

Anti-inflammatory activities of 8-benzylaminoxanthines showing potent adenosine A_{2A} receptor antagonistic properties

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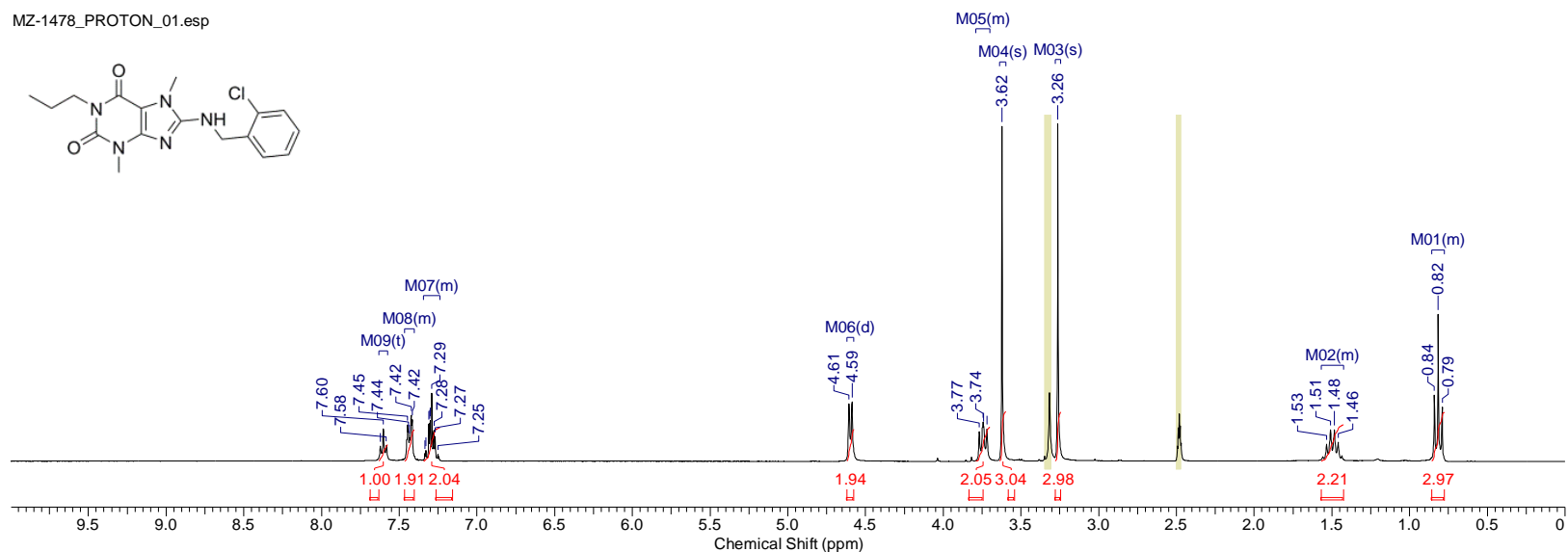


Figure 1S. ¹H NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (5)

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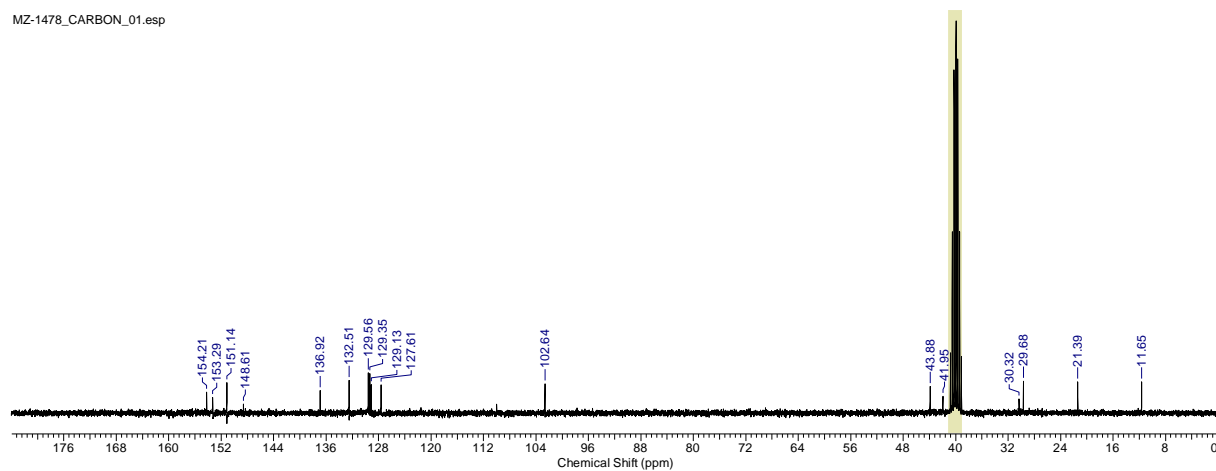
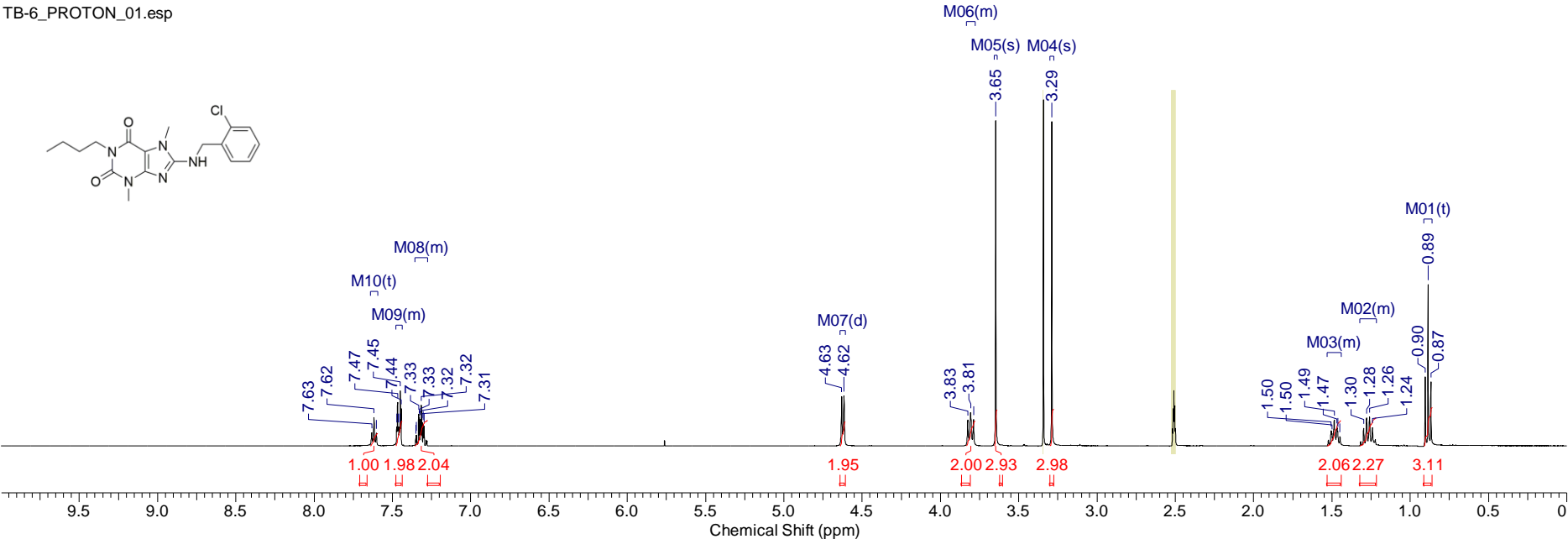
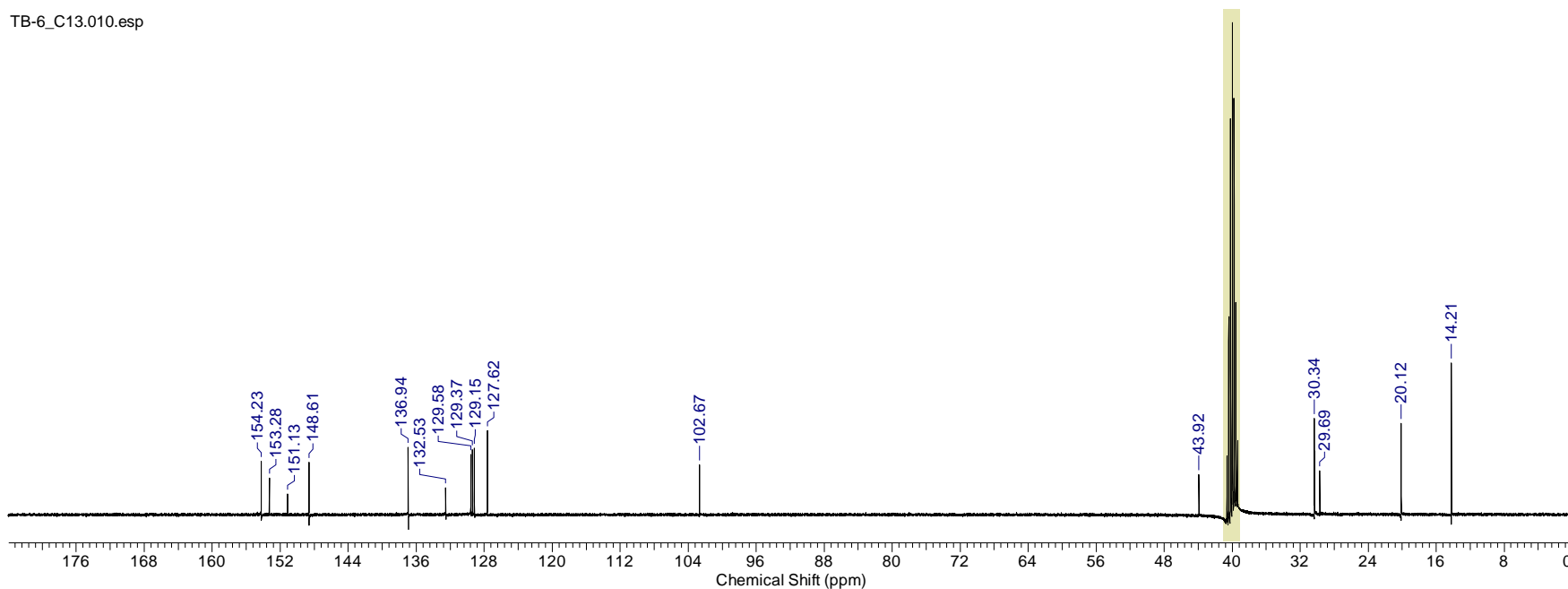


Figure 2S. ¹³C NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (5)

Figure 3S. ¹H NMR spectrum of 1-butyl-8-((2-chlorobenzyl)amino)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (6)Figure 4S. ¹³C NMR spectrum of 1-butyl-8-((2-chlorobenzyl)amino)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (6)

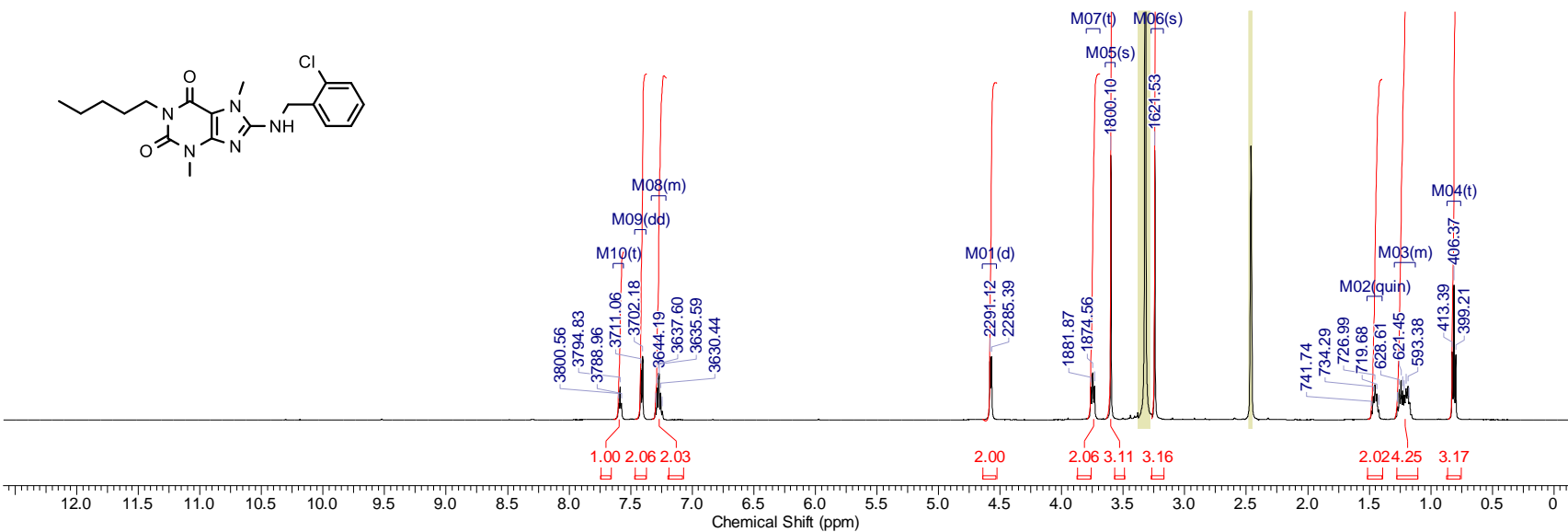
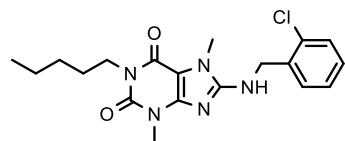


Figure 5S. ^1H NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-pentyl-3,7-dihydro-1H-purine-2,6-dione (**7**)

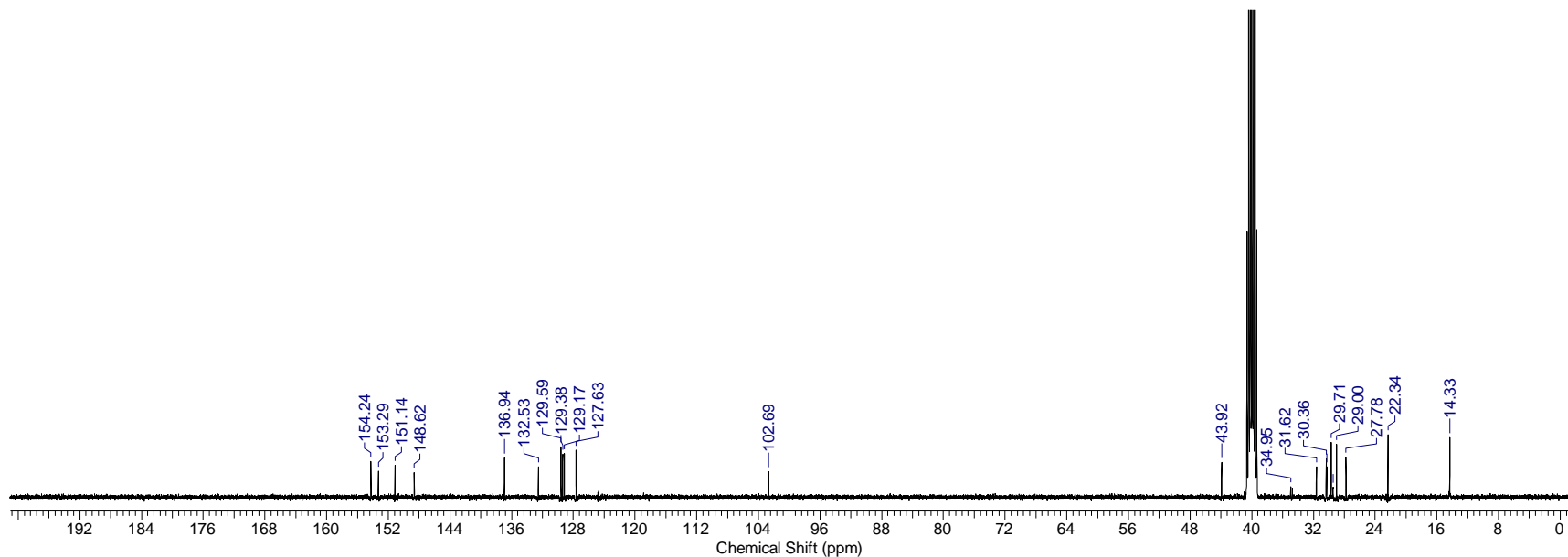


Figure 6S. ^{13}C NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-pentyl-3,7-dihydro-1H-purine-2,6-dione (**7**)

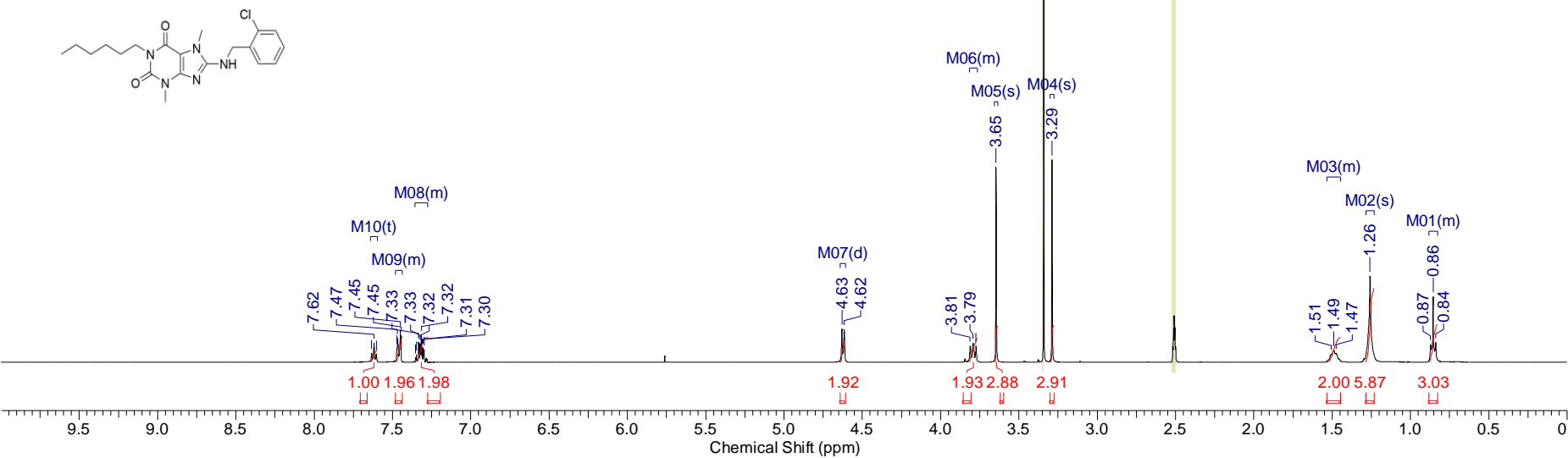


Figure 7S. ^1H NMR spectrum of 8-((2-chlorobenzyl)amino)-1-hexyl-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (**8**)

