₁ 2 ₁	P-1
Z / Z'	4 / 1	4 / 1	2 / 1
<i>a</i> , Å	10.4431(7)	9.5788(2)	8.8678(4)
<i>b</i> , Å	15.6683(11)	16.7852(3)	9.6639(5)
<i>c</i> , Å	13.1324(9)	18.1337(3)	13.3198(5)
α , °	90	90	87.1340(10)
β , °	109.1969(14)	90	70.557(2)
γ , °	90	90	80.6250(10)
<i>V</i> , Å ³	2029.3(2)	2915.57(9)	1061.99(8)
<i>d</i> _{calc} (g cm ⁻³)	1.445	1.307	1.431
μ , cm ⁻¹	1.99	1.6	2.84
F(000)	928	1224	480
2 θ _{max} , °	61.4	61.1	61.2
Refls collected	27883	44223	14488
Independent refls [Rint]	6271 [0.0431]	8926 [0.0869]	6495 [0.0164]
Observed refls [<i>I</i> > 2 σ (<i>I</i>)]	5148	4752	5733
Parameters	288	408	288
<i>R</i> 1	0.0399	0.0562	0.0323
w <i>R</i> 2	0.1075	0.1332	0.0860
GOF	1.035	1.015	1.022
Residual density, $\Delta\rho_{\max}/\Delta\rho_{\min}$ (e Å ⁻³)	0.525/-0.252	0.402/-0.211	0.466/-0.274

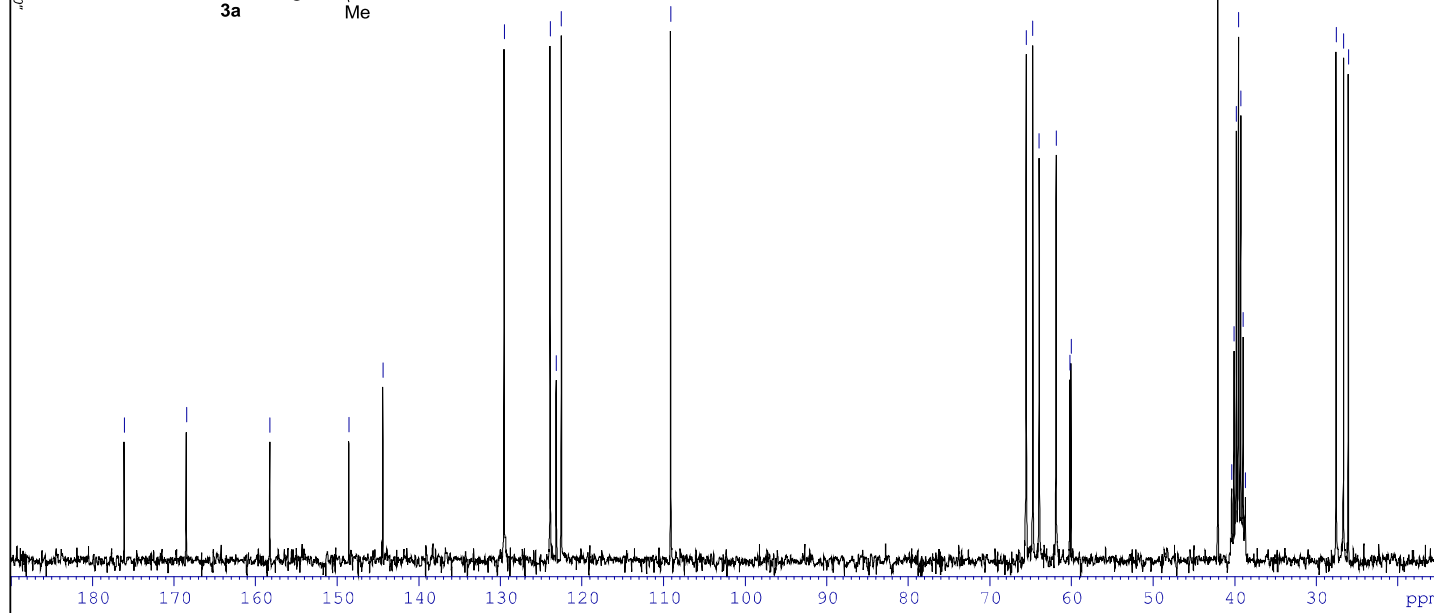
