

Supplementary Material

Iodocyclisation of Electronically-Resistant Alkynes: Synthesis of 2-Carboxy(and sulfoxy)-3-iodobenzo[*b*]thiophenes

Shuqi Chen^A and Bernard L. Flynn^{A,B}

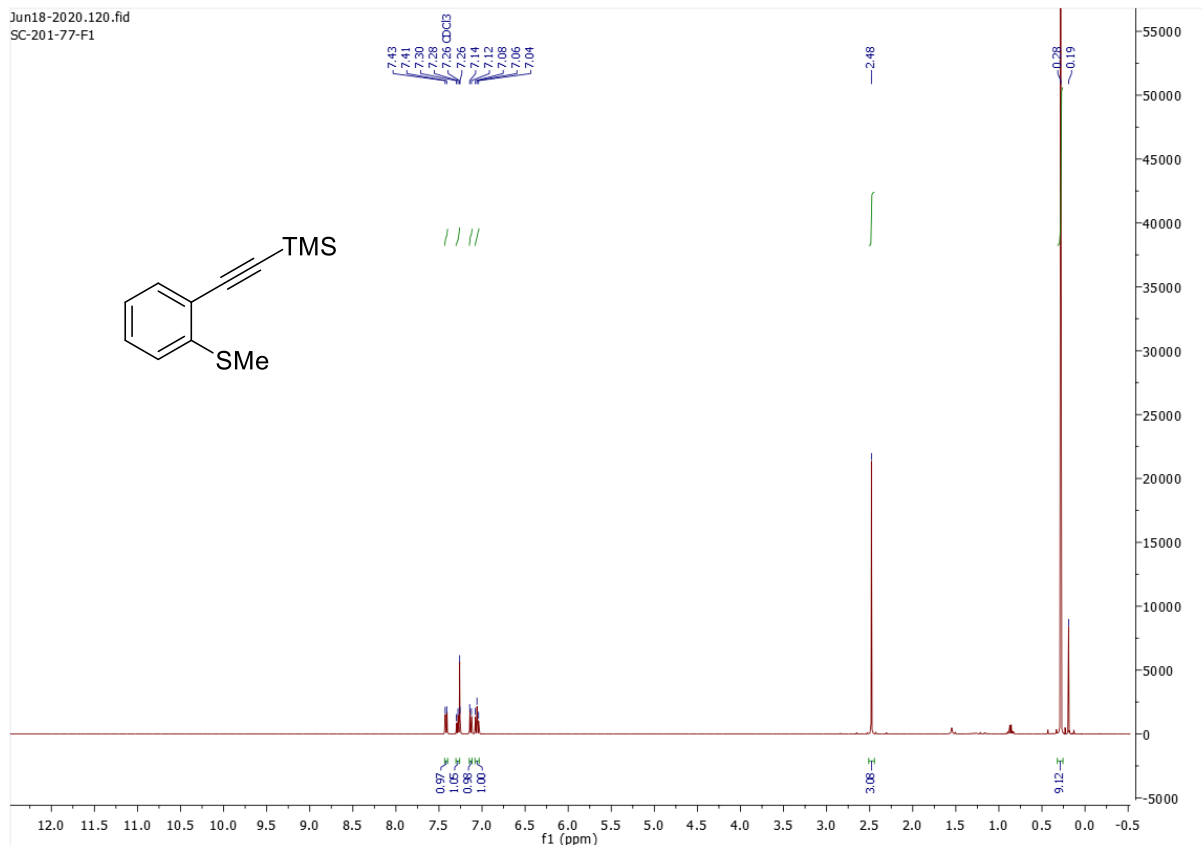
^AMonash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, Vic. 3052, Australia.

^BCorresponding author. Email: bernard.flynn@monash.edu

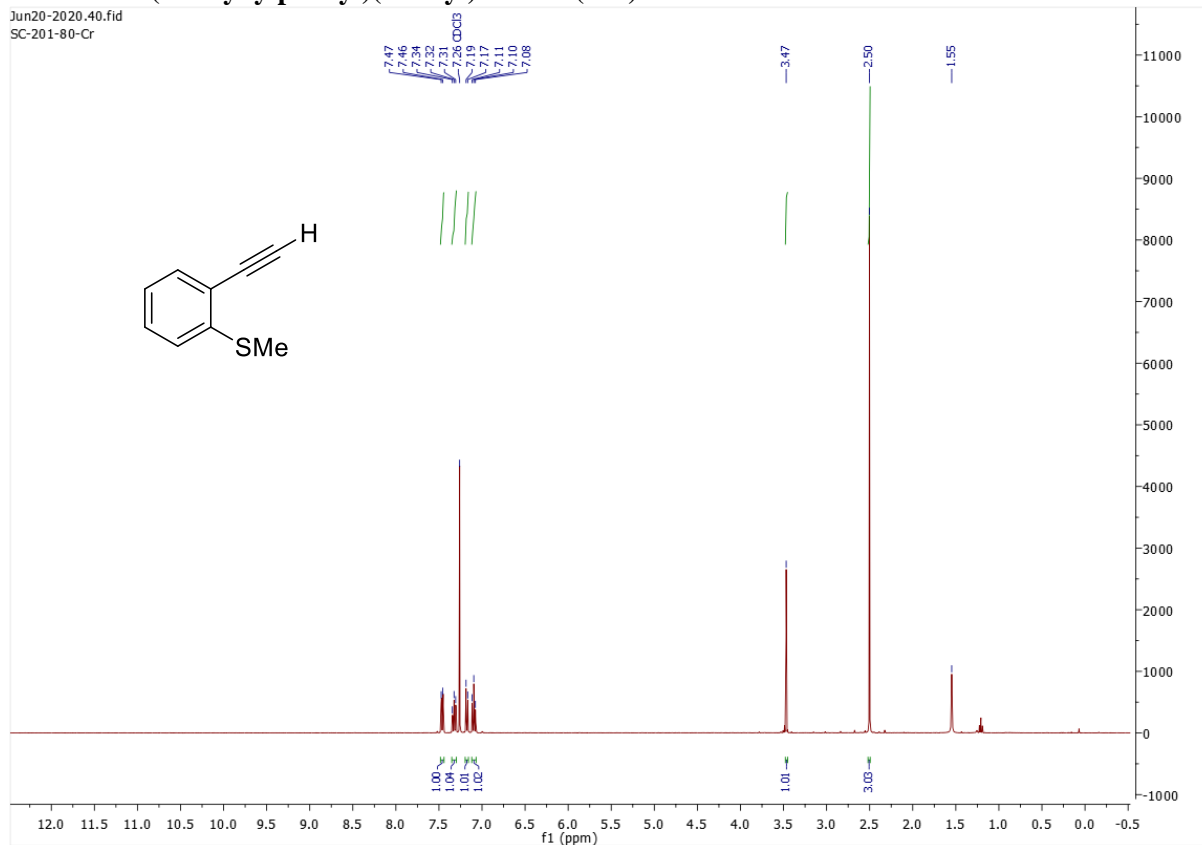
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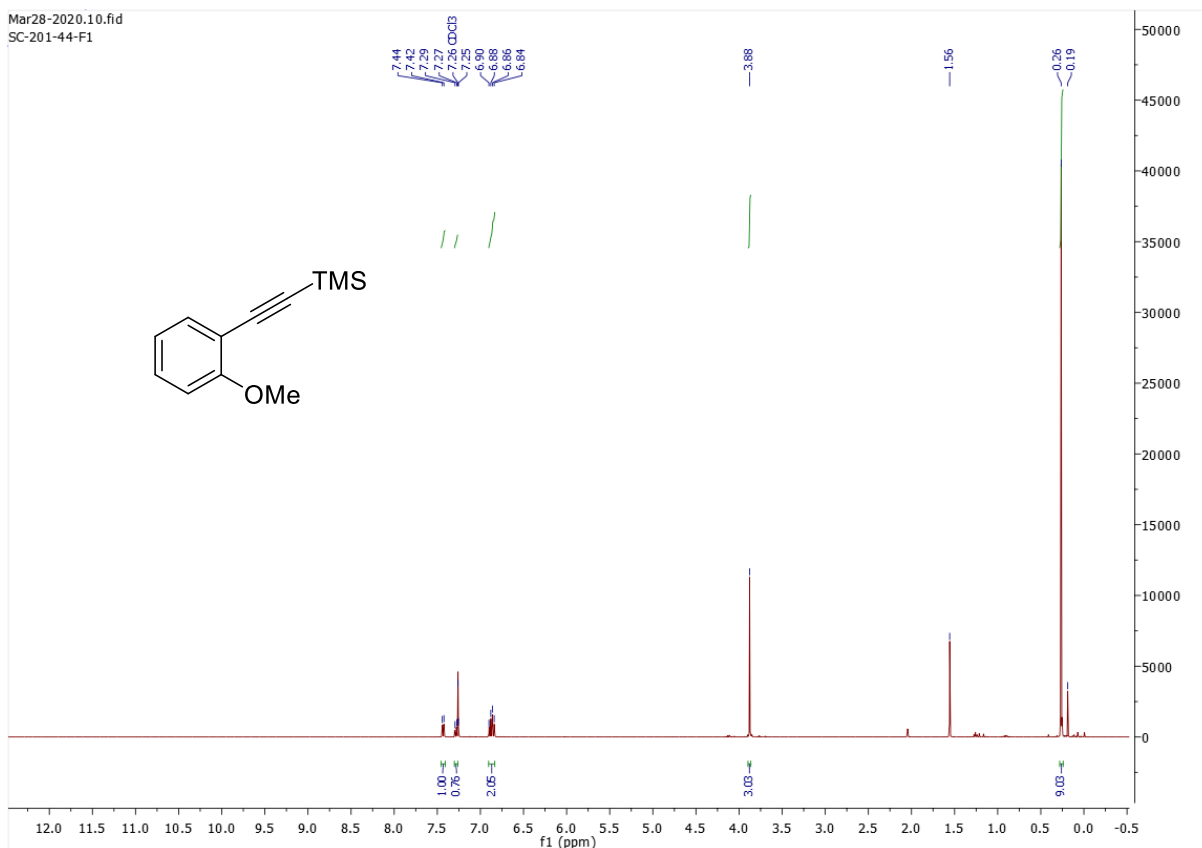
¹H NMR of trimethyl((2-(methylthio)phenyl)ethynyl)silane:



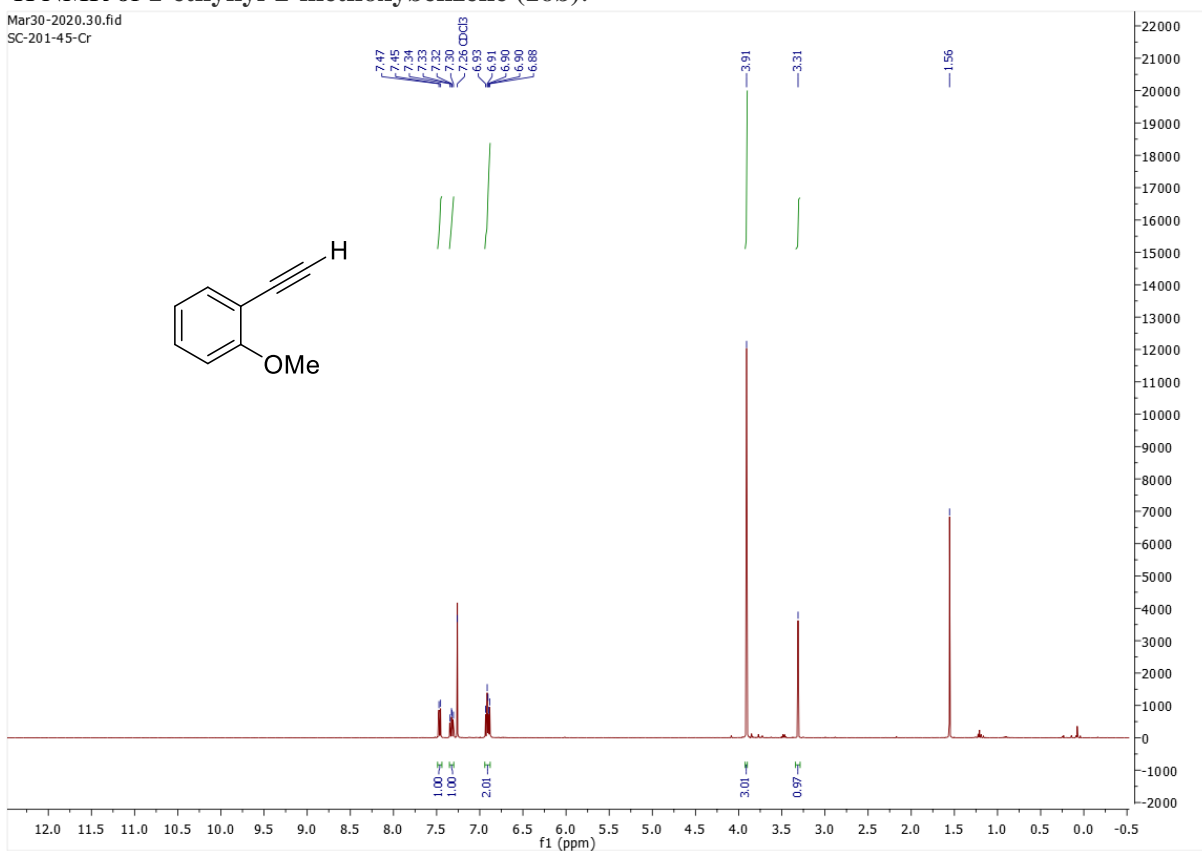
¹H NMR of (2-ethynylphenyl)(methyl)sulfane (16a):



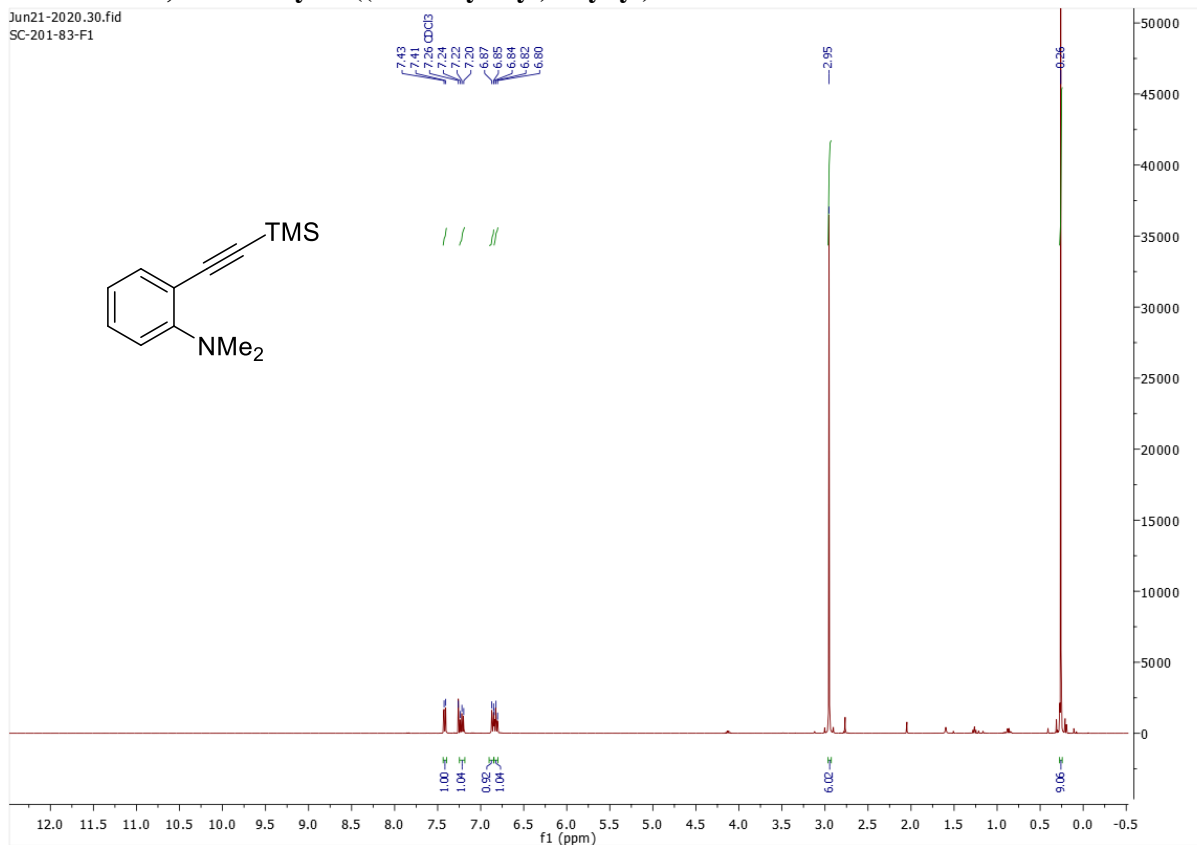
¹H NMR of ((2-methoxyphenyl)ethynyl)trimethylsilane:



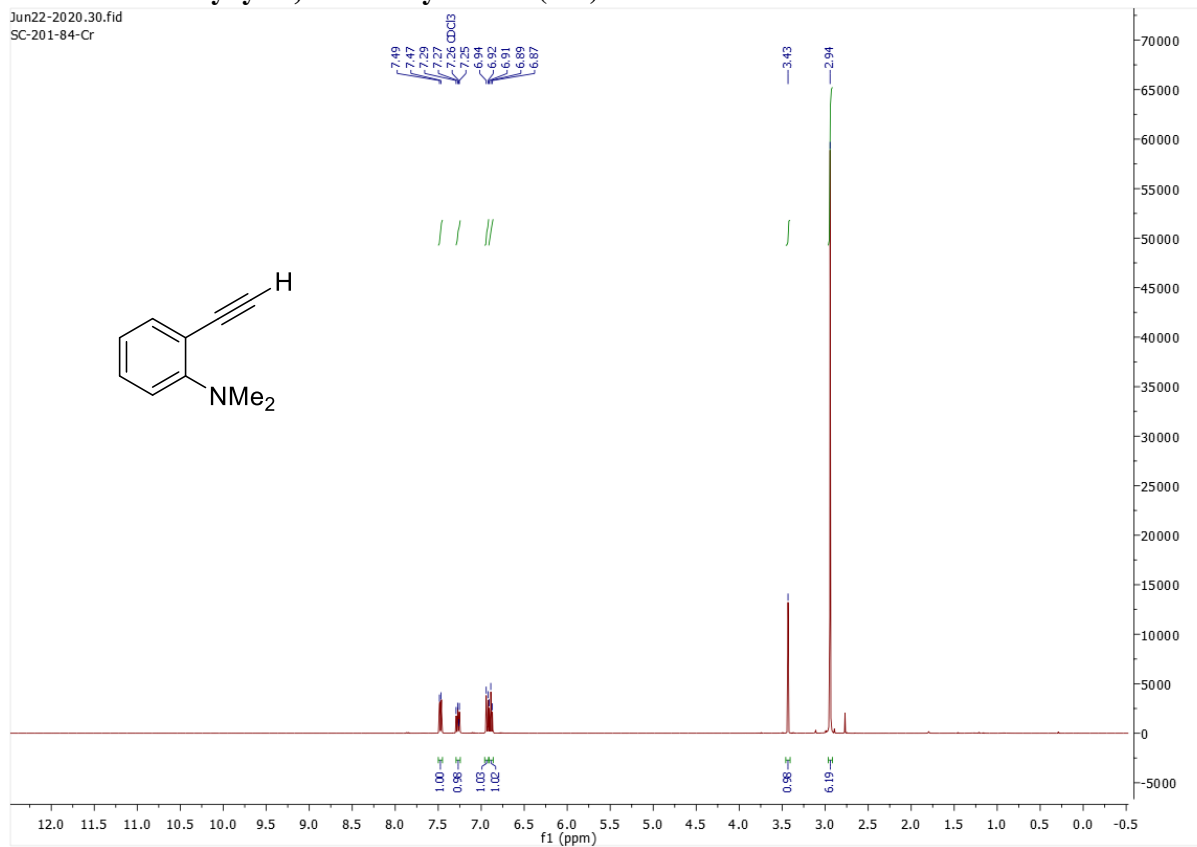
¹H NMR of 1-ethynyl-2-methoxybenzene (16b):



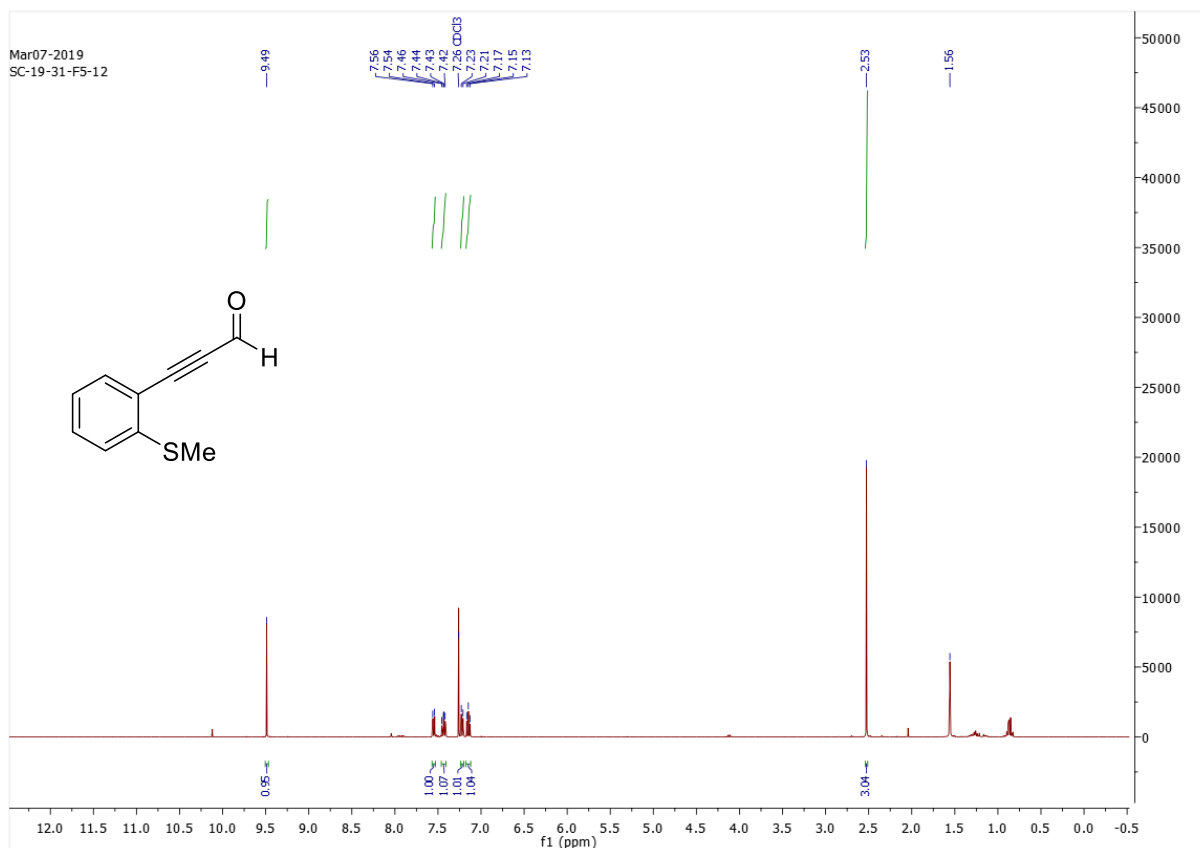
¹H NMR of *N,N*-dimethyl-2-((trimethylsilyl)ethynyl)aniline:



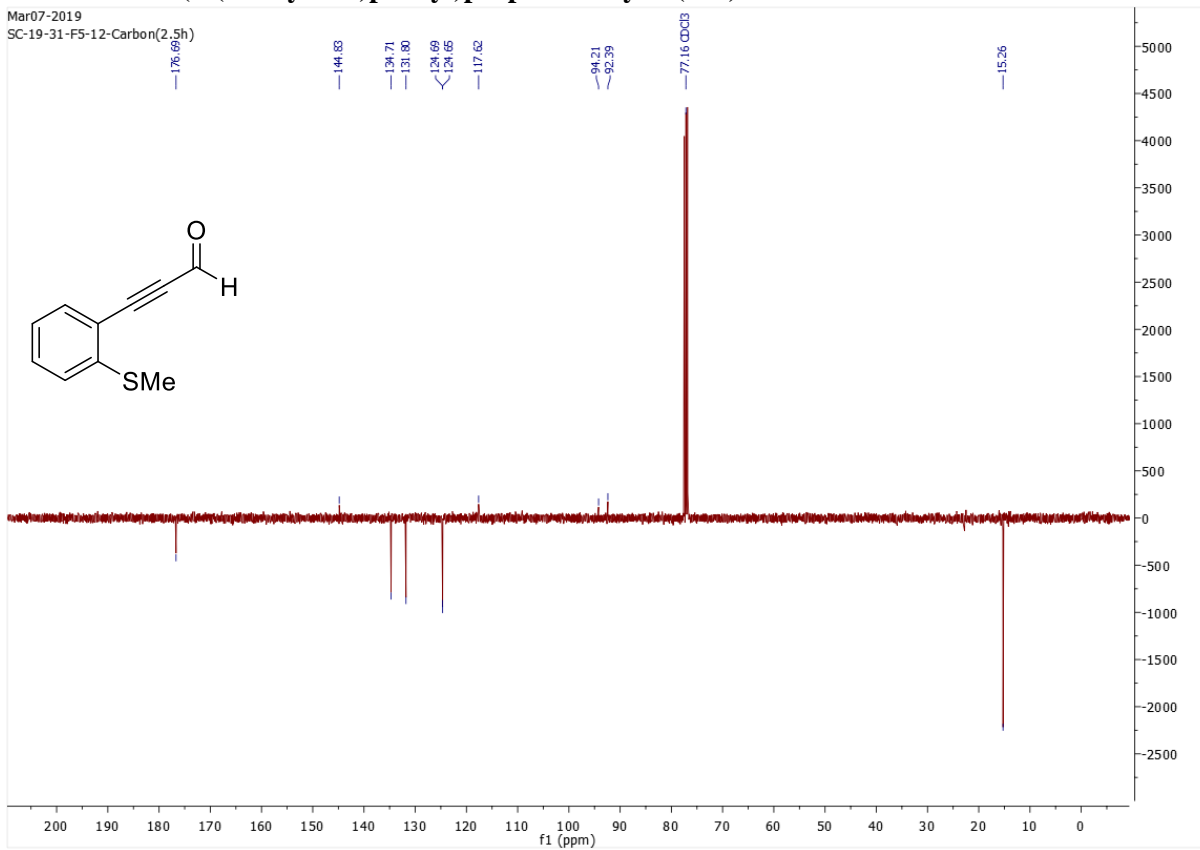
¹H NMR of 2-ethynyl-*N,N*-dimethylaniline (16c):



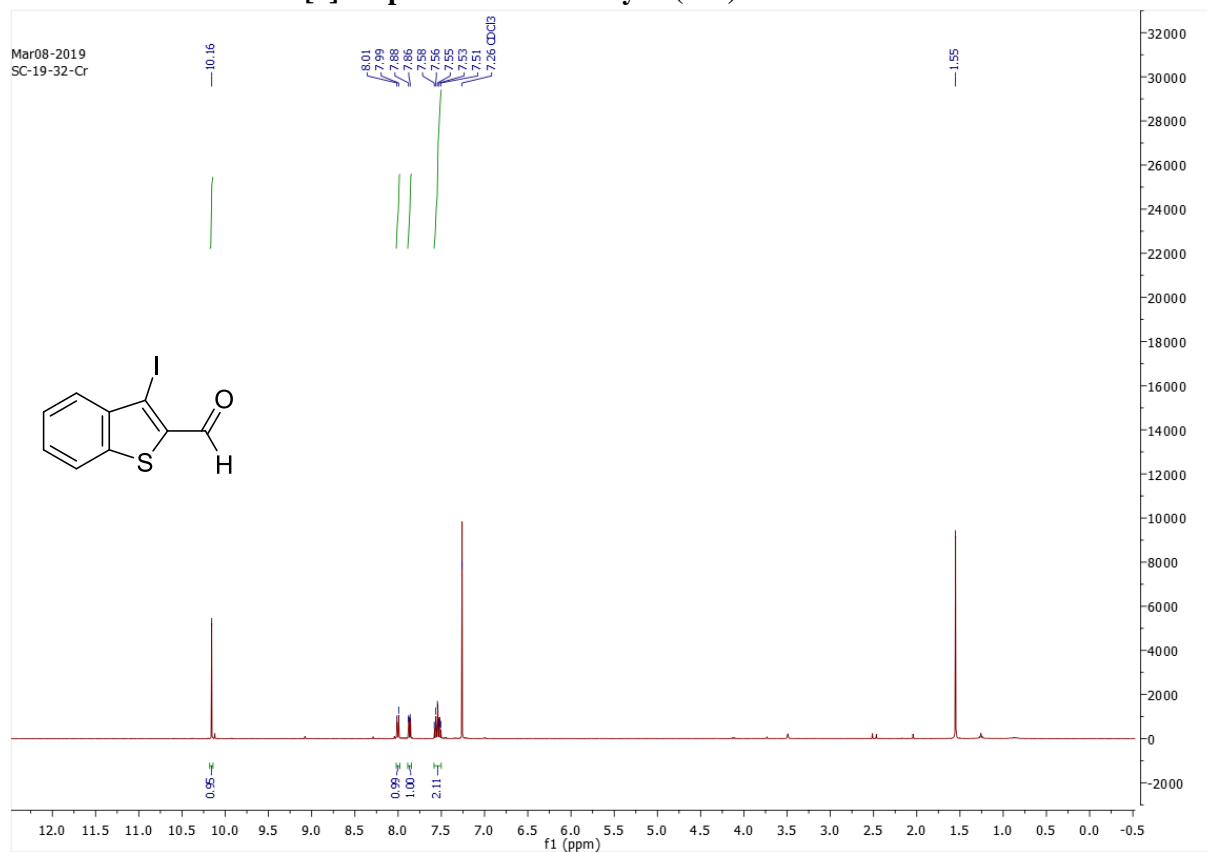
¹H NMR of 3-(2-(methylthio)phenyl)propionaldehyde (8aa):



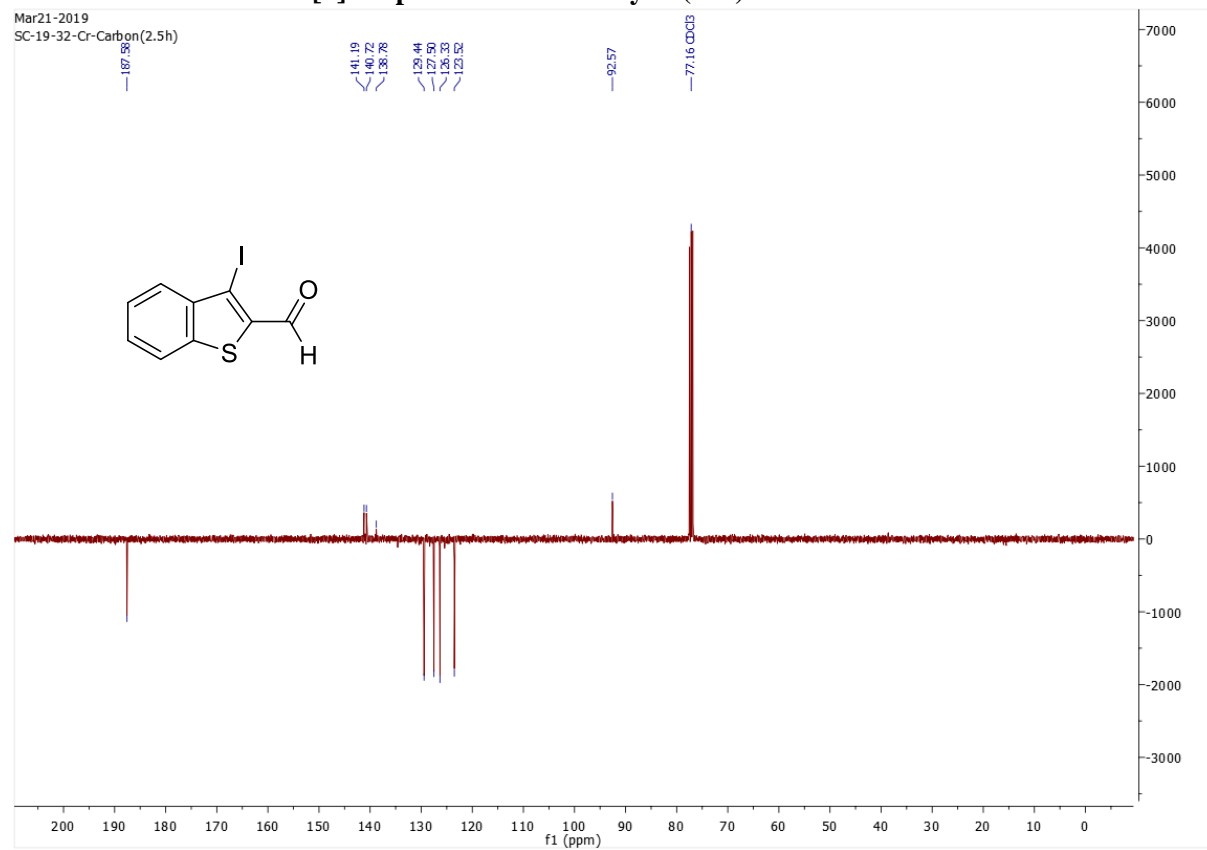
¹³C NMR of 3-(2-(methylthio)phenyl)propionaldehyde (8aa):



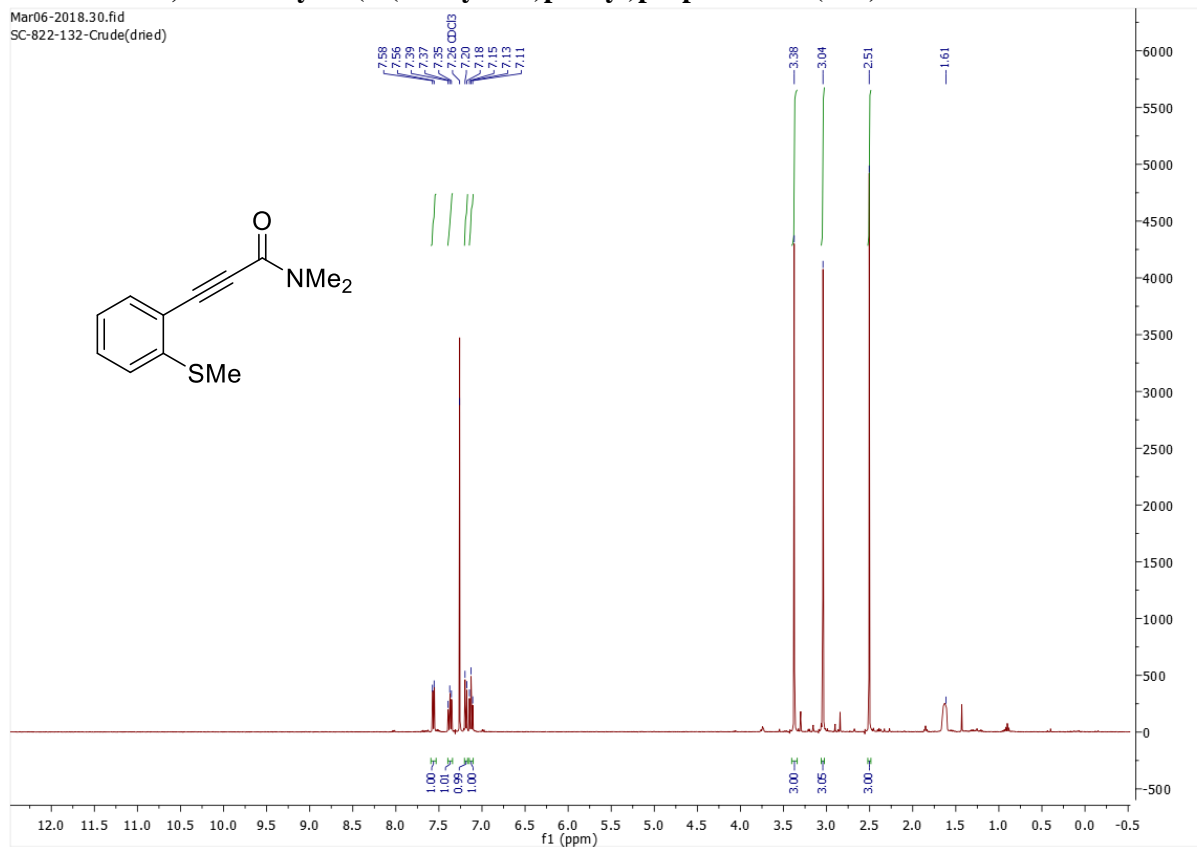
¹H NMR of 3-iodobenzo[*b*]thiophene-2-carbaldehyde (9aa):



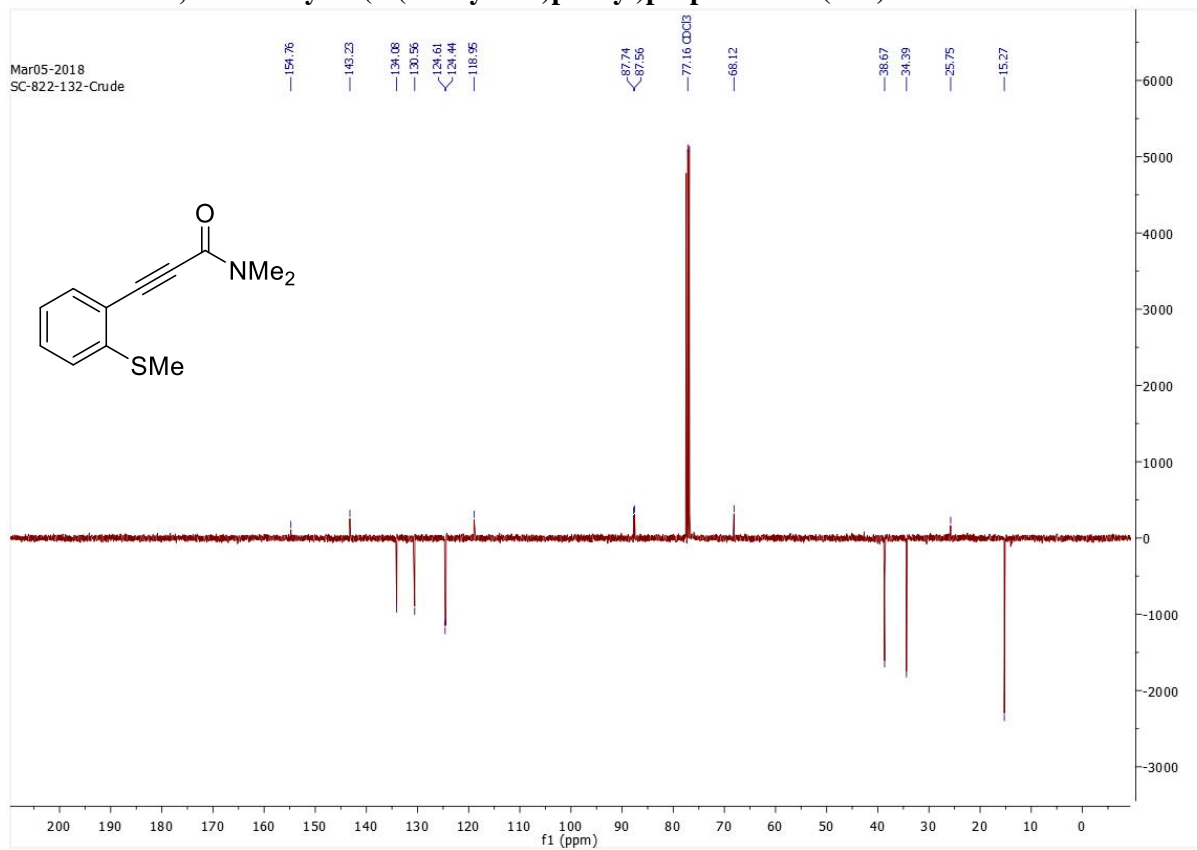
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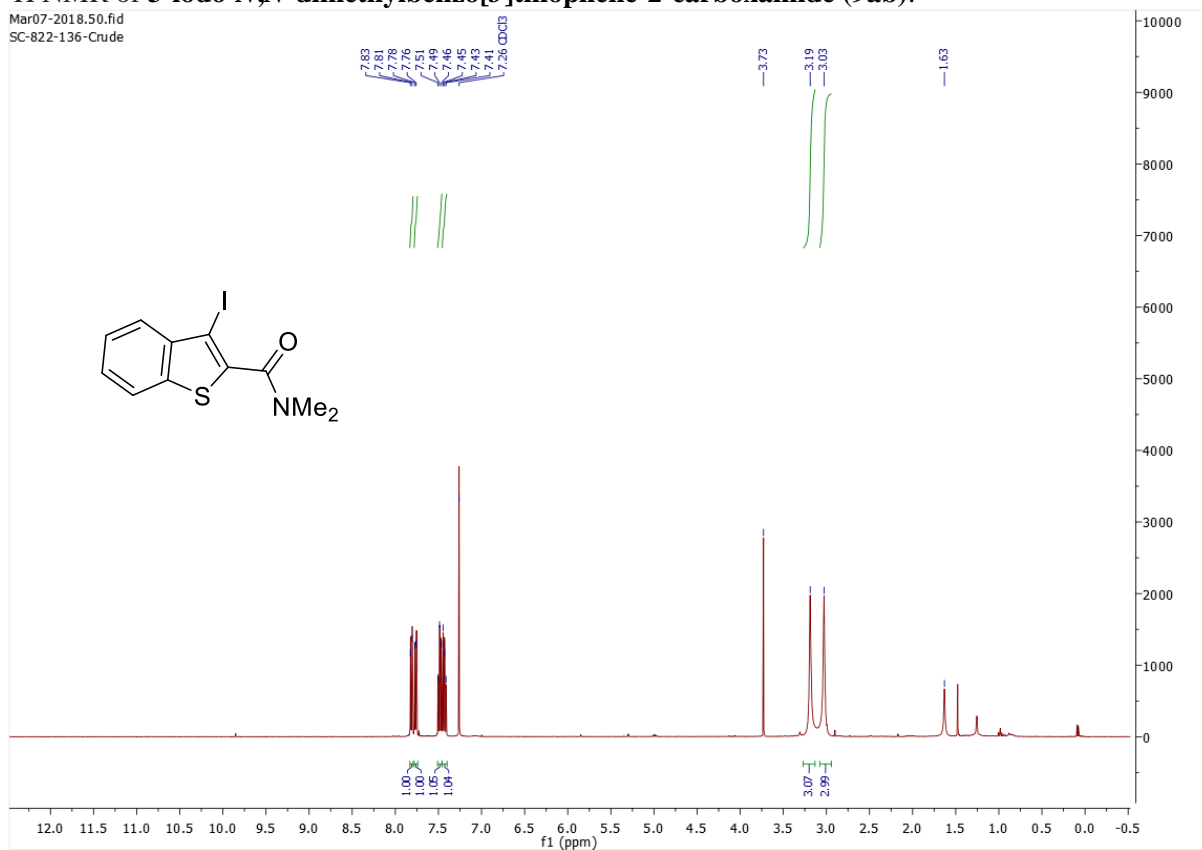
¹H NMR of *N,N*-dimethyl-3-(2-(methylthio)phenyl)propiolamide (8ab):