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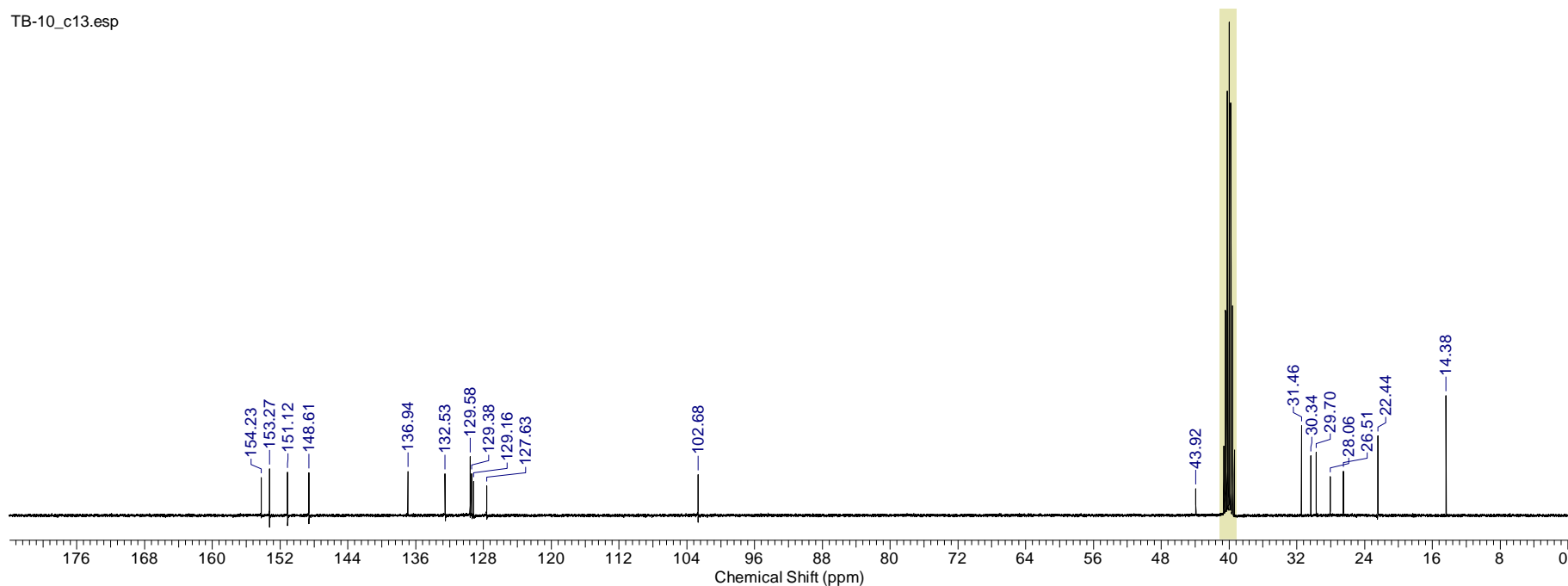
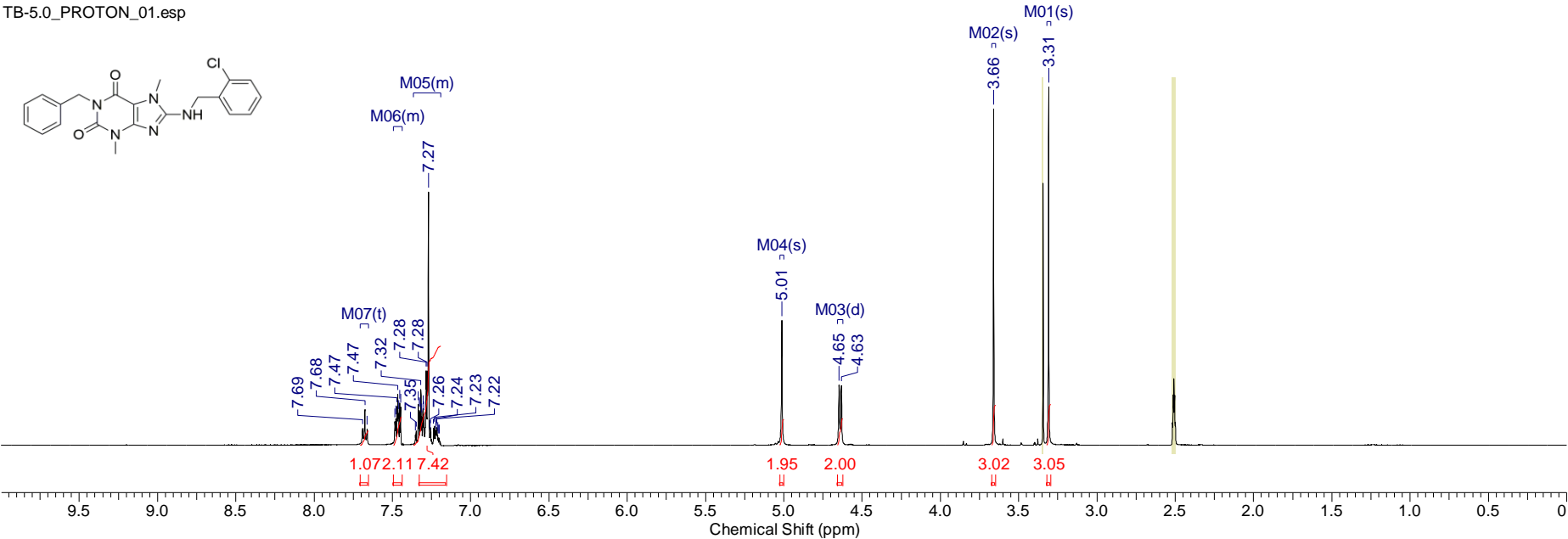
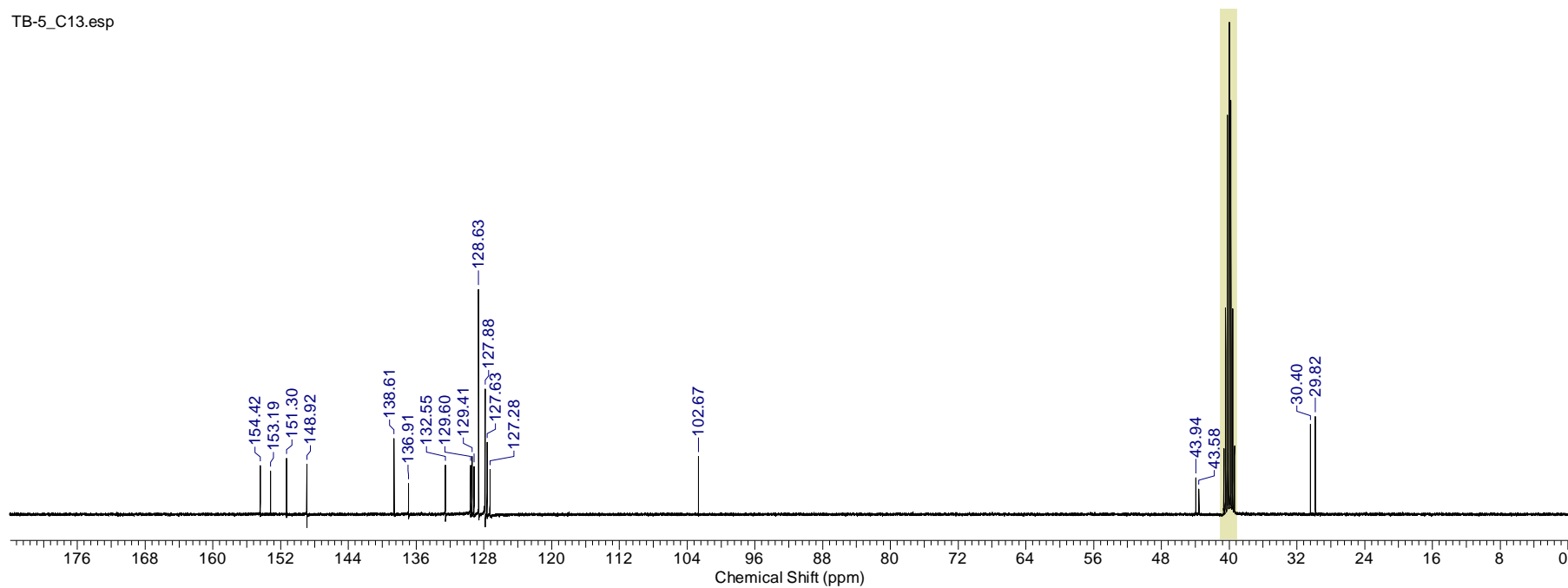


Figure 8S. ^{13}C NMR spectrum of 8-((2-chlorobenzyl)amino)-1-hexyl-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (**8**)

Figure 9S. ¹H NMR spectrum of 1-benzyl-8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**9**)Figure 10S. ¹³C NMR spectrum of 1-benzyl-8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**9**)

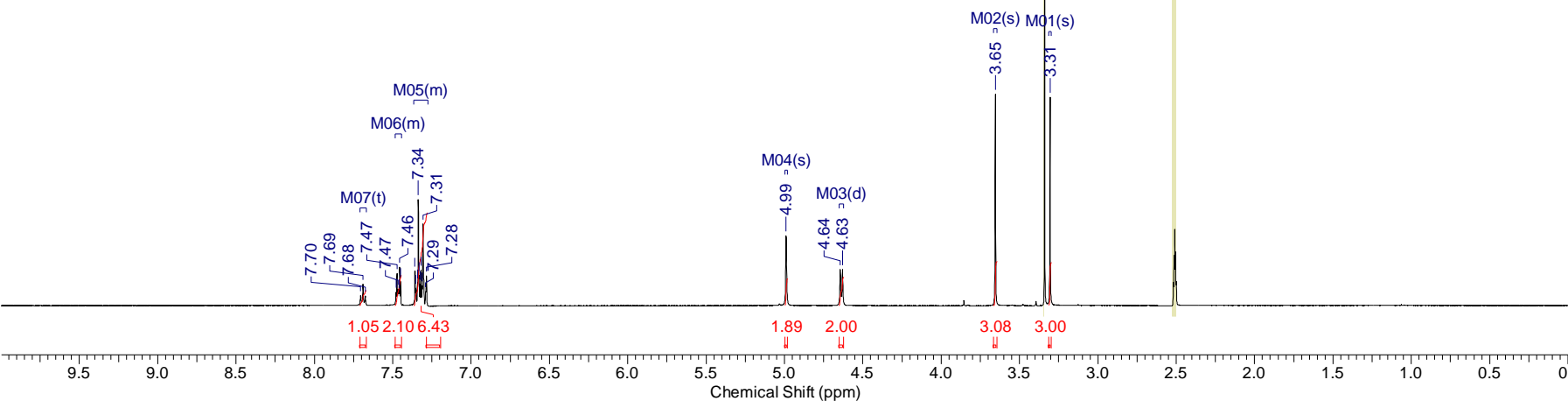
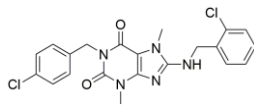


Figure 11S. ^1H NMR spectrum of 1-(4-chlorobenzyl)-8-((2-chlorobenzyl)amino)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (**10**)

