Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Application of Nazarov cyclization to access [6-5-6]and[6-5-5]tricyclic core embedded New Heterocycles : An easy entry to structures related to Taiwaniaquinoids

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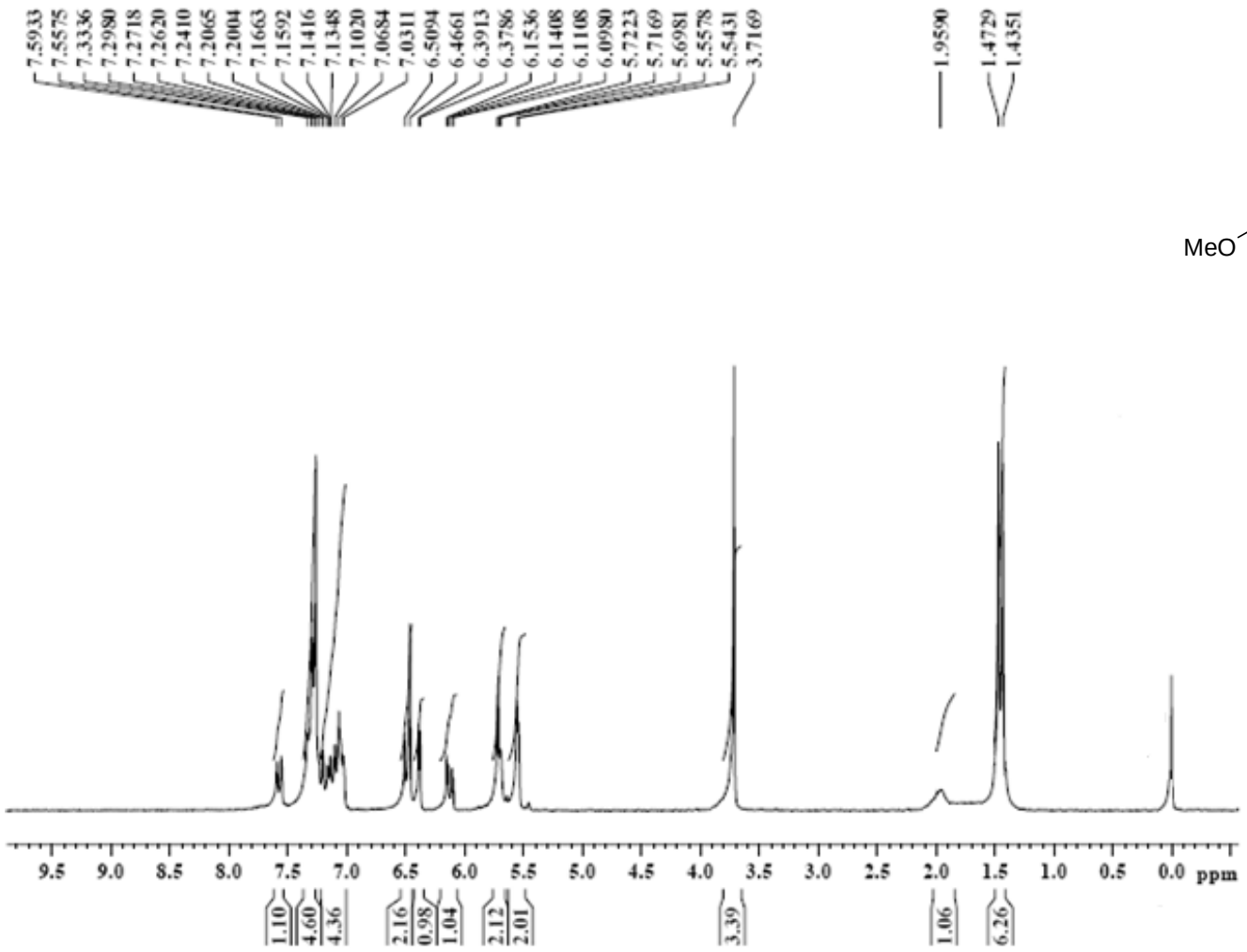


Fig. S-2: ^{1}H NMR of (1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanol (13b)

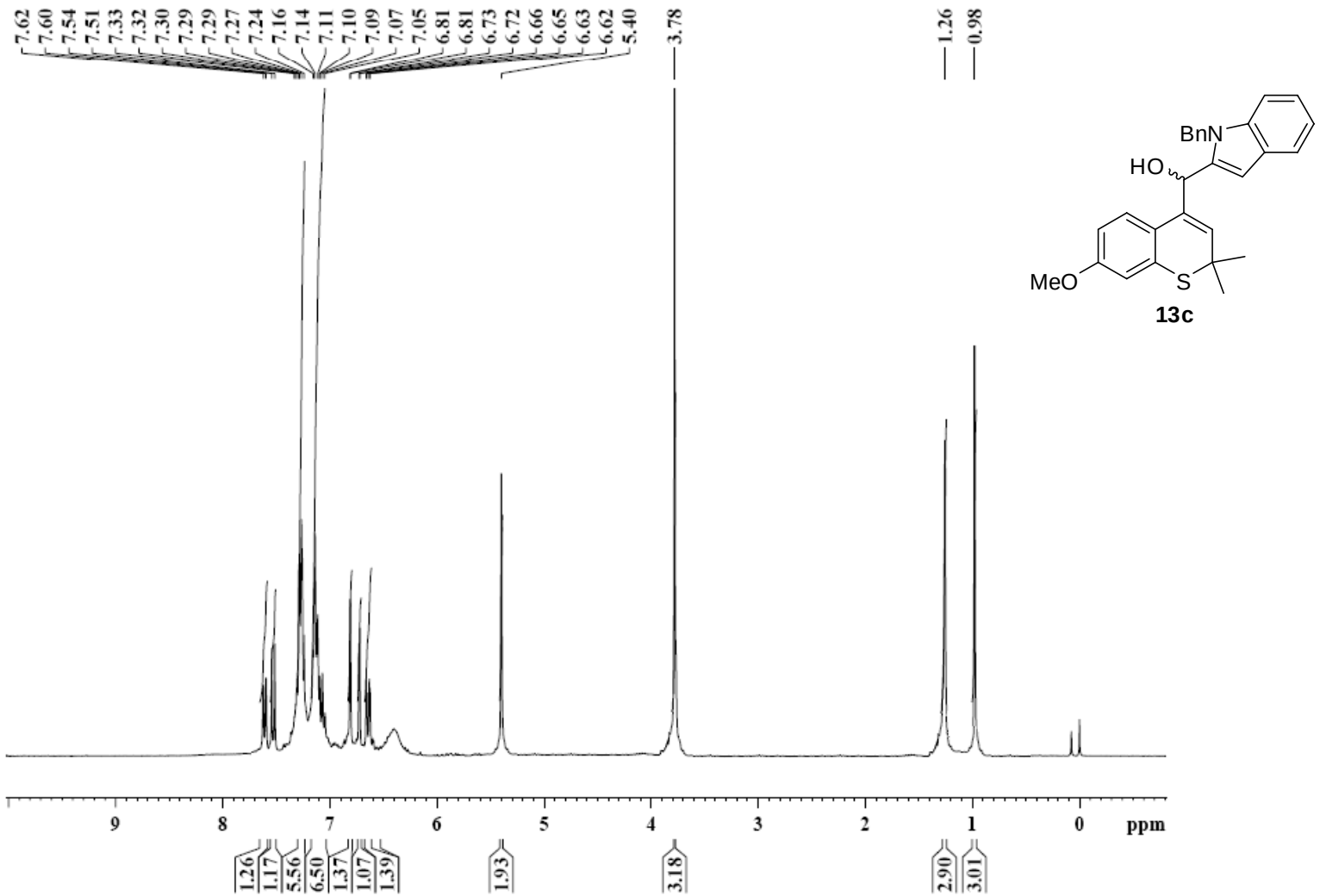


Fig. S-3: ^{1}H NMR of (1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanol (13c)

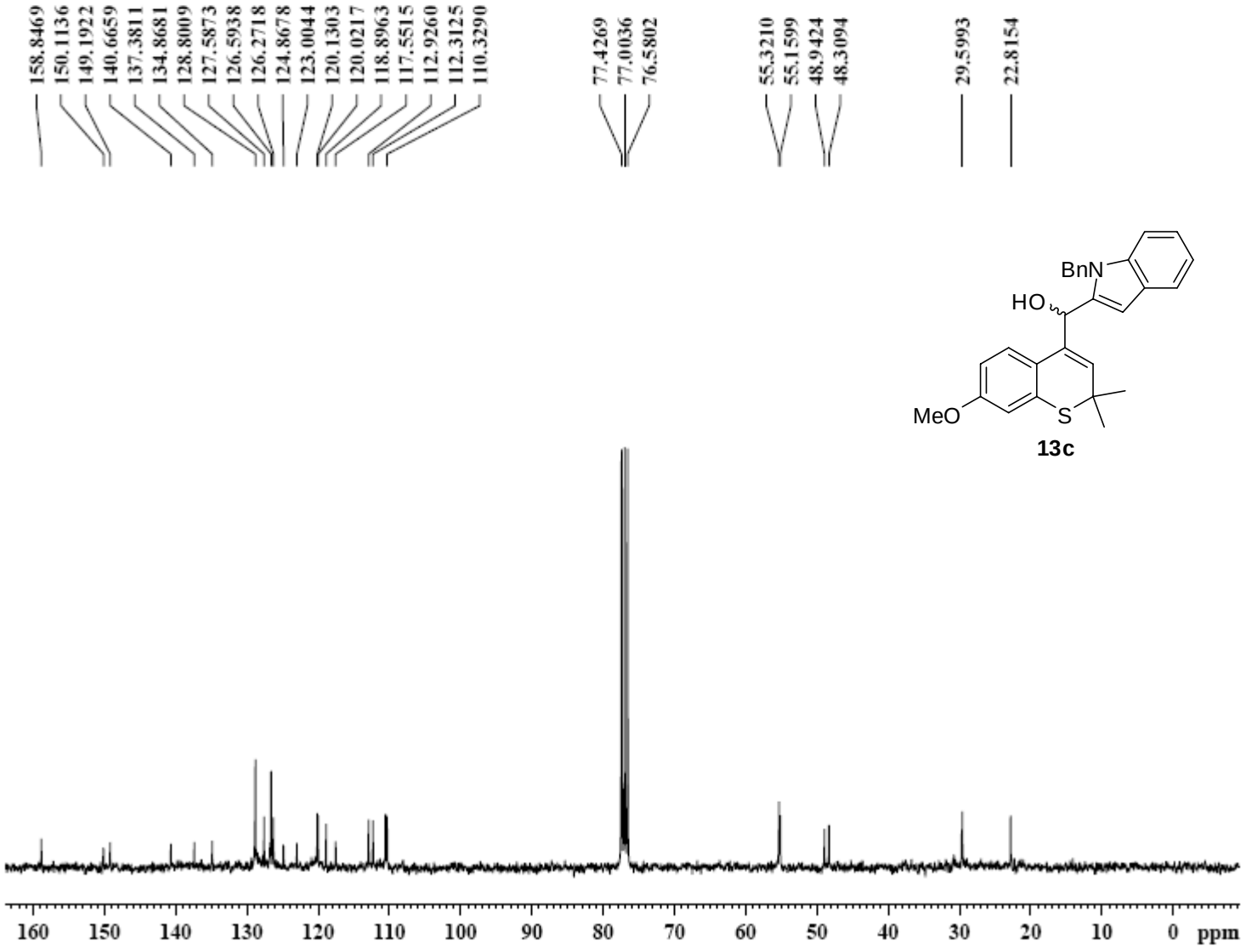


Fig. S-4: : ^{13}C NMR of (1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanol (13c)

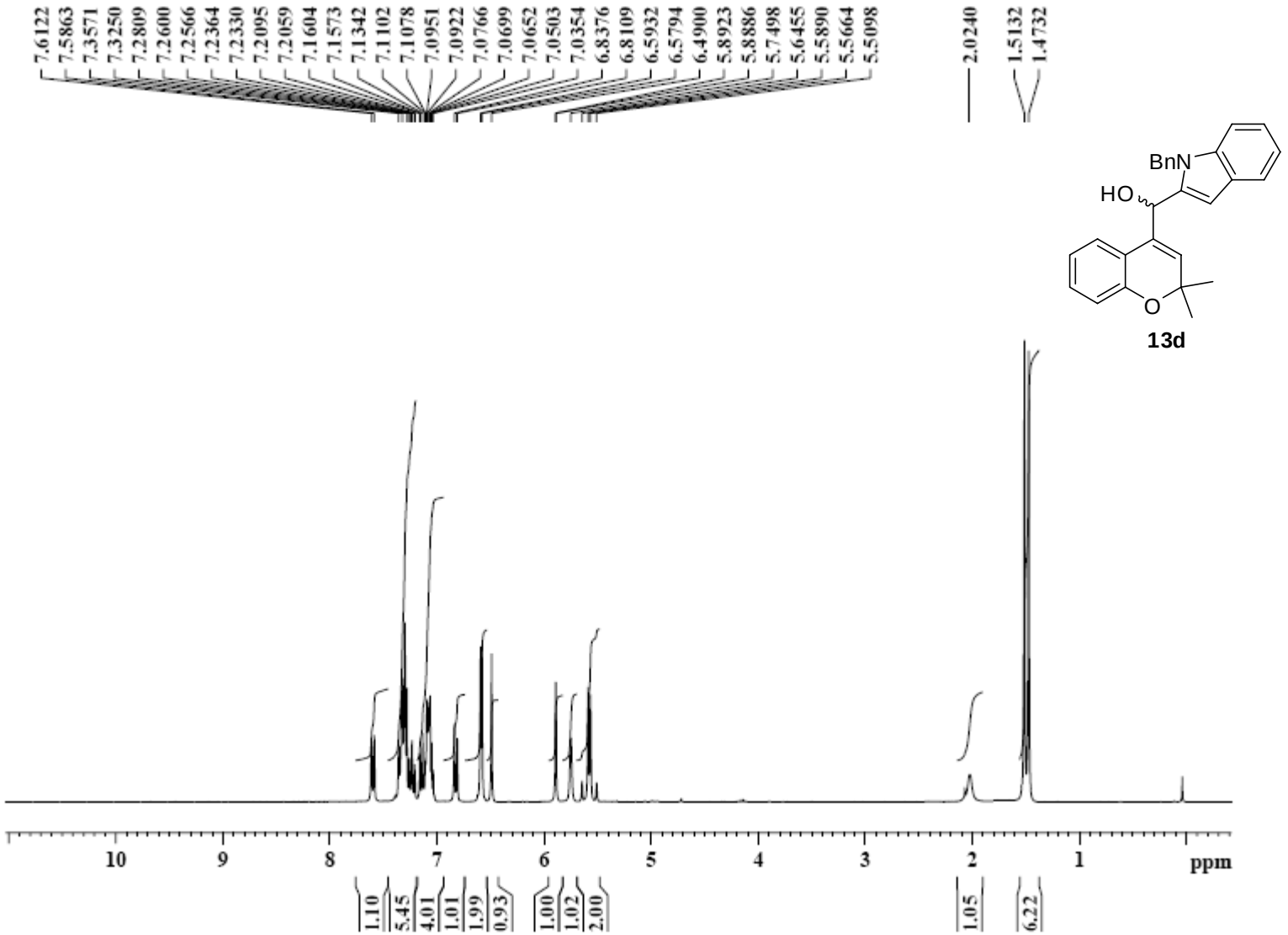


Fig. S-5: ^{1}H NMR of (1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-chromen-4-yl)methanol (13d)

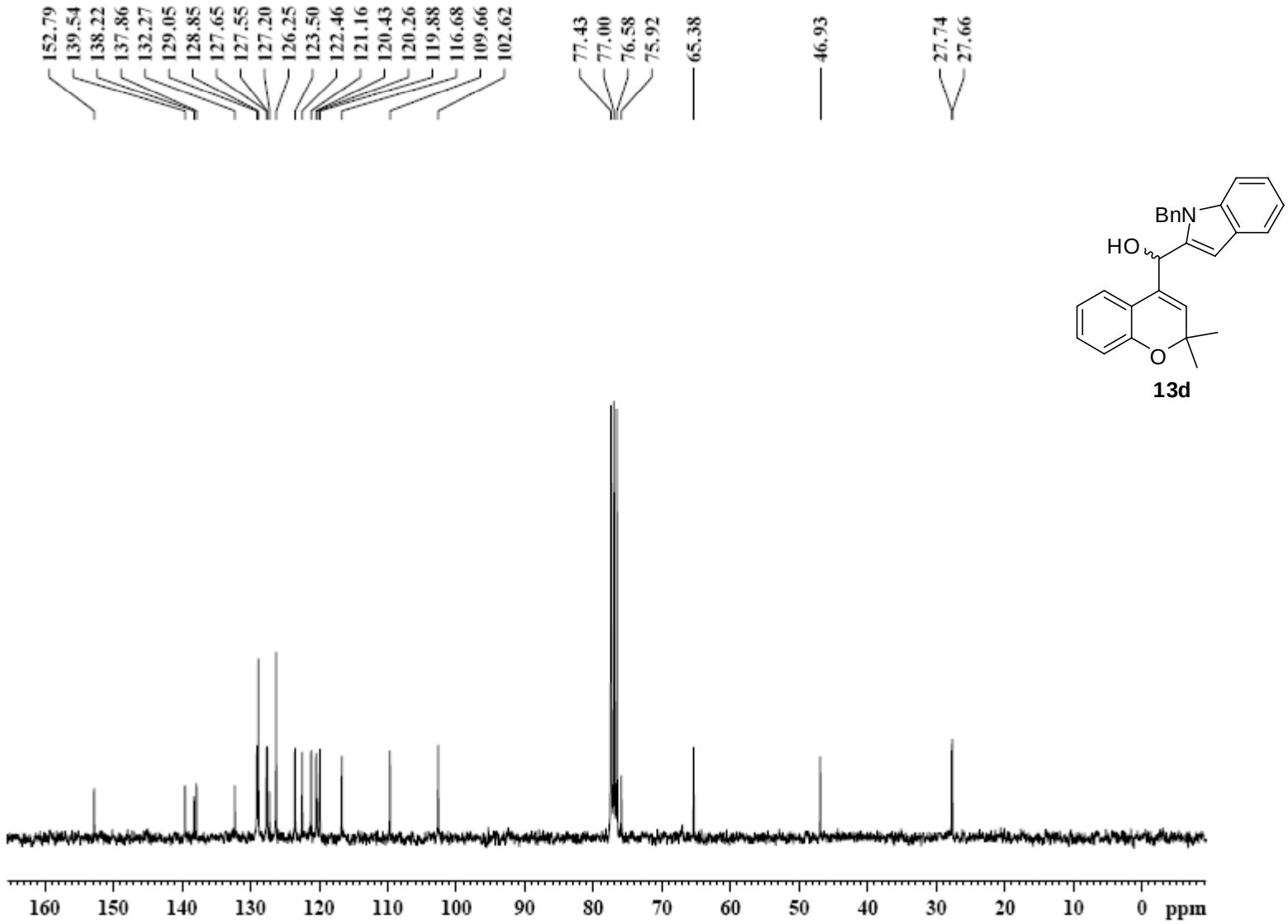


Fig. S-6: : ^{13}C NMR of (1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-chromen-4-yl)methanol (13d)

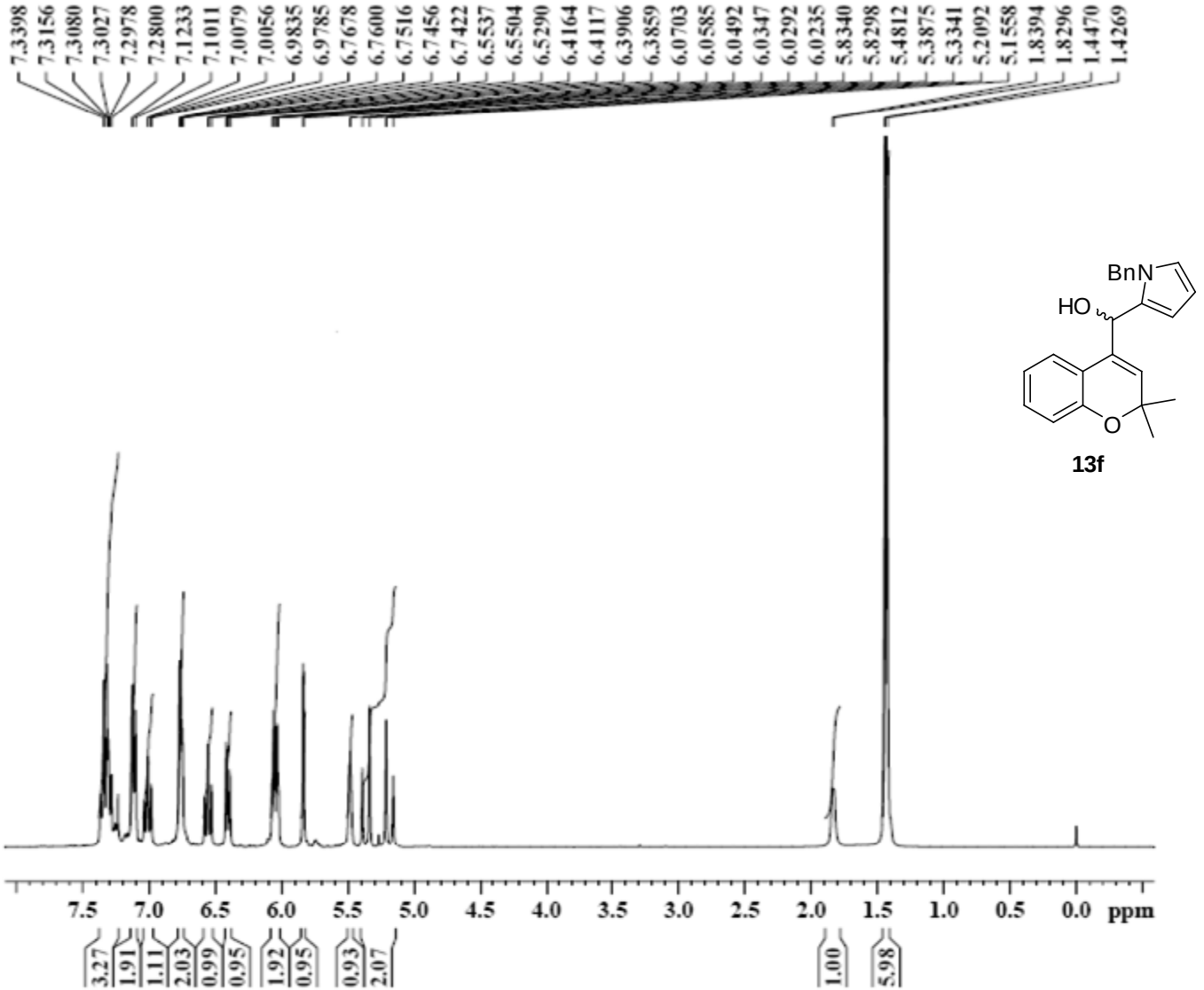


Fig. S-7: ^{1}H NMR of (1-Benzyl-1H-pyrrol-2-yl)(2,2-dimethyl-2H-chromen-4-yl)methanol (13f)

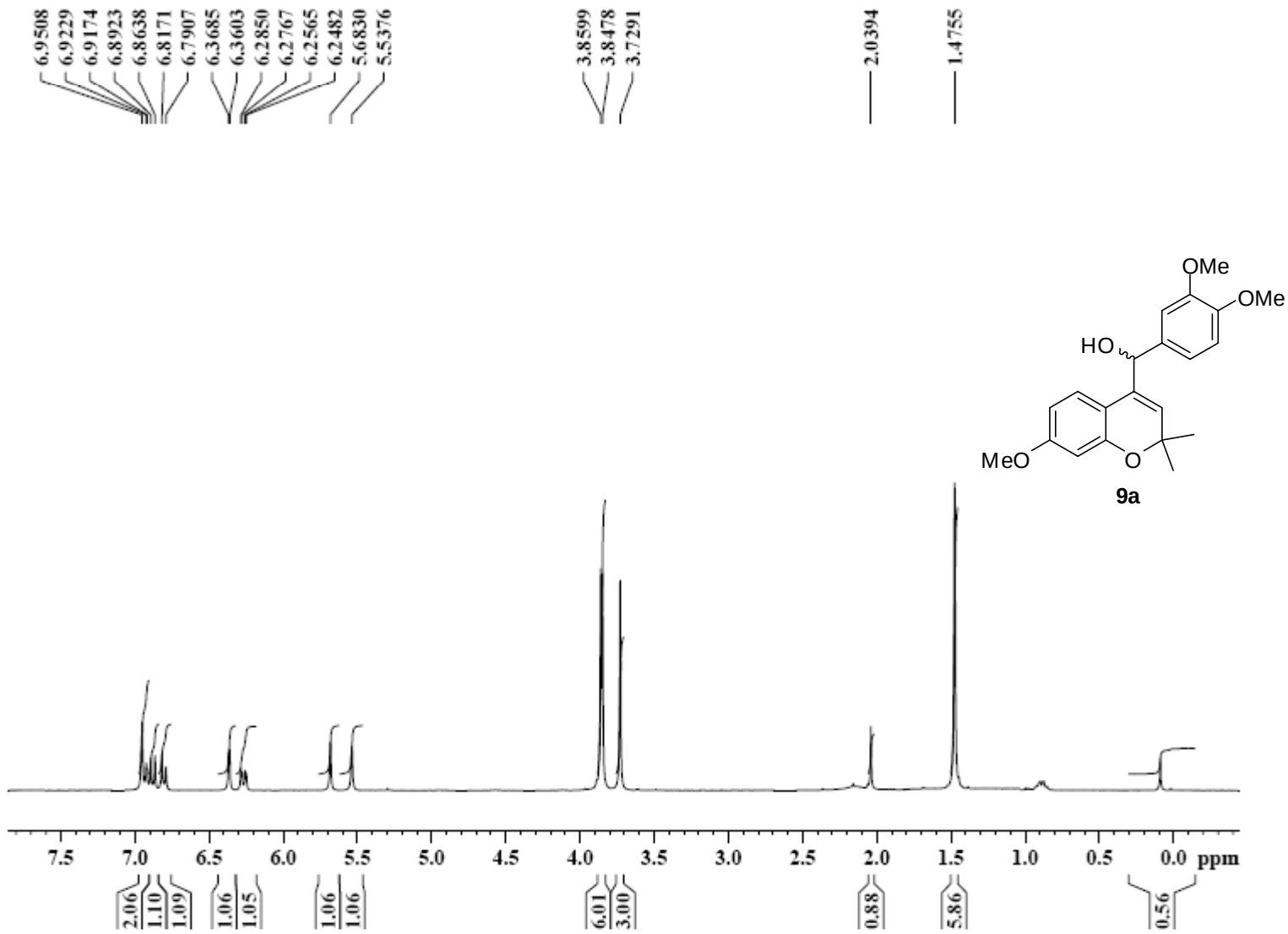


Fig. S-8: ^{1}H NMR of (3,4-Dimethoxyphenyl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanol (9a)

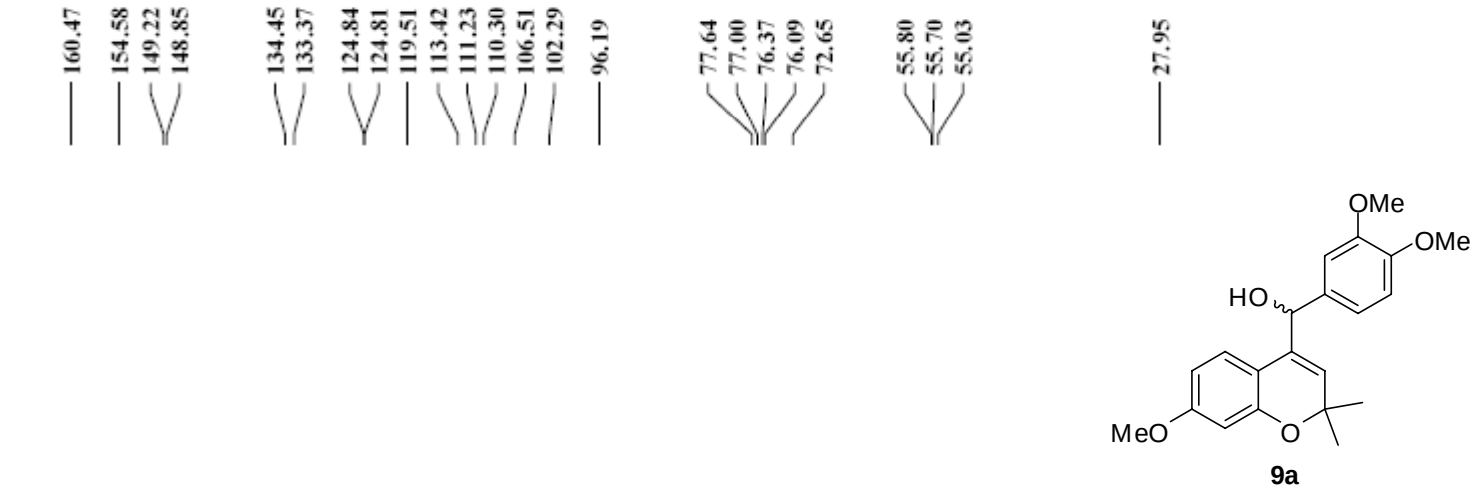


Fig. S-9: ^{13}C NMR of (3,4-Dimethoxyphenyl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanol (9a)

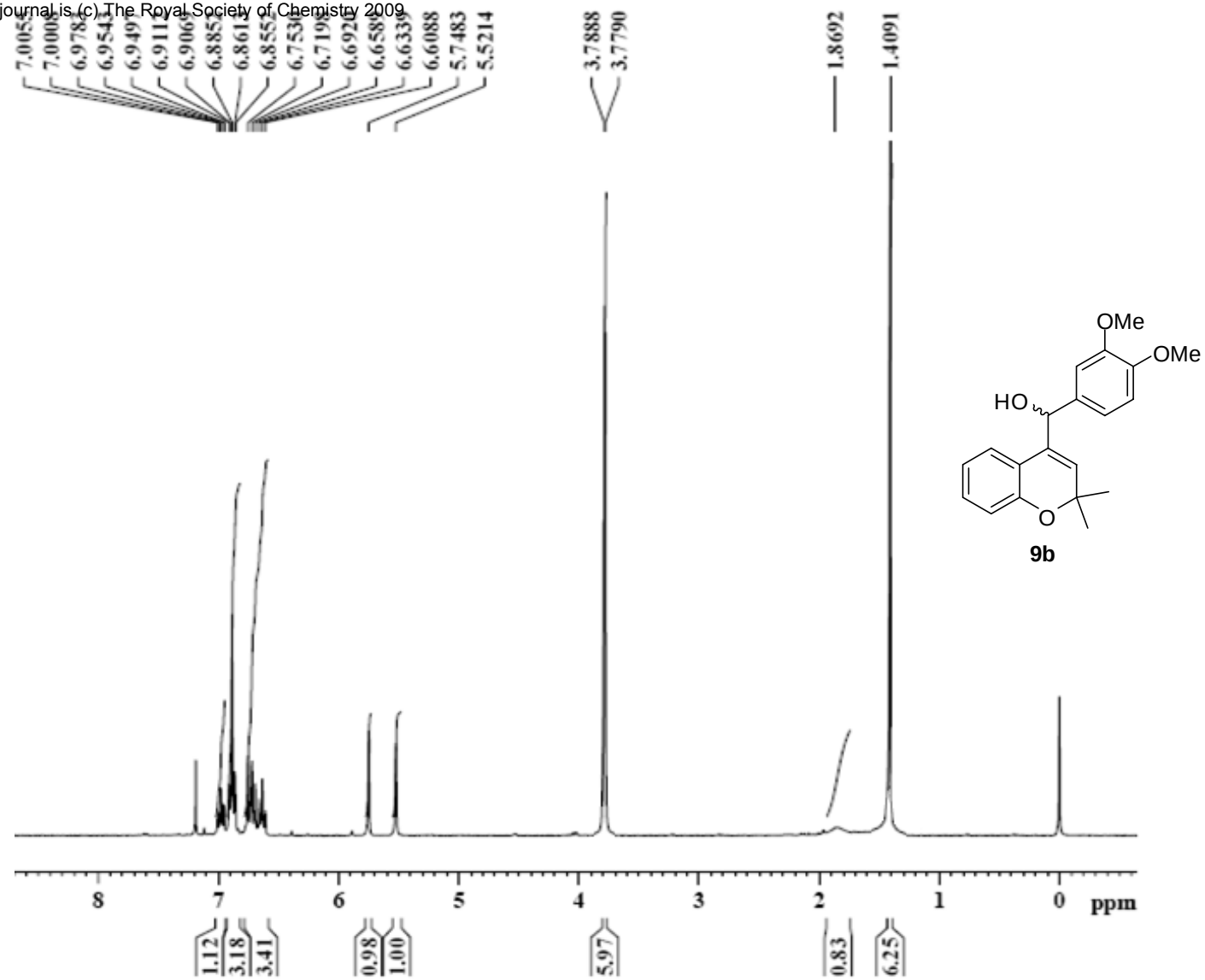


Fig. S-10: ^{1}H NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-chromen-4-yl)methanol (9b)

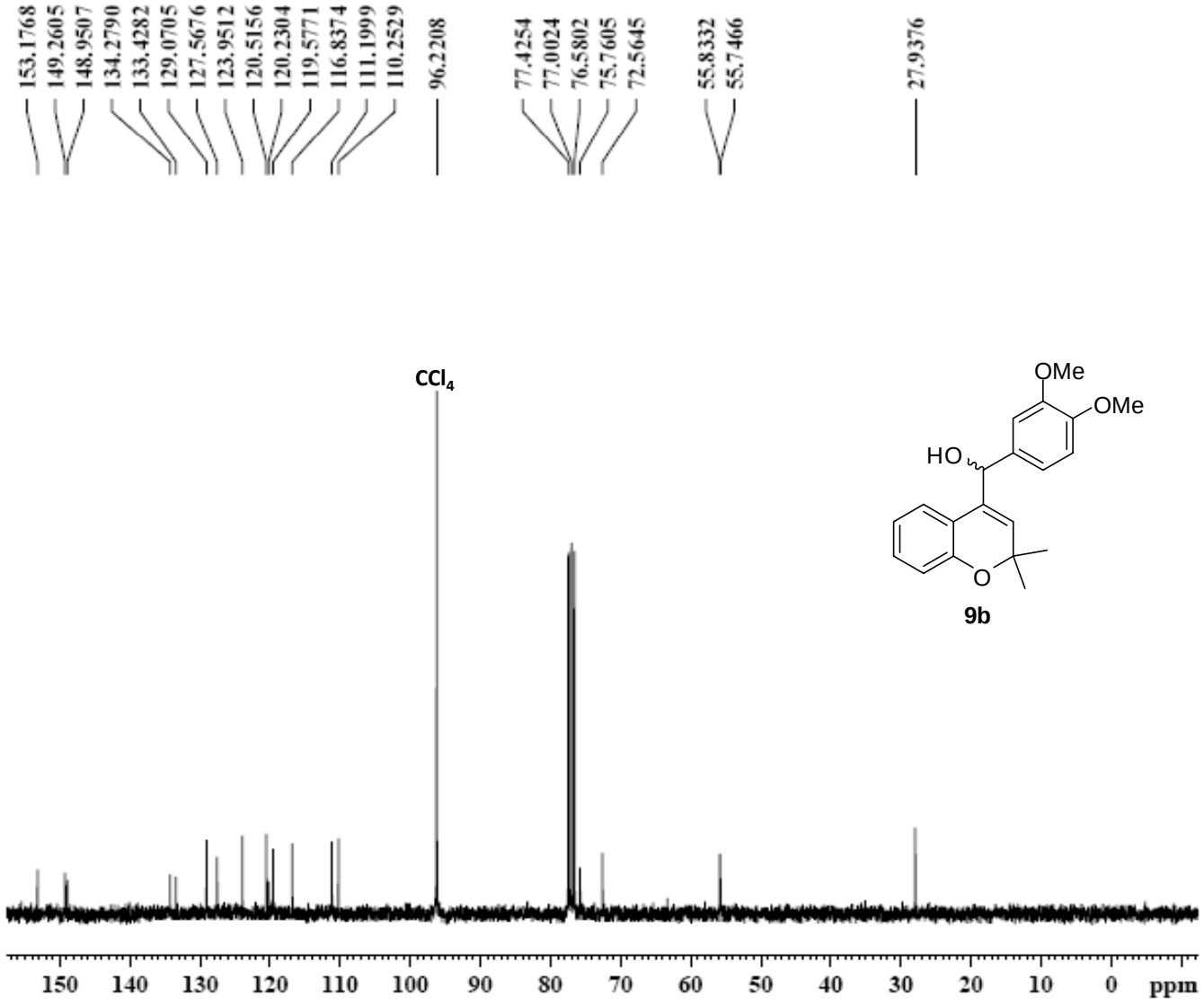


Fig. S-11: ^{13}C NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-chromen-4-yl)methanol (9b)

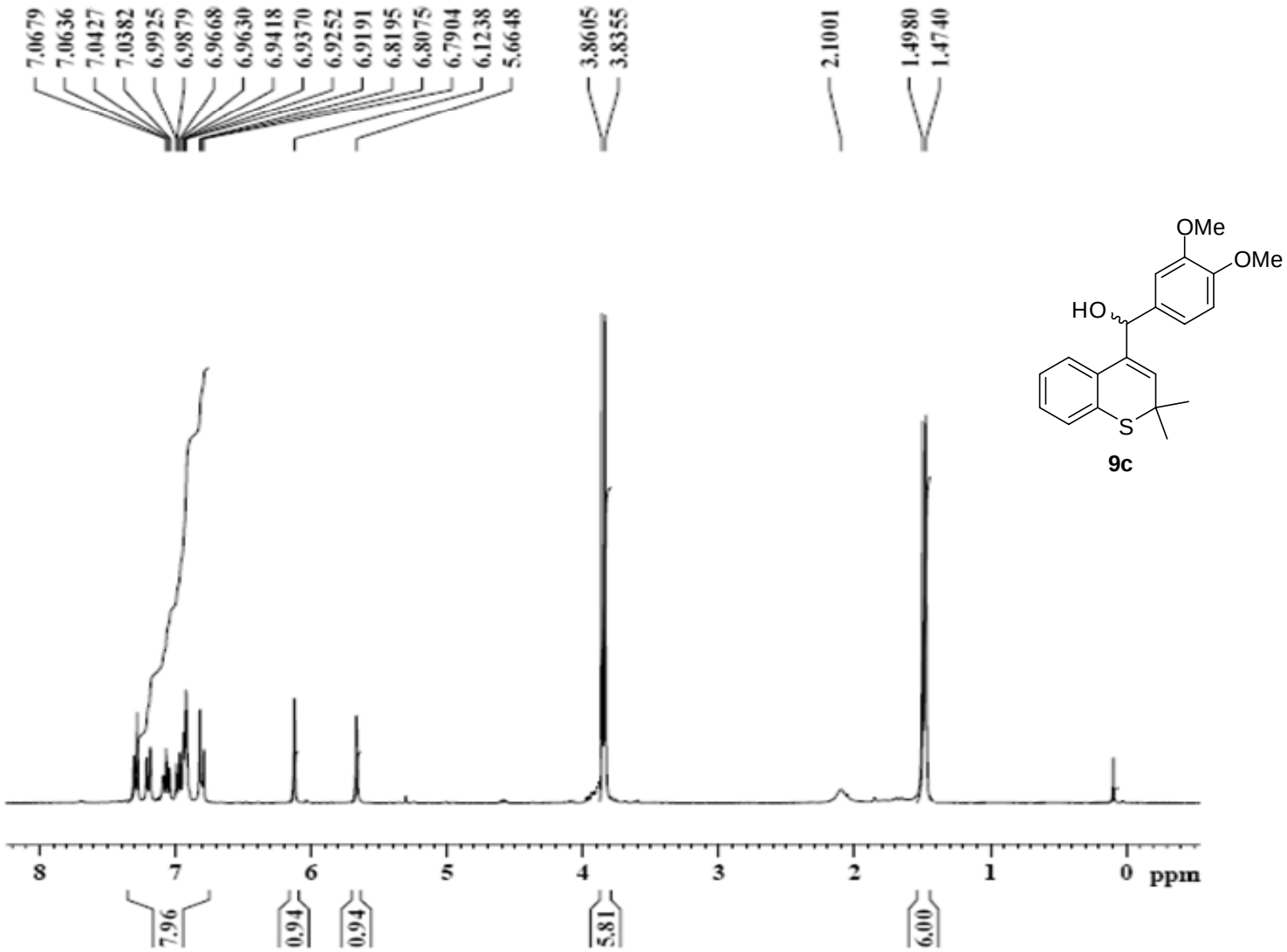
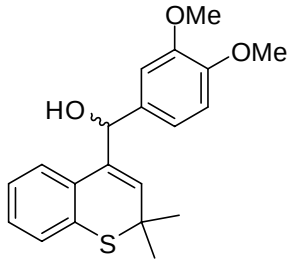