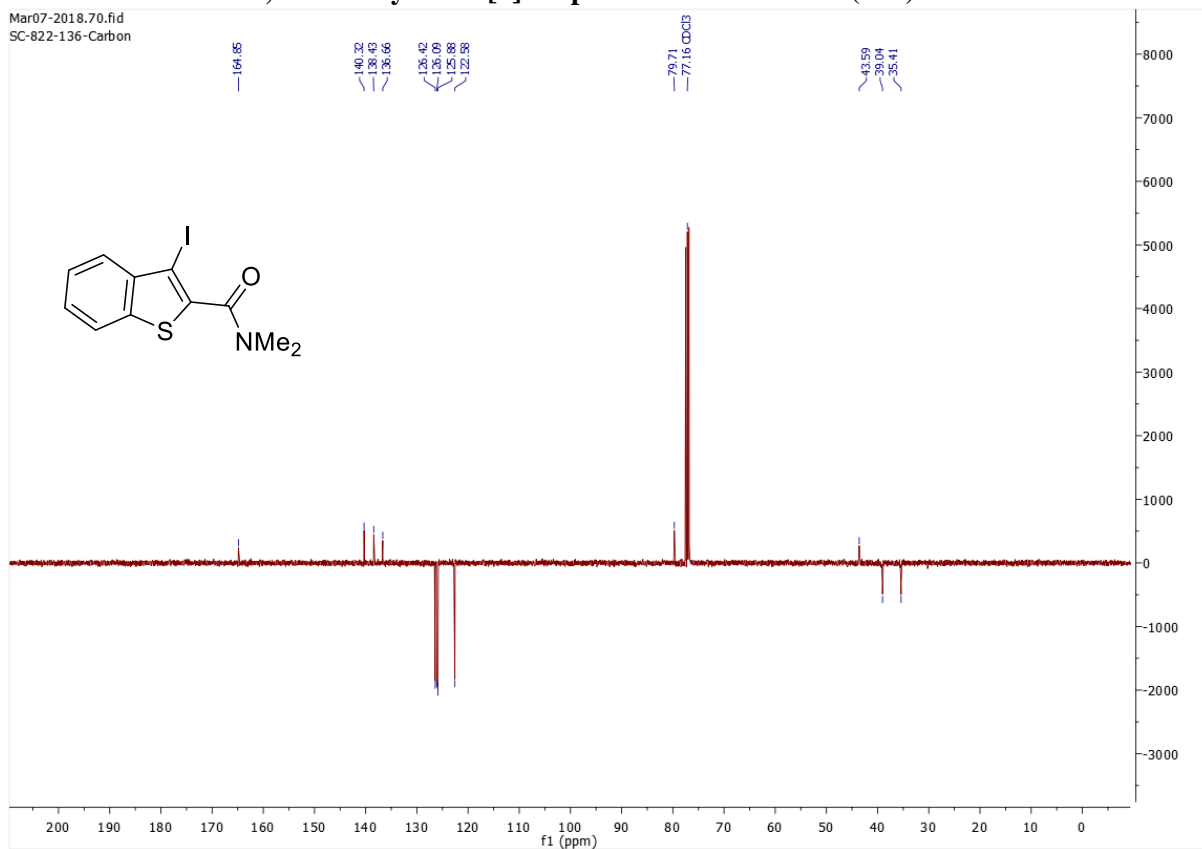
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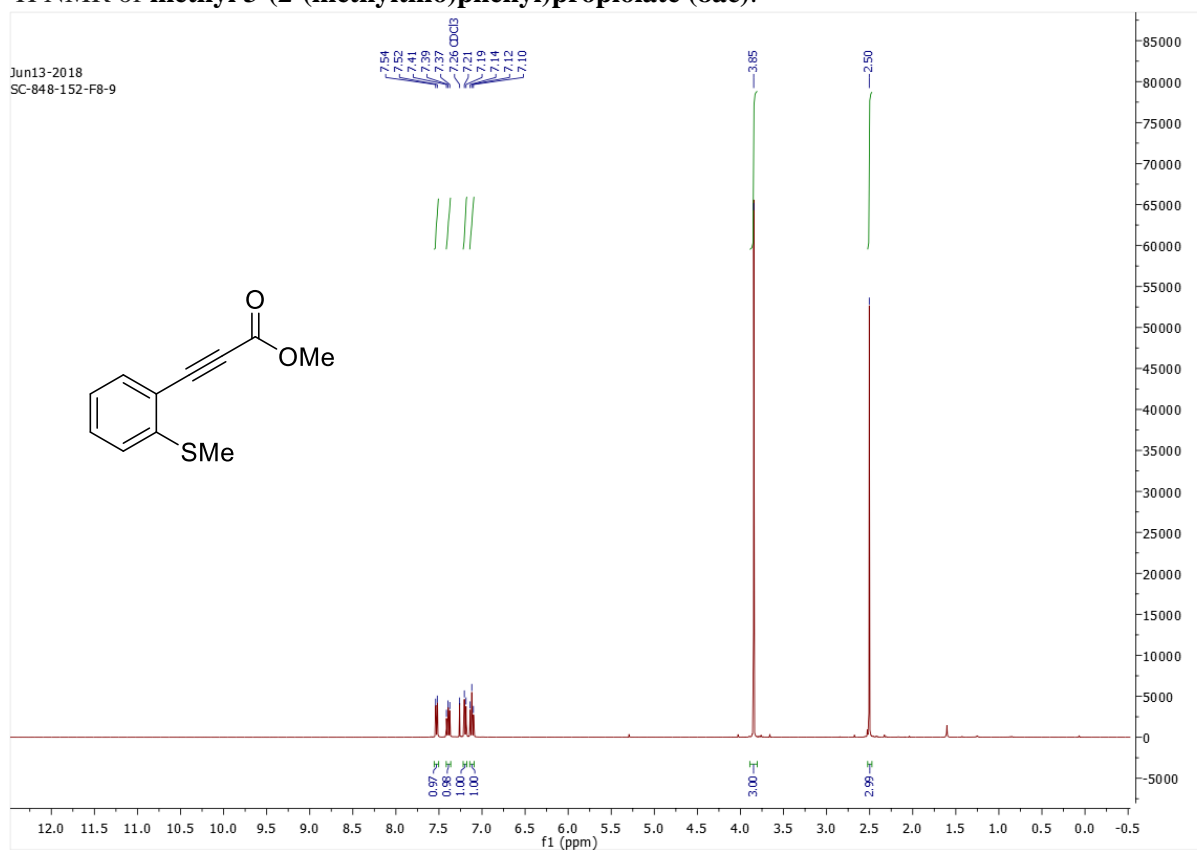
¹H NMR of 3-iodo-*N,N*-dimethylbenzo[*b*]thiophene-2-carboxamide (9ab):



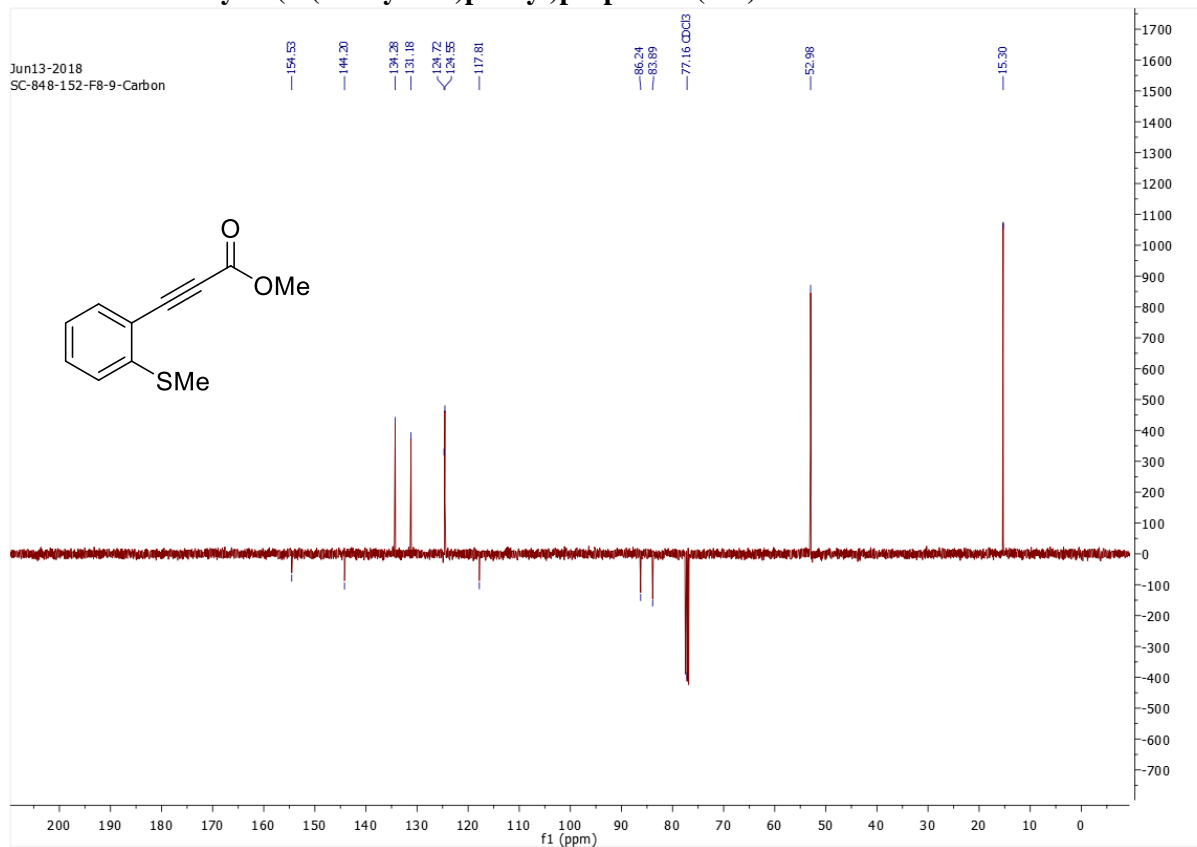
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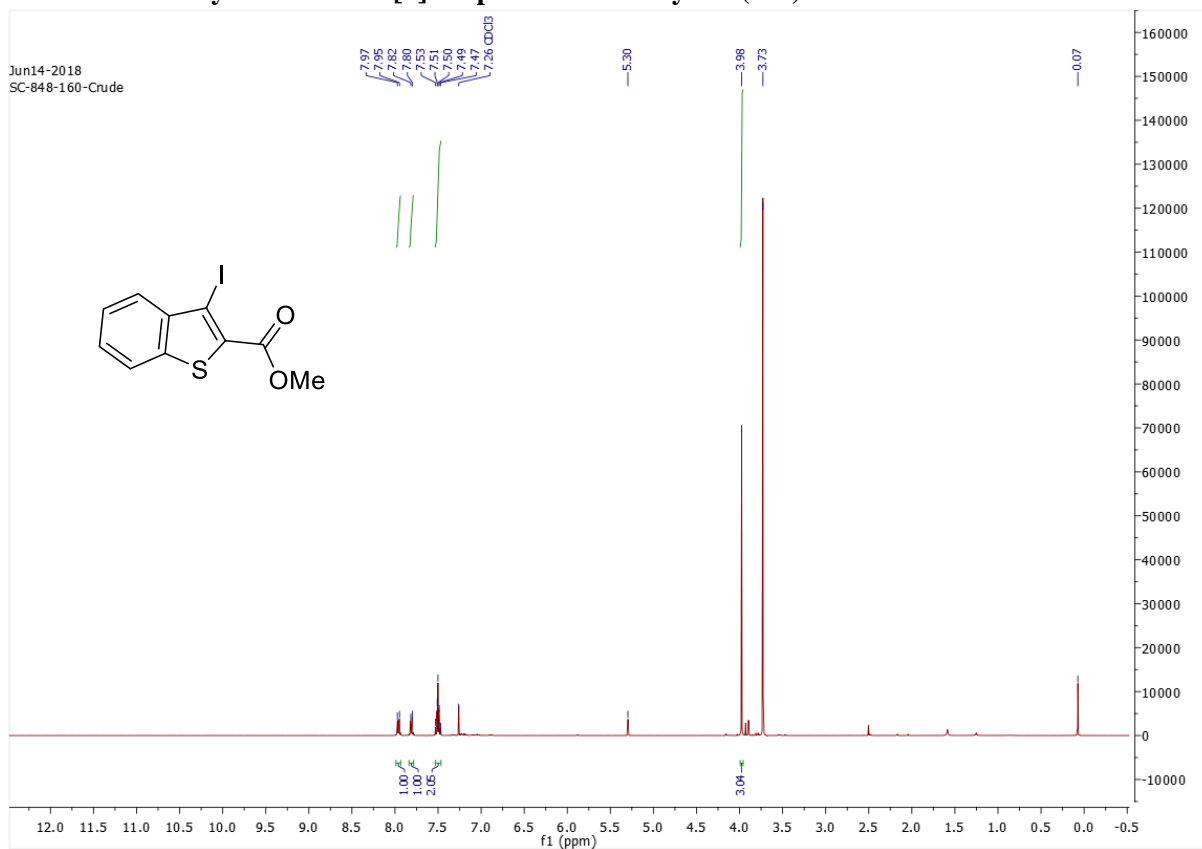
¹H NMR of methyl 3-(2-(methylthio)phenyl)propiolate (8ac):



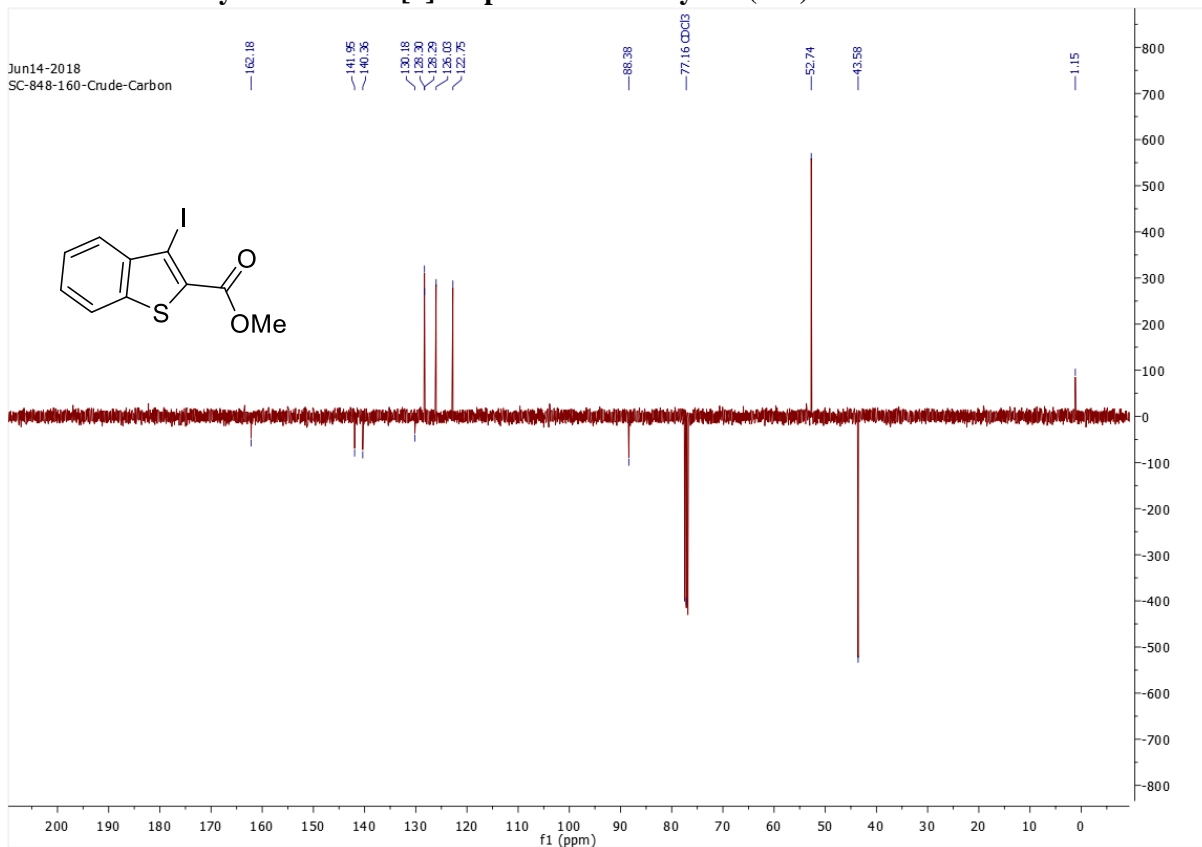
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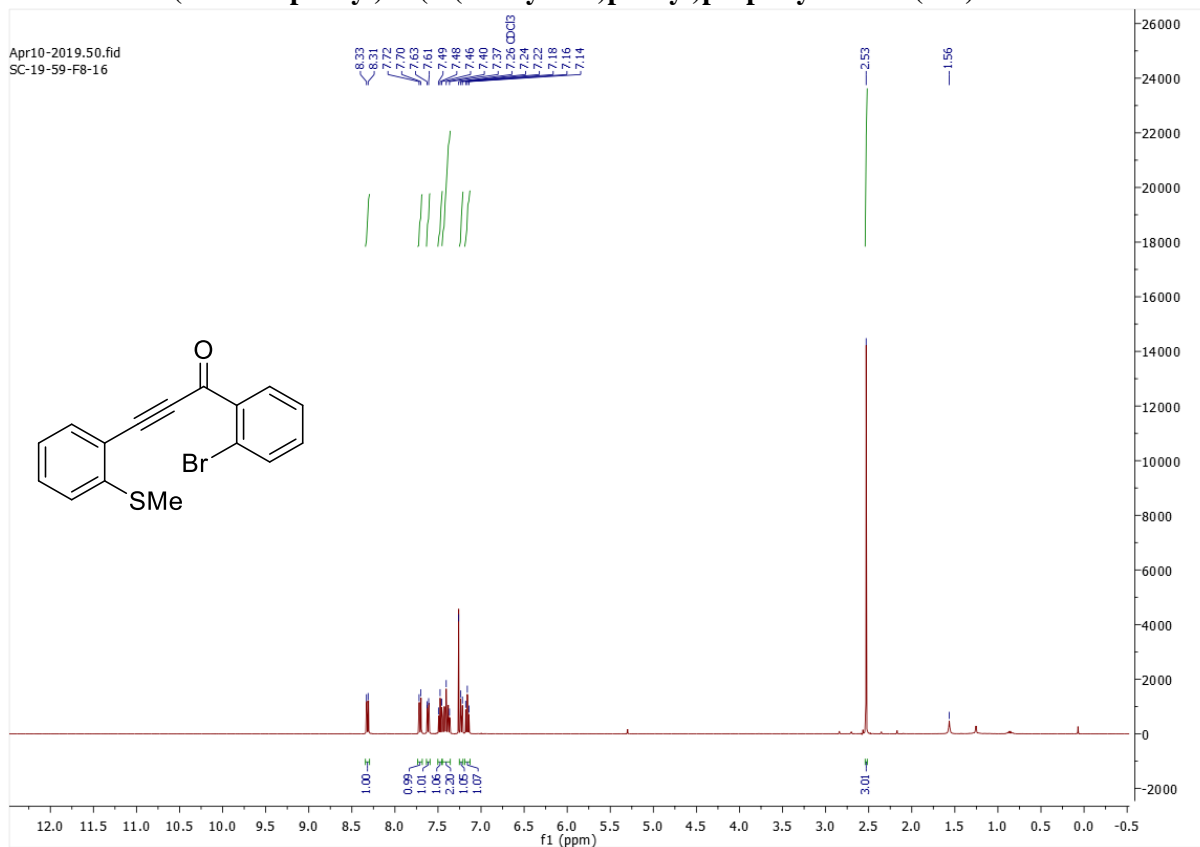
¹H NMR of methyl 3-iodobenzo[*b*]thiophene-2-carboxylate (9ac):



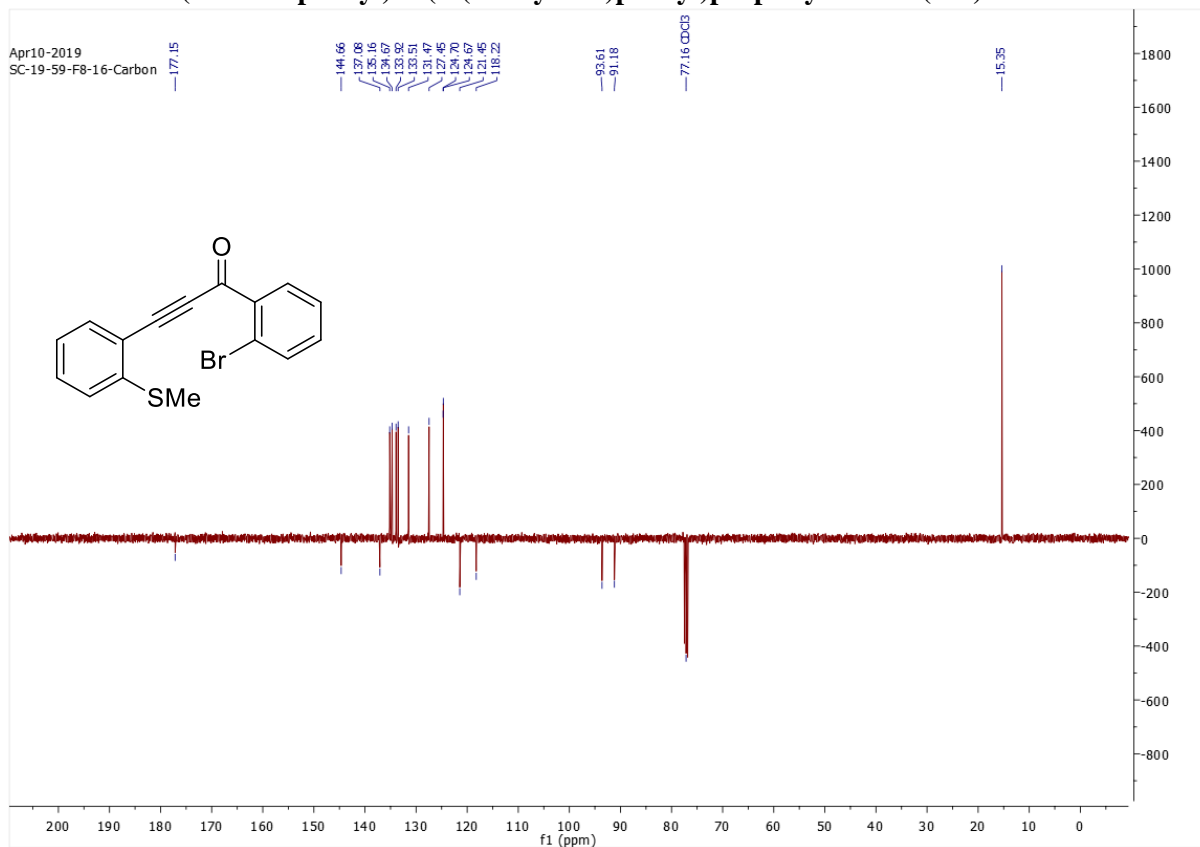
¹³C NMR of methyl 3-iodobenzo[*b*]thiophene-2-carboxylate (9ac):



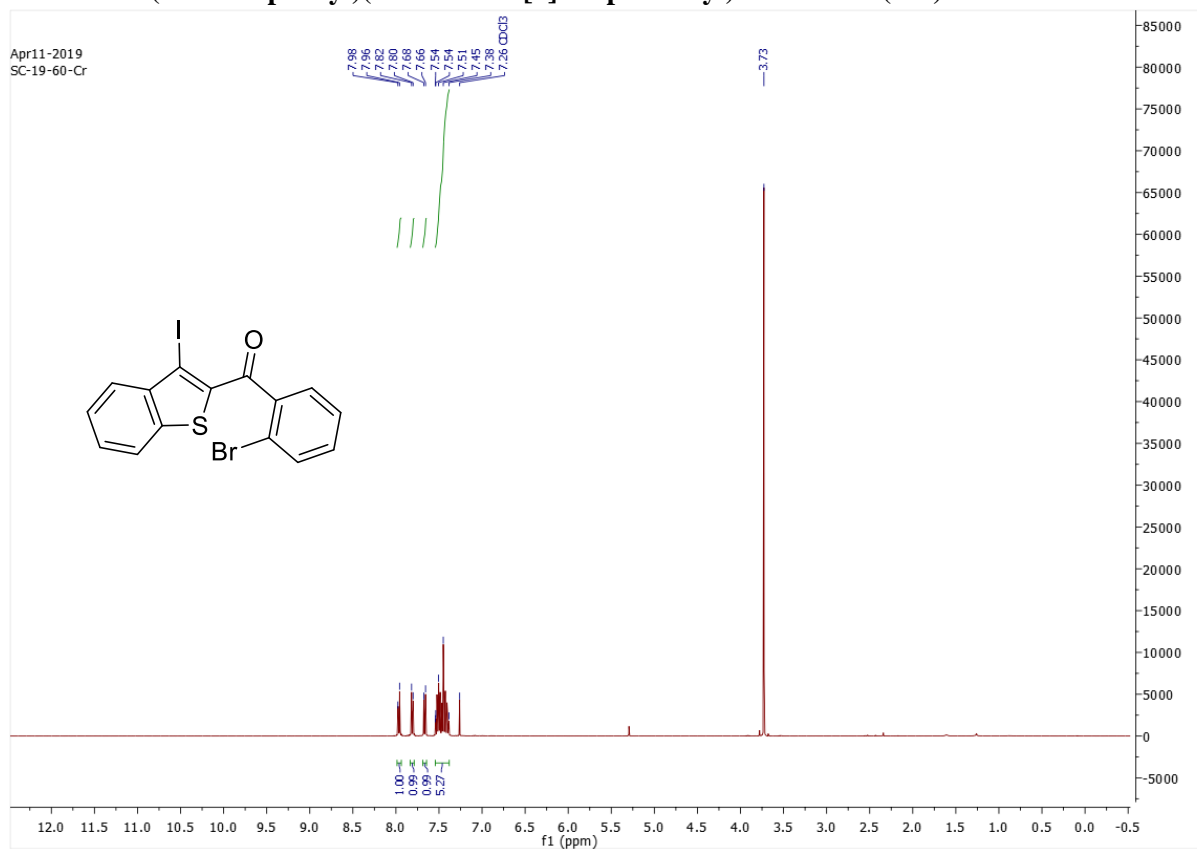
¹H NMR of 1-(2-bromophenyl)-3-(2-(methylthio)phenyl)prop-2-yn-1-one (8ae):