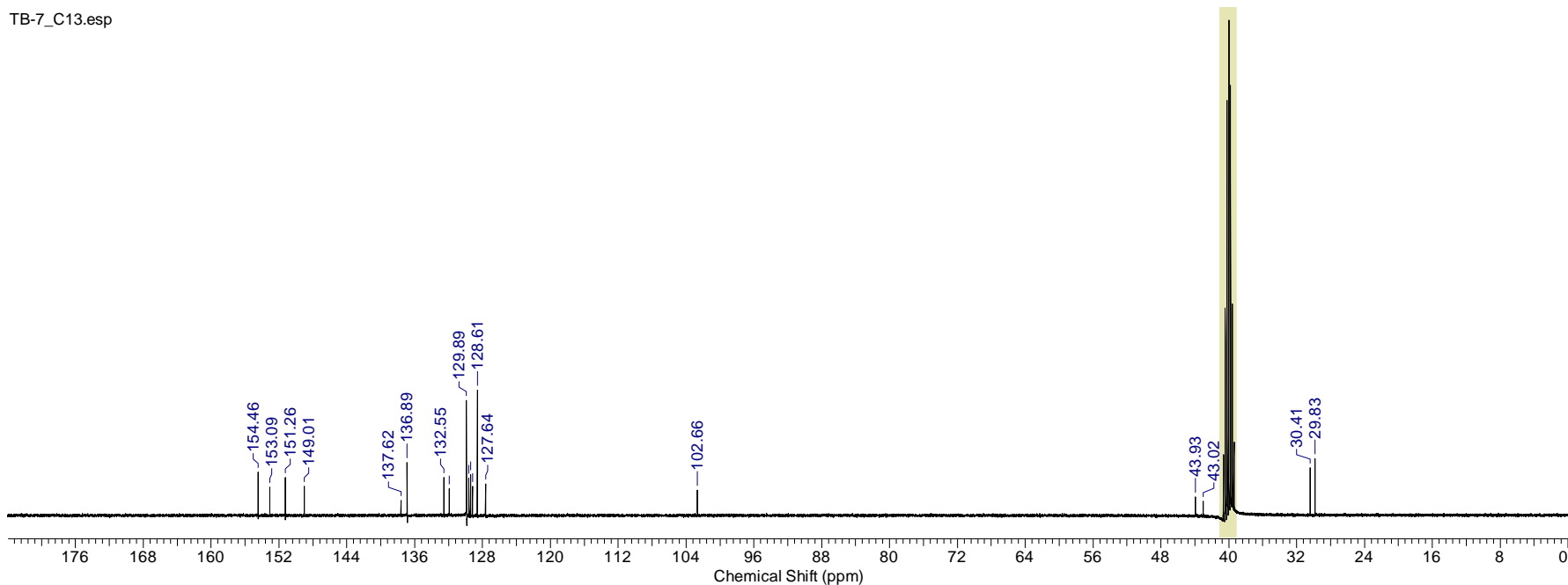
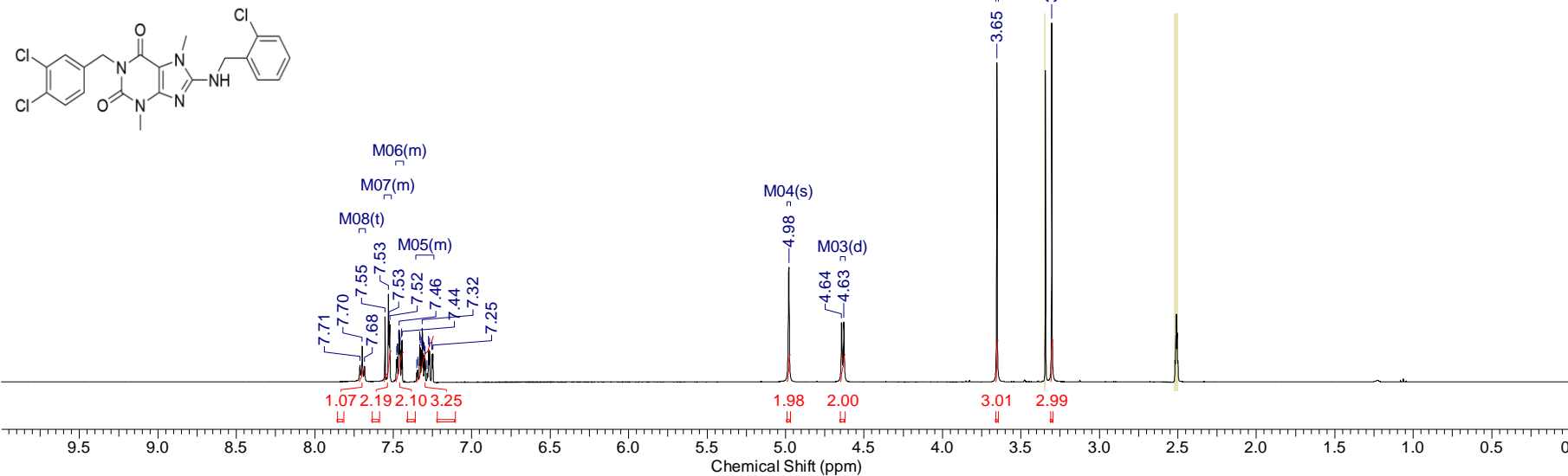
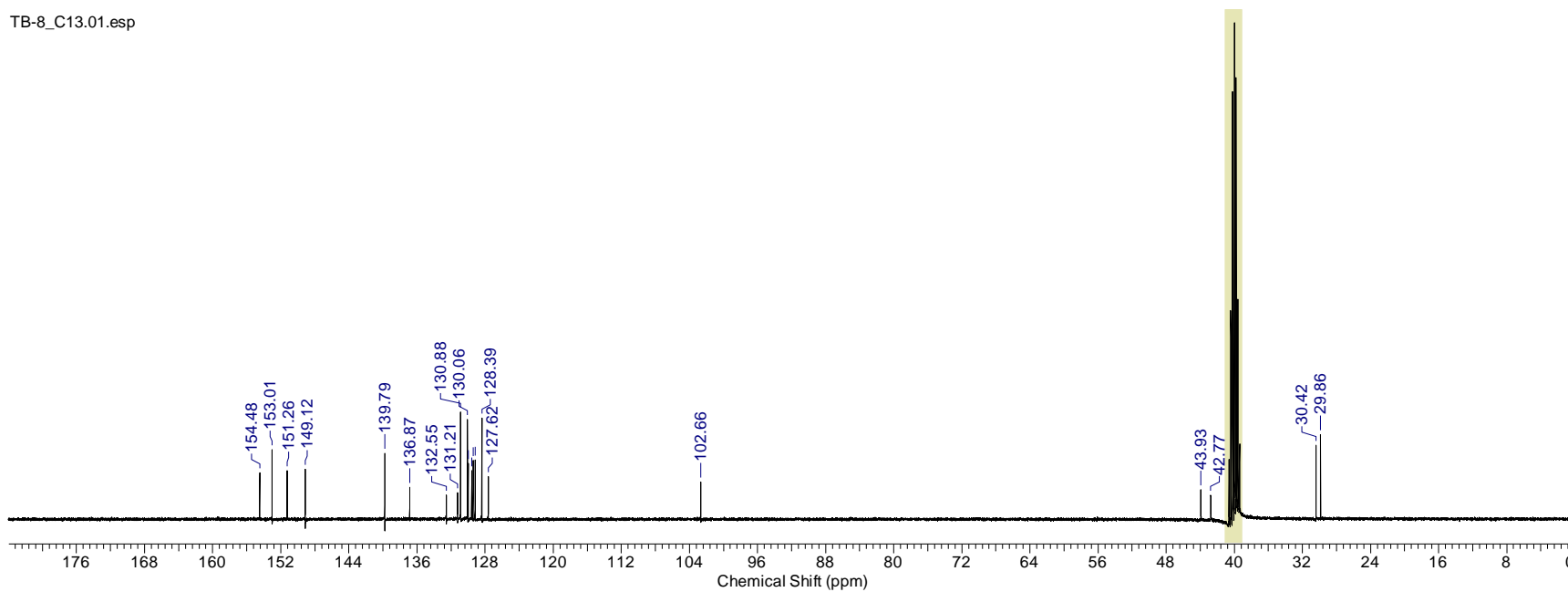
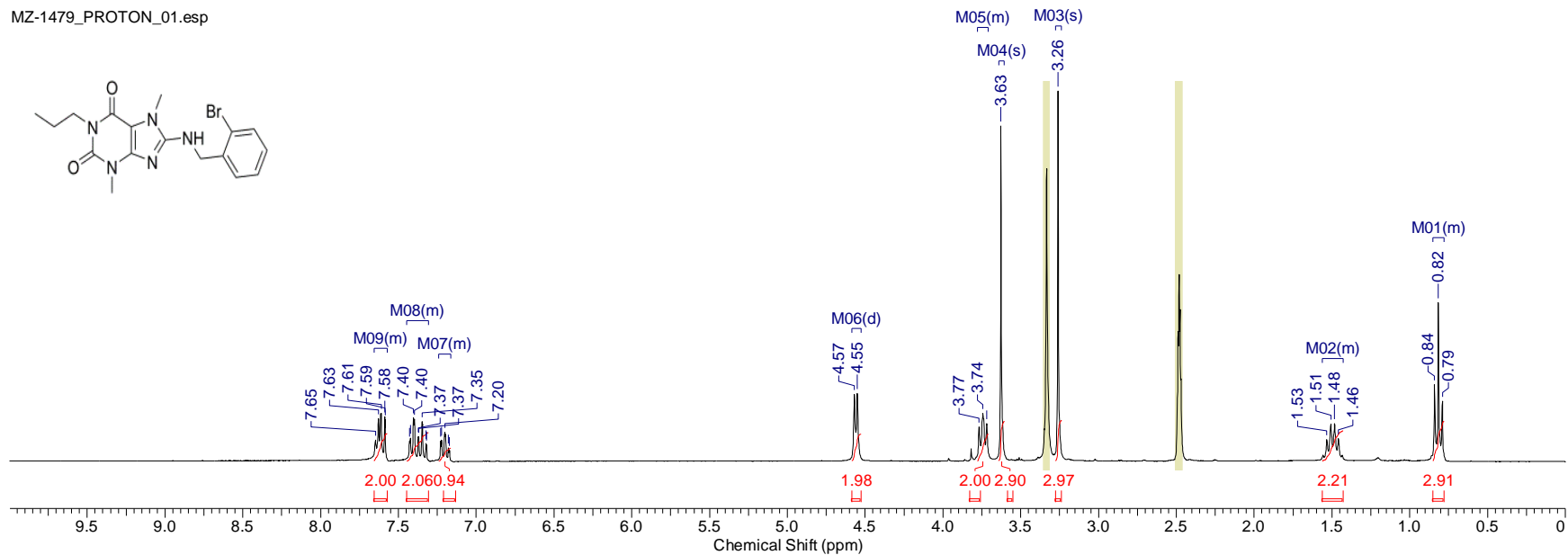
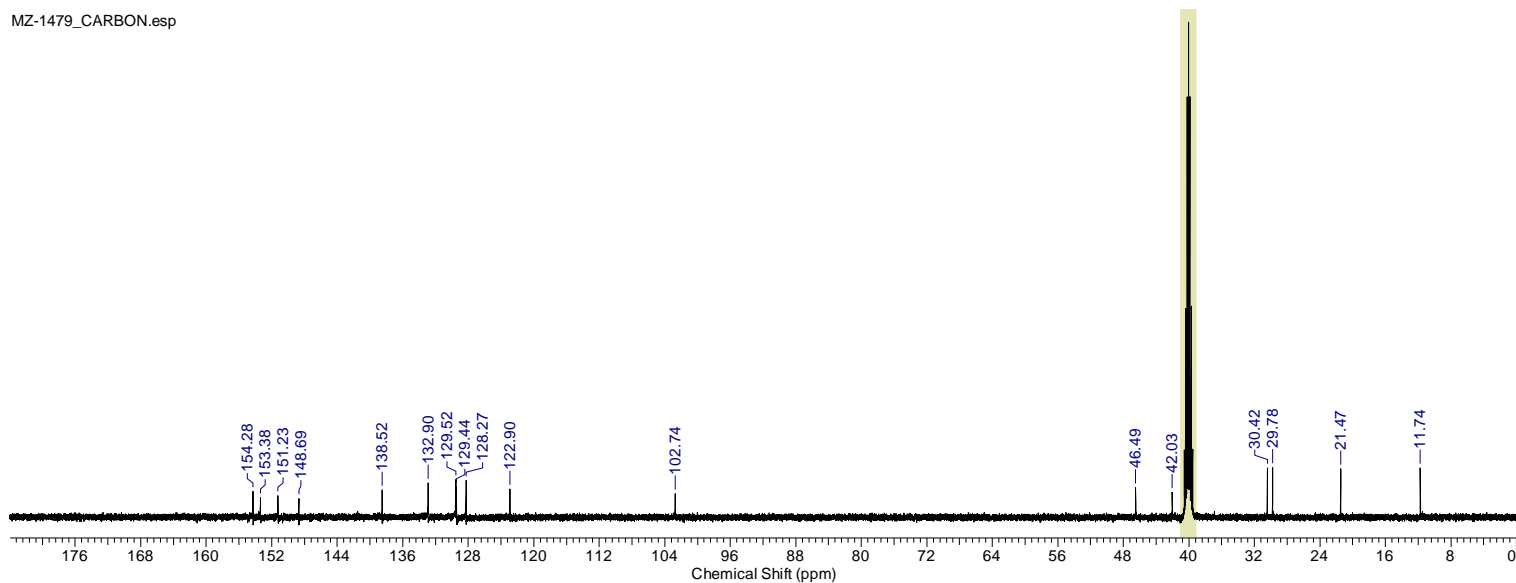


Figure 12S. ^{13}C NMR spectrum of 1-(4-chlorobenzyl)-8-((2-chlorobenzyl)amino)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (**10**)

Figure 13S. ¹H NMR spectrum of 8-((2-chlorobenzyl)amino)-1-(3,4-dichlorobenzyl)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (11)Figure 14S. ¹³C NMR spectrum of 8-((2-chlorobenzyl)amino)-1-(3,4-dichlorobenzyl)-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione (11)

Figure 15S. ¹H NMR spectrum of 8-((2-bromobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (12)Figure 16S. ¹³C NMR spectrum of 8-((2-bromobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (12)

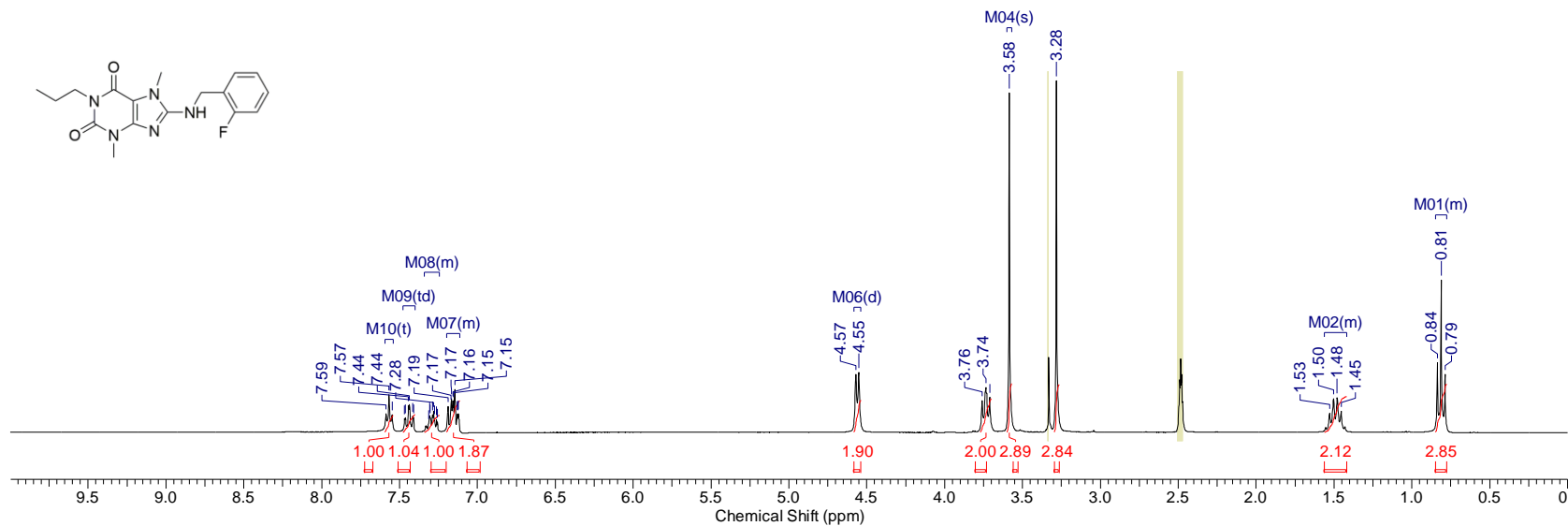


Figure 17S. ¹H NMR spectrum of 8-((2-fluorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**13**)

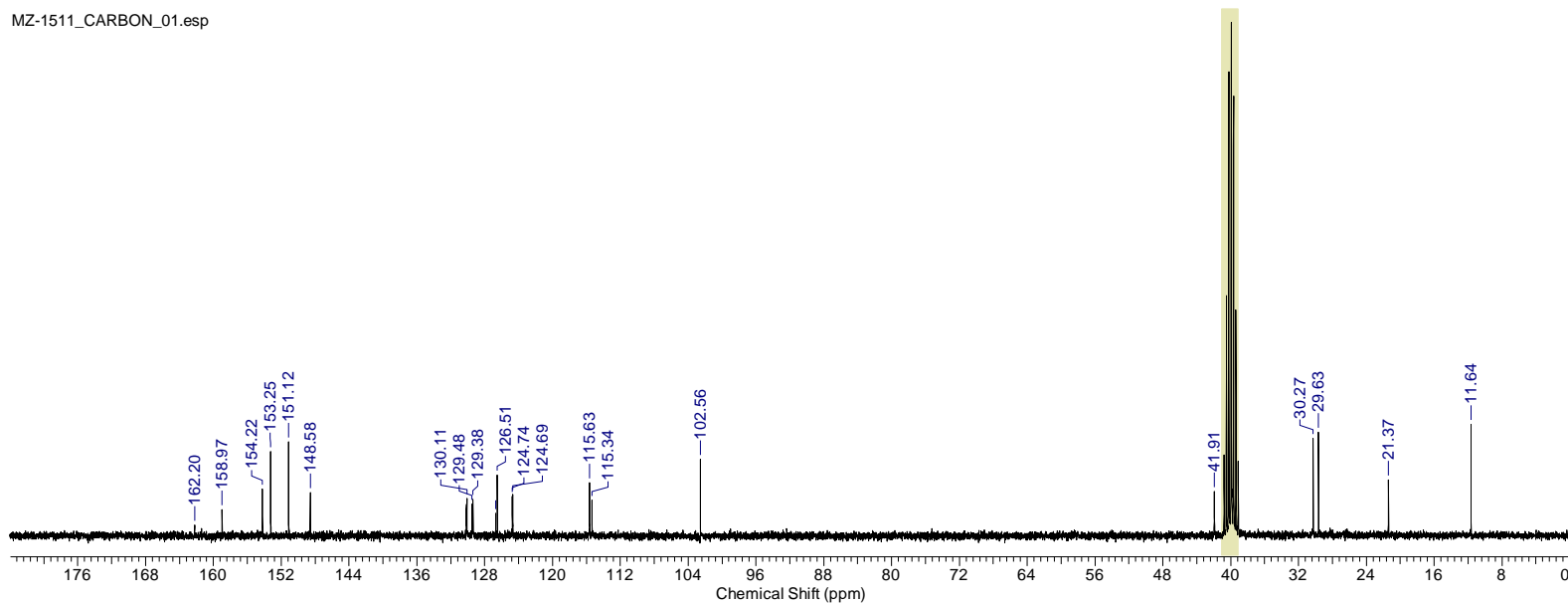


Figure 18S. ¹³C NMR spectrum of 8-((2-fluorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**13**)

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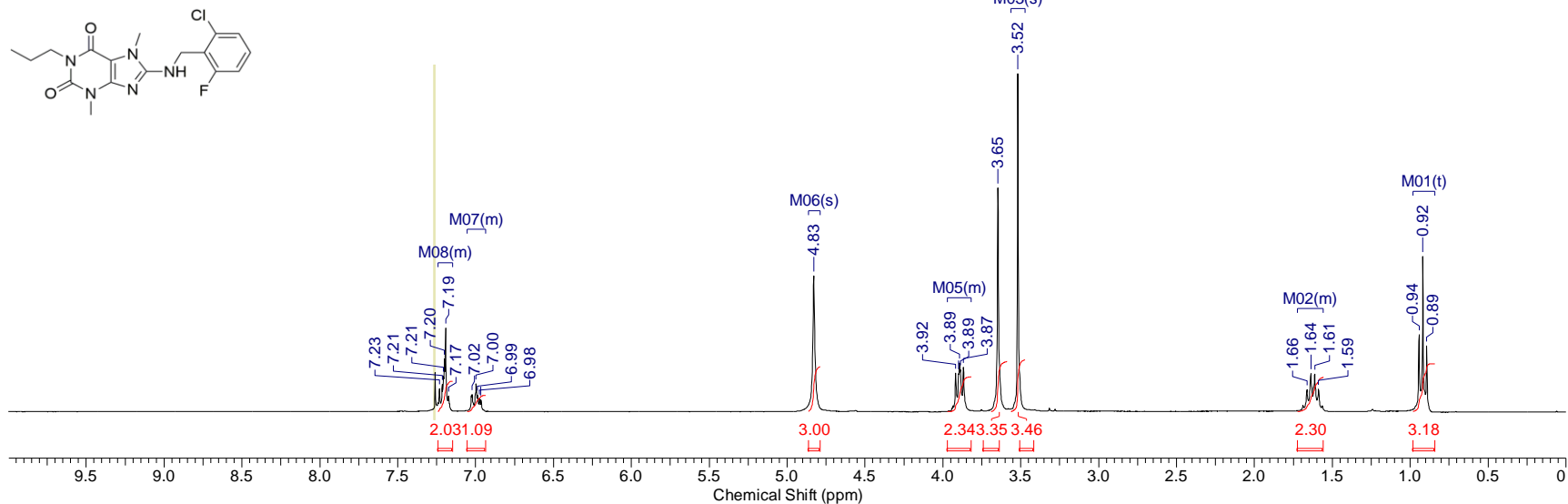


Figure 19S. ¹H NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**14**)

