

Supporting information

Synthesis and Tautomerization of Hydroxylated Isoflavones Bearing Heterocyclic Hemi-Aminals

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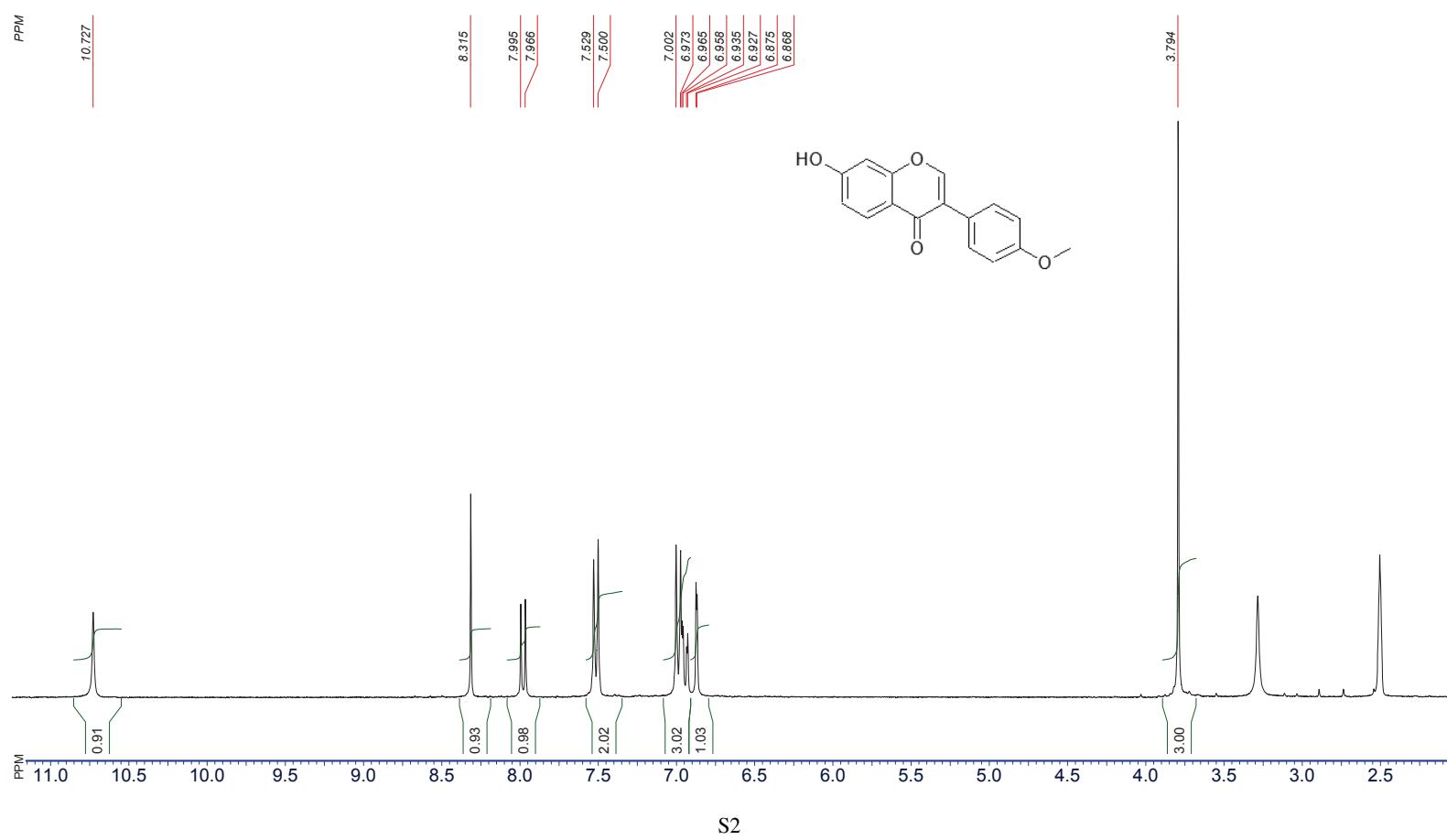
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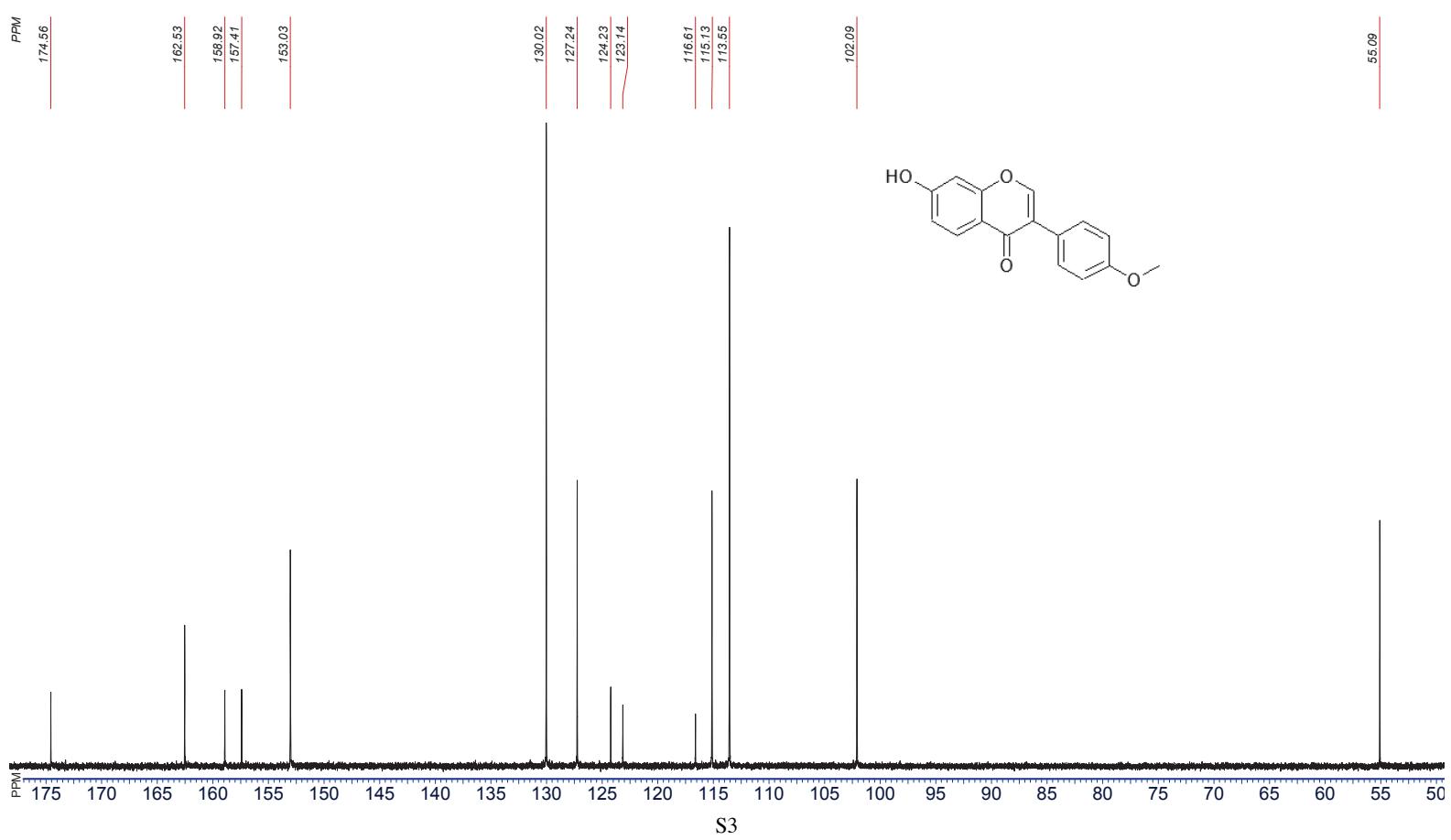
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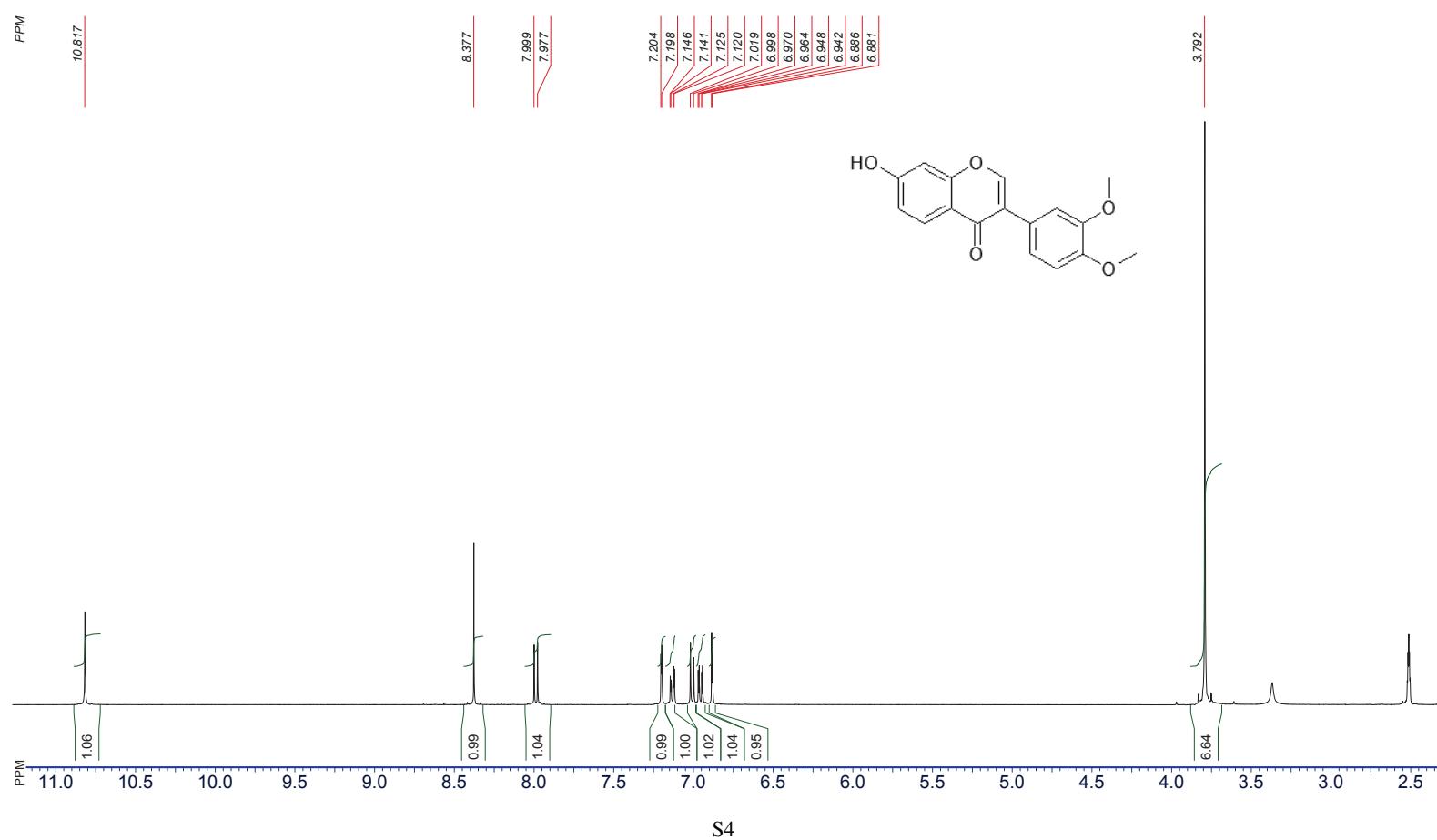
¹H NMR spectrum of NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-4*H*-chromen-4-one (**3a**) in DMSO-d6



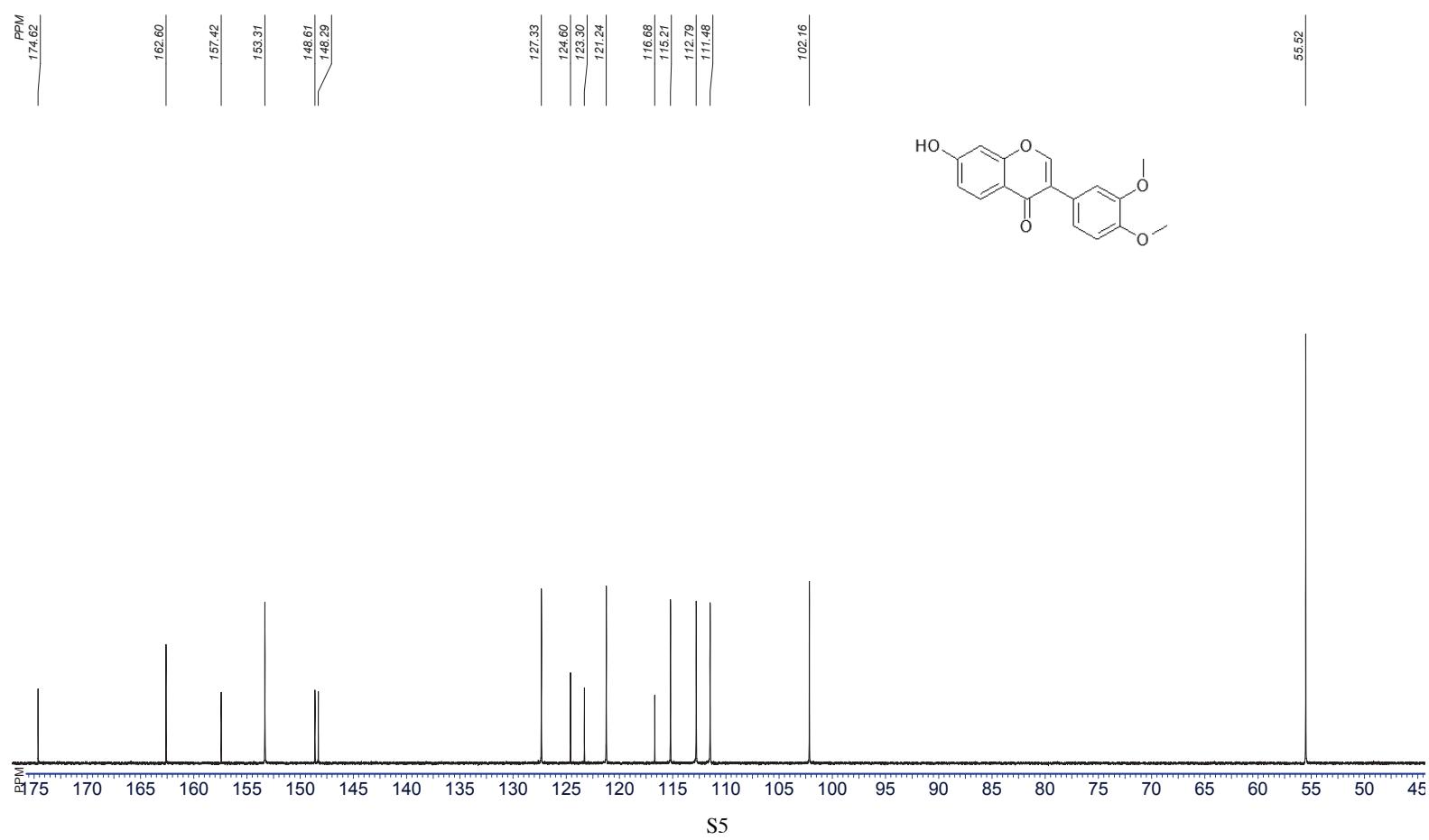
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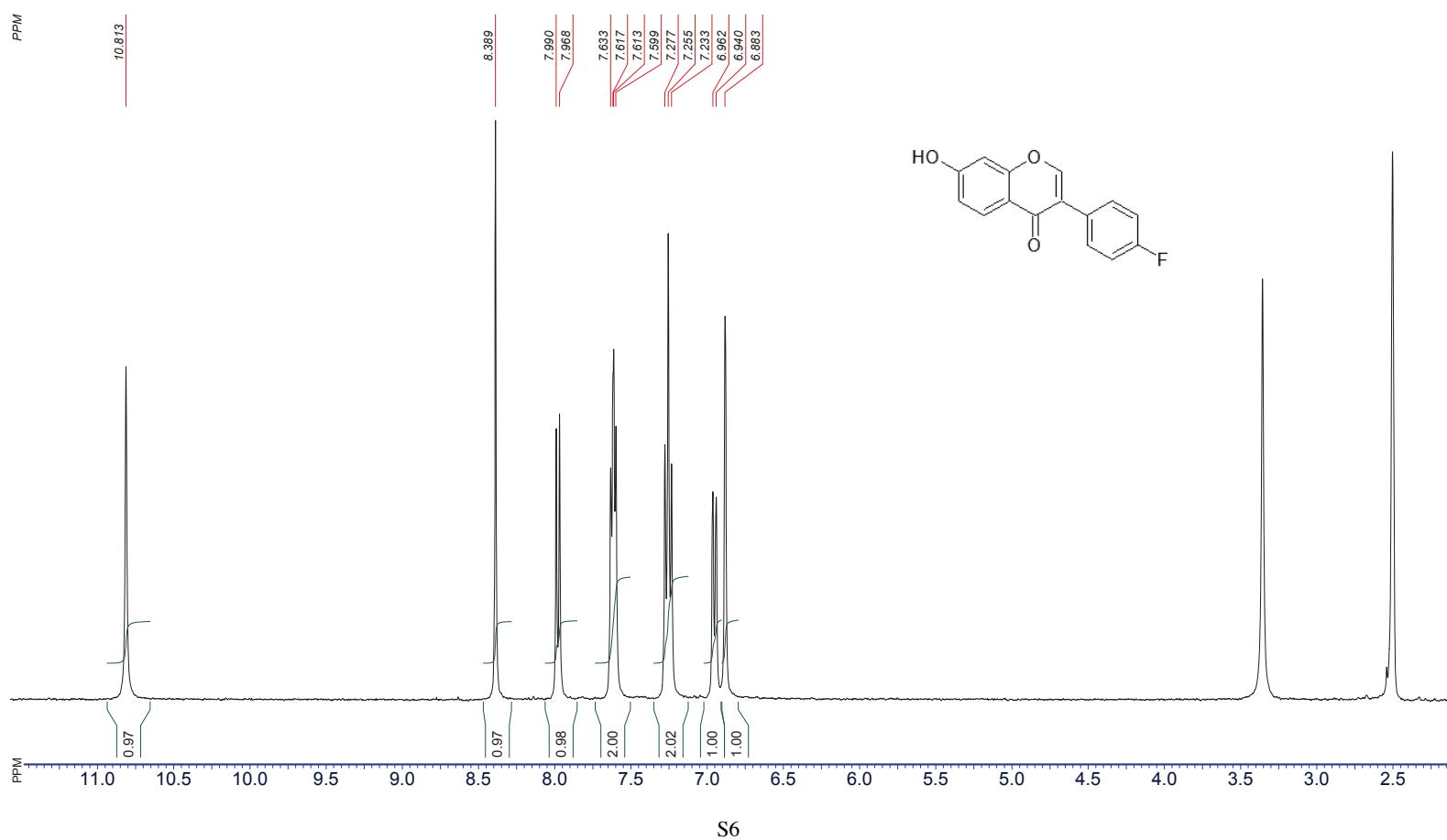
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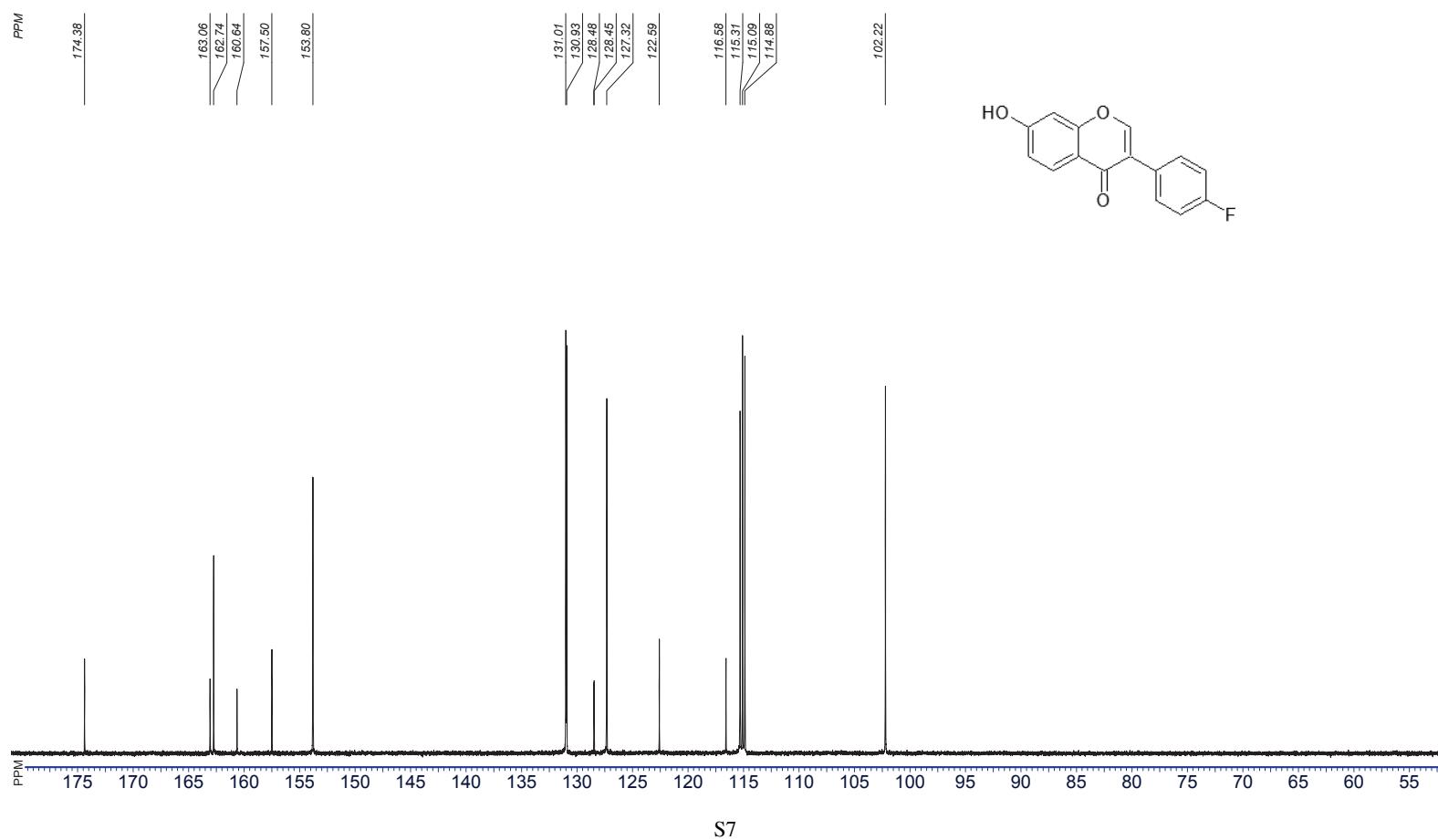
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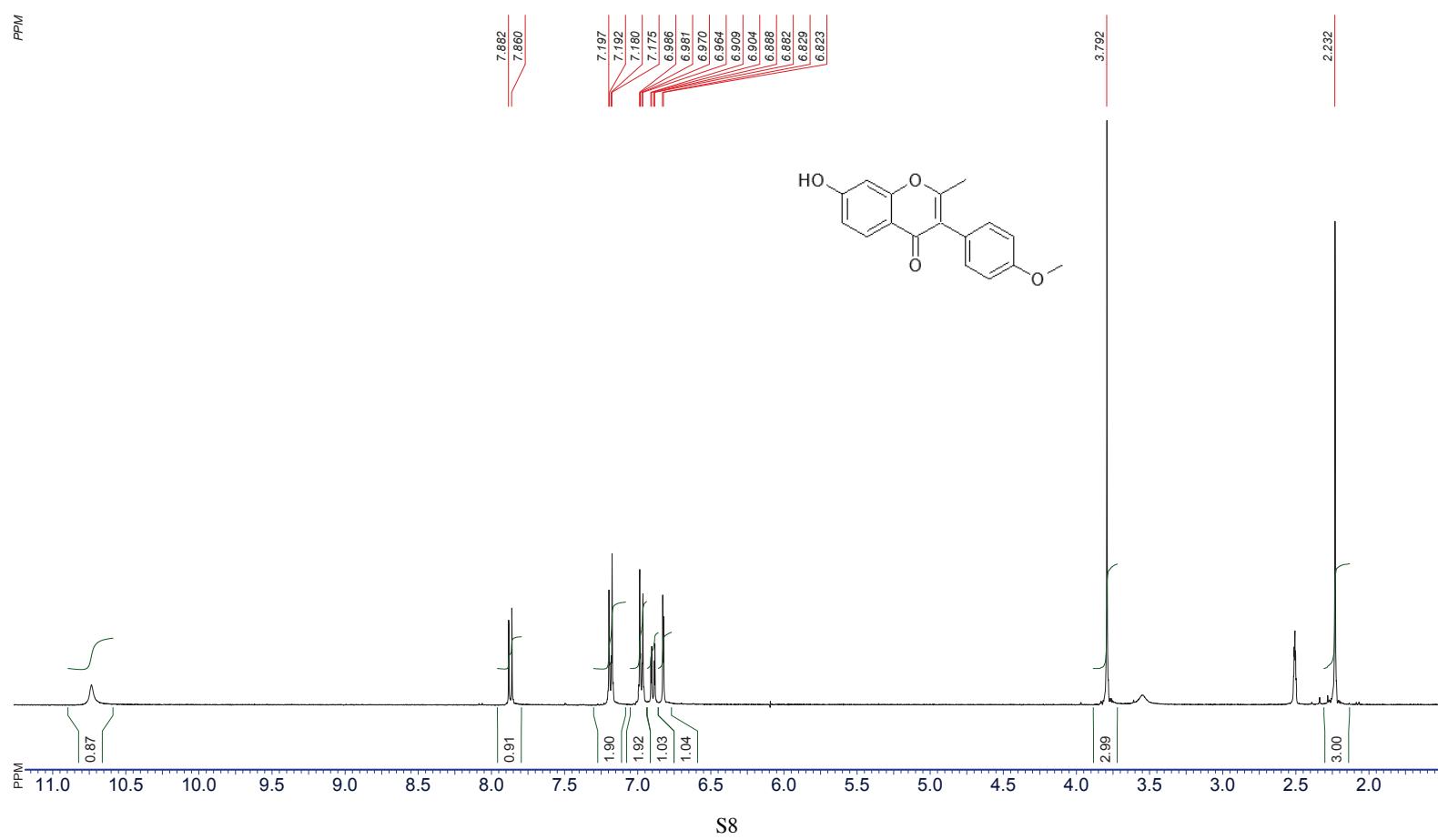
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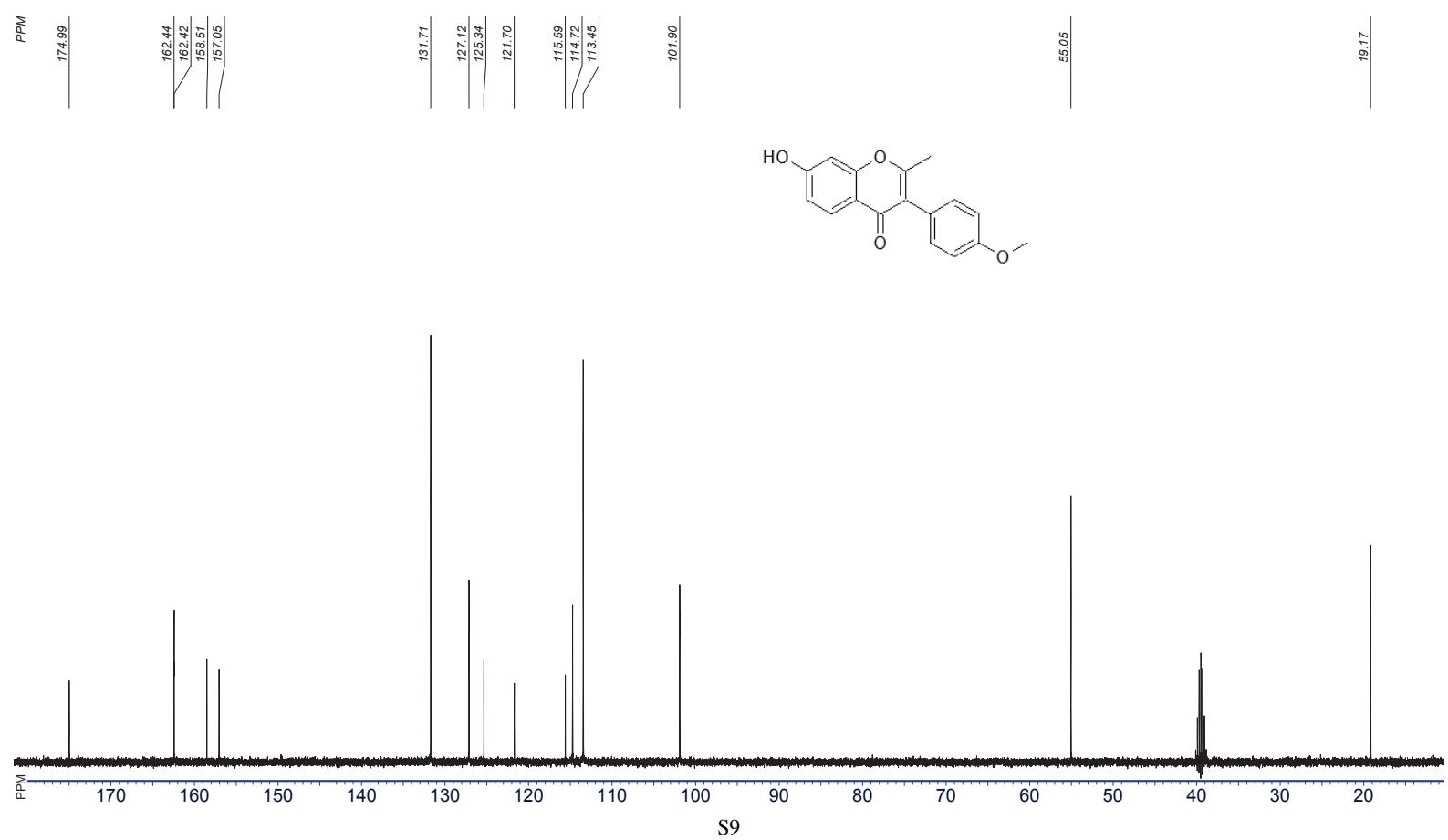
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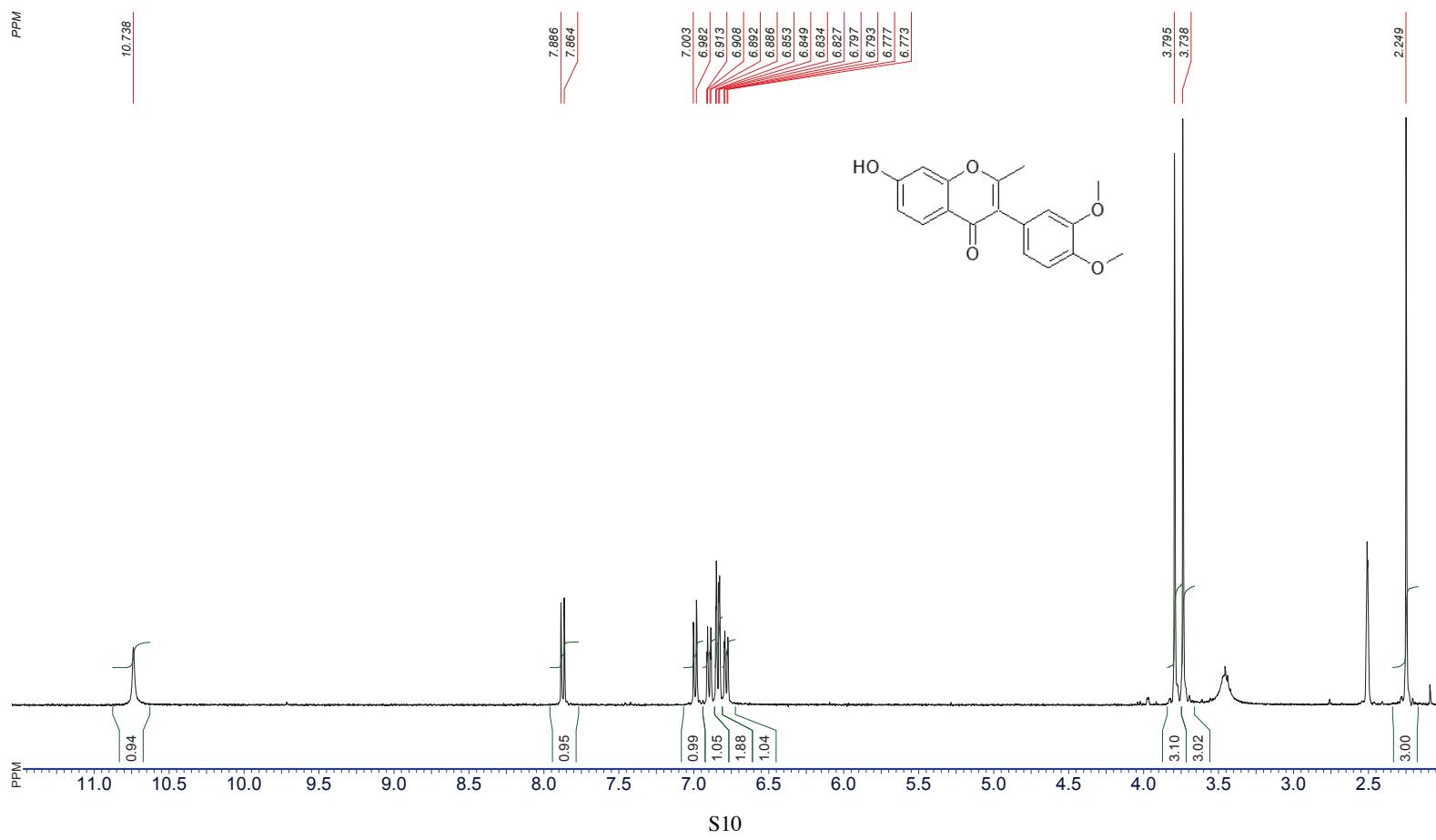
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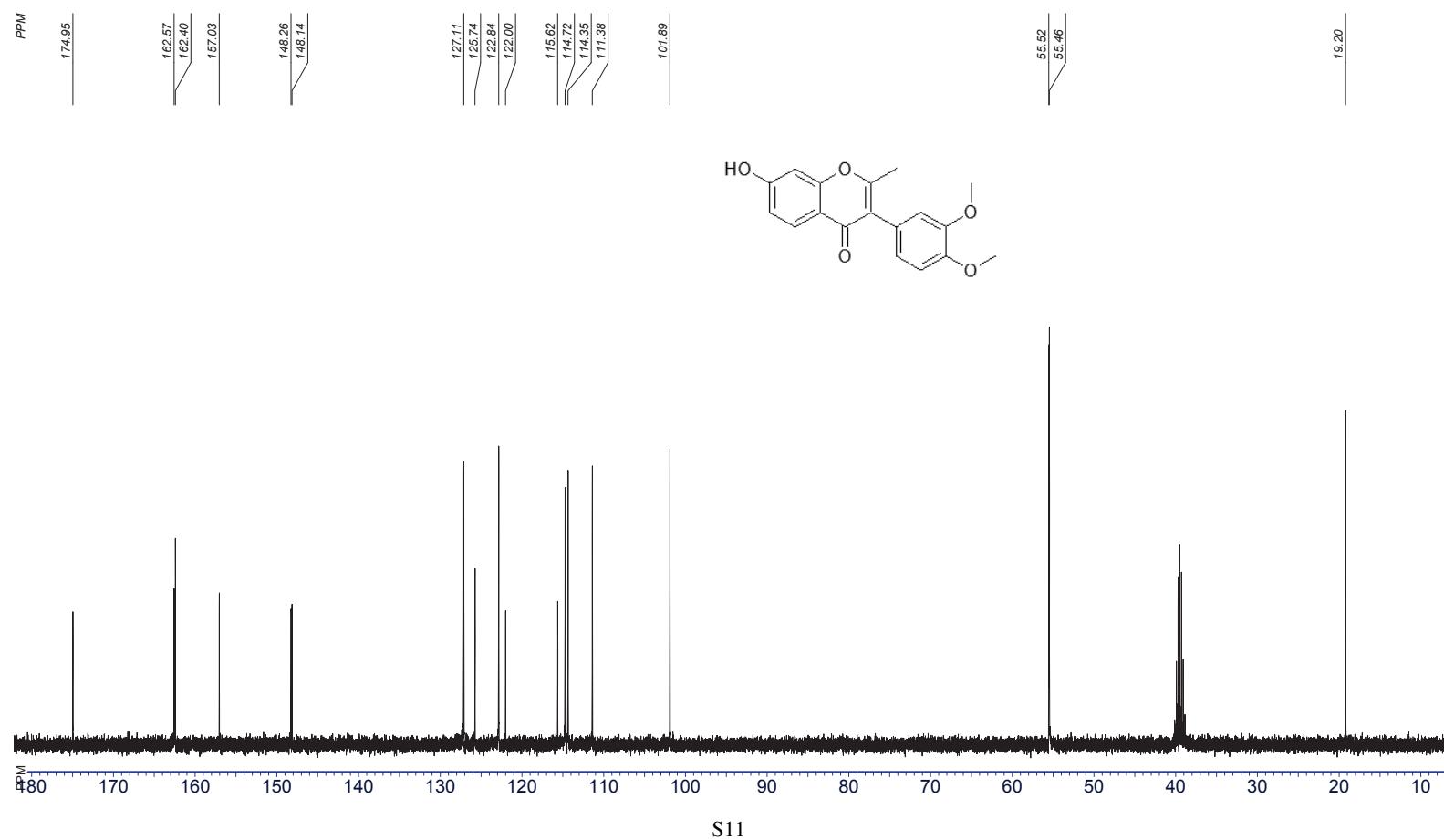
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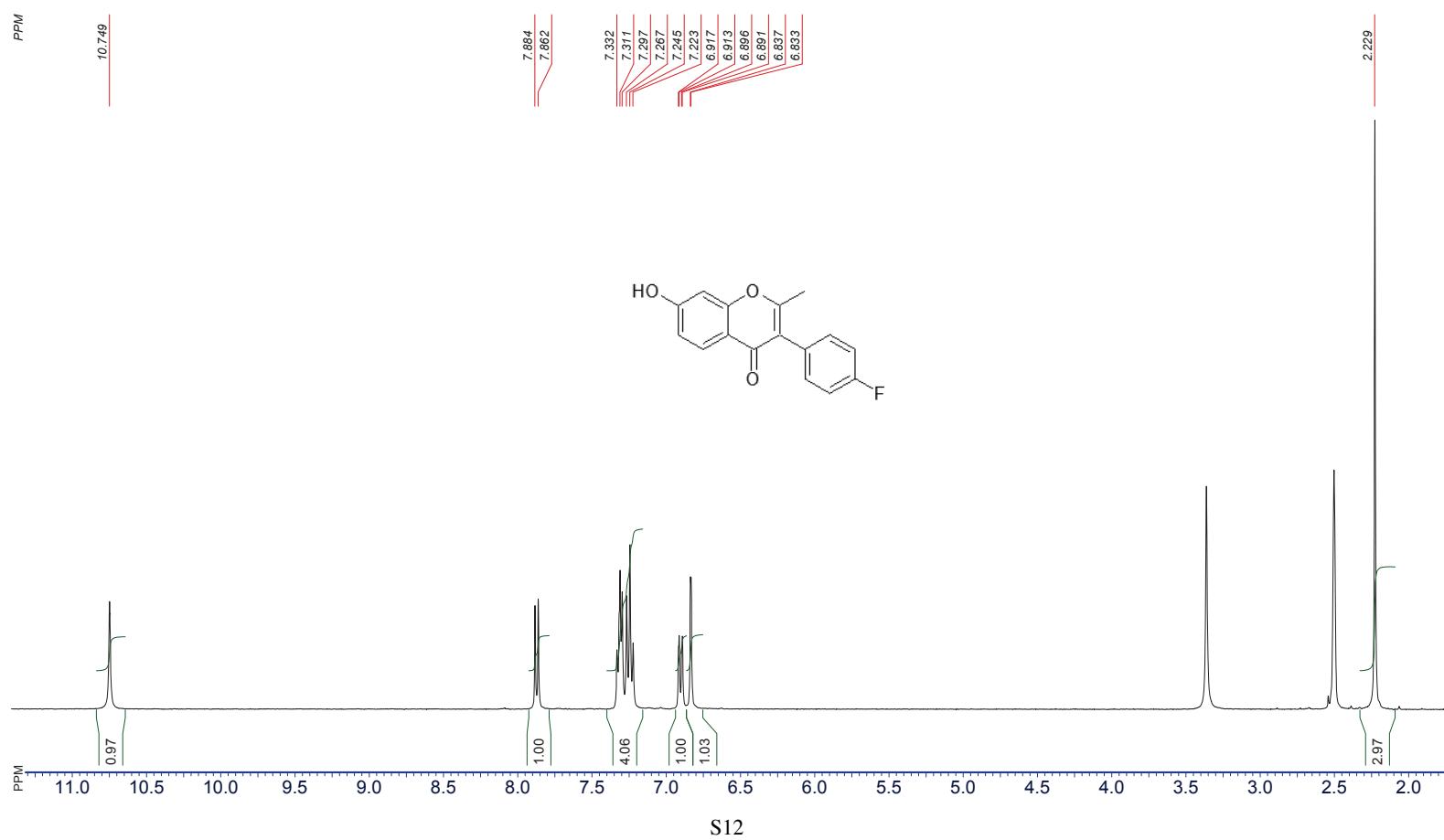
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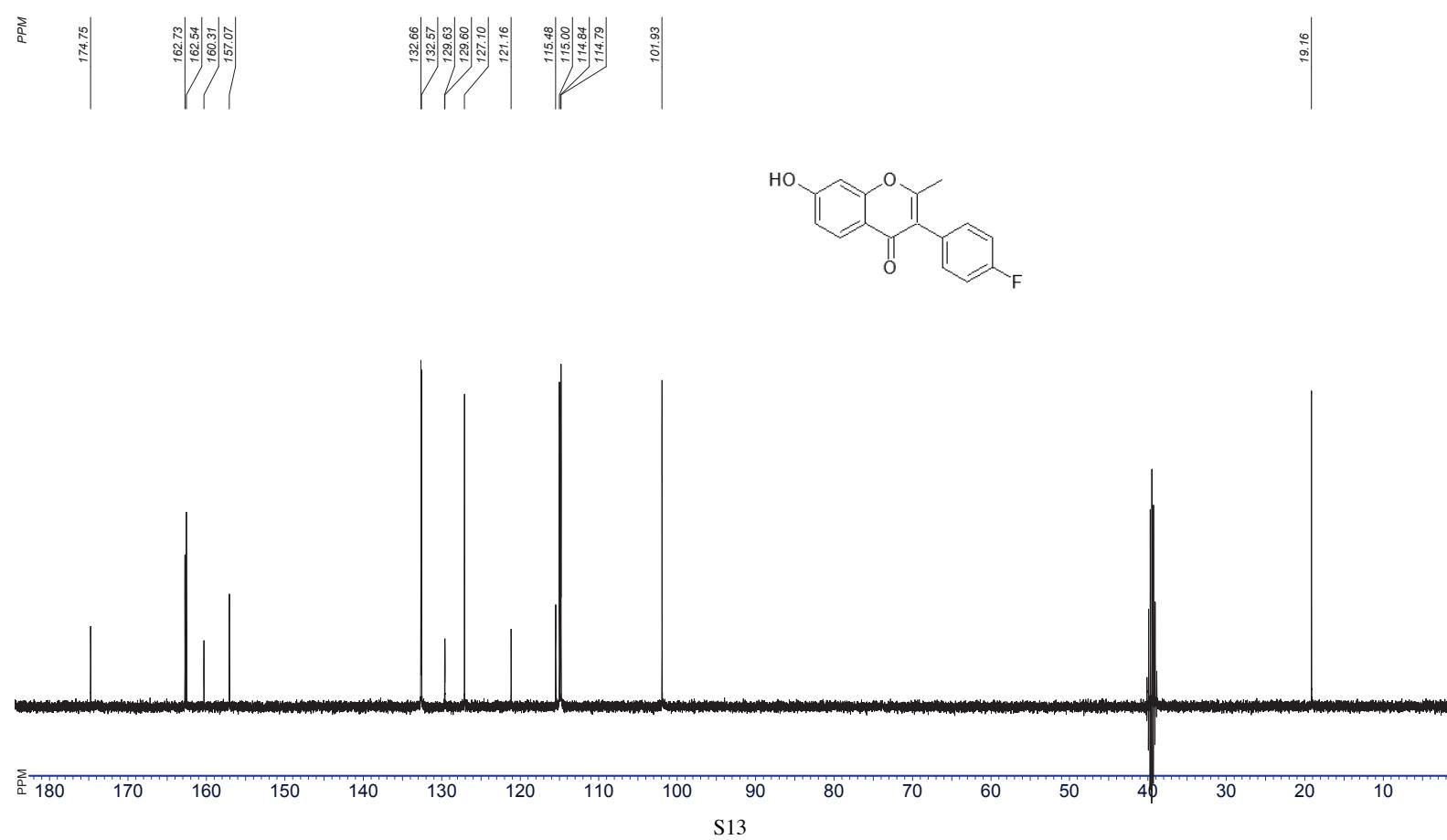
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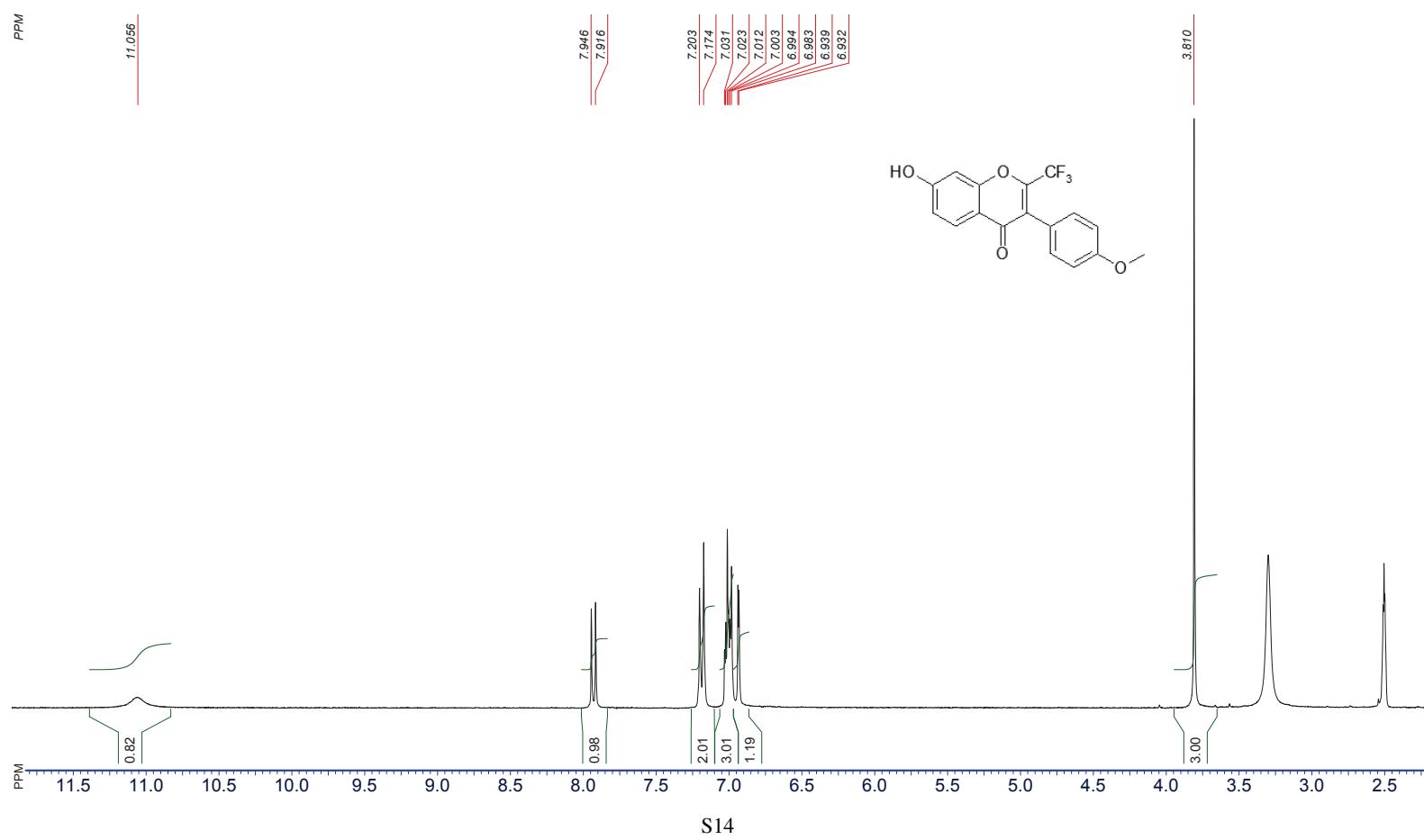
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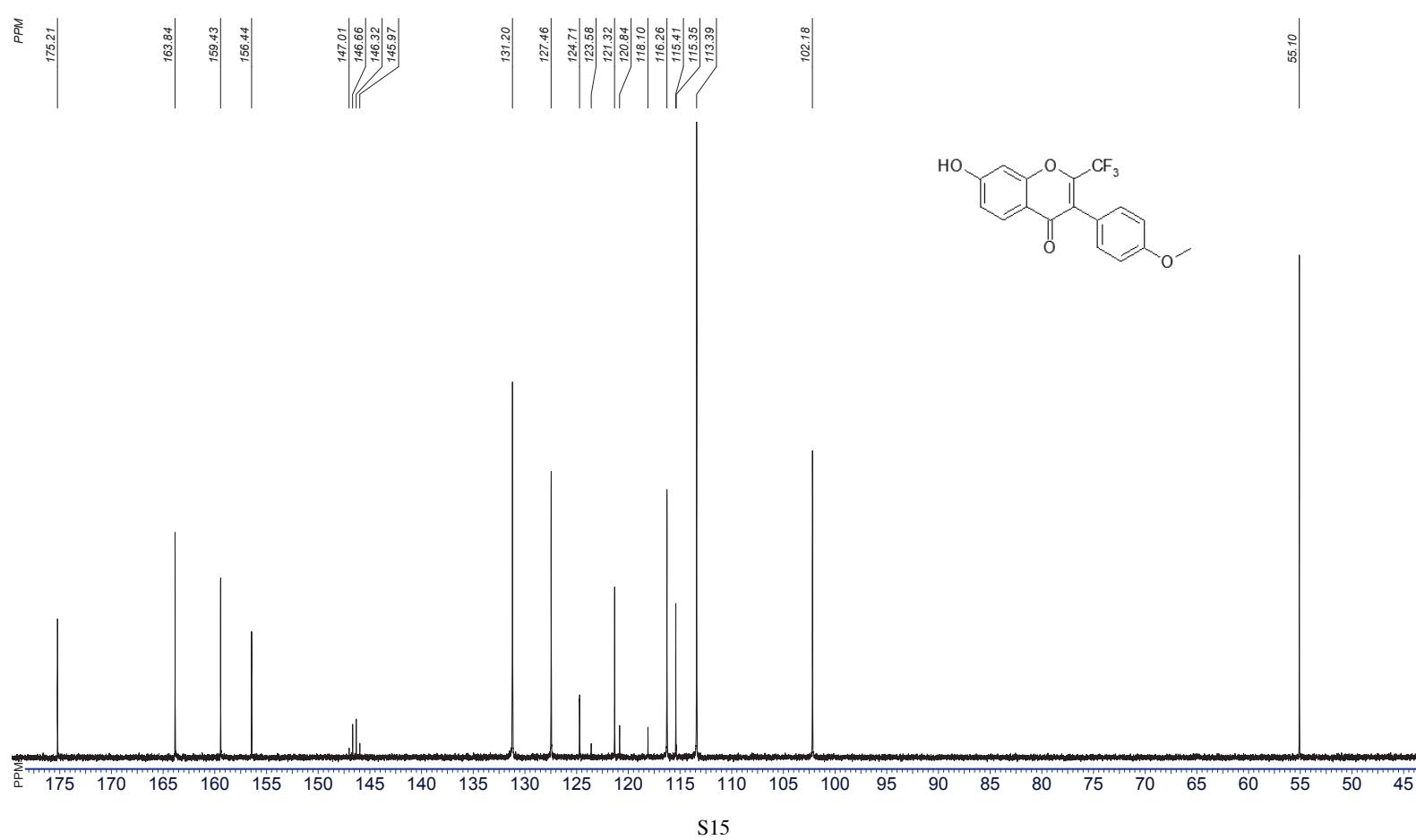
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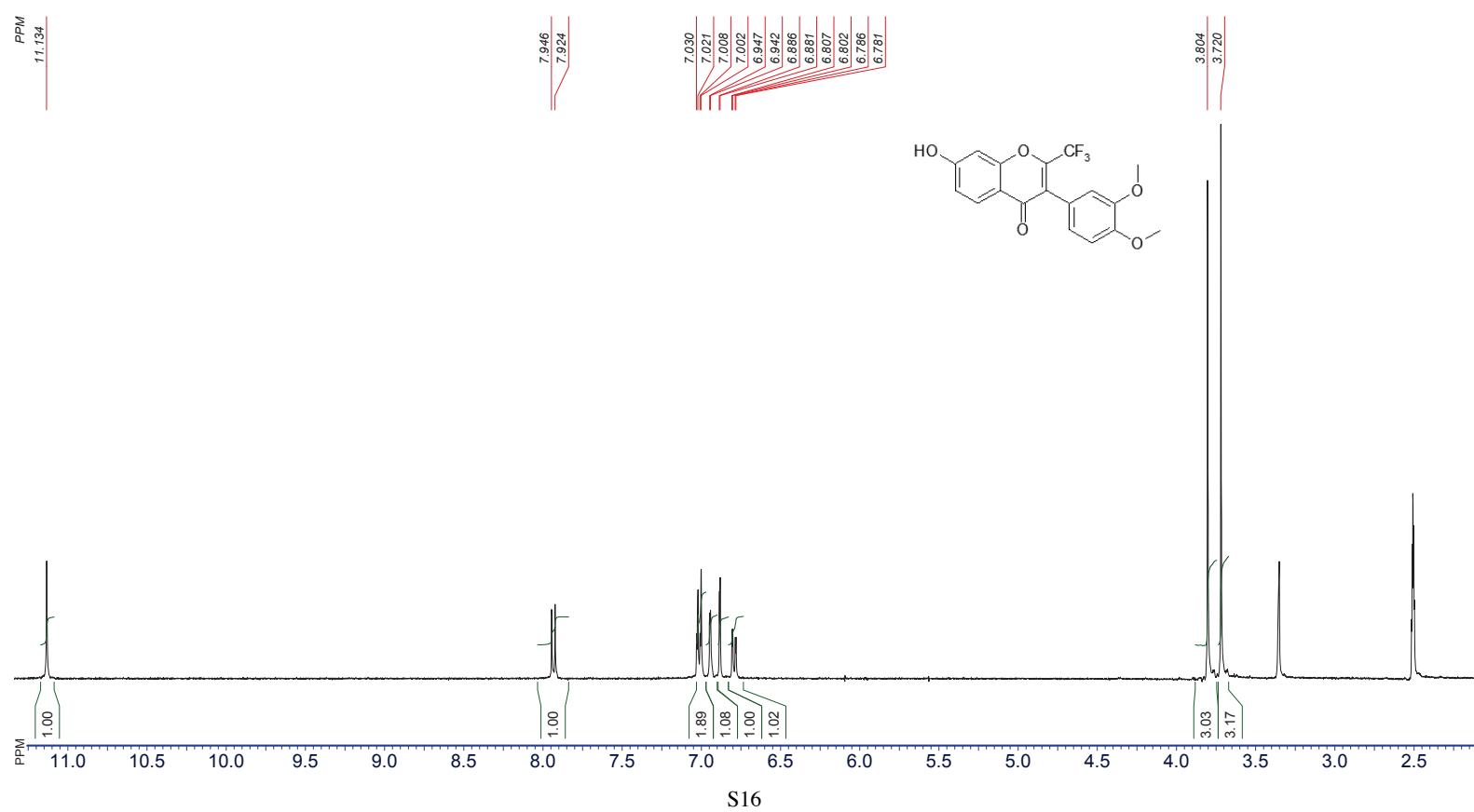
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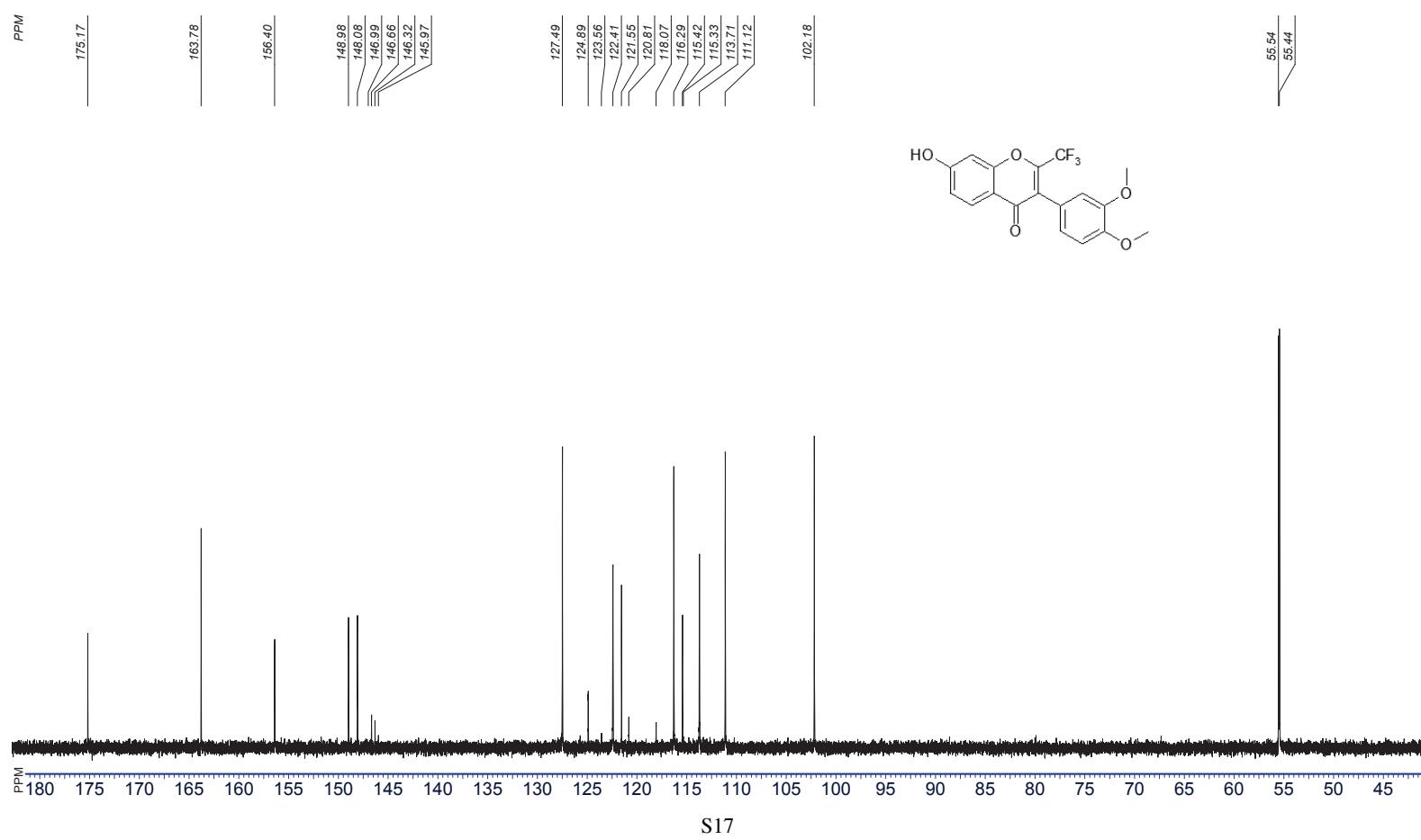
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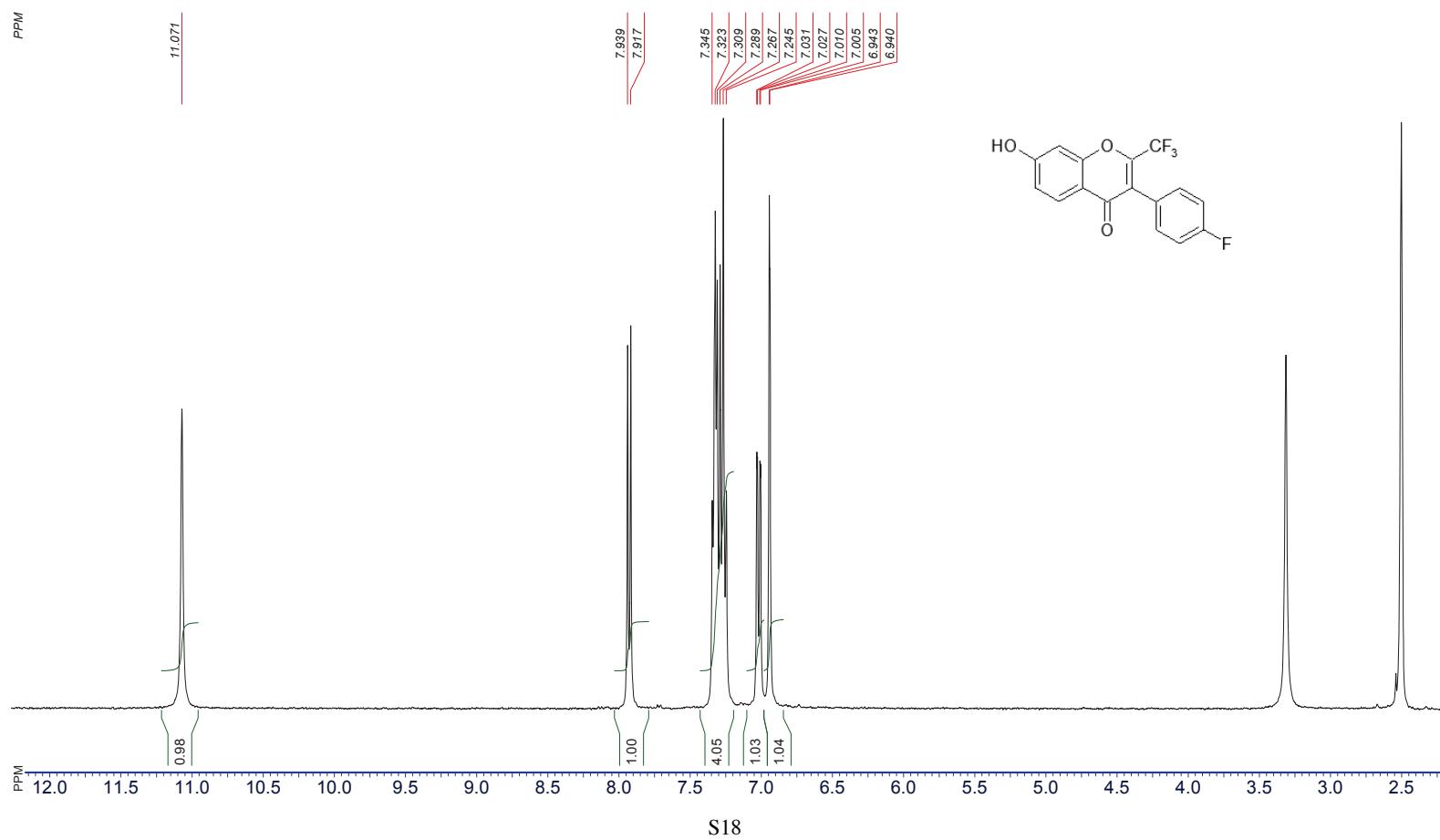
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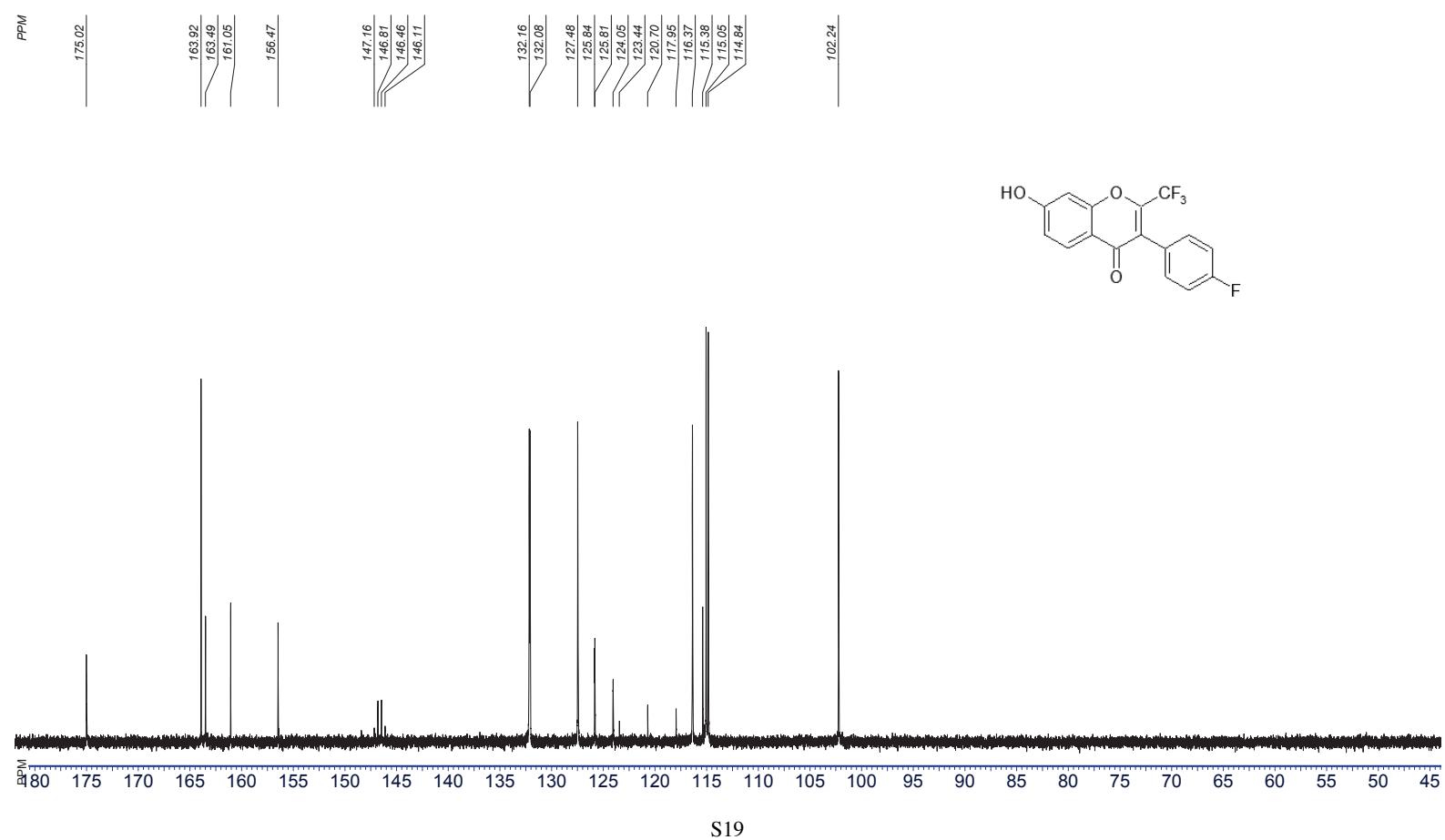
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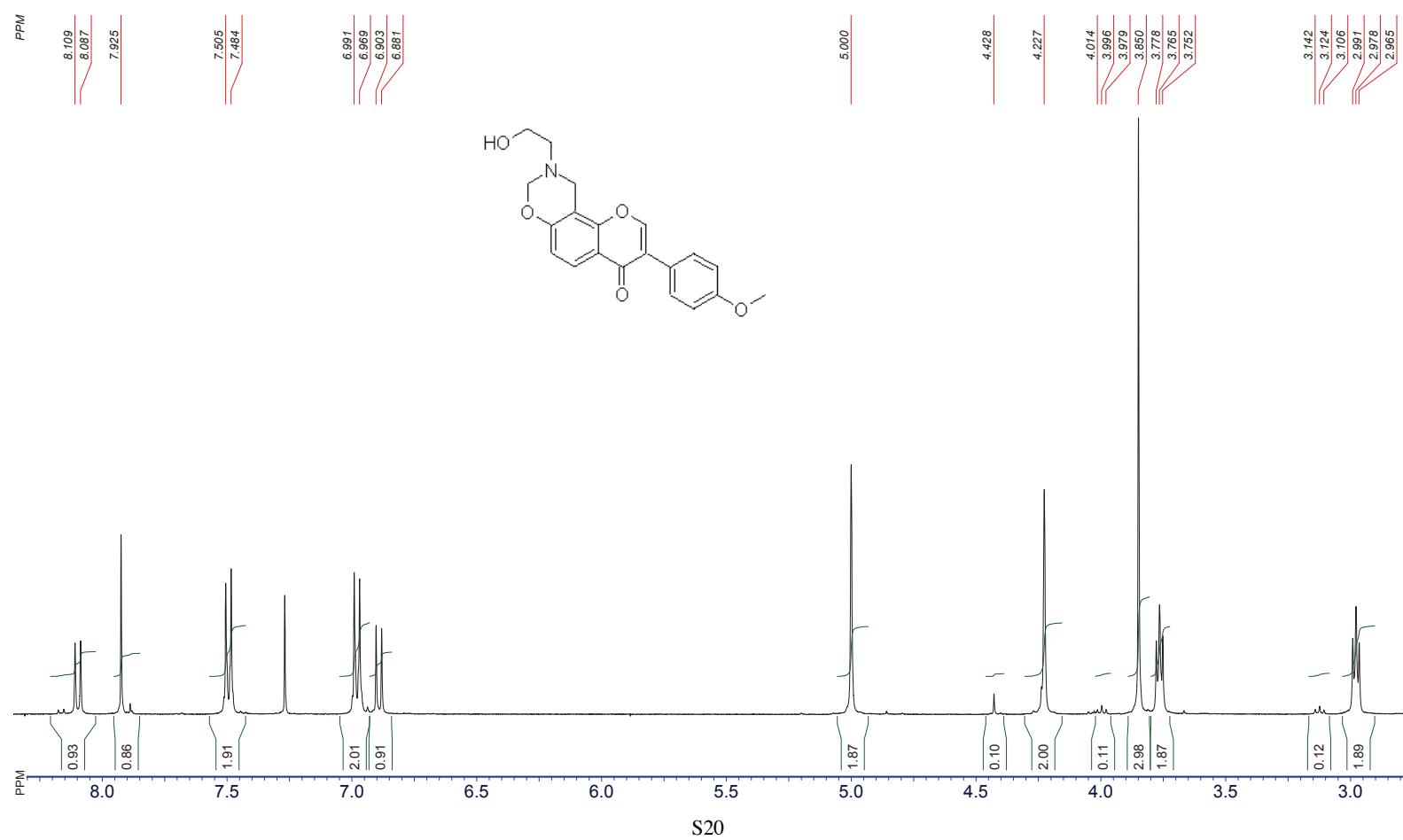
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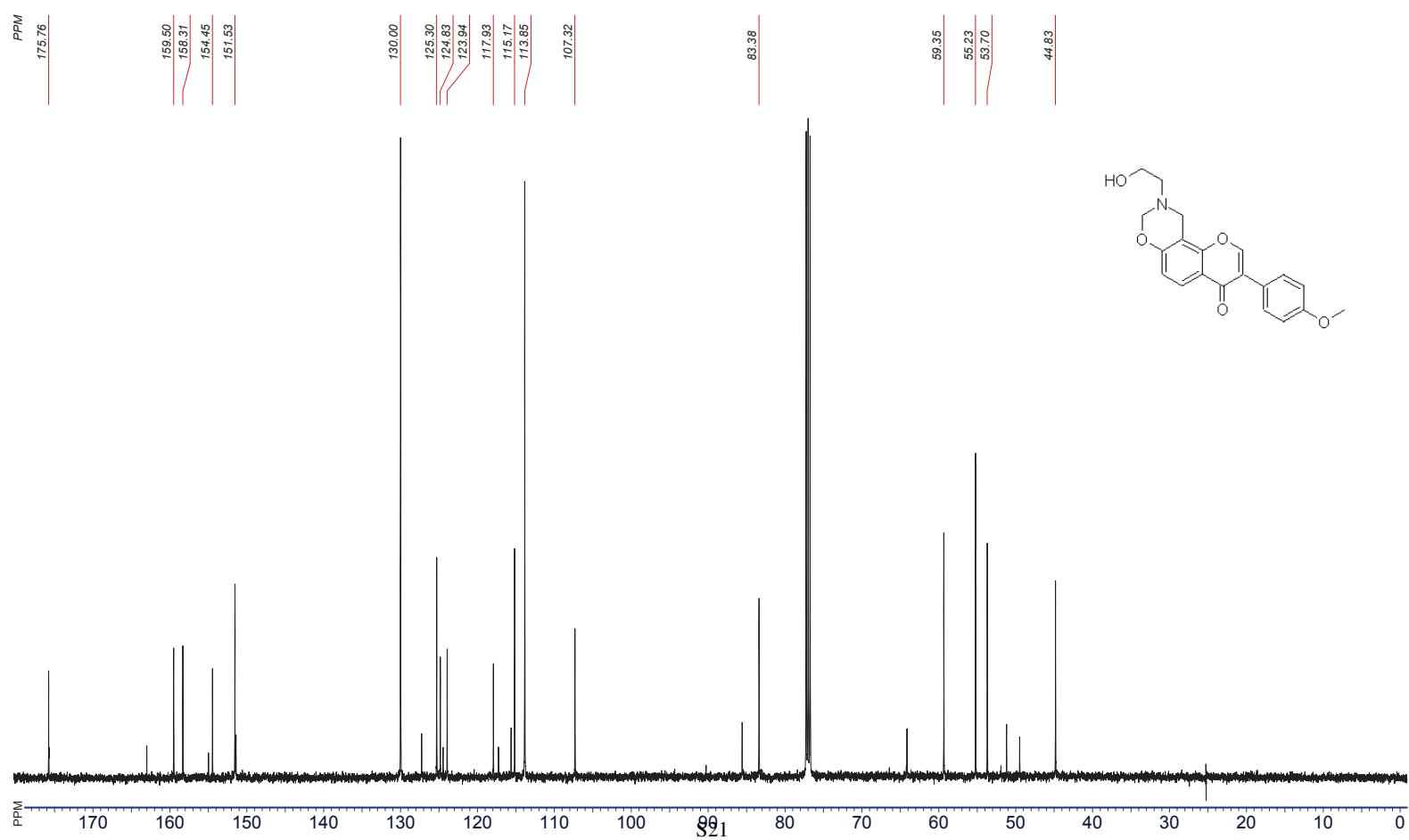
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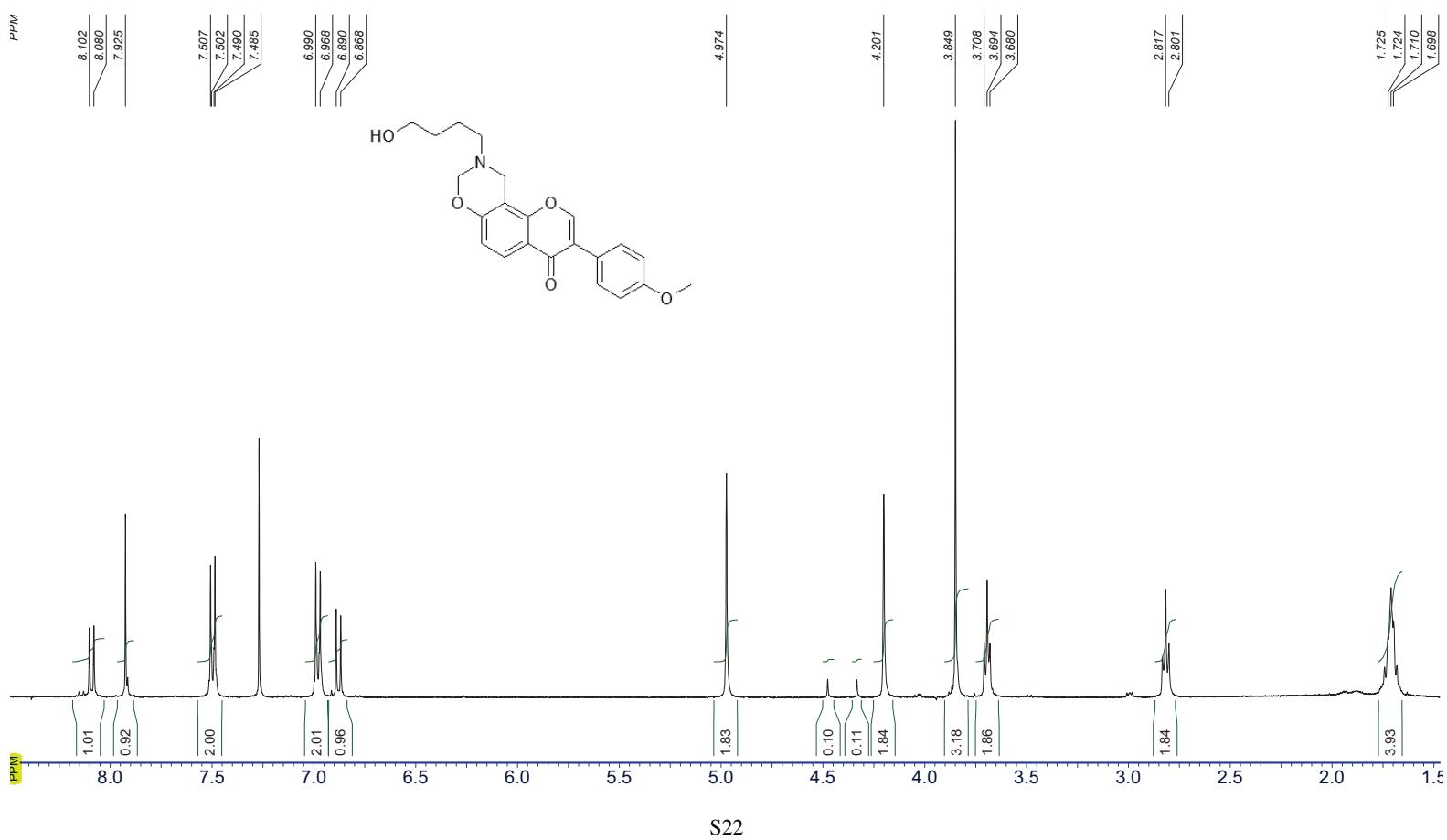
¹H NMR spectrum of 9-(2-hydroxyethyl)-3-(4-methoxyphenyl)-9,10-dihydro-4*H,8H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4a, n=1**) in CDCl₃