Fig. S-12: ^{1}H NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-thiochromen-4-yl)methanol (9c)



9c

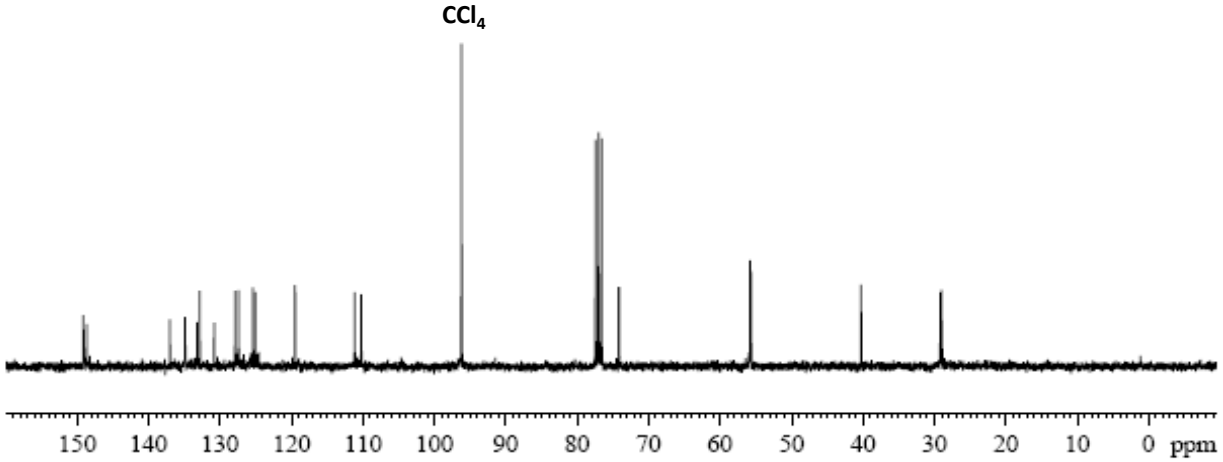


Fig. S-13: ^{13}C NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-thiochromen-4-yl)methanol (9c)

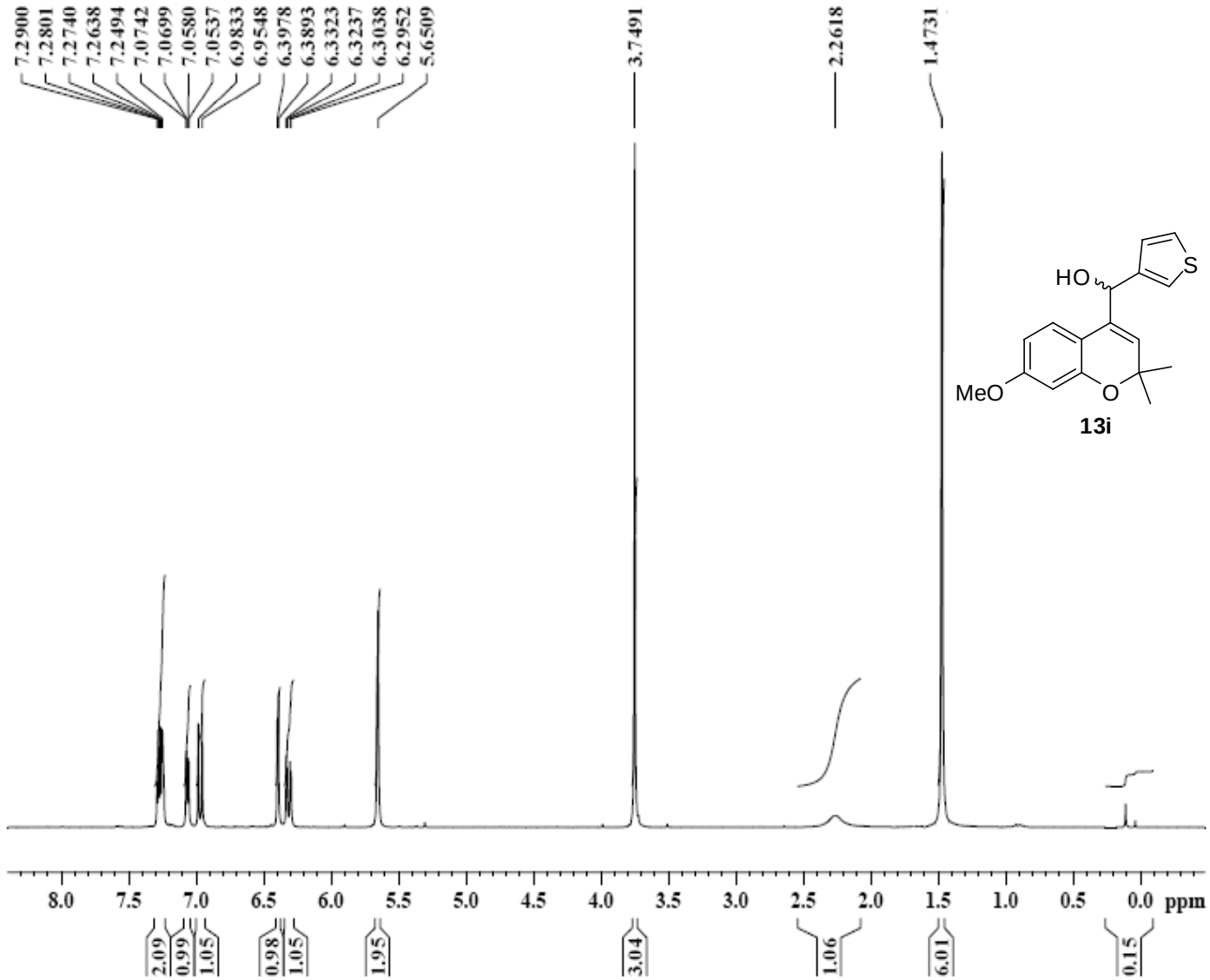


Fig. S-14: ^{1}H NMR of (Thiophen-3-yl-(2,2,7-trimethyl-2H-chromen-4-yl)methanol (13i)

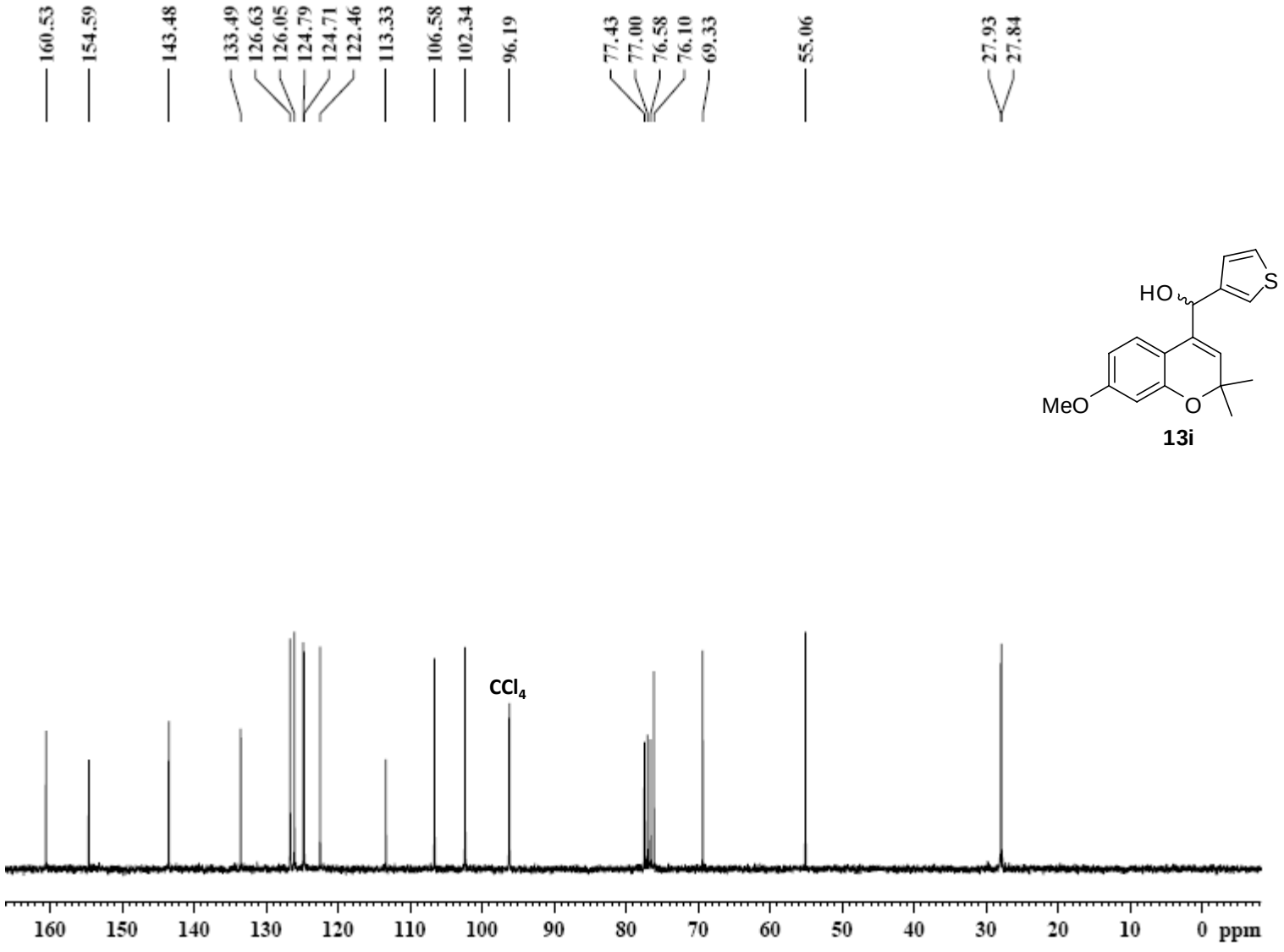


Fig. S-15: ^{13}C NMR of (Thiophen-3-yl-(2,2,7-trimethyl-2H-chromen-4-yl)methanol (13i)

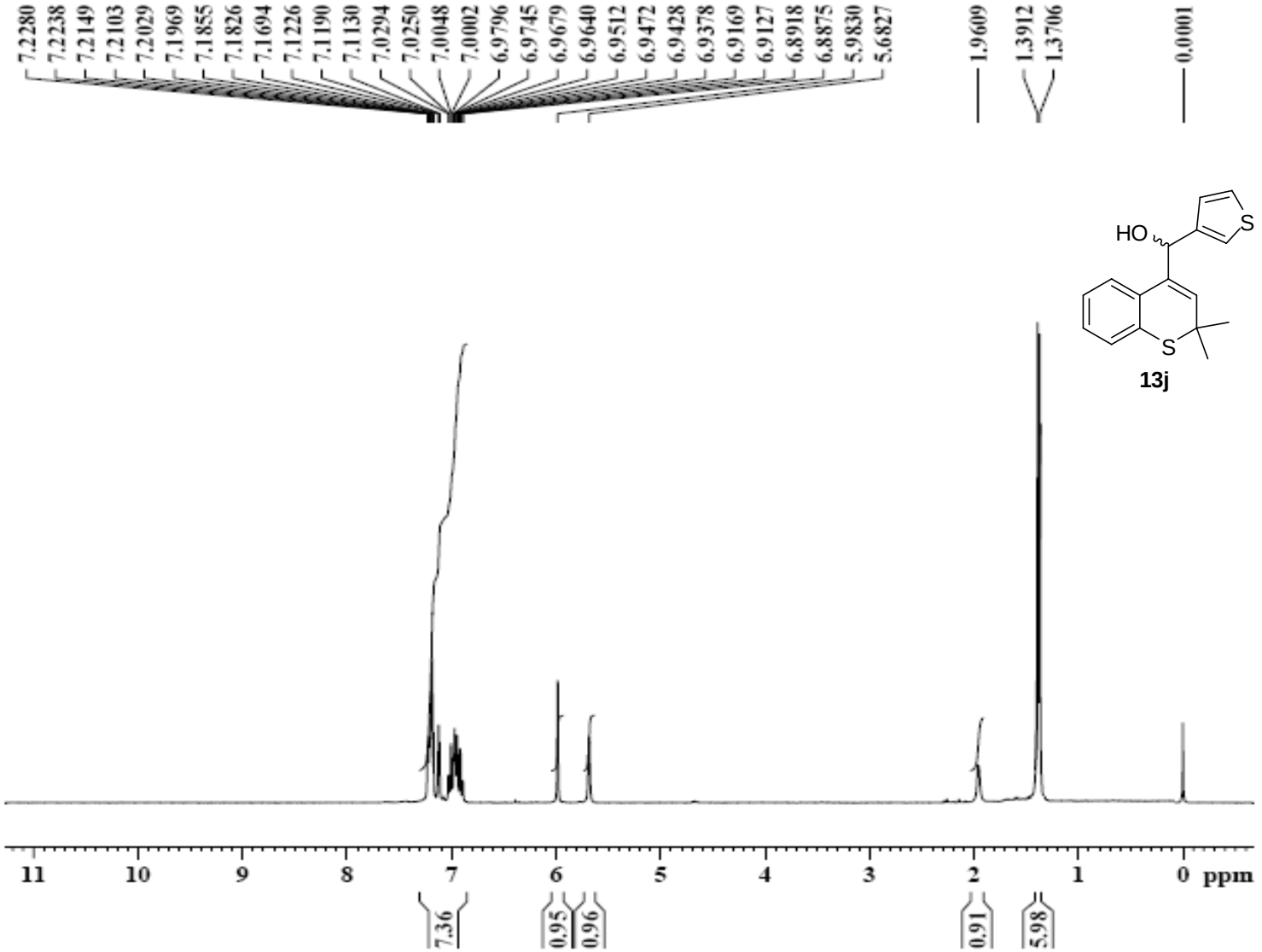


Fig. S-16: ^{1}H NMR of (2,2-Dimethyl-2H-thiochromen-4-yl)thiophen-3-ylmethanol (13j)

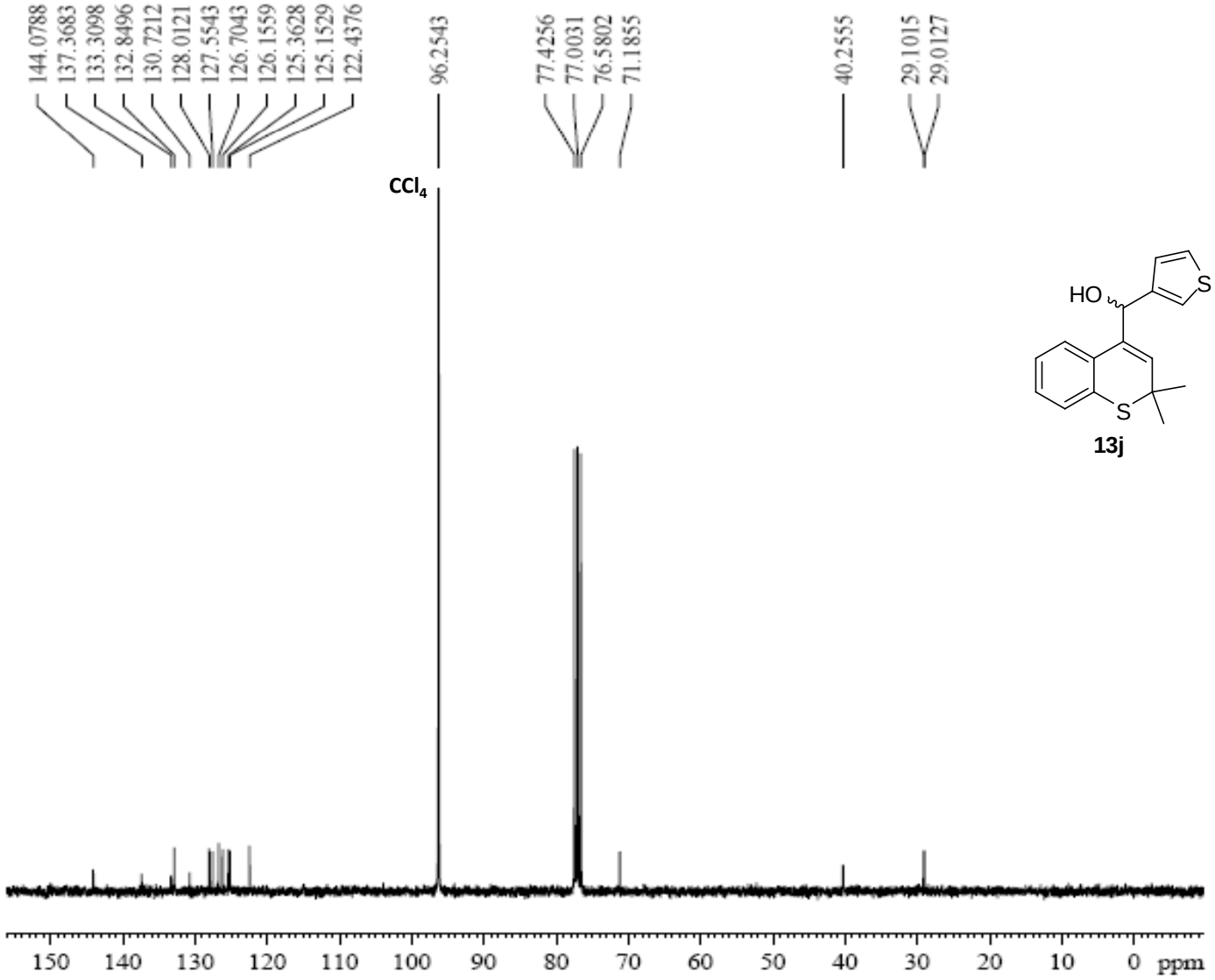


Fig. S-17: ^{13}C NMR of (2,2-Dimethyl-2H-thiochromen-4-yl)thiophen-3-ylmethanol (13j)

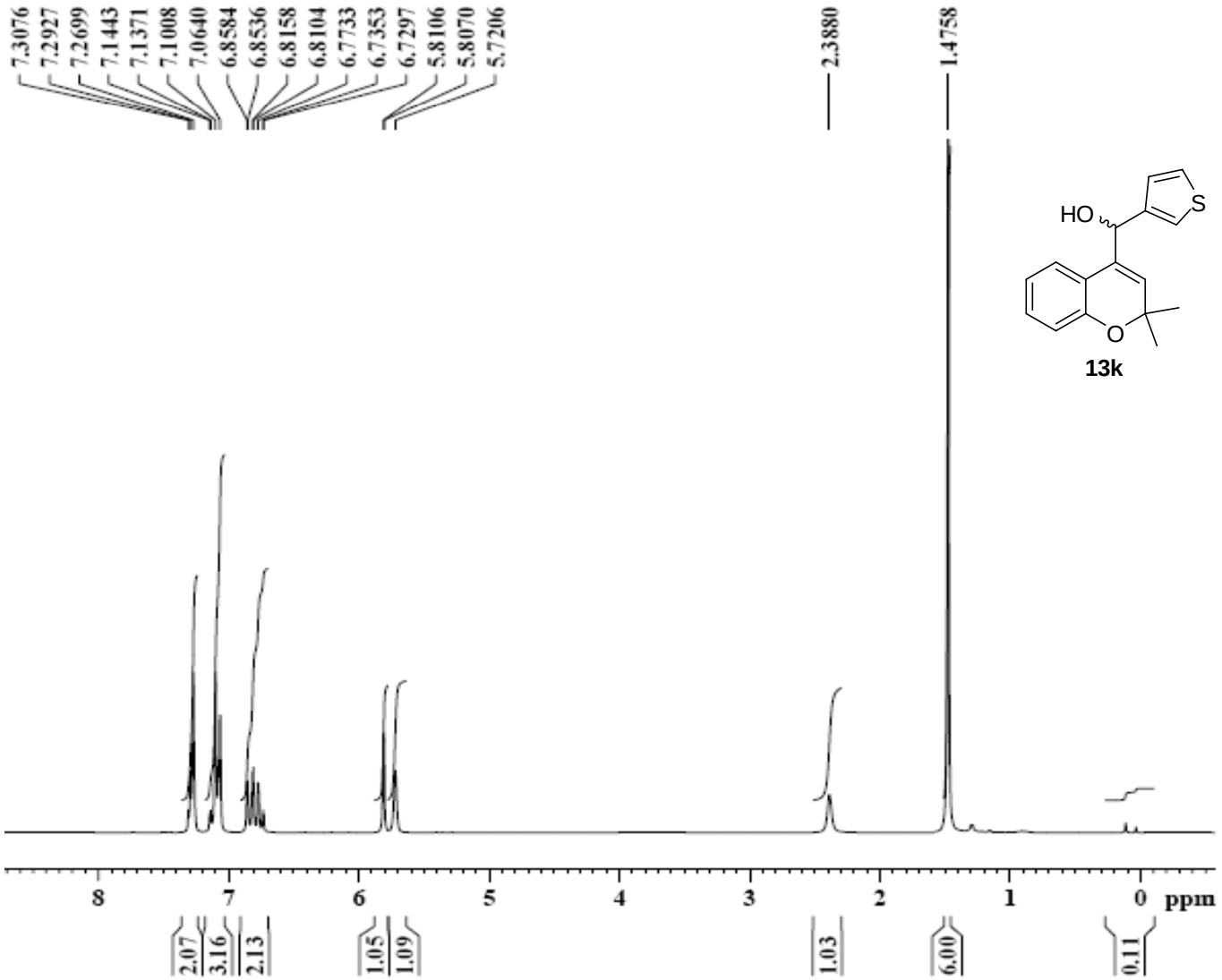


Fig. S-18: ^{1}H NMR of (2,2-Dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanol (13k)

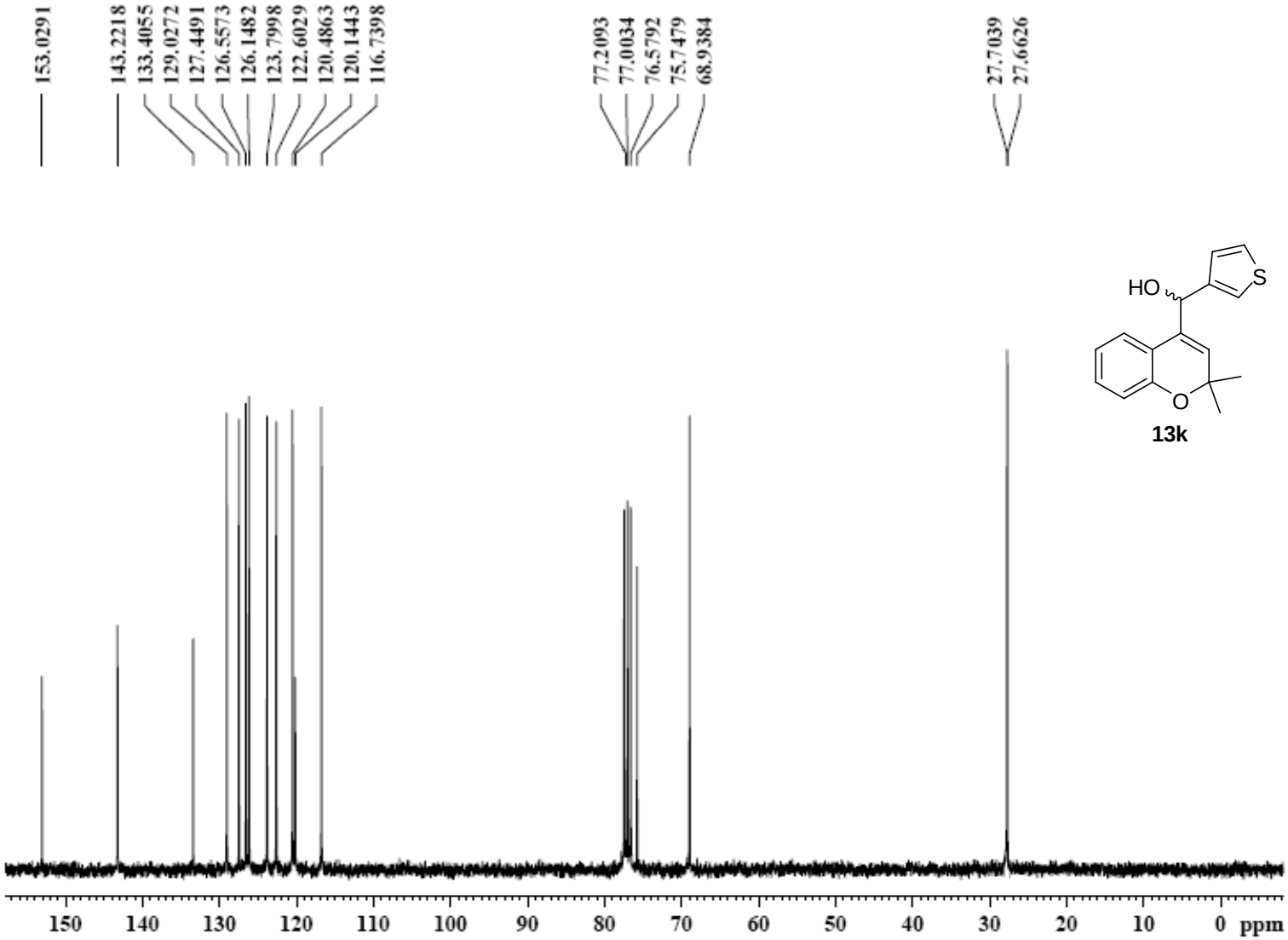


Fig. S-19: ^{13}C NMR of (2,2-Dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanol (13k)

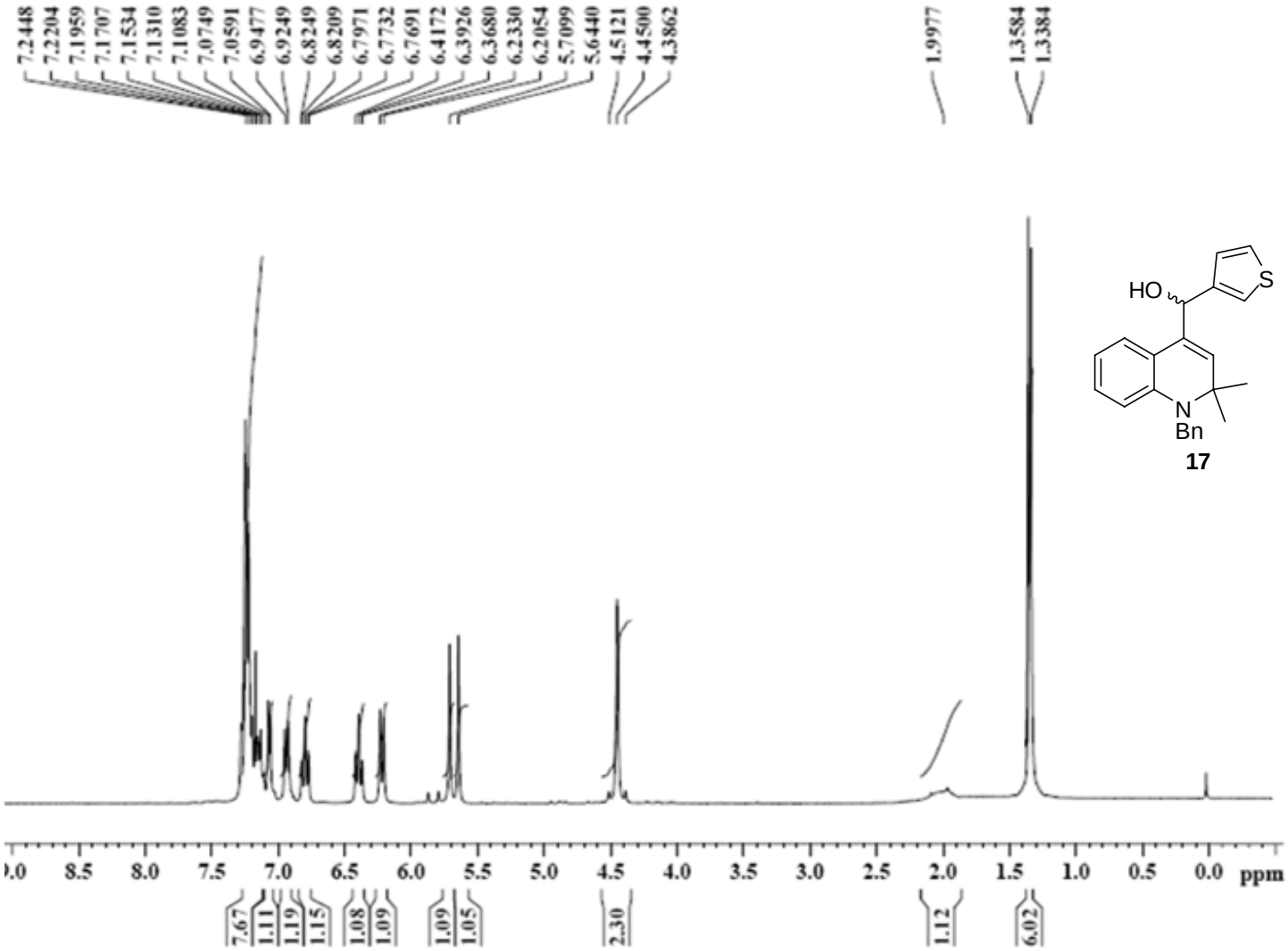


Fig. S-20: ^{1}H NMR of (1-Benzyl-2,2-dimethyl-1,2-dihydroquinolin-4-yl)thiophen-3-ylmethanol (17)

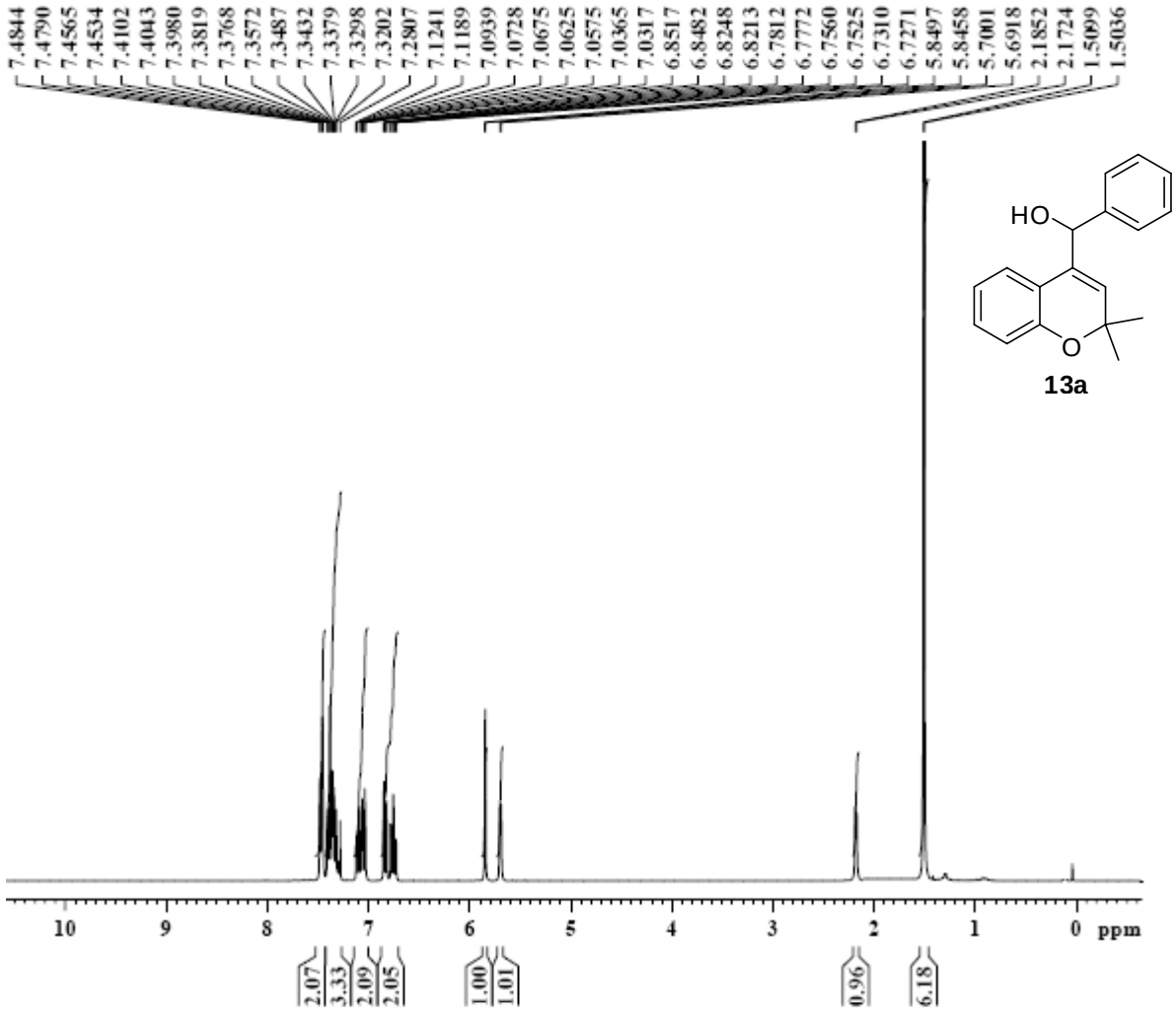


Fig. S-21: ^{1}H NMR of (2,2-dimethyl-2H-chromen-4-yl)(phenyl)methanol(13a)

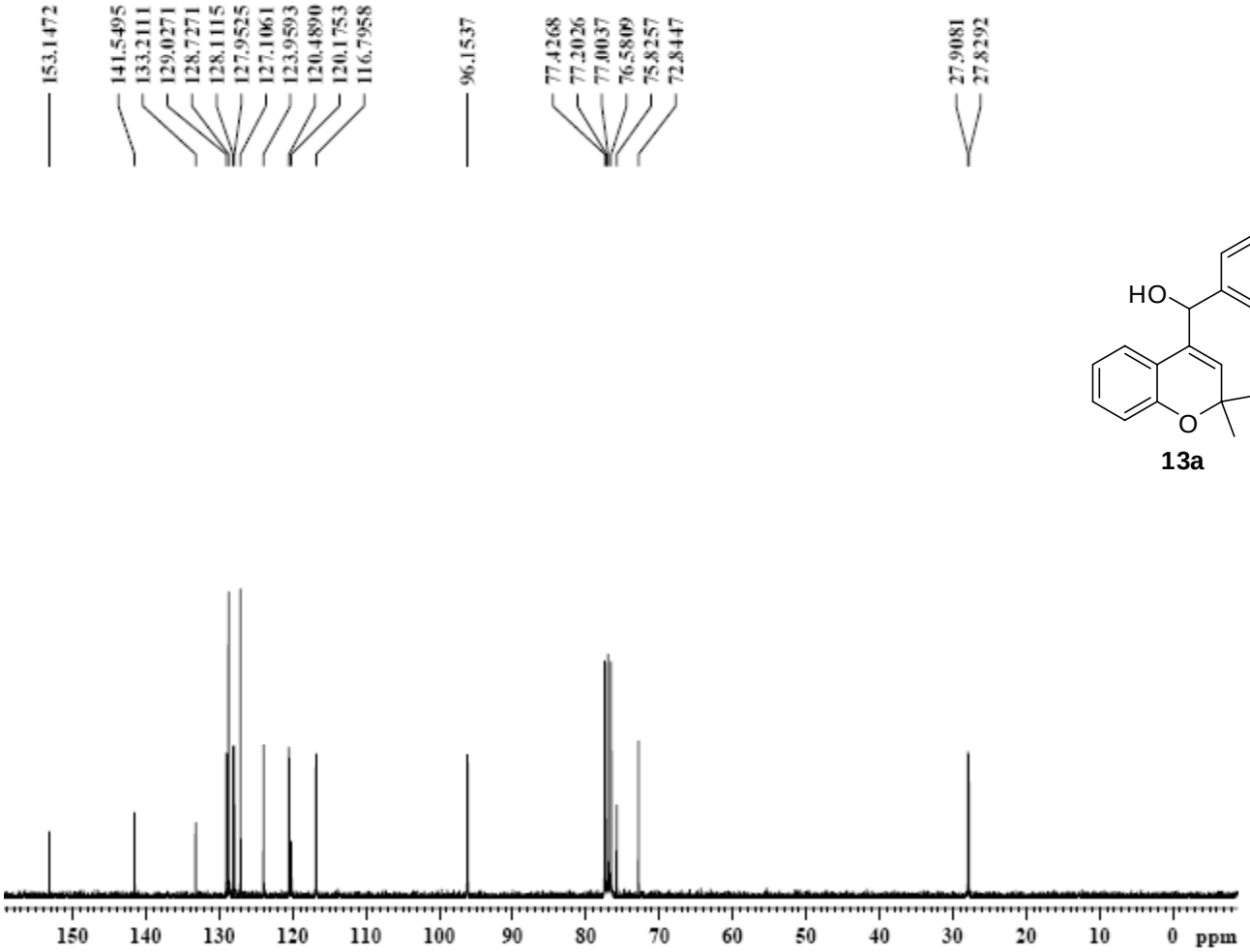


Fig. S-22: ^{1}H NMR of (2,2-dimethyl-2H-chromen-4-yl)(phenyl)methanol(13a)

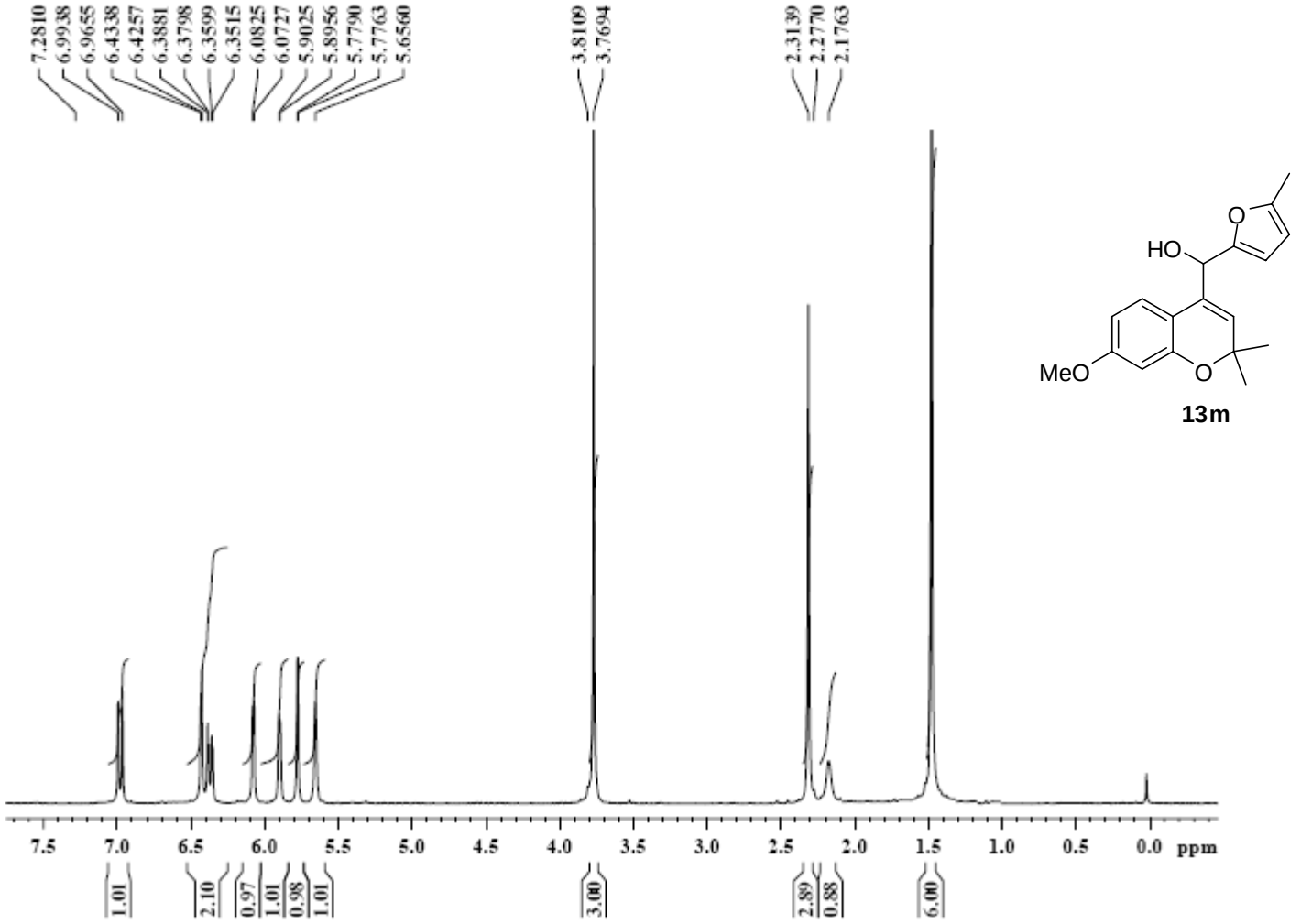


Fig. S-23: ^{1}H NMR of (7-methoxy-2,2-dimethyl-2H-chromen-4-yl)(5-methylfuran-2-yl)methanol (13m)

