

SUPPORTING INFORMATION

Diastereoselective Synthesis of Functionalised Carbazoles via a Sequential Diels-Alder/Ene Reaction

Strategy

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General experimental information

S4

¹H and ¹³C NMR Spectra:

2a - (3aS*,10aS*,10bS*)-2-methyl-10-tosyl-4,10,10a,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione	S5
2b - 2-phenyl-11-tosyl-11,11a-dihydro-1H,5H-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4-b]indole-1,3(2H)-dione	S7
2c - ethyl 3-((3aS*,4R*,10aS*,10bS*)-2-methyl-1,3-dioxo-10-tosyl-1,2,3,3a,4,10,10a,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S9
2d - ethyl 3-((3aS*,4R*,10aS*,10bS*)-1,3-dioxo-10-tosyl-1,2,3,3a,4,10,10a,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S11
2e - ethyl 3-((3aS*,4R*,10aS*,10bS*)-1,3-dioxo-2-phenyl-10-tosyl-1,2,3,3a,4,10,10a,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S13
3a - (3aS*,5S*,10bS*)-5-(hydroxy(phenyl)amino)-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione	S15
3b - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione	S17
3c - (3aS*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione	S19
3d - (3aS*,5S*,10bS*)-5-((<i>S</i> *)-hydroxy(perfluorophenyl)methyl)-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione and (3aS*,5S*,10bS*)-5-((<i>R</i> *)-hydroxy(perfluorophenyl)methyl)-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione	S21
3e - 6-(hydroxy(phenyl)amino)-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4-b]indole-1,3(2H,11H)-dione	S23
3f - 6-(hydroxy(<i>o</i> -tolyl)amino)-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4-b]indole-1,3(2H,11H)-dione	S25
3g - ethyl 3-((3aS*,4S*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-2-methyl-1,3-dioxo-10-tosyl-1,2,3,3a,4,5,10,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S27
3h - ethyl 3-((3aS*,4S*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-1,3-dioxo-2-phenyl-10-tosyl-1,2,3,3a,4,5,10,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S29
3i - ethyl 3-((3aS*,4S*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methyl-1,3-dioxo-10-tosyl-1,2,3,3a,4,5,10,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S31
3j - ethyl 3-((3aS*,4S*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-1,3-dioxo-10-tosyl-1,2,3,3a,4,5,10,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate	S33

3k - (3aS*,5S*,10bS*)-5-(hydroxy(phenyl)amino)-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S35
3l - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S37
3m - (3aS*,5S*,10bS*)-5-((<i>S</i> *)-hydroxy(perfluorophenyl)methyl)-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S39
3n - (3aS*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S41
3o - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-7-methoxy-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S43
3p - (3aS*,5S*,10bS*)-5-((<i>S</i> *)-hydroxy(perfluorophenyl)methyl)-7-methoxy-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione and (3aS*,5S*,10bS*)-5-((<i>R</i> *)-hydroxy(perfluorophenyl)methyl)-7-methoxy-2-methyl-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S45
3q - (3aS*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-7-methoxy-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2H,3a <i>H</i>)-dione	S47
3r - 6-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2H,11 <i>H</i>)-dione	S49
3s - 6-(hydroxy(<i>o</i> -tolyl)amino)-8-methoxy-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2H,11 <i>H</i>)-dione	S51
3t - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)- <i>N,N</i> ,2-trimethyl-1,3-dioxo-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S53
3u - (3aS*,5S*,10bS*)-5-((2,6-dibromophenyl)(hydroxy)amino)- <i>N,N</i> -dimethyl-1,3-dioxo-2-phenyl-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S55
3v - (3aS*,5S*,10bS*)-5-((<i>S</i> *)-hydroxy(perfluorophenyl)methyl)- <i>N,N</i> -dimethyl-1,3-dioxo-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S57
3w - 6-(hydroxy(<i>o</i> -tolyl)amino)- <i>N,N</i> -dimethyl-1,3-dioxo-2-phenyl-2,3,5,6-tetrahydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-11(1 <i>H</i>)-sulfonamide	S59
3x - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)- <i>N,N</i> -dimethyl-1,3-dioxo-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S61
3y - (3aS*,5S*,10bS*)-benzyl 5-(hydroxy(phenyl)amino)-2-methyl-1,3-dioxo-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-carboxylate	S63
3z - (3aS*,5S*,10bS*)-benzyl 5-(hydroxy(<i>o</i> -tolyl)amino)-2-methyl-1,3-dioxo-1,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-carboxylate	S65
3aa - (3aS*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methyl-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S67
3bb - benzyl (3aS*,5S*,10bS*)-5-(hydroxy(phenyl)amino)-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S69
3cc - benzyl (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S71
3dd - benzyl (3aS*,5S*,10bS*)-5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S73
3ee - benzyl (<i>R</i> *)-6-(hydroxy(phenyl)amino)-1,3-dioxo-2-phenyl-2,3,5,6-tetrahydro-1 <i>H</i> ,11 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-11-carboxylate	S75
3ff - benzyl (<i>R</i> *)-6-(hydroxy(<i>o</i> -tolyl)amino)-1,3-dioxo-2-phenyl-2,3,5,6-tetrahydro-1 <i>H</i> ,11 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-11-carboxylate	S77
3gg - benzyl (3aS*,5S*,10bS*)-5-(hydroxy(phenyl)amino)-7-methoxy-2-methyl-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S79
3hh - benzyl (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-7-methoxy-2-methyl-	S81

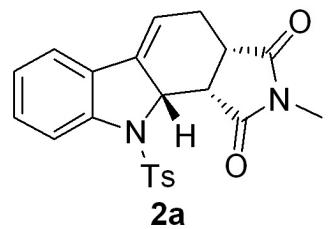
1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate 3ii - benzyl (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(phenyl)amino)-7-methoxy-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S83
3jj - benzyl (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(<i>o</i> -tolyl)amino)-7-methoxy-1,3-dioxo-2,3,3a,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(1 <i>H</i>)-carboxylate	S85
3kk - benzyl (<i>R</i> [*])-6-(hydroxy(phenyl)amino)-8-methoxy-1,3-dioxo-2-phenyl-2,3,5,6-tetrahydro-1 <i>H</i> ,11 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-11-carboxylate	S87
3ll - benzyl (<i>R</i> [*])-6-(hydroxy(<i>o</i> -tolyl)amino)-8-methoxy-1,3-dioxo-2-phenyl-2,3,5,6-tetrahydro-1 <i>H</i> ,11 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-11-carboxylate	S89
4a - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S91
4b - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-ethoxy-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S93
4c - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(phenyl)amino)-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S95
4d - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(<i>o</i> -tolyl)amino)-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S97
4e - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S99
4f - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(phenyl)amino)-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S101
4g - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(<i>o</i> -tolyl)amino)-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S103
4h - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S105
4i - (<i>R</i> [*])-6-(hydroxy(phenyl)amino)-2-phenyl-6,11-dihydro-1 <i>H</i> ,5 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i>)-dione	S107
4j - (<i>R</i> [*])-6-(hydroxy(<i>o</i> -tolyl)amino)-2-phenyl-6,11-dihydro-1 <i>H</i> ,5 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i>)-dione	S109
4k - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(phenyl)amino)-7-methoxy-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S111
4l - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(<i>o</i> -tolyl)amino)-7-methoxy-2-methyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S113
4m - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(phenyl)amino)-7-methoxy-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S115
4n - (3a <i>S</i> ^{*,5<i>S</i>^{*,10b<i>S</i>[*]}} -5-(hydroxy(<i>o</i> -tolyl)amino)-7-methoxy-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S117
4o - (<i>R</i> [*])-6-(hydroxy(phenyl)amino)-8-methoxy-2-phenyl-6,11-dihydro-1 <i>H</i> ,5 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i>)-dione	S119
4p - (<i>R</i> [*])-6-(hydroxy(<i>o</i> -tolyl)amino)-8-methoxy-2-phenyl-6,11-dihydro-1 <i>H</i> ,5 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i>)-dione	S121

Crystal Data and Structure Refinement Tables

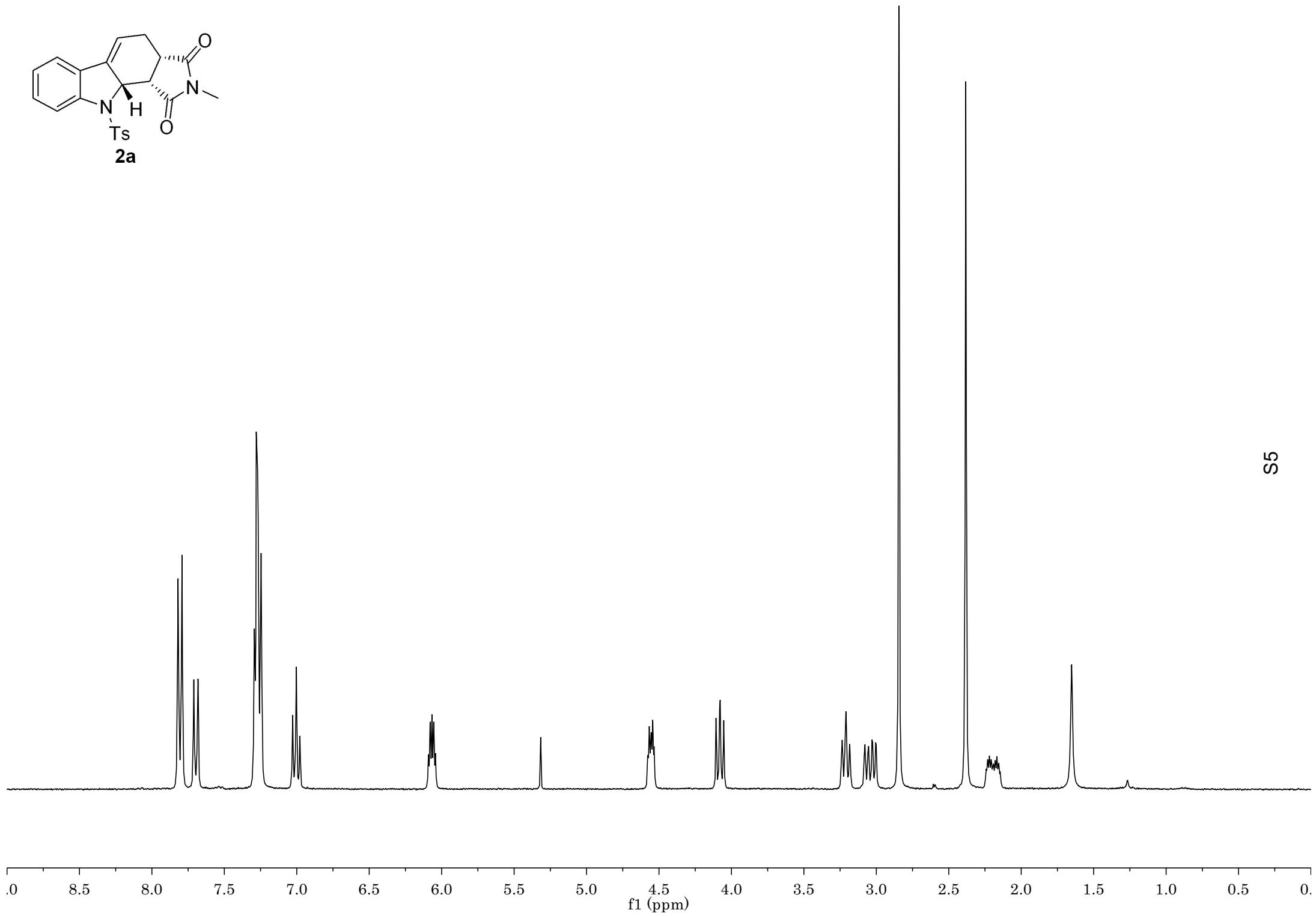
2a - (3aS*,10aS*,10bS*)-2-methyl-10-tosyl-4,10,10a,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S123
2b - 2-phenyl-11-tosyl-11,11 <i>a</i> -dihydro-1 <i>H</i> ,5 <i>H</i> -[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i>)-dione	S125
2d - ethyl 3-((3aS*,4 <i>R</i> *,10aS*,10bS*)-1,3-dioxo-10-tosyl-1,2,3,3 <i>a</i> ,4,10,10a,10b-octahydropyrrolo[3,4- <i>a</i>]carbazol-4-yl)propanoate	S127
3l - (3aS*,5S*,10bS*)-5-(hydroxy(<i>o</i> -tolyl)amino)-10-tosyl-4,5,10,10b-tetrahydropyrrolo[3,4- <i>a</i>]carbazole-1,3(2 <i>H</i> ,3 <i>aH</i>)-dione	S128
3r - 6-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4- <i>b</i>]indole-1,3(2 <i>H</i> ,11 <i>H</i>)-dione	S130
3u - (3aS*,5S*,10bS*)-5-((2,6-dibromophenyl)(hydroxy)amino)- <i>N,N</i> -dimethyl-1,3-dioxo-2-phenyl-1,3,3 <i>a</i> ,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S132
3v - (3aS*,5S*,10bS*)-5-((<i>S</i> *)-hydroxy(perfluorophenyl)methyl)- <i>N,N</i> -dimethyl-1,3-dioxo-1,3,3 <i>a</i> ,4,5,10b-hexahydropyrrolo[3,4- <i>a</i>]carbazole-10(2 <i>H</i>)-sulfonamide	S134

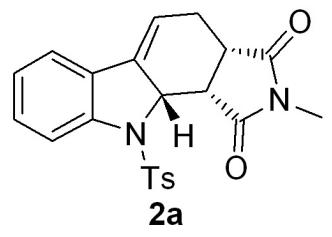
General experimental information

¹H and ¹³C NMR spectra were recorded directly with a Jeol Lambda 500 MHz, Jeol ECS-400 MHz or Bruker Avance 300 MHz. HRMS data were provided by the EPSRC National Mass Spectrometry Service (University of Swansea). X-ray diffraction data was obtained on an Oxford Diffraction Gemini. IR spectra were obtained as neat samples using a Varian 800 FT-IR Scimitar Series spectrometer scanning from 4000-600 cm⁻¹. THF and Et₂O were distilled from sodium/benzophenone and used directly. DCM was distilled from calcium hydride and used directly.

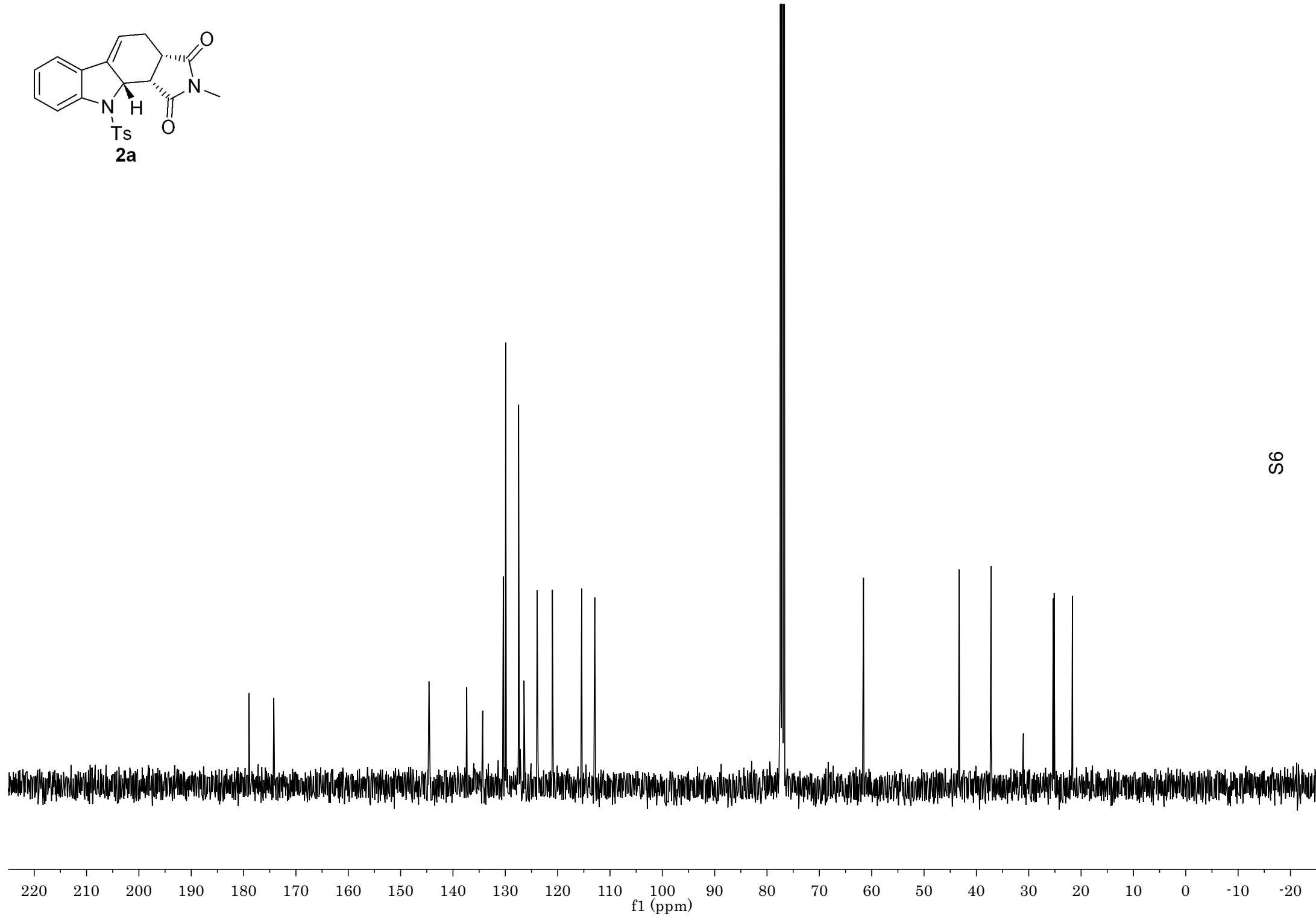


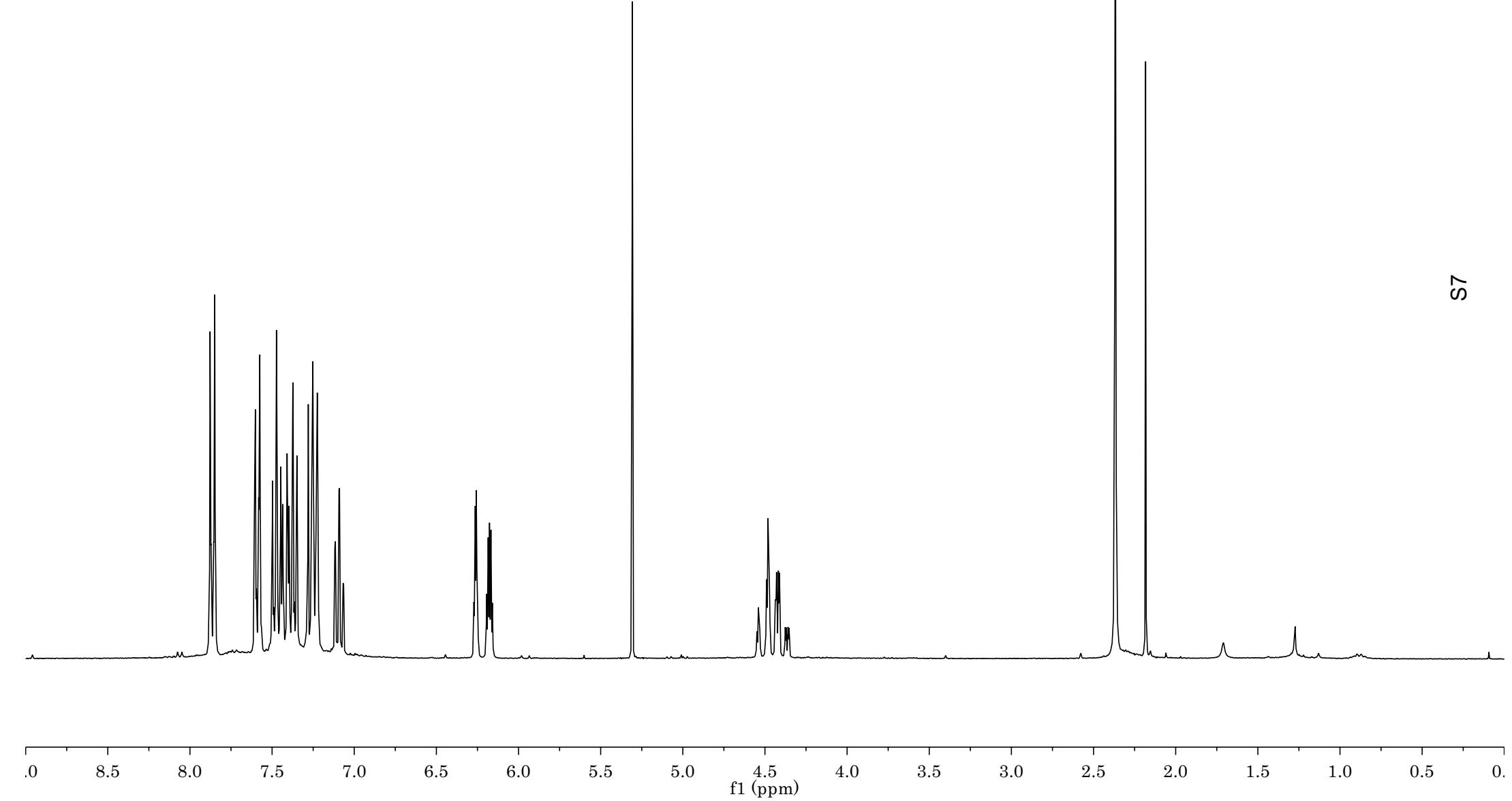
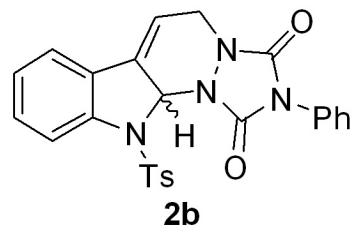
S5

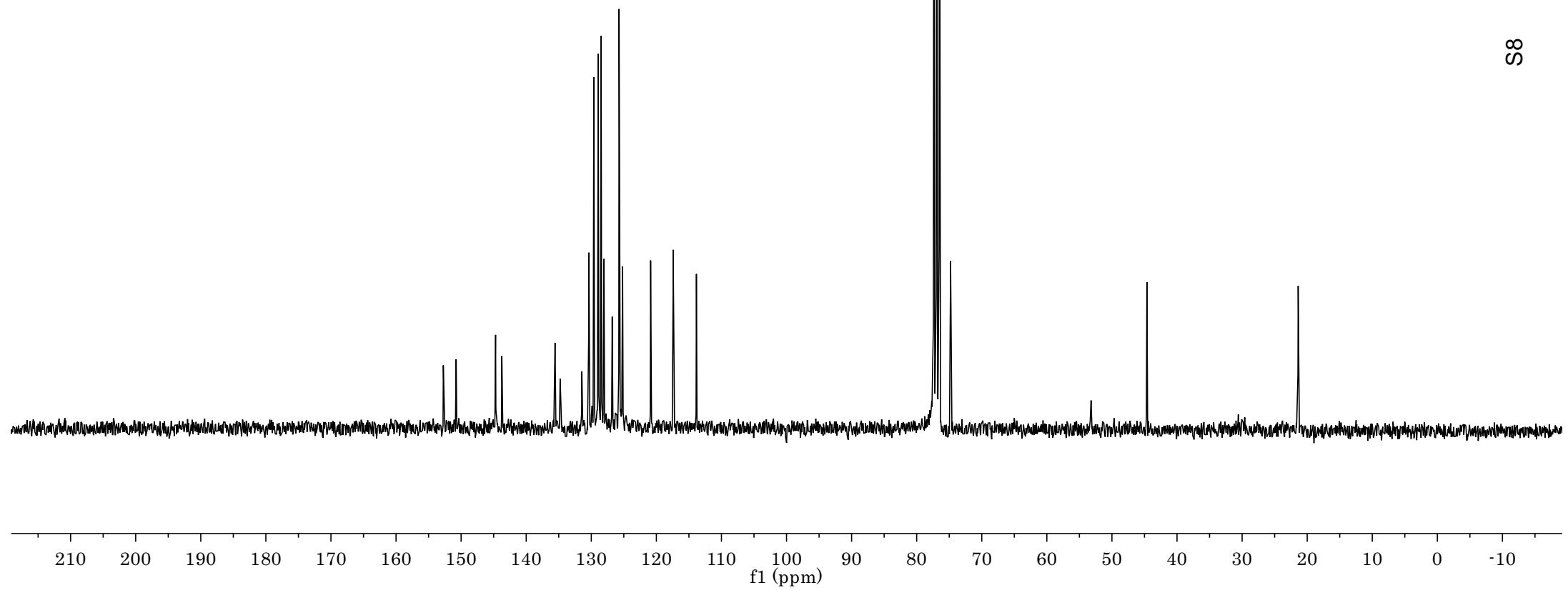
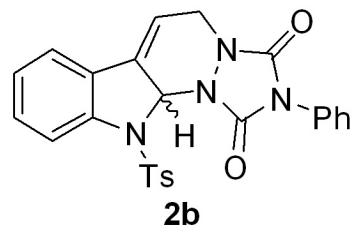


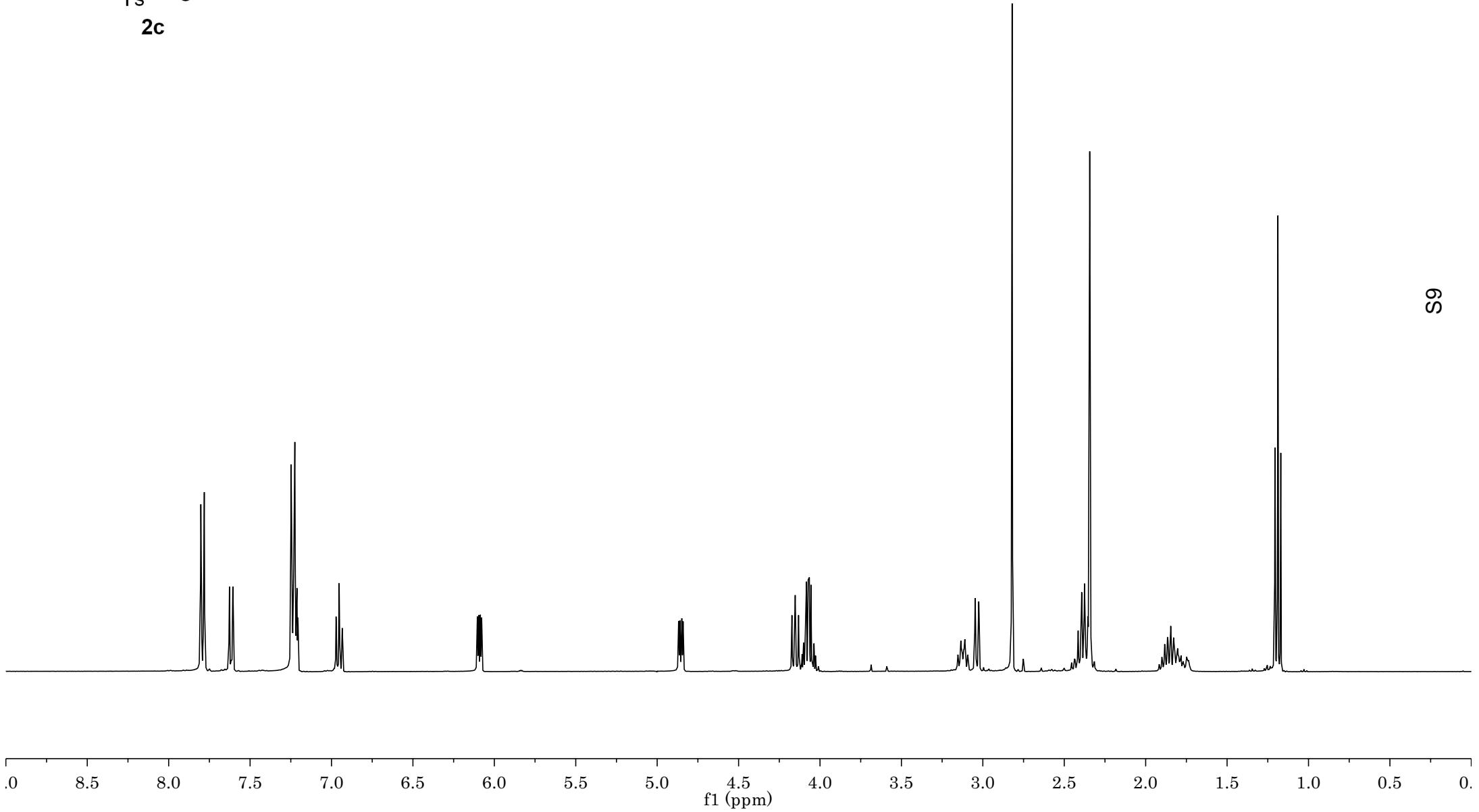
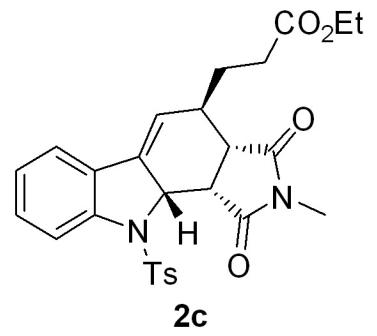


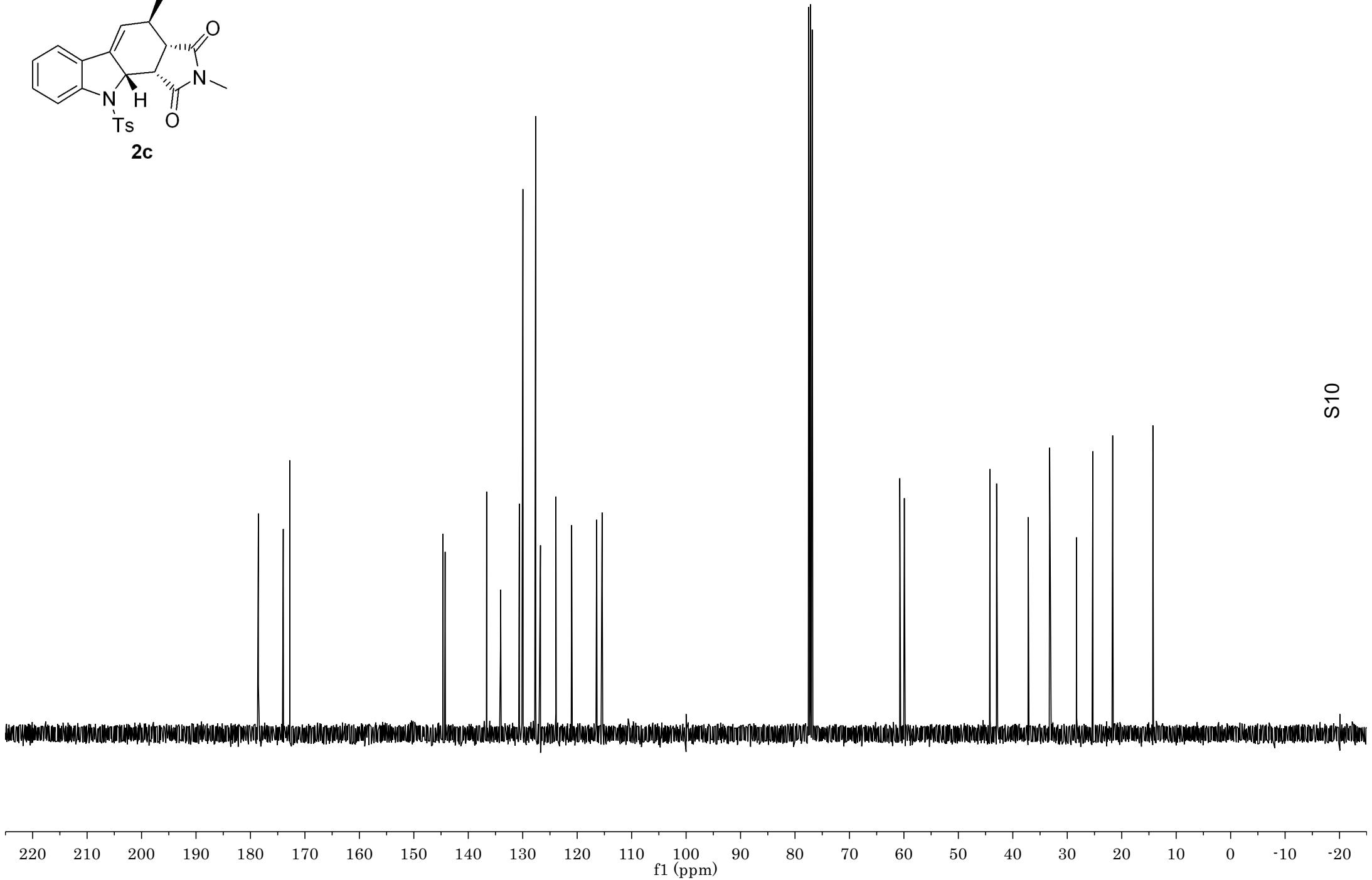
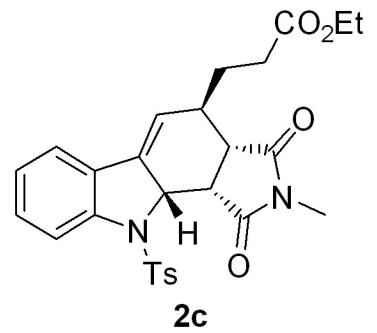
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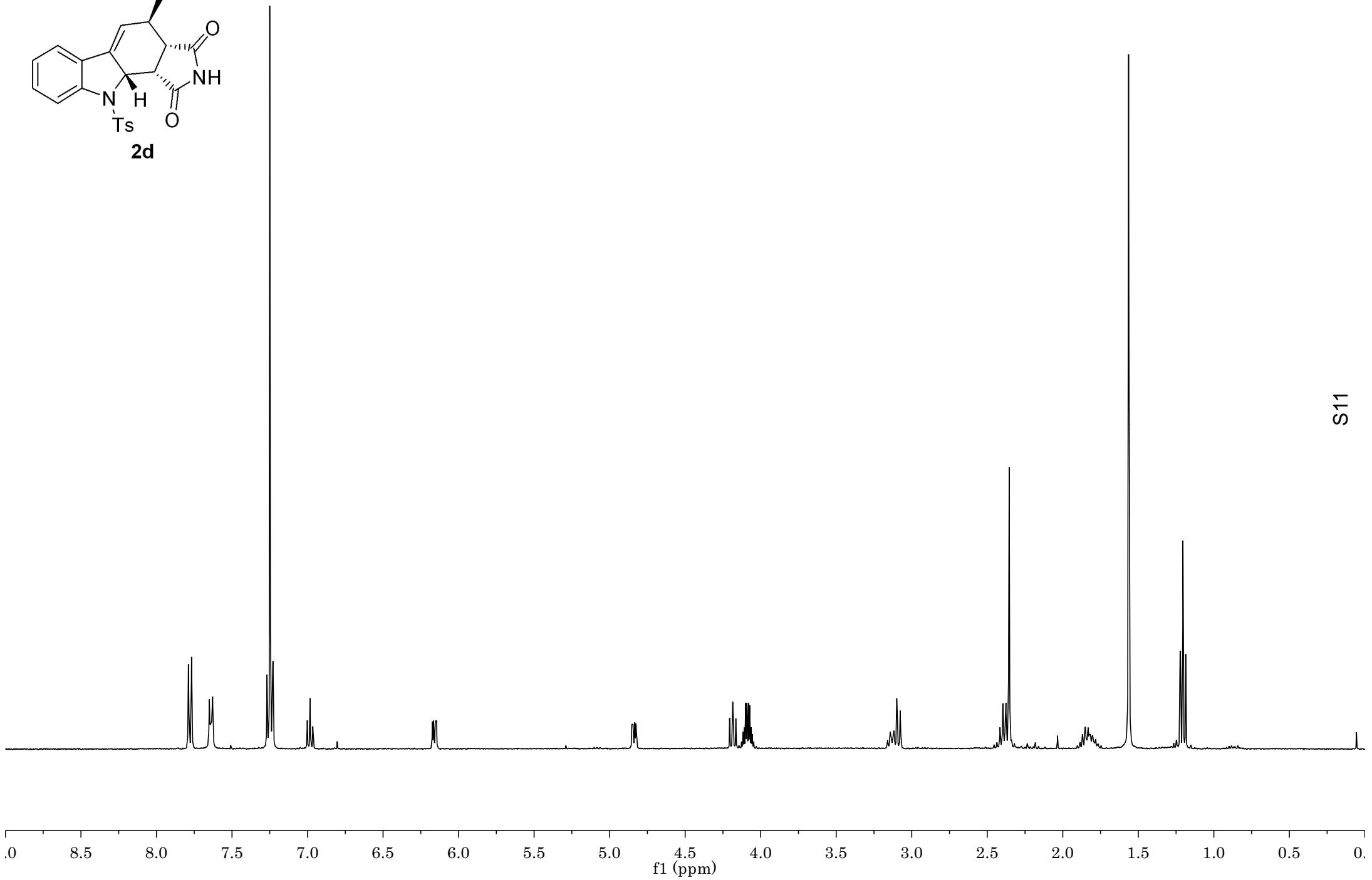
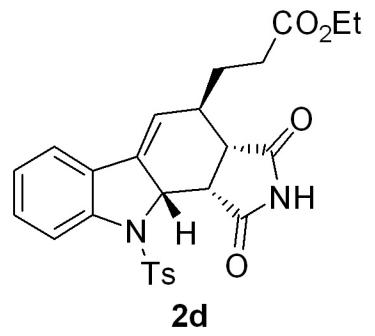


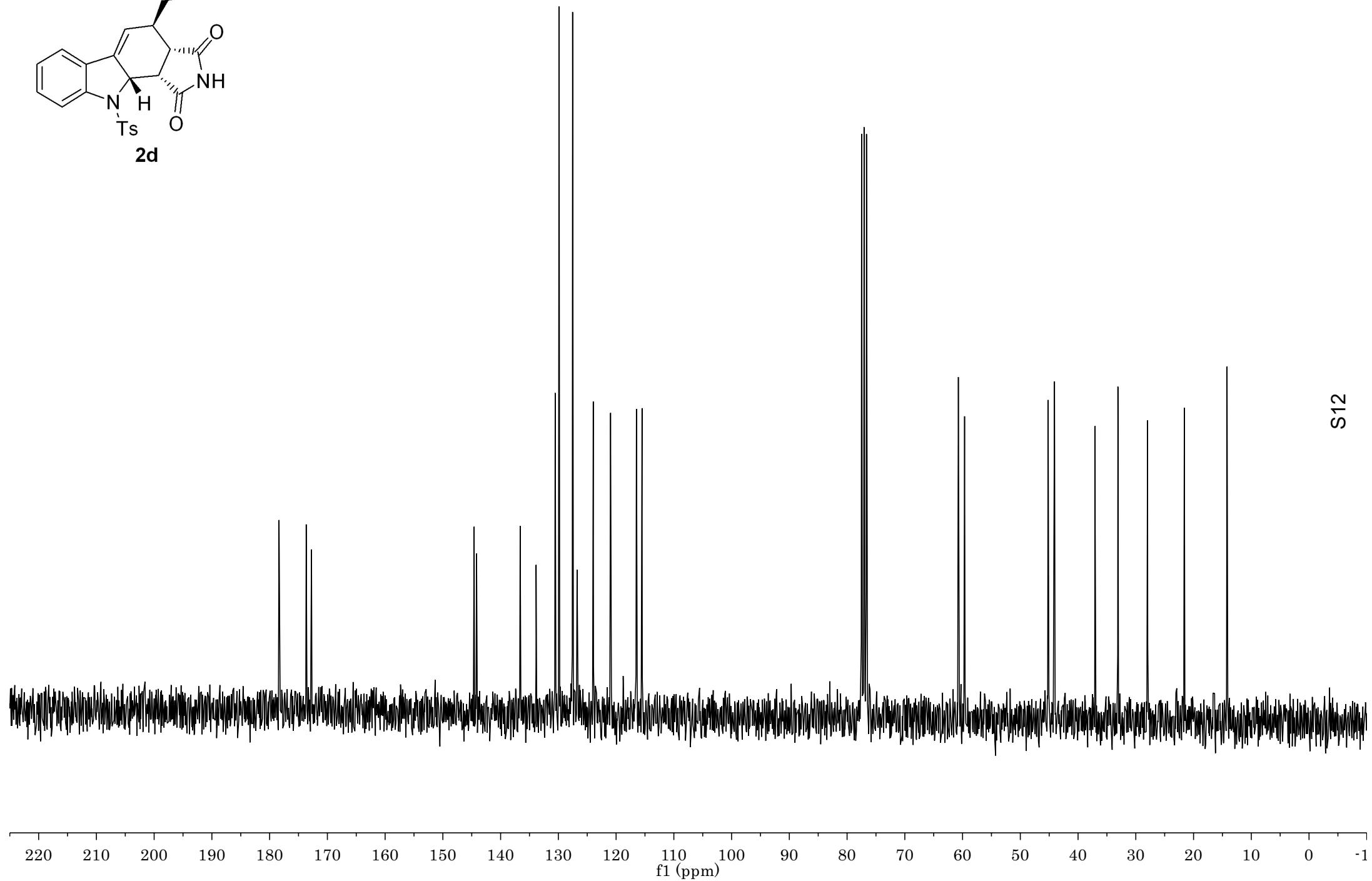
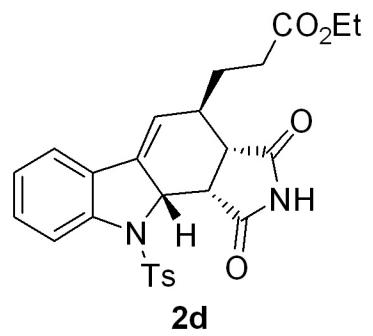


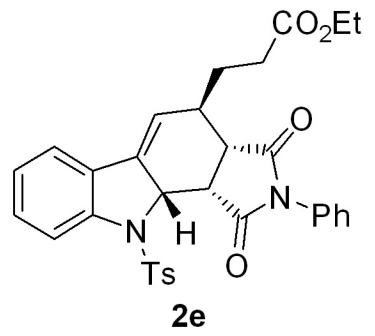




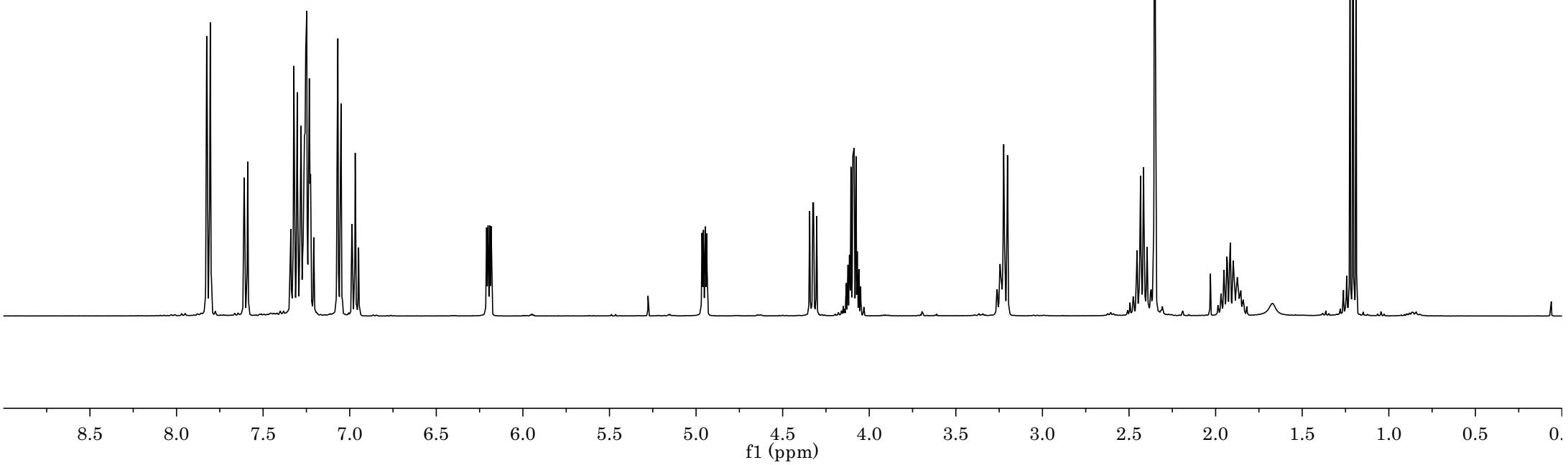


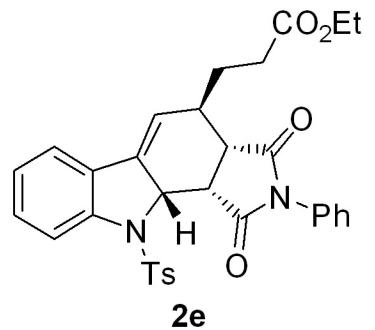




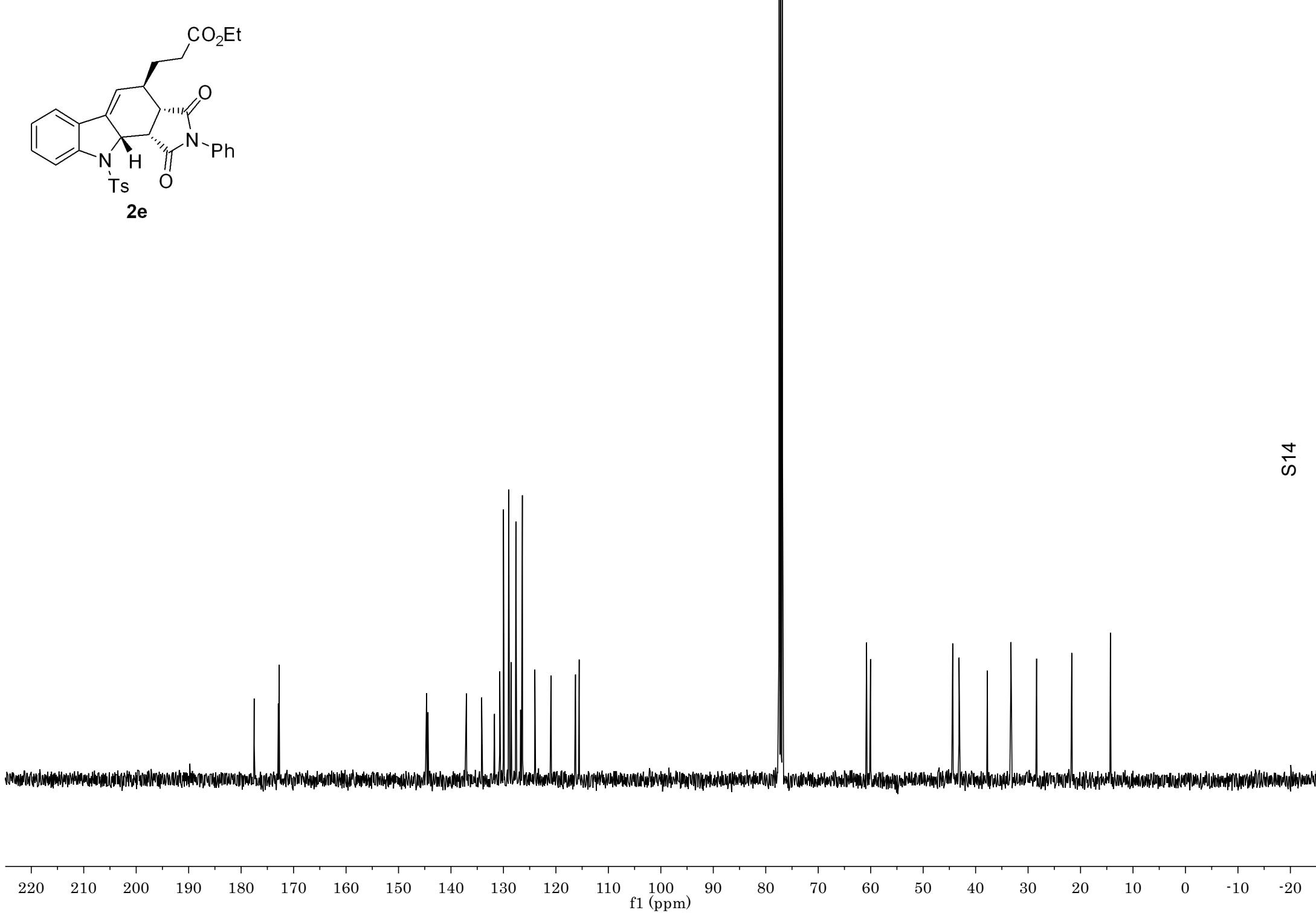


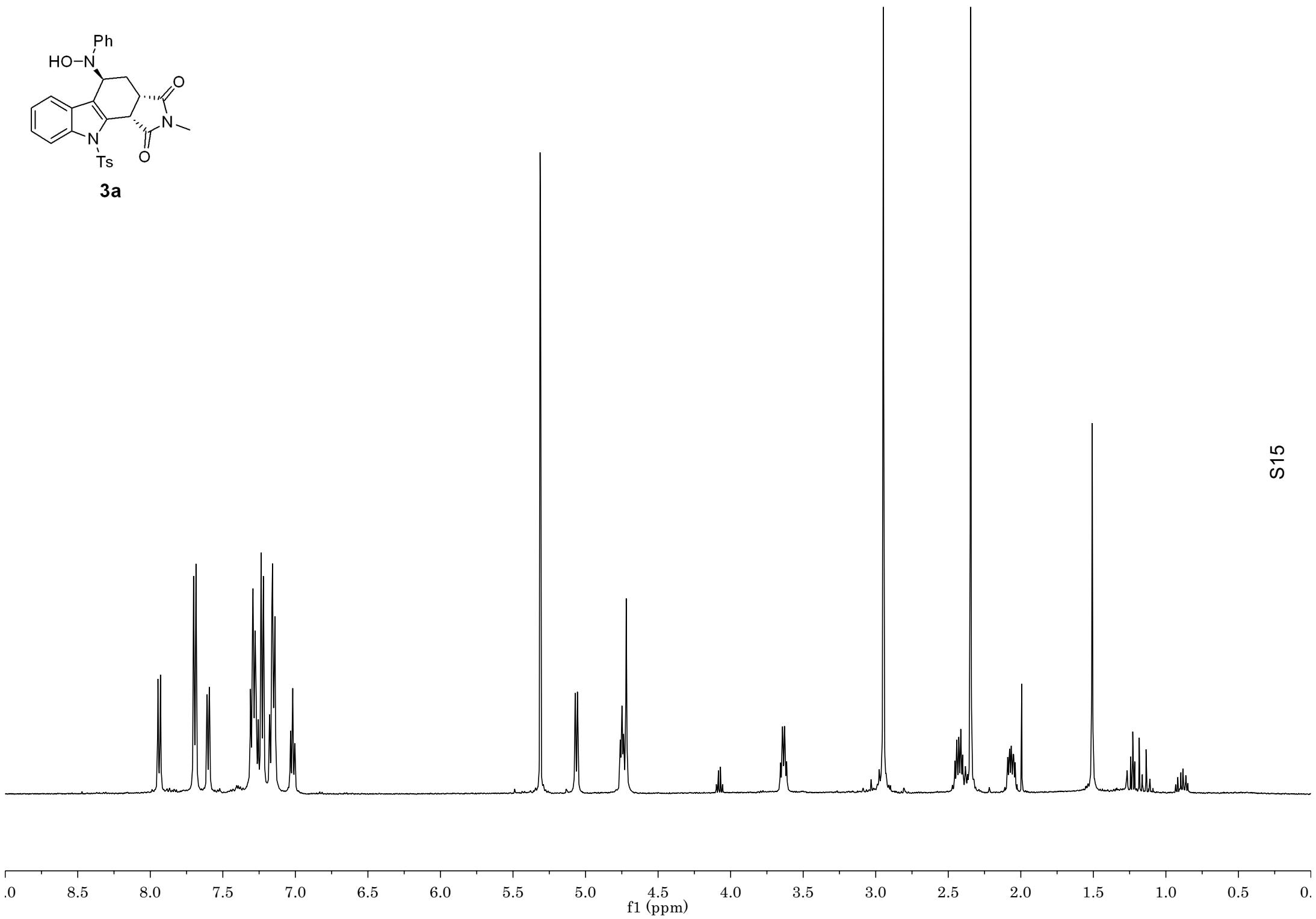
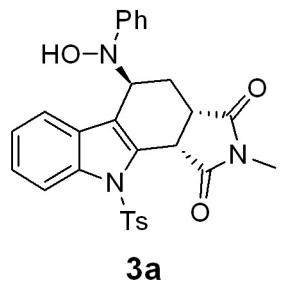
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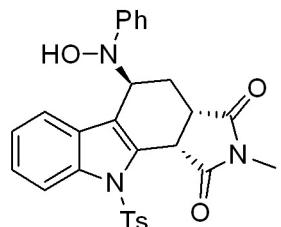




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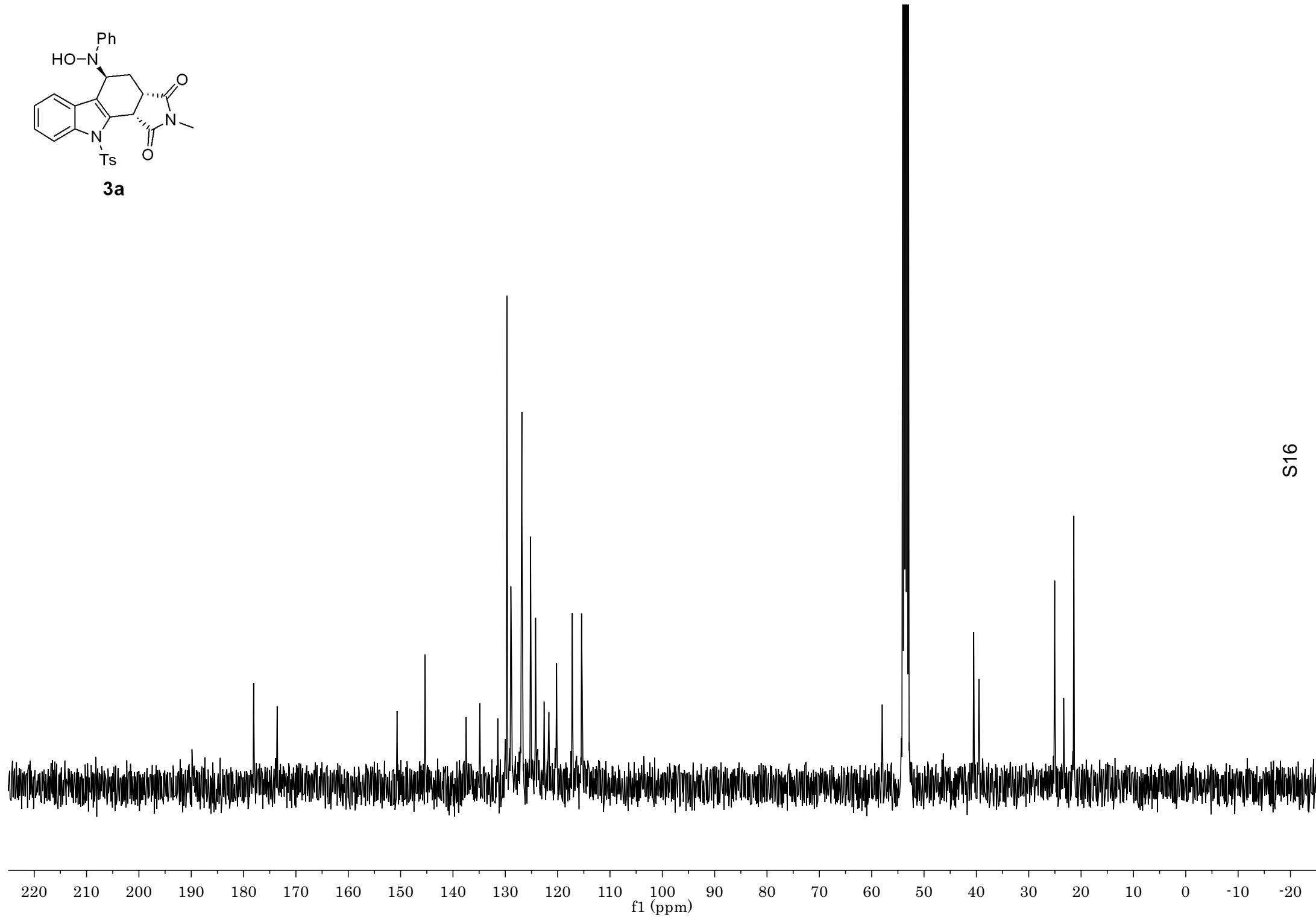


