

Supporting Information

IDENTIFICATION OF A NOVEL INDOLEAMINE 2,3-DIOXYGENASE INHIBITOR BEARING AN EIGHT-MEMBERED RING FUSED INDOLE SCAFFOLD AND ITS STRUCTURE ACTIVITY RELATIONSHIP

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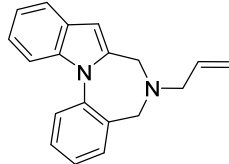
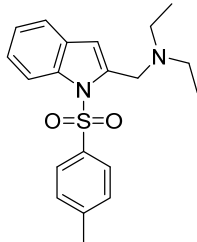
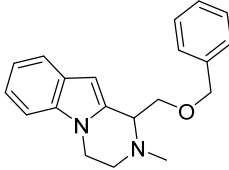
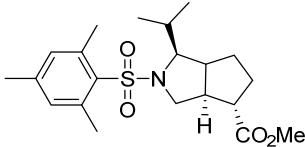
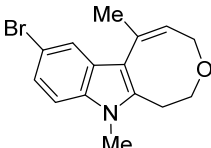
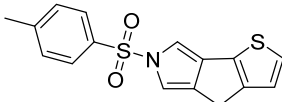
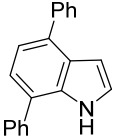
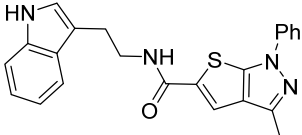
e-mail: sinuki@pharm.kyoto-u.ac.jp (Shinsuke Inuki)

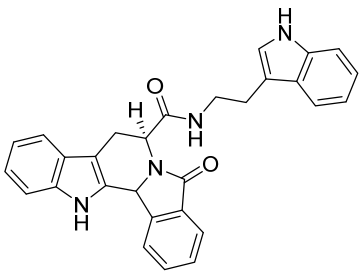
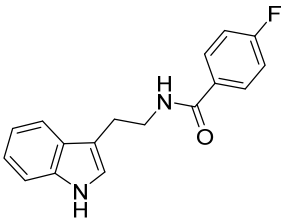
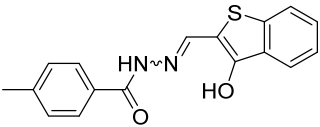
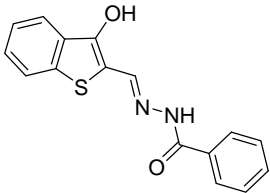
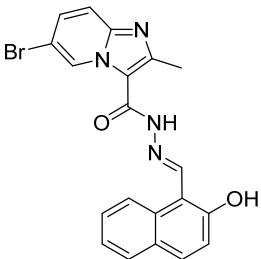
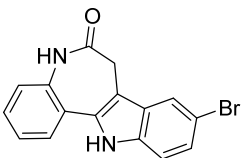
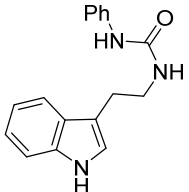
e-mail: hohno@pharm.kyoto-u.ac.jp (Hiroaki Ohno)

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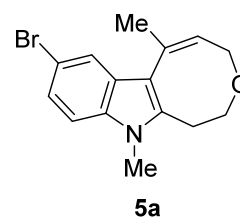
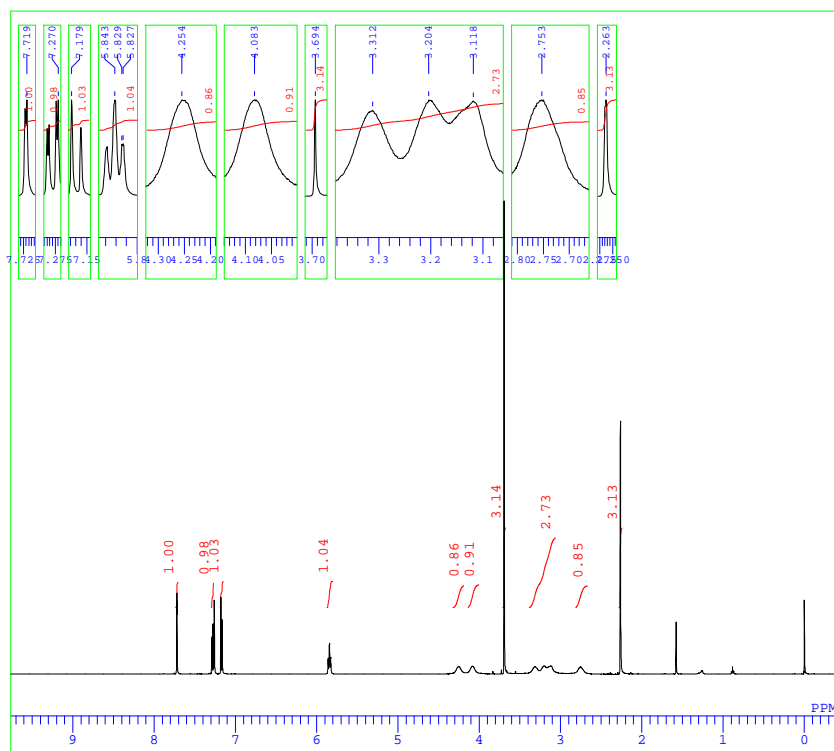
Structures and Biological Activities of 15 Hit Compounds	S2
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Table S1. Structures and Biological Activities of 15 Hit Compounds

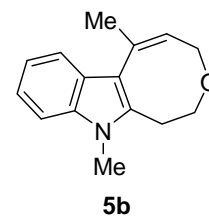
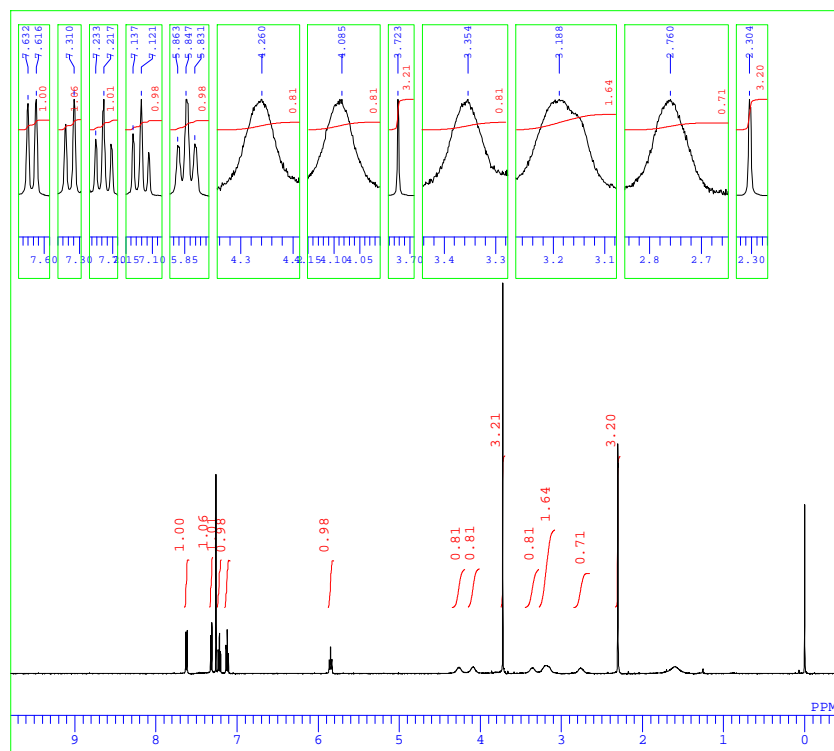
Structure	A431 cell % inhibition at 10 μ M	A431 cell viability at 10 μ M	rhIDO % inhibition at 30 μ M
	54%	96%	13%
	66%	100%	14%
	73%	100%	18%
	65%	89%	20%
	68%	109%	47%
	67%	82%	20%
	88%	97%	33%
	64%	108%	37%

Structure	A431 cell % inhibition at 10 μ M	A431 cell viability at 10 μ M	rhIDO % inhibition at 30 μ M
	99%	110%	34%
	55%	101%	19%
	100%	91%	22%
	63%	86%	19%
	57%	87%	0%
	68%	94%	26%
	72%	96%	33%

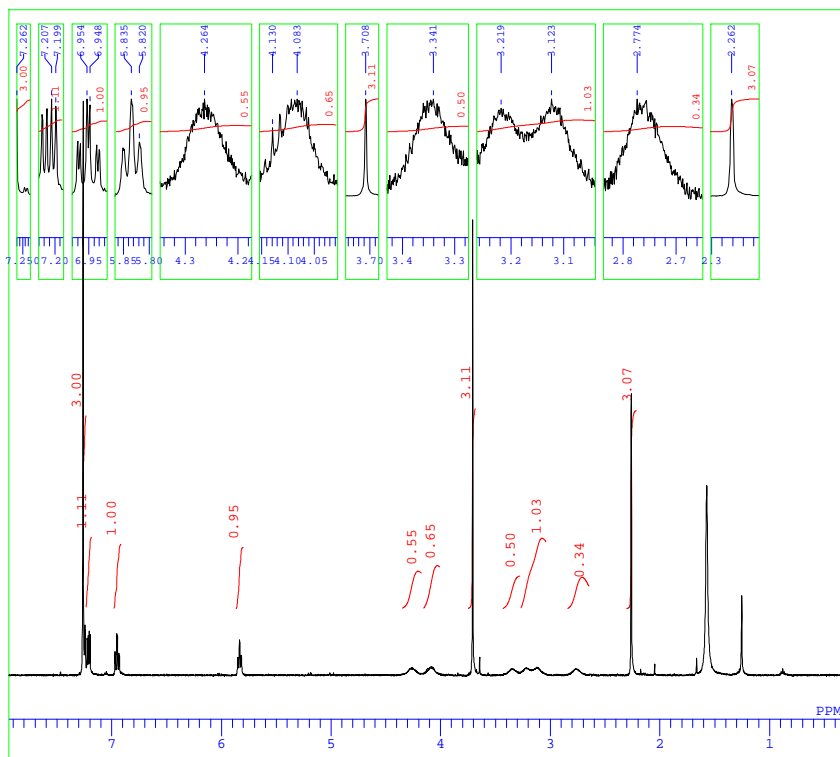
¹H NMR spectrum for compound 5a (500 MHz, CDCl₃)



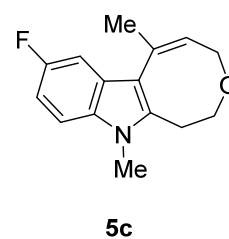
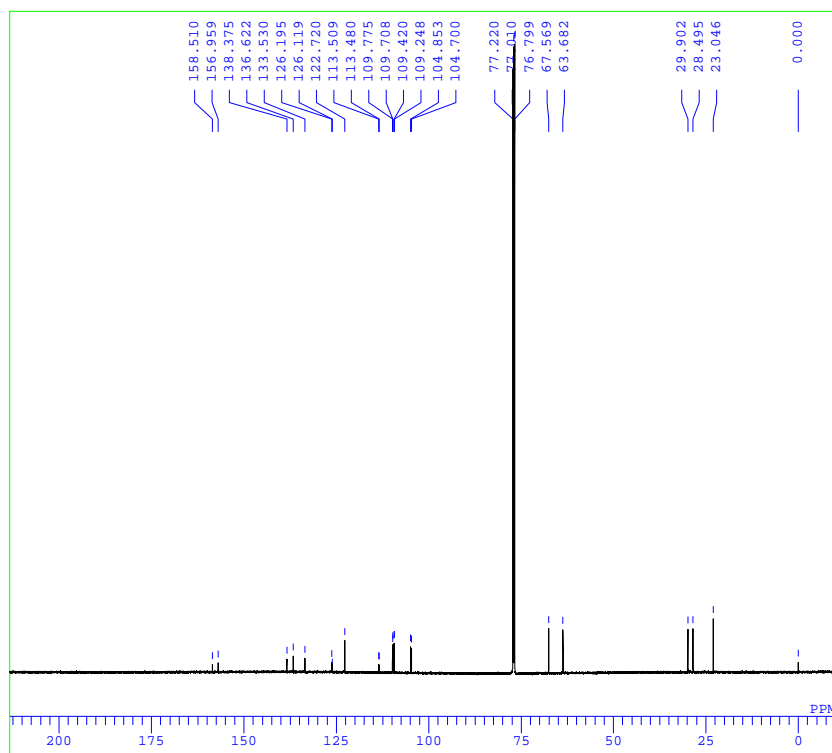
¹H NMR spectrum for compound 5b (500 MHz, CDCl₃)