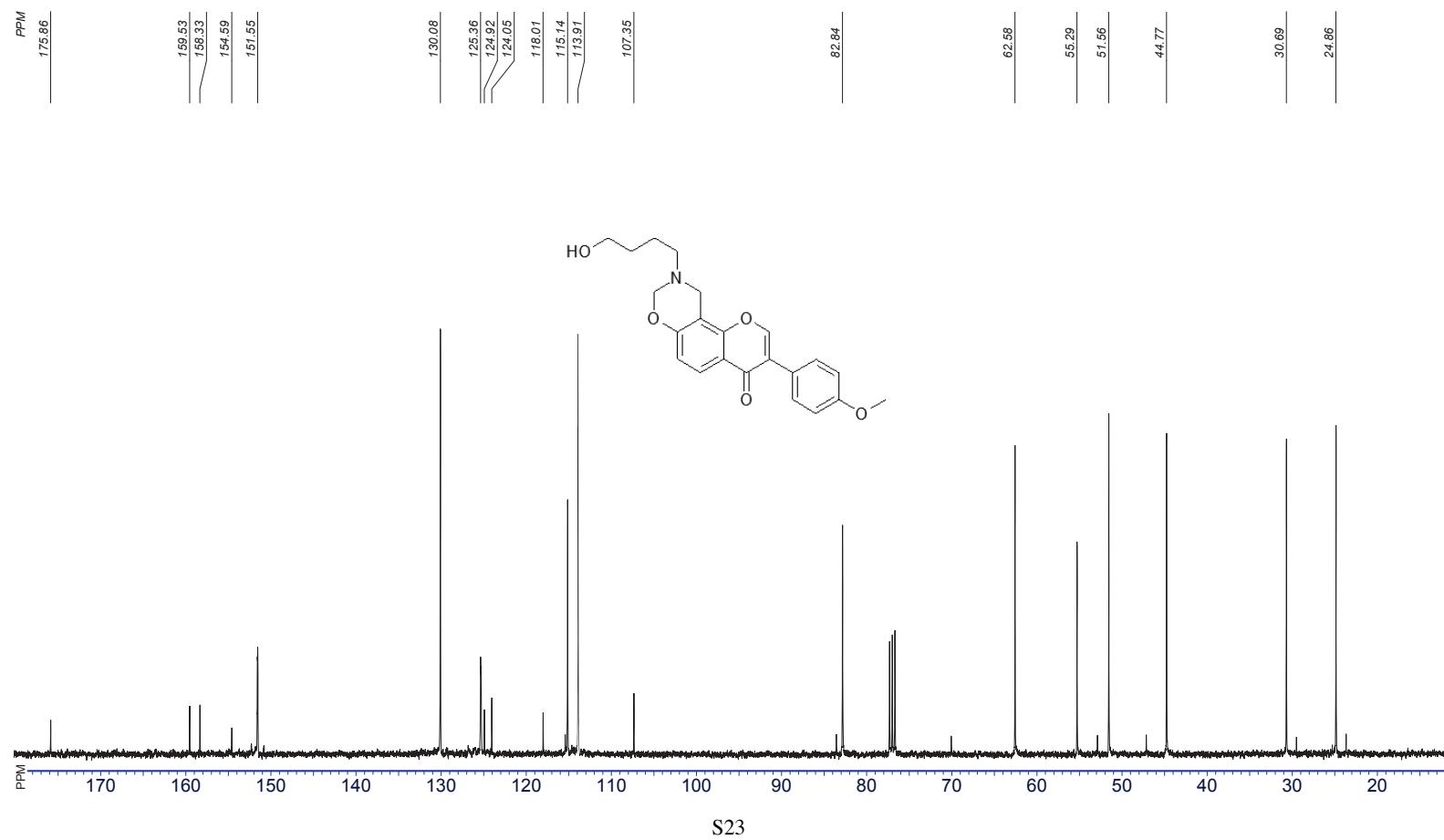
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¹H NMR spectrum of 9-(4-hydroxybutyl)-3-(4-methoxyphenyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4a, n = 3**) in CDCl₃

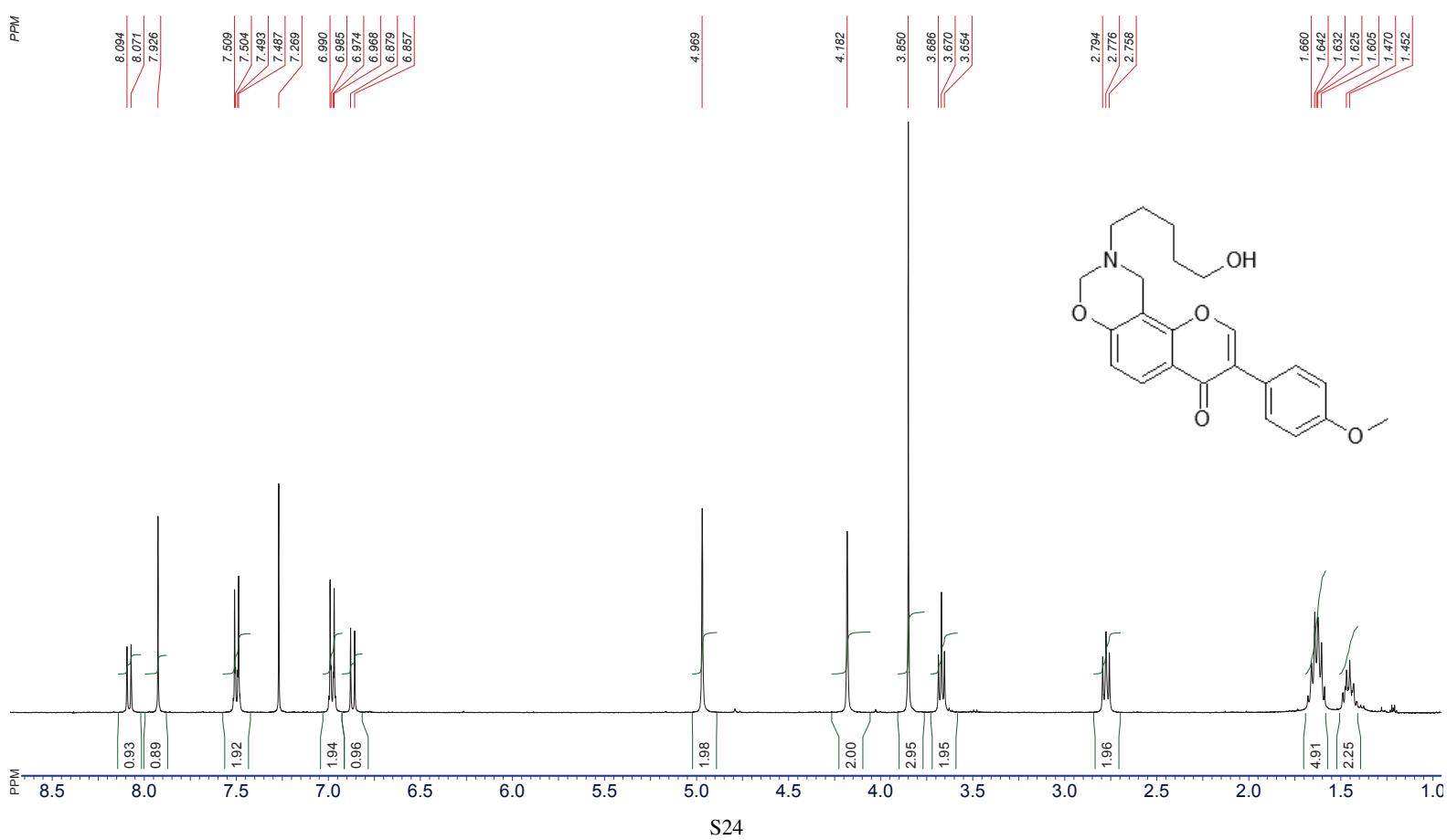


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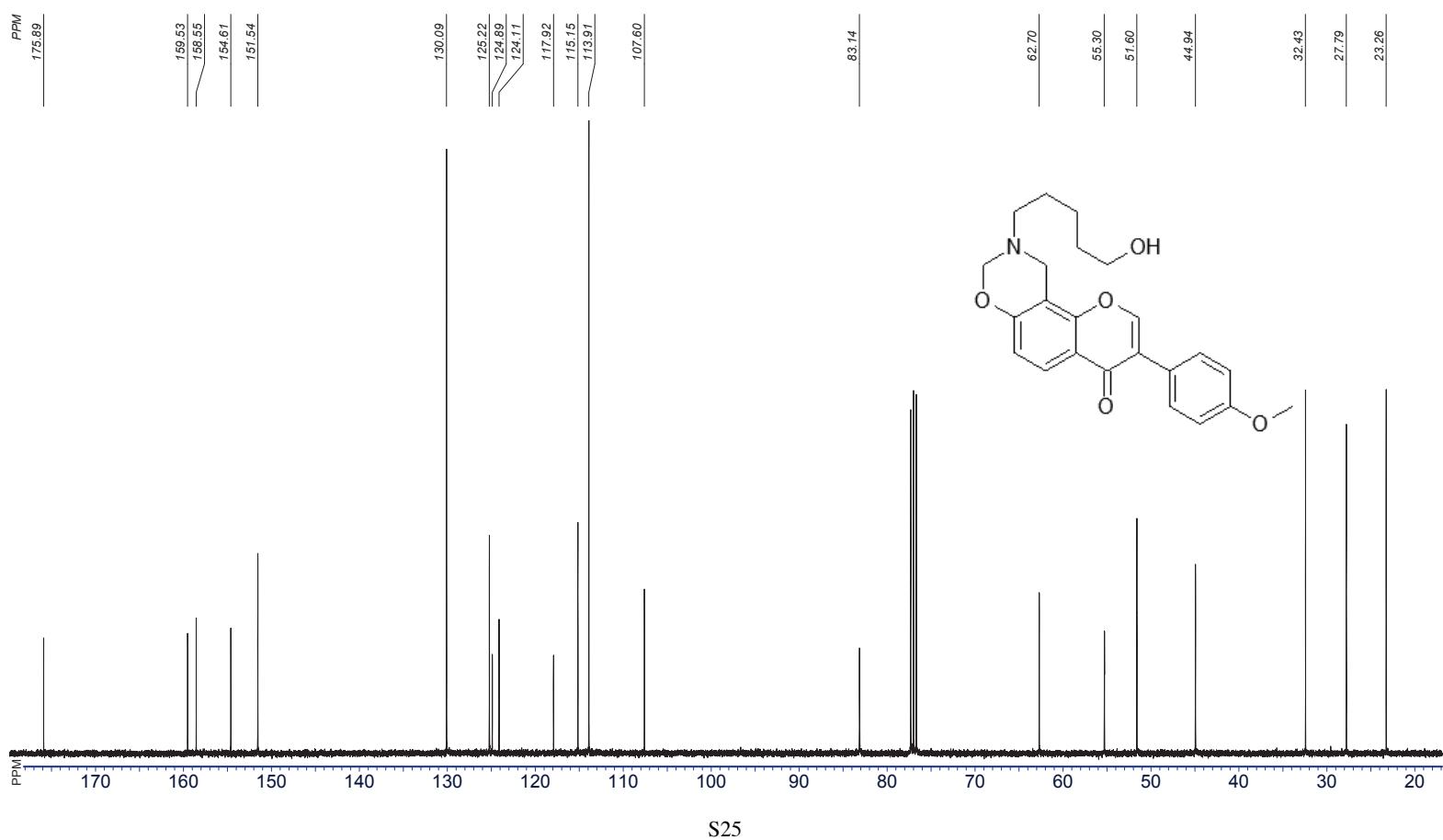