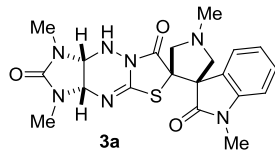
Table S2. Sum of CNN, CNC, NNH and CNH angles (°) for **3a**, **4e** and **7c**

	3a	4e	7c
N(1)	351.06	354.39	359.4
N(2)	354.39	351.93	358.31
N(3)	330.04	327.83	340.06
N(4)	334.77	333.51	337.69

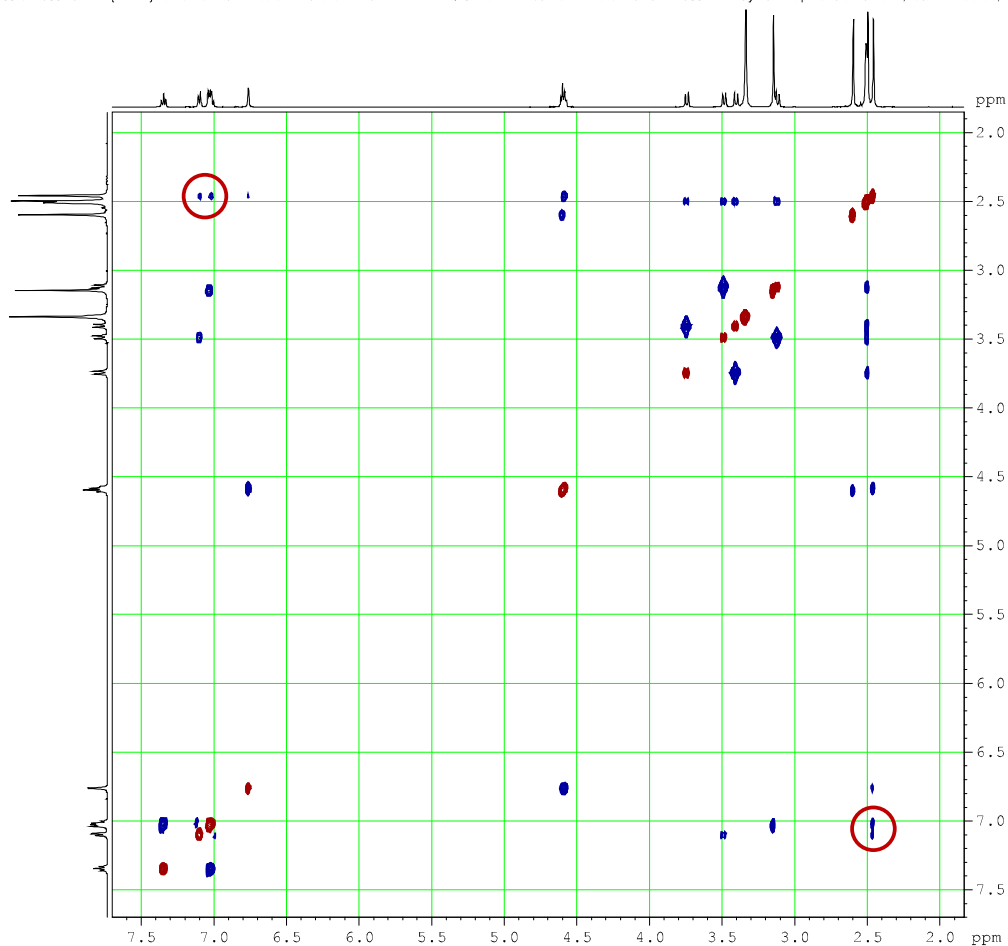
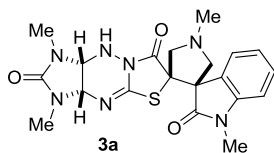
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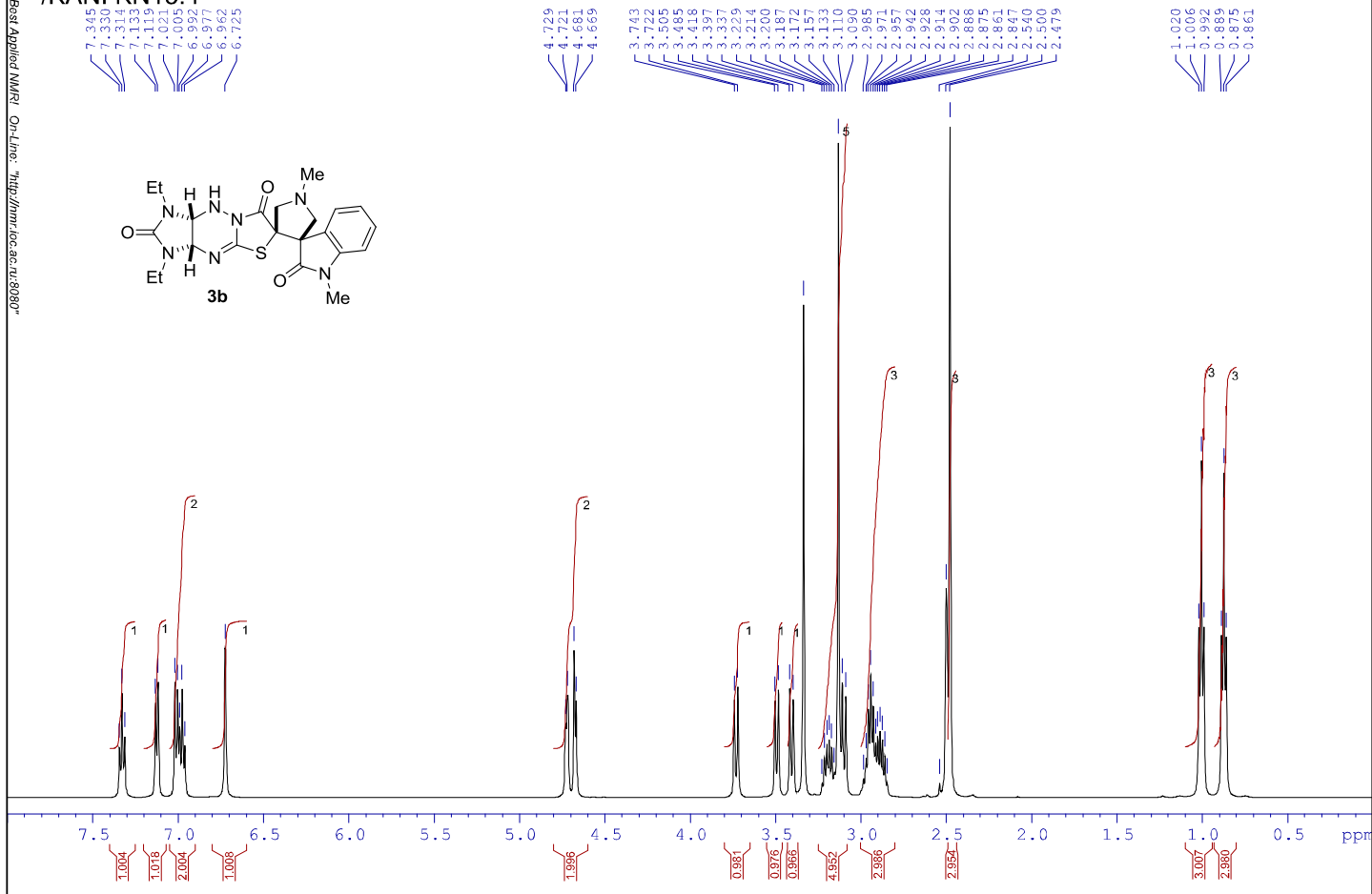
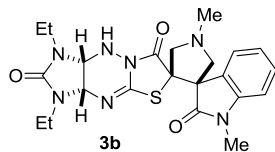
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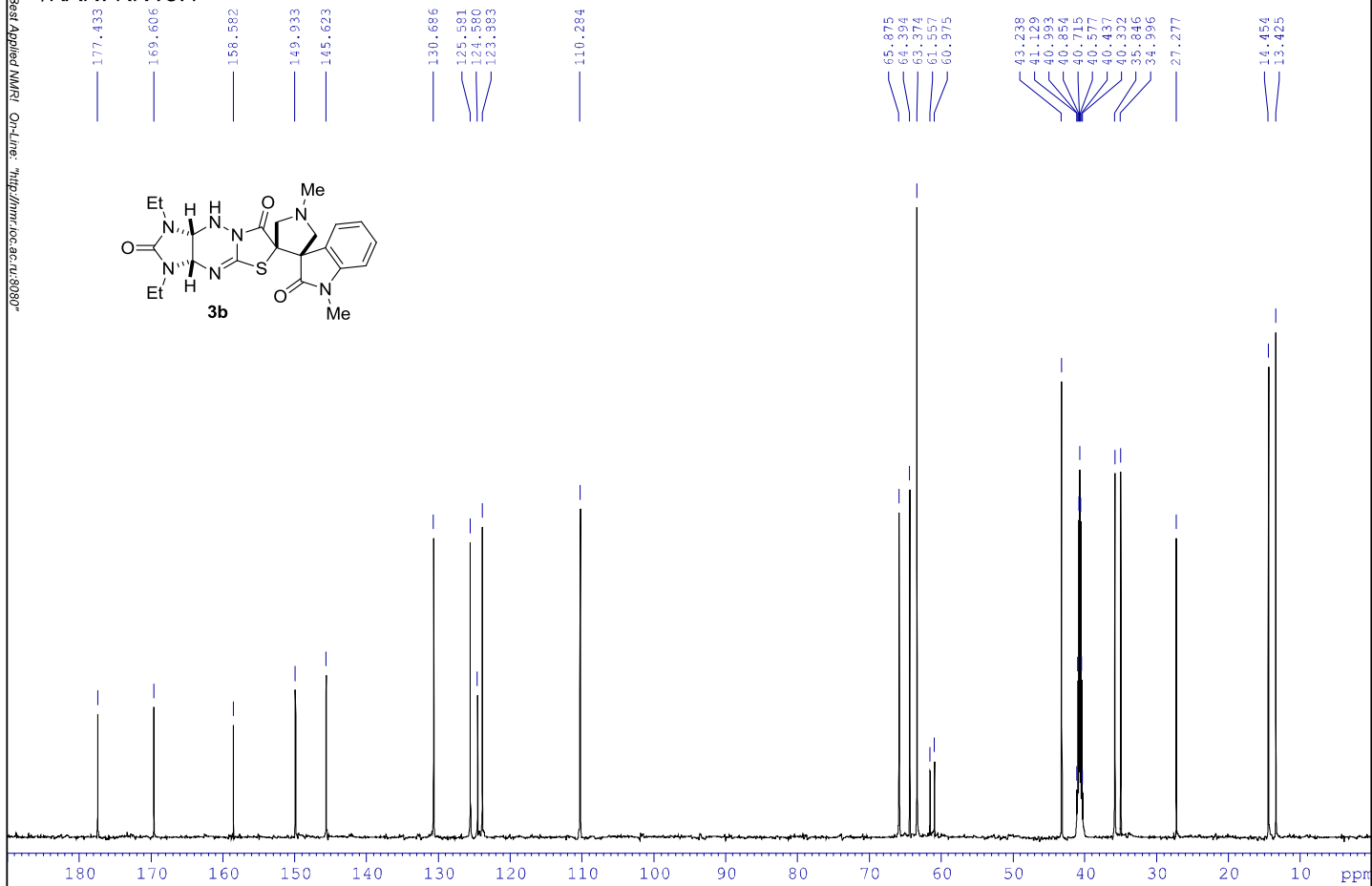
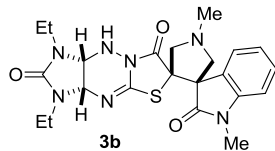
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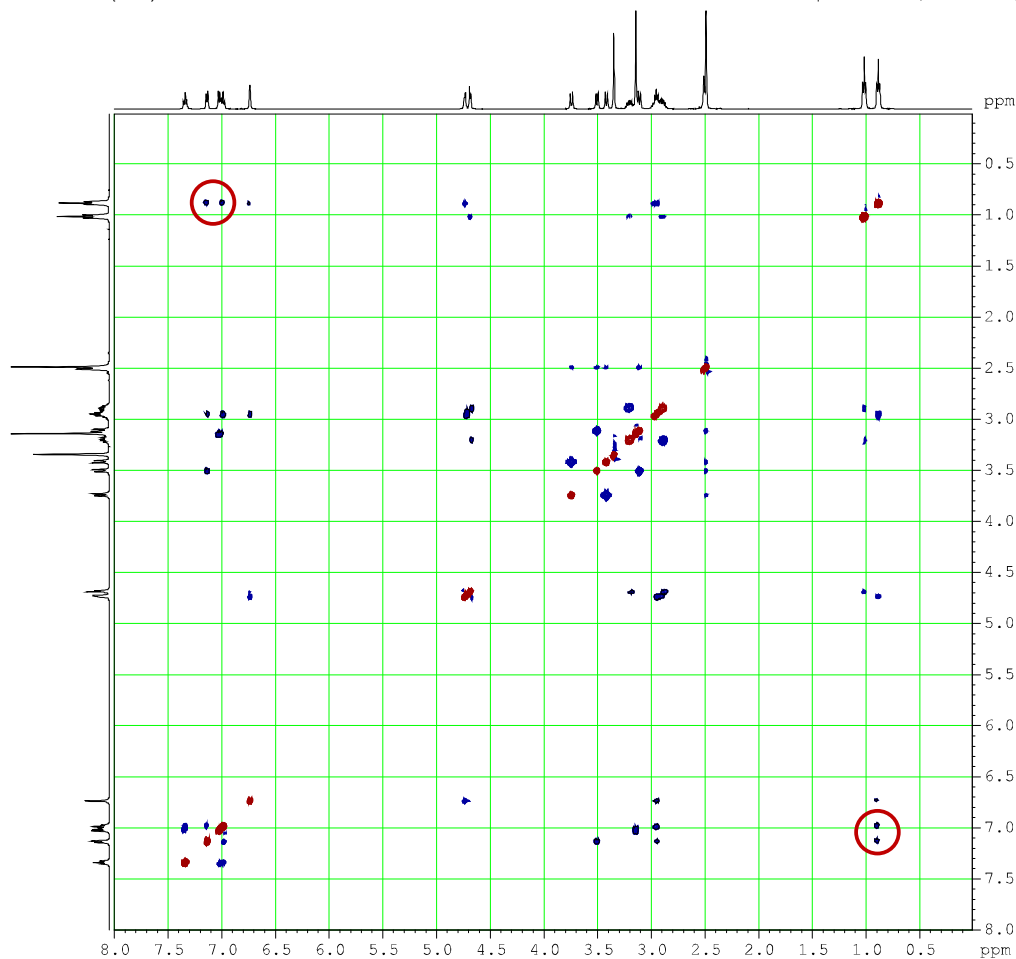
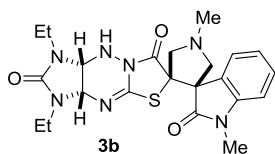
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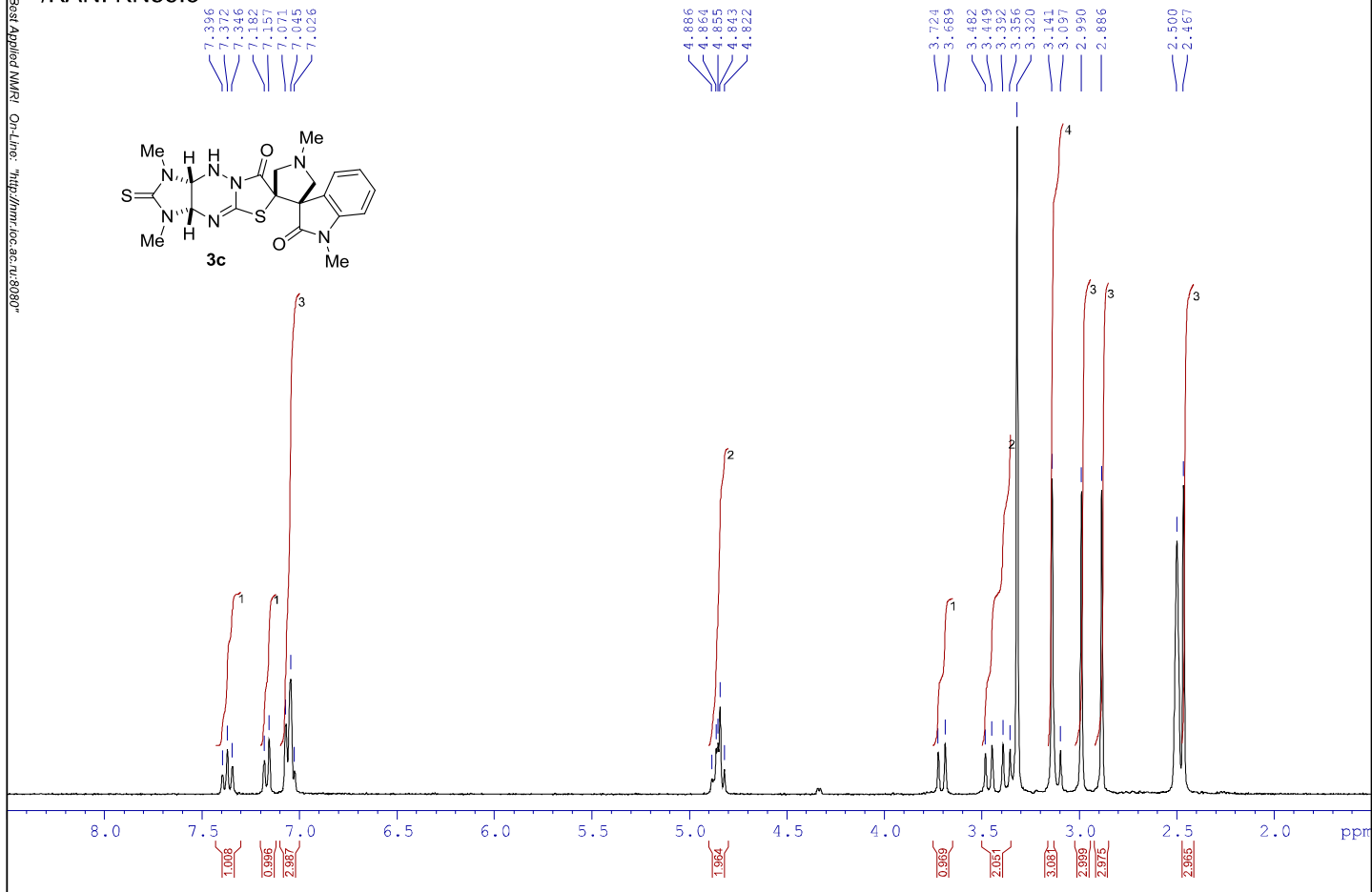
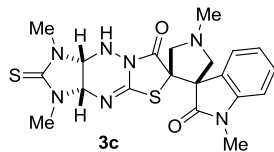