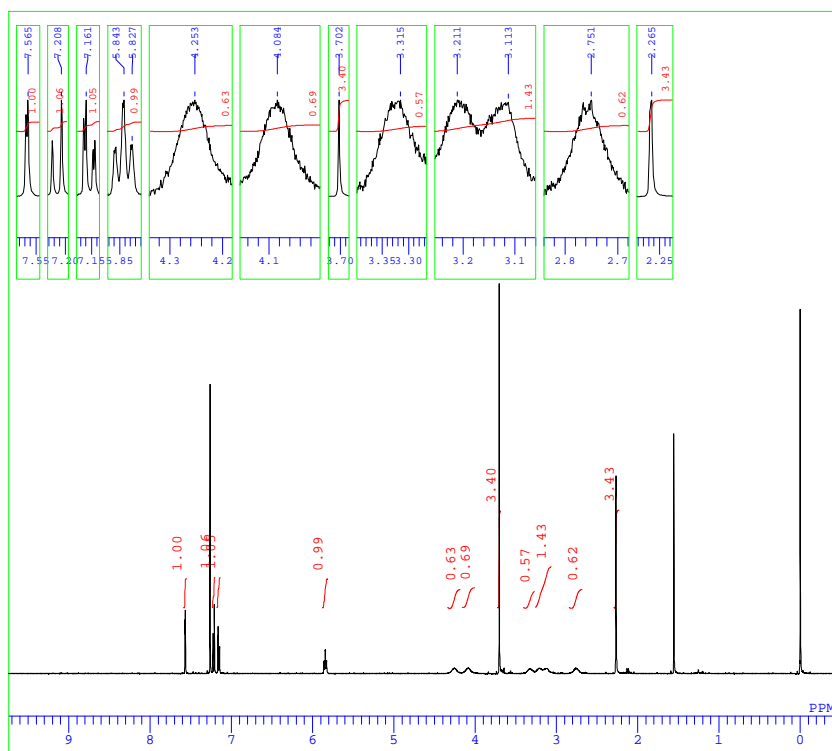
¹H NMR spectrum for compound 5c (500 MHz, CDCl₃)



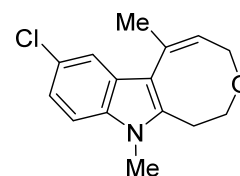
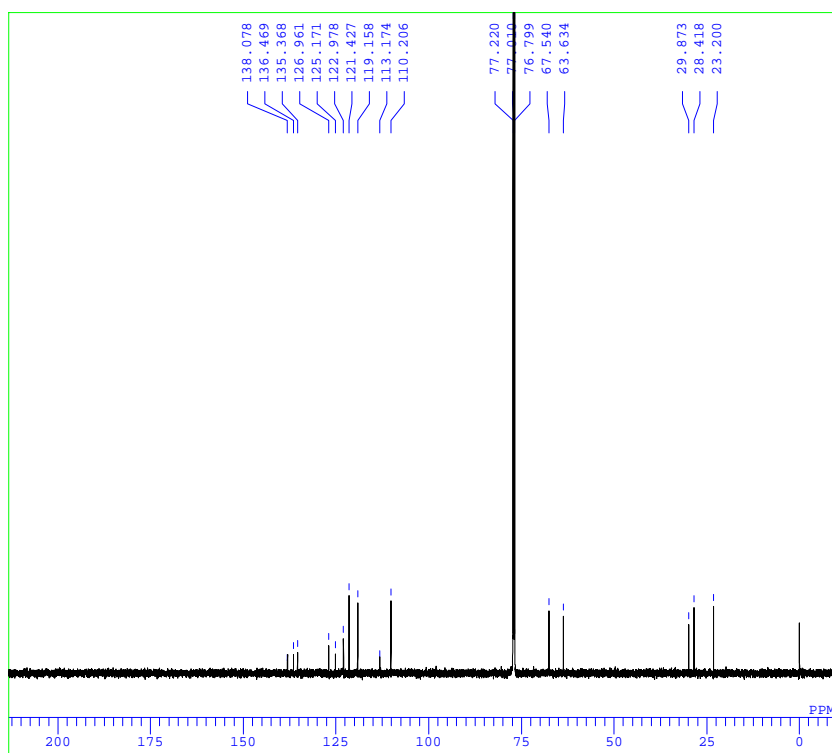
¹³C NMR spectrum for compound 5c (150 MHz, CDCl₃)



¹H NMR spectrum for compound 5d (500 MHz, CDCl₃)

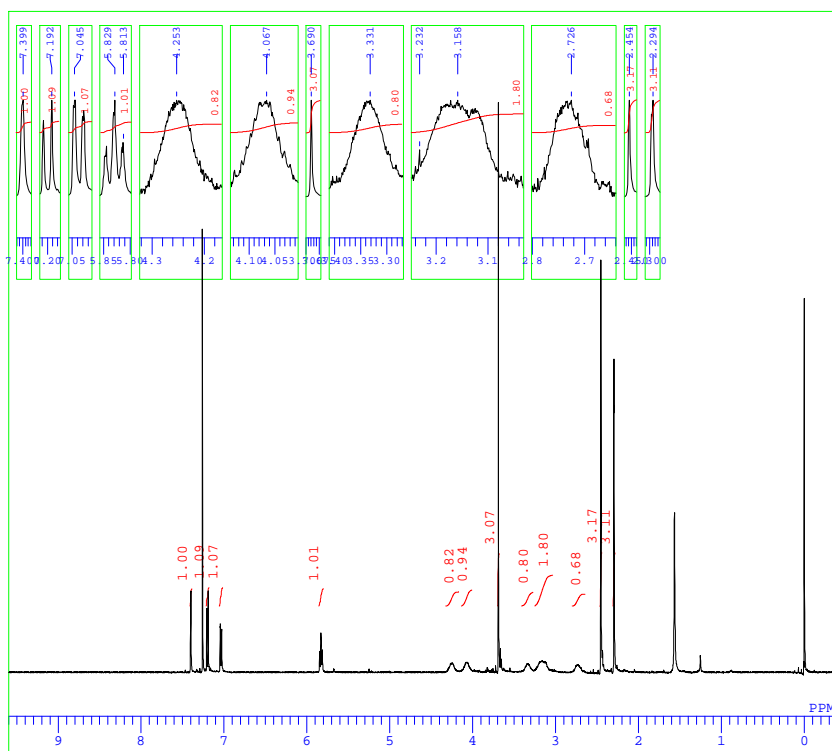


¹³C NMR spectrum for compound 5d (150 MHz, CDCl₃)

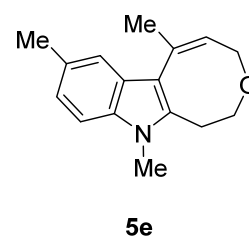
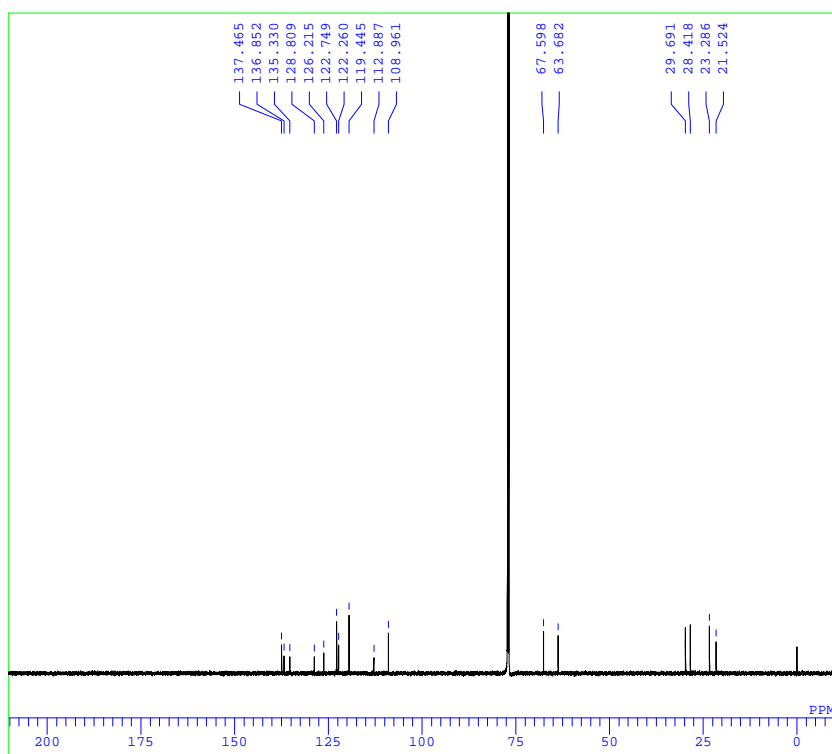


5d

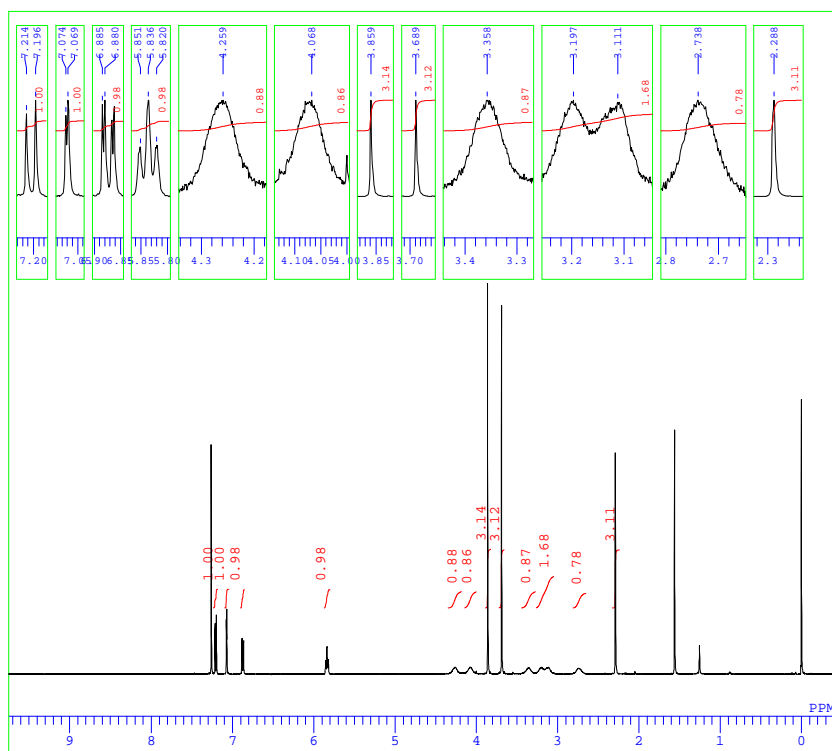
¹H NMR spectrum for compound 5e (500 MHz, CDCl₃)



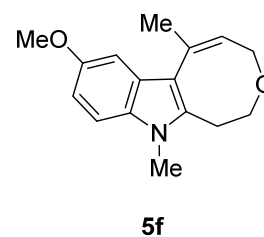
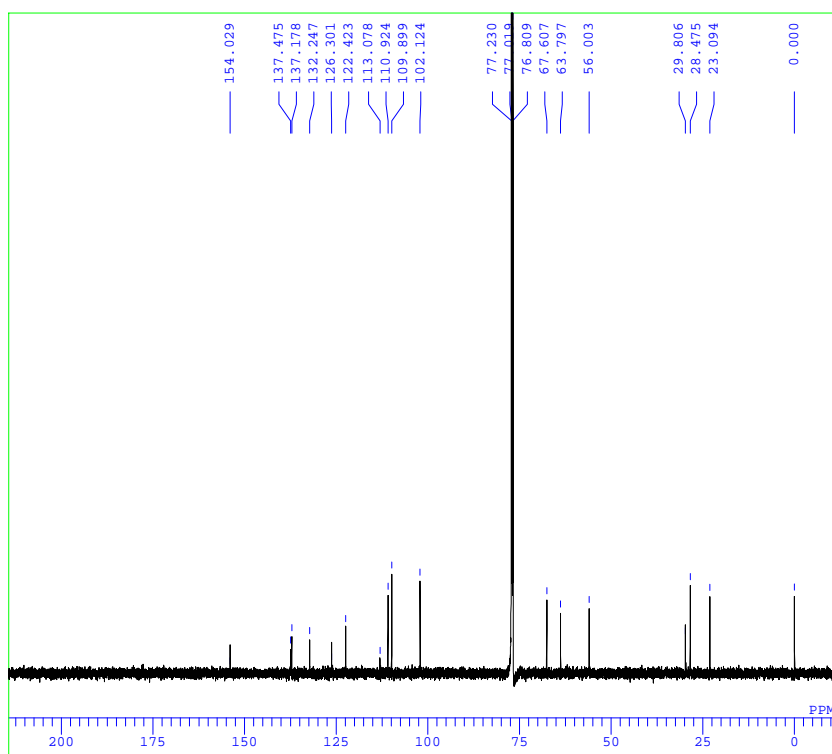
¹³C NMR spectrum for compound 5e (150 MHz, CDCl₃)