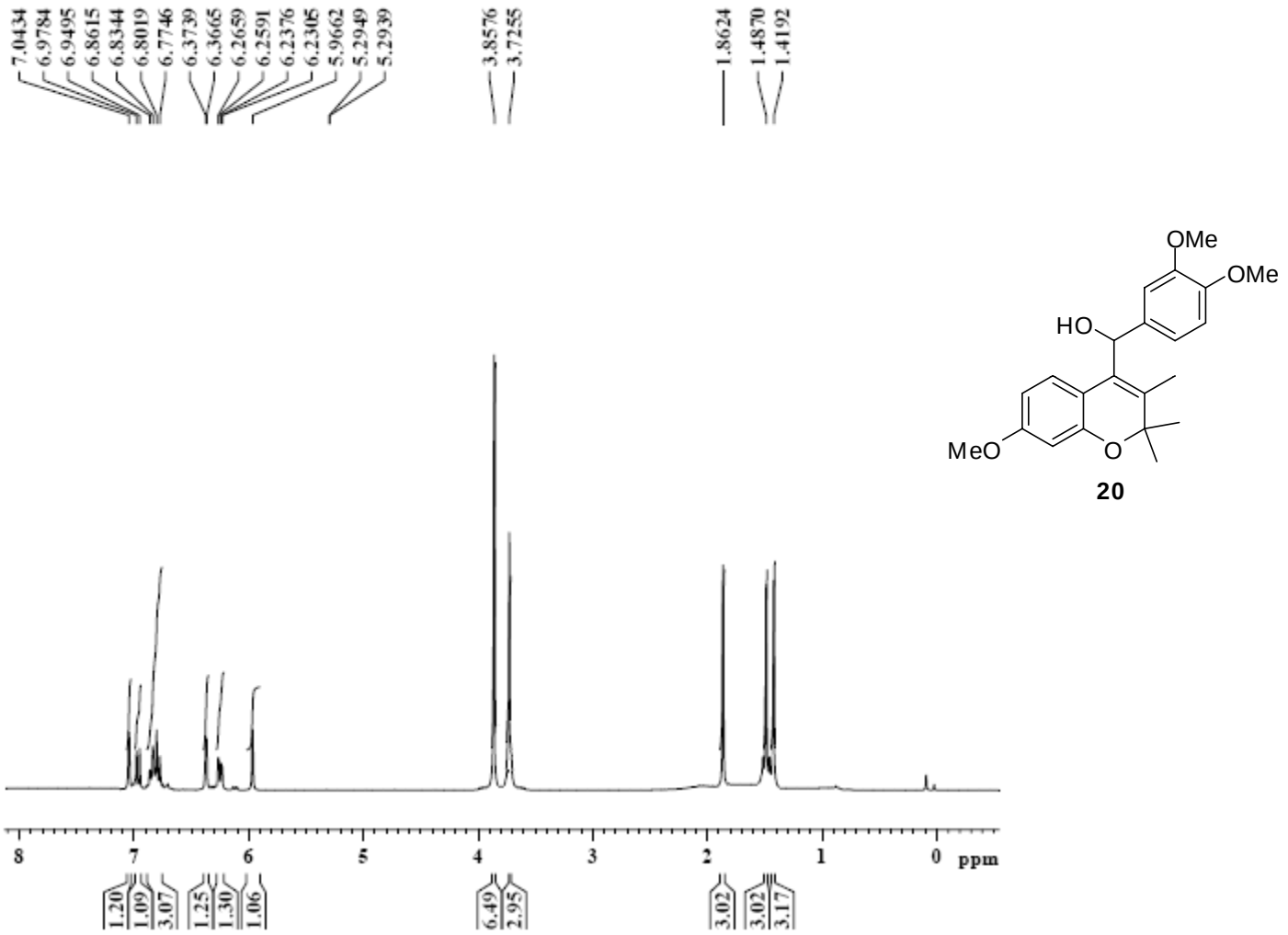


Fig. S-24: ^{1}H NMR of (3,4-dimethoxyphenyl)(7-methoxy-2,2,3-trimethyl-2H-chromen-4-yl)methanol (20)

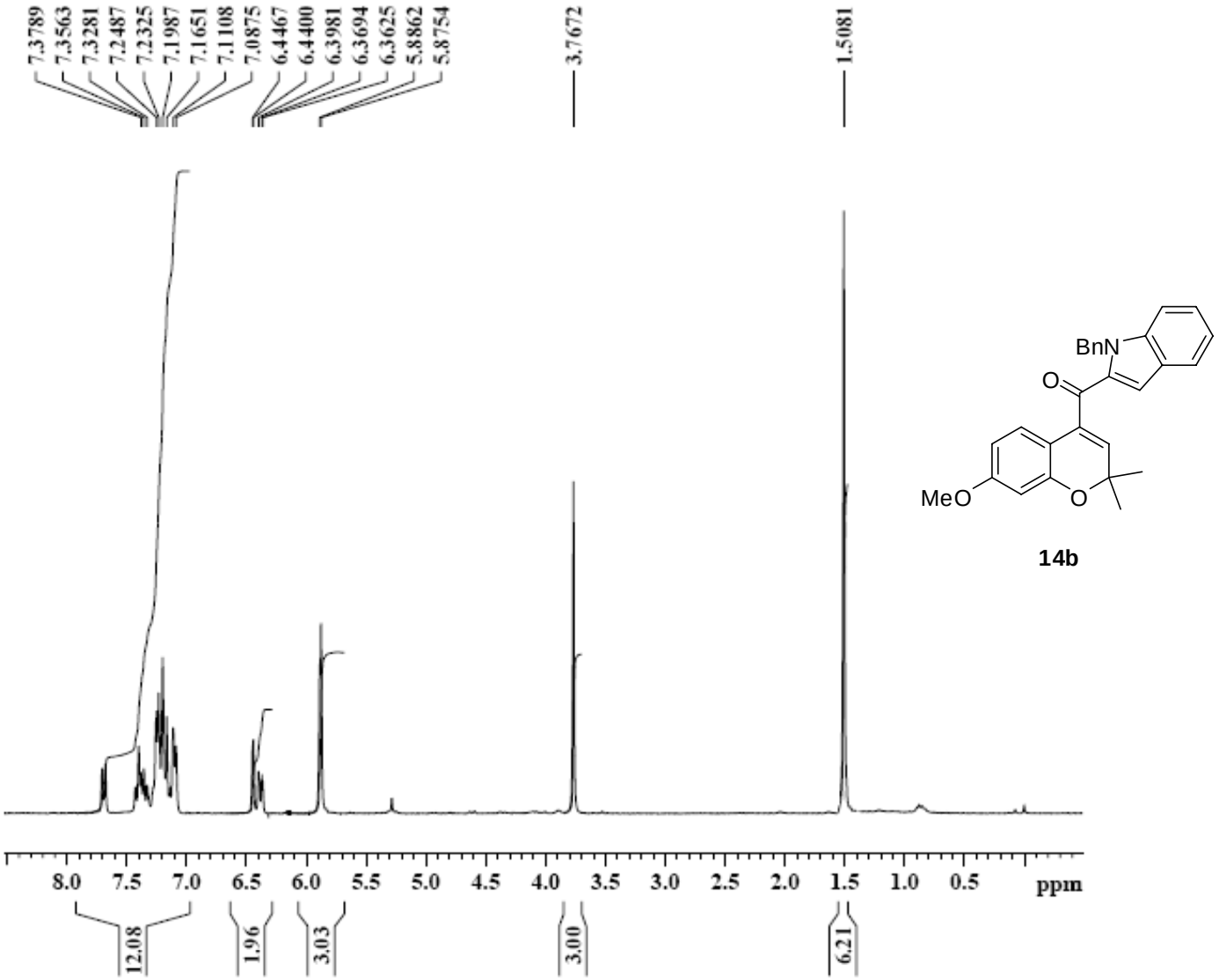


Fig. S-25: ^{1}H NMR of 2H-Chromen(1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl--4-yl) methanone (14b)

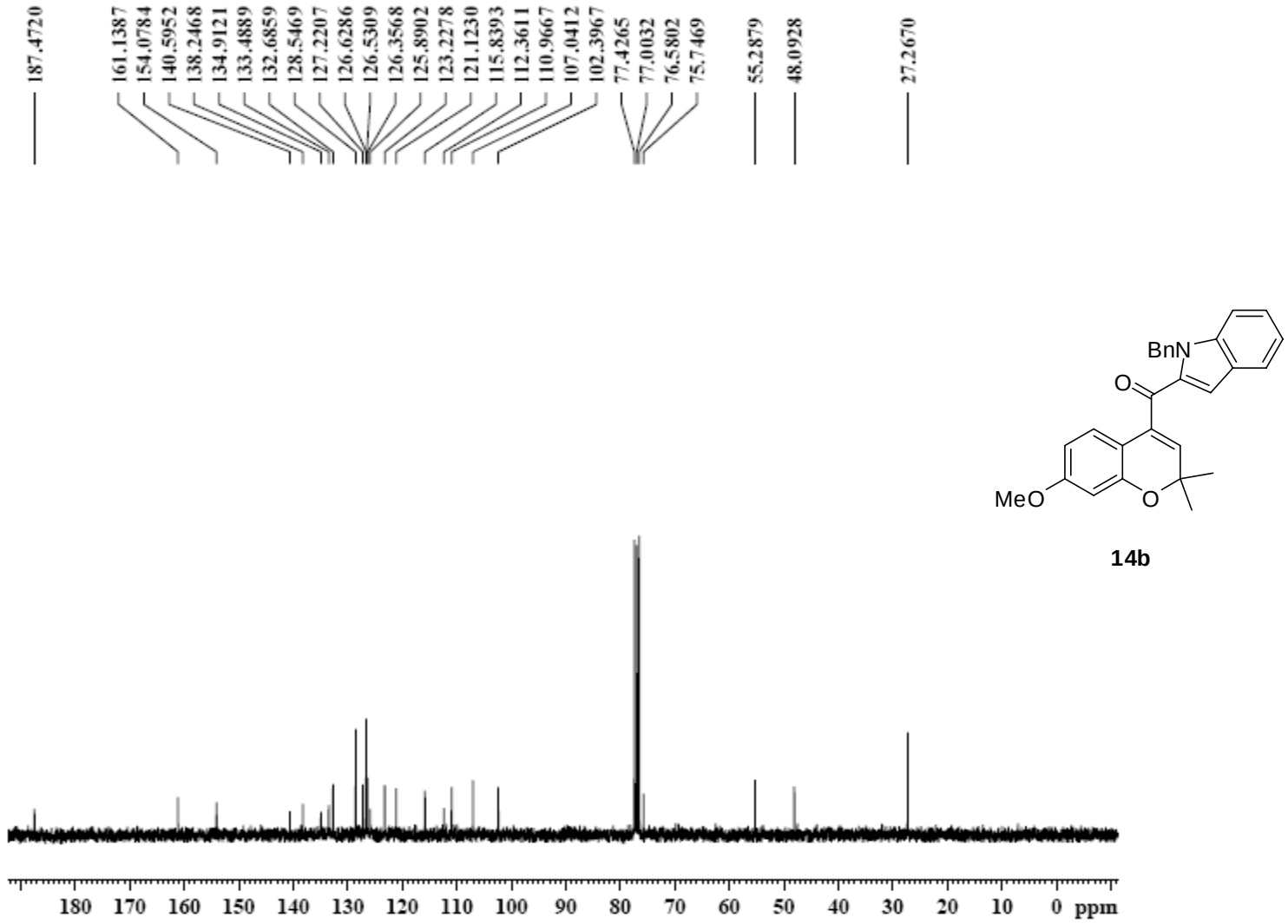


Fig. S-26: ^{13}C NMR of 2H-Chromen(1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl--4-yl)methanone (14b)

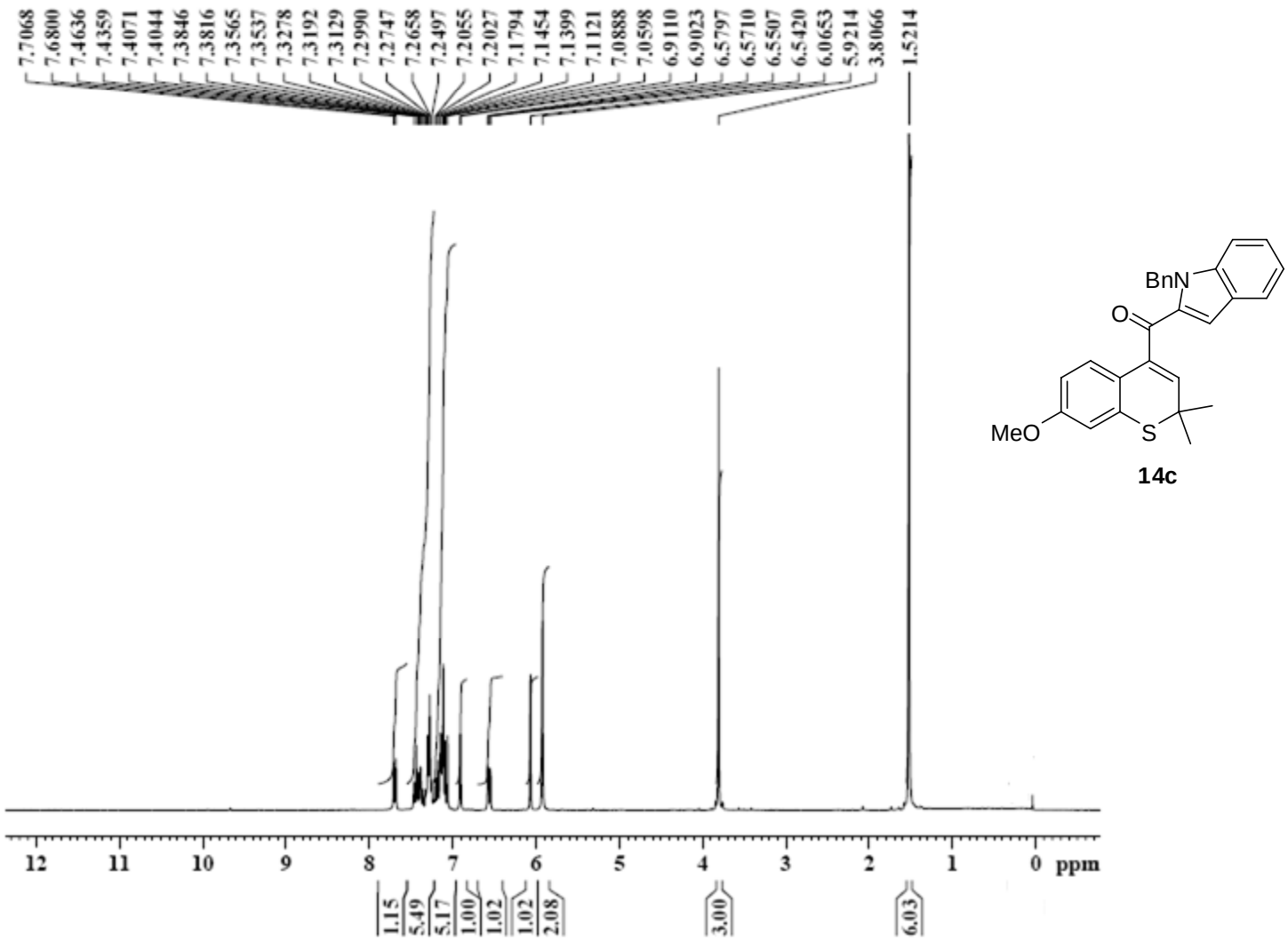


Fig. S-27: ^{1}H NMR of (1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanone (14c)

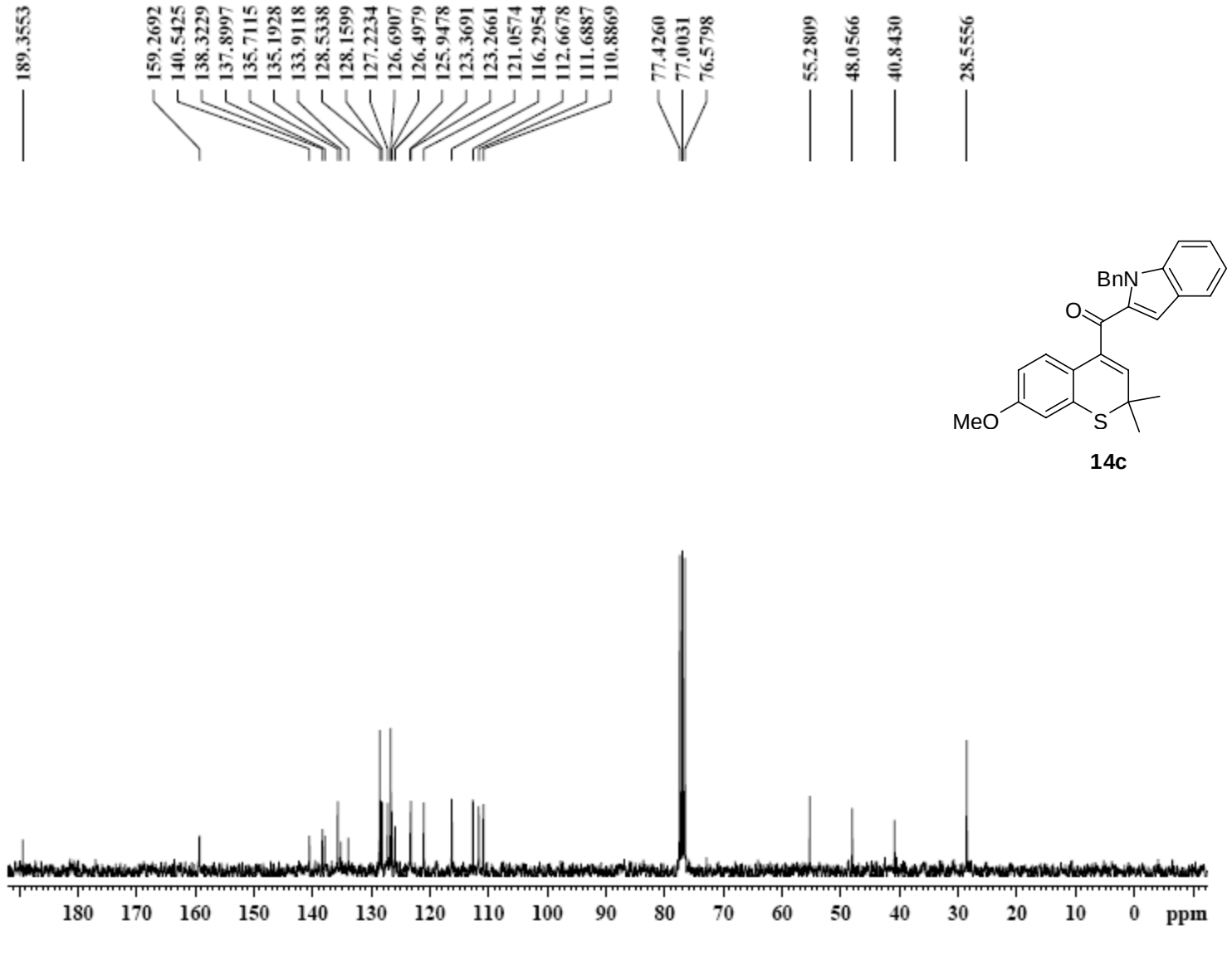


Fig. S-28: ^{13}C NMR of (1-Benzyl-1H-indol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanone (14c)

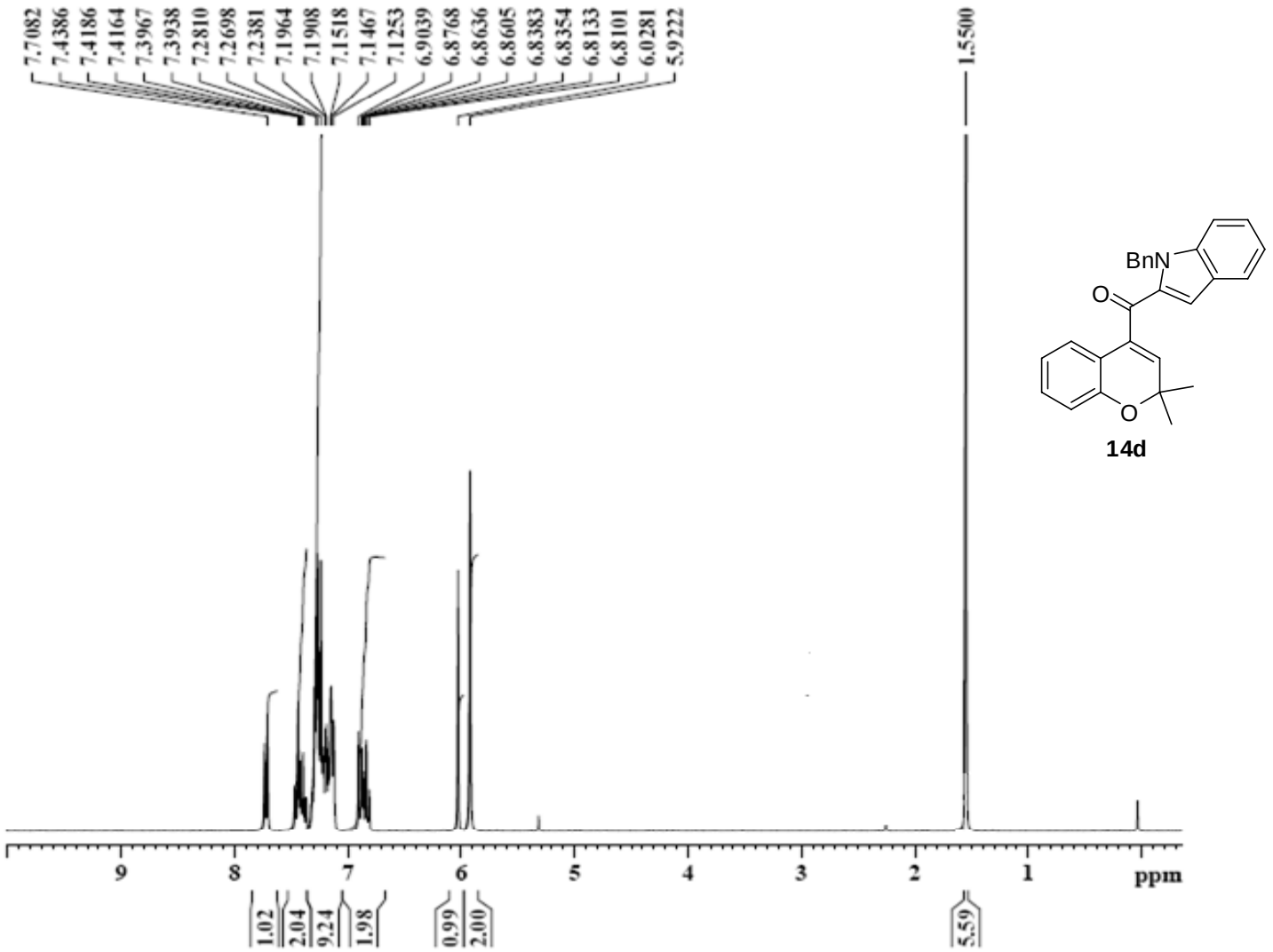


Fig. S-29: ^{1}H NMR of (1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-chromen-4-yl)methanone (14d)

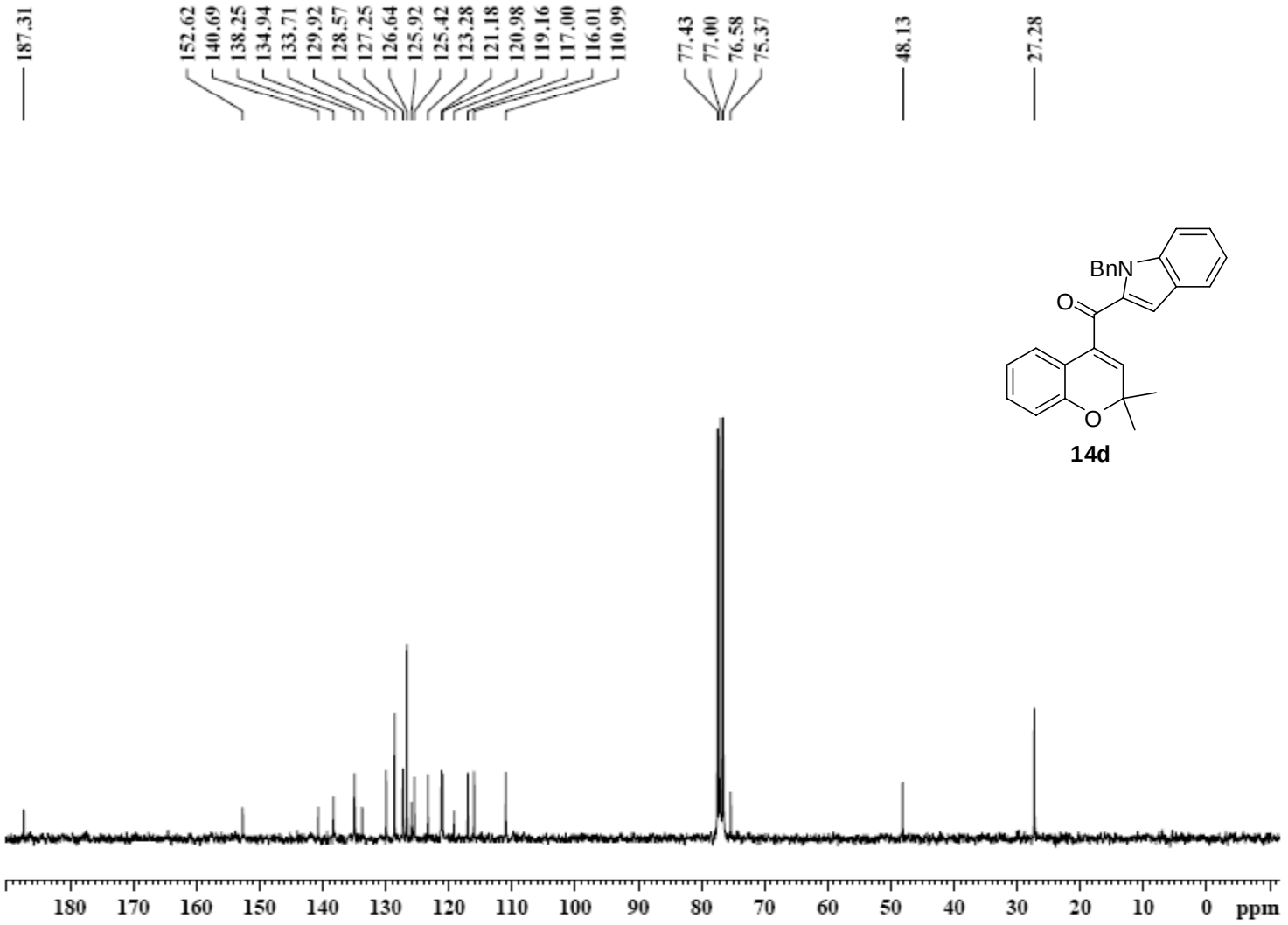


Fig. S-30: ^{13}C NMR of(1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-chromen-4-yl)methanone (14d)

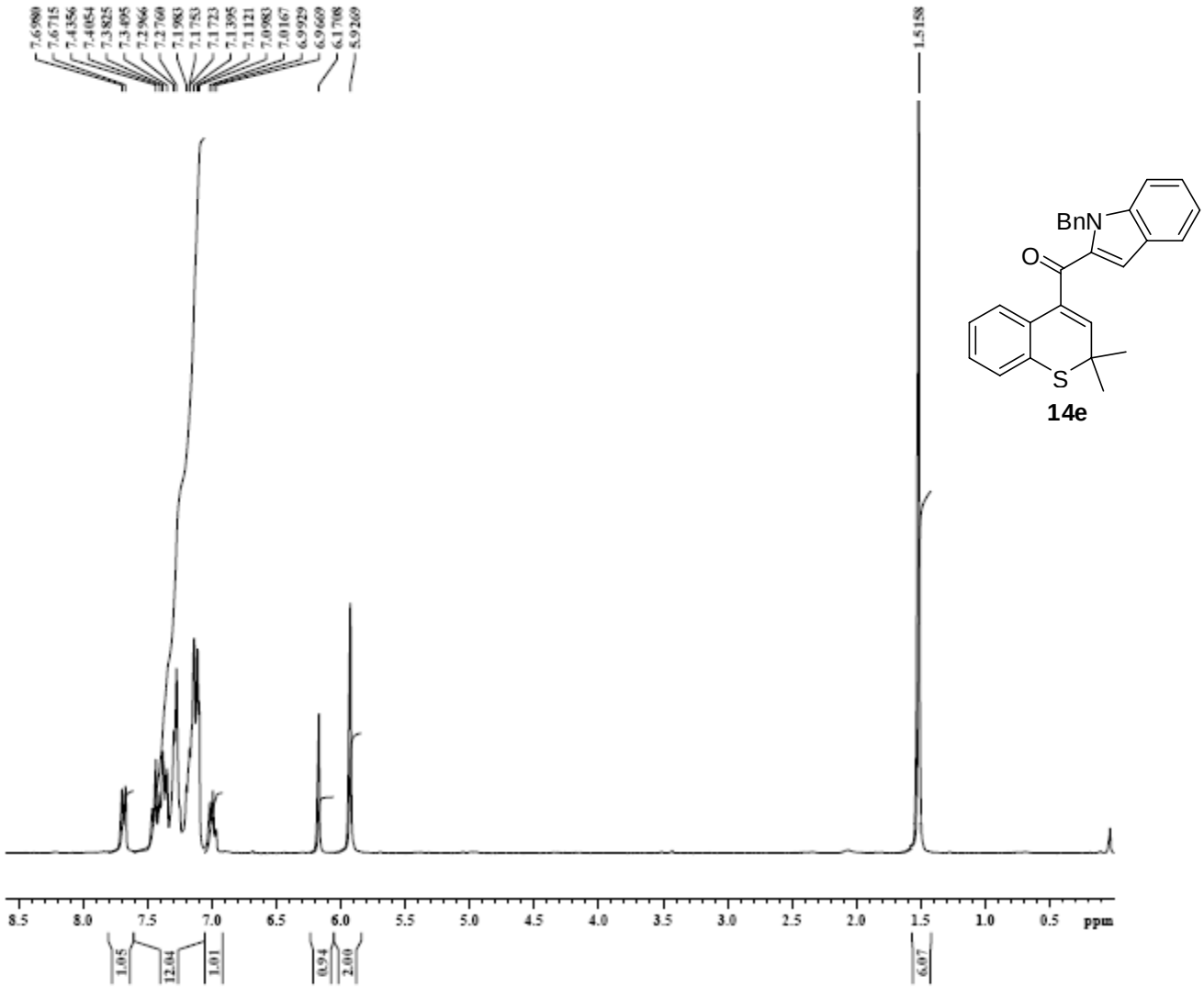


Fig. S-31: ^{1}H NMR (1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-thiochromen-4-yl)methanone (14e)

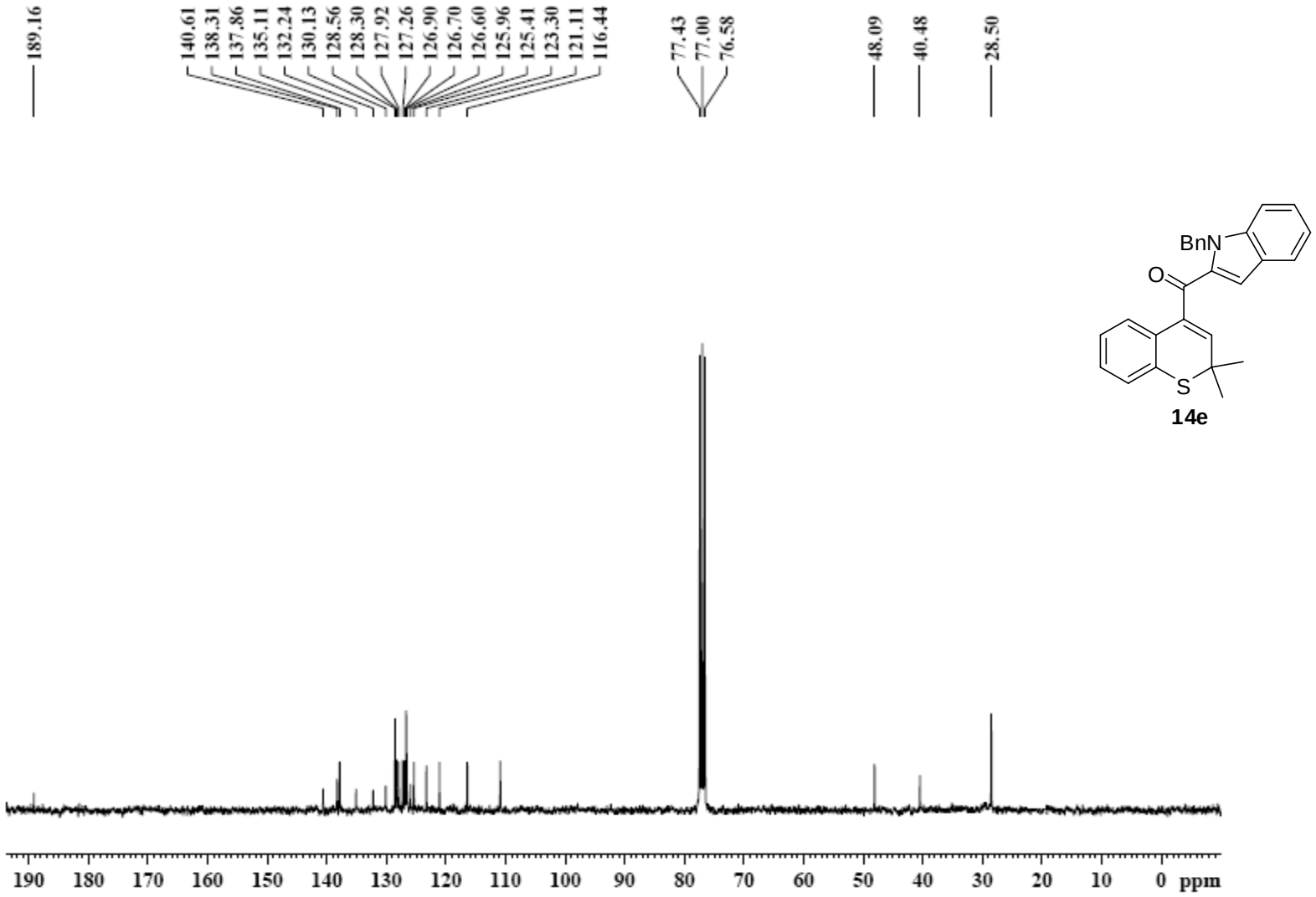


Fig. S-32: ^{13}C NMR of (1-Benzyl-1H-indol-2-yl)(2,2-dimethyl-2H-thiochromen-4-yl)methanone (14e)

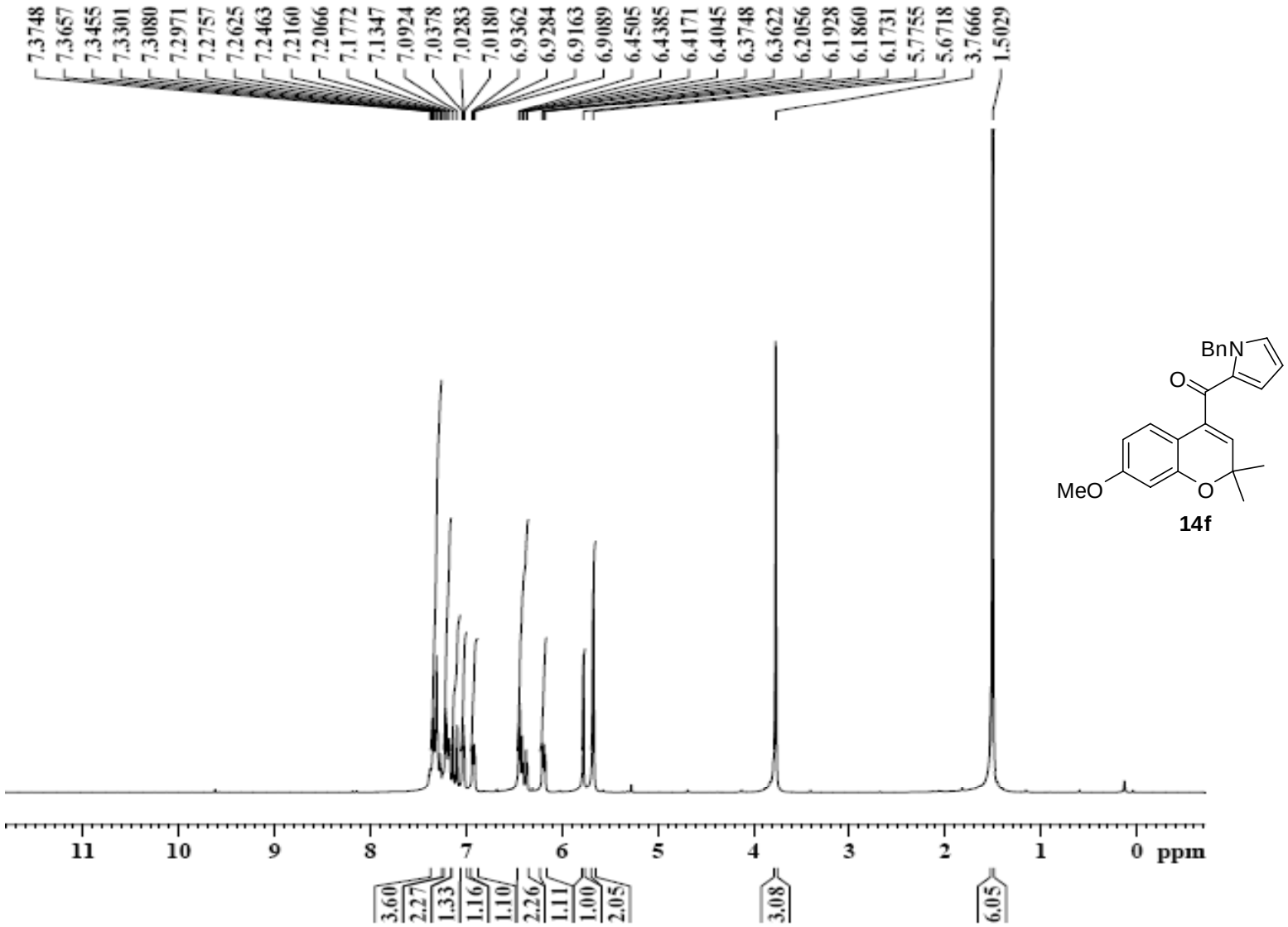


Fig. S-33: ^{1}H NMR of (1-Benzyl-1H-pyrrol-2-yl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanone (14f)

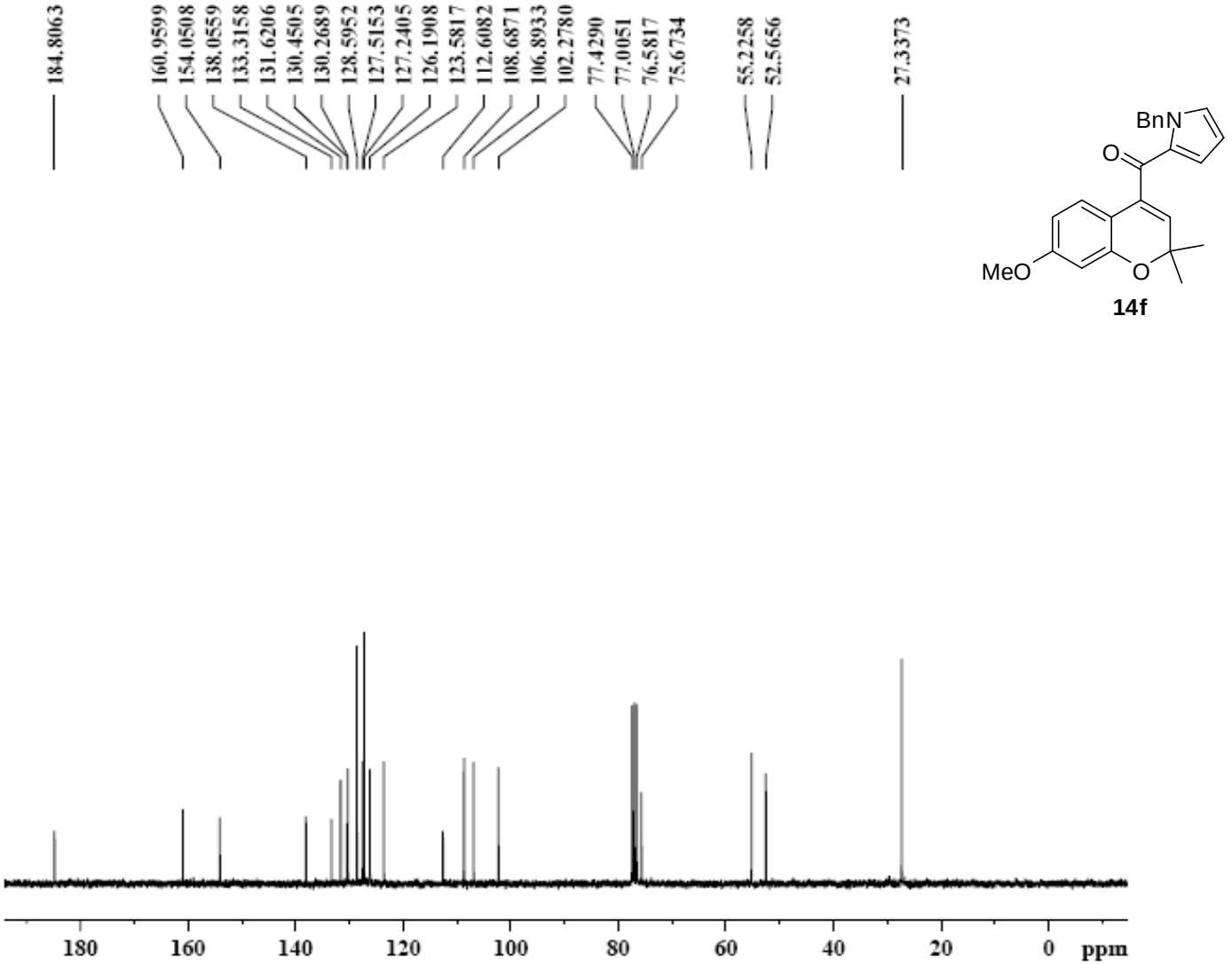


Fig. S-34: ^{13}C NMR of (1-Benzyl-1H-pyrrol-2-yl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanone (14f)