S23

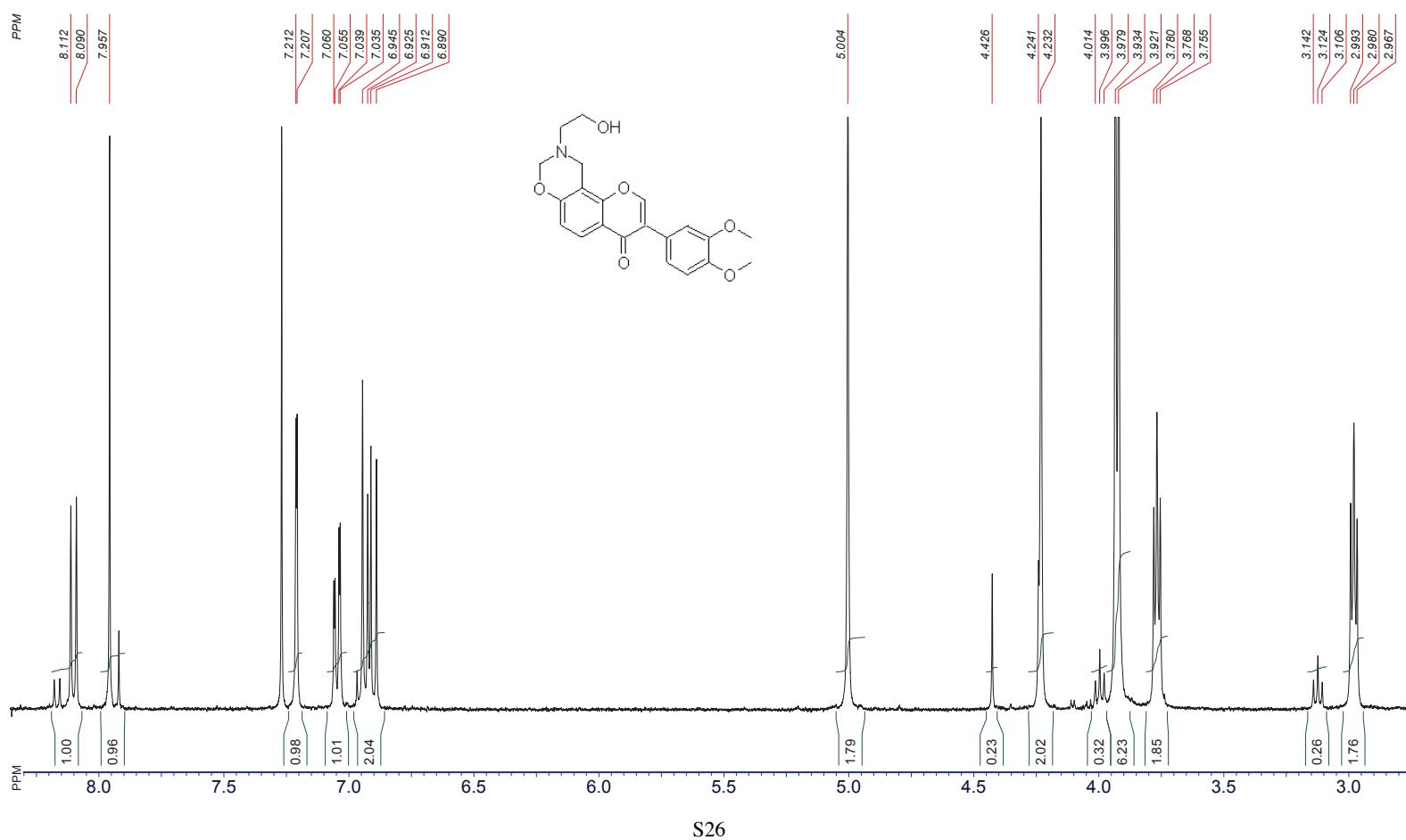
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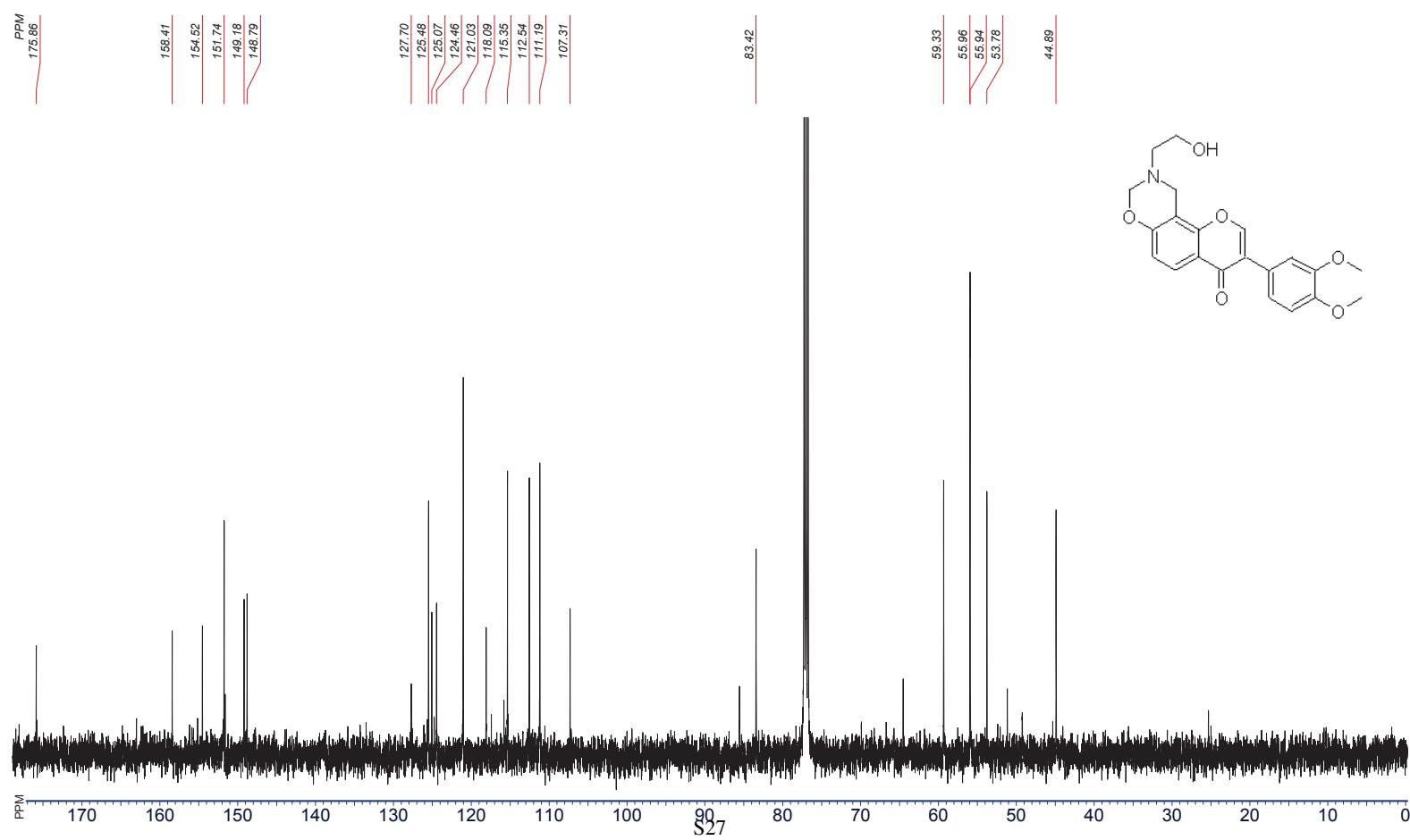
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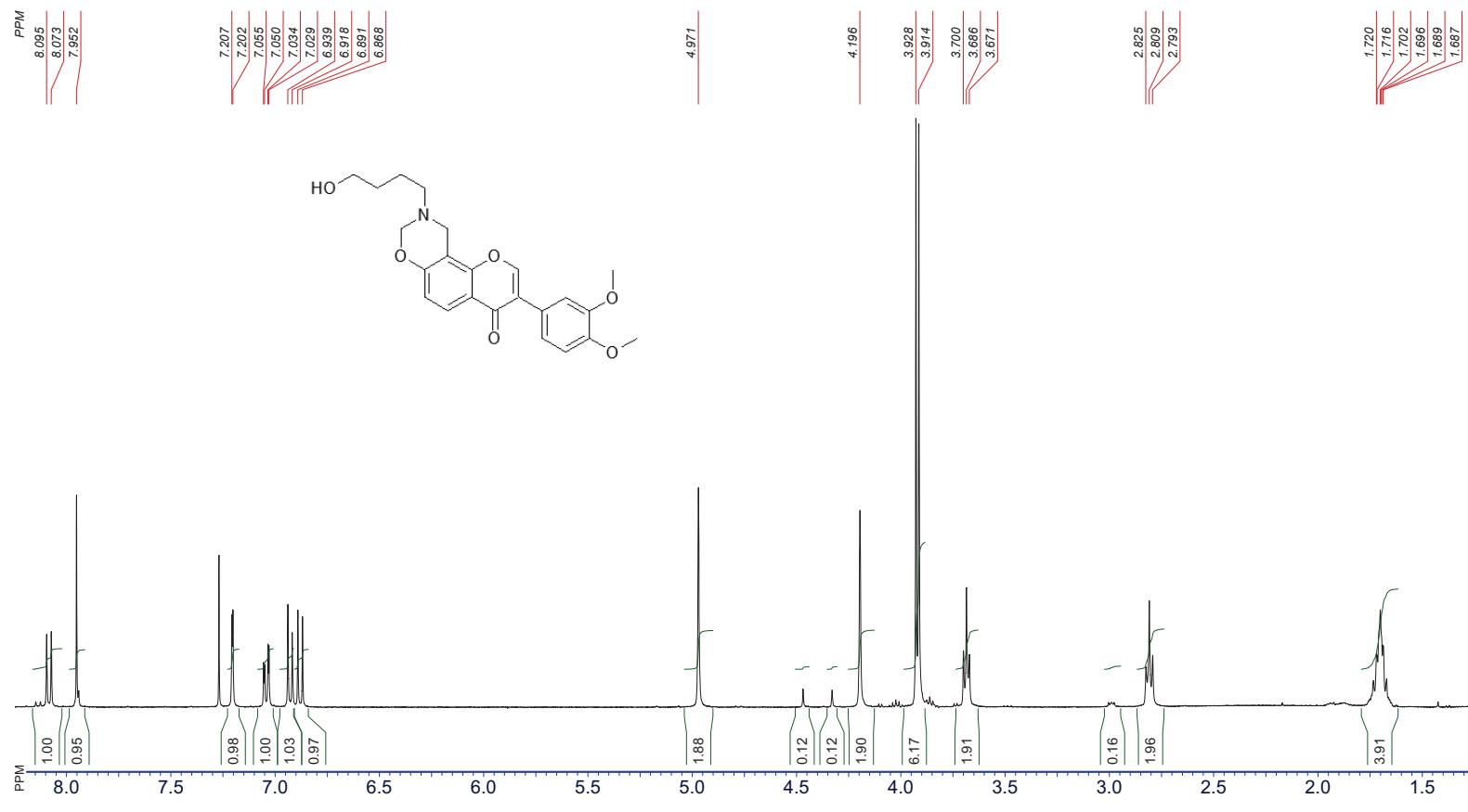
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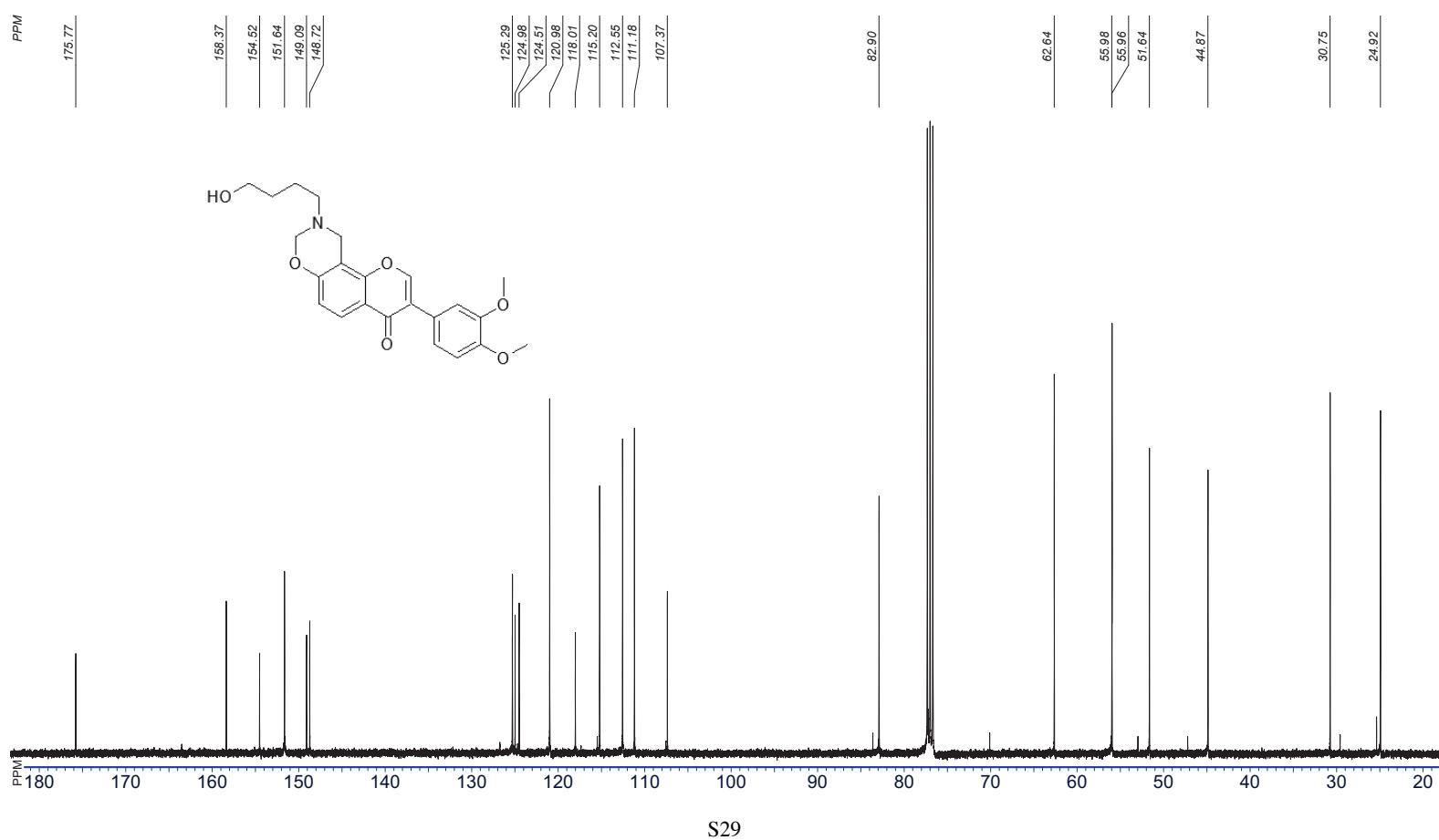
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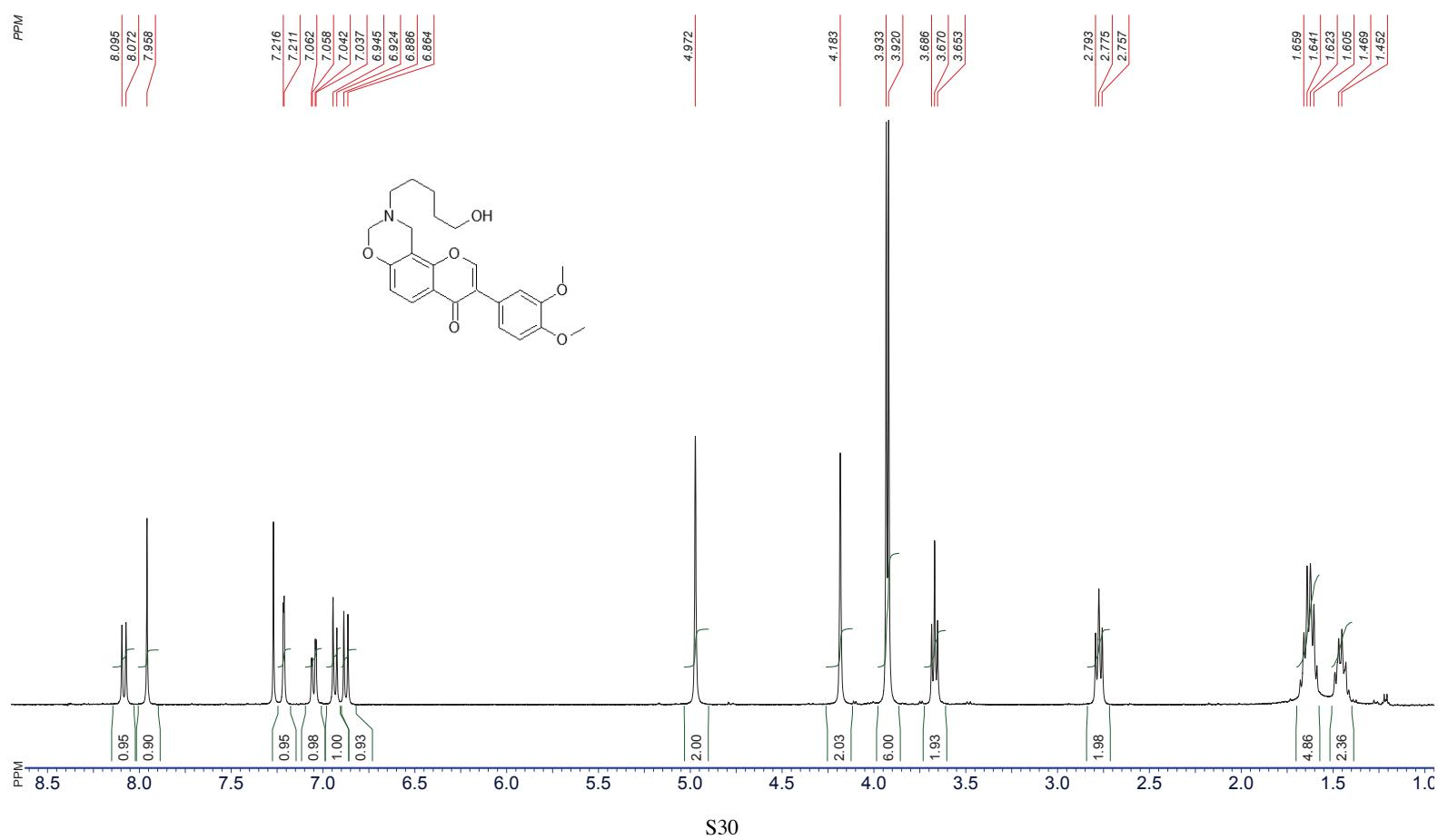
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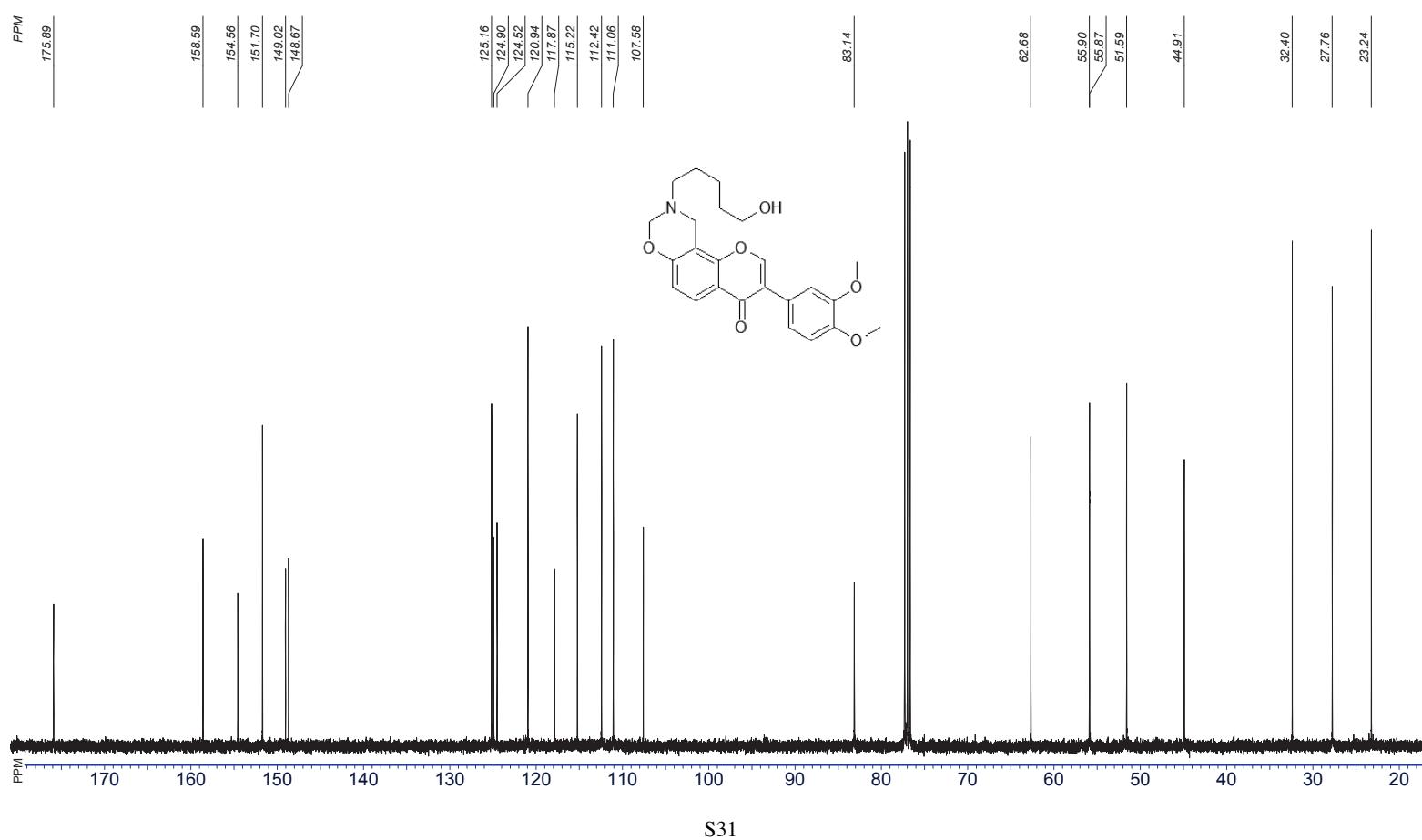
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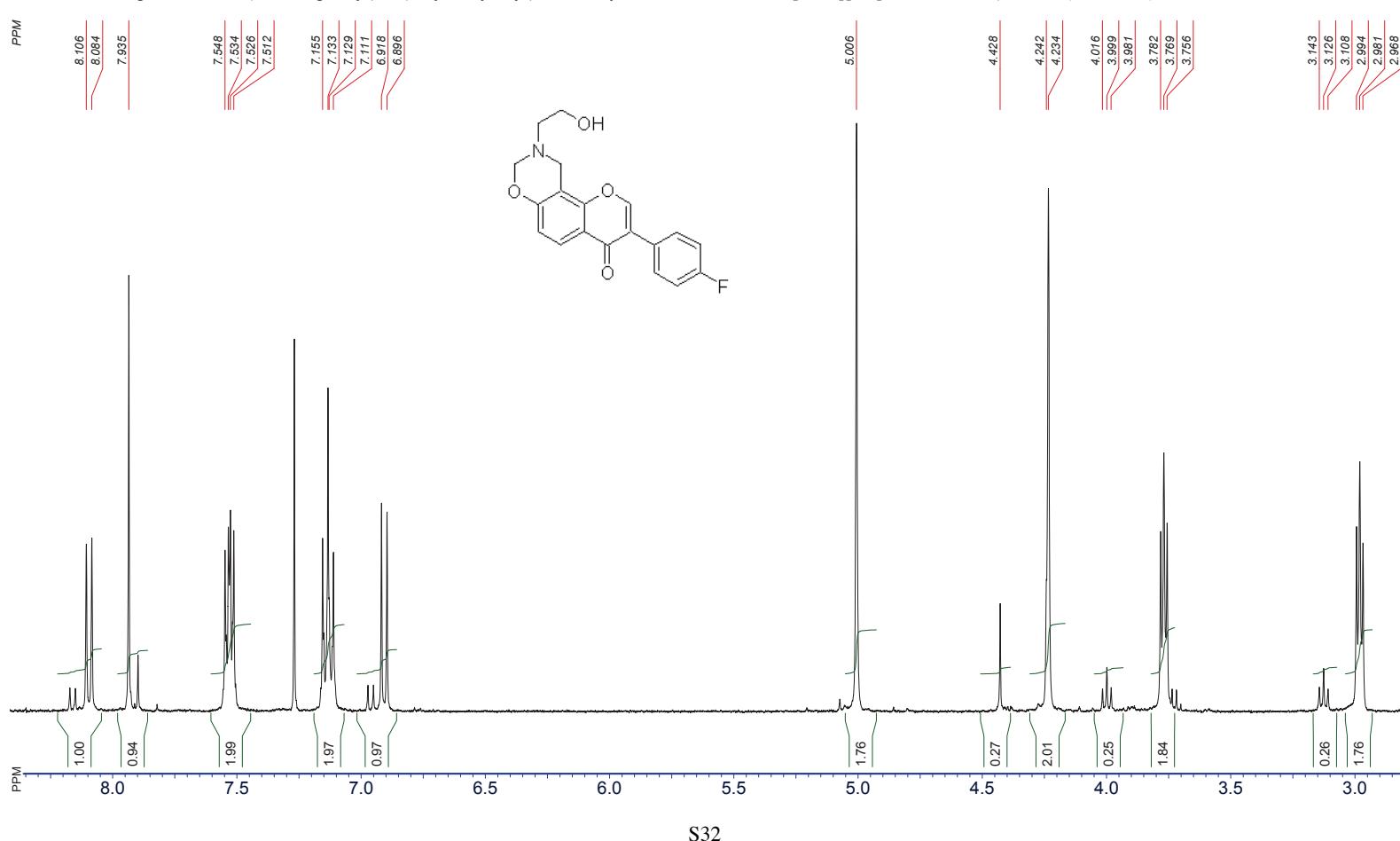
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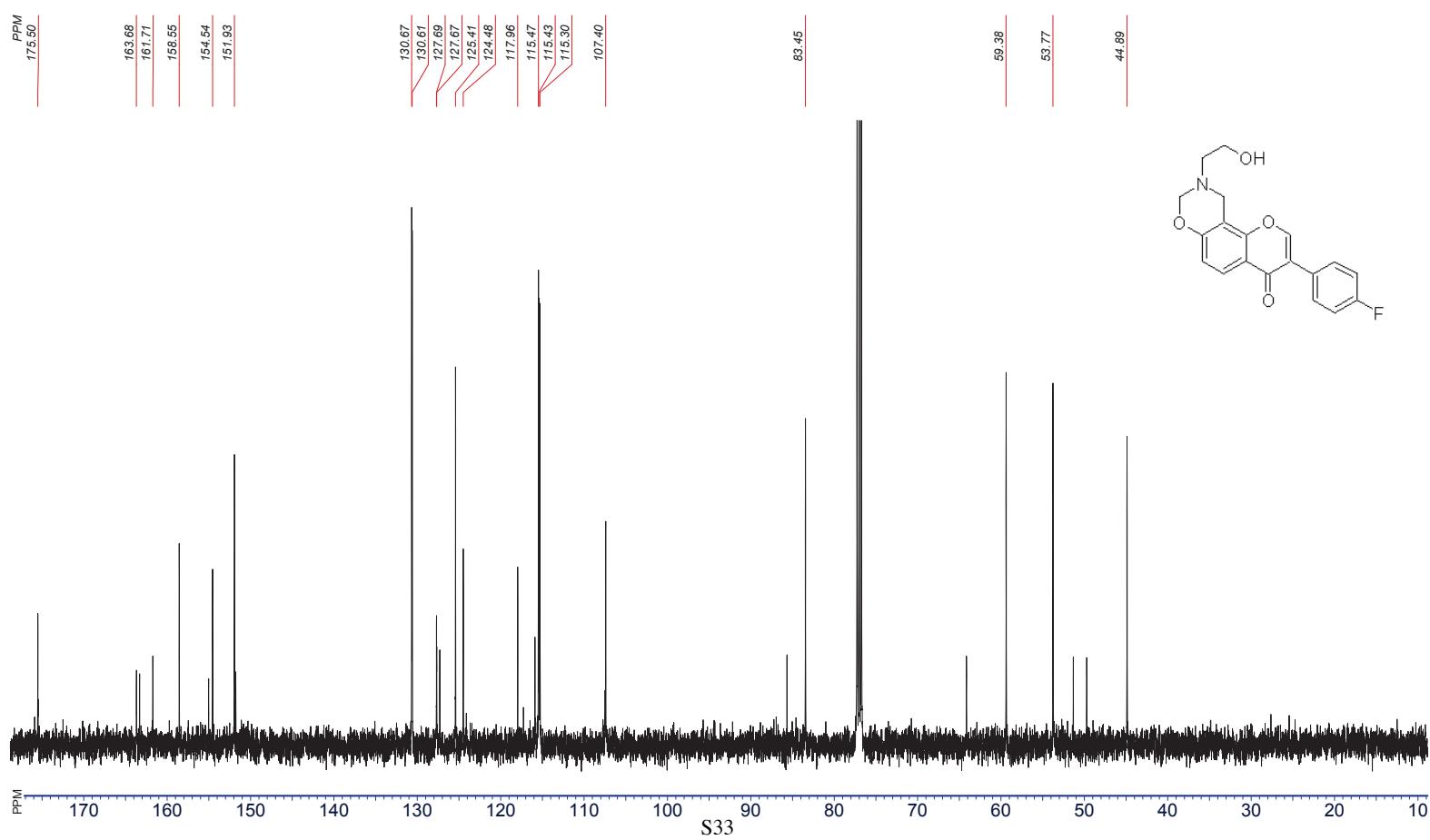
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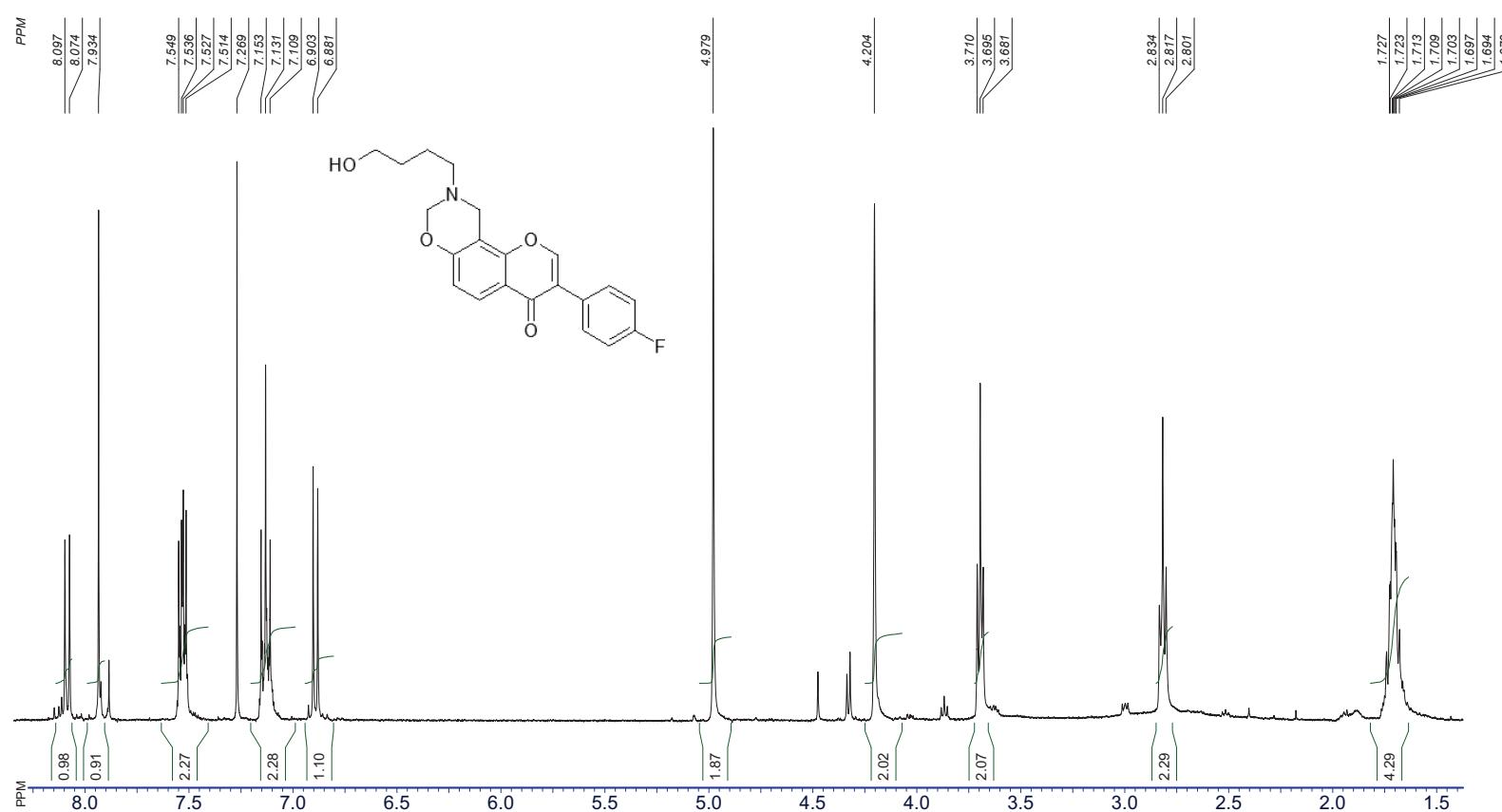
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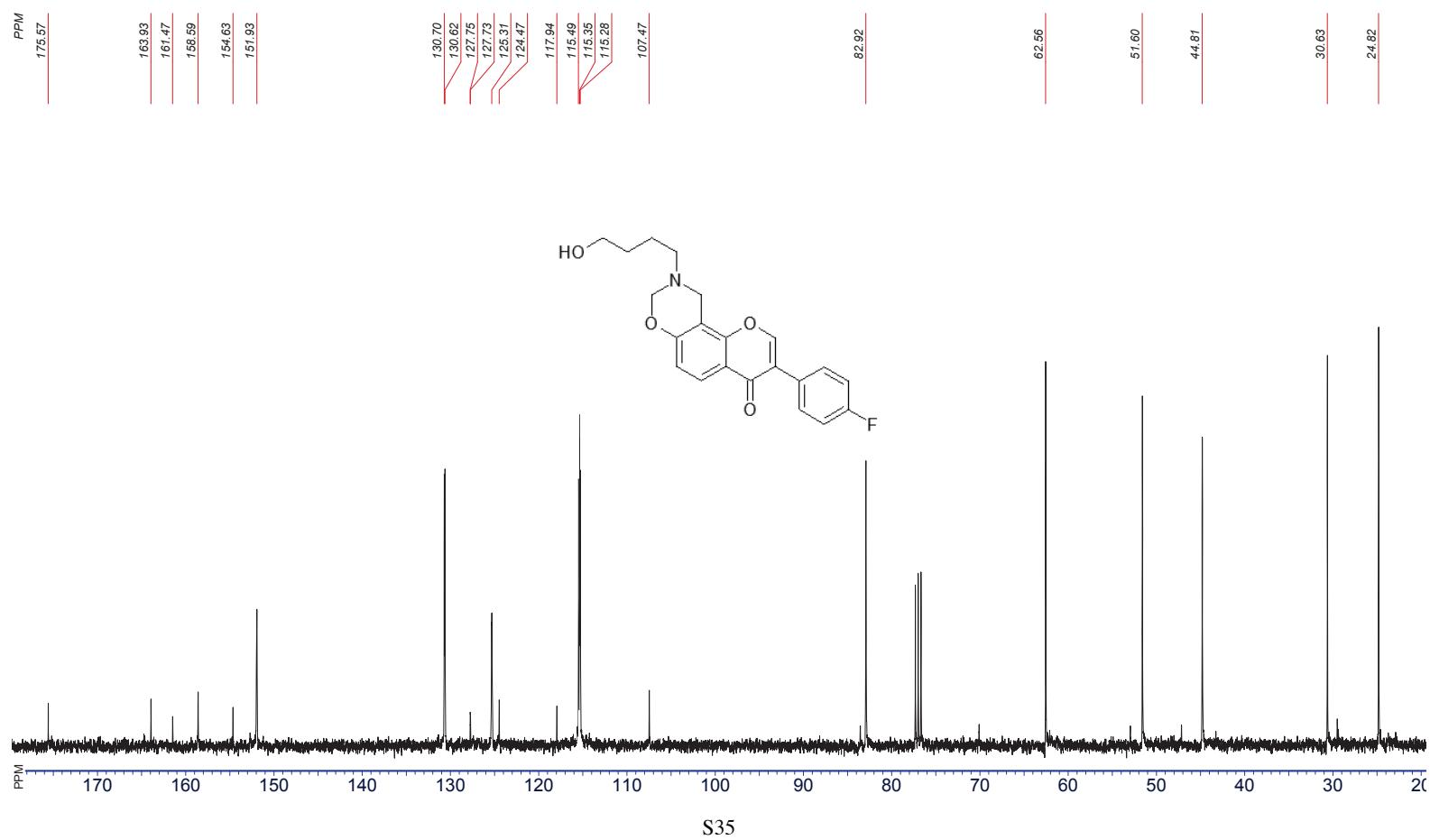
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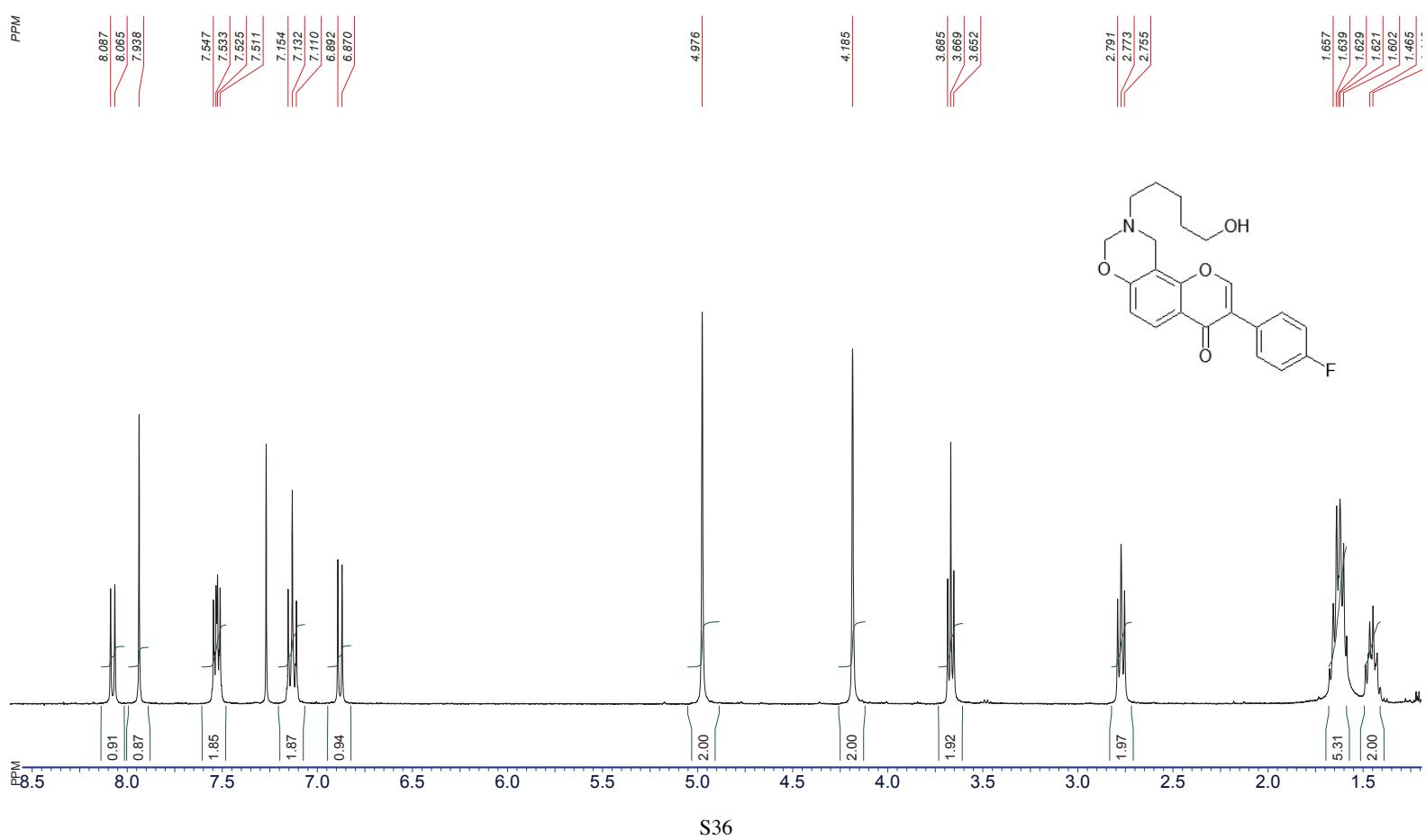
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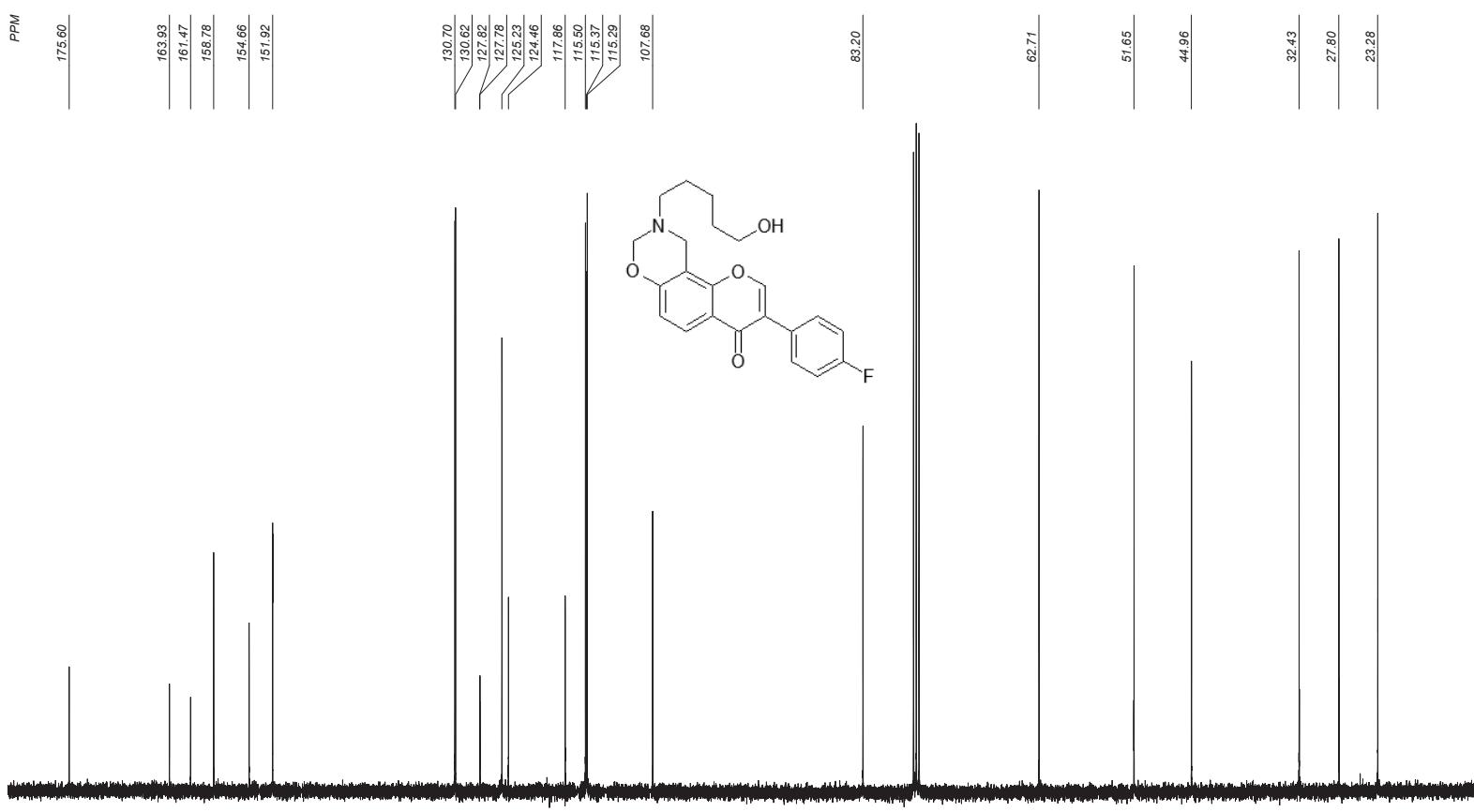
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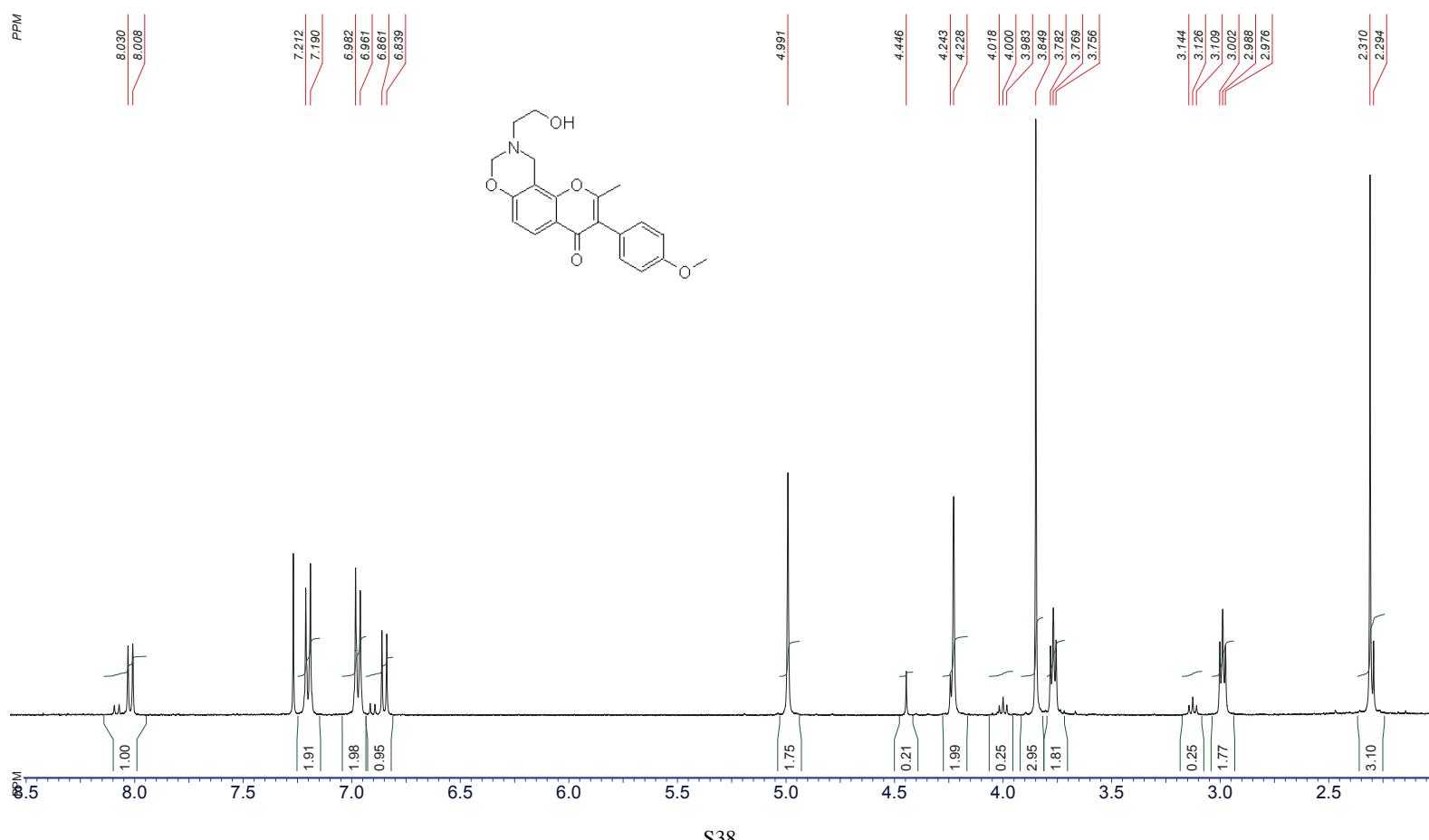
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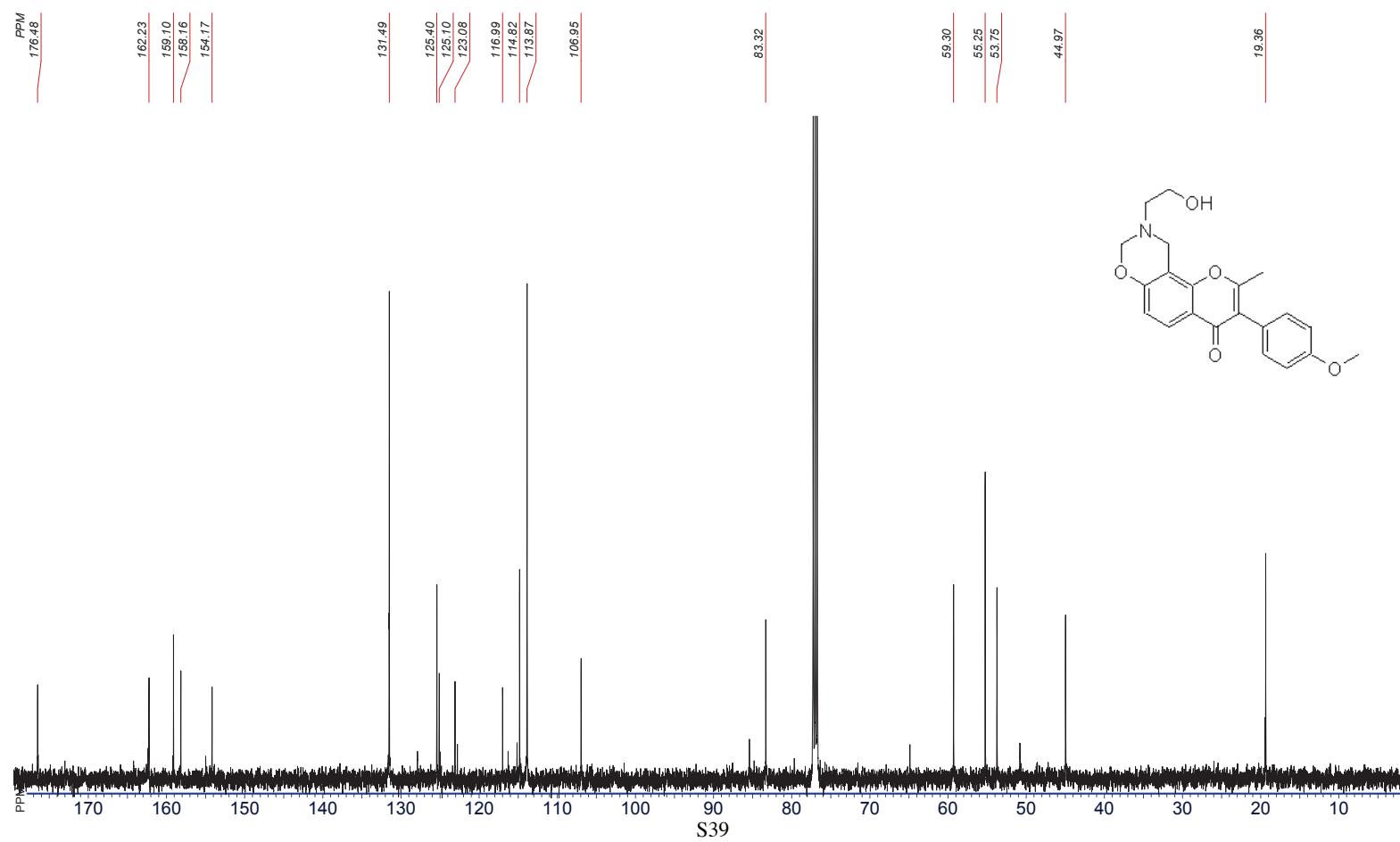
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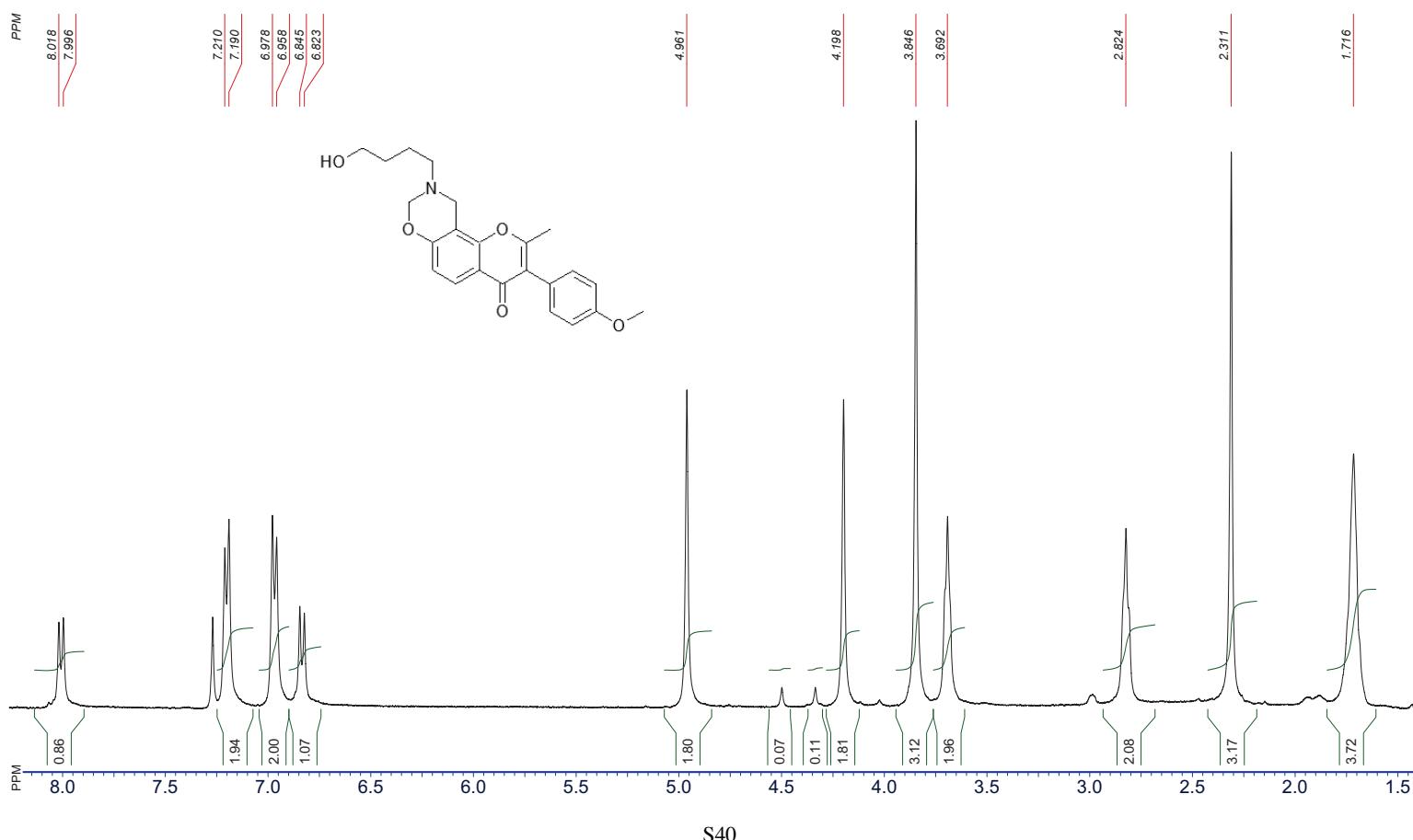
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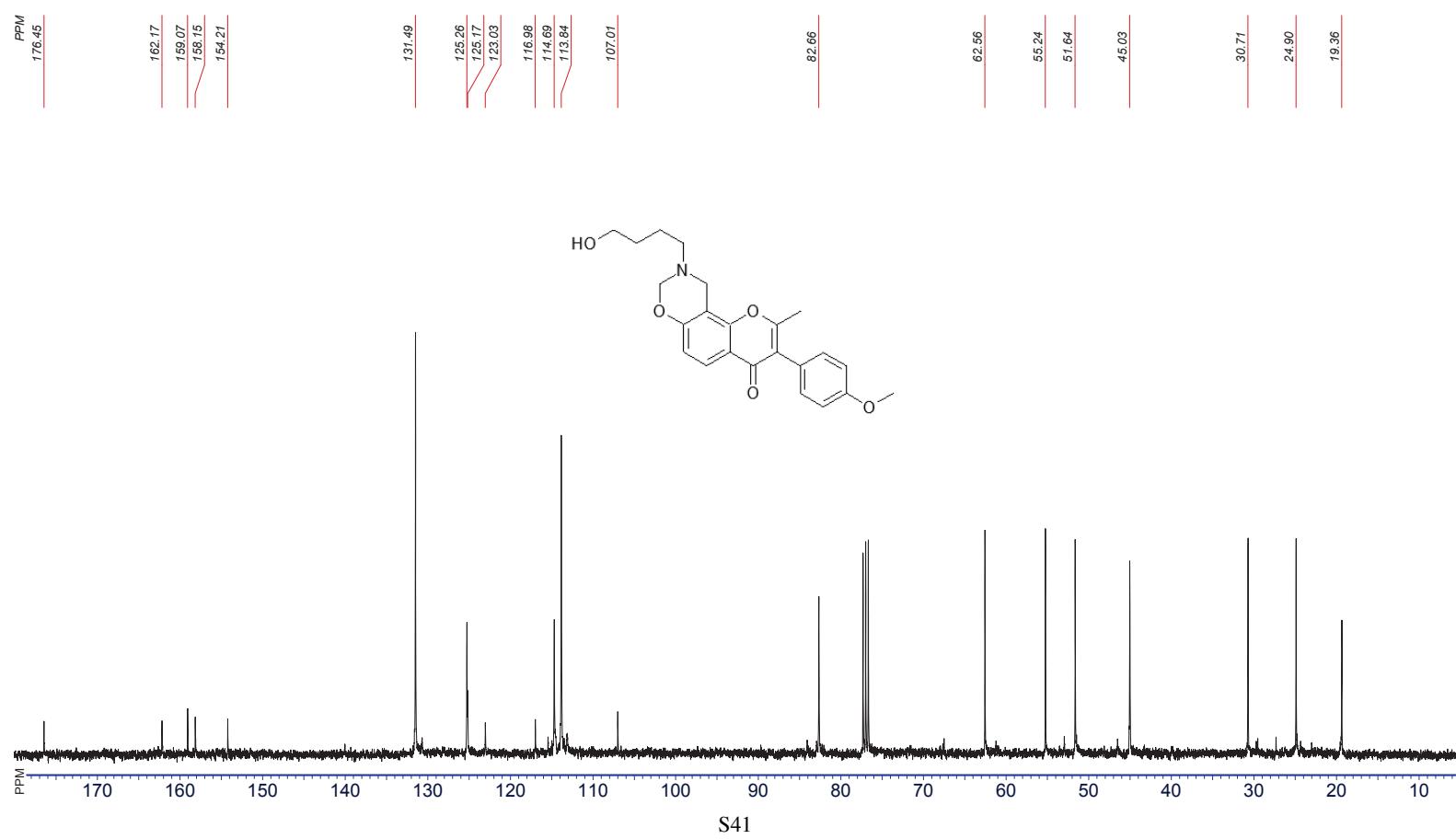
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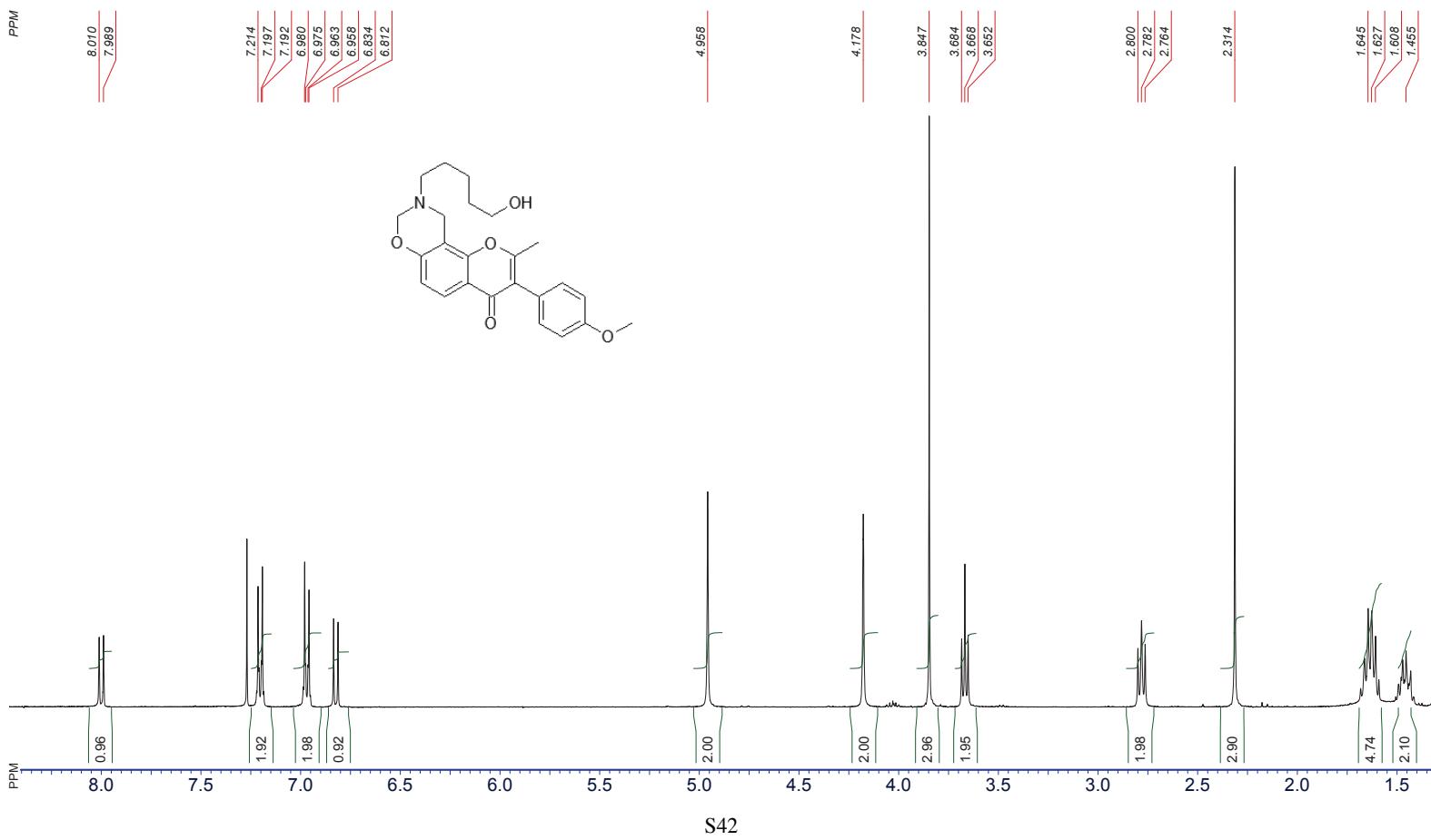
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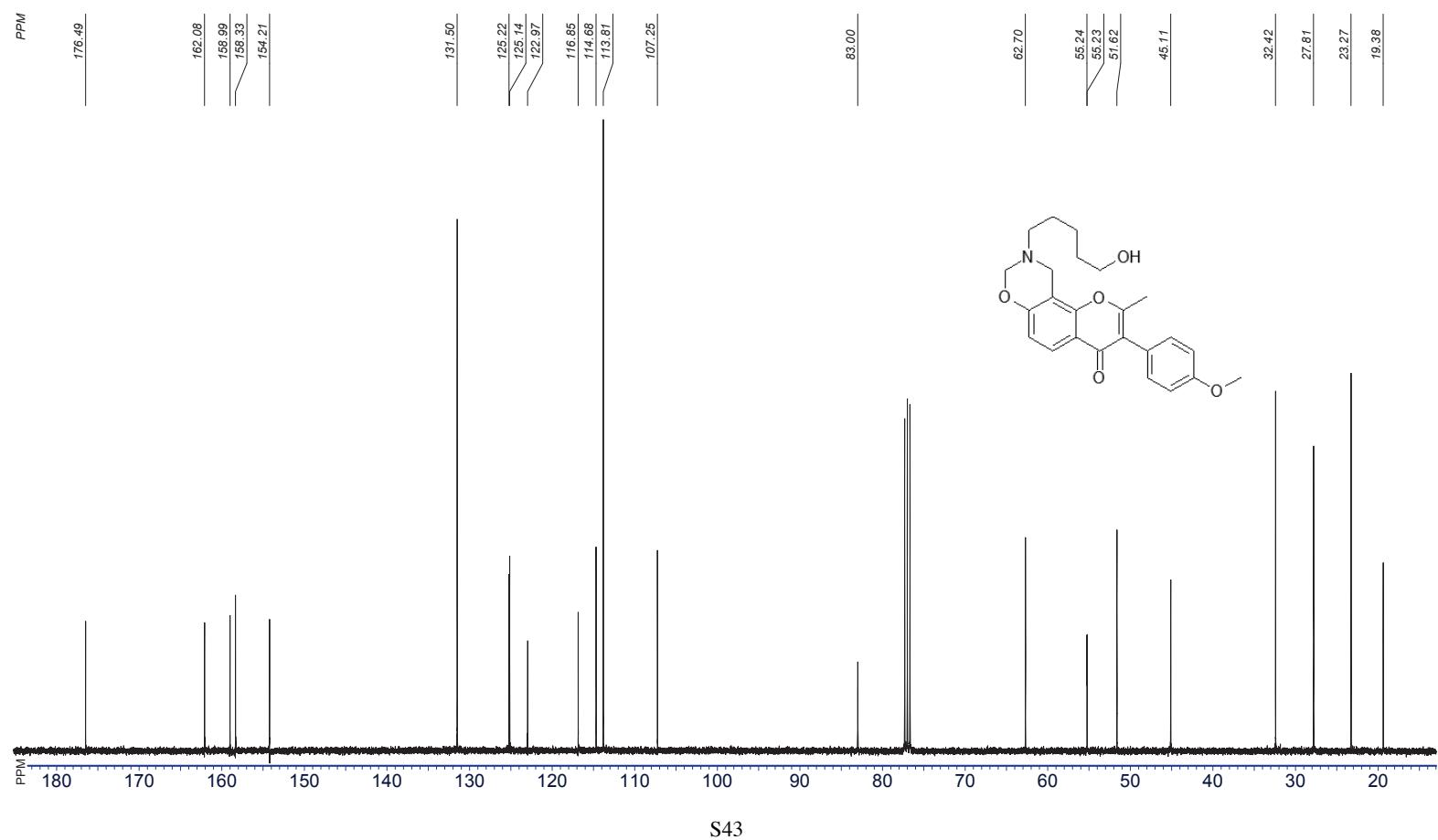
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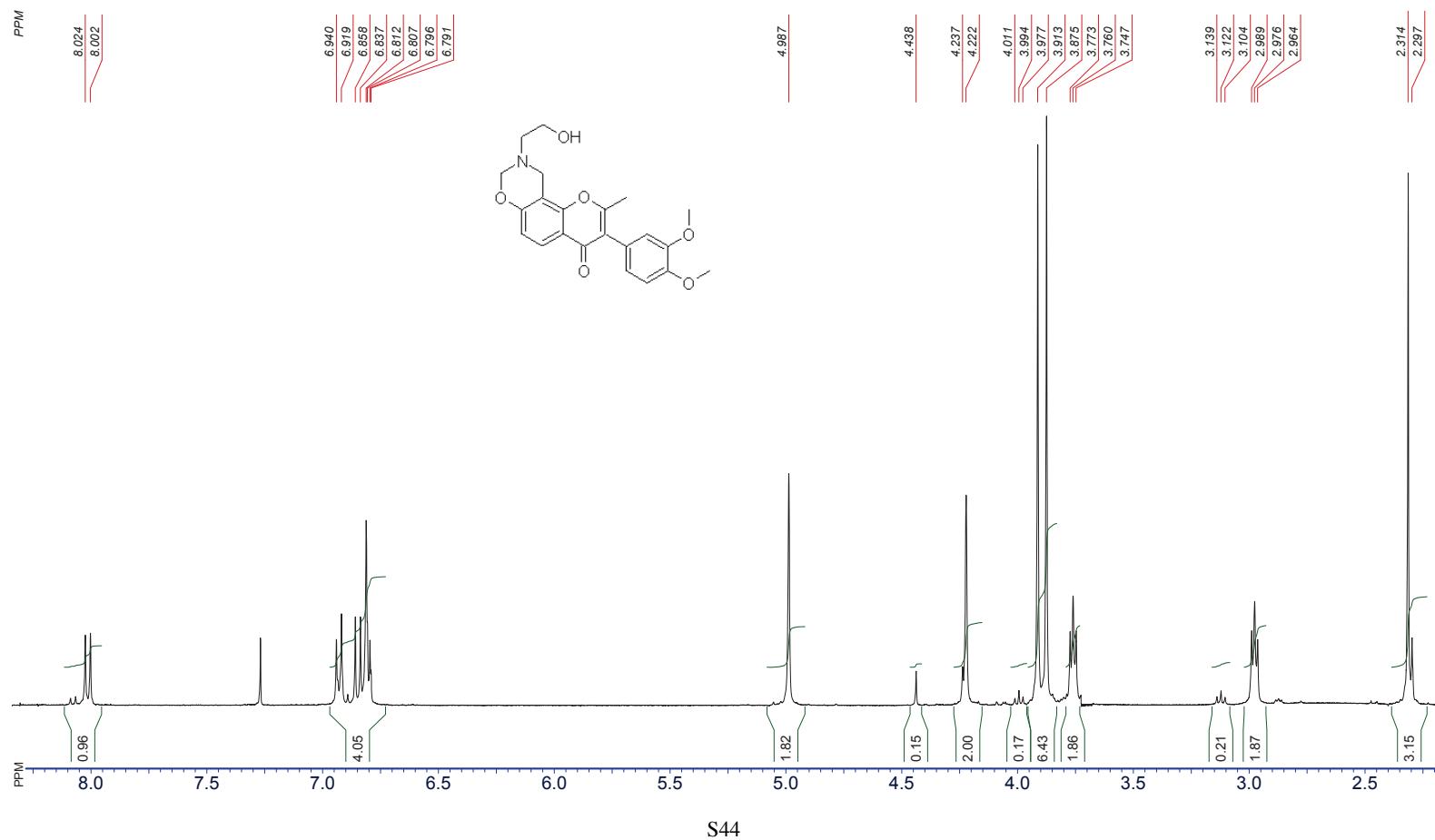
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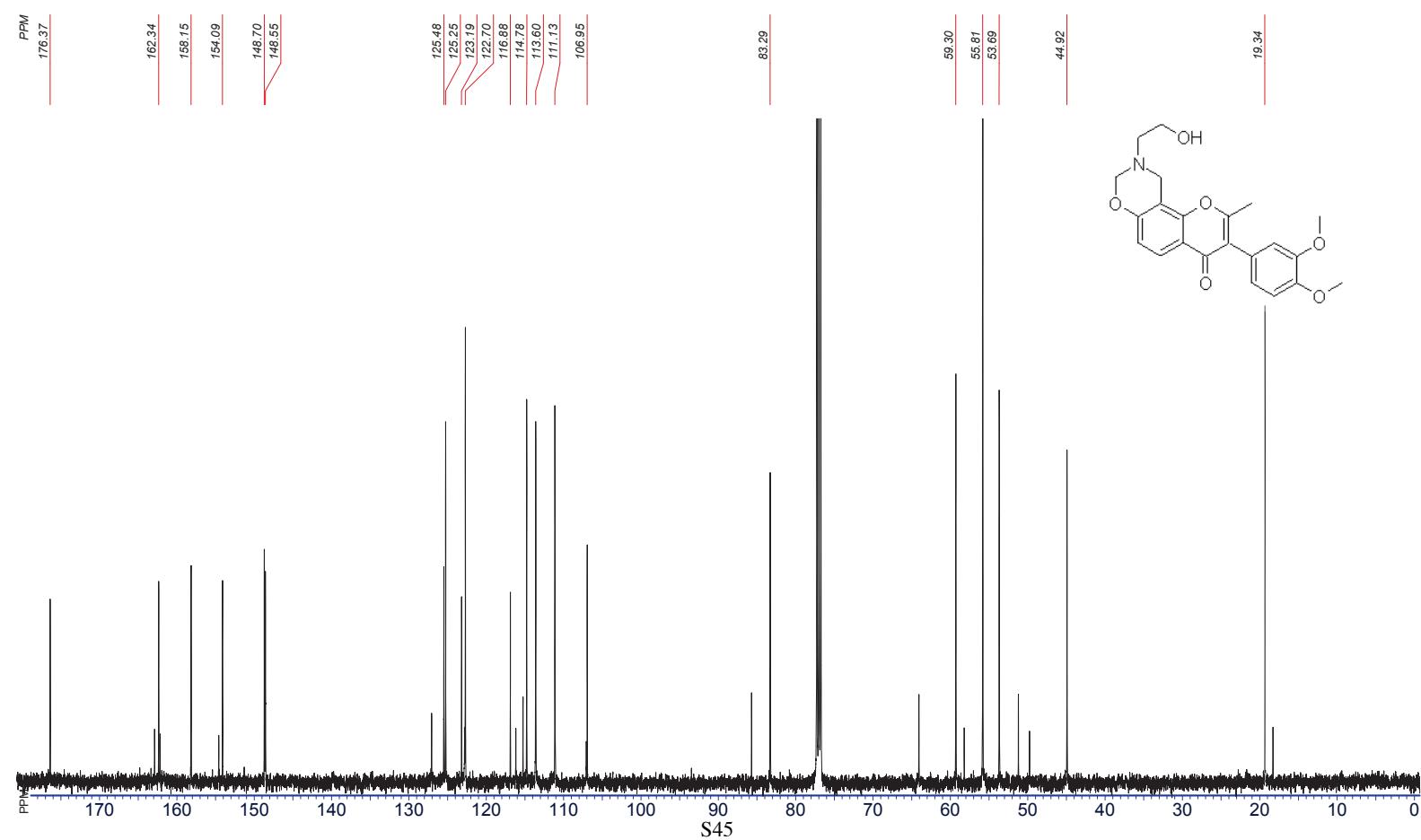
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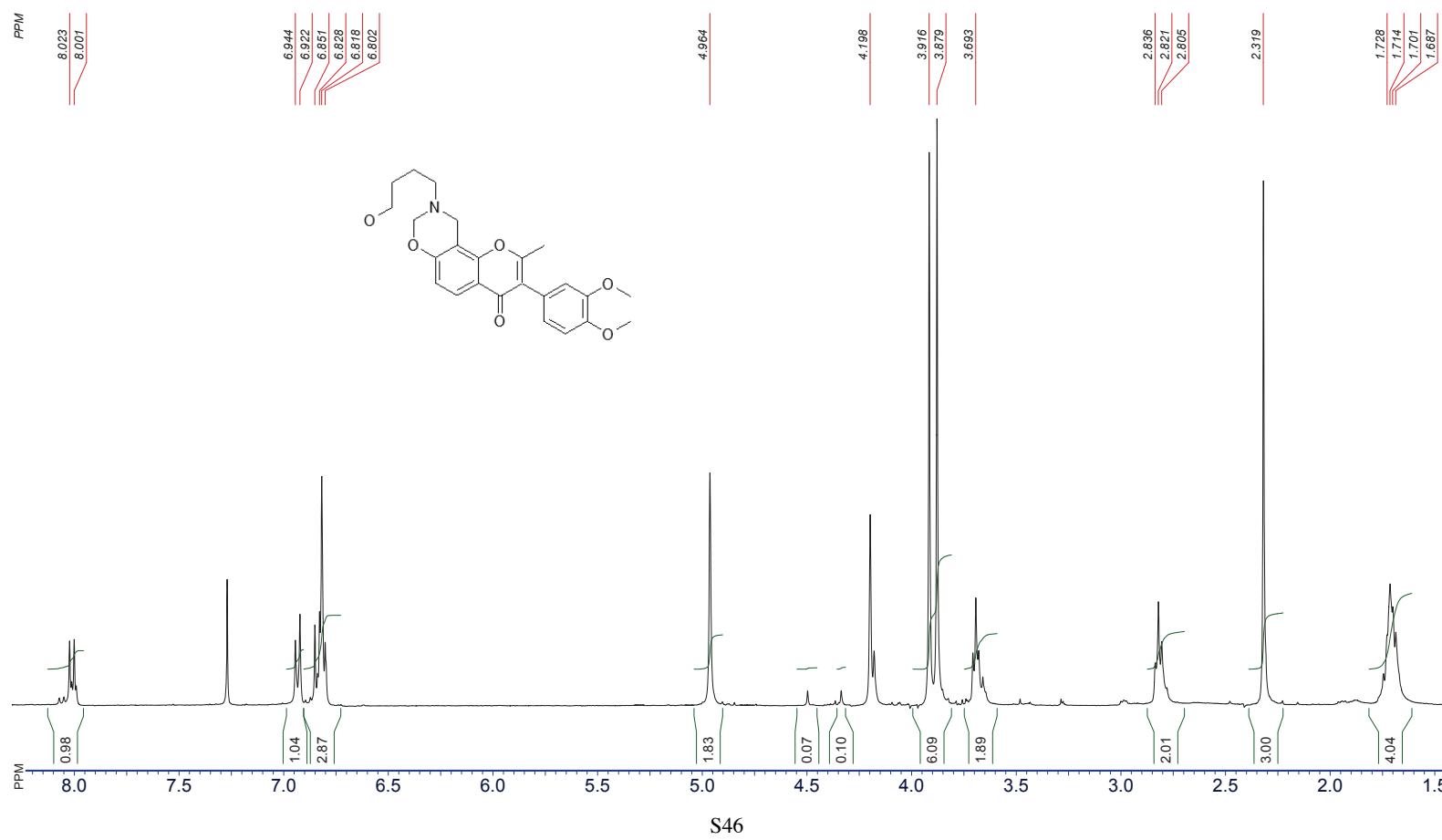
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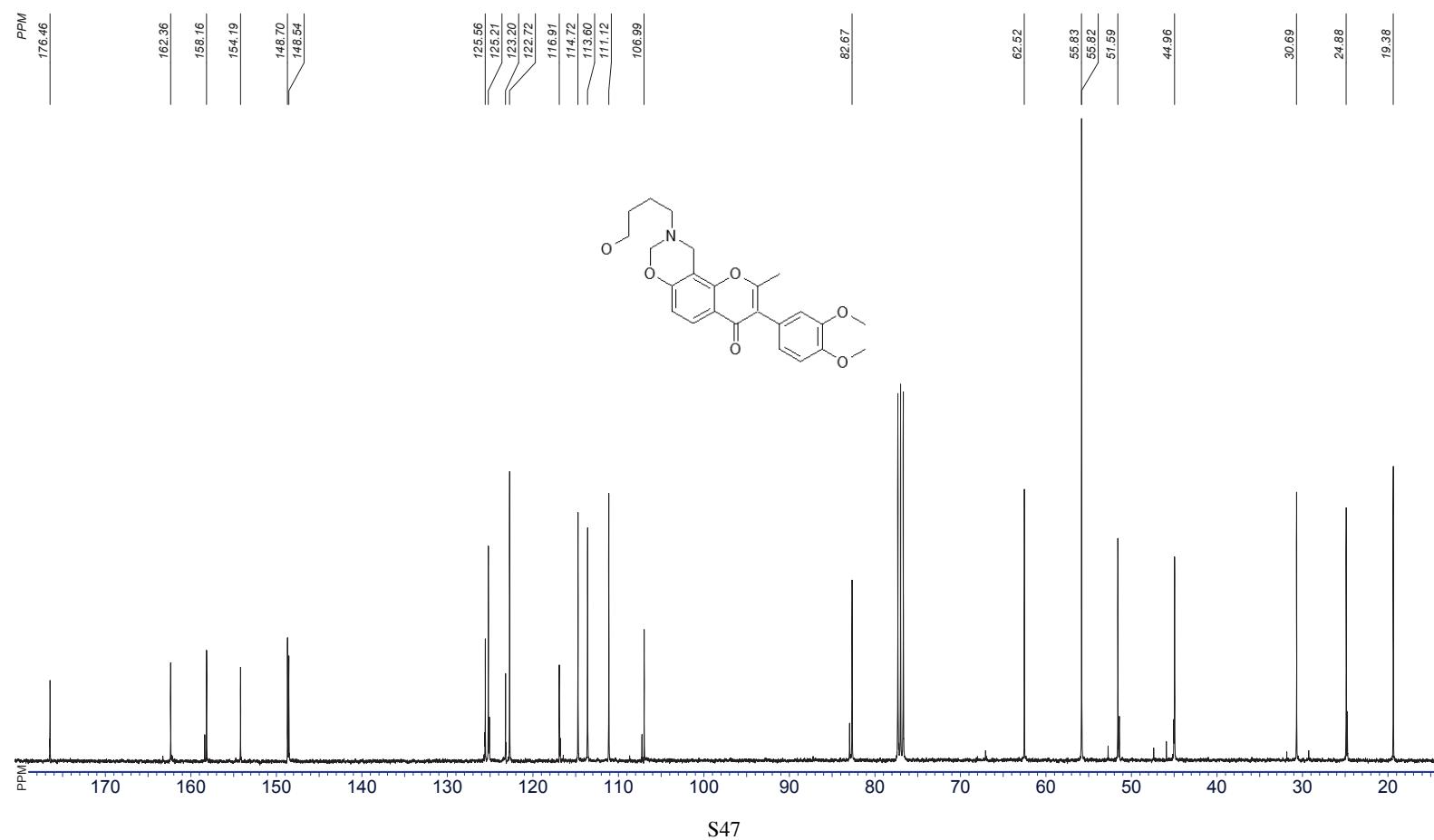
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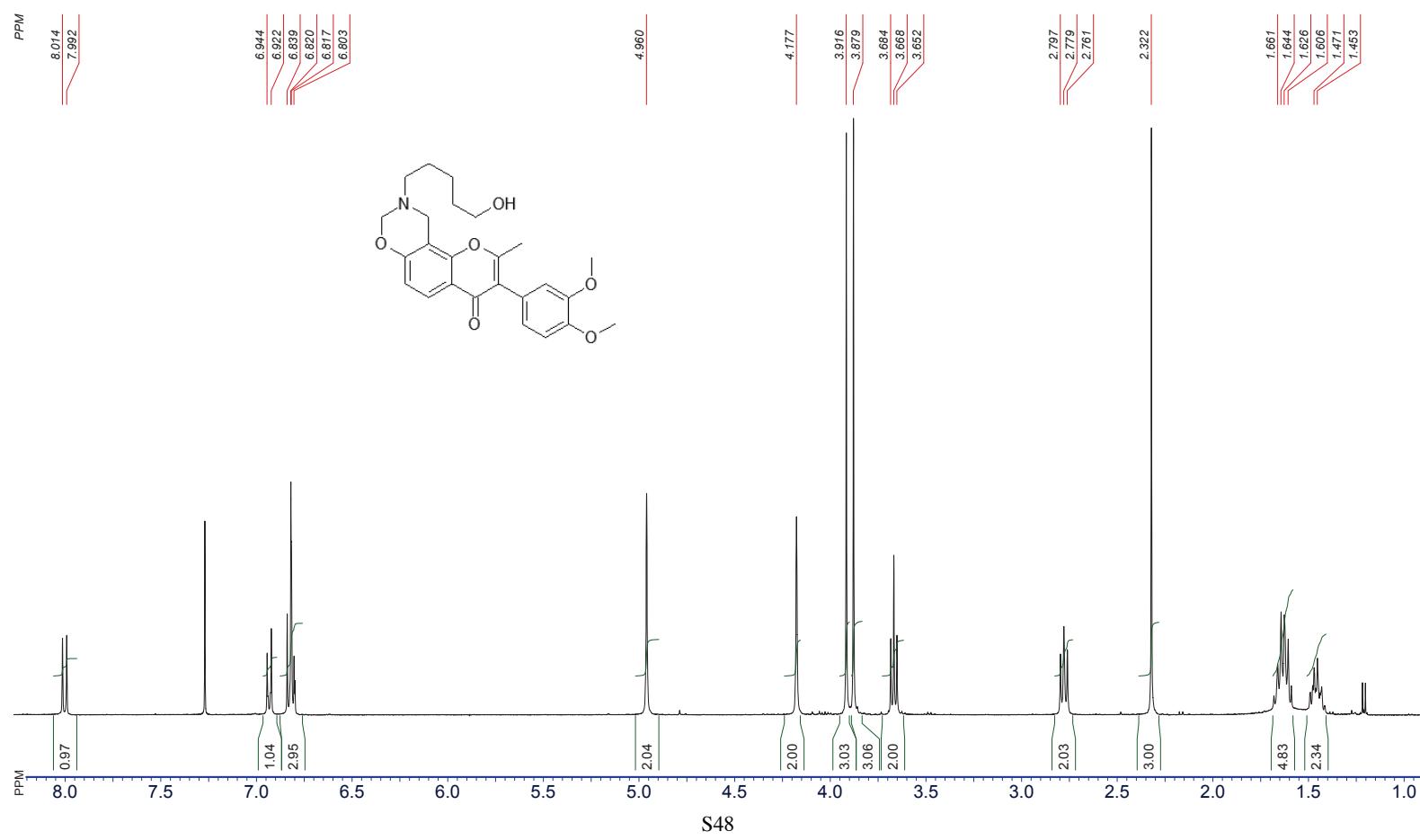
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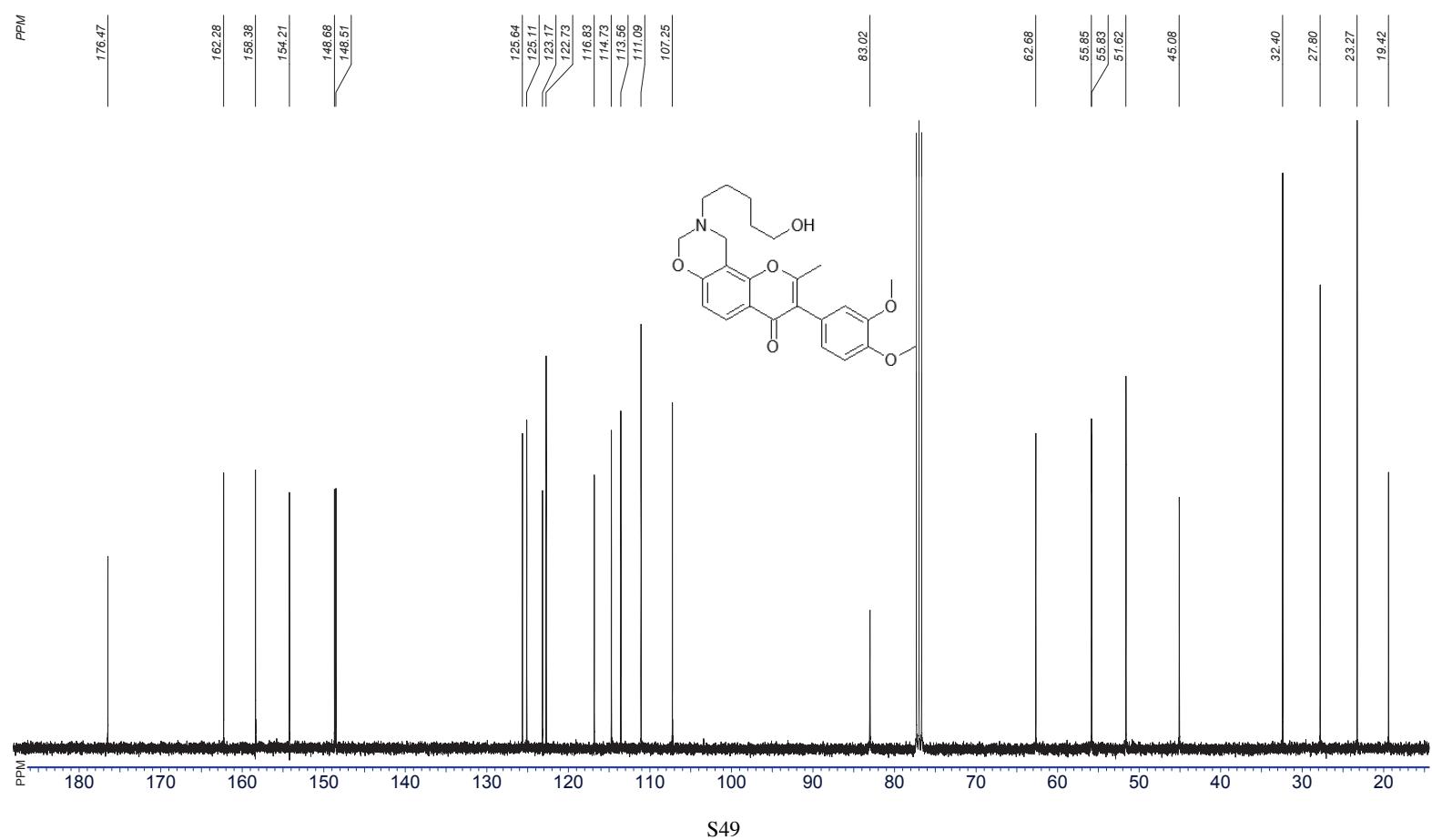
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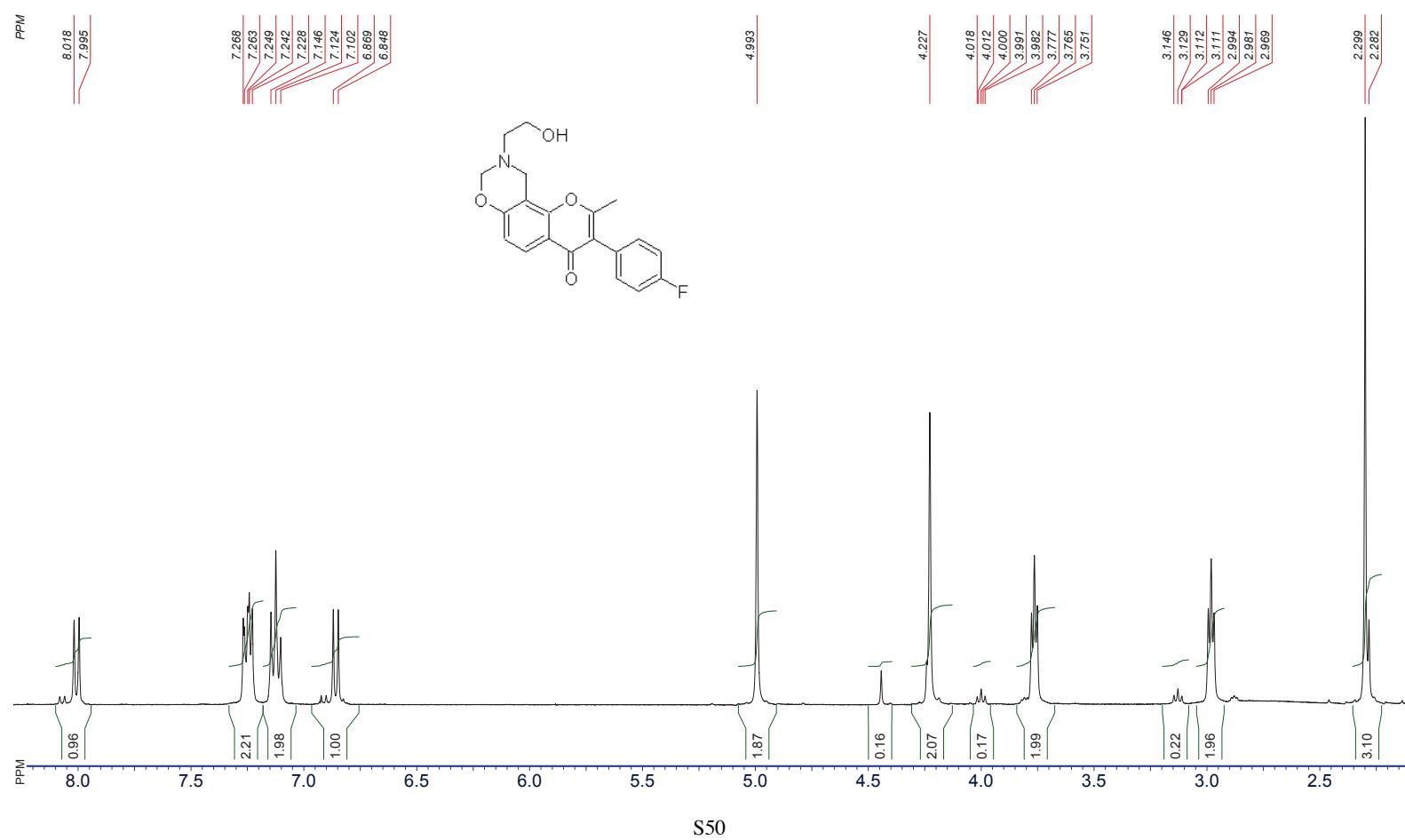
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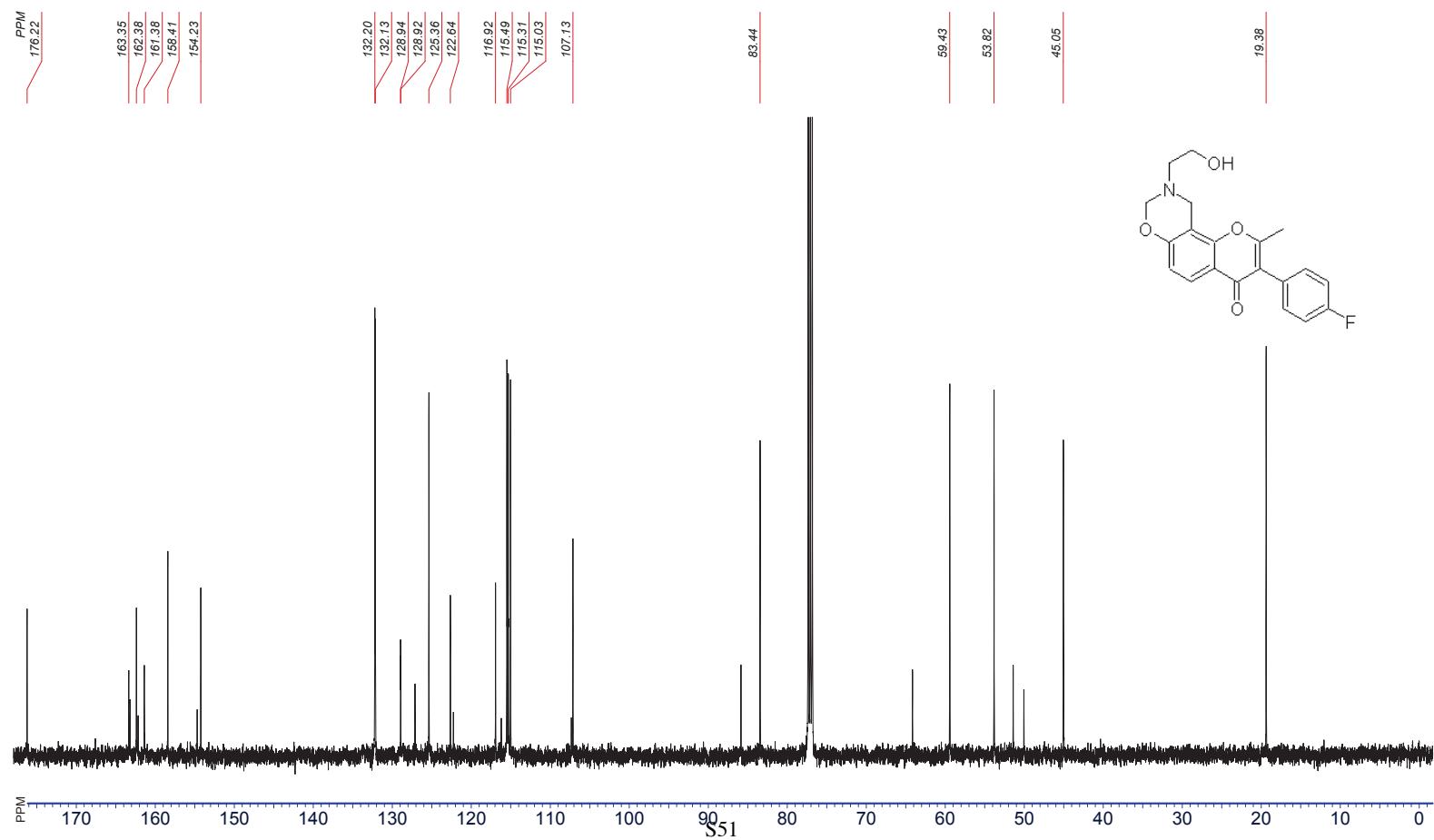
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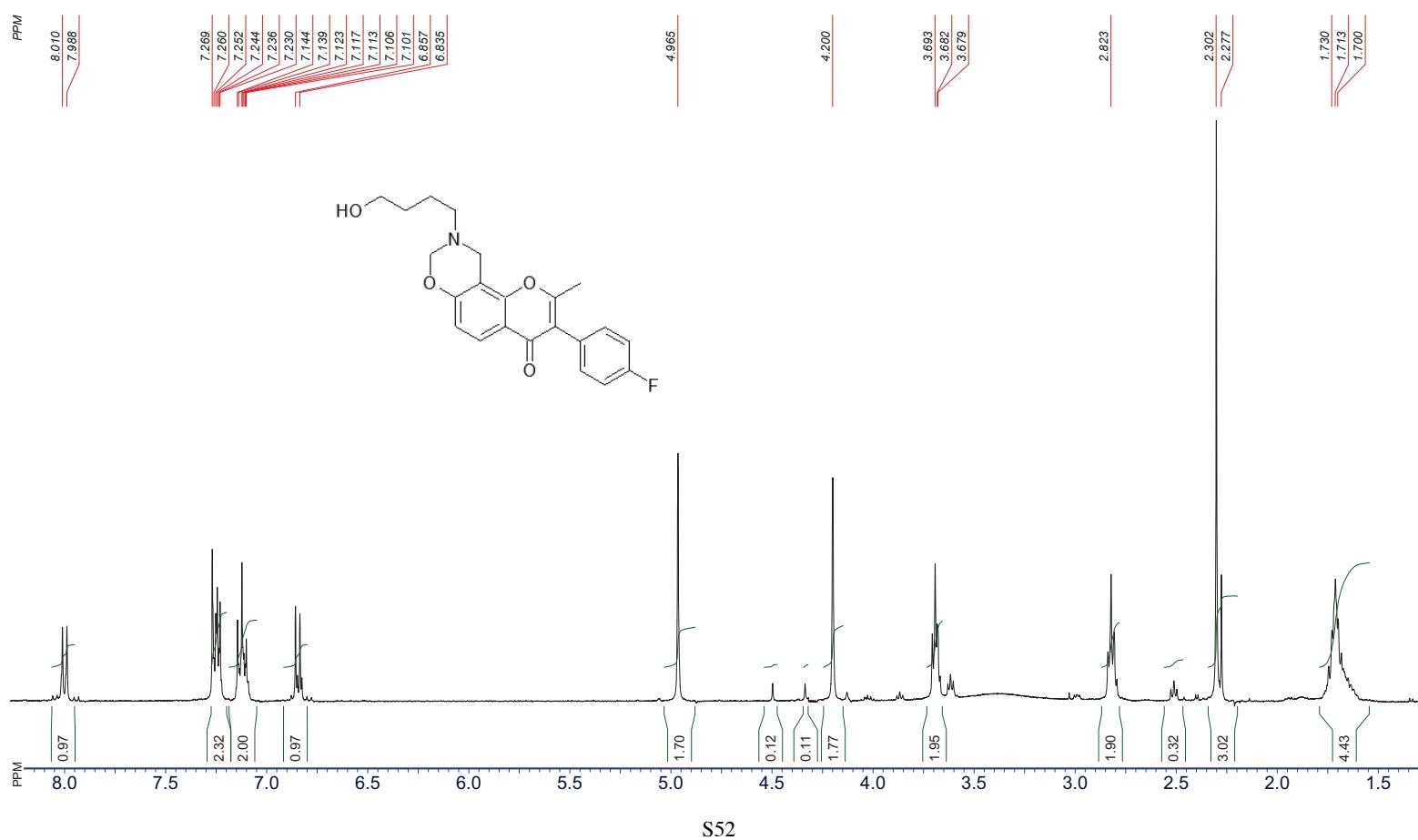
¹H NMR spectrum of 3-(4-fluorophenyl)-9-(2-hydroxyethyl)-2-methyl-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4f, n = 1**) in CDCl₃