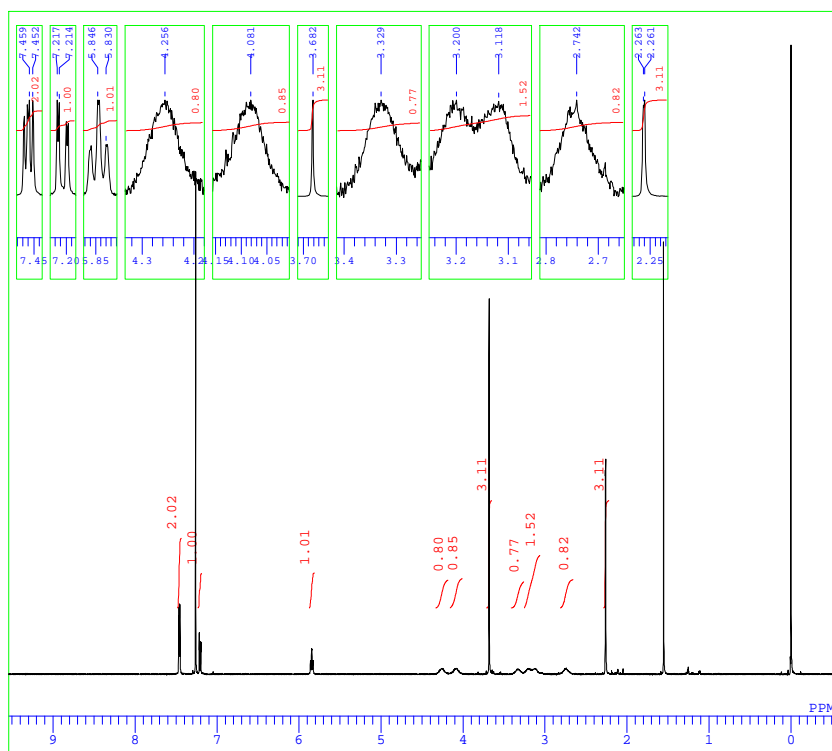
¹H NMR spectrum for compound 5f (500 MHz, CDCl₃)



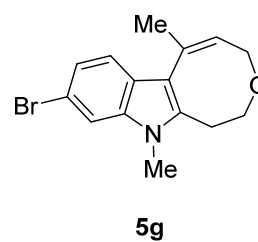
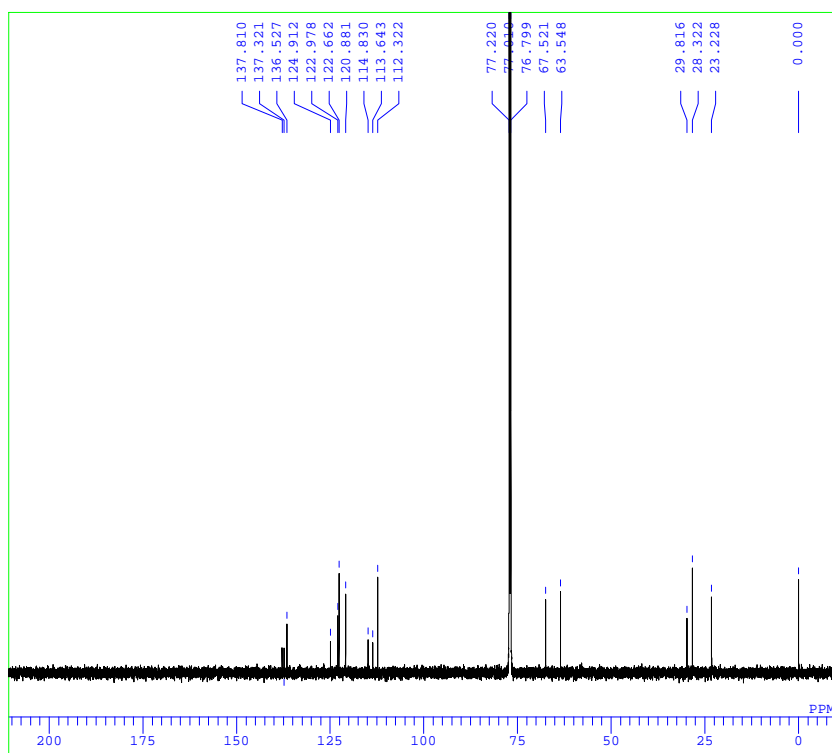
¹³C NMR spectrum for compound 5f (150 MHz, CDCl₃)



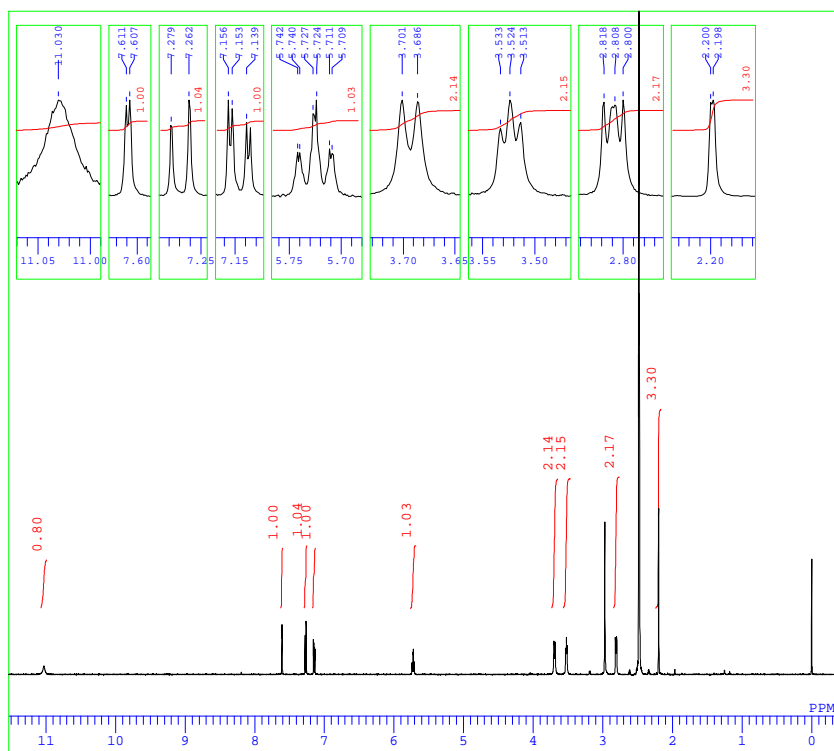
¹H NMR spectrum for compound 5g (500 MHz, CDCl₃)



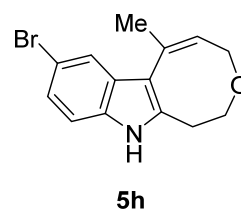
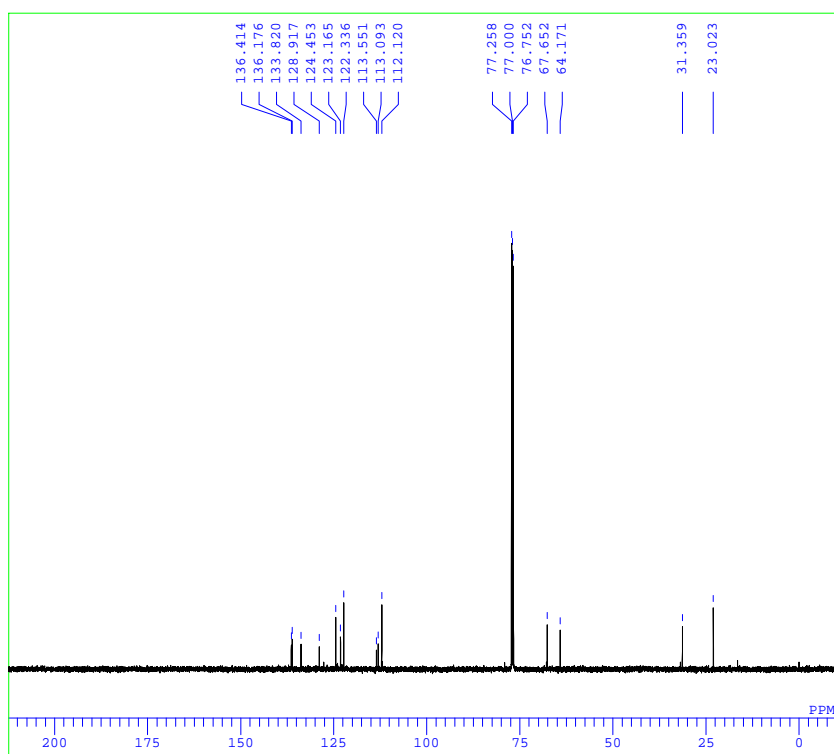
¹³C NMR spectrum for compound 5g (150 MHz, CDCl₃)



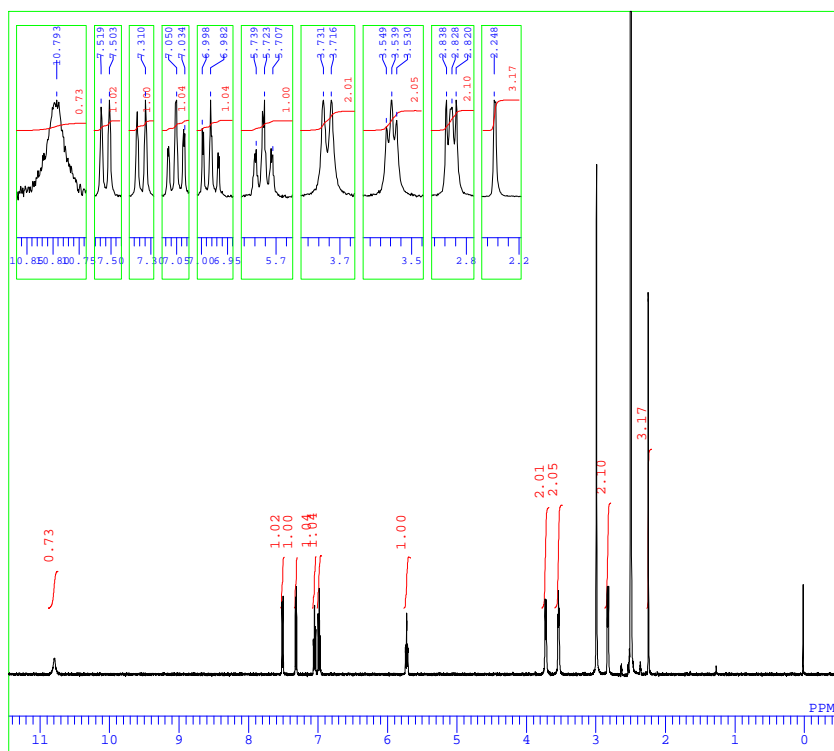
¹H NMR spectrum for compound 5h (500 MHz, DMSO-*d*₆, 100 °C)



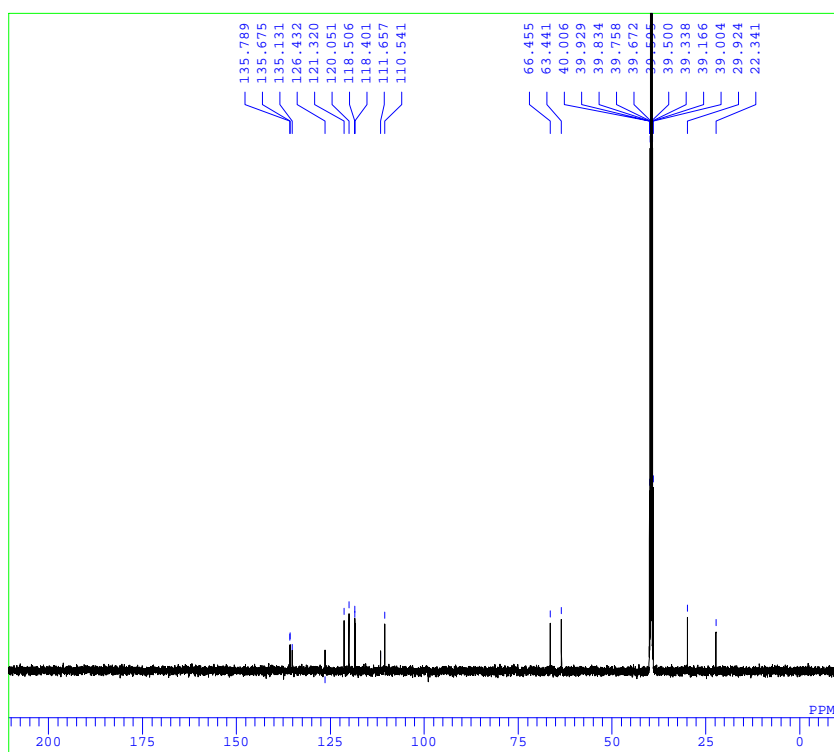
¹³C NMR spectrum for compound 5h (125 MHz, CDCl₃)