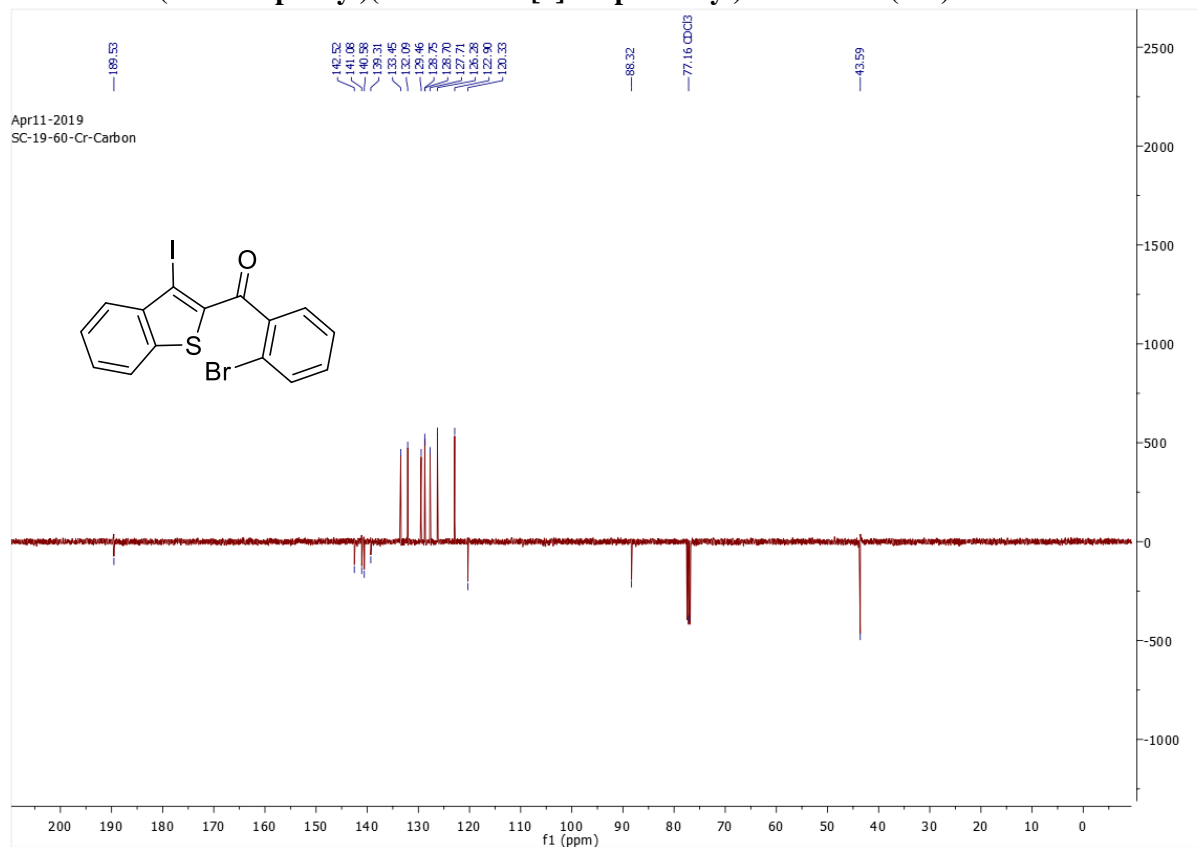
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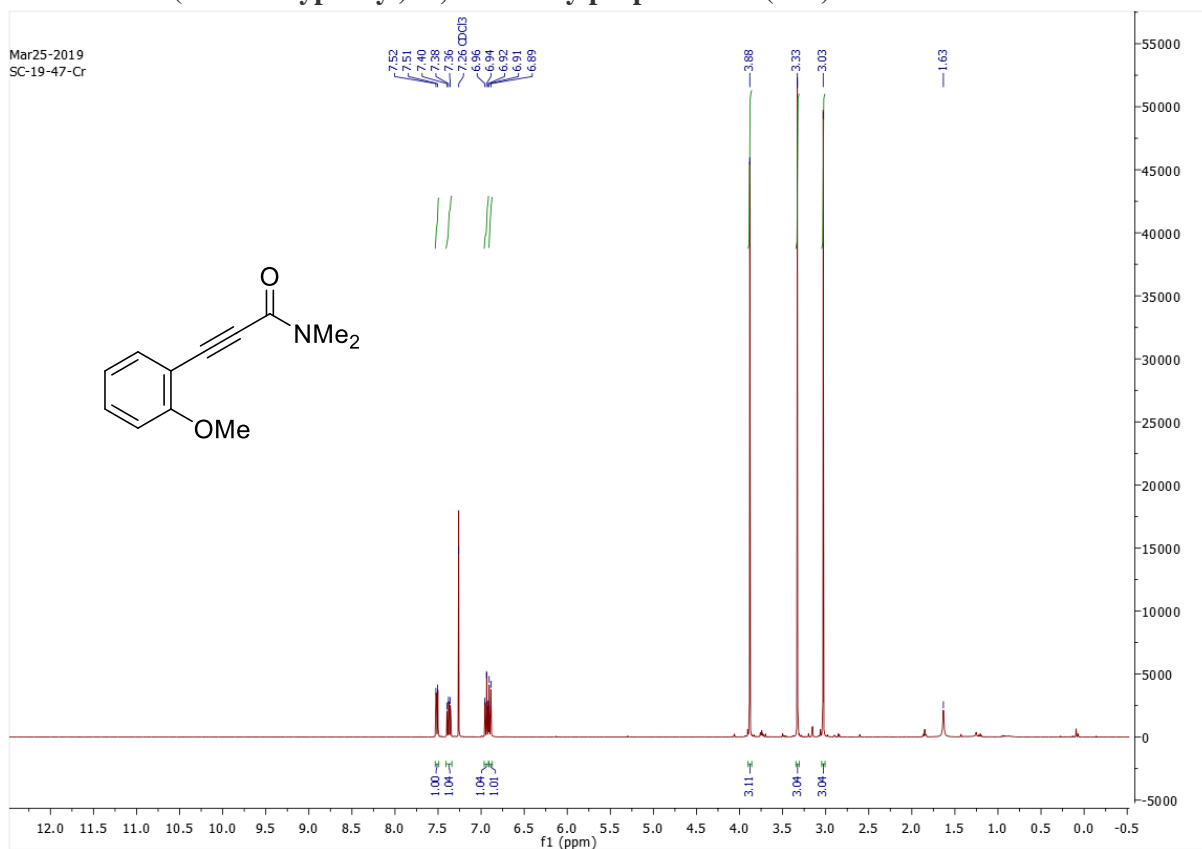
¹H NMR of (2-bromophenyl)(3-iodobenzo[*b*]thiophen-2-yl)methanone (9ae):



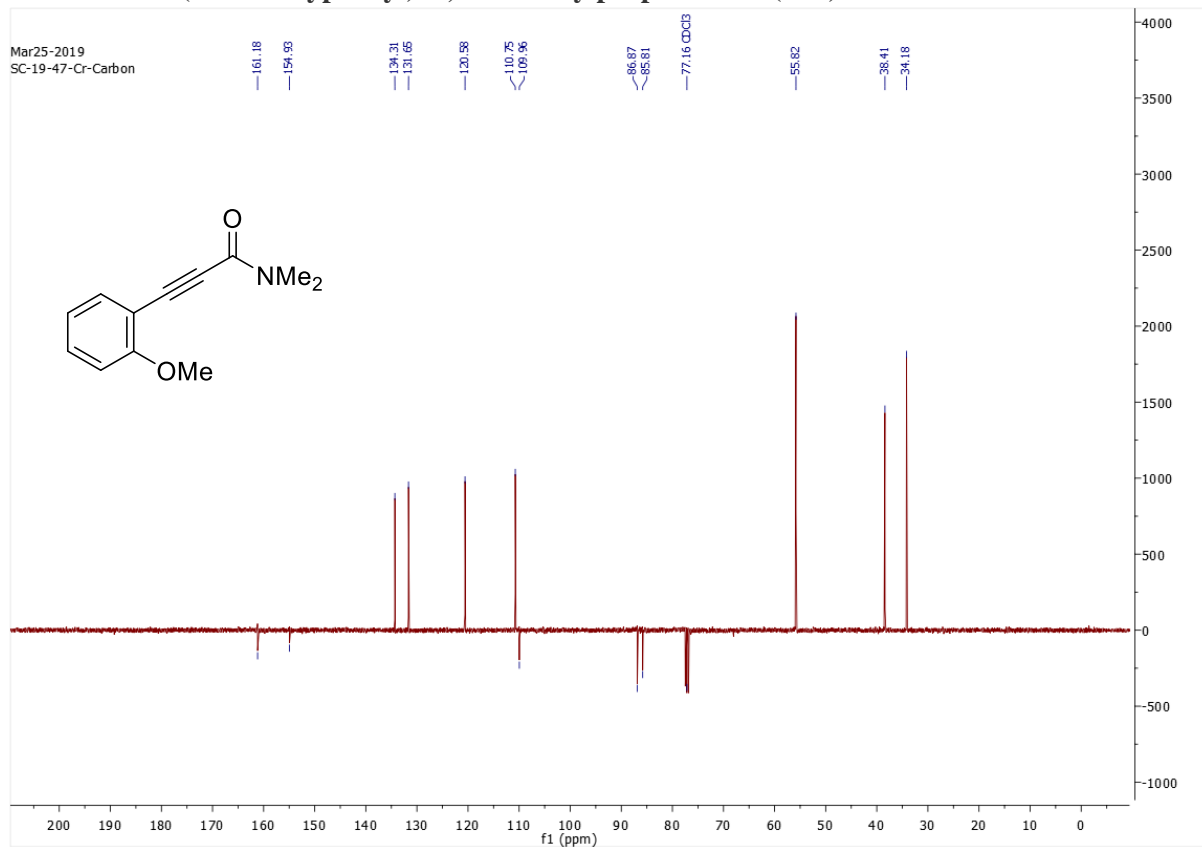
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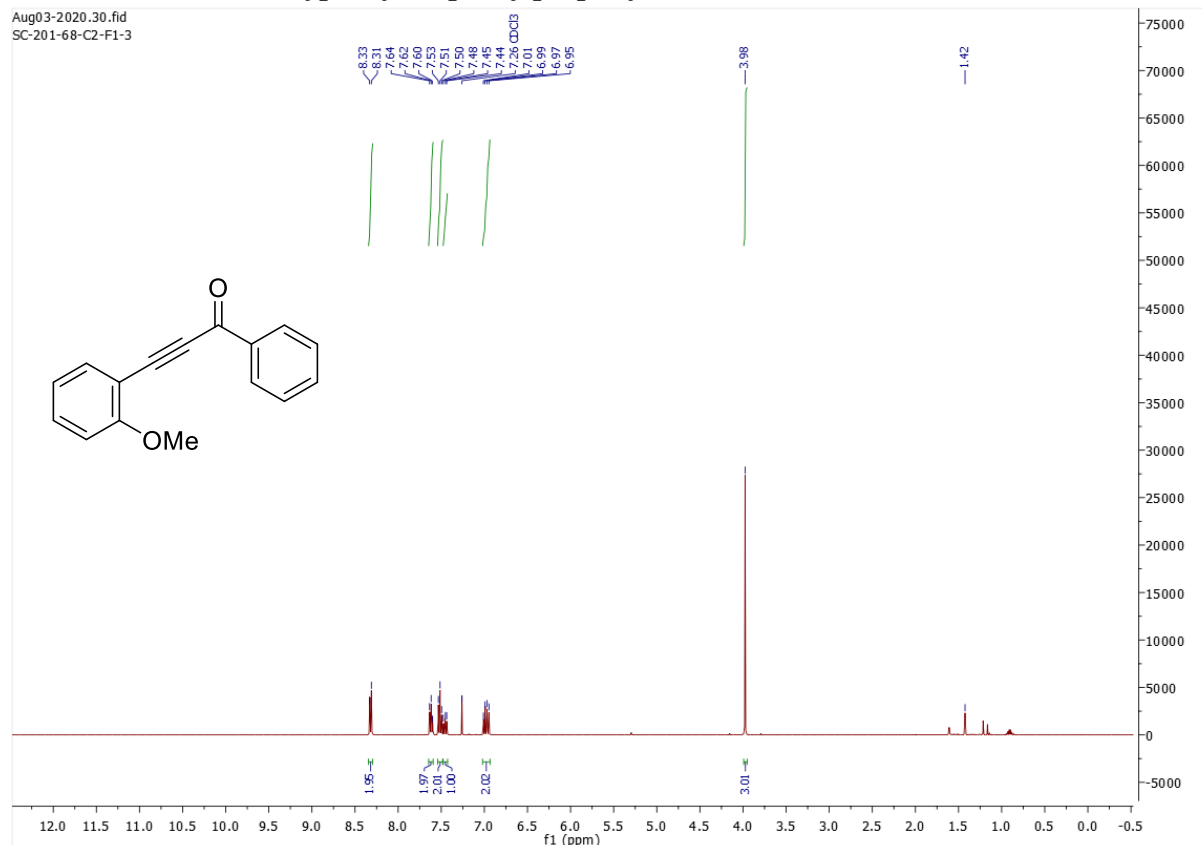
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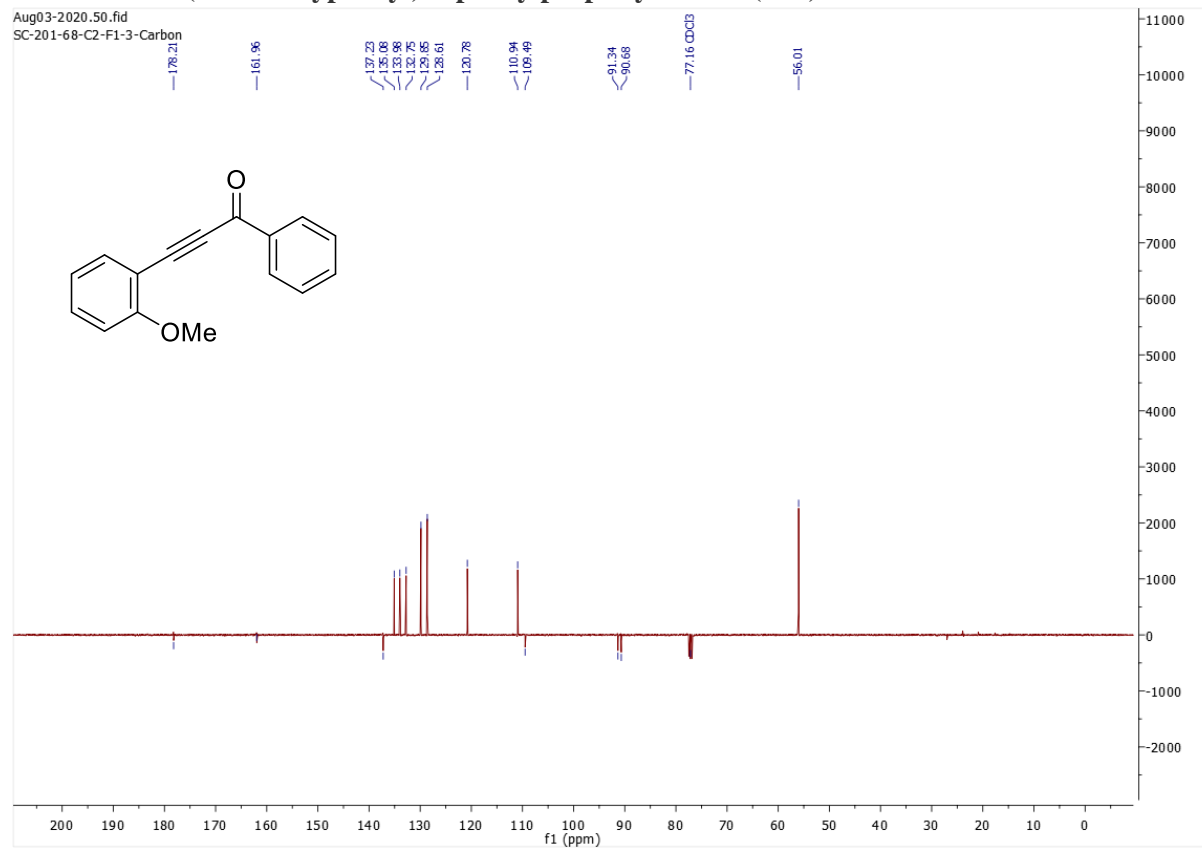
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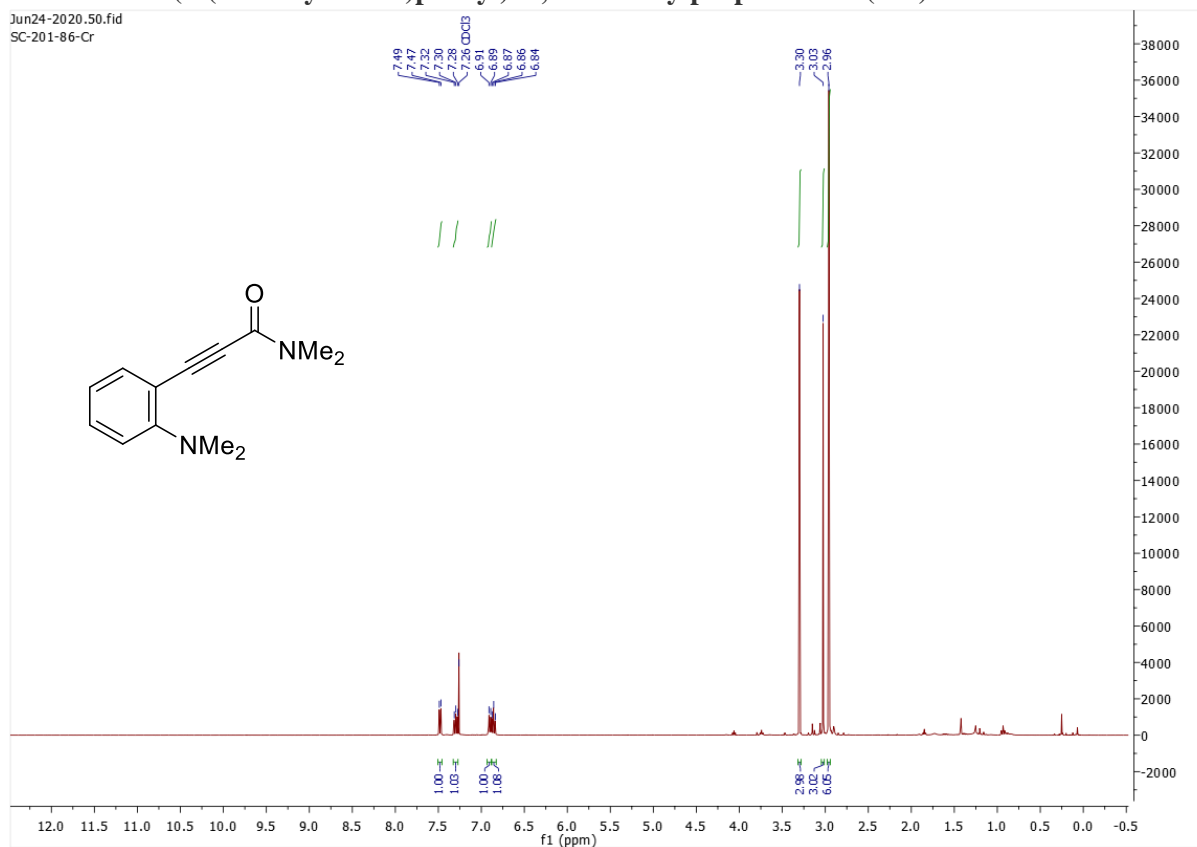
¹H NMR of 3-(2-methoxyphenyl)-1-phenylprop-2-yn-1-one (8bd):