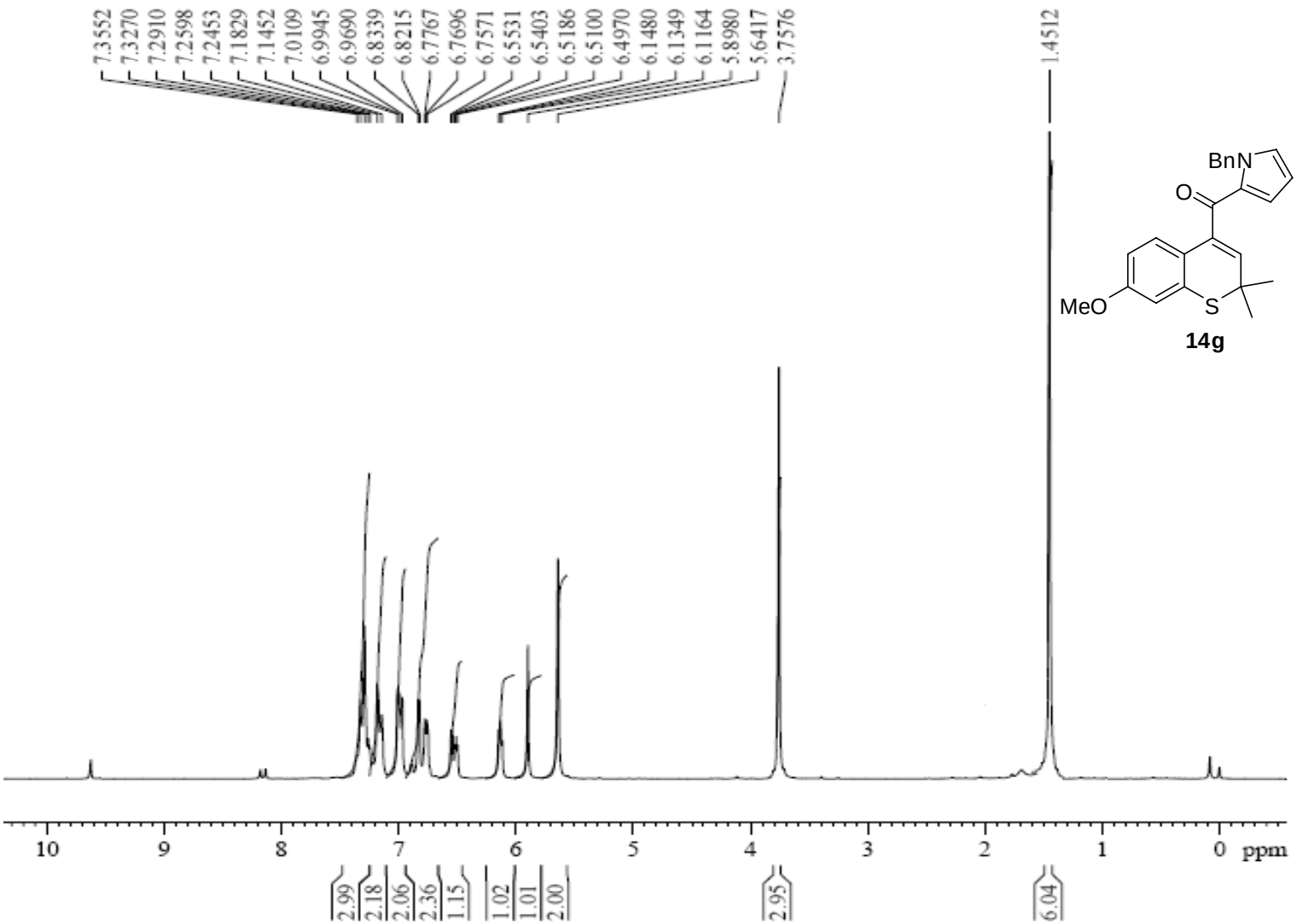


Fig. S-35: ^{1}H NMR of (1-Benzyl-1H-pyrrol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanone (14g)

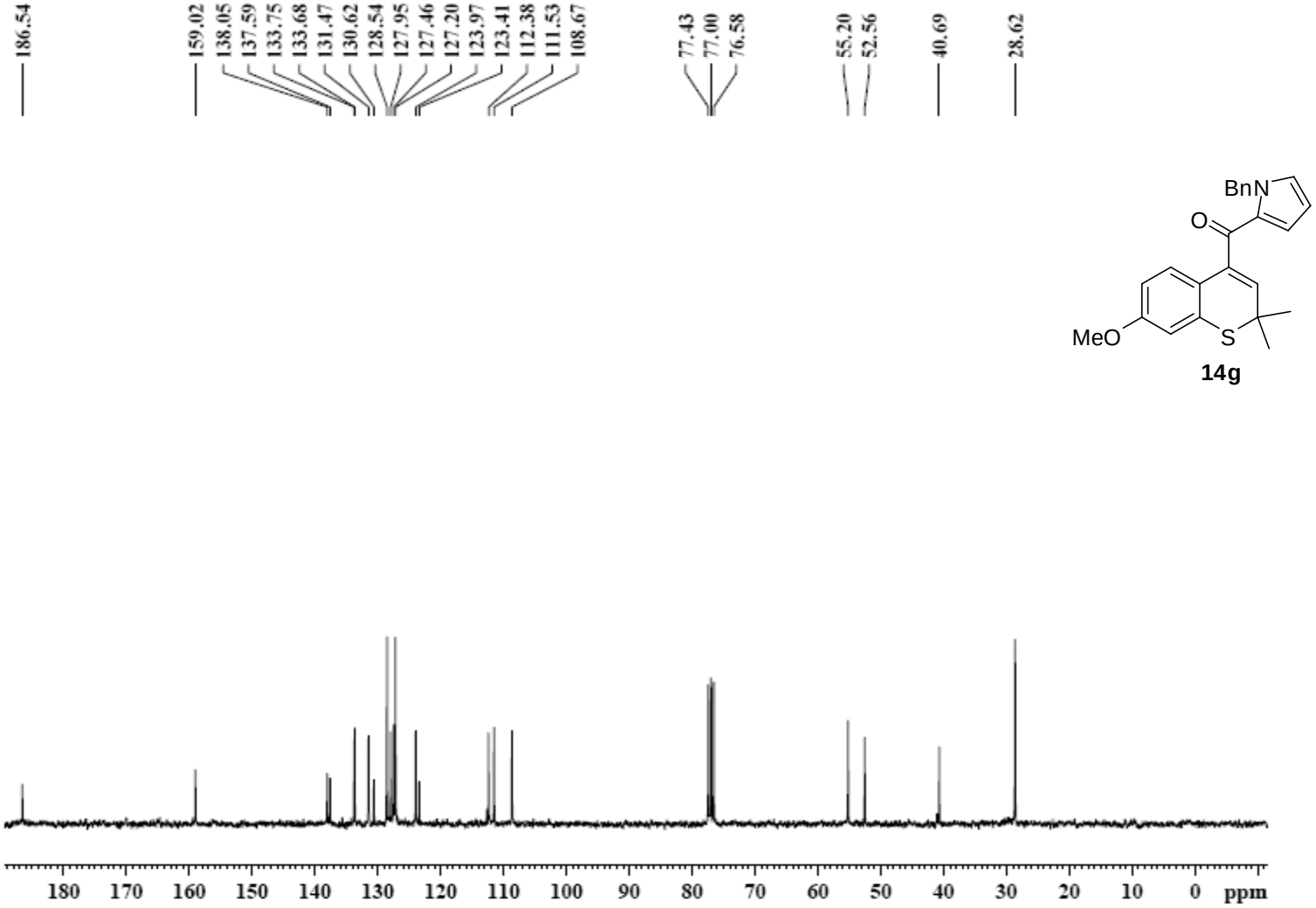


Fig. S-36: ^{13}C NMR of (1-Benzyl-1H-pyrrol-2-yl)(7-methoxy-2,2-dimethyl-2H-thiochromen-4-yl)methanone (14g)

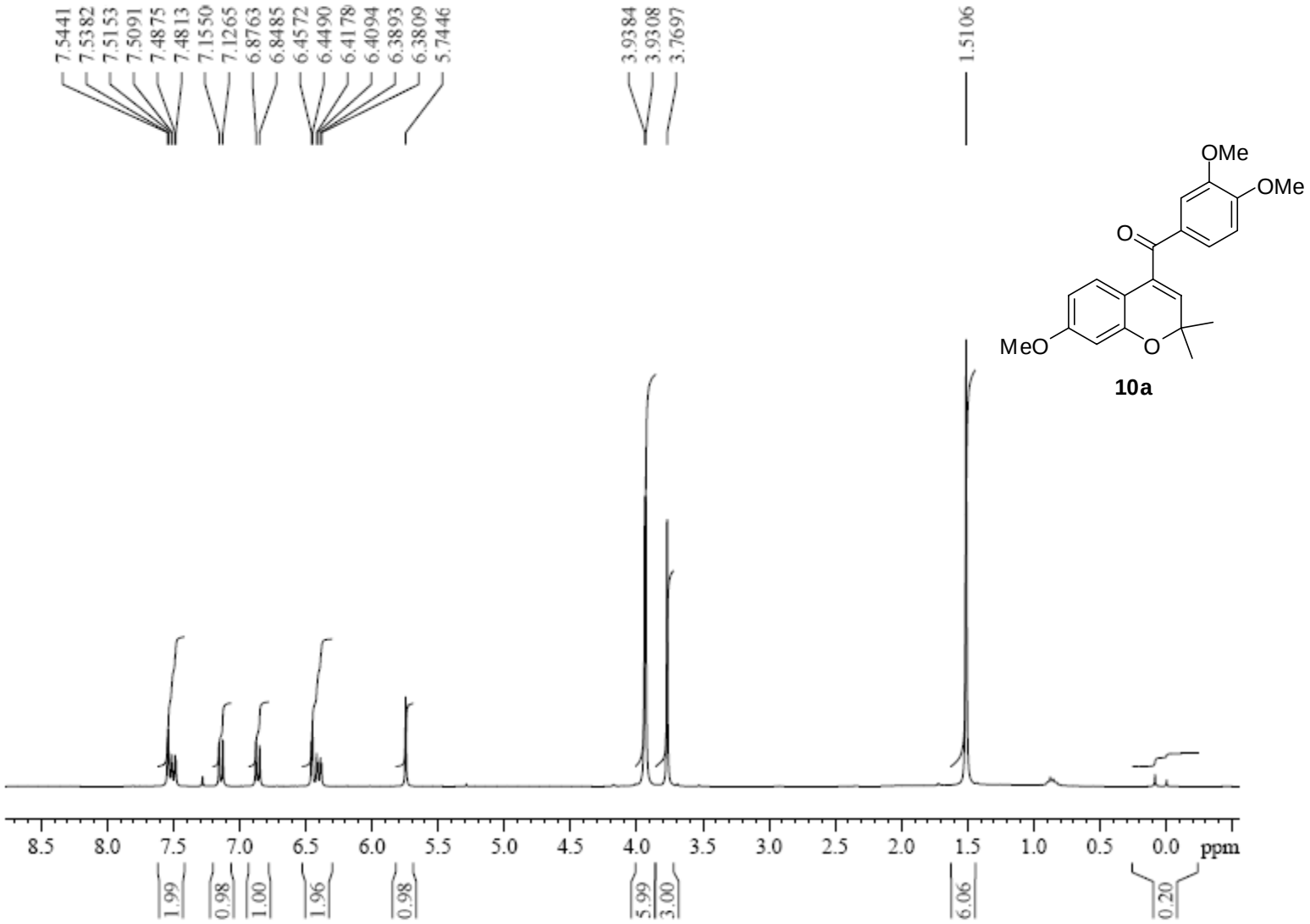


Fig. S-37: ^{1}H NMR of (3,4-Dimethoxyphenyl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanone (10a)

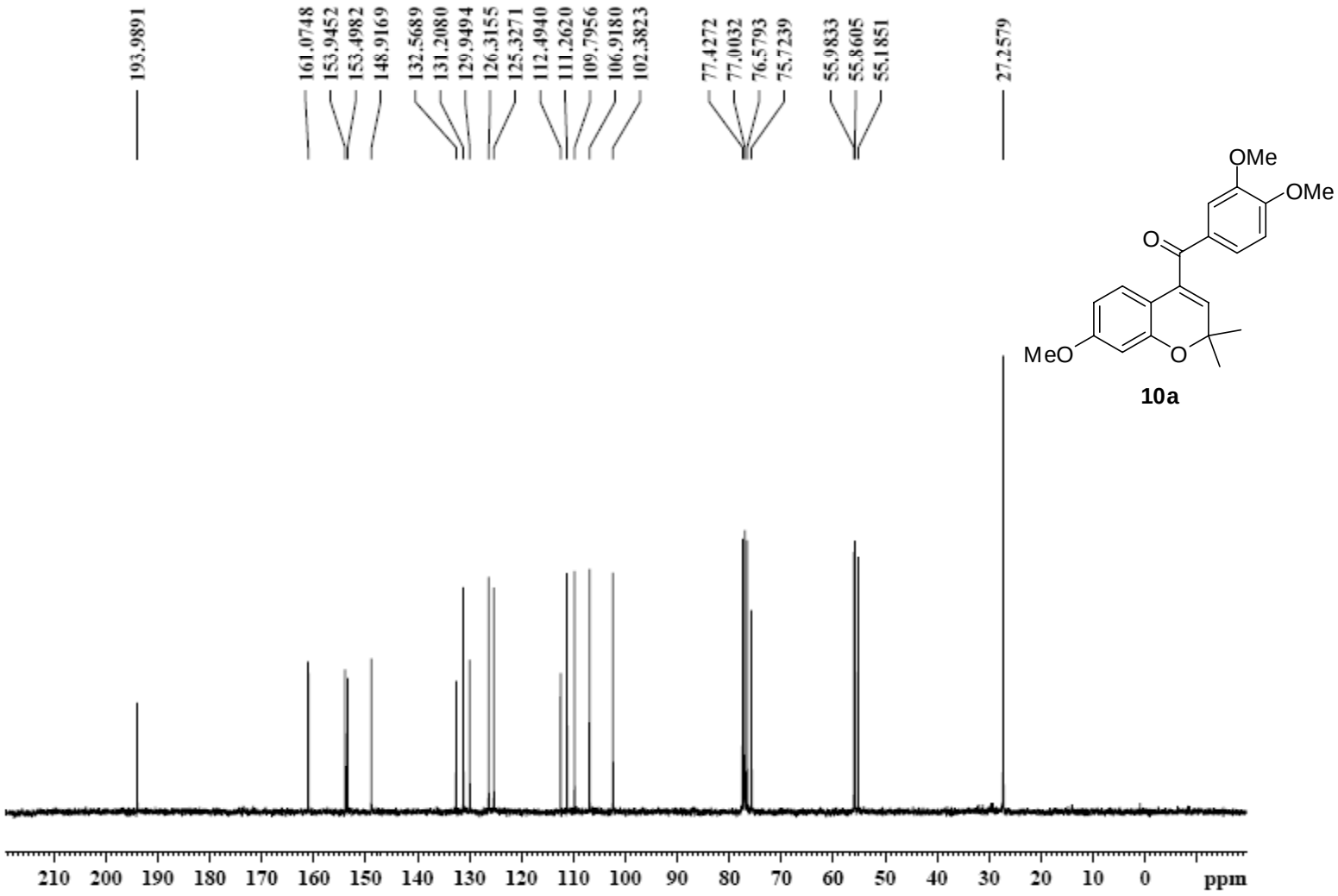


Fig. S-38 : ^{13}C NMR of (3,4-Dimethoxyphenyl)(7-methoxy-2,2-dimethyl-2H-chromen-4-yl)methanone (10a)

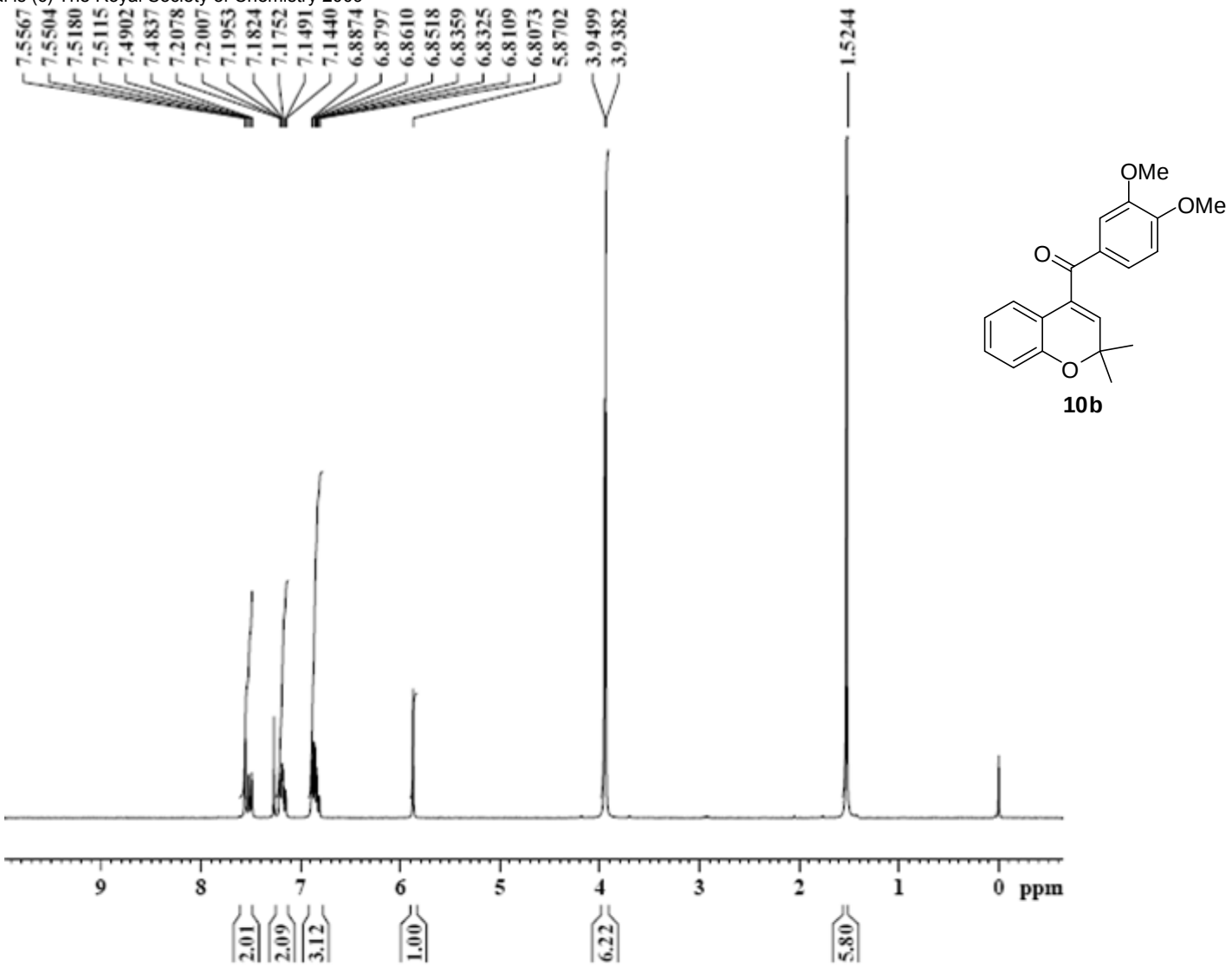


Fig. S-39: ^{1}H NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-chromen-4-yl)methanone (10b)

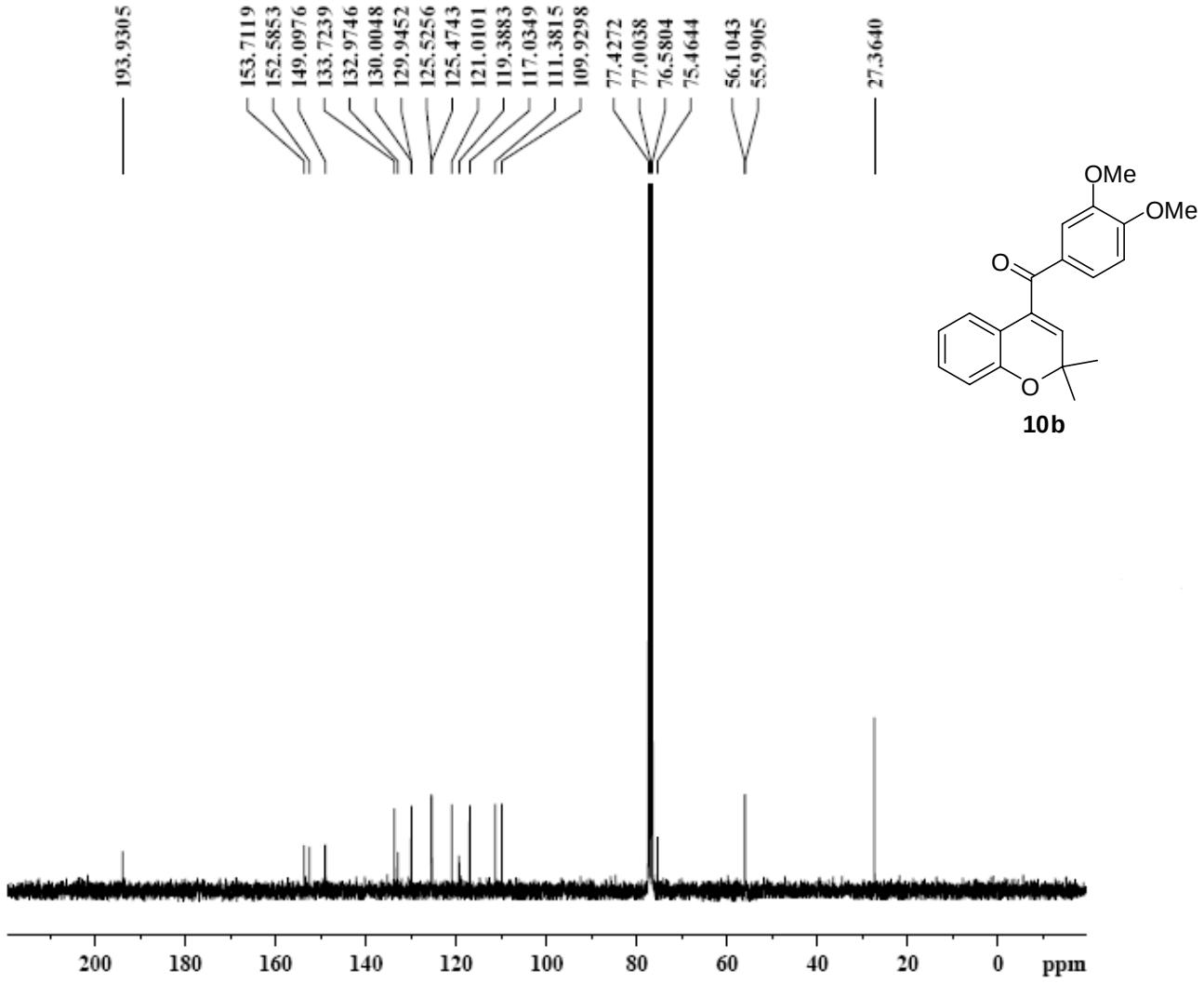


Fig. S-40: ^{13}C NMR of (3,4-Dimethoxyphenyl)(2,2-dimethyl-2H-chromen-4-yl) methanone (10b)

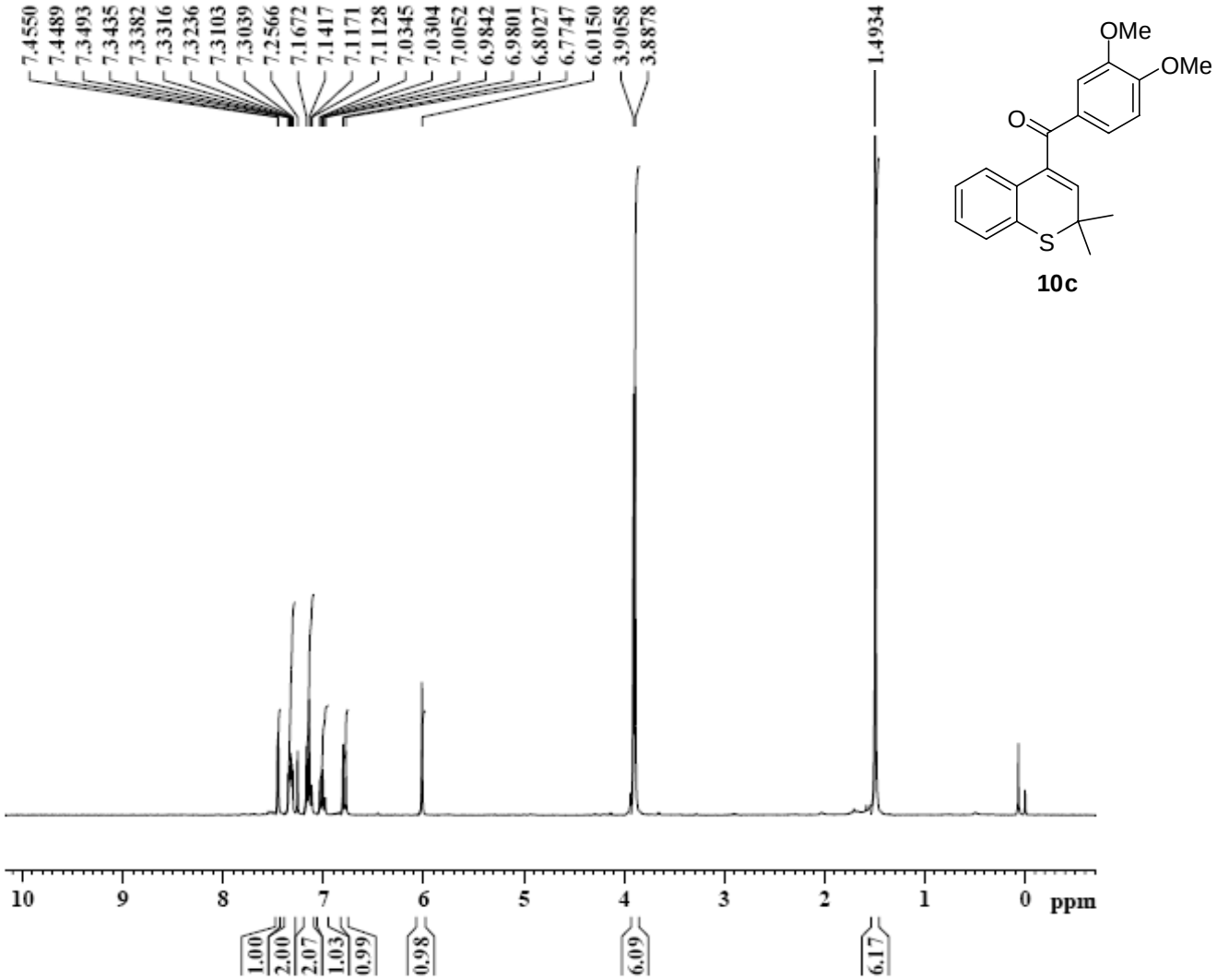


Fig. S-41: ^{1}H NMR of (3,4-Dimethoxyphenyl)-(2,2-dimethyl-2H-thiochromen-4-yl)methanone (10c)

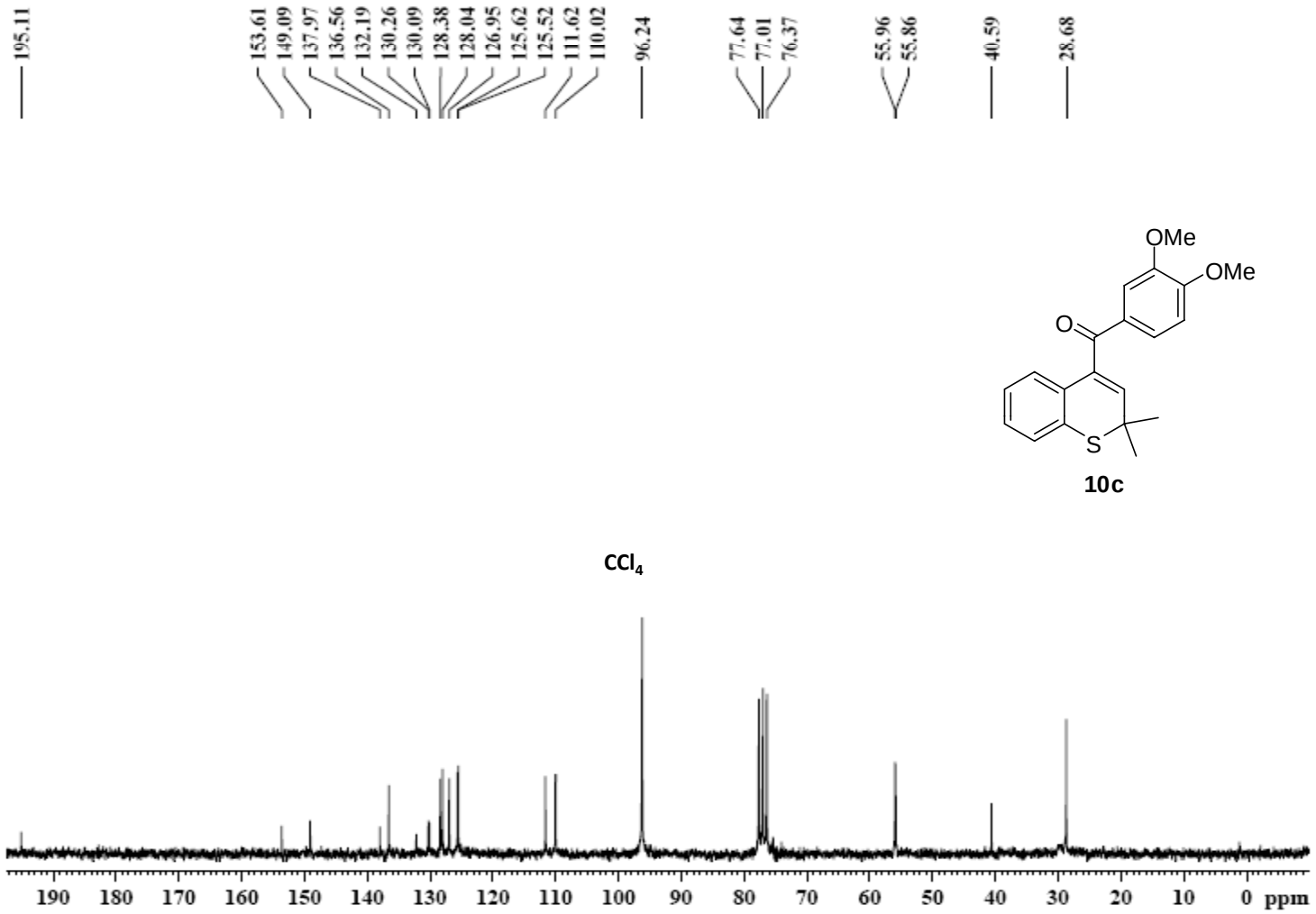


Fig. S-42: ^{13}C NMR of (3,4-Dimethoxyphenyl)-(2,2-dimethyl-2H-thiochromen-4-yl)methanone (10c)

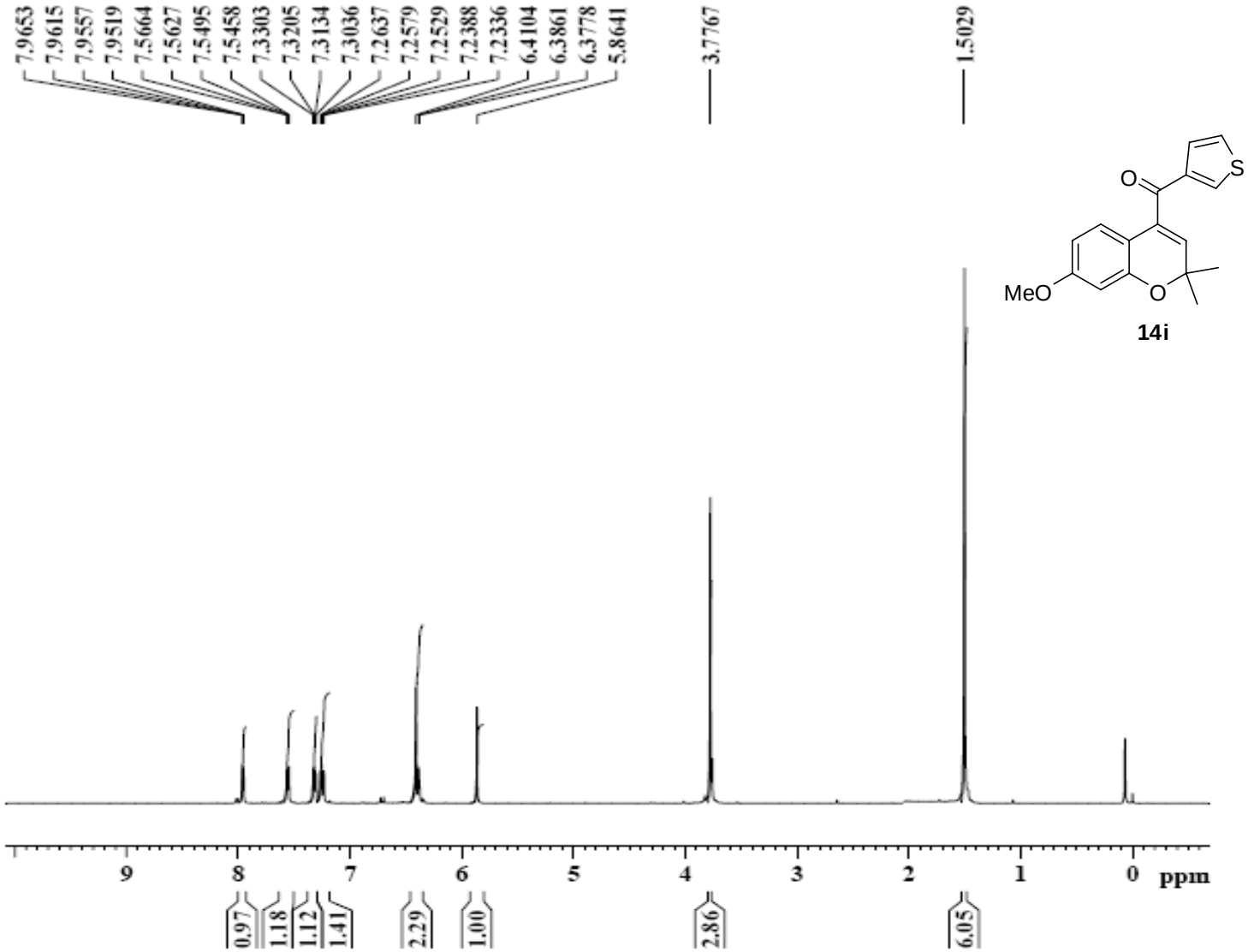


Fig. S-43: ^{1}H NMR of (7-Methoxy-2,2-dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanone (14i)

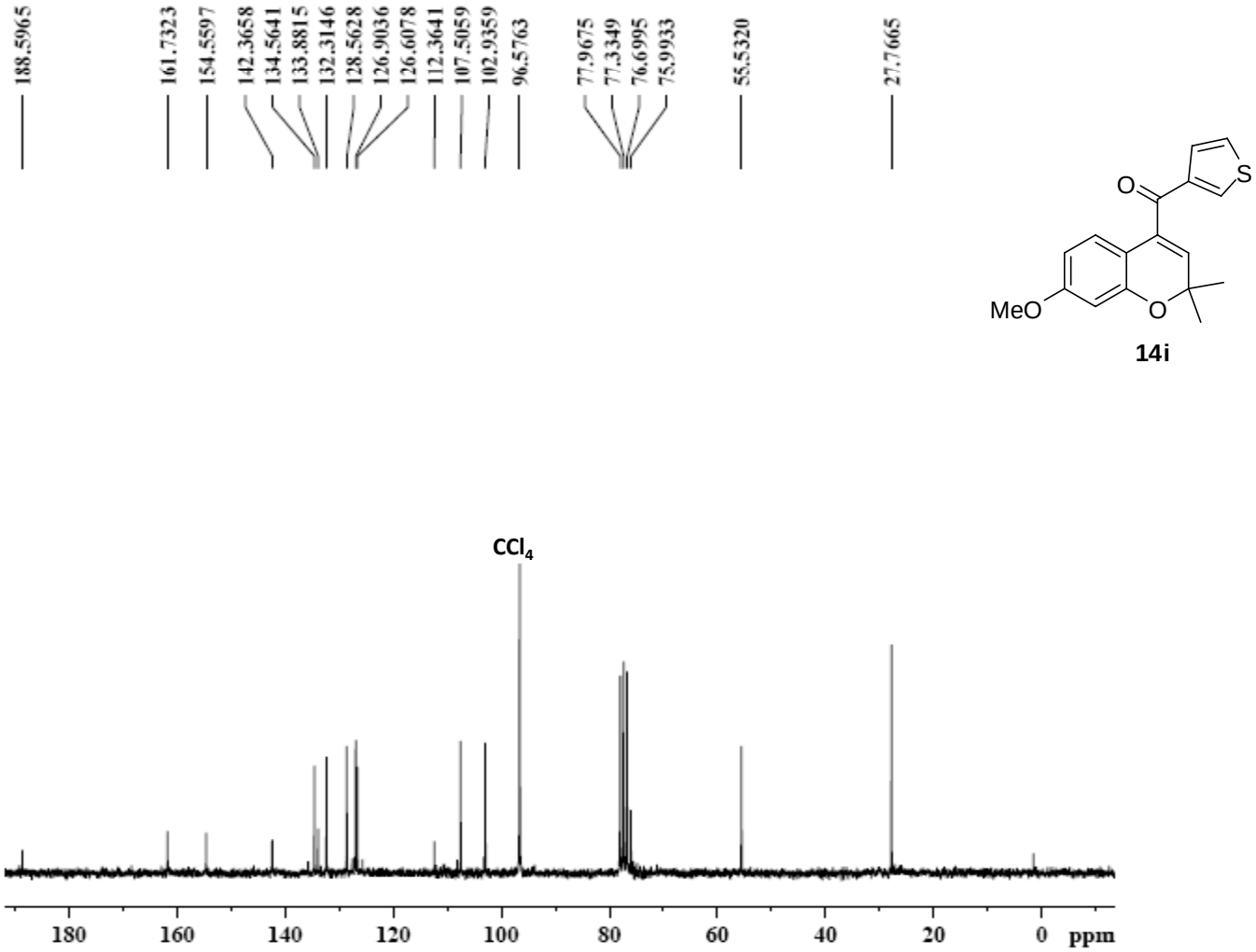


Fig. S-44: ^{13}C NMR of (7-Methoxy-2,2-dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanone (14i)