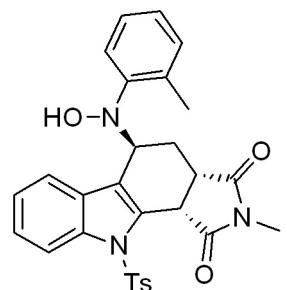




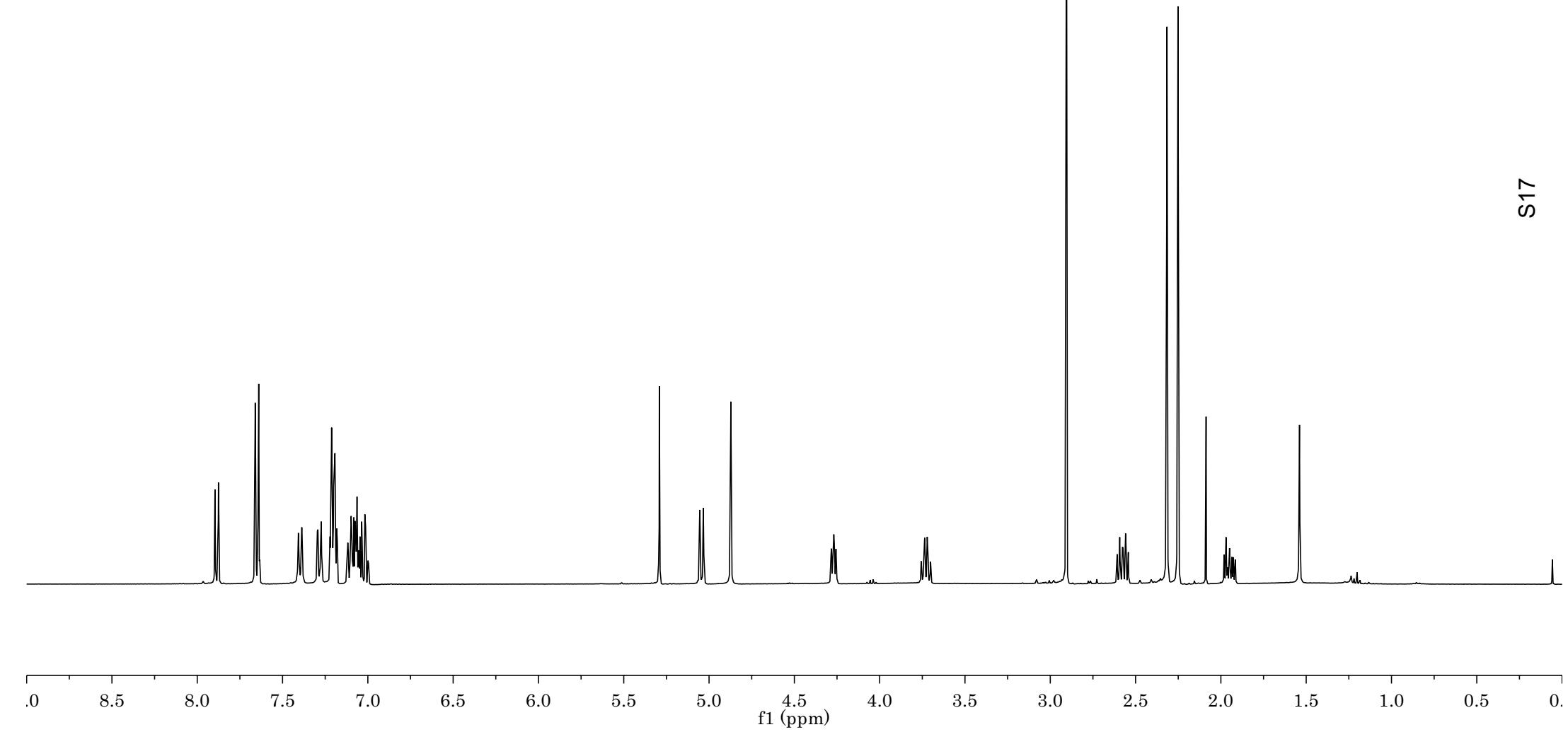
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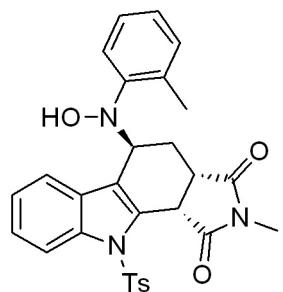
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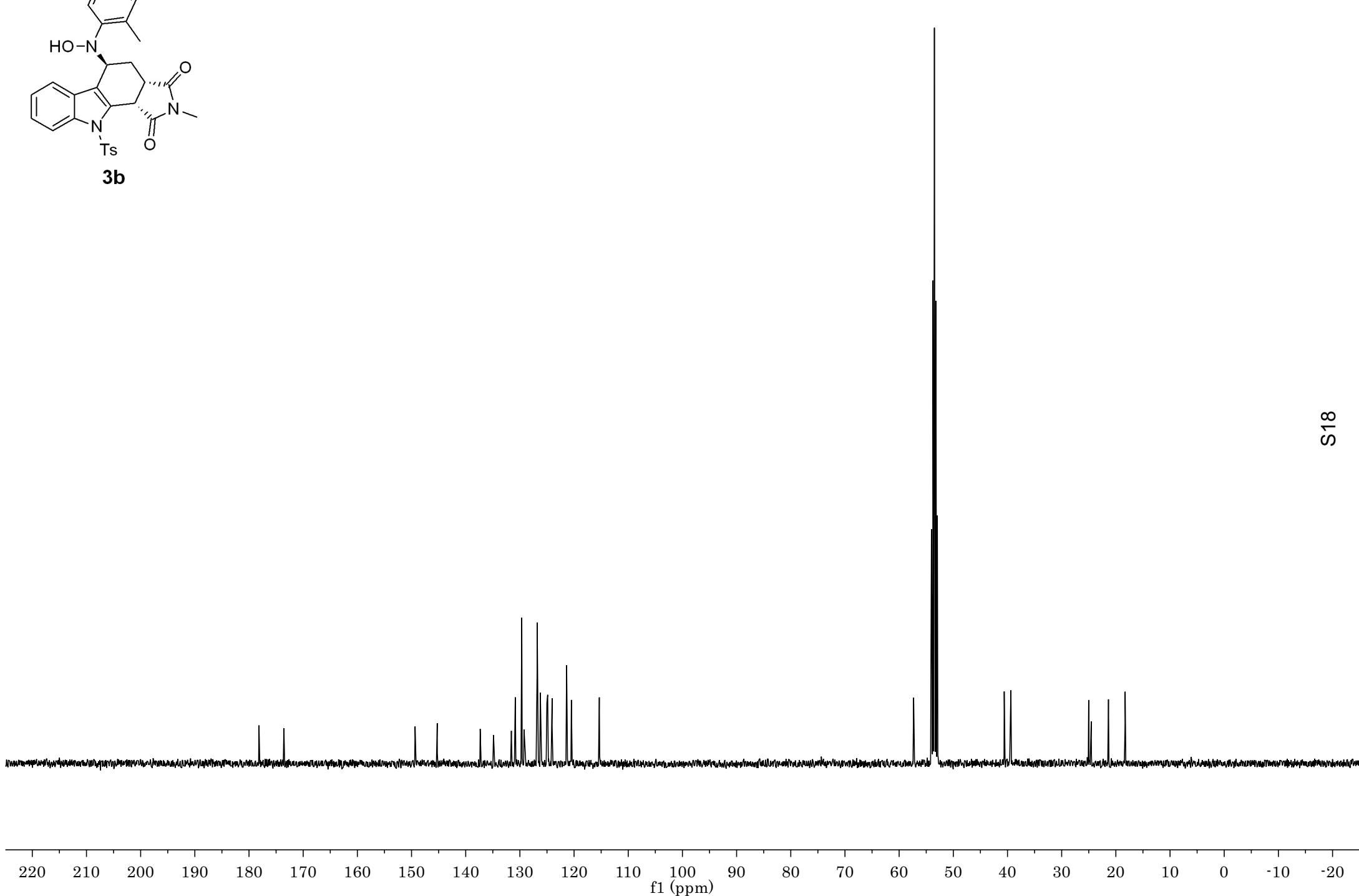
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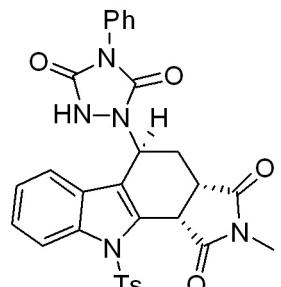




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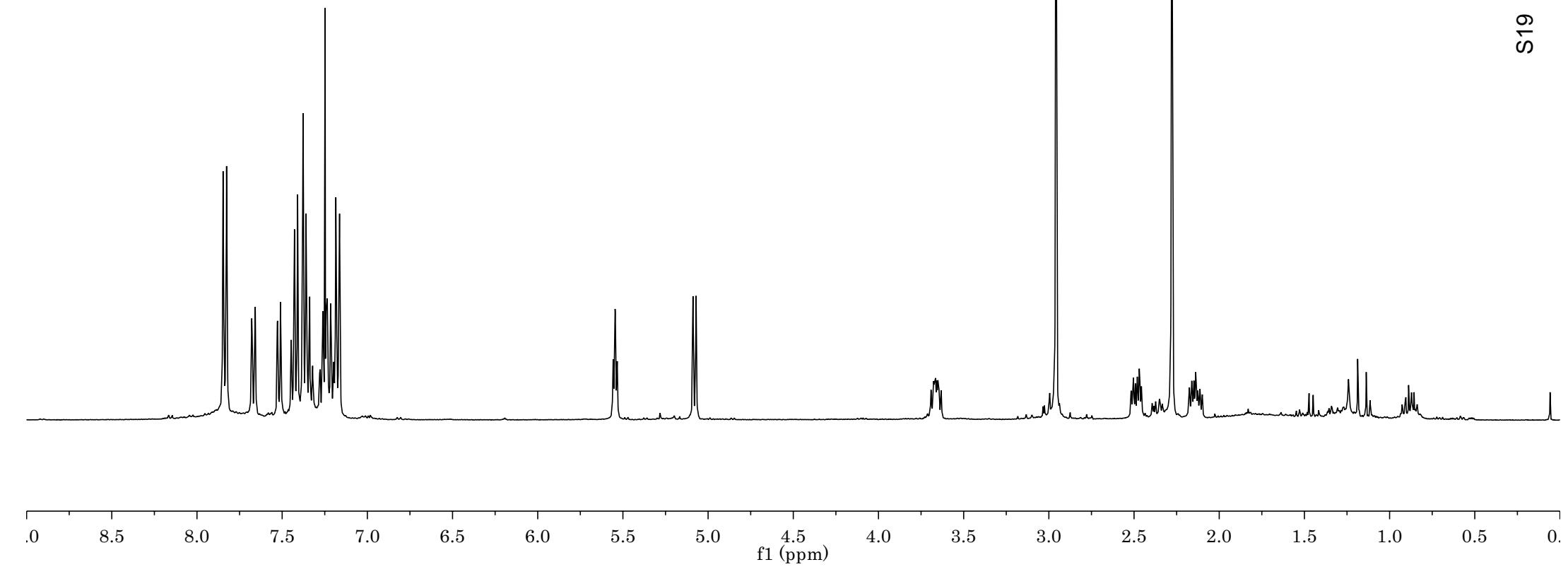
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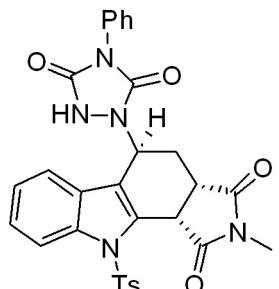




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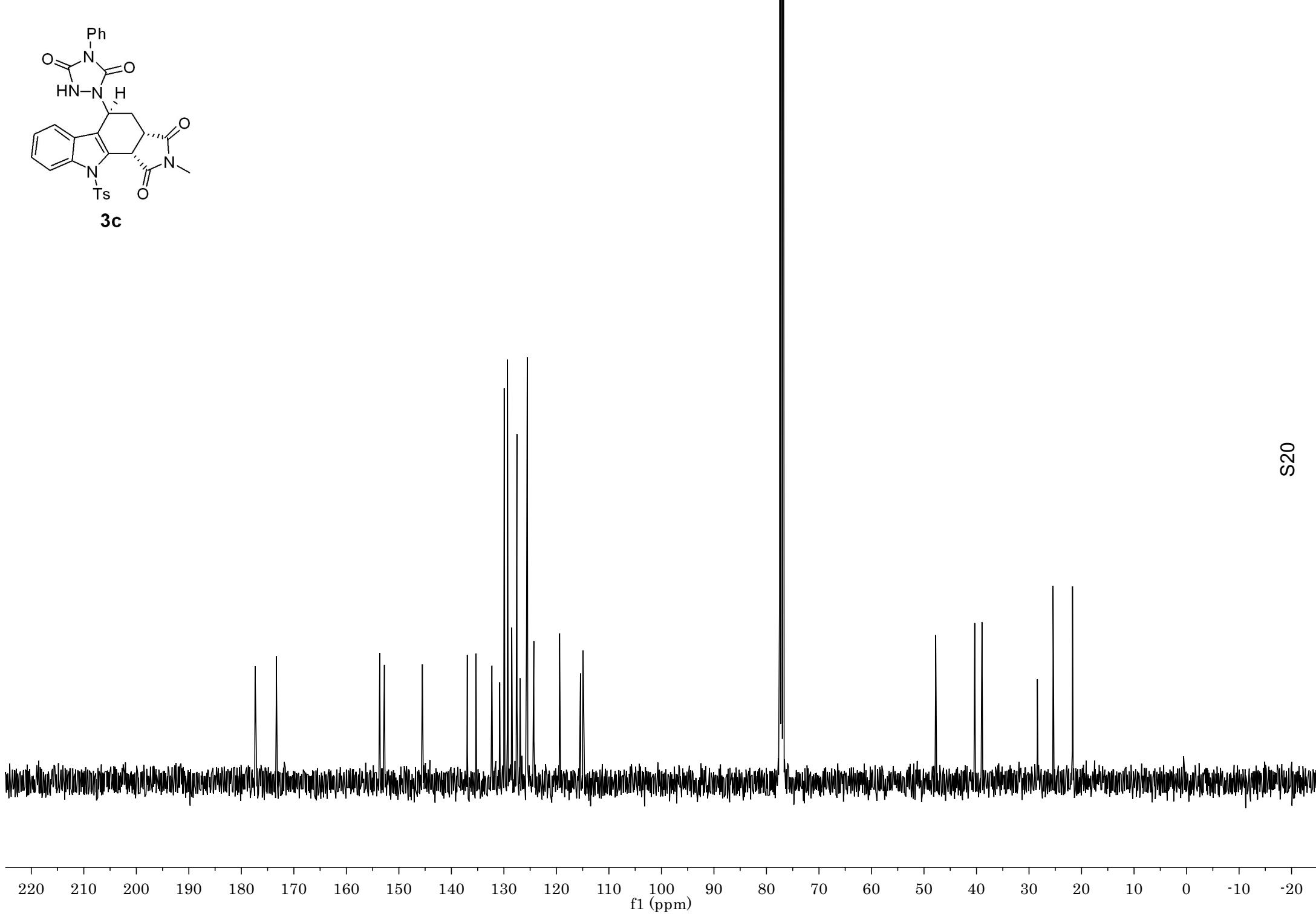
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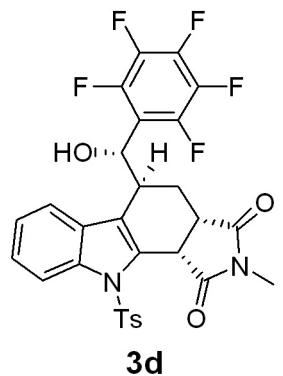




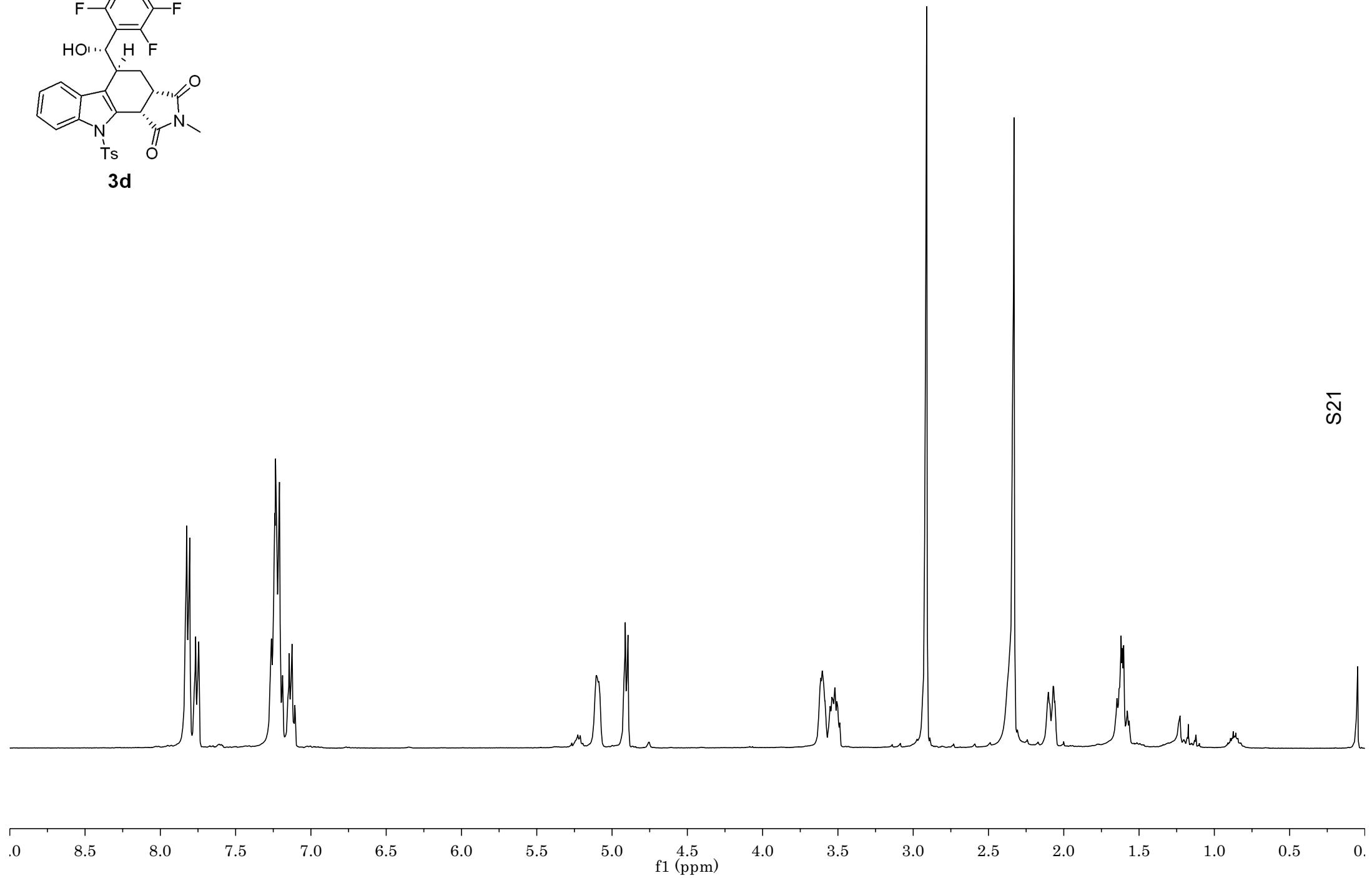
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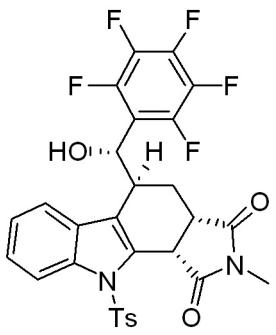
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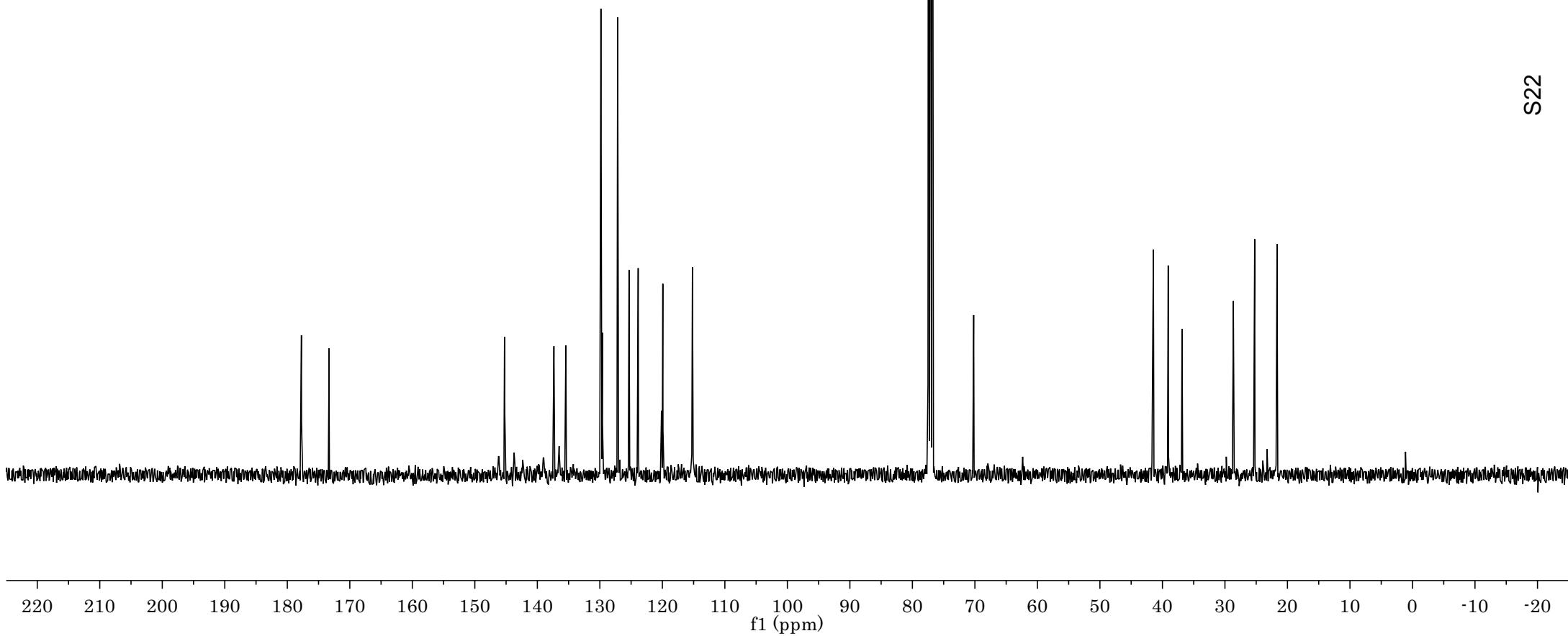


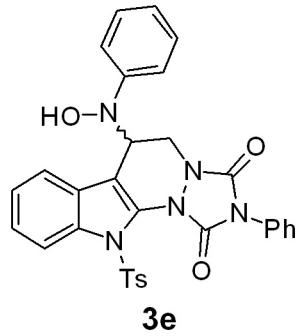
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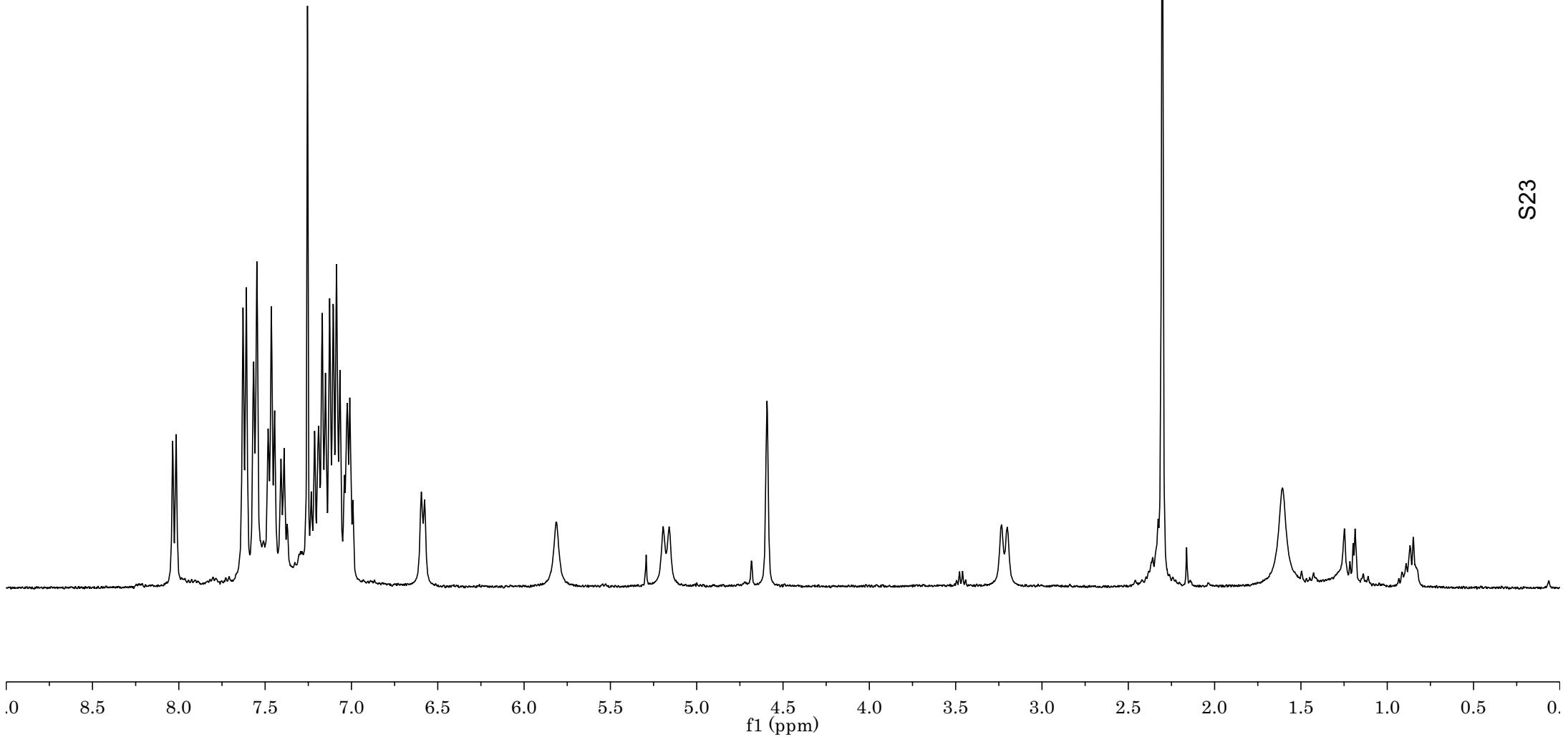


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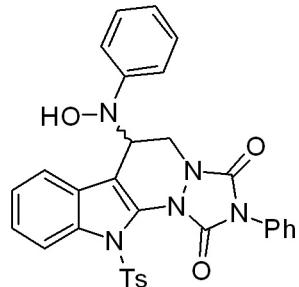




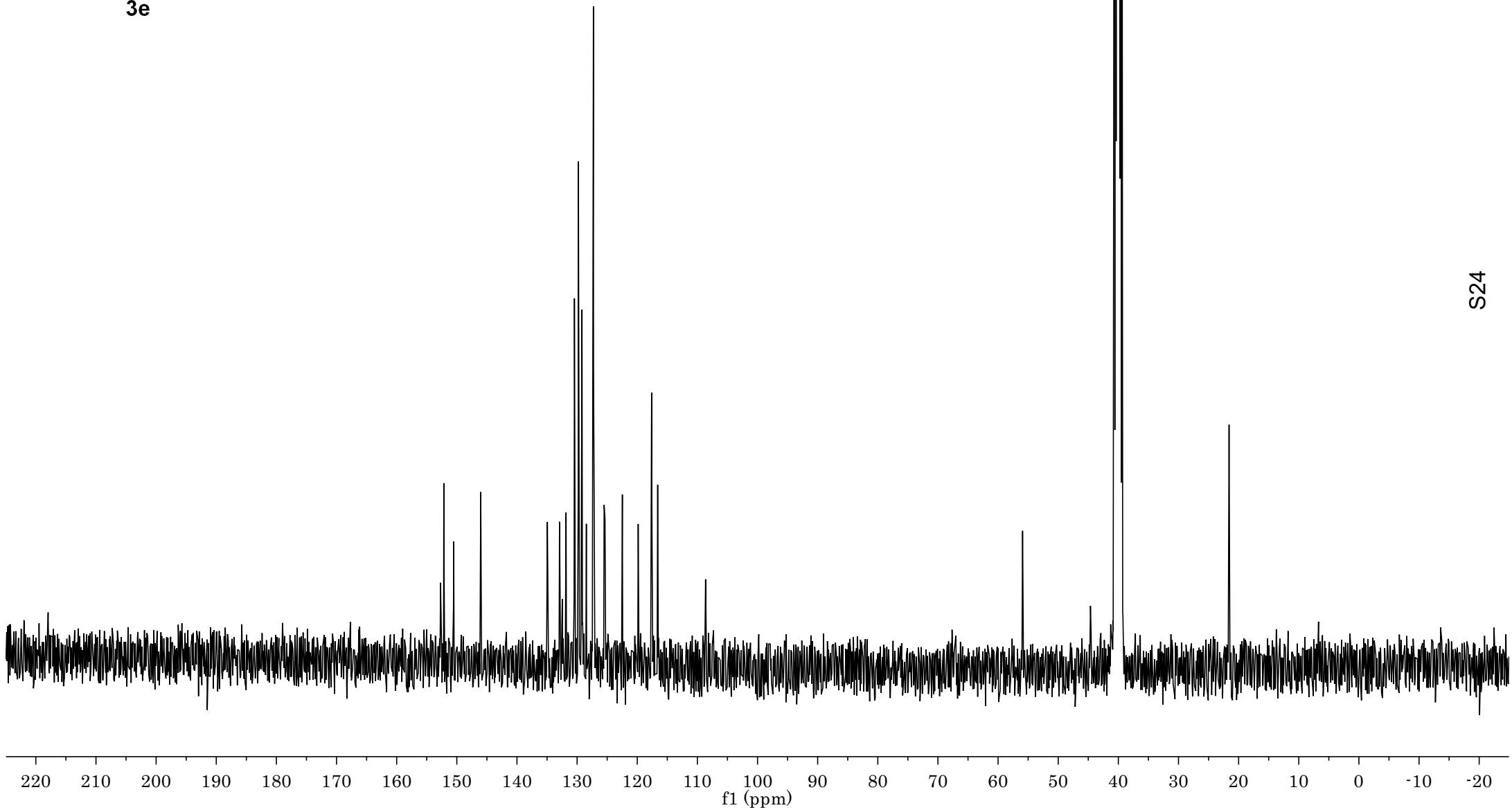
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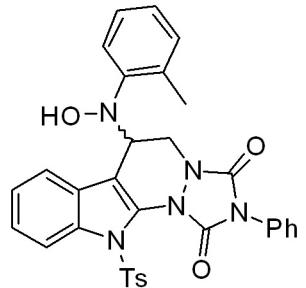


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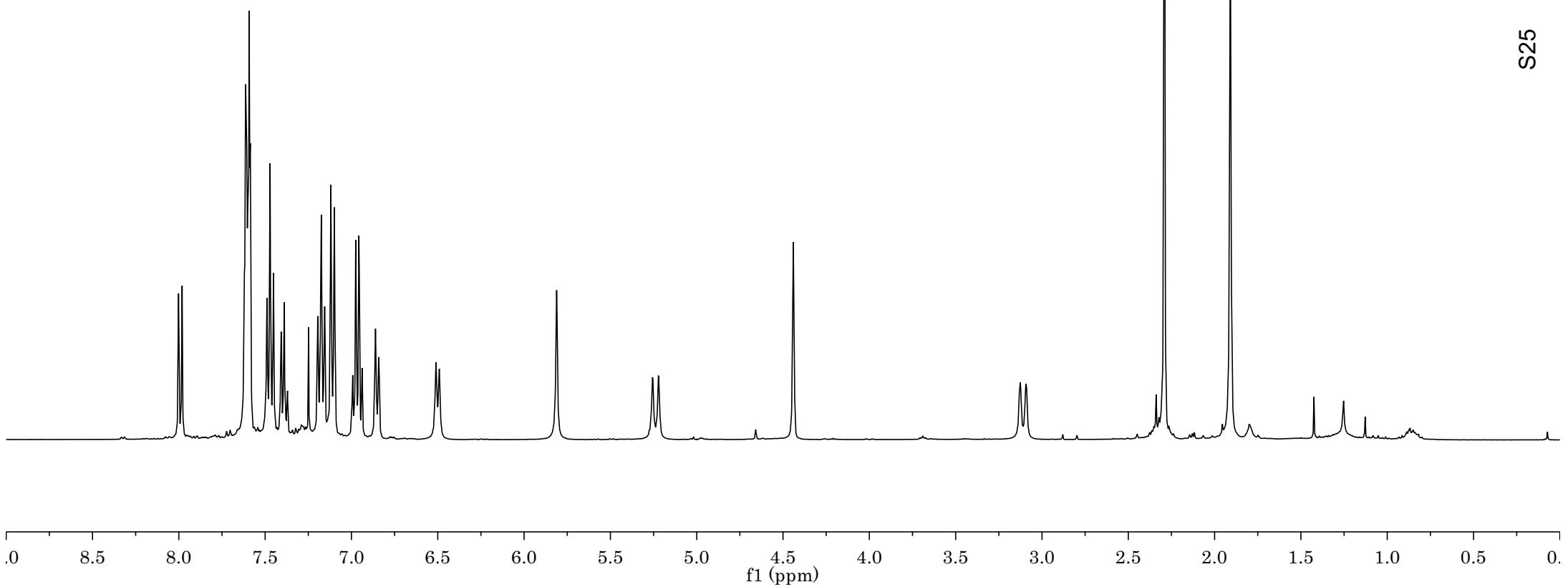


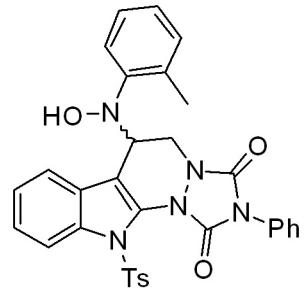
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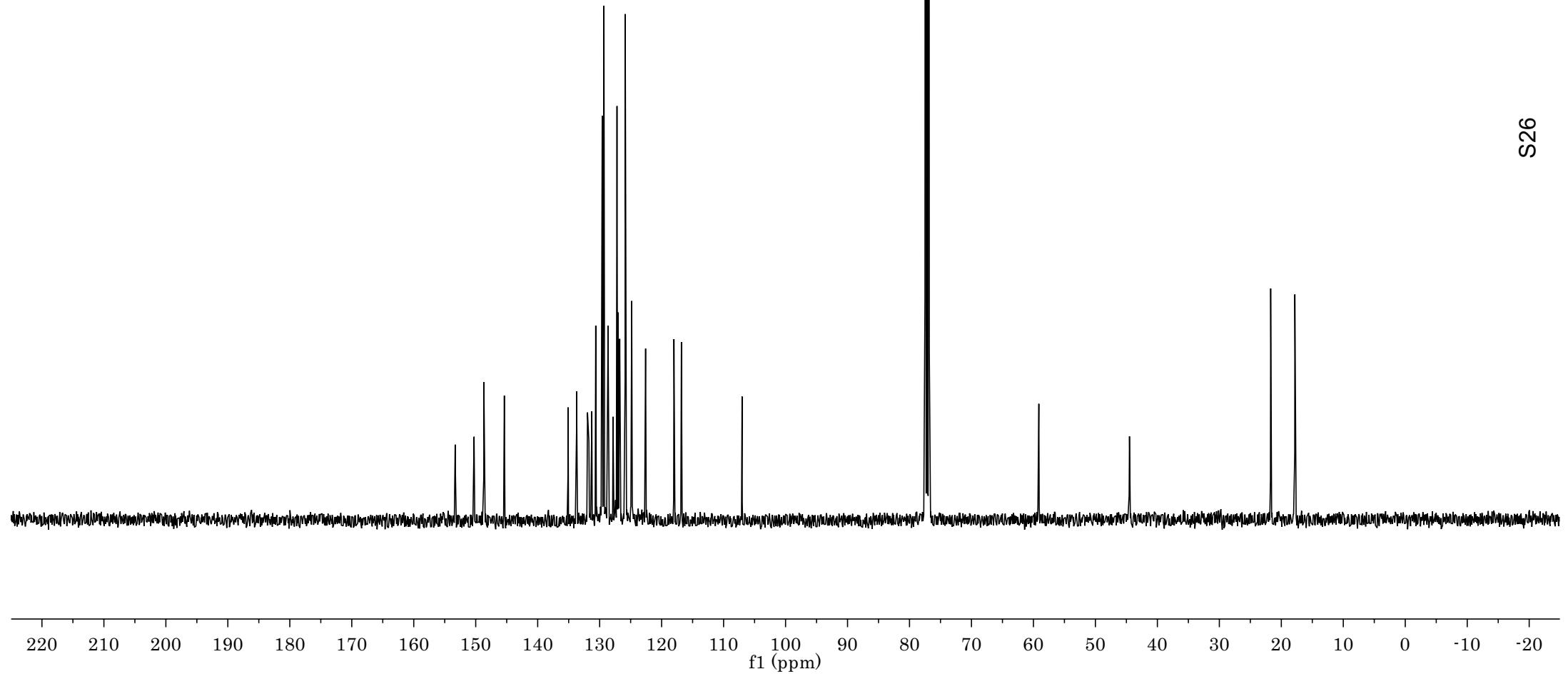


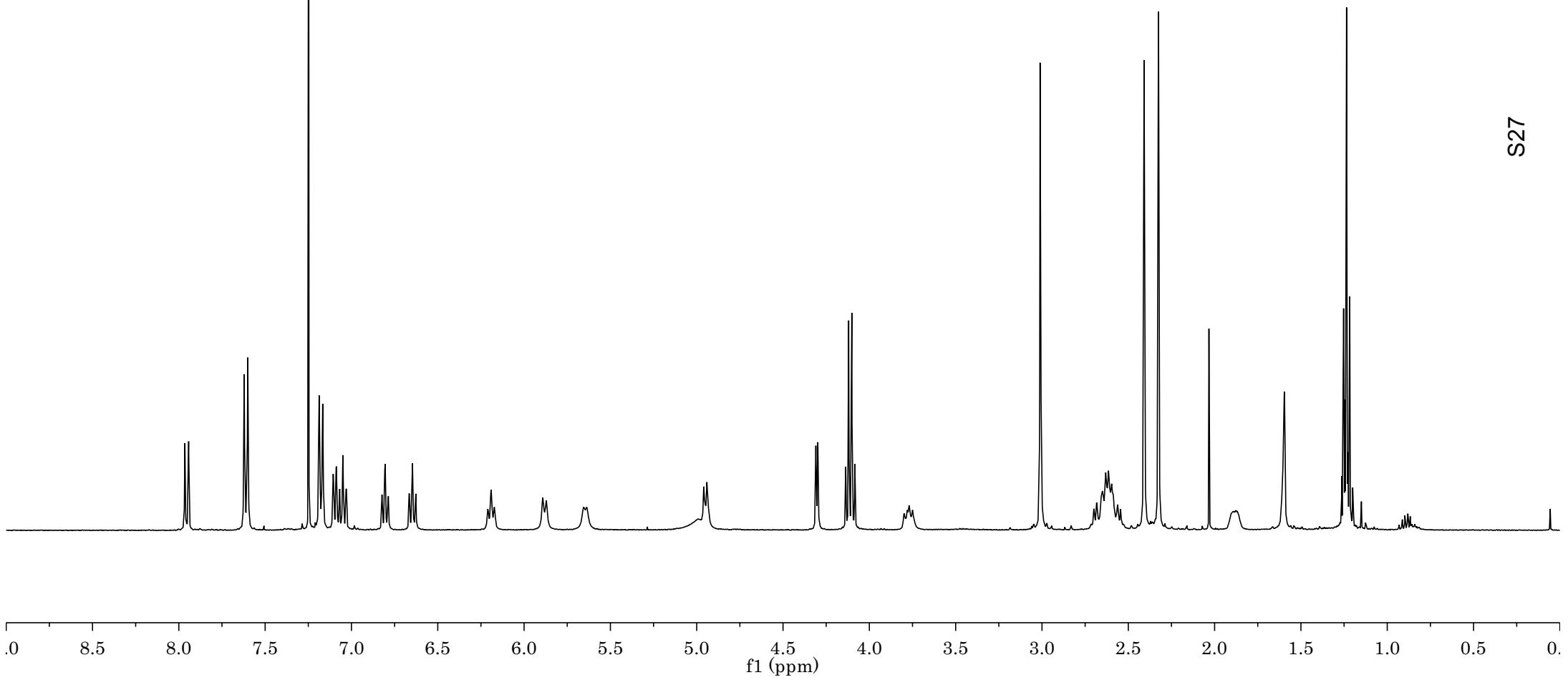
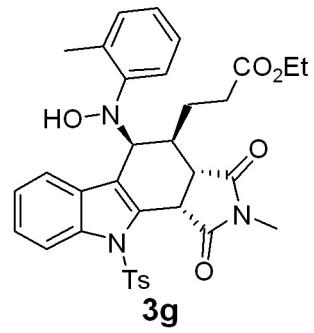
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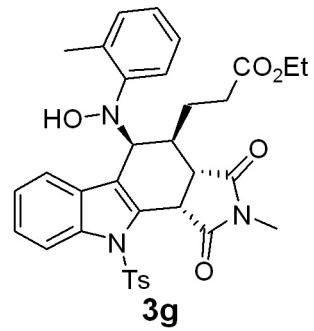




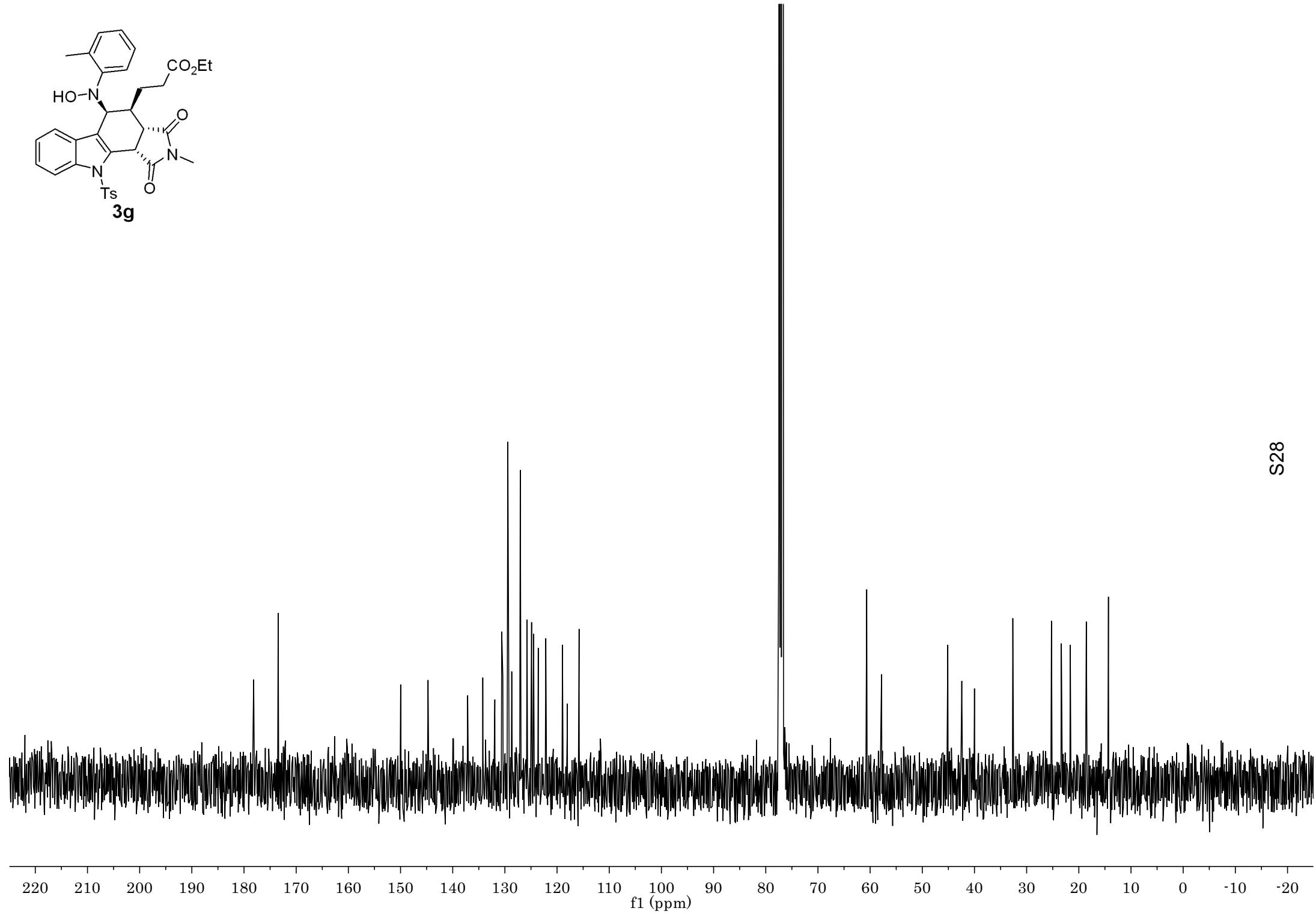
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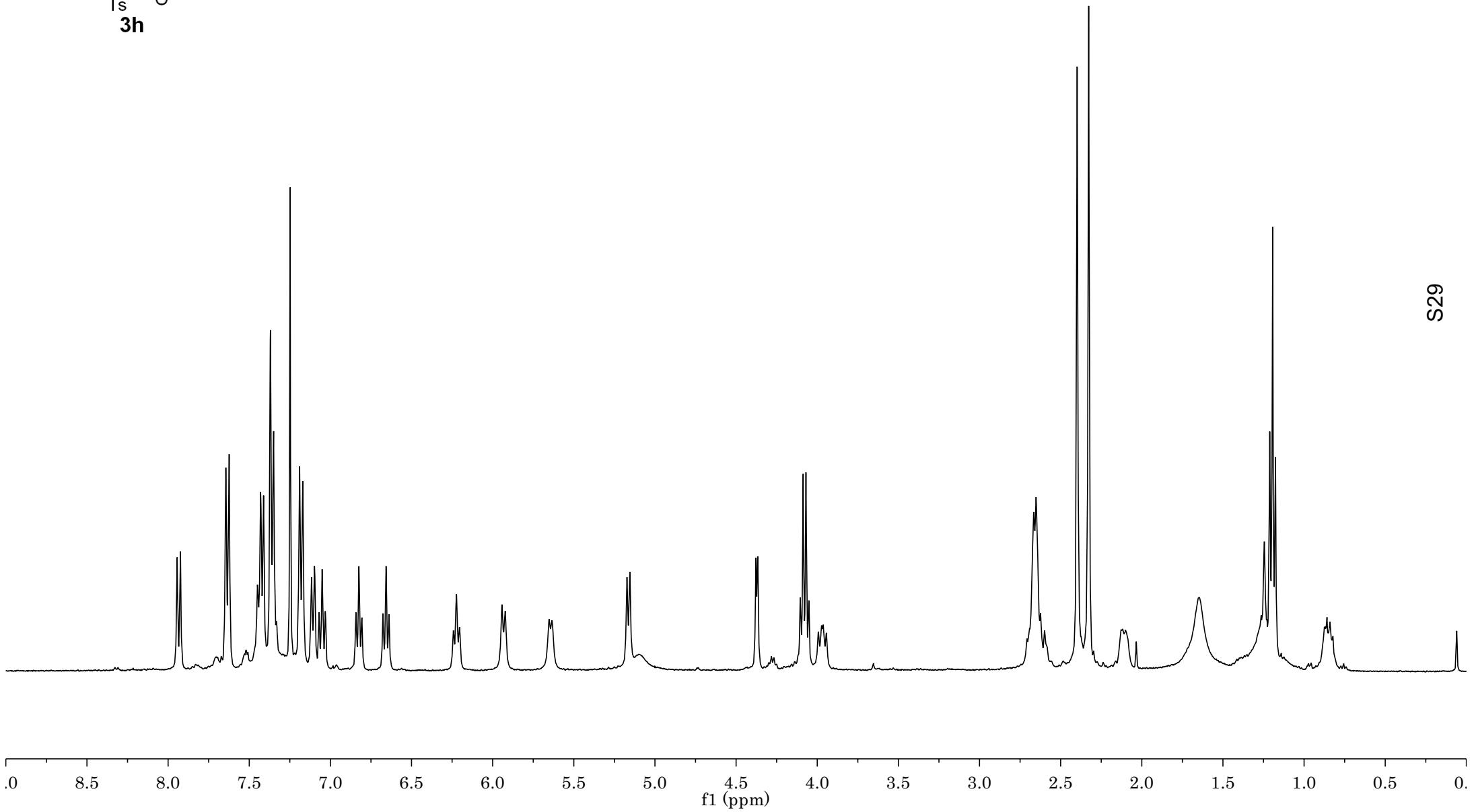
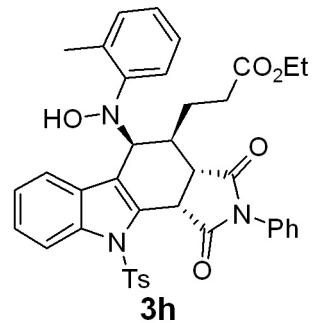




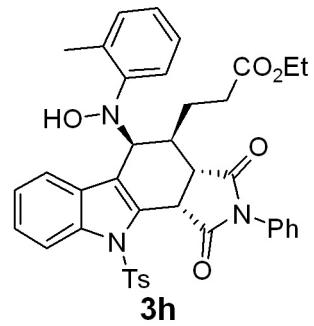


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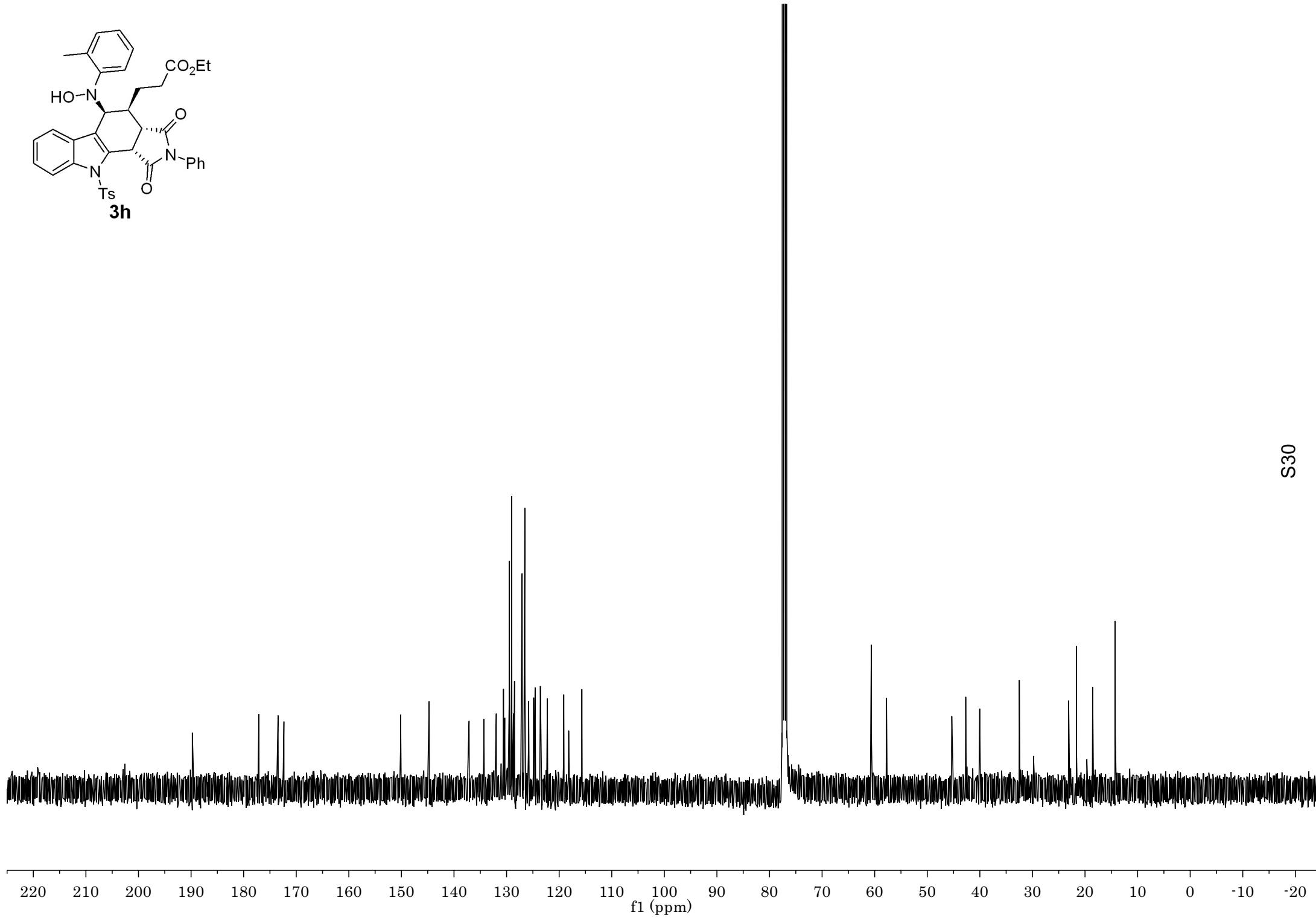


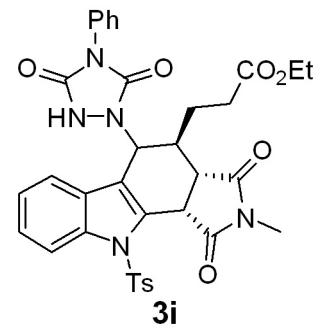


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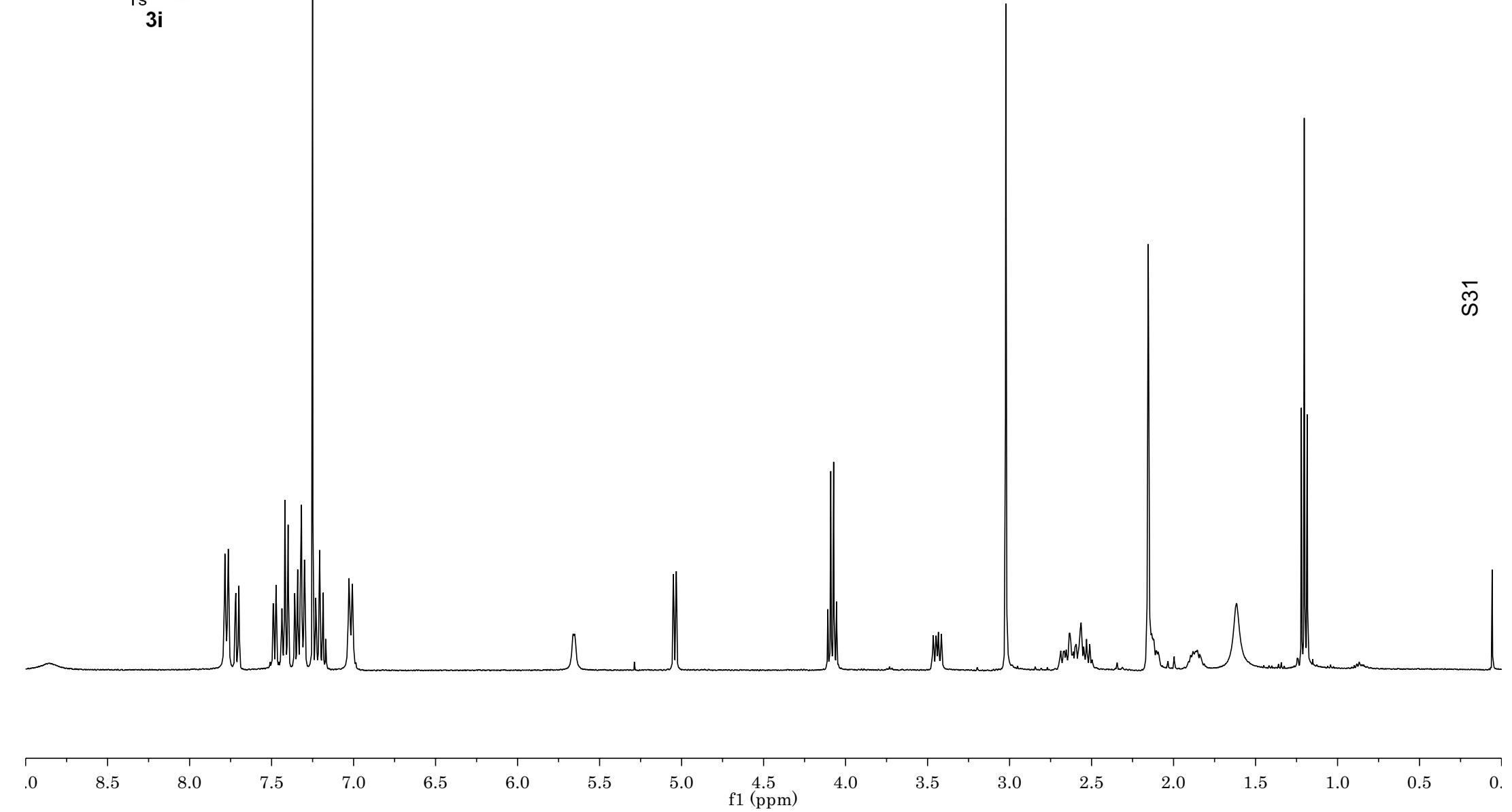
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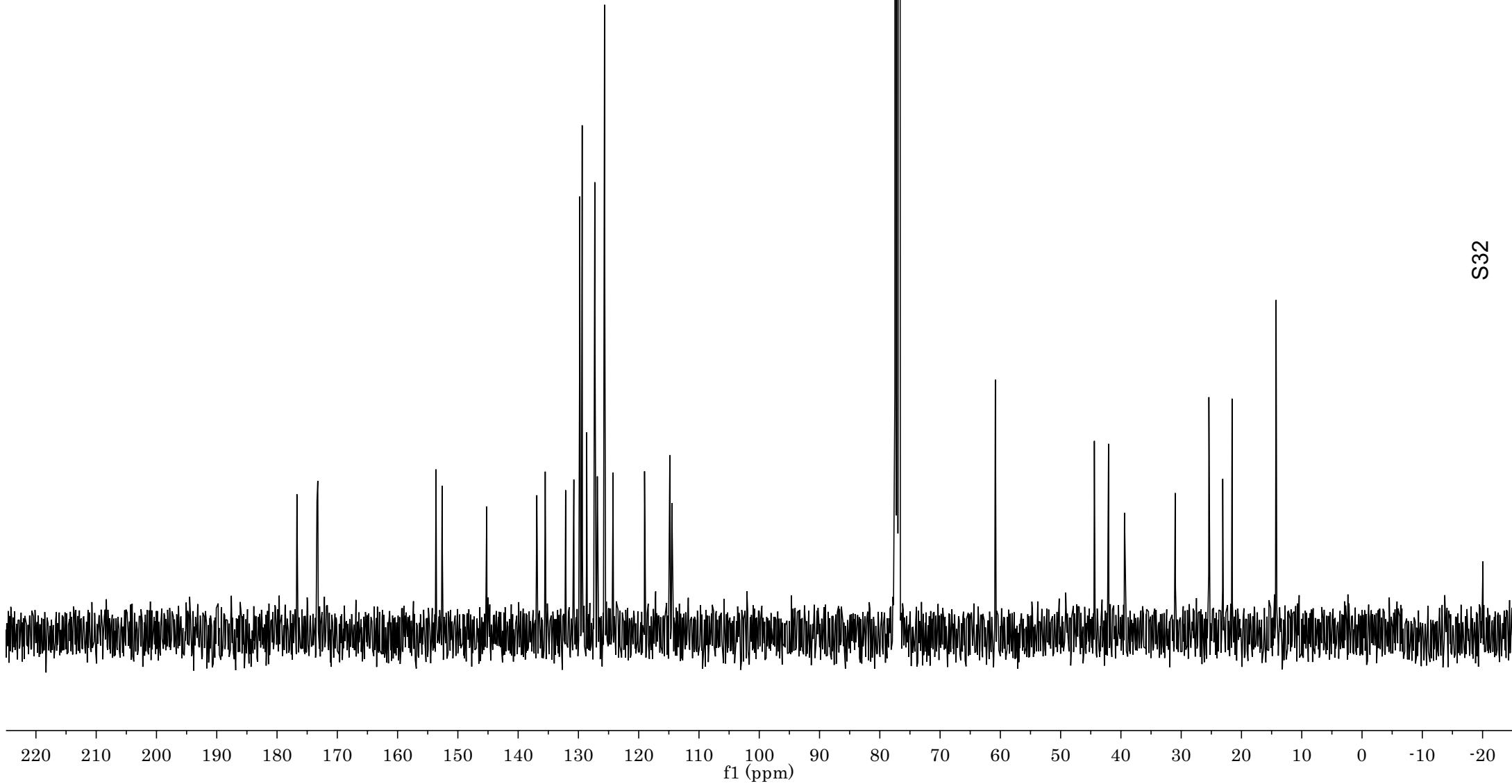
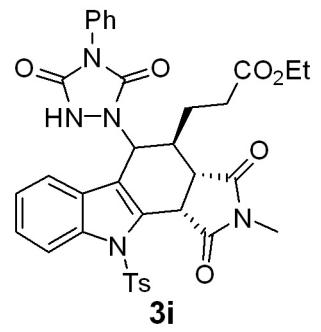