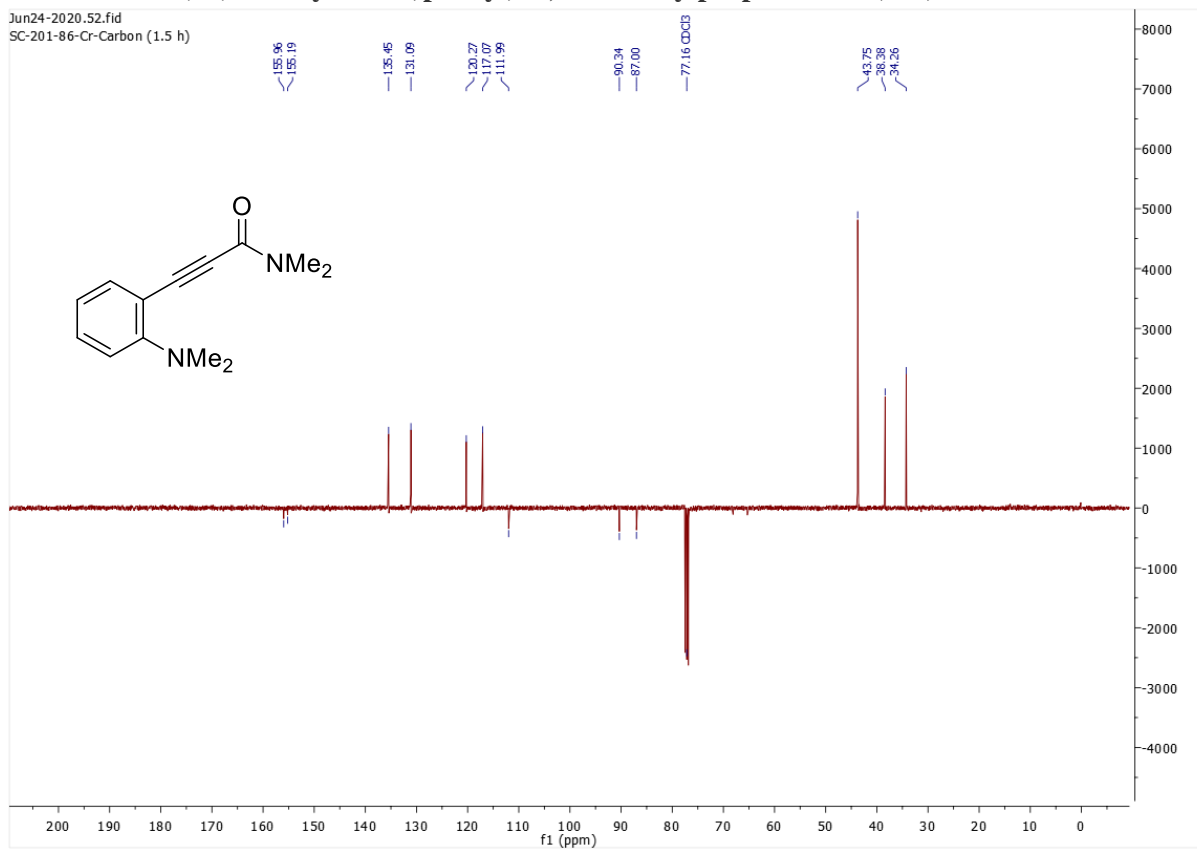
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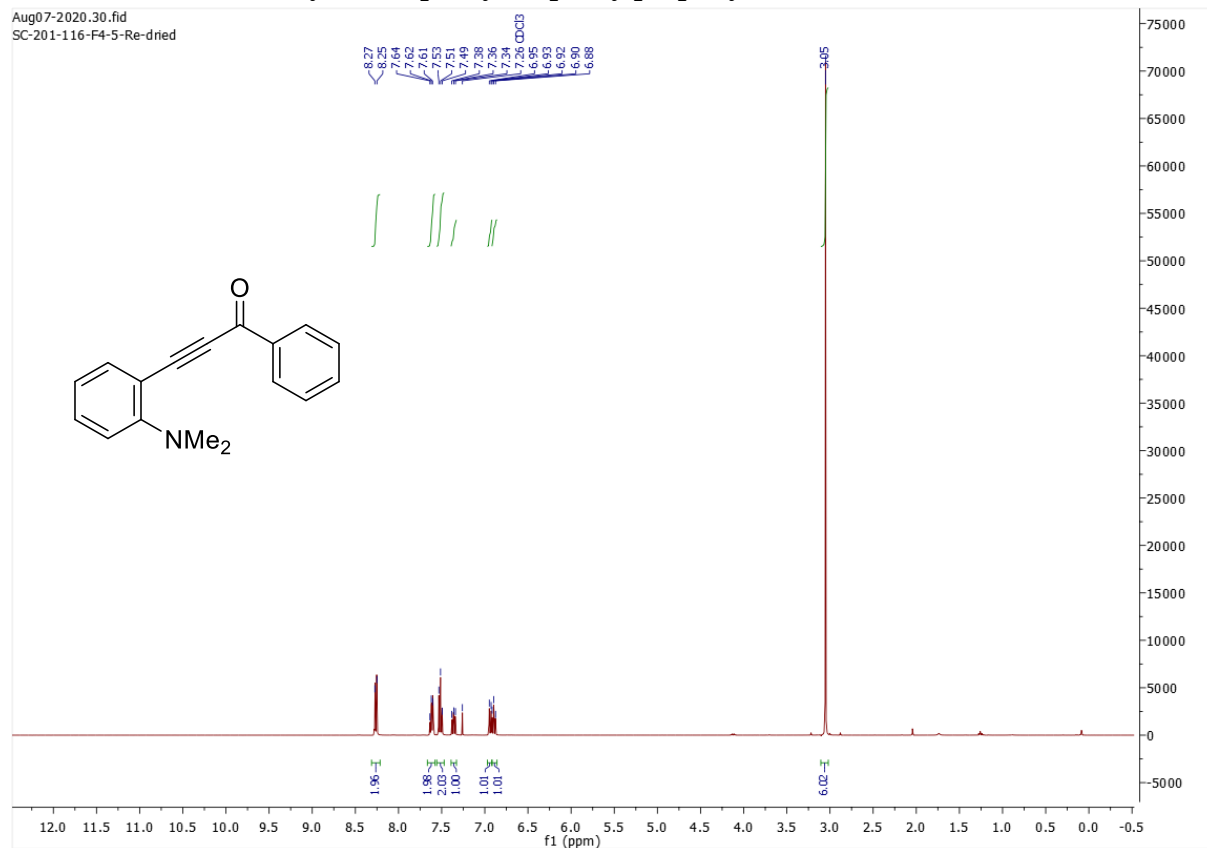
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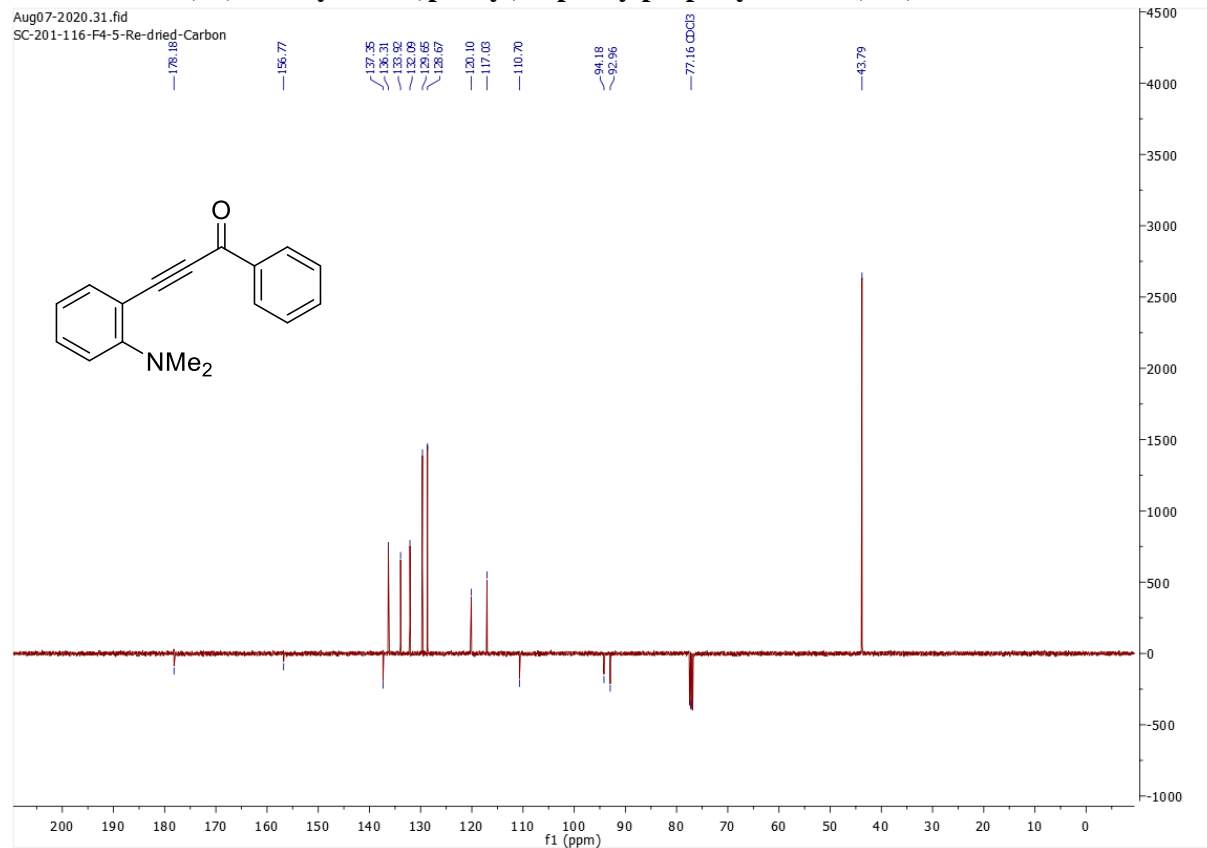
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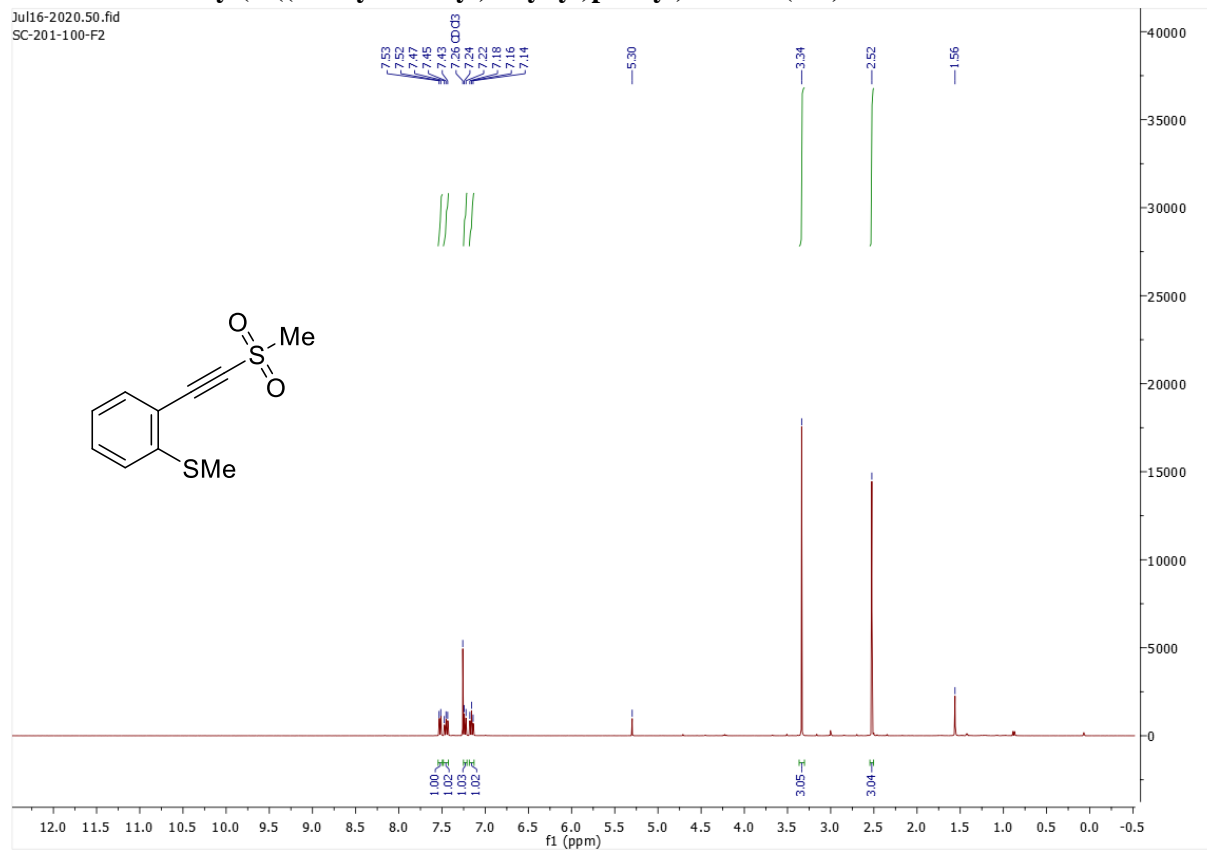
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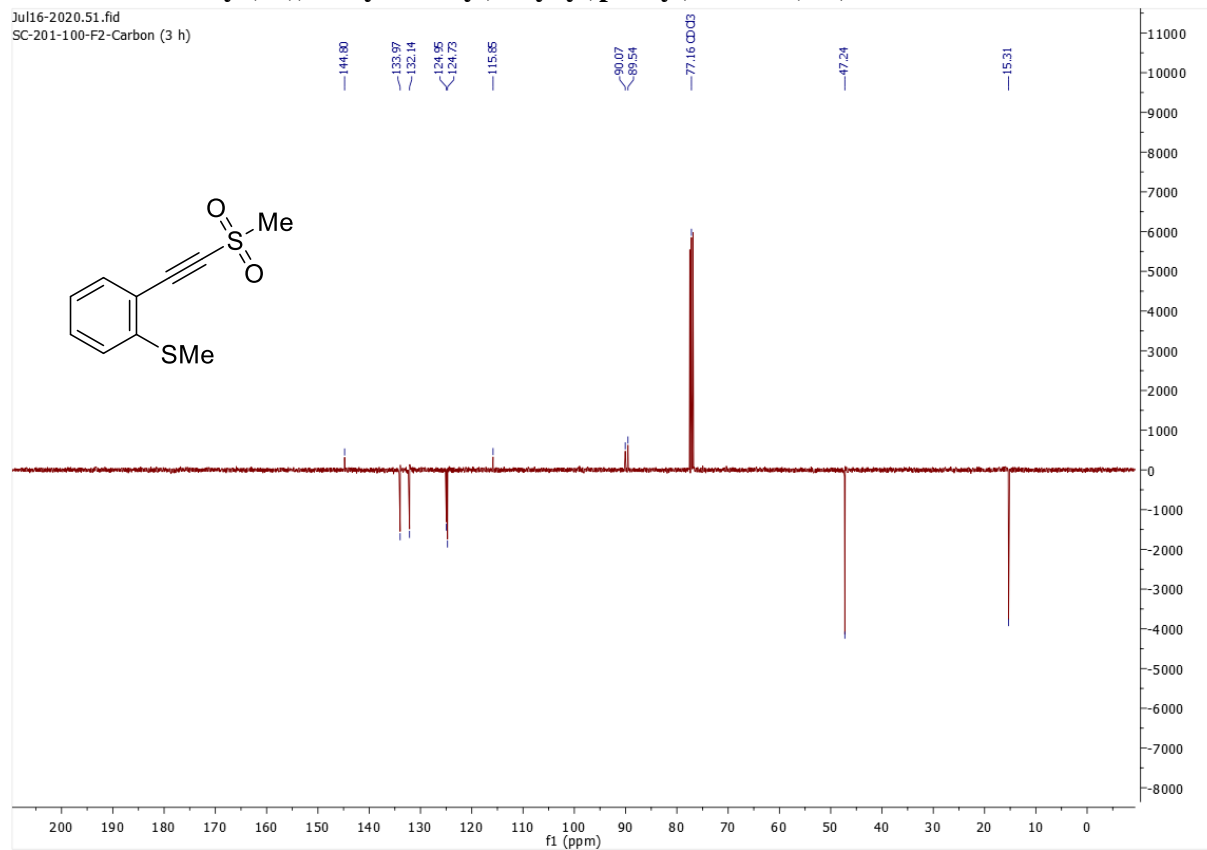
¹³C NMR of 3-(2-(dimethylamino)phenyl)-1-phenylprop-2-yn-1-one (8cd):



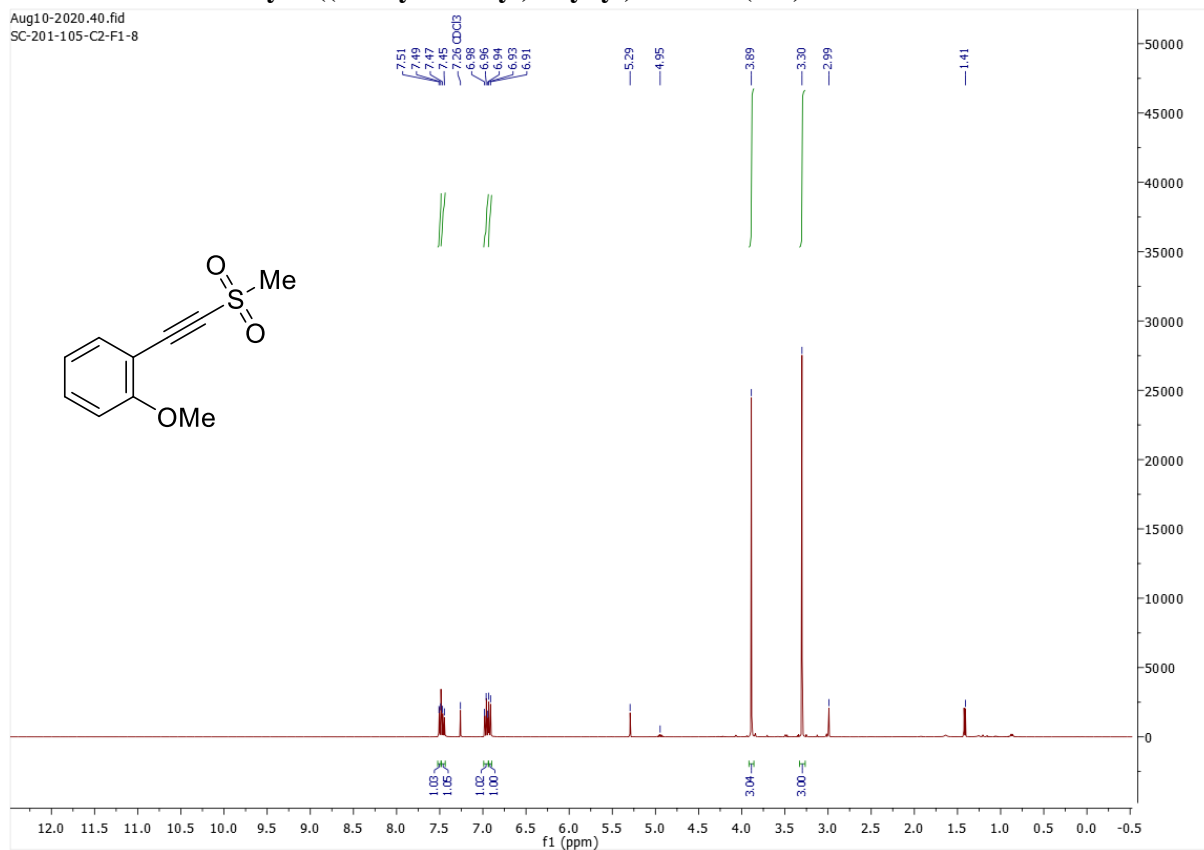
¹H NMR of methyl(2-((methylsulfonyl)ethynyl)phenyl)sulfane (8af):