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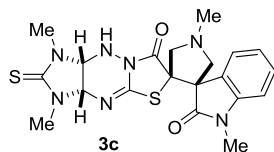
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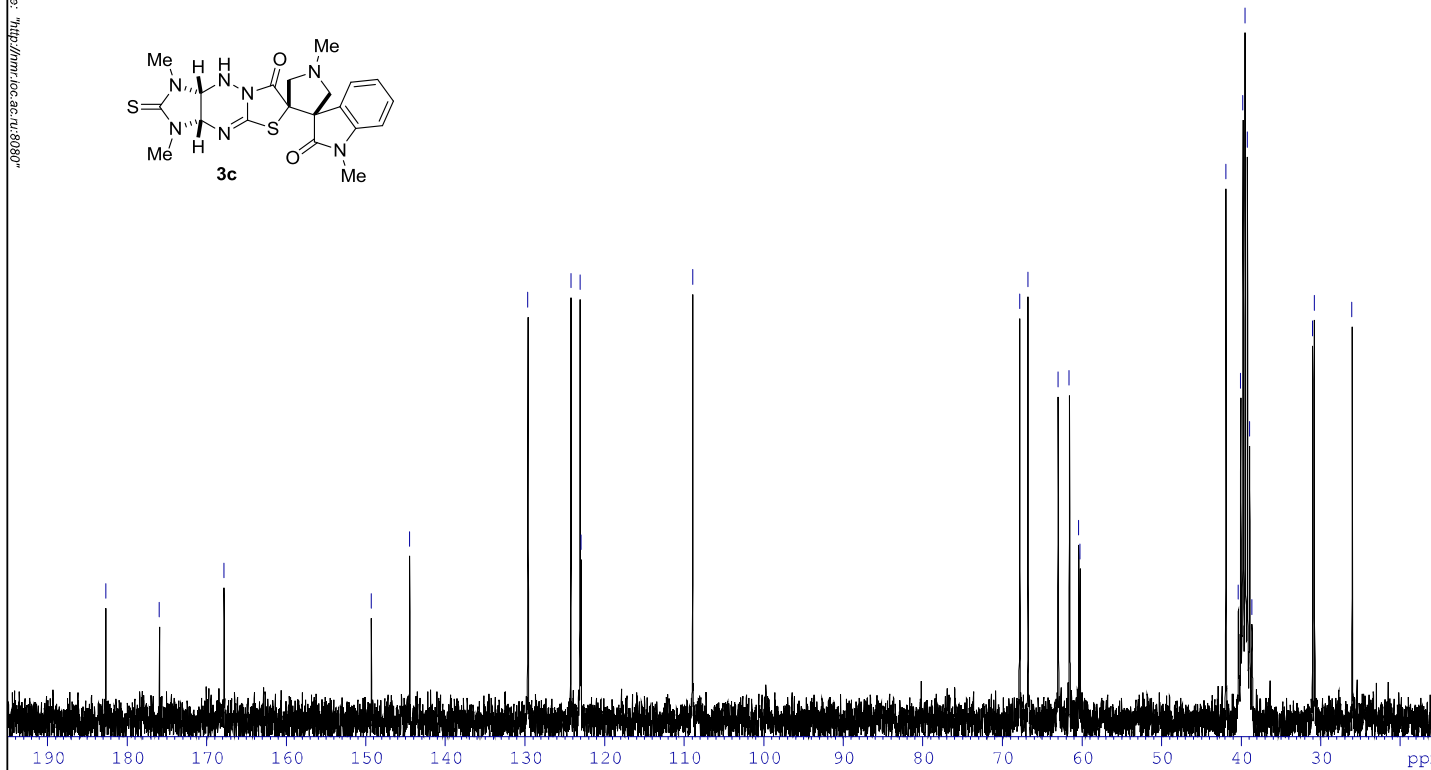
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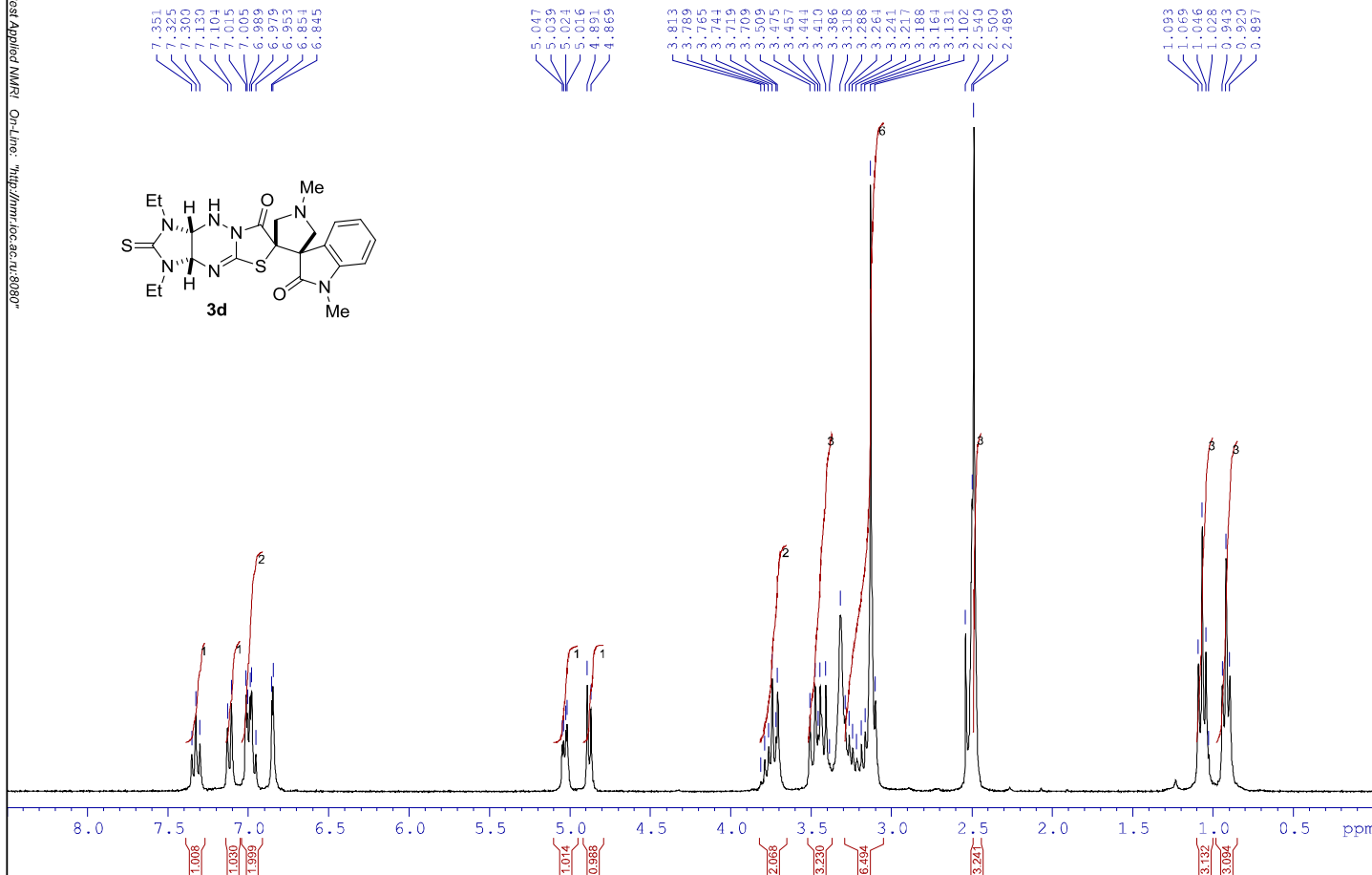
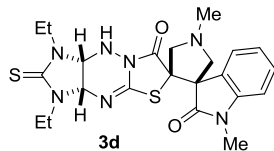
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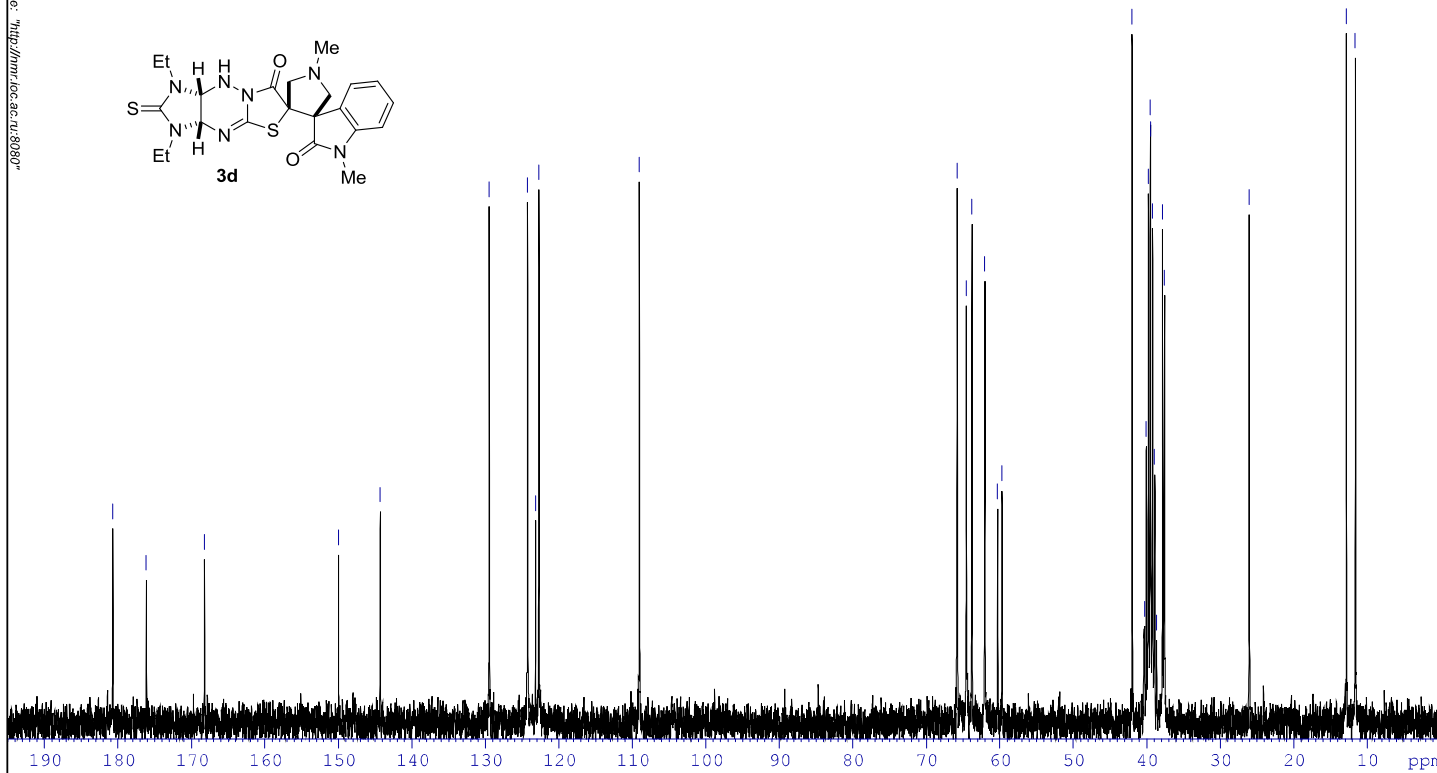
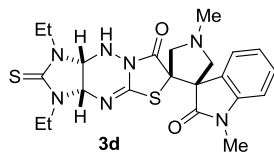
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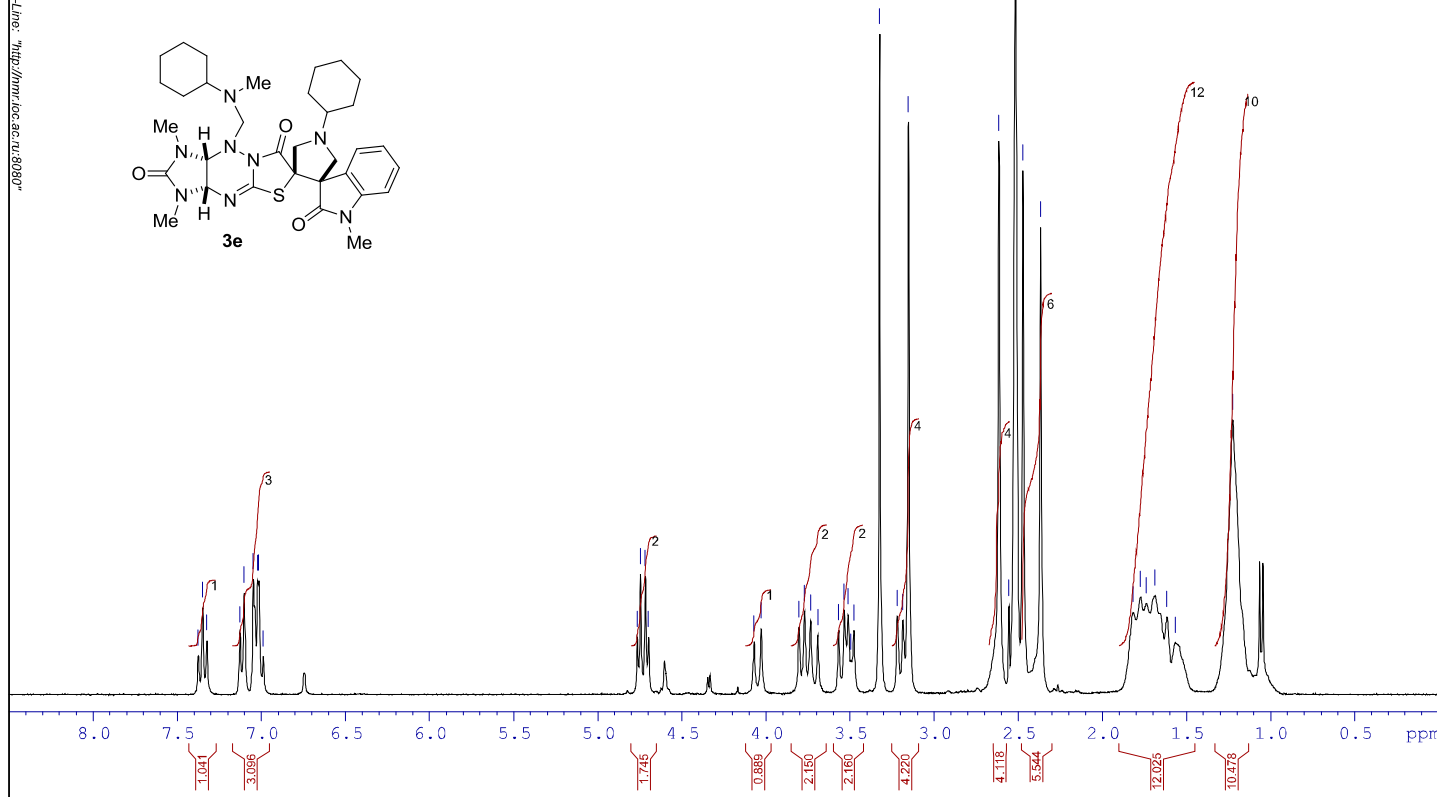
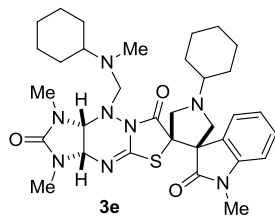
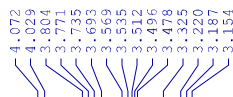
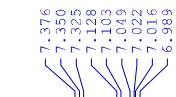
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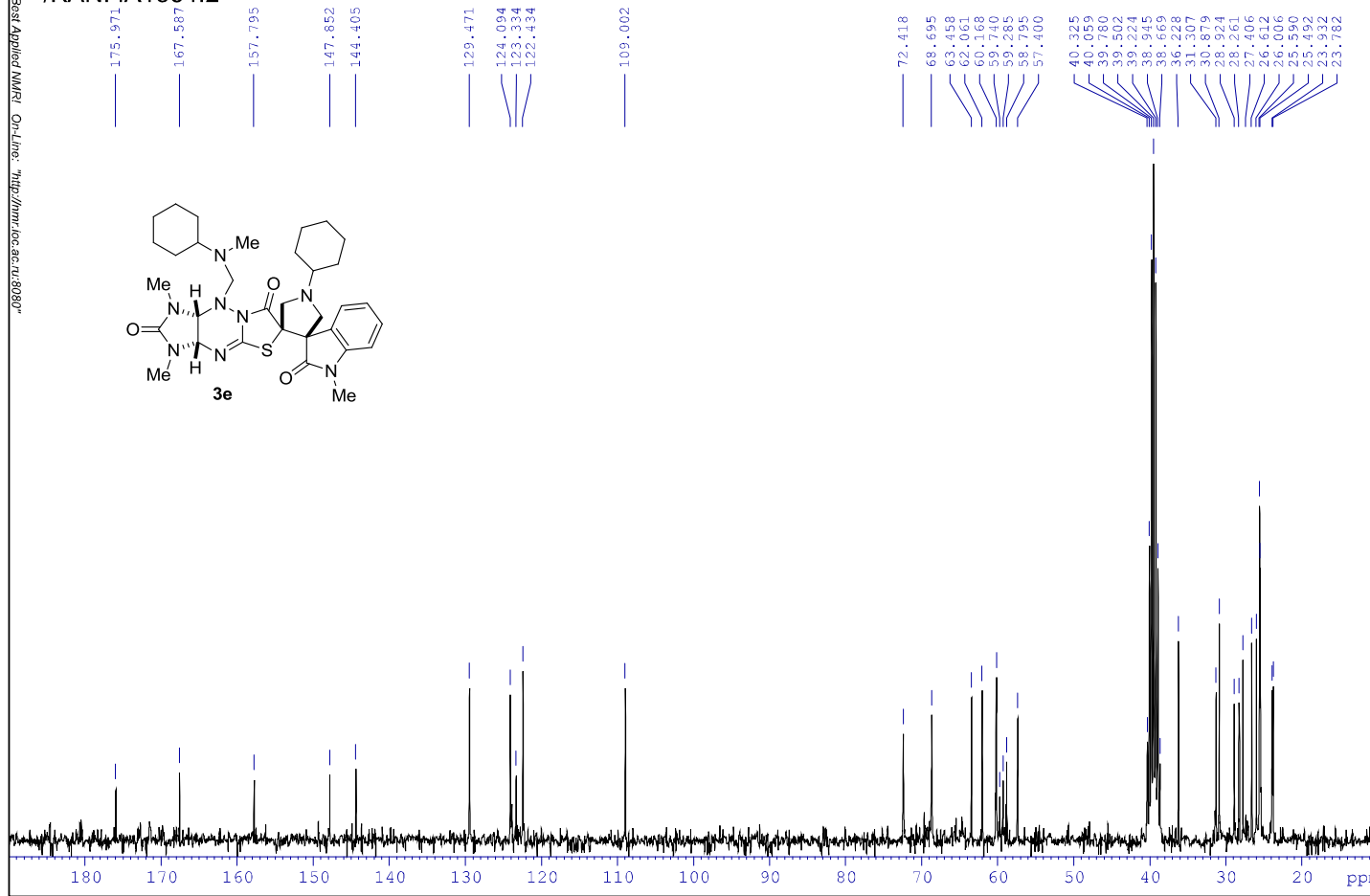
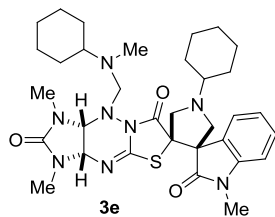