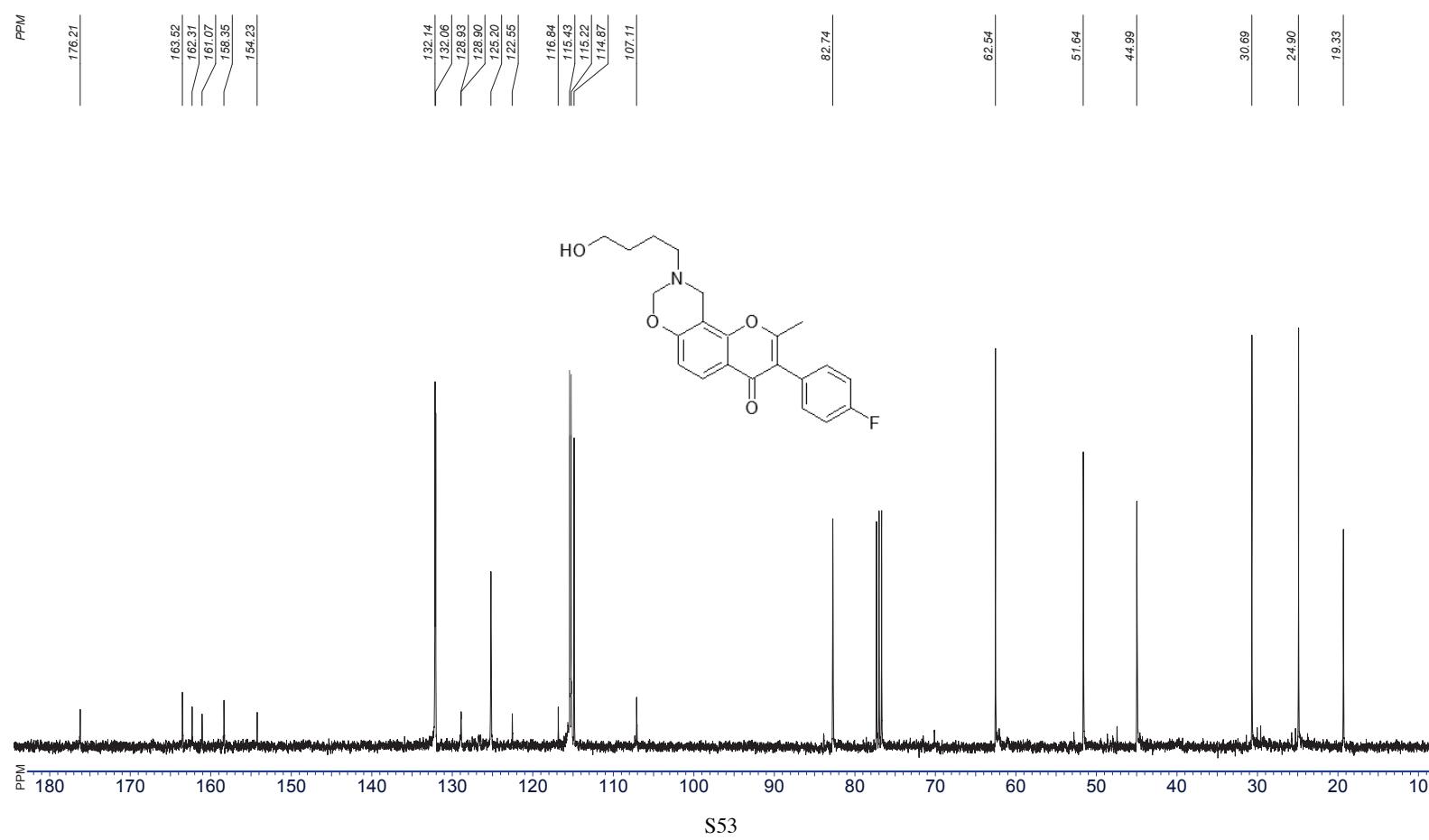
^{13}C NMR spectrum of 3-(4-fluorophenyl)-9-(2-hydroxyethyl)-2-methyl-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4f, n = 1**) in CDCl_3



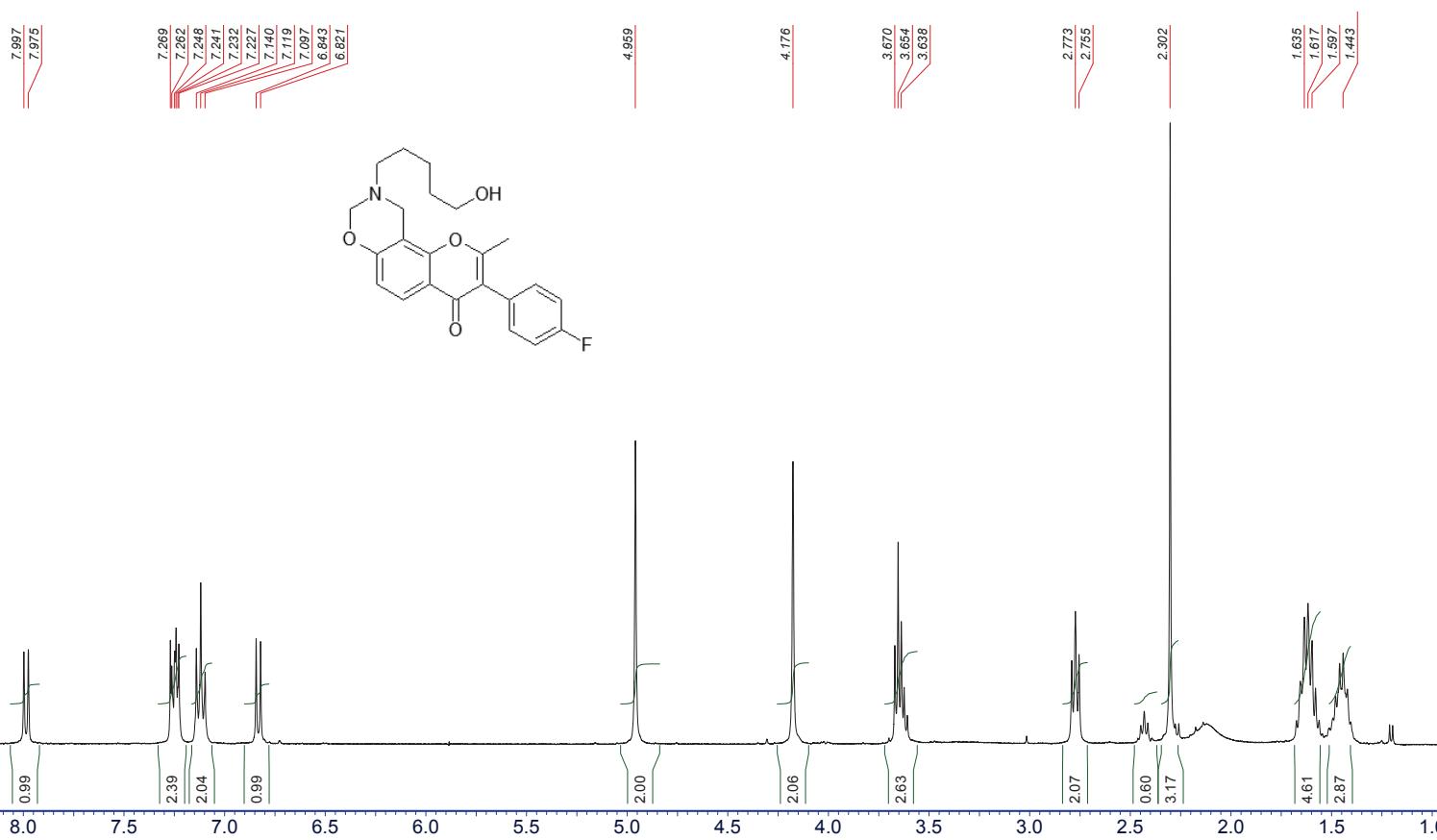
¹H NMR spectrum of 3-(4-fluorophenyl)-9-(4-hydroxybutyl)-2-methyl-9,10-dihydro-4H,8H-chromeno[8,7-e][1,3]oxazin-4-one (**4f, n = 3**) in CDCl₃