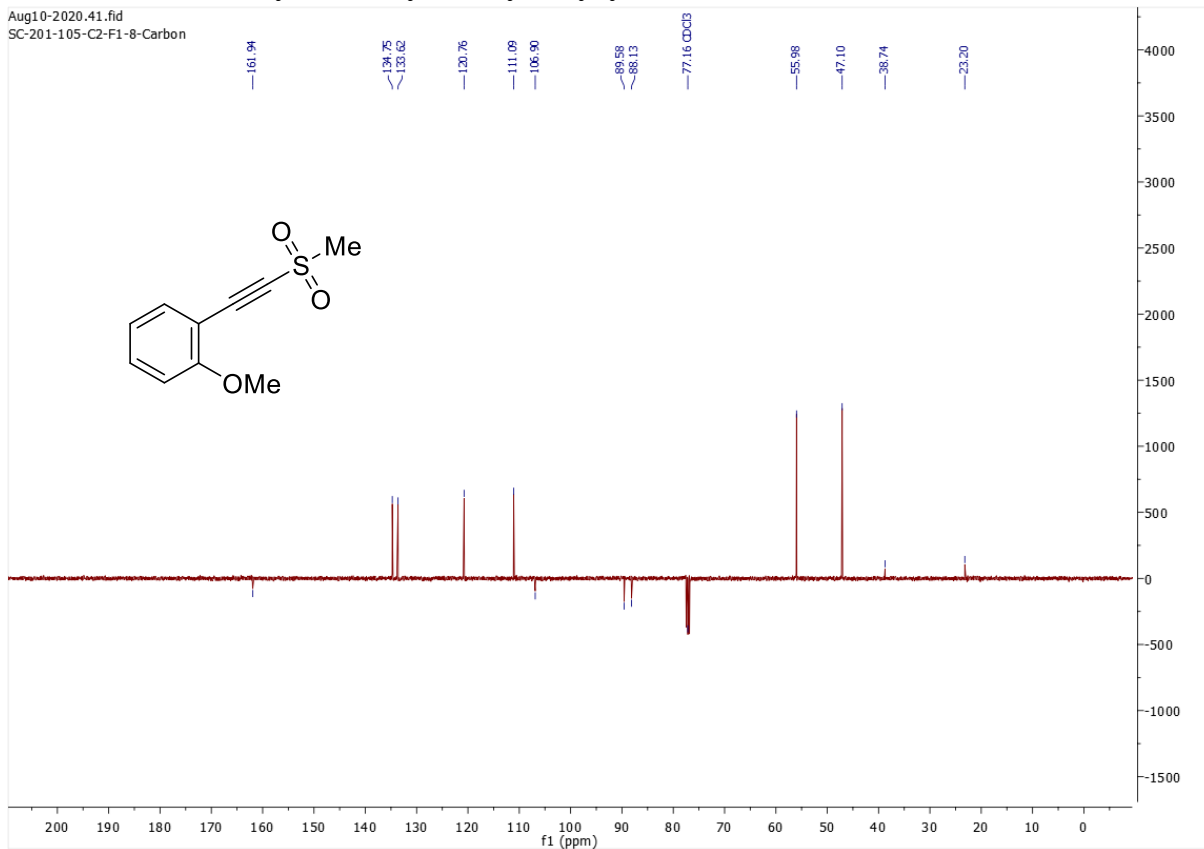
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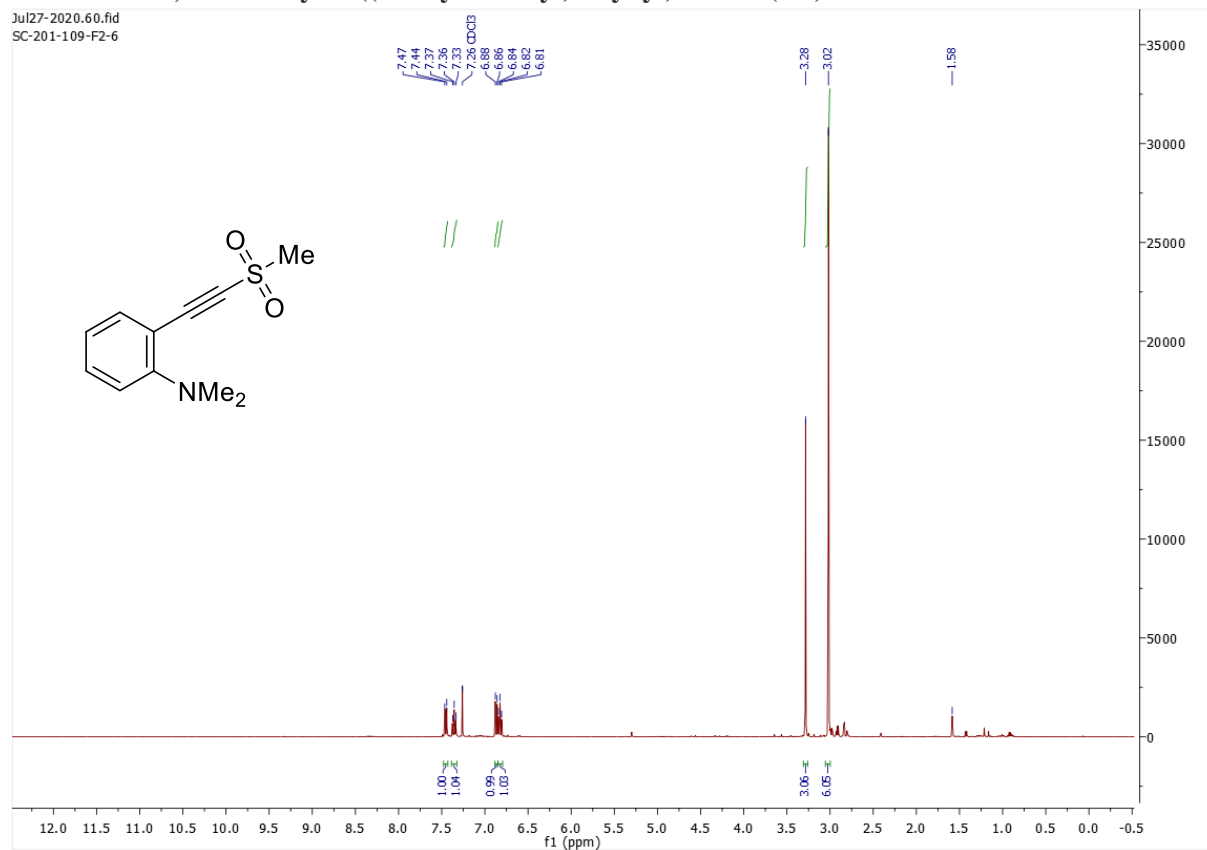
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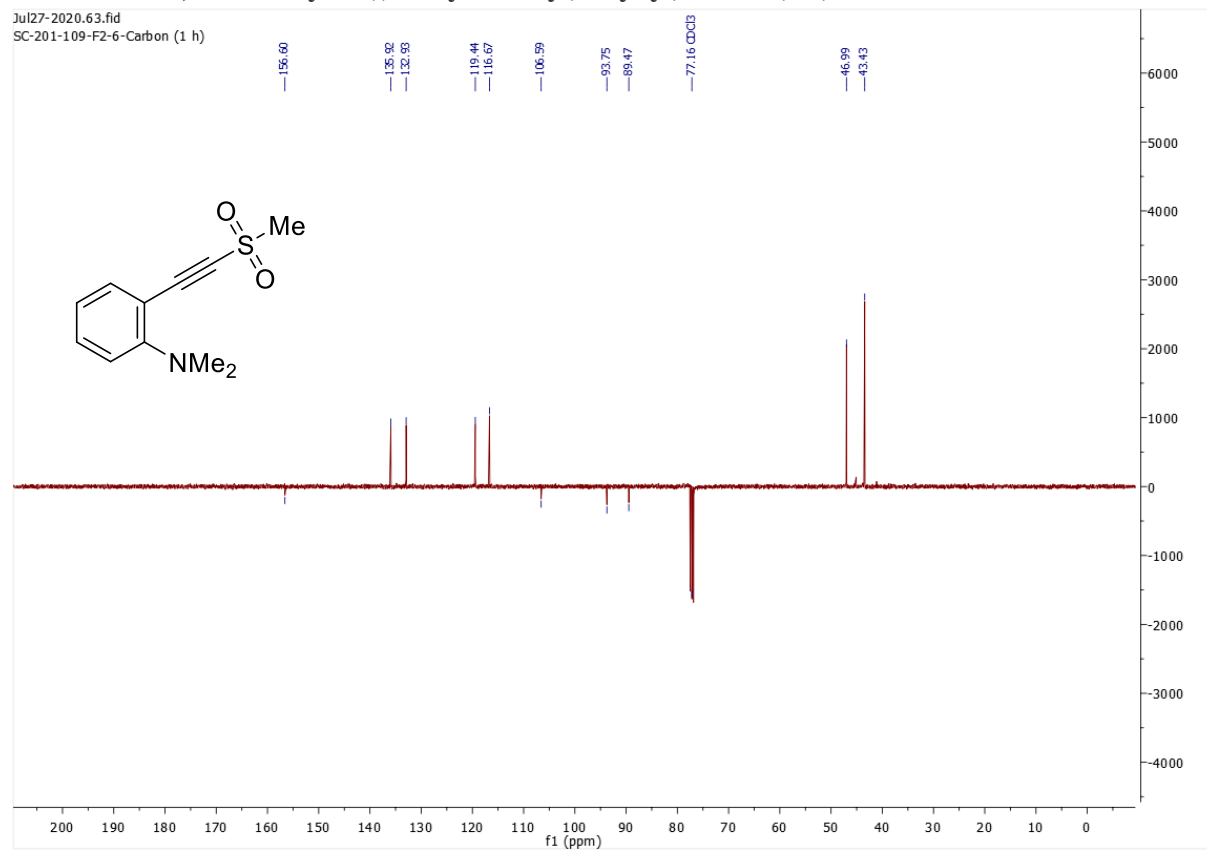
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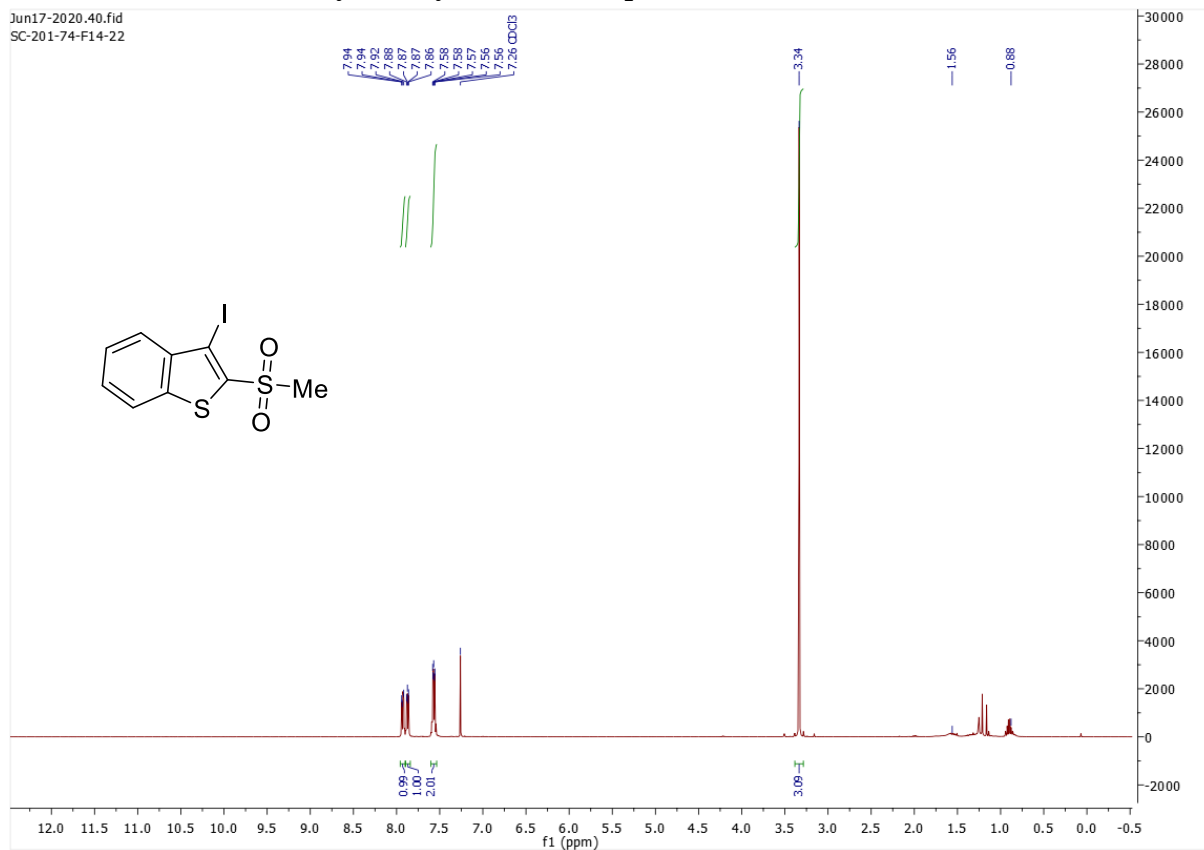
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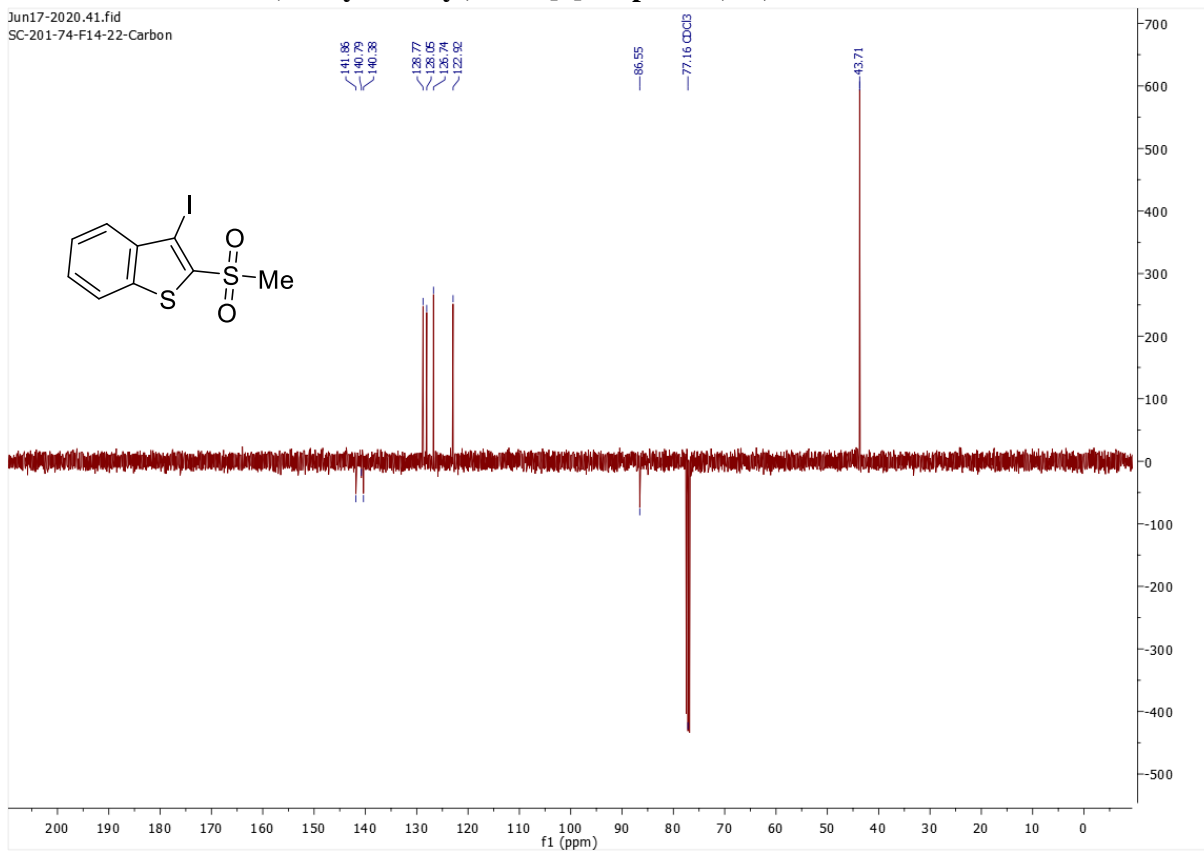
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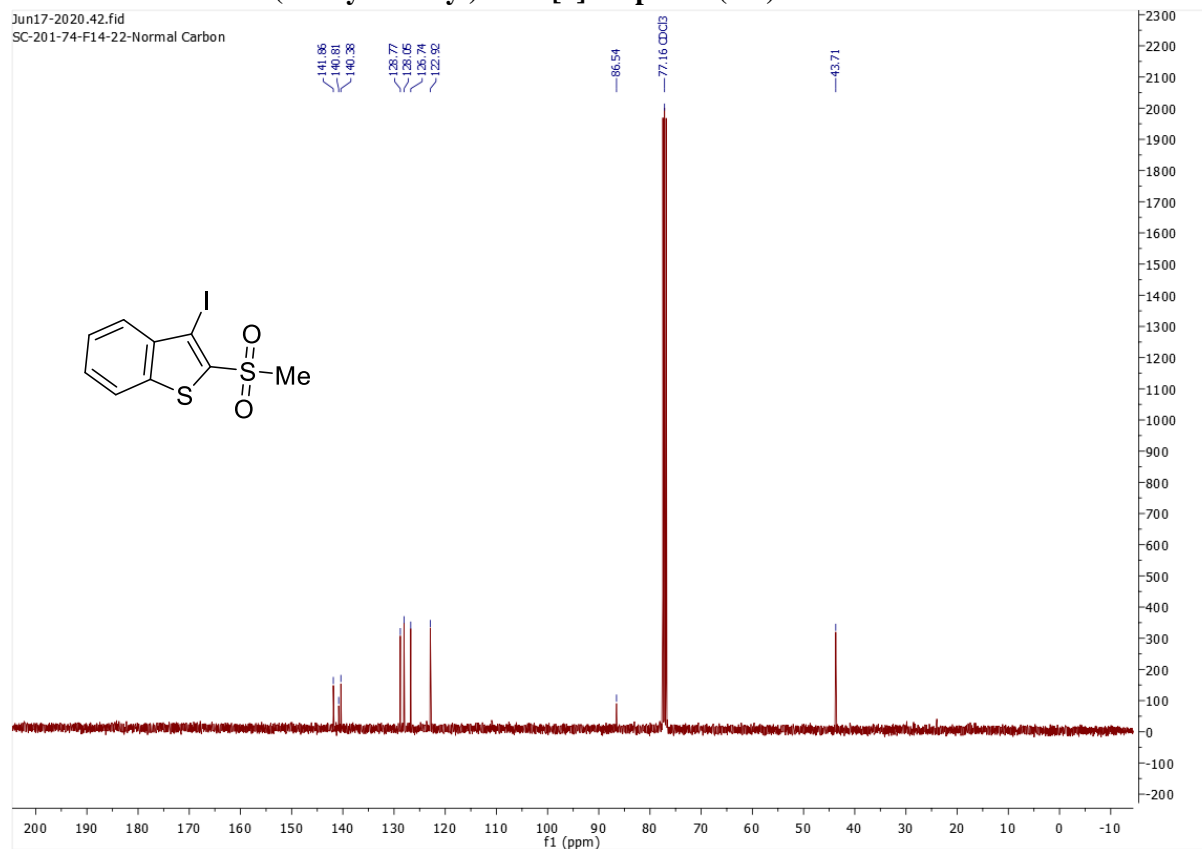
¹H NMR of 3-iodo-2-(methylsulfonyl)benzo[*b*]thiophene (9af):



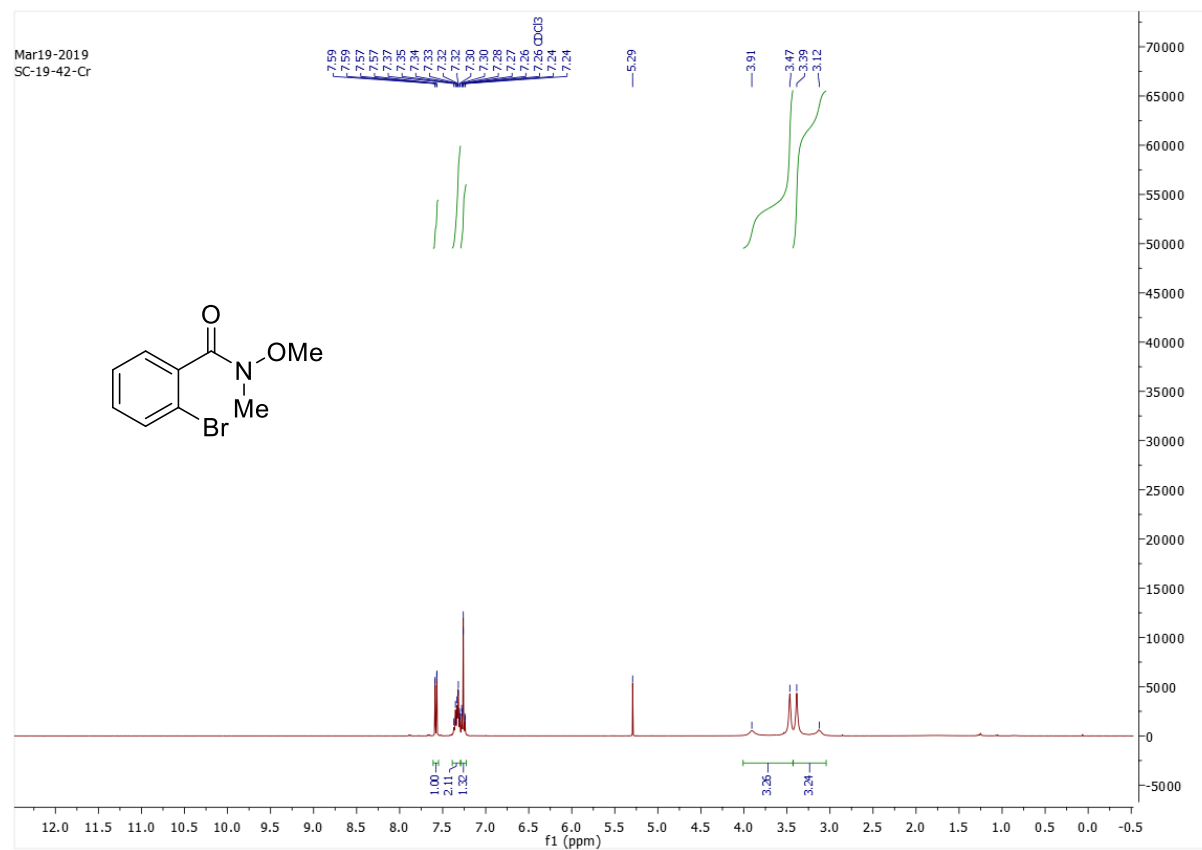
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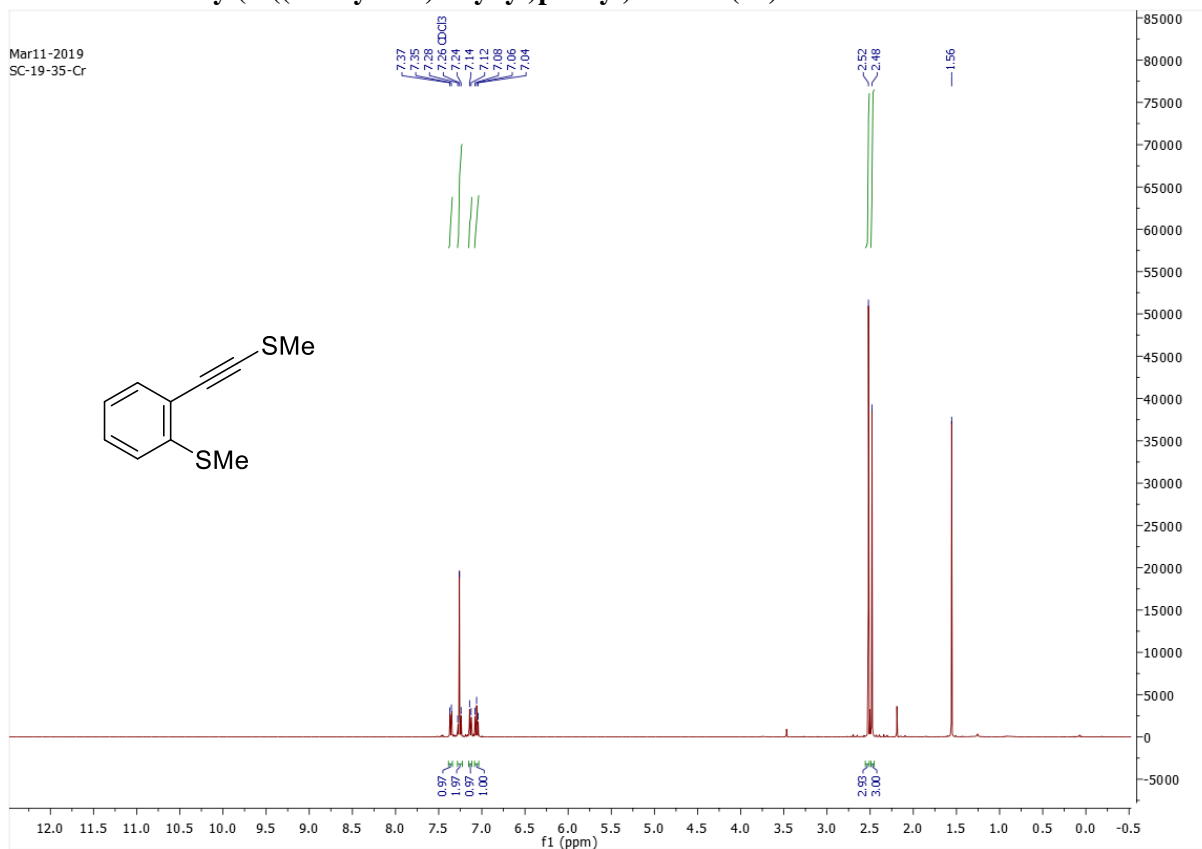
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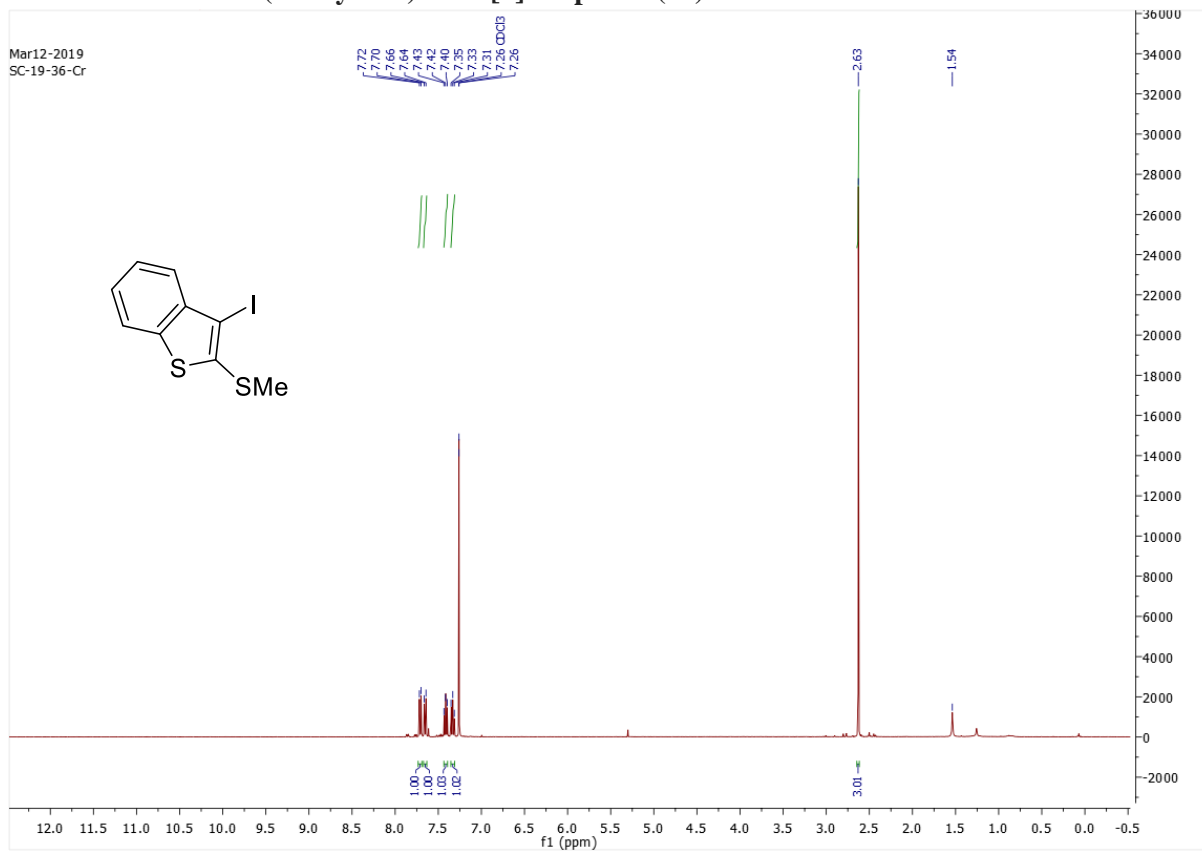
^1H NMR of 2-bromo-*N*-methoxy-*N*-methylbenzamide (17e):