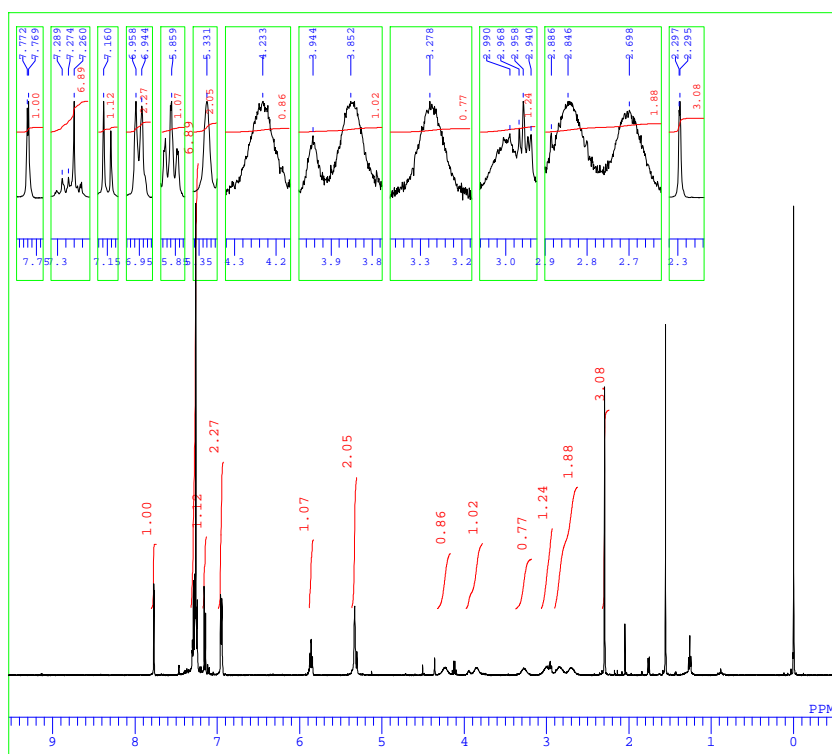
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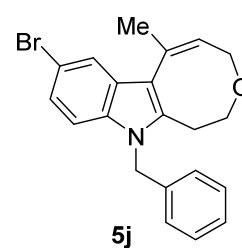
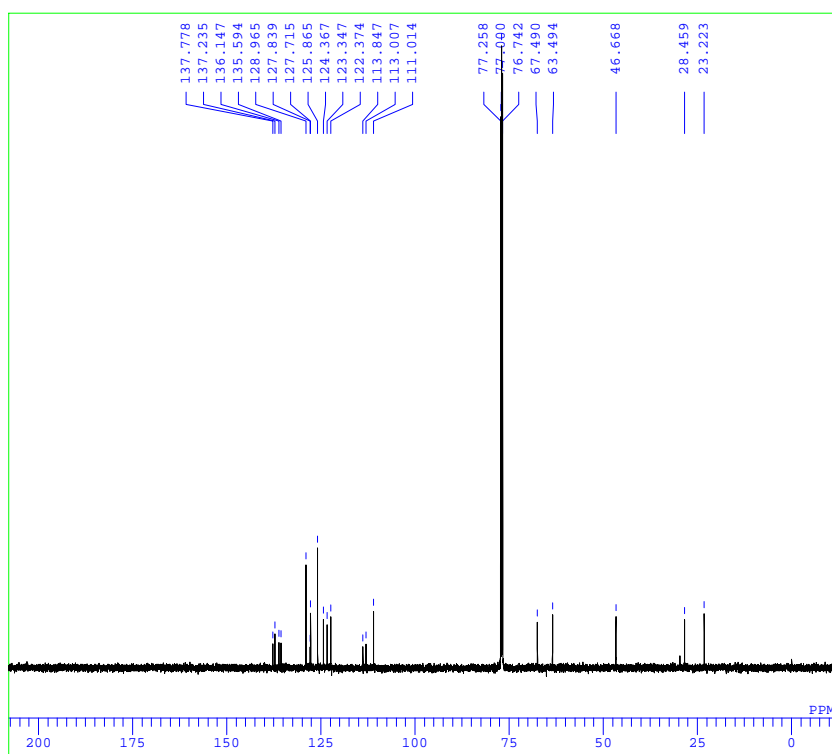
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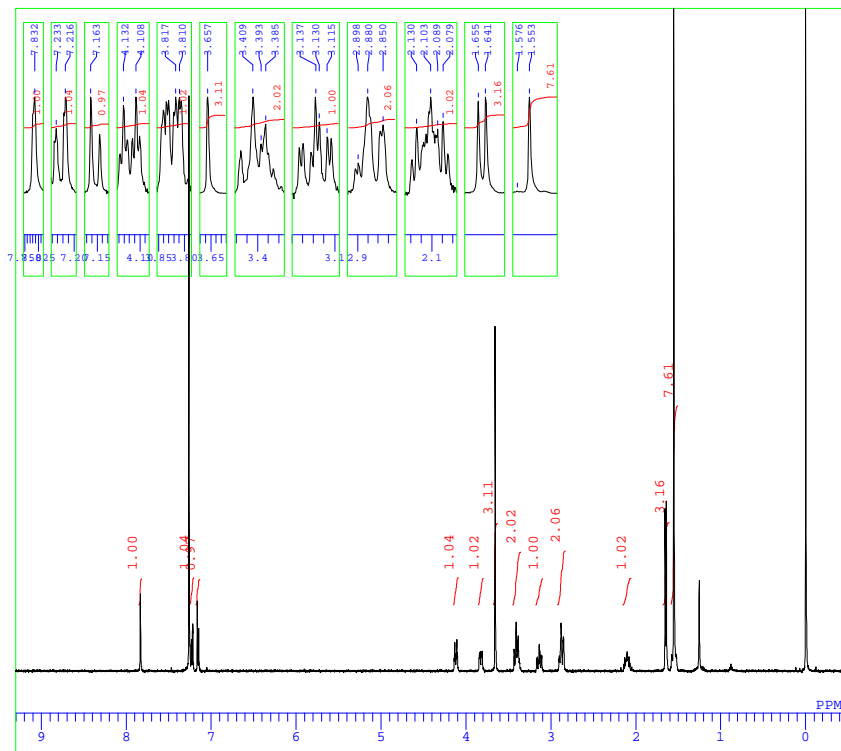
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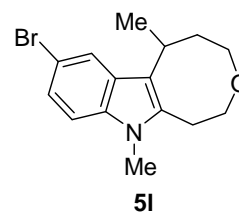
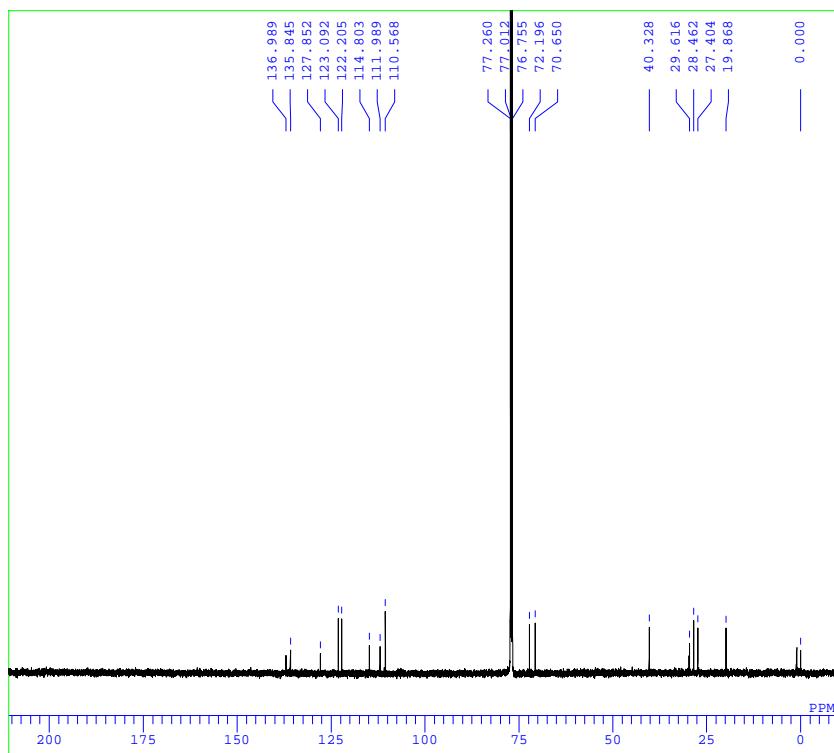
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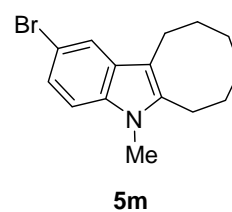
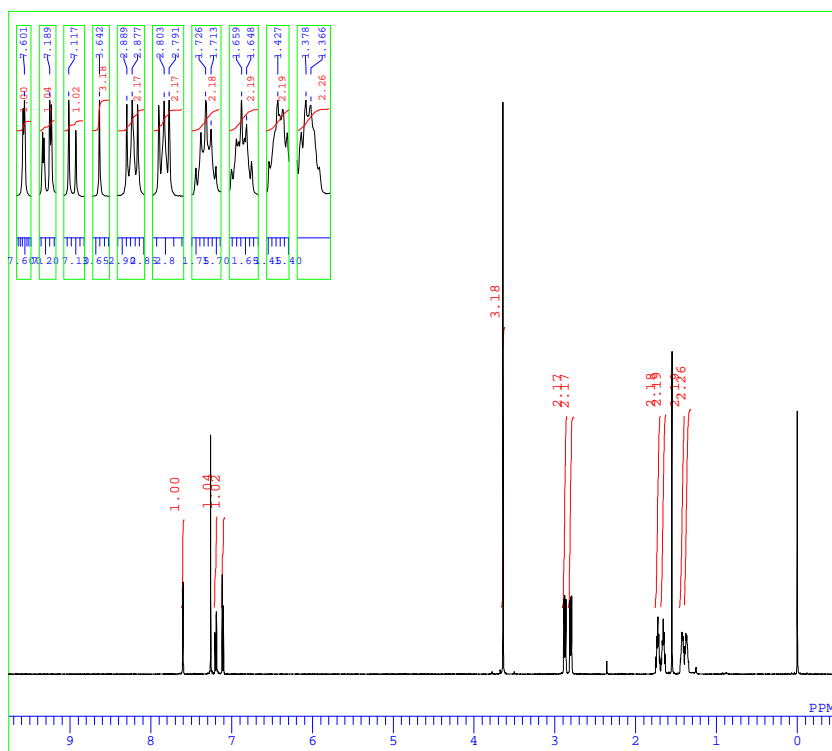
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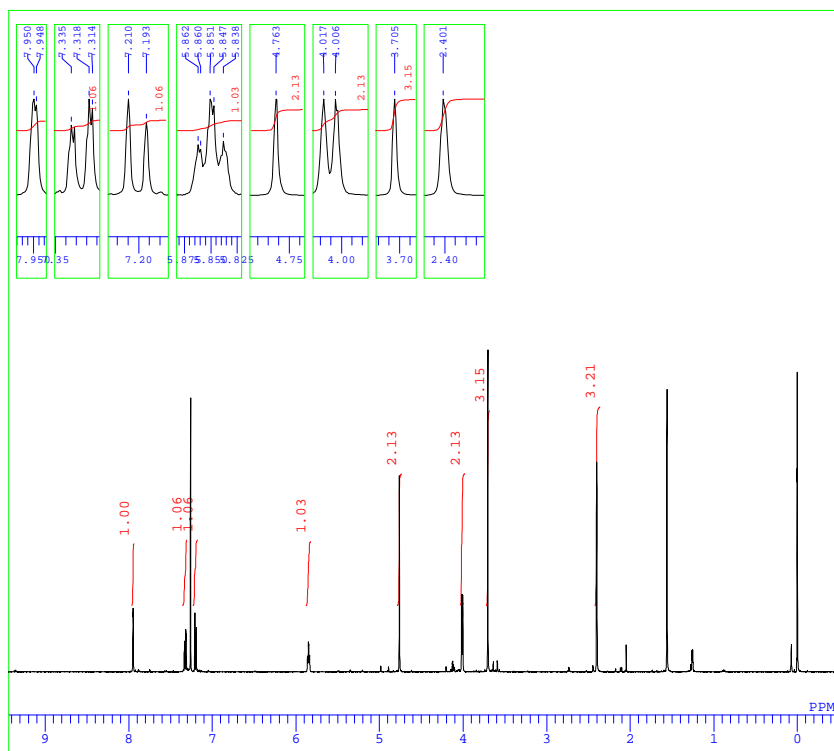
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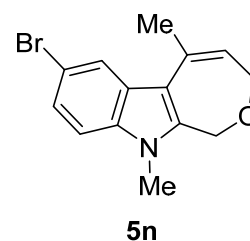
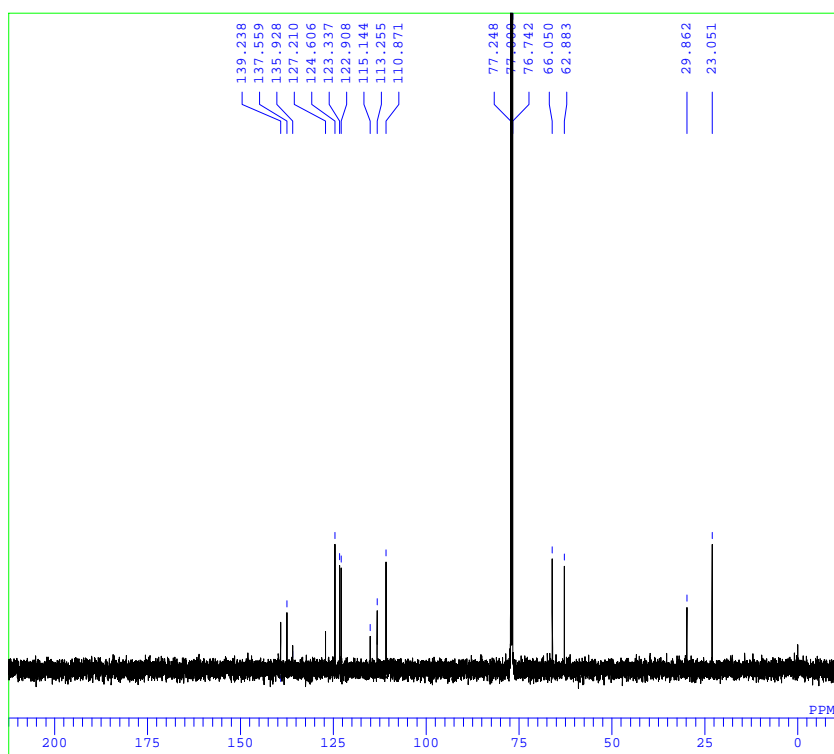
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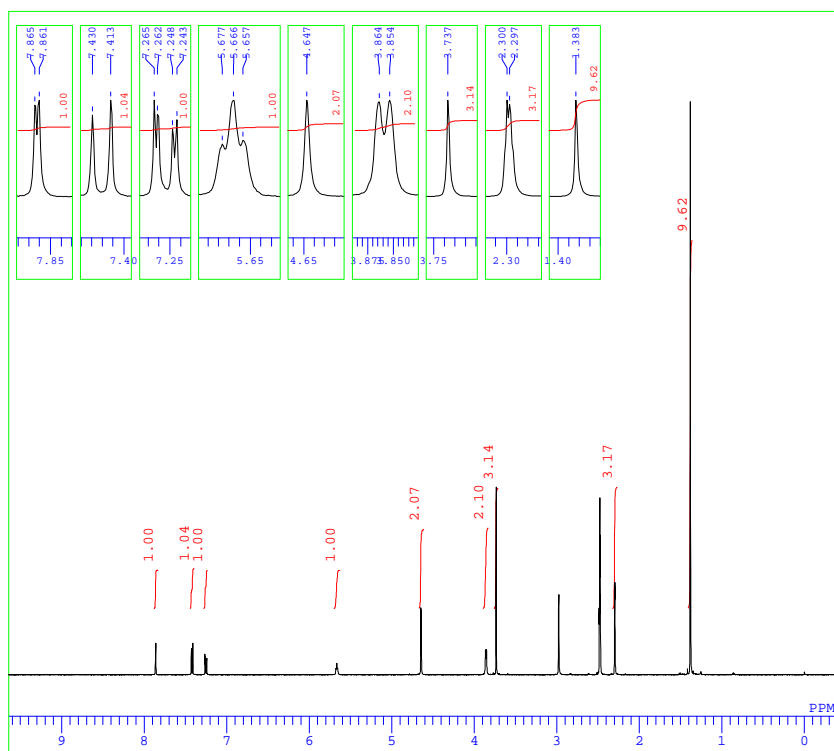
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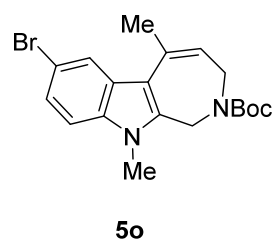
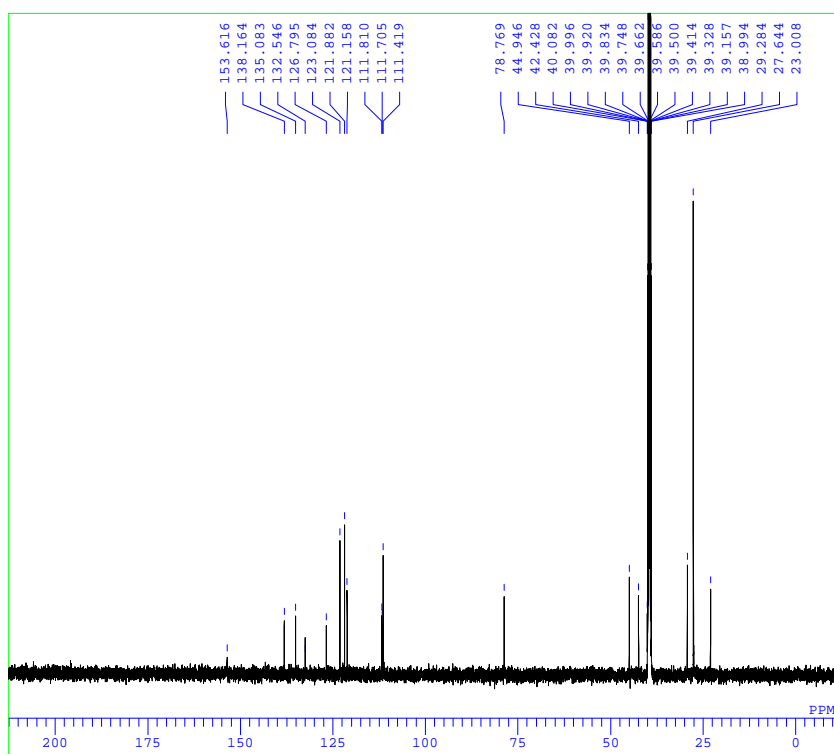
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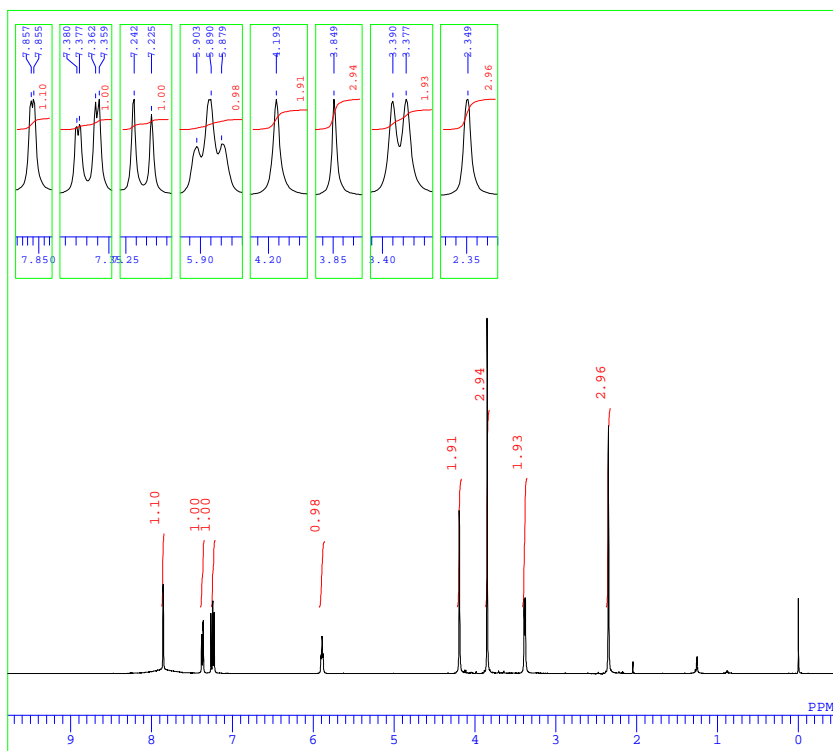
¹H NMR spectrum for compound 5o (500 MHz, DMSO-*d*₆, 100 °C)