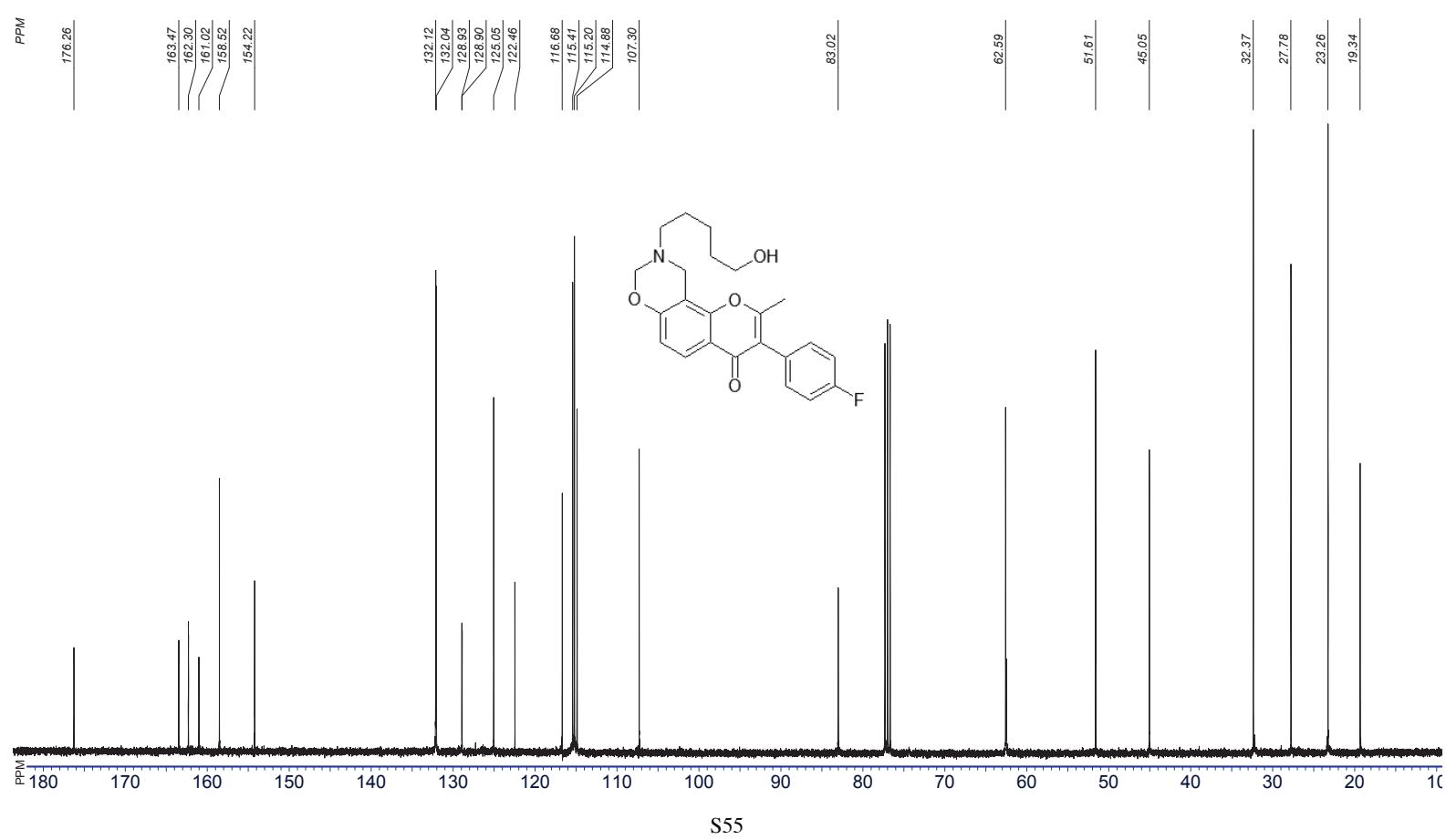
^{13}C NMR spectrum of 3-(4-fluorophenyl)-9-(4-hydroxybutyl)-2-methyl-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4f, n = 3**) in CDCl_3



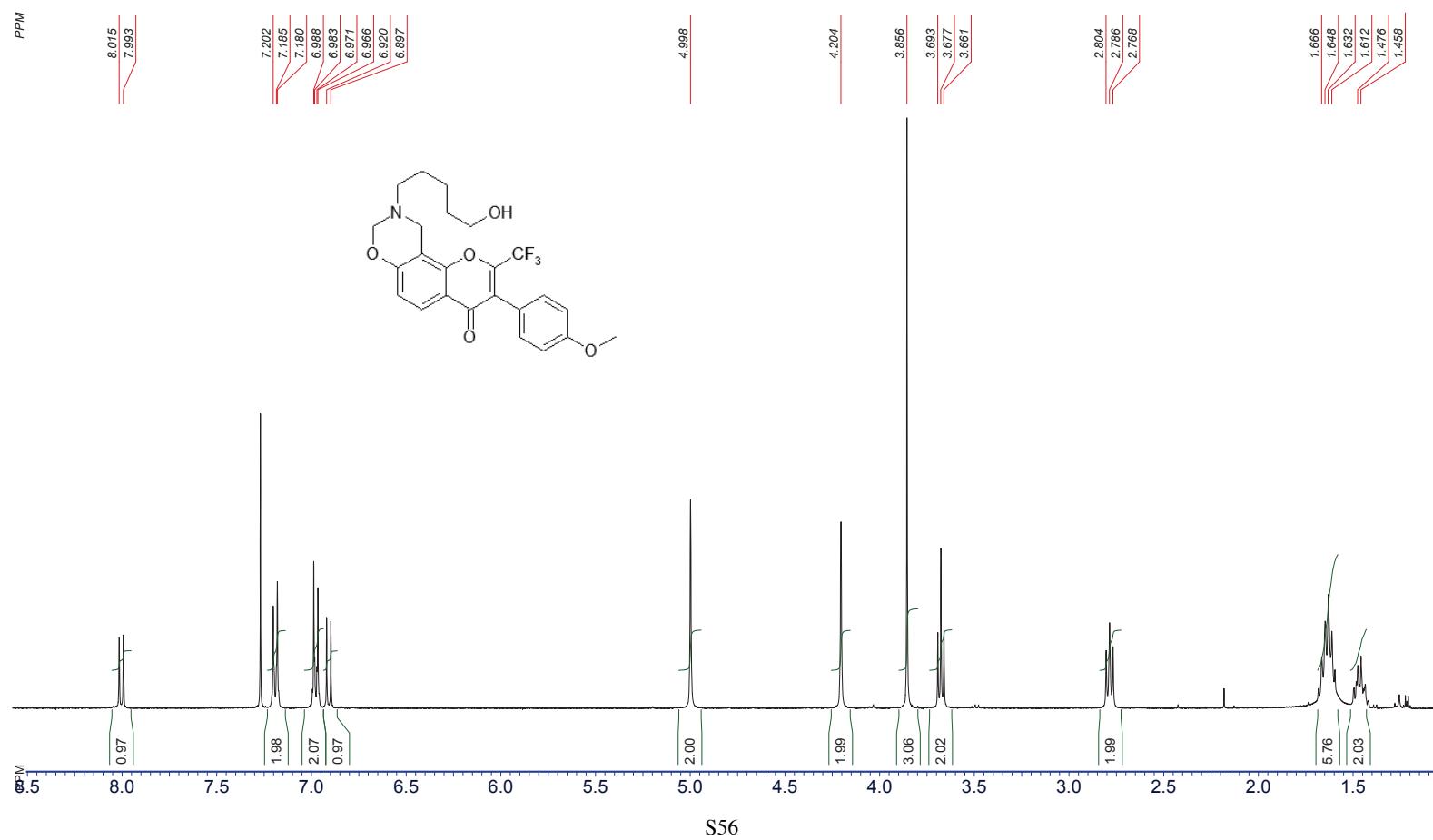
¹H NMR spectrum of 3-(4-fluorophenyl)-9-(5-hydroxypentyl)-2-methyl-9,10-dihydro-4H,8H-chromeno[8,7-*e*][1,3]oxazin-4-one (**4f, n = 4**) in CDCl₃



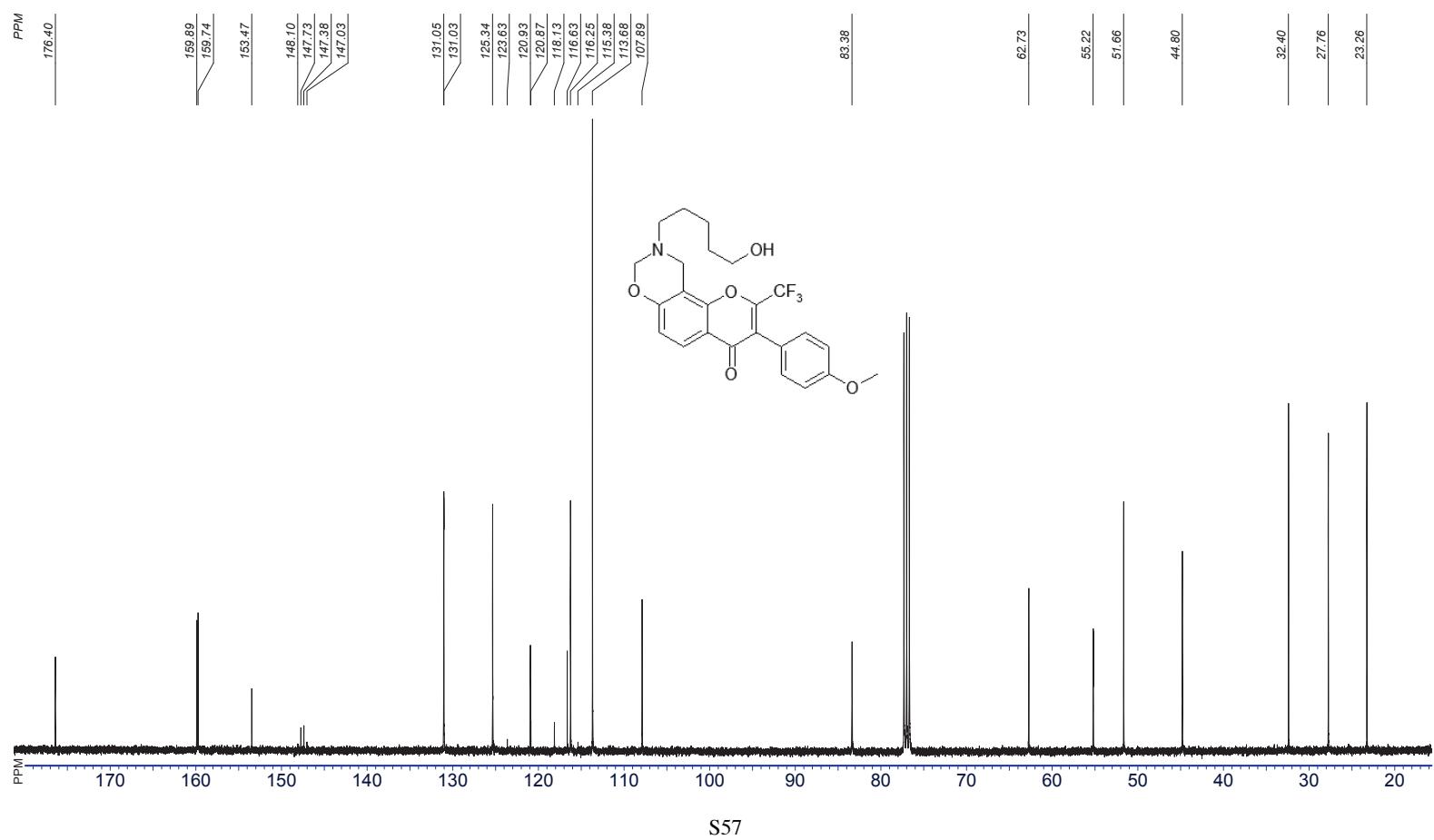
¹³C NMR spectrum of 3-(4-fluorophenyl)-9-(5-hydroxypentyl)-2-methyl-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4f, n = 4**) in CDCl₃



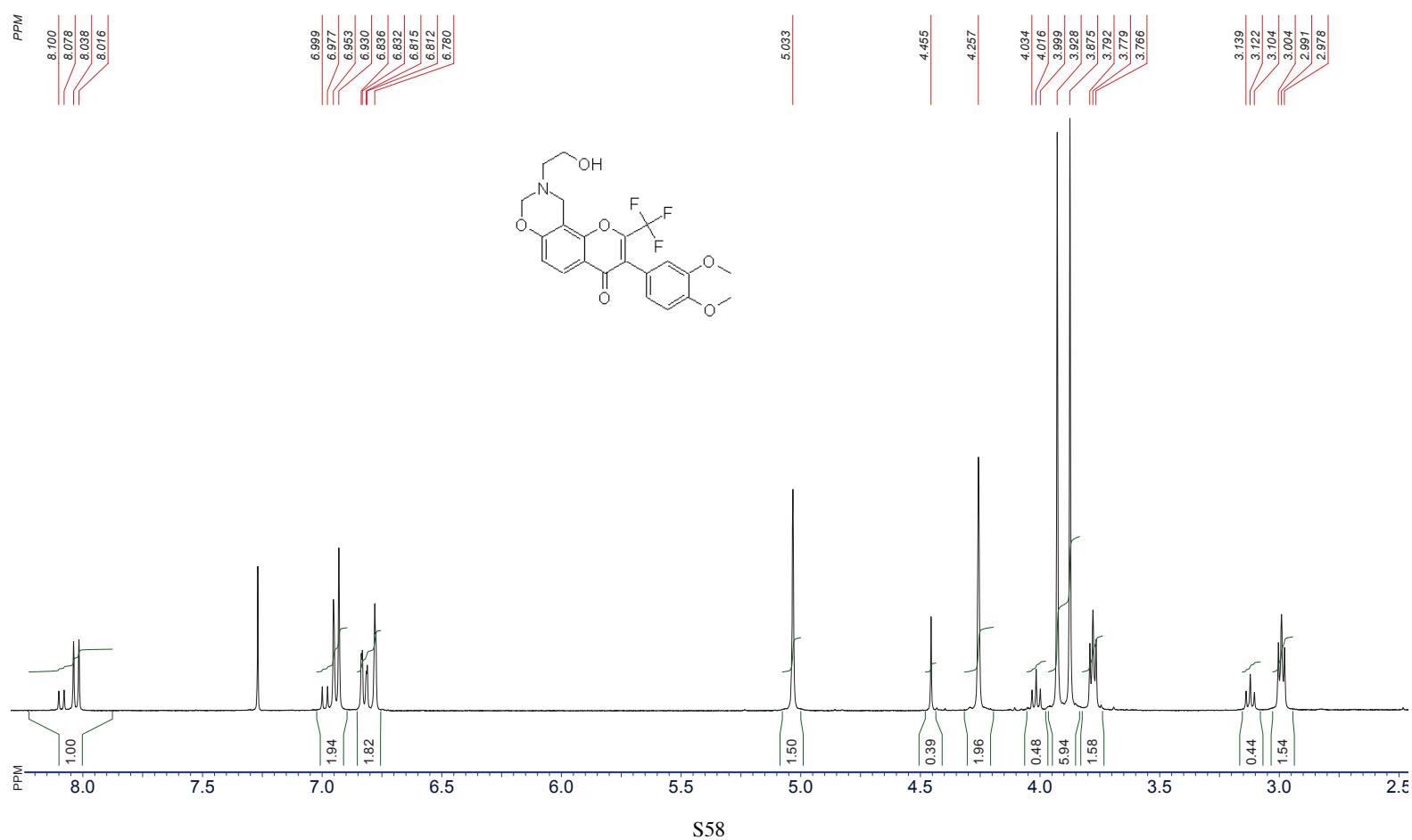
¹H NMR spectrum of 9-(5-hydroxypentyl)-3-(4-methoxyphenyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4g, n = 4**) in CDCl₃



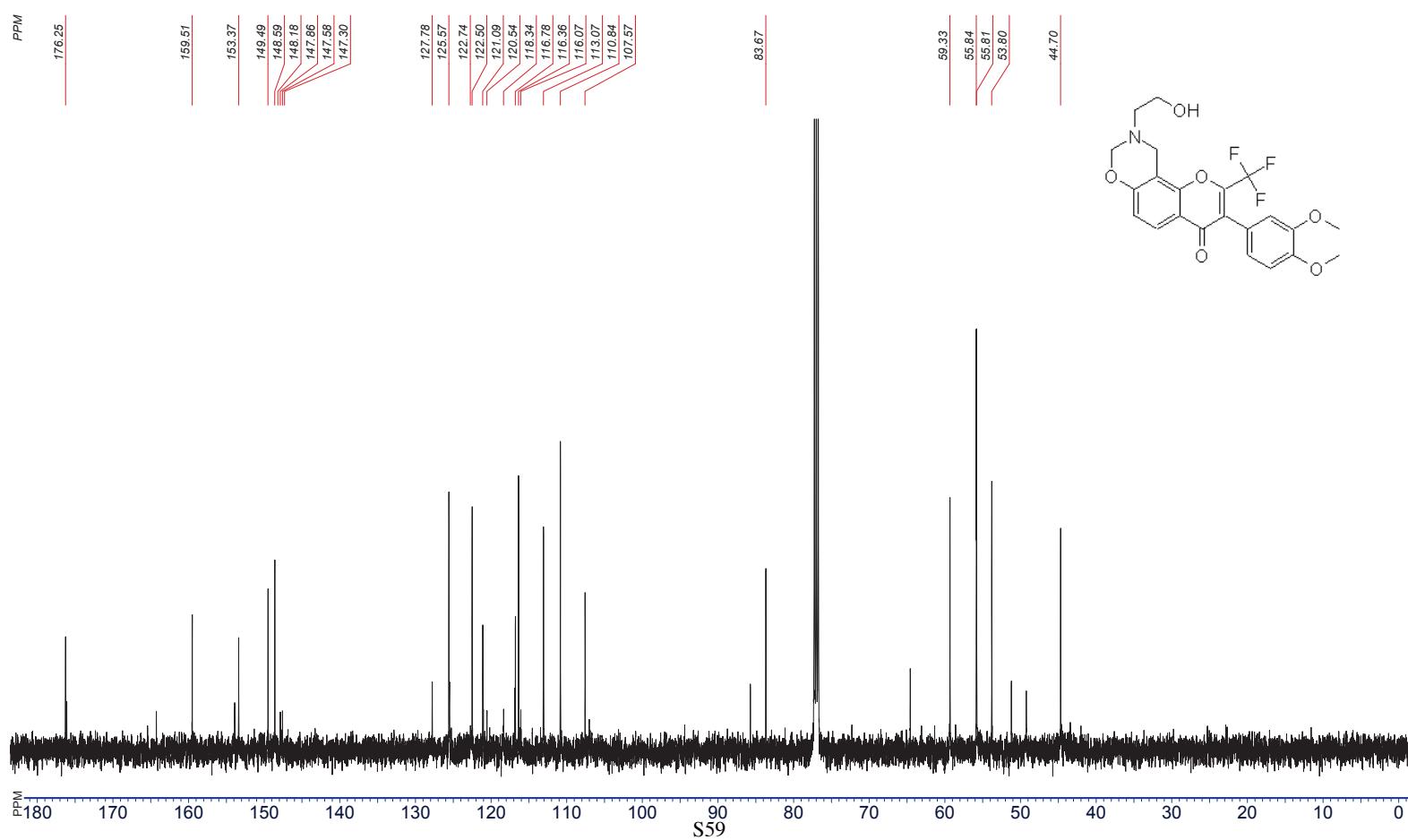
¹³C NMR spectrum of 9-(5-hydroxypentyl)-3-(4-methoxyphenyl)-2-(trifluoromethyl)-9,10-dihydro-4H,8H-chromeno[8,7-*e*][1,3]oxazin-4-one (**4g, n = 4**) in CDCl₃



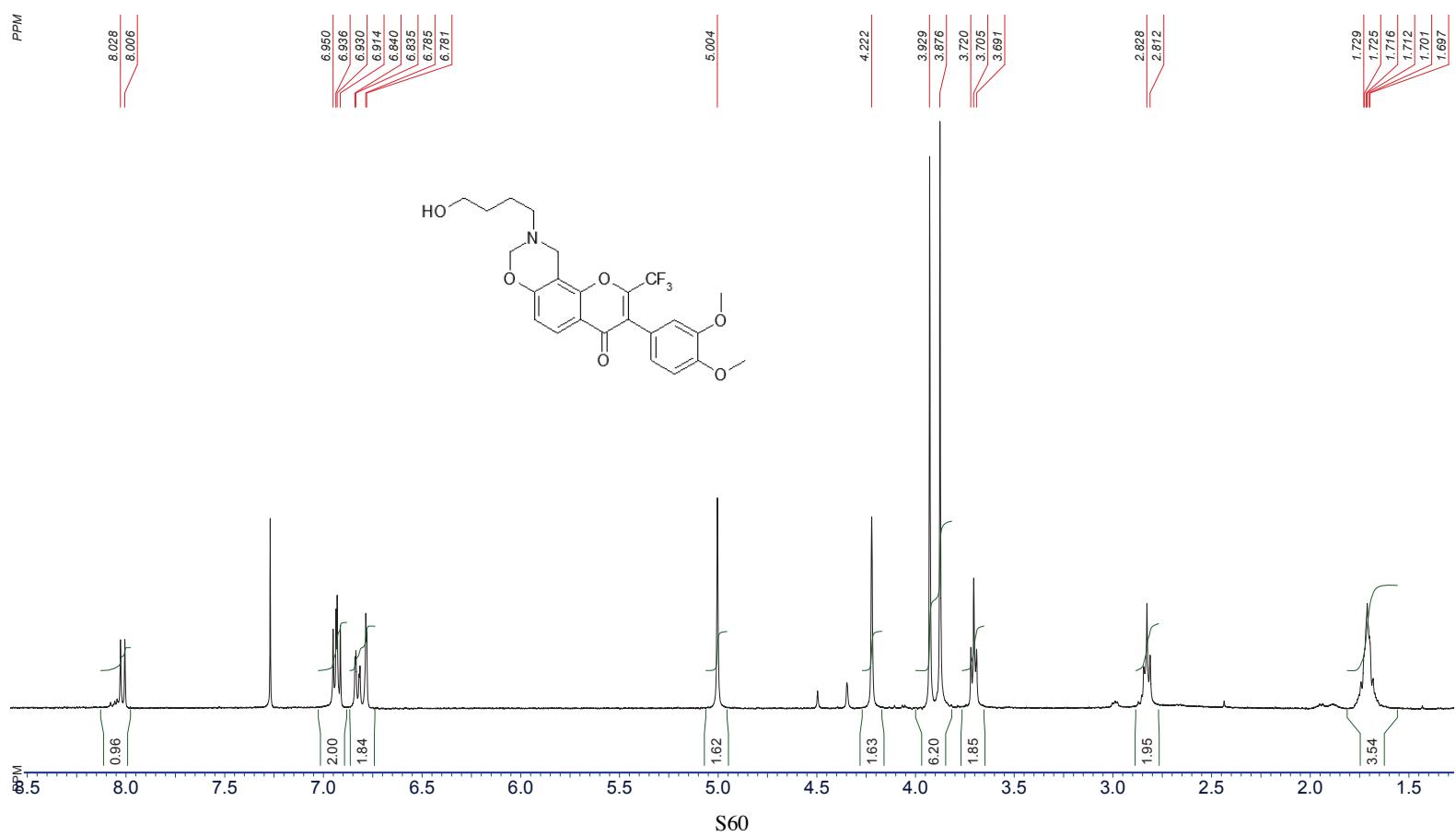
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-9-(2-hydroxyethyl)-2-(trifluoromethyl)-9,10-dihydro-4H,8H-chromeno[8,7-*e*][1,3]oxazin-4-one (**4h, n = 1**) in CDCl₃



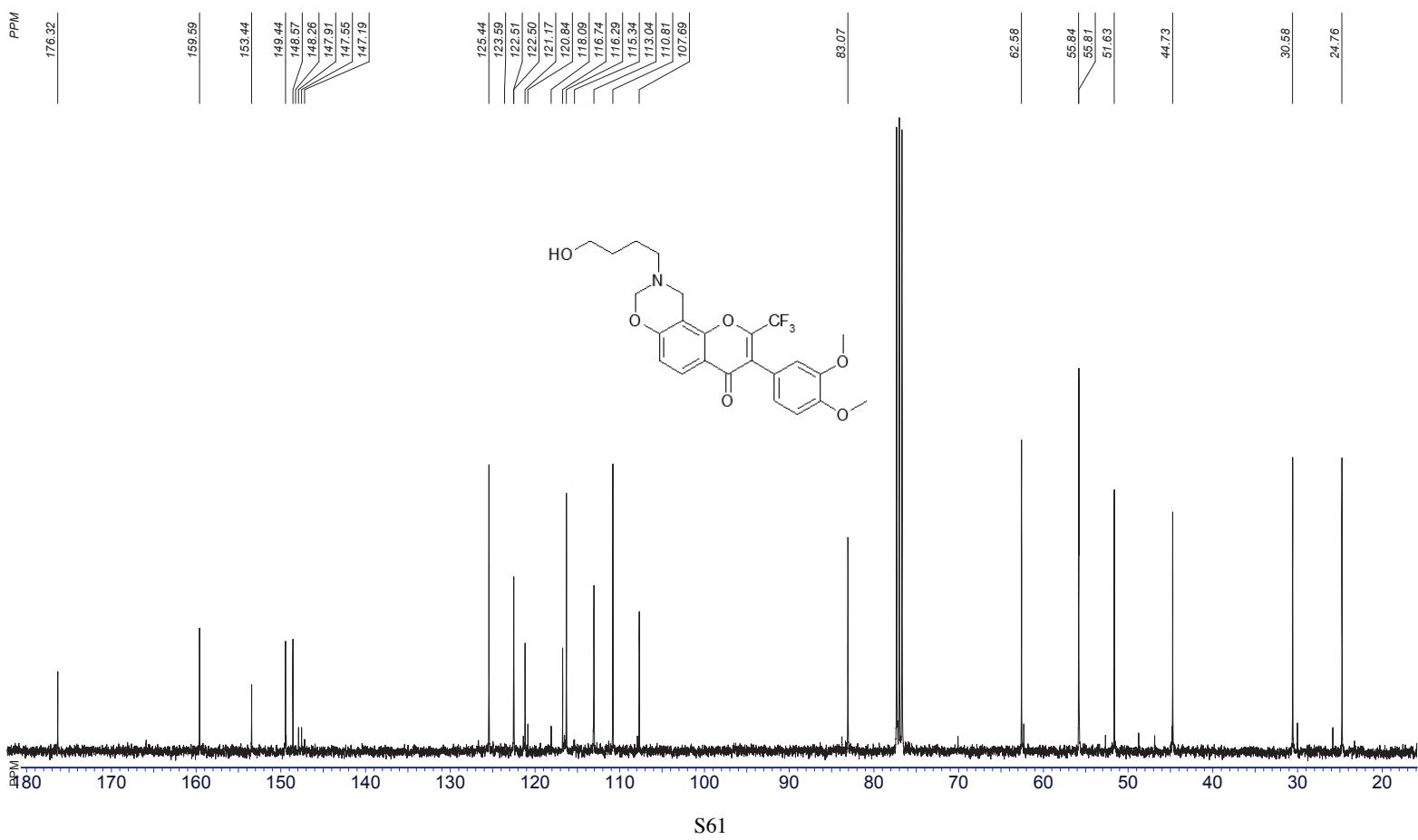
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-9-(2-hydroxyethyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4h, n = 1**) in CDCl₃



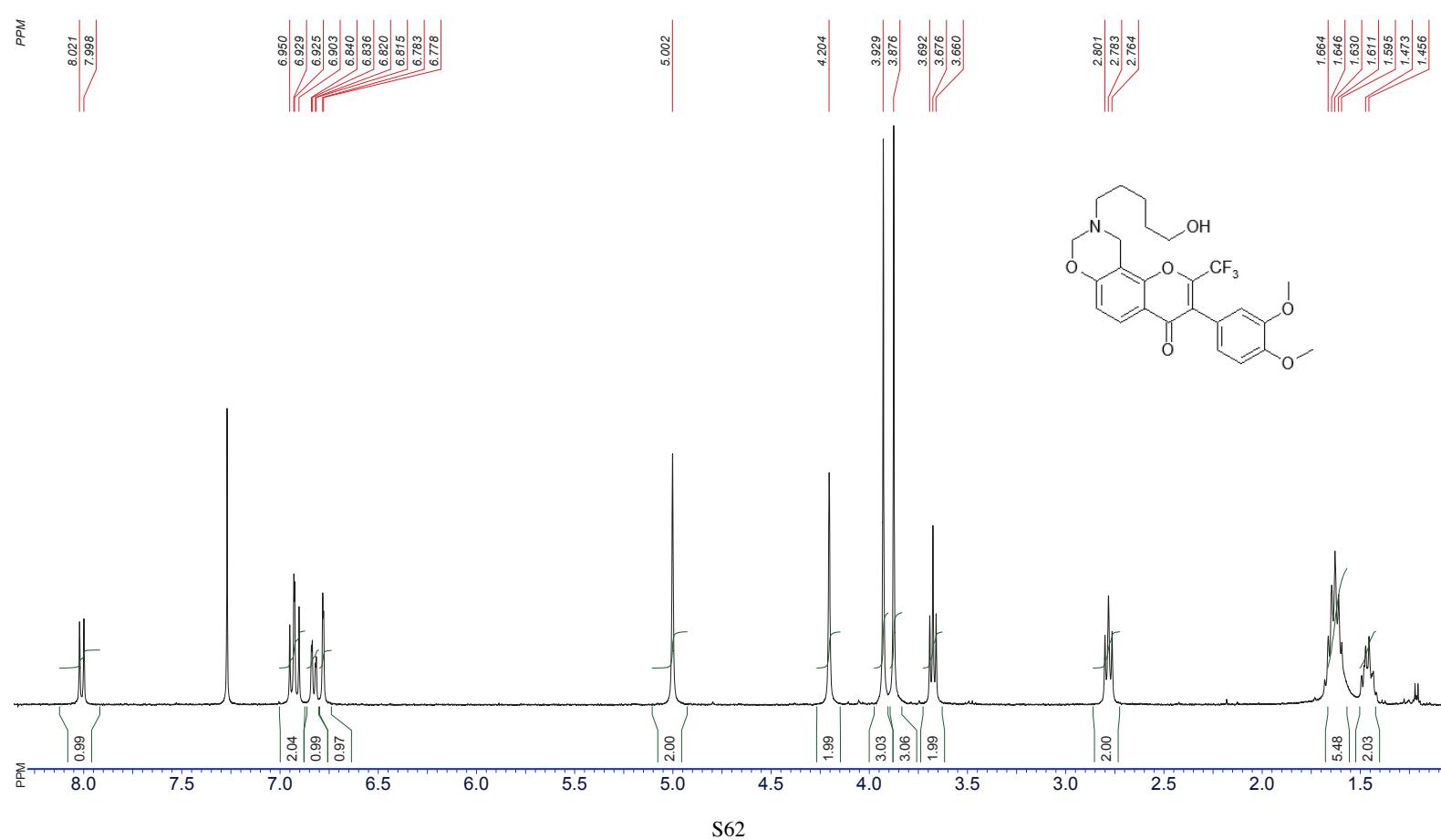
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-9-(4-hydroxybutyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4h, n = 3**) in CDCl₃



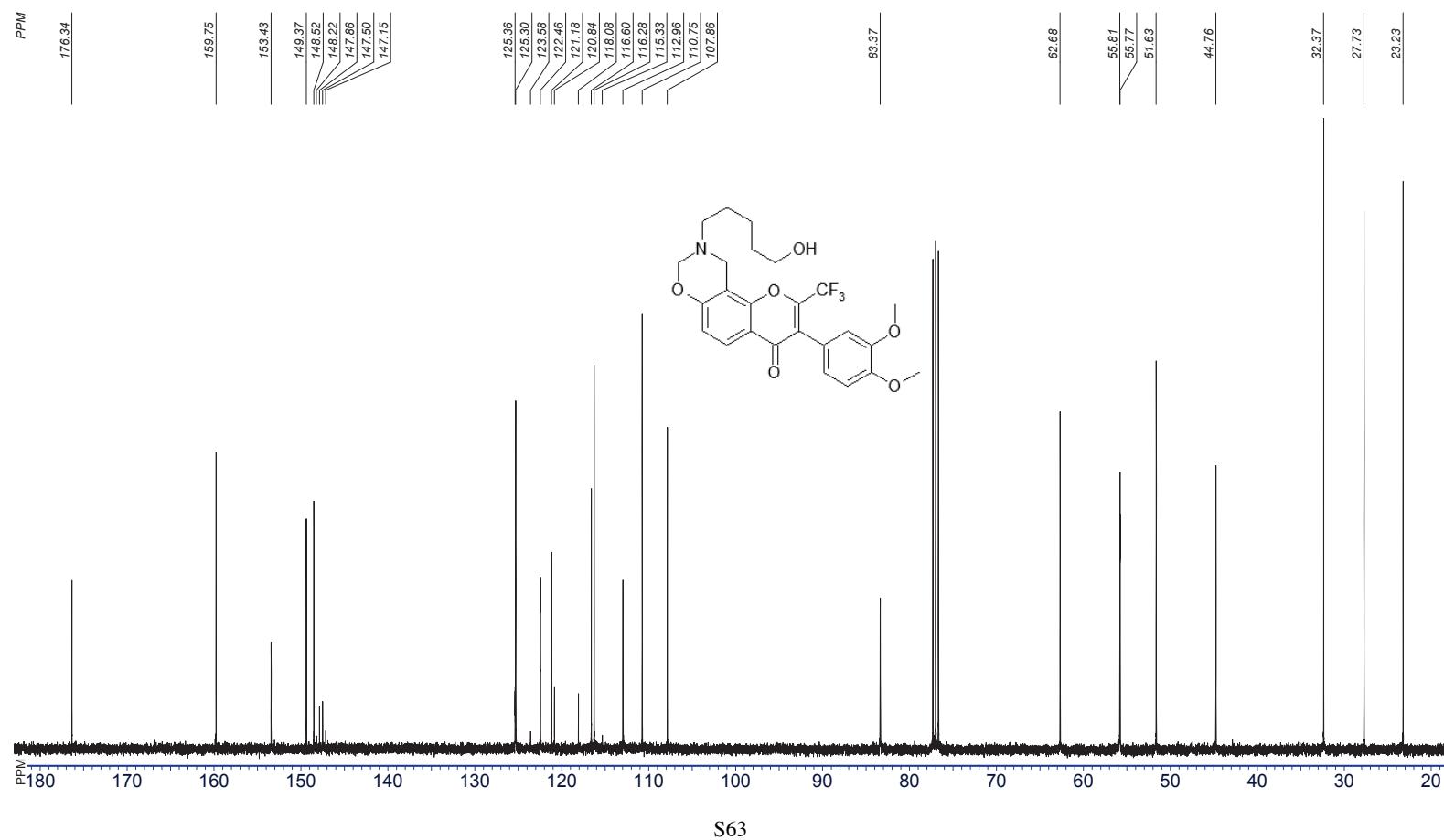
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-9-(4-hydroxybutyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4h, n = 3**) in CDCl₃



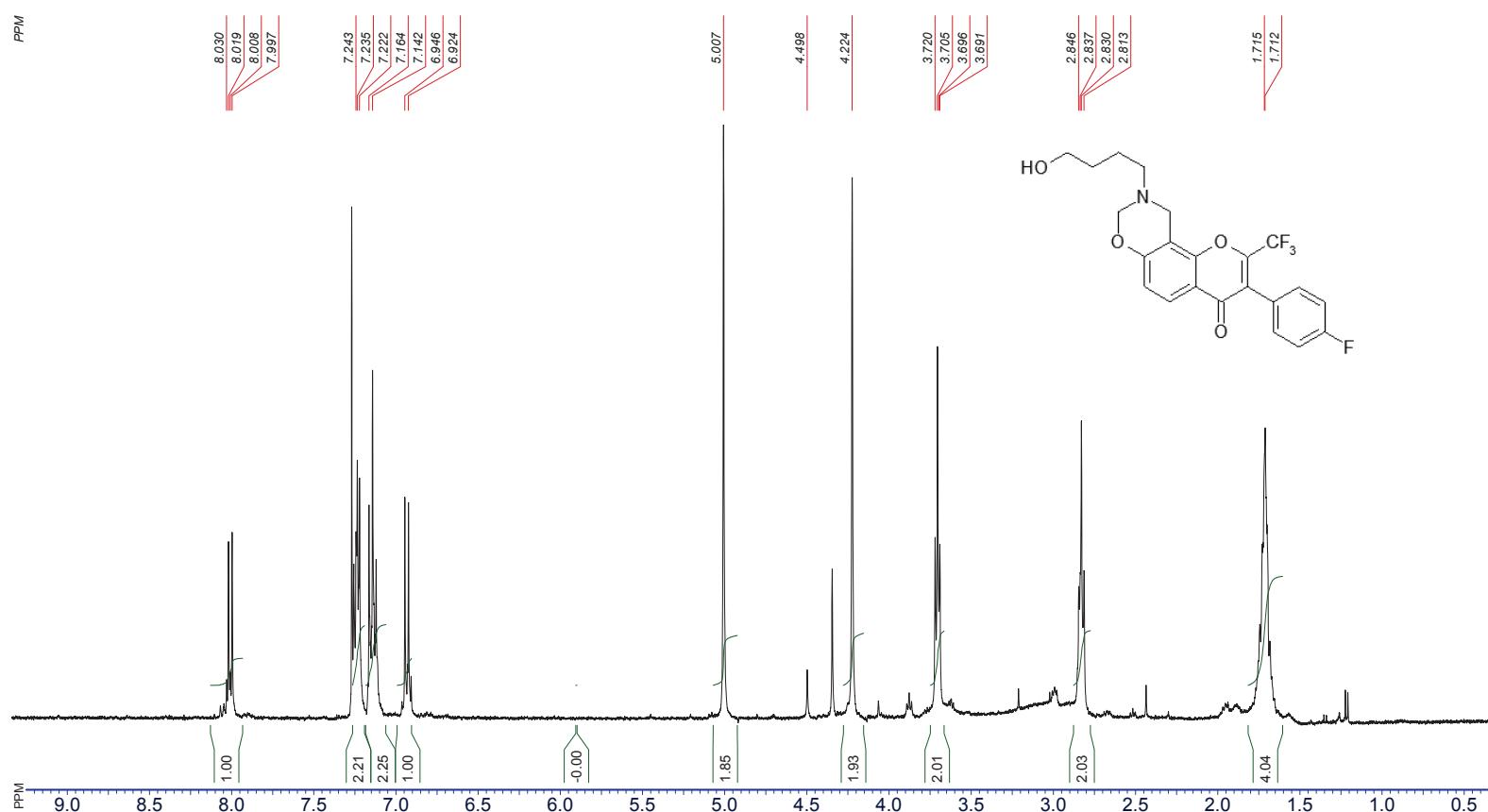
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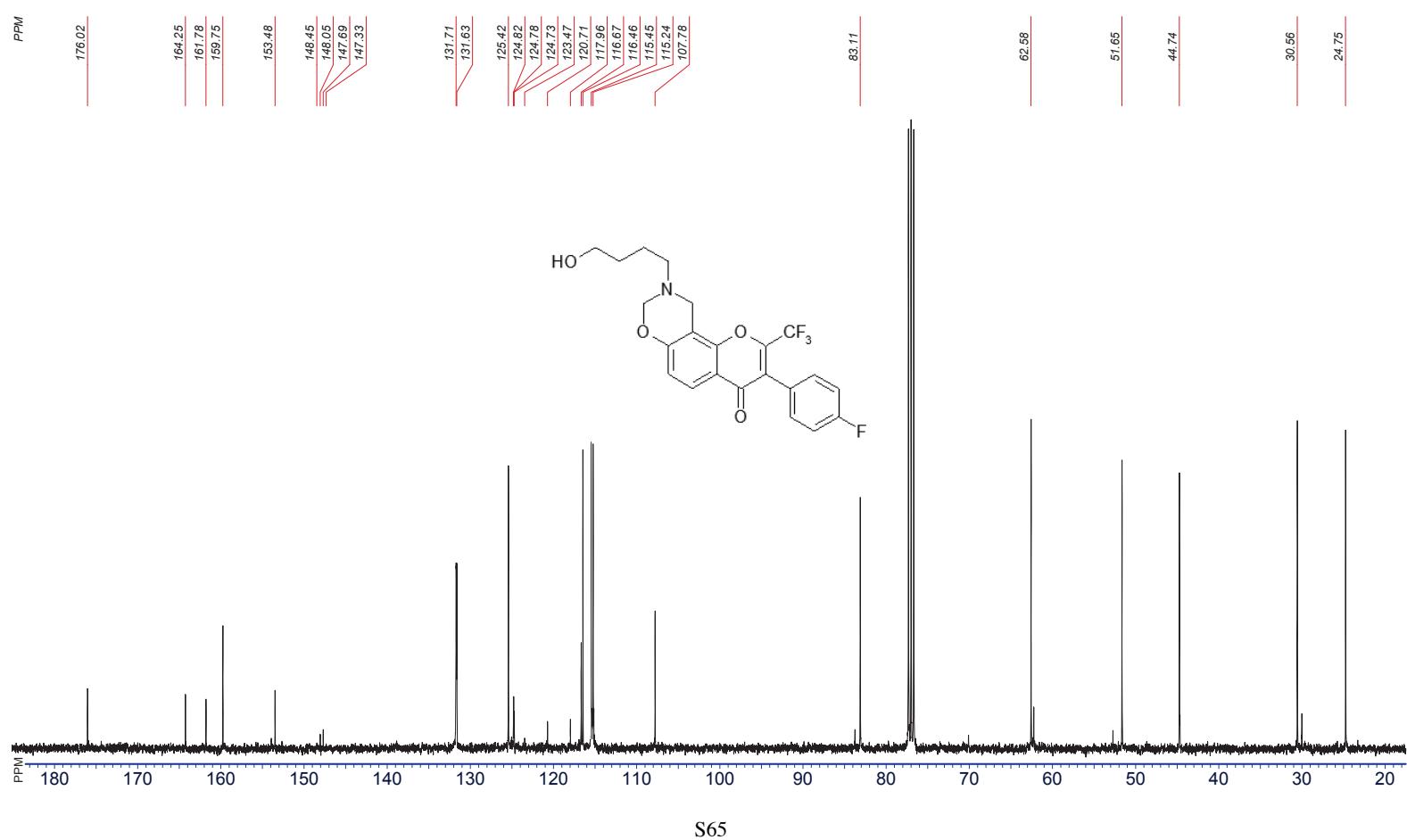
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-9-(5-hydroxypentyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4h, n = 4**) in CDCl₃



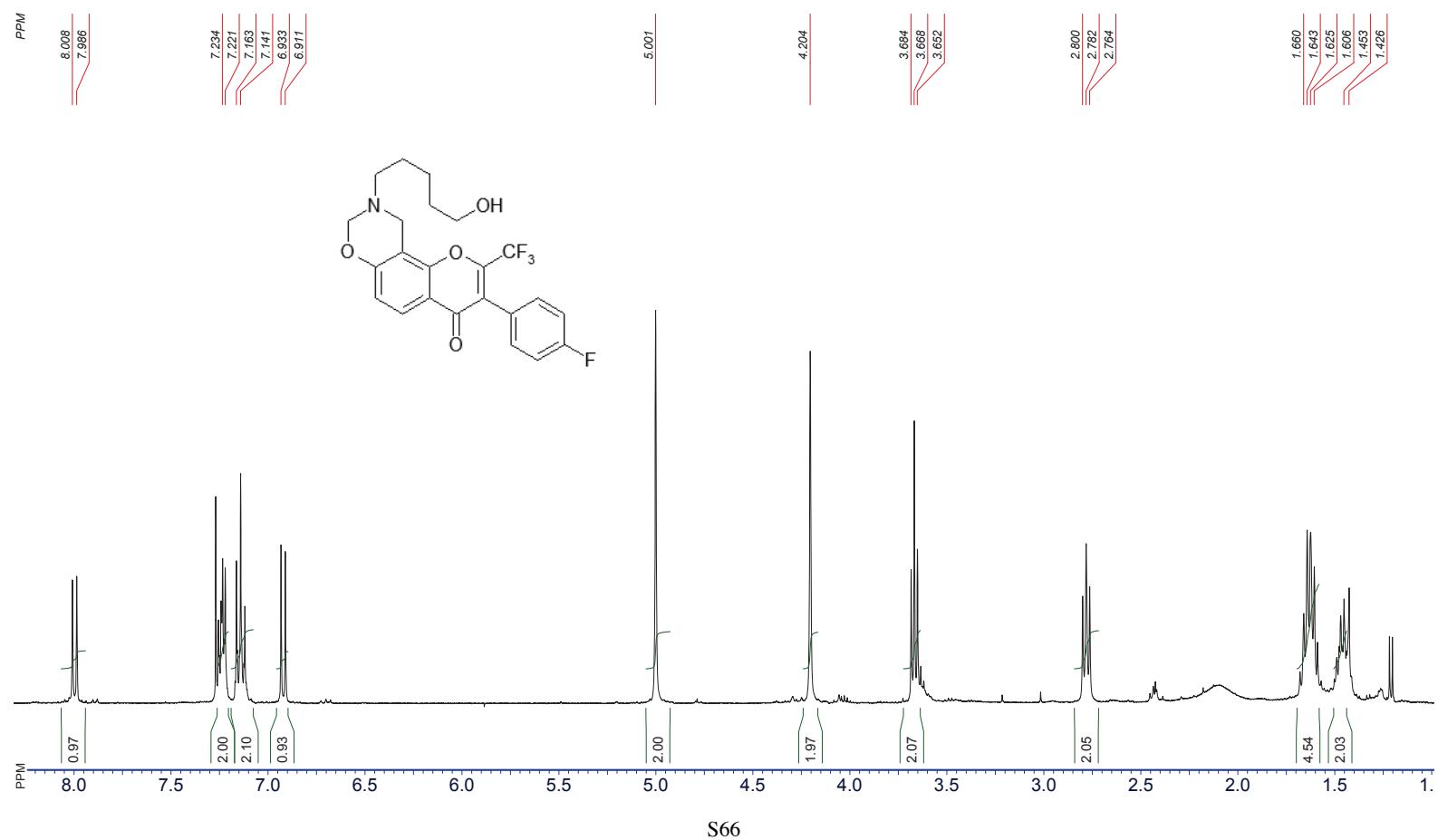
¹H NMR spectrum of 3-(4-fluorophenyl)-9-(4-hydroxybutyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4i, n = 3**) in CDCl₃



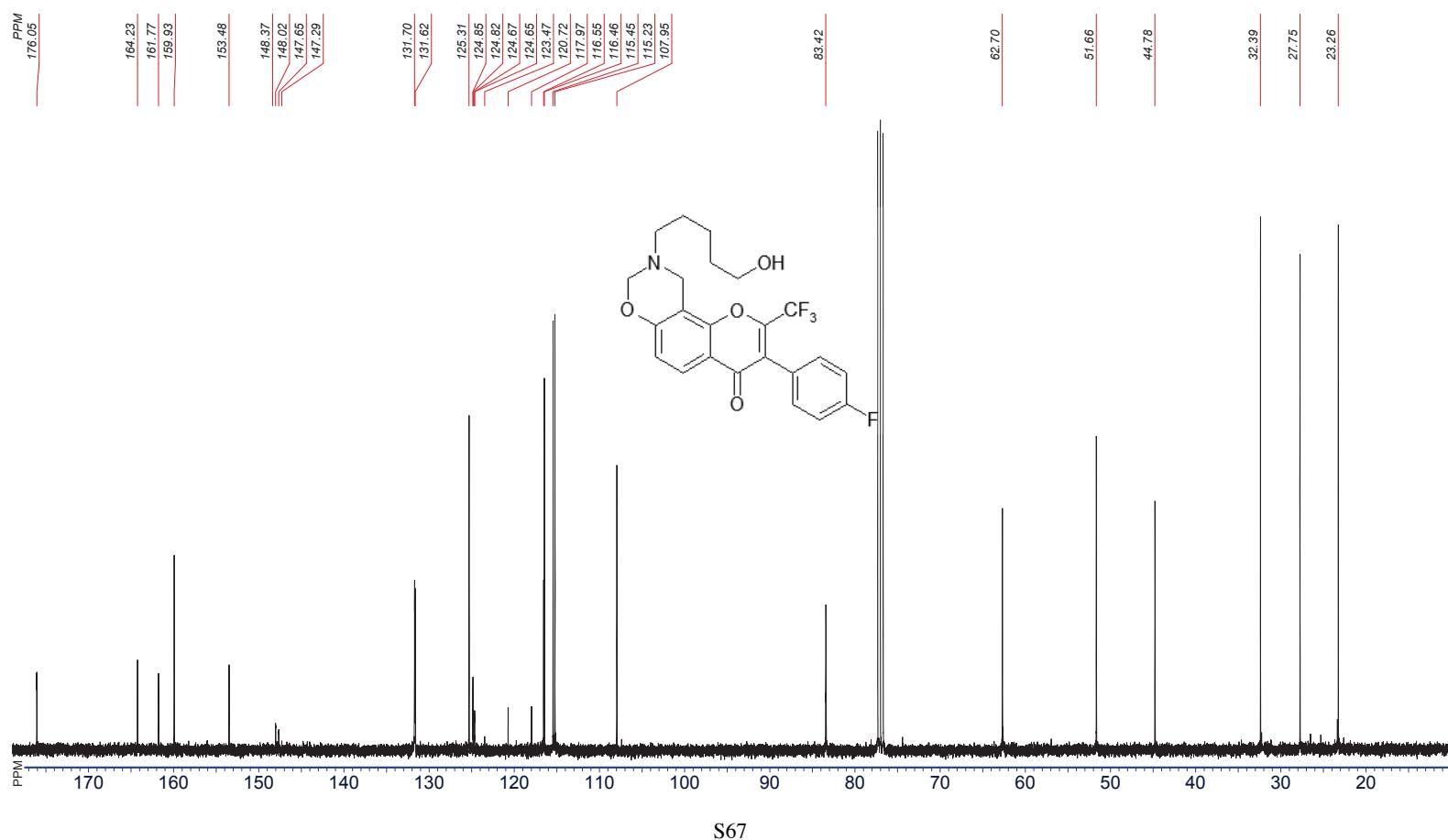
¹³C NMR spectrum of 3-(4-fluorophenyl)-9-(4-hydroxybutyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4i, n = 3**) in CDCl₃