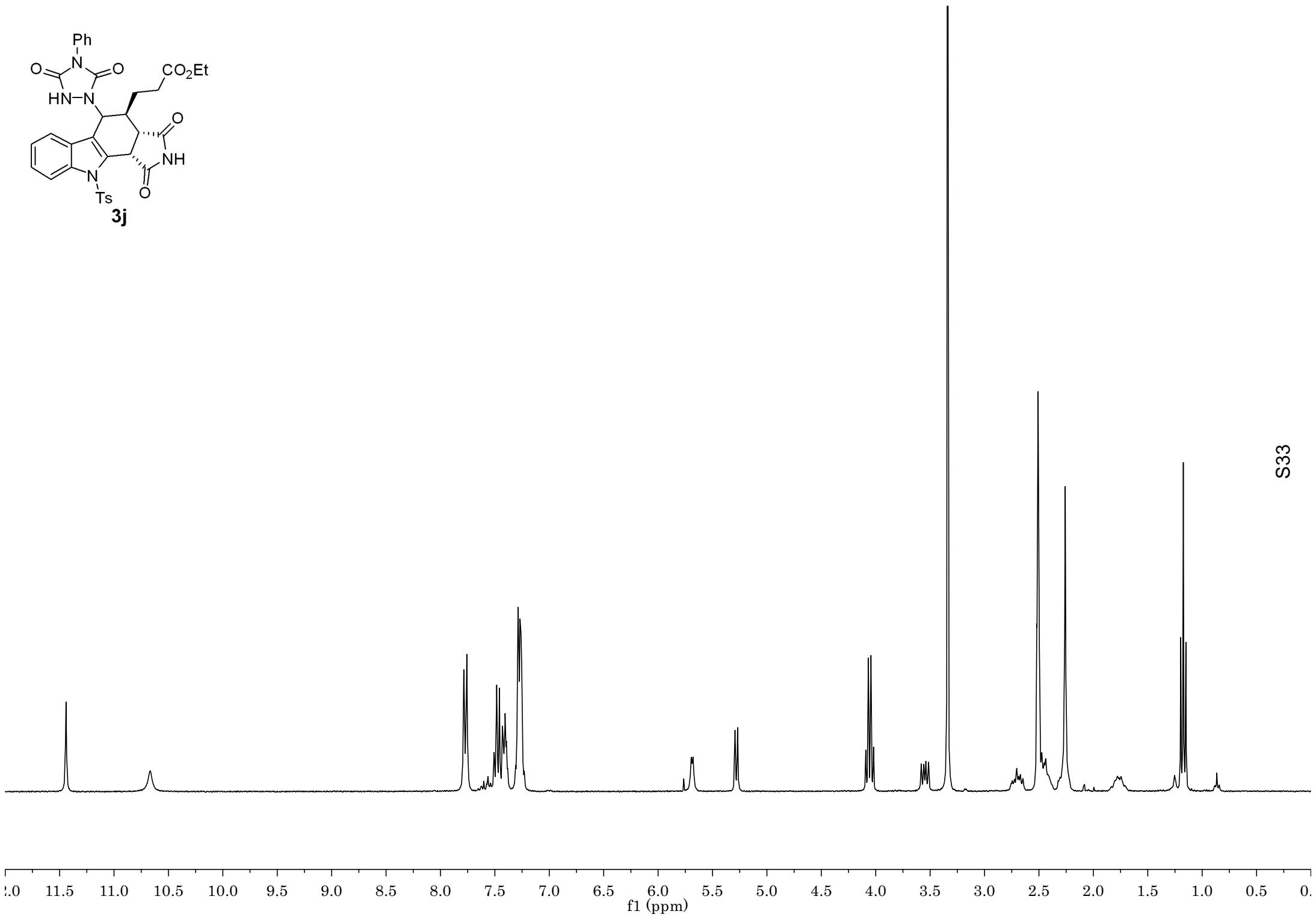
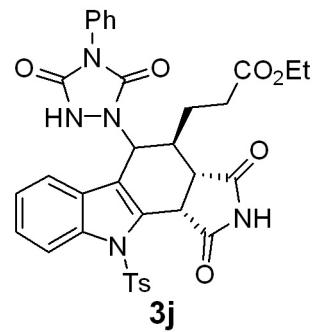
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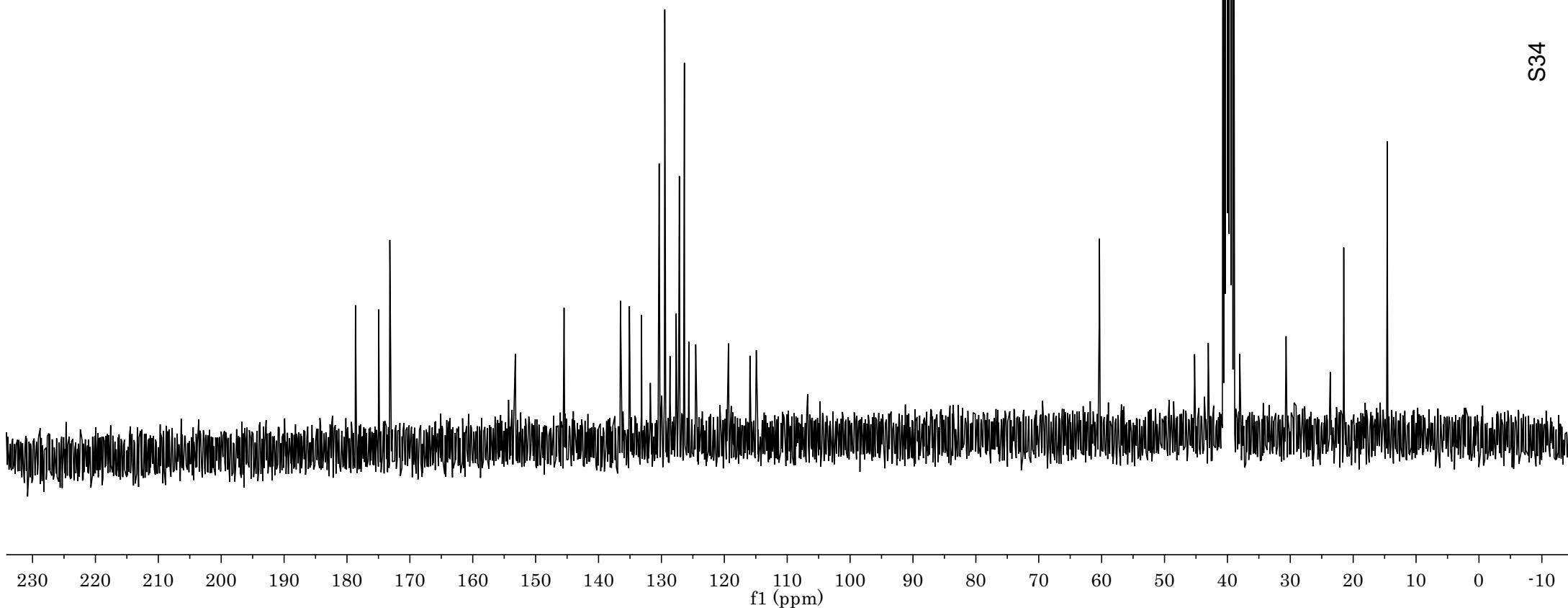
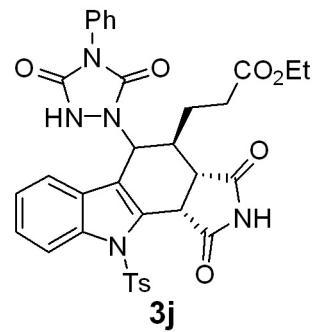
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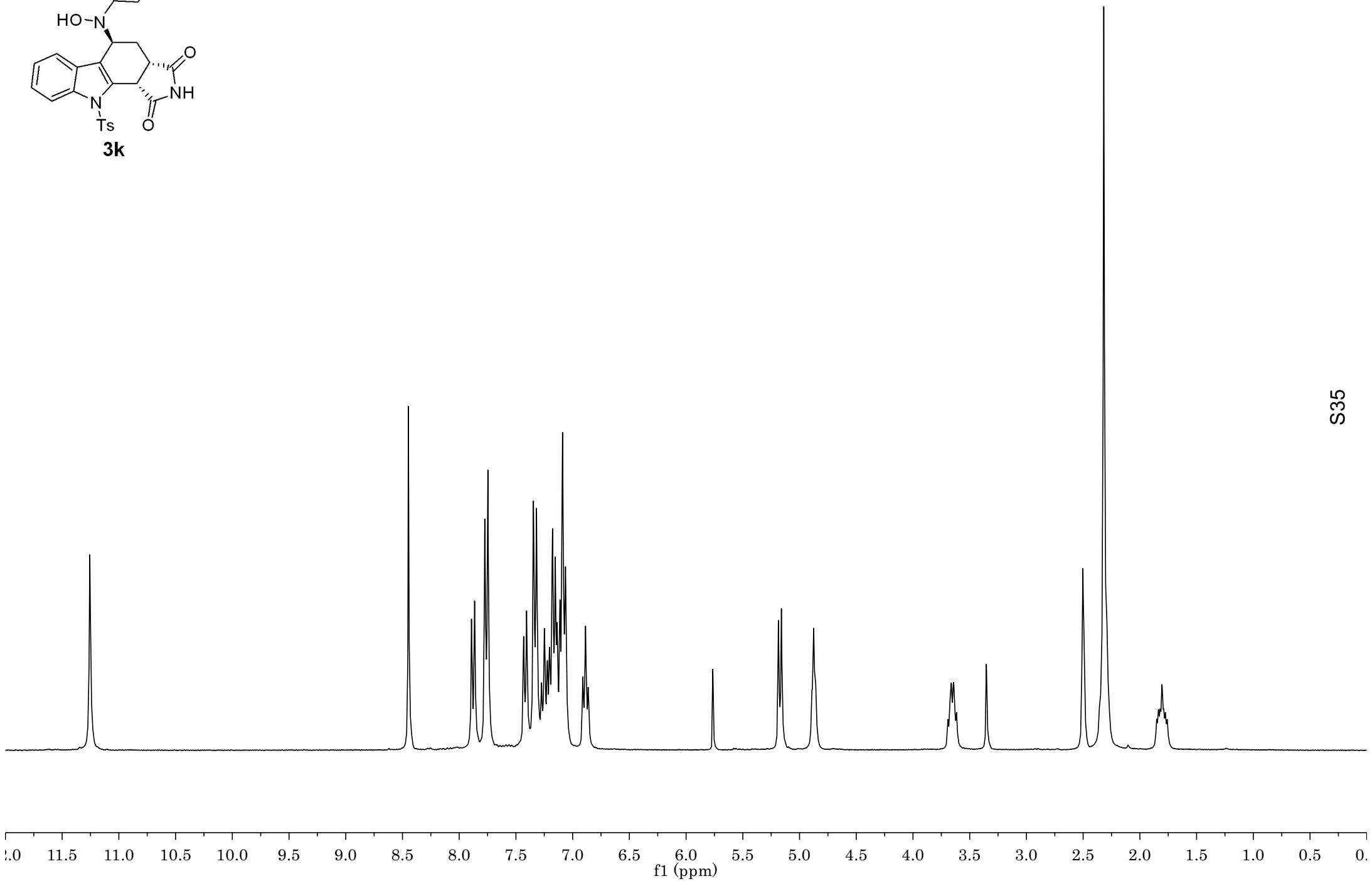
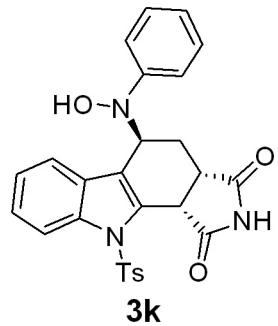


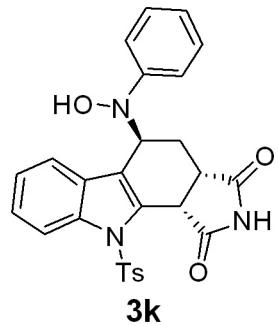


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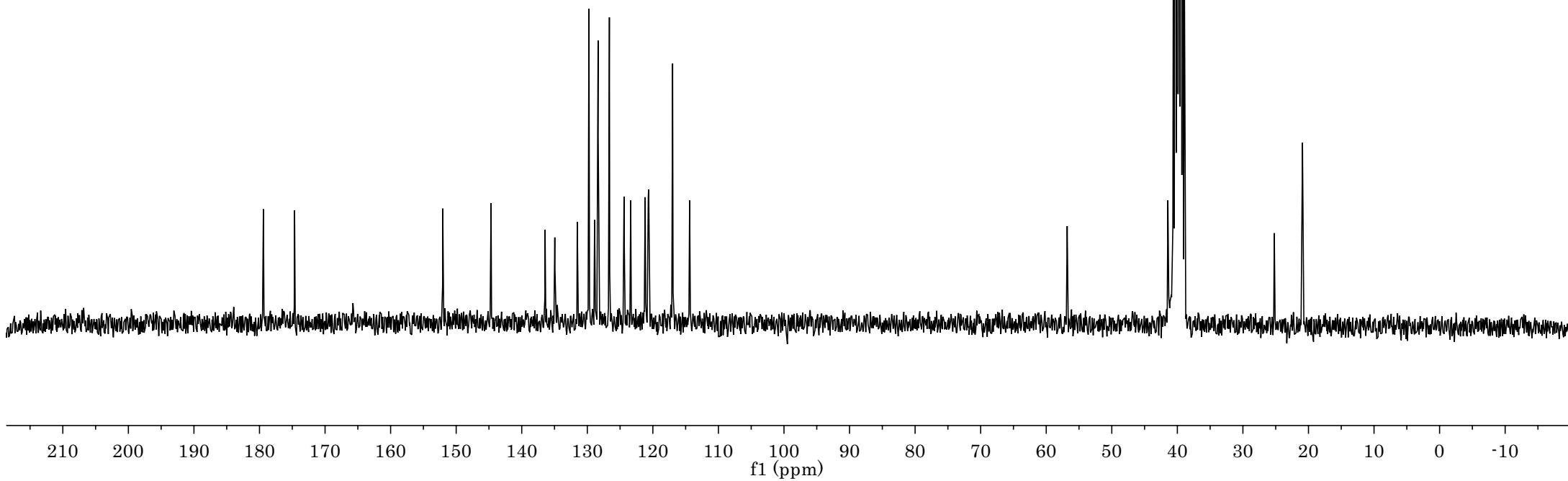


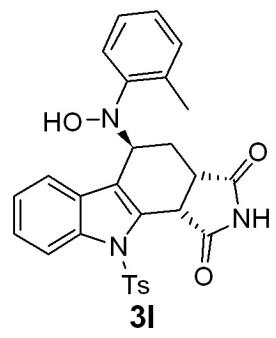




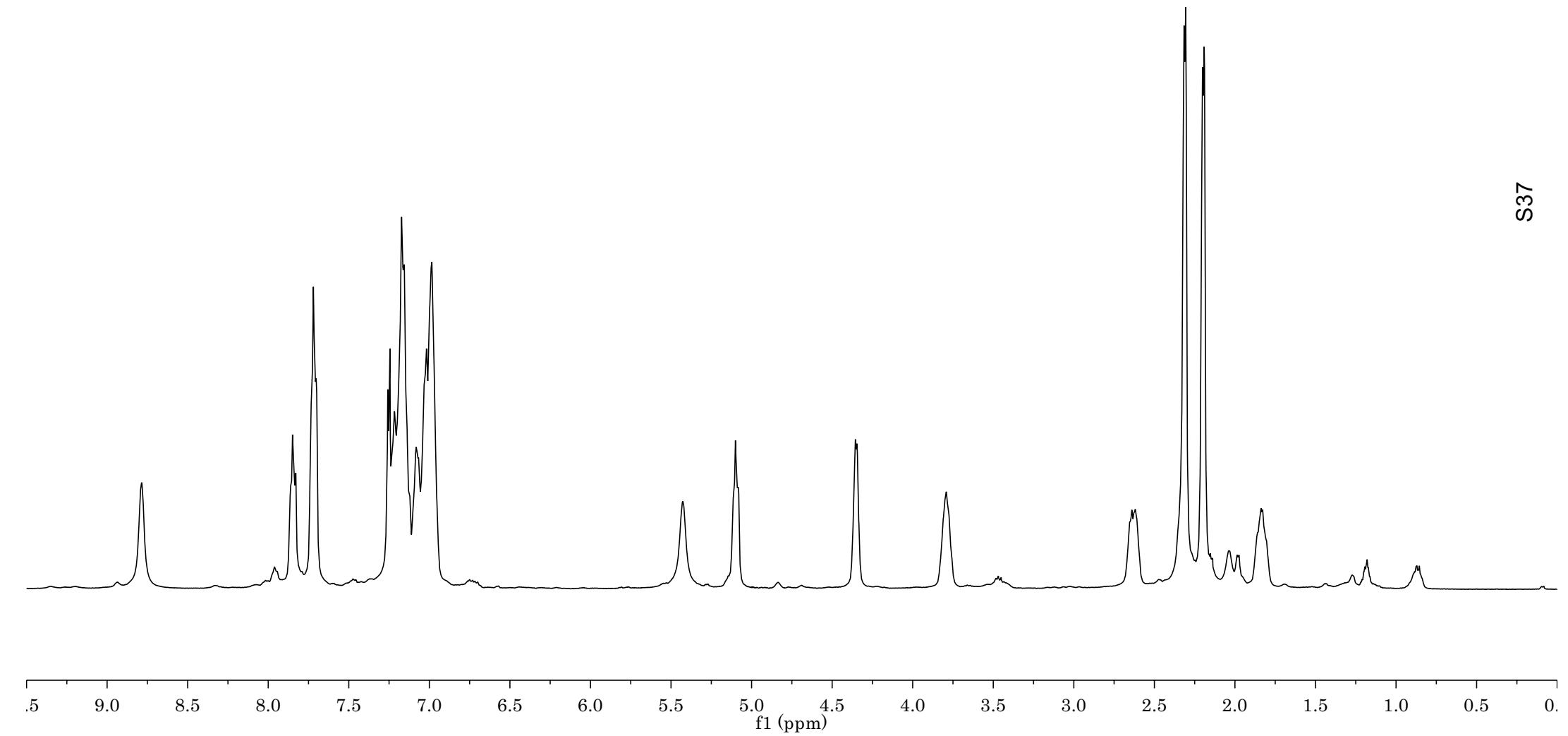


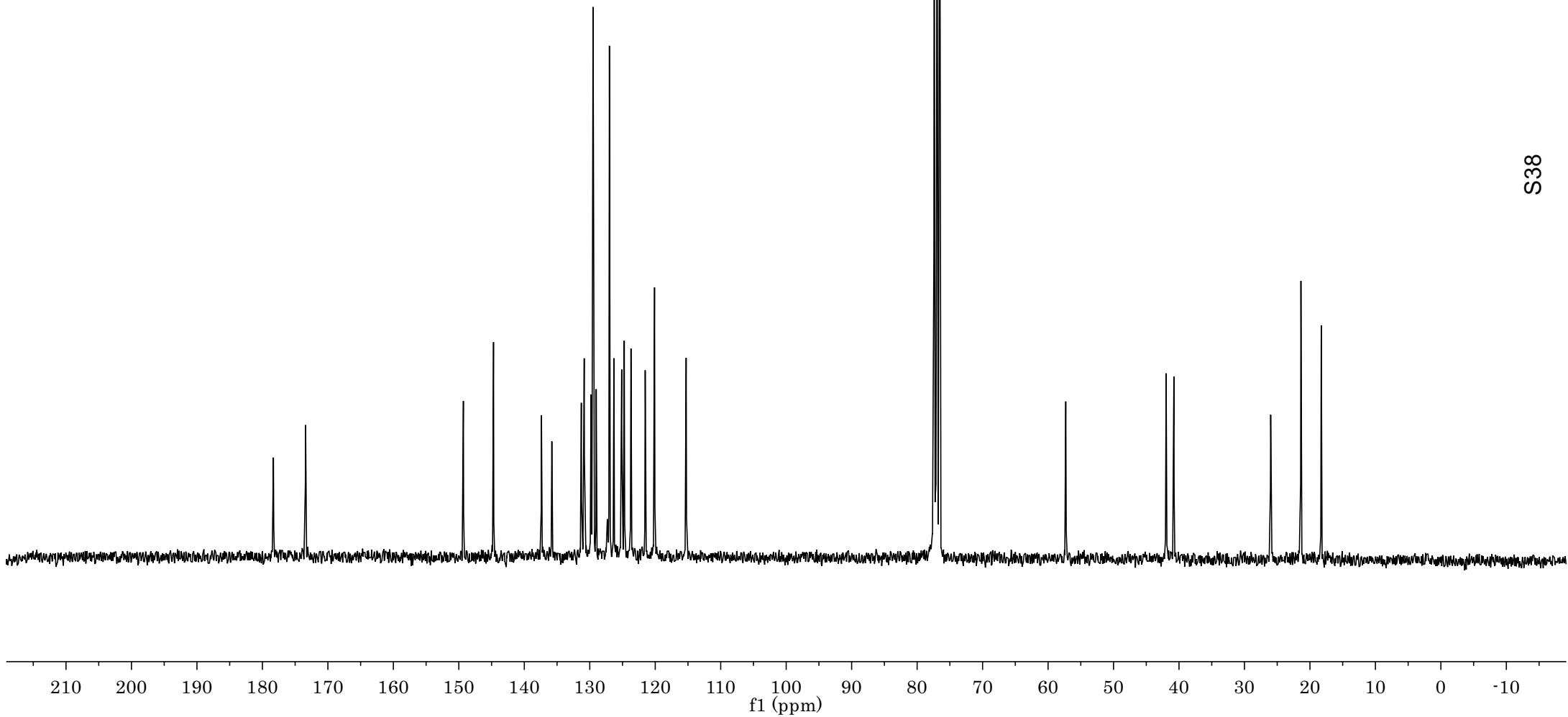
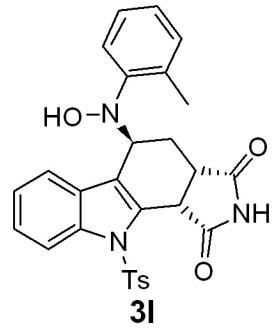
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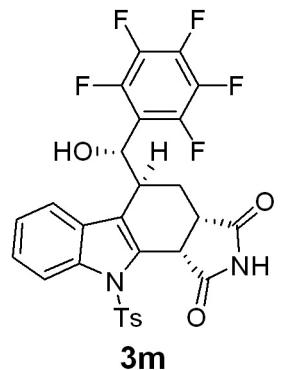




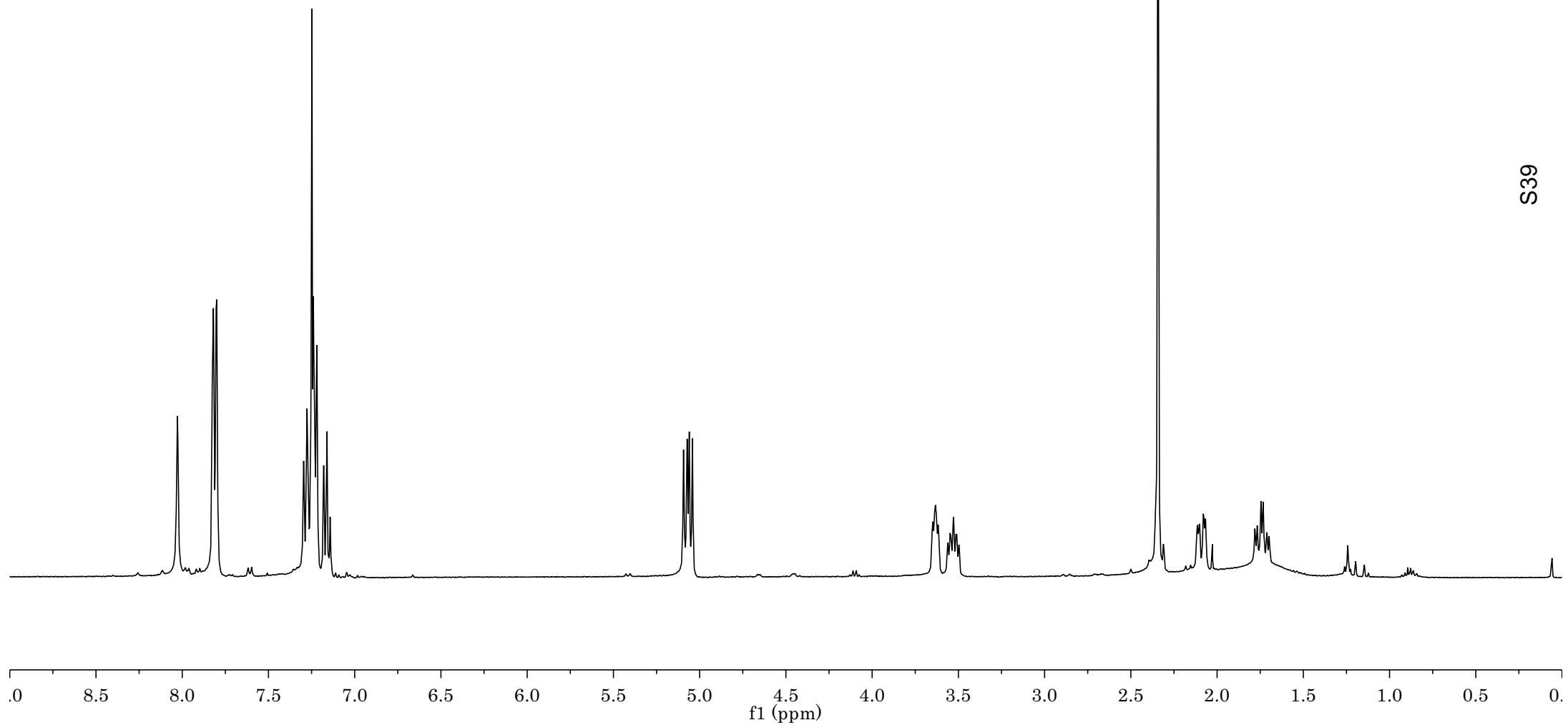
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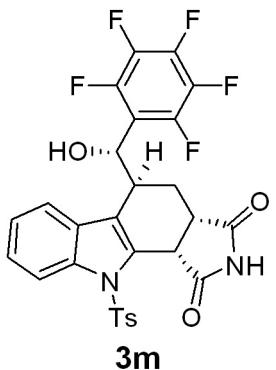




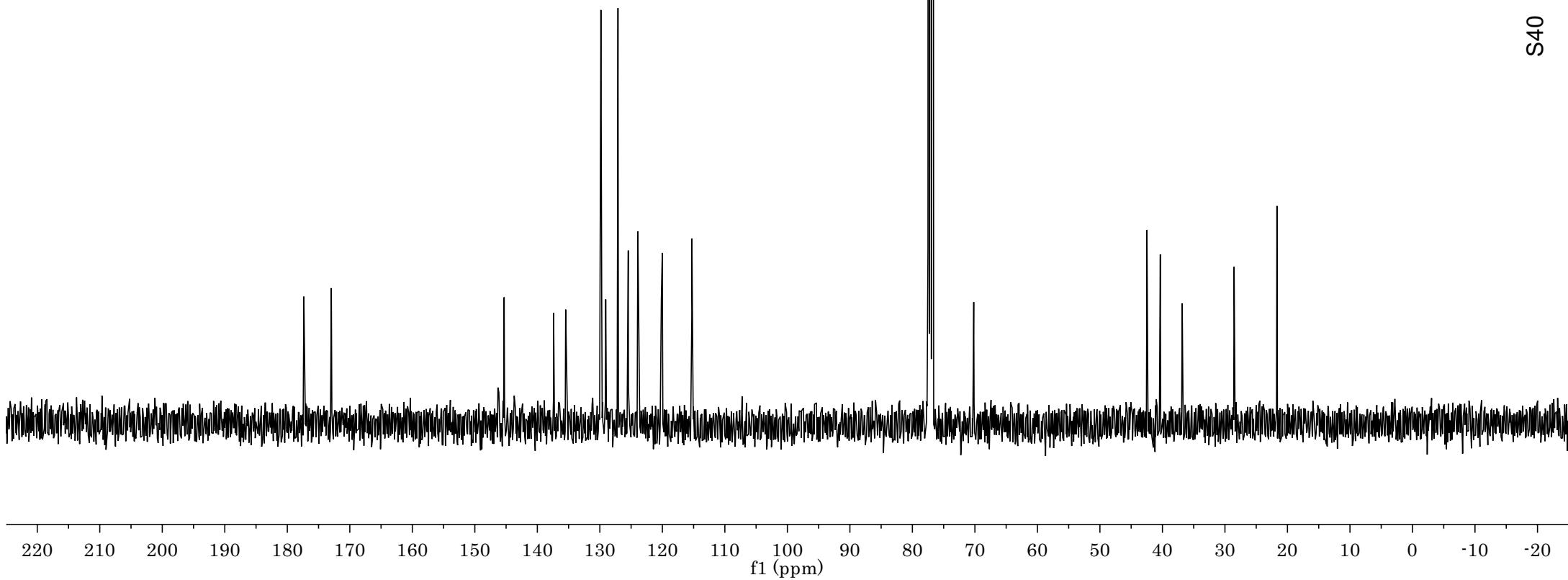


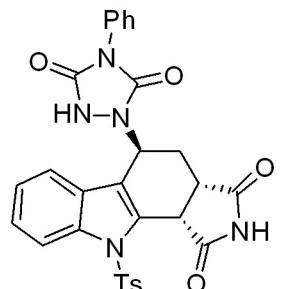
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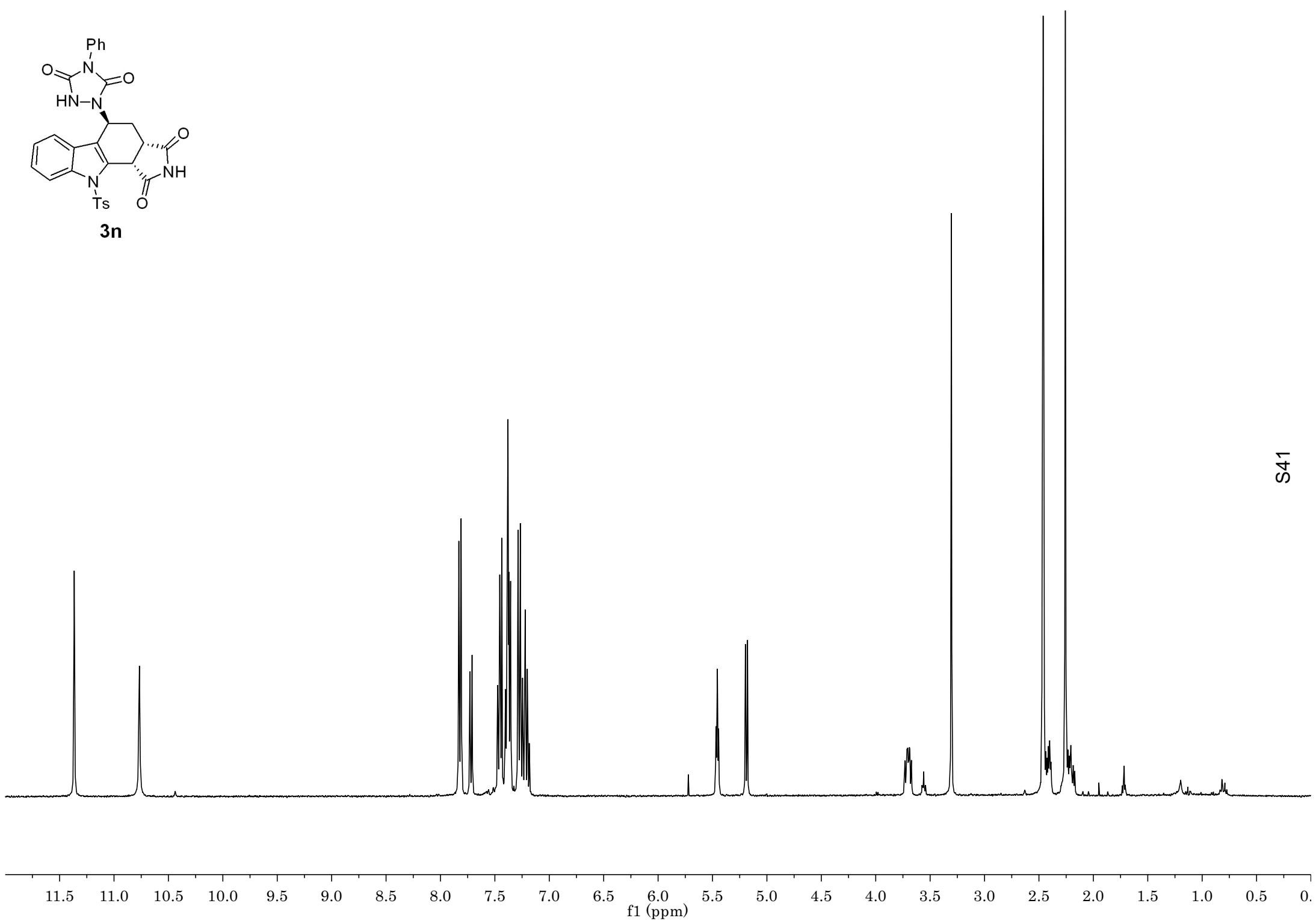


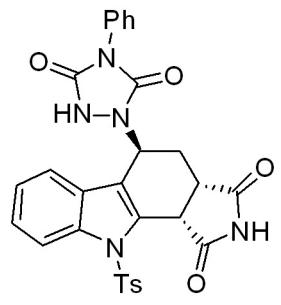
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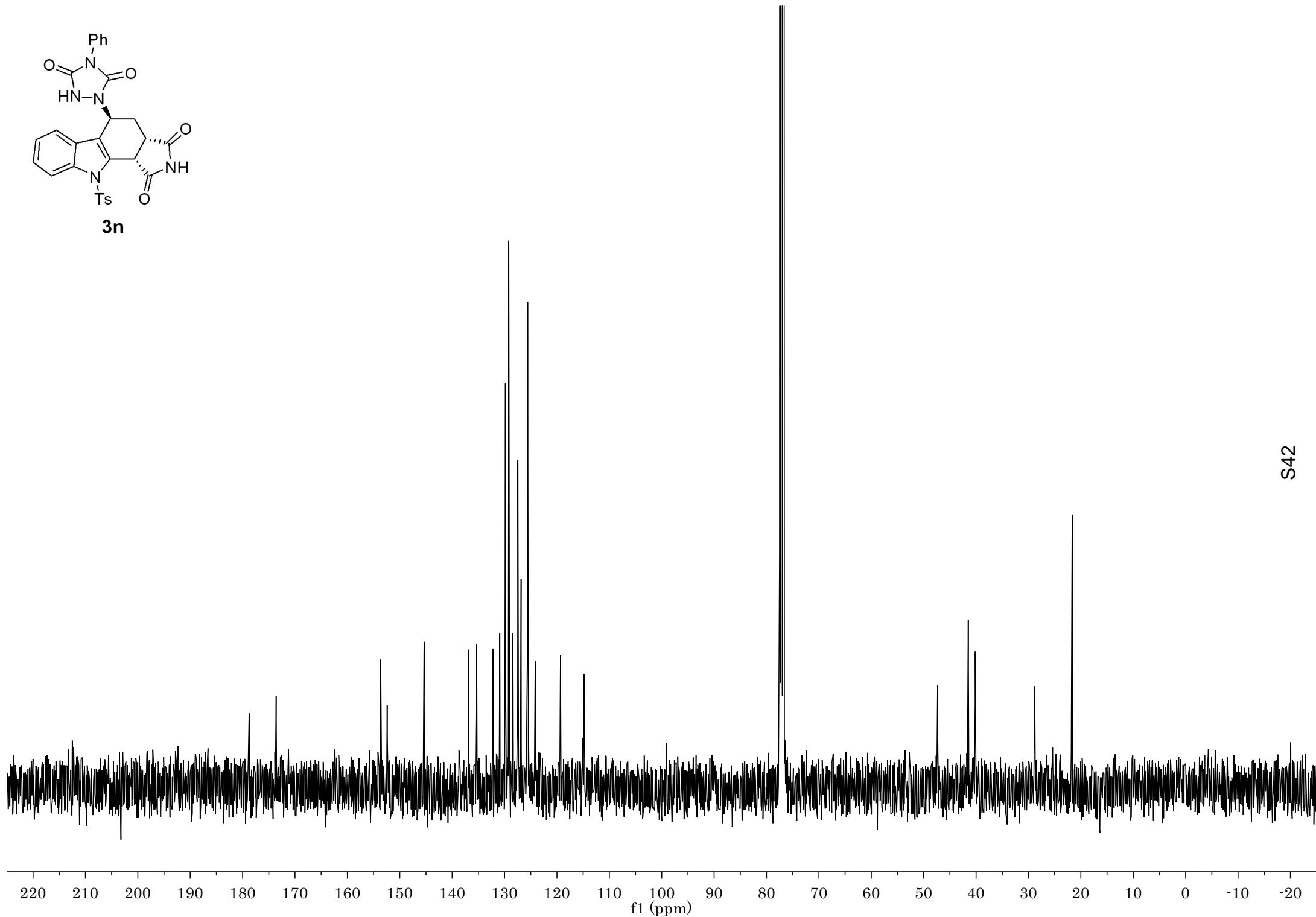


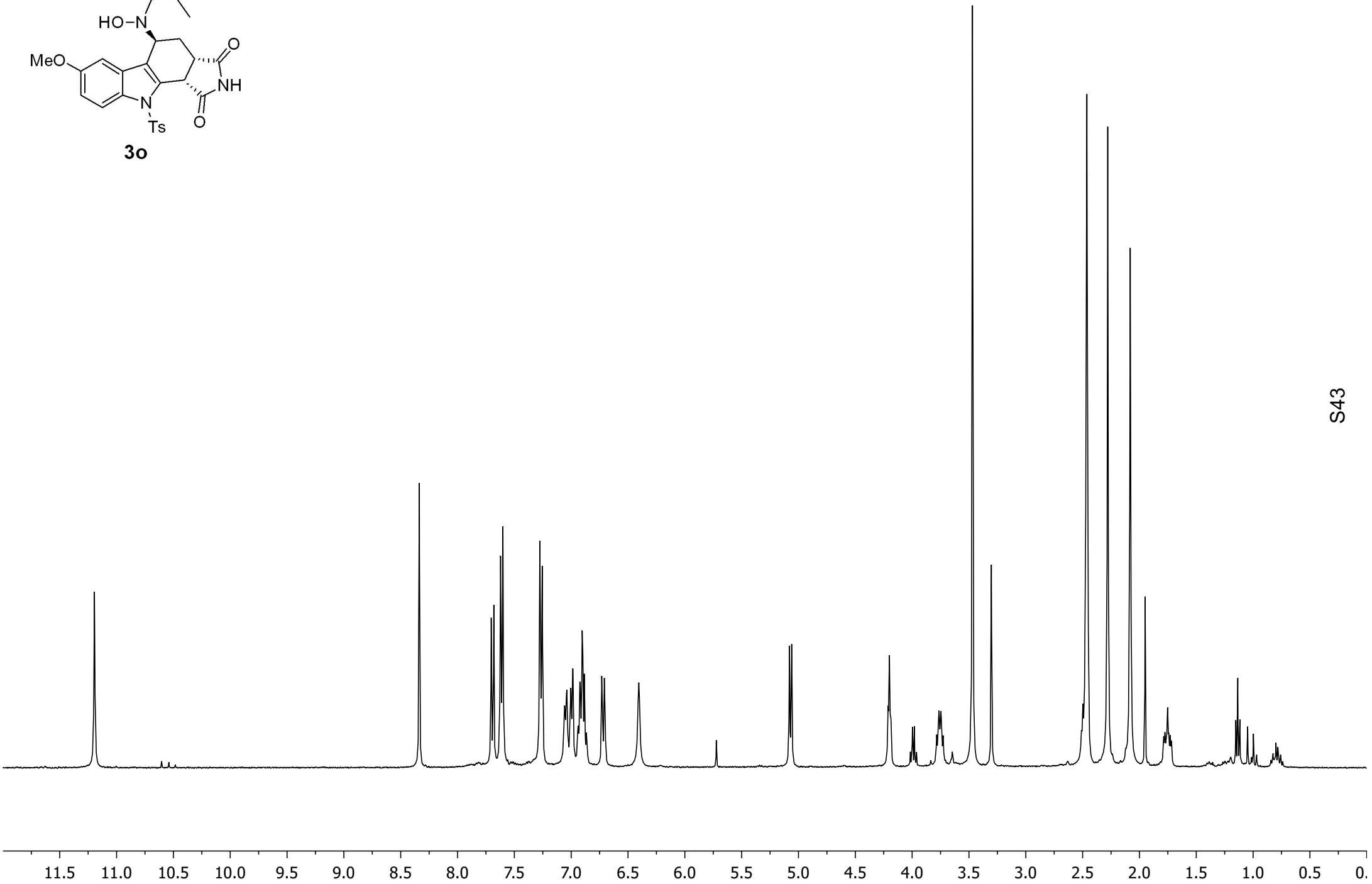
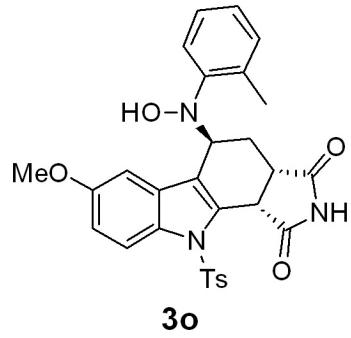
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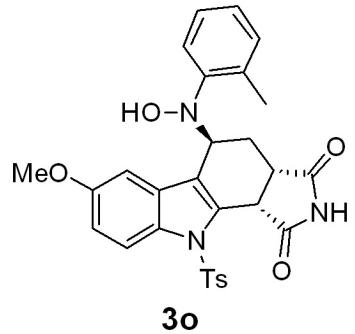




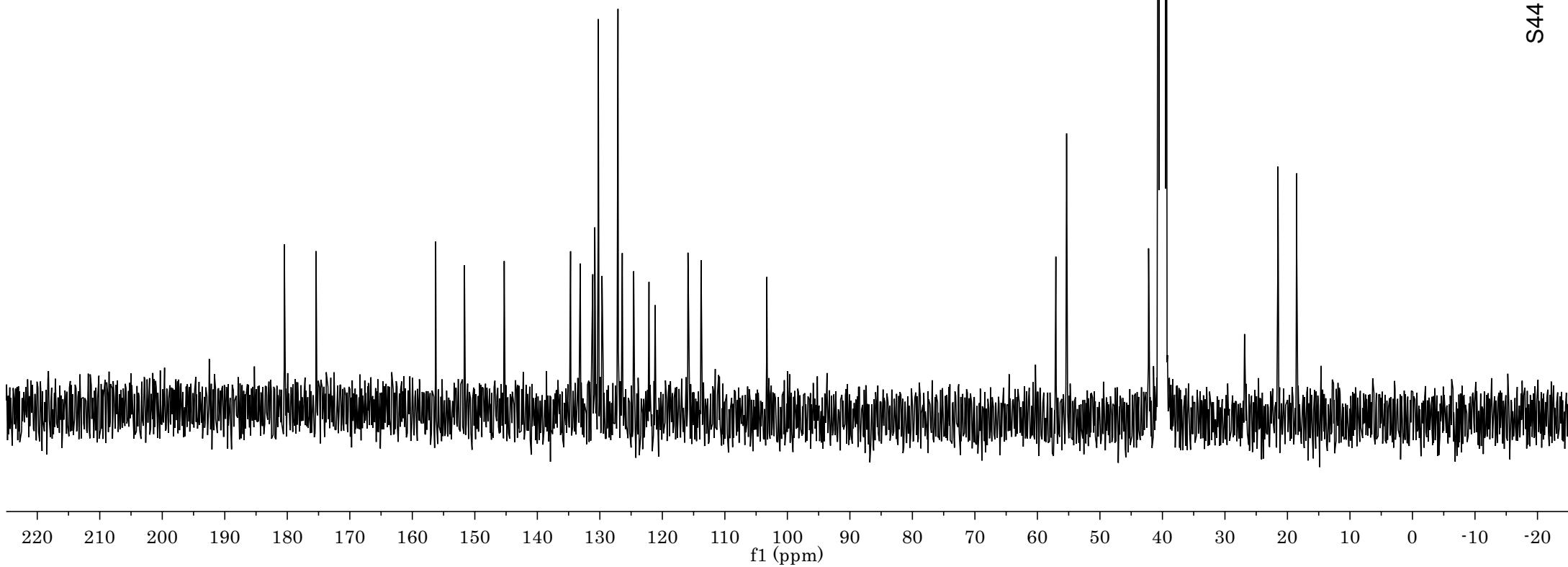
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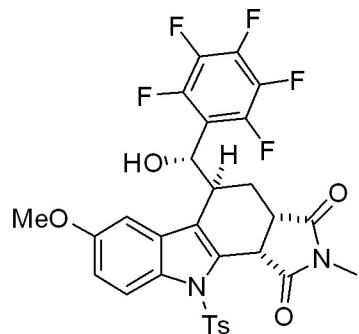




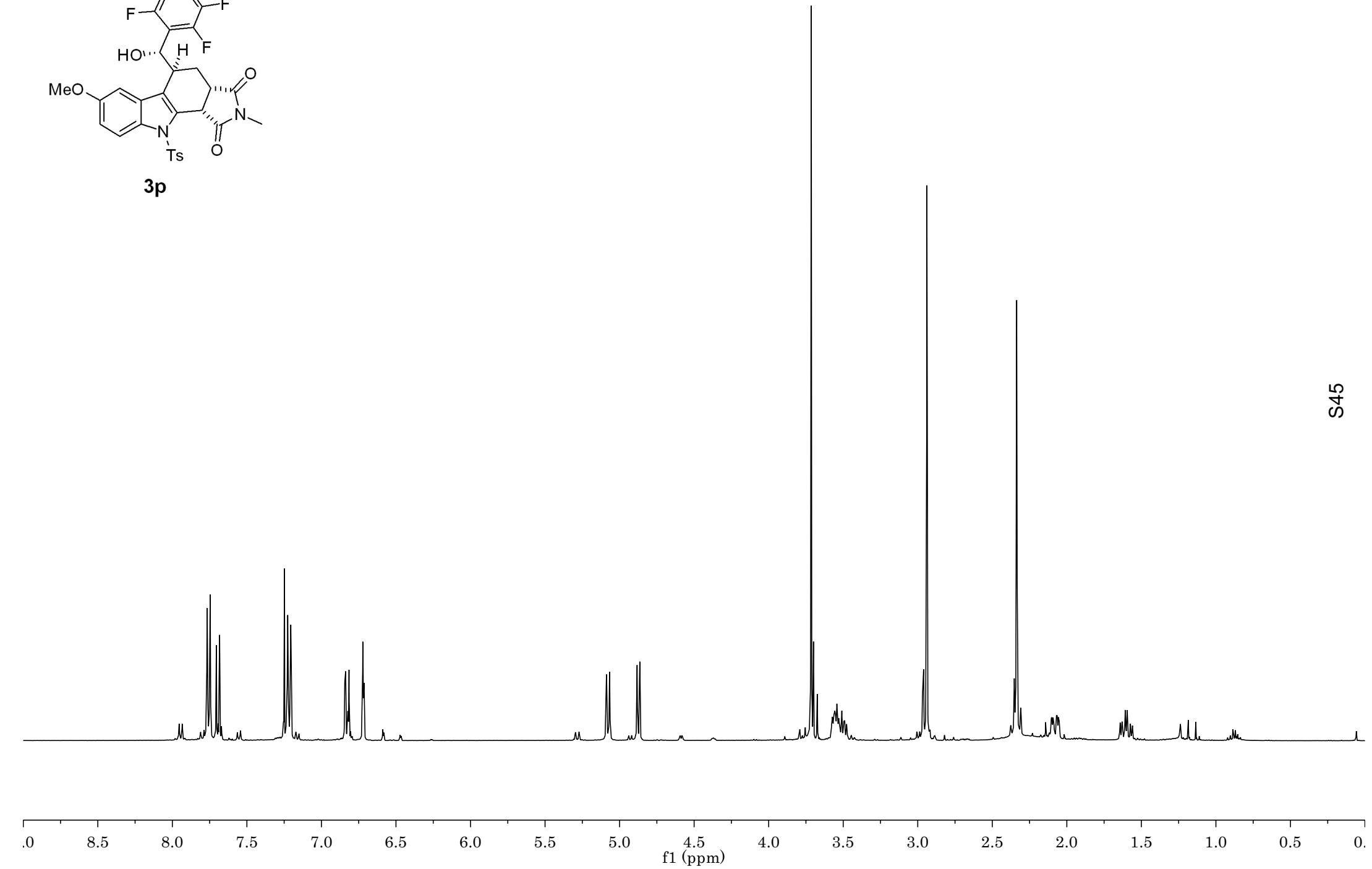


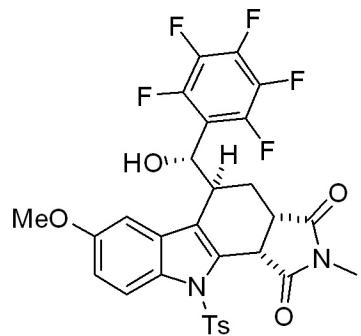
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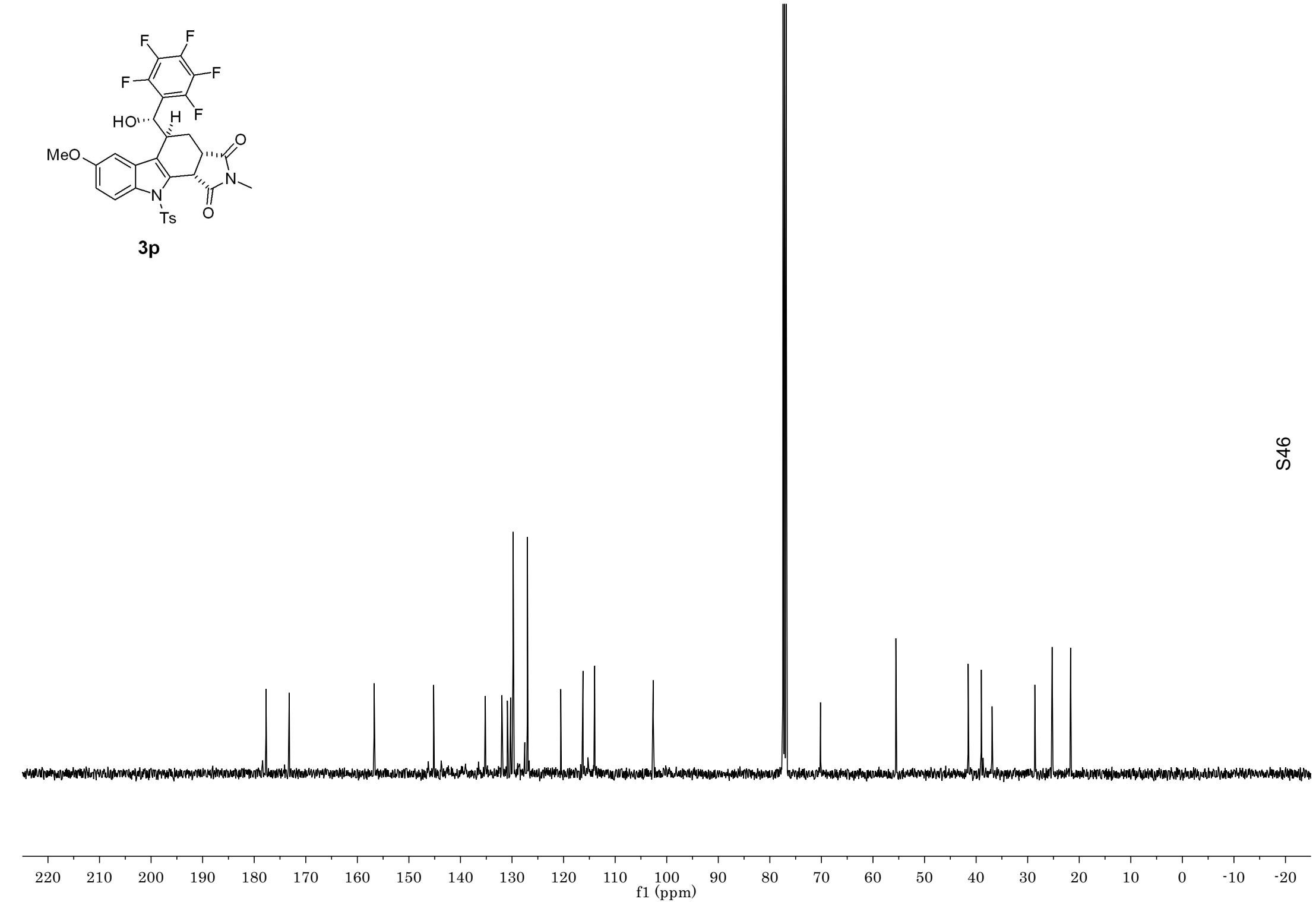
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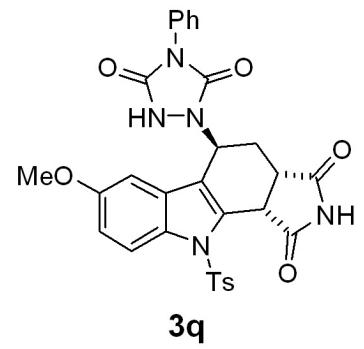




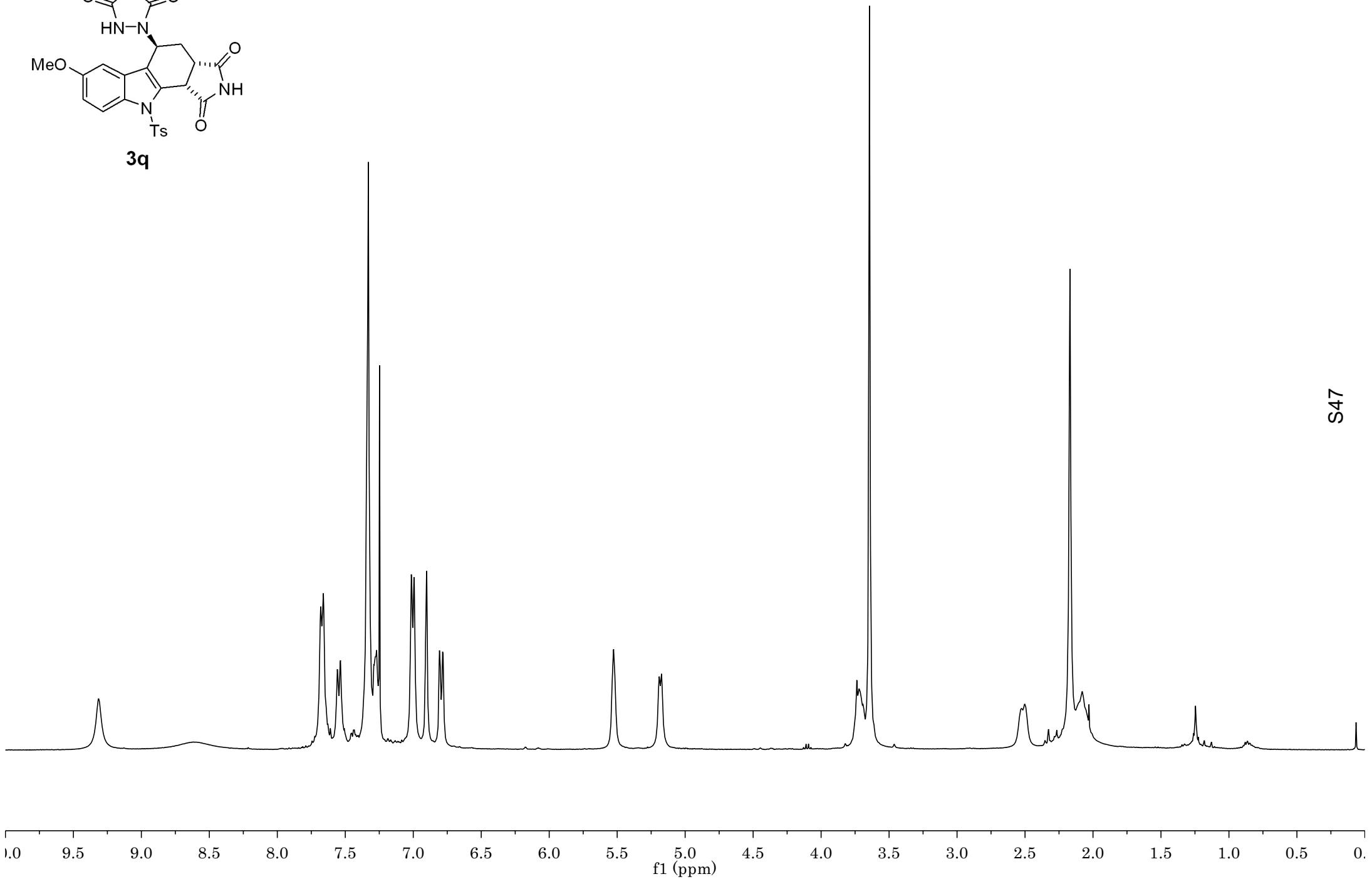
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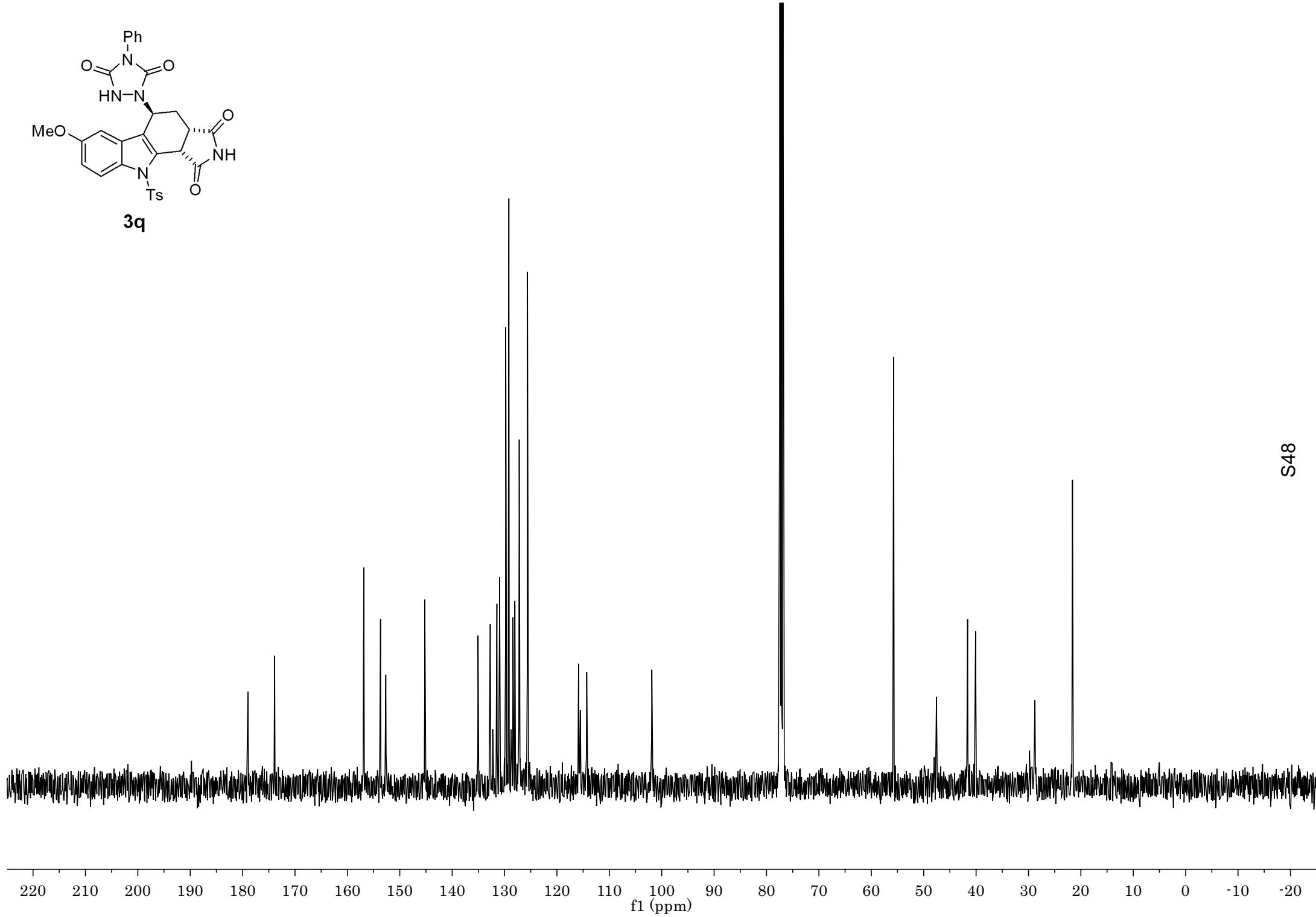
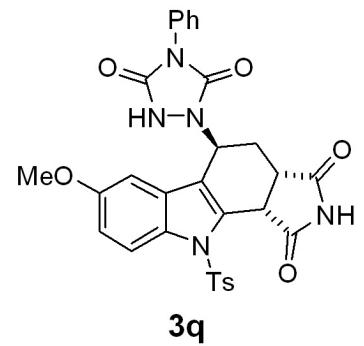
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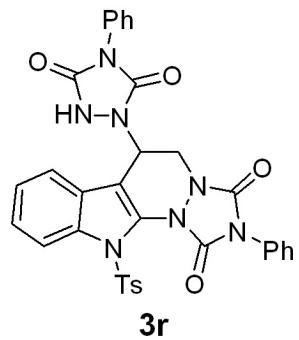