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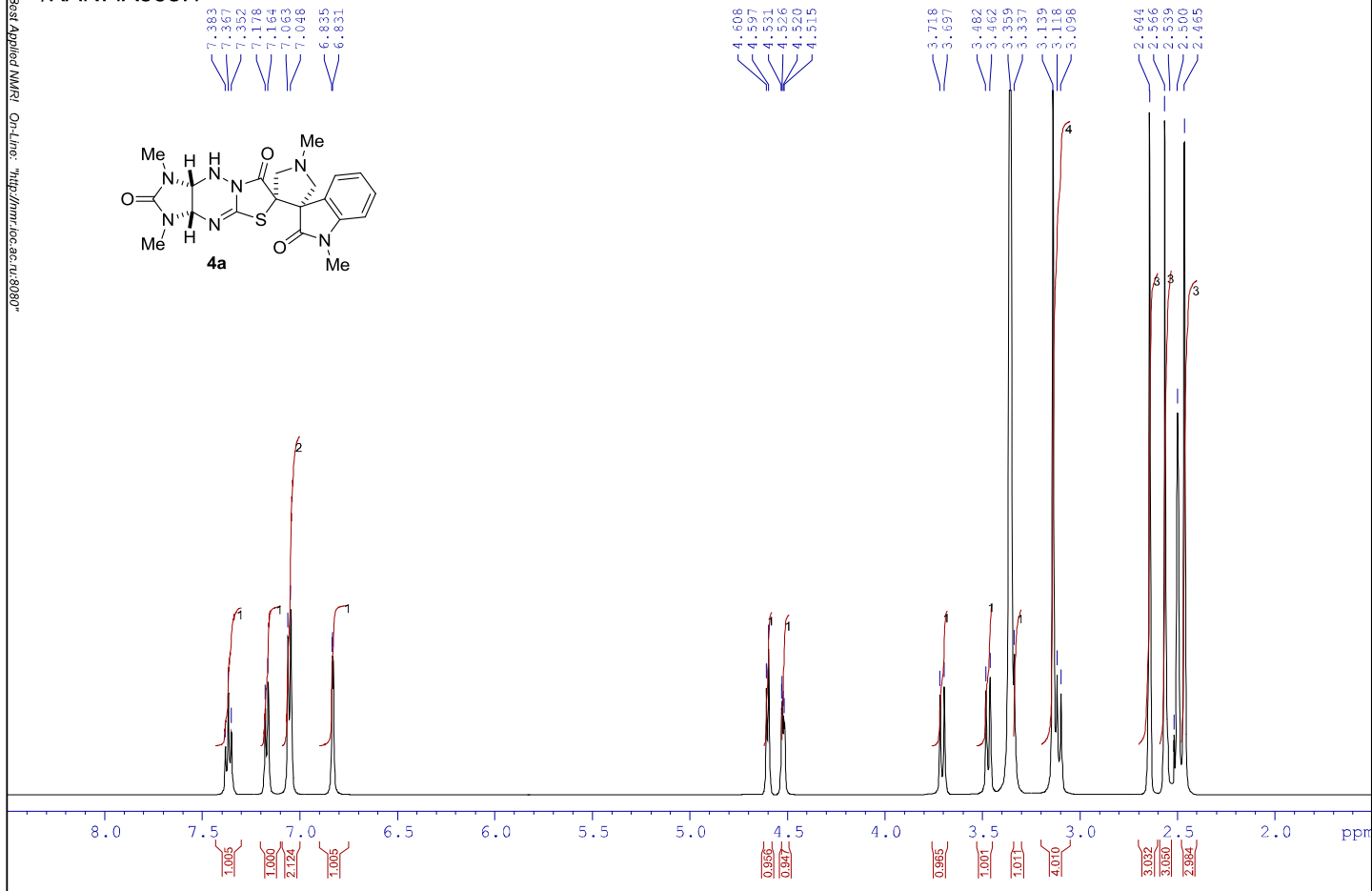
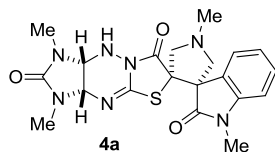
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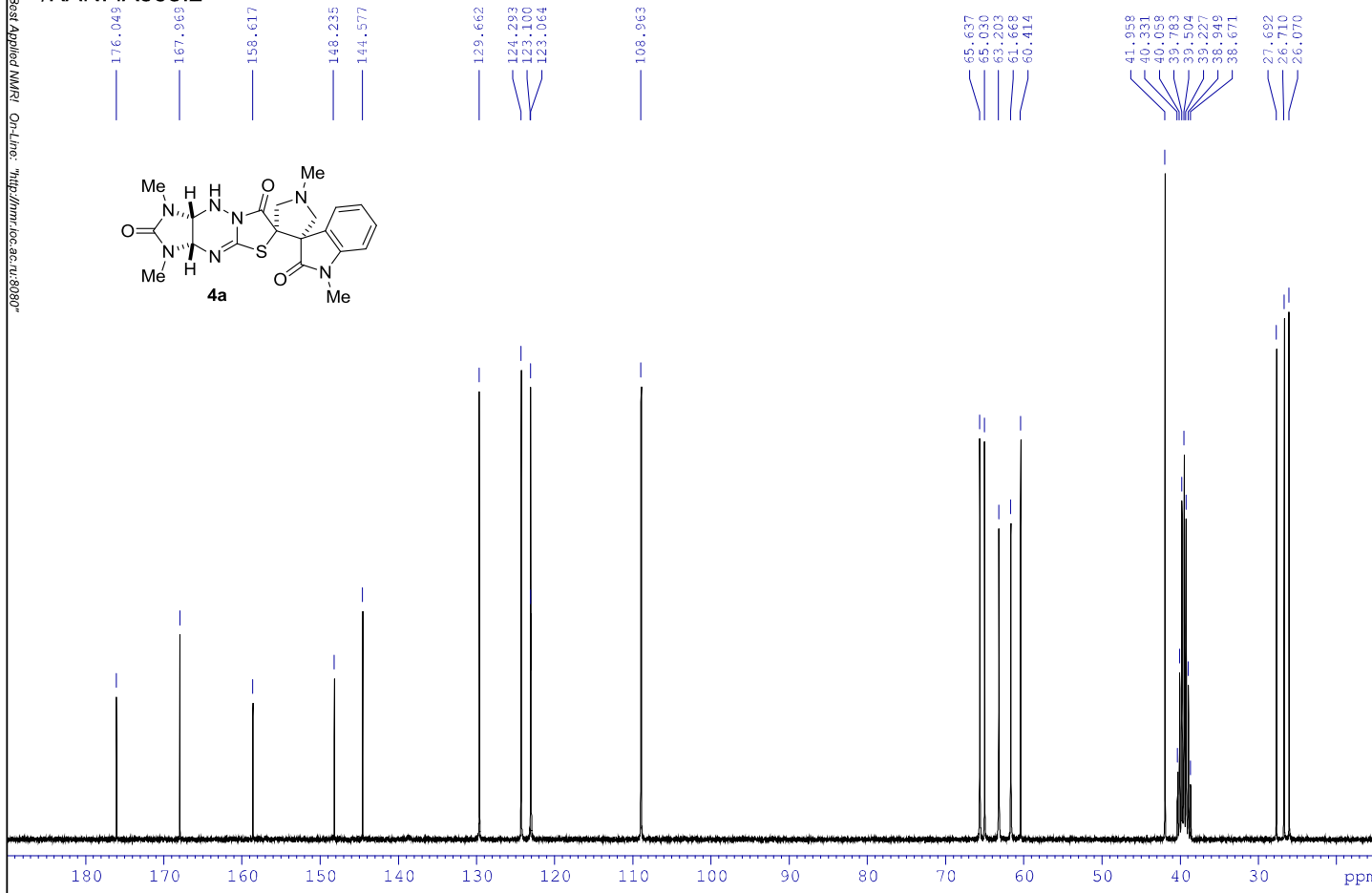
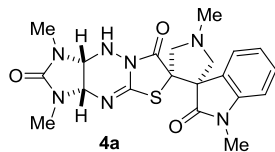
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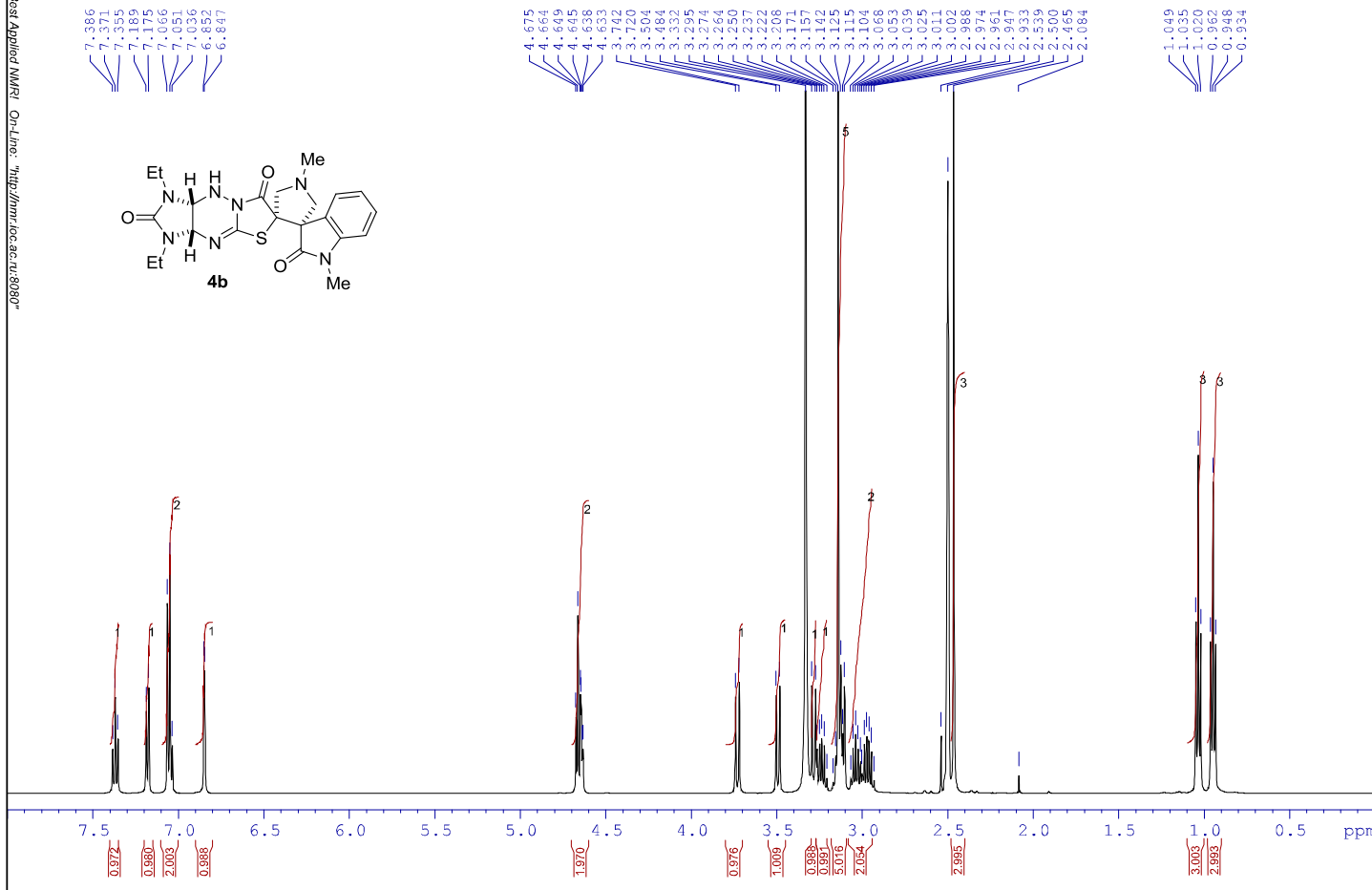
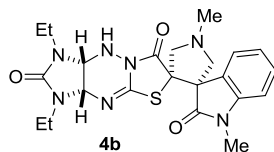
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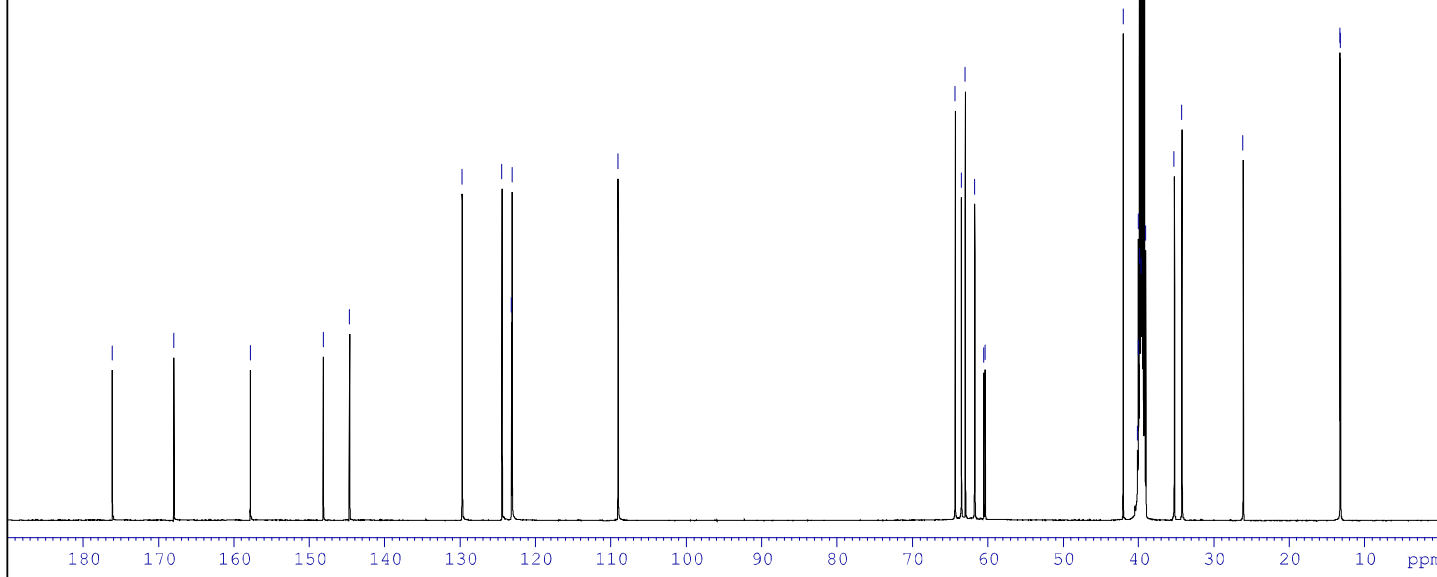
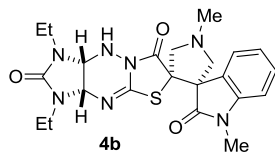
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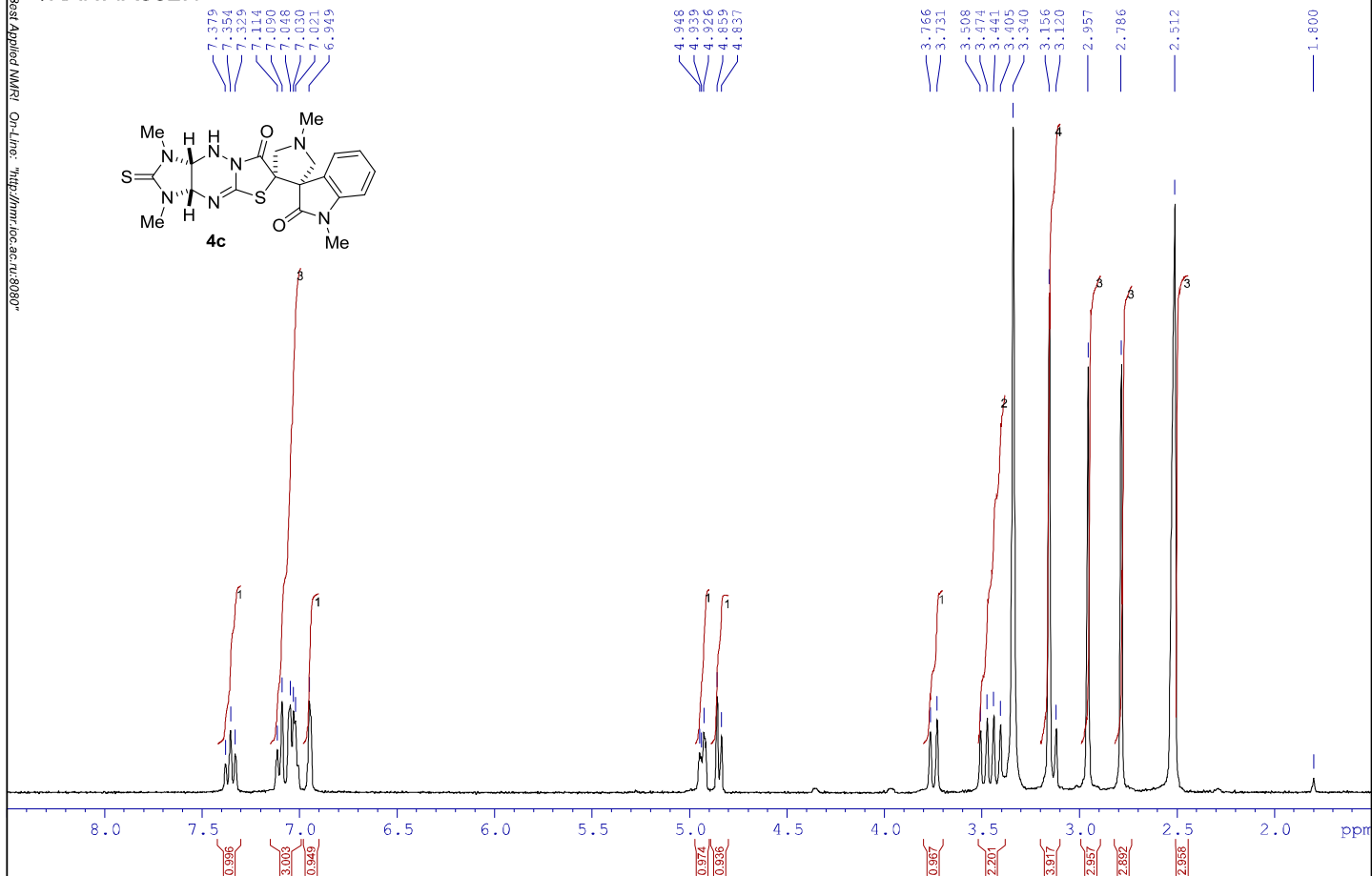
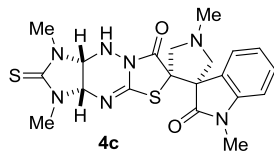
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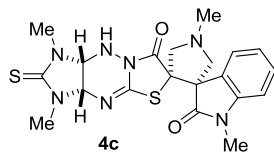
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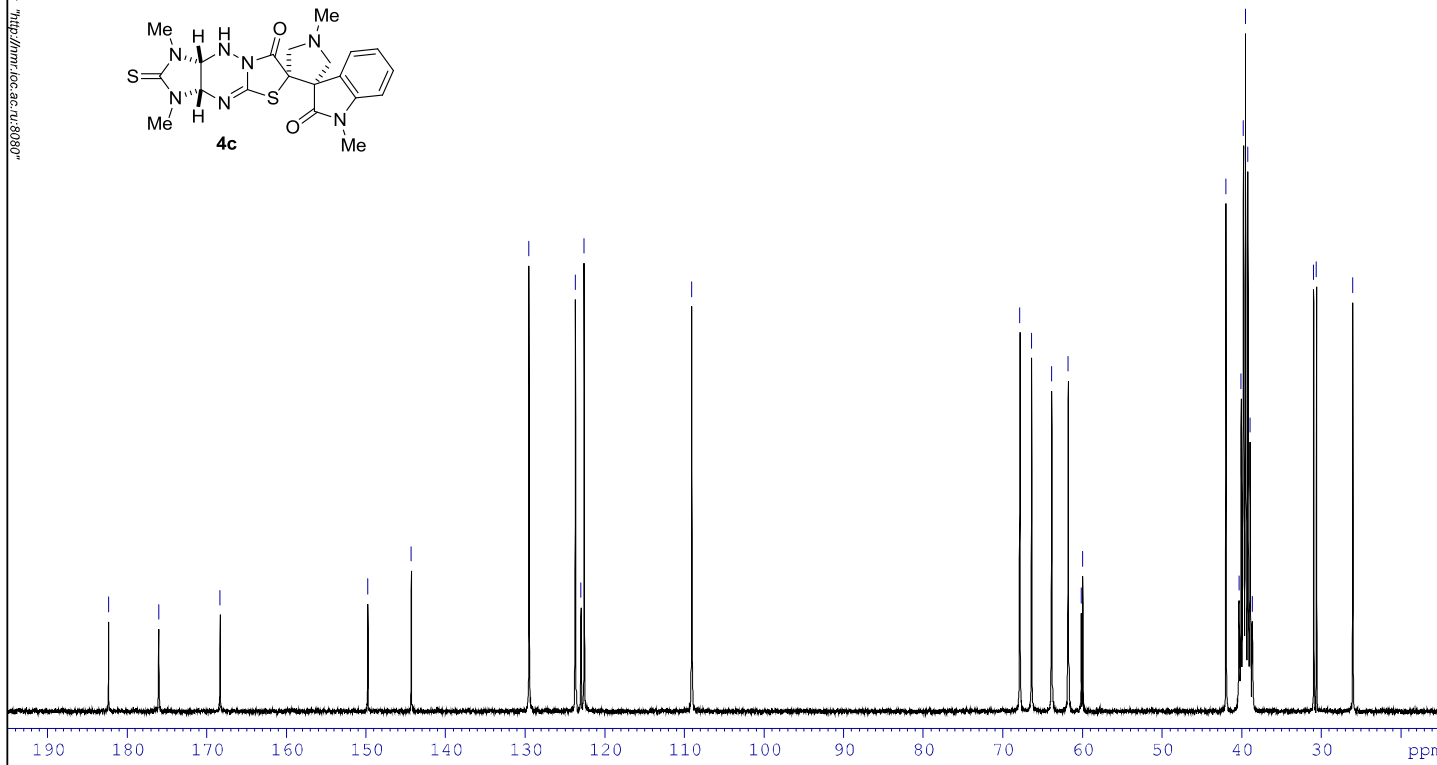