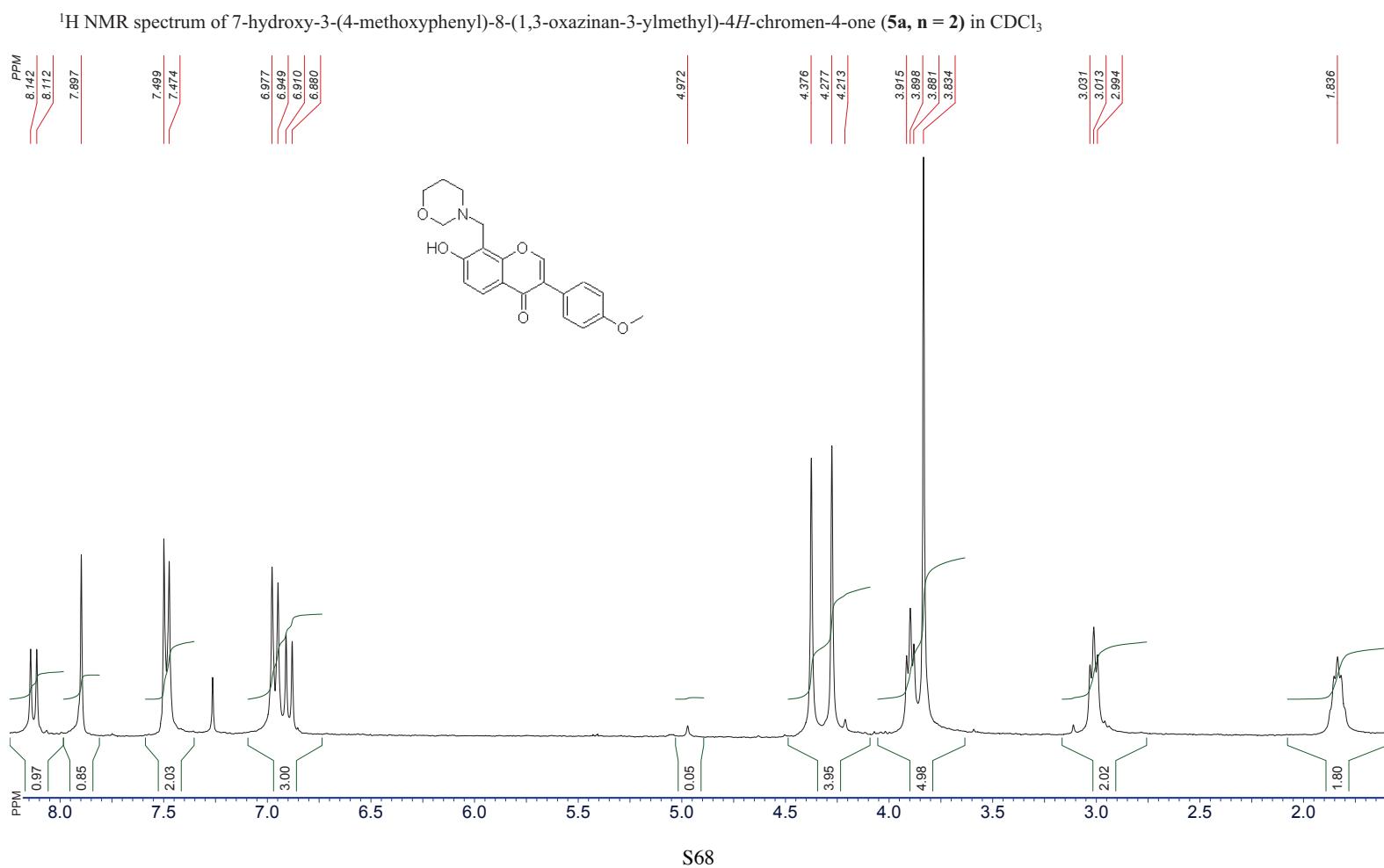


¹H NMR spectrum of 3-(4-fluorophenyl)-9-(5-hydroxypentyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4i, n = 4**) in CDCl₃

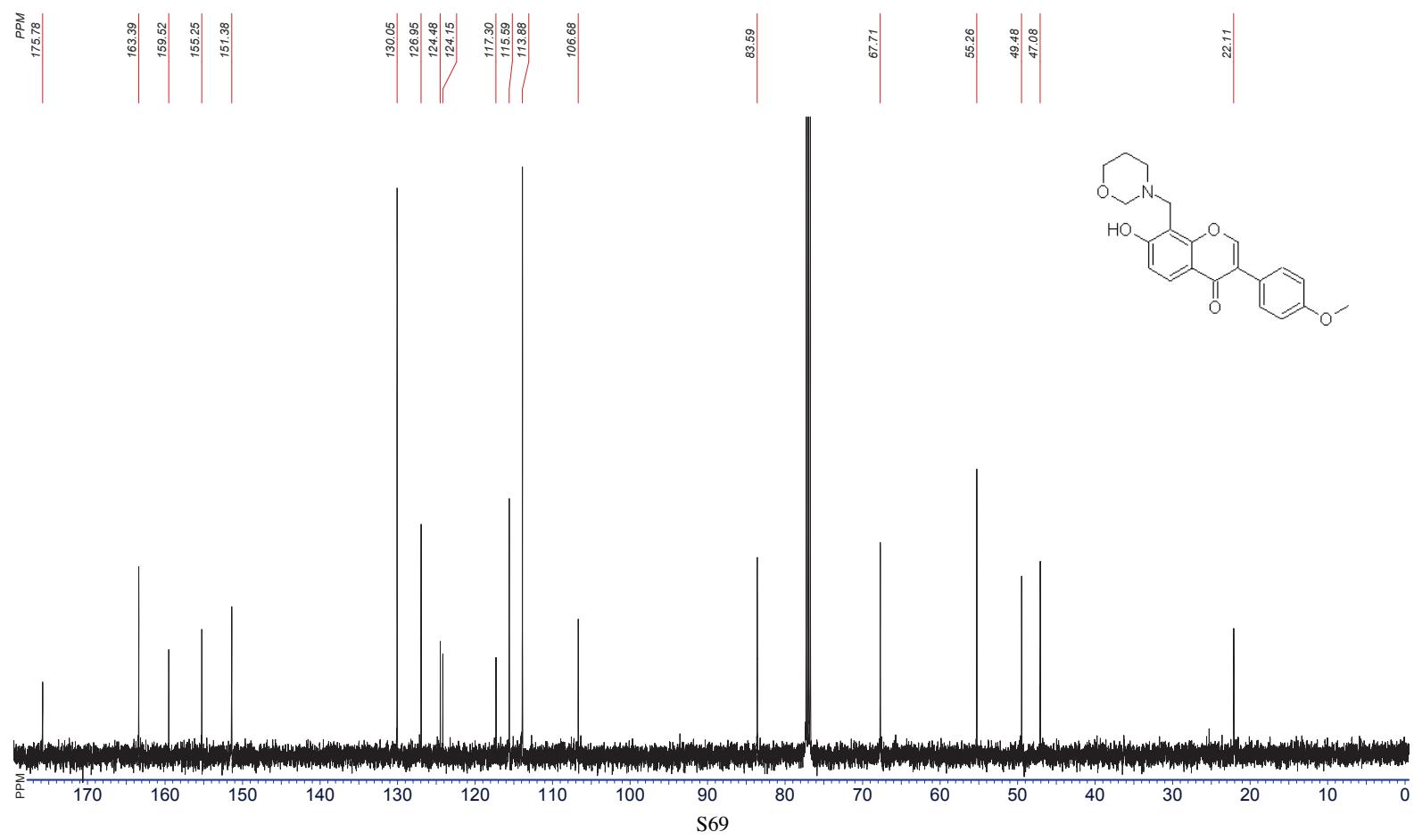


¹³C NMR spectrum of 3-(4-fluorophenyl)-9-(5-hydroxypentyl)-2-(trifluoromethyl)-9,10-dihydro-4*H*,8*H*-chromeno[8,7-*e*][1,3]oxazin-4-one (**4i, n = 4**) in CDCl₃

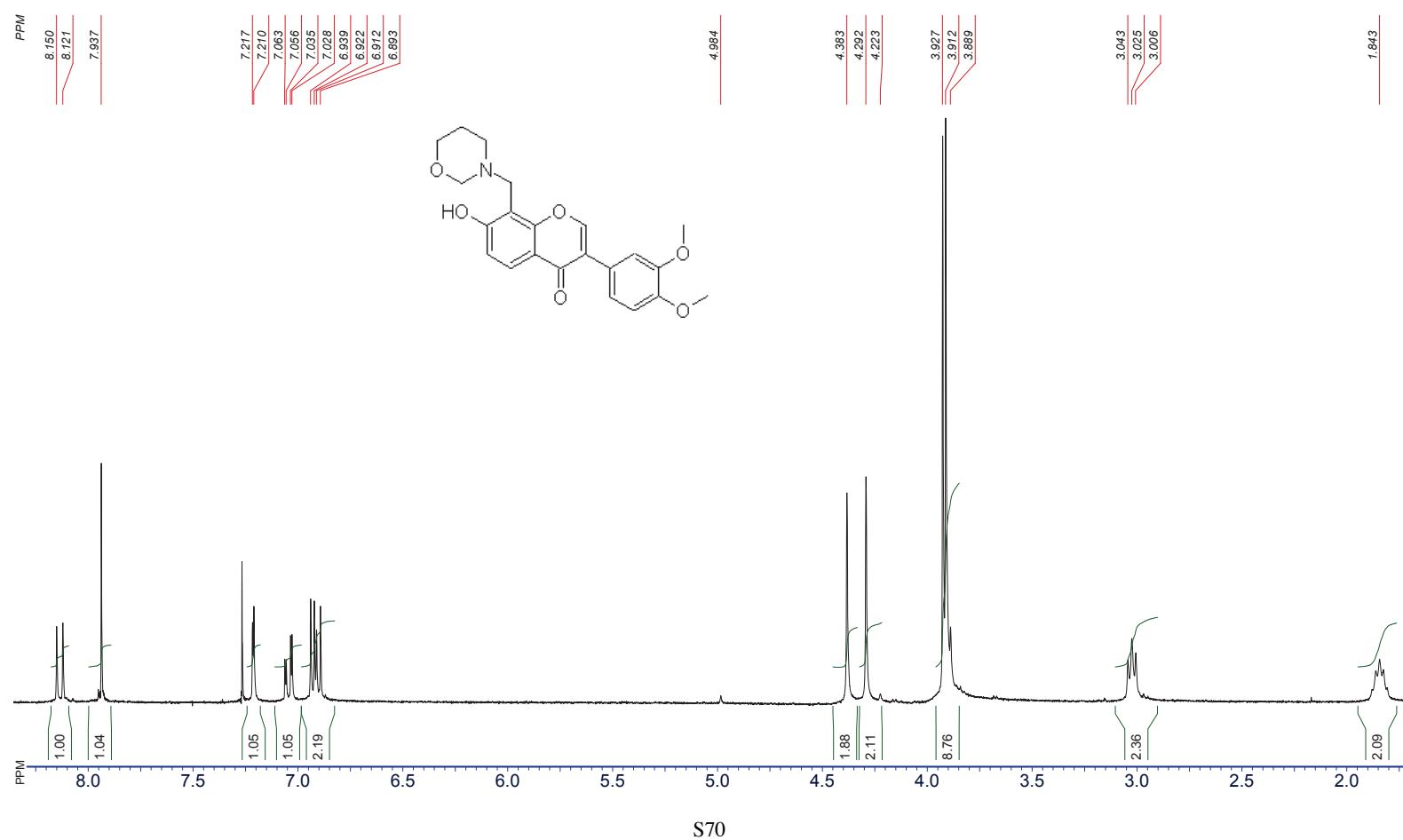




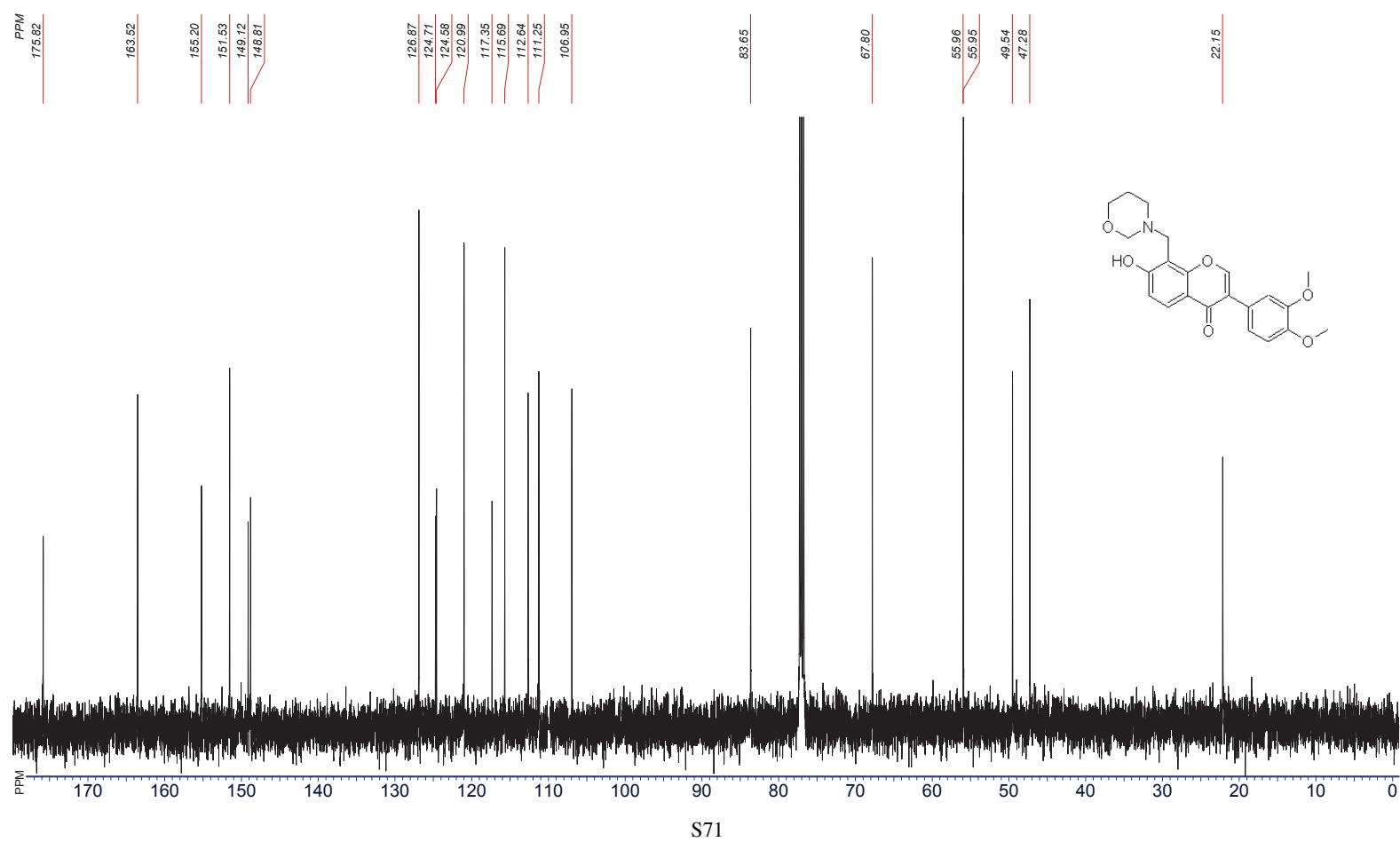
¹³C NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5a, n = 2**) in CDCl₃



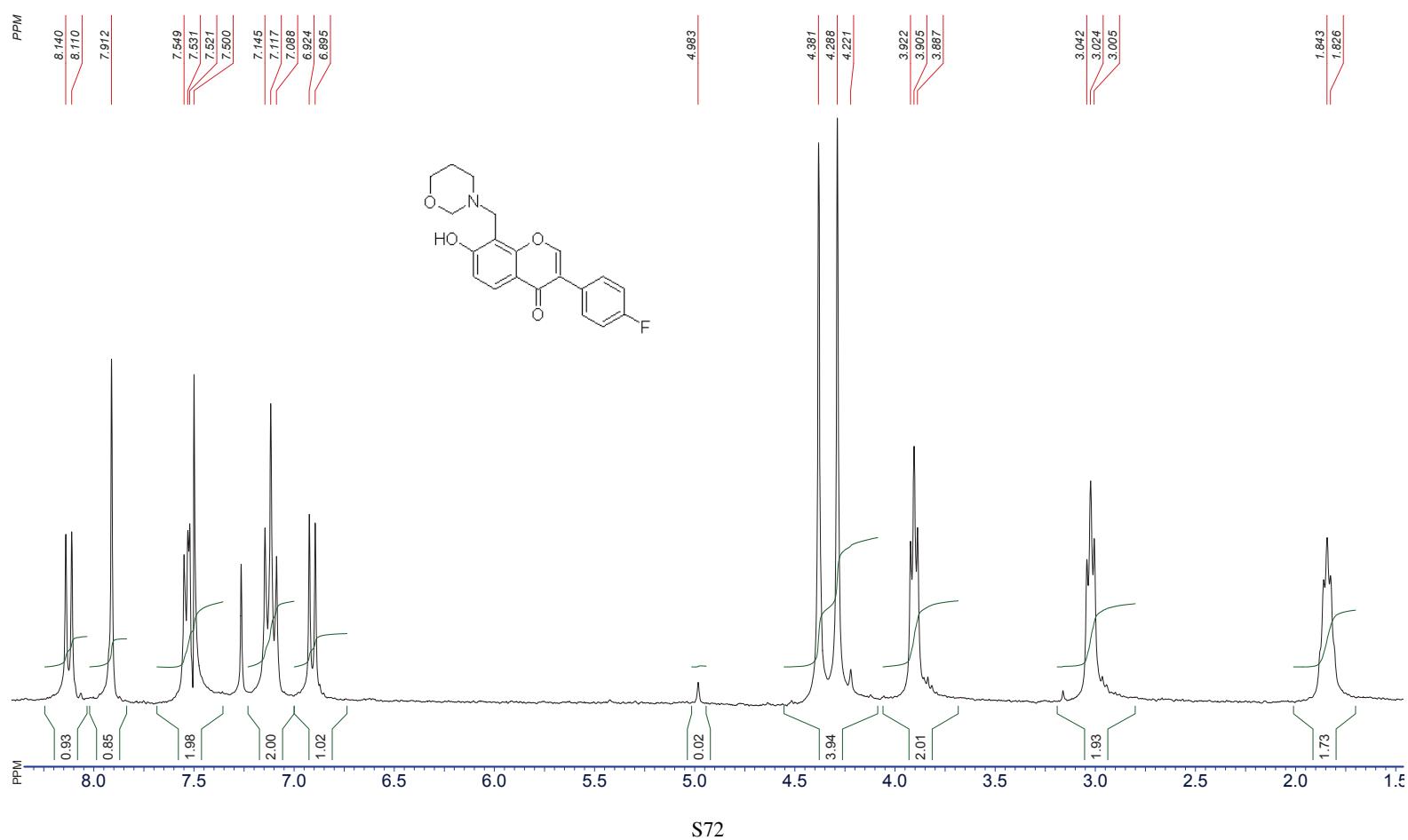
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-4*H*-chromen-4-one (**5b, n = 2**) in CDCl₃



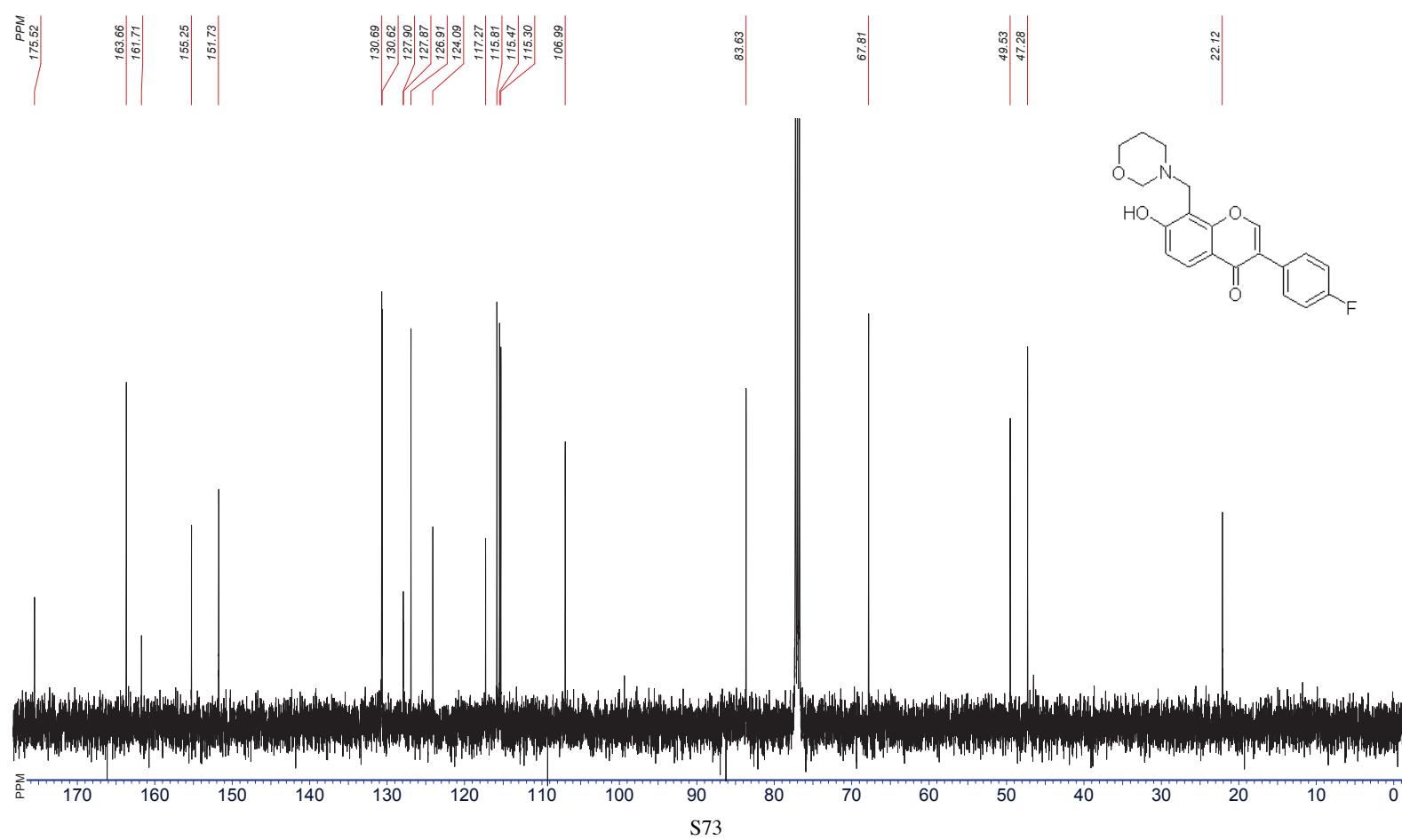
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5b, n = 2**) in CDCl₃



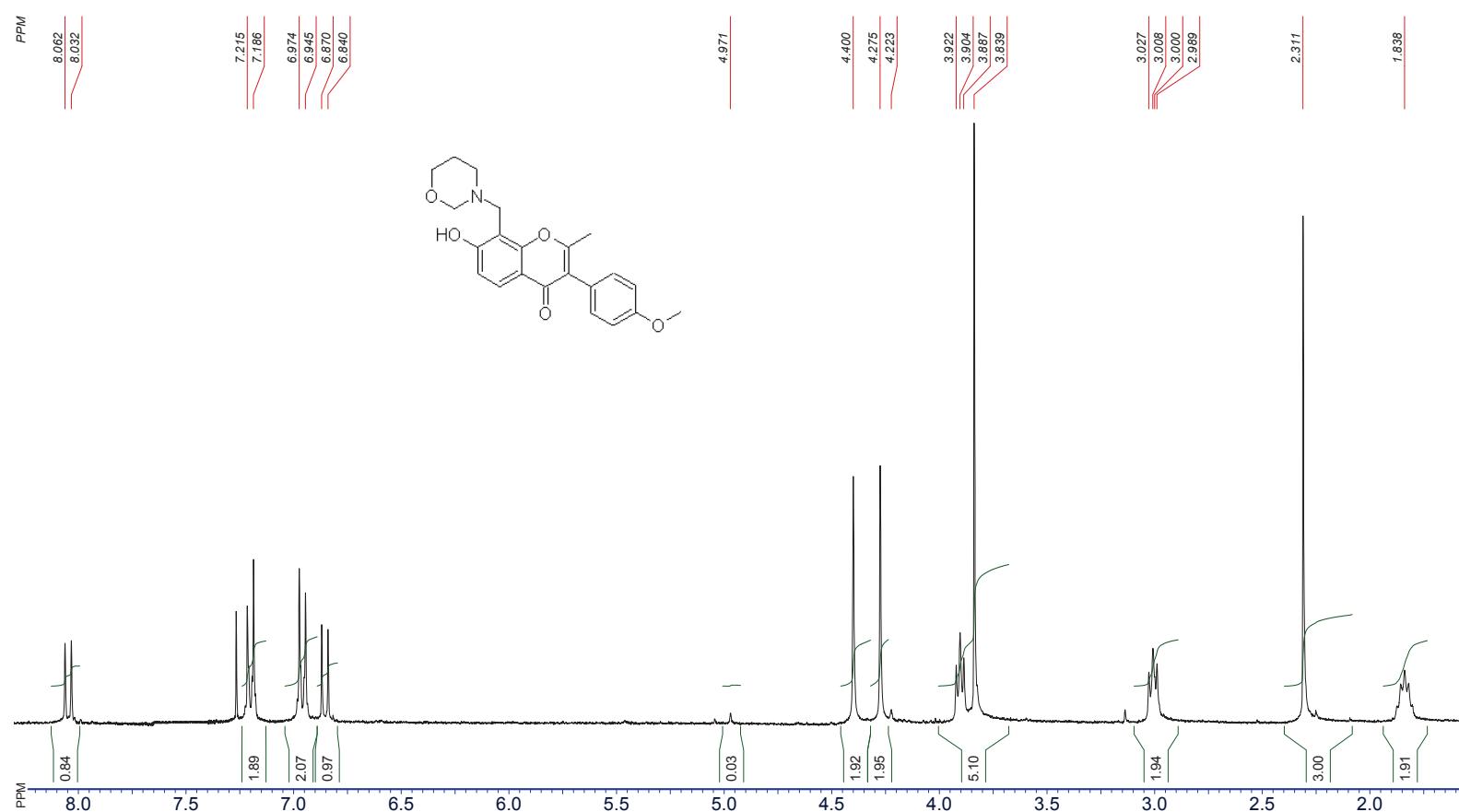
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5c, n = 2**) in CDCl₃



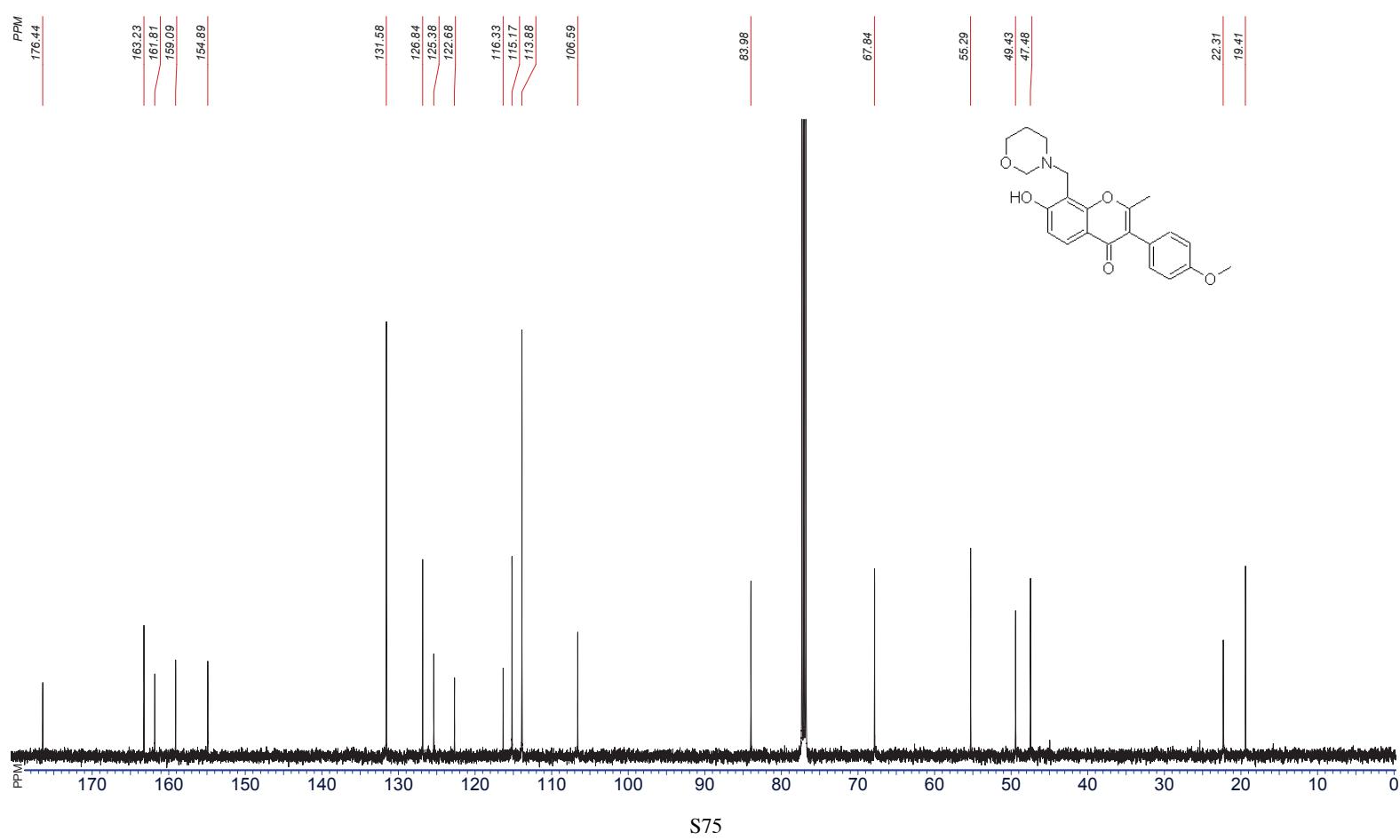
¹³C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5c, n = 2**) in CDCl₃



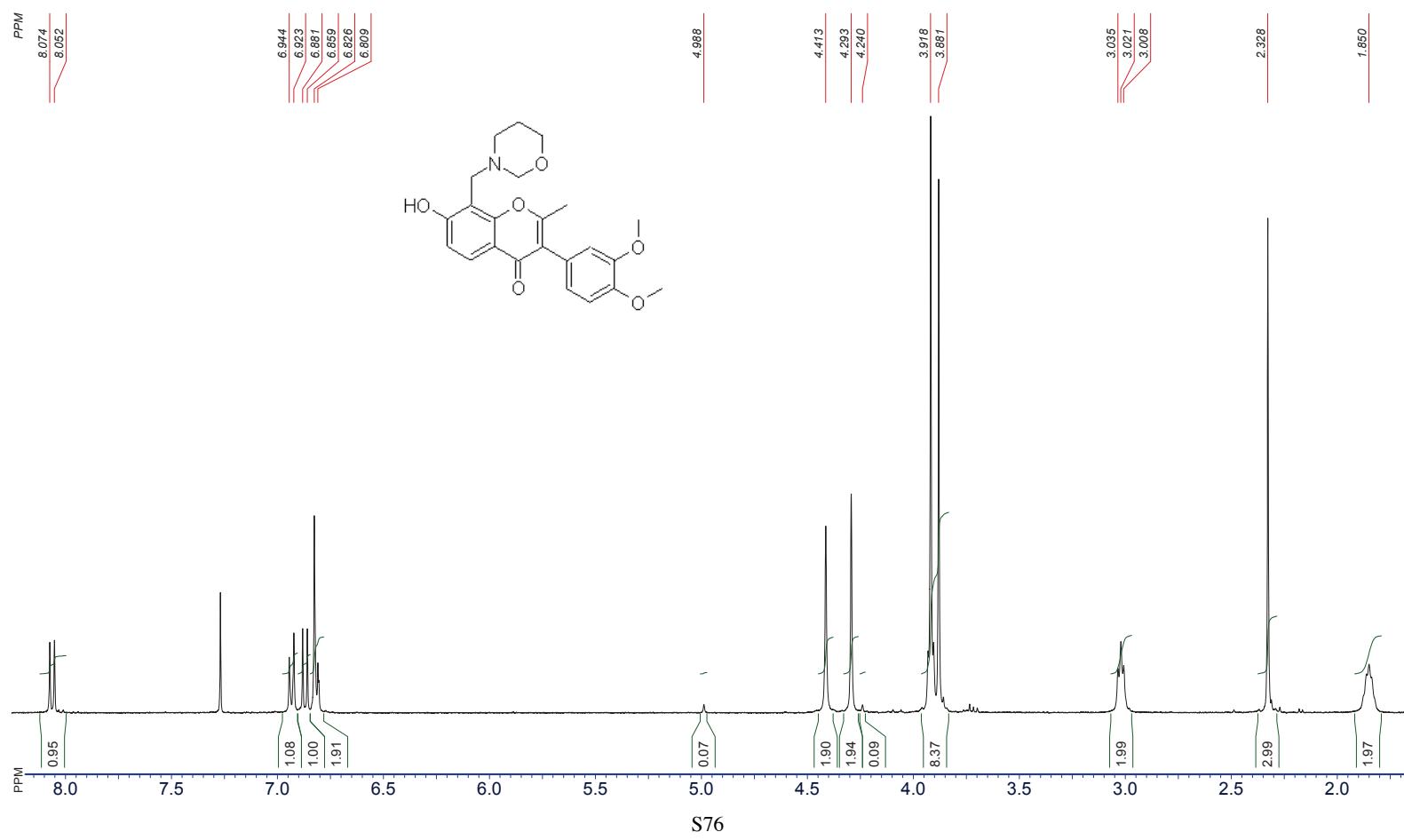
¹H NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5d, n = 2**) in CDCl₃



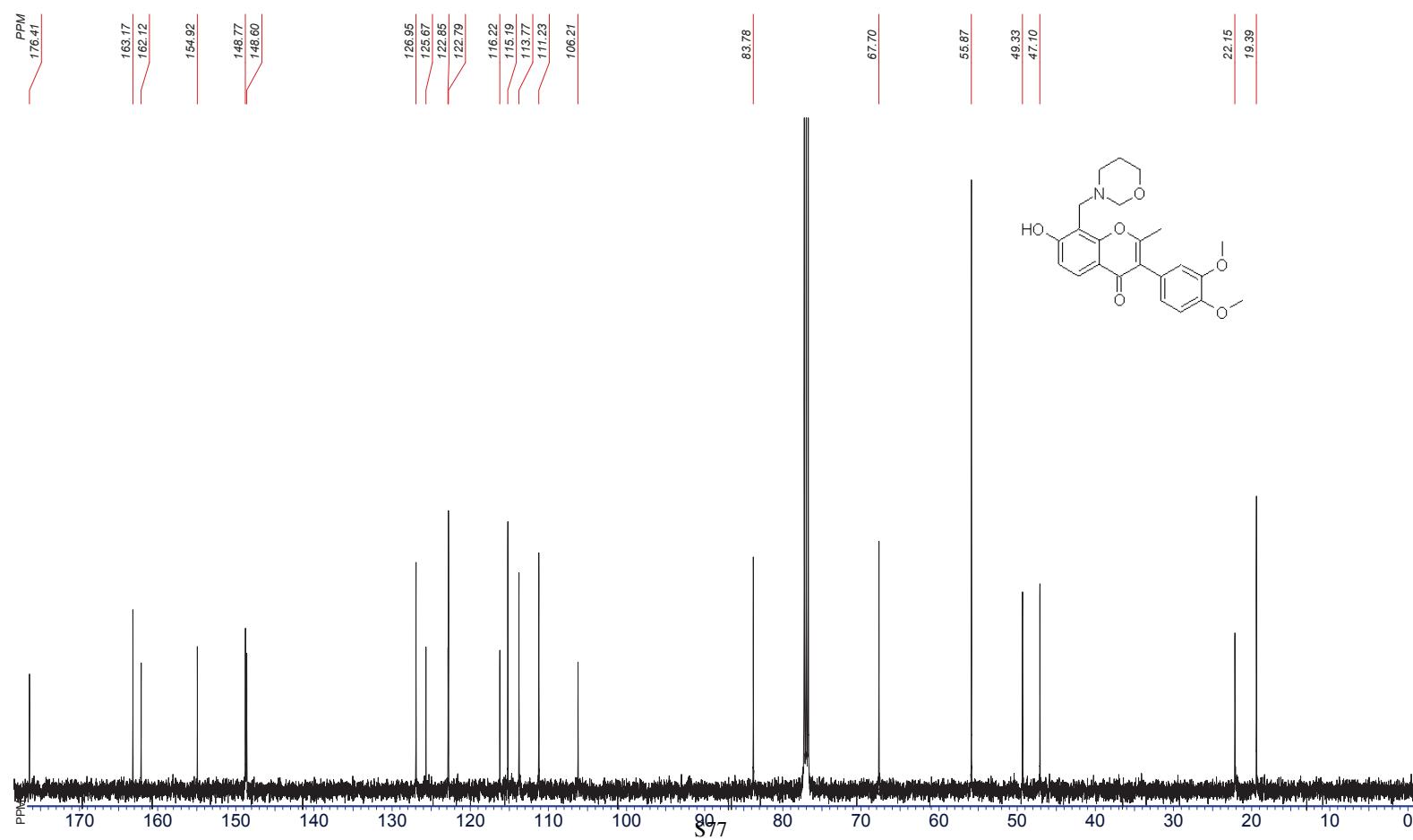
¹³C NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5d, n = 2**) in CDCl₃



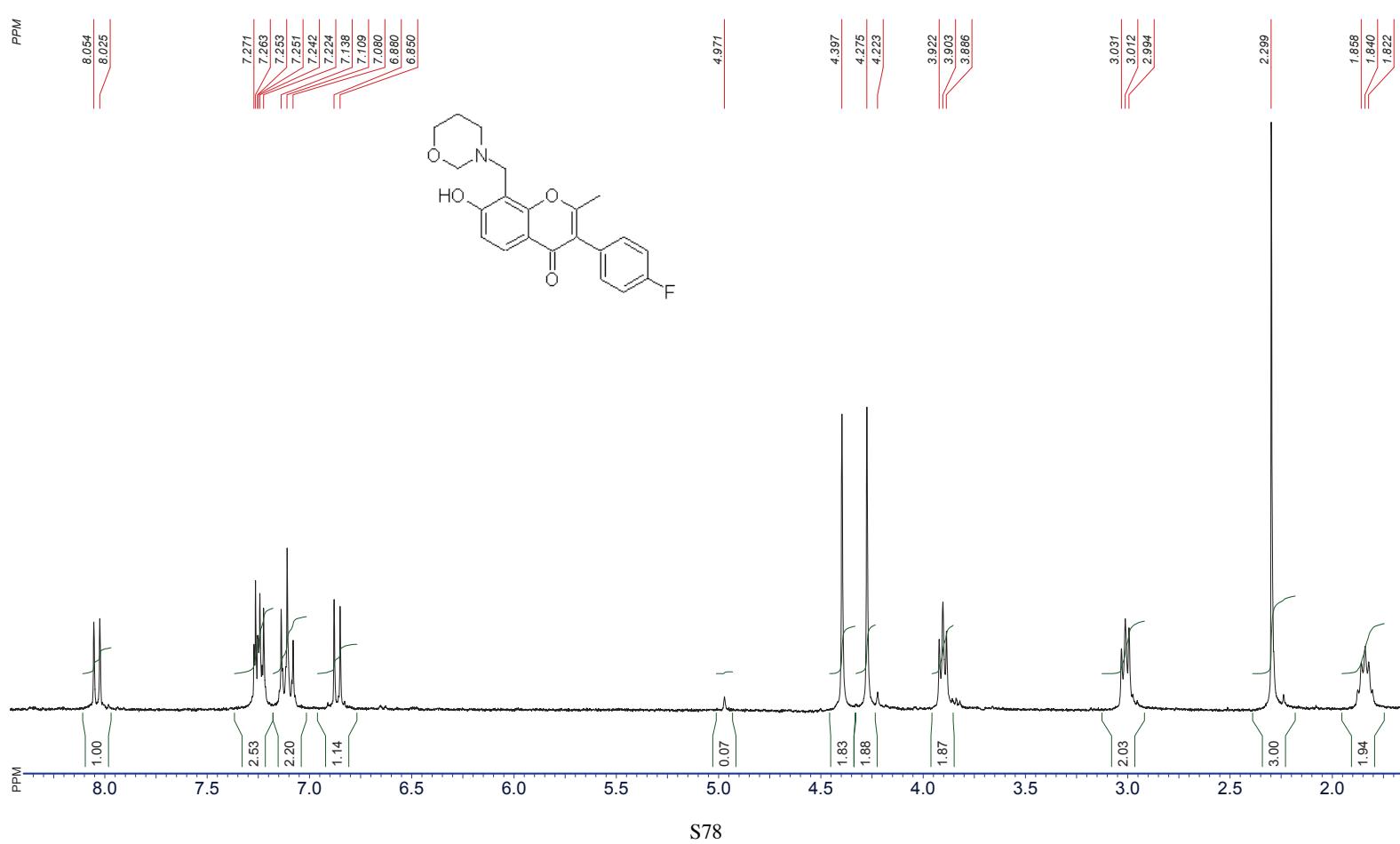
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5e, n = 2**) in CDCl₃



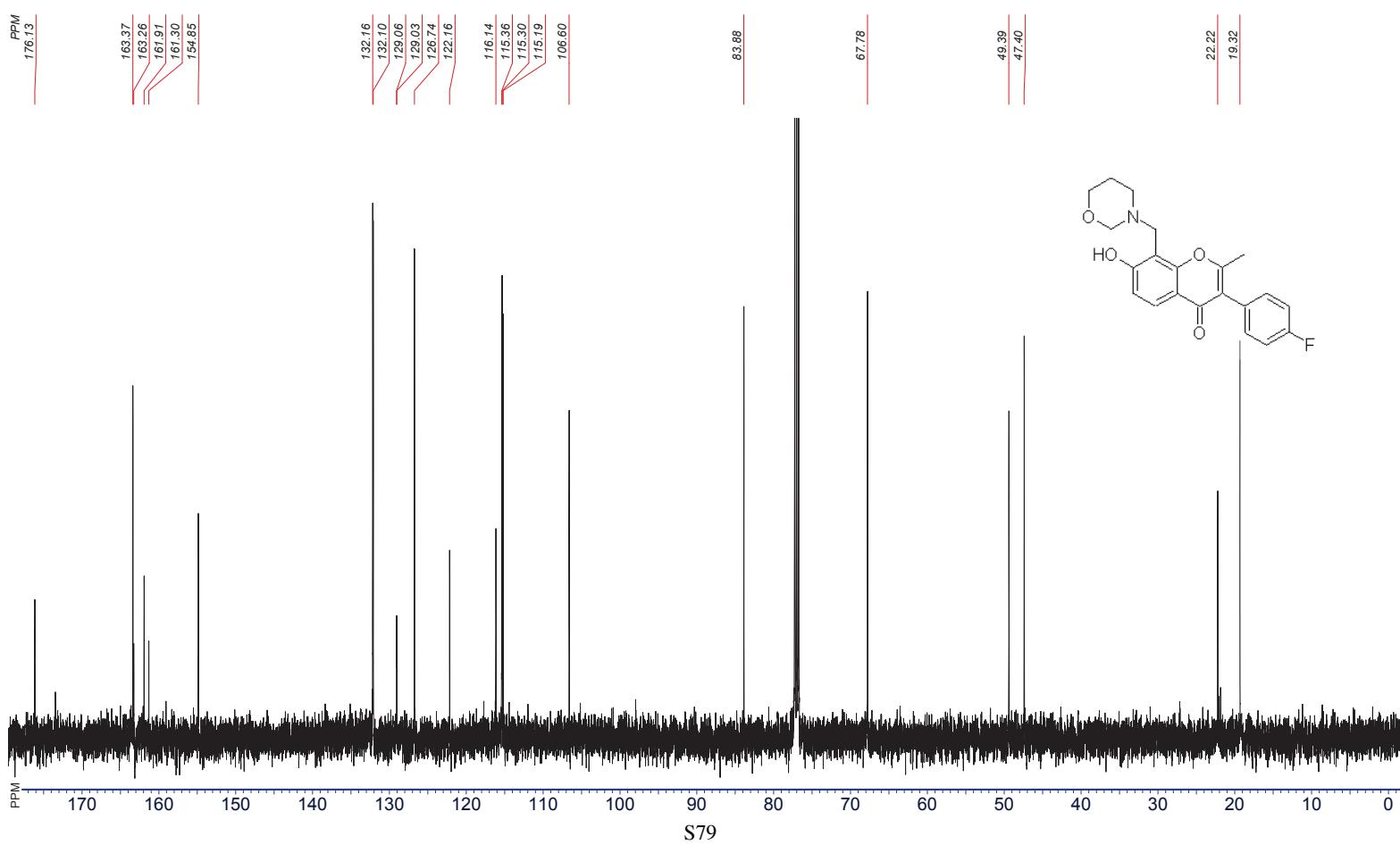
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5e, n = 2**) in CDCl₃



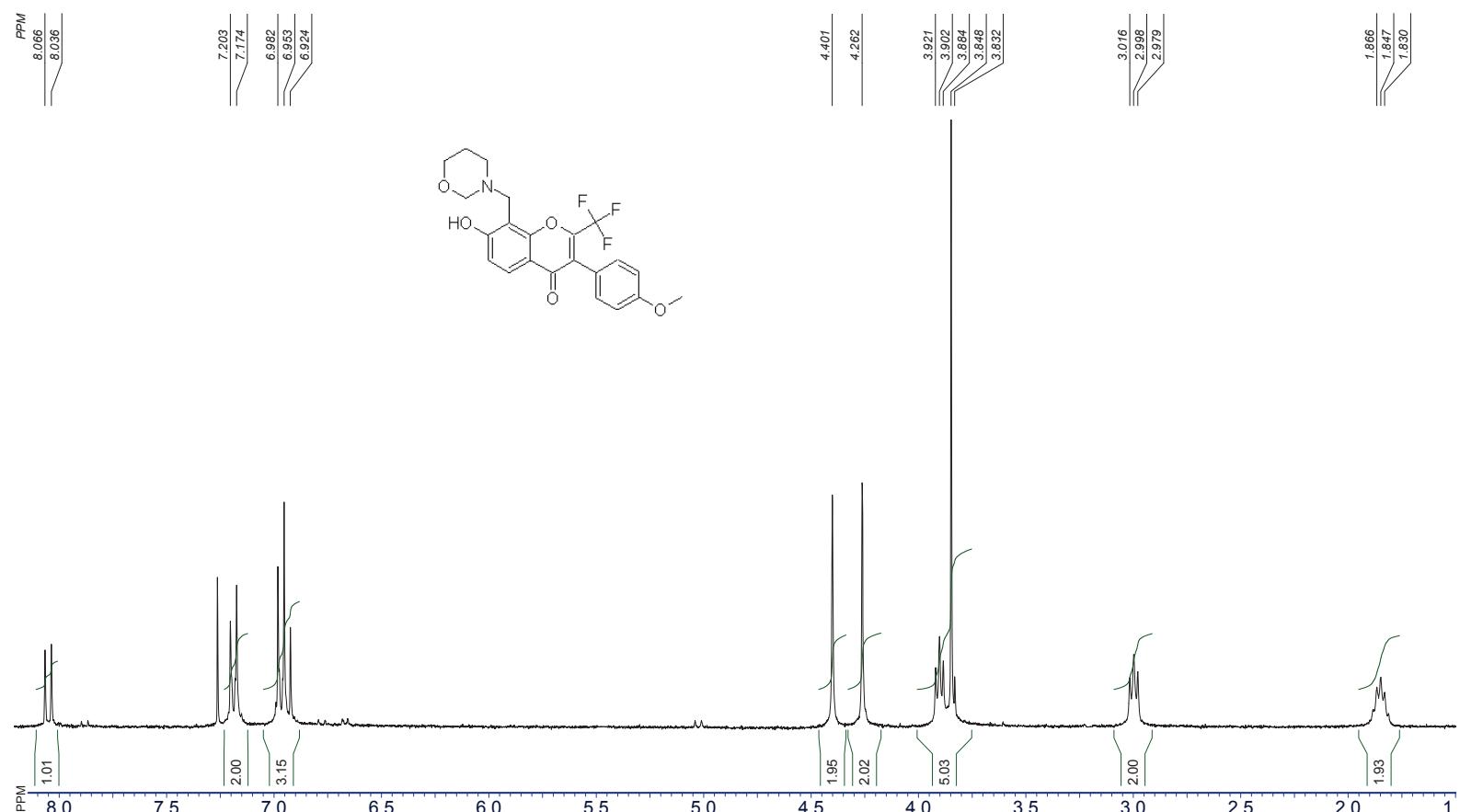
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4H-chromen-4-one (**5f, n = 2**) in CDCl₃