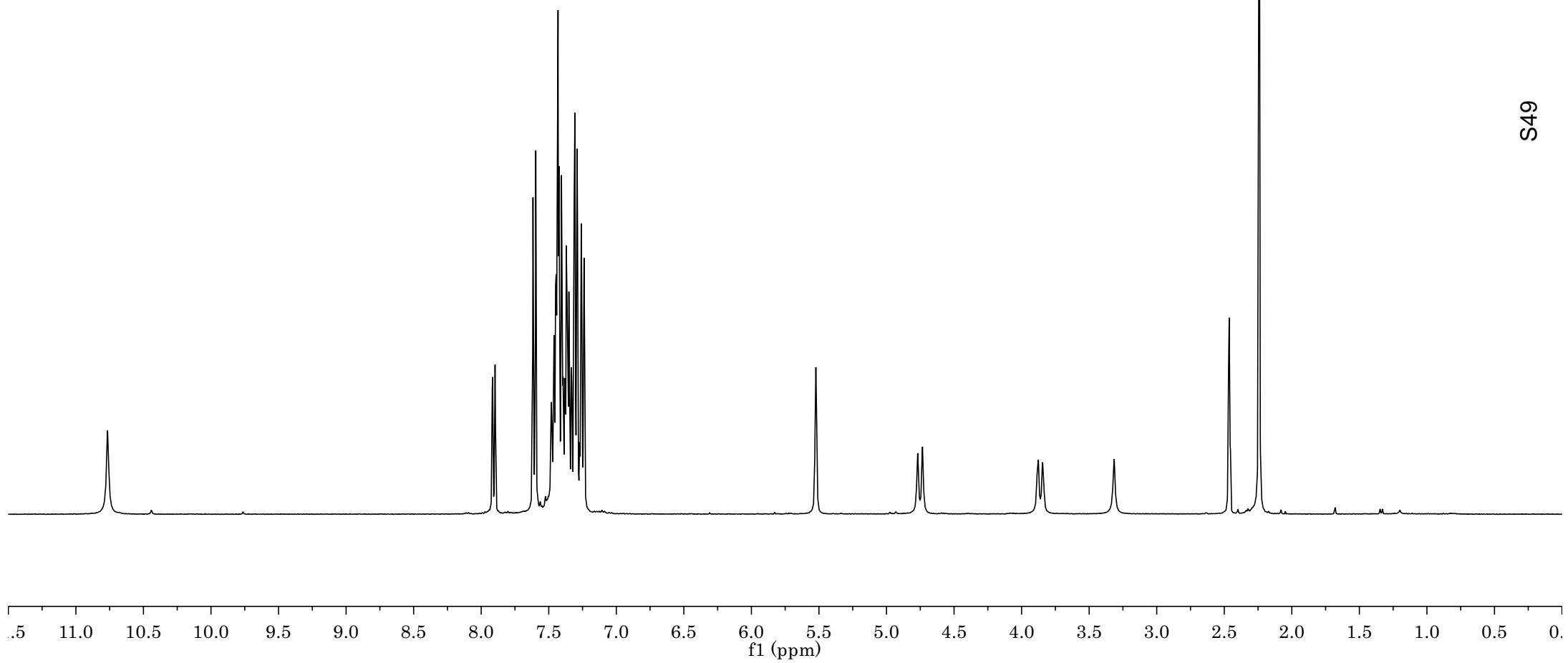
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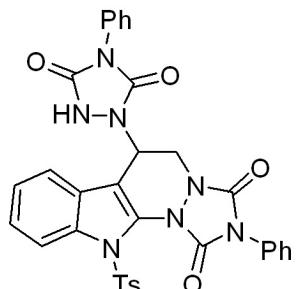






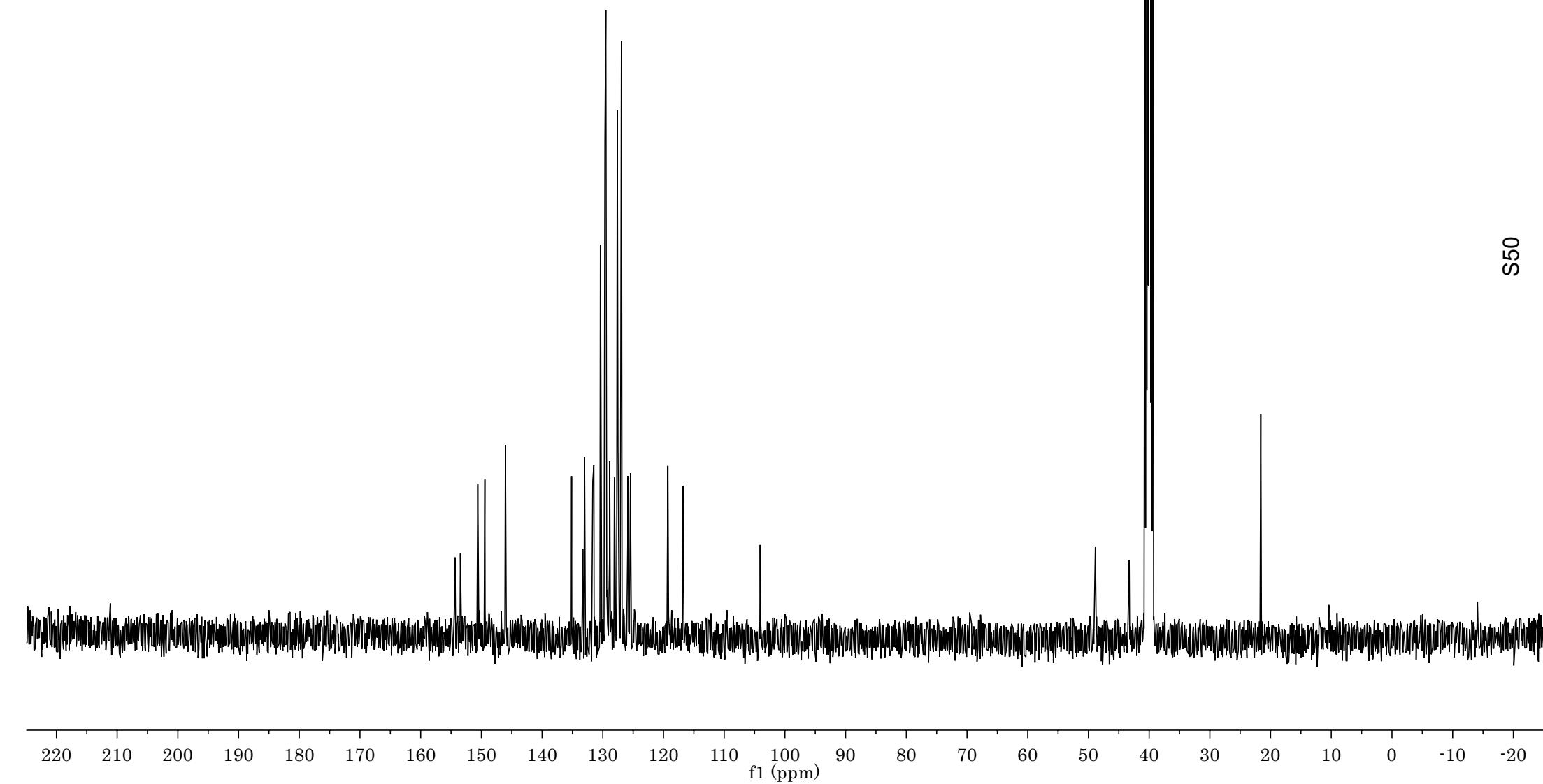
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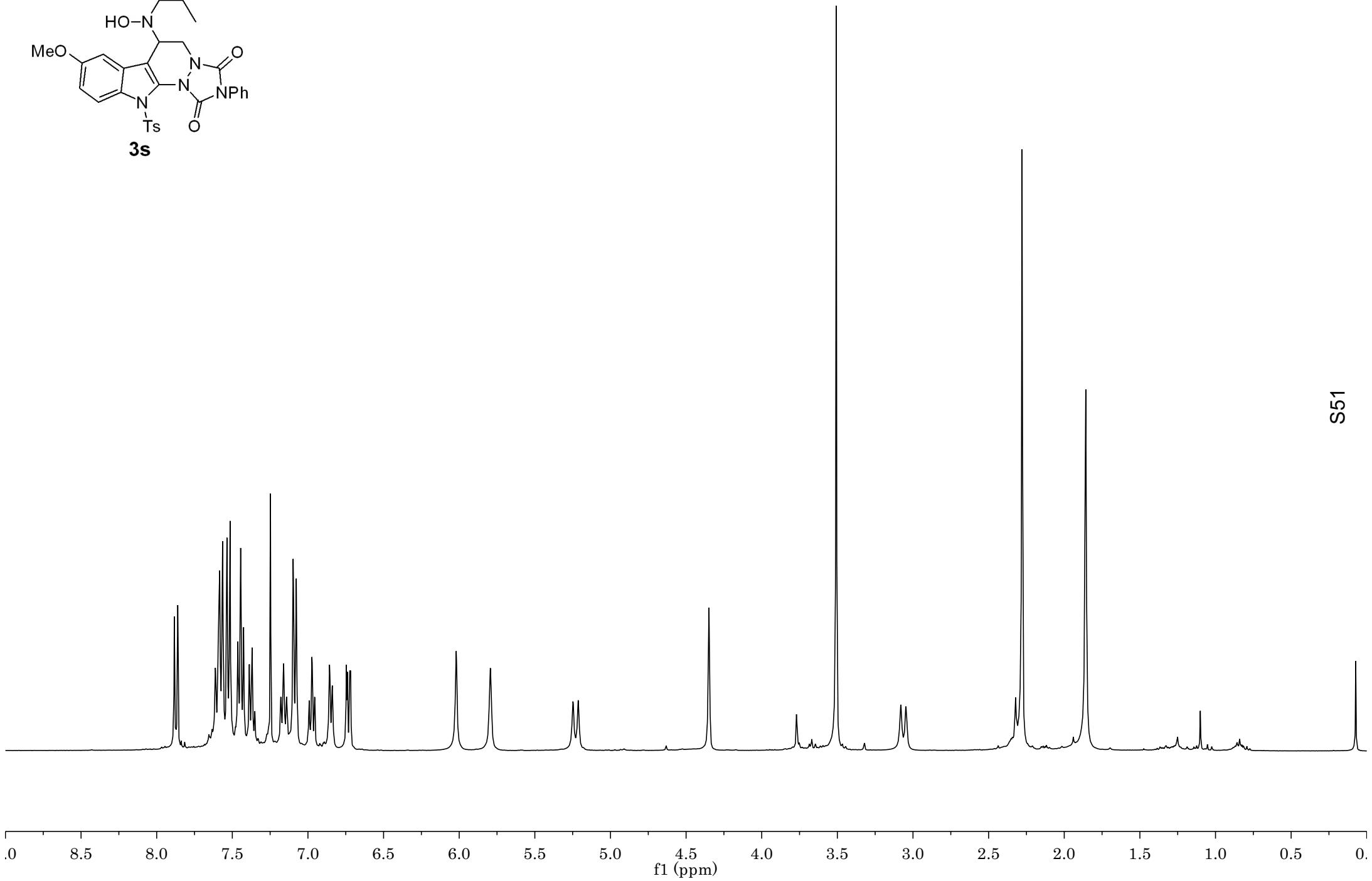
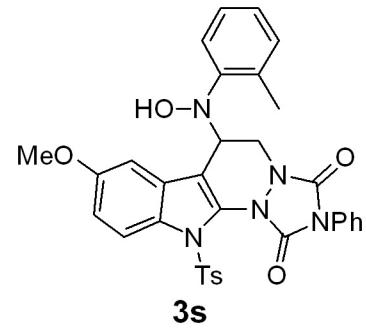


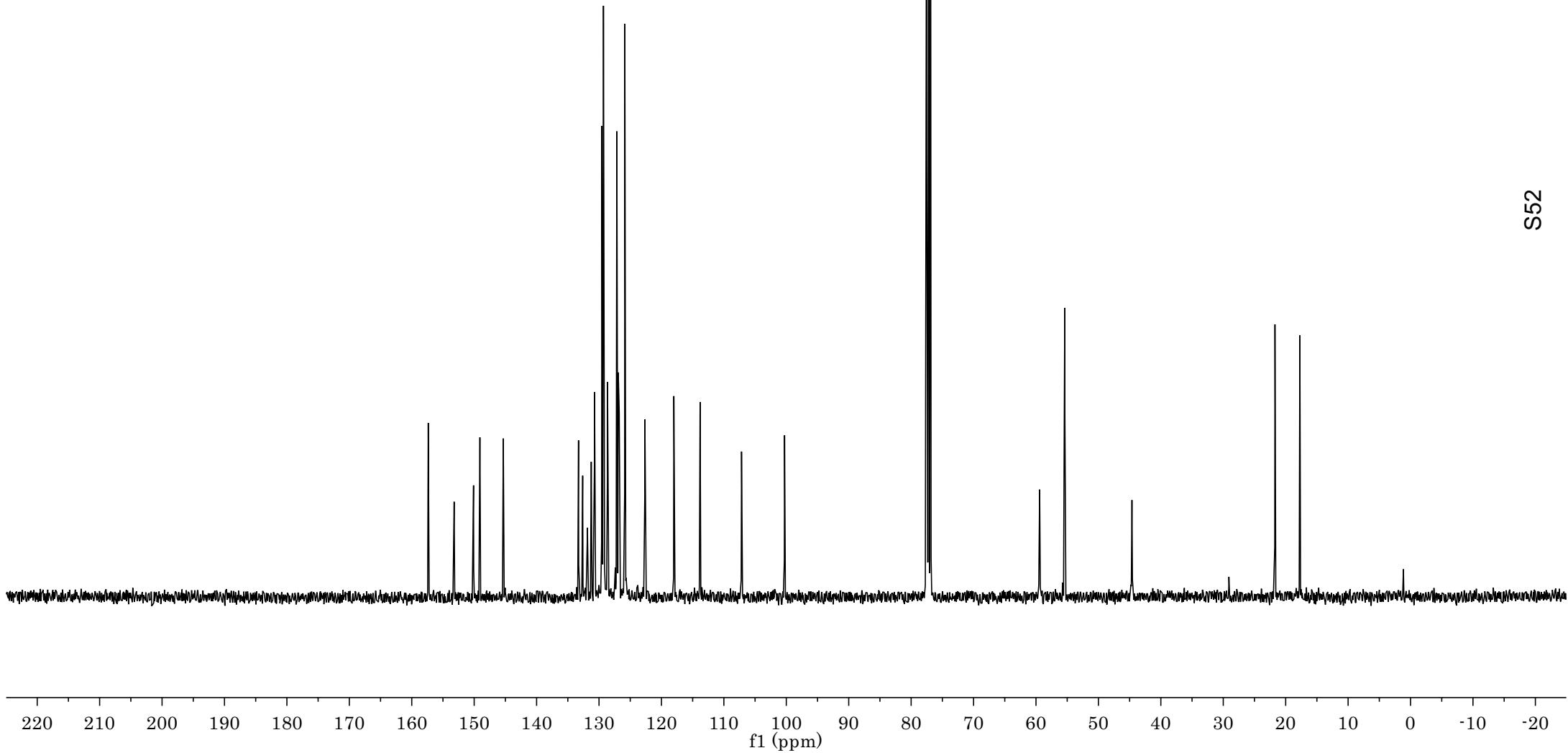
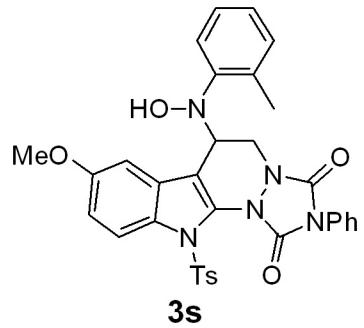


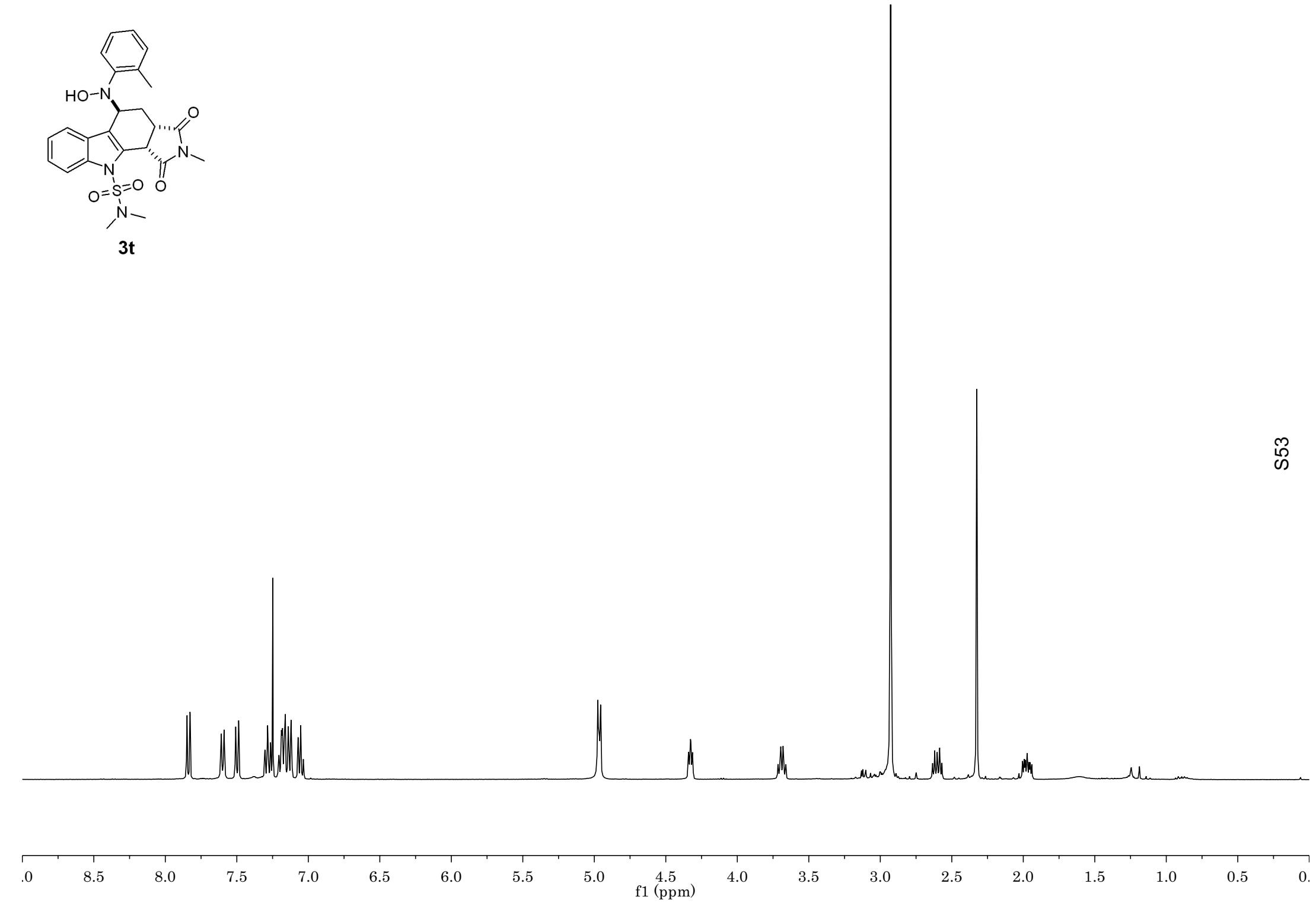
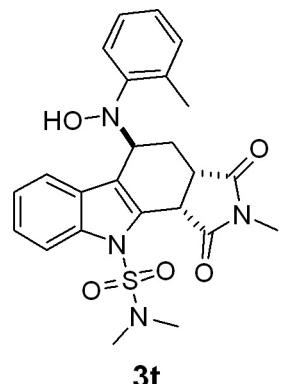
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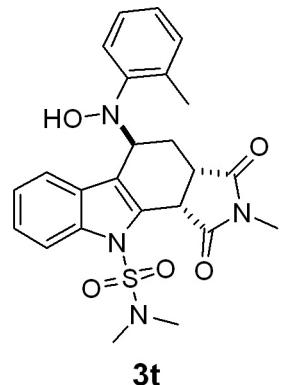
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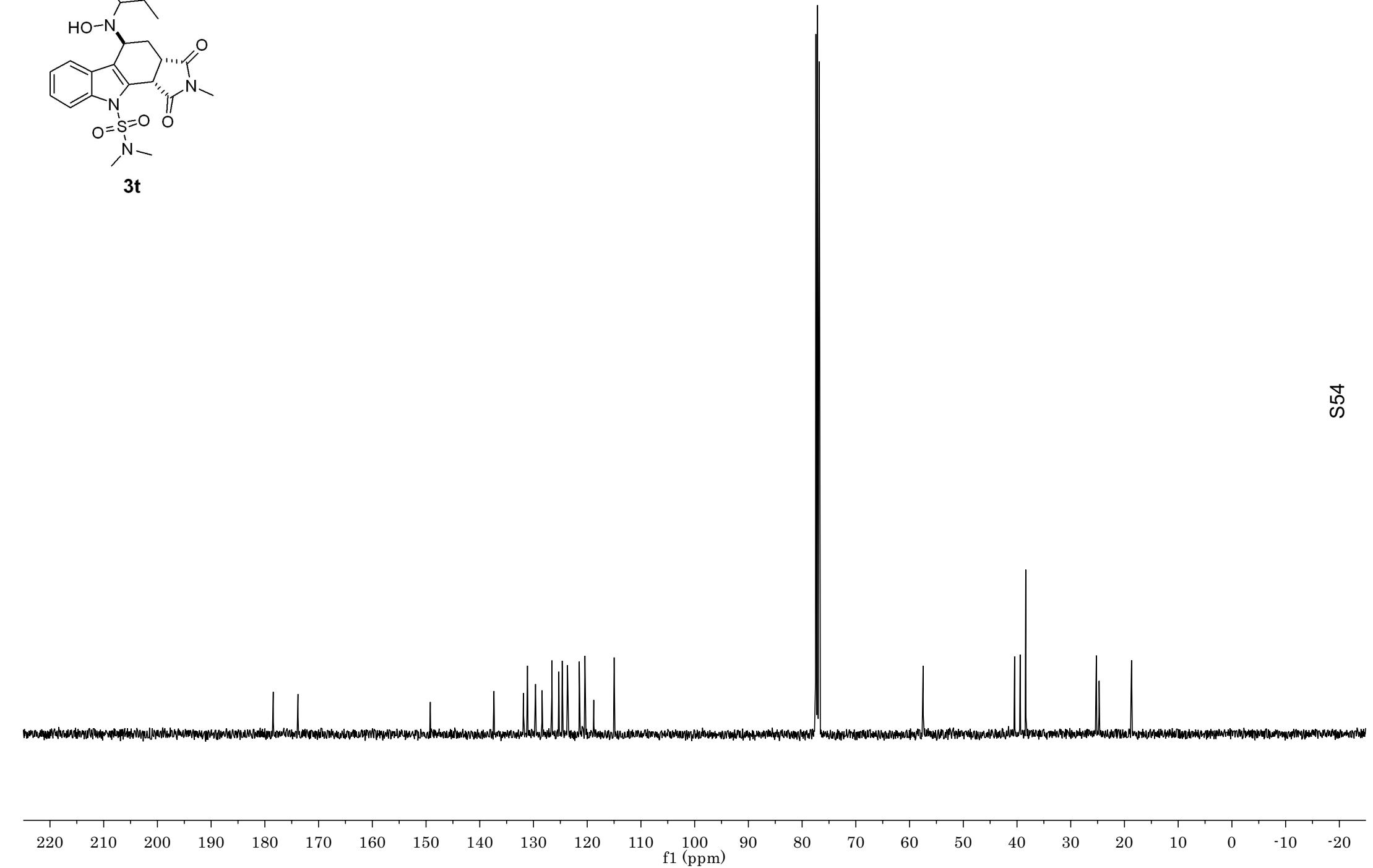


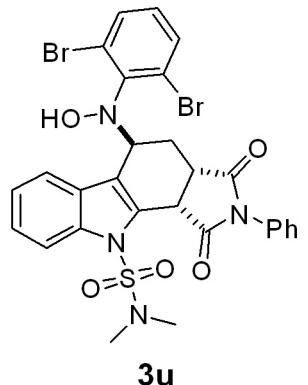






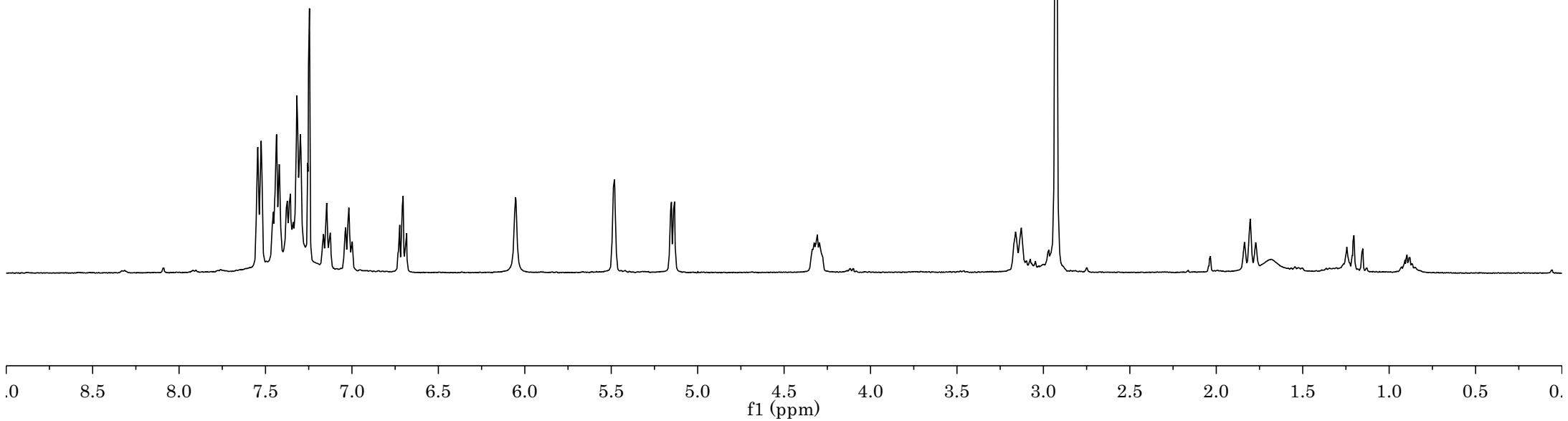
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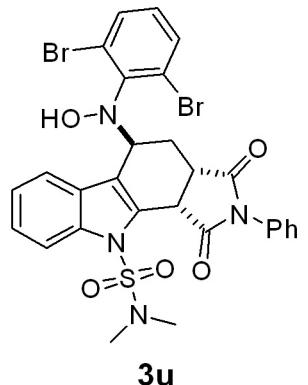




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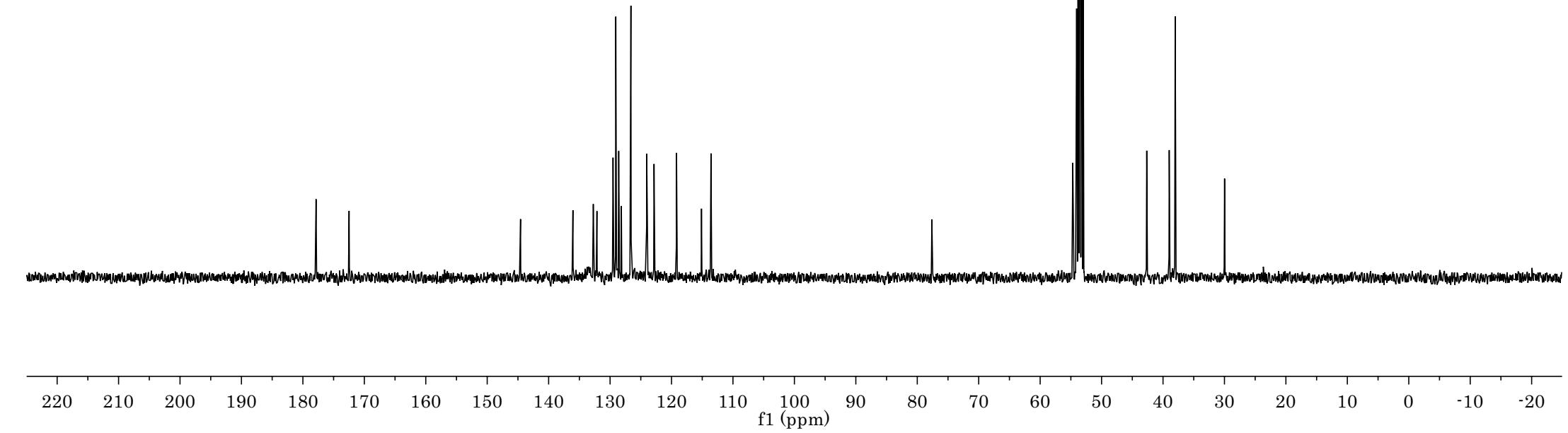
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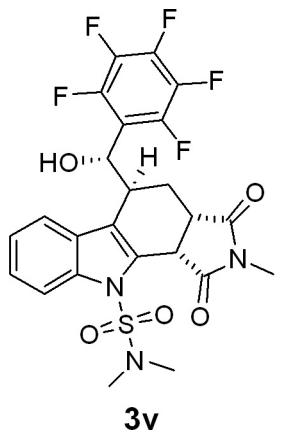




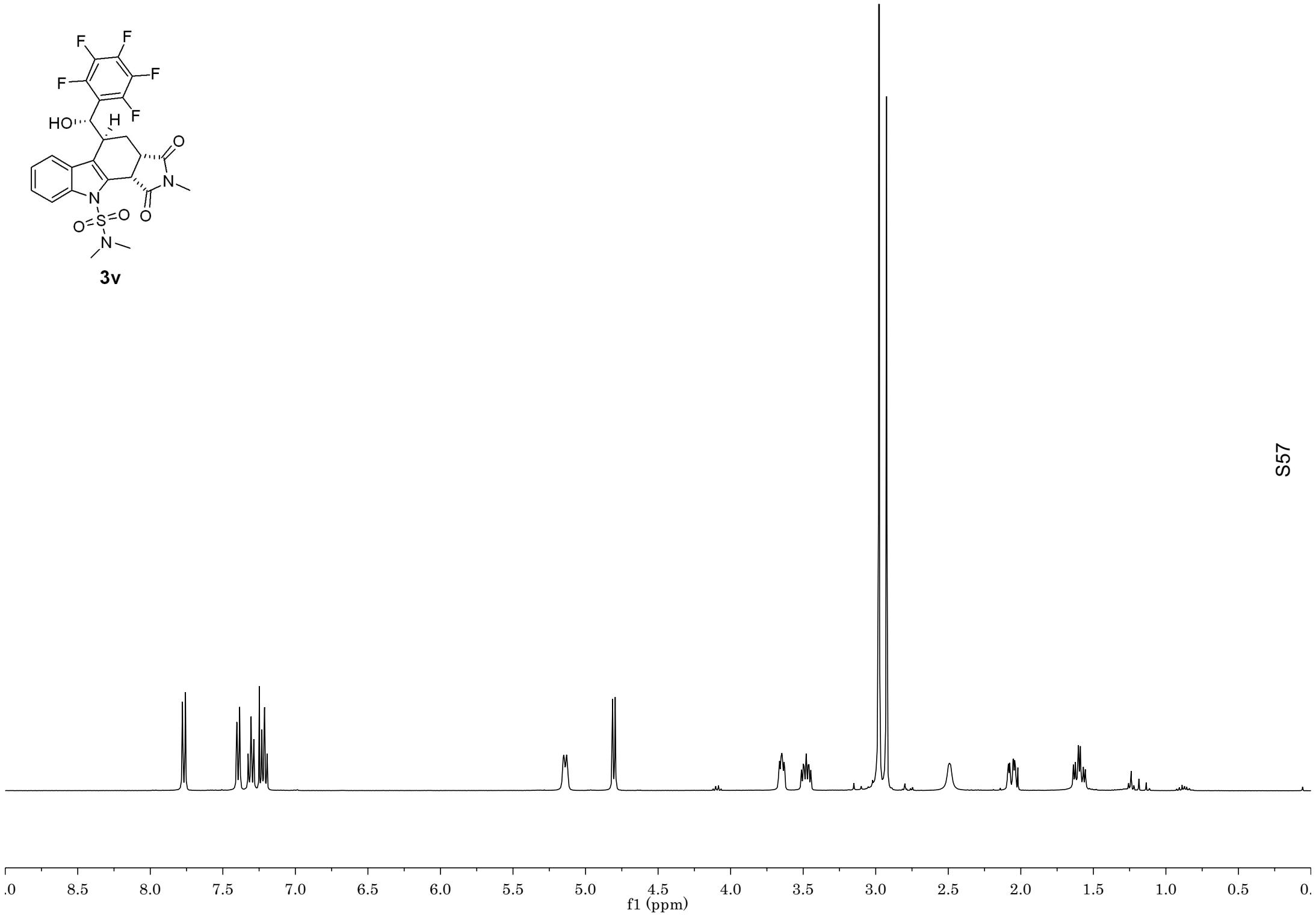
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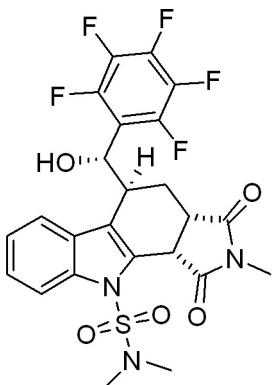
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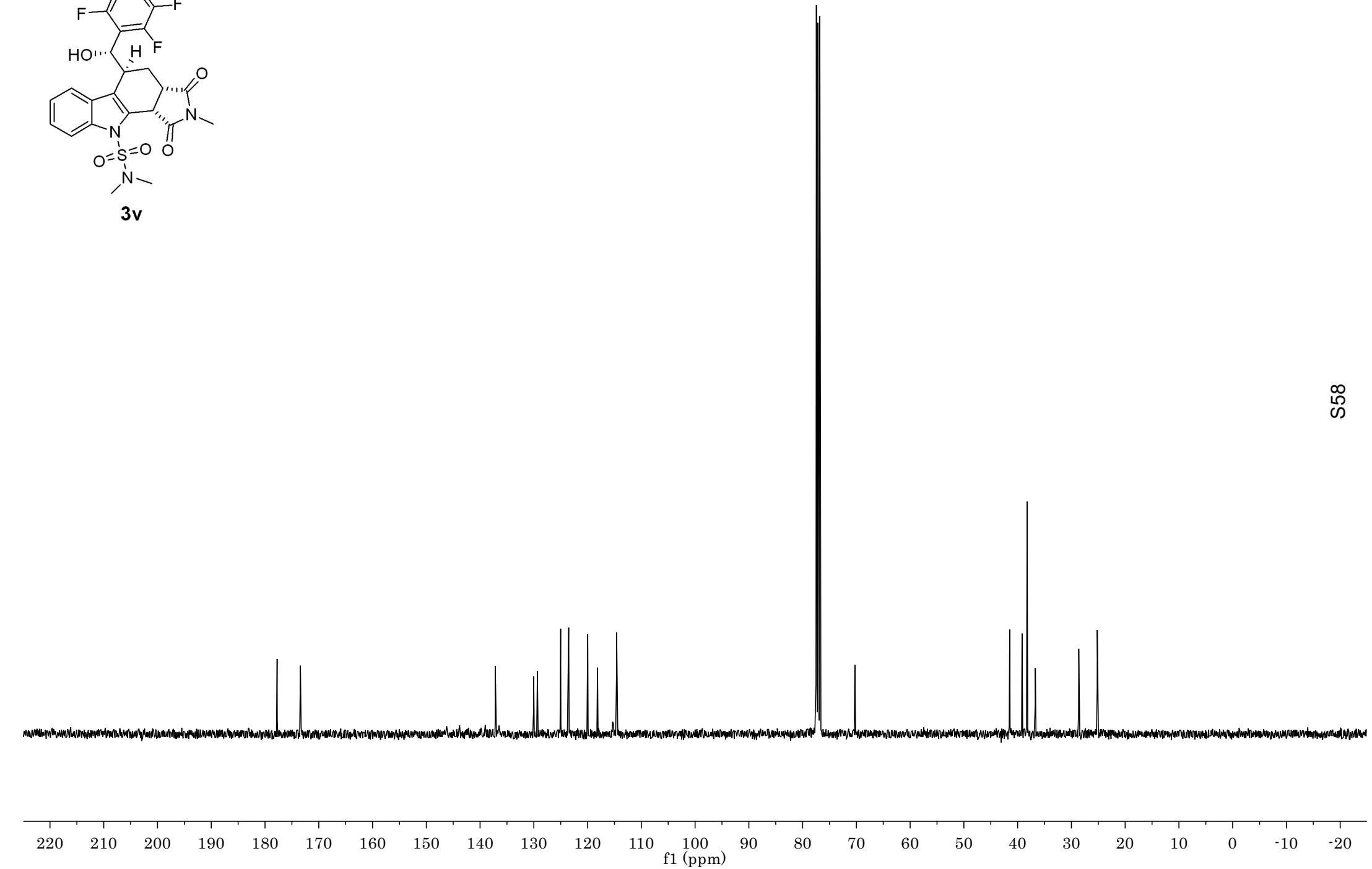


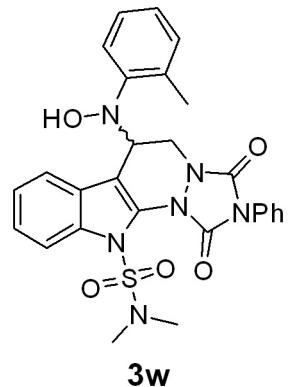
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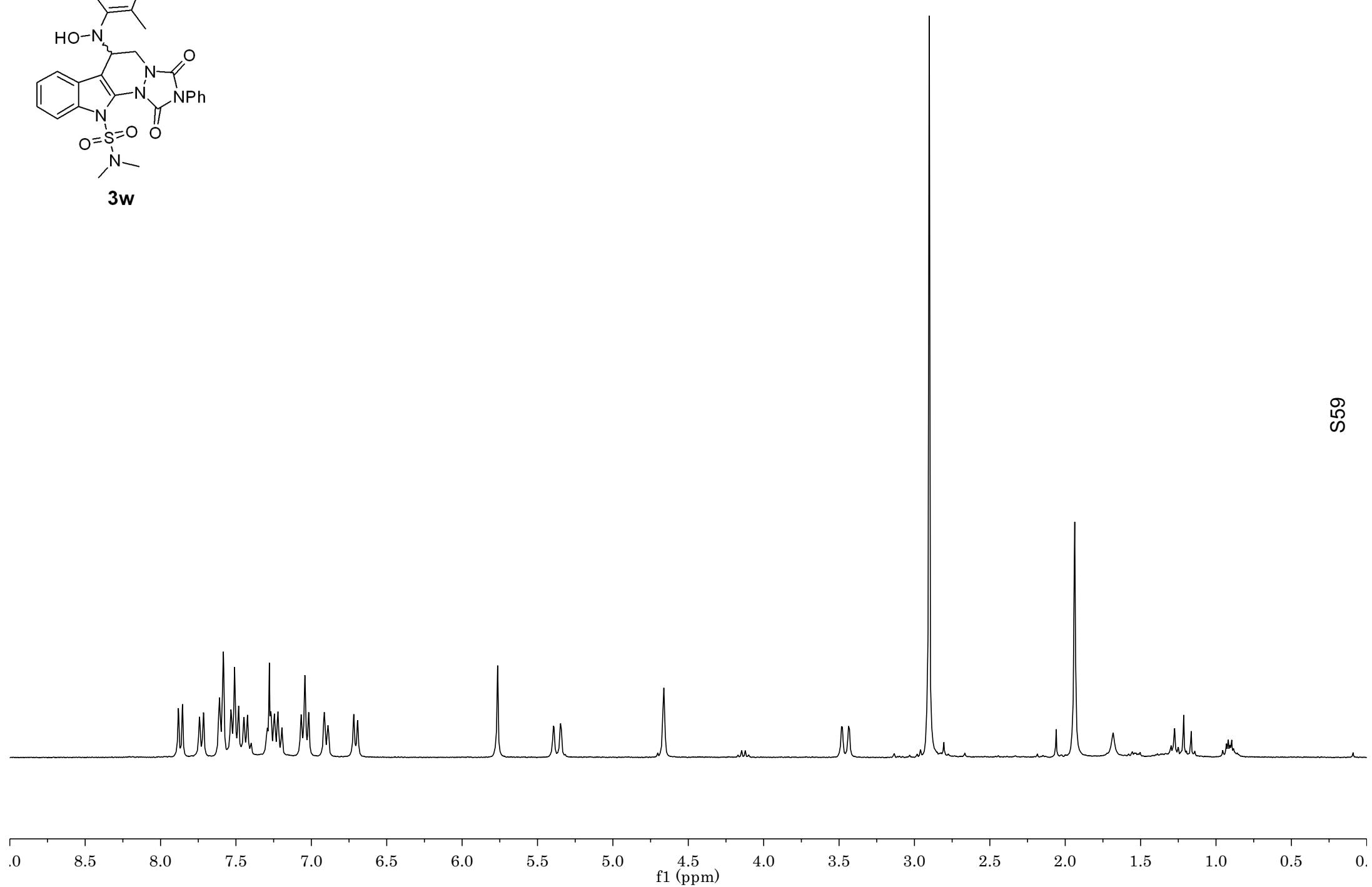


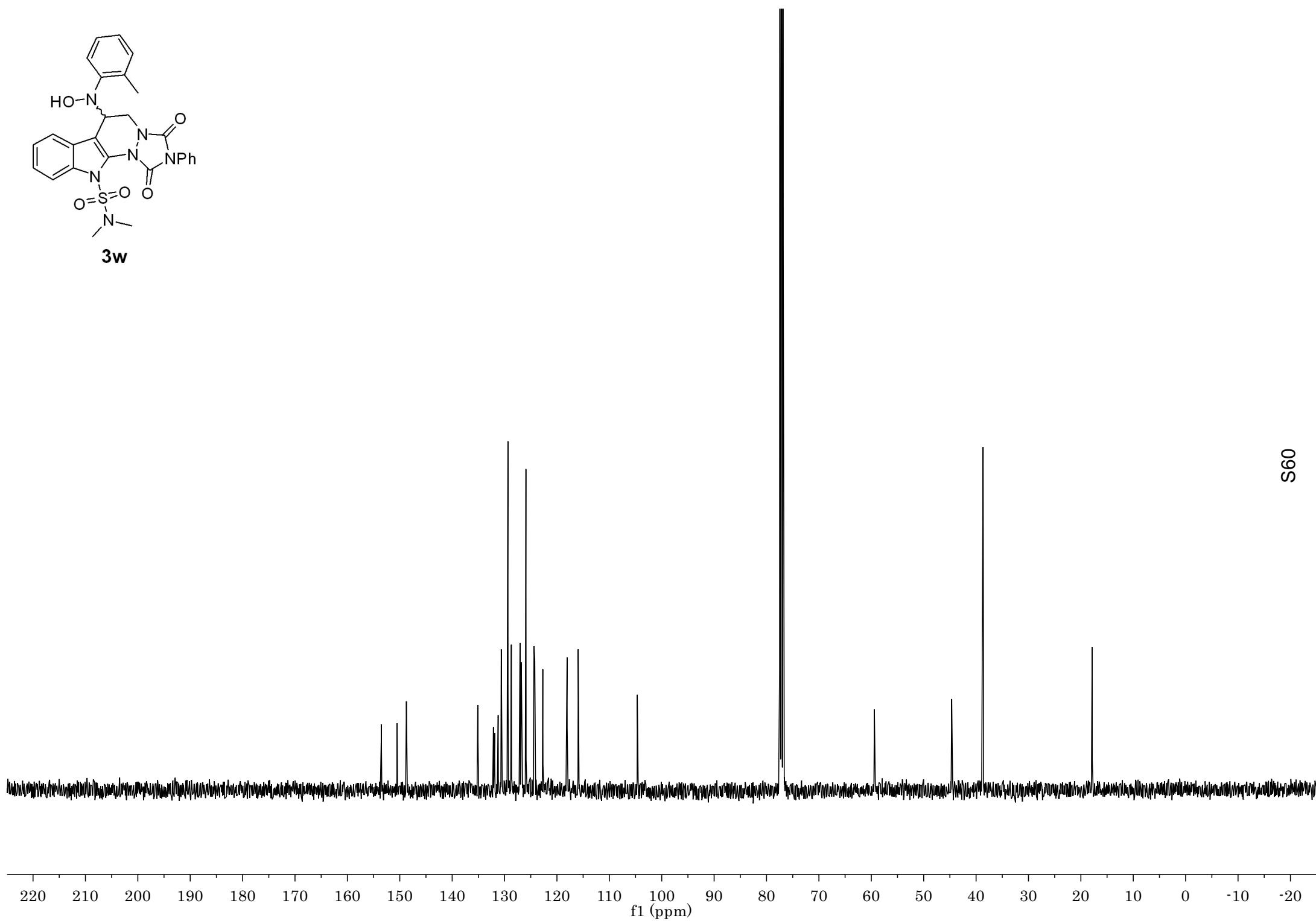
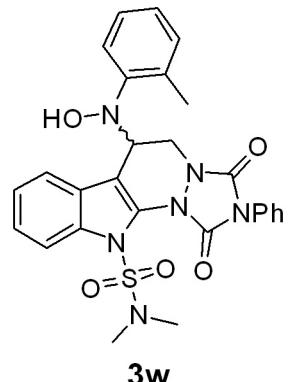
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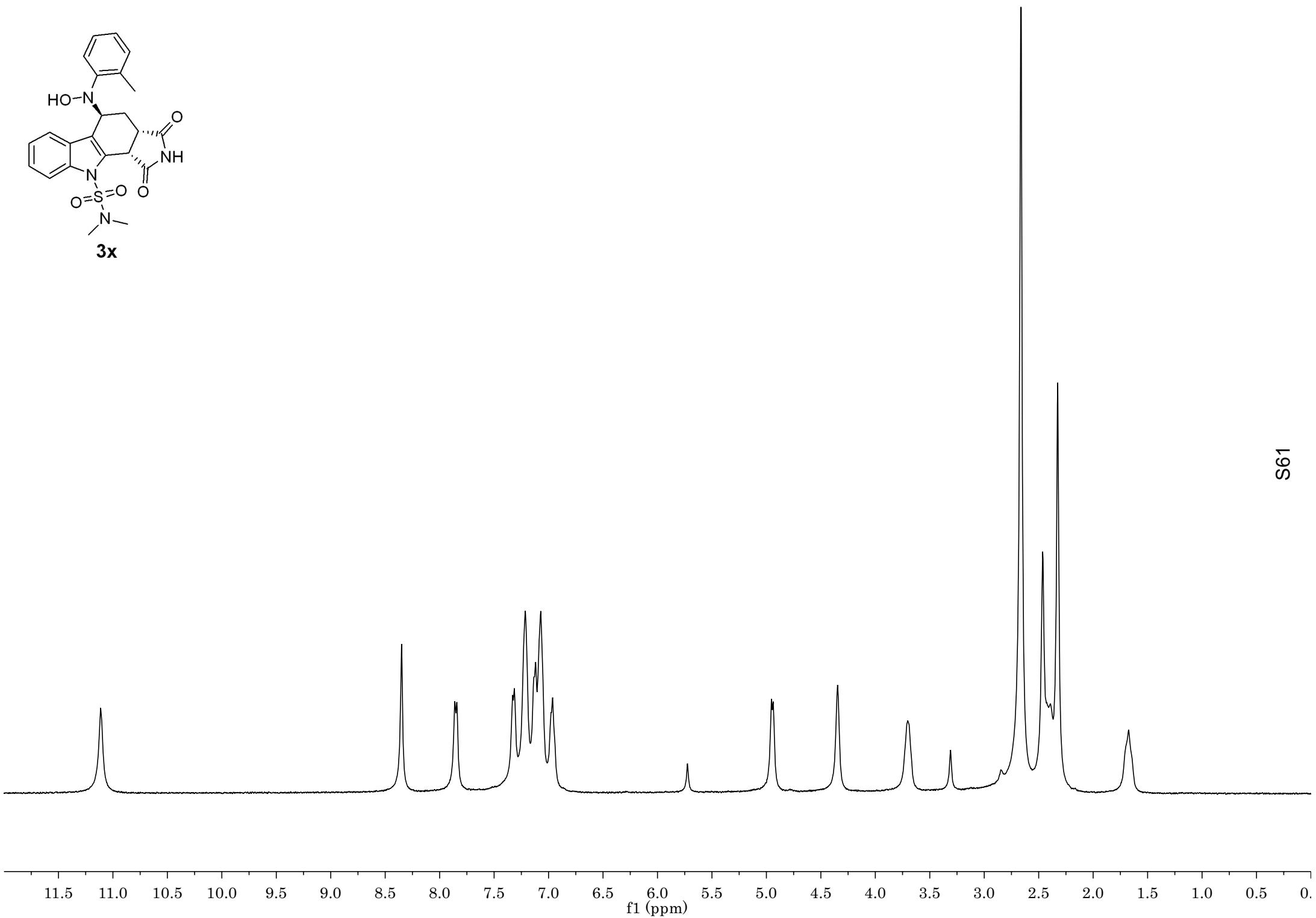
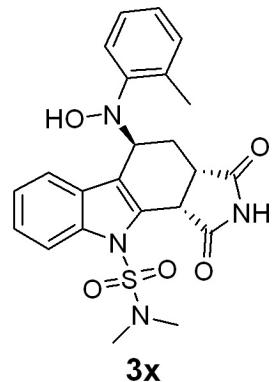




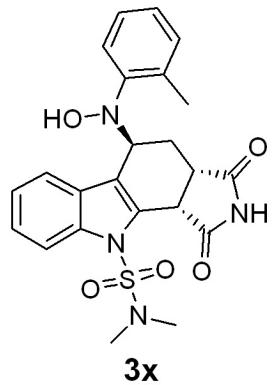
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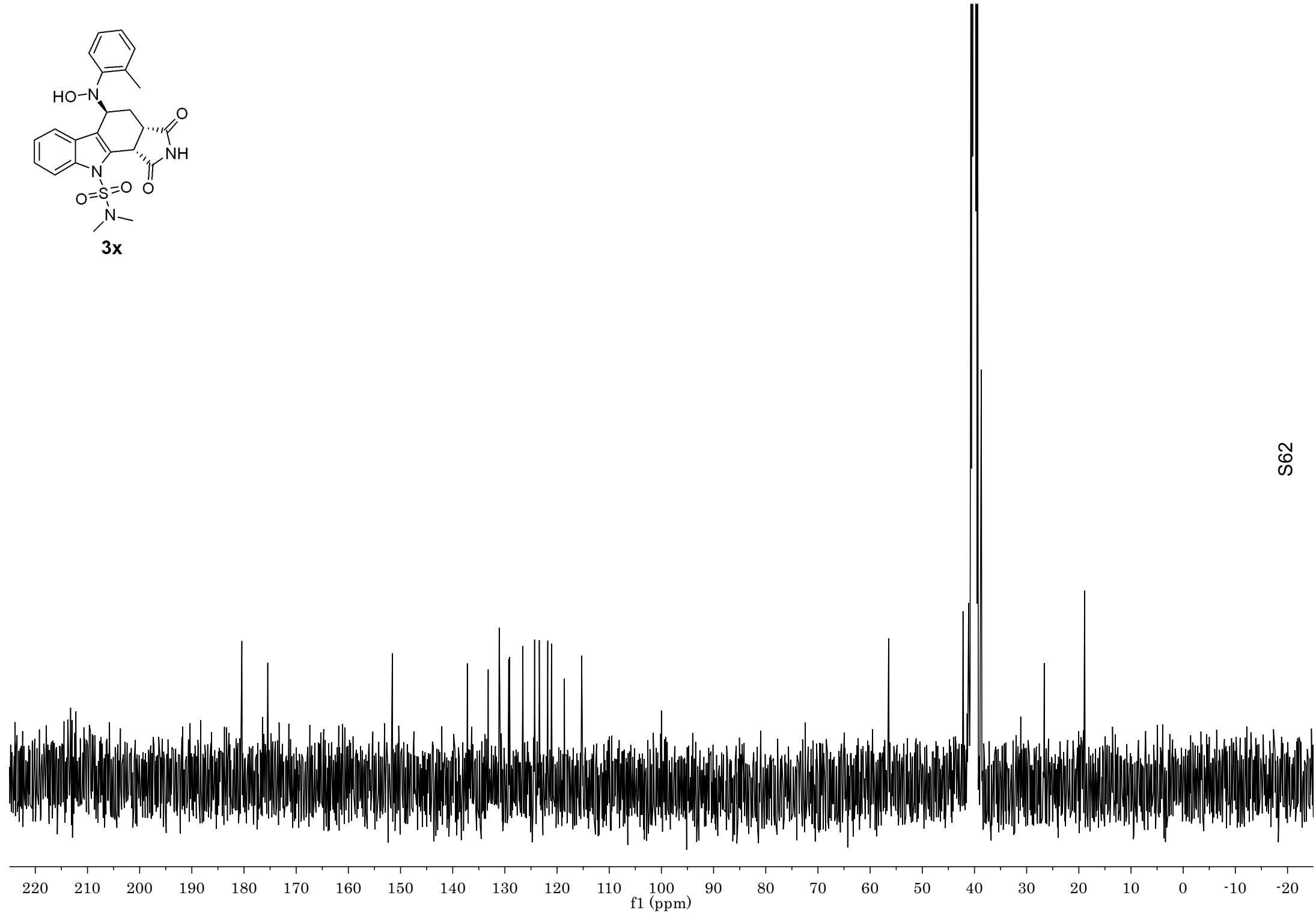


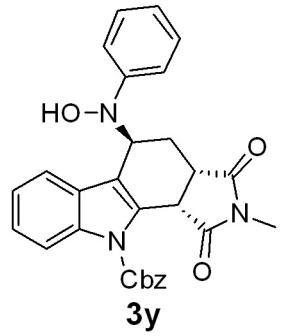


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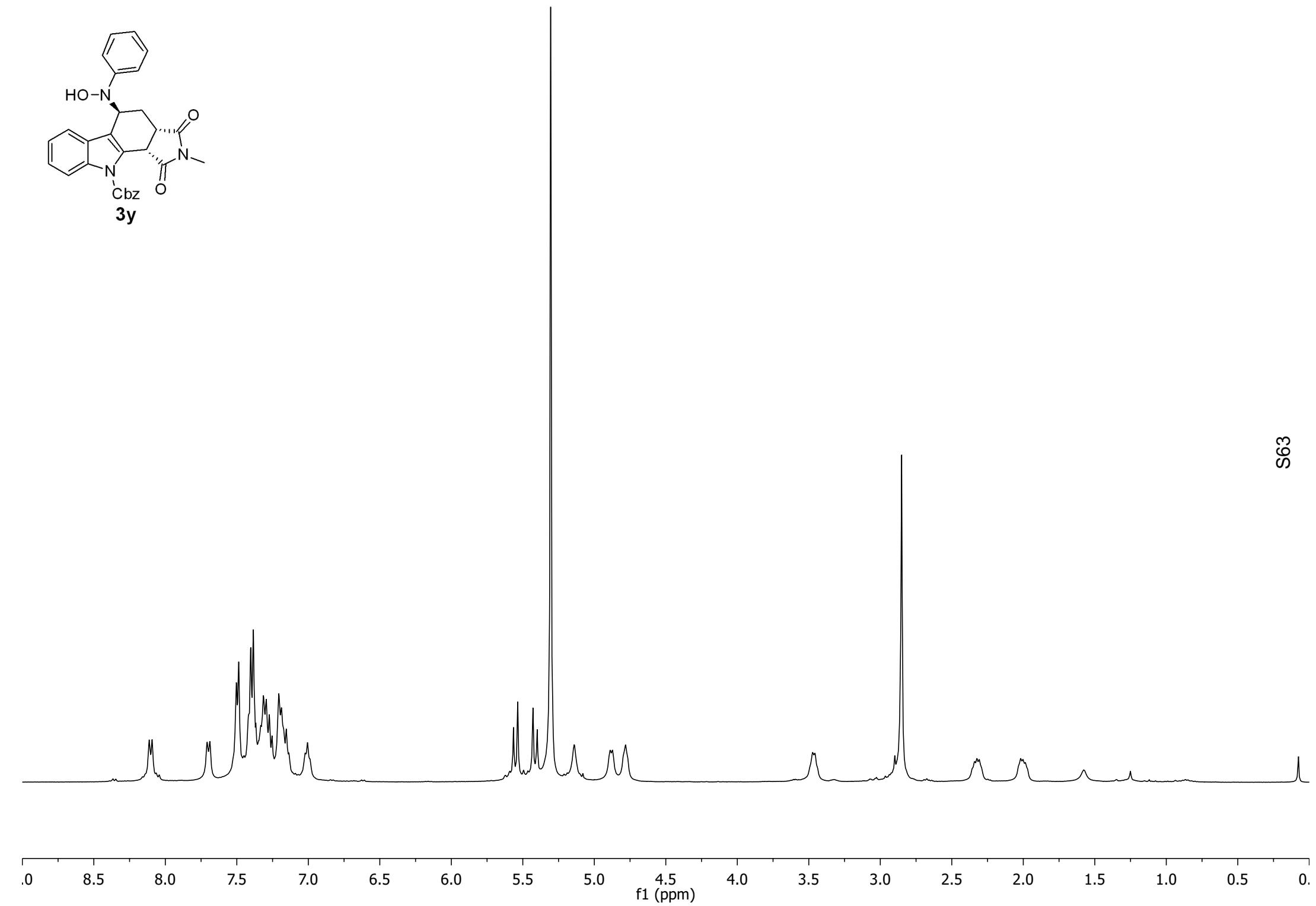


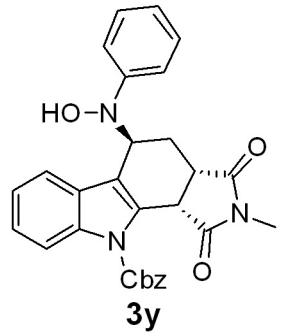
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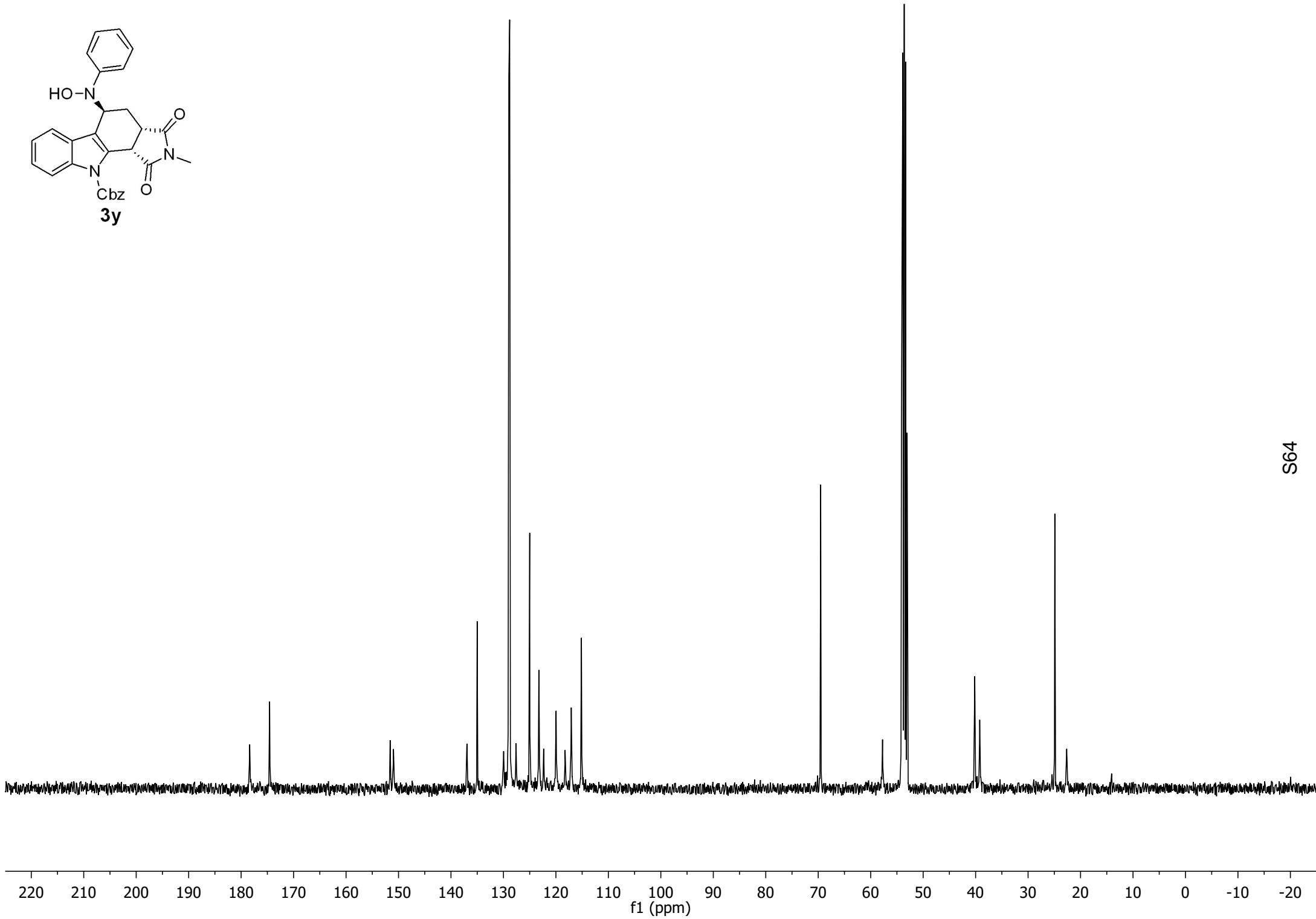