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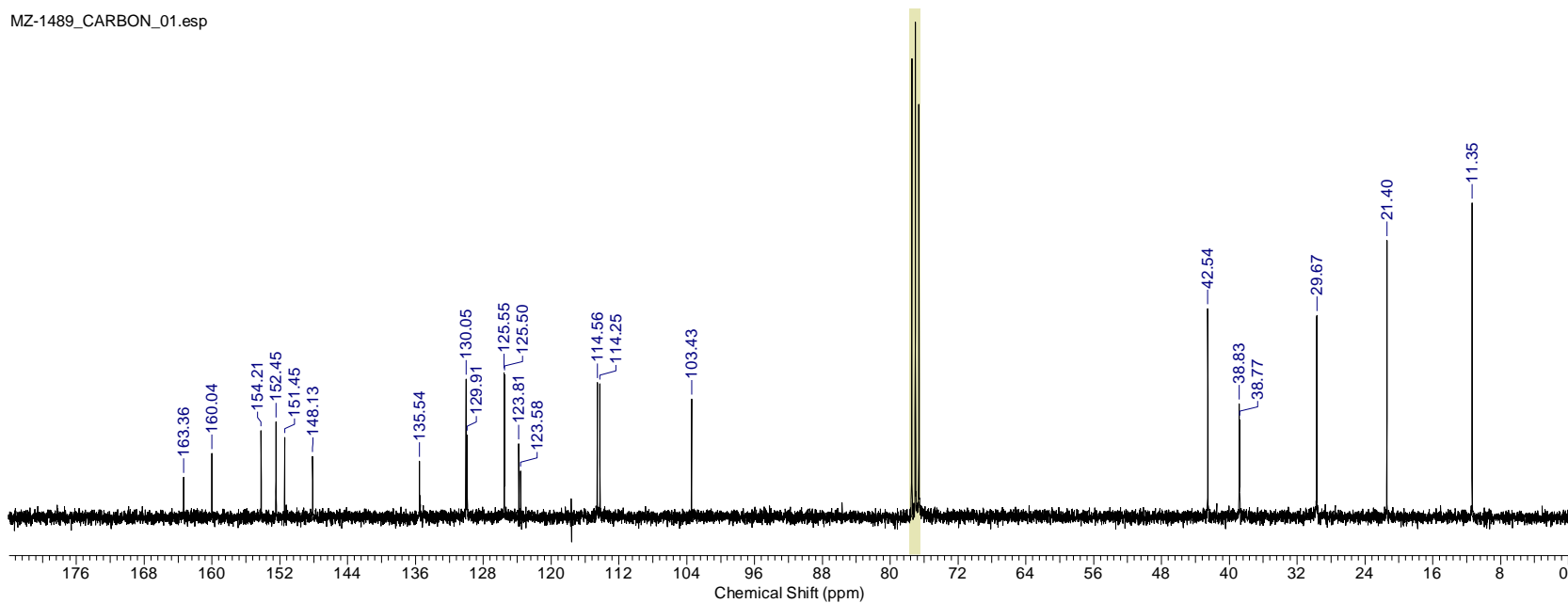


Figure 20S. ¹³C NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**14**)

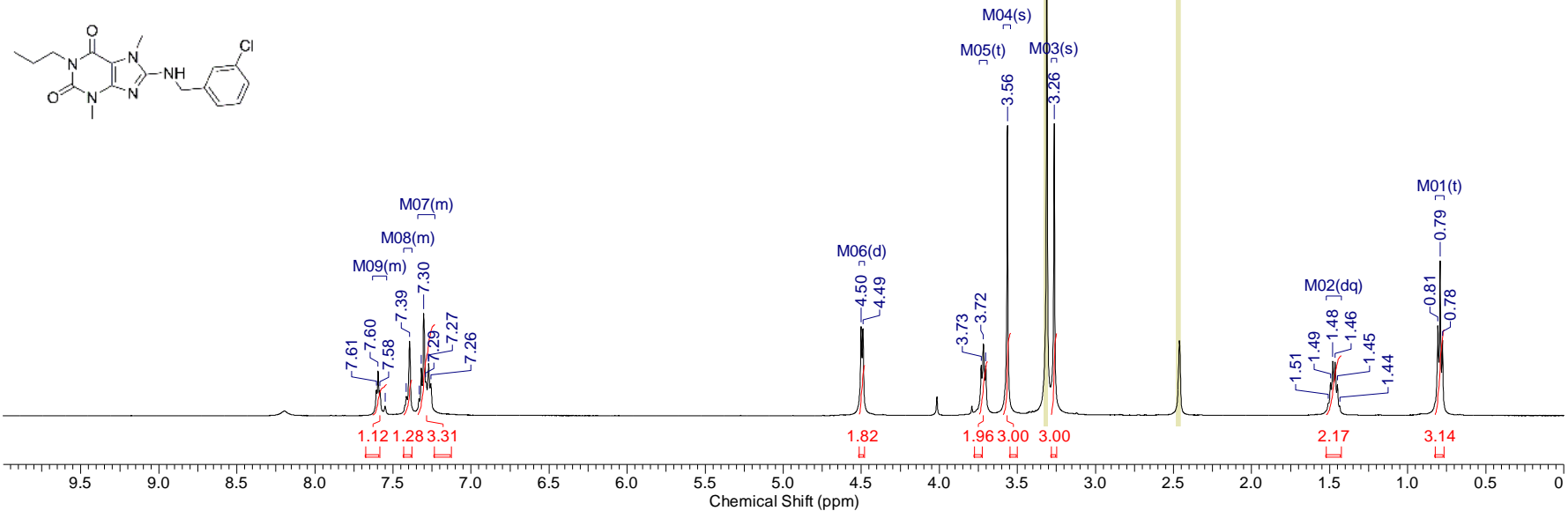


Figure 21S. ¹H NMR spectrum of 8-((3-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (15)

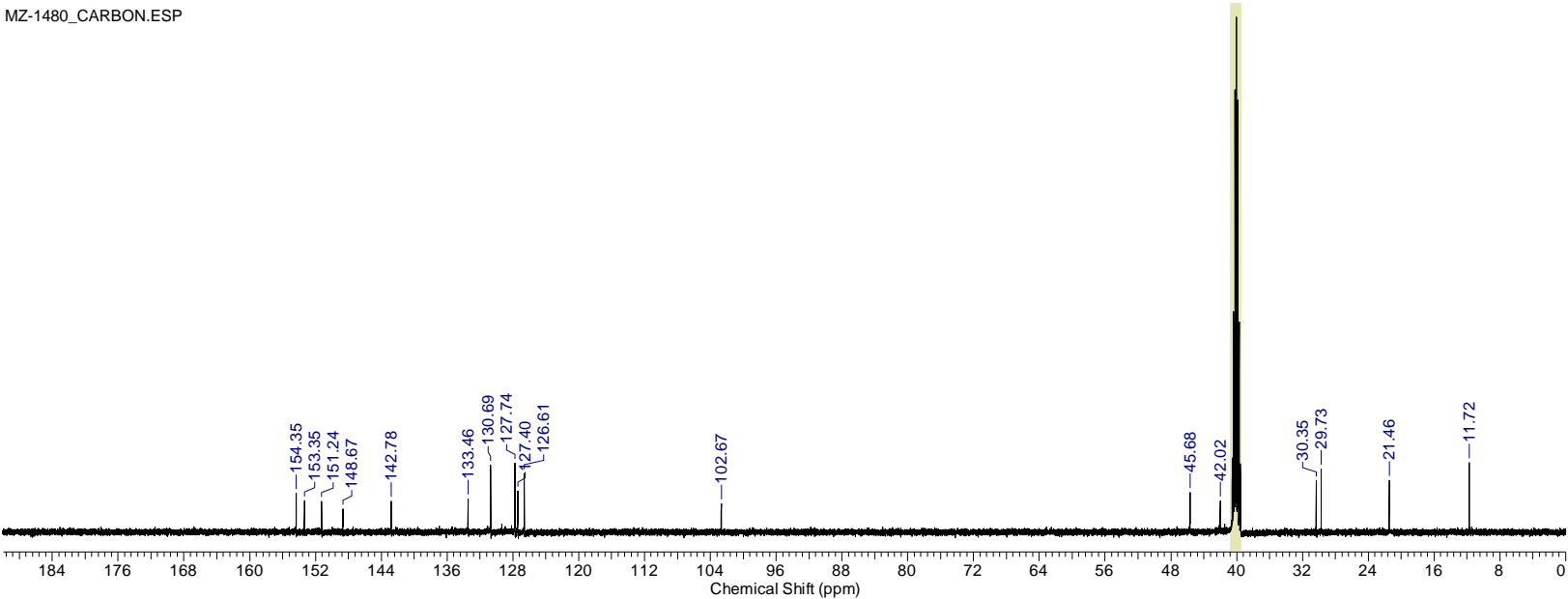


Figure 22S. ¹³C NMR spectrum of 8-((3-chlorobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (15)

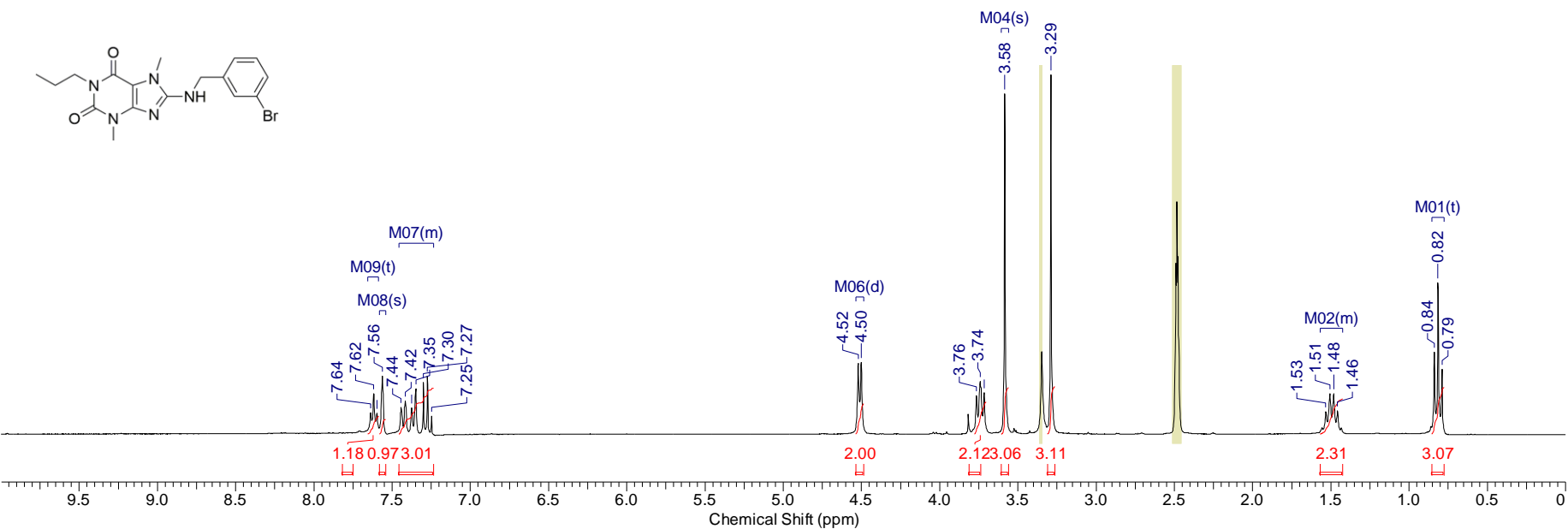
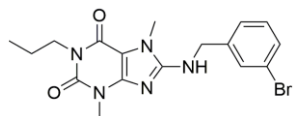


Figure 23S. ^1H NMR spectrum of 8-((3-bromobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**16**)

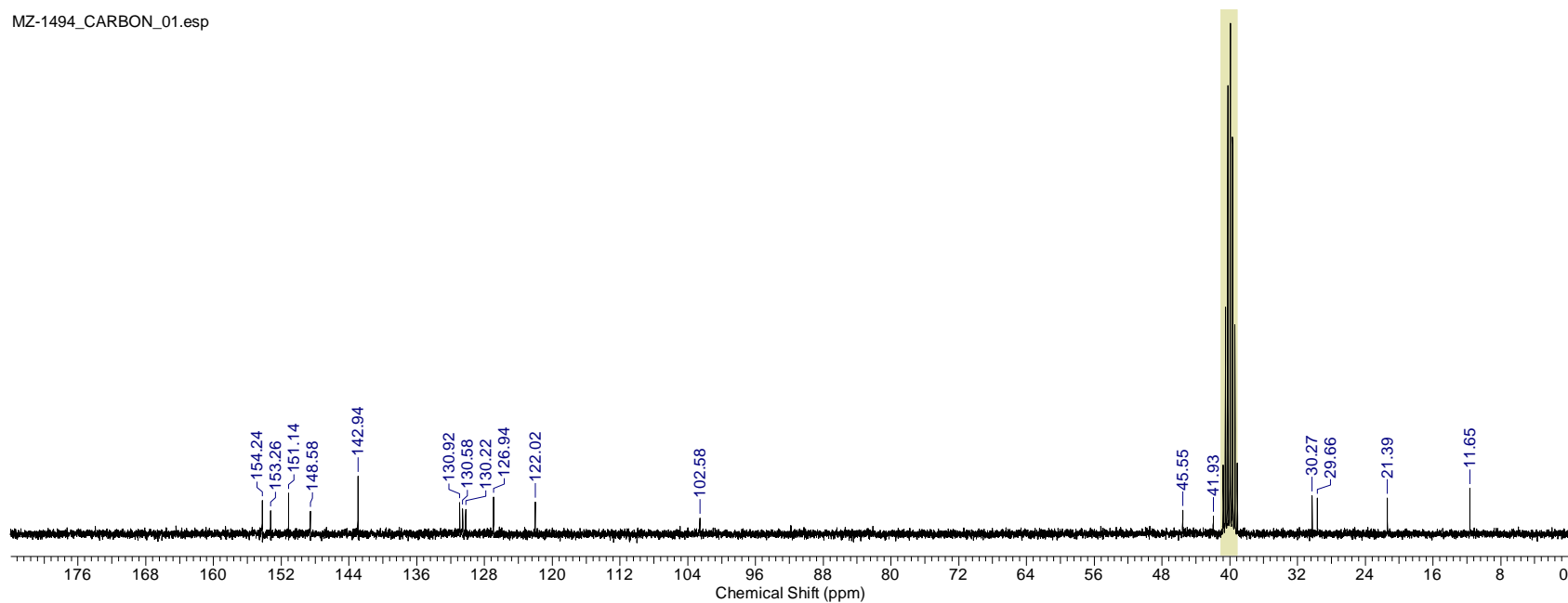


Figure 24S. ^{13}C NMR spectrum of 8-((3-bromobenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**16**)