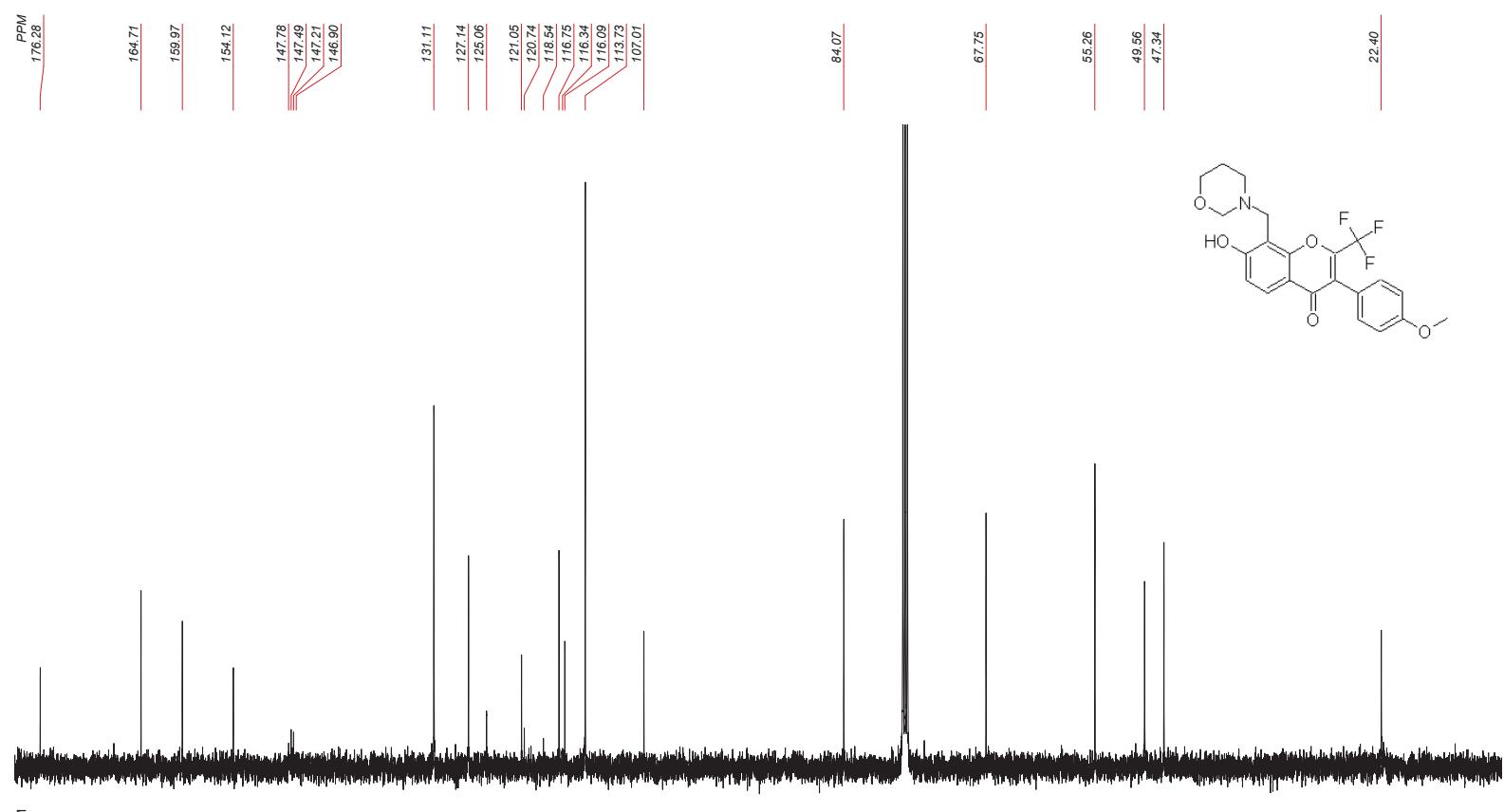
^{13}C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-2-methyl-8-(1,3-oxazinan-3-ylmethyl)-4*H*-chromen-4-one (**5f, n = 2**) in CDCl_3



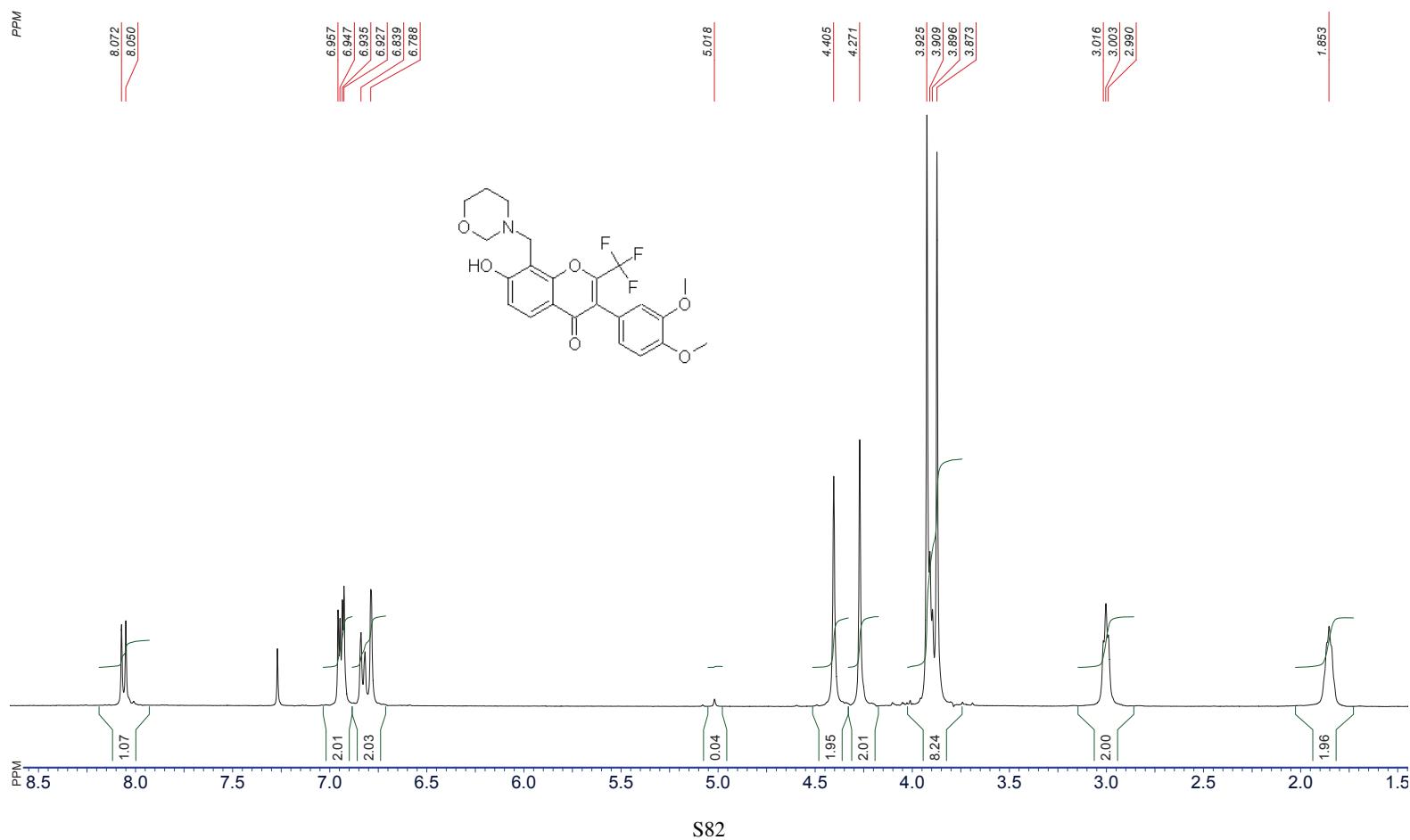
¹H NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-8-(1,3-oxazinan-3-ylmethyl)-2-(trifluoromethyl)-4H-chromen-4-one (**5g, n = 2**) in CDCl₃



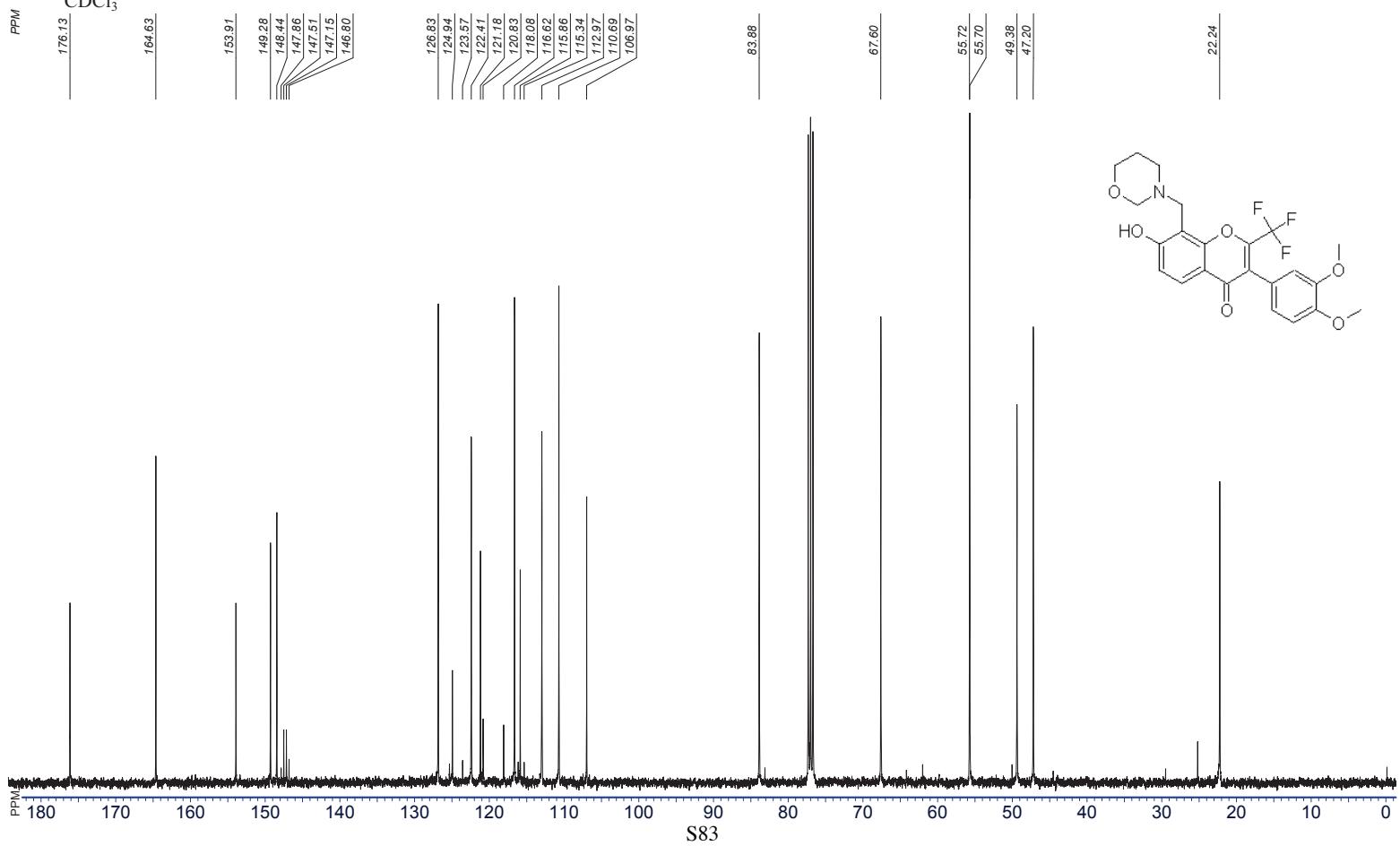
¹³C NMR spectrum of 7-hydroxy-3-(4-methoxyphenyl)-8-(1,3-oxazinan-3-ylmethyl)-2-(trifluoromethyl)-4H-chromen-4-one (**5g, n = 2**) in CDCl₃



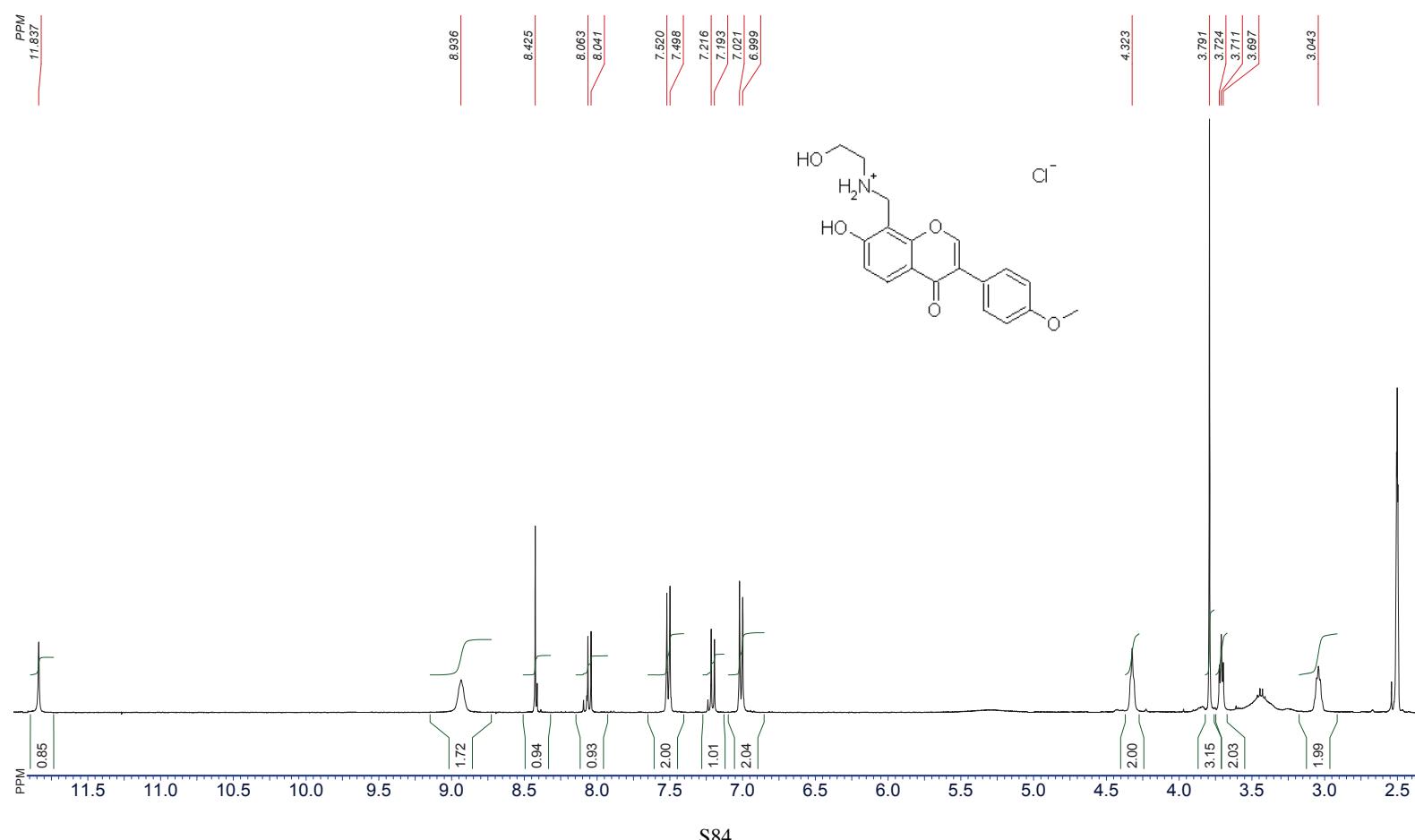
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-2-(trifluoromethyl)-4*H*-chromen-4-one (**5h, n = 2**) in CDCl₃



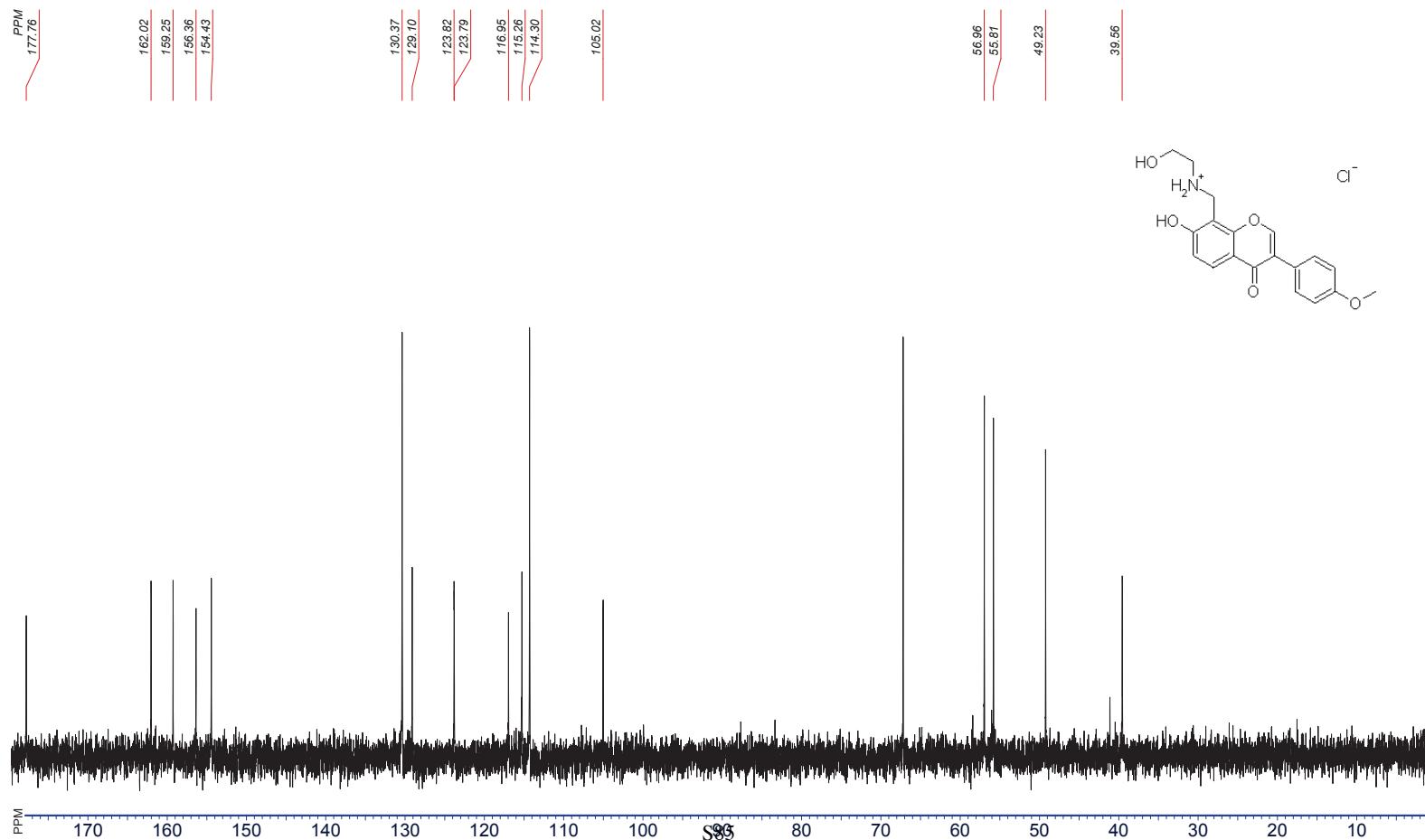
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-(1,3-oxazinan-3-ylmethyl)-2-(trifluoromethyl)-4H-chromen-4-one (**5h, n = 2**) in CDCl₃



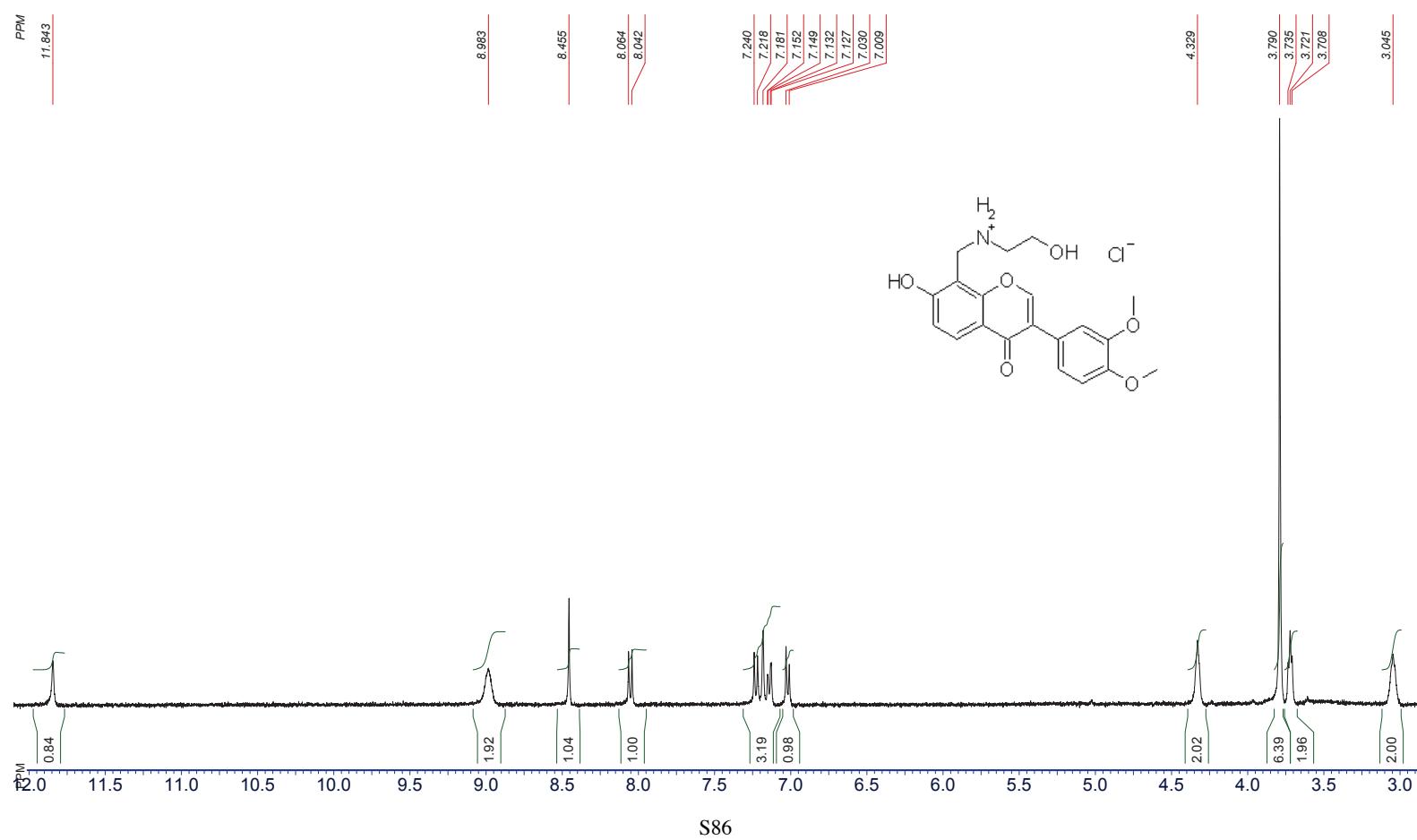
¹H NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-4H-chromen-4-one hydrochloride (**6a, n = 1**) in DMSO-d₆



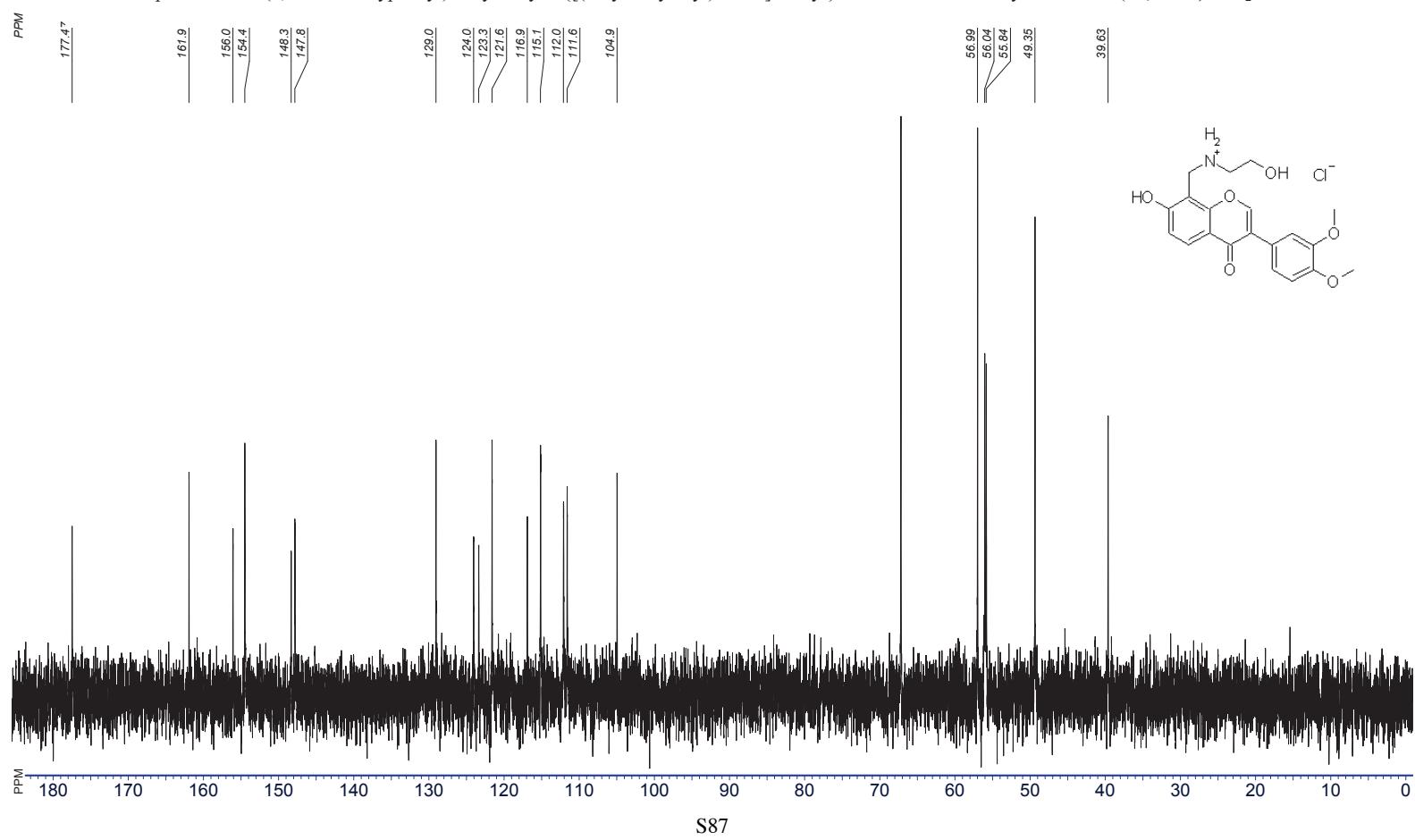
¹³C NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-4H-chromen-4-one hydrochloride (**6a, n = 1**) in D₂O



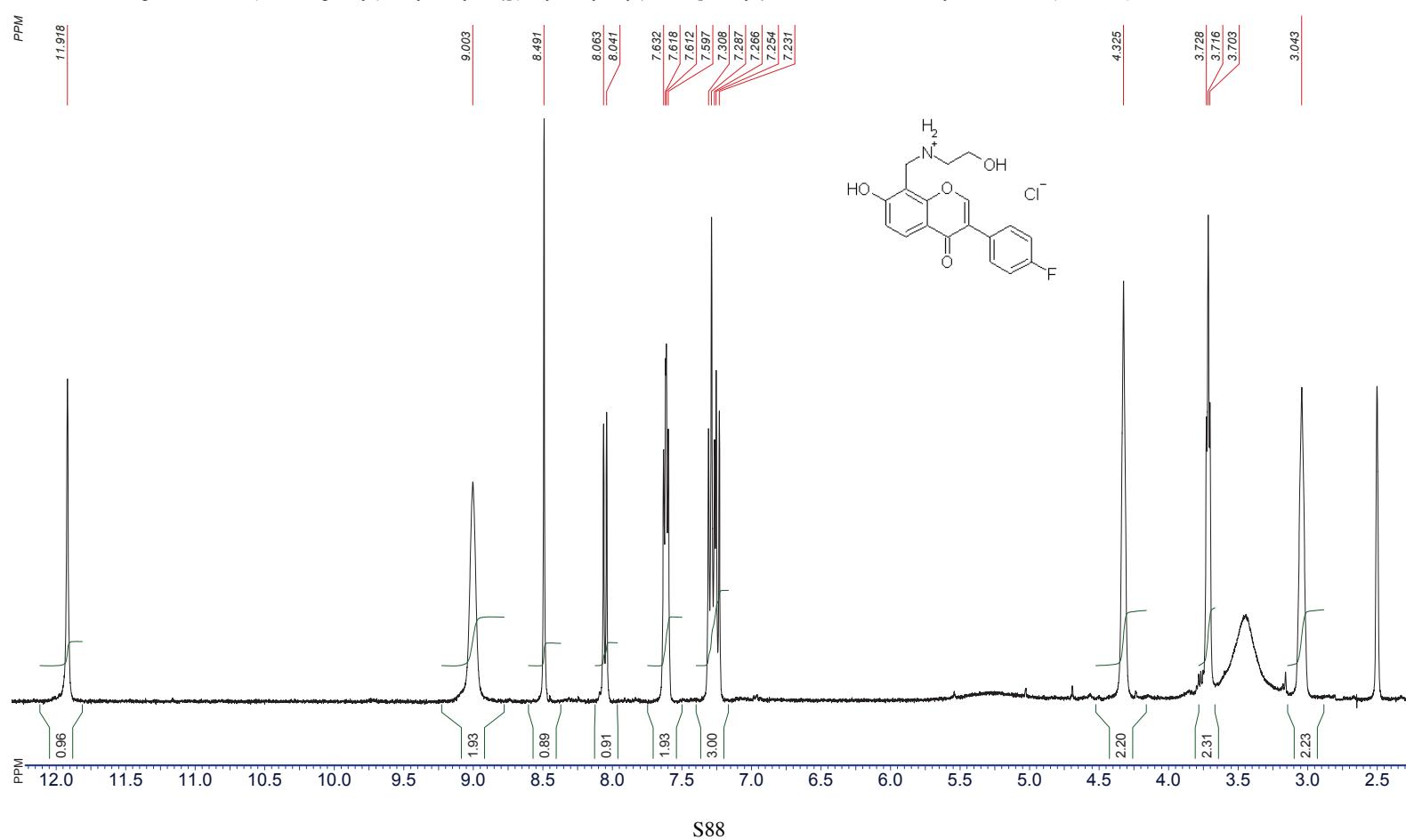
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-4*H*-chromen-4-one hydrochloride (**6b, n = 1**) in DMSO-d₆



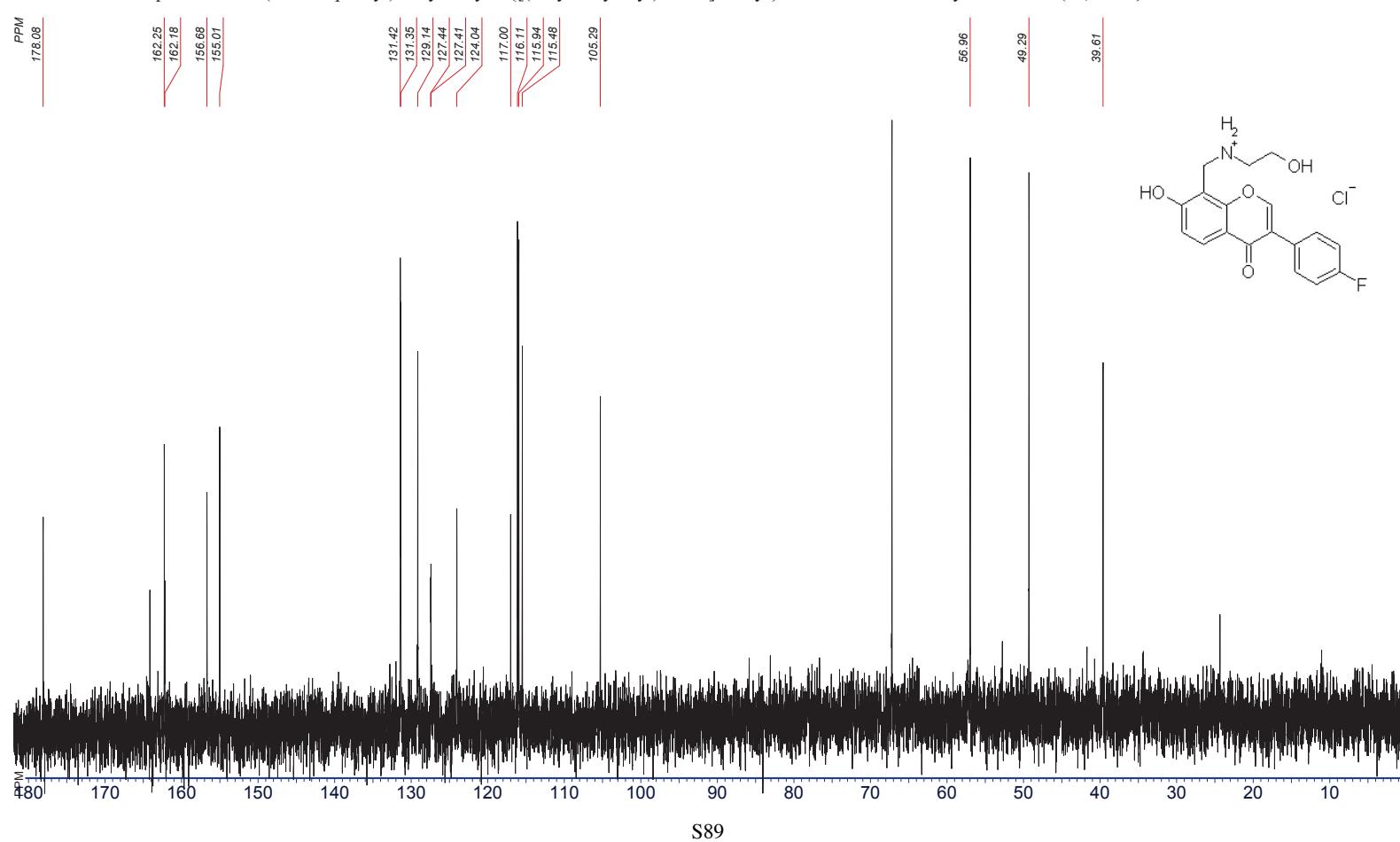
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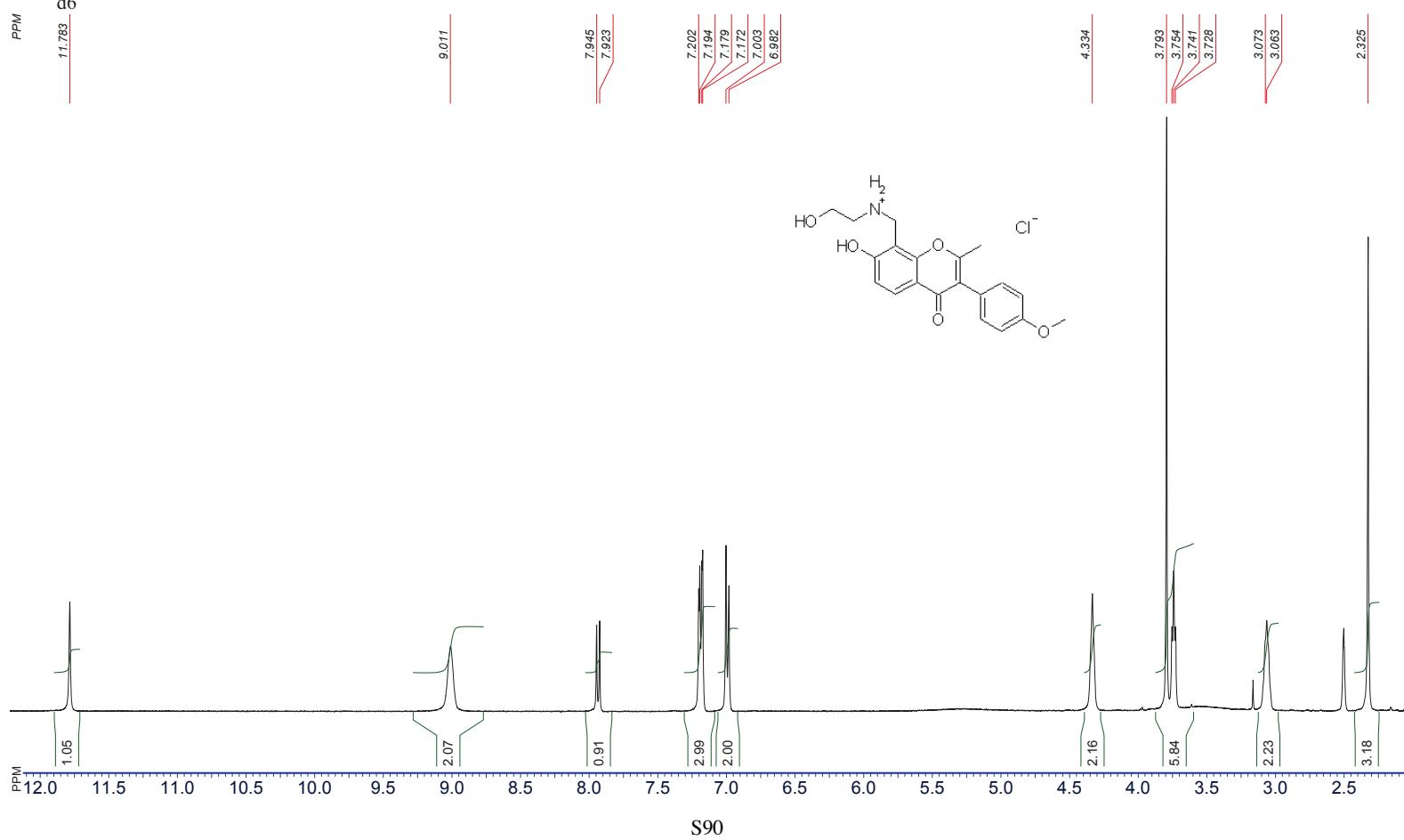
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-4H-chromen-4-one hydrochloride (**6c, n = 1**) in DMSO-d₆



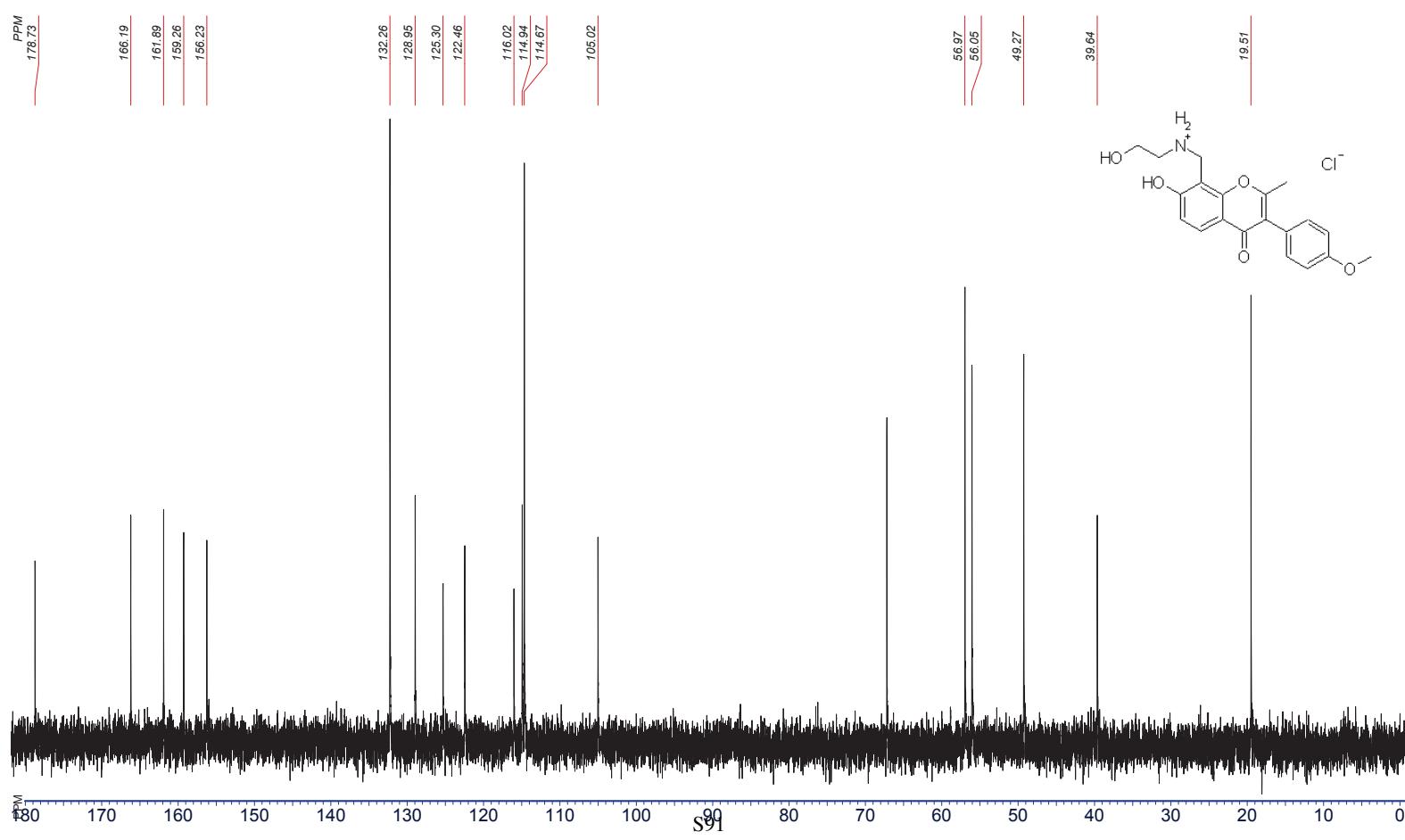
¹³C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-4H-chromen-4-one hydrochloride (**6c, n = 1**) in D₂O



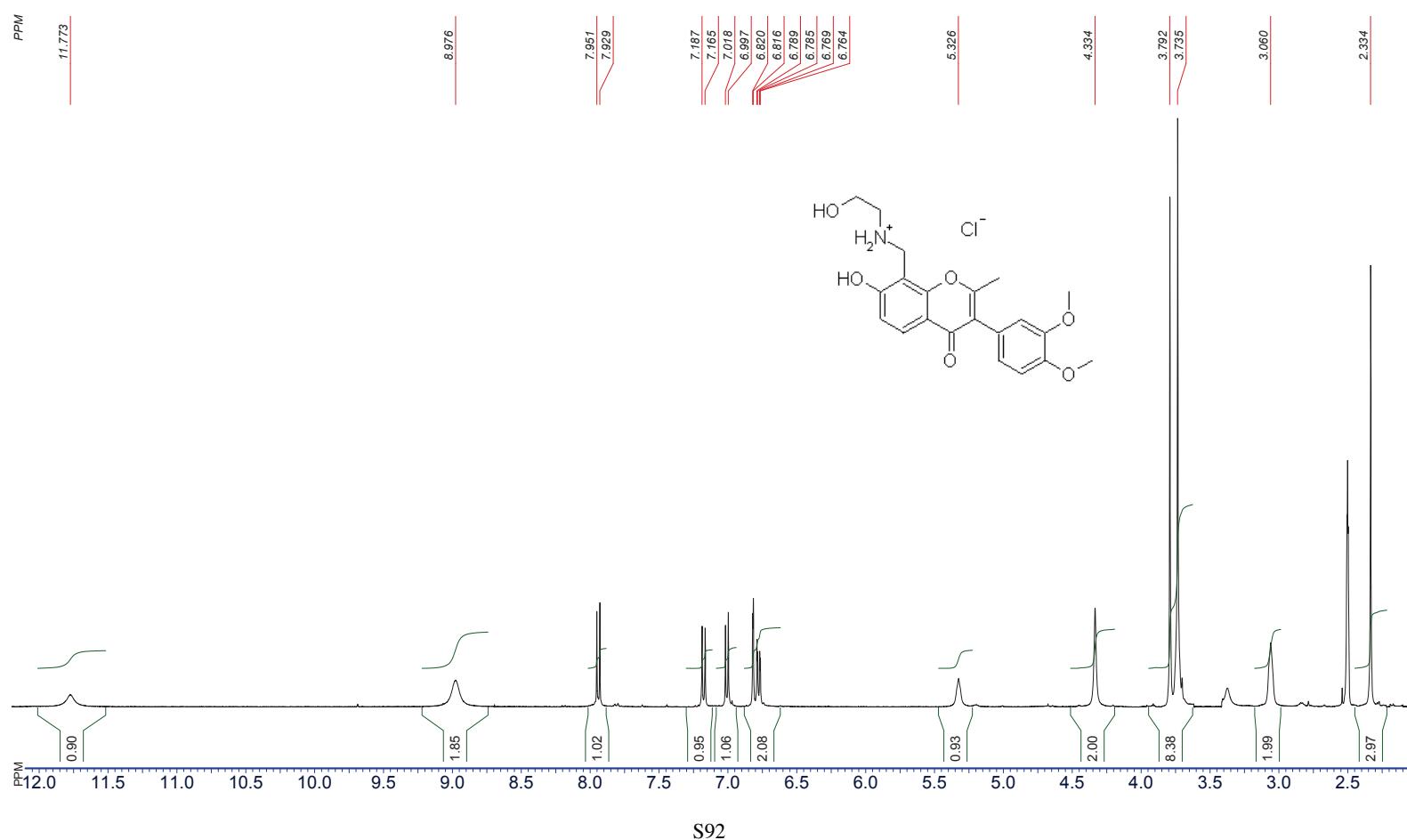
¹H NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-2-methyl-4*H*-chromen-4-one hydrochloride (**6d, n = 1**) in DMSO-d₆



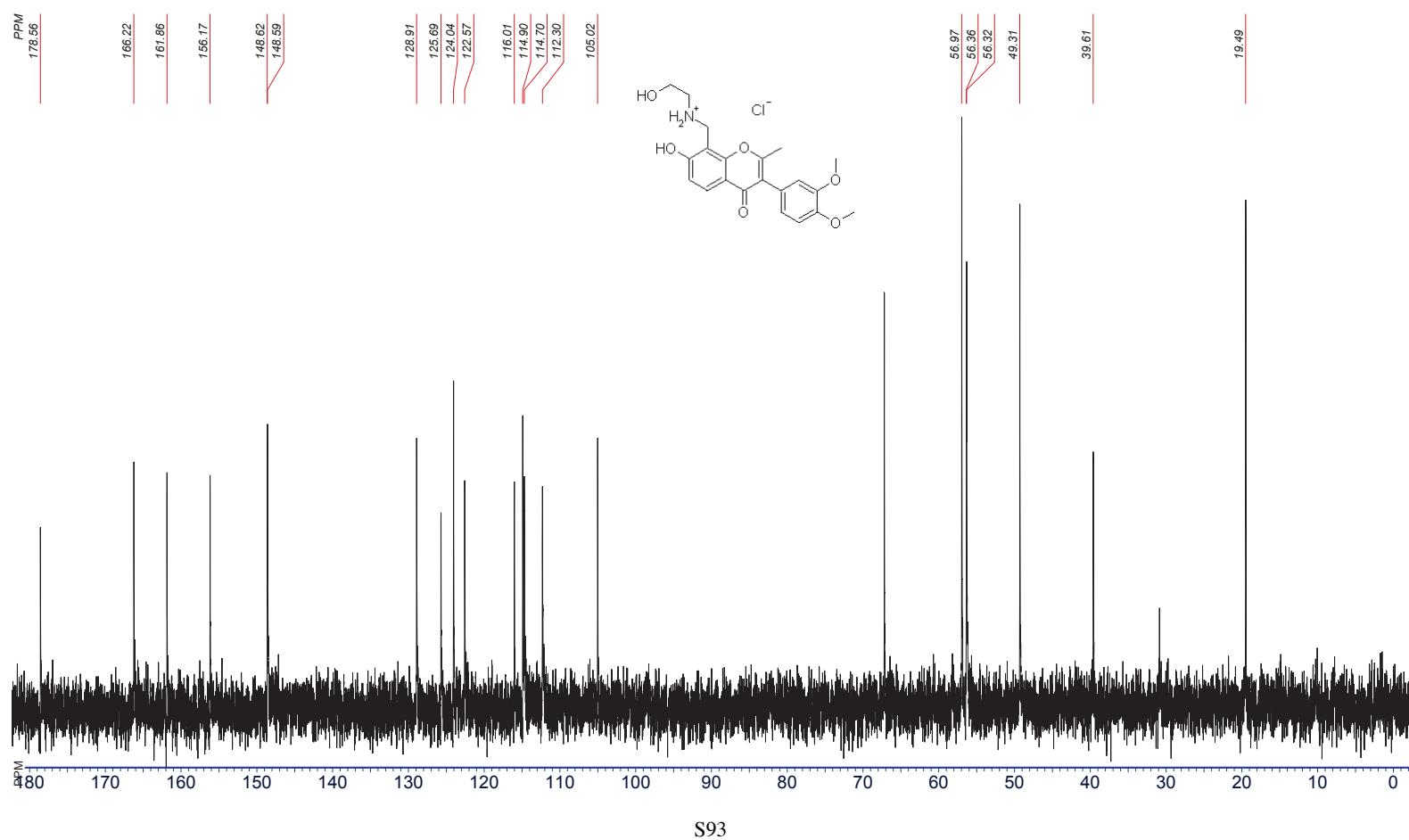
¹³C NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-2-methyl-4H-chromen-4-one hydrochloride (**6d, n = 1**) in D₂O