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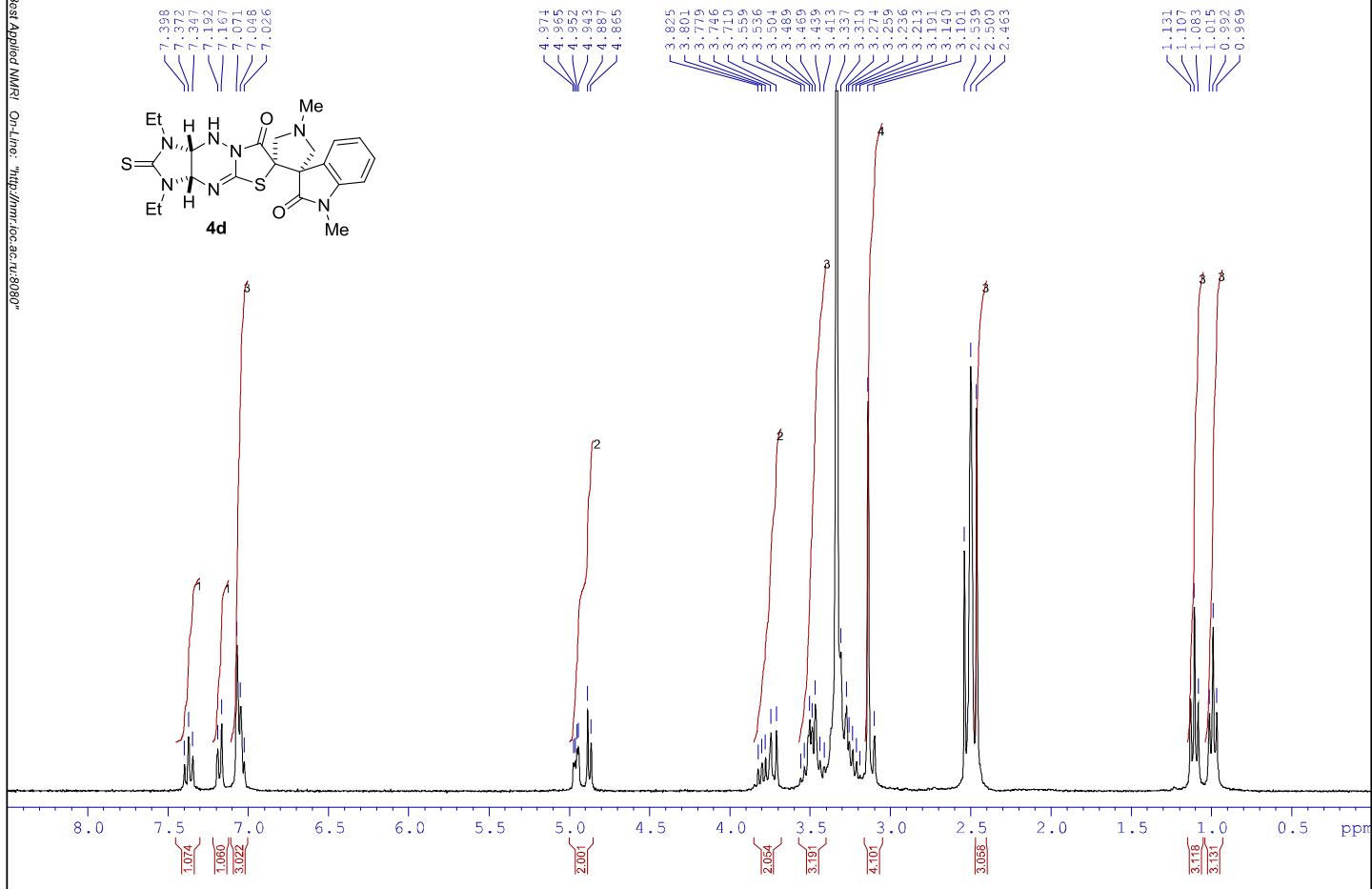
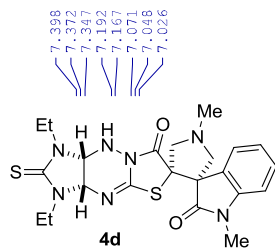
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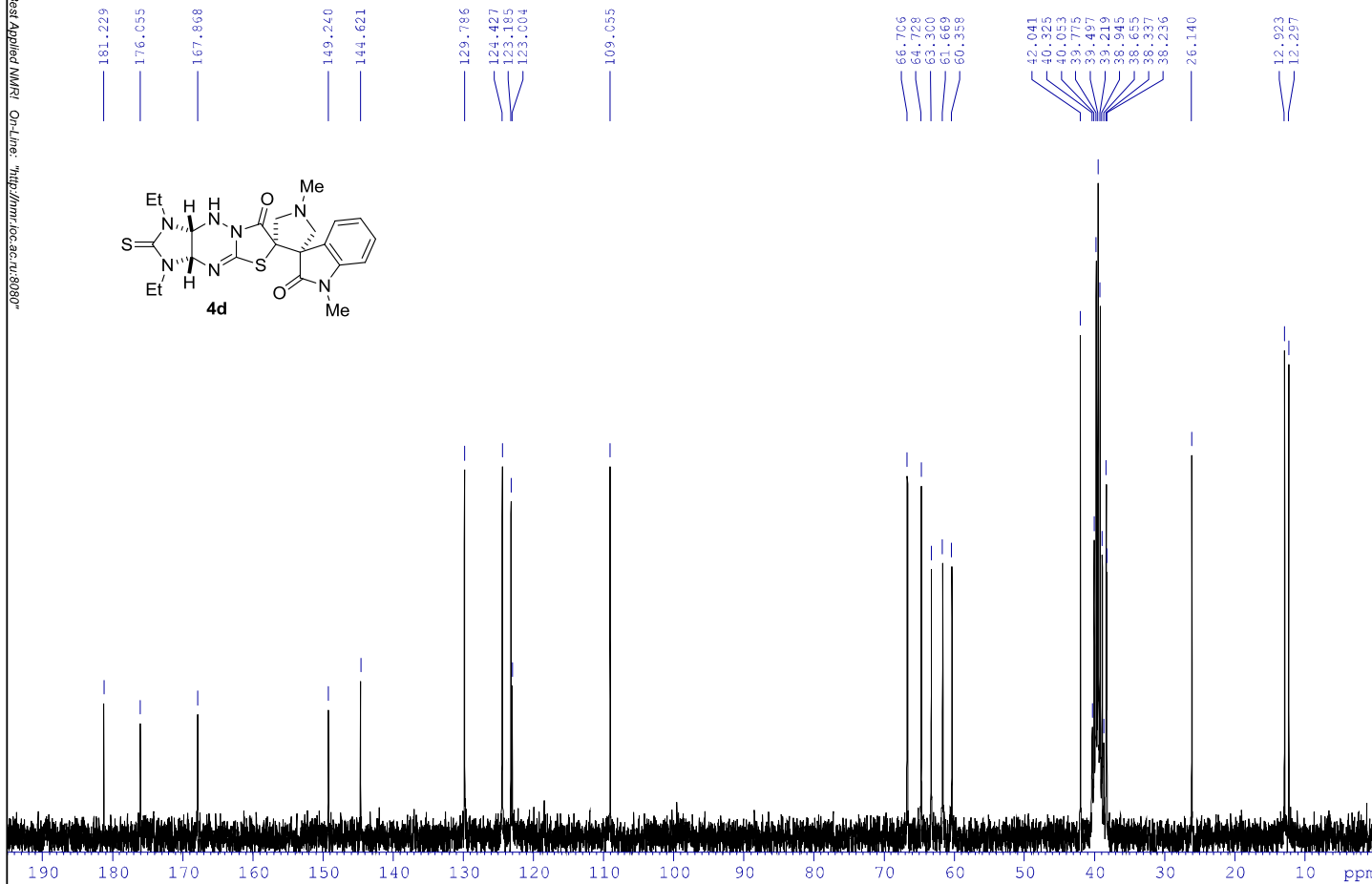
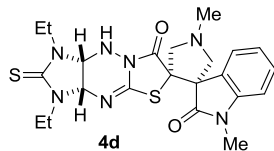
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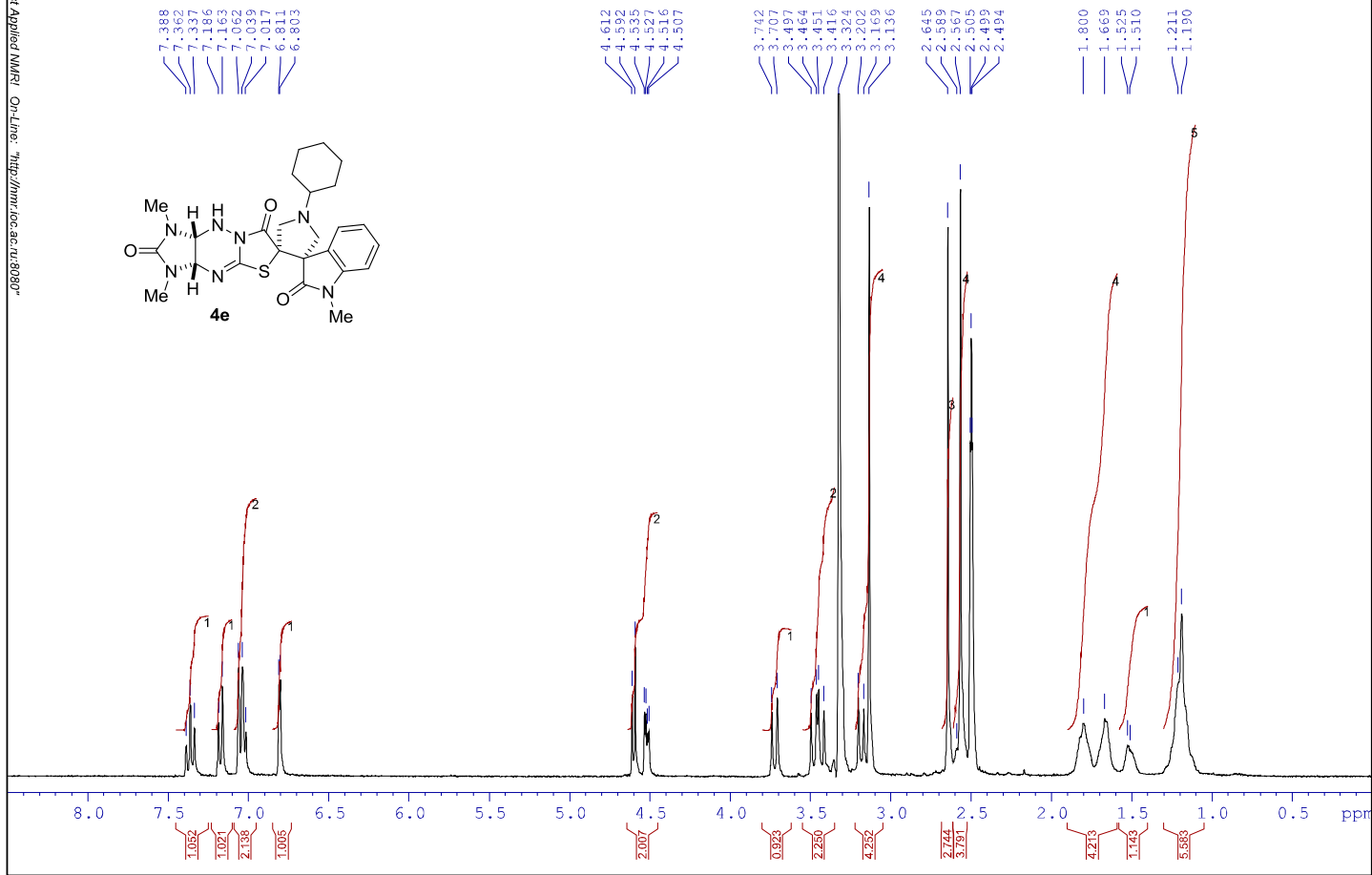
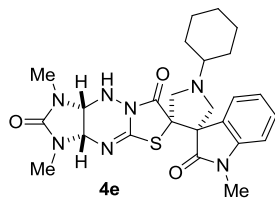
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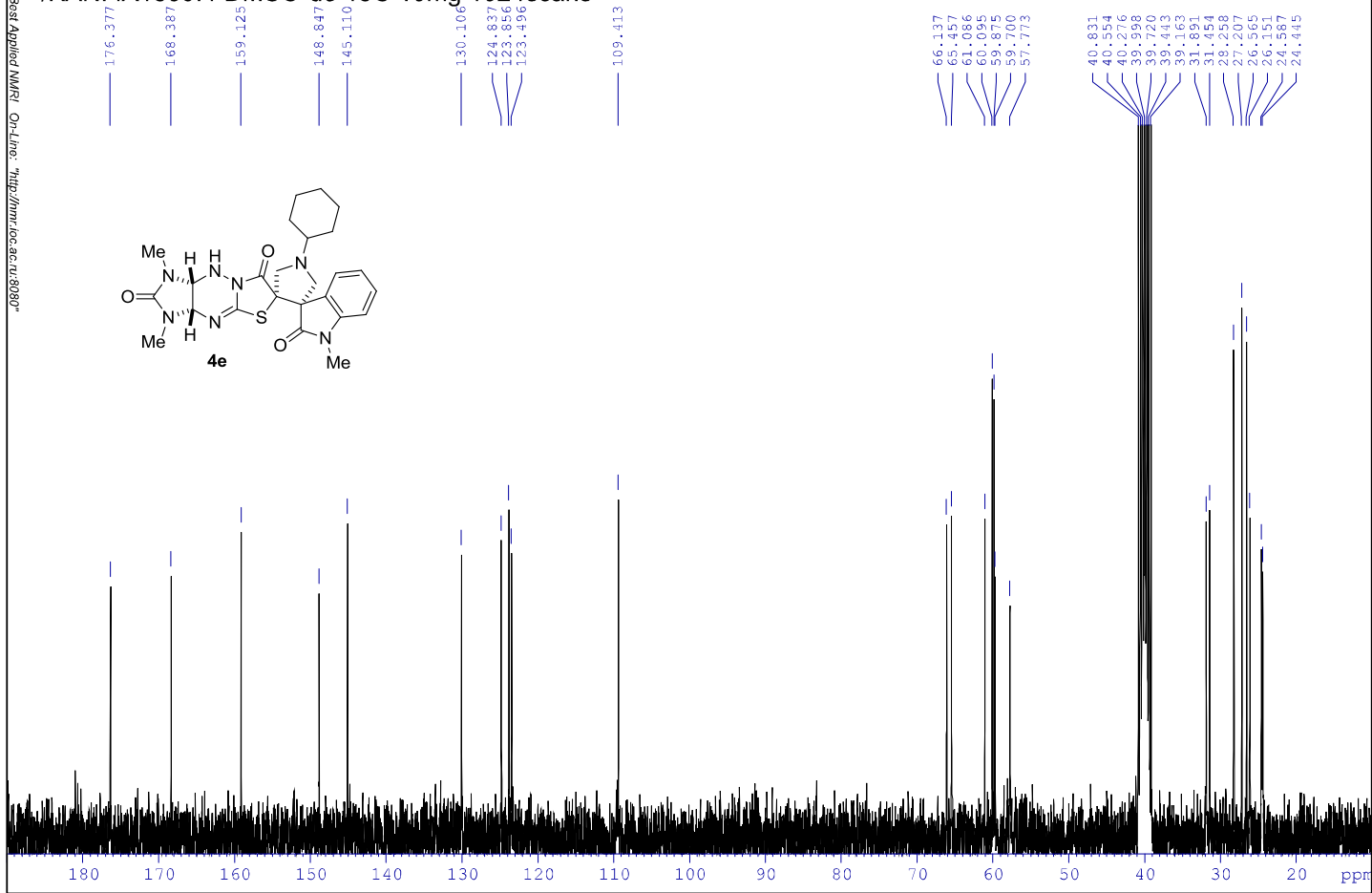
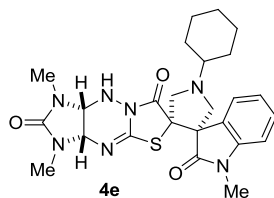
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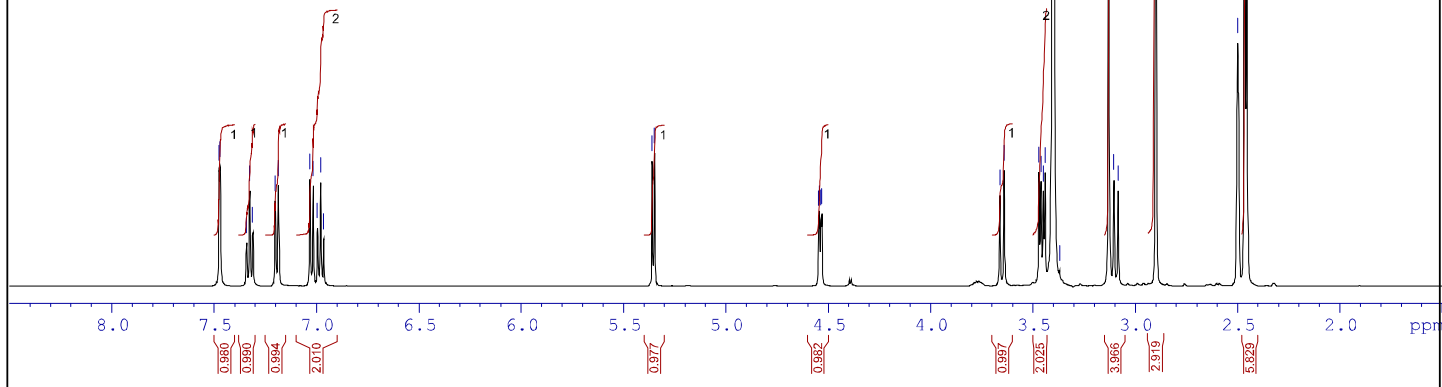
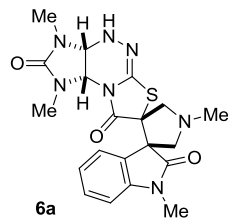
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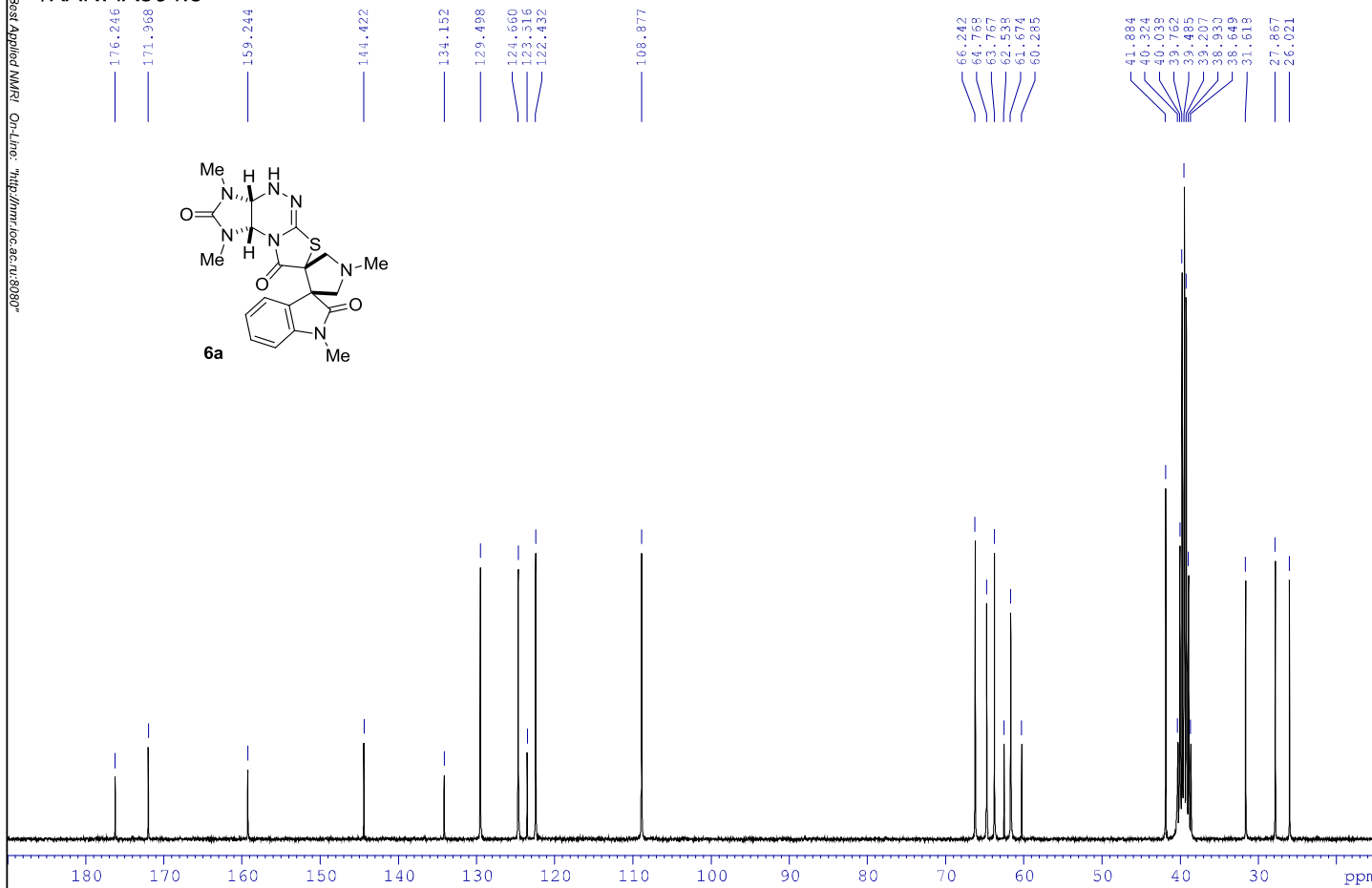
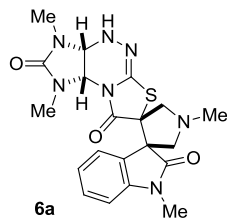