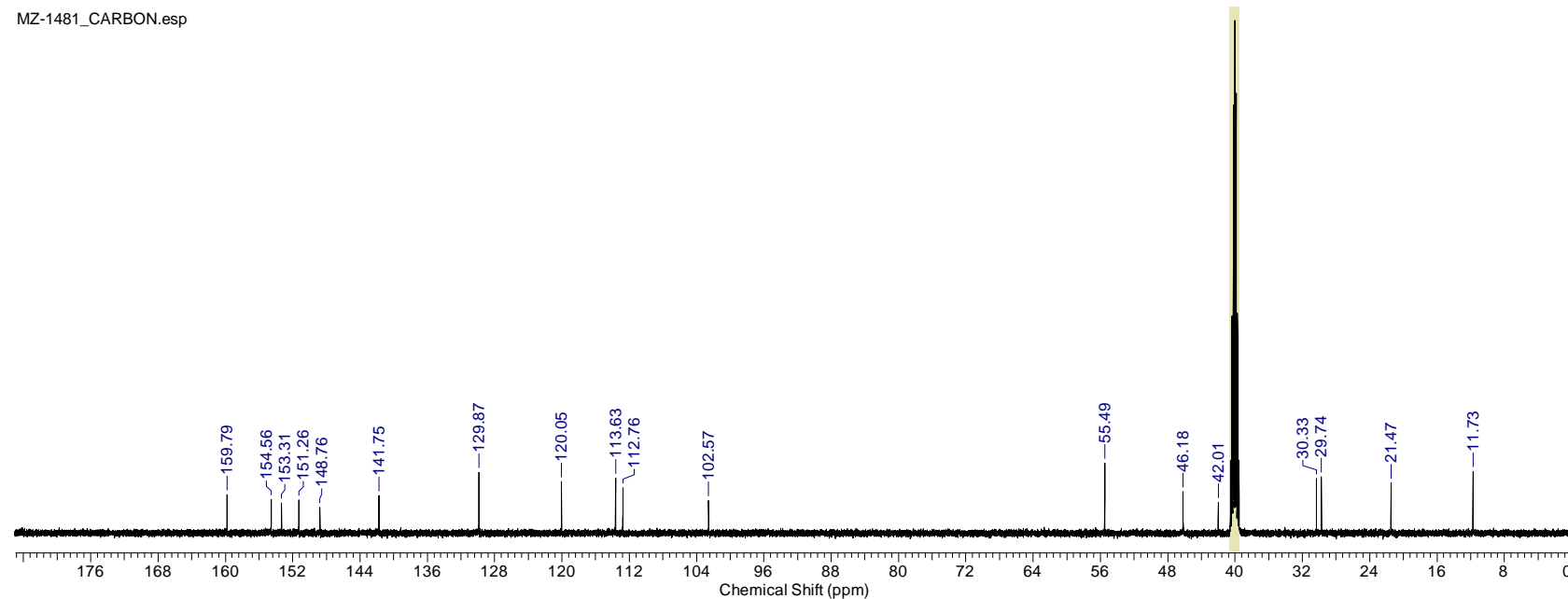
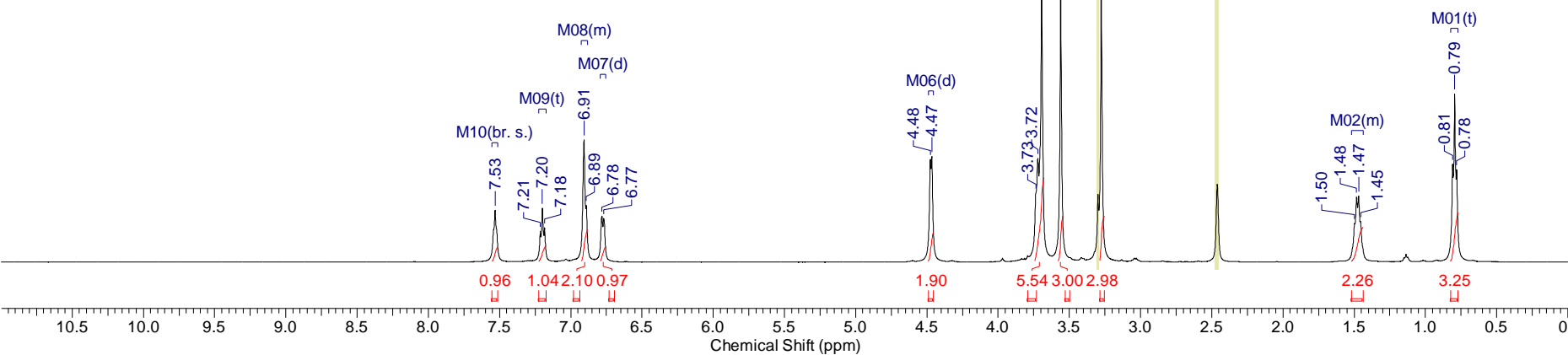
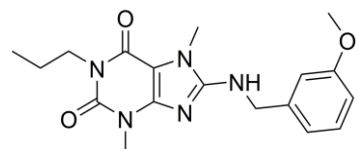
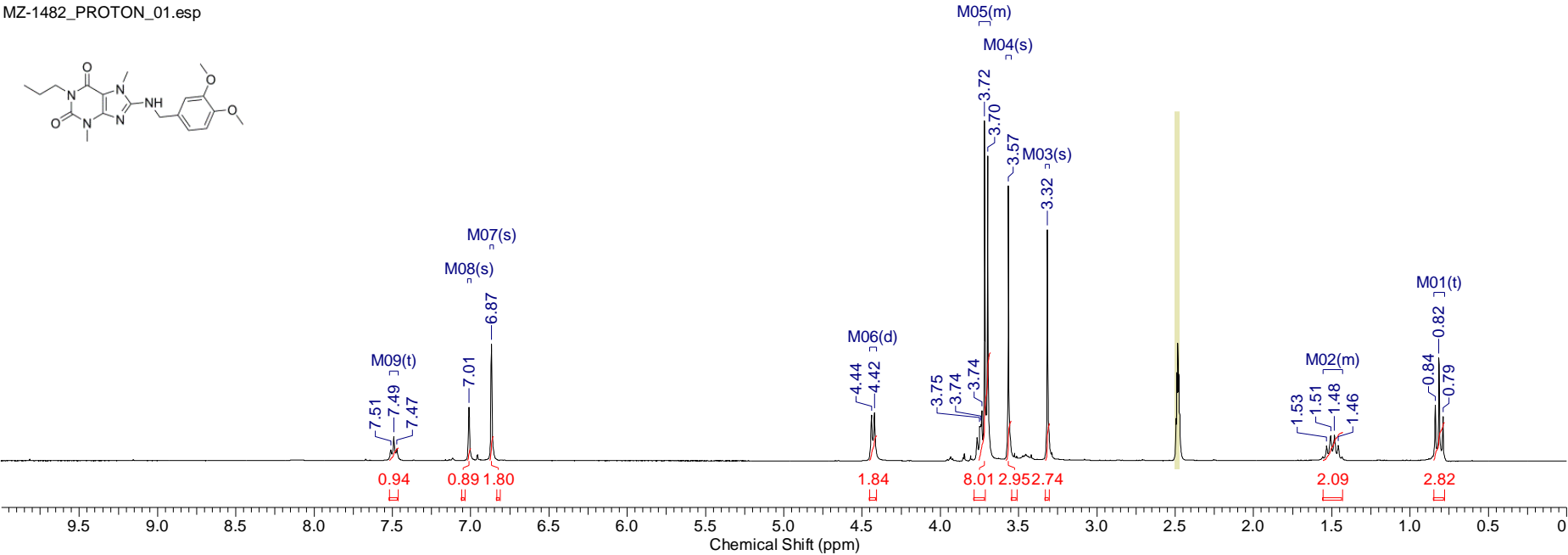
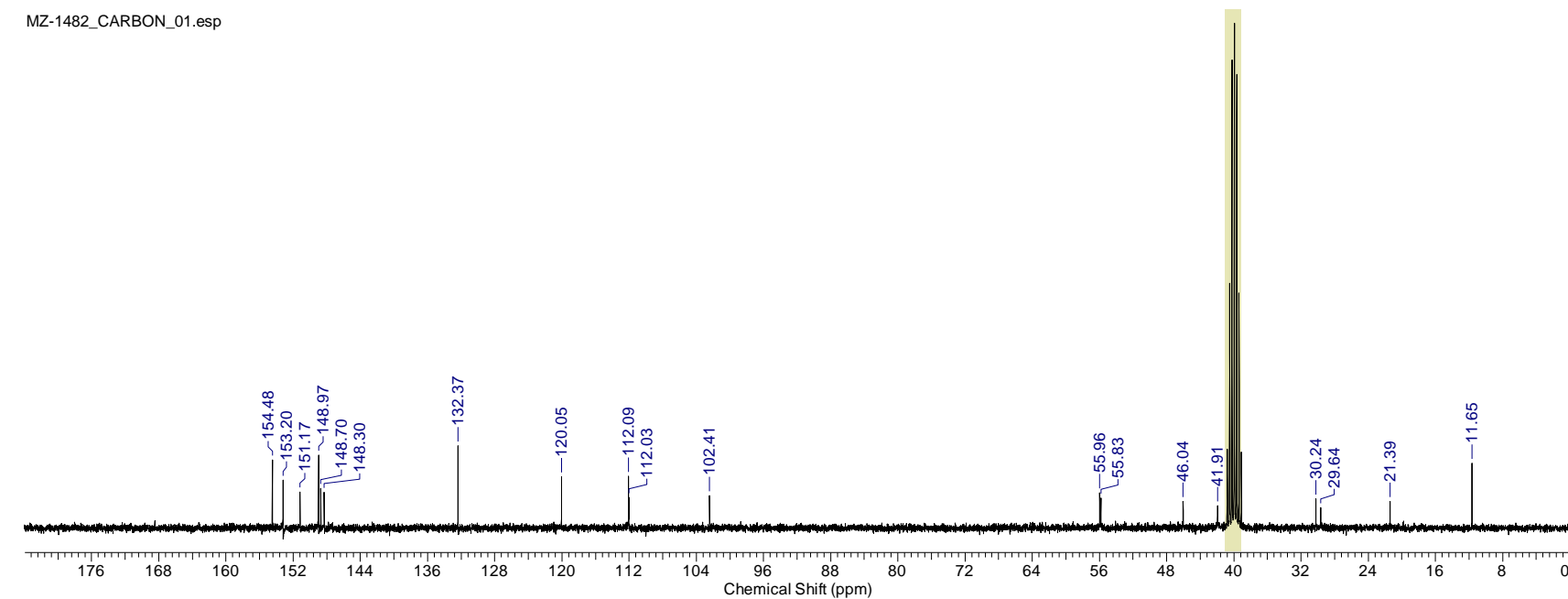
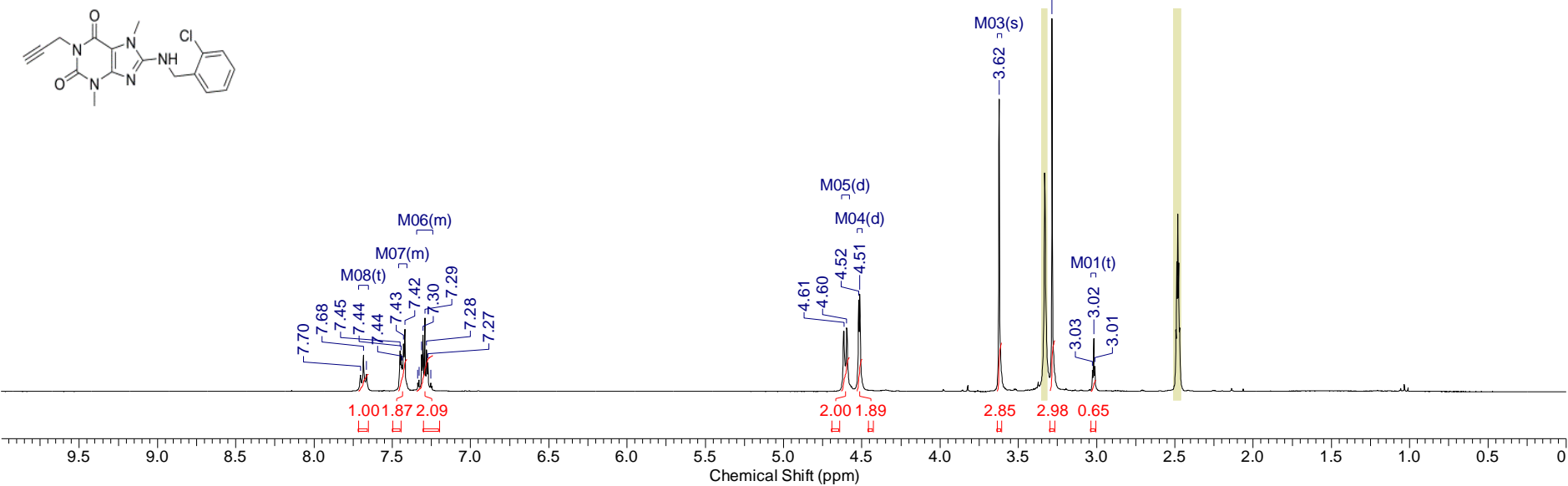
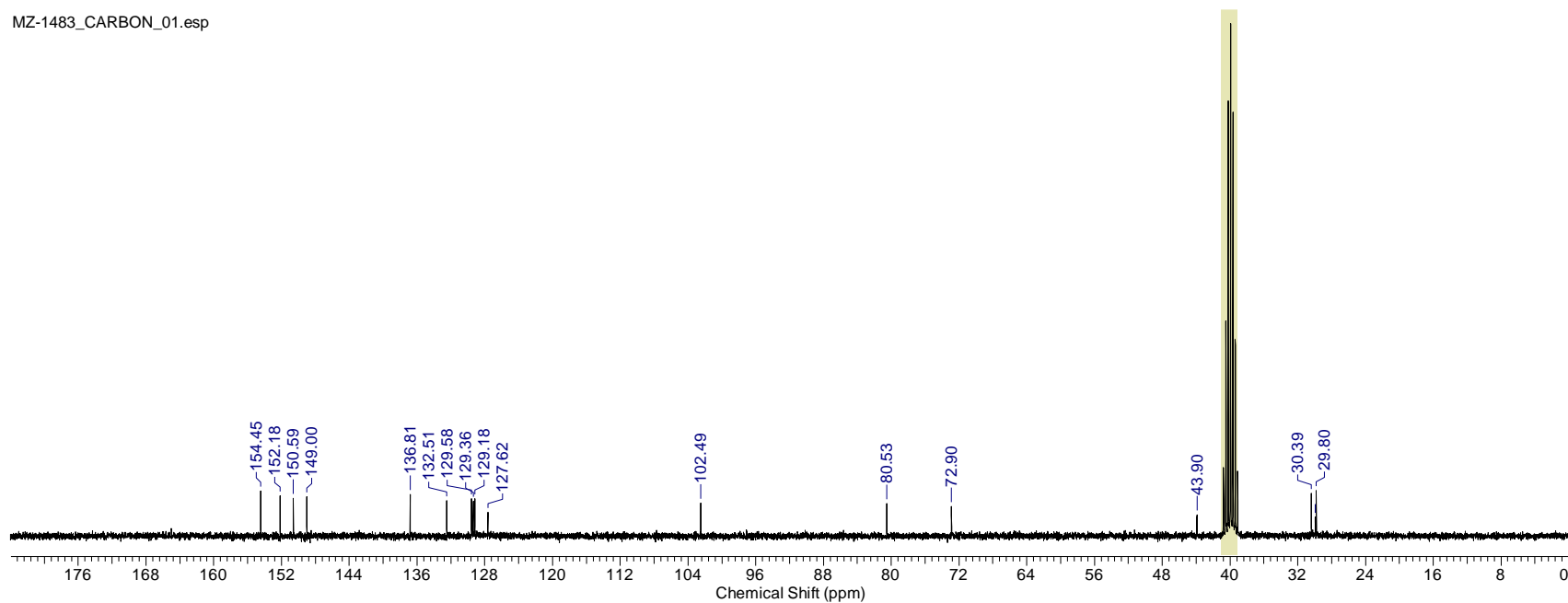
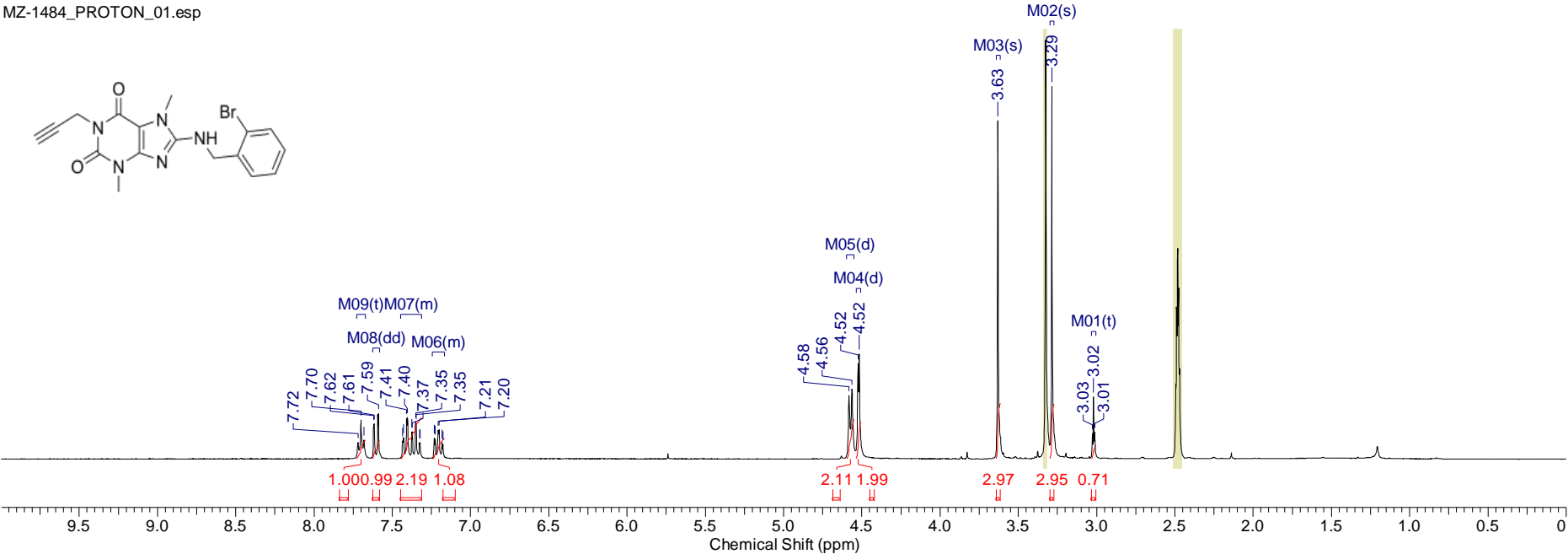
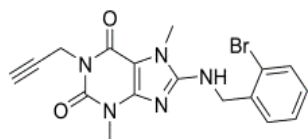
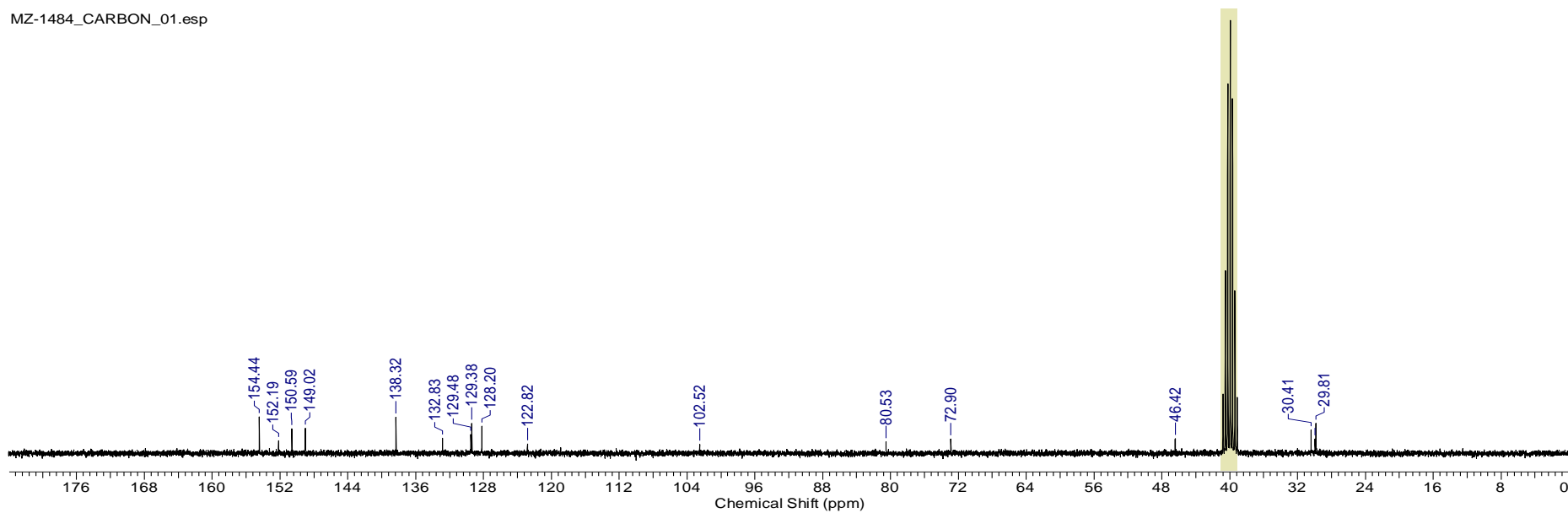


Figure 26S. ^{13}C NMR spectrum of 8-((3-methoxybenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (17)

Figure 27S. ¹H NMR spectrum of 8-((3,4-dimethoxybenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**18**)Figure 28S. ¹³C NMR spectrum of 8-((3,4-dimethoxybenzyl)amino)-3,7-dimethyl-1-propyl-3,7-dihydro-1H-purine-2,6-dione (**18**)