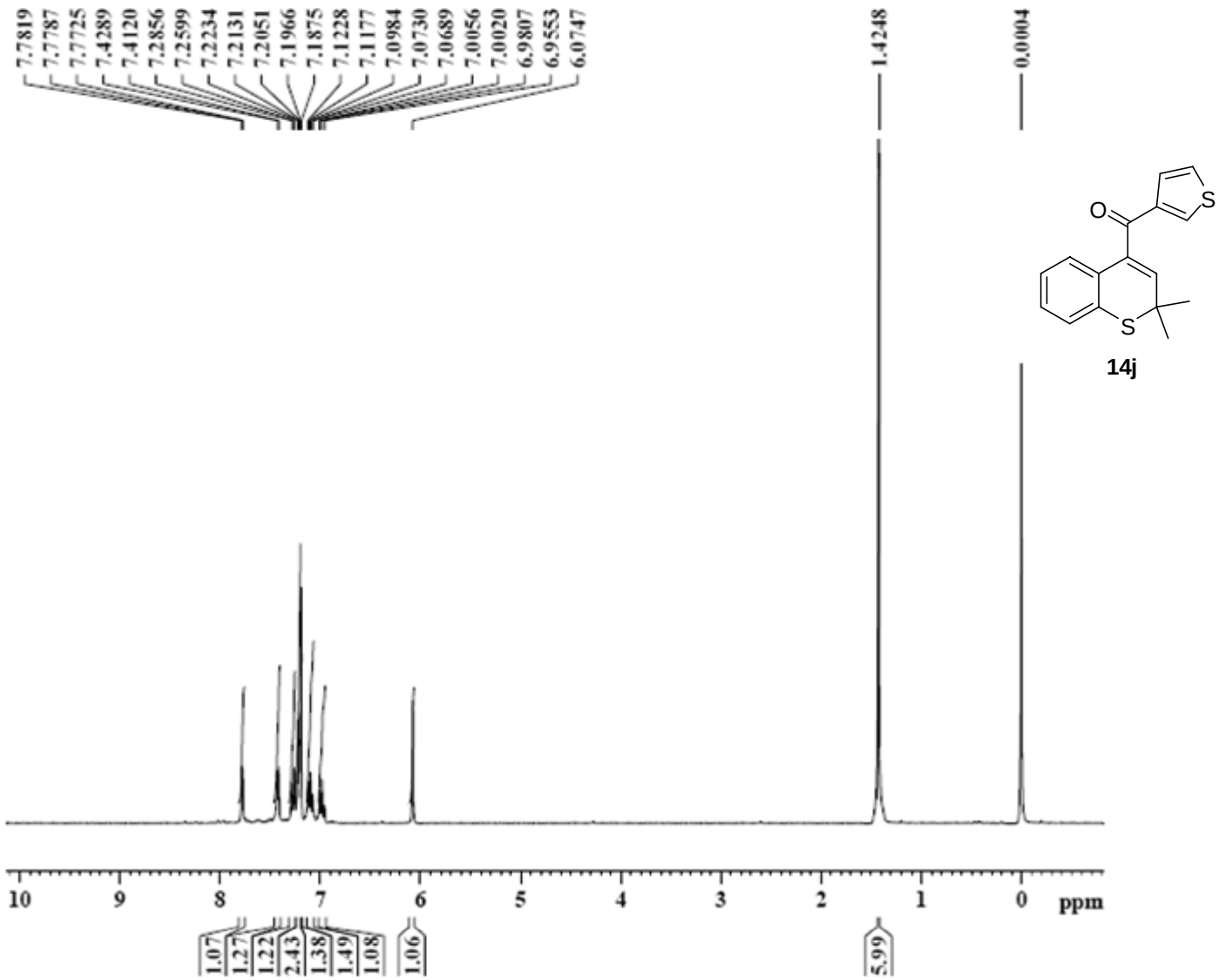


Fig. S-45: ^{1}H NMR of (2,2-Dimethyl-2H-thiochromen-4-yl) (thiophen-3-yl)methanone (l4j)

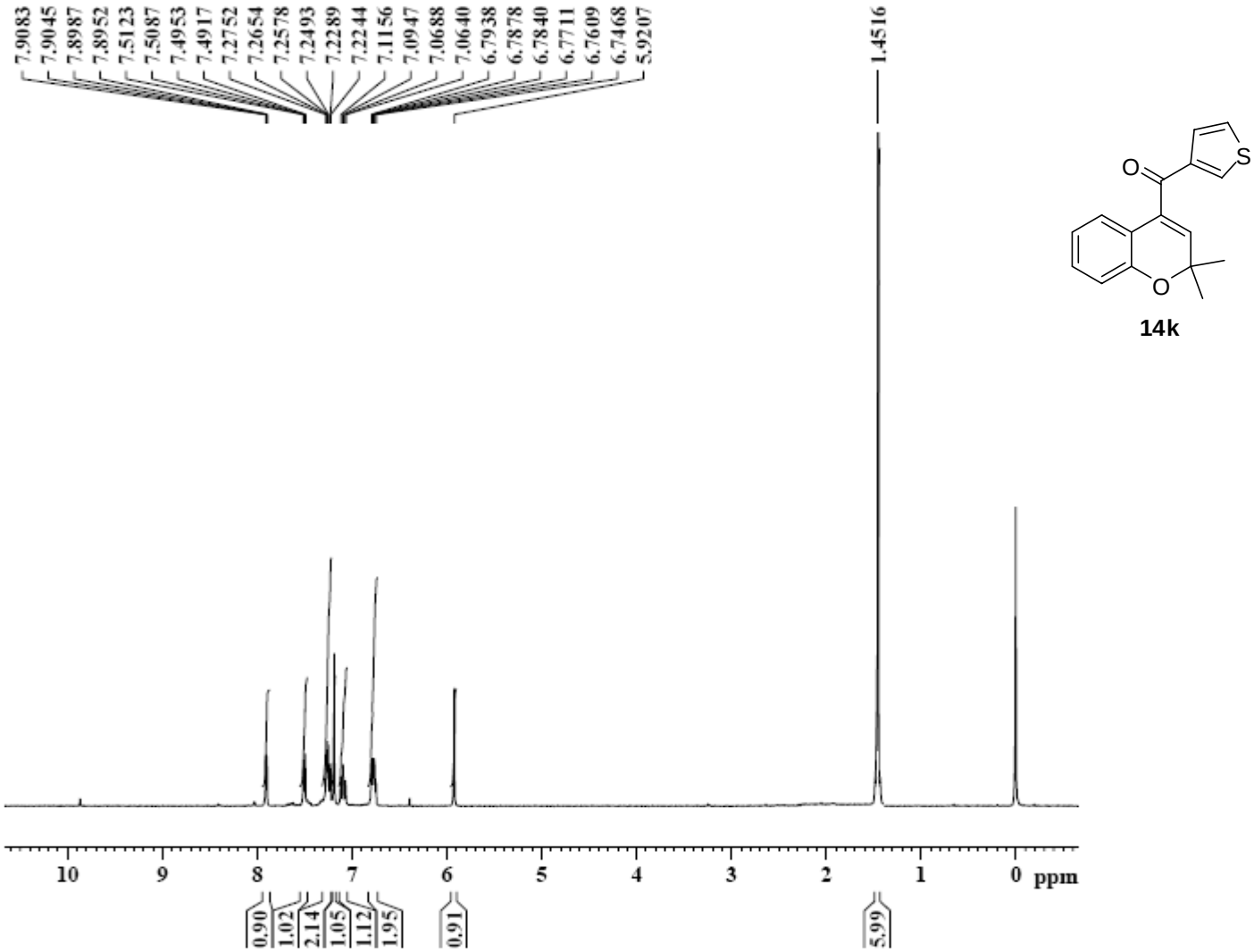


Fig. S-46: ^{1}H NMR of (2,2-Dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanone (14k)

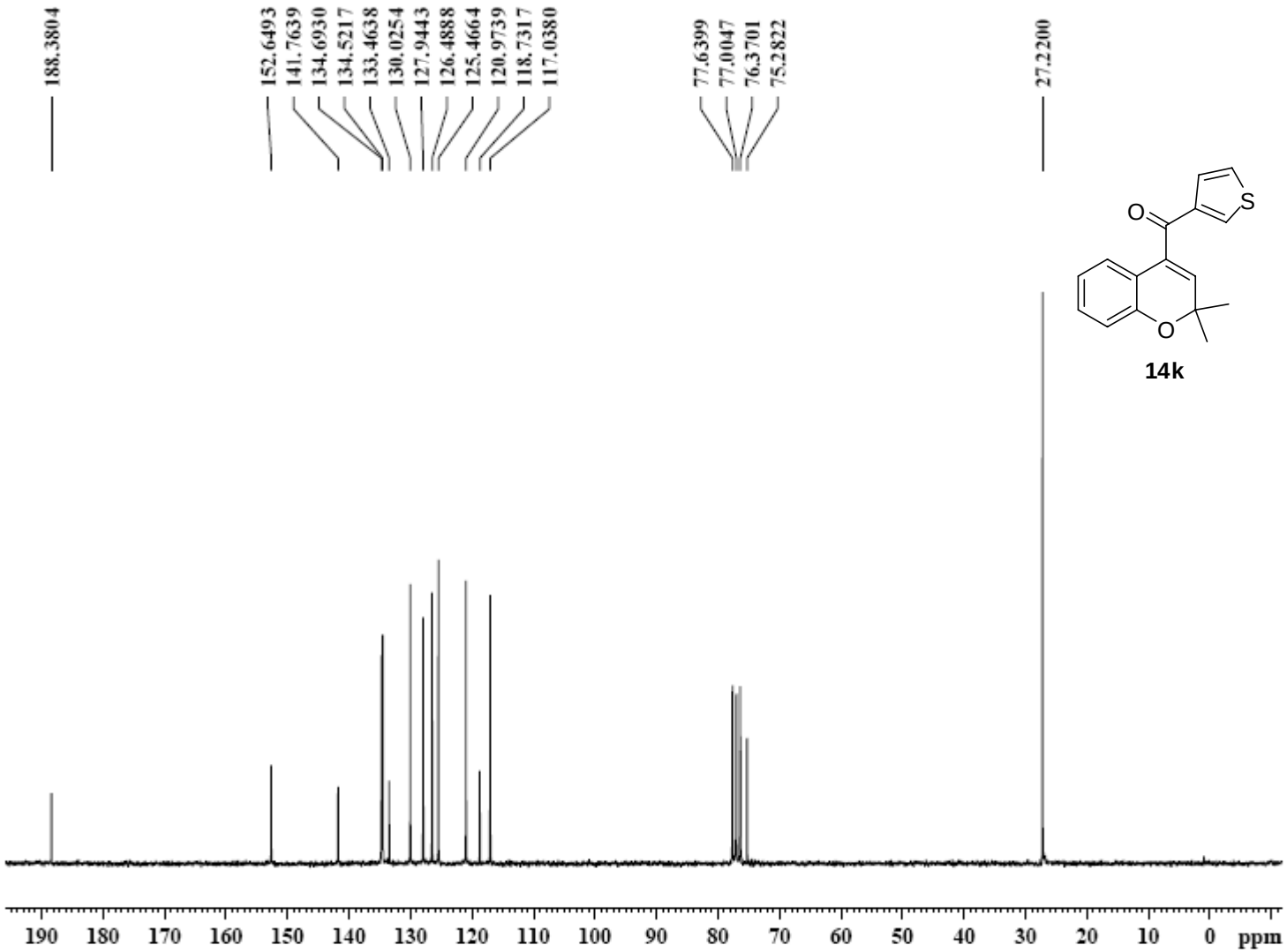


Fig. S-47: ^{13}C NMR of (2,2-Dimethyl-2H-chromen-4-yl)(thiophen-3-yl)methanone (14k)

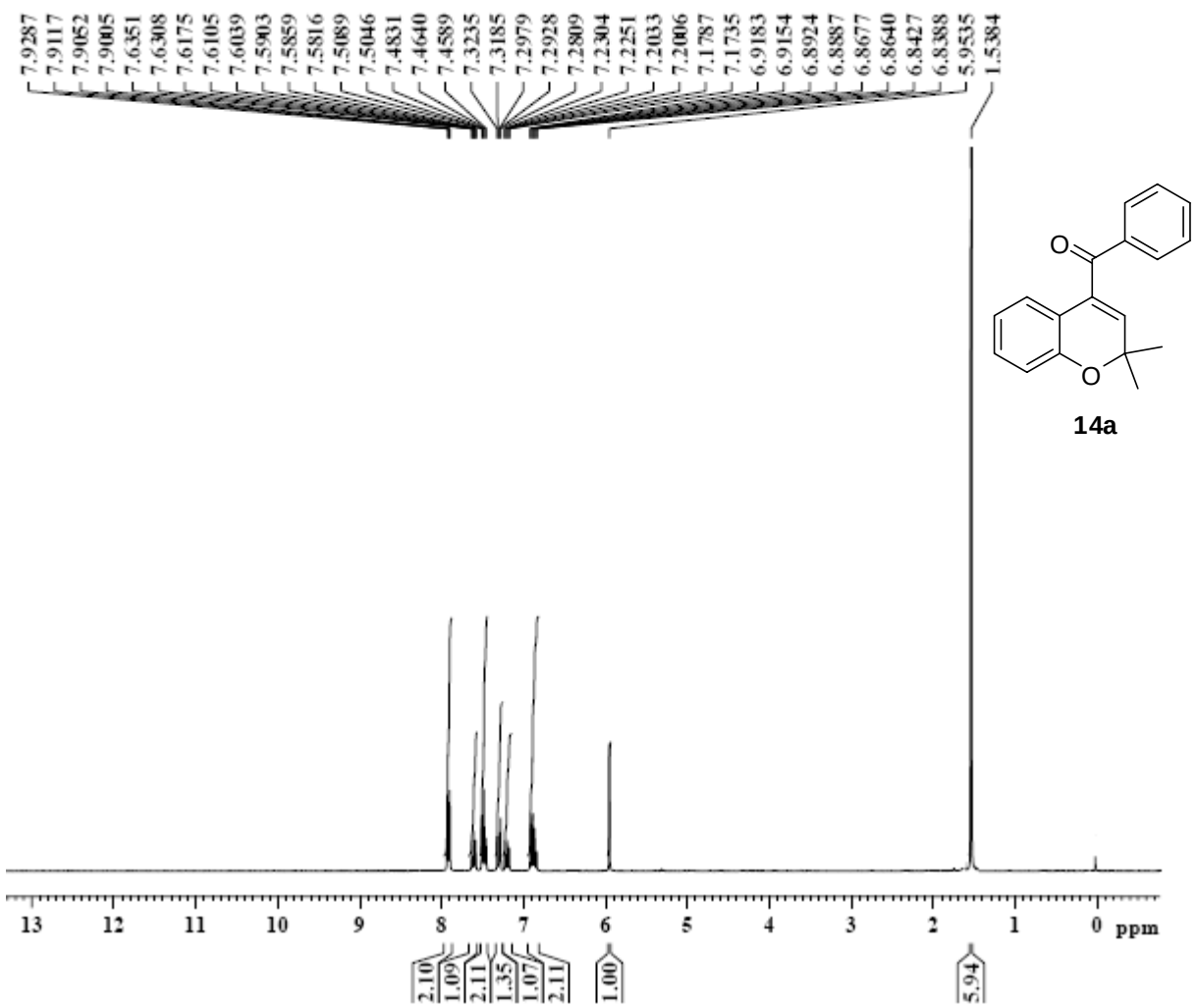


Fig. S-48: ^{1}H NMR of (2,2-dimethyl-2H-chromen-4-yl)(phenyl)methanone (14a)

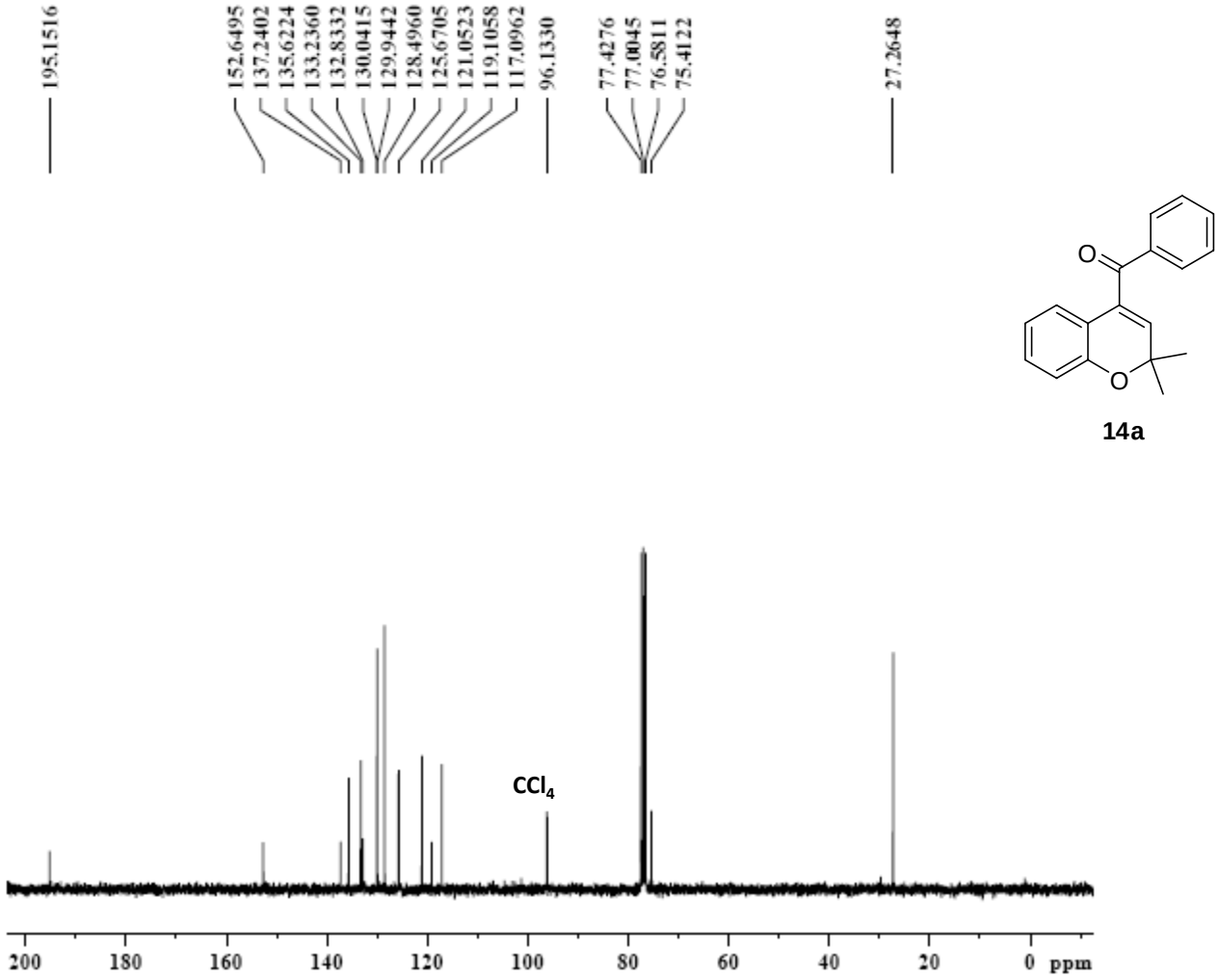


Fig. S-49: ^{13}C NMR of (2,2-dimethyl-2H-chromen-4-yl)(phenyl) methanone)(14a)

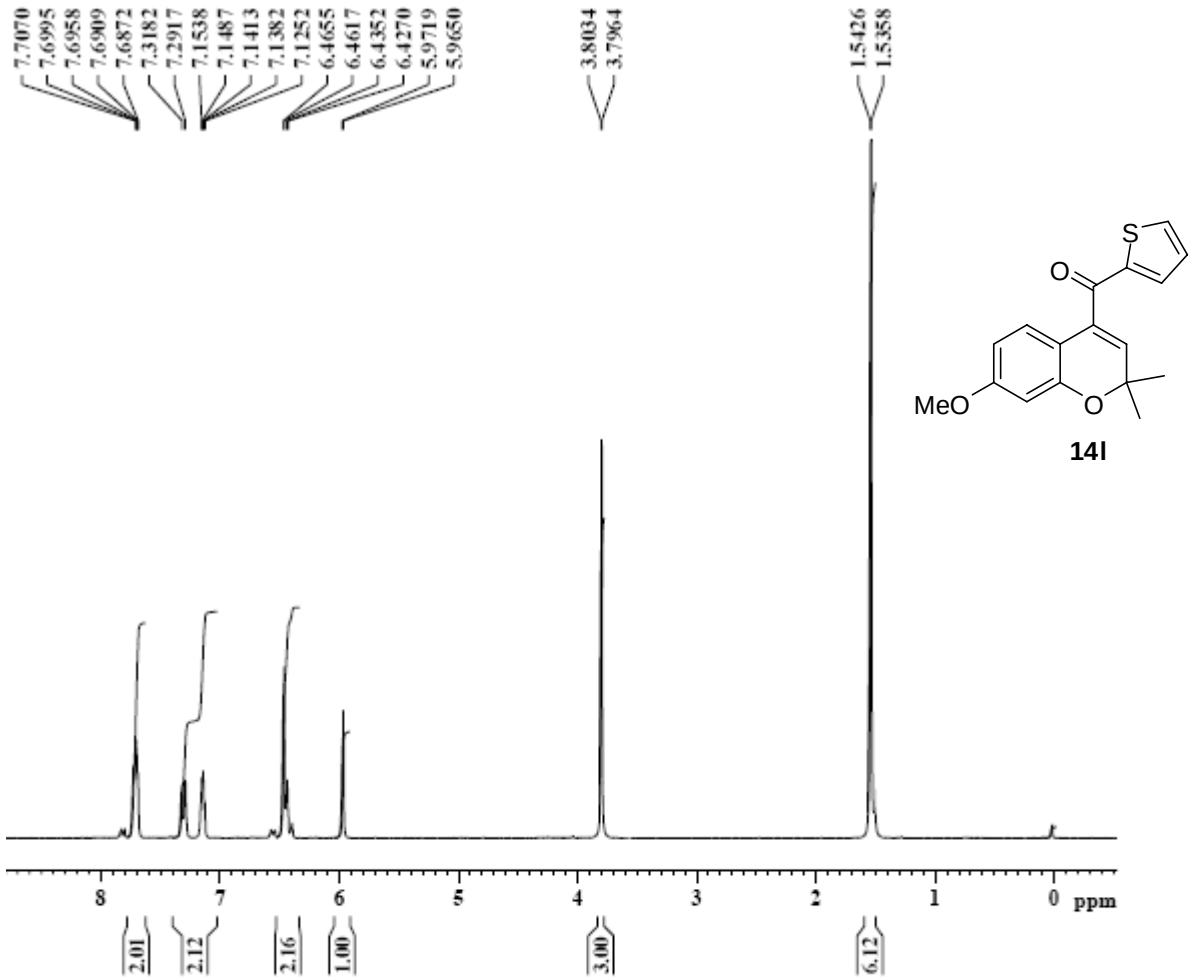


Fig. S-50: ^{1}H NMR of (7-methoxy-2,2-dimethyl-2H-chromen-4-yl)(thiophen-2-yl)methanone(14l)

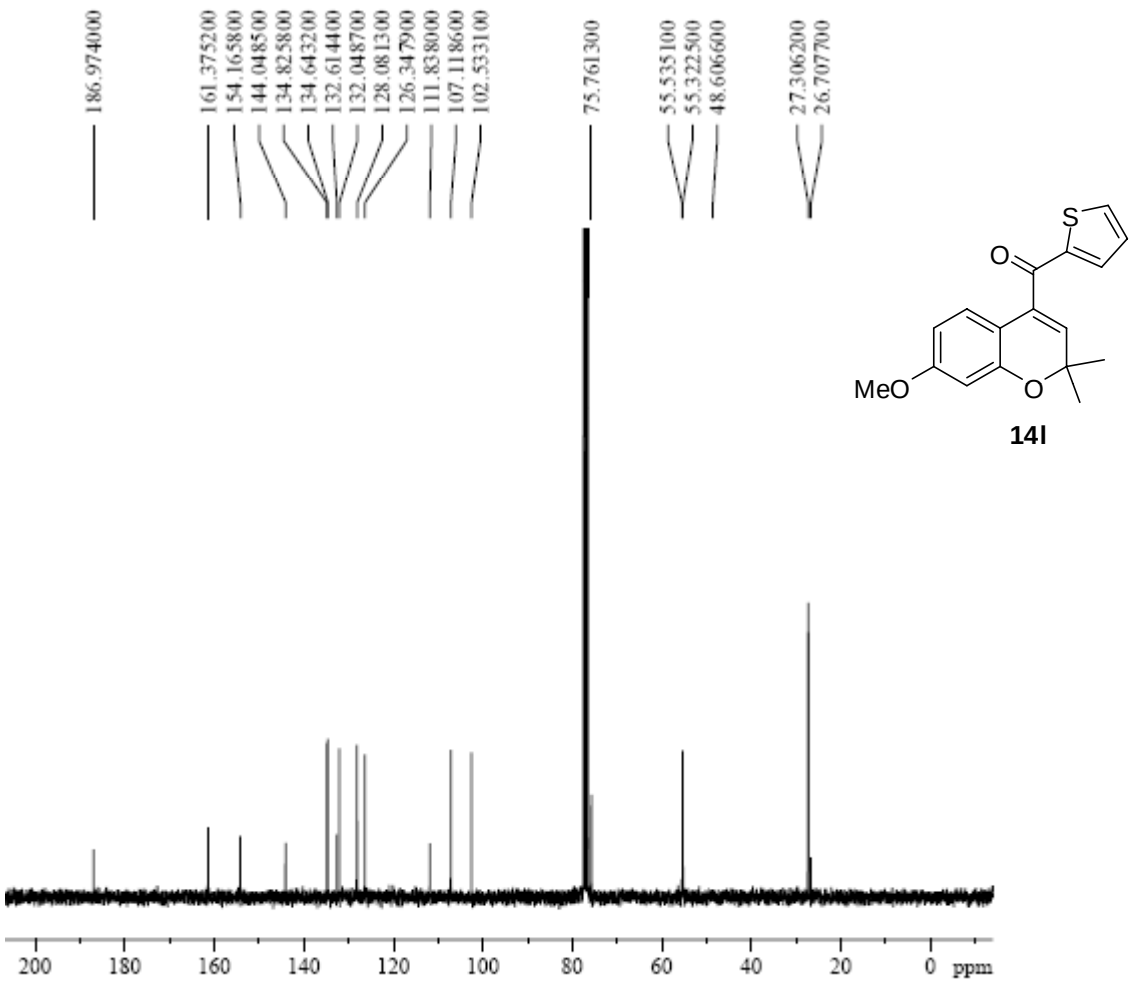


Fig. S-51: ^{13} C NMR of (7-methoxy-2,2-dimethyl-2H-chromen-4-yl)(thiophen-2-yl)methanone(14l)

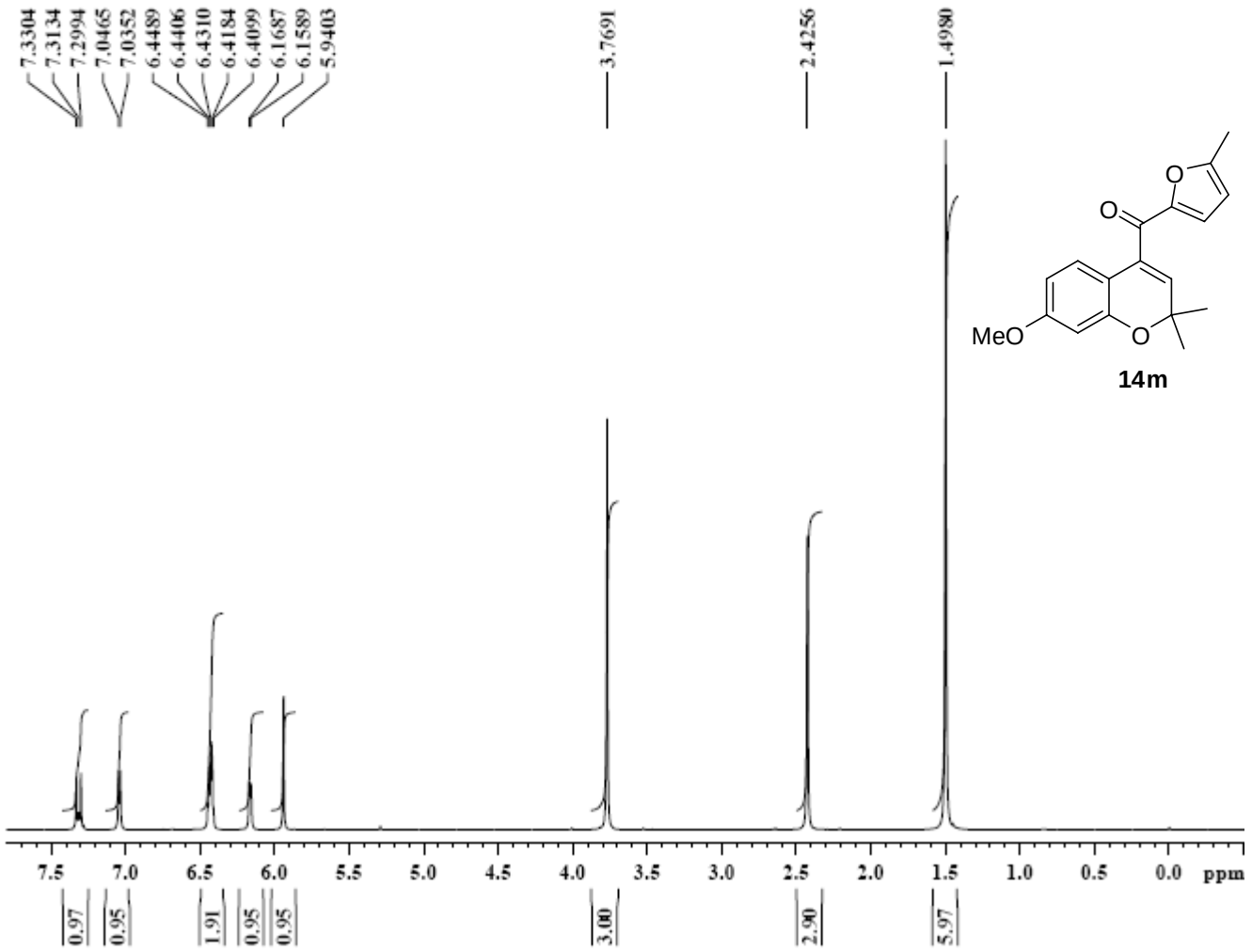


Fig. S-52: ^{1}H NMR of (7-methoxy-2,2-dimethyl-2H-chromen-4-yl)(5-methylfuran-2-yl) methanone(14m)

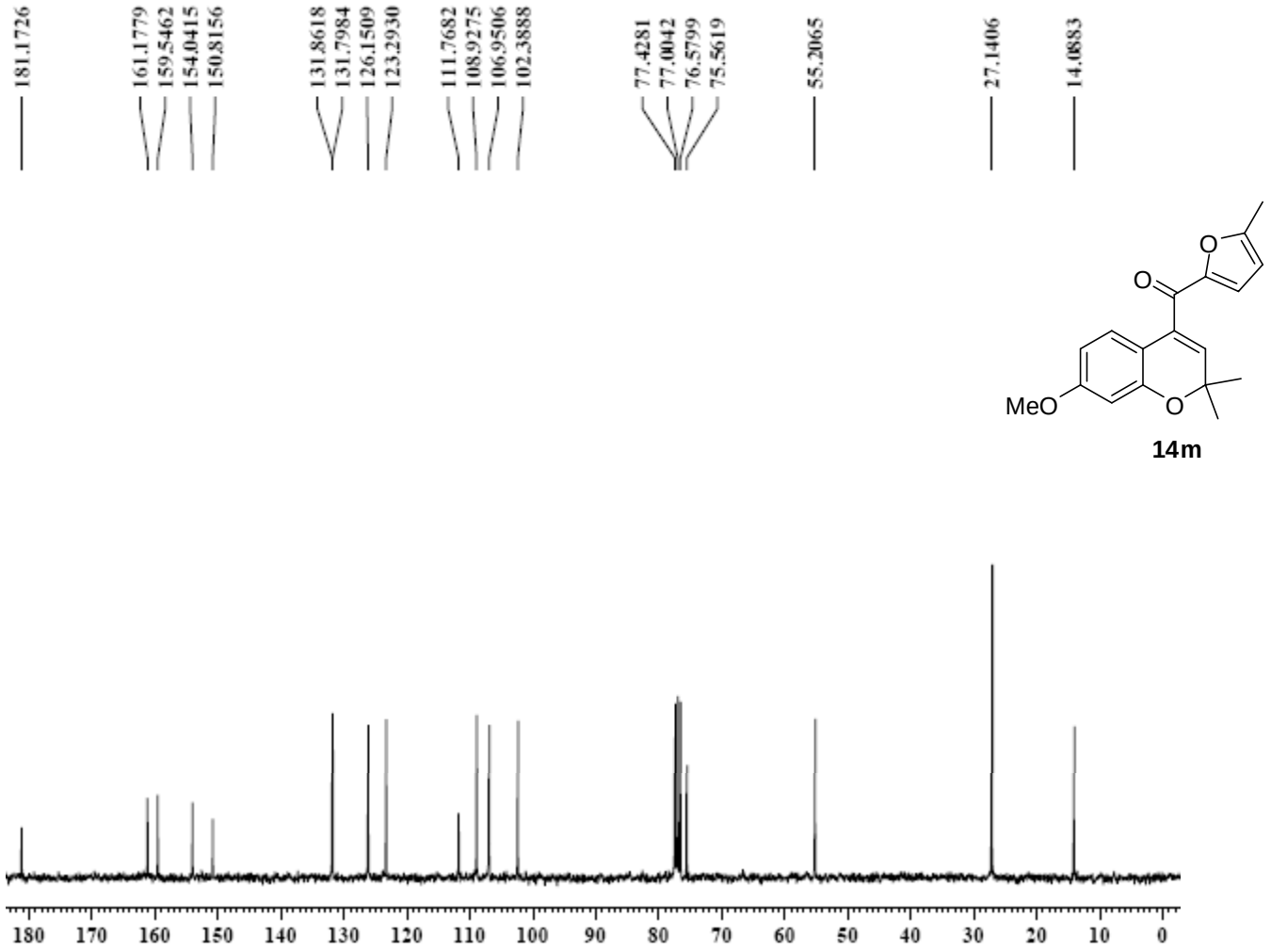


Fig. S-53: ^{1}H NMR of (7-methoxy-2,2-dimethyl-2H-chromen-4-yl)(5-methylfuran-2-yl)methanone(14m)

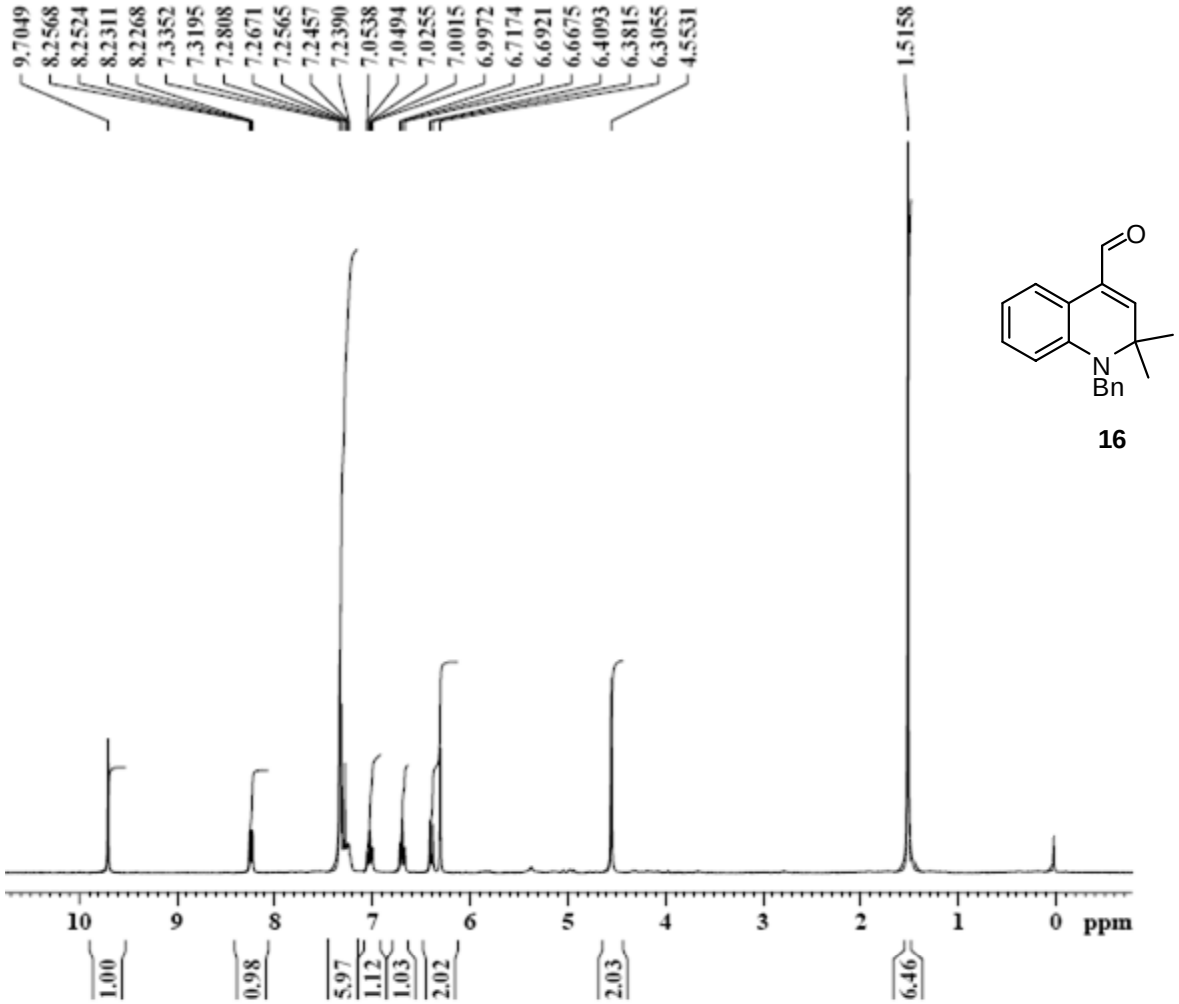


Fig. S-54: ^{1}H NMR of 1-Benzyl-2,2-dimethyl-1,2-dihydroquinoline-4-carbaldehyde (16)

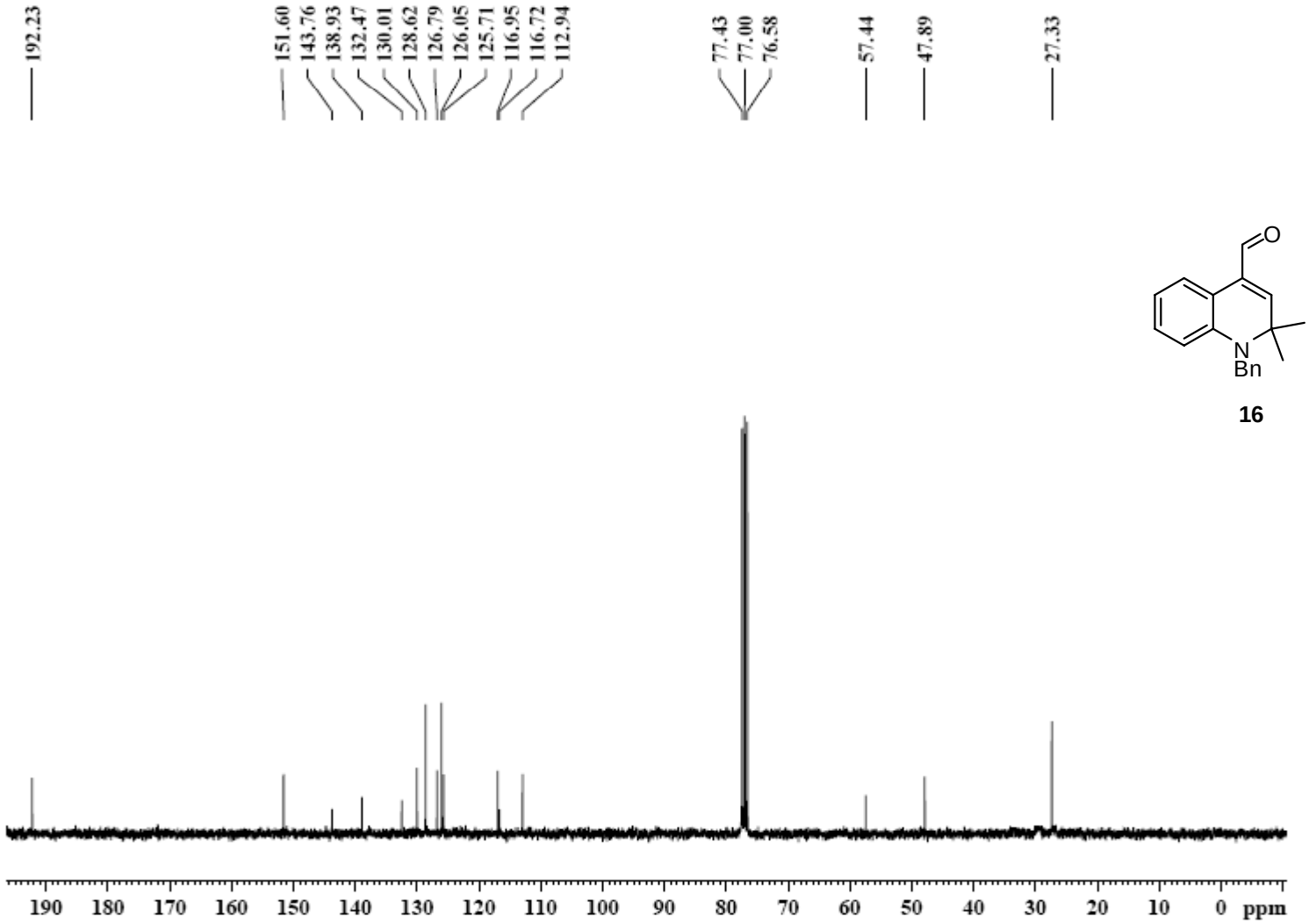


Fig. S-55: ^{13}C NMR of 1-Benzyl-2,2-dimethyl-1,2-dihydroquinoline-4-carbaldehyde (16)