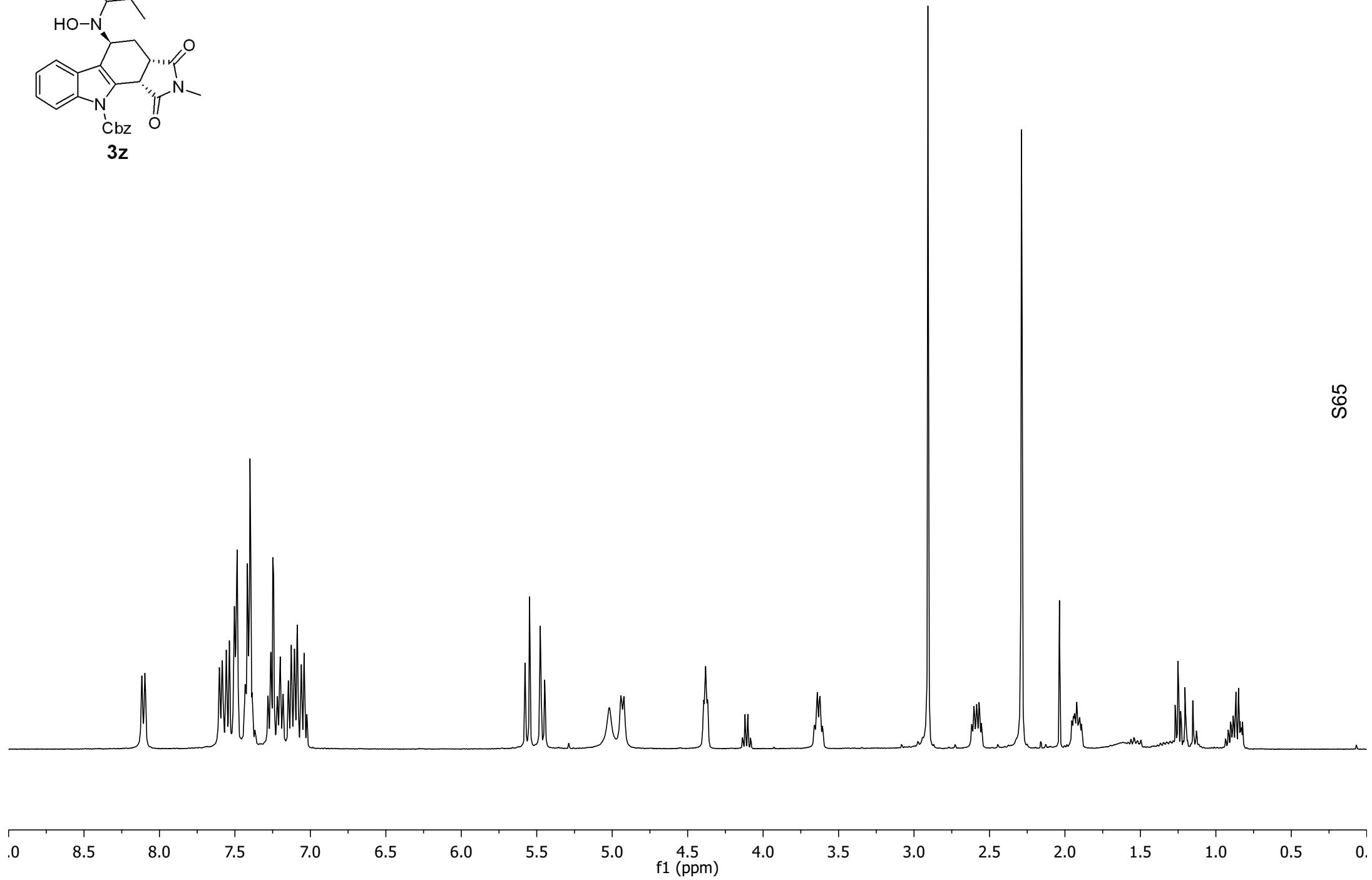
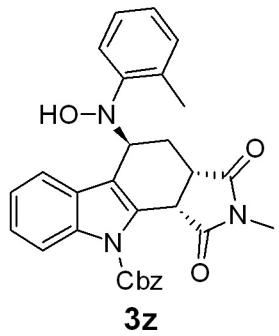
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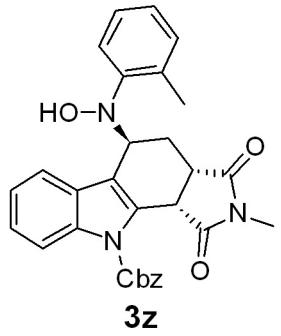




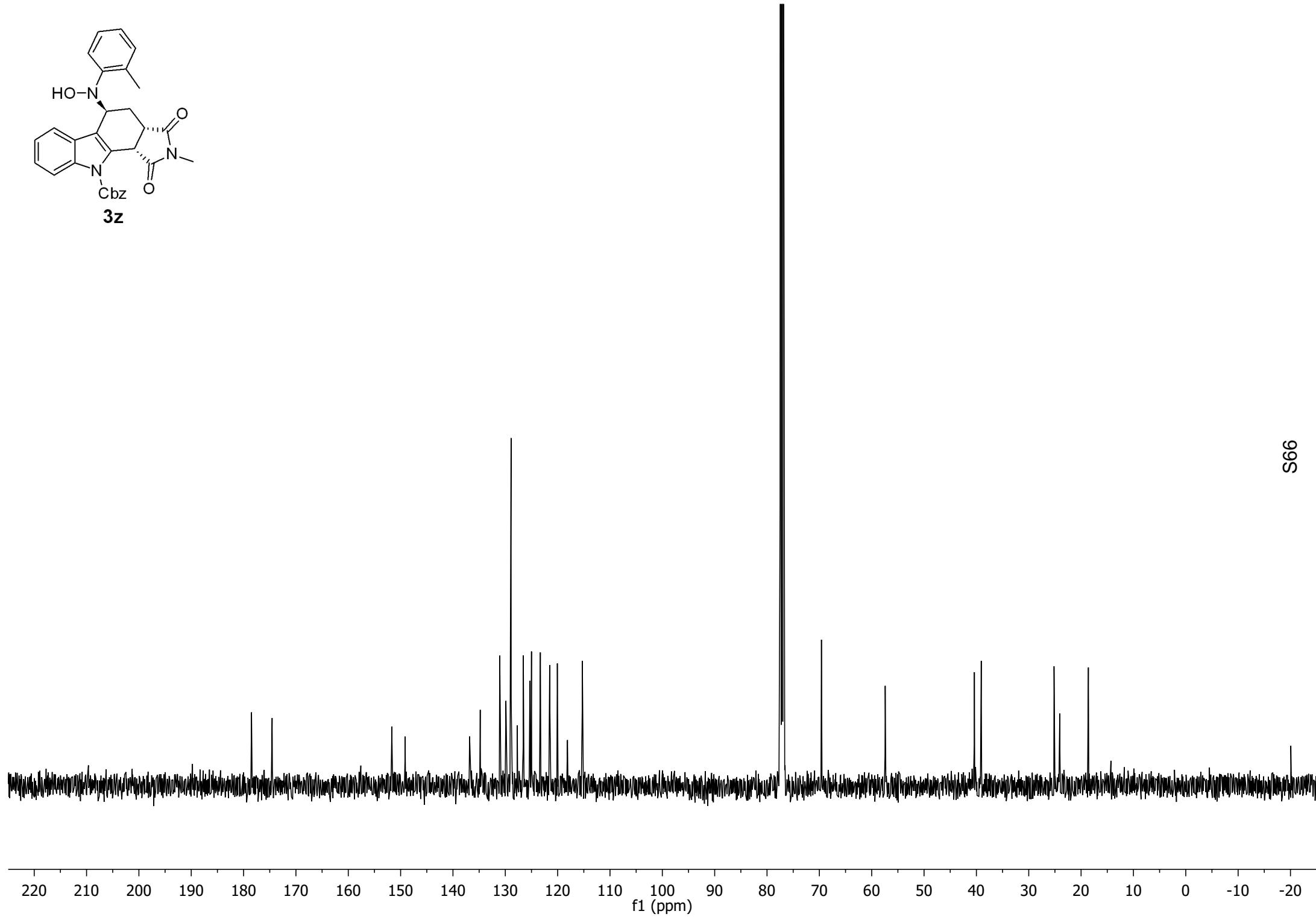
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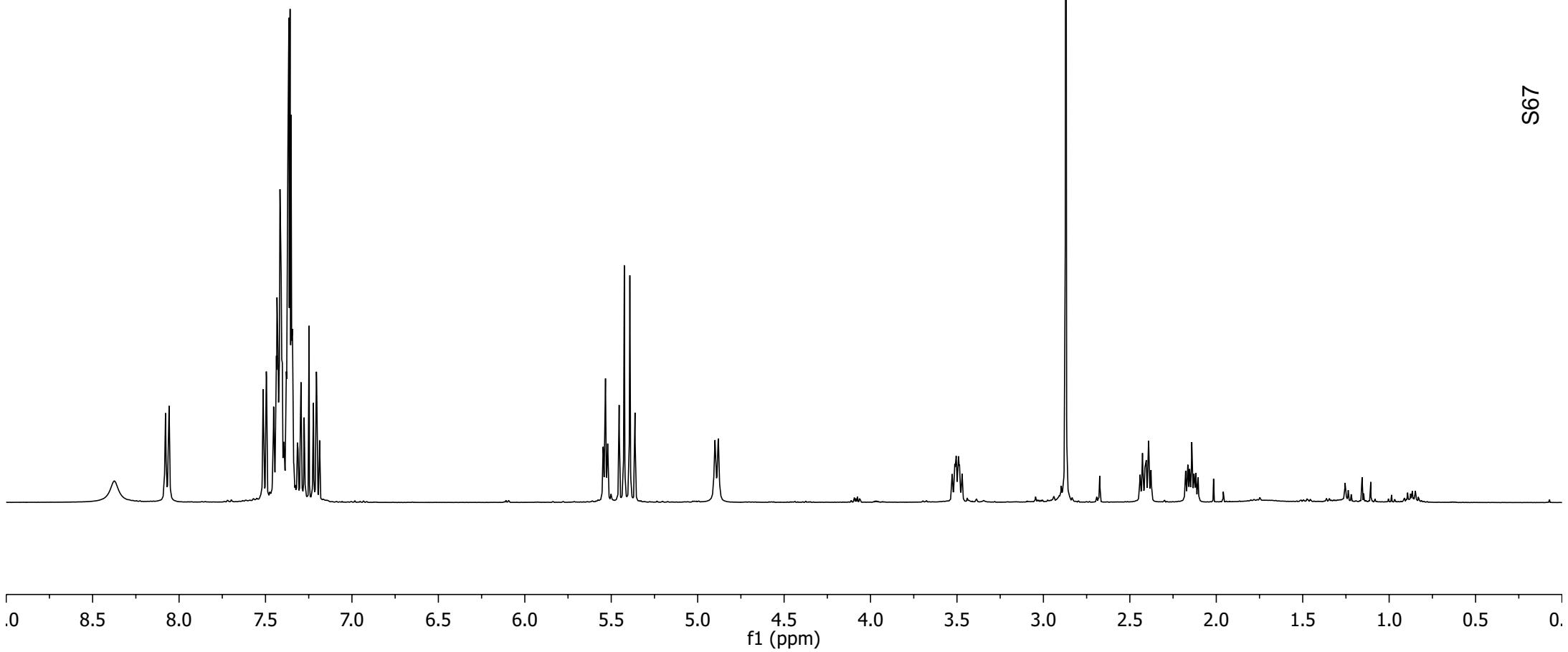
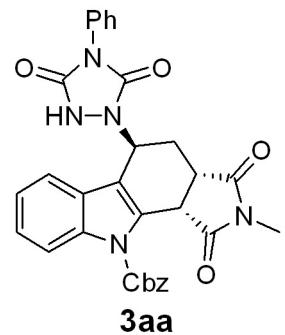


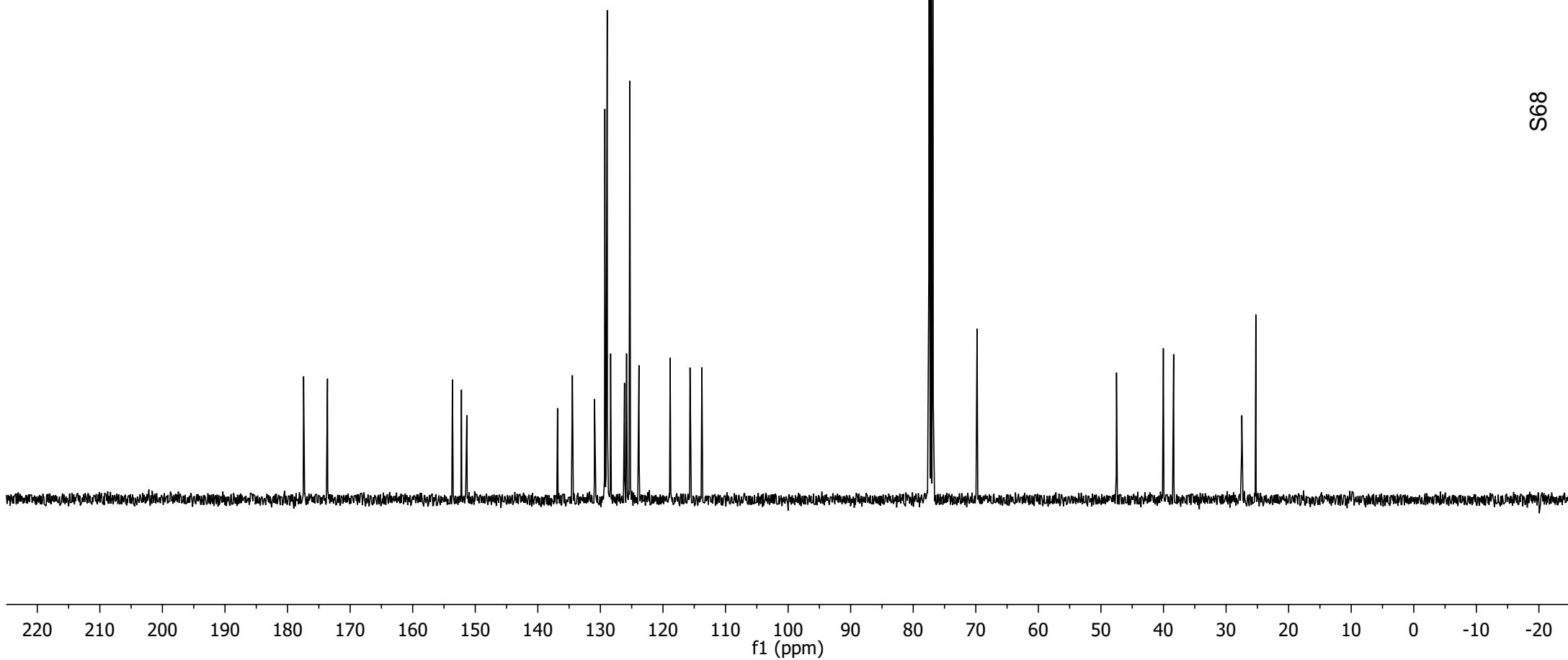
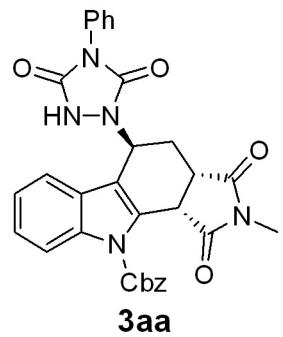


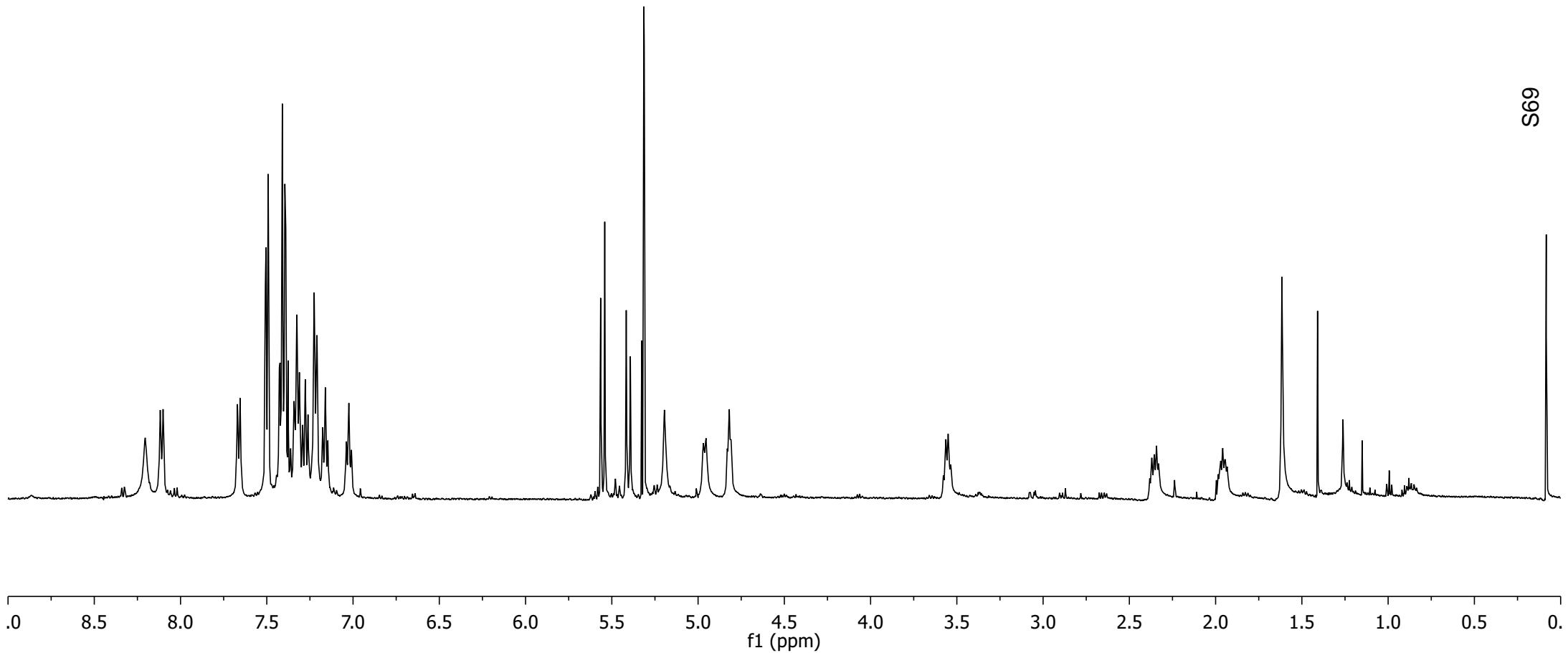
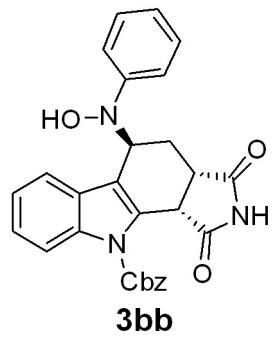


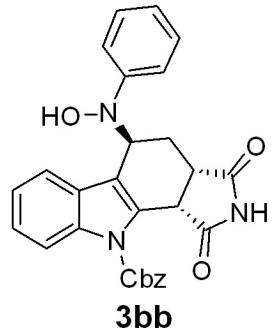
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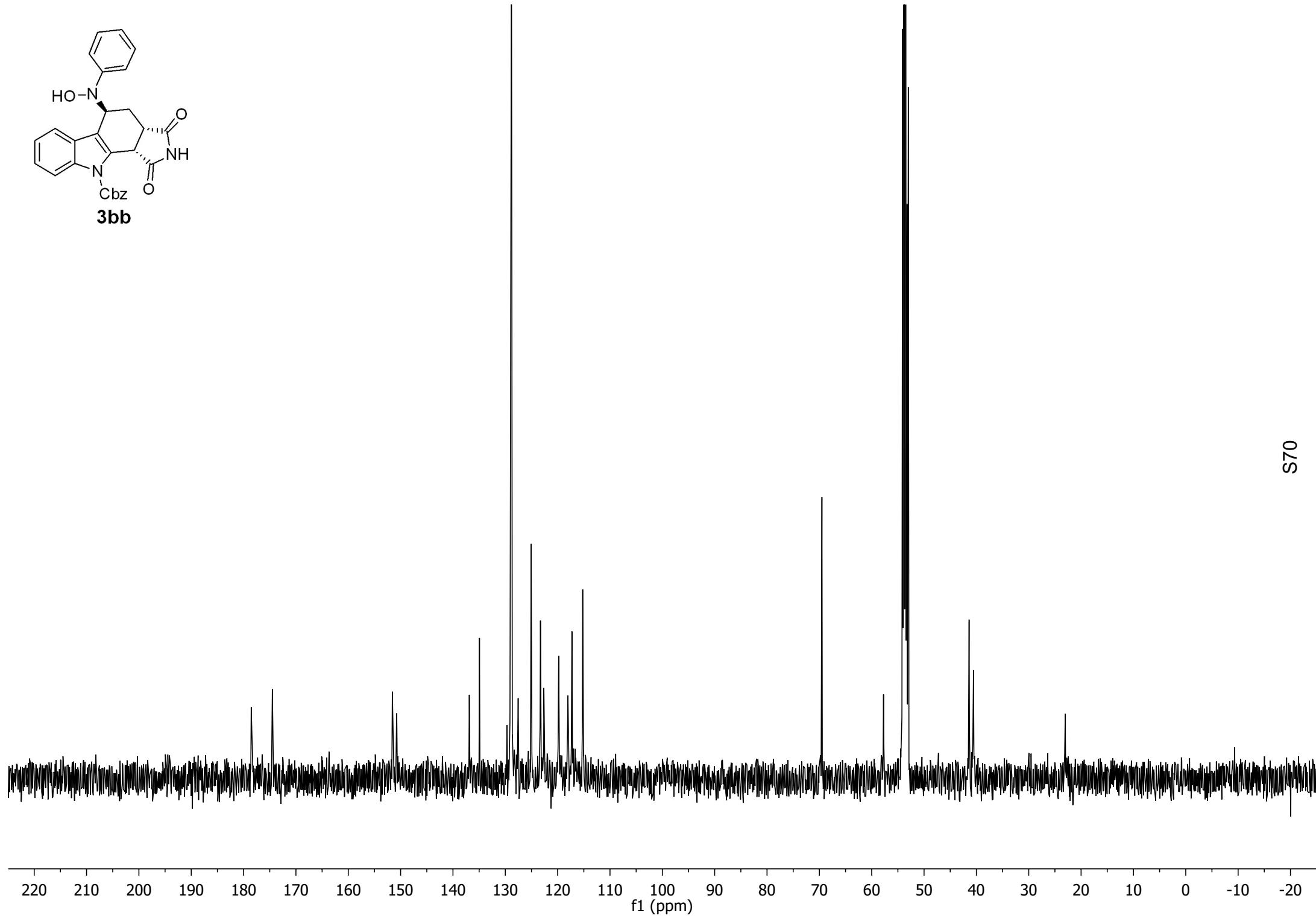


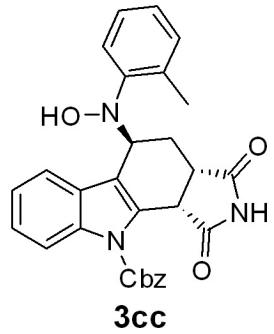




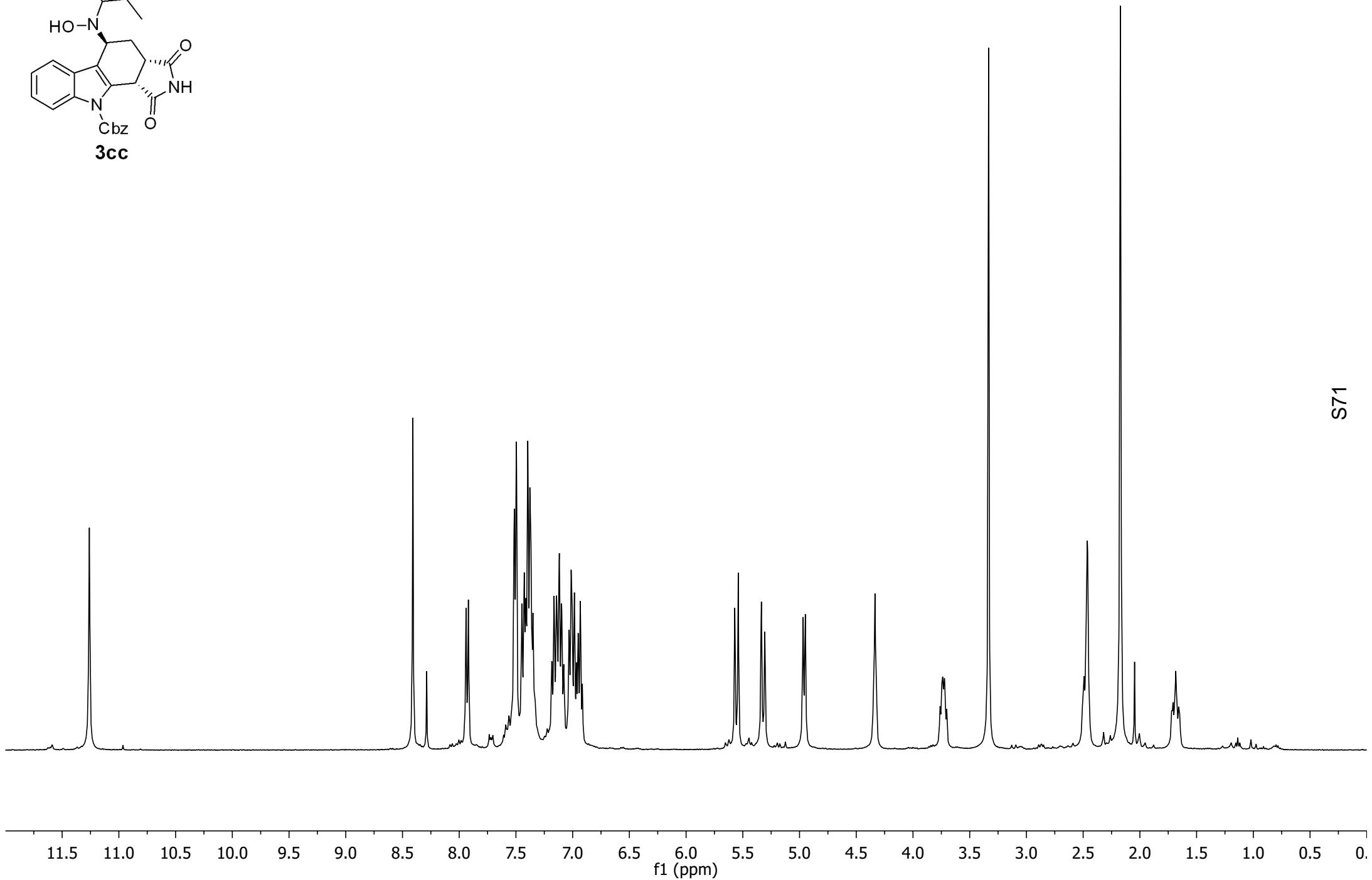


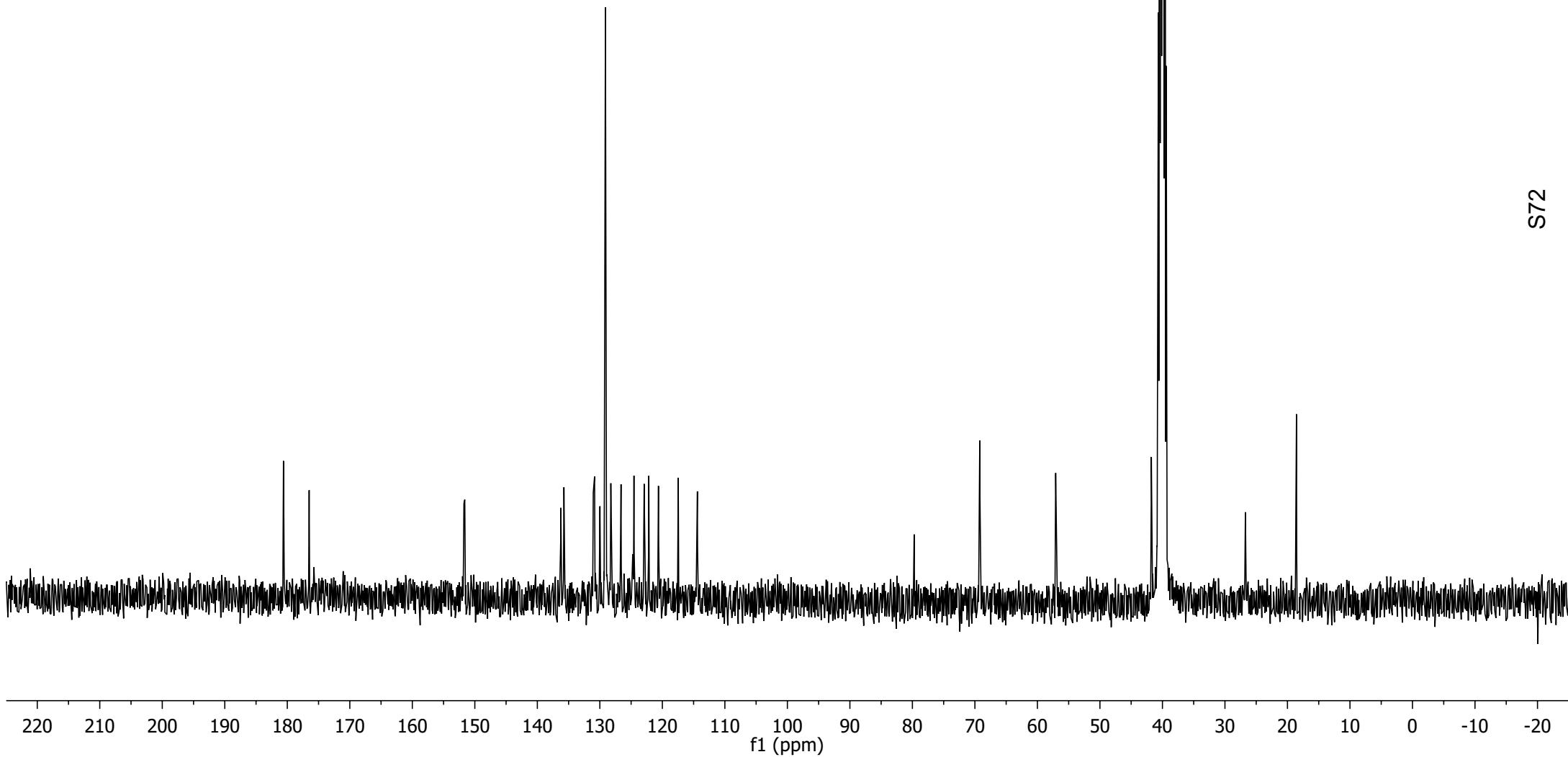
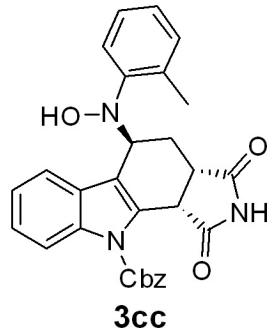
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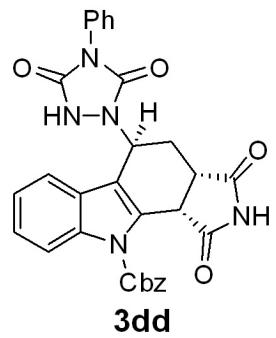




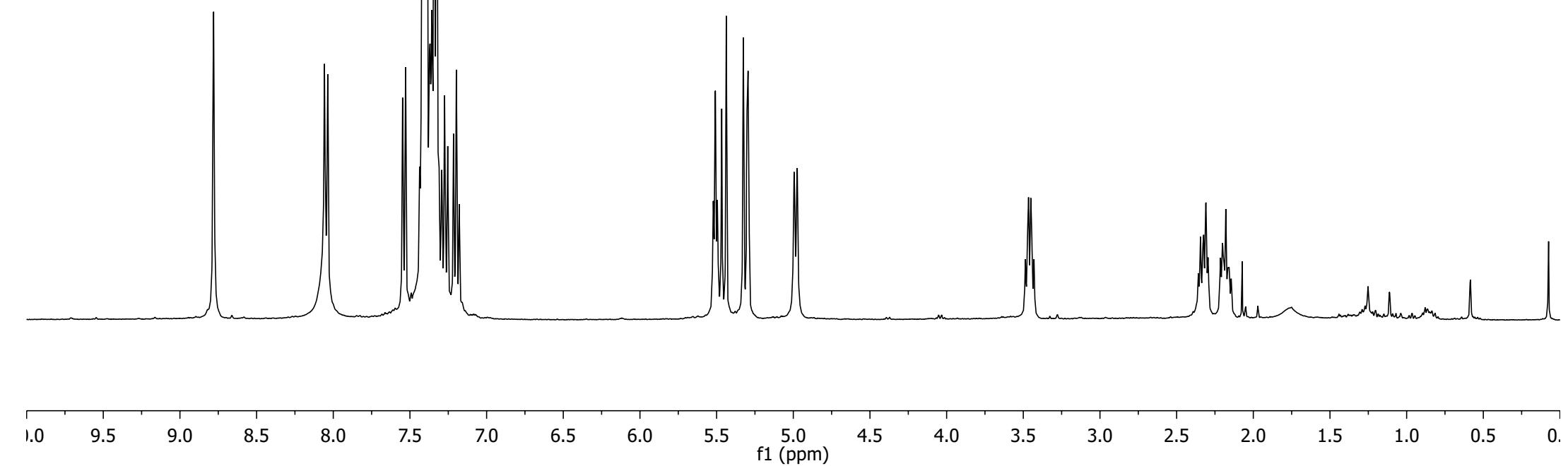
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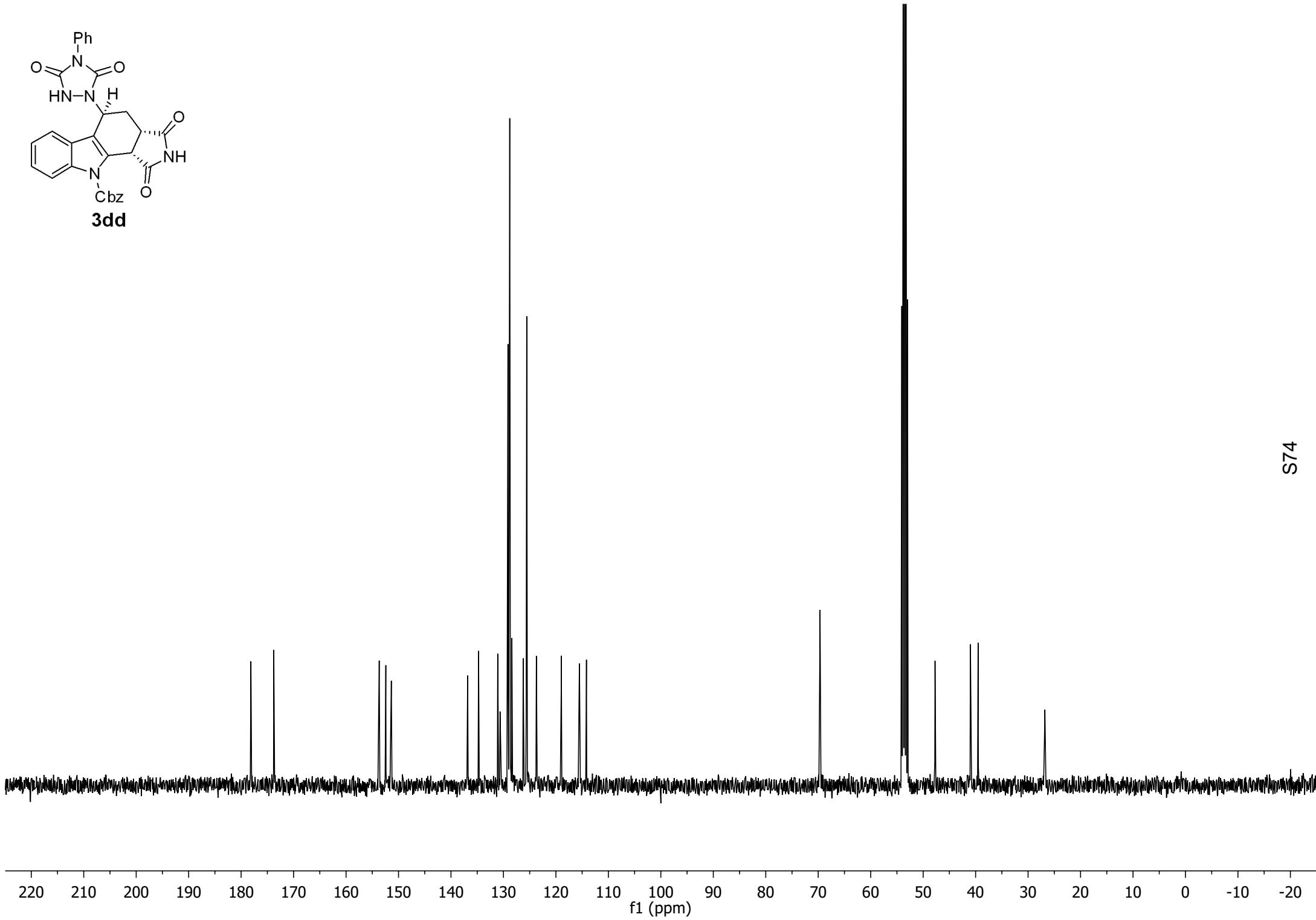
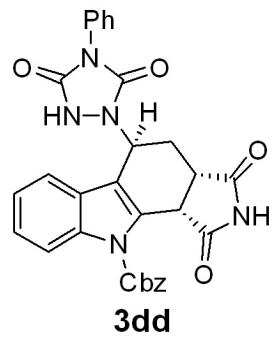


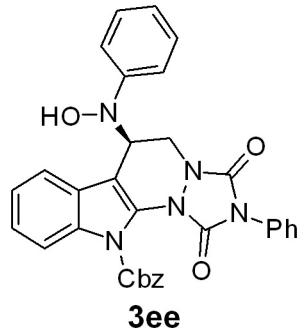




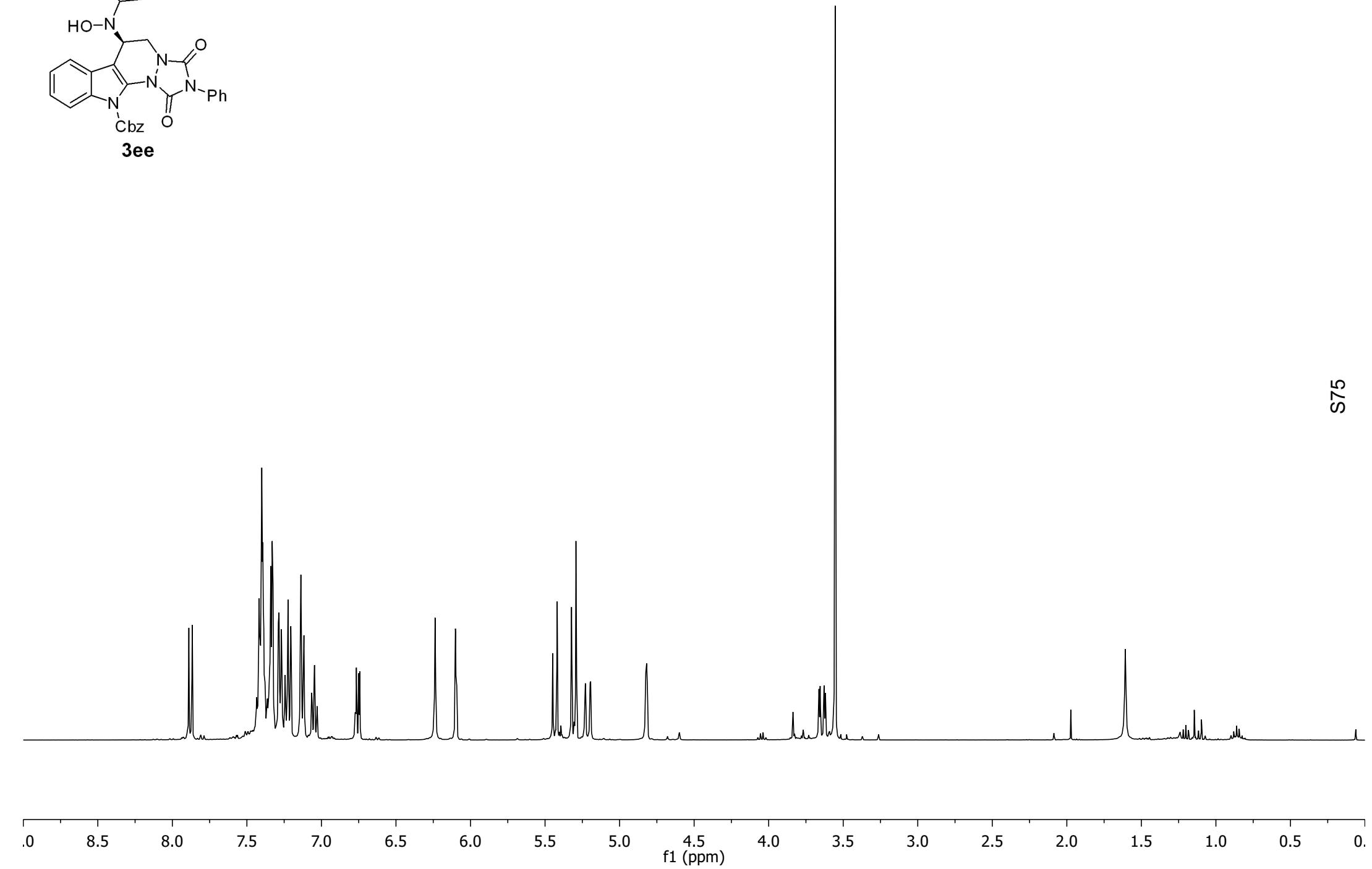
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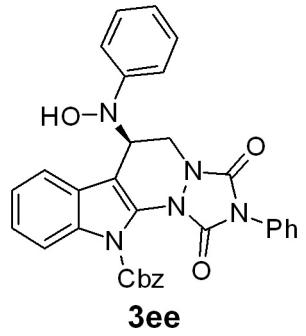




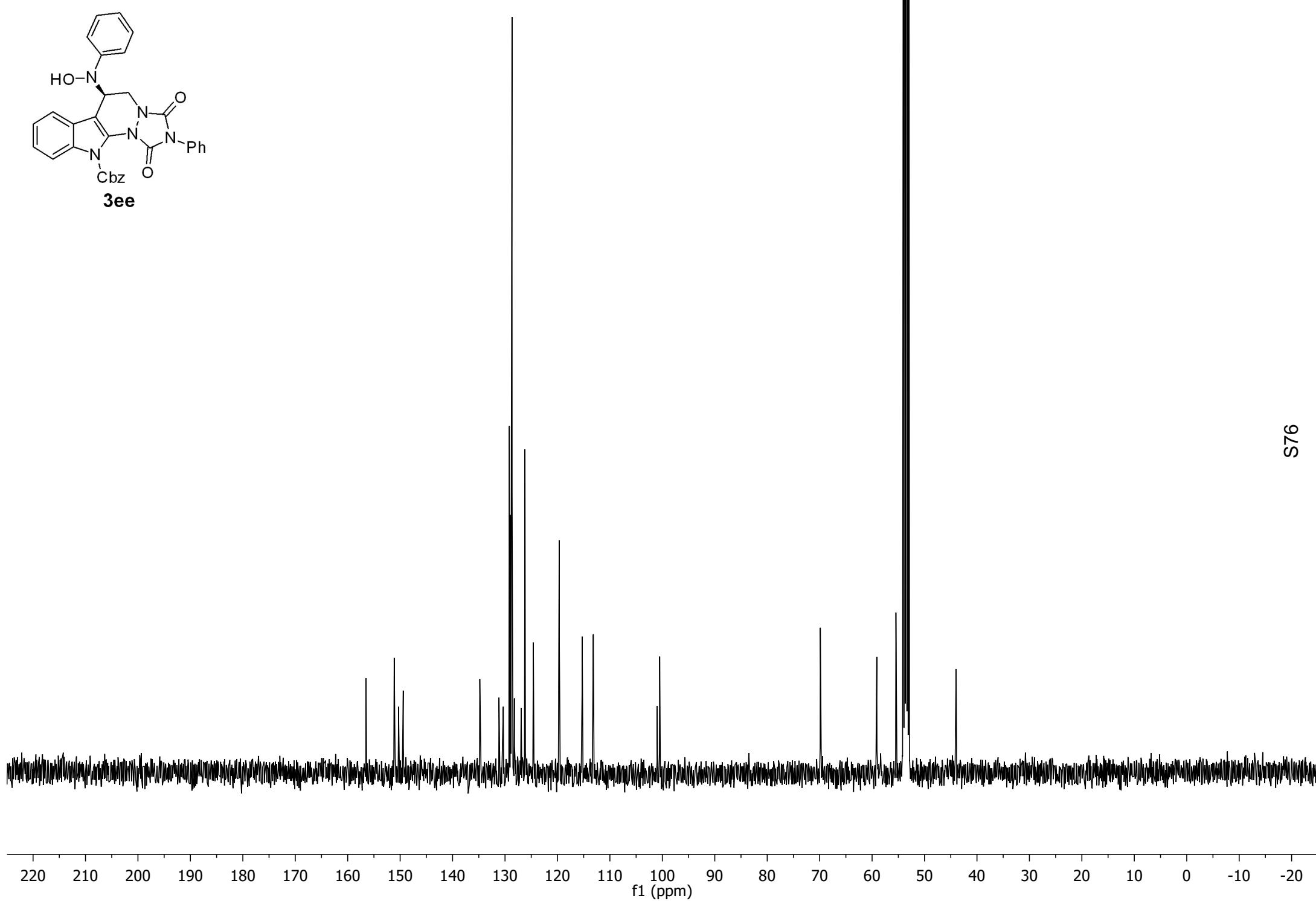


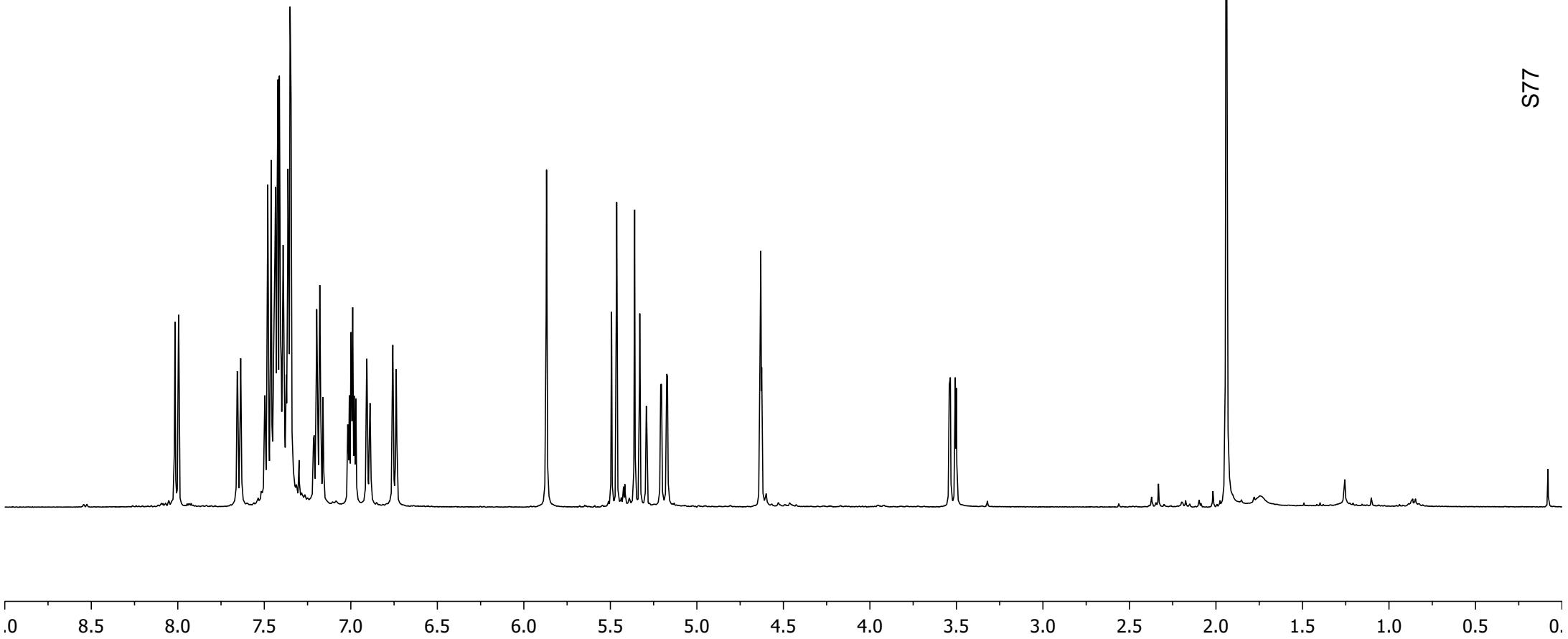
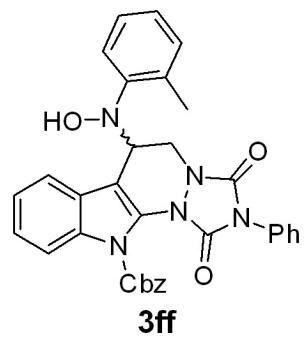
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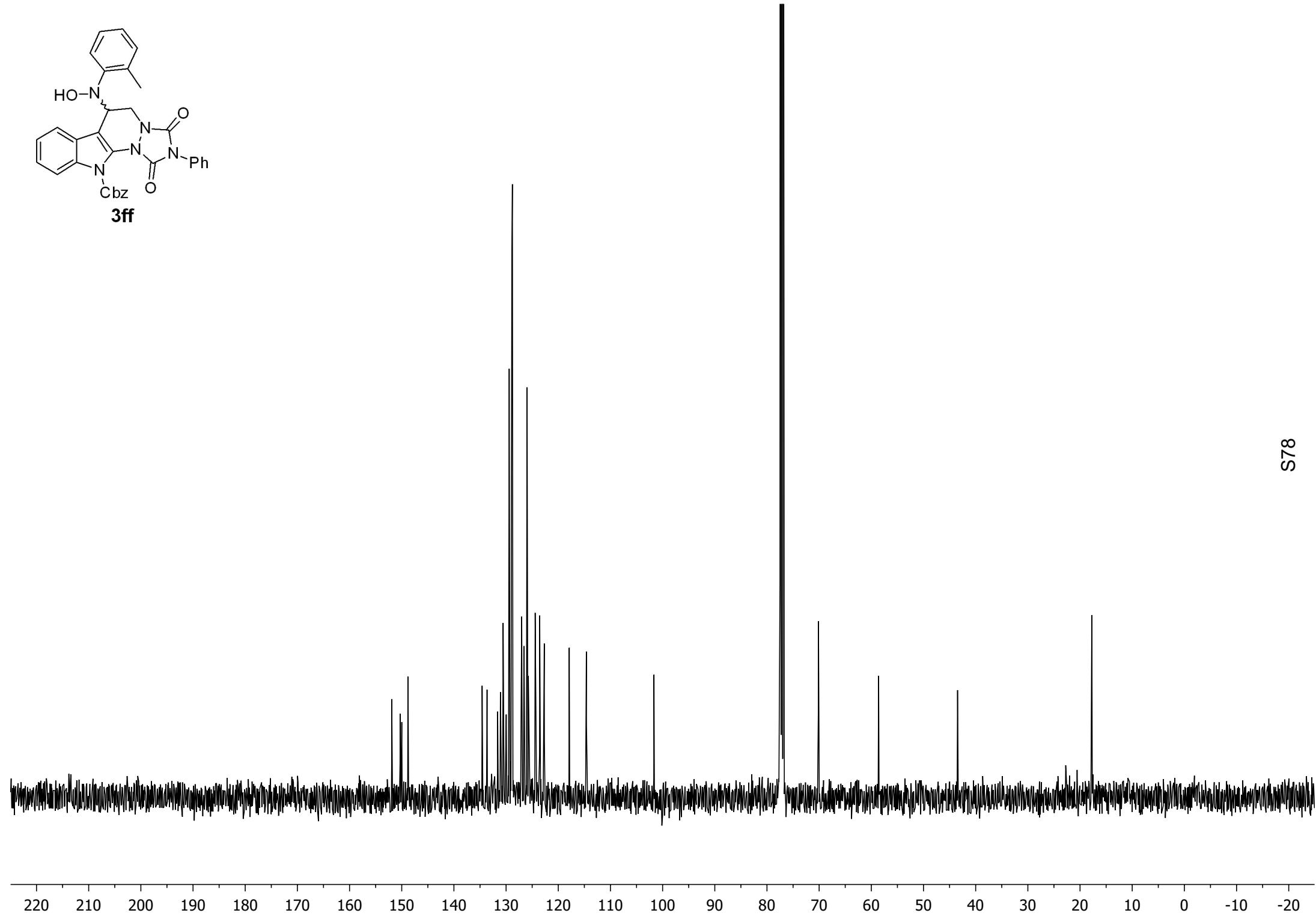
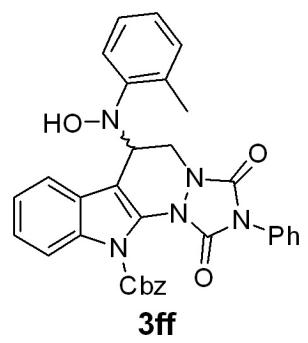


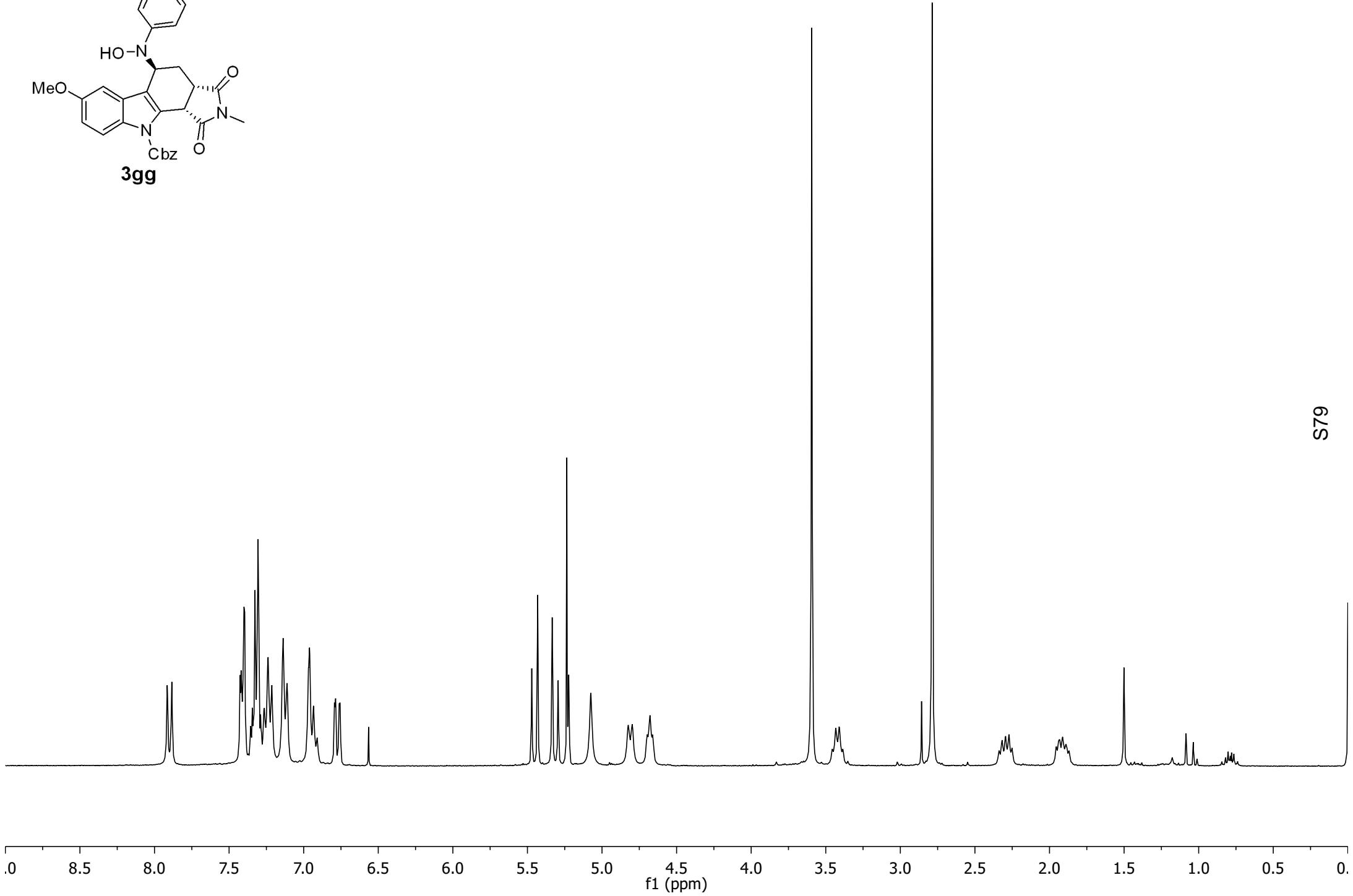
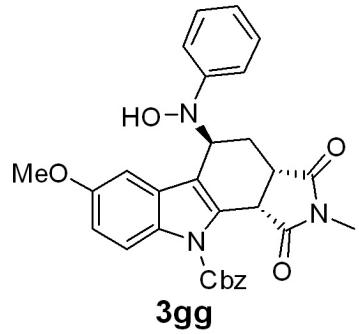


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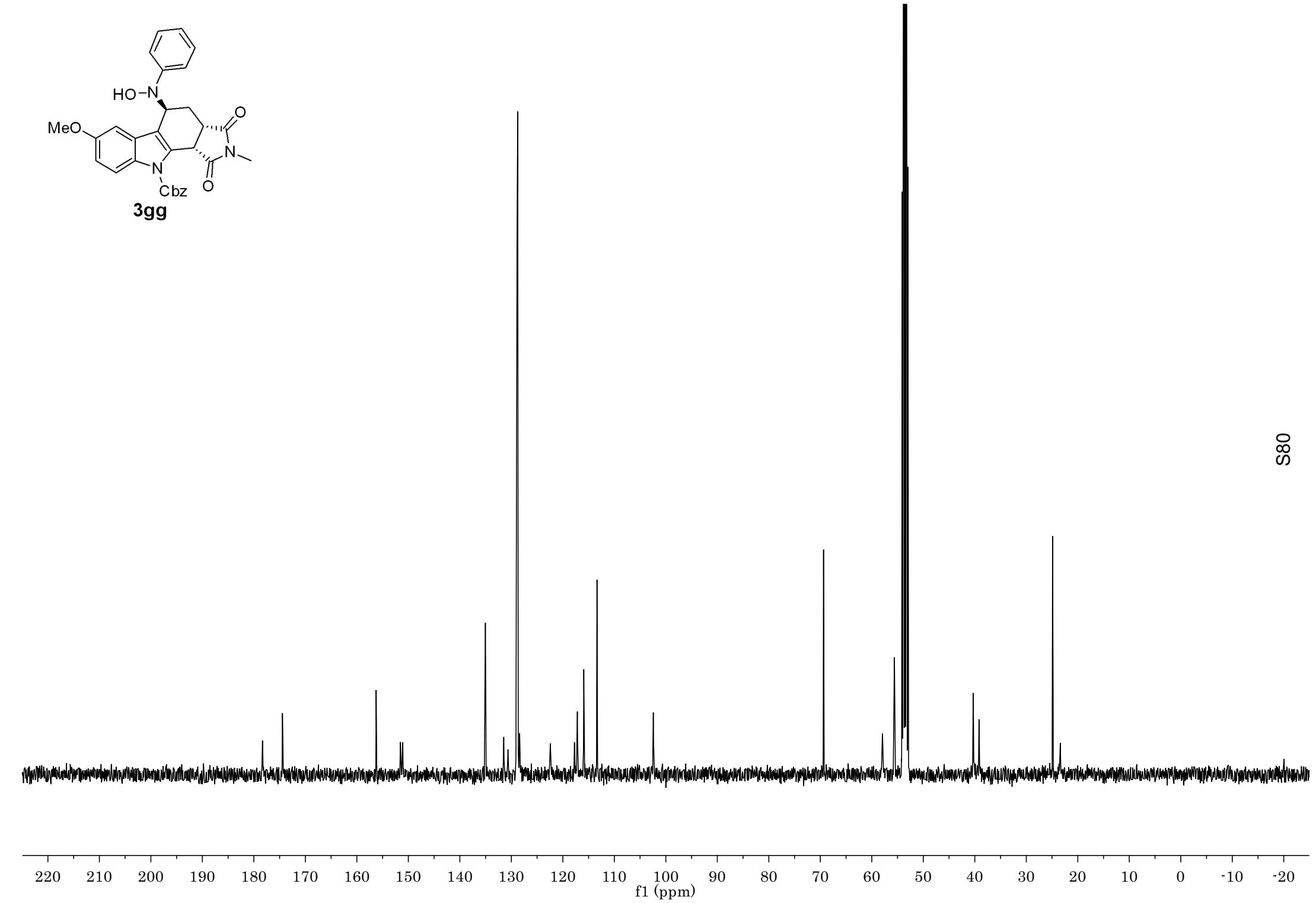
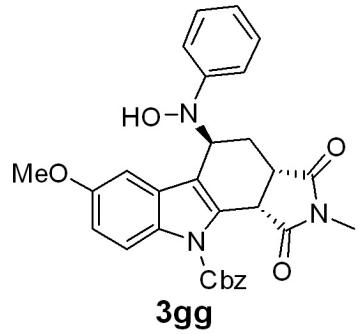