Figure 29S. ¹H NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (19)Figure 30S. ¹³C NMR spectrum of 8-((2-chlorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (19)

Figure 31S. ¹H NMR spectrum of 8-((2-bromobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**20**)Figure 32S. ¹³C NMR spectrum of 8-((2-bromobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**20**)

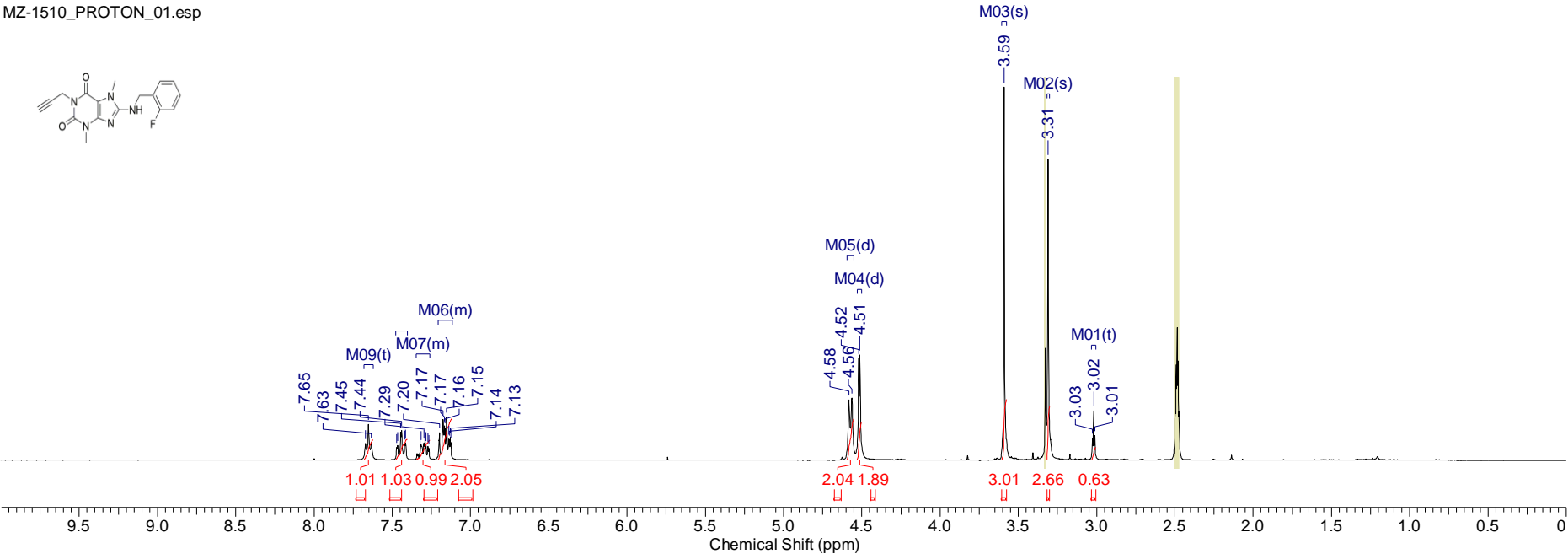
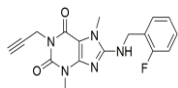


Figure 33S. ¹H NMR spectrum of 8-((2-fluorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**21**)

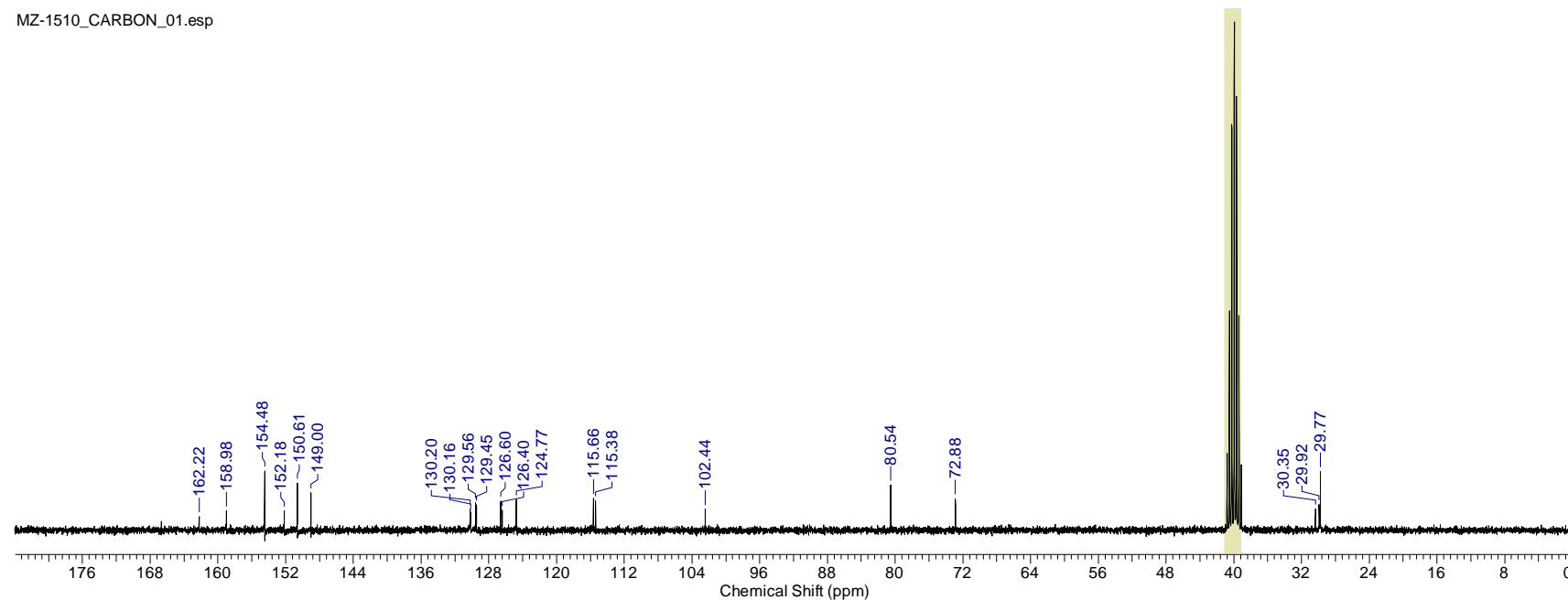


Figure 34S. ¹³C NMR spectrum of 8-((2-fluorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**21**)

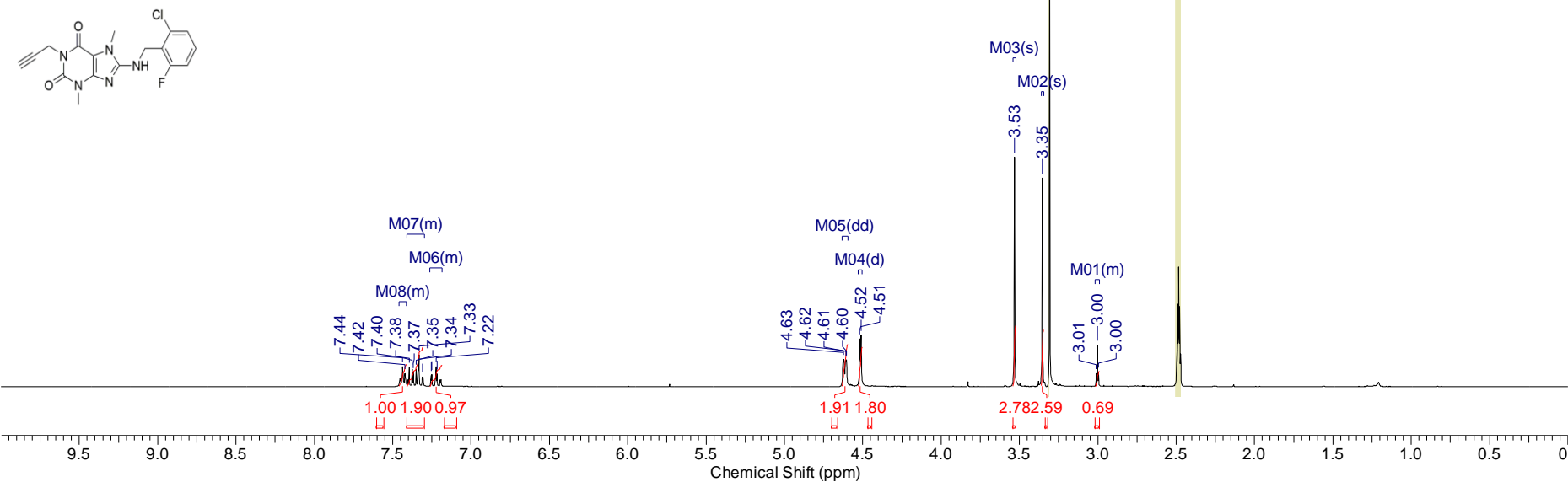


Figure 35S. ¹H NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**22**)

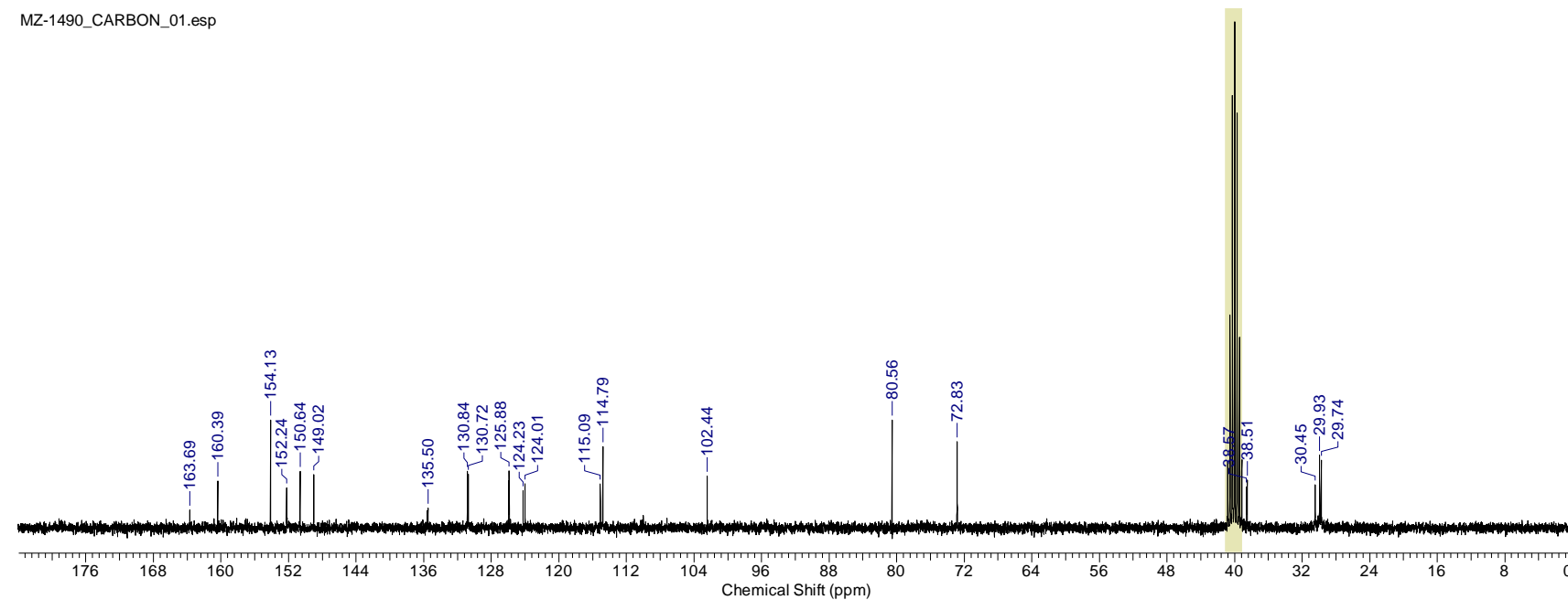


Figure 36S. ¹³C NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**22**)

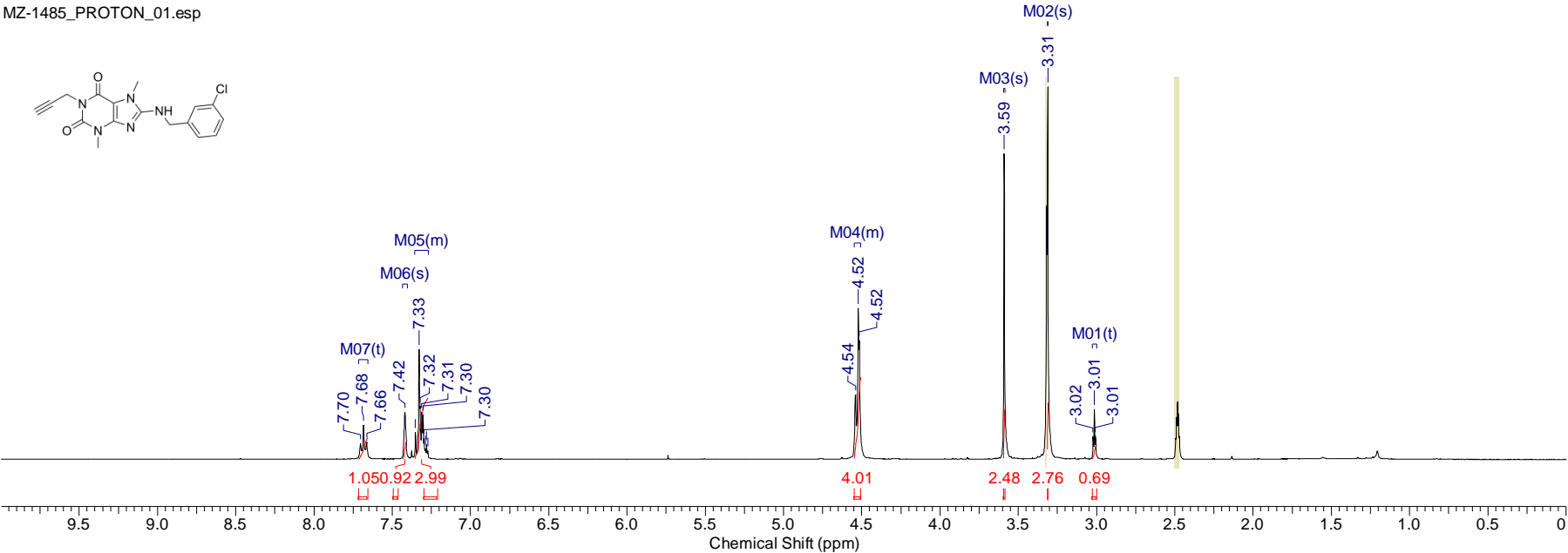
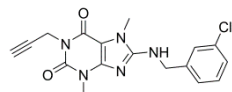


Figure 37S. ¹H NMR spectrum of 8-((3-chlorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**23**)