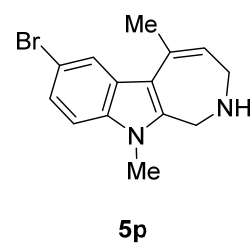
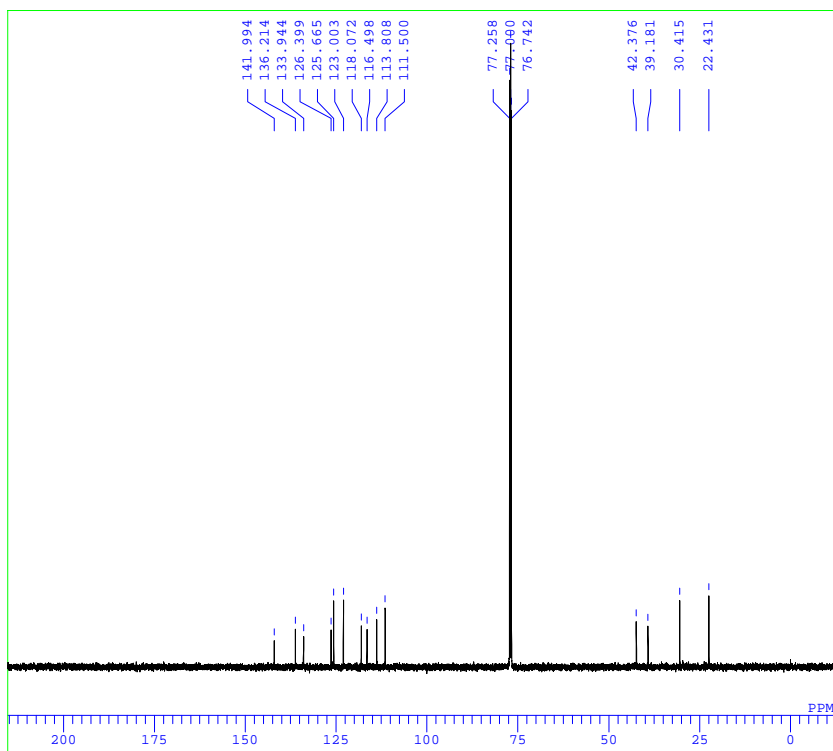
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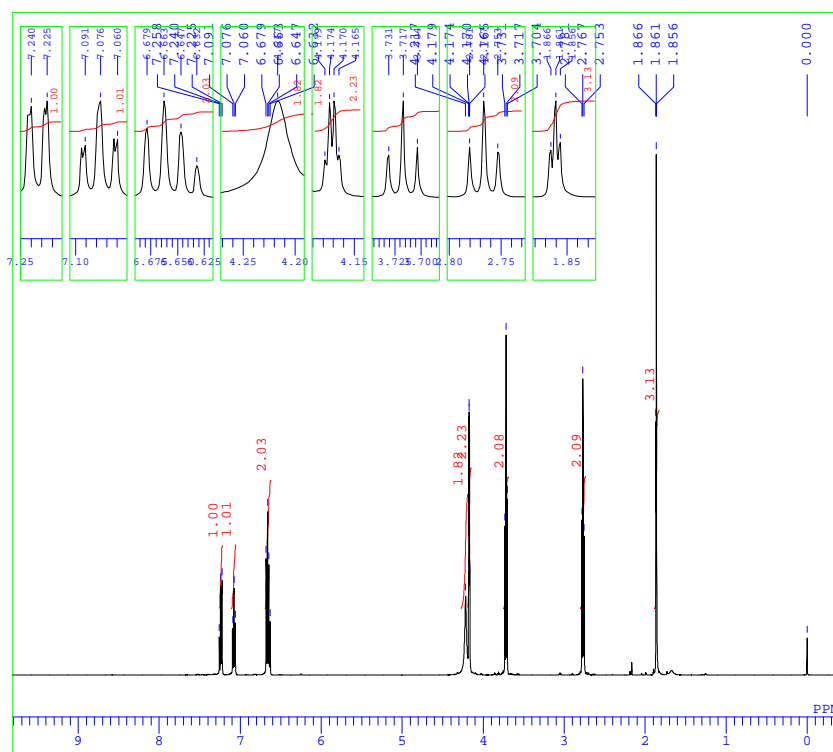
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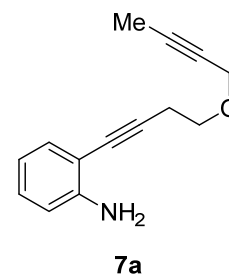
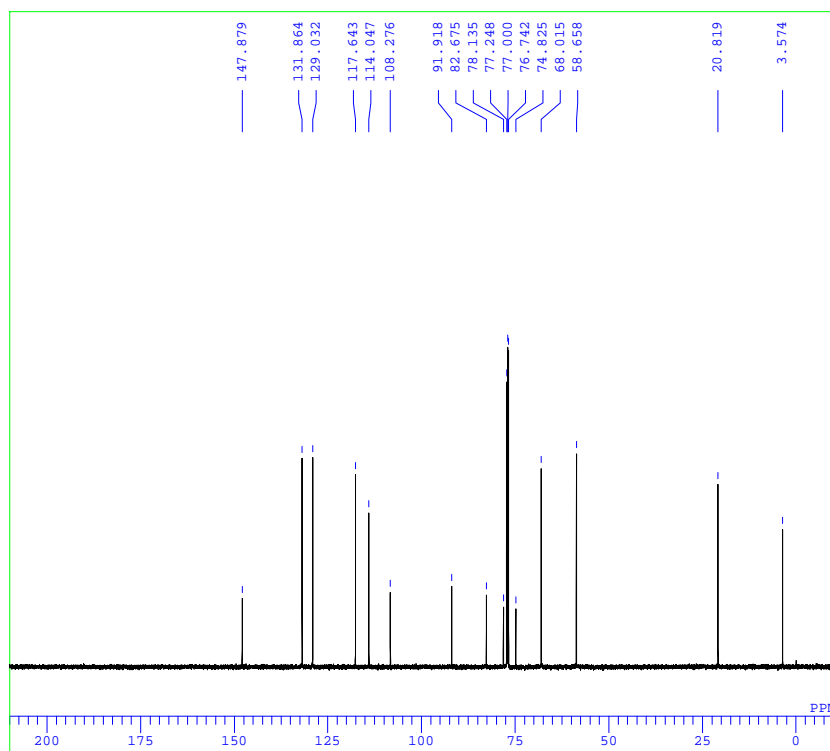
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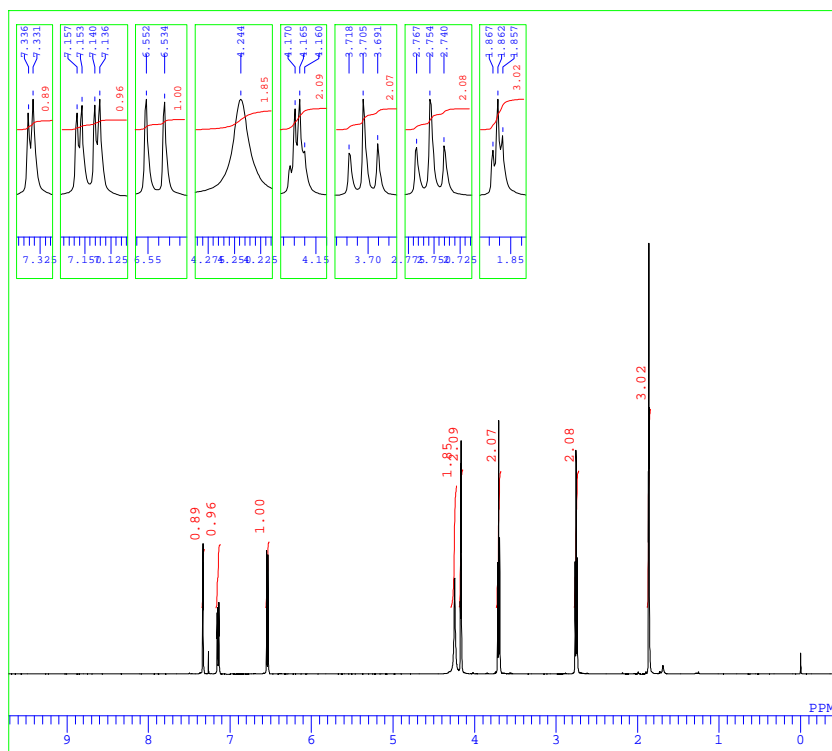
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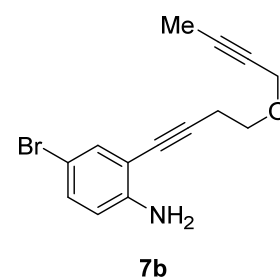
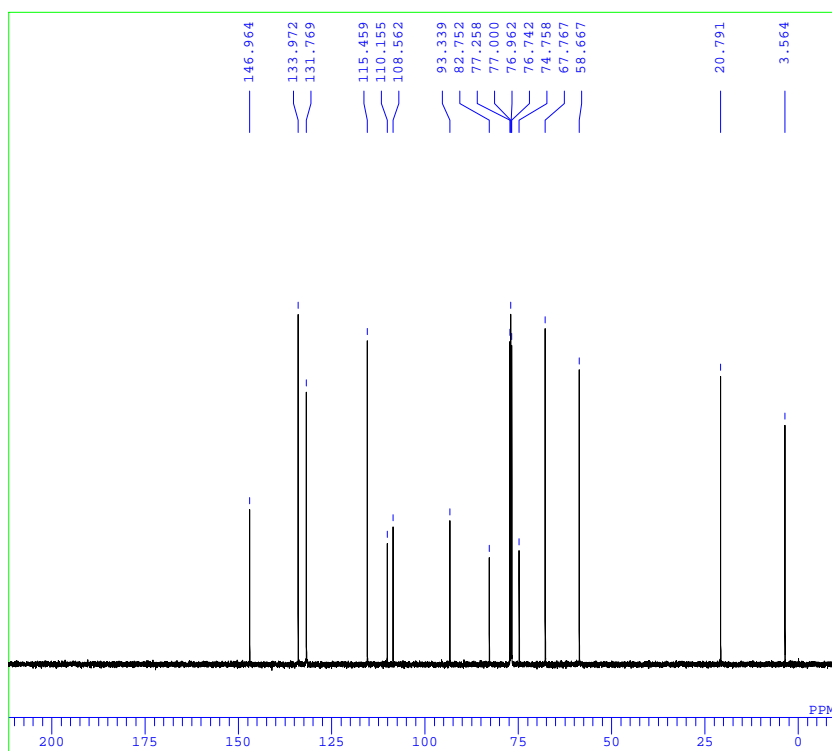
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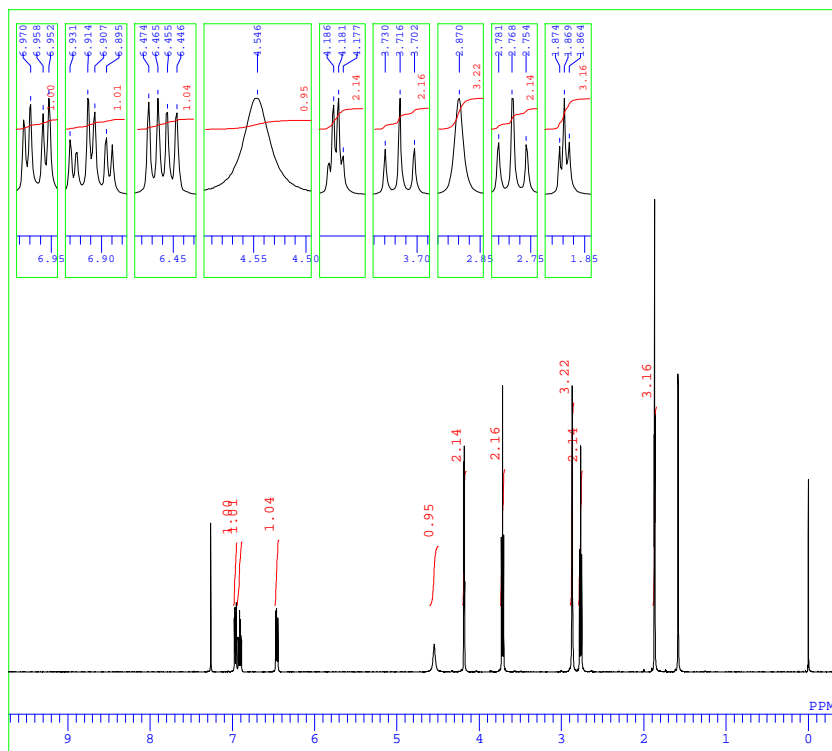
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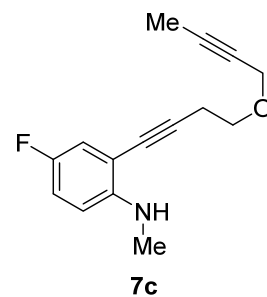
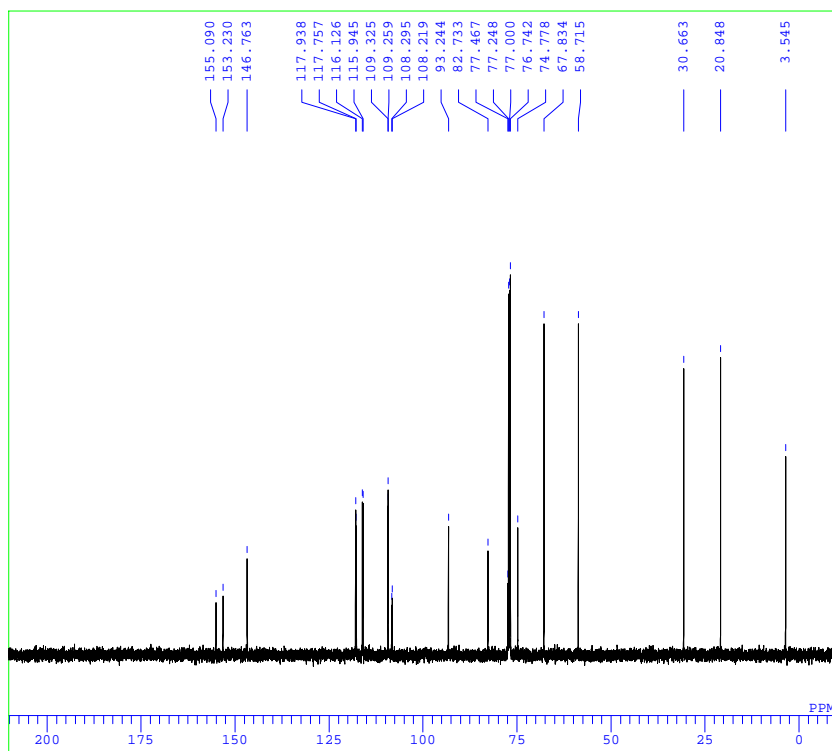
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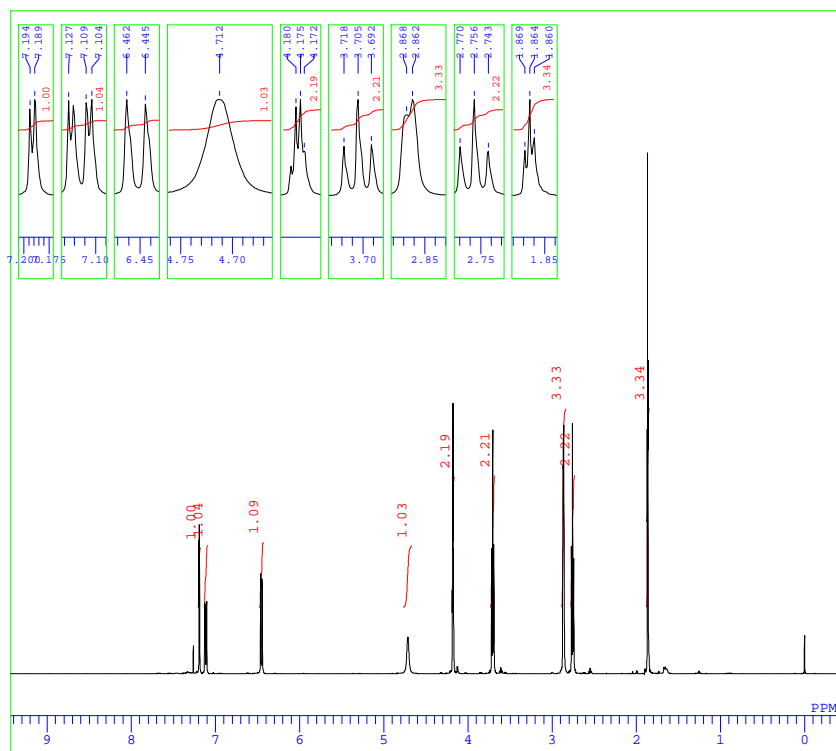
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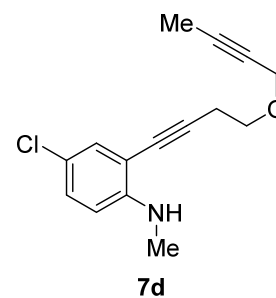
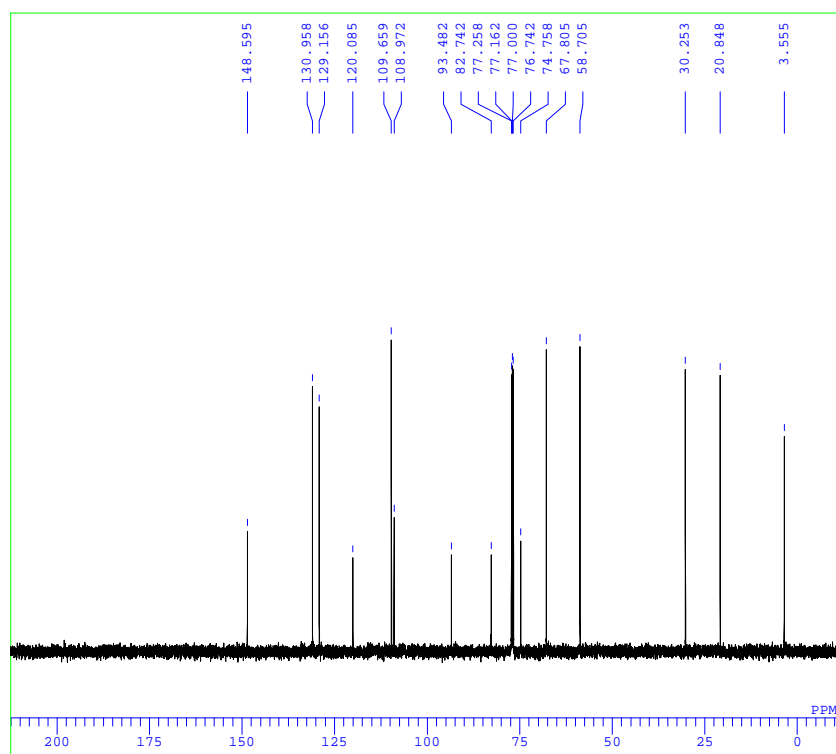
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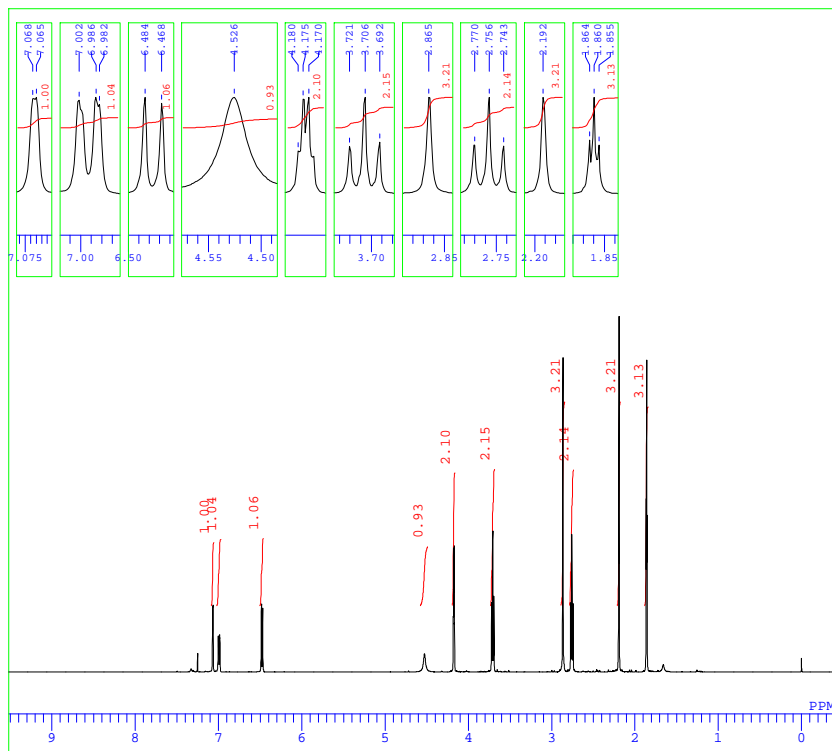
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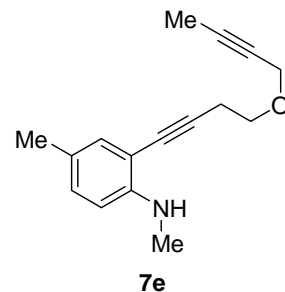
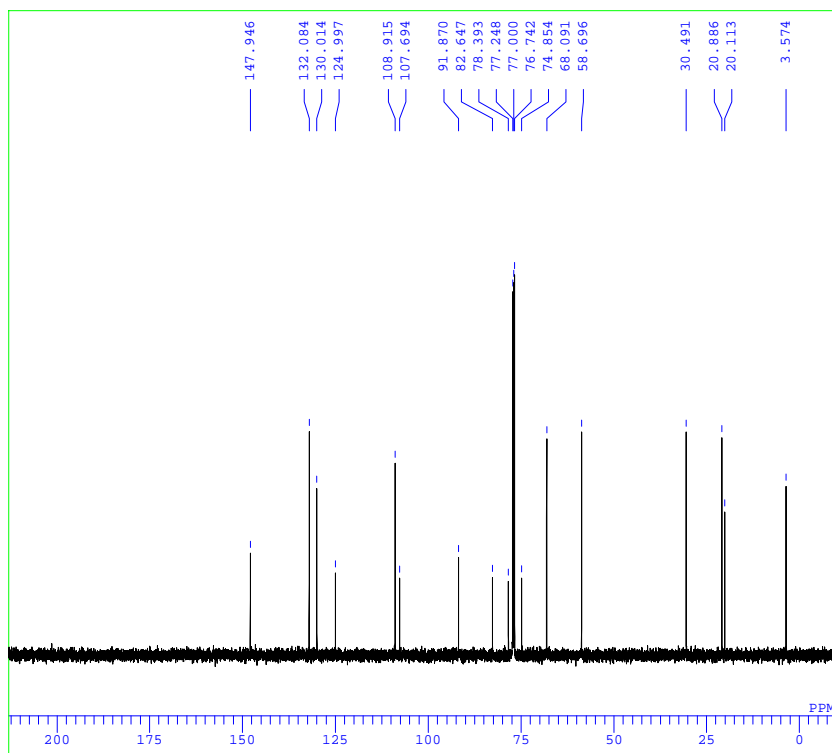
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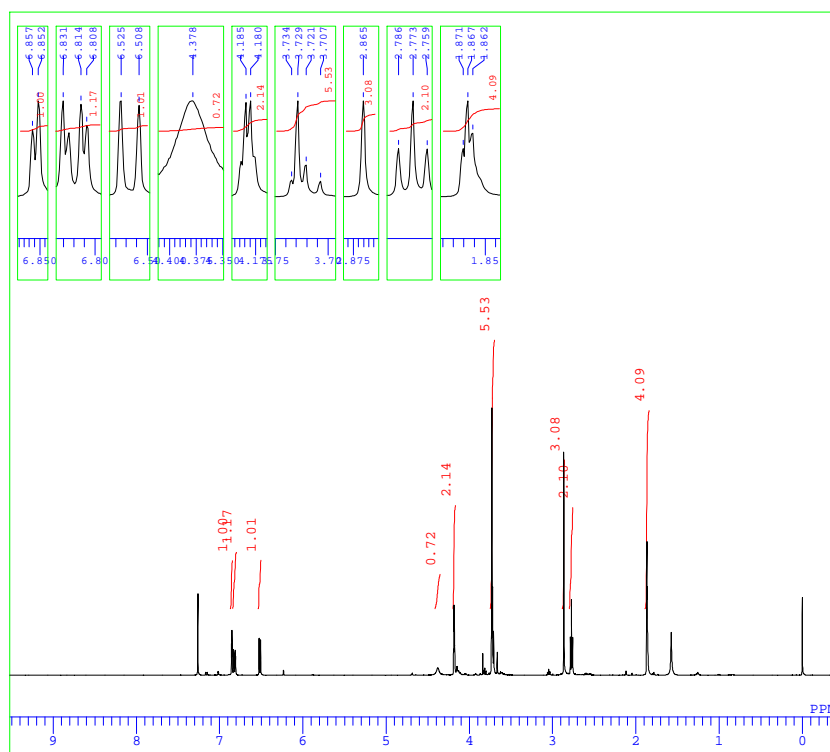
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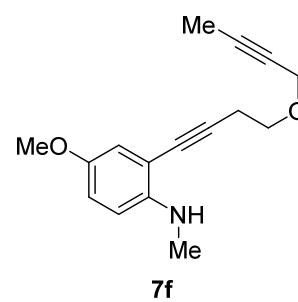
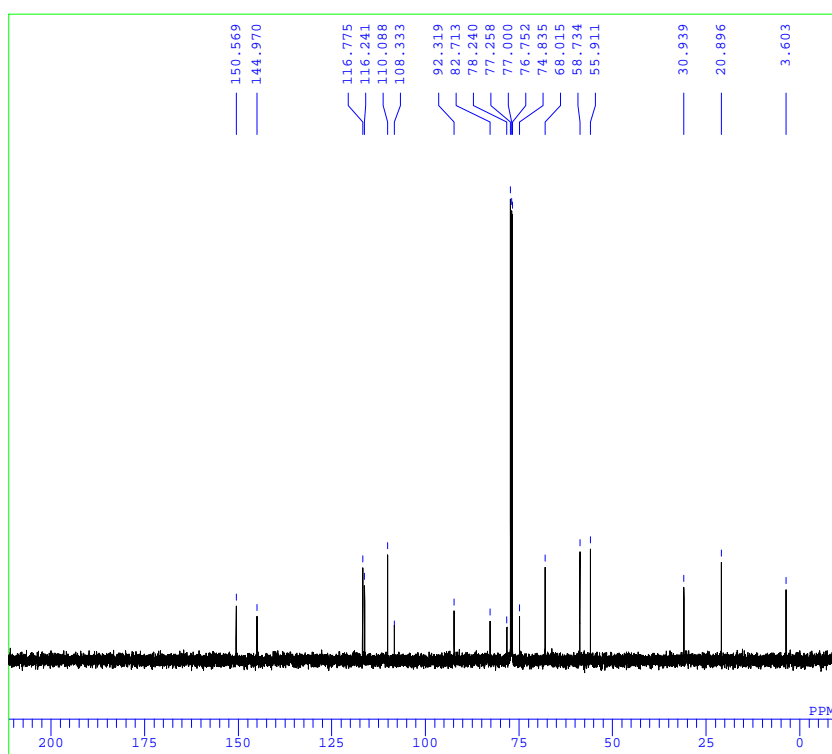
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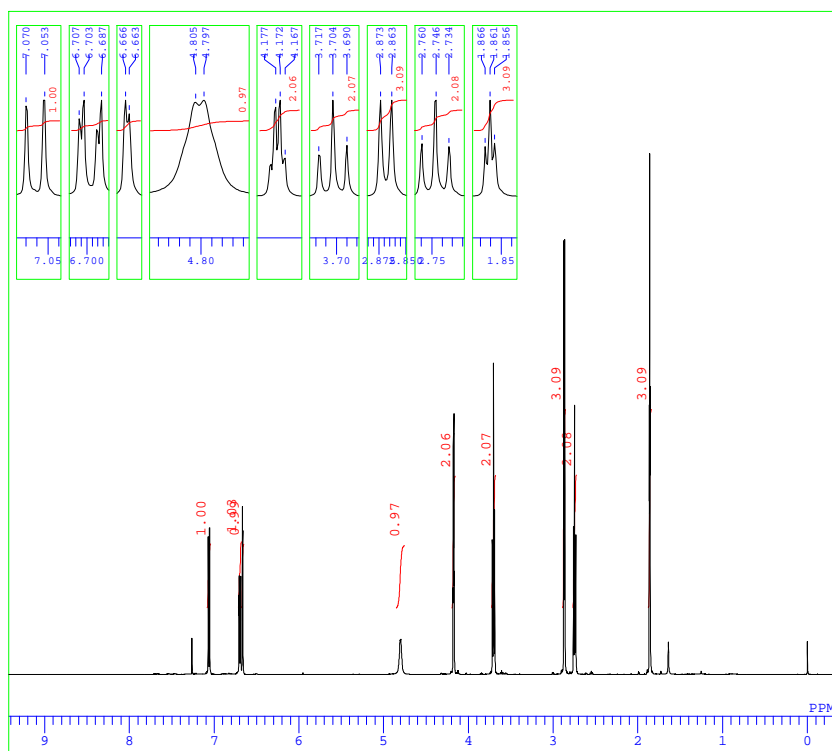
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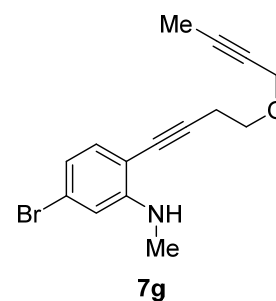
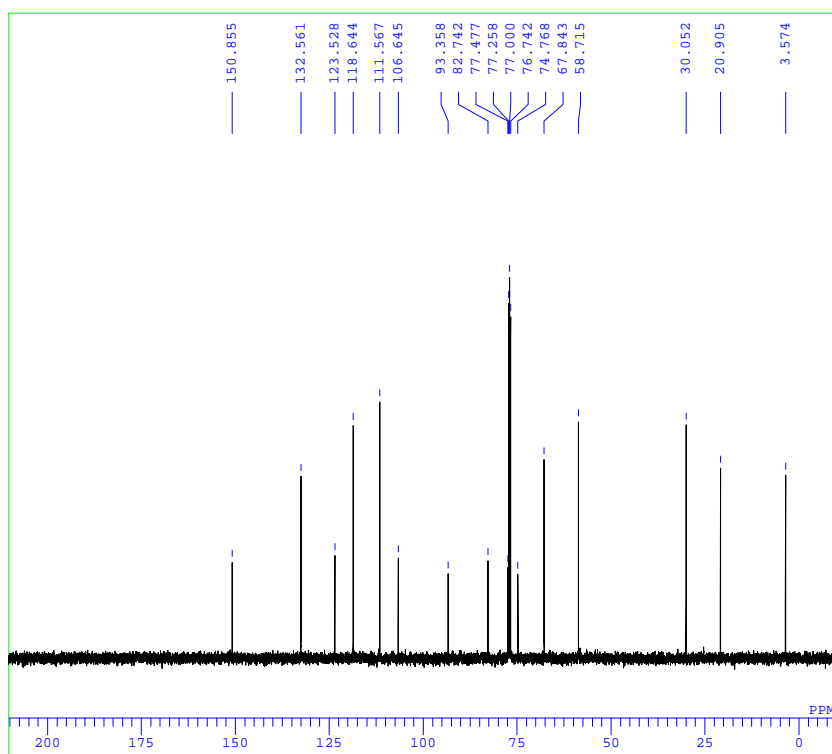
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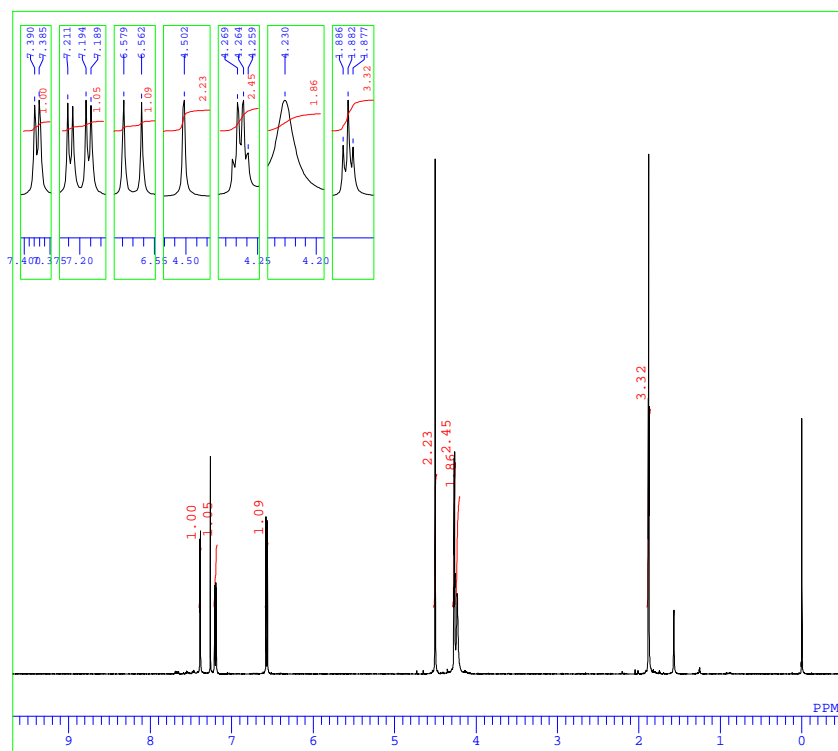
¹H NMR spectrum for compound 7g (500 MHz, CDCl₃)