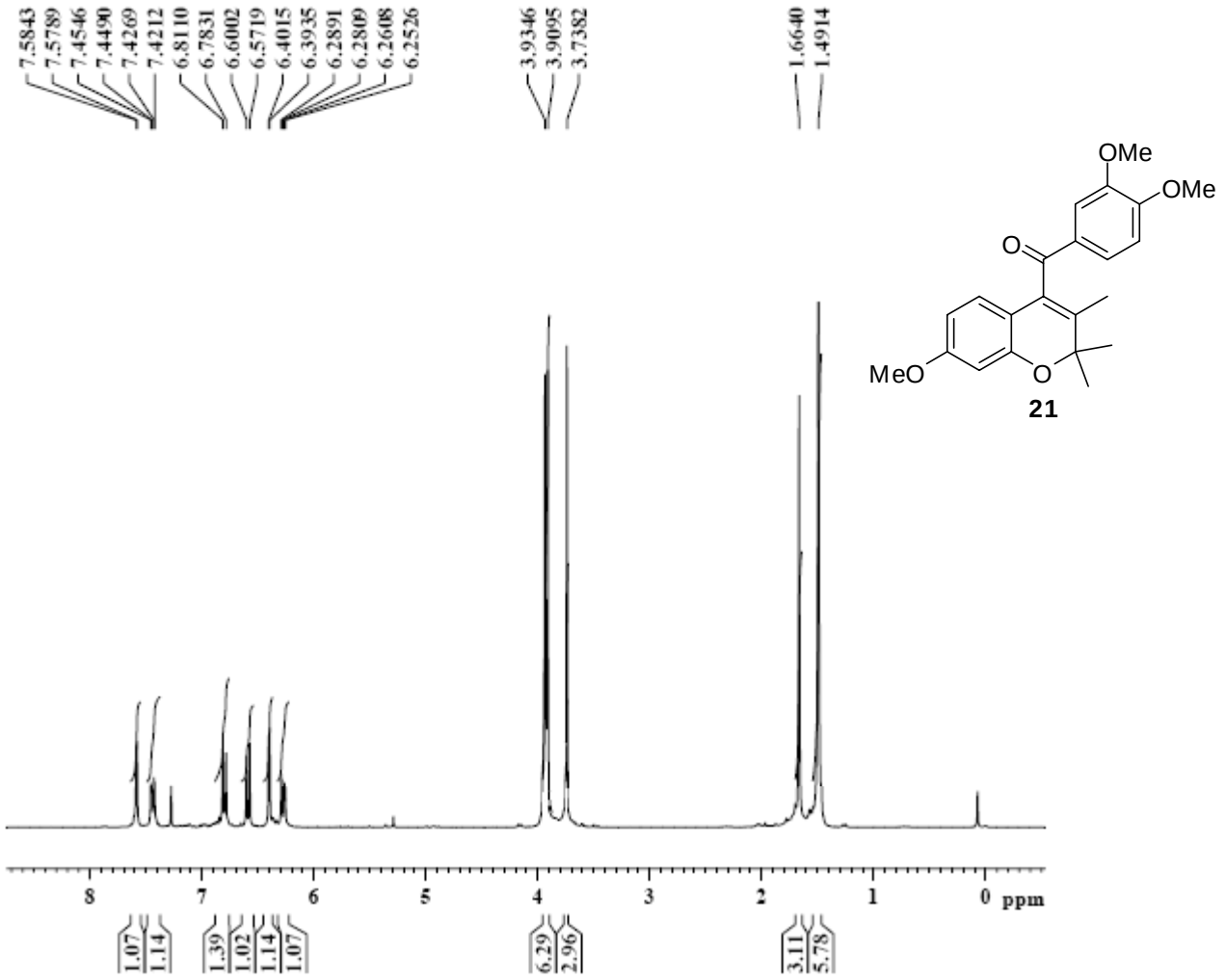


Fig. S-56: ^{1} H NMR of (3,4-dimethoxyphenyl)(7-methoxy-2,2,3-trimethyl-2H-chromen-4-yl)methanone (21)

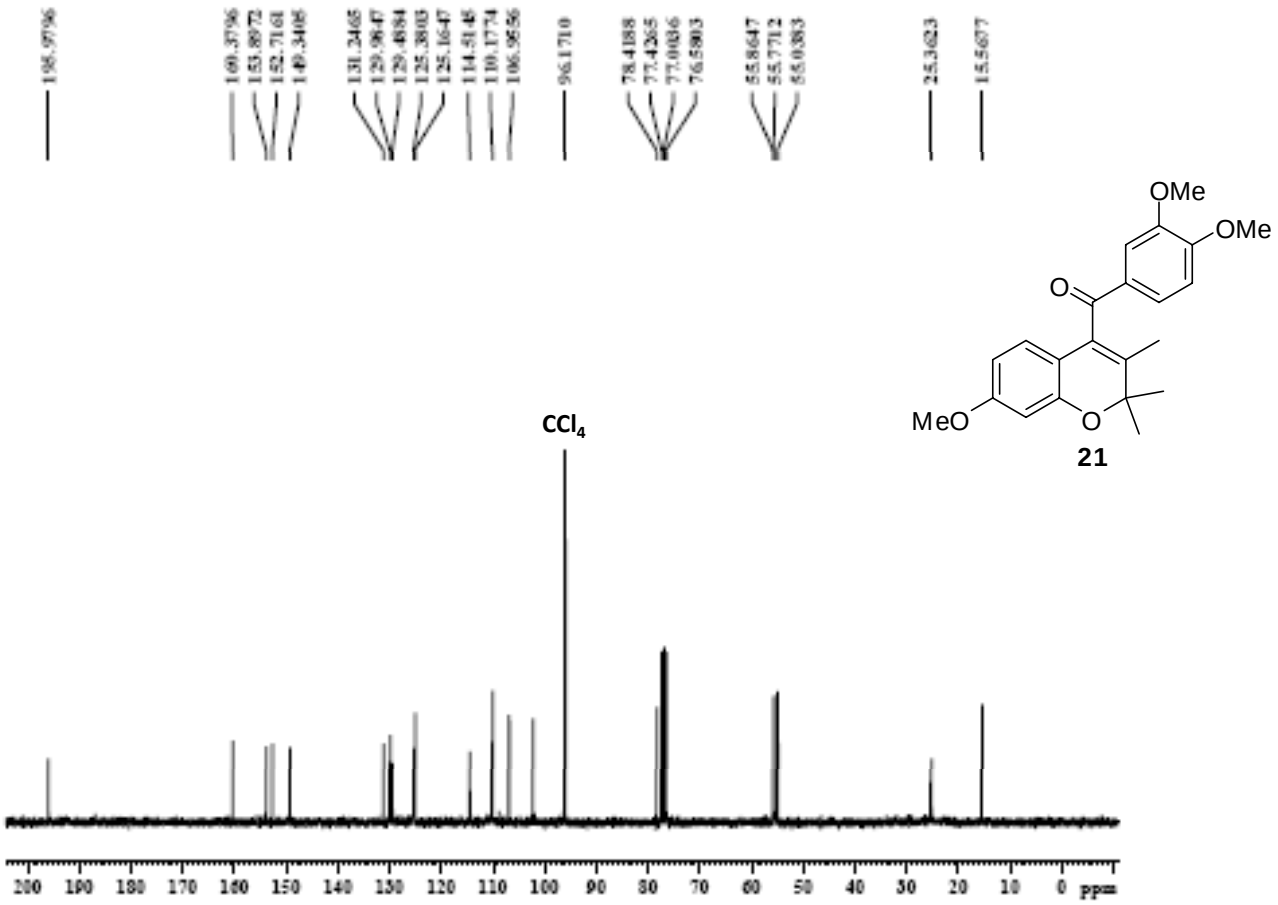


Fig. S-57: ^{13} C NMR of (3,4-dimethoxyphenyl)(7-methoxy-2,2,3-trimethyl-2H-chromen-4-yl)methanone (21)

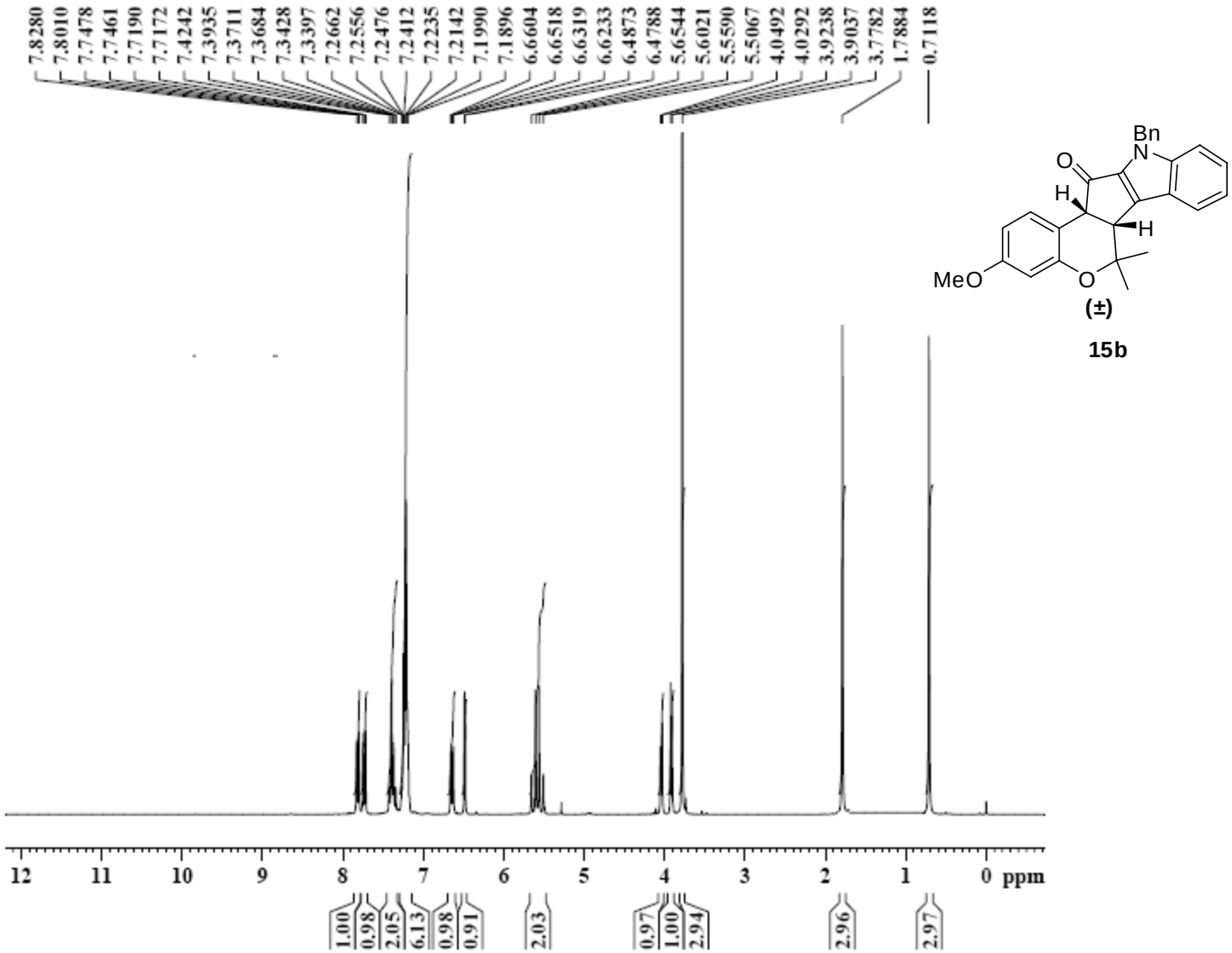


Fig. S-58: ^{1}H Spectra of (±)-11-Benzyl-3-methoxy-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-oxa-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15b)

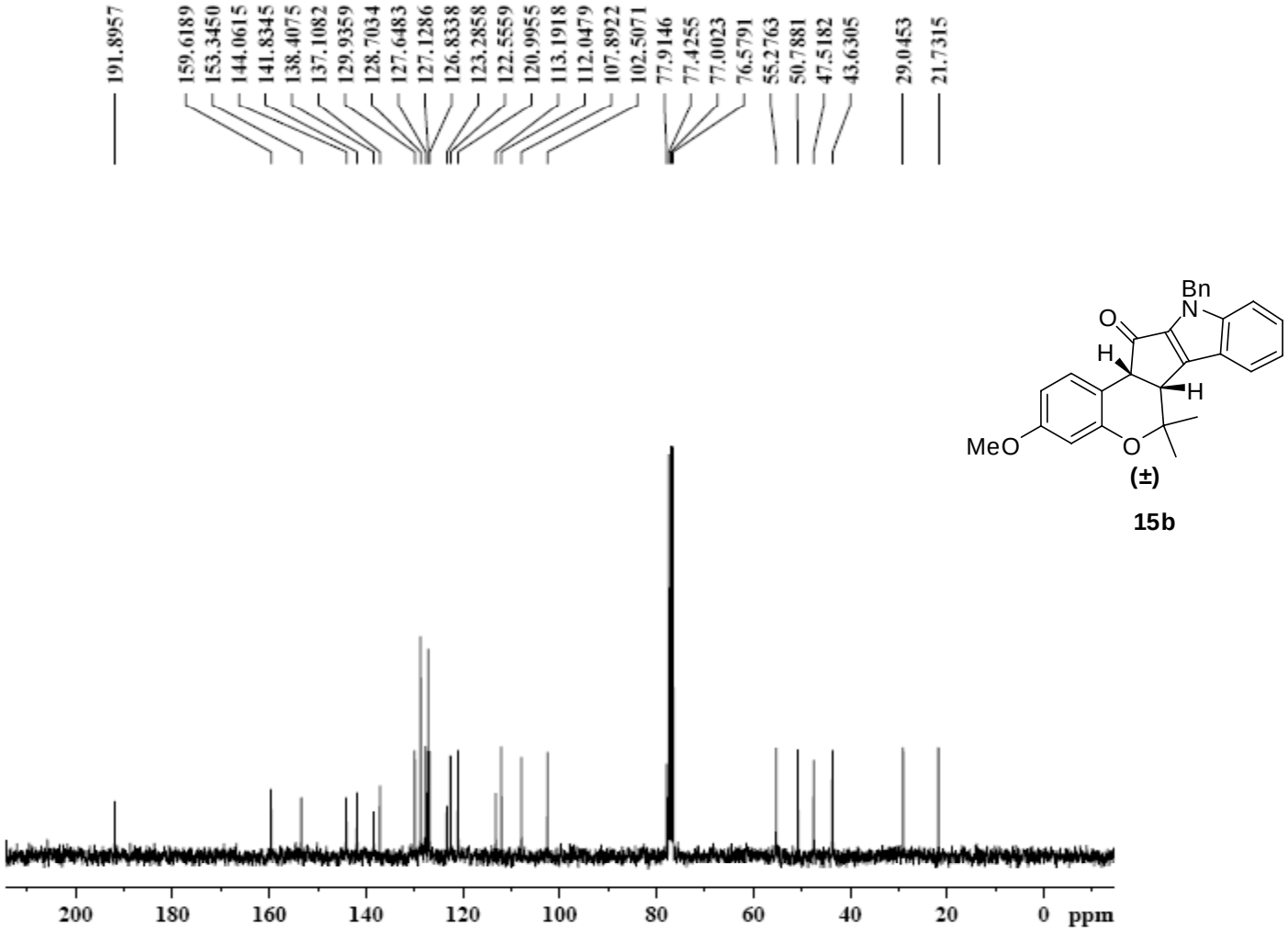


Fig. S-59: ^{13}C Spectra of (±)-11-Benzyl-3-methoxy-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-oxa-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15b)

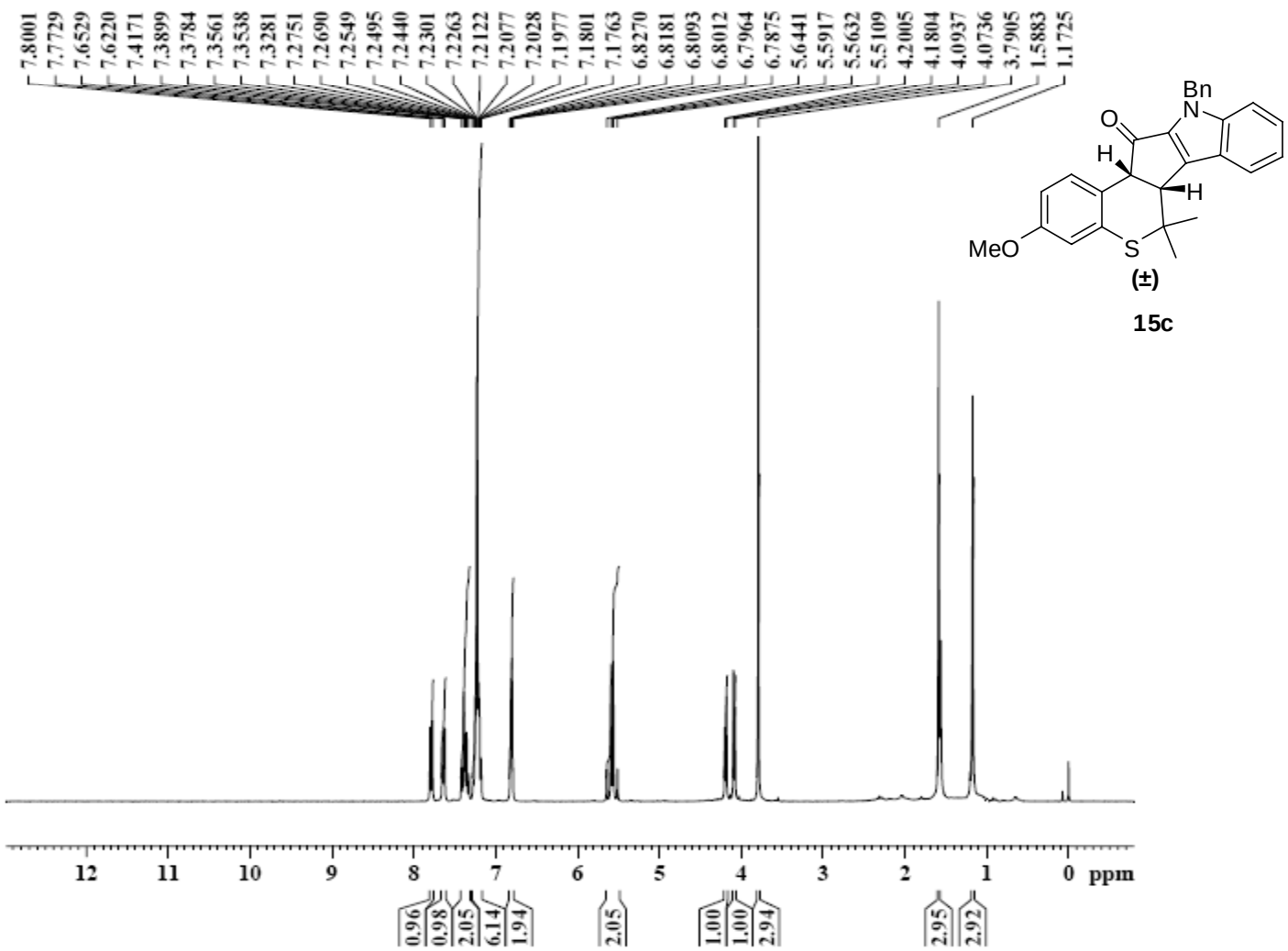


Fig. S-60: ^{1}H NMR of (±)-11-Benzyl-3-methoxy-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-thia-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15c)

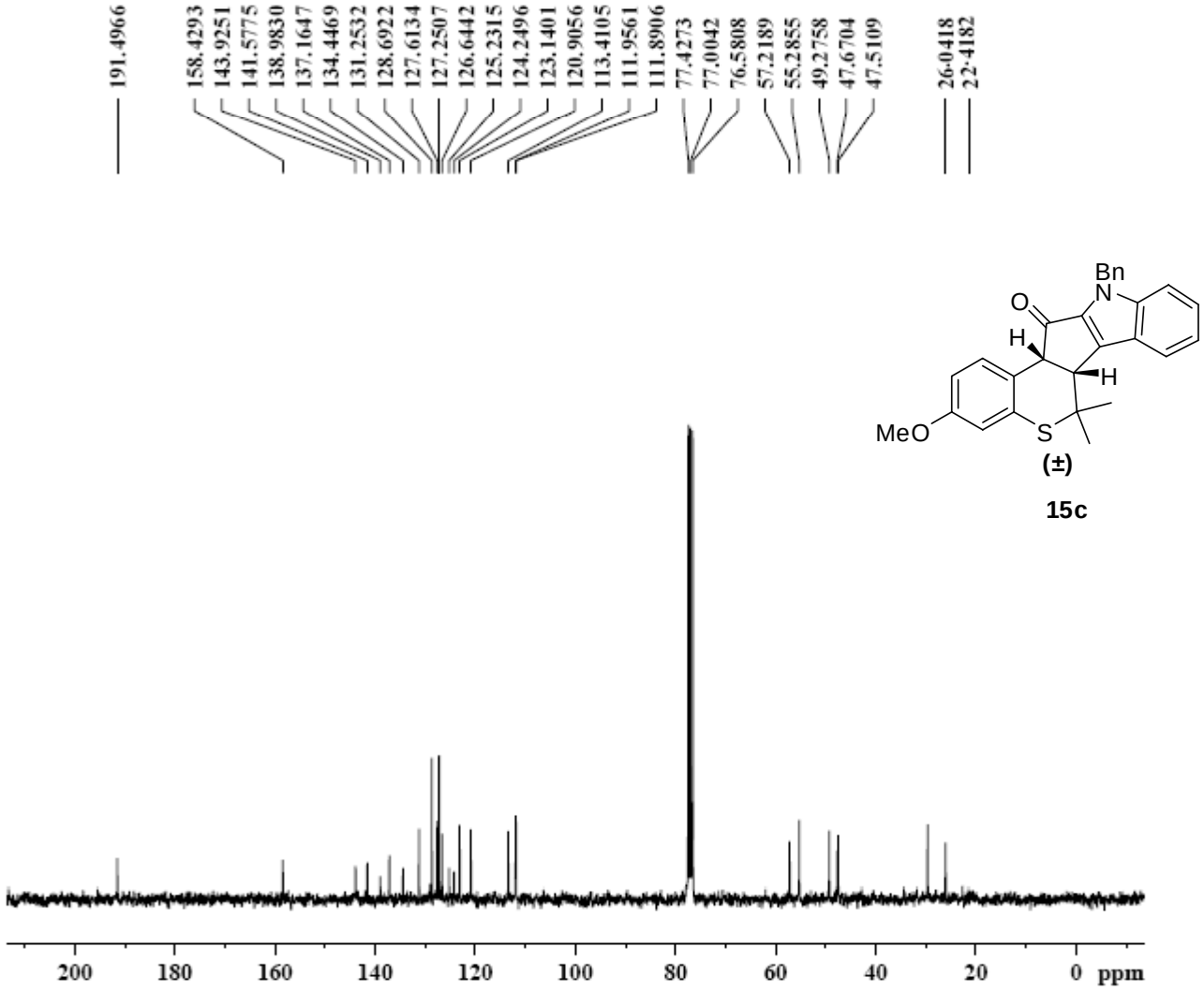


Fig. S-61: ^{13}C NMR of (±)-11-Benzyl-3-methoxy-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-thia-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15c)

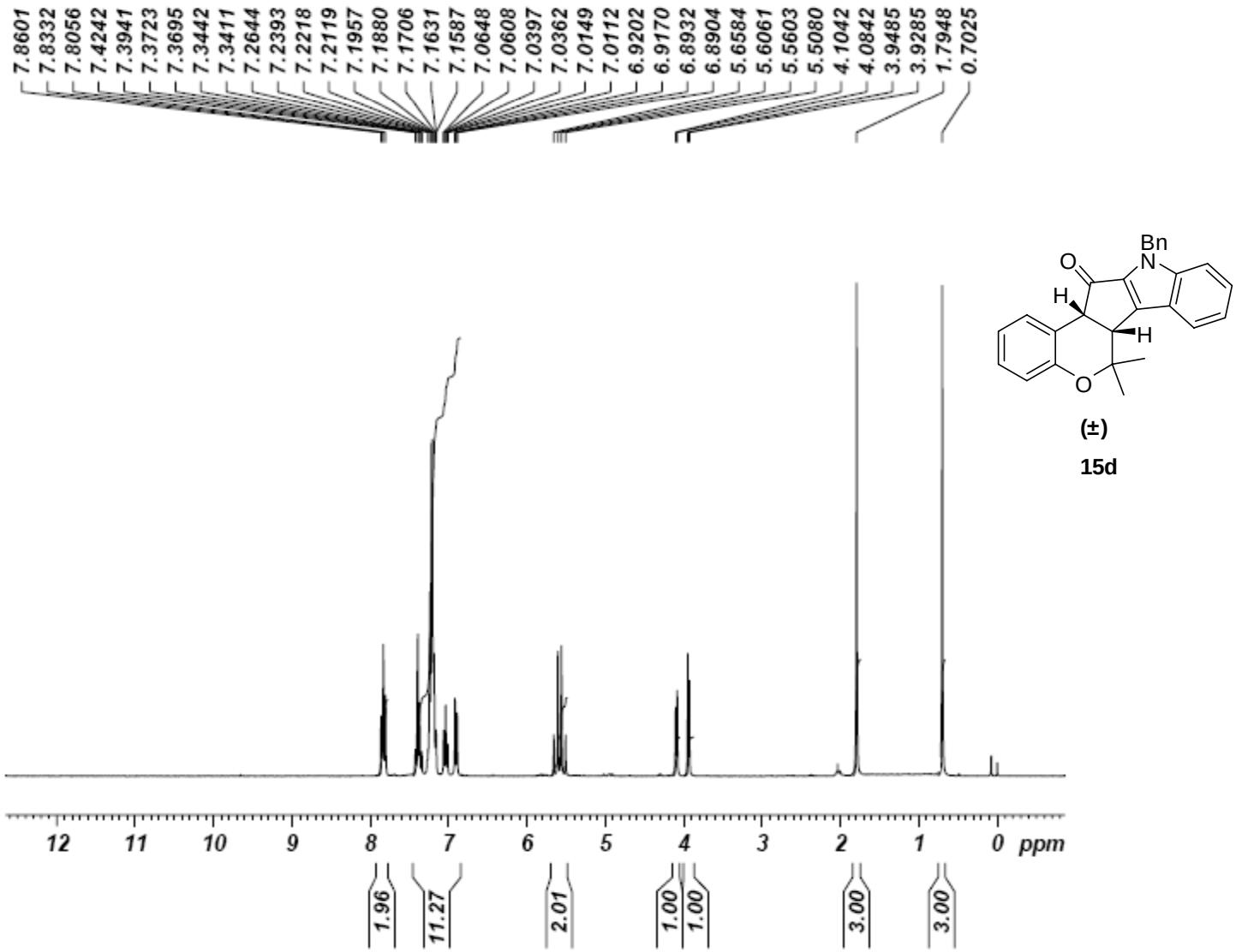


Fig. S-62: ^{1}H NMR of (±)11-Benzyl-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-oxa-11-azabenzo[5,6]pentaleno[2,1-b]naphthalene (15d)

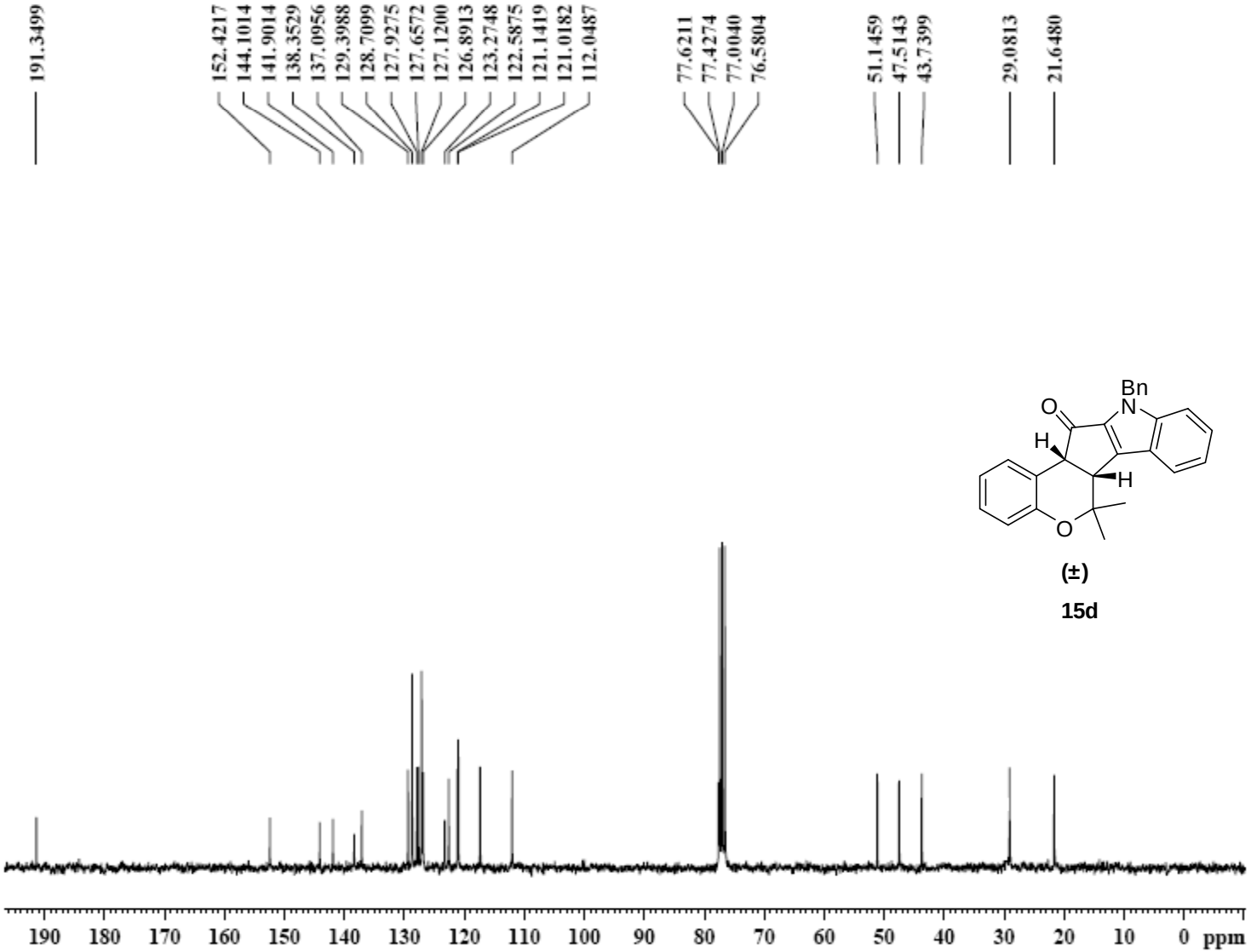


Fig. S-63: ^{13}C NMR of (±)11-Benzyl-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-oxa-11-azabenzo[5,6]pentaleno[2,1-b]naphthalene (15d)

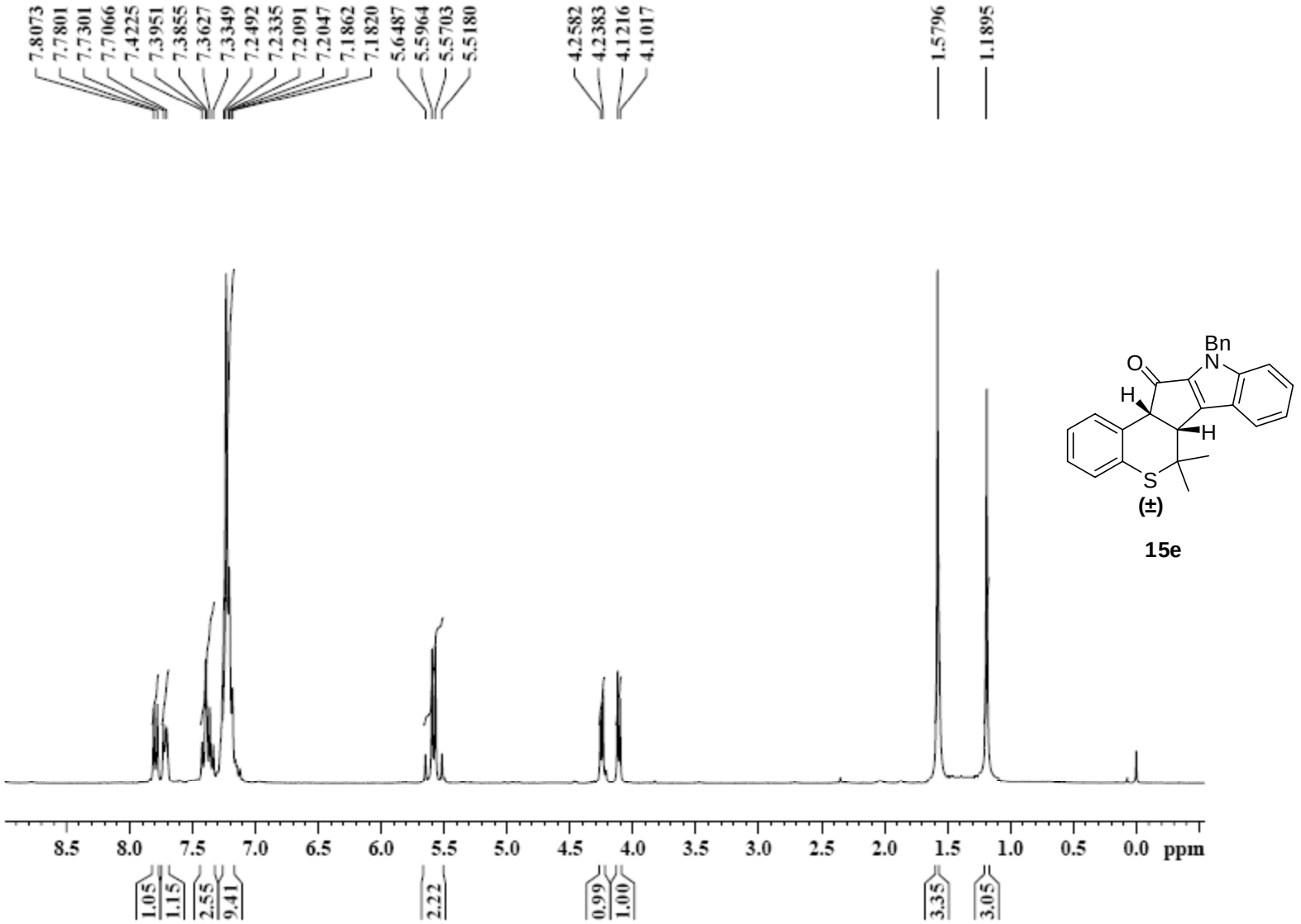


Fig. S-64: ^{1}H NMR of (±)-11-Benzyl-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-thia-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15e)

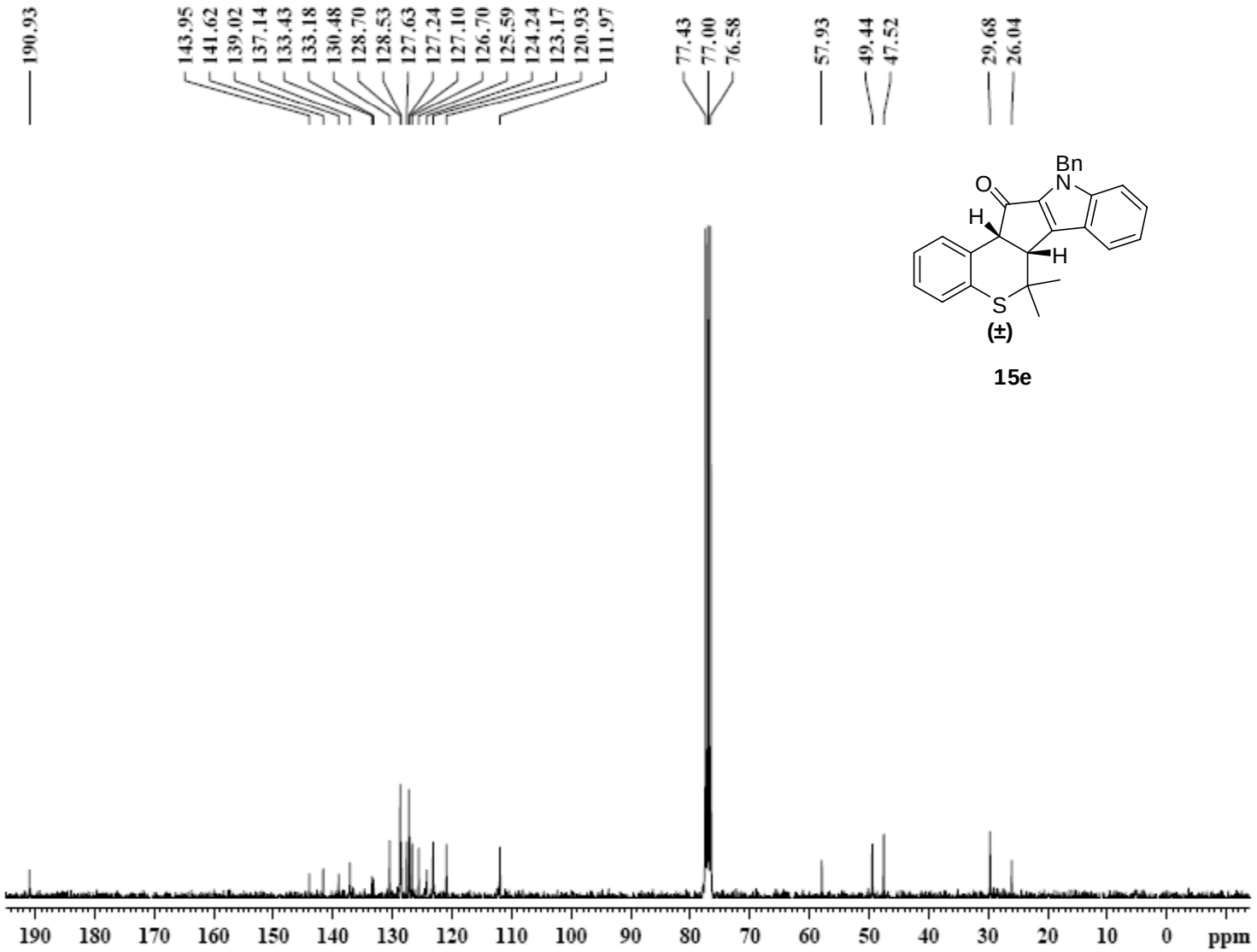


Fig. S-65: ^{13}C NMR of (±)-11-Benzyl-6,6-dimethyl-6a,11-dihydro-6H,12aH-5-thia-11-azabenzo[5,6]pentaleno[2,1-b]naphthalen-12-one (15e)