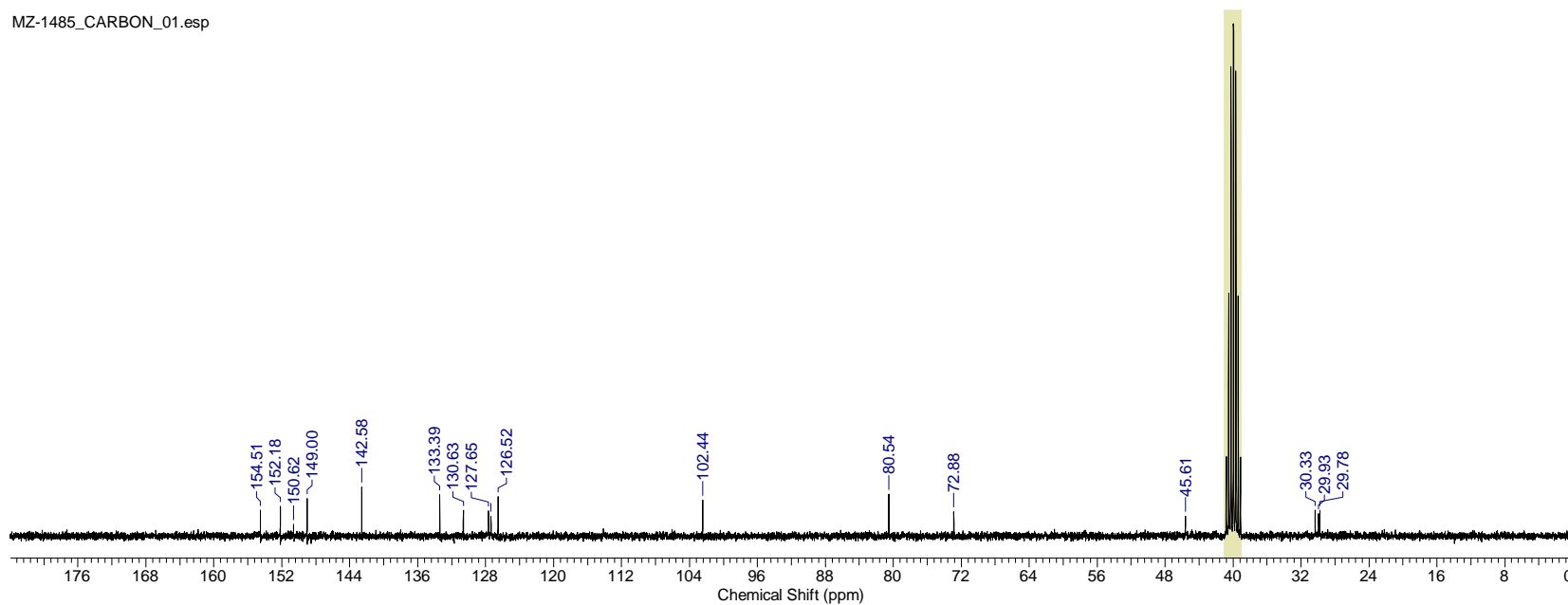
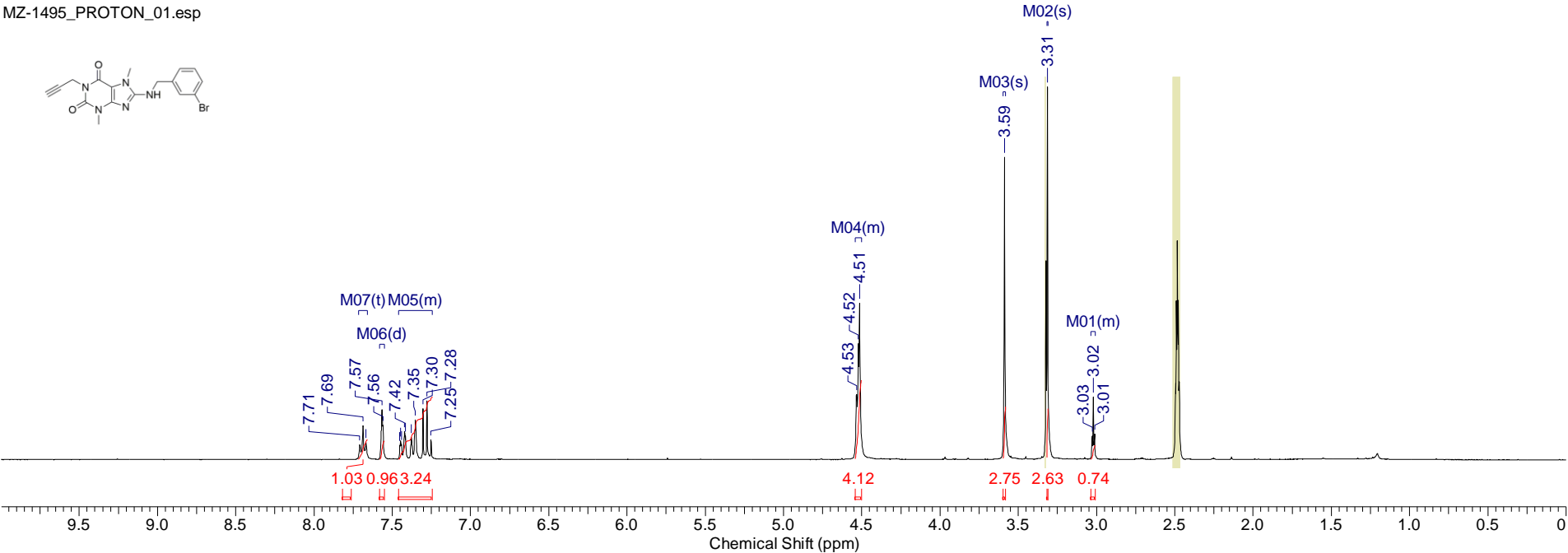
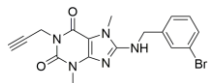
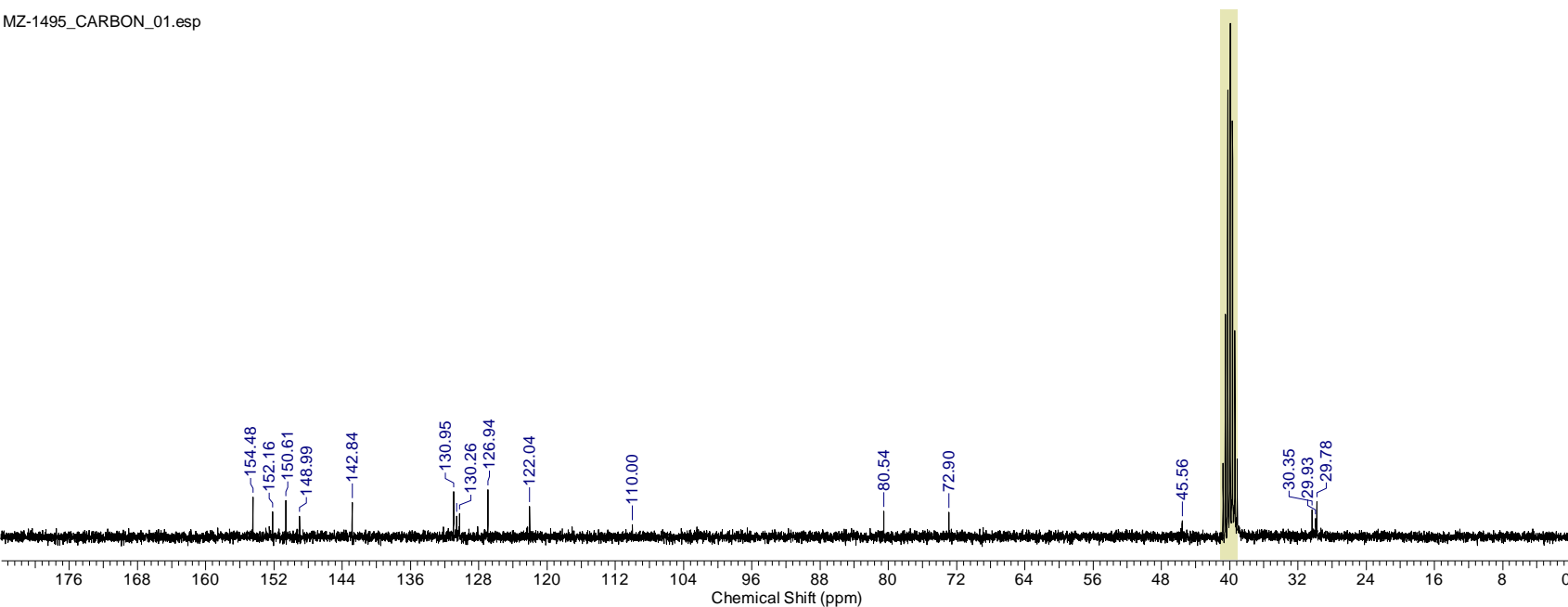
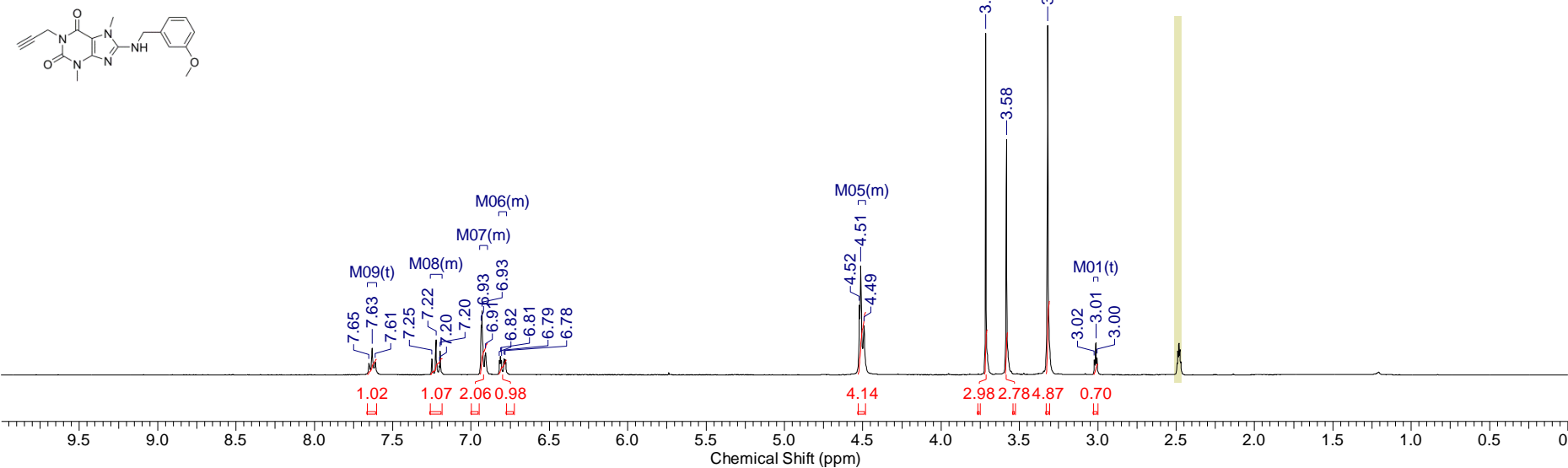
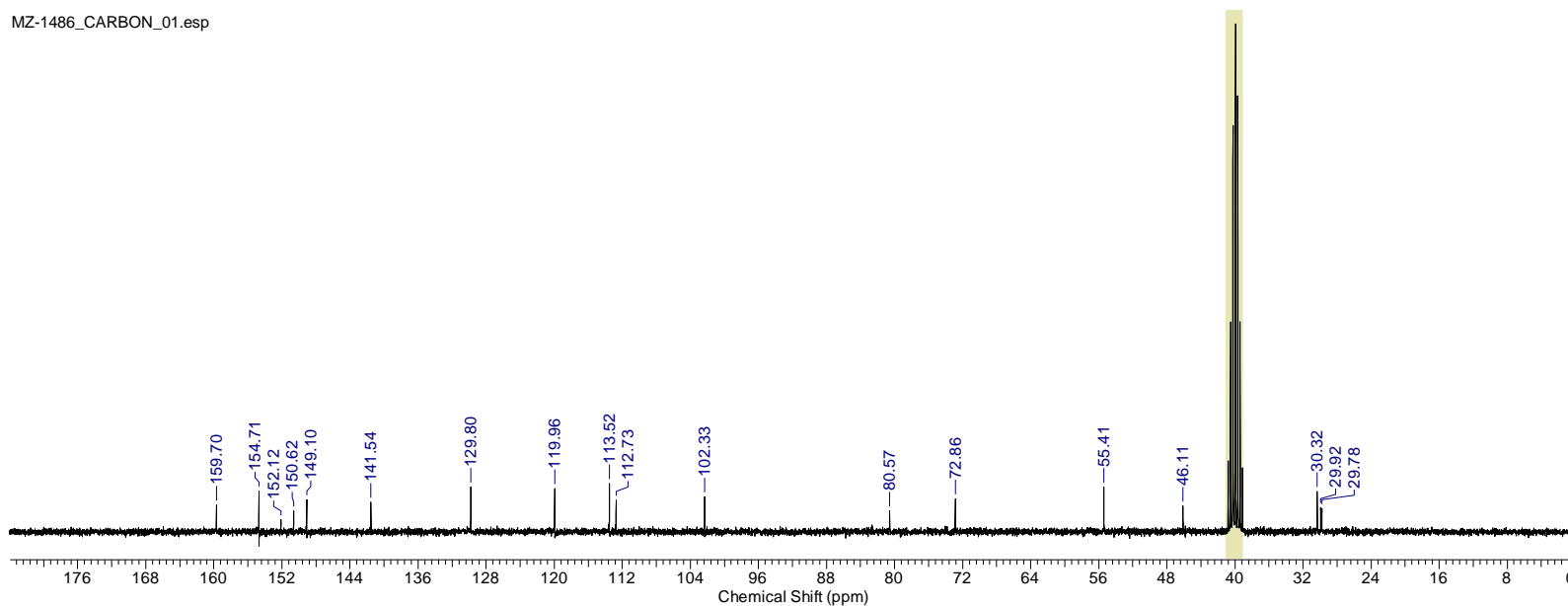


Figure 38S. ¹³C NMR spectrum of 8-((3-chlorobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**23**)

Figure 39S. ¹H NMR spectrum of 8-((3-bromobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**24**)Figure 40S. ¹³C NMR spectrum of 8-((3-bromobenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**24**)

Figure 41S. ¹H NMR spectrum of 8-((3-methoxybenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**25**)Figure 42S. ¹³C NMR spectrum of 8-((3-methoxybenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**25**)

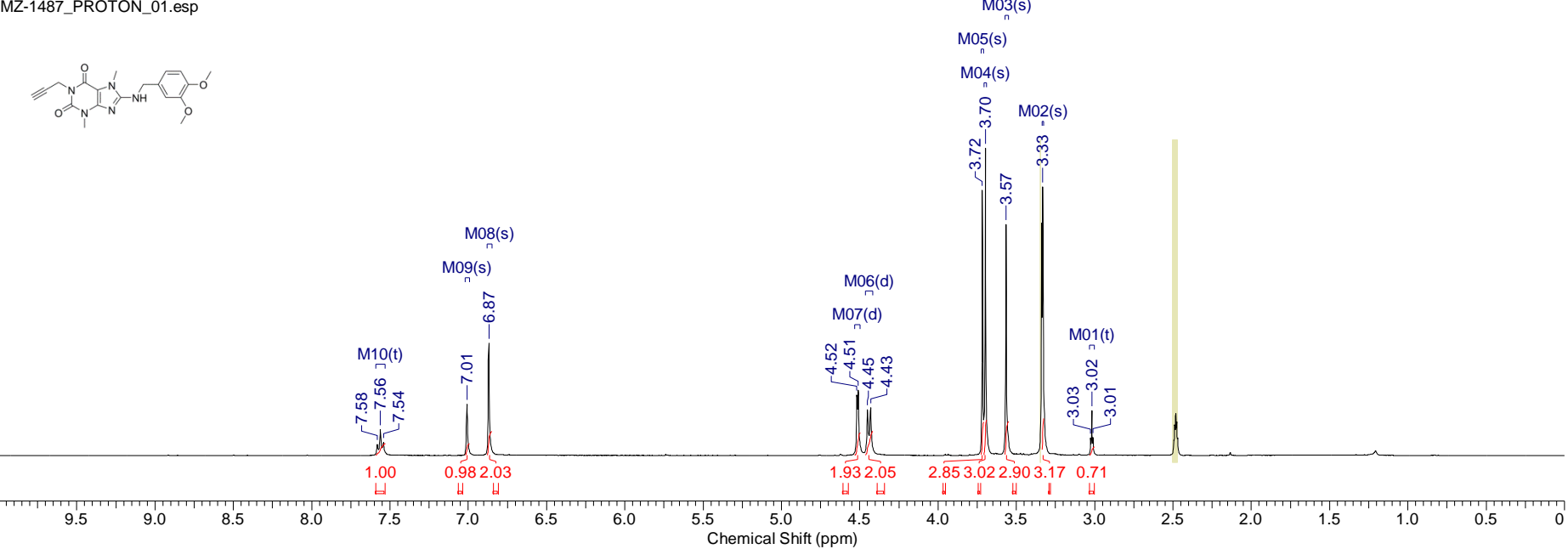
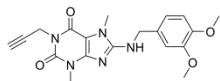


Figure 43S. ¹H NMR spectrum of 8-((3,4-dimethoxybenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**26**)

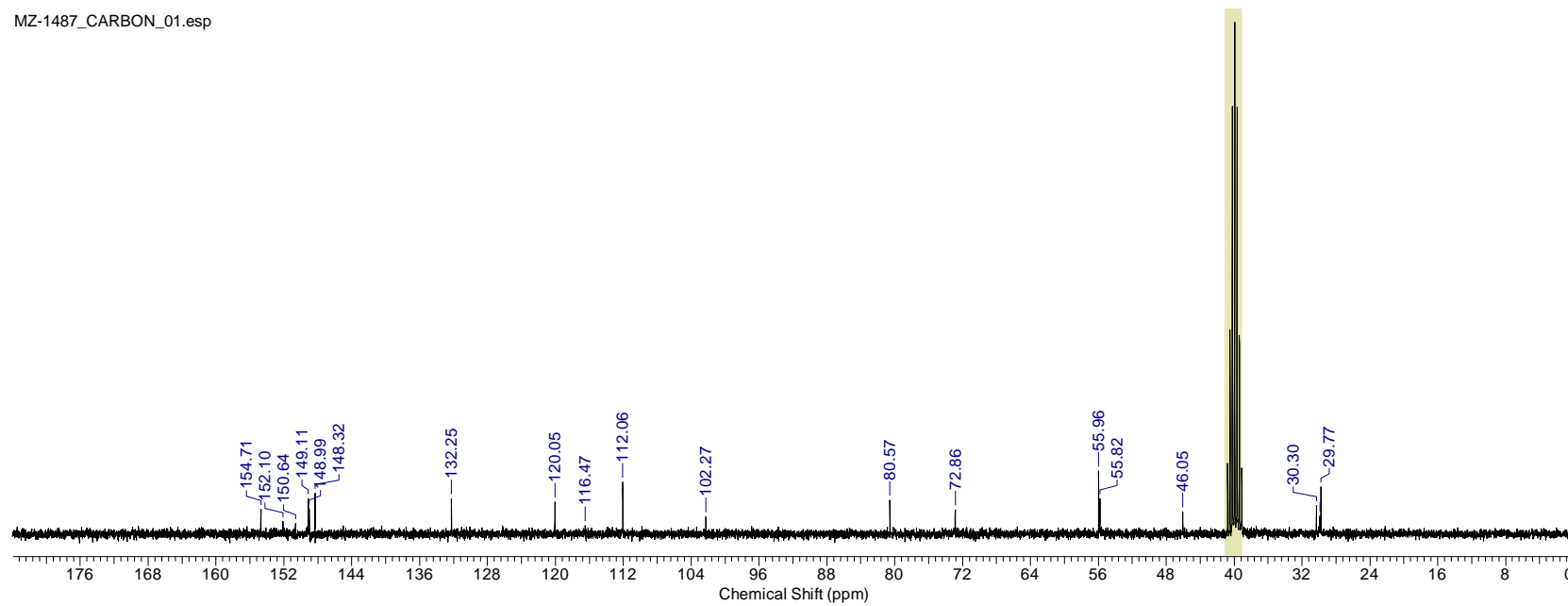


Figure 44S. ¹³C NMR spectrum of 8-((3,4-dimethoxybenzyl)amino)-3,7-dimethyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**26**)