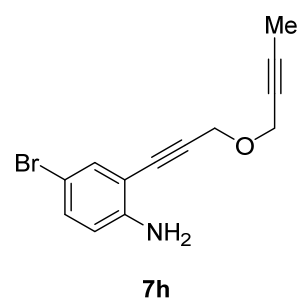
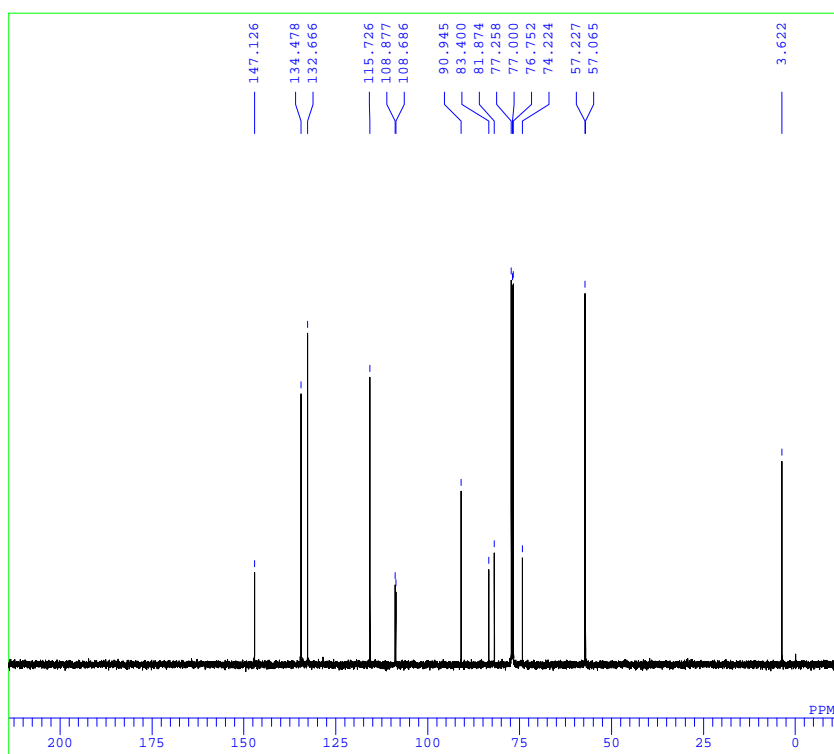
¹³C NMR spectrum for compound 7g (125 MHz, CDCl₃)