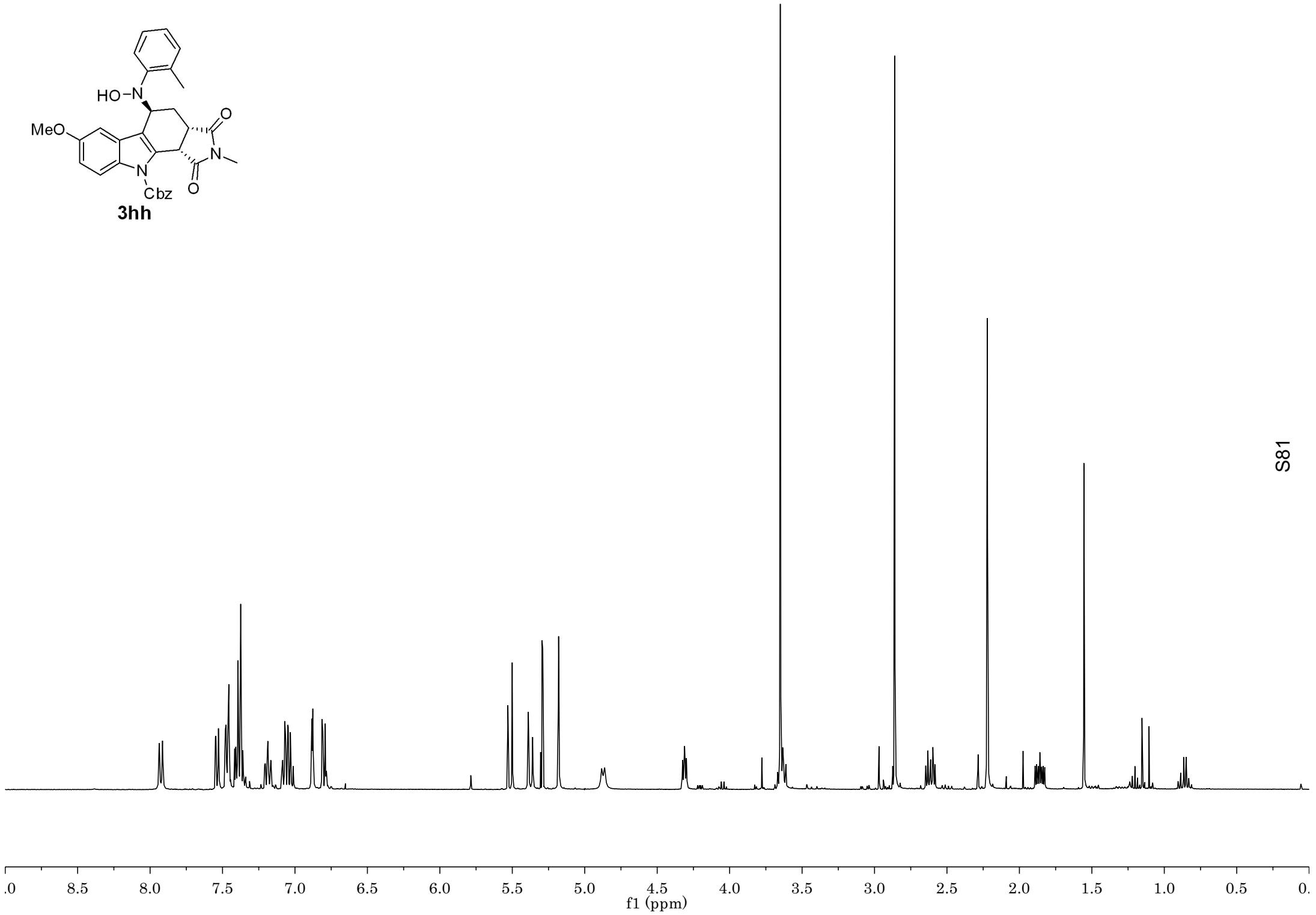
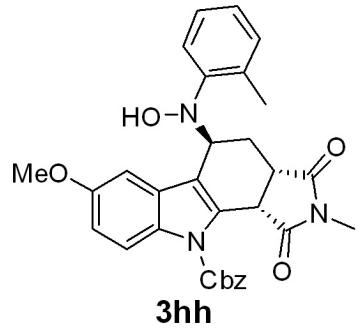




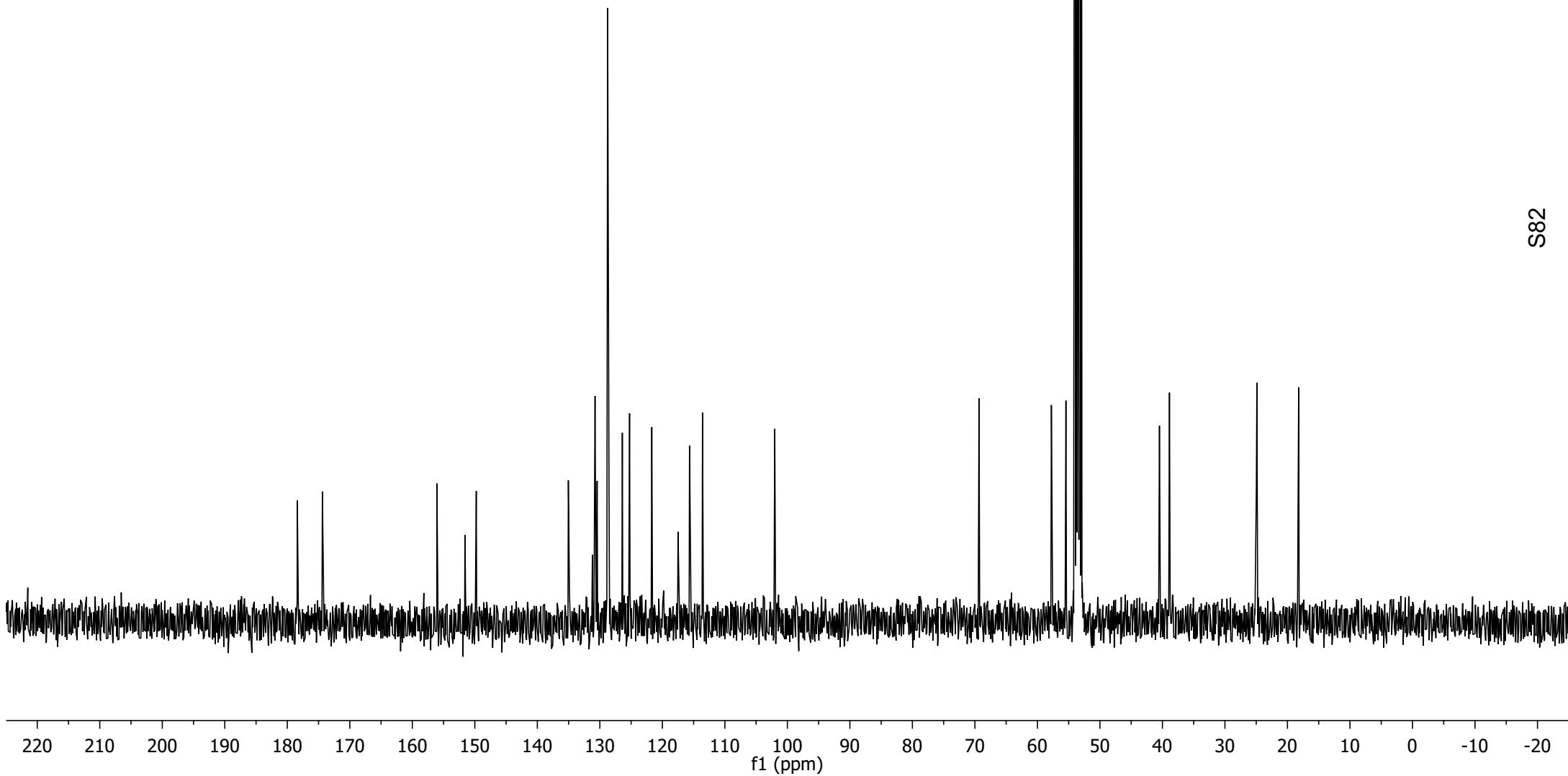
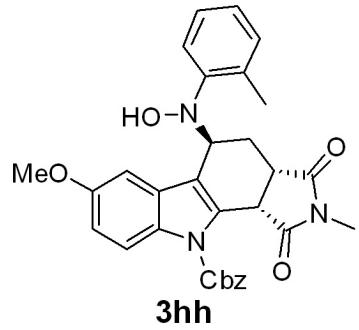
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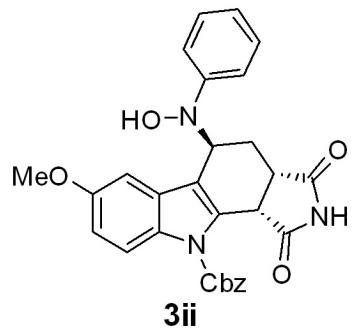


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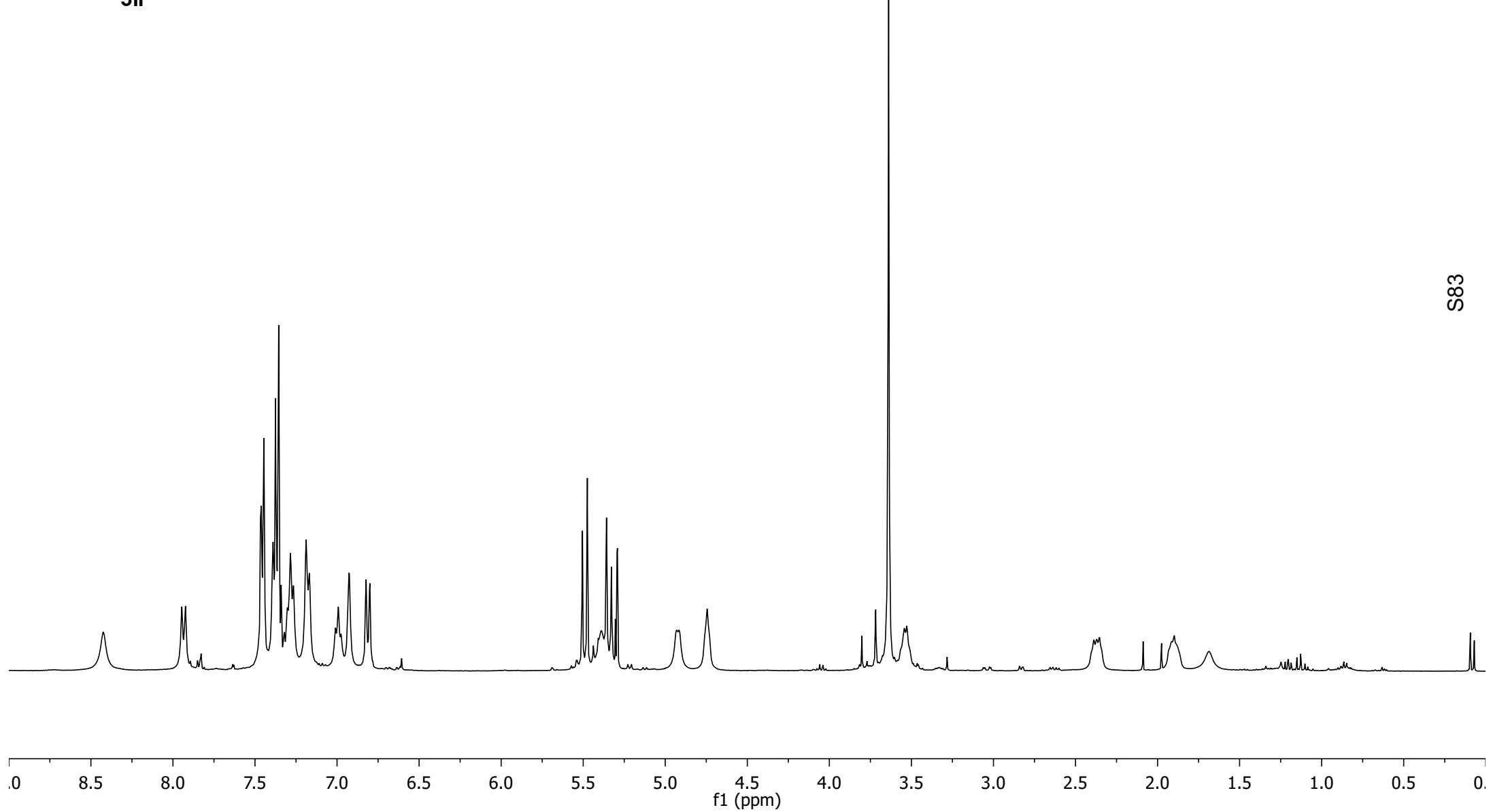


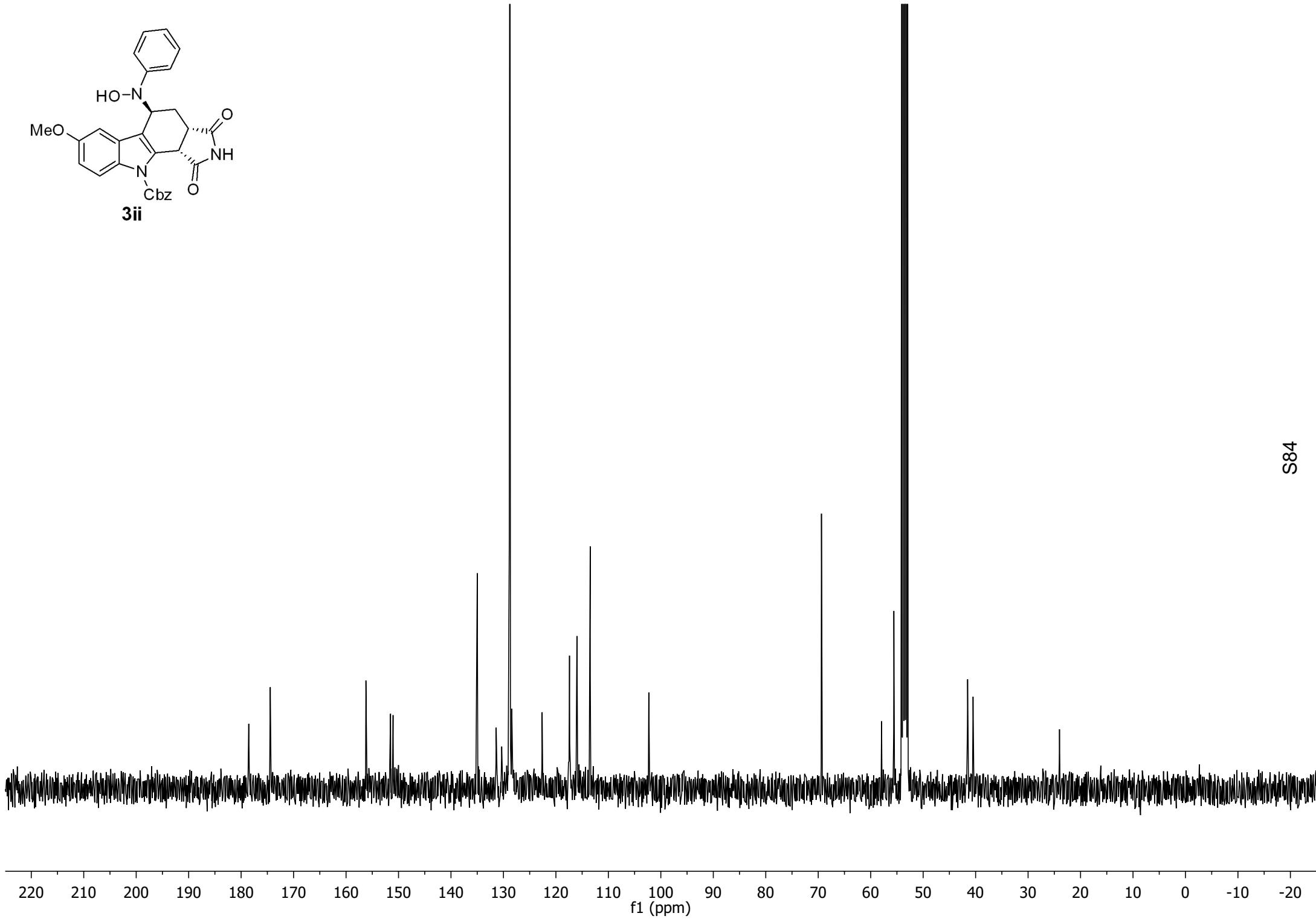
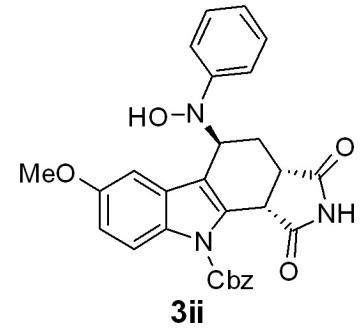
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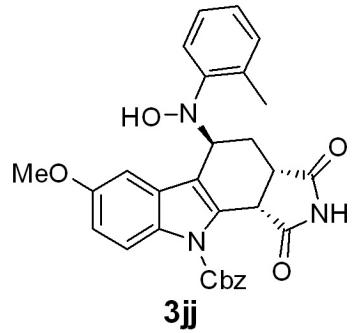




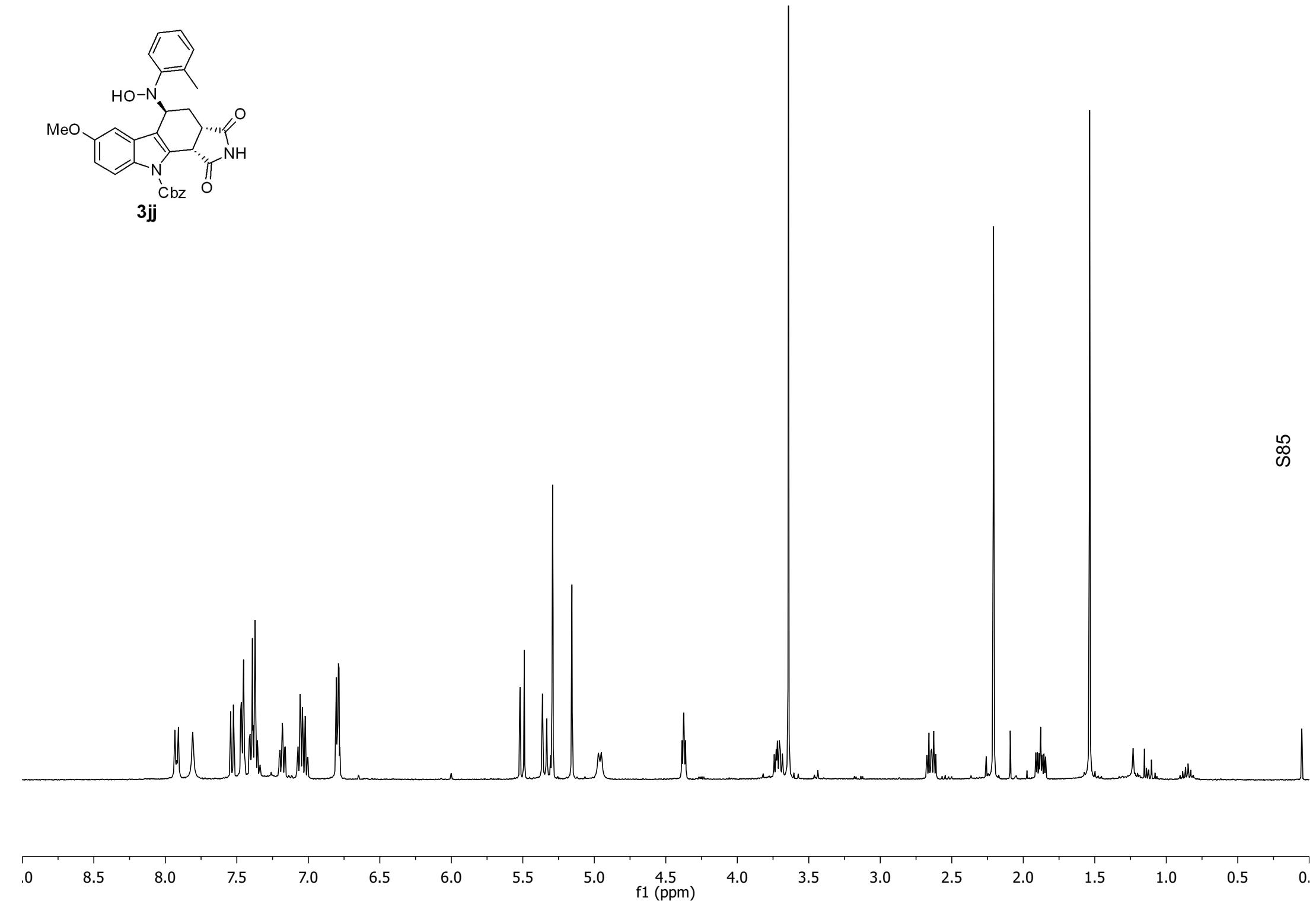
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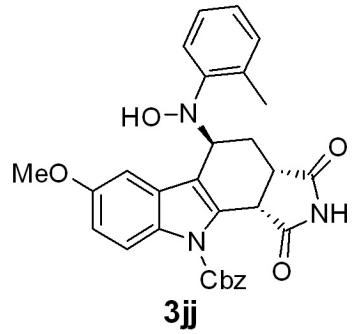




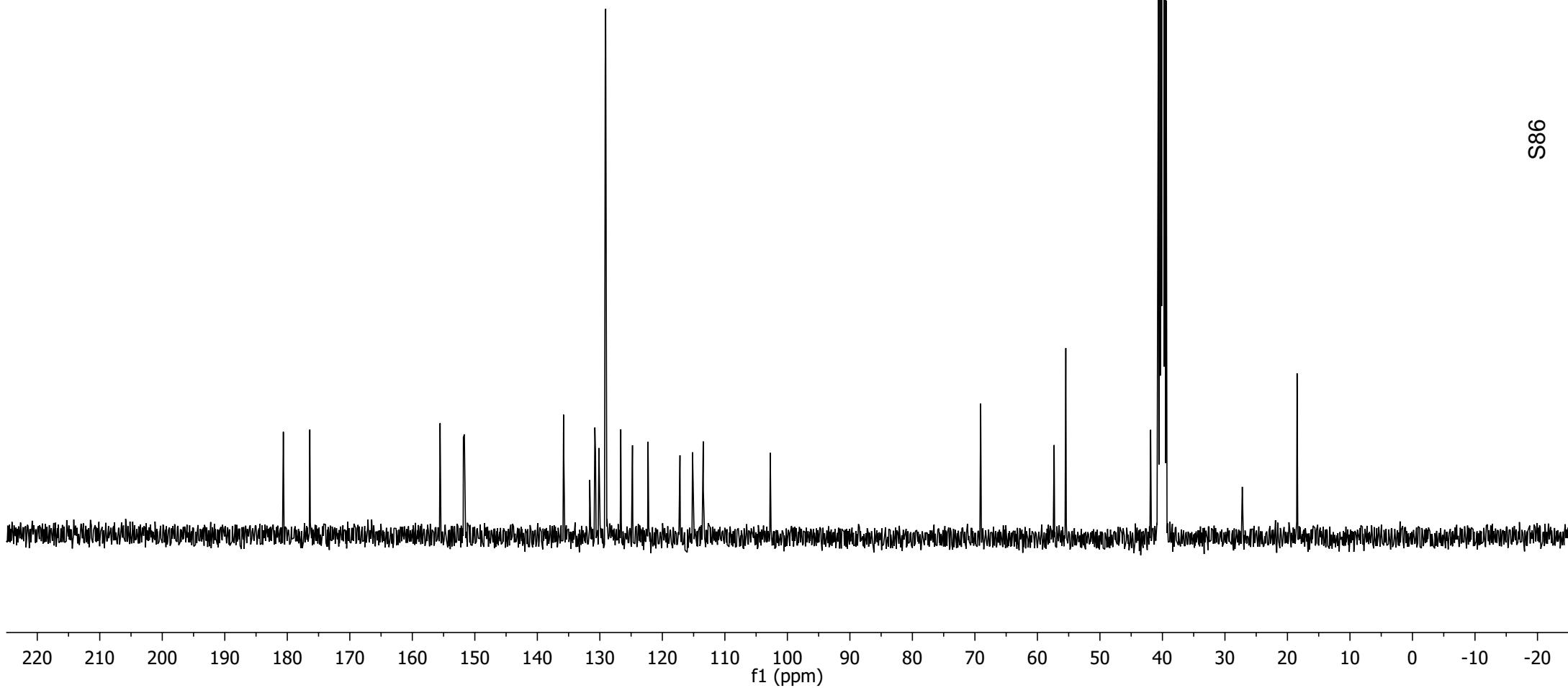


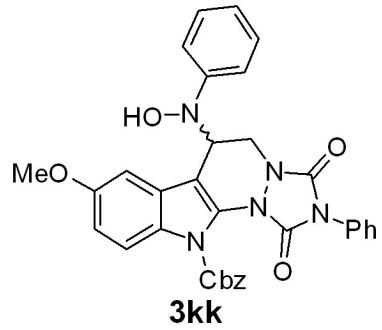
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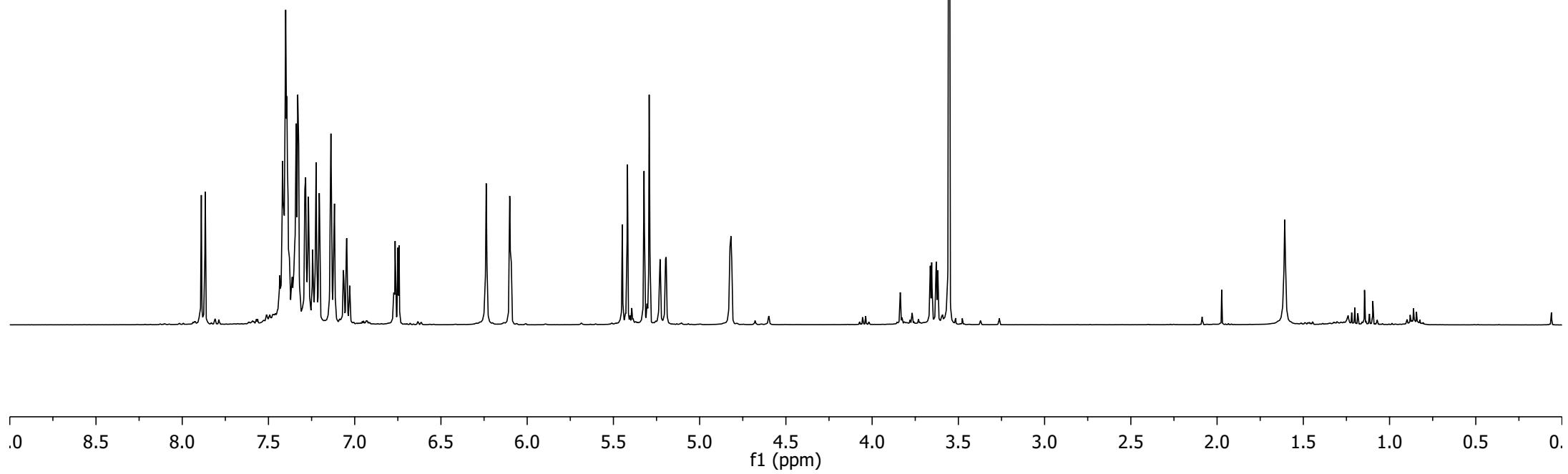


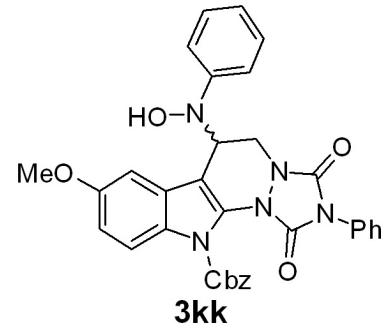
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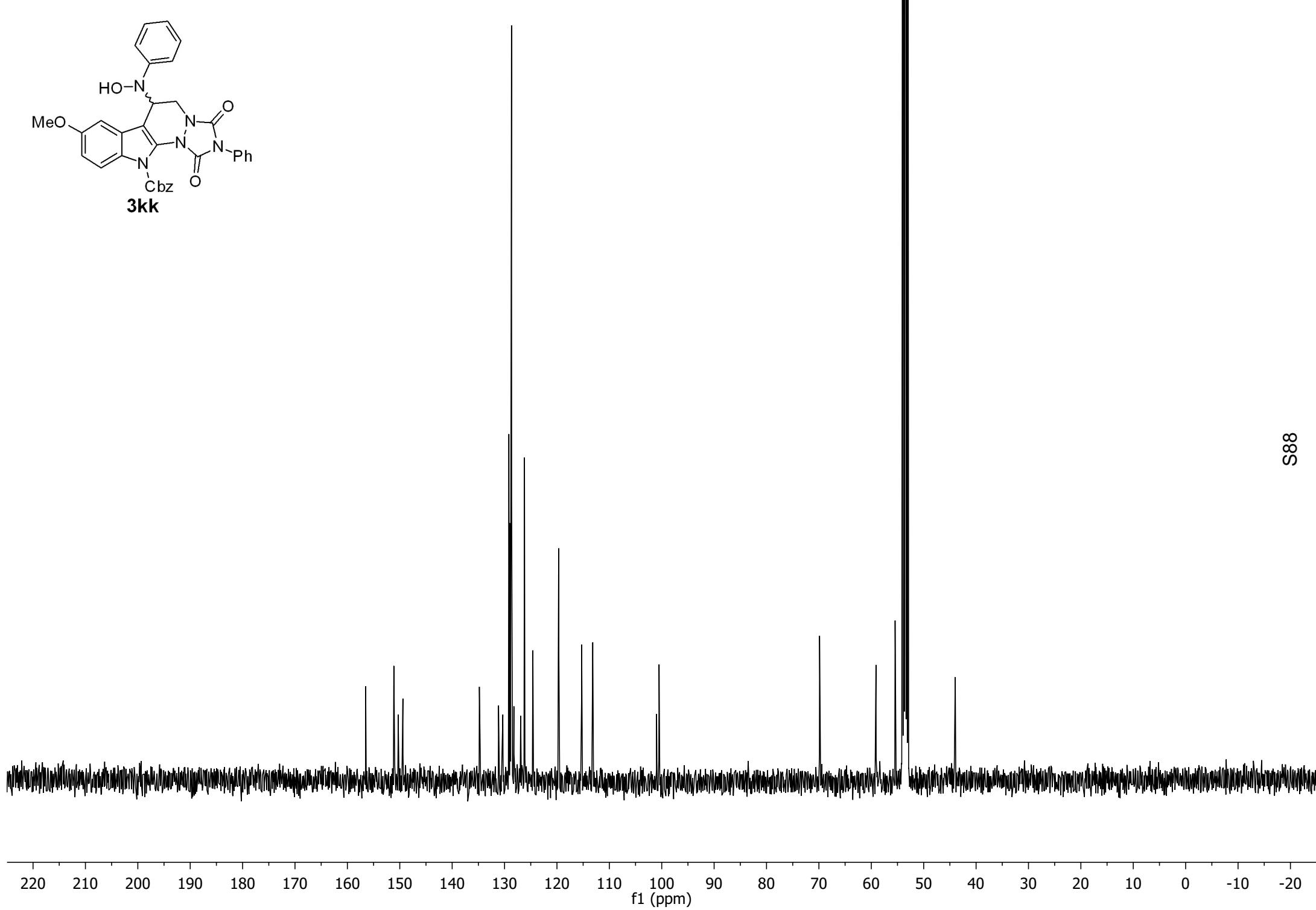


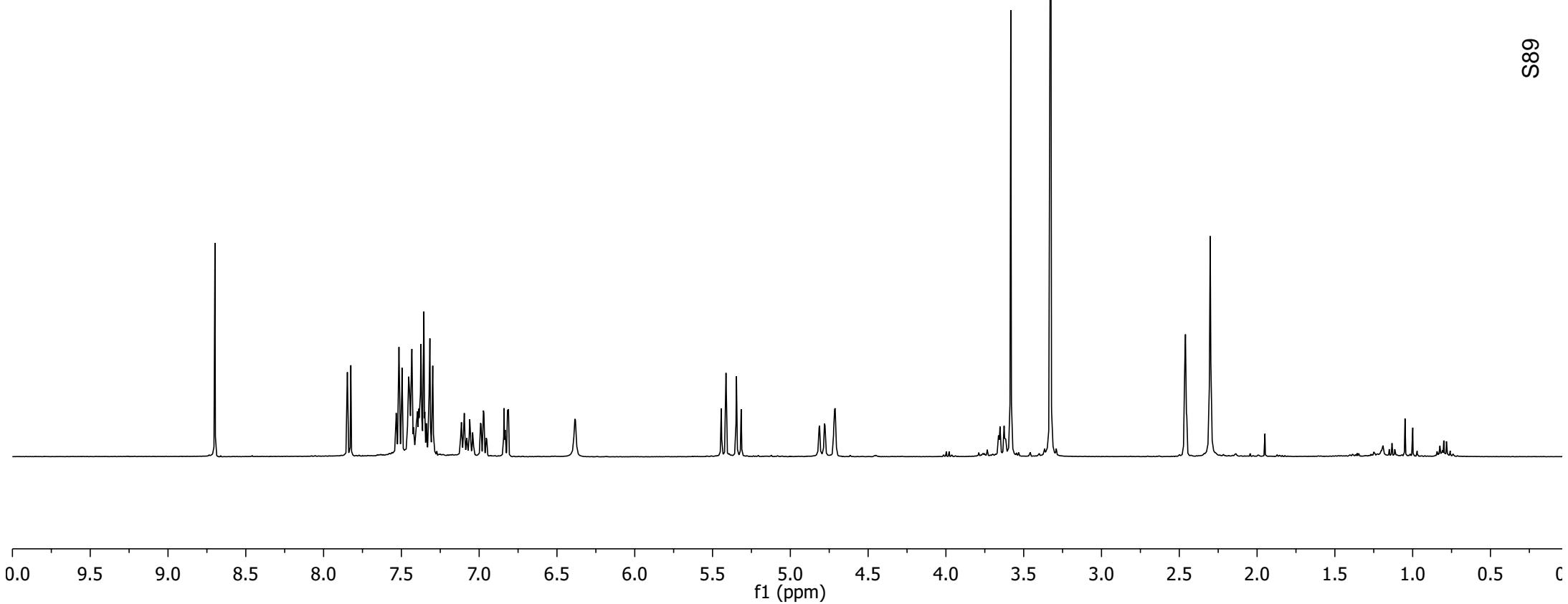
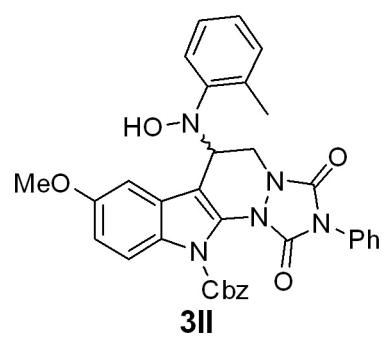
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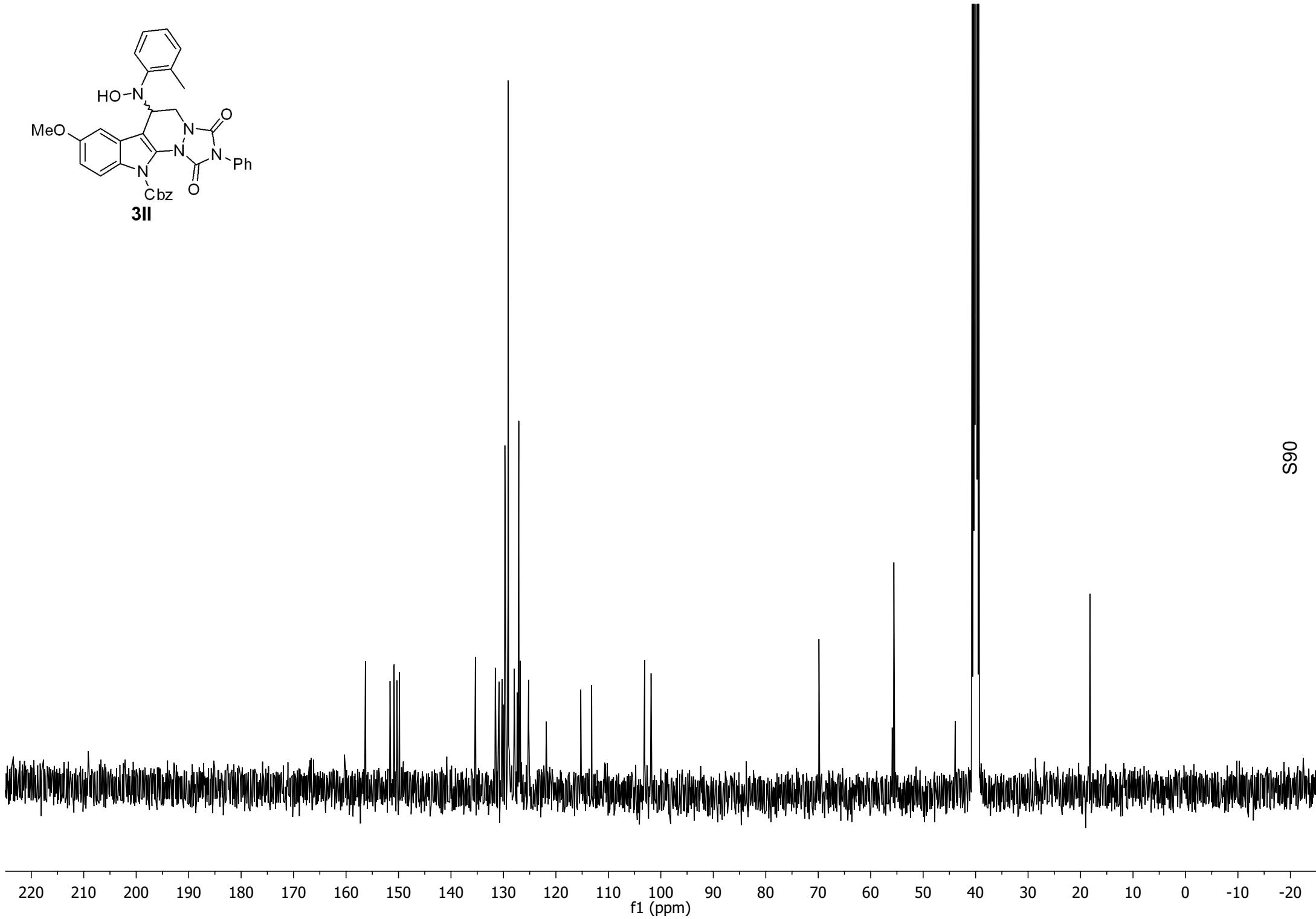
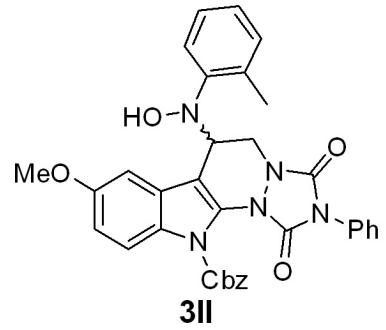


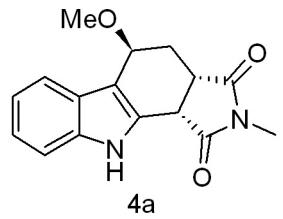


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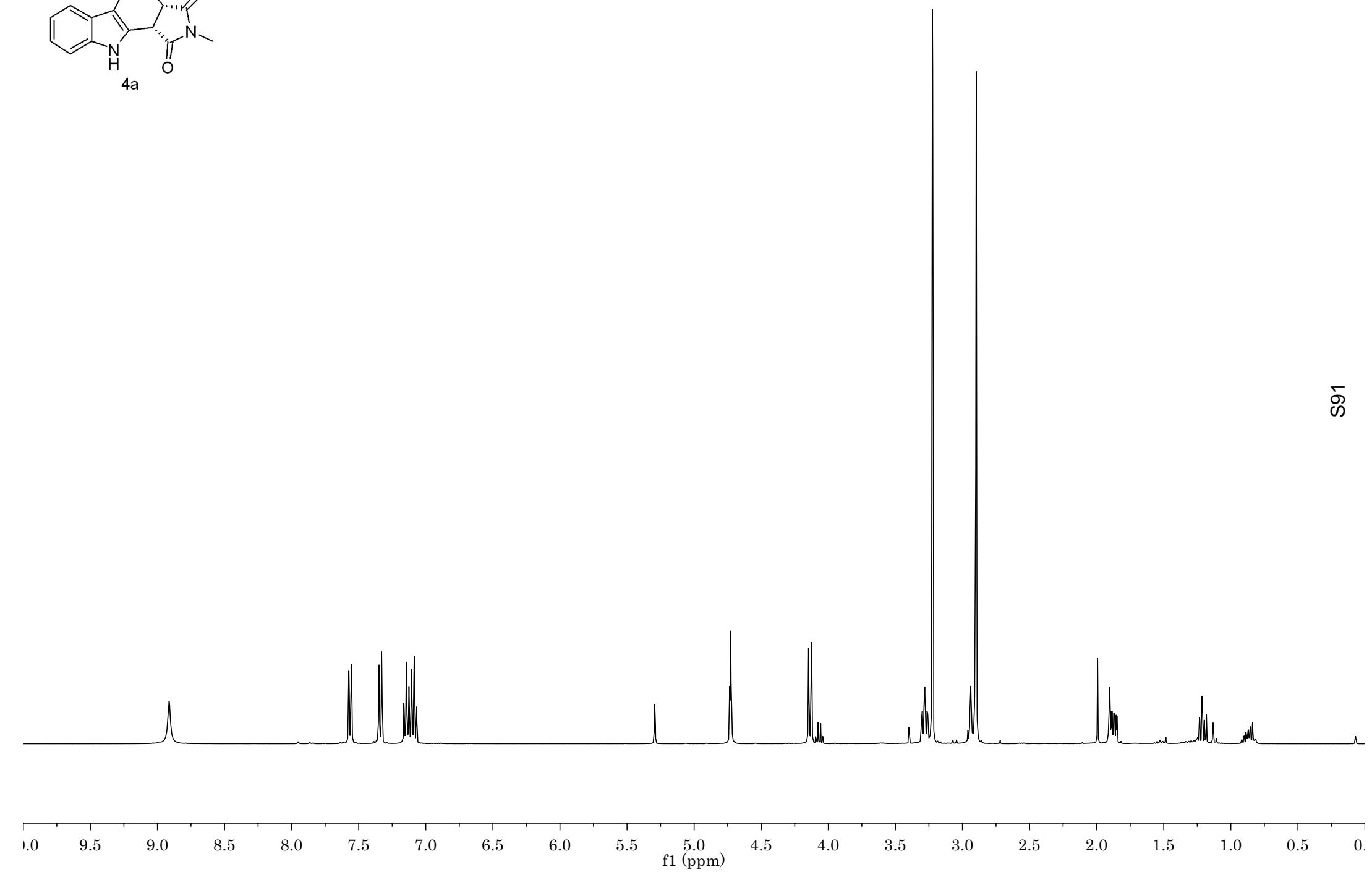


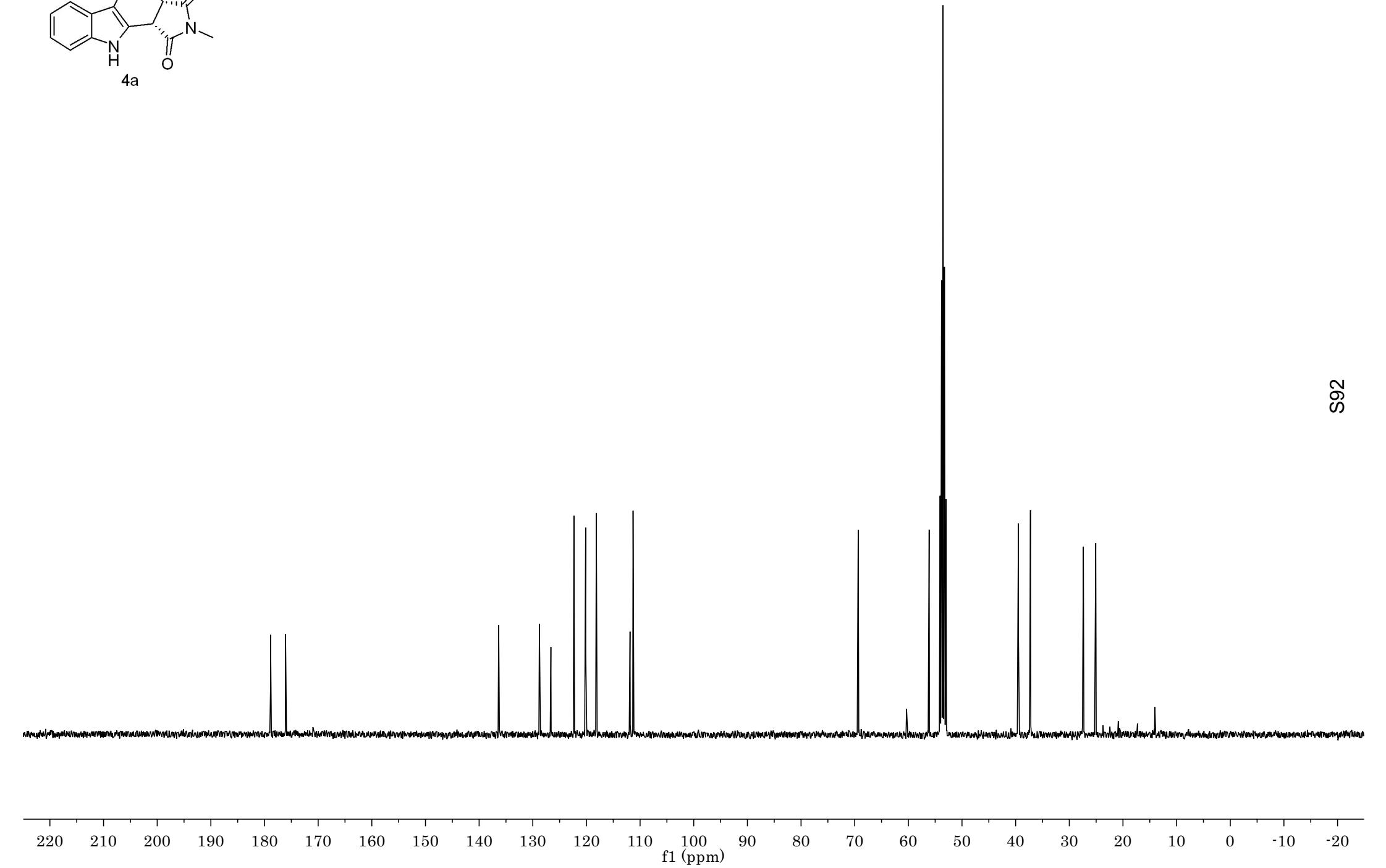
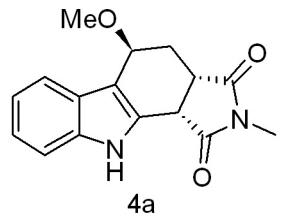


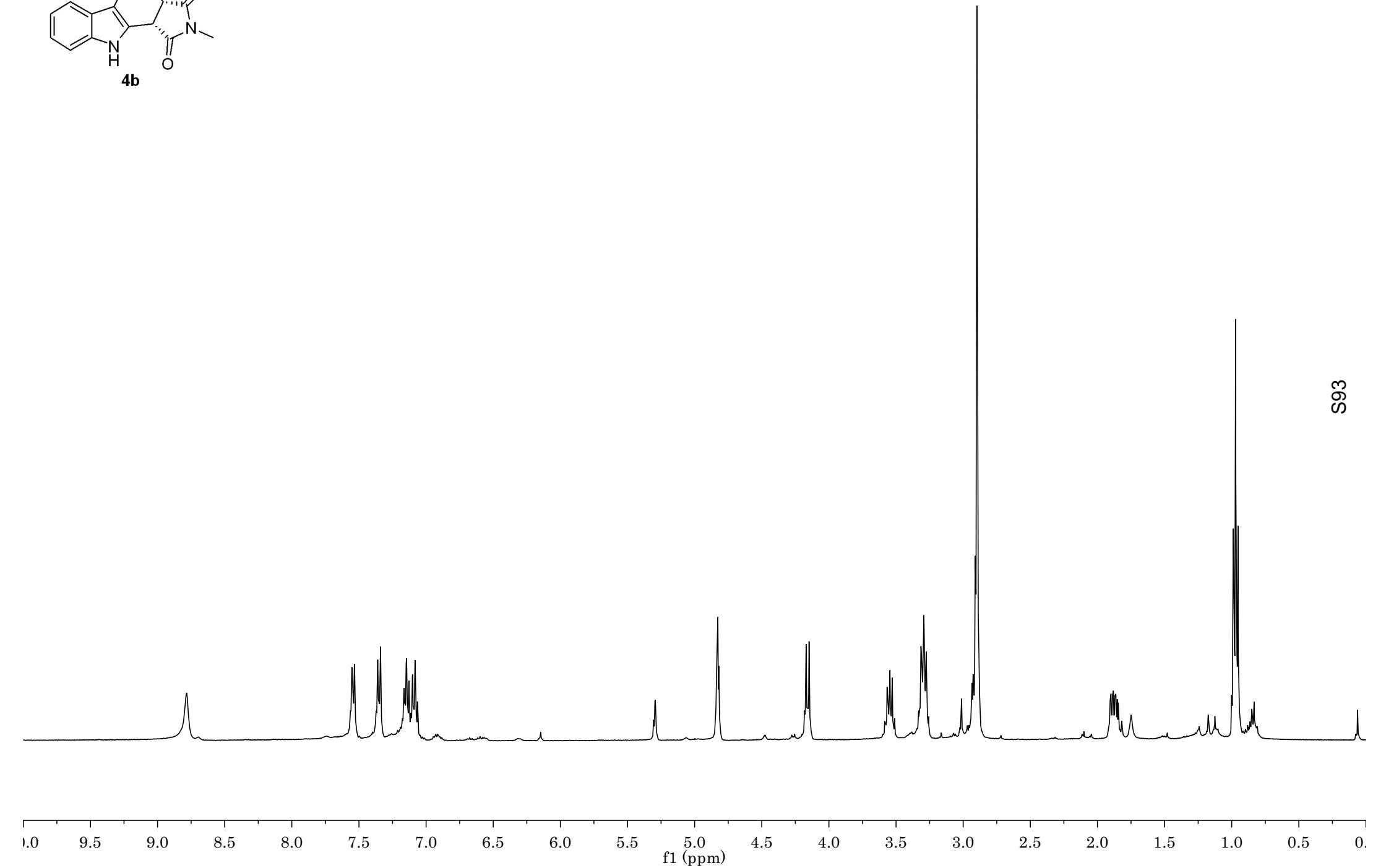
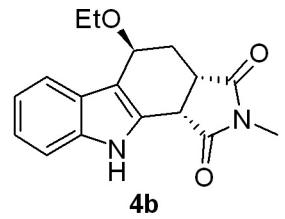




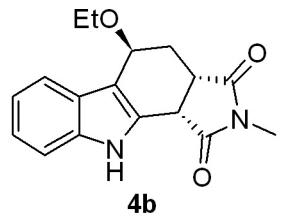
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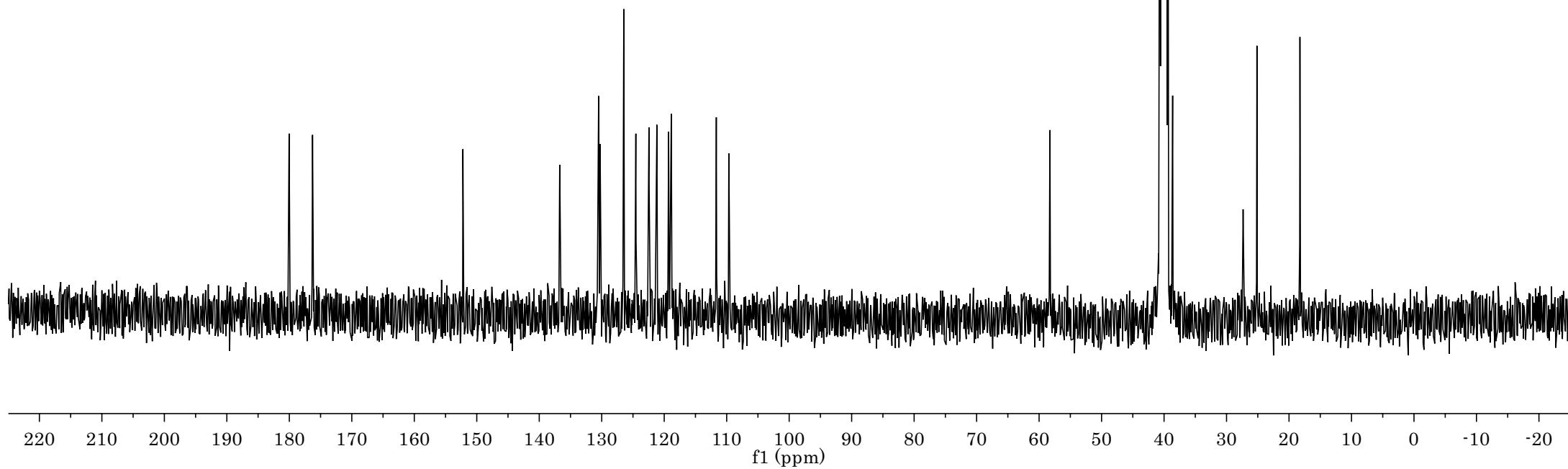


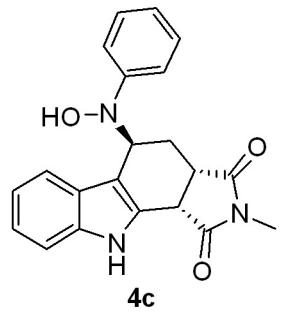


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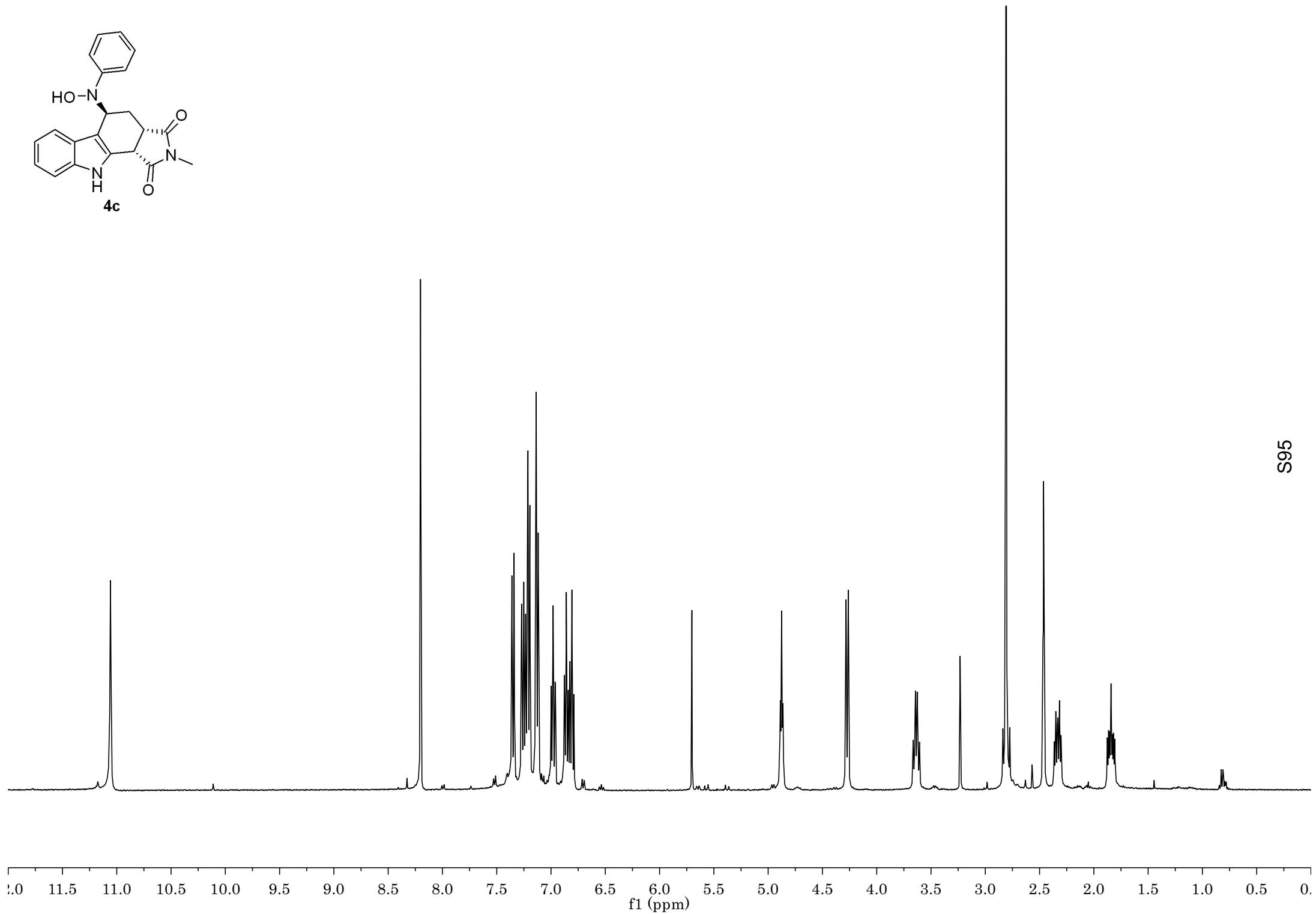