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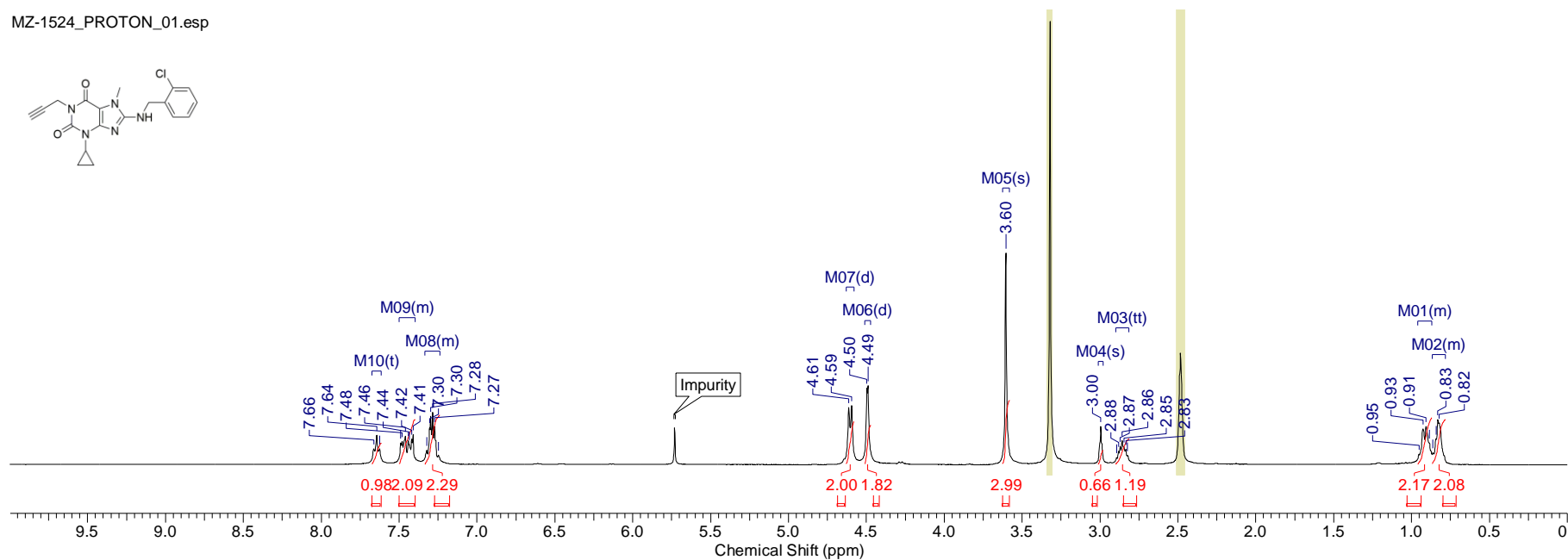
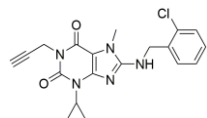


Figure 45S. ^1H NMR spectrum of 8-((2-chlorobenzyl)amino)-3-cyclopropyl-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**27**)

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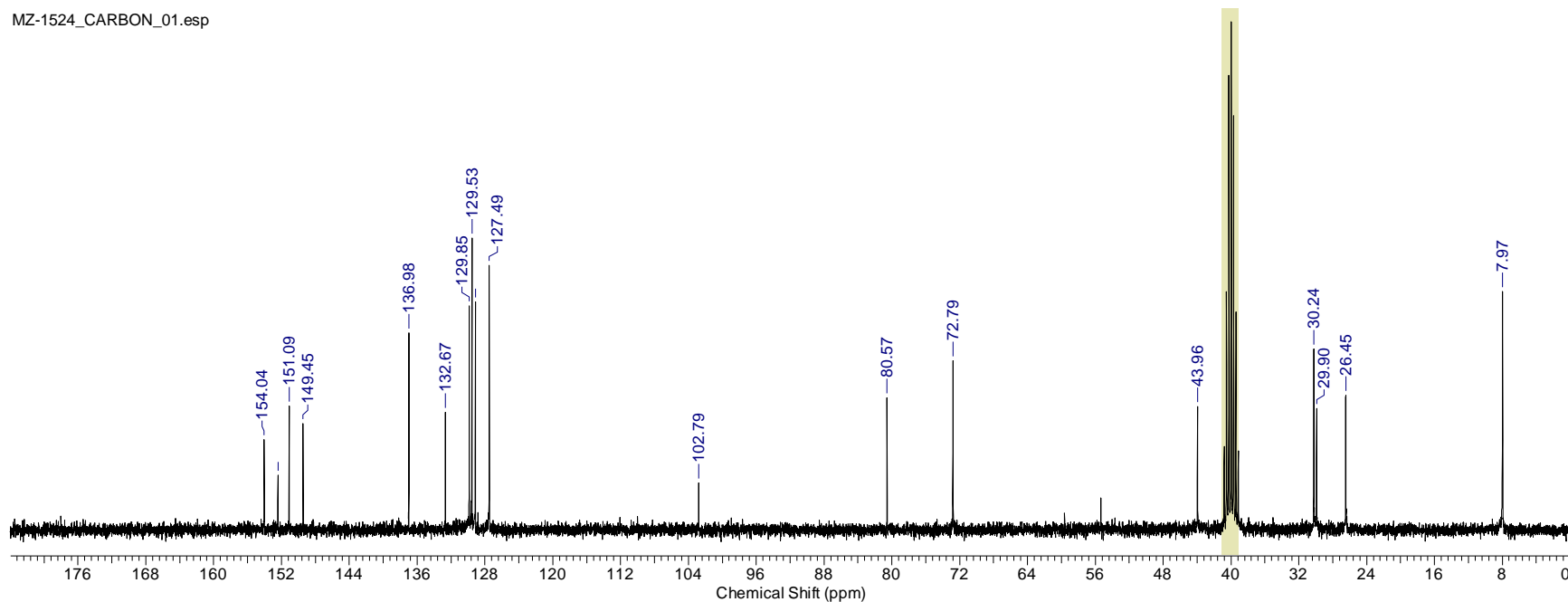


Figure 46S. ^{13}C NMR spectrum of 8-((2-chlorobenzyl)amino)-3-cyclopropyl-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**27**)

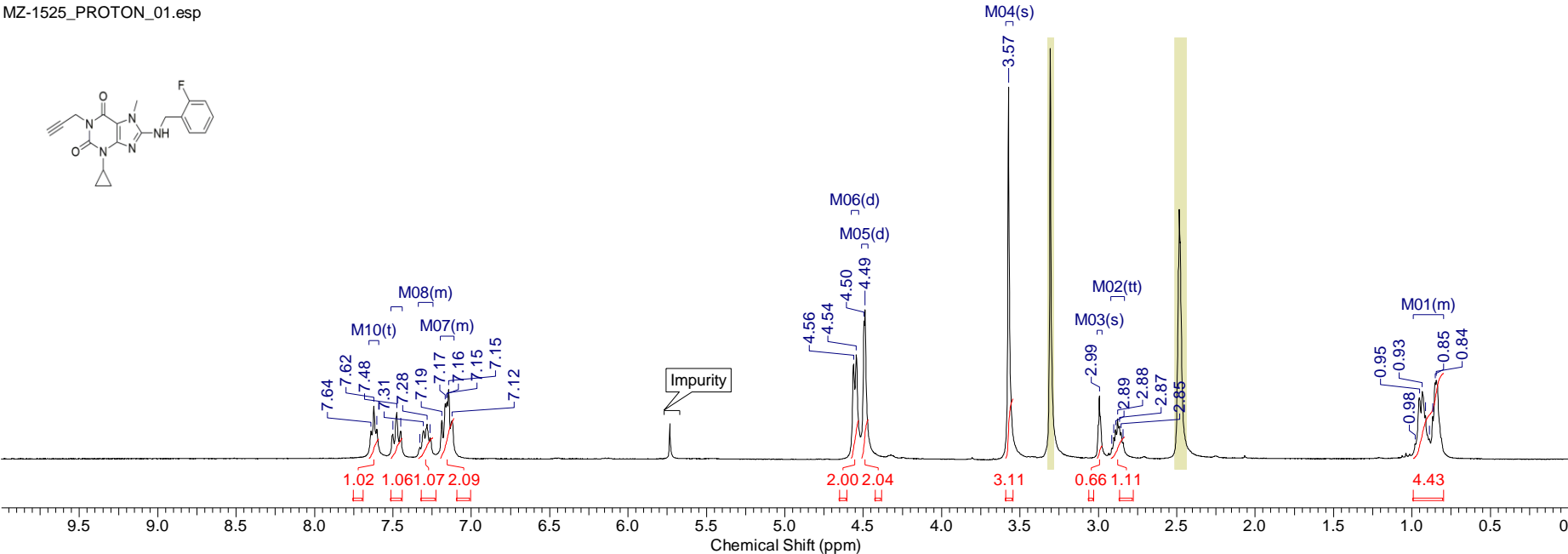


Figure 47S. ¹H NMR spectrum of 3-cyclopropyl-8-((2-fluorobenzyl)amino)-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**28**)

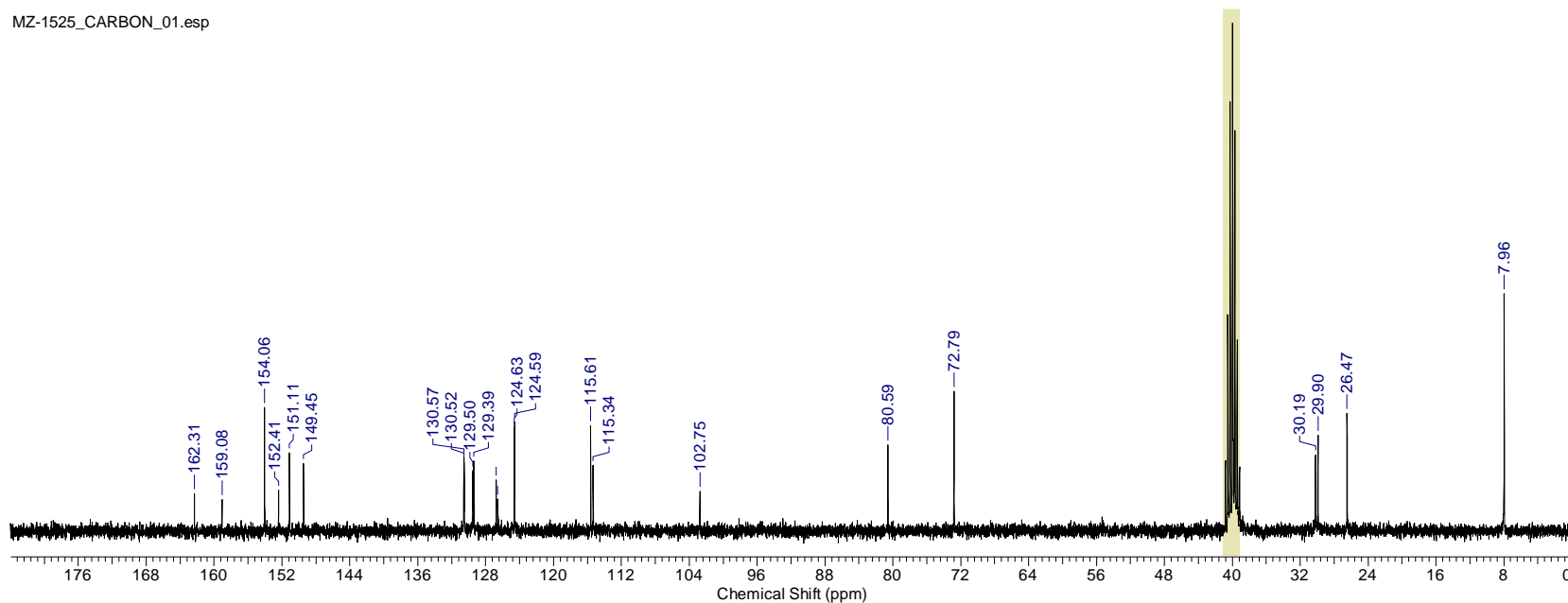


Figure 48S. ¹³C NMR spectrum of 3-cyclopropyl-8-((2-fluorobenzyl)amino)-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**28**)

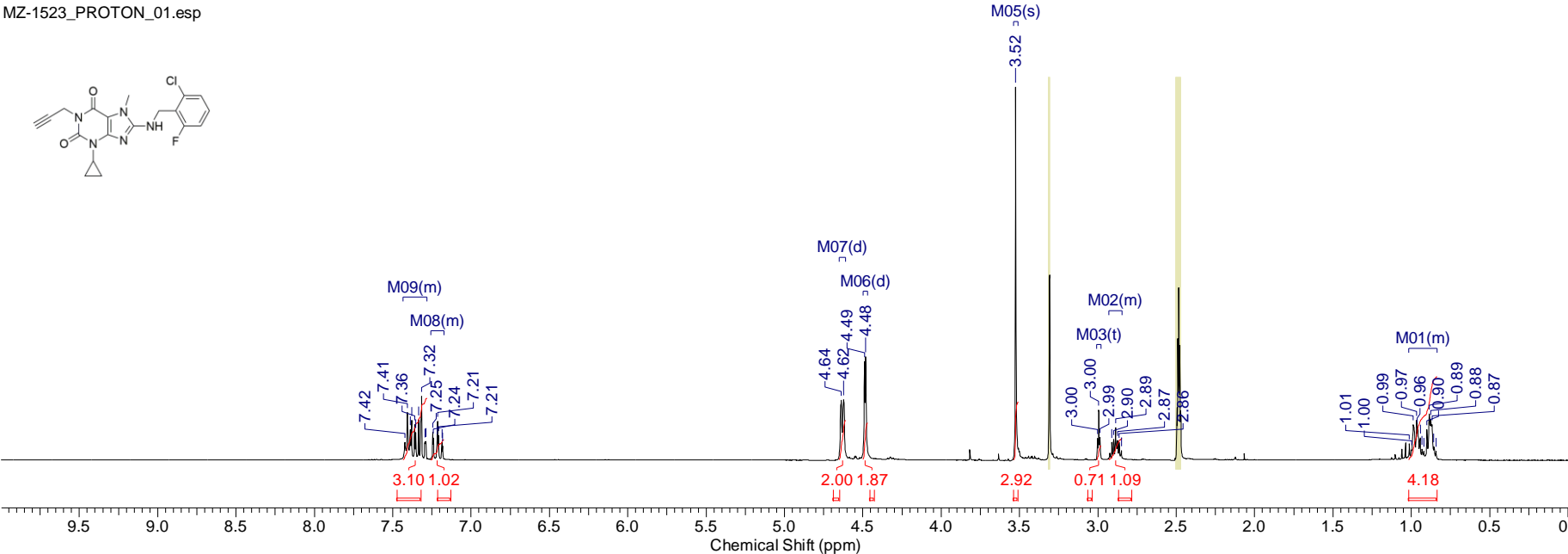
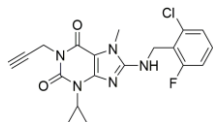


Figure 49S. ¹H NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3-cyclopropyl-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**29**)

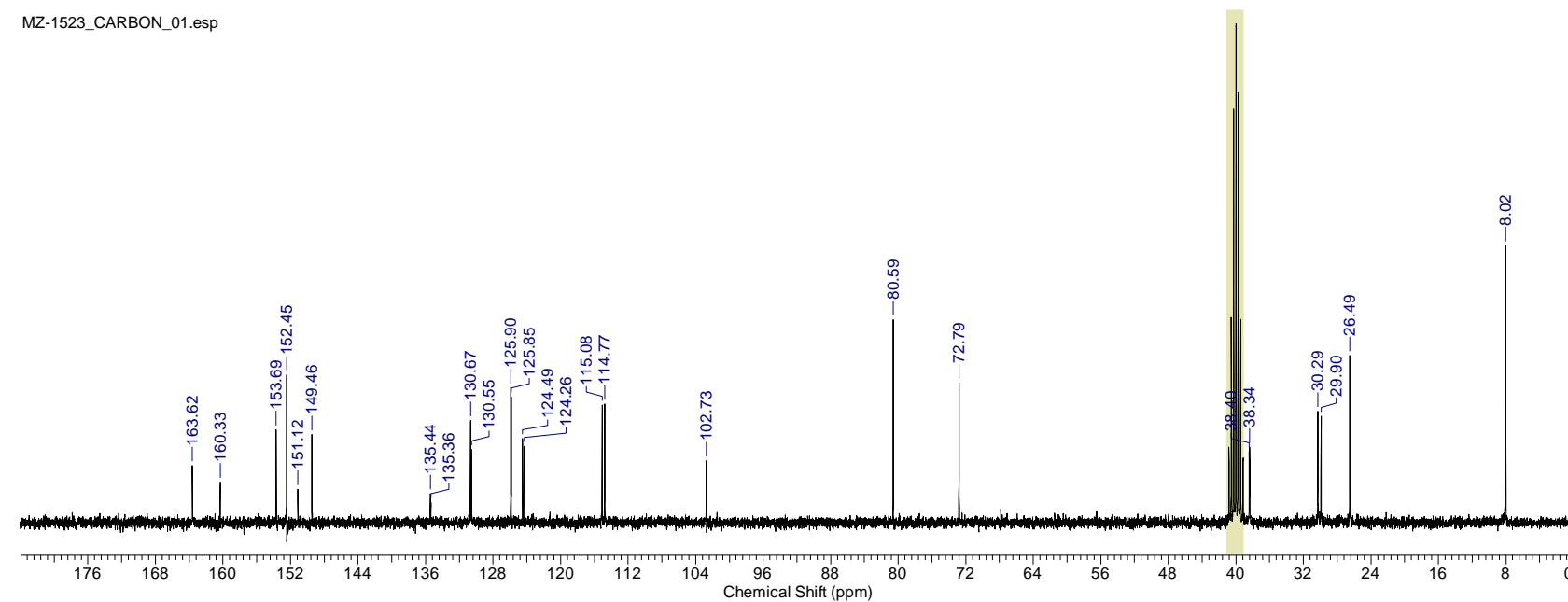


Figure 50S. ¹³C NMR spectrum of 8-((2-chloro-6-fluorobenzyl)amino)-3-cyclopropyl-7-methyl-1-(prop-2-yn-1-yl)-3,7-dihydro-1H-purine-2,6-dione (**29**)