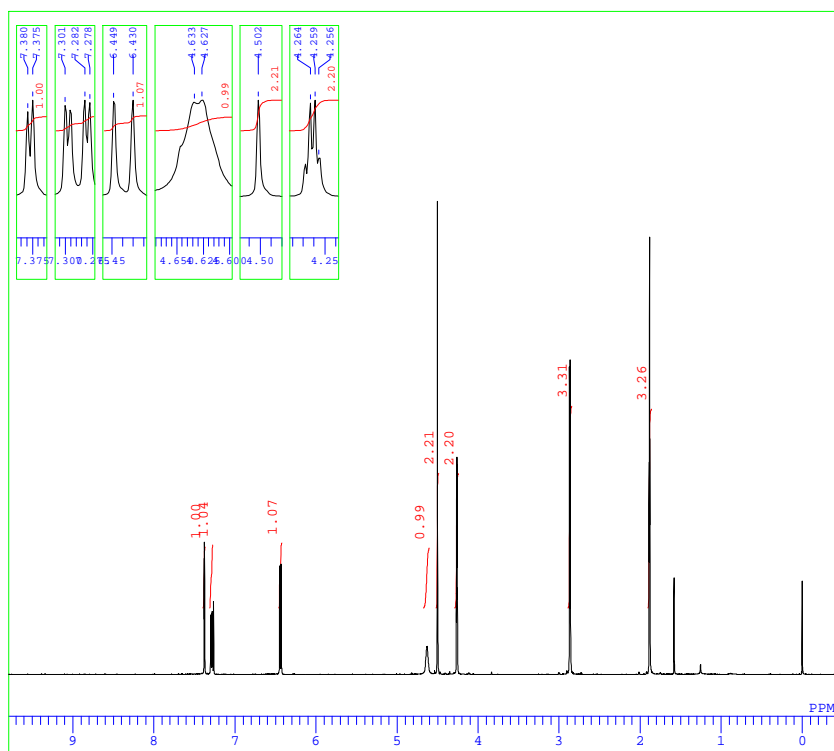
¹H NMR spectrum for compound 7h (500 MHz, CDCl₃)