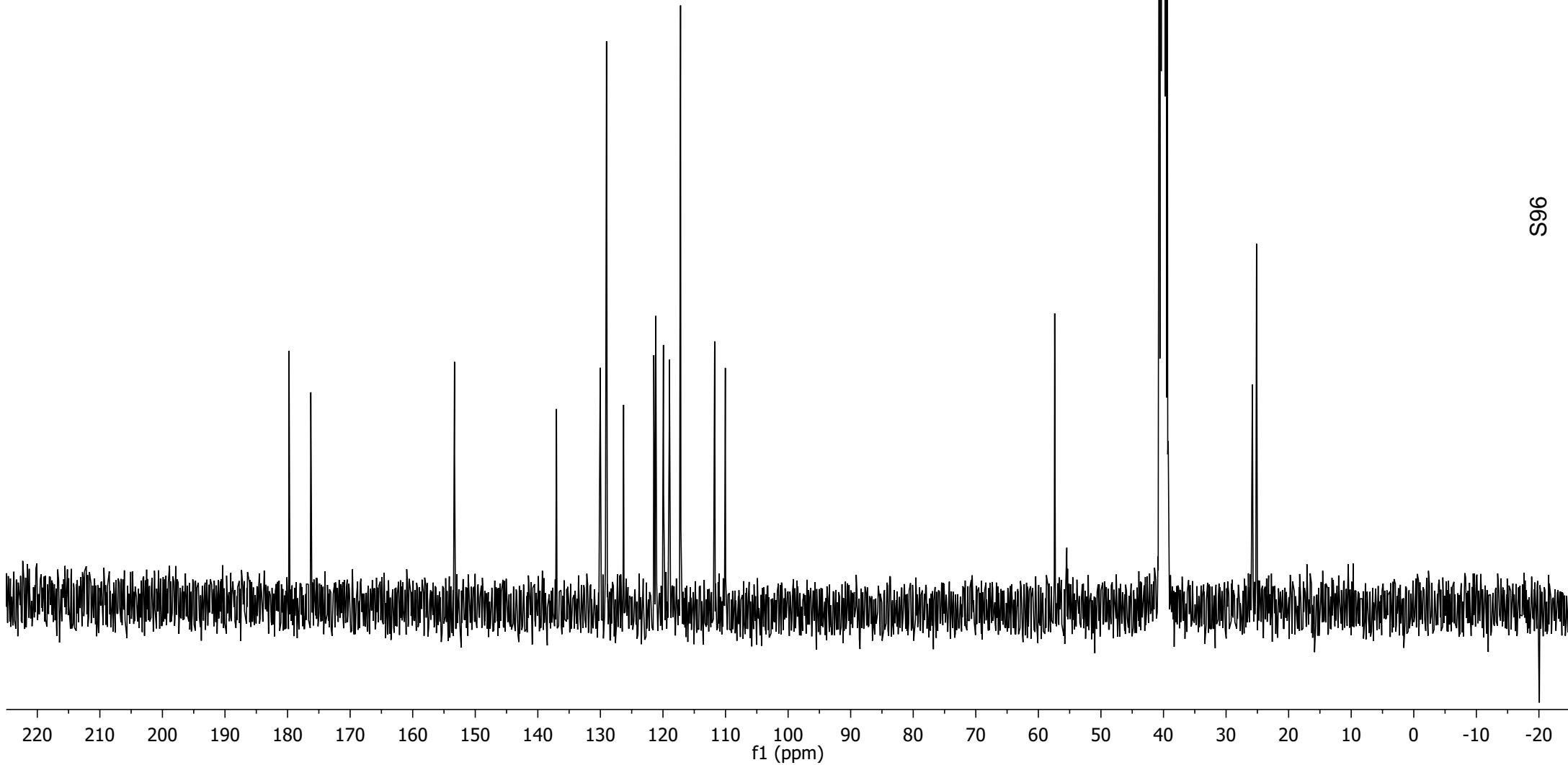
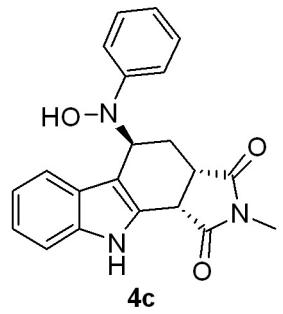
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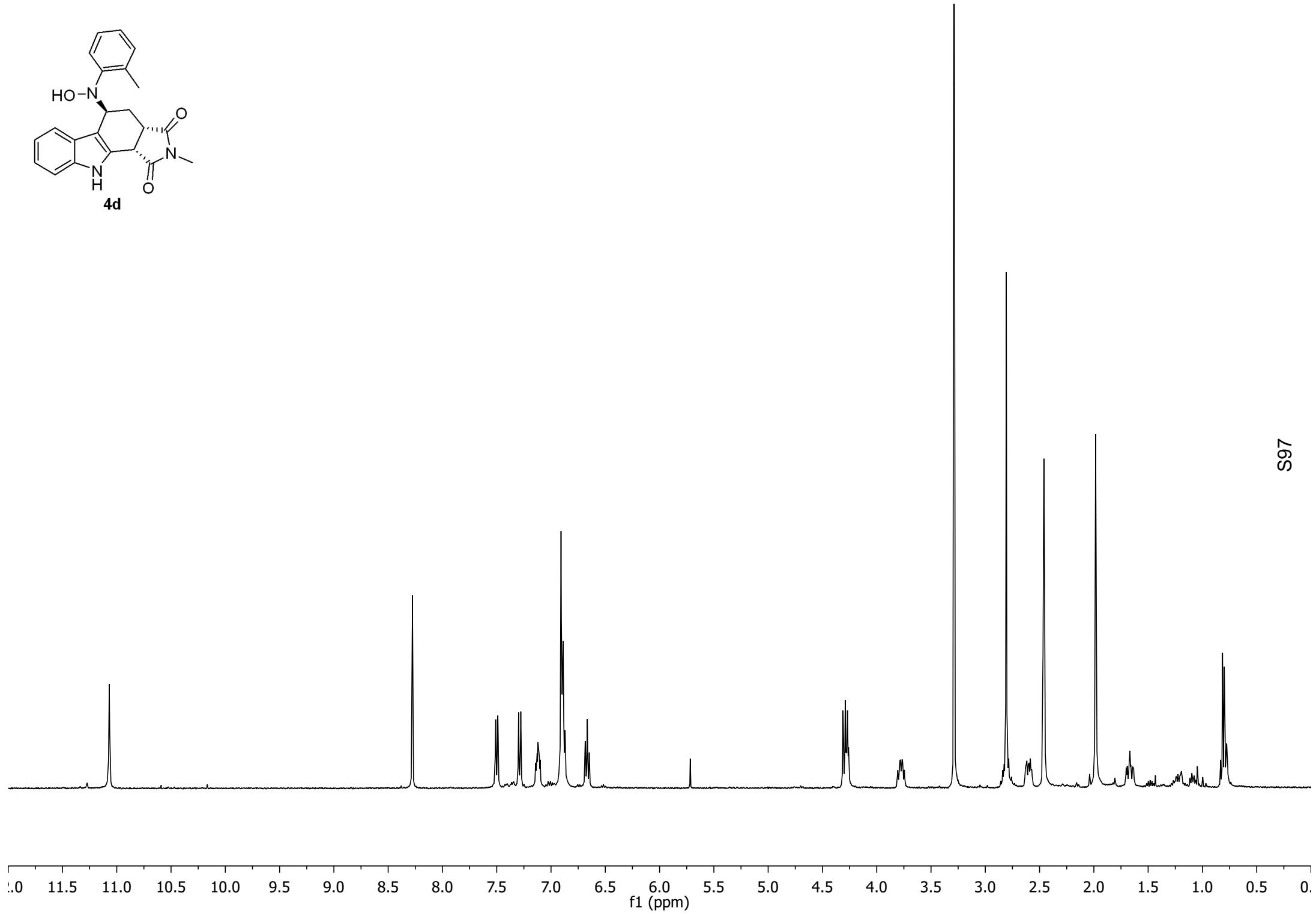
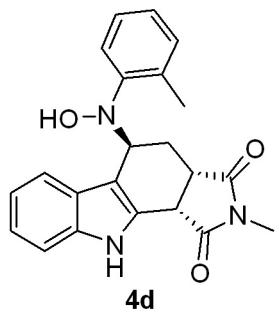


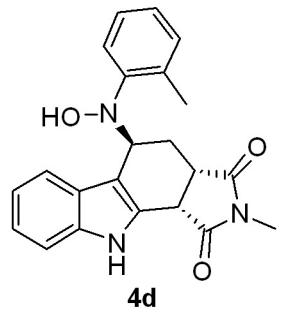


S95

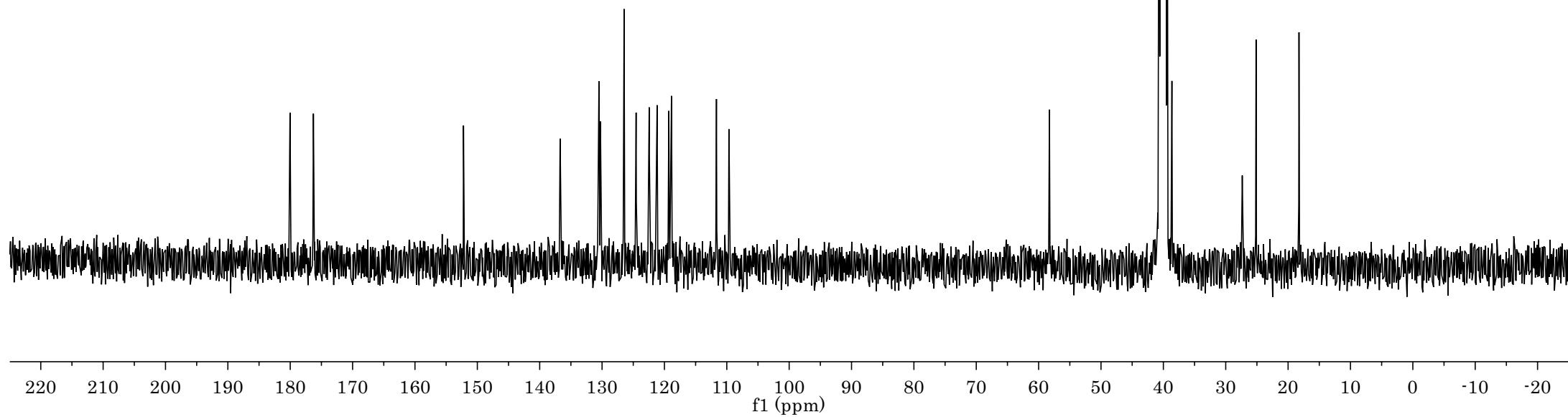


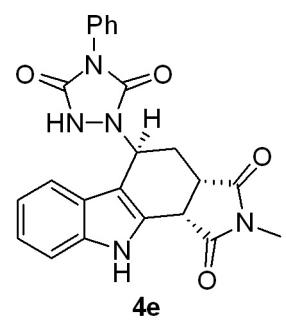




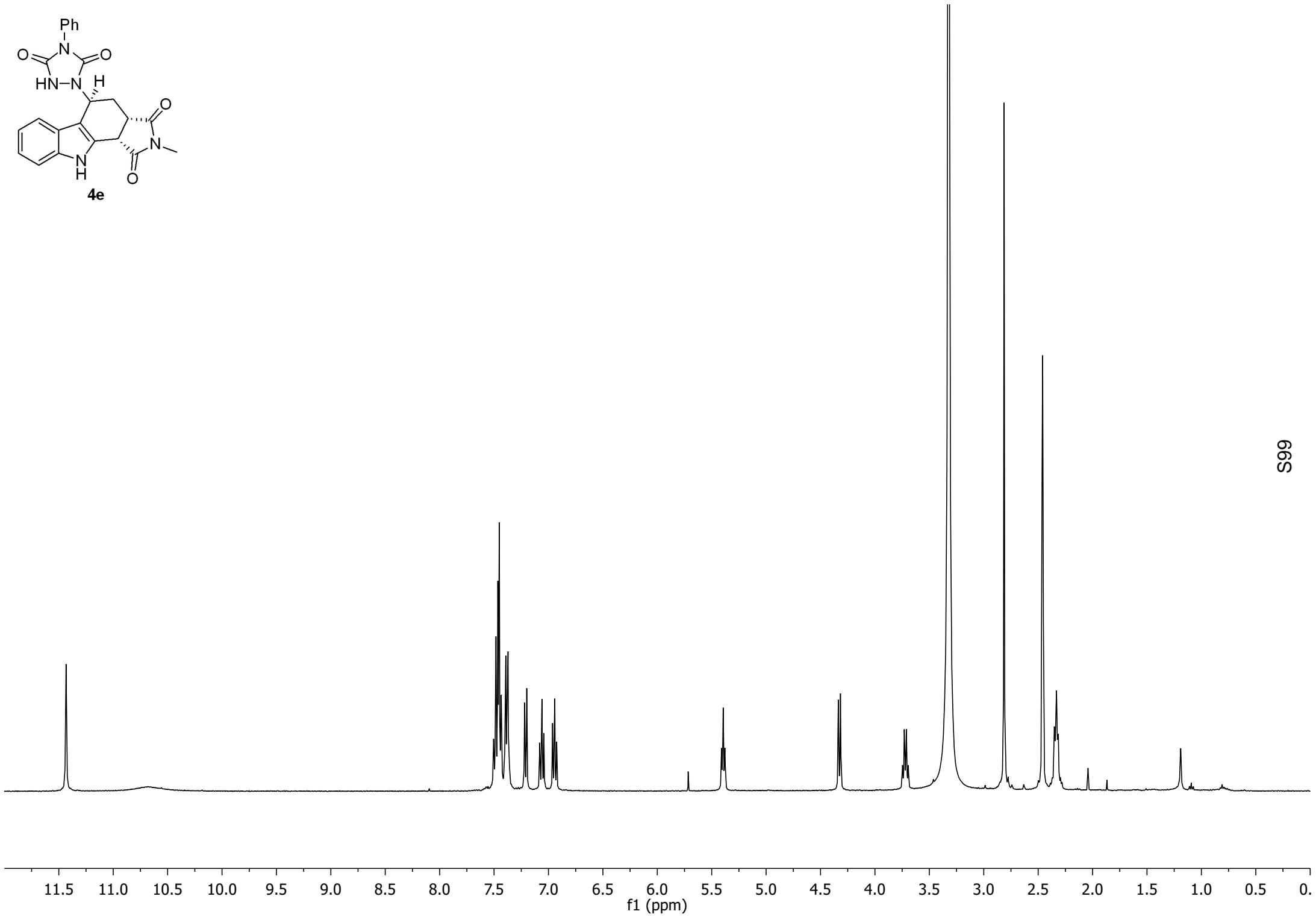


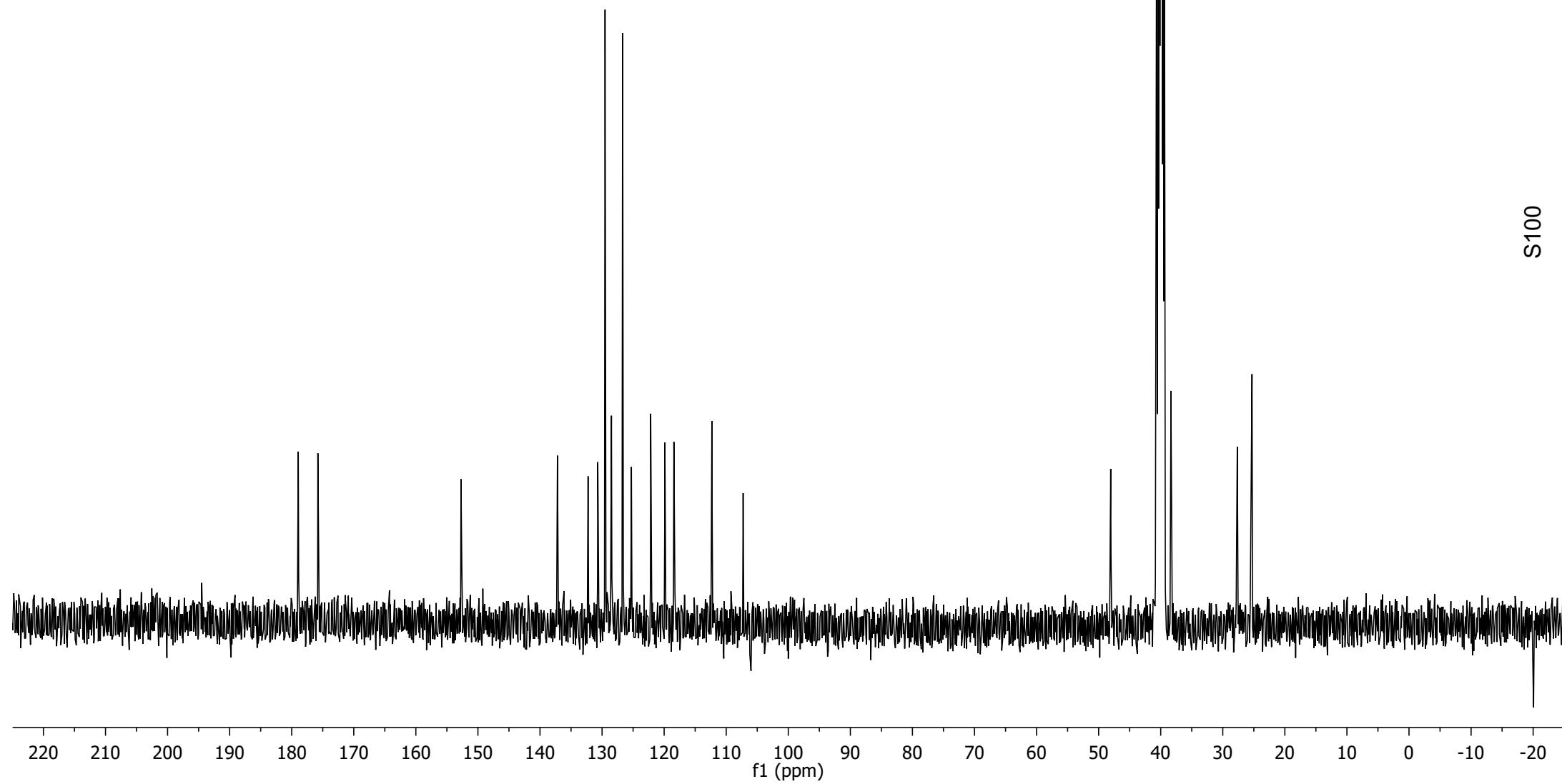
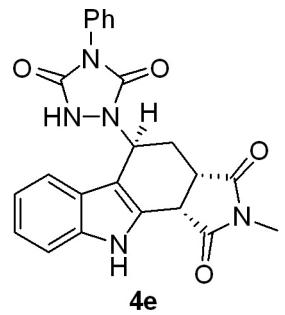
S98



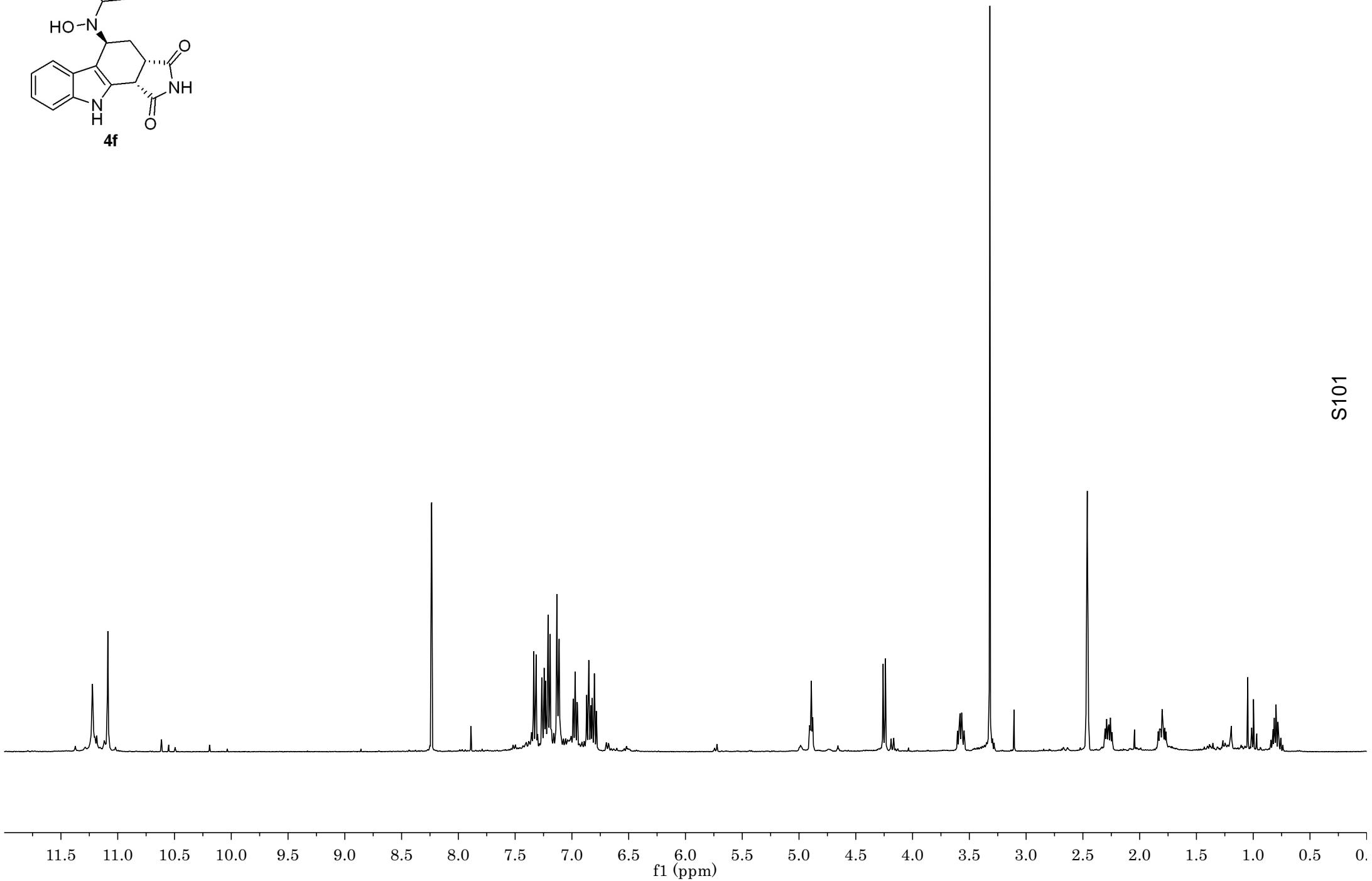
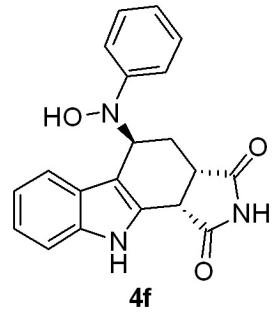


S99

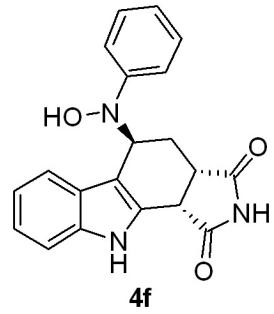




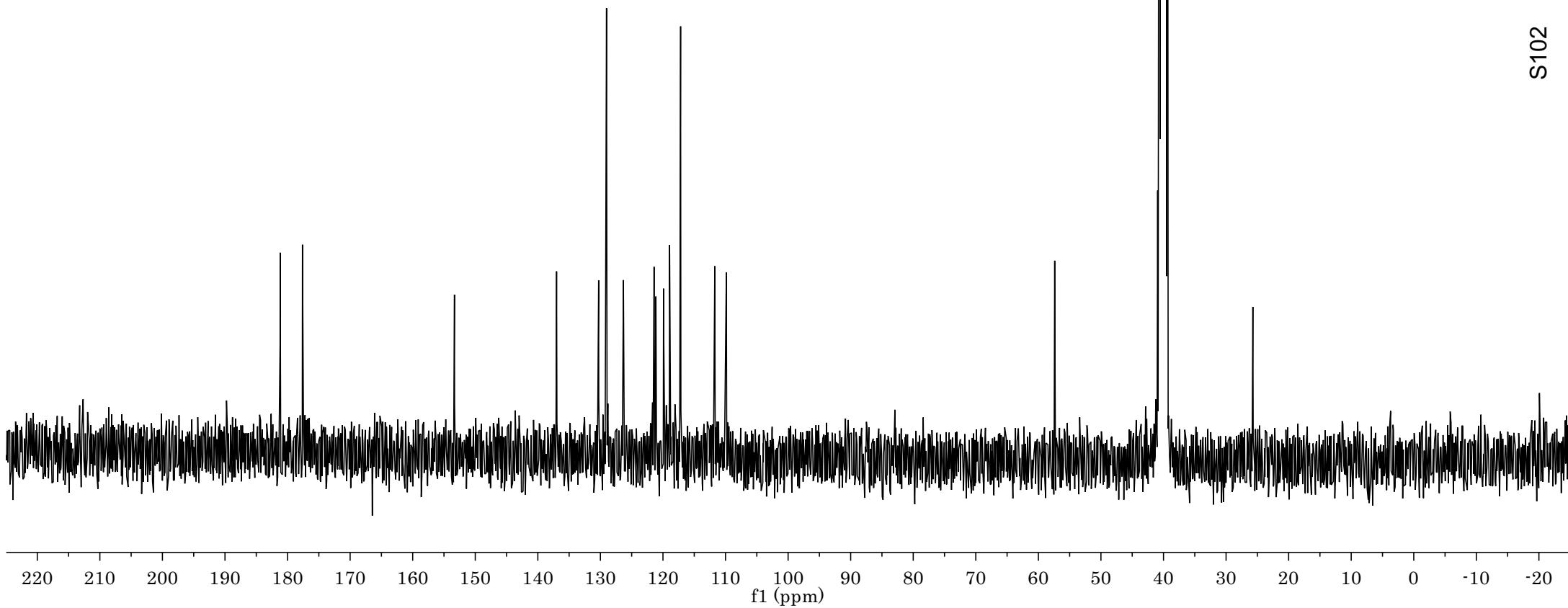
S100

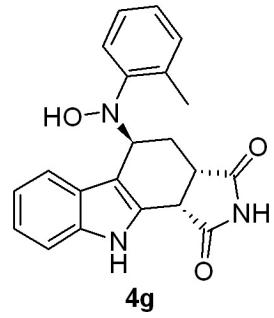


S101

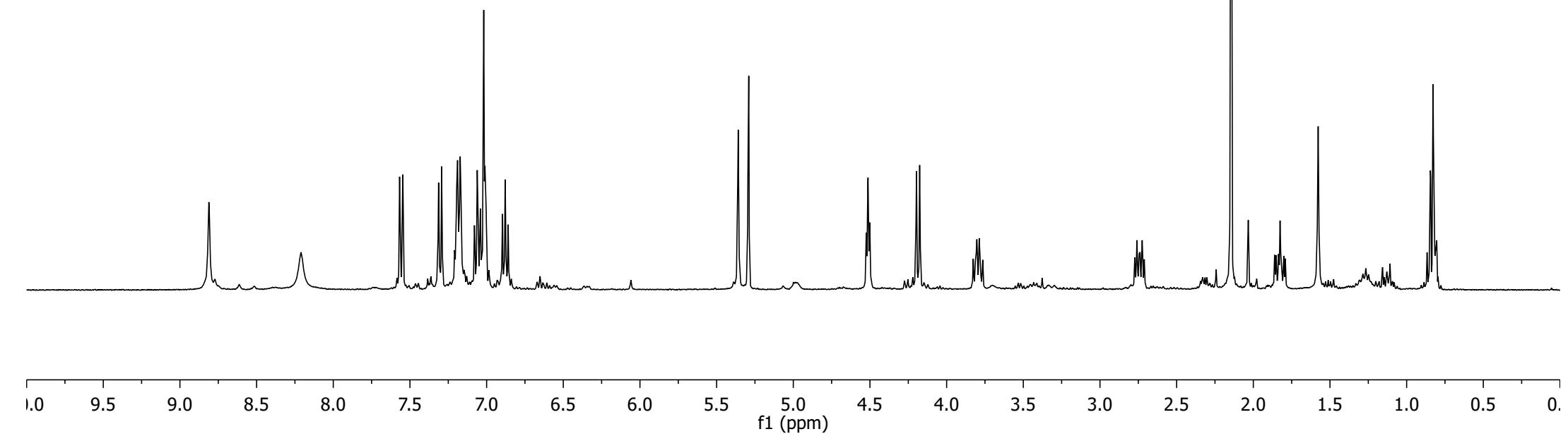


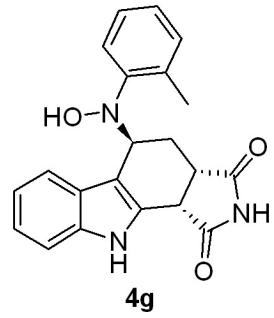
S102



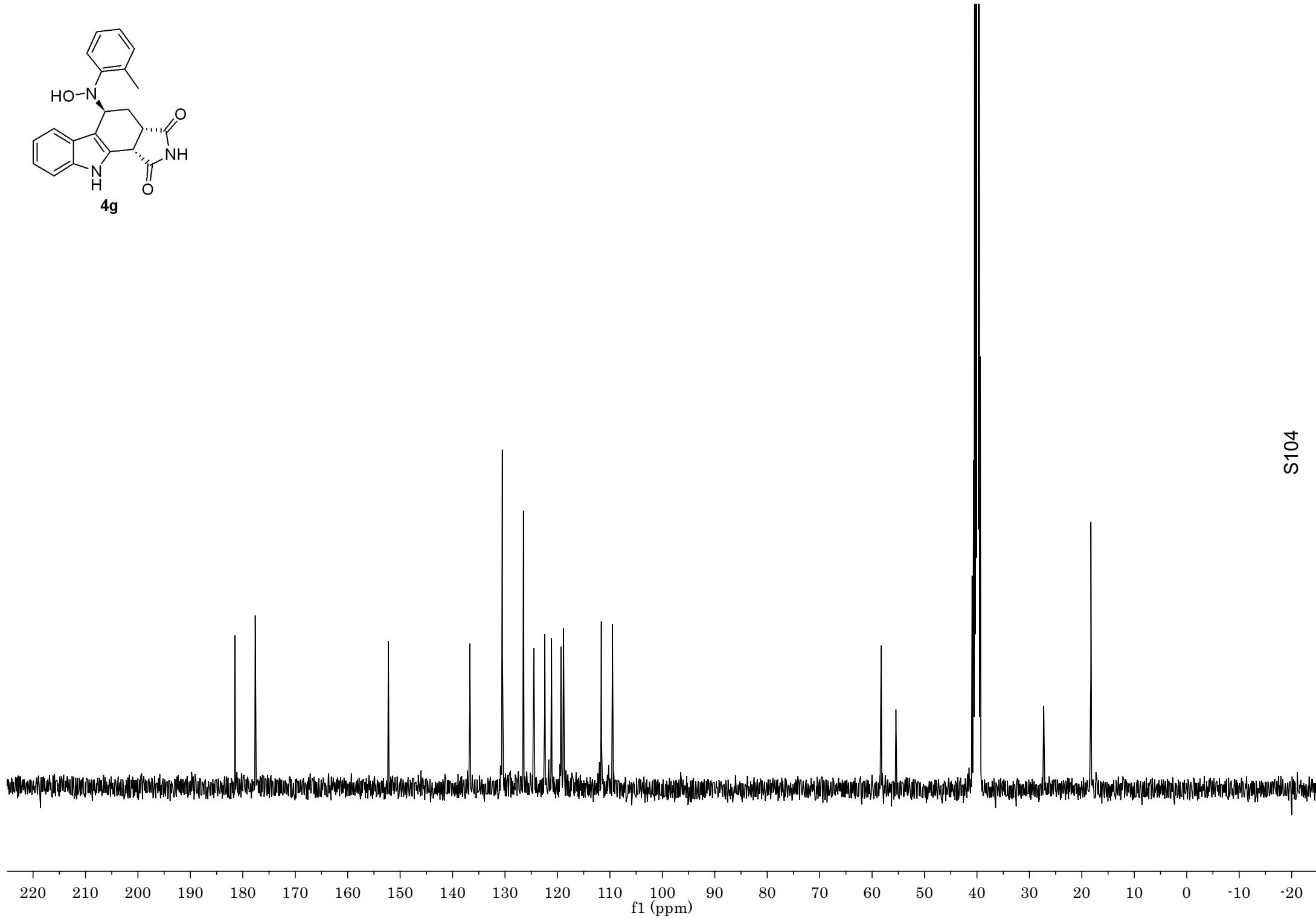


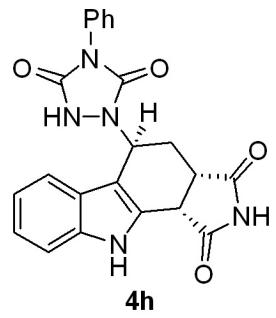
S103



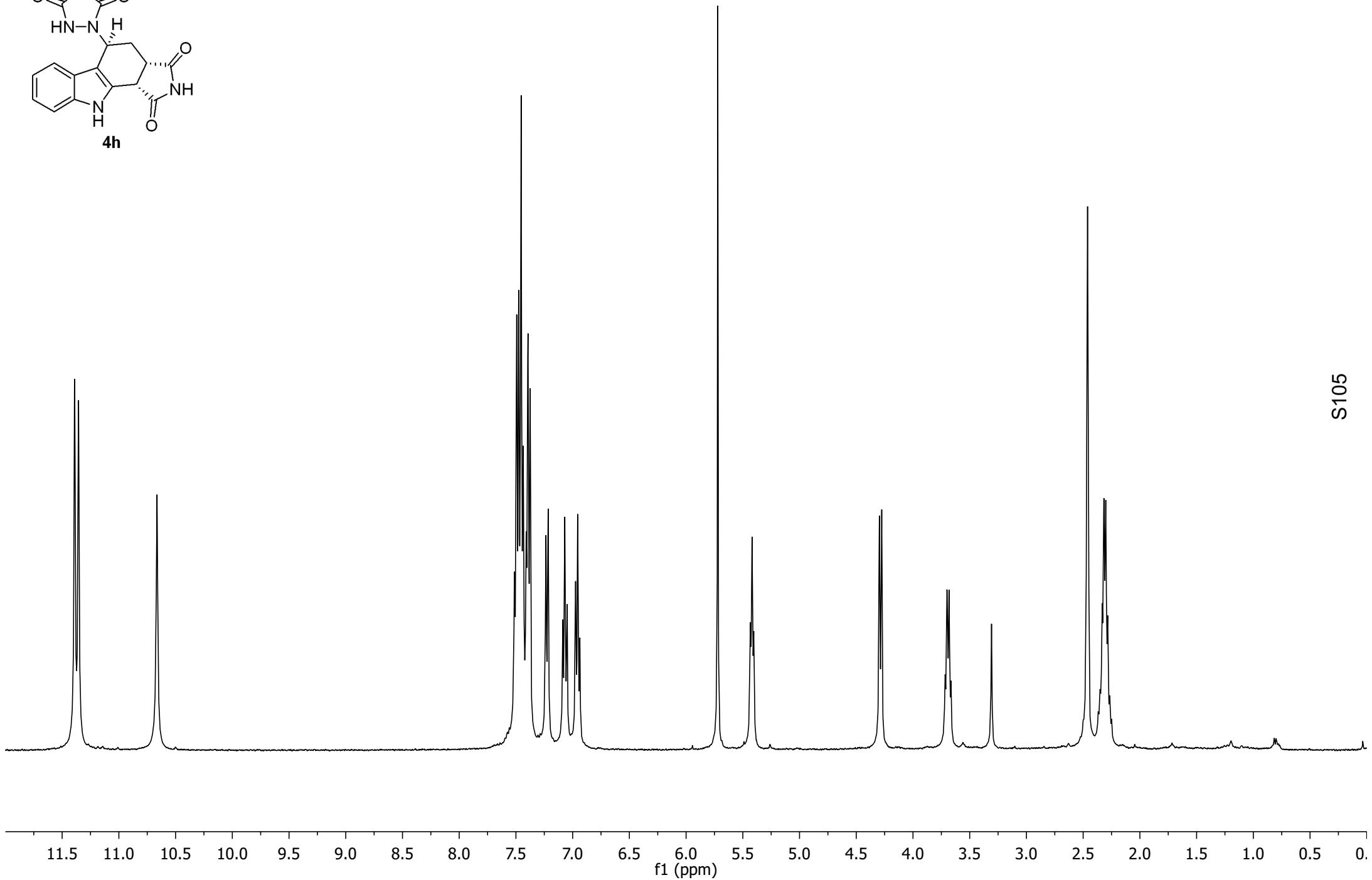


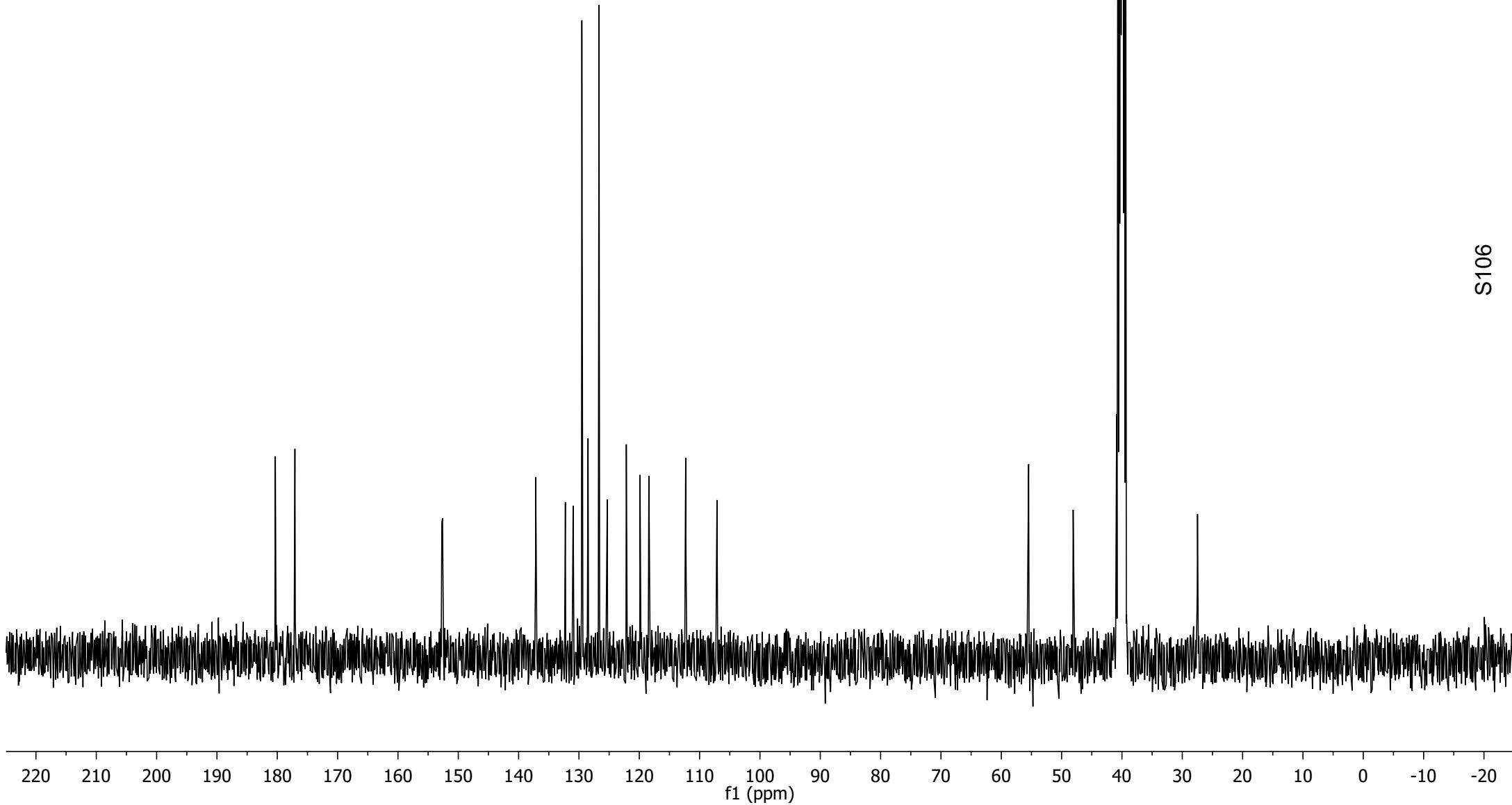
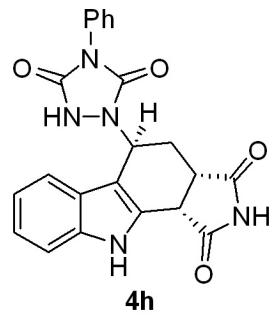
S104



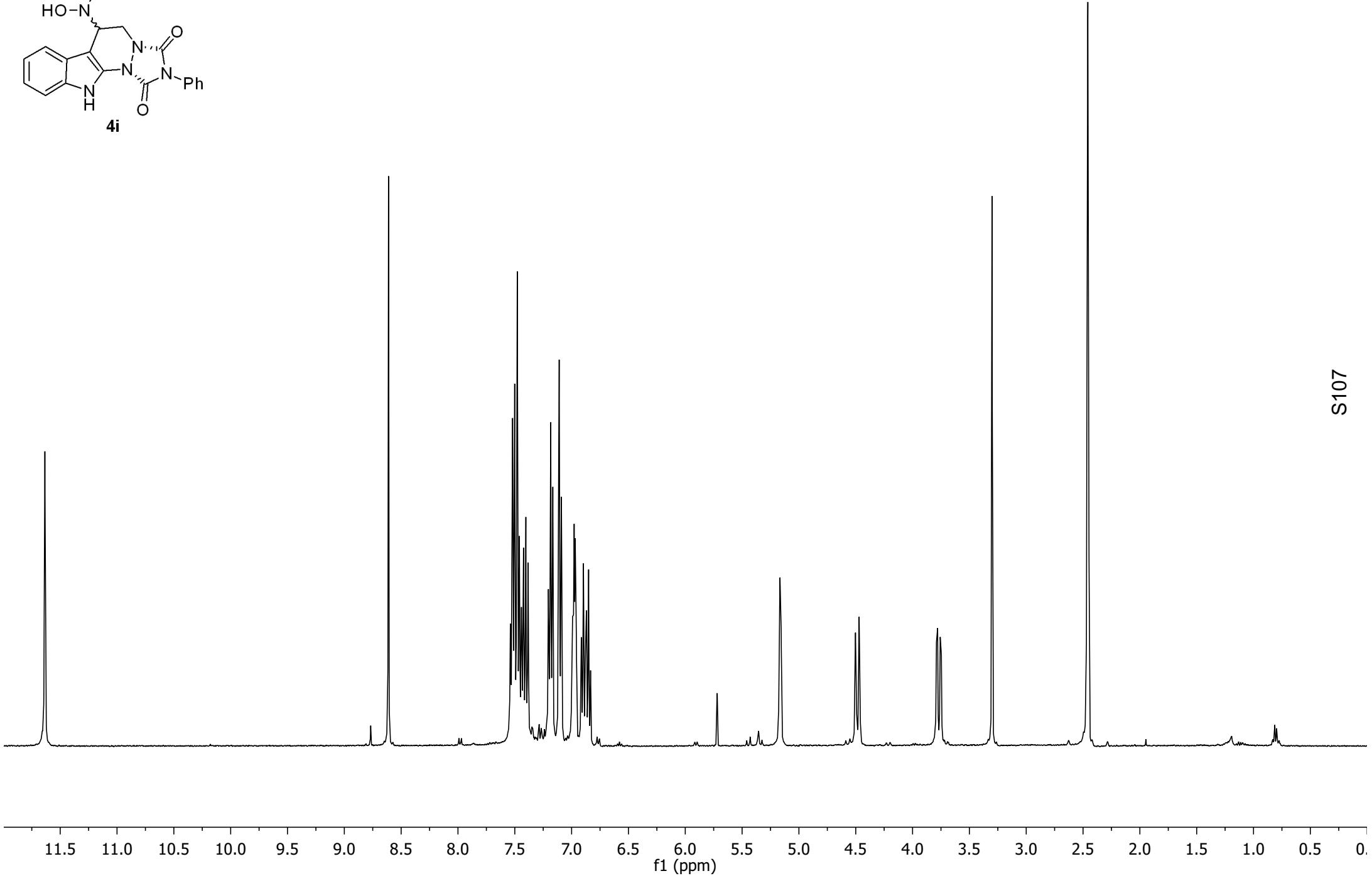
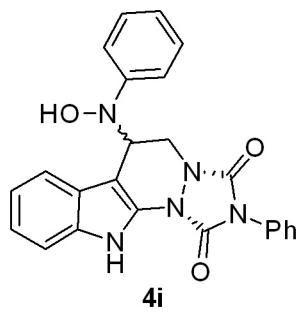


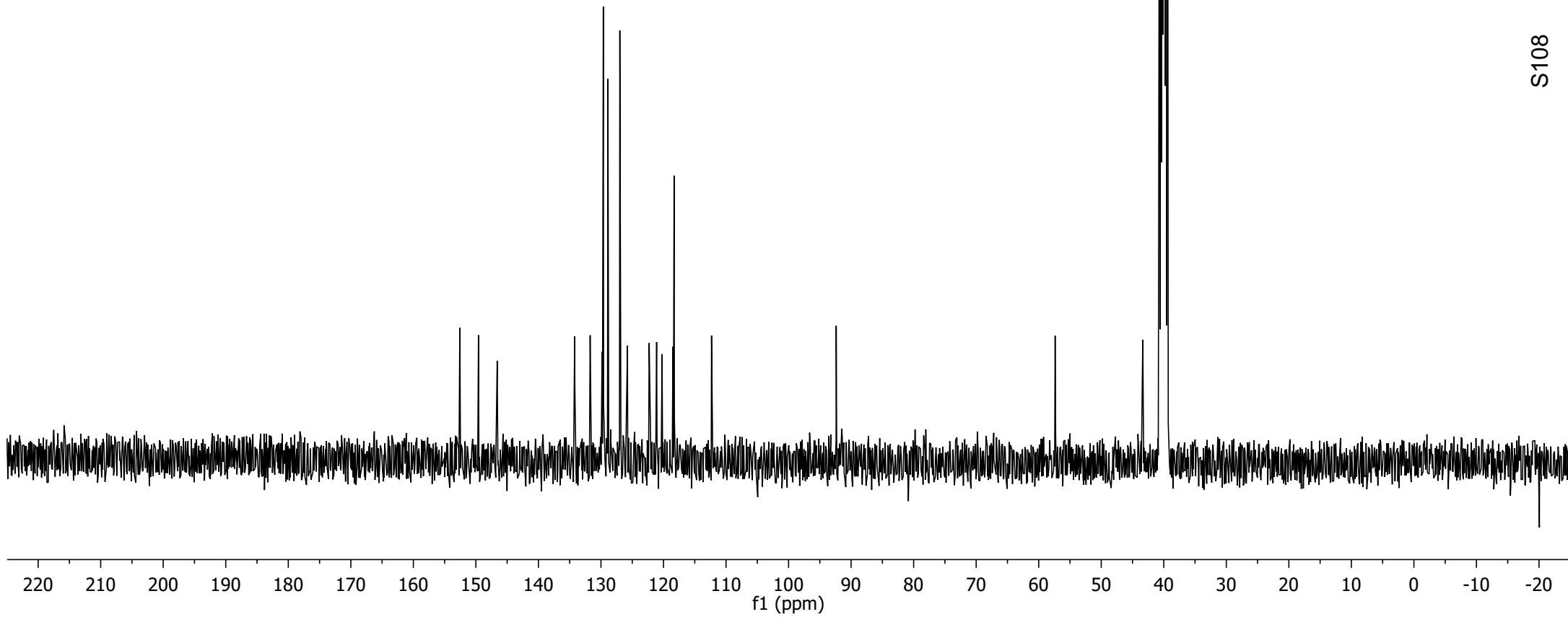
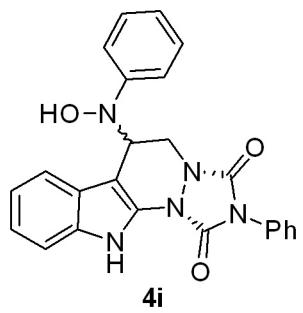
S105

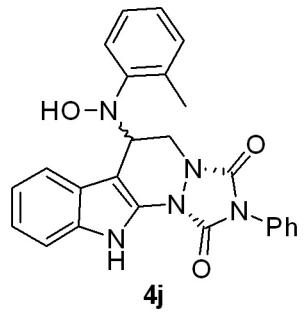




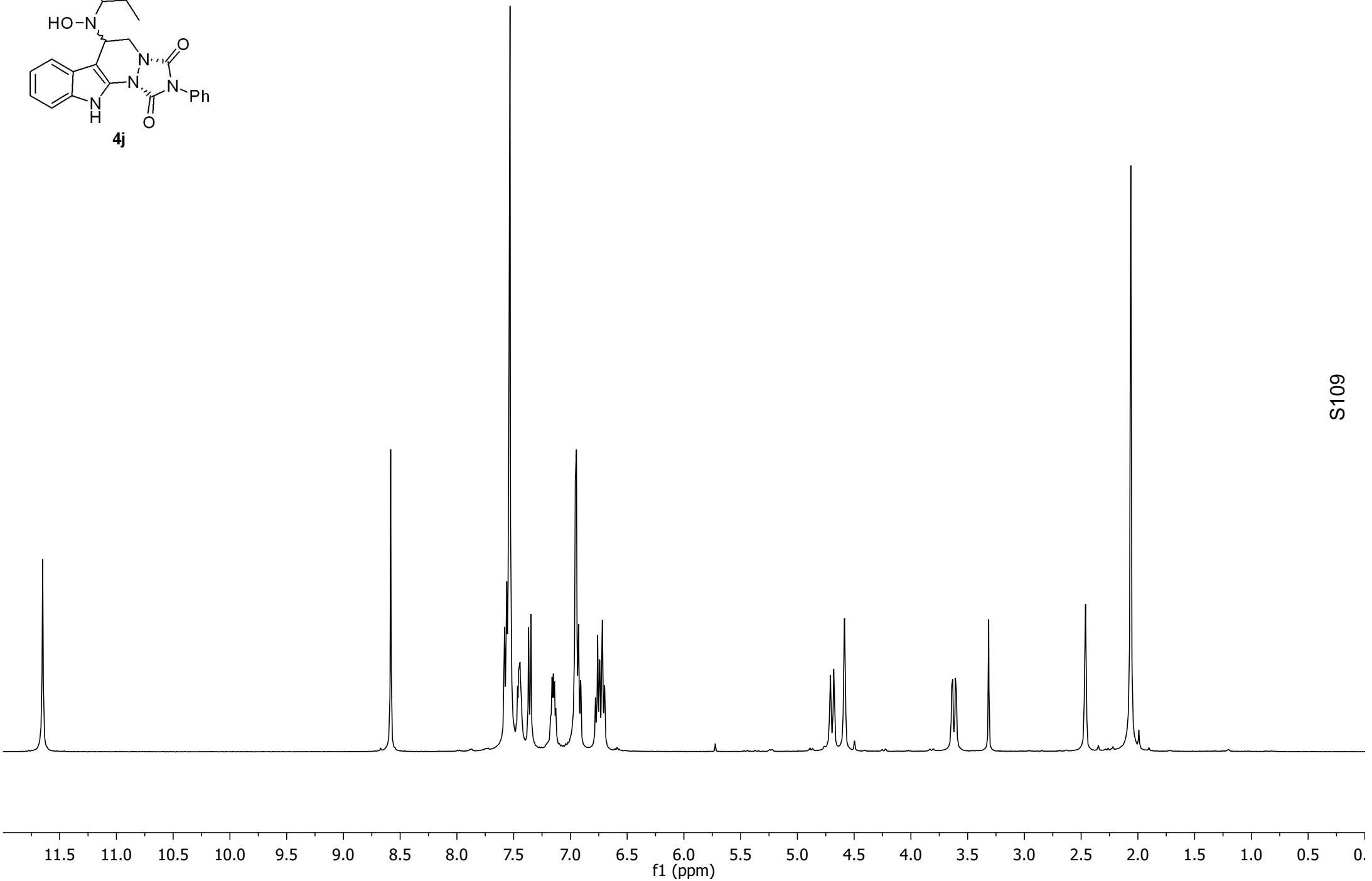
S106



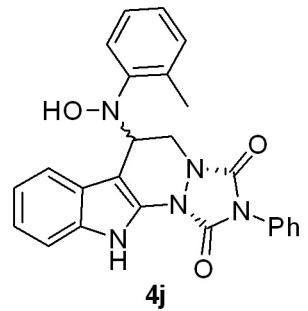




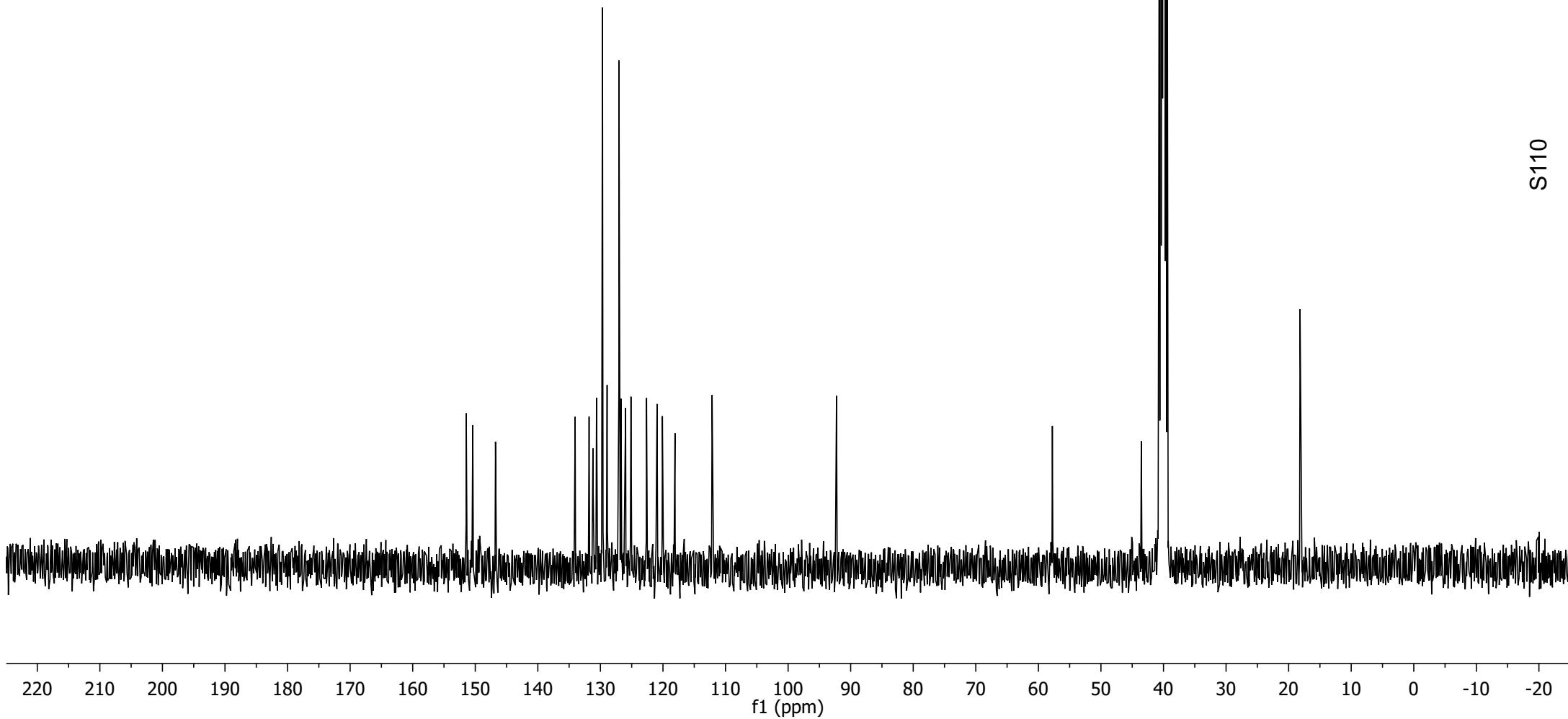
4j



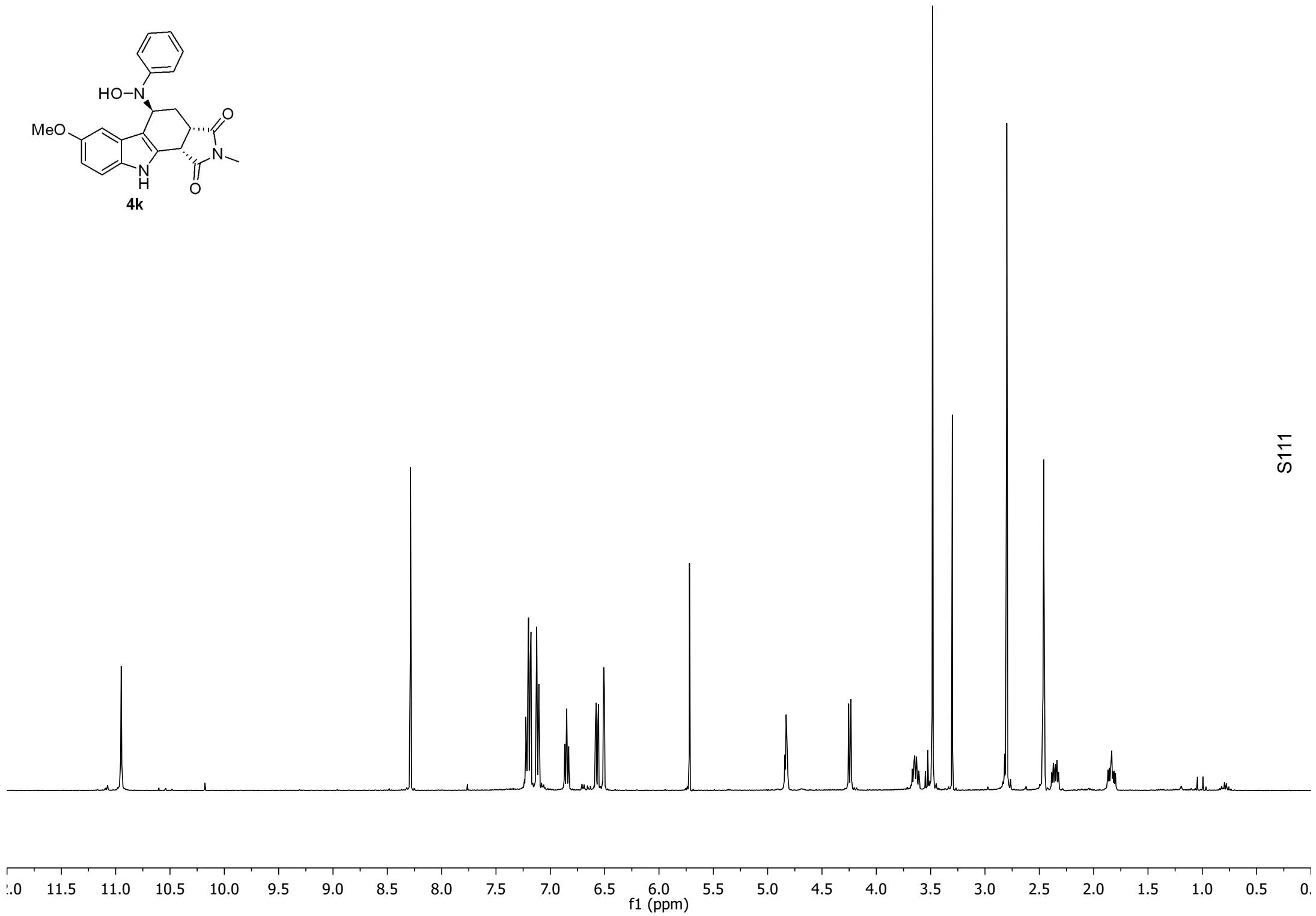
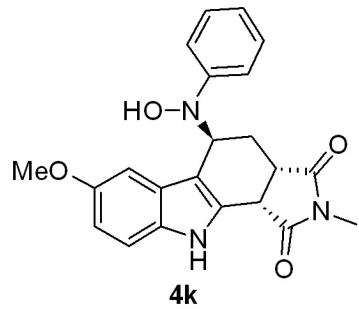
S109