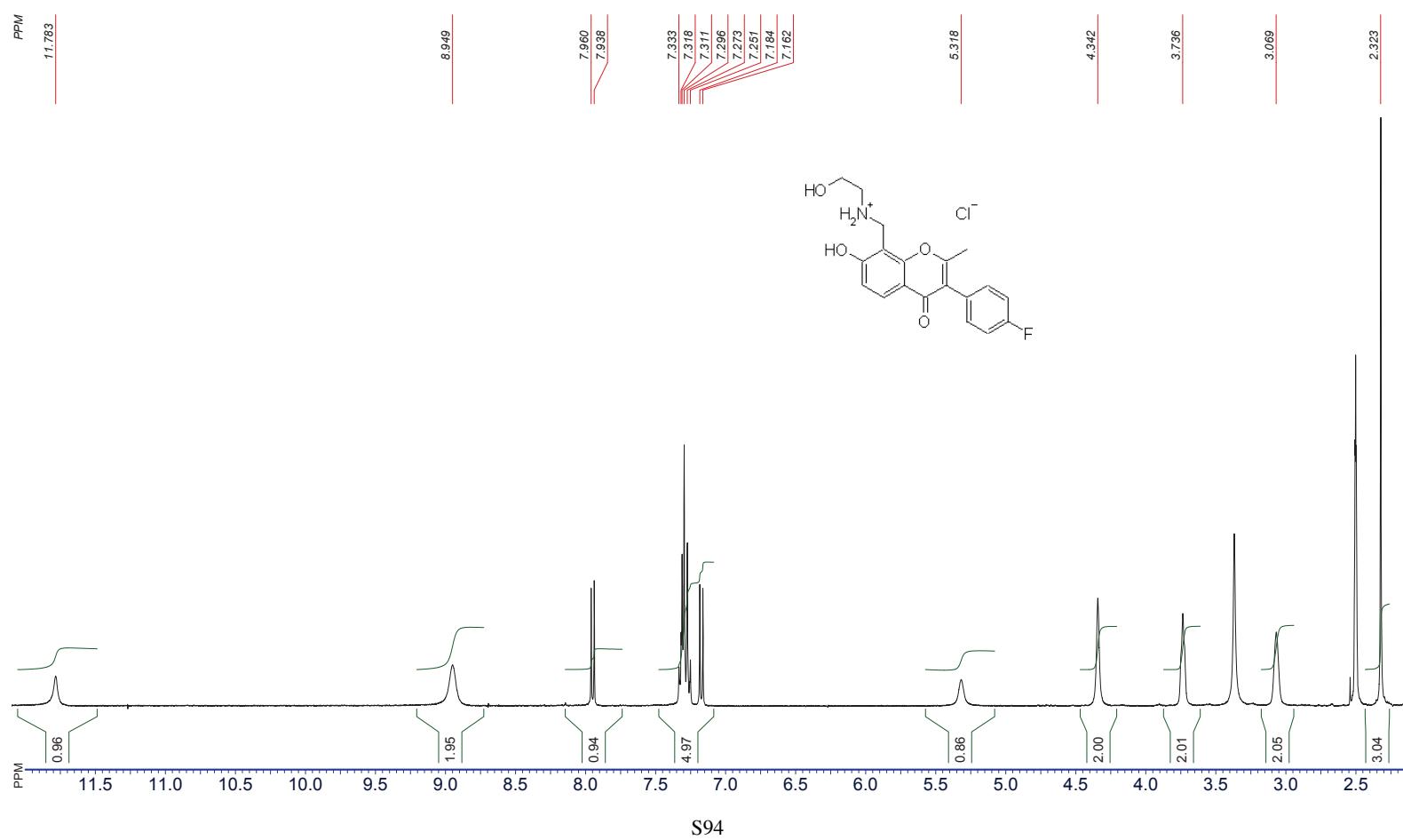
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-2-methyl-4*H*-chromen-4-one hydrochloride (**6e, n = 1**) in DMSO-d₆



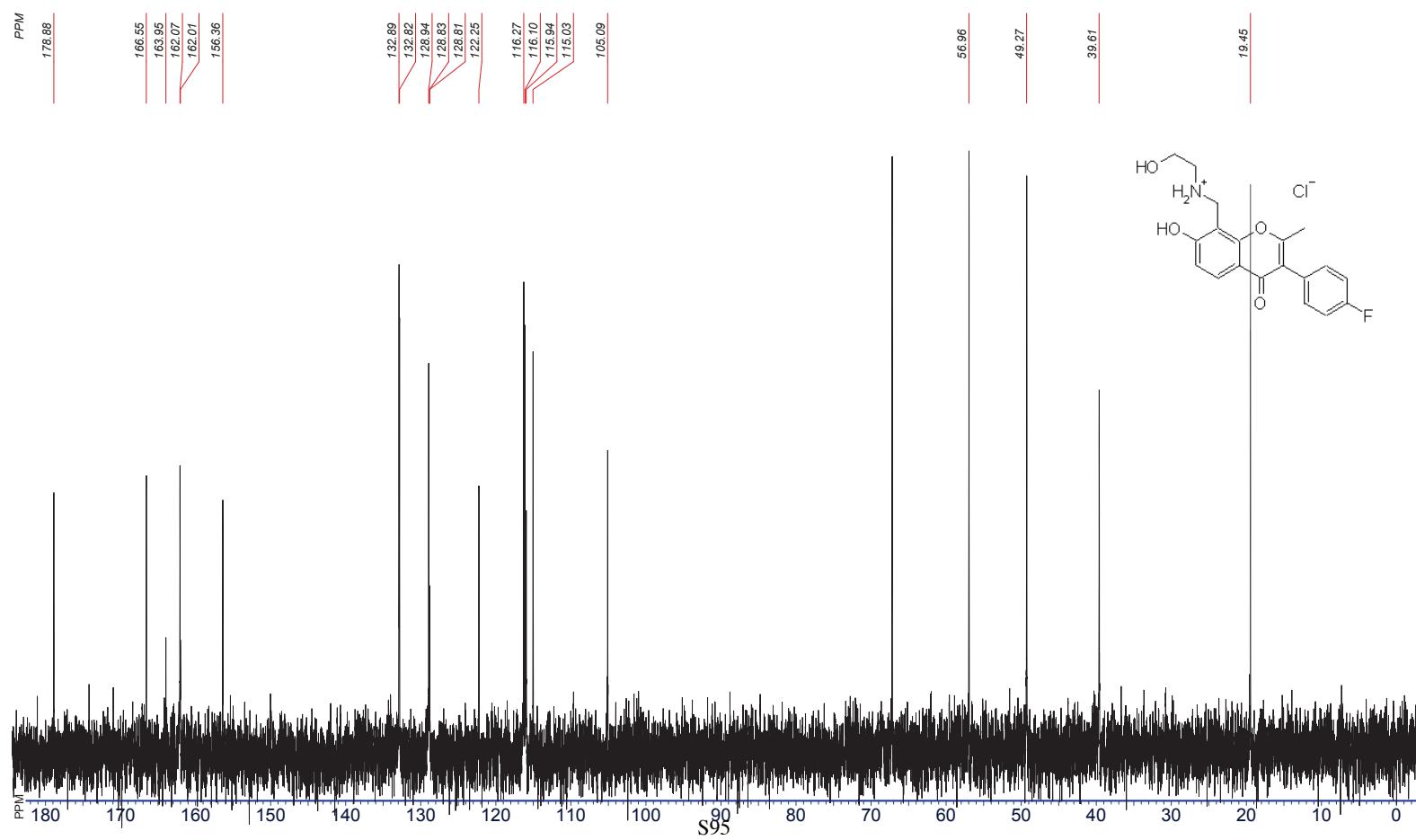
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-2-methyl-4*H*-chromen-4-one hydrochloride (**6e, n = 1**) in D₂O



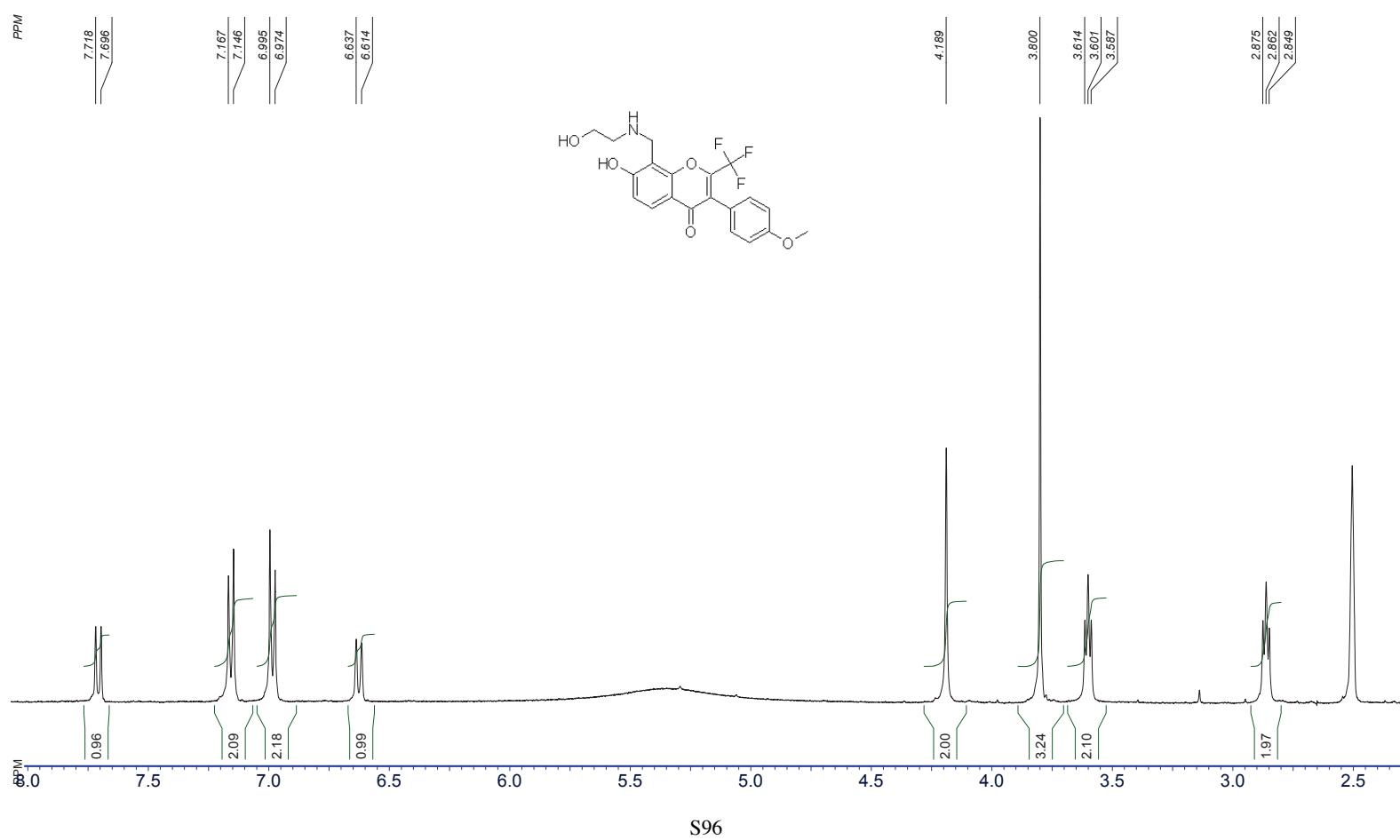
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-2-methyl-4*H*-chromen-4-one hydrochloride (**6f, n = 1**) in DMSO-d₆



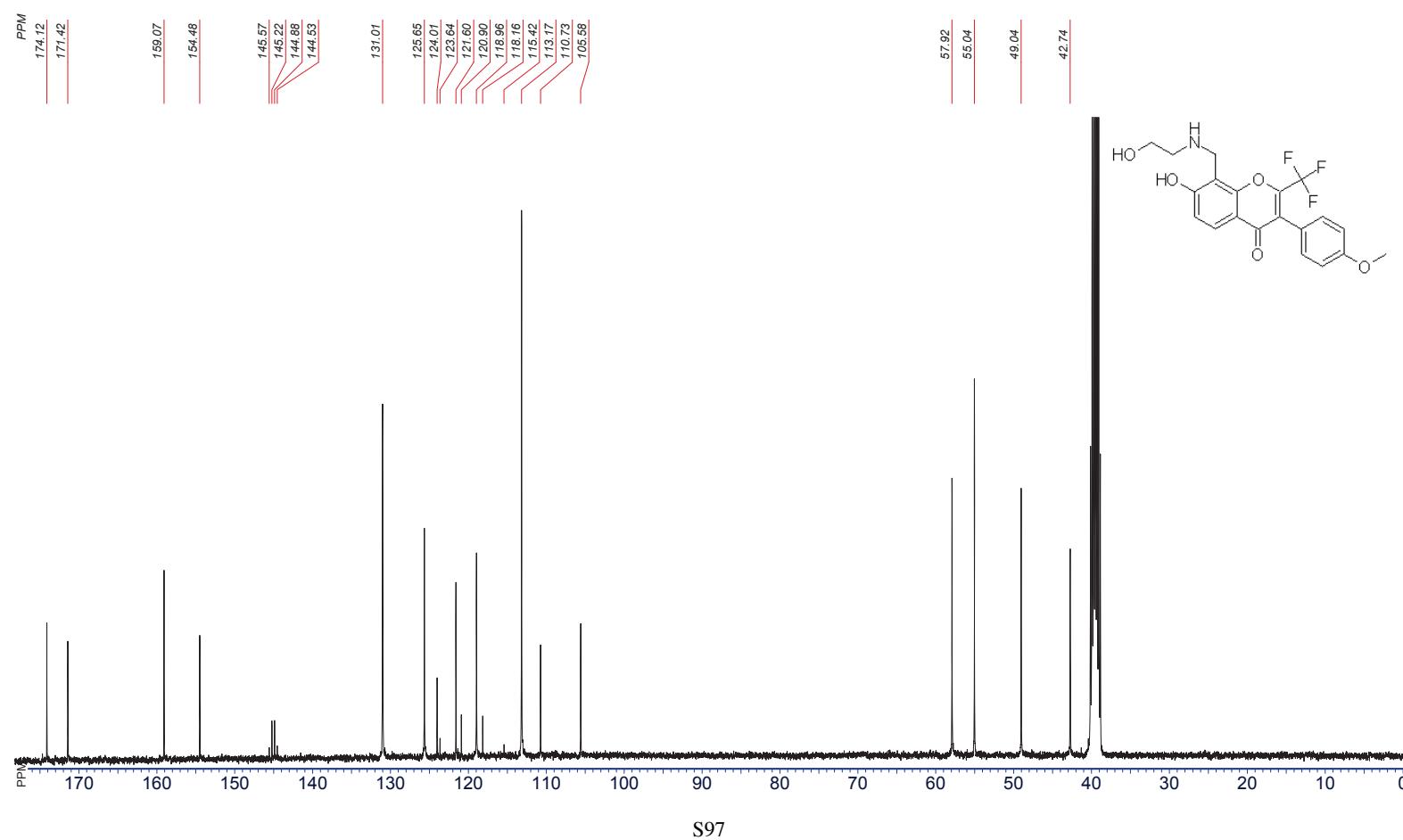
¹³C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-2-methyl-4H-chromen-4-one hydrochloride (**6f, n = 1**) in D₂O



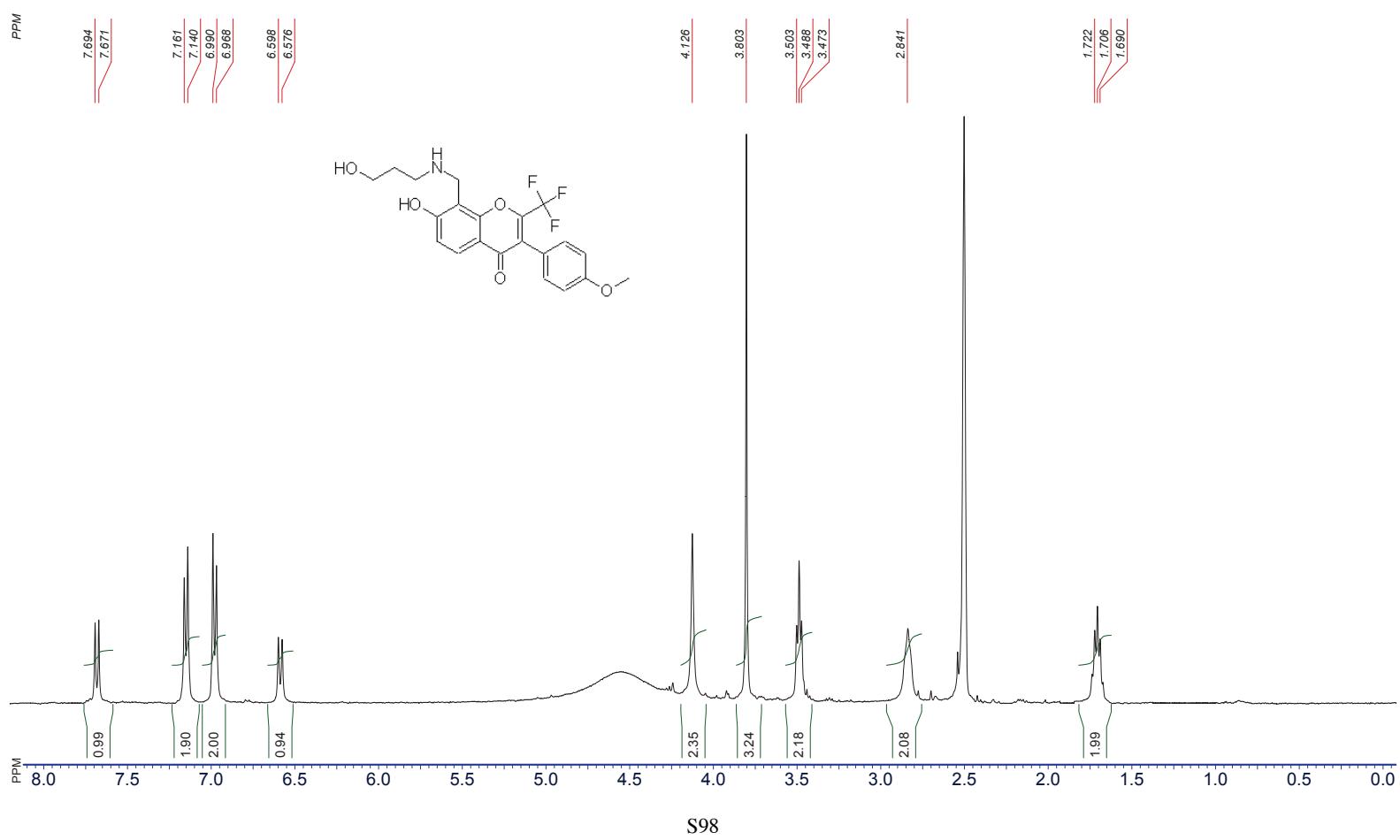
¹H NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-2-(trifluoromethyl)-4*H*-chromen-4-one (**6g, n = 1**) in DMSO-d₆



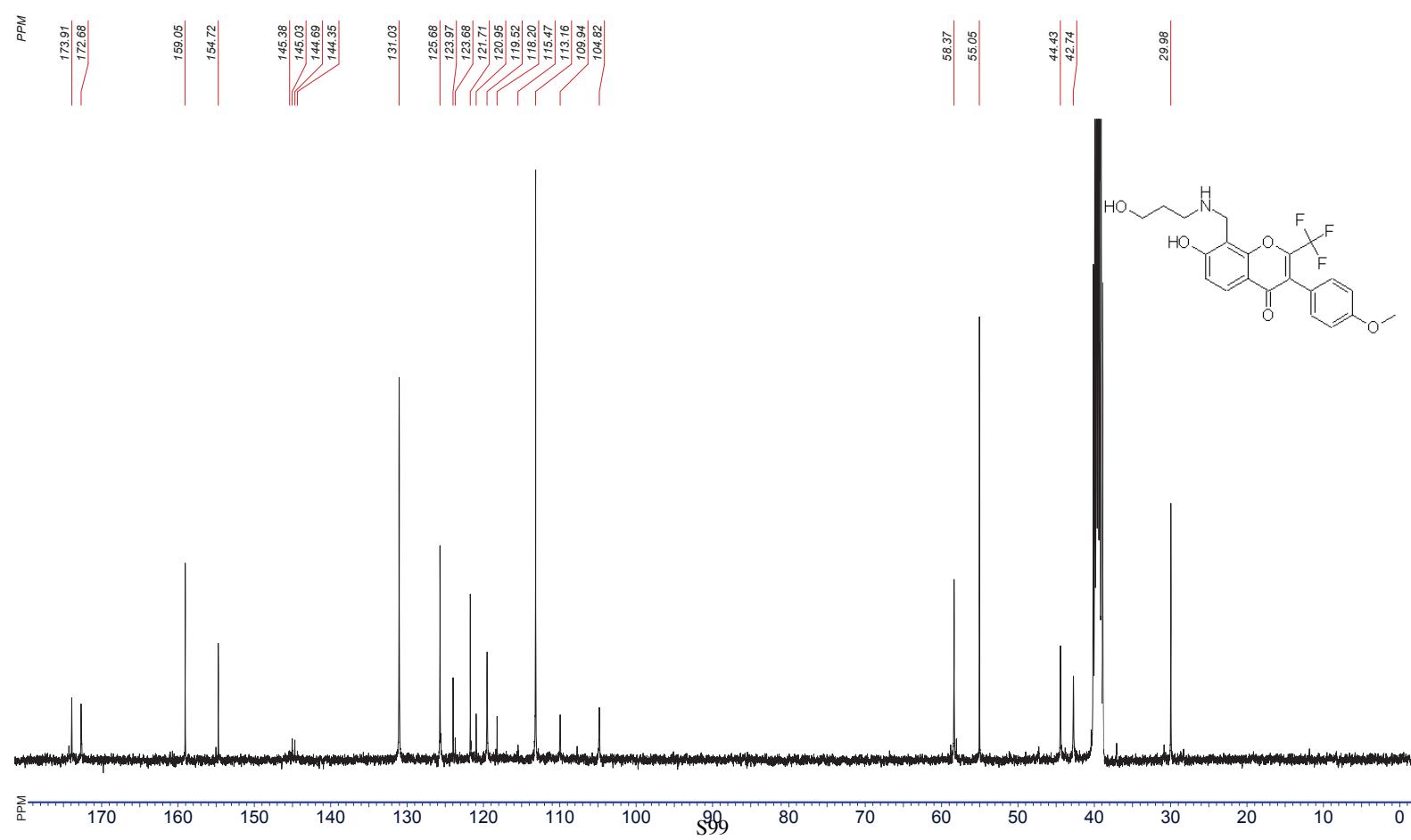
¹³C NMR spectrum of 7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-3-(4-methoxyphenyl)-2-(trifluoromethyl)-4H-chromen-4-one (**6g, n = 1**) in DMSO-d₆



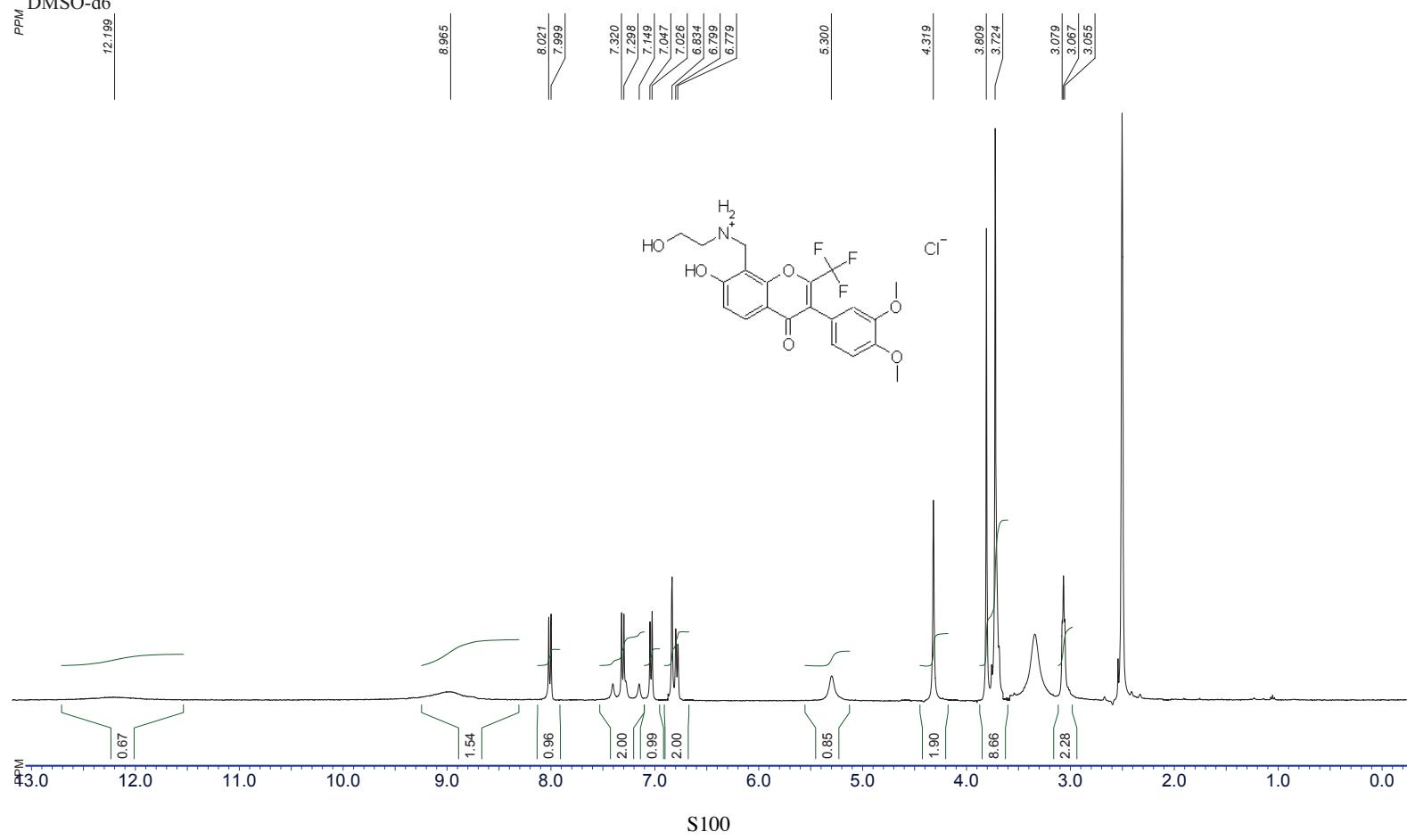
¹H NMR spectrum of 7-hydroxy-8-[(3-hydroxypropyl)amino]methyl-3-(4-methoxyphenyl)-2-(trifluoromethyl)-4H-chromen-4-one (**6g, n = 2**) in DMSO-d₆



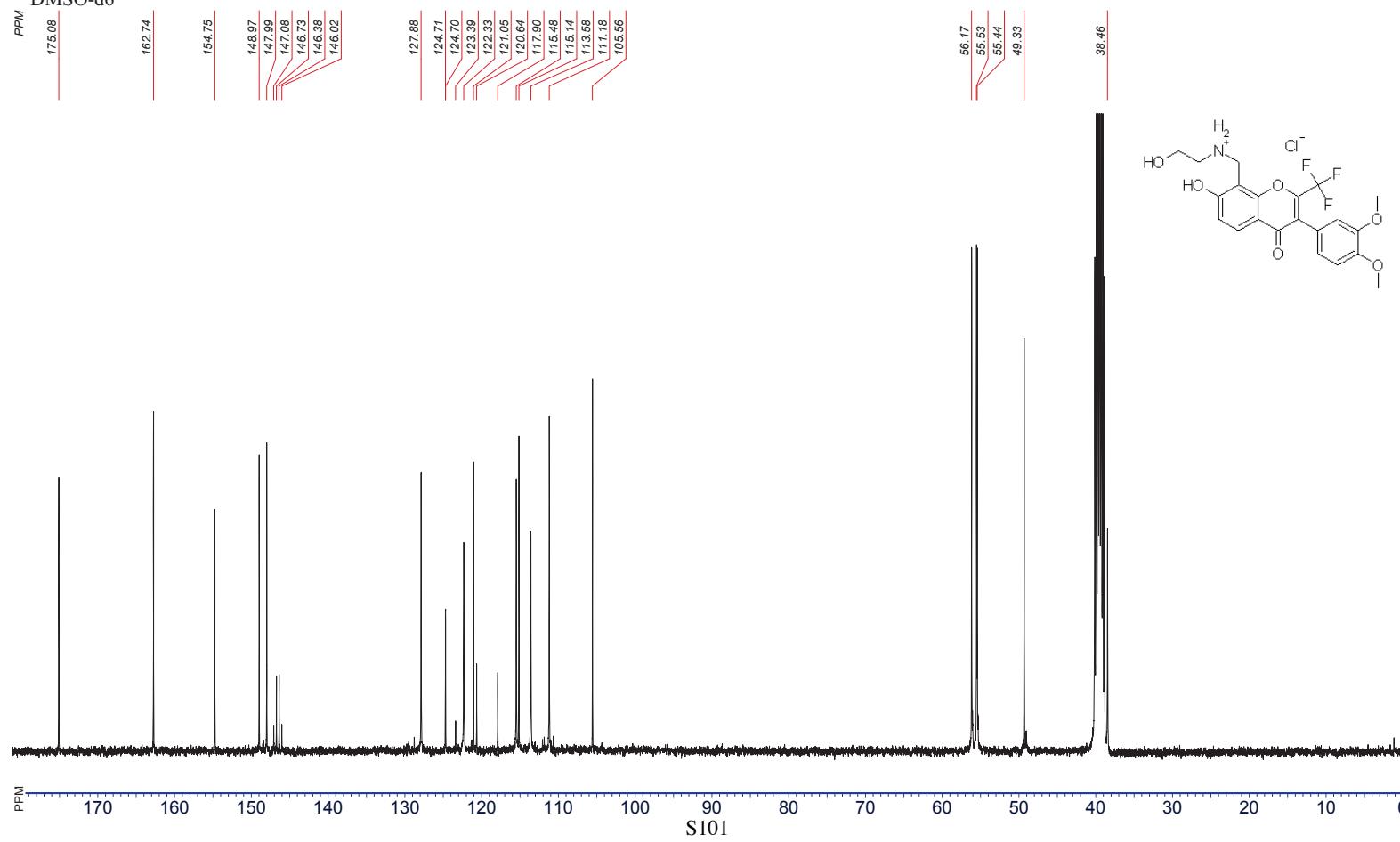
¹³C NMR spectrum of 7-hydroxy-8-{{[(3-hydroxypropyl)amino]methyl}-3-(4-methoxyphenyl)-2-(trifluoromethyl)-4H-chromen-4-one (**6g, n = 2**) in DMSO-d₆



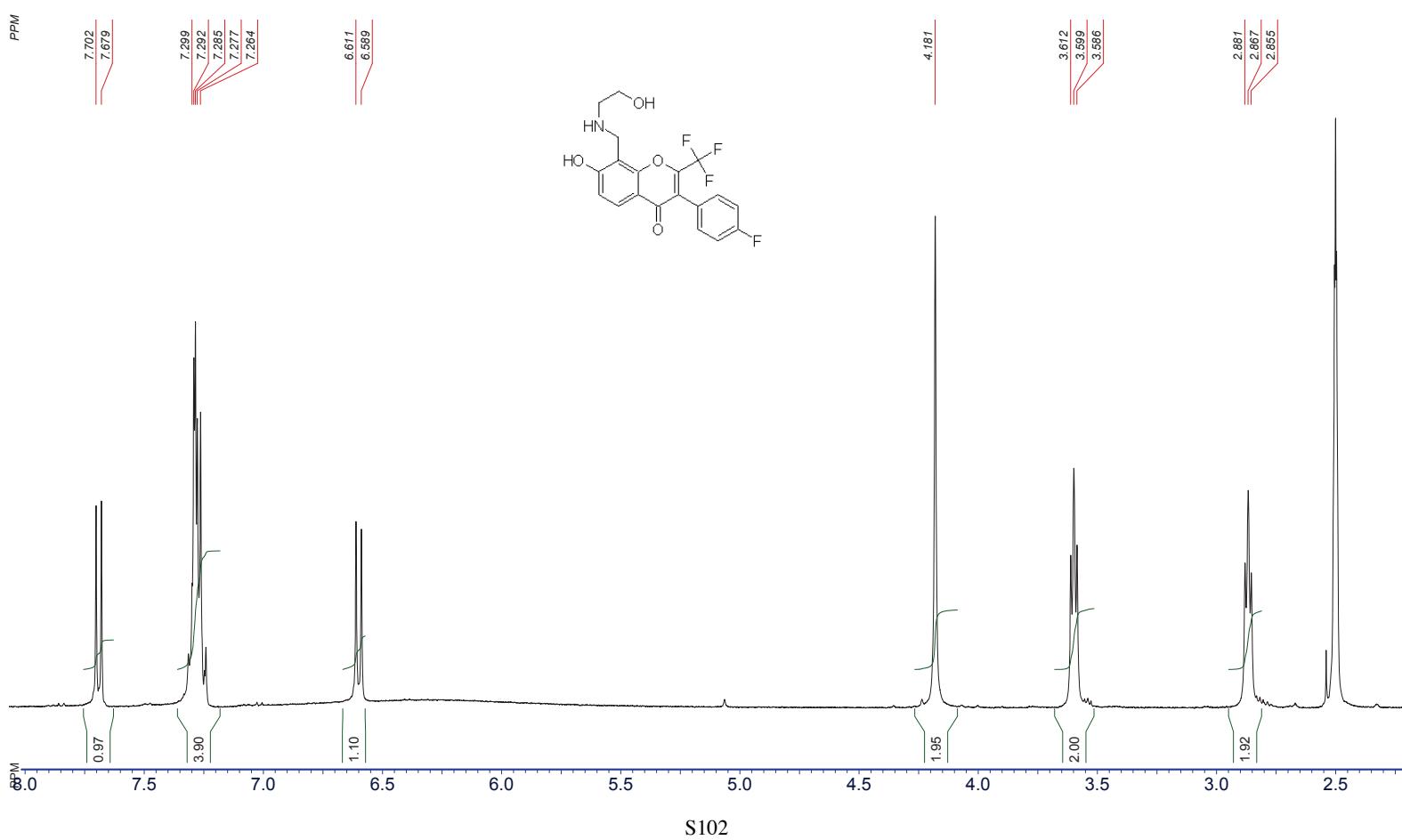
¹H NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-{[(2-hydroxyethyl)amino]methyl}-2-(trifluoromethyl)-4*H*-chromen-4-one hydrochloride (**6h, n = 1**) in DMSO-d₆



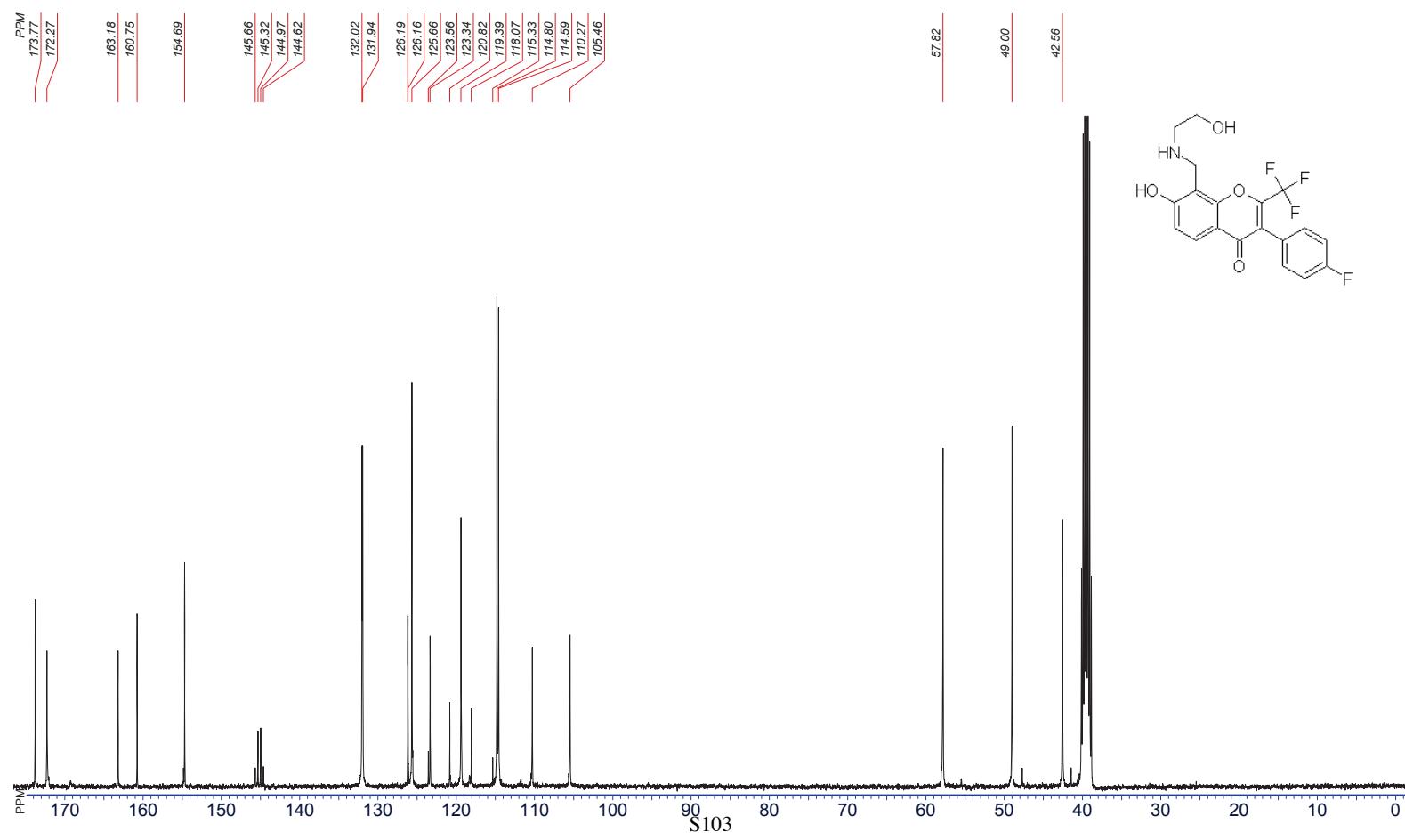
¹³C NMR spectrum of 3-(3,4-dimethoxyphenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-2-(trifluoromethyl)-4H-chromen-4-one hydrochloride (**6h, n = 1**) in DMSO-d₆



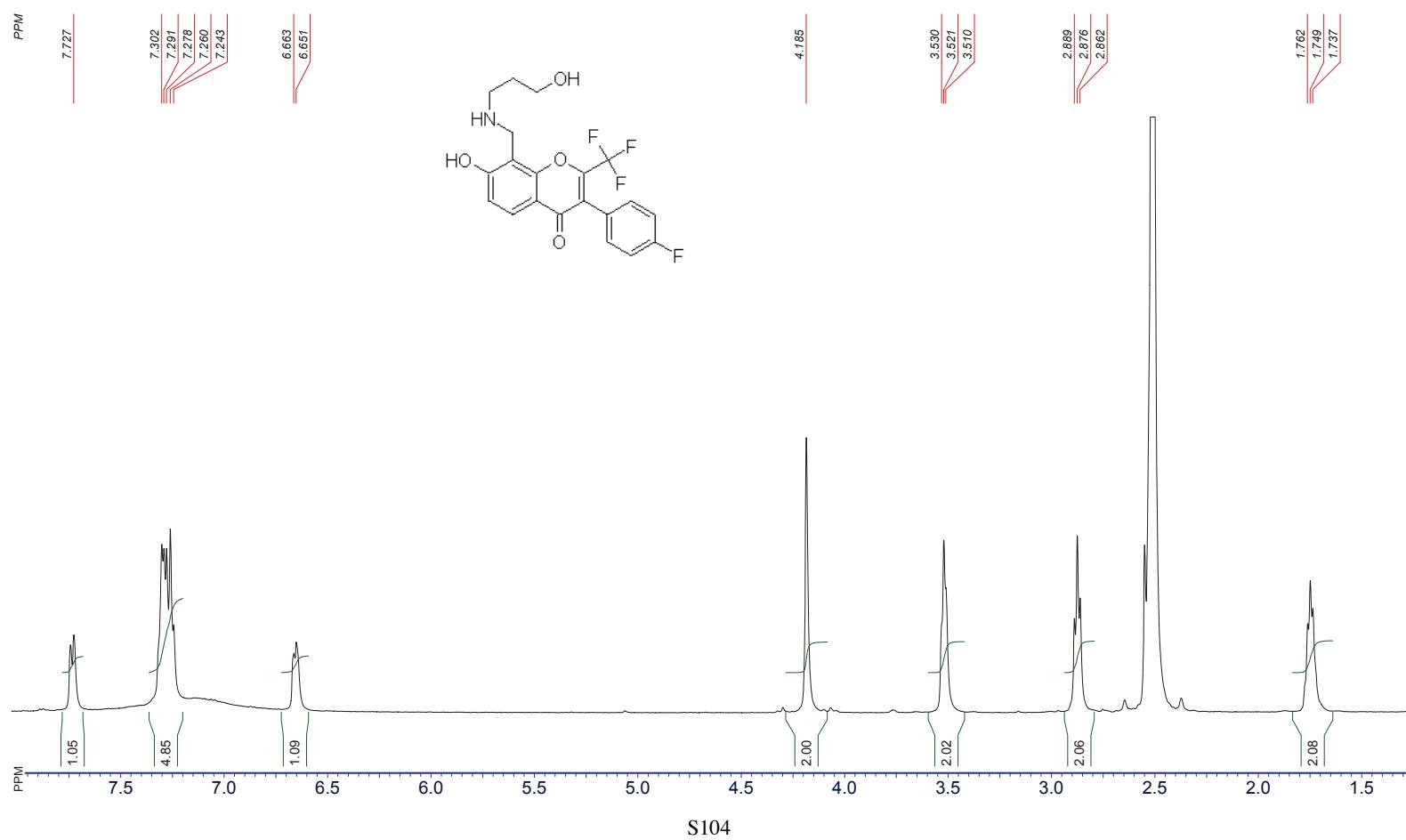
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl-2-(trifluoromethyl)-4H-chromen-4-one (**6i**, **n = 1**) in DMSO-d₆



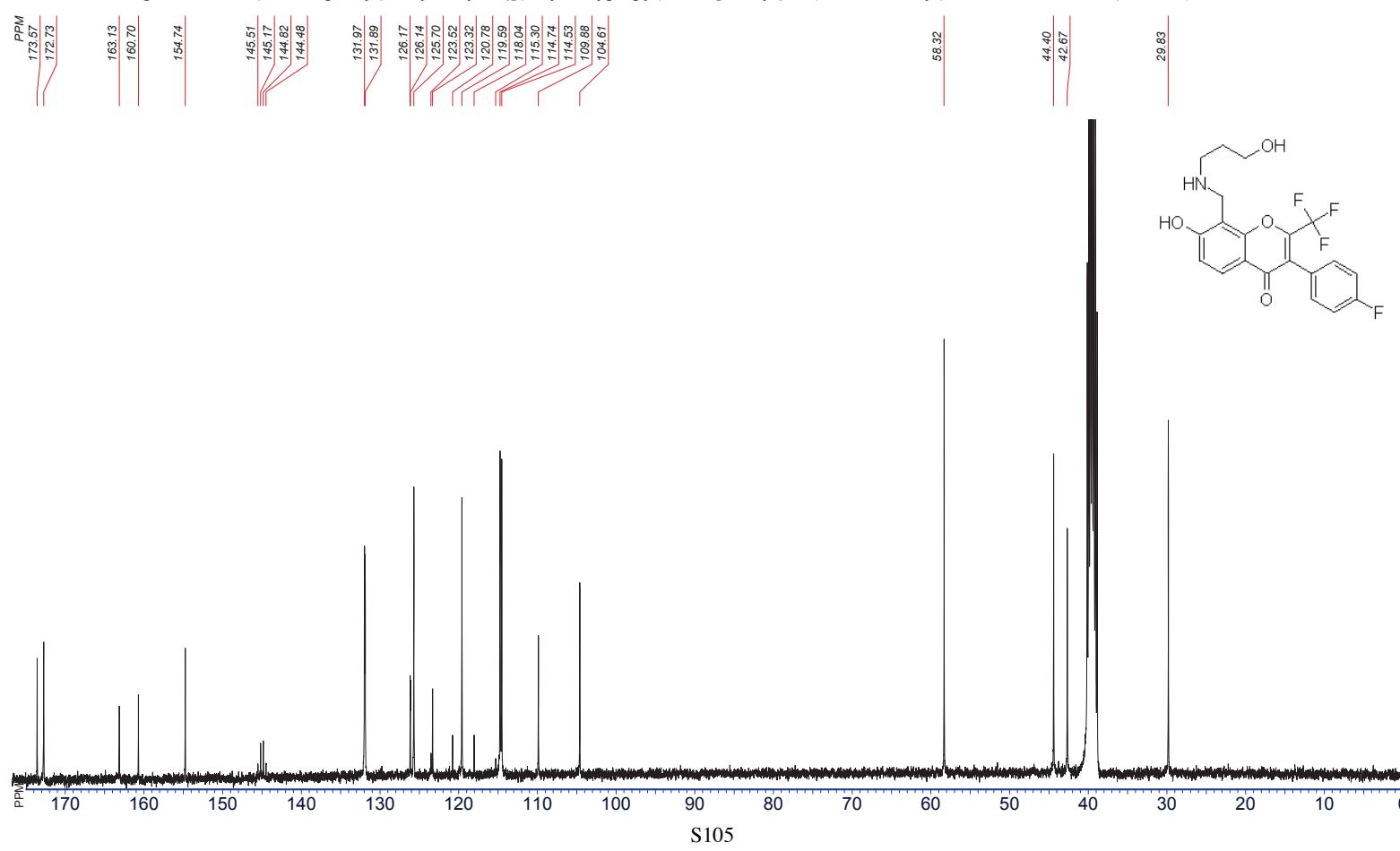
¹³C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(2-hydroxyethyl)amino]methyl]-2-(trifluoromethyl)-4H-chromen-4-one (**6i, n = 1**) in DMSO-d₆



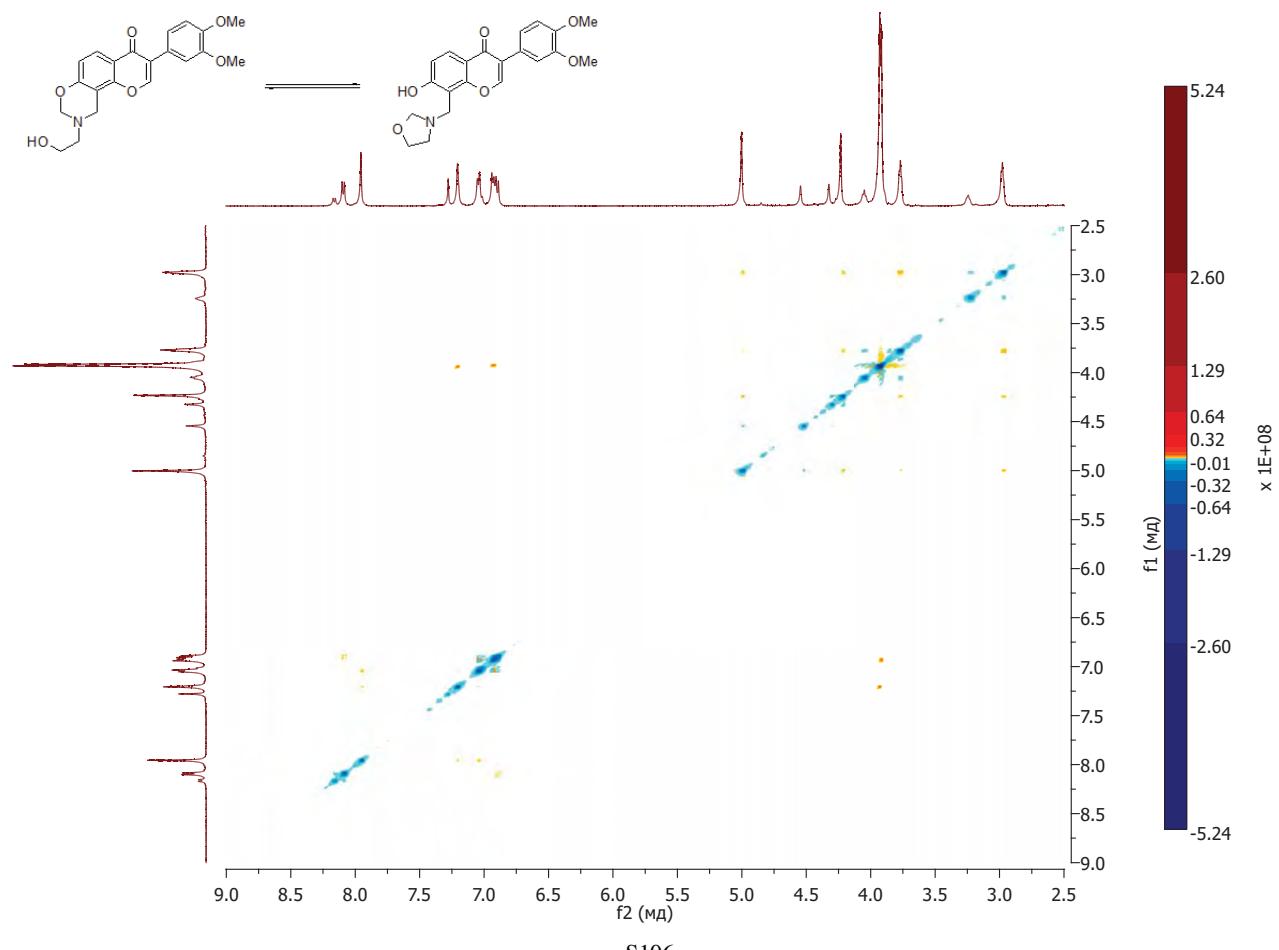
¹H NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-[(3-hydroxypropyl)amino]methyl-2-(trifluoromethyl)-4H-chromen-4-one (**6i, n = 2**) in DMSO-d₆



¹³C NMR spectrum of 3-(4-fluorophenyl)-7-hydroxy-8-{{[(3-hydroxypropyl)amino]methyl}-2-(trifluoromethyl)-4H-chromen-4-one (**6i, n = 2**) in DMSO-d₆



2D NOESY spectrum of **4b, n = 1** in CDCl_3



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