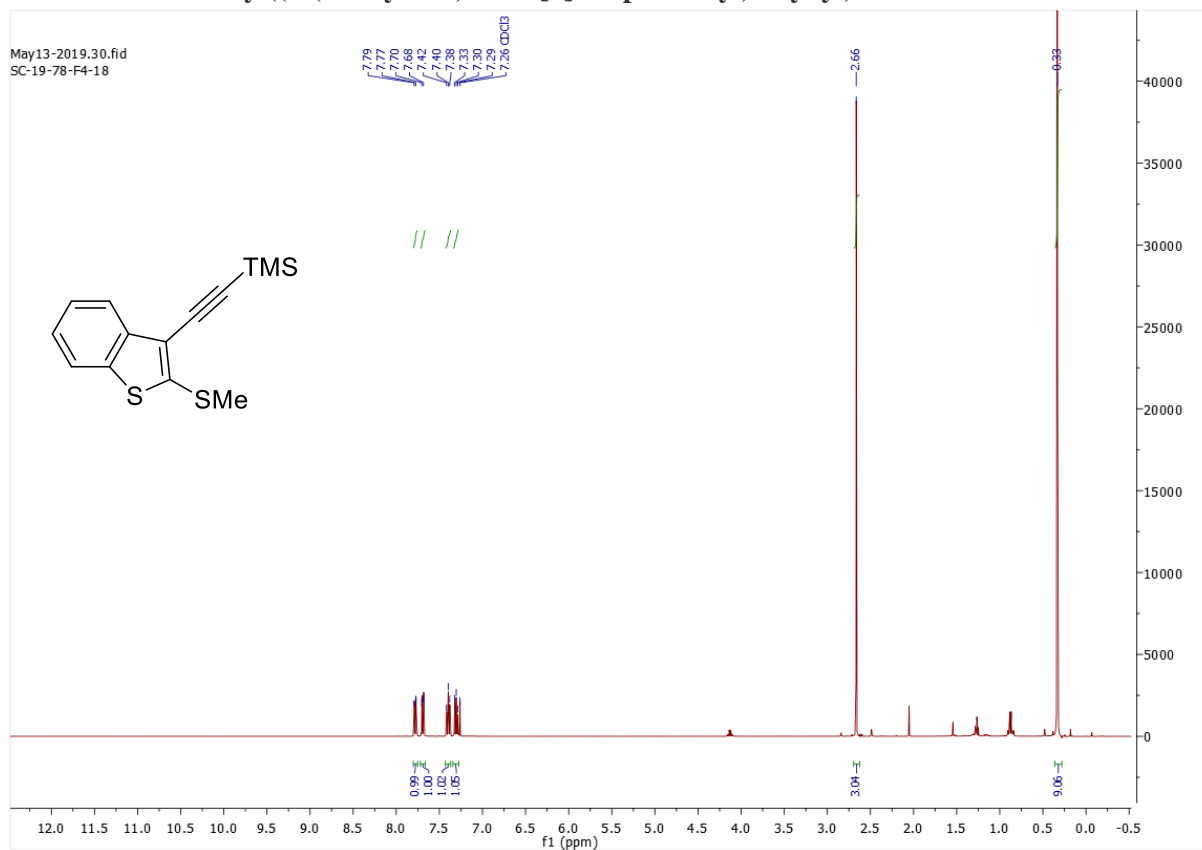
¹H NMR of methyl(2-((methylthio)ethynyl)phenyl)sulfane (18):



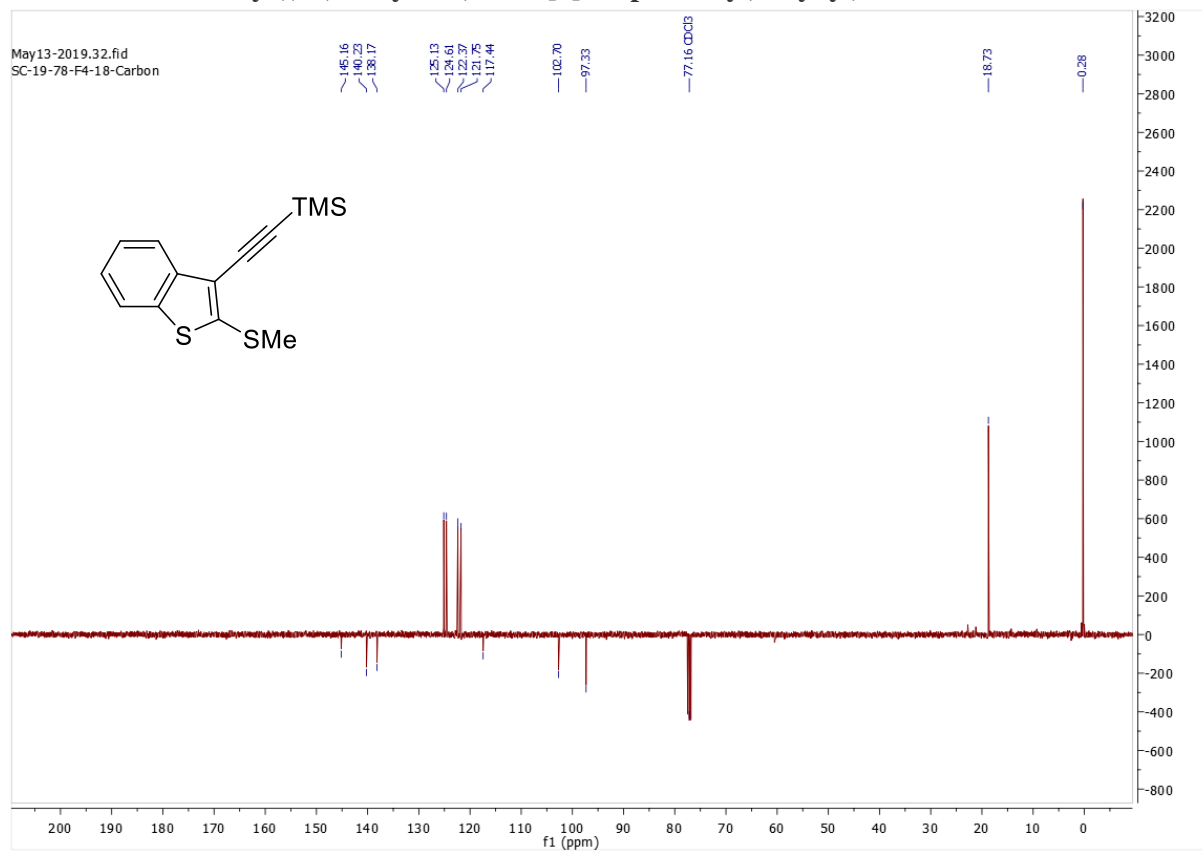
¹H NMR of 3-iodo-2-(methylthio)benzo[*b*]thiophene (19):



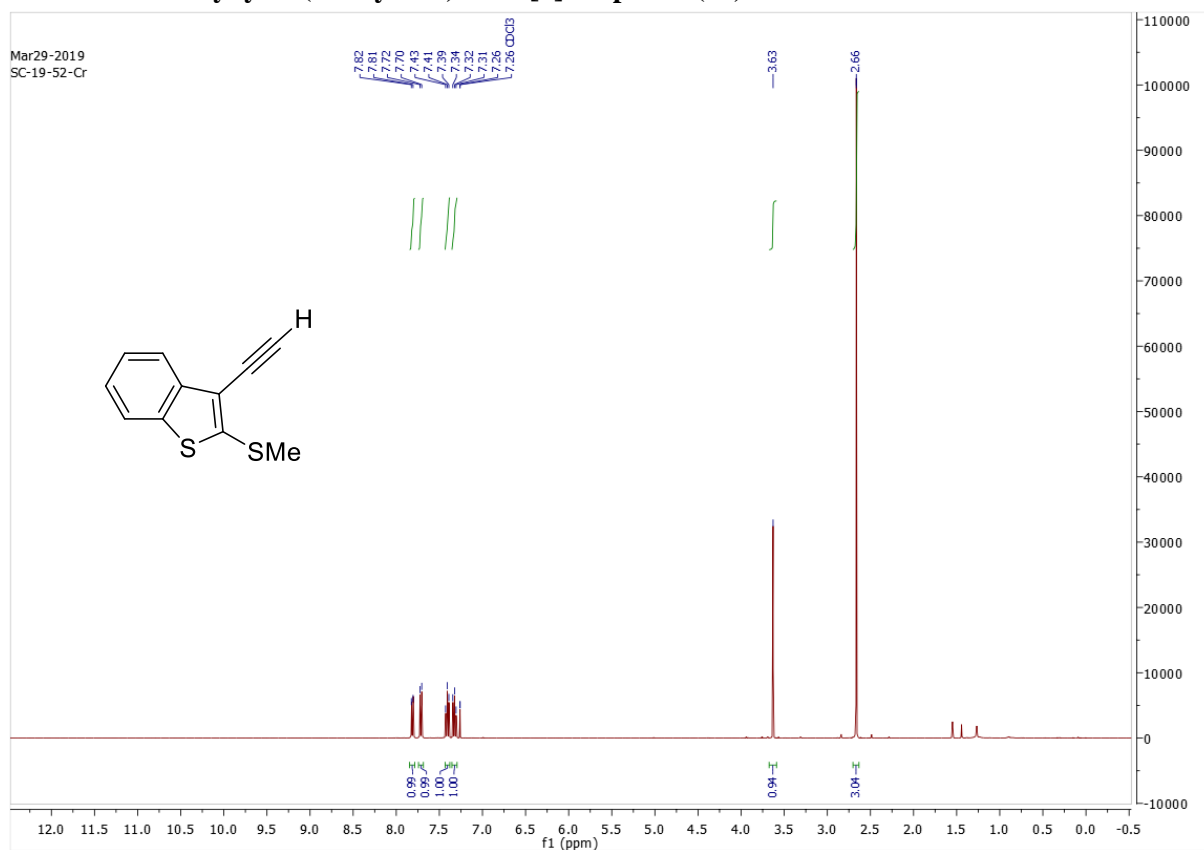
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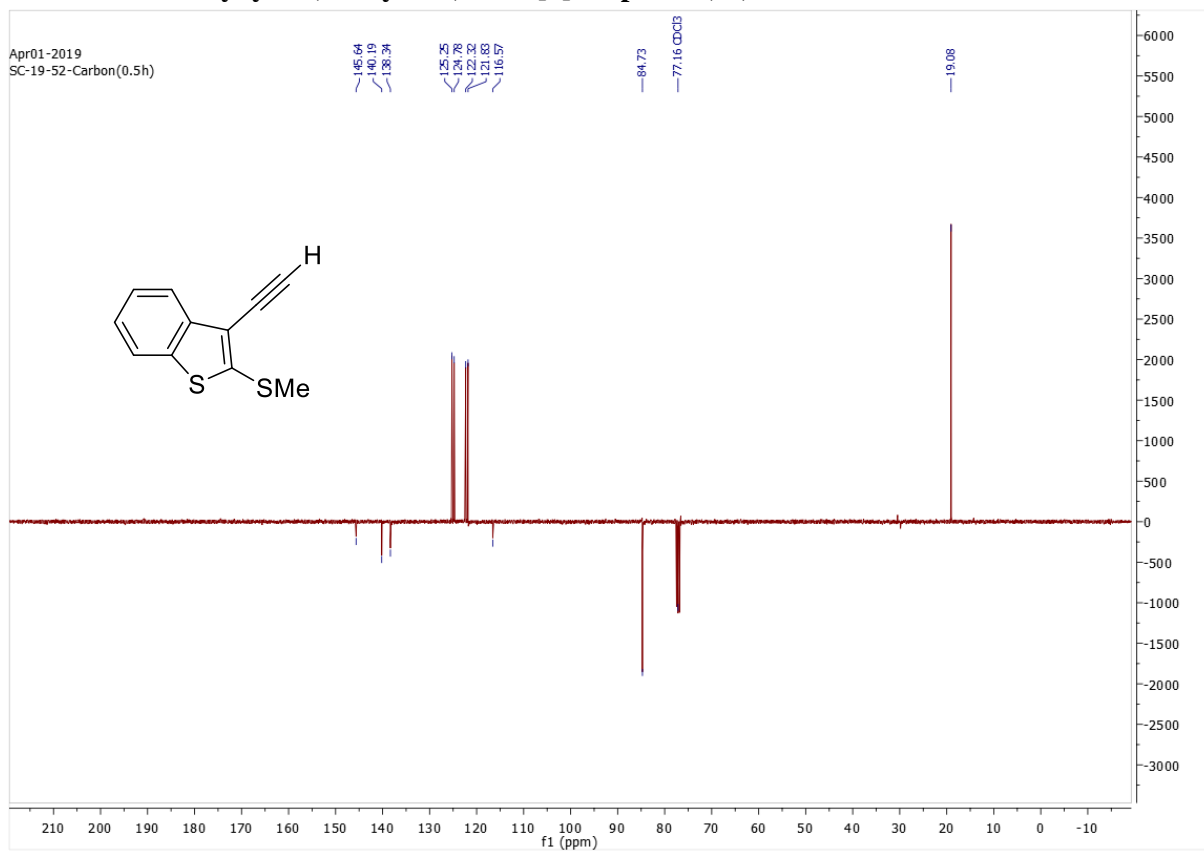
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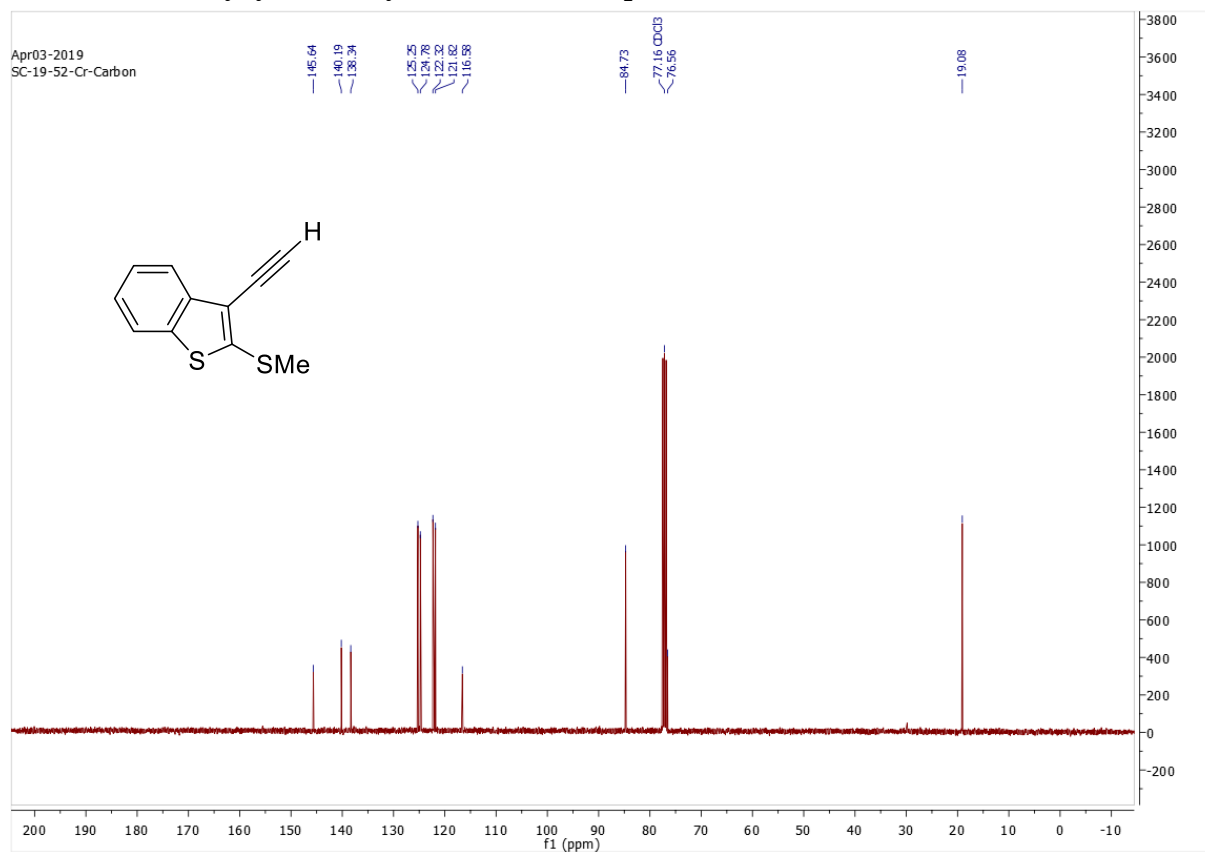
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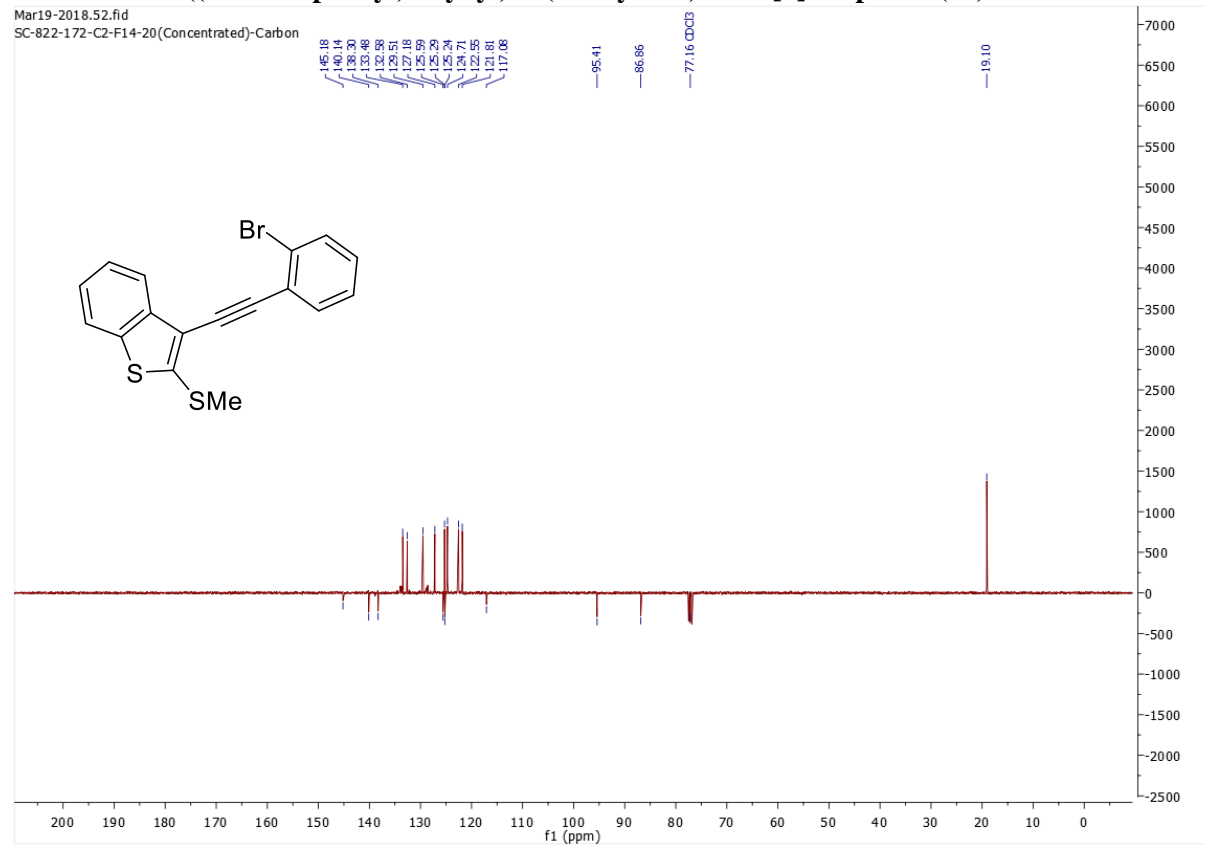
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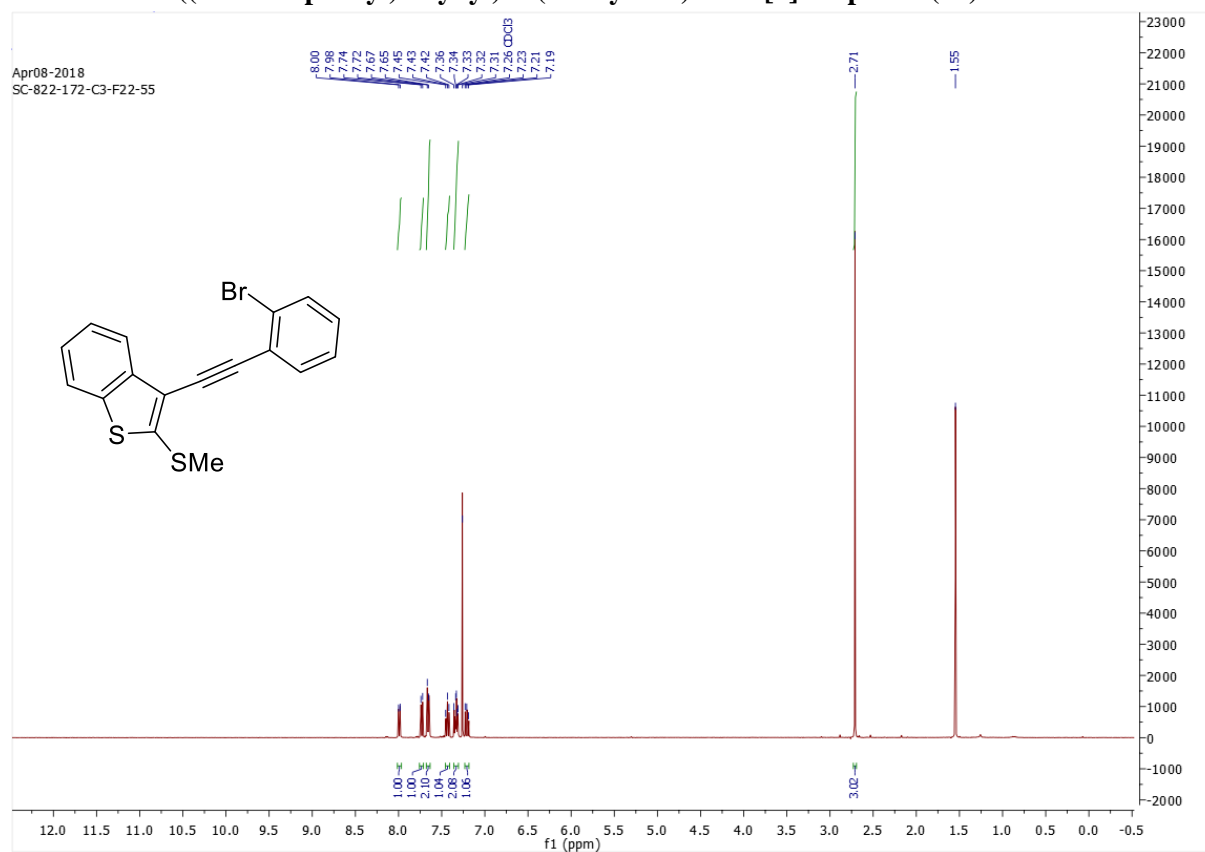
¹³C NMR of 3-ethynyl-2-(methylthio)benzo[*b*]thiophene (20):