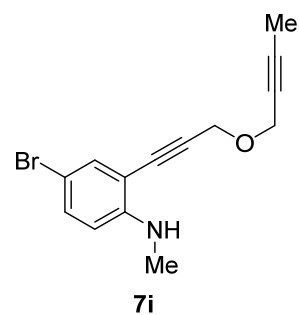
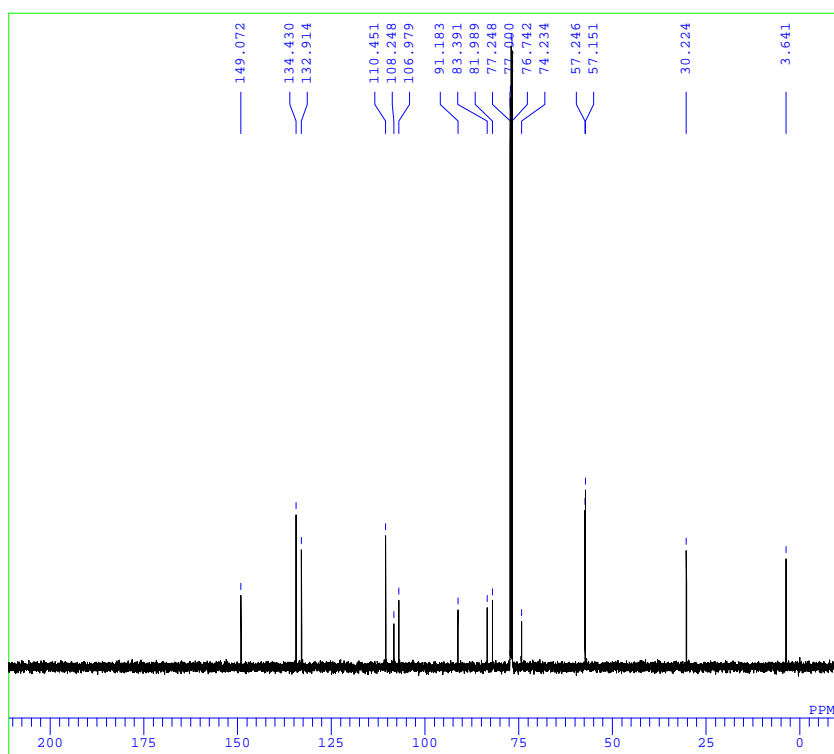
¹³C NMR spectrum for compound 7h (125 MHz, CDCl₃)



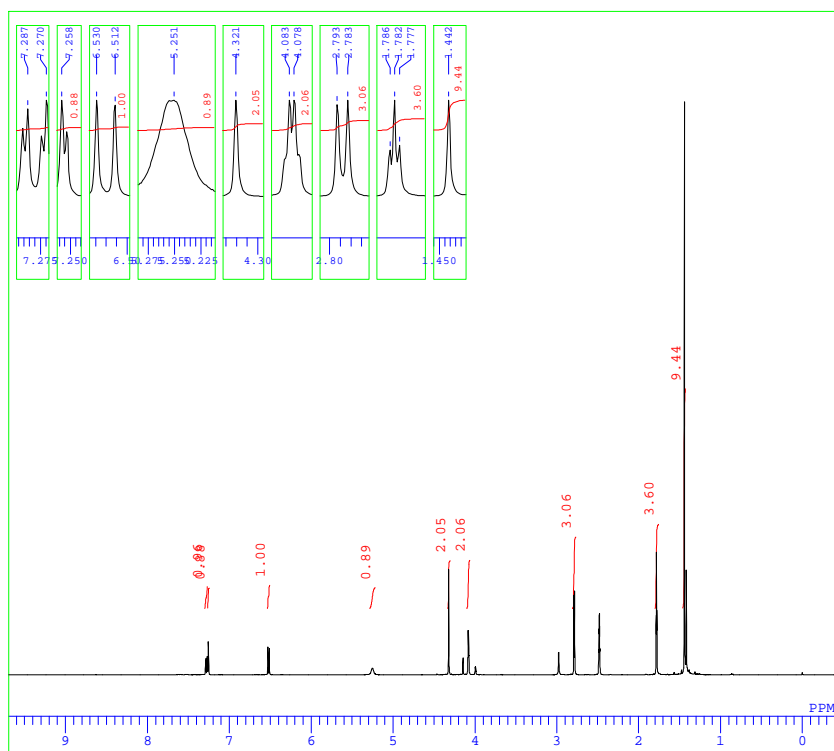
¹H NMR spectrum for compound 7i (500 MHz, CDCl₃)



¹³C NMR spectrum for compound 7i (125 MHz, CDCl₃)



¹H NMR spectrum for compound 7j (500 MHz, DMSO-*d*₆, 100 °C)



¹³C NMR spectrum for compound 7j (125 MHz, DMSO-*d*₆, 100 °C)