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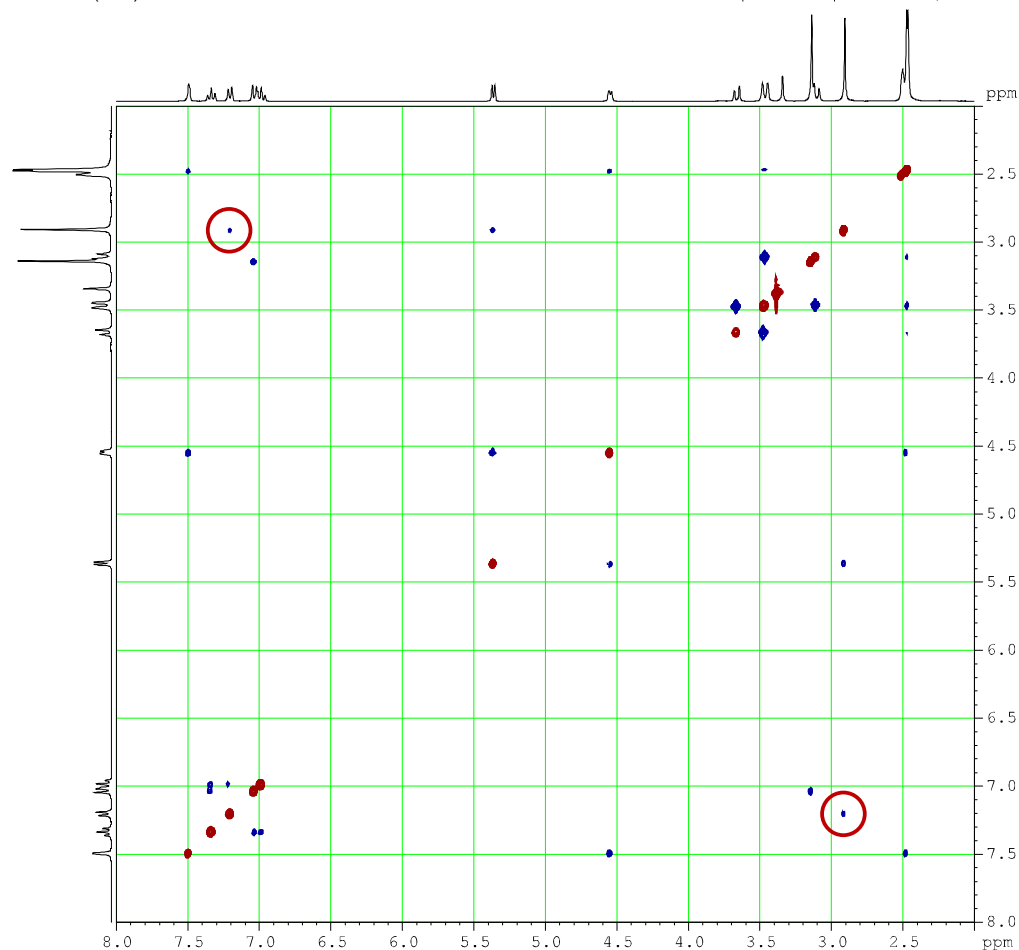
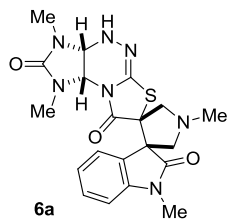
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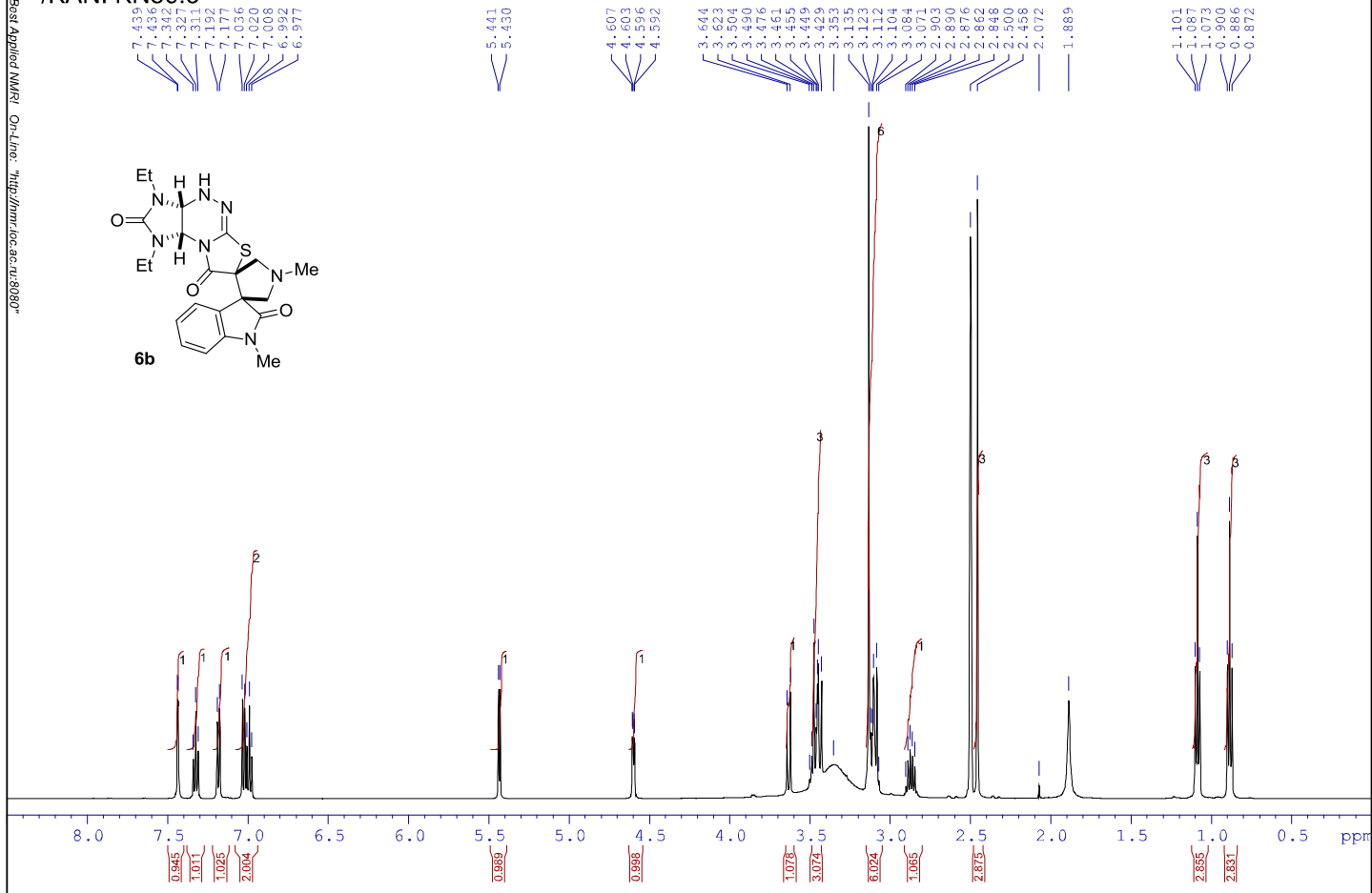
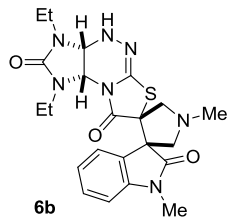
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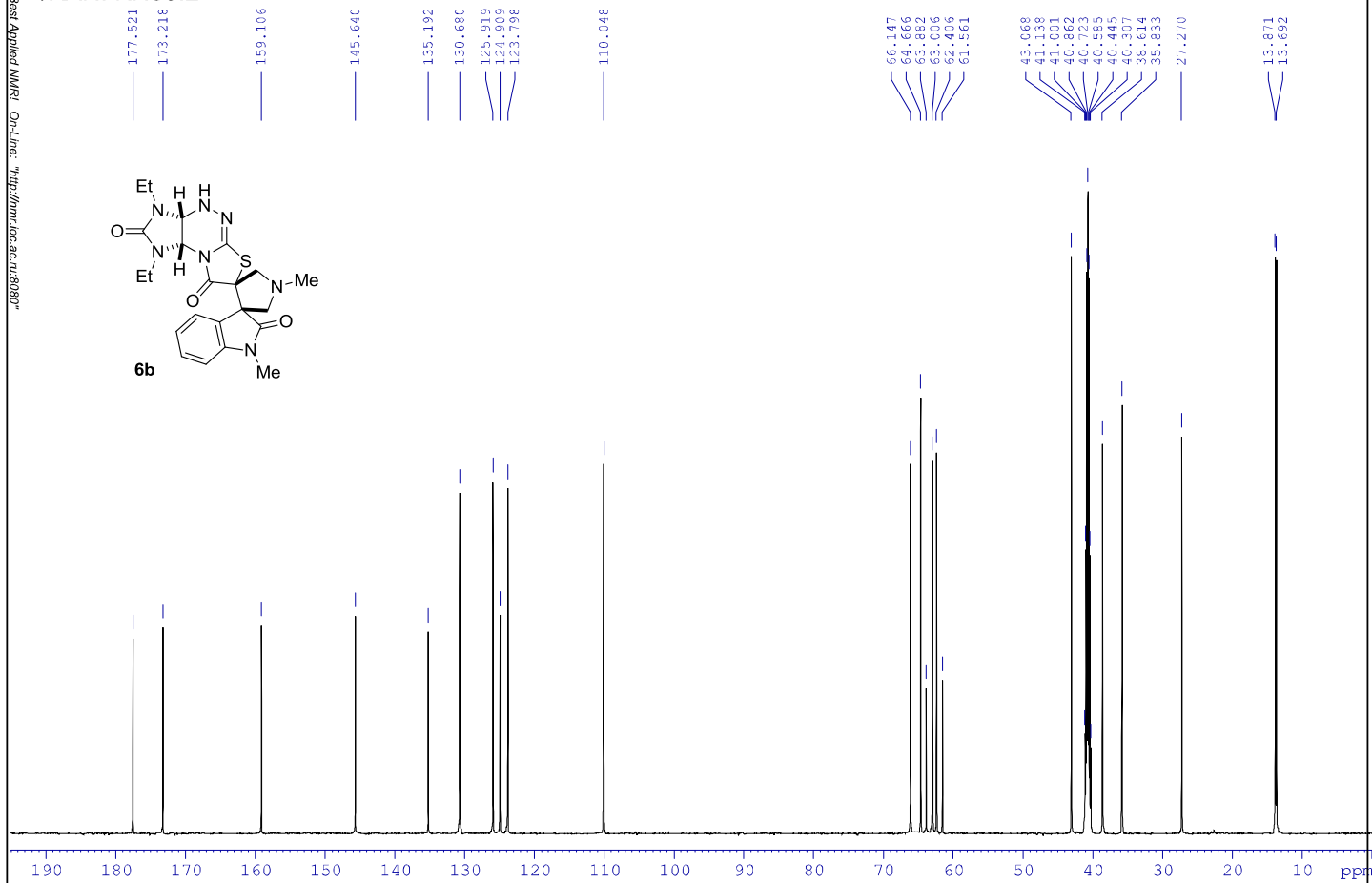
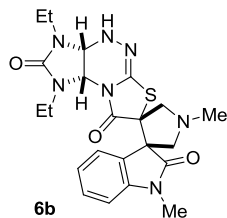
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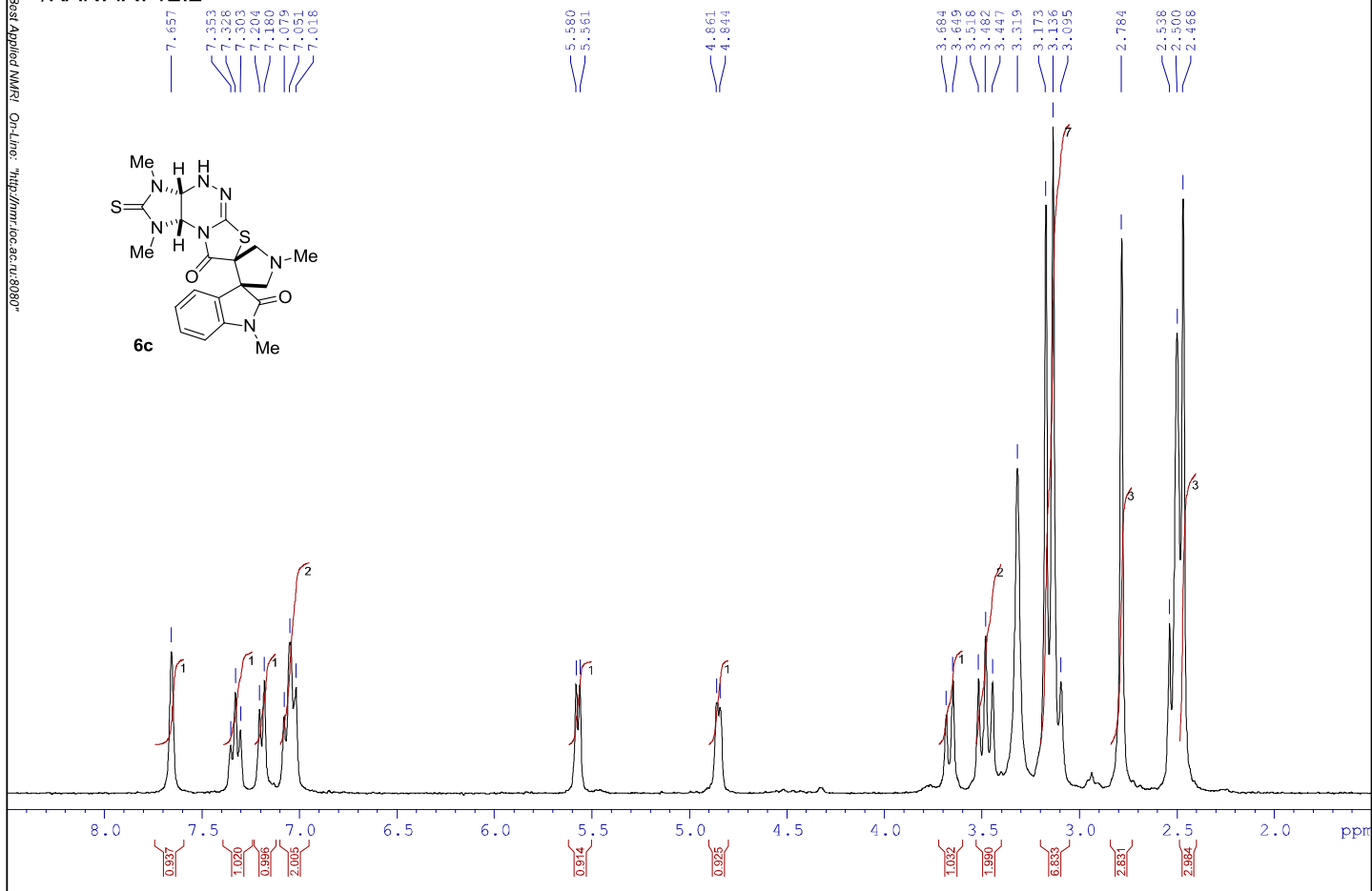
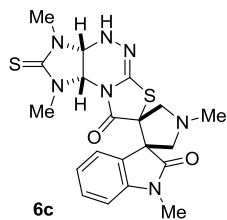
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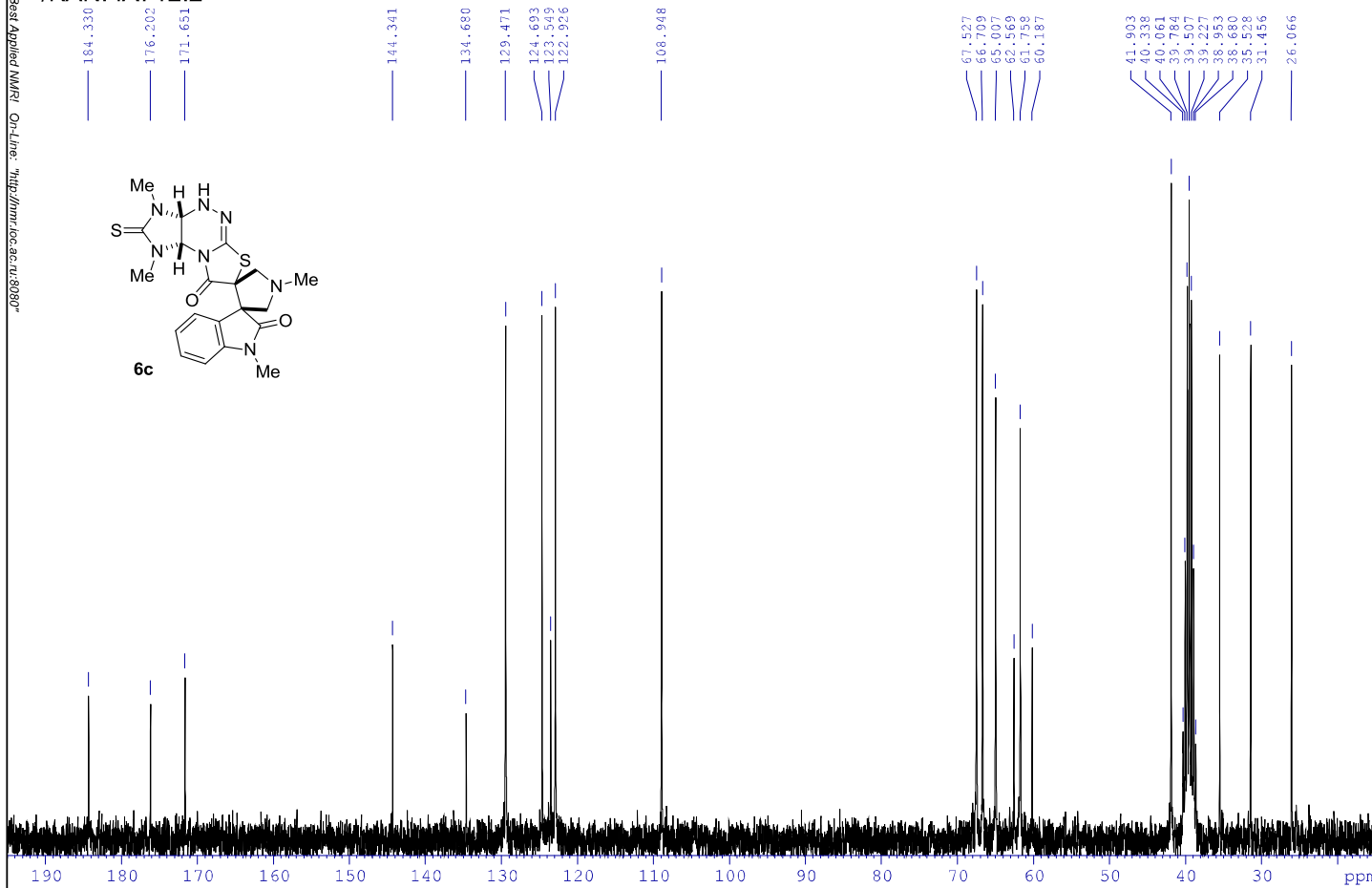
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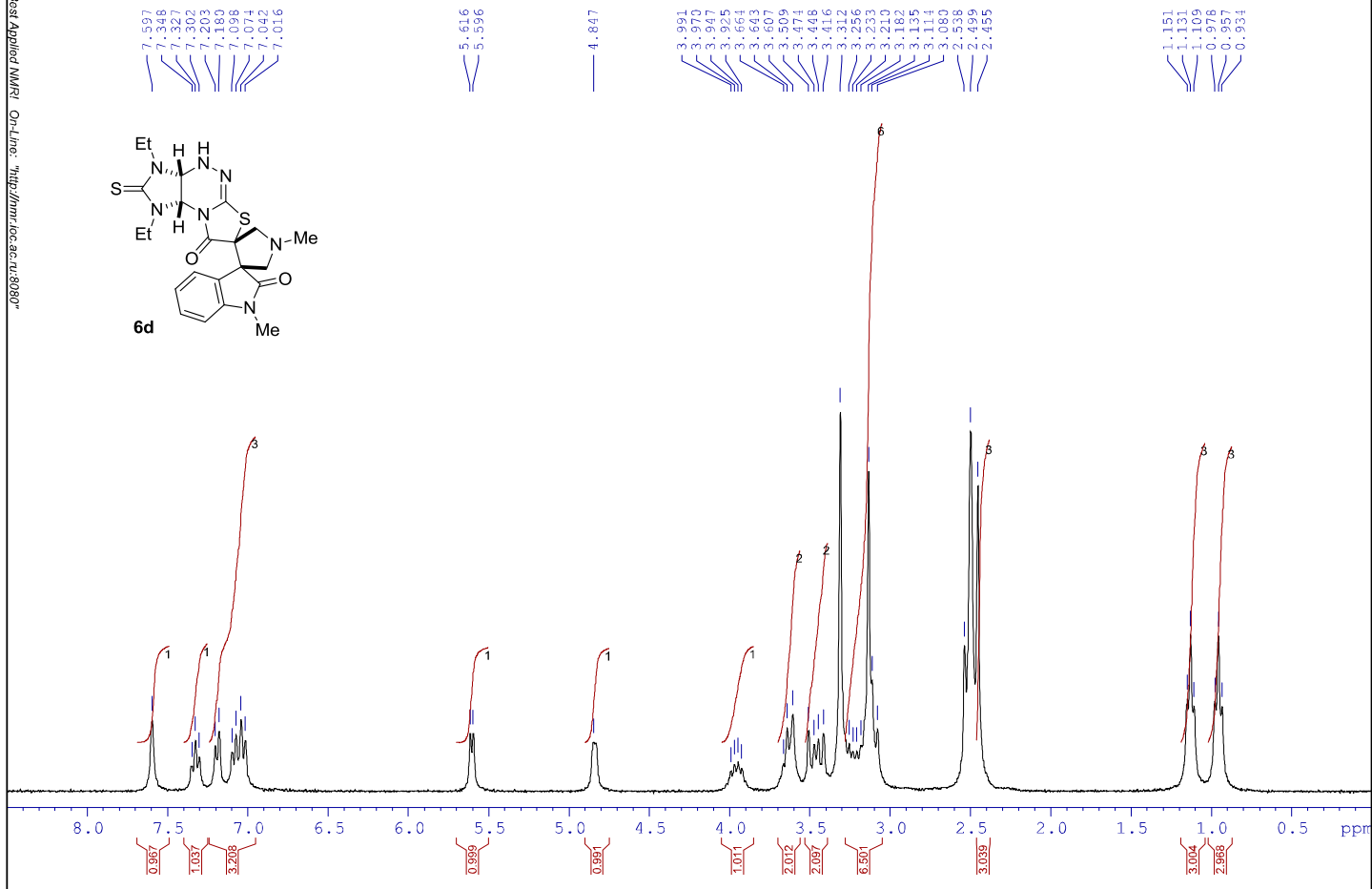
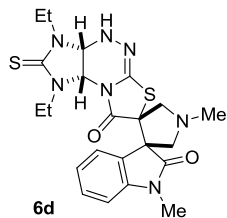
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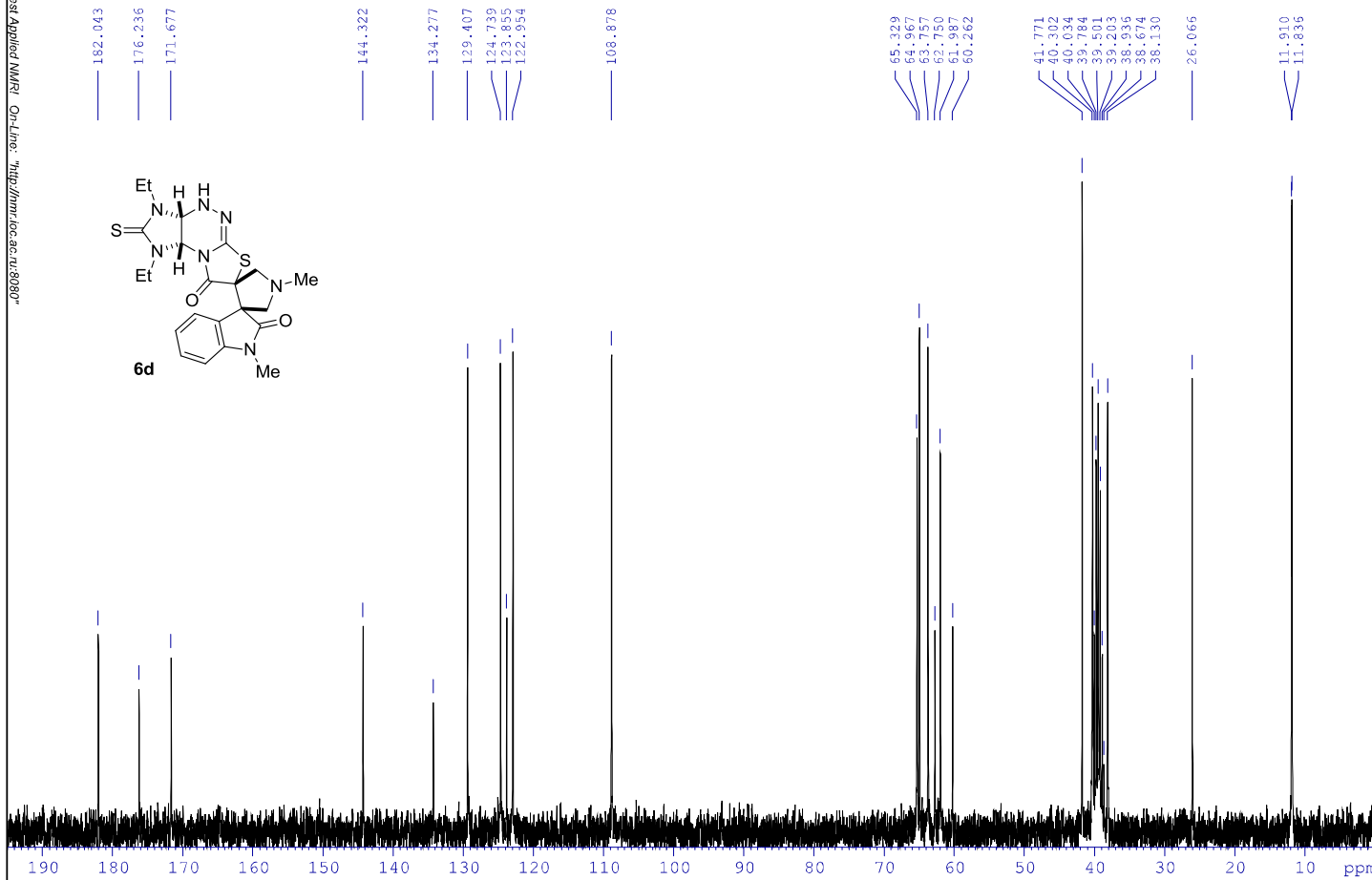