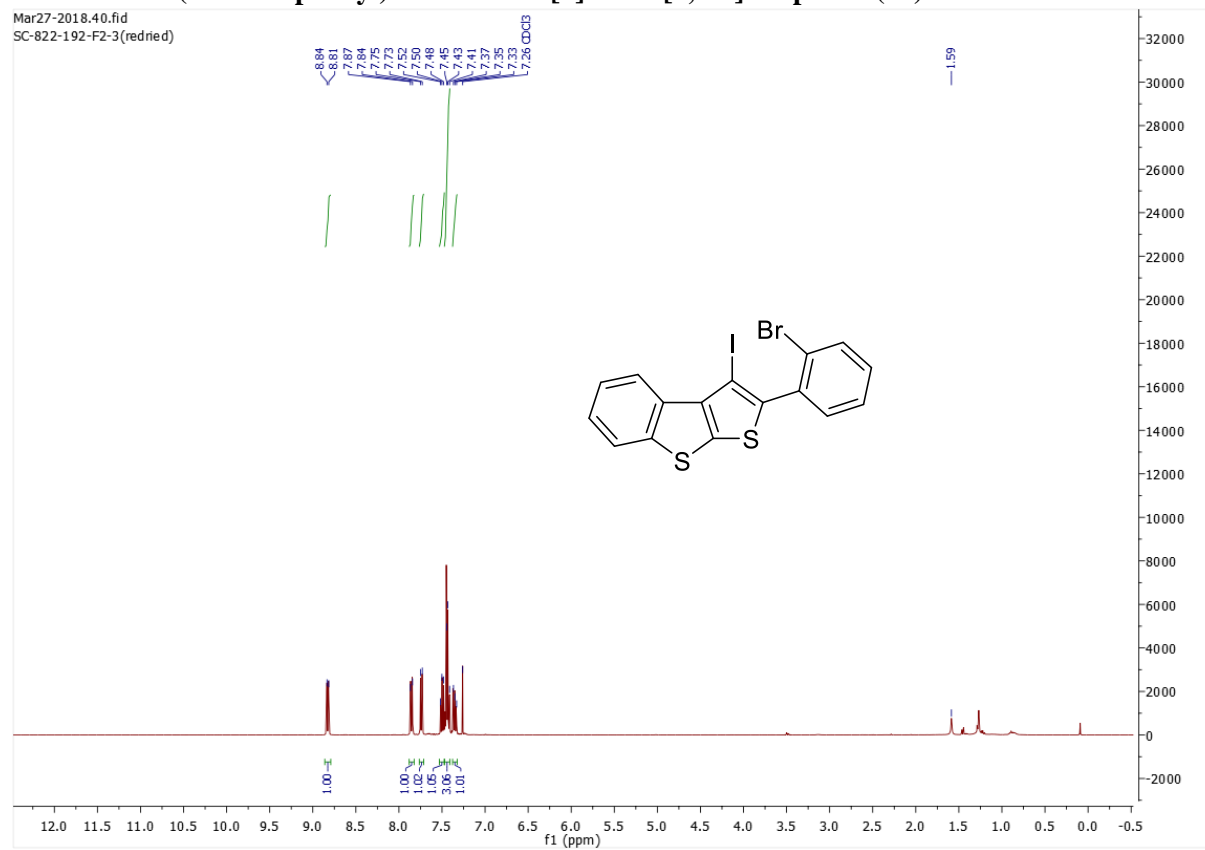
¹³C NMR of 3-((2-bromophenyl)ethynyl)-2-(methylthio)benzo[*b*]thiophene (21):



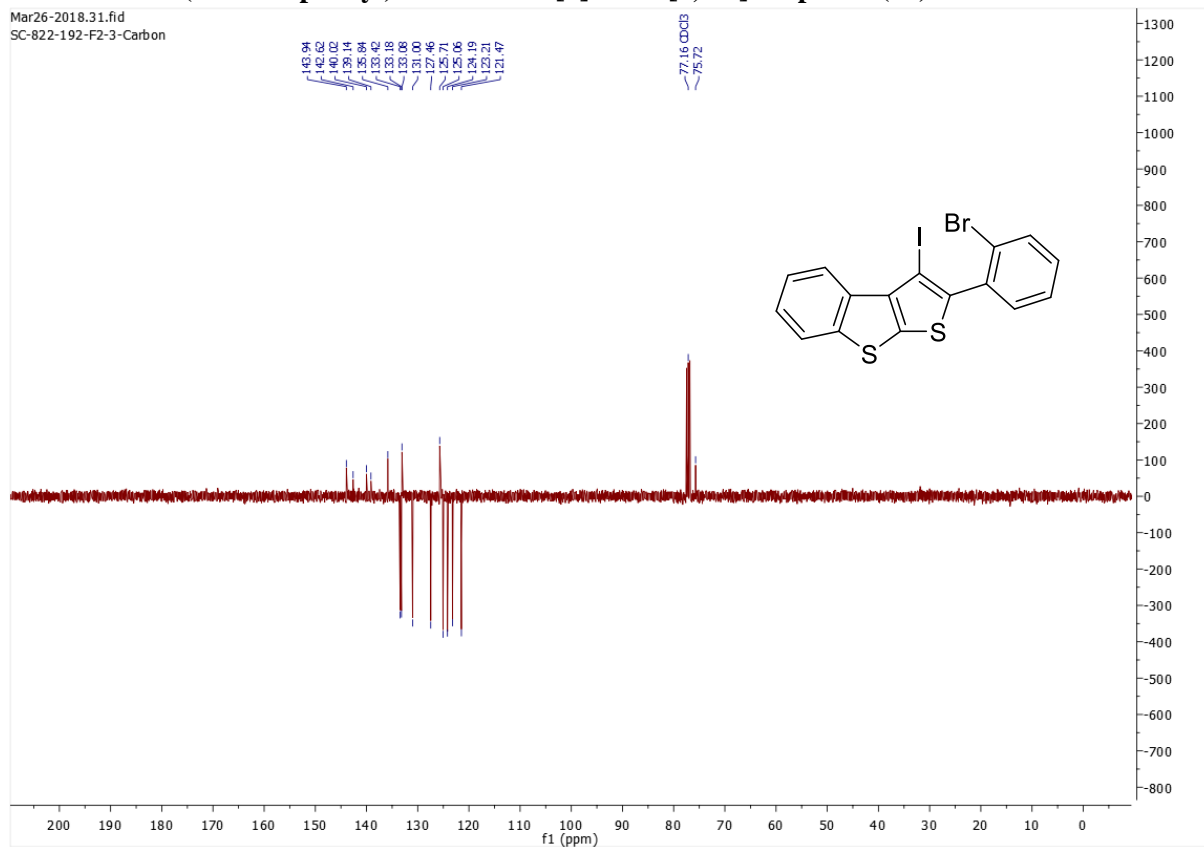
¹H NMR of 3-((2-bromophenyl)ethynyl)-2-(methylthio)benzo[b]thiophene (21):



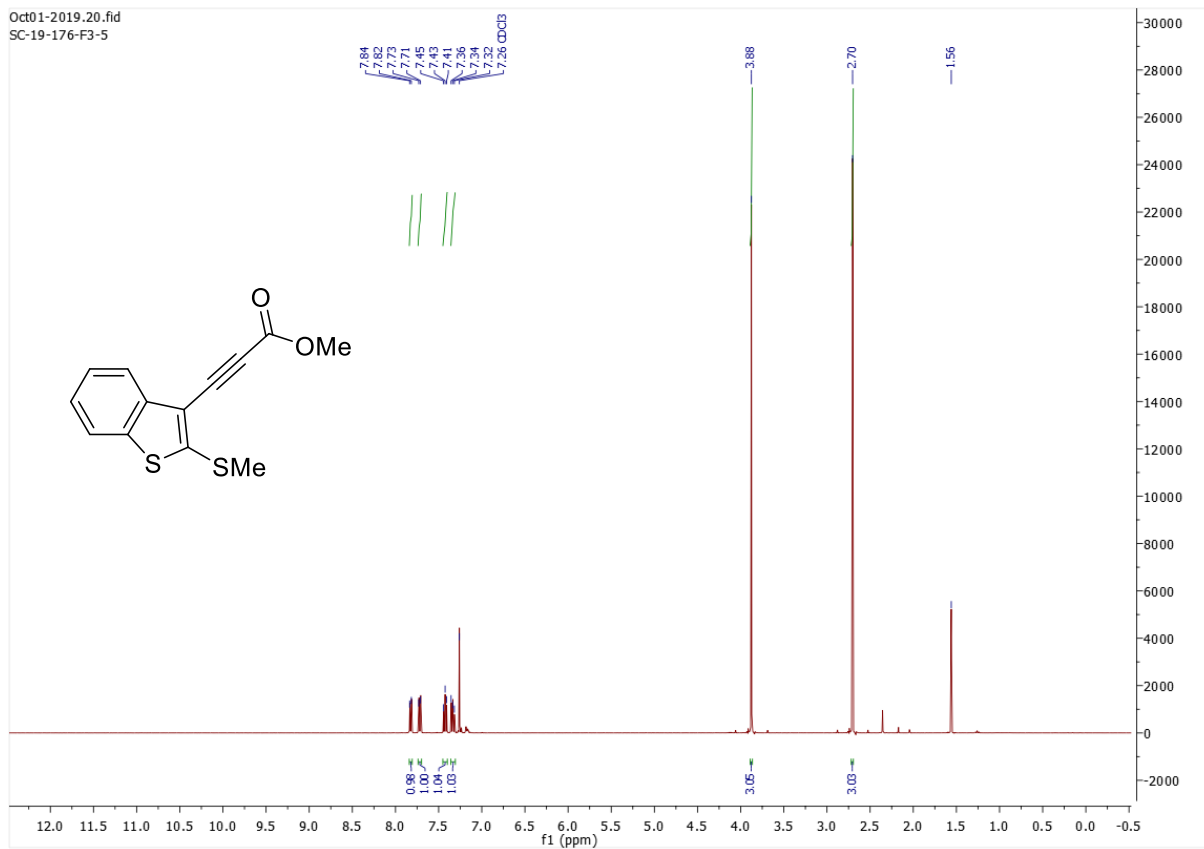
¹H NMR of 2-(2-bromophenyl)-3-iodobenzo[b]thieno[3,2-d]thiophene (24):



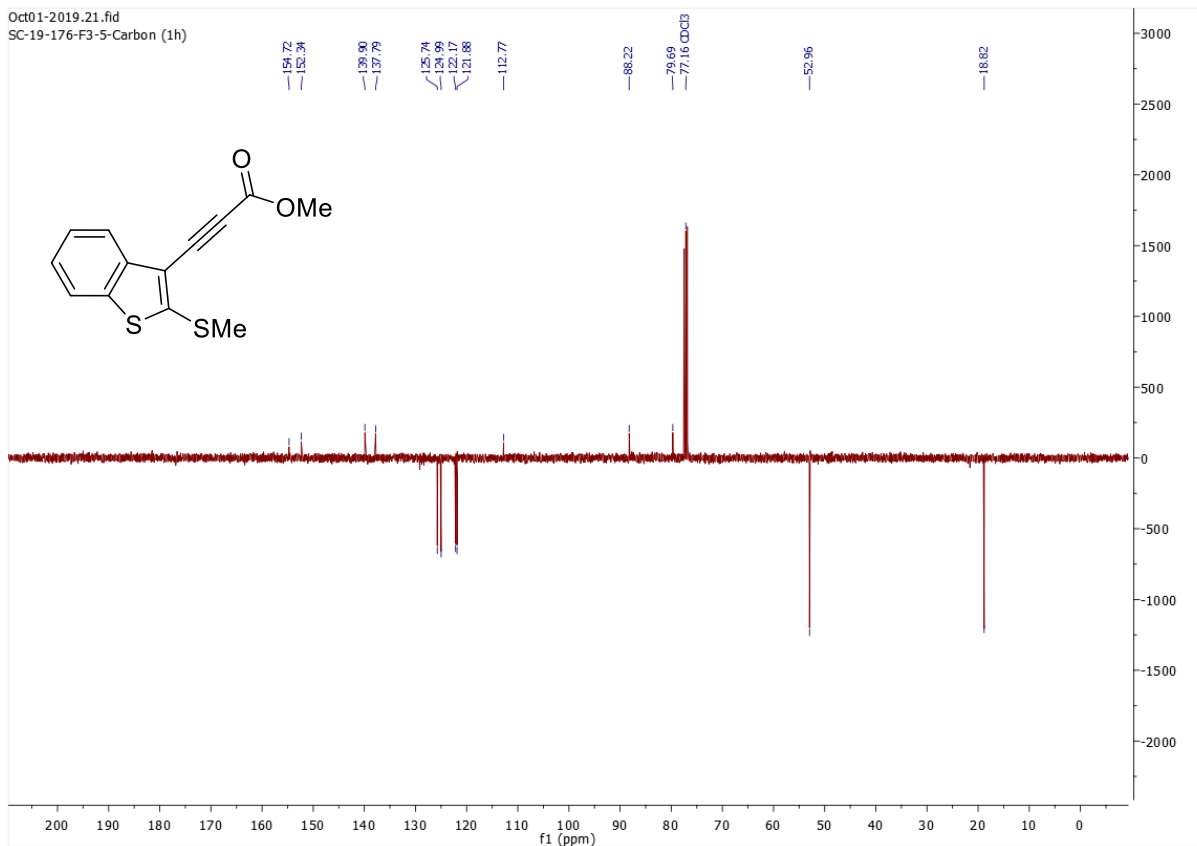
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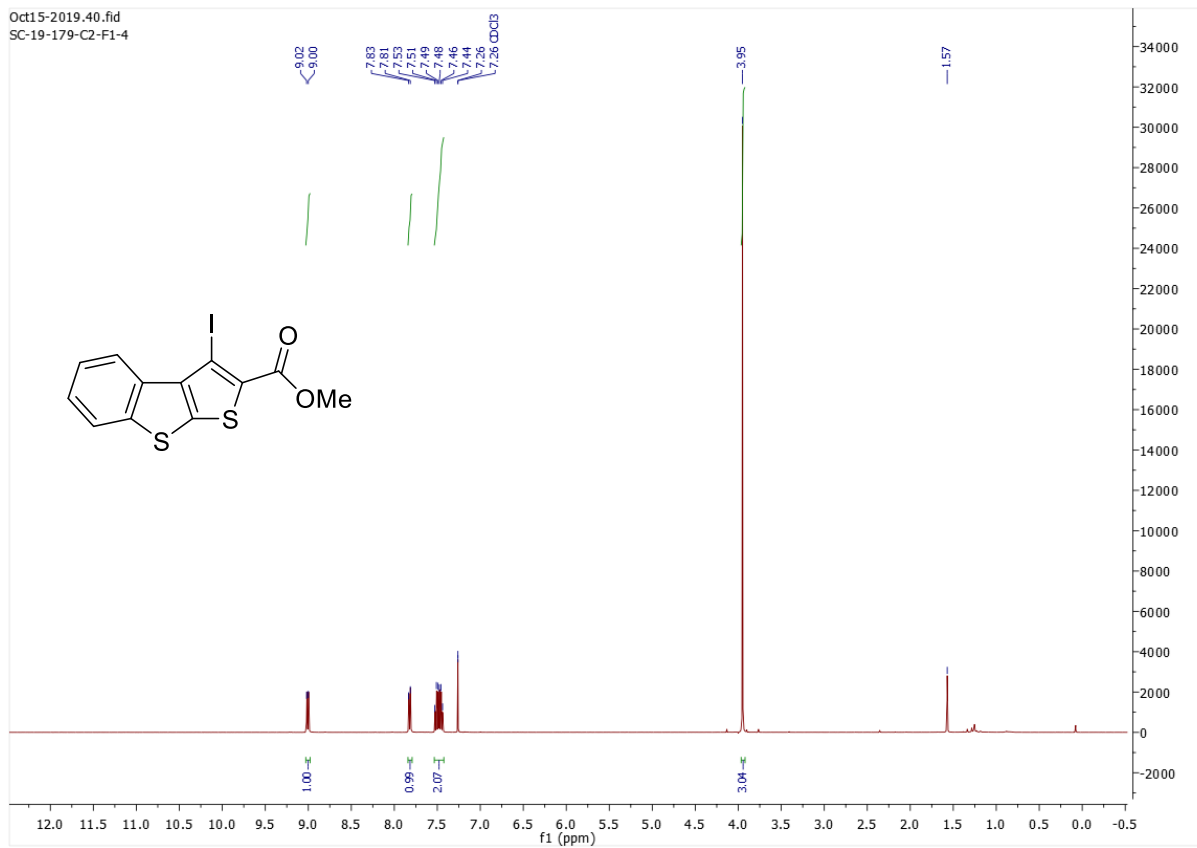
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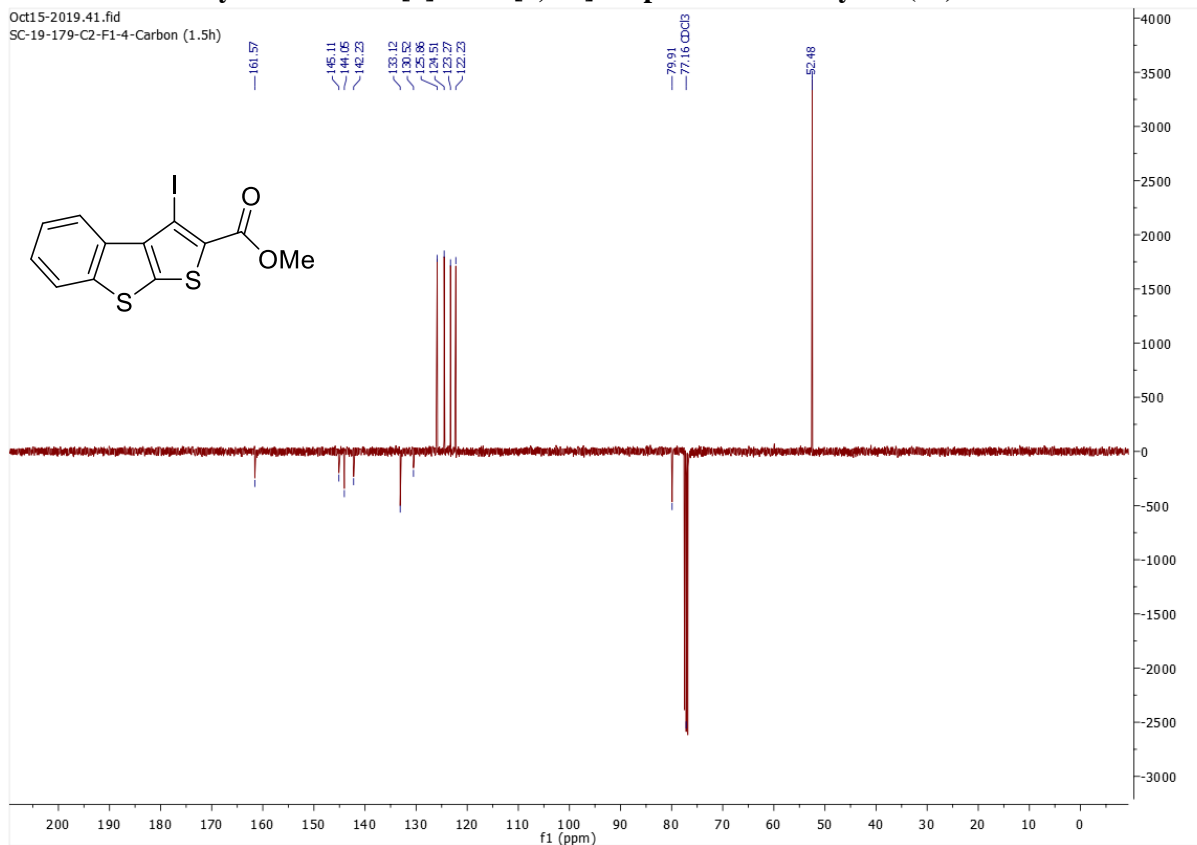
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