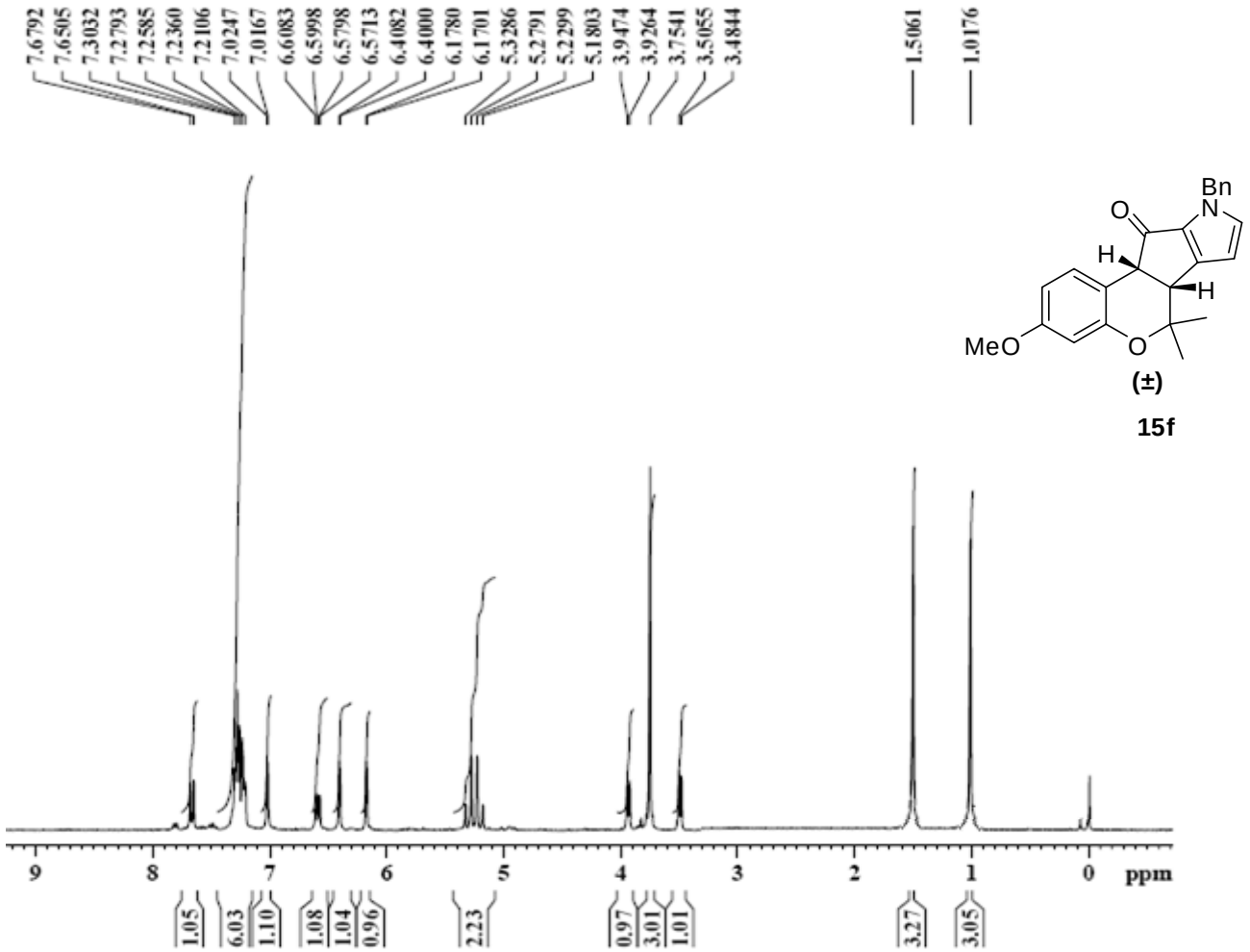


Fig. S-66: ^{1}H NMR of (±) -(9-Benzyl-3-methoxy-6,6-dimethyl-6a,9-dihydro-6H,10aH-5-oxa-9-azapentaleno[2,1-a]naphthalen-10-one (15f)

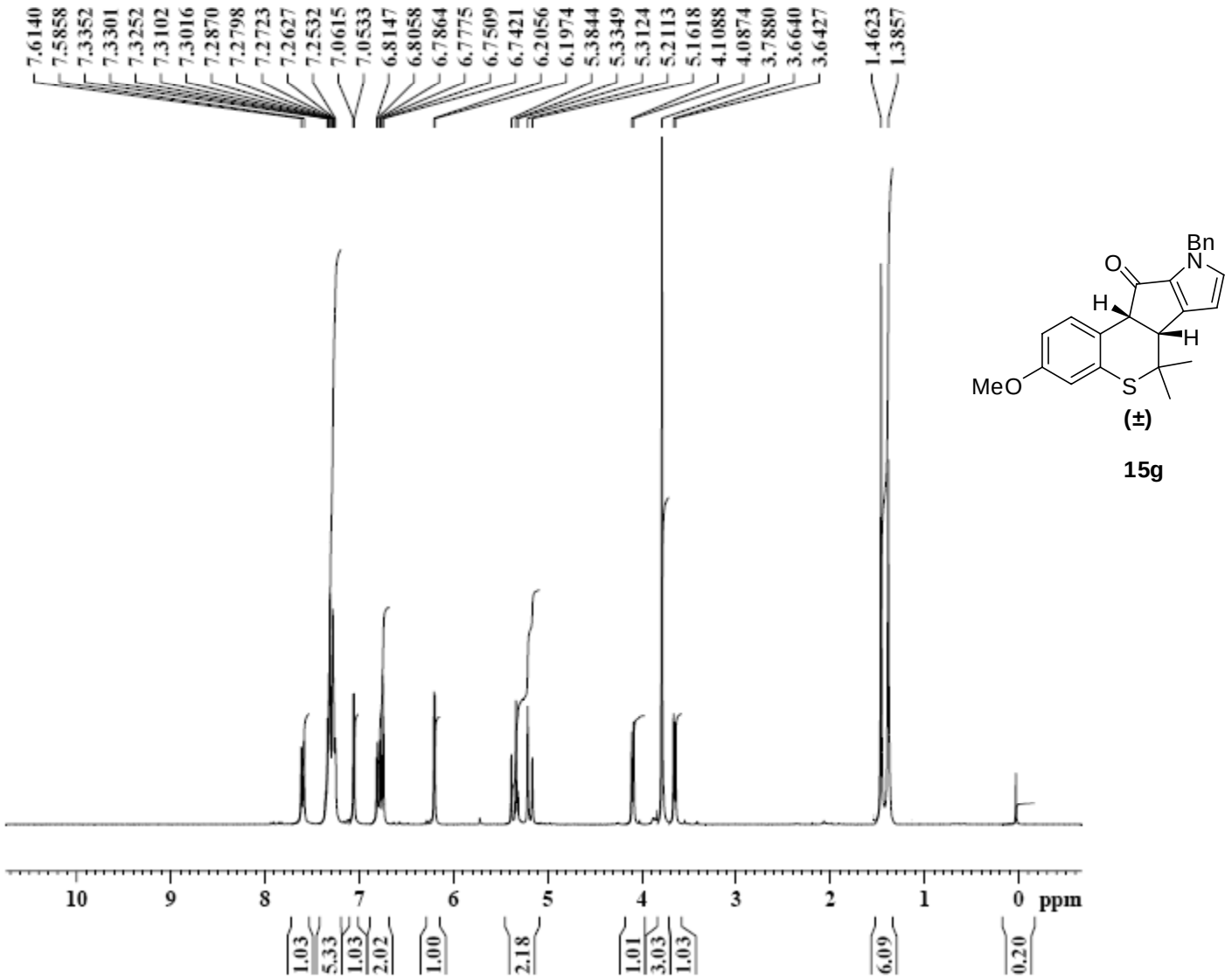


Fig. S-67: ^{1}H NMR of (±)-9-Benzyl-3-methoxy-6,6-dimethyl-6a,9-dihydro-6H,10aH-5-thia-9-azapentaleno[2,1-a]naphthalen-10-one (15g)

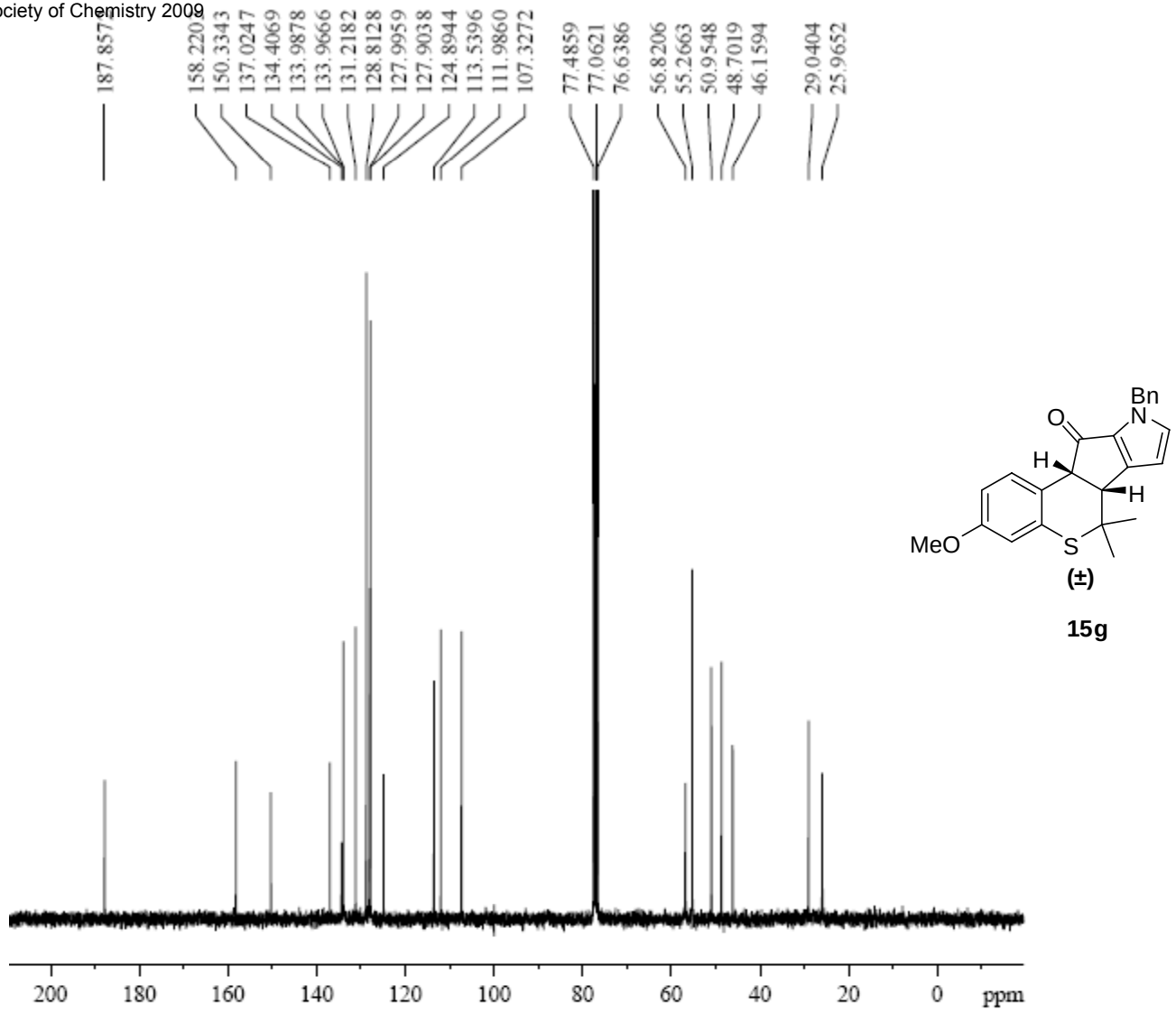


Fig. S-68: ^{13}C NMR of (±)-9-Benzyl-3-methoxy-6,6-dimethyl-6a,9-dihydro-6H,10aH-5-thia-9-azapentaleno[2,1-a]naphthalen-10-one (15g)

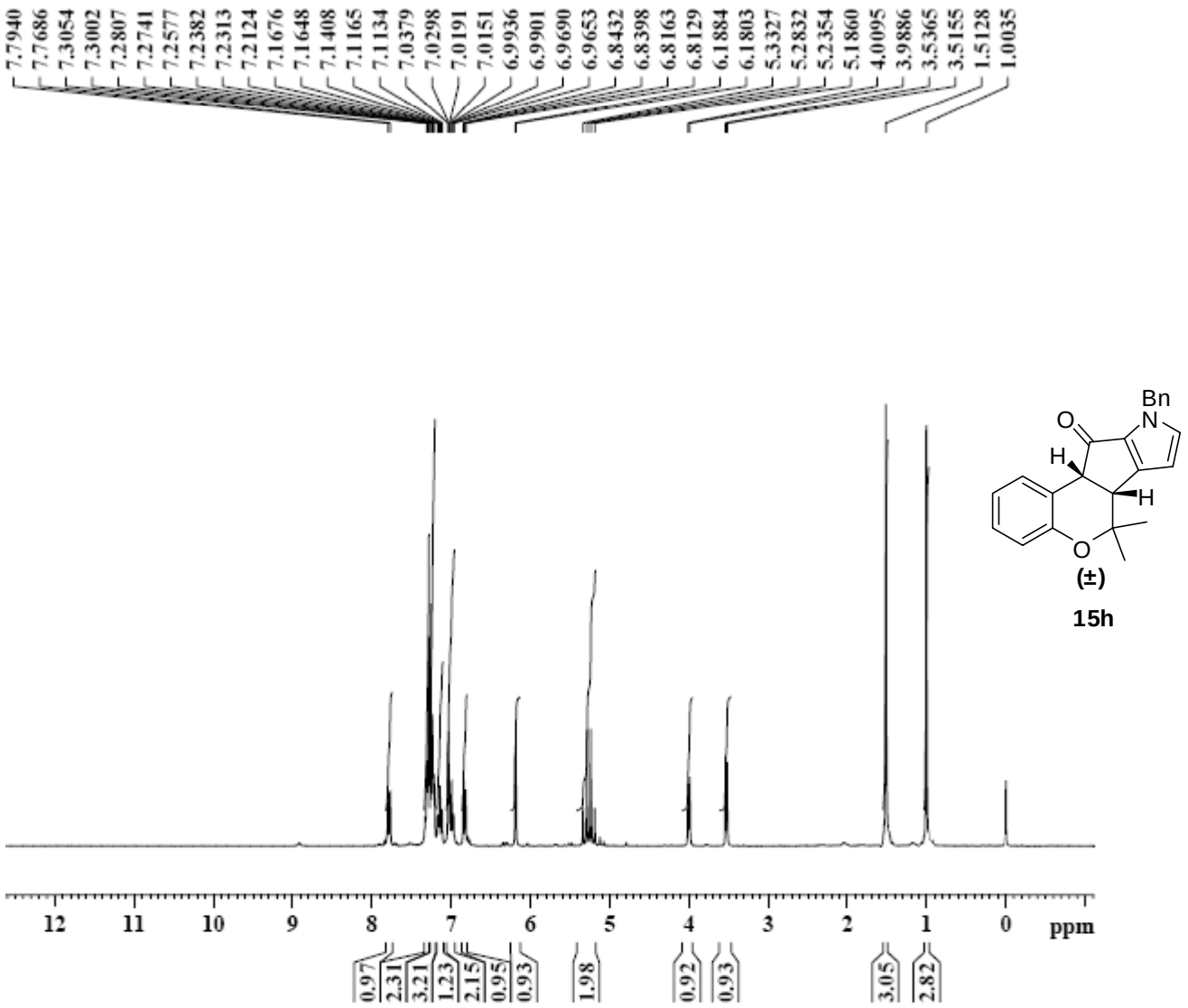


Fig. S-69: ^{1}H NMR of (±)-9-Benzyl-6,6-dimethyl-6a,9-dihydro-6H,10aH-5-oxa-9-azapentaleno[2,1-a]naphthalen-10-one (15h)

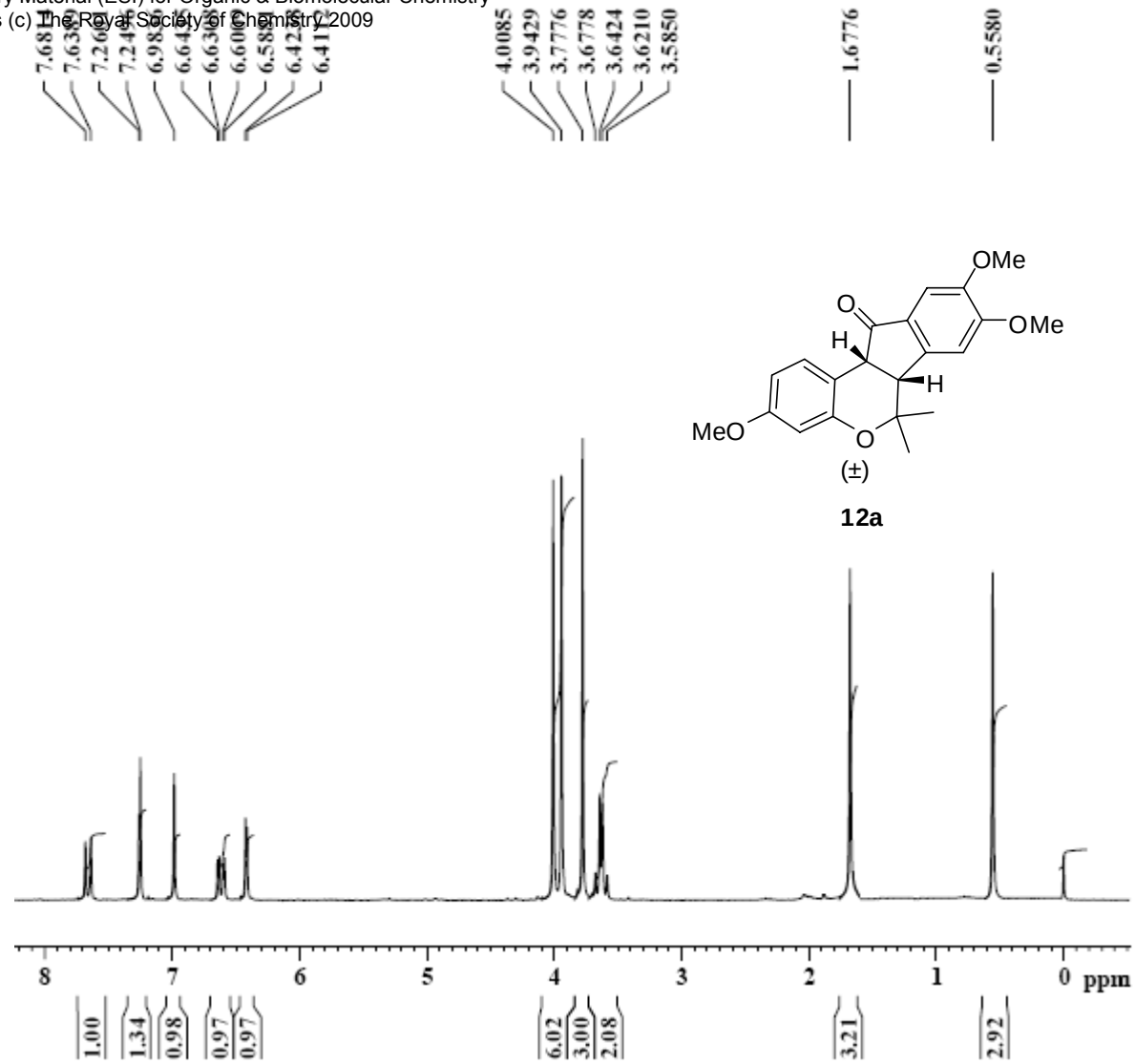


Fig. S-70: ^{1}H NMR of (±)-3,8,9-Trimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-indeno[1,2-c]chromen-11-one (12a)

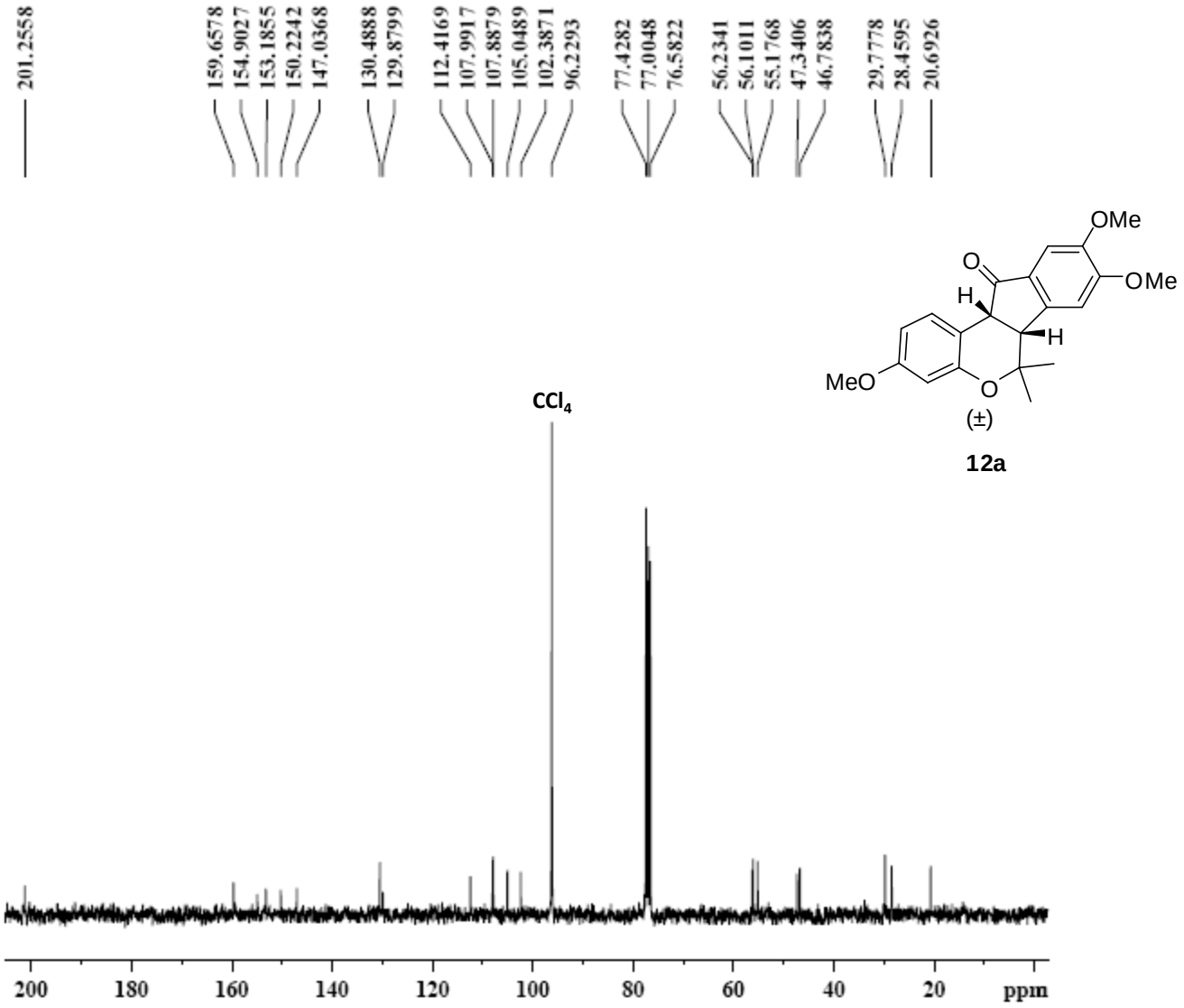


Fig. S-71: ^{13}C NMR of (±)-3,8,9-Trimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-indeno[1,2-c]chromen-11-one (12a)

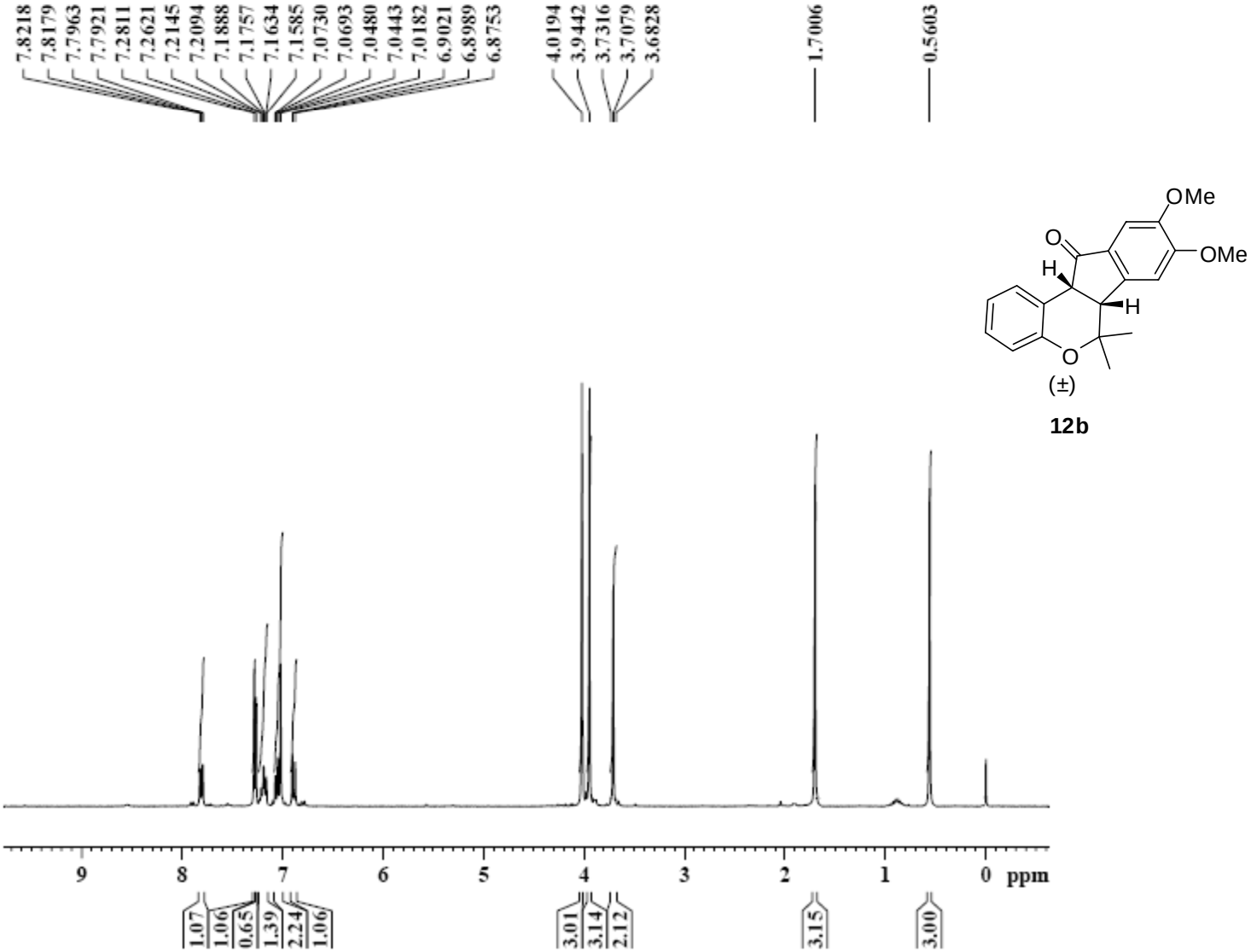


Fig. S-72: ^{1}H NMR of (±)- (8,9-Dimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-indeno[1,2-c]chromen-11- one (12b)

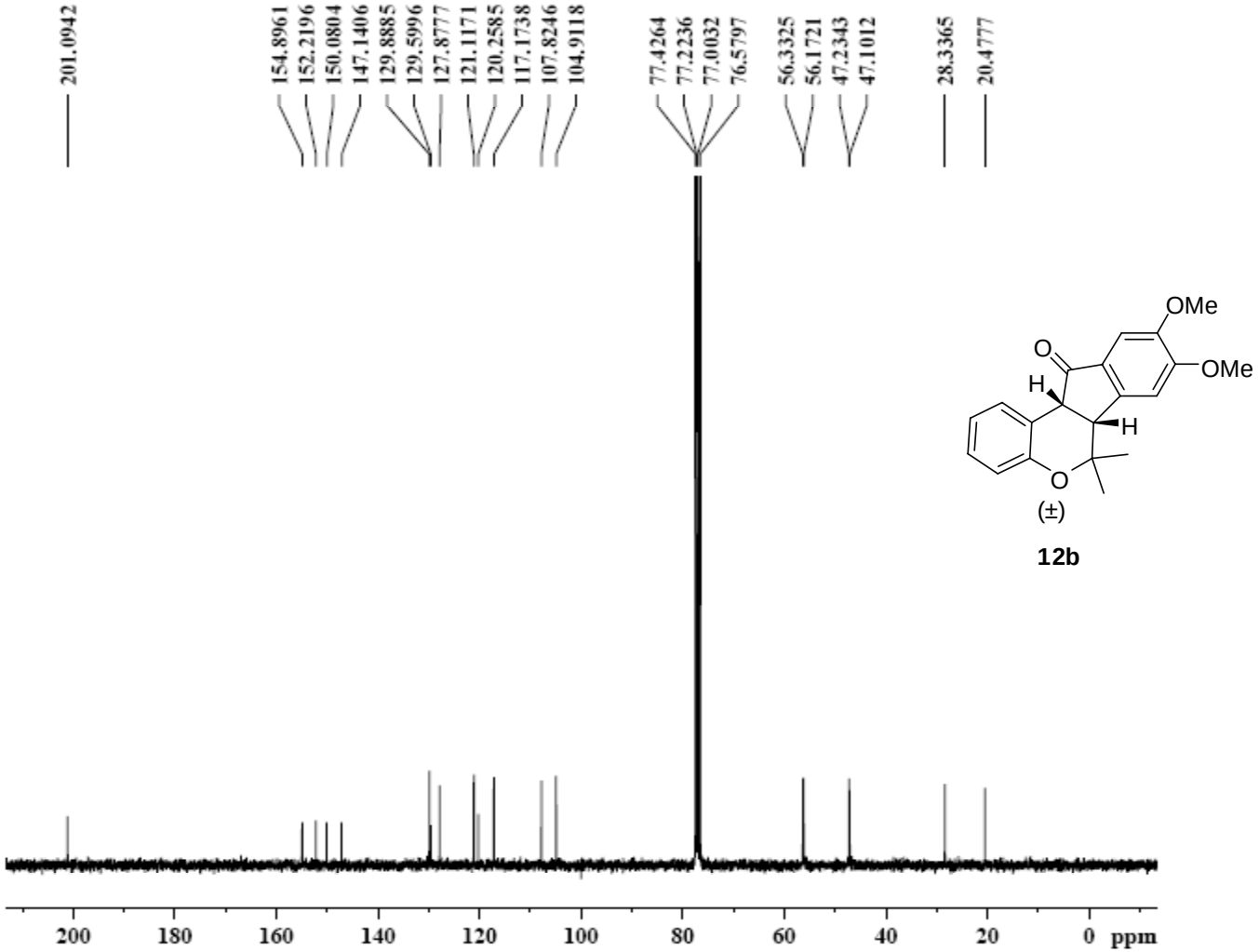


Fig. S-73: ^{13}C NMR of (±)- (8,9-Dimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-indeno[1,2-c]chromen-11- one (12b)

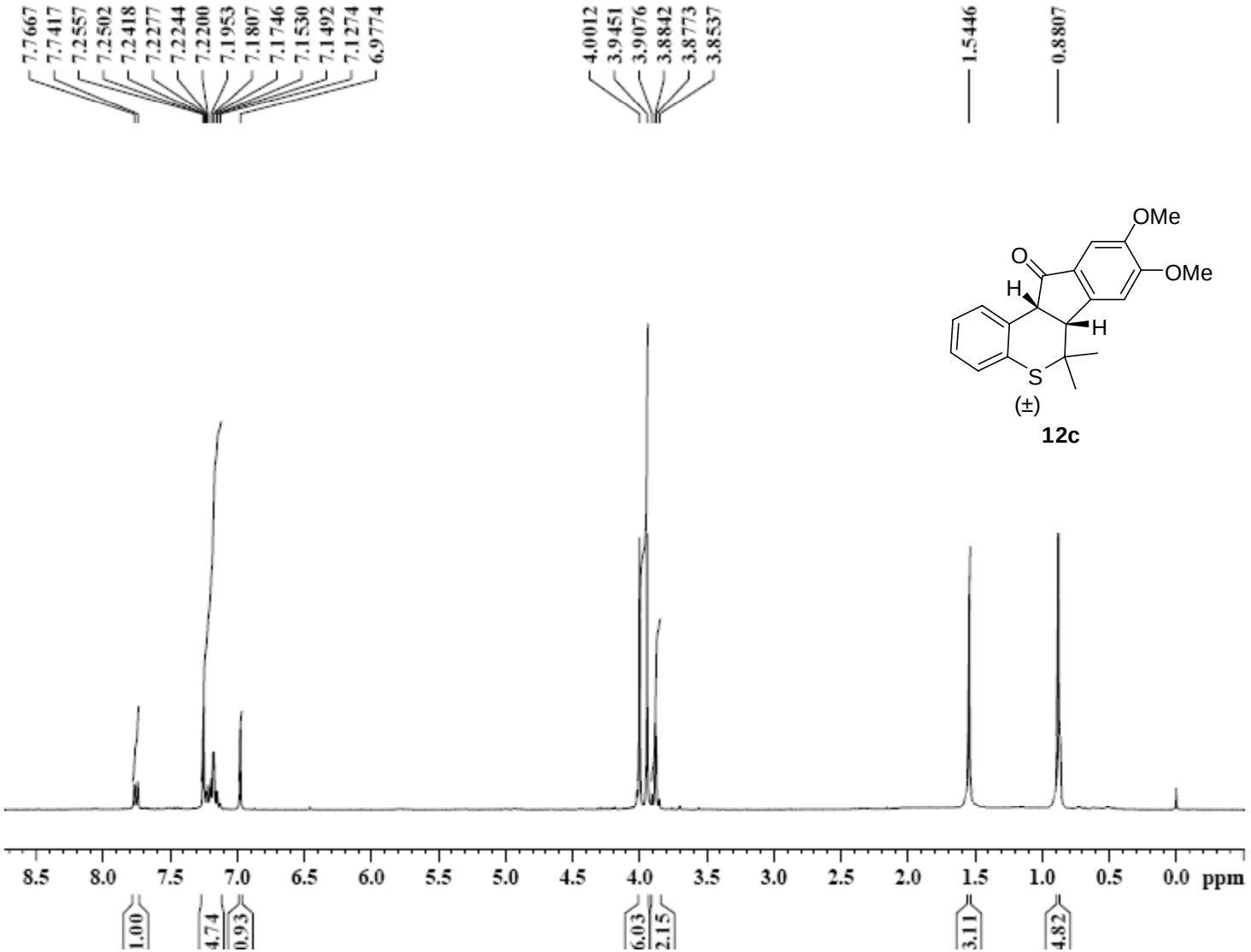


Fig. S-74: ^{1}H NMR of (±)-8,9-Dimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-5-thiabenzo[a]fluoren-11-one (12c)

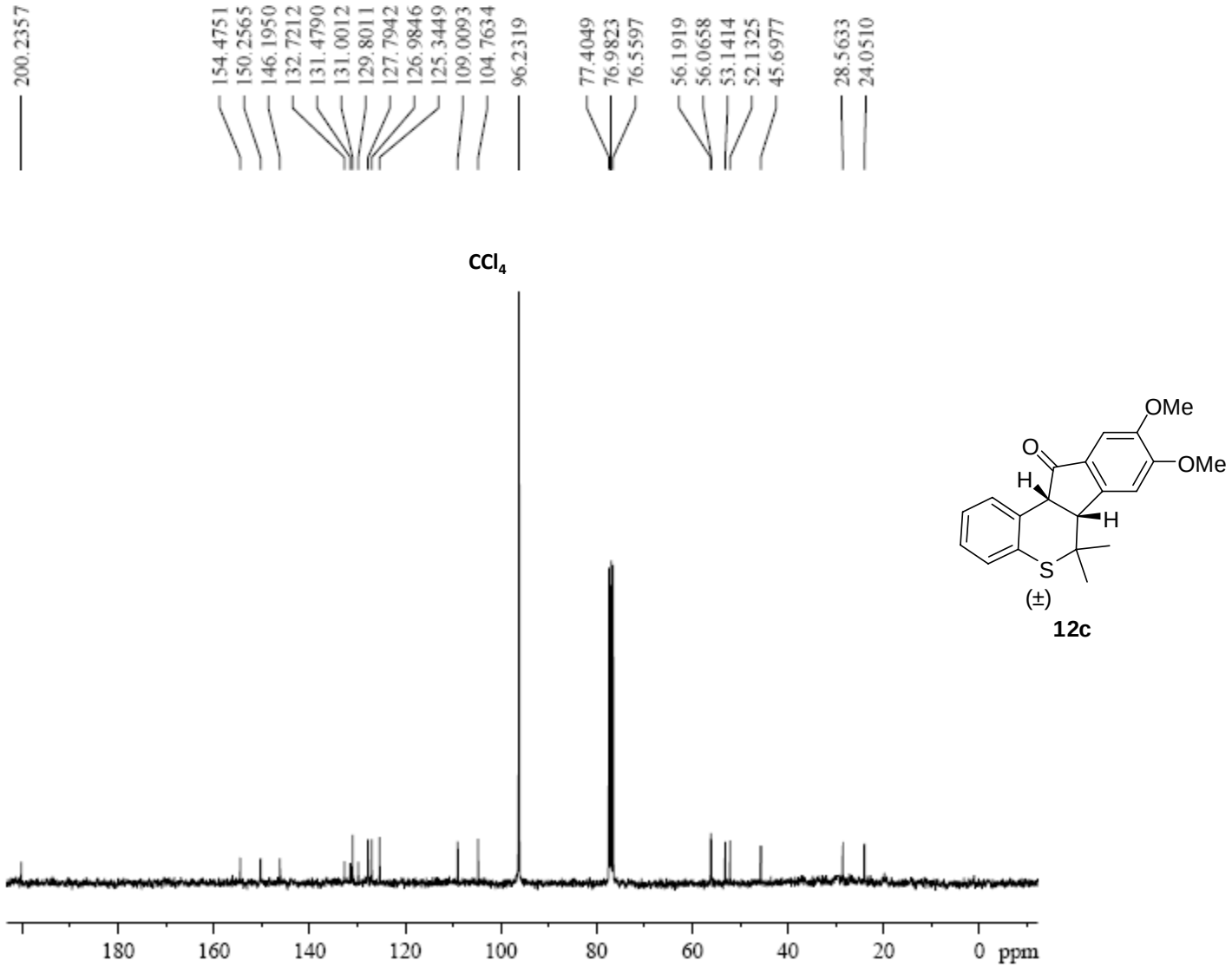


Fig. S-75: ^{13}C NMR of (±)-8,9-Dimethoxy-6,6-dimethyl-6a,11a-dihydro-6H-5-thiabenzo[a]fluoren-11-one (12c)

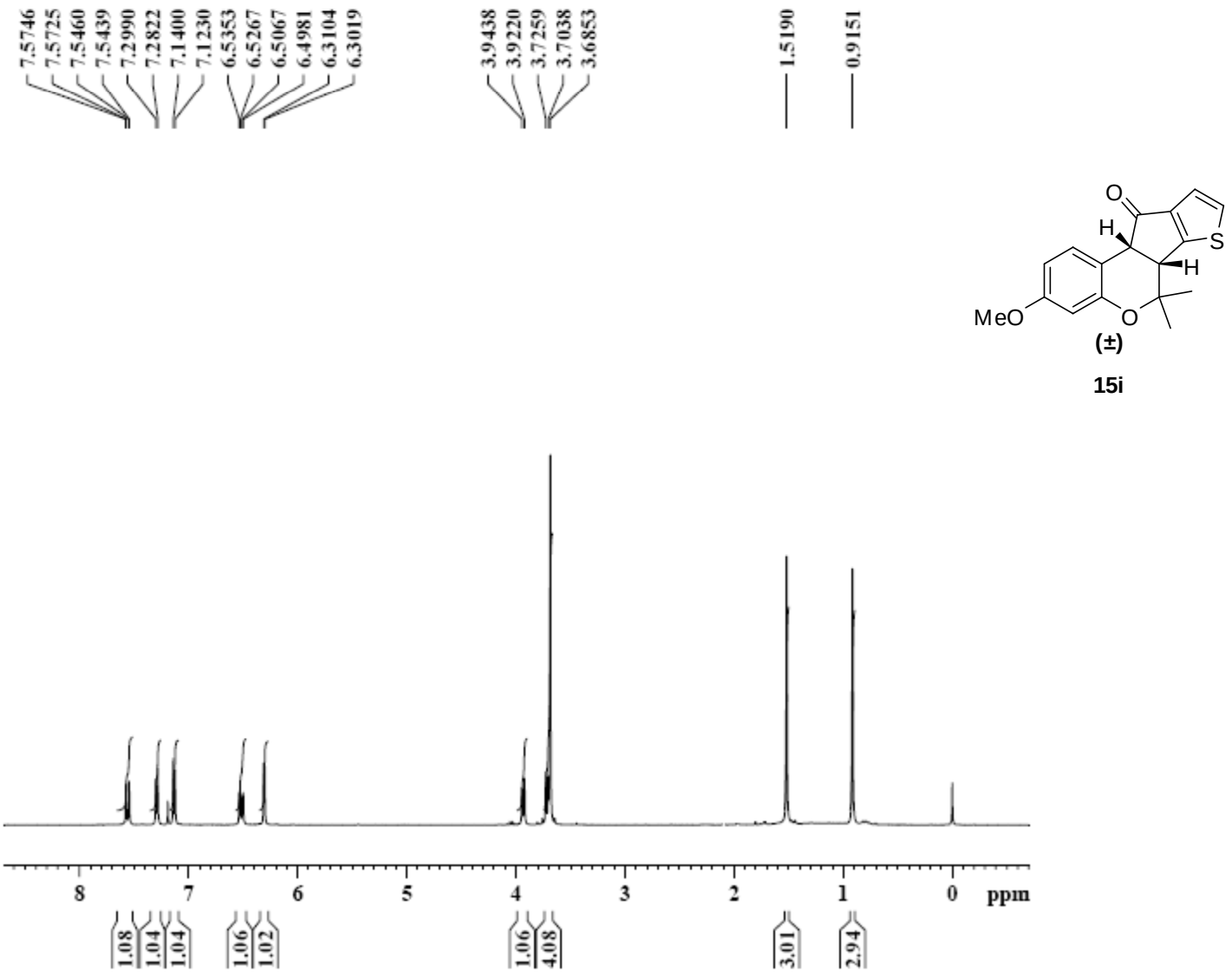


Fig. S-76: ^{1}H NMR of (±)-3-Methoxy-6,6-dimethyl-6a,10a-dihydro-6H-5-oxa-7-thiapentaleno[2,1-a]naphthalen-10-one (15i)