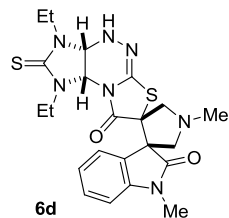
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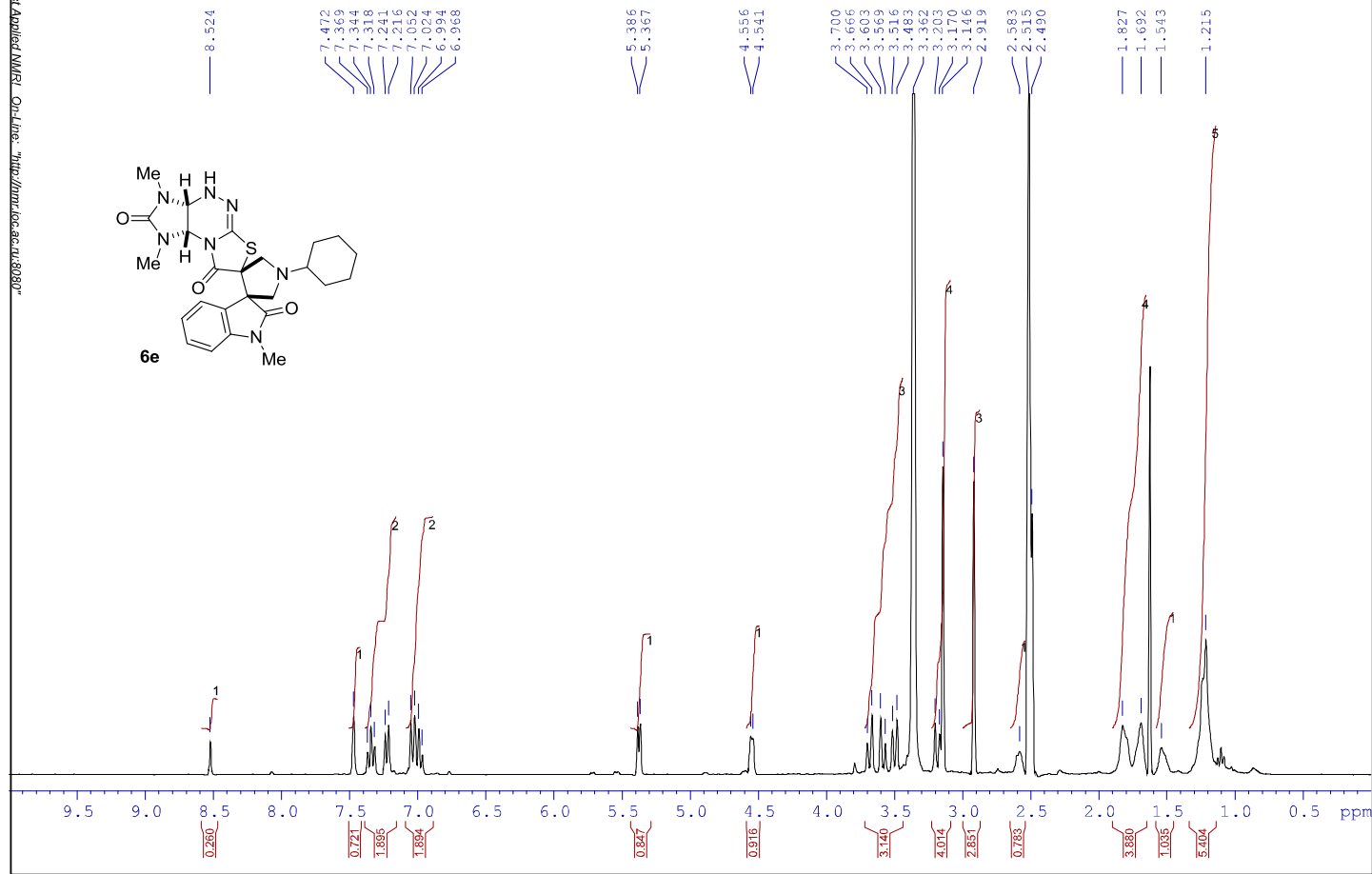
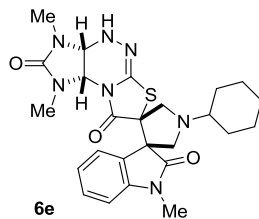
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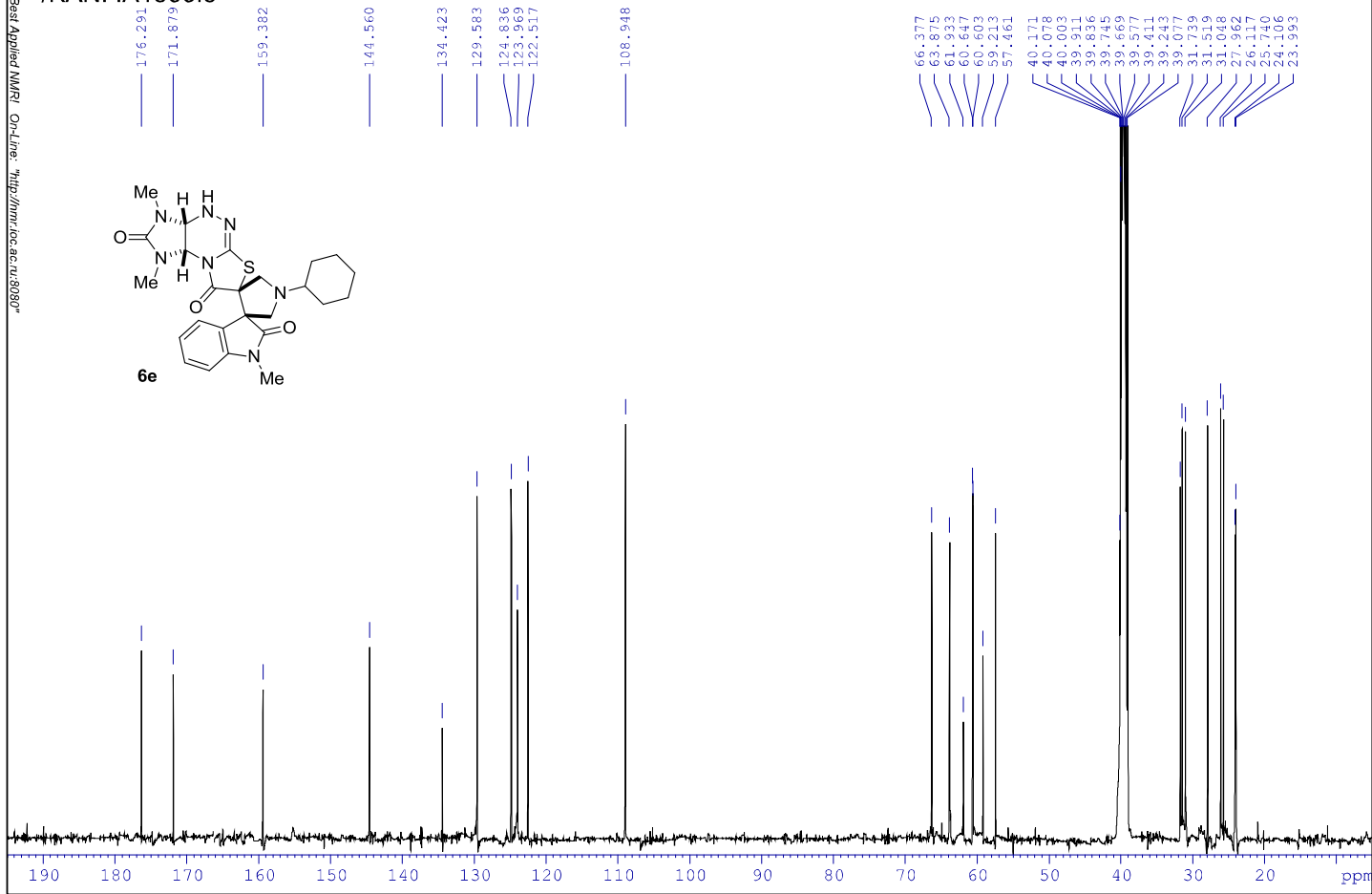
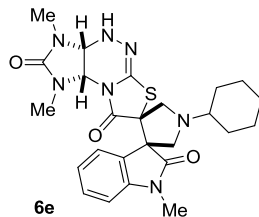
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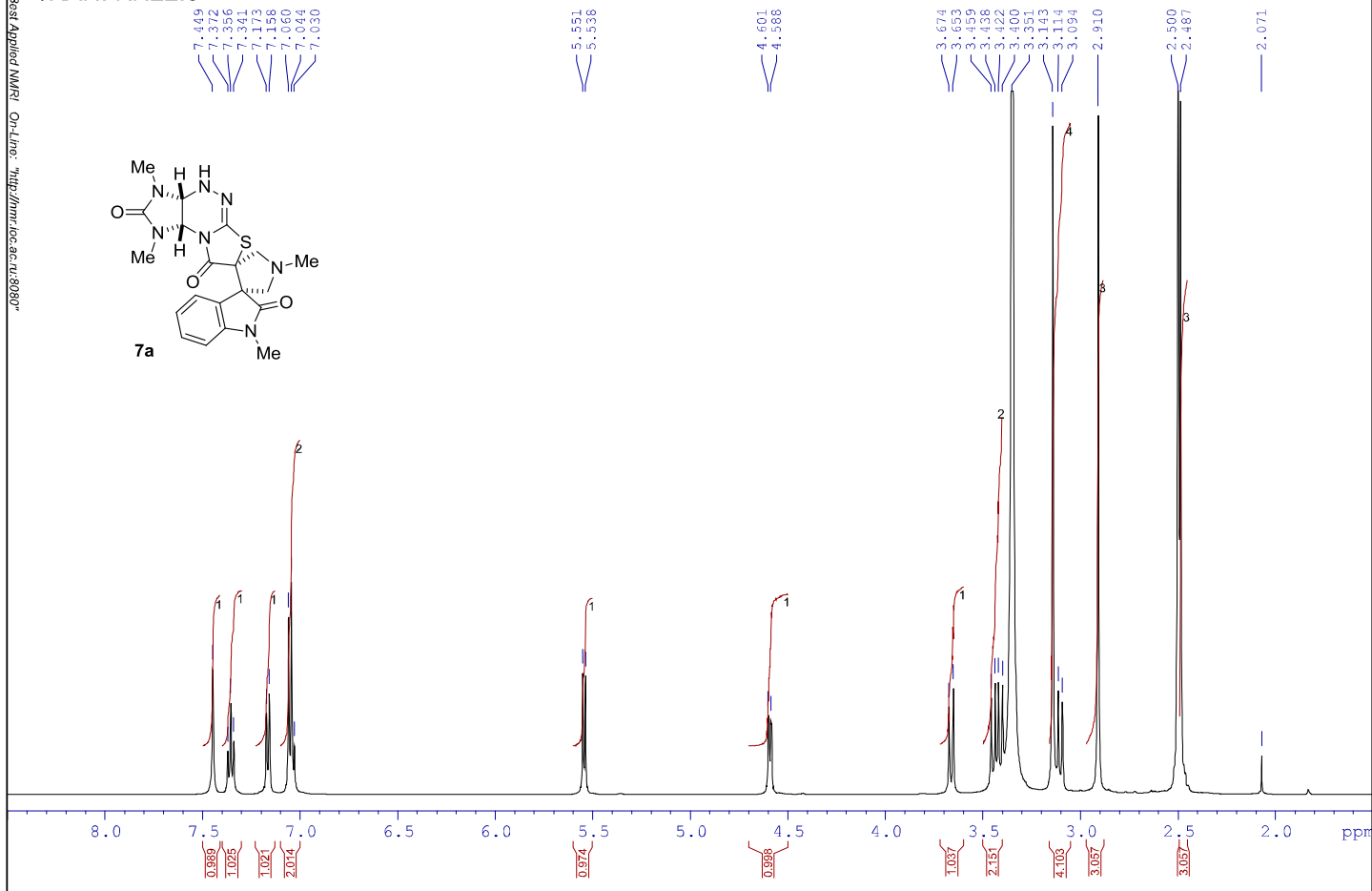
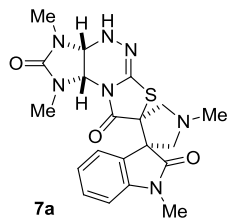
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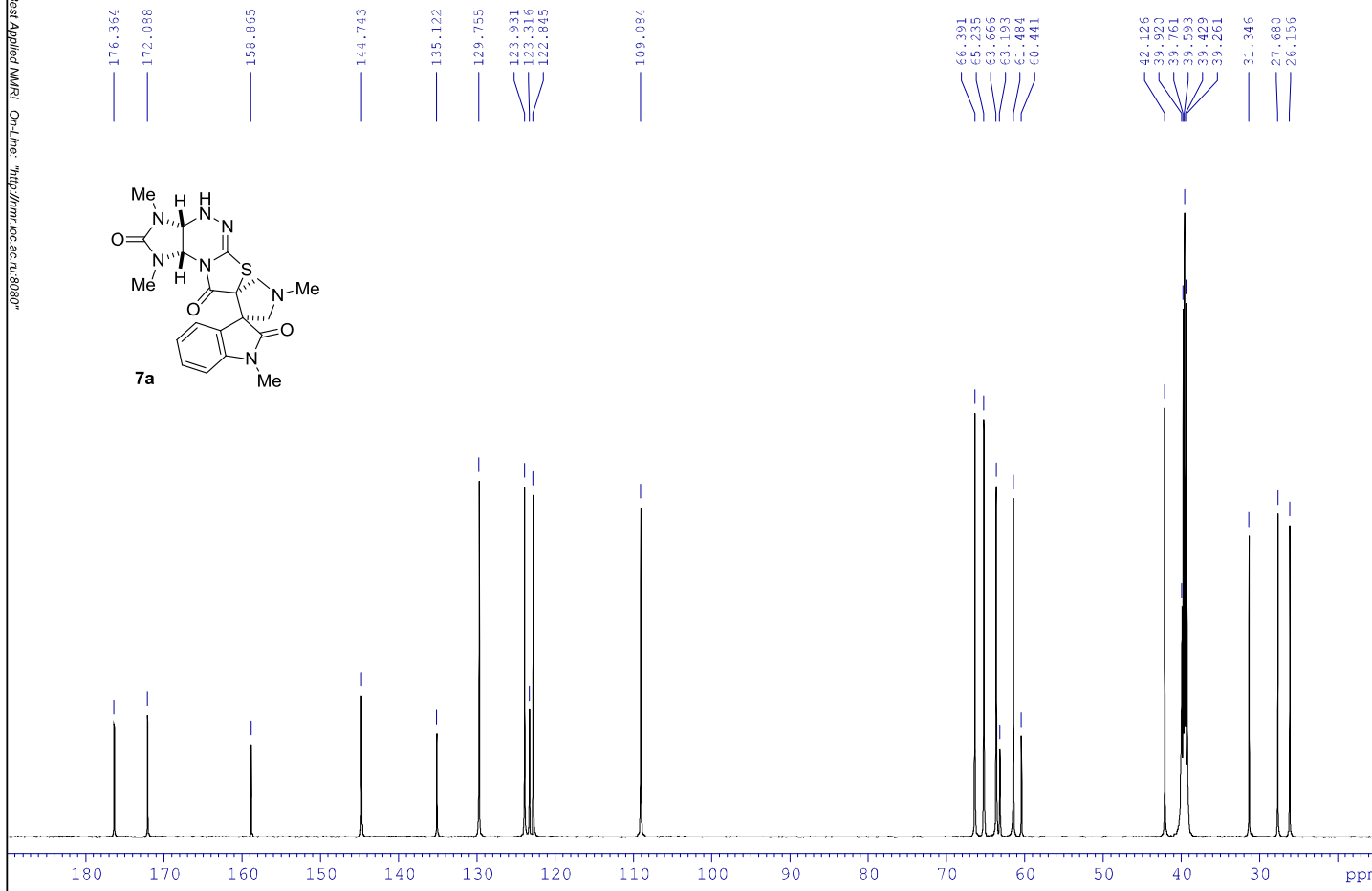
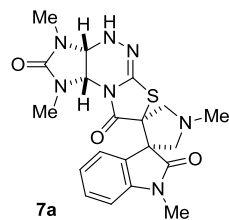
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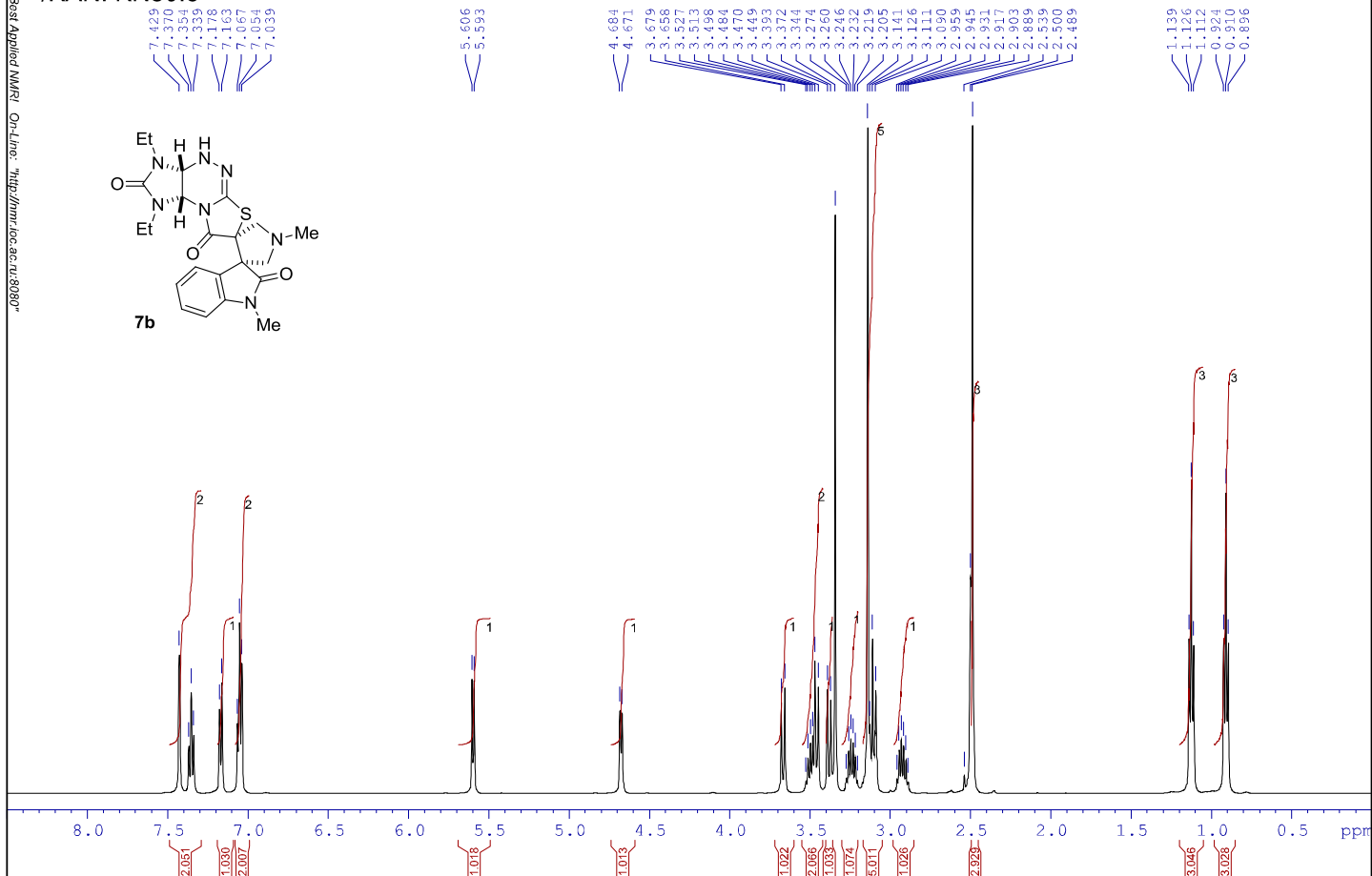
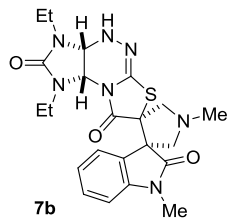
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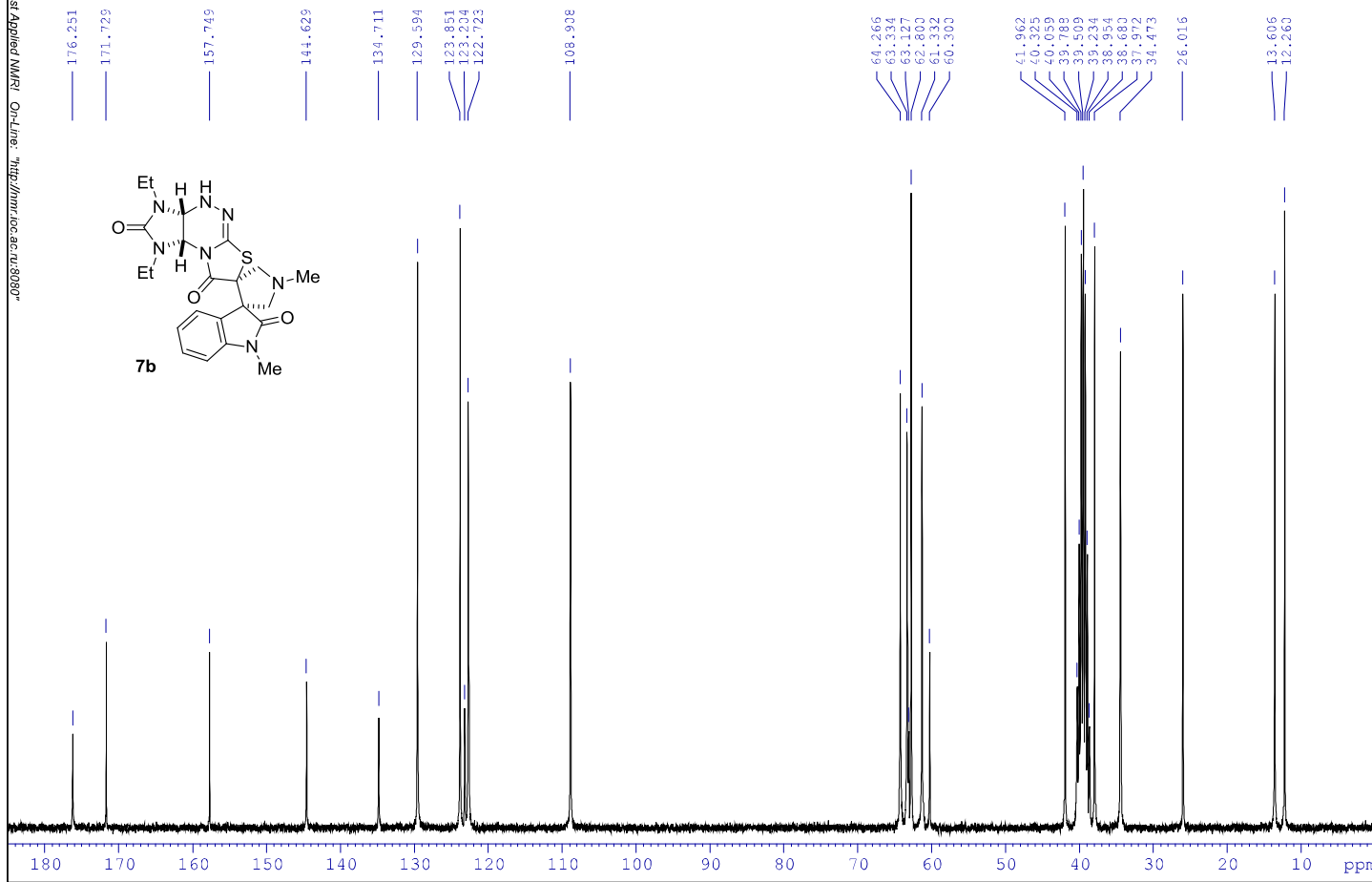