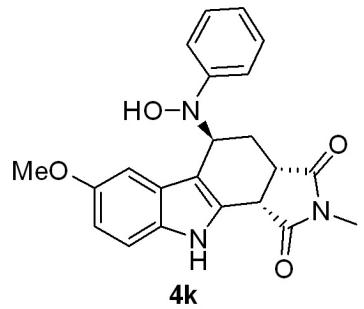


4j

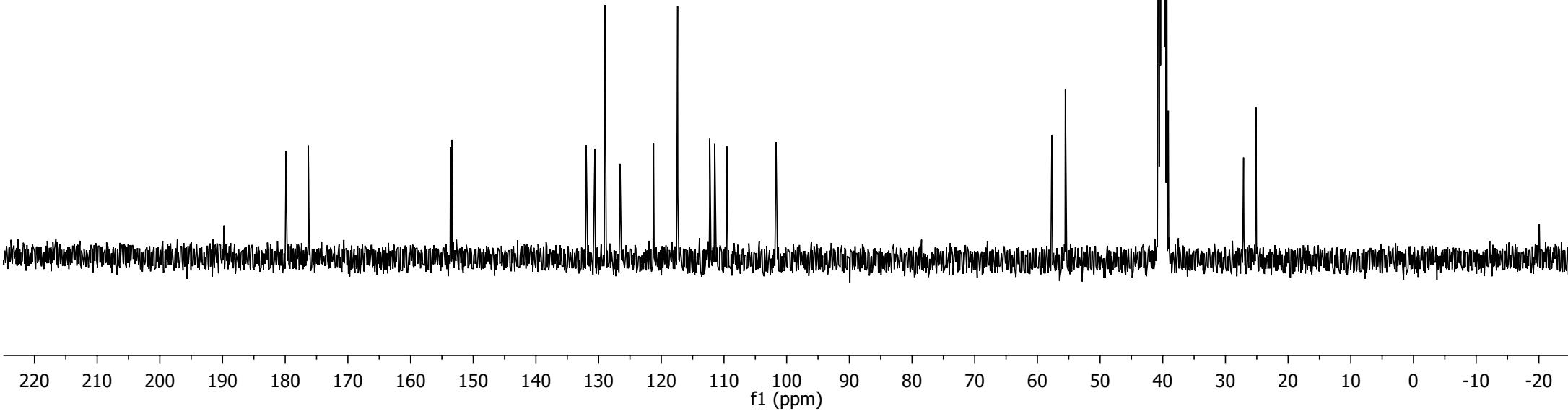


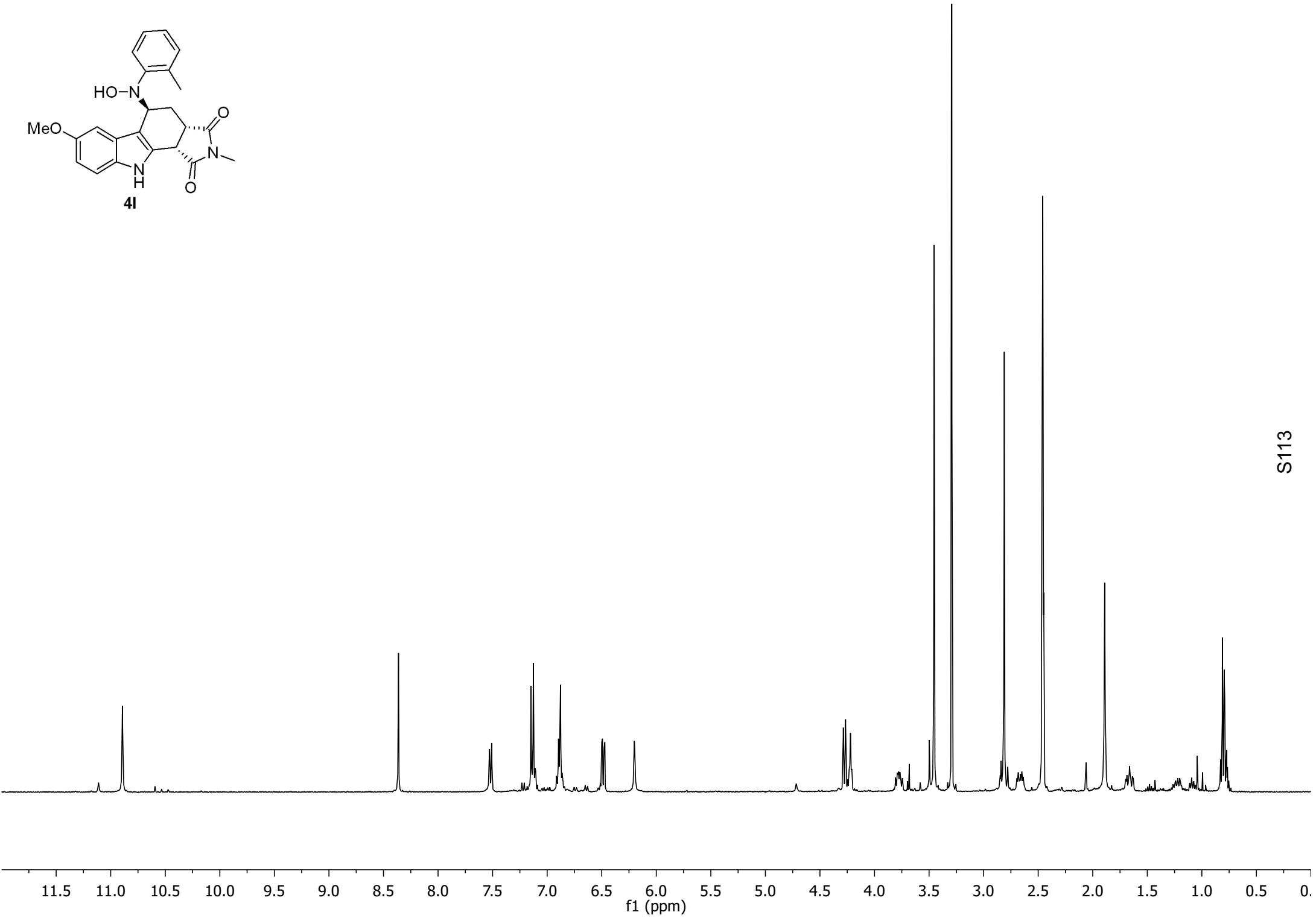
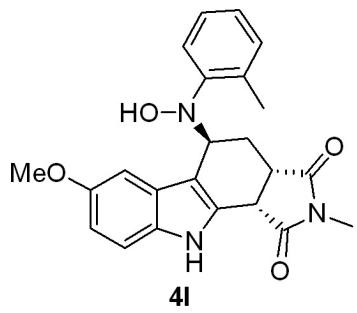
S110

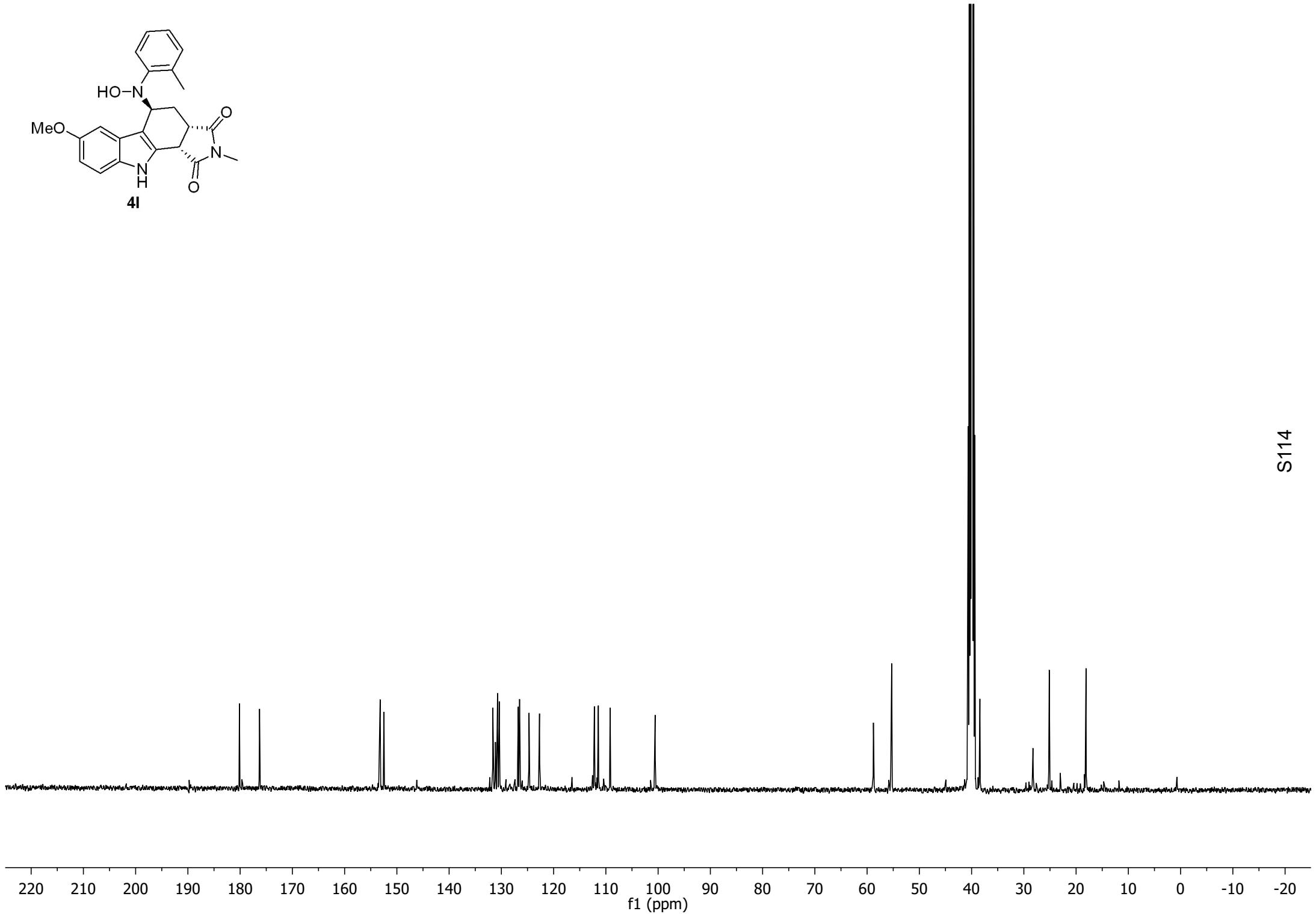
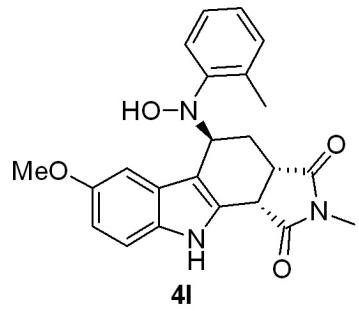


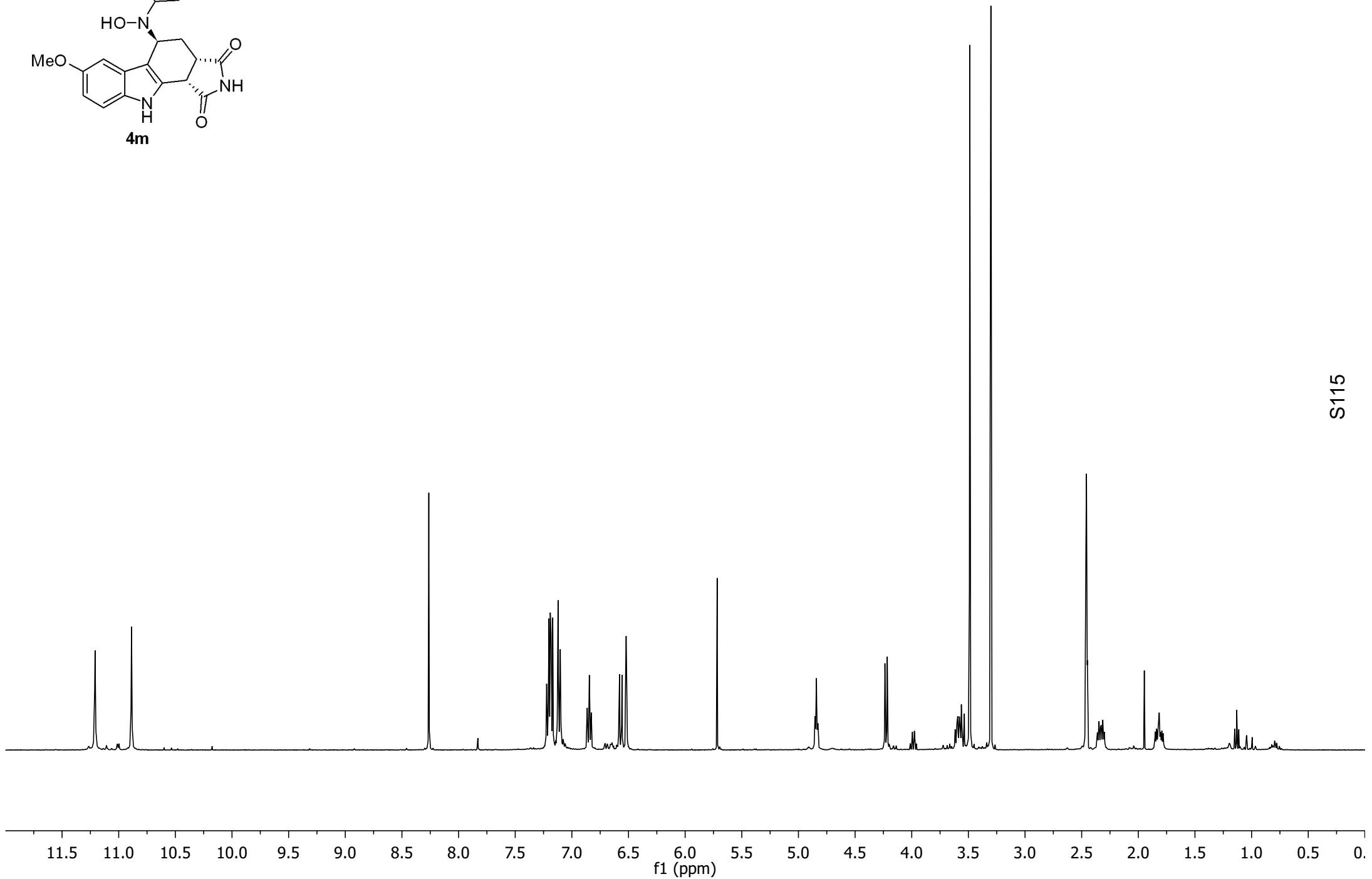
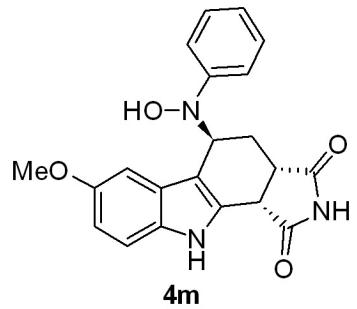


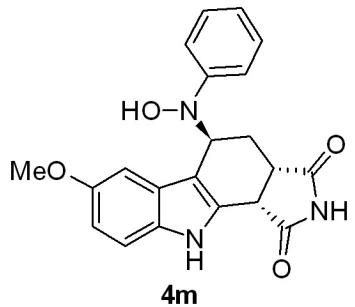
S112



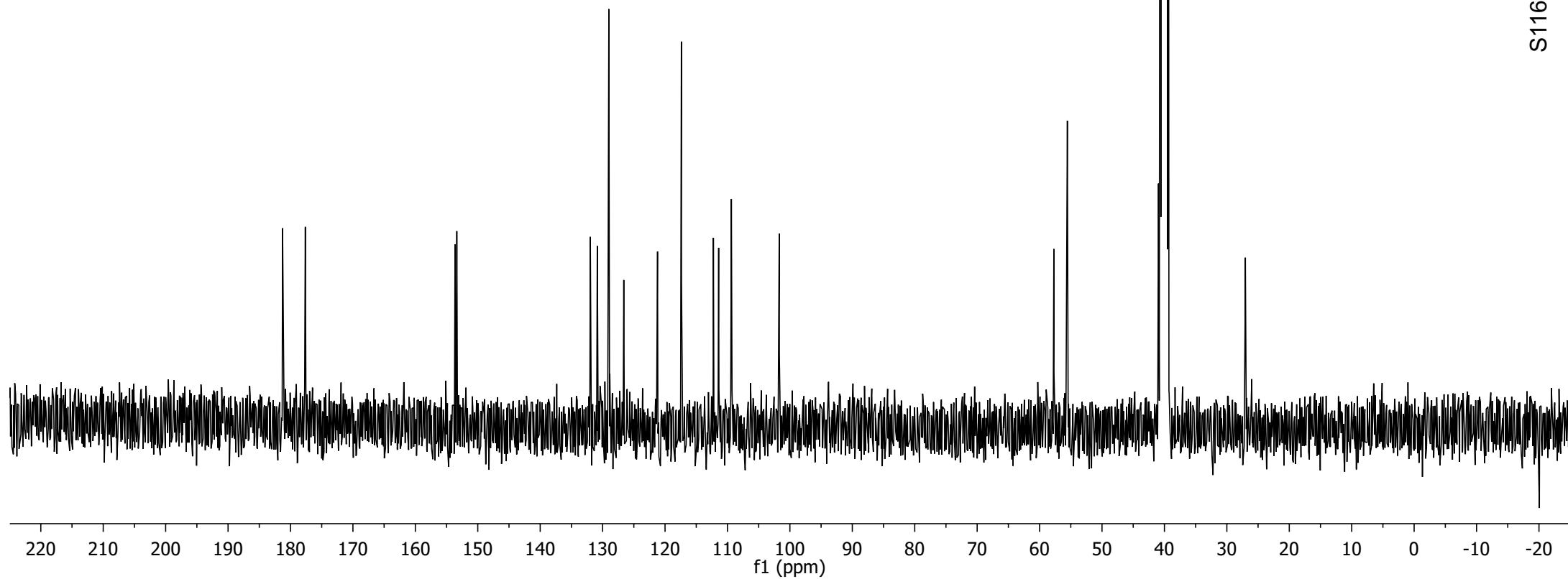


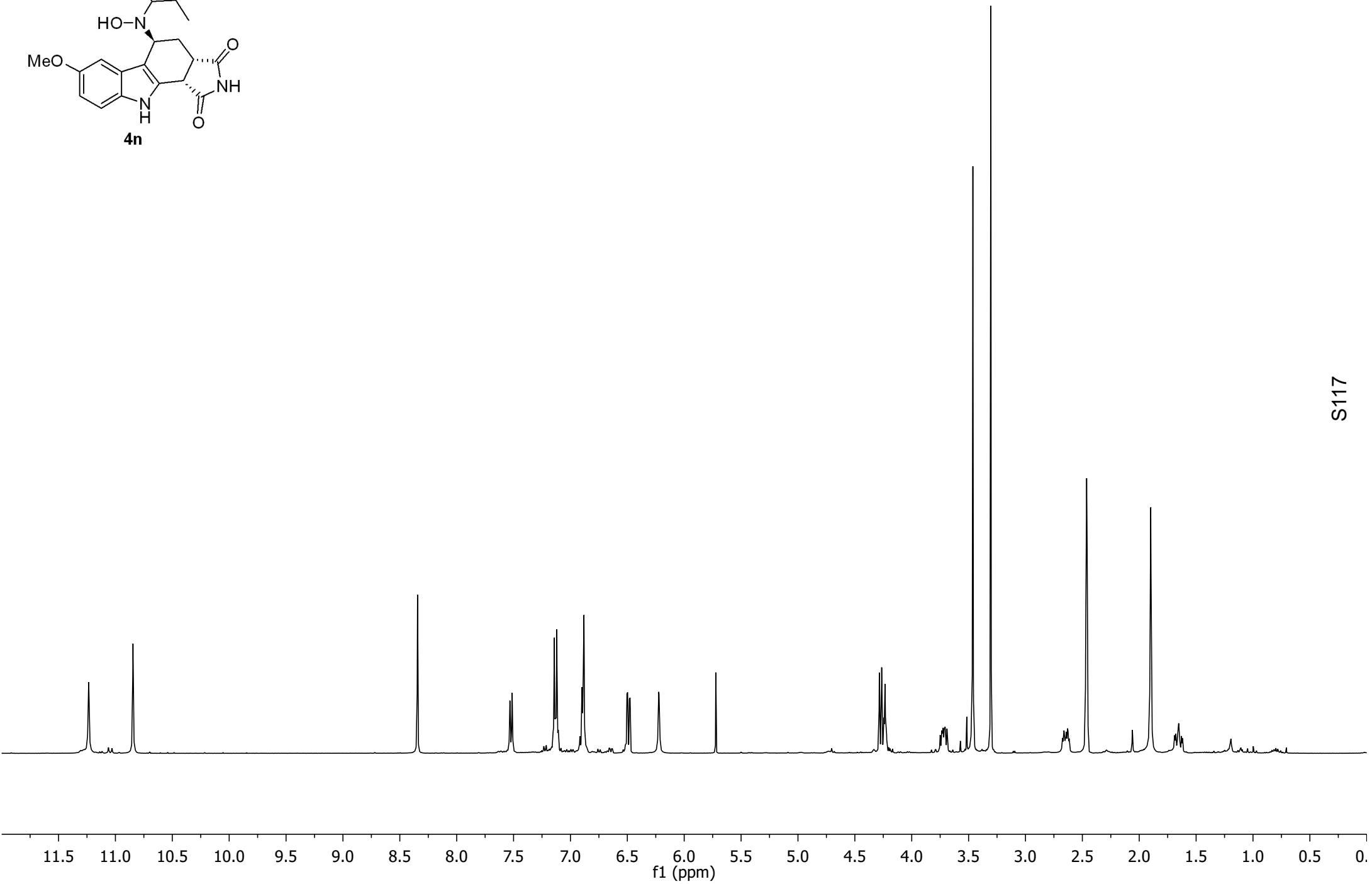
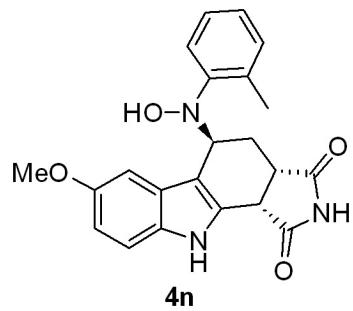




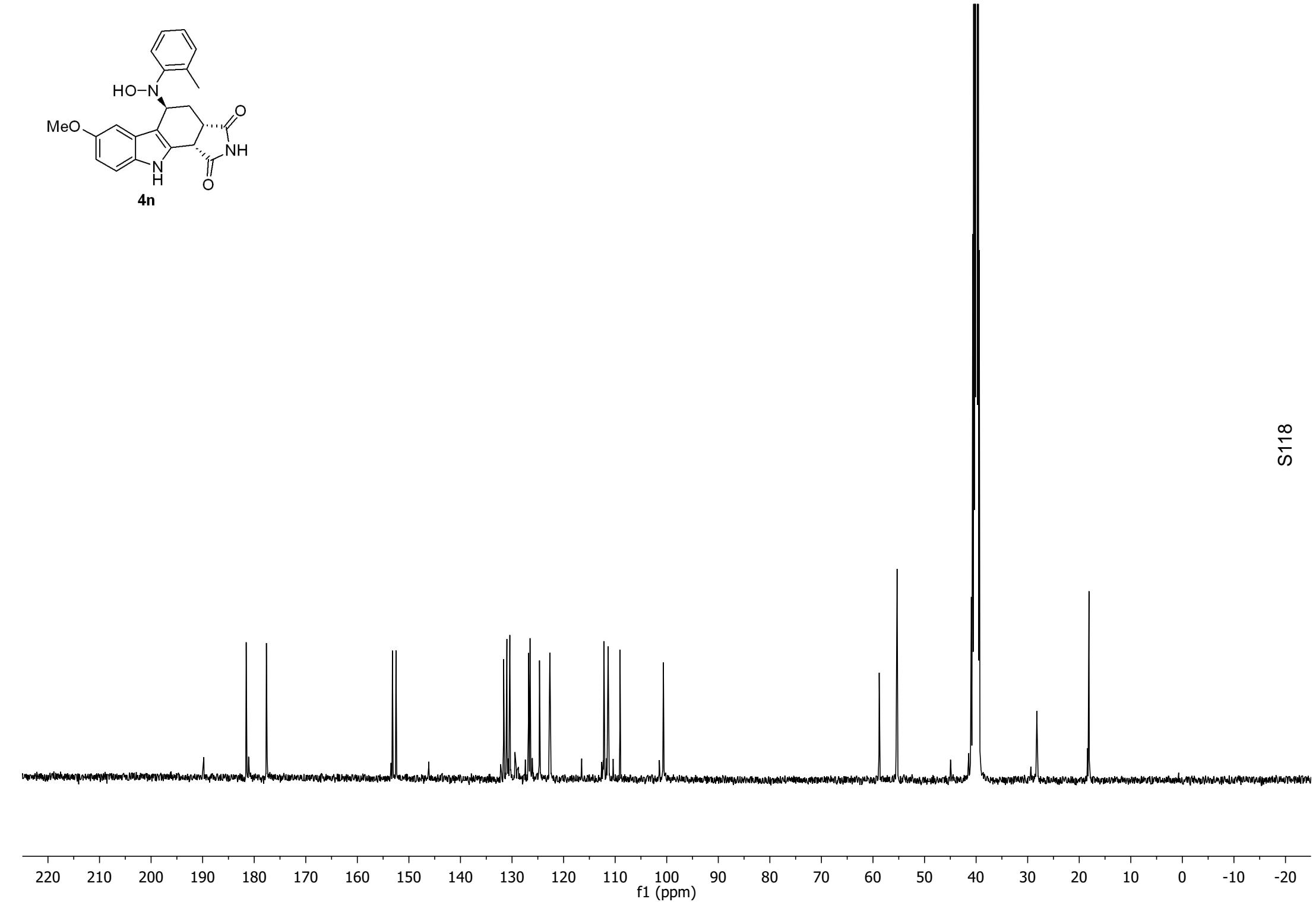
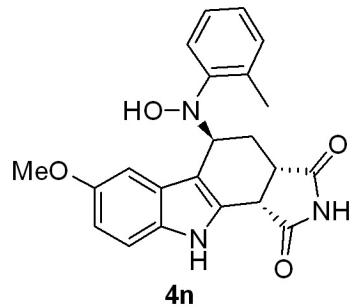


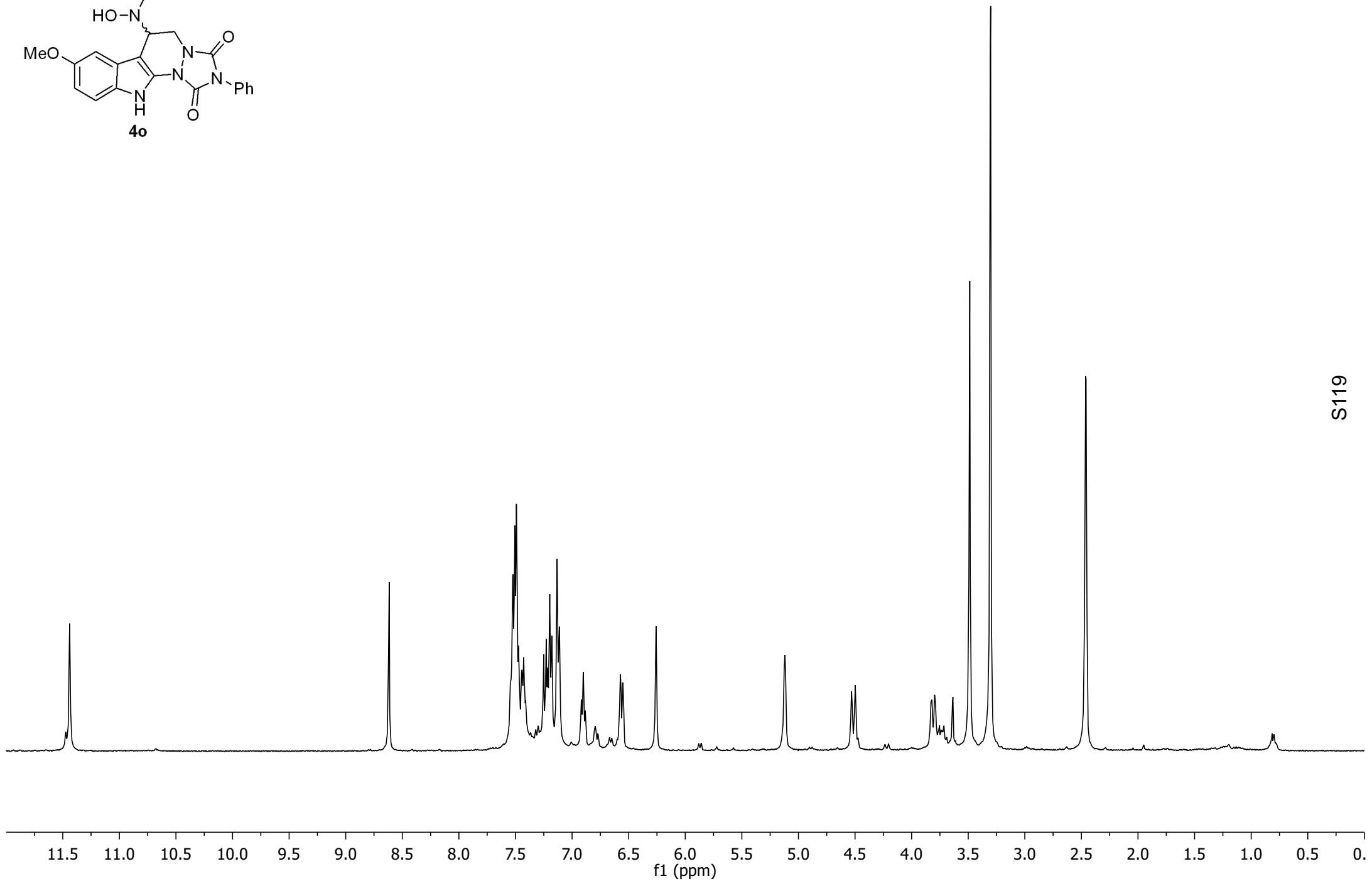
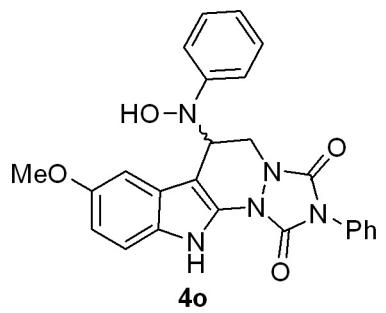
S116

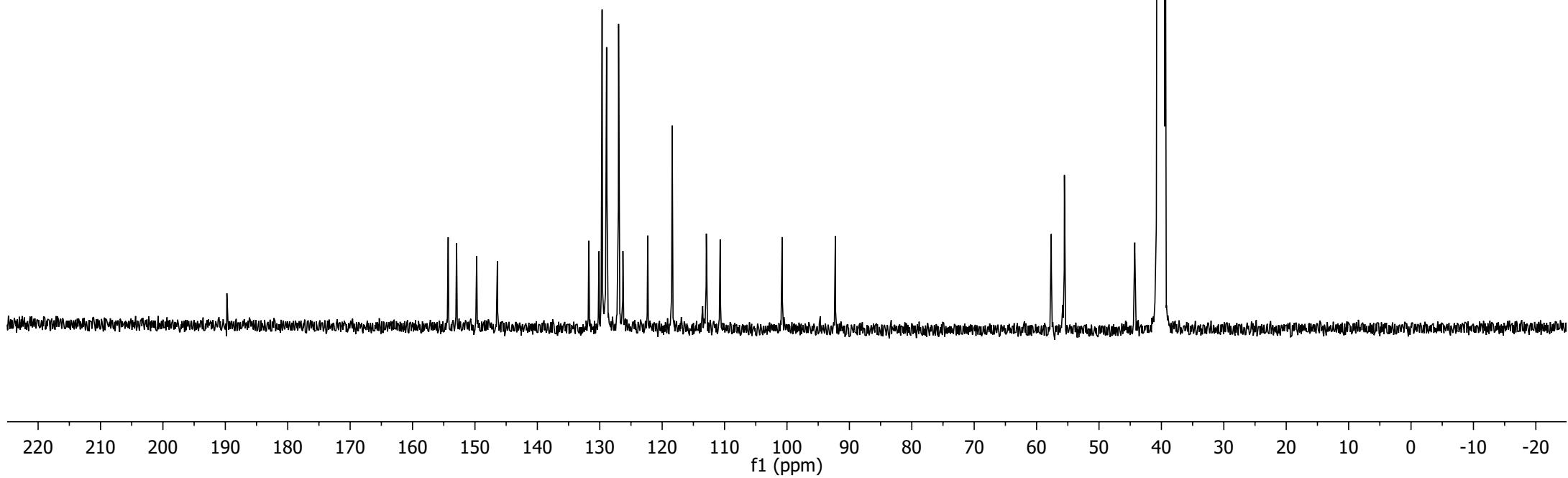
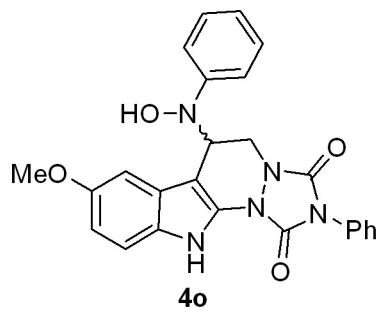




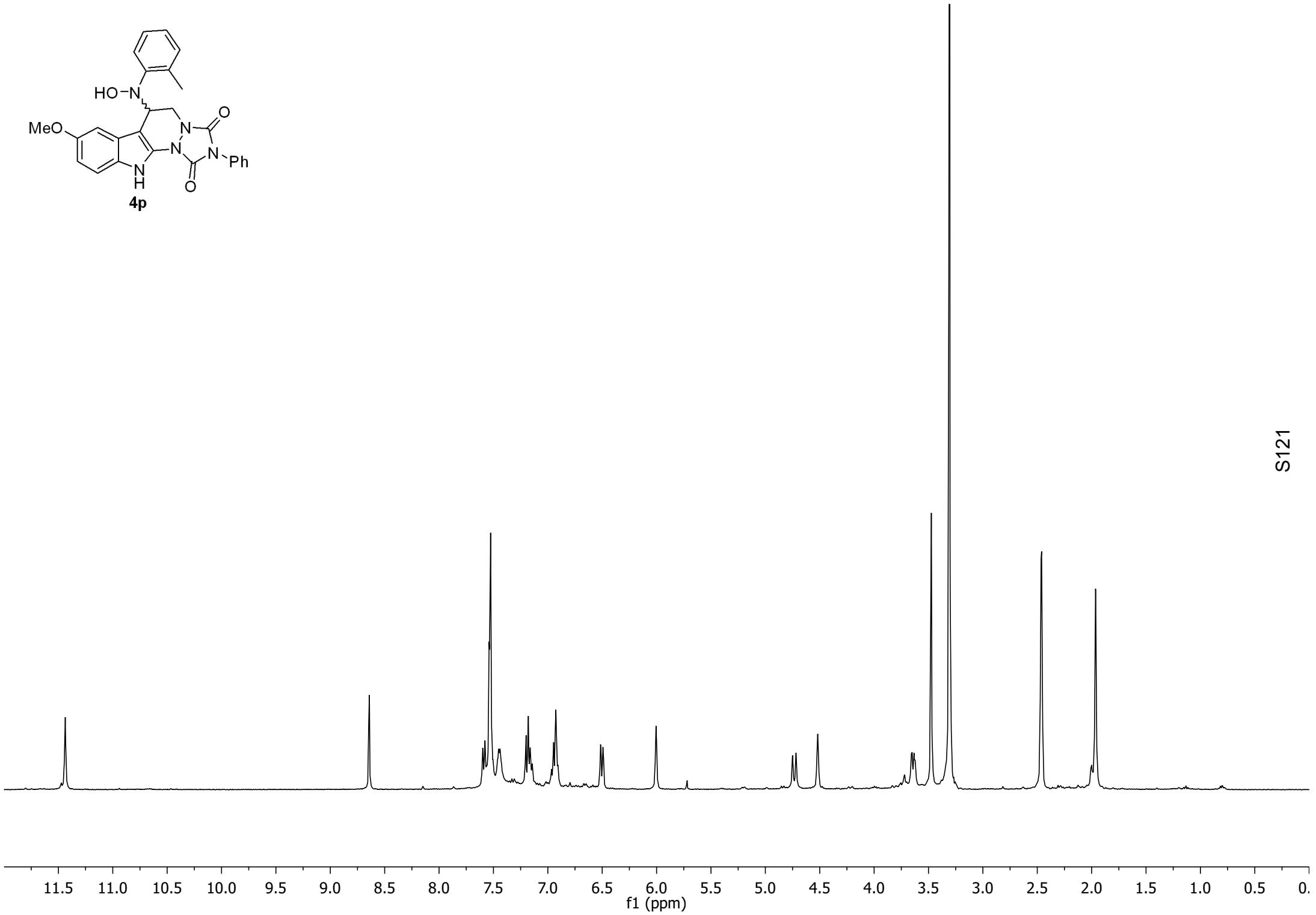
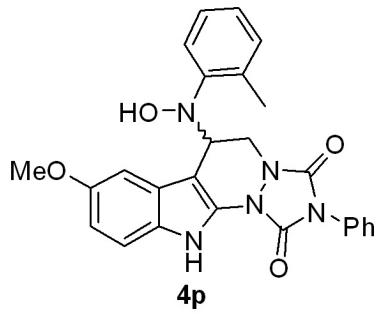
S117

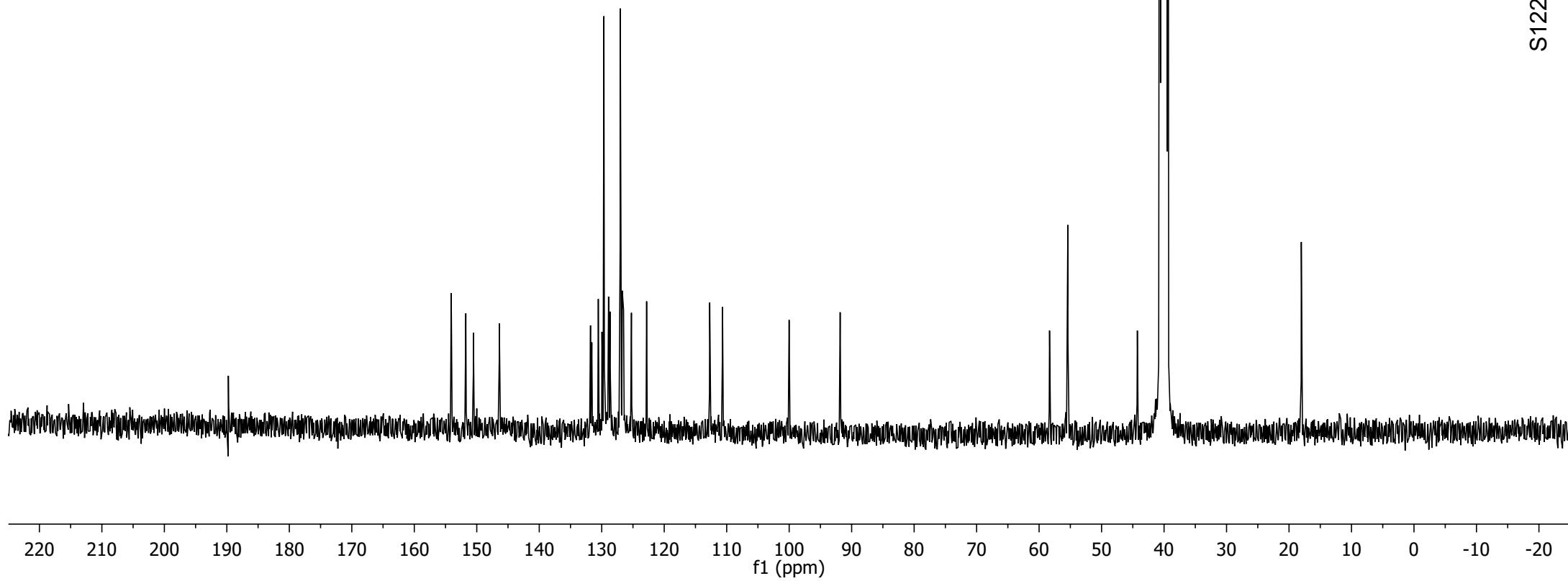
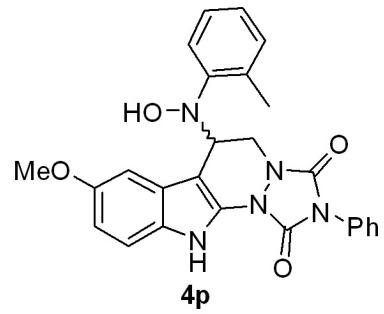






S120





2a - (3aS*,10aS*,10bS*)-2-methyl-10-tosyl-4,10,10a,10b-tetrahydropyrrolo[3,4-a]carbazole-1,3(2H,3aH)-dione

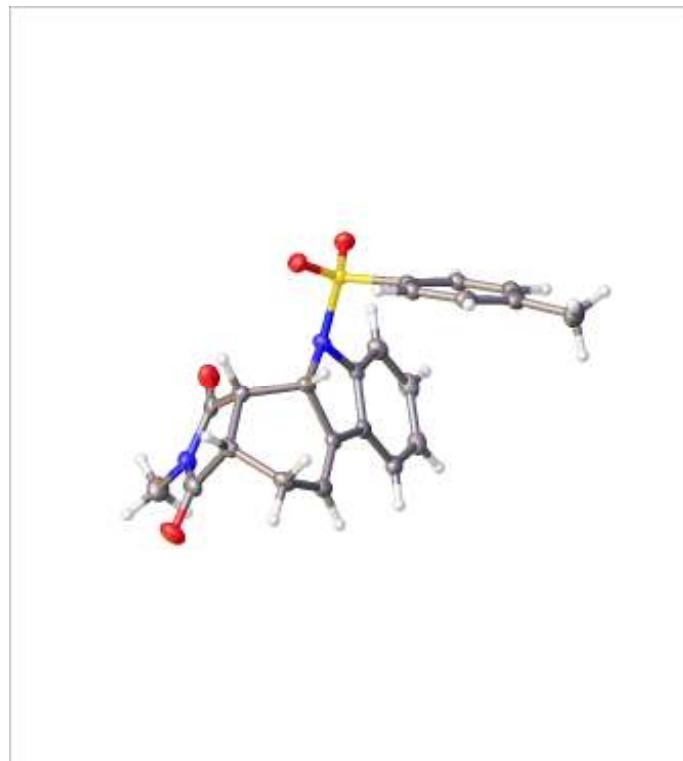


Table 1 Crystal data and structure refinement for MJH80.

Identification code	MJH80
Empirical formula	C ₂₂ H ₂₀ N ₂ O ₄ S
Formula weight	408.46
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	10.5141(8)
b/Å	17.9454(11)
c/Å	11.0976(8)
α/°	90
β/°	113.865(9)
γ/°	90
Volume/Å ³	1914.9(3)
Z	4
ρ _{calc} g/cm ³	1.417
μ/mm ⁻¹	0.202
F(000)	856.0
Crystal size/mm ³	0.3 × 0.3 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.06 to 56.914
Index ranges	-13 ≤ h ≤ 10, -23 ≤ k ≤ 21, -14 ≤ l ≤ 13
Reflections collected	10008

Independent reflections	4083 [R _{int} = 0.0256, R _{sigma} = 0.0354]
Data/restraints/parameters	4083/0/264
Goodness-of-fit on F ²	1.040
Final R indexes [I>=2σ (I)]	R ₁ = 0.0409, wR ₂ = 0.0943
Final R indexes [all data]	R ₁ = 0.0525, wR ₂ = 0.1019
Largest diff. peak/hole / e Å ⁻³	0.34/-0.46

2b - 2-phenyl-11-tosyl-11,11a-dihydro-1*H*,5*H*-[1',2':1,2]triazolo[1',2':1,2]pyridazino[3,4-*b*]indole-1,3(2*H*)-dione

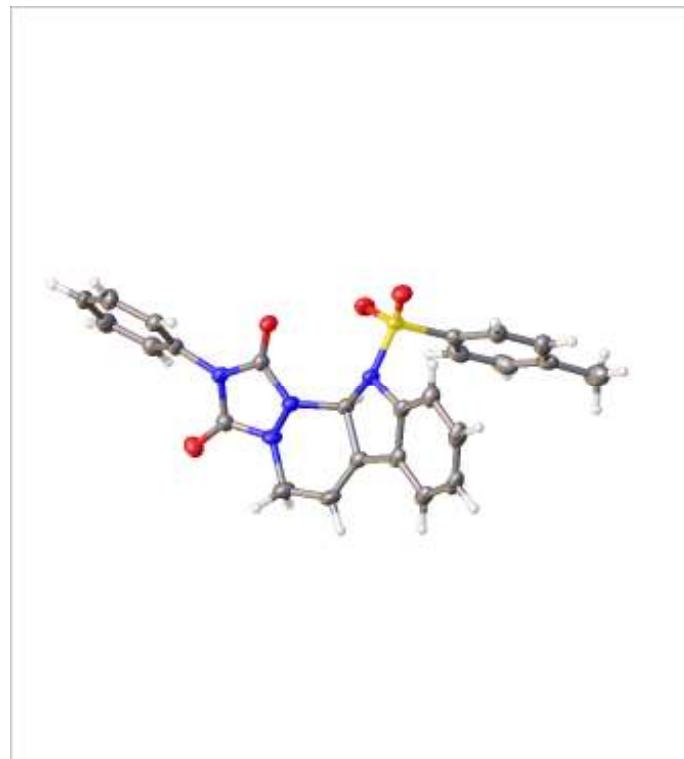


Table 1 Crystal data and structure refinement for MJH105.

Identification code	MJH105
Empirical formula	C _{25.5} H ₂₁ O ₄ SN ₄ Cl
Formula weight	514.97
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	6.2586(2)
b/Å	43.8481(9)
c/Å	17.0987(3)
α/°	90
β/°	93.143(2)
γ/°	90
Volume/Å ³	4685.3(2)
Z	8
ρ _{calc} g/cm ³	1.460
μ/mm ⁻¹	2.634
F(000)	2136.0
Crystal size/mm ³	0.3 × 0.3 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.03 to 124.68
Index ranges	-3 ≤ h ≤ 6, -41 ≤ k ≤ 49, -19 ≤ l ≤ 19
Reflections collected	13831

Independent reflections	7203 [R _{int} = 0.0228, R _{sigma} = 0.0341]
Data/restraints/parameters	7203/0/640
Goodness-of-fit on F ²	1.076
Final R indexes [I>=2σ (I)]	R ₁ = 0.0560, wR ₂ = 0.1441
Final R indexes [all data]	R ₁ = 0.0702, wR ₂ = 0.1528
Largest diff. peak/hole / e Å ⁻³	0.39/-0.42

2d - ethyl 3-((3aS*,4R*,10aS*,10bS*)-1,3-dioxo-10-tosyl-1,2,3,3a,4,10,10a,10b-octahydropyrrolo[3,4-a]carbazol-4-yl)propanoate

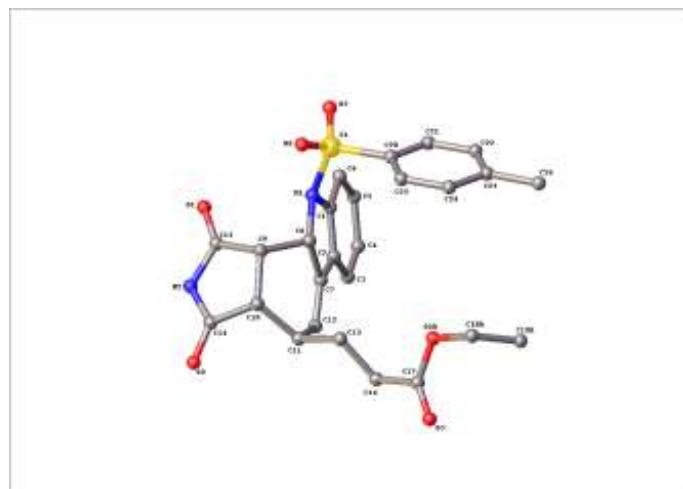


Table 1 Crystal data and structure refinement for mjh140029_fa.

Identification code	mjh140029_fa
Empirical formula	C ₂₆ H ₂₆ N ₂ O ₆ S
Formula weight	494.55
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	16.0840(2)
b/Å	8.84163(10)
c/Å	18.0999(2)
α/°	90
β/°	106.2054(14)
γ/°	90
Volume/Å ³	2471.70(6)
Z	4
ρ _{calc} g/cm ³	1.329
μ/mm ⁻¹	1.537
F(000)	1040.0
Crystal size/mm ³	0.2871 × 0.2849 × 0.1359
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	6.51 to 133.56
Index ranges	-19 ≤ h ≤ 19, -10 ≤ k ≤ 10, -21 ≤ l ≤ 21
Reflections collected	65129
Independent reflections	4373 [R _{int} = 0.0518, R _{sigma} = 0.0153]
Data/restraints/parameters	4373/345/341
Goodness-of-fit on F ²	1.031
Final R indexes [I>=2σ (I)]	R ₁ = 0.0351, wR ₂ = 0.0896
Final R indexes [all data]	R ₁ = 0.0392, wR ₂ = 0.0929
Largest diff. peak/hole / e Å ⁻³	0.32/-0.48

3I - (3aS*,5S*,10bS*)-5-(hydroxy(*o*-tolyl)amino)-10-tosyl-4,5,10b-tetrahydropyrrolo[3,4-*a*]carbazole-1,3(2*H*,3*aH*)-dione

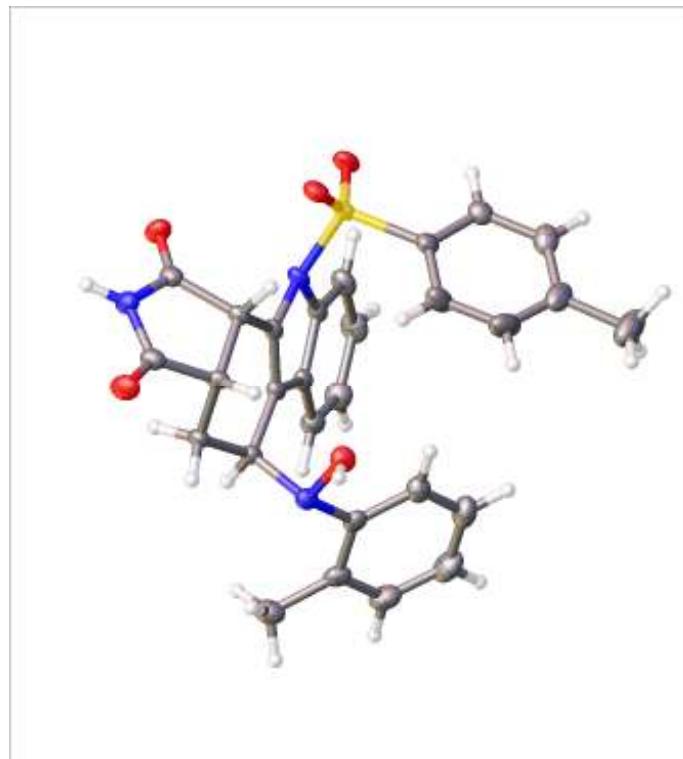


Table 1 Crystal data and structure refinement for mjh120026.

Identification code	mjh120026
Empirical formula	C ₂₉ H ₂₆ O ₅ SN ₃ Cl ₃
Formula weight	634.94
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	10.0614(5)
b/Å	10.2208(5)
c/Å	15.2649(7)
α/°	104.231(4)
β/°	95.071(4)
γ/°	109.240(4)
Volume/Å ³	1411.79(12)
Z	2
ρ _{calc} g/cm ³	1.494
μ/mm ⁻¹	4.017
F(000)	656.0
Crystal size/mm ³	0.15 × 0.13 × 0.12
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	6.078 to 133.94
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 12, -17 ≤ l ≤ 18
Reflections collected	13047

Independent reflections	4955 [R _{int} = 0.0264, R _{sigma} = 0.0239]
Data/restraints/parameters	4955/411/397
Goodness-of-fit on F ²	1.050
Final R indexes [I>=2σ (I)]	R ₁ = 0.0490, wR ₂ = 0.1265
Final R indexes [all data]	R ₁ = 0.0537, wR ₂ = 0.1296
Largest diff. peak/hole / e Å ⁻³	0.93/-0.69

3r - 6-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-phenyl-11-tosyl-5,6-dihydro-[1,2,4]triazolo[1',2':1,2]pyridazino[3,4-*b*]indole-1,3(2*H*,11*H*)-dione

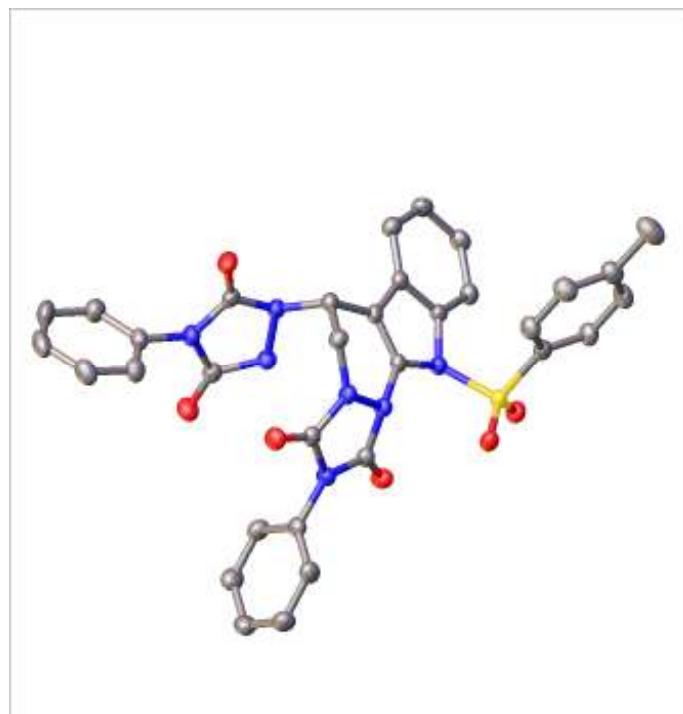


Table 1 Crystal data and structure refinement for mjh140002.

Identification code	mjh140002
Empirical formula	C ₃₃ H ₂₅ N ₇ O ₆ S
Formula weight	647.66
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	13.1236(3)
b/Å	20.8432(5)
c/Å	12.0391(2)
α/°	90
β/°	100.991(2)
γ/°	90
Volume/Å ³	3232.74(13)
Z	4
ρ _{calc} mg/mm ³	1.331
m/mm ⁻¹	1.360
F(000)	1344.0
Crystal size/mm ³	0.25 × 0.1 × 0.06
Radiation	CuKα (λ = 1.54184)
2θ range for data collection	6.862 to 132.494°
Index ranges	-14 ≤ h ≤ 15, -24 ≤ k ≤ 24, -14 ≤ l ≤ 10
Reflections collected	23327
Independent reflections	5646 [R _{int} = 0.0383, R _{sigma} = 0.0297]
Data/restraints/parameters	5646/0/428

Goodness-of-fit on F^2	1.036
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0357, wR_2 = 0.0863$
Final R indexes [all data]	$R_1 = 0.0464, wR_2 = 0.0927$
Largest diff. peak/hole / e Å ⁻³	0.35/-0.36

3u - (3a*S*^{*},5*S*^{*},10b*S*^{*})-5-((2,6-dibromophenyl)(hydroxy)amino)-*N,N*-dimethyl-1,3-dioxo-2-phenyl-1,3,3a,4,5,10b-hexahdropyrrolo[3,4-*a*]carbazole-10(2*H*)-sulfonamide

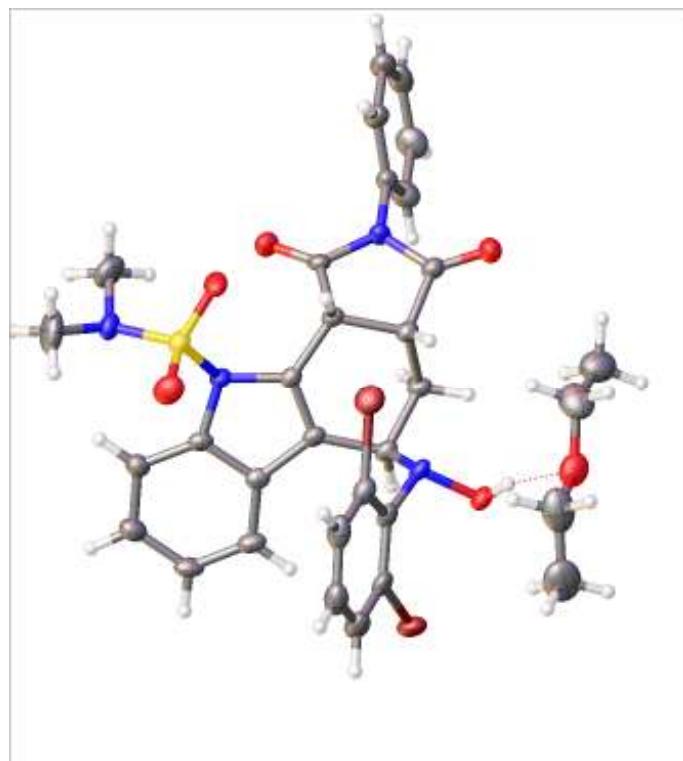


Table 1 Crystal data and structure refinement for mjh69.

Identification code	mjh69
Empirical formula	C ₃₂ H ₃₄ O ₆ SBr ₂ N ₄
Formula weight	762.51
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.0627(11)
b/Å	12.5064(17)
c/Å	13.7858(16)
α/°	87.321(10)
β/°	78.605(10)
γ/°	70.030(11)
Volume/Å ³	1598.0(4)
Z	2
ρ _{calc} g/cm ³	1.585
μ/mm ⁻¹	2.653
F(000)	776.0
Crystal size/mm ³	0.7113 × 0.156 × 0.1482
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.788 to 53.596
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 9, -17 ≤ l ≤ 15
Reflections collected	10012

Independent reflections	6056 [R _{int} = 0.0263, R _{sigma} = 0.0504]
Data/restraints/parameters	6056/366/414
Goodness-of-fit on F ²	1.037
Final R indexes [I>=2σ (I)]	R ₁ = 0.0604, wR ₂ = 0.1457
Final R indexes [all data]	R ₁ = 0.0755, wR ₂ = 0.1595
Largest diff. peak/hole / e Å ⁻³	3.75/-0.92

3v - (3aS*,5S*,10bS*)-5-((S*)-hydroxy(perfluorophenyl)methyl)-N,N-dimethyl-1,3-dioxo-1,3,3a,4,5,10b-hexahdropyrrolo[3,4-a]carbazole-10(2H)-sulfonamide

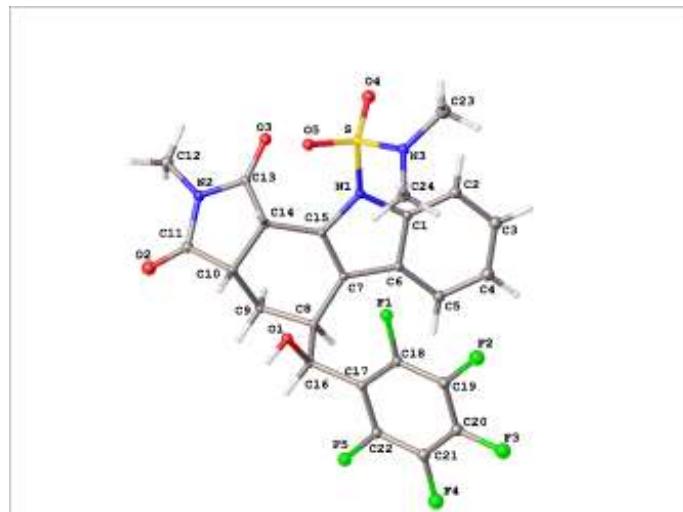


Table 1 Crystal data and structure refinement for mjh120042.

Identification code	mjh120042
Empirical formula	C ₂₄ H ₂₀ N ₃ O ₅ F ₅ S
Formula weight	557.49
Temperature/K	150.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	7.9070(4)
b/Å	14.2862(7)
c/Å	20.6839(10)
α/°	90
β/°	101.016(5)
γ/°	90
Volume/Å ³	2293.4(2)
Z	4
ρ _{calc} g/cm ³	1.615
μ/mm ⁻¹	0.227
F(000)	1144.0
Crystal size/mm ³	0.15 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.704 to 57.17
Index ranges	-10 ≤ h ≤ 10, -18 ≤ k ≤ 18, -26 ≤ l ≤ 24
Reflections collected	23890
Independent reflections	5125 [R _{int} = 0.0596, R _{sigma} = 0.0600]
Data/restraints/parameters	5125/0/350
Goodness-of-fit on F ²	1.027
Final R indexes [I>=2σ (I)]	R ₁ = 0.0492, wR ₂ = 0.0954
Final R indexes [all data]	R ₁ = 0.0864, wR ₂ = 0.1108
Largest diff. peak/hole / e Å ⁻³	0.34/-0.37