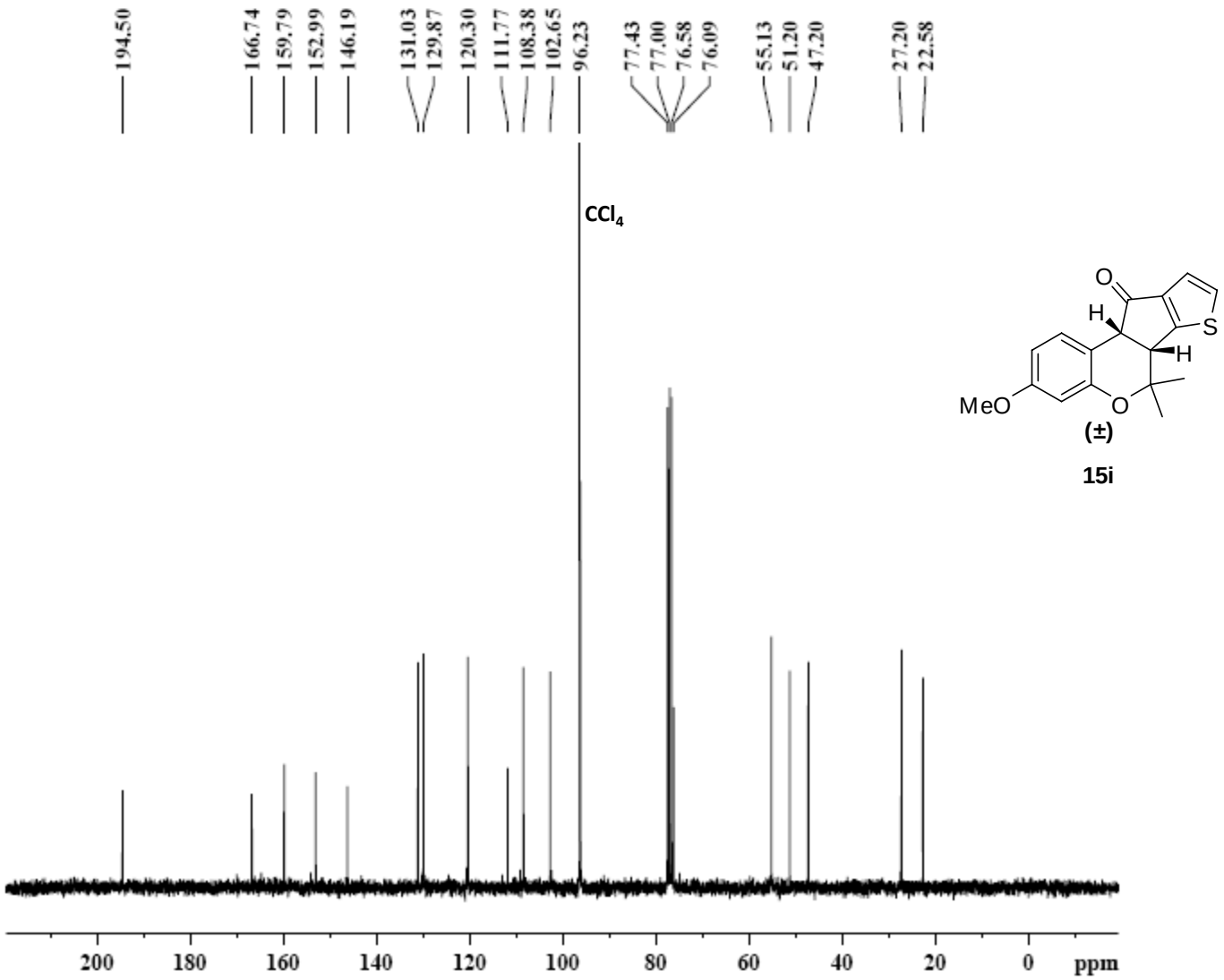


Fig. S-77: ^{13}C NMR of (±)-3-Methoxy-6,6-dimethyl-6a,10a-dihydro-6H-5-oxa-7-thiapentaleno[2,1-a]naphthalen-10-one (15i)

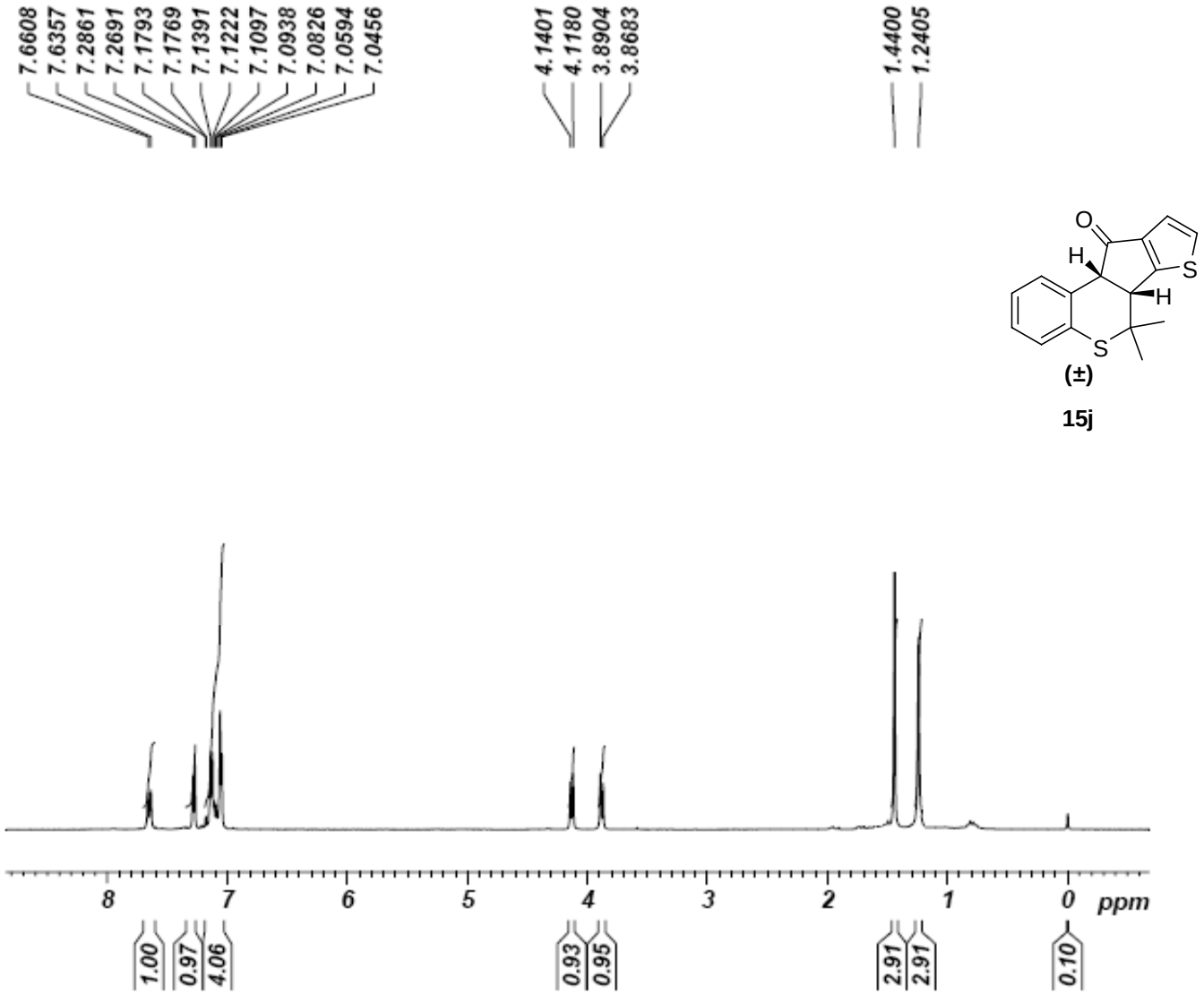


Fig. S-78: ^{1}H NMR of (±)-6,6-Dimethyl-6a,11a-dihydro-6H,7H-5,8-dithiacyclopenta[b]phenanthren-11- one (15j)

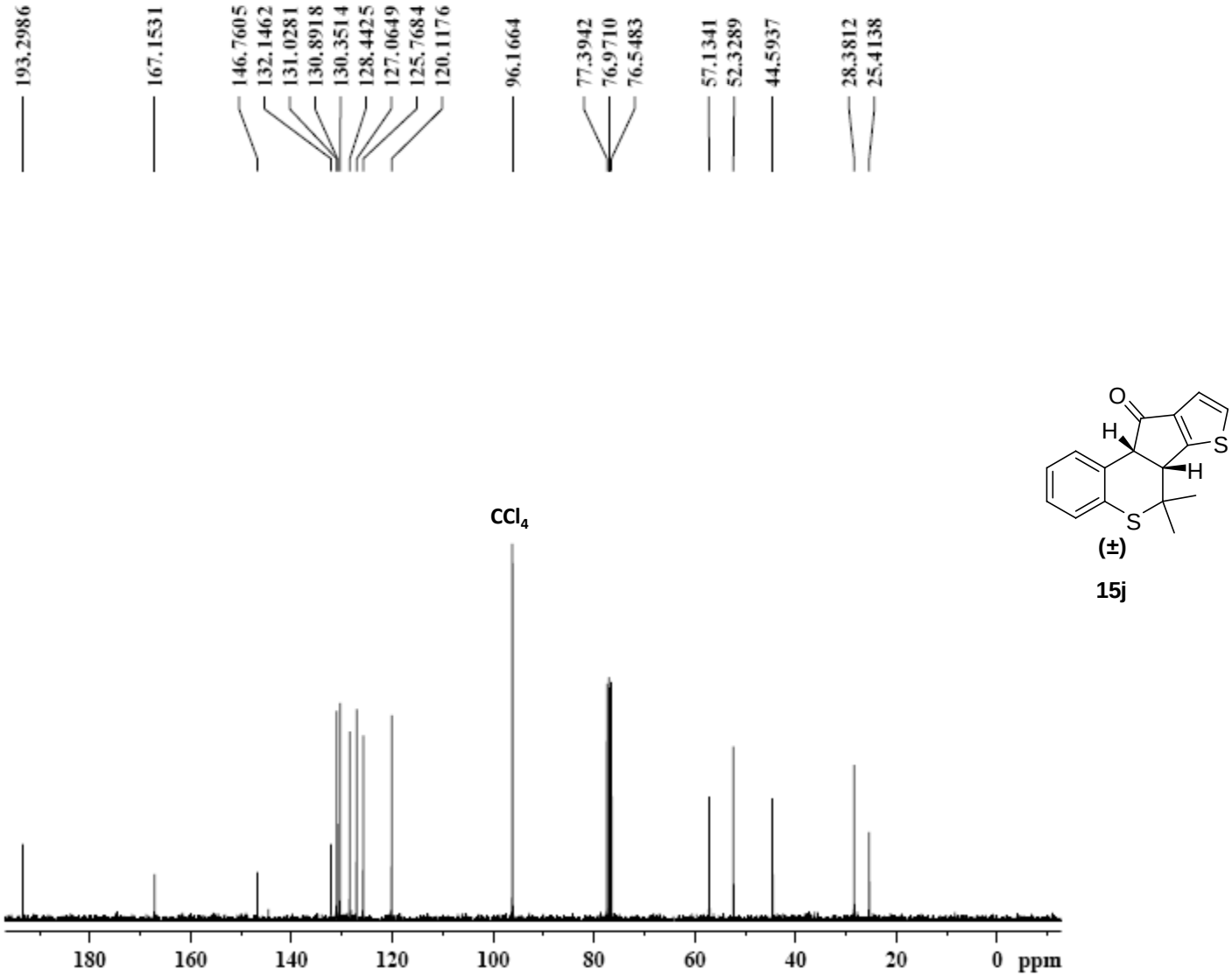


Fig. S-79: ^{13}C NMR of (±)-6,6-Dimethyl-6a,11a-dihydro-6H,7H-5,8-dithiacyclopenta[b]phenanthren-11- one (15j)

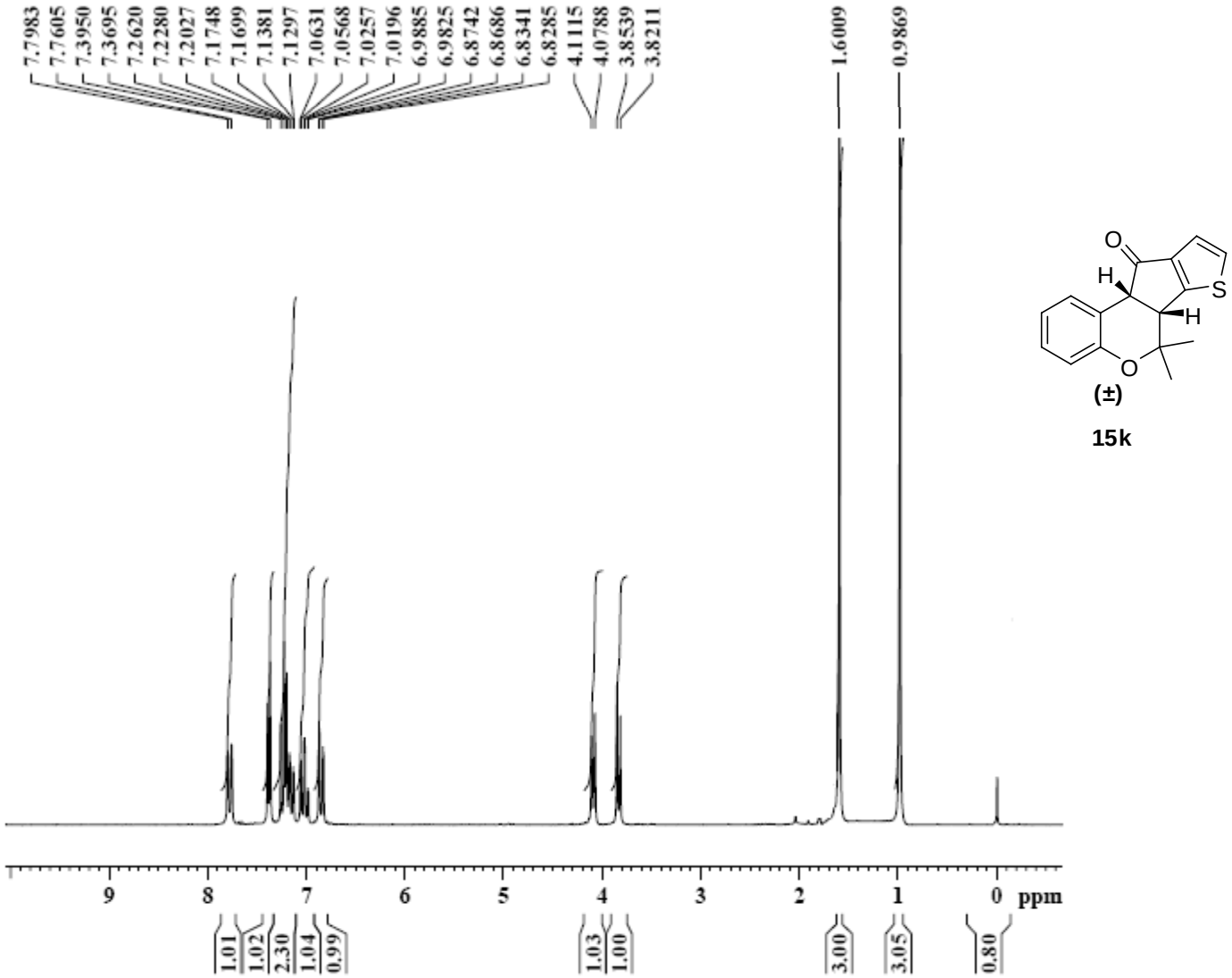


Fig. S-80: ^{1}H NMR of (±)-6,6-Dimethyl-6a,10a-dihydro-6H-5-oxa-7-thiapentaleno[2,1-a]naphthalen-10-one (15k)

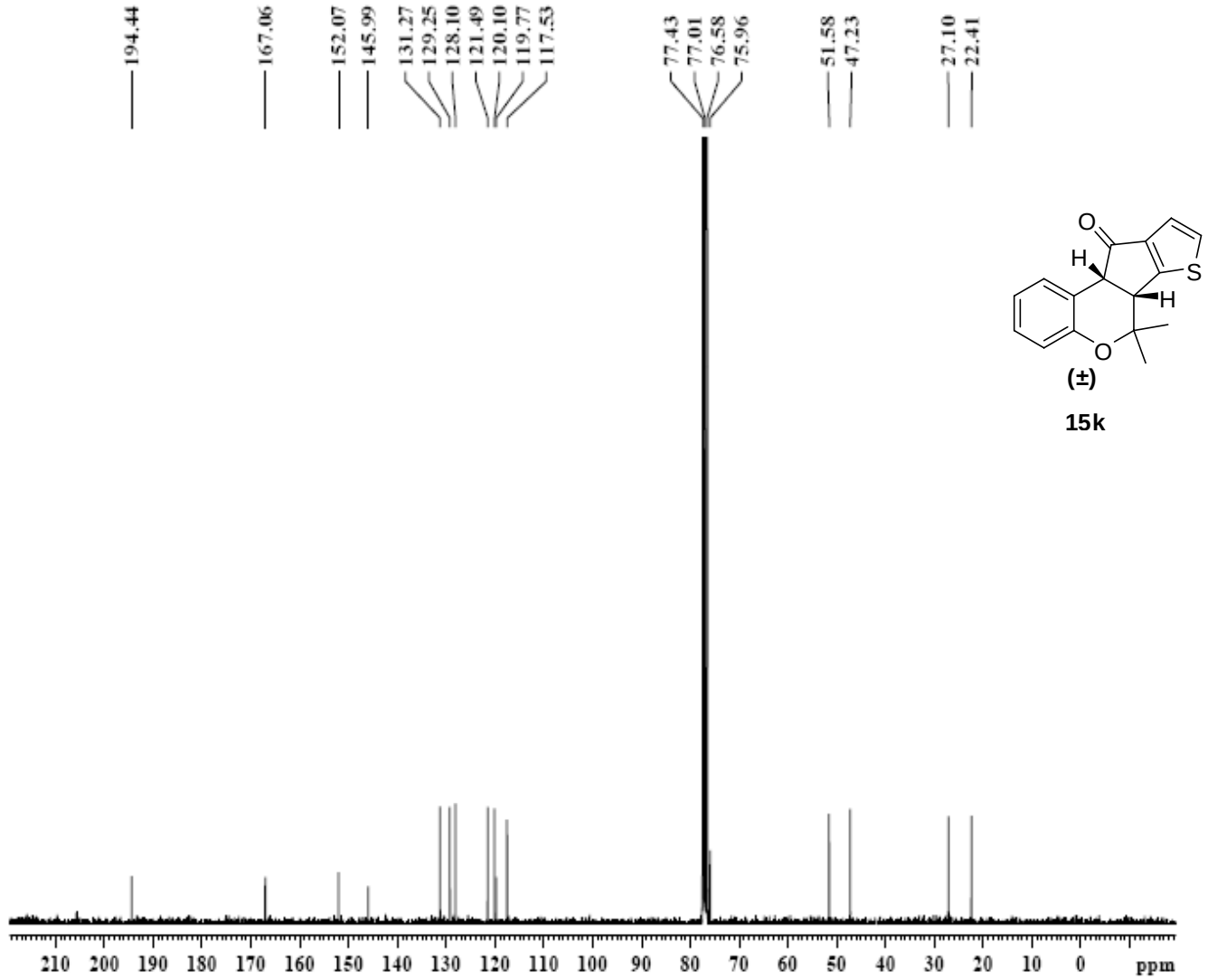


Fig. S-81: ^{13}C NMR of (±)-6,6-Dimethyl-6a,10a-dihydro-6H-5-oxa-7-thiapentaleno[2,1-a]naphthalen-10-one (15k)

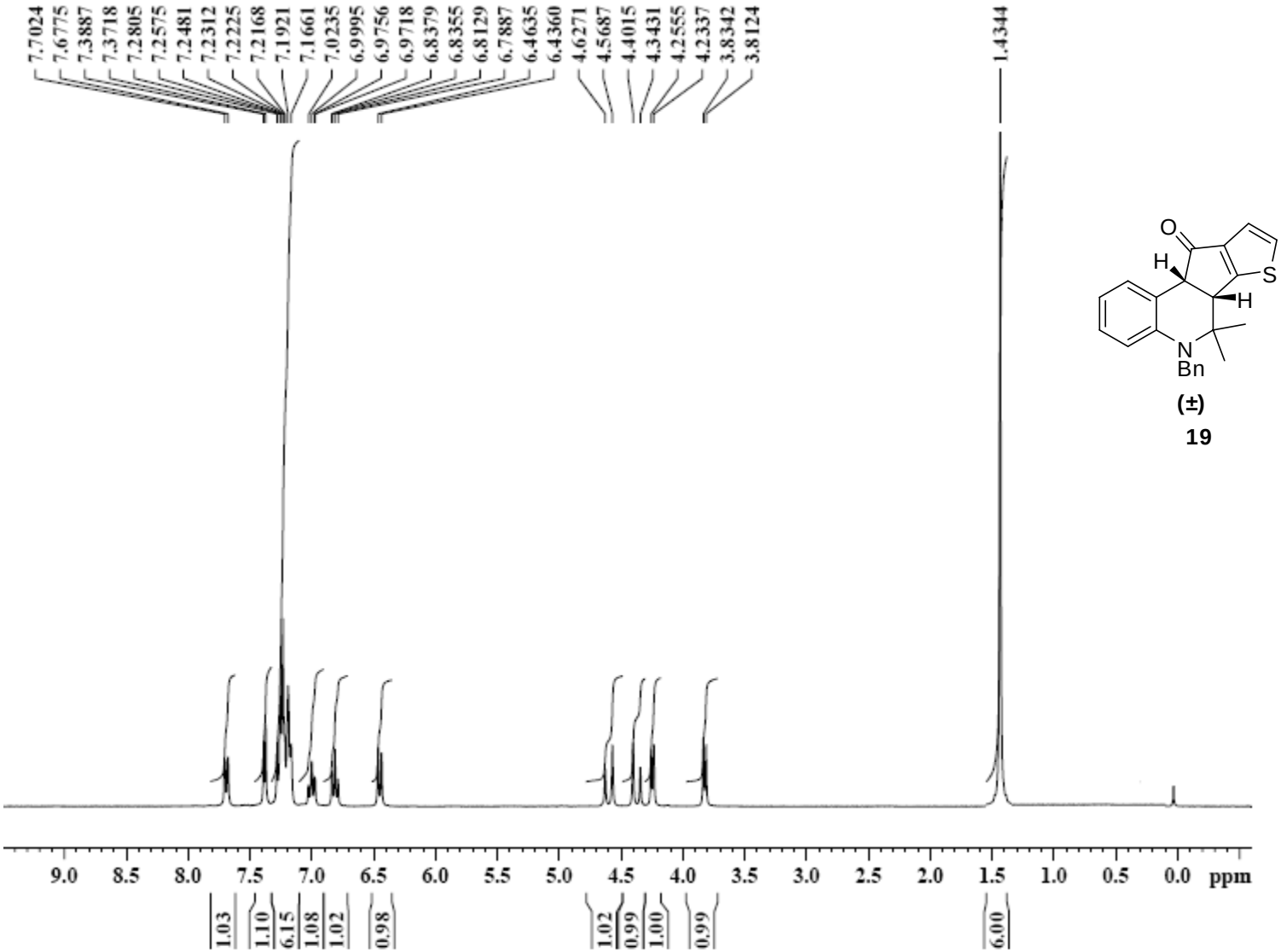


Fig. S-82: ^{1}H NMR of (±)-5-Benzyl-6,6-dimethyl-5,6,6a,10a-tetrahydro-7-thia-5-azapentaleno[2,1-a]naphthalen-10-one (19)

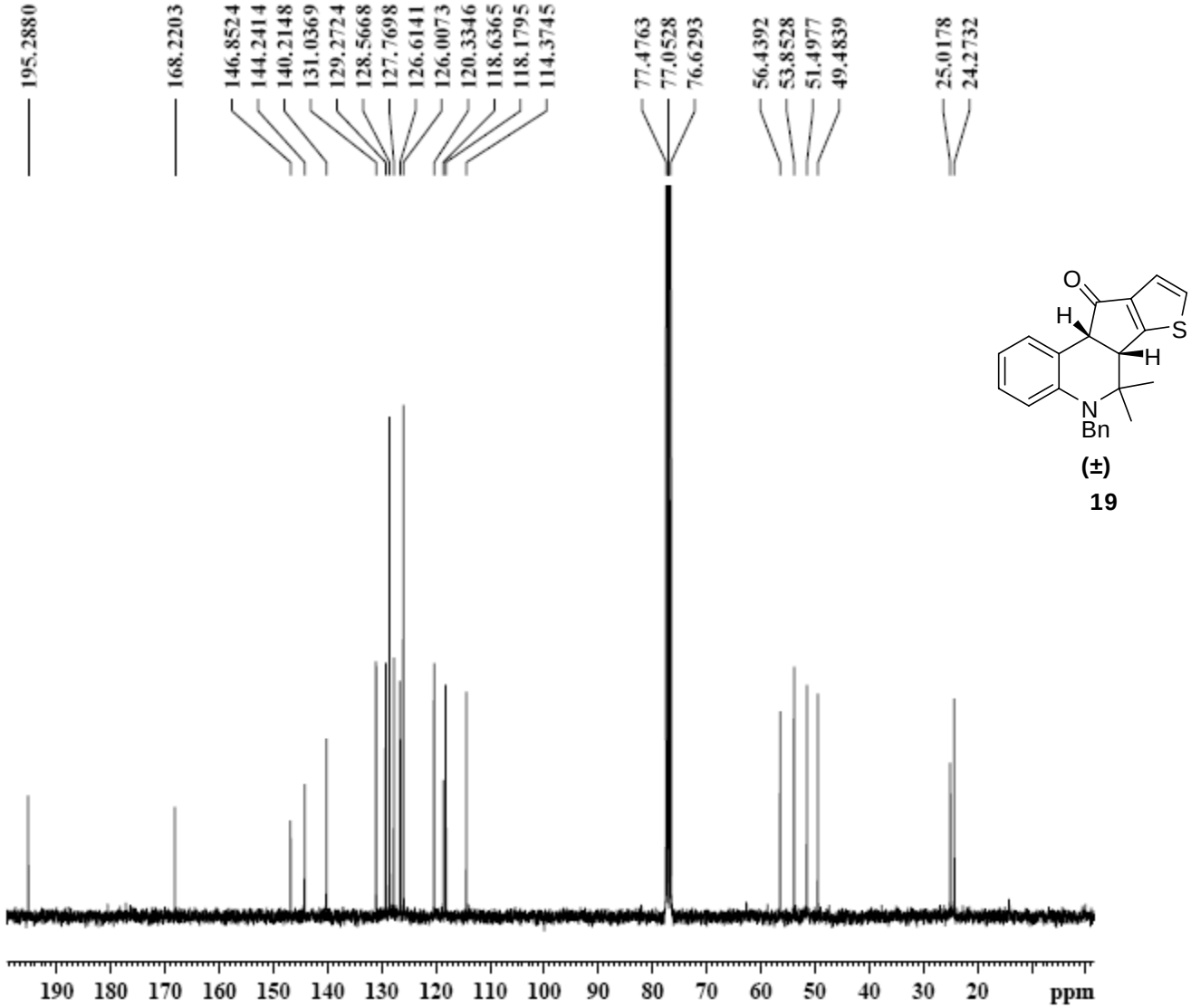
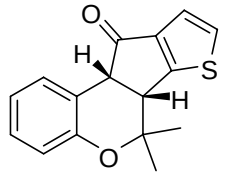
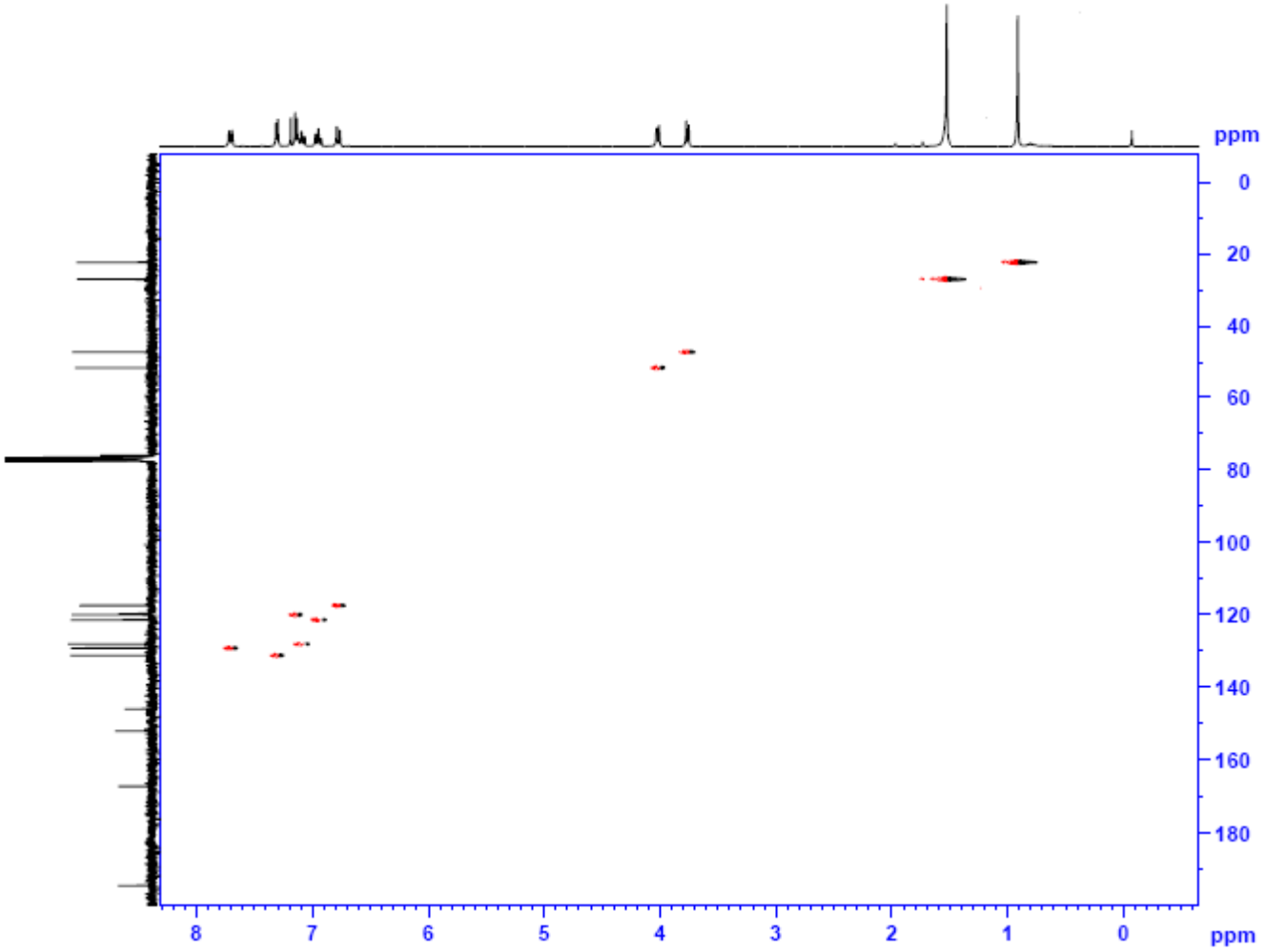


Fig. S-83: ^{13}C Spectra of (±)-5-Benzyl-6,6-dimethyl-5,6,6a,10a-tetrahydro-7-thia-5-azapentaleno[2,1-a]naphthalen-10-one (19)

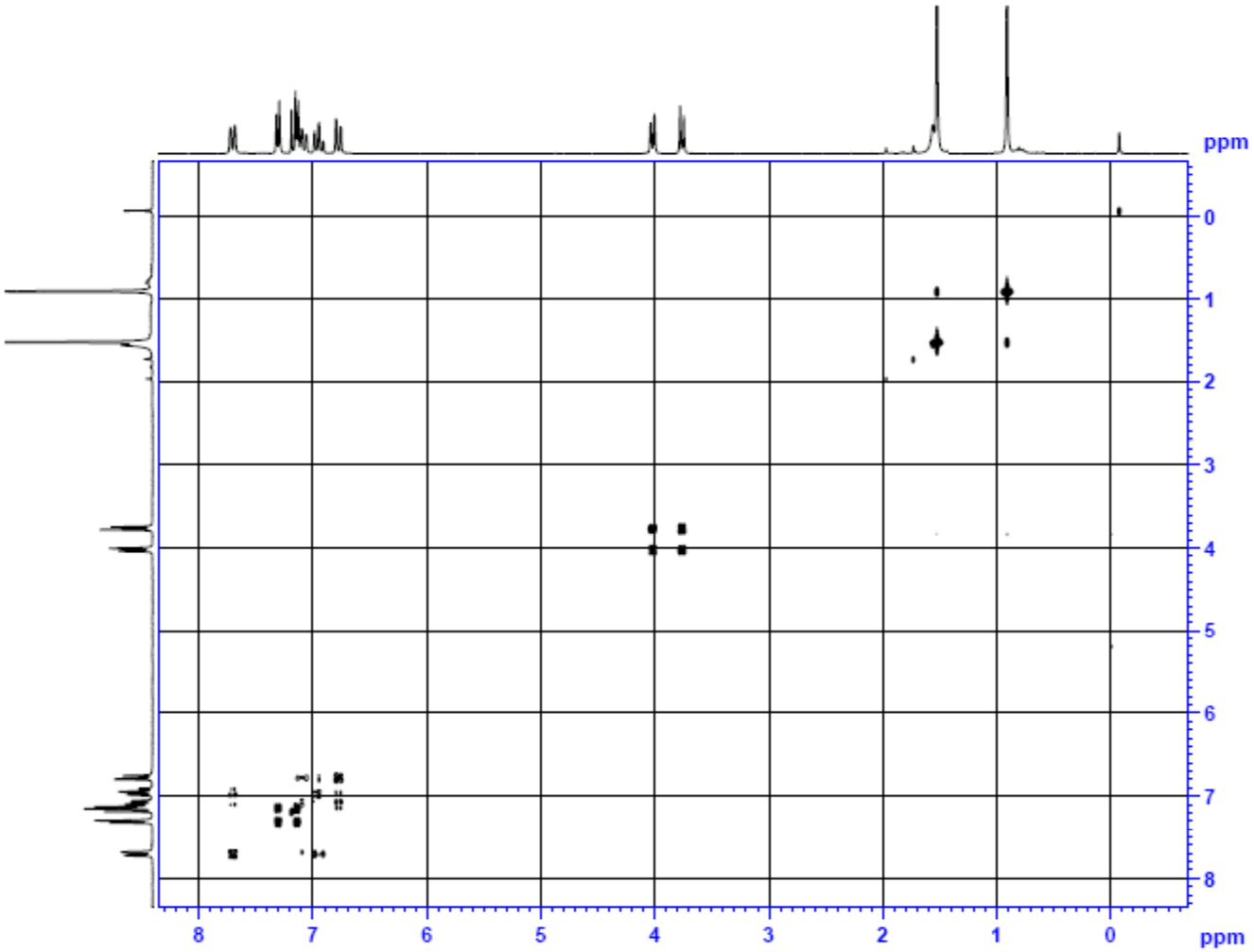


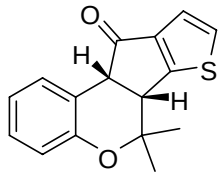
(±)

15k



HSQC

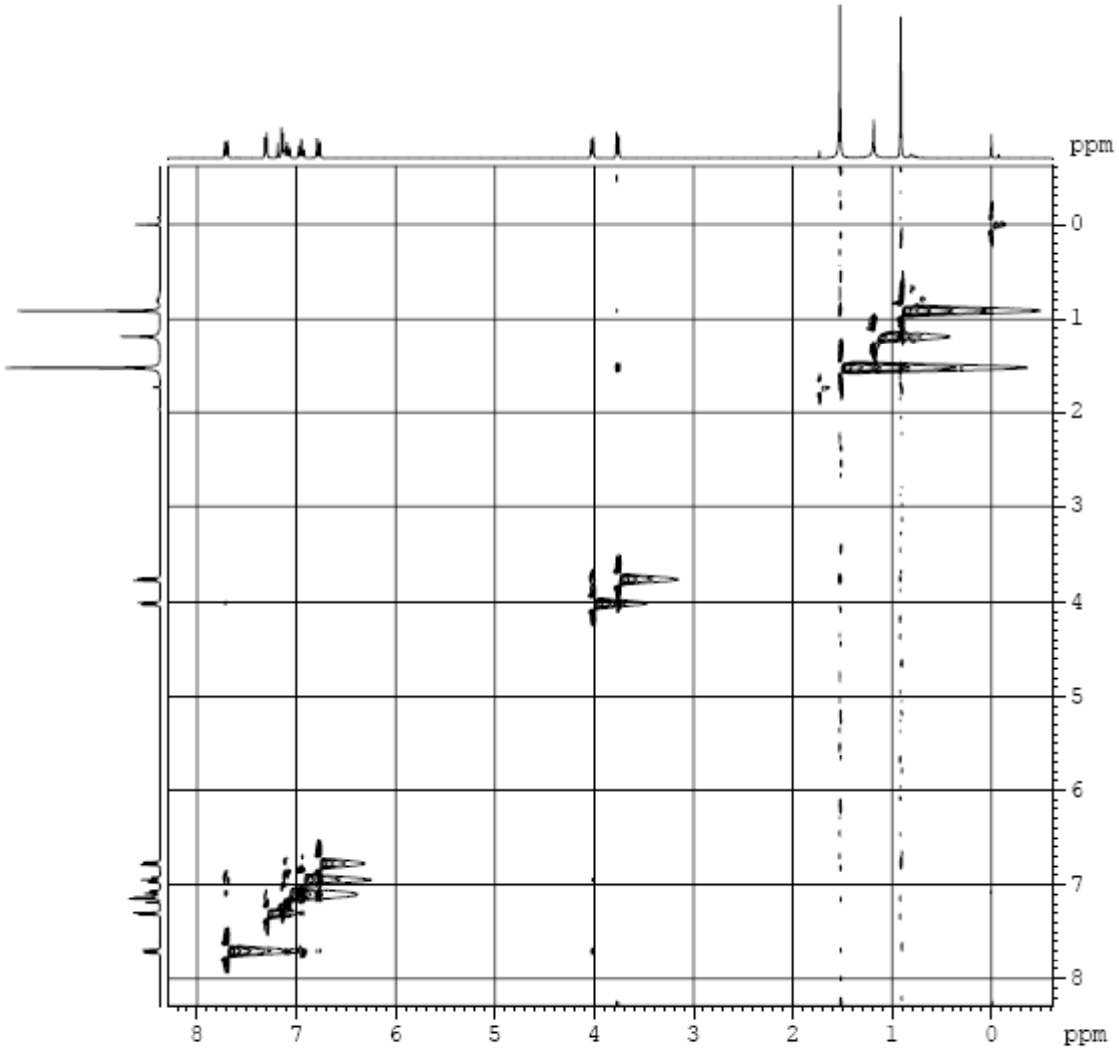


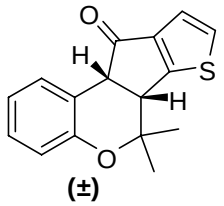


(±)

15k

1H- 1H COSY



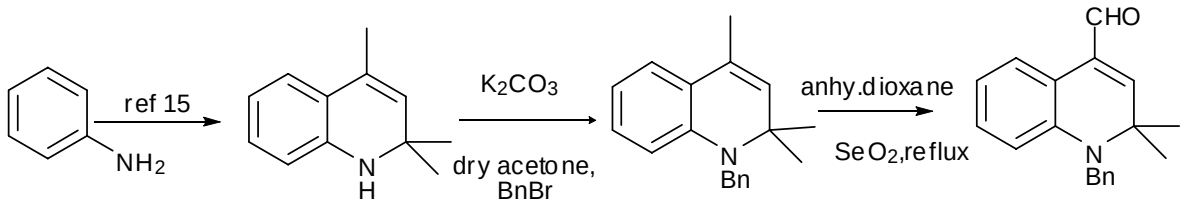


(±)

15k

NOESY

Scheme for synthesis of 16 as mentioned in the paper



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