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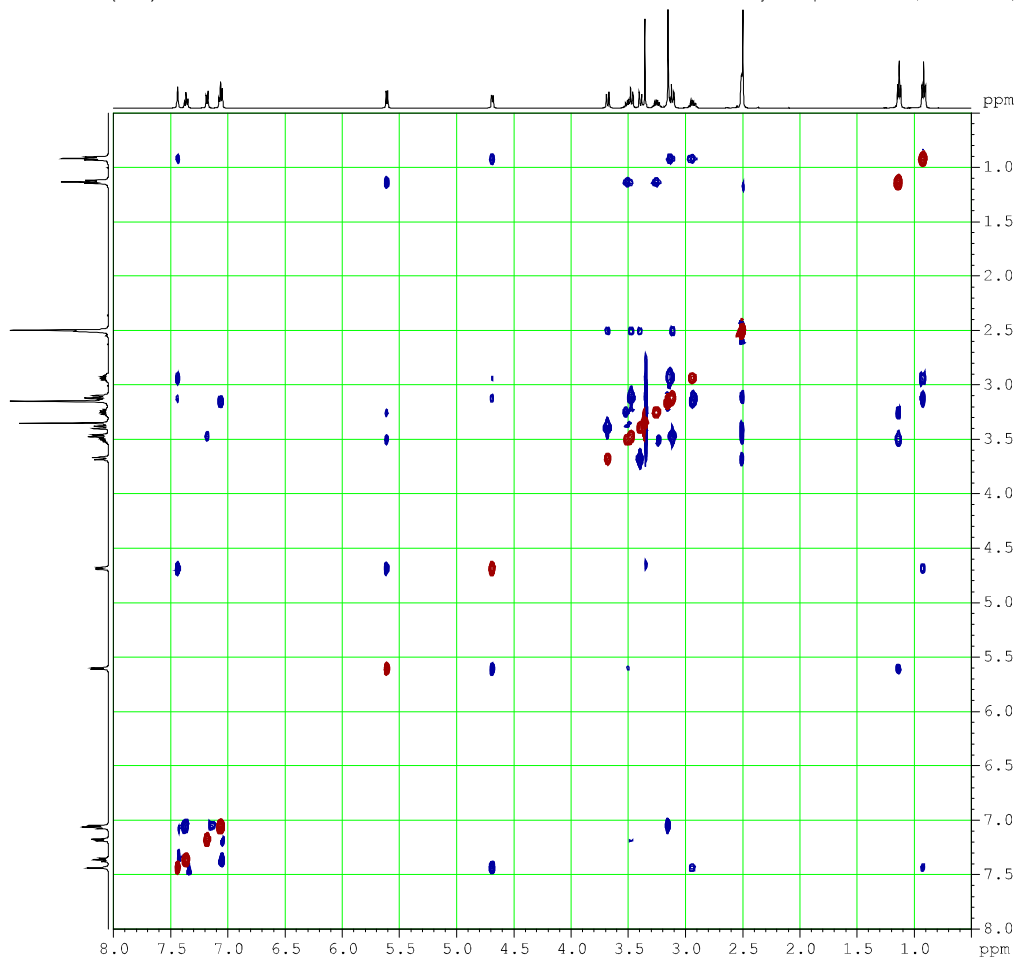
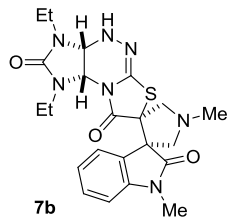
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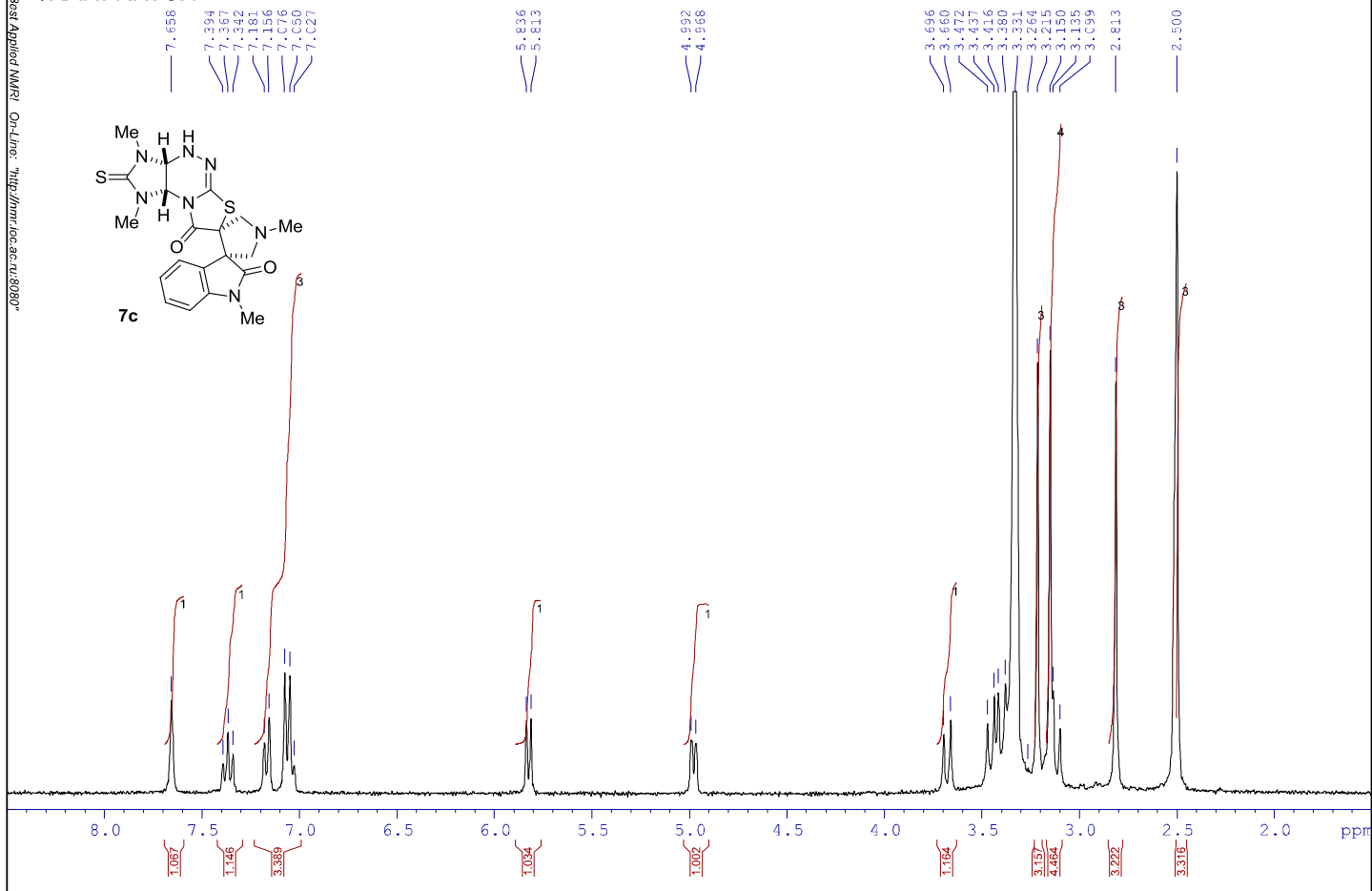
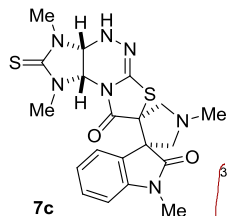
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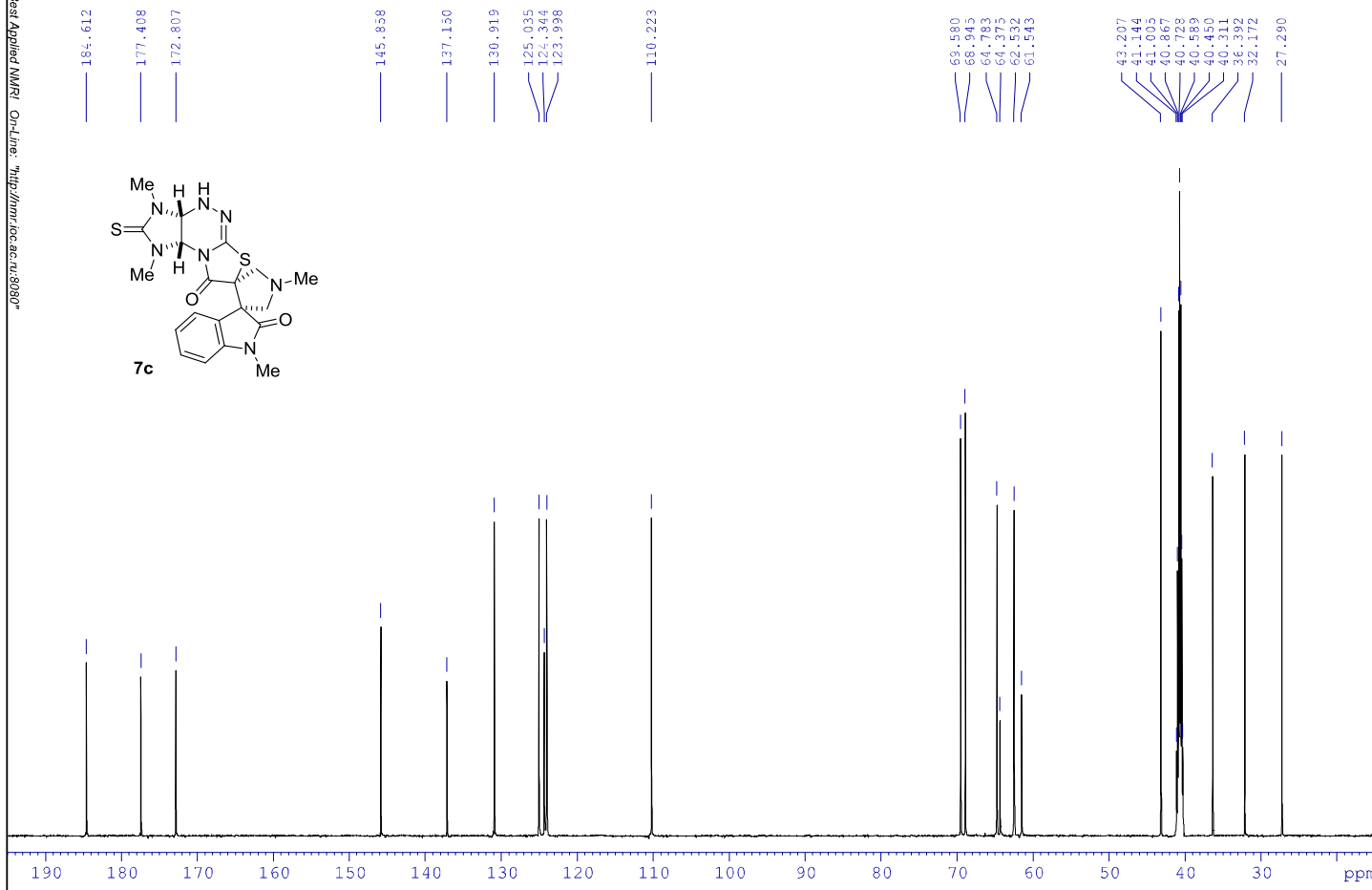
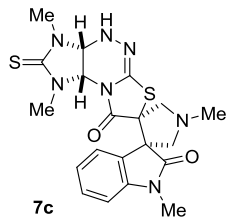
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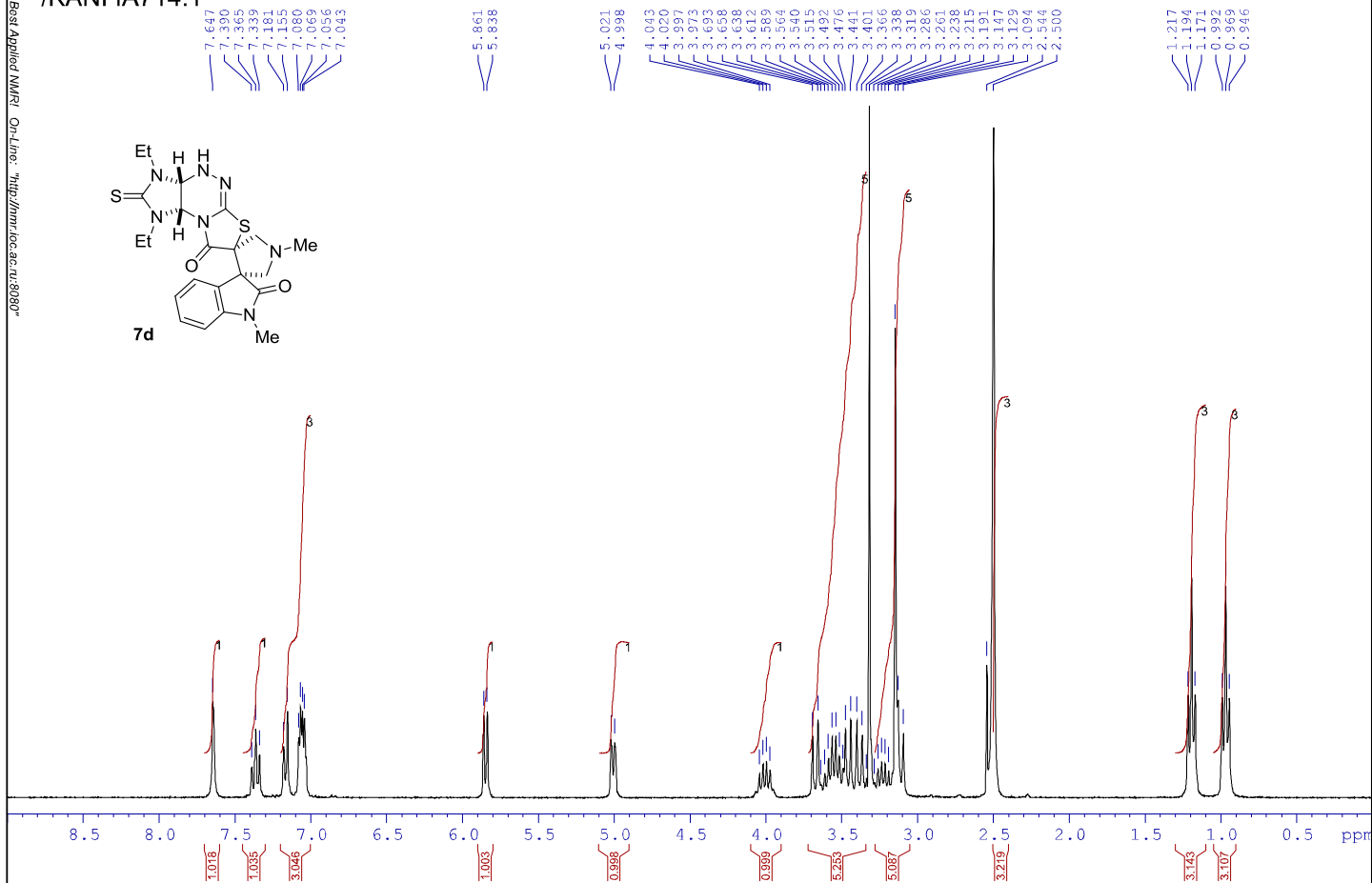
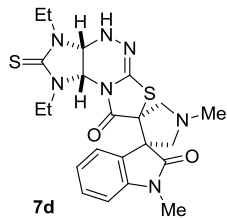
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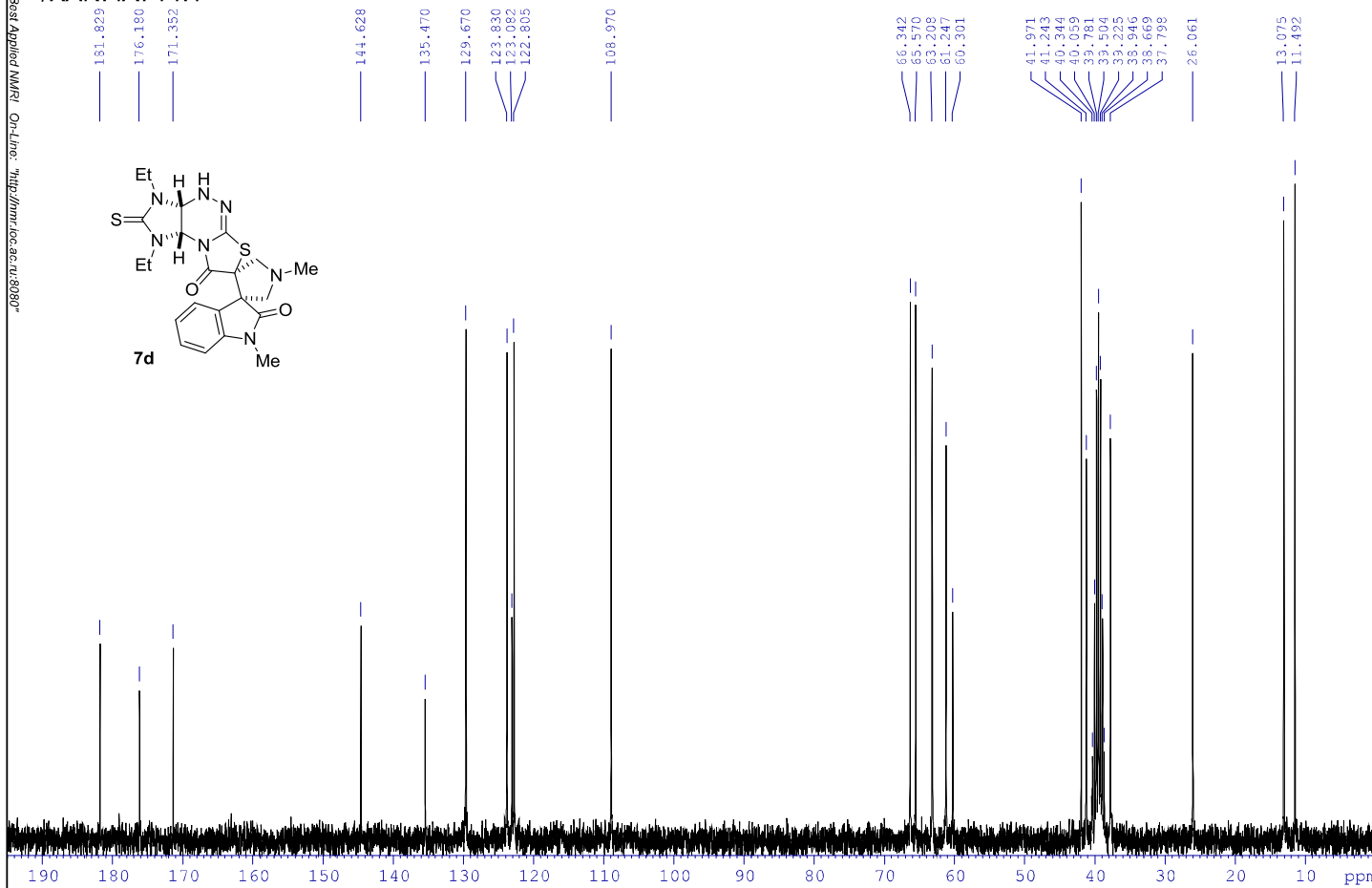
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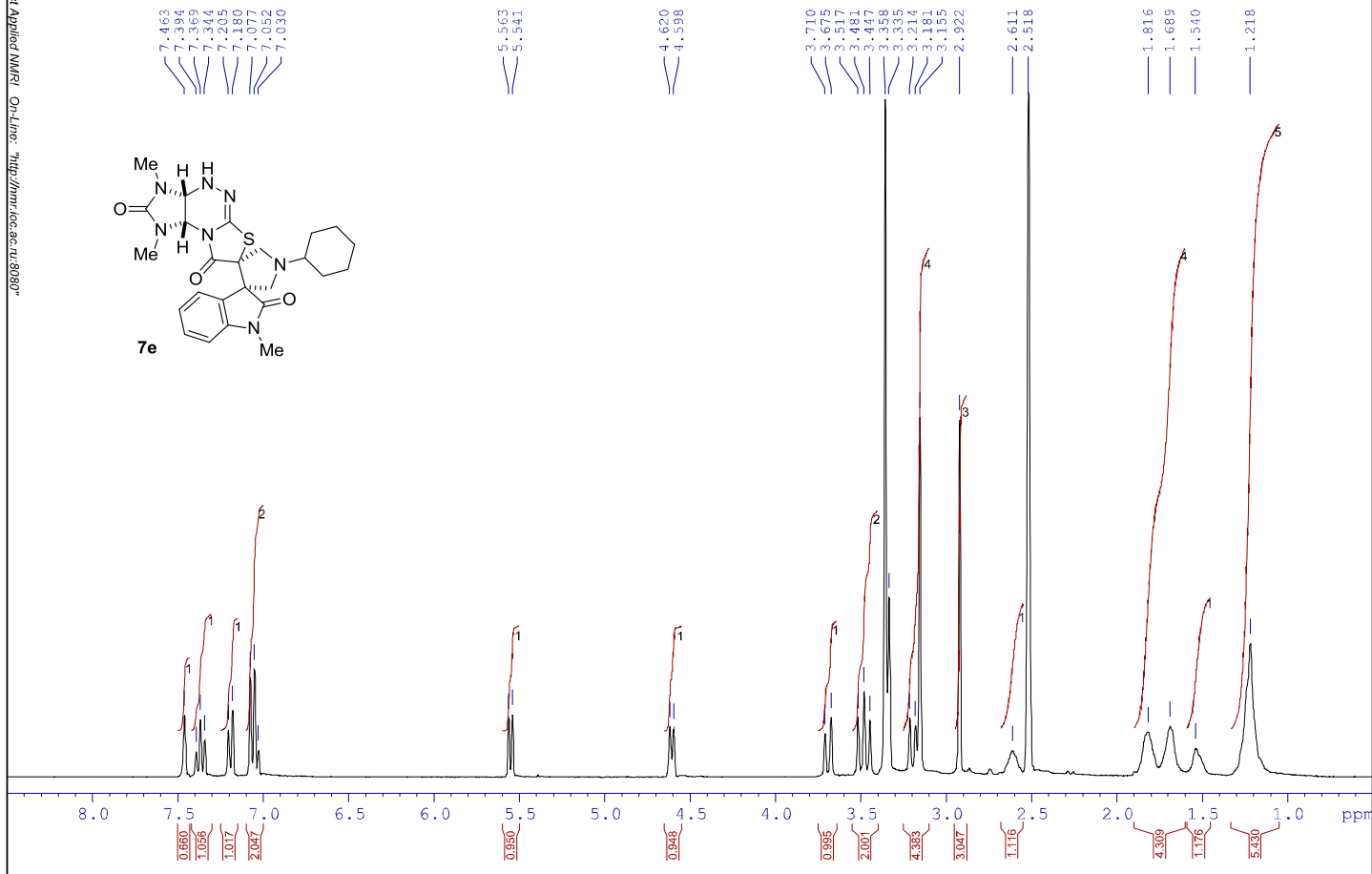
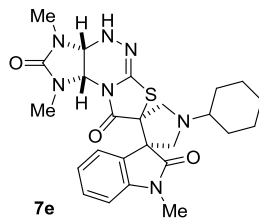
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/KANI IA714.1



/KANI IA1557.4



/KANI IA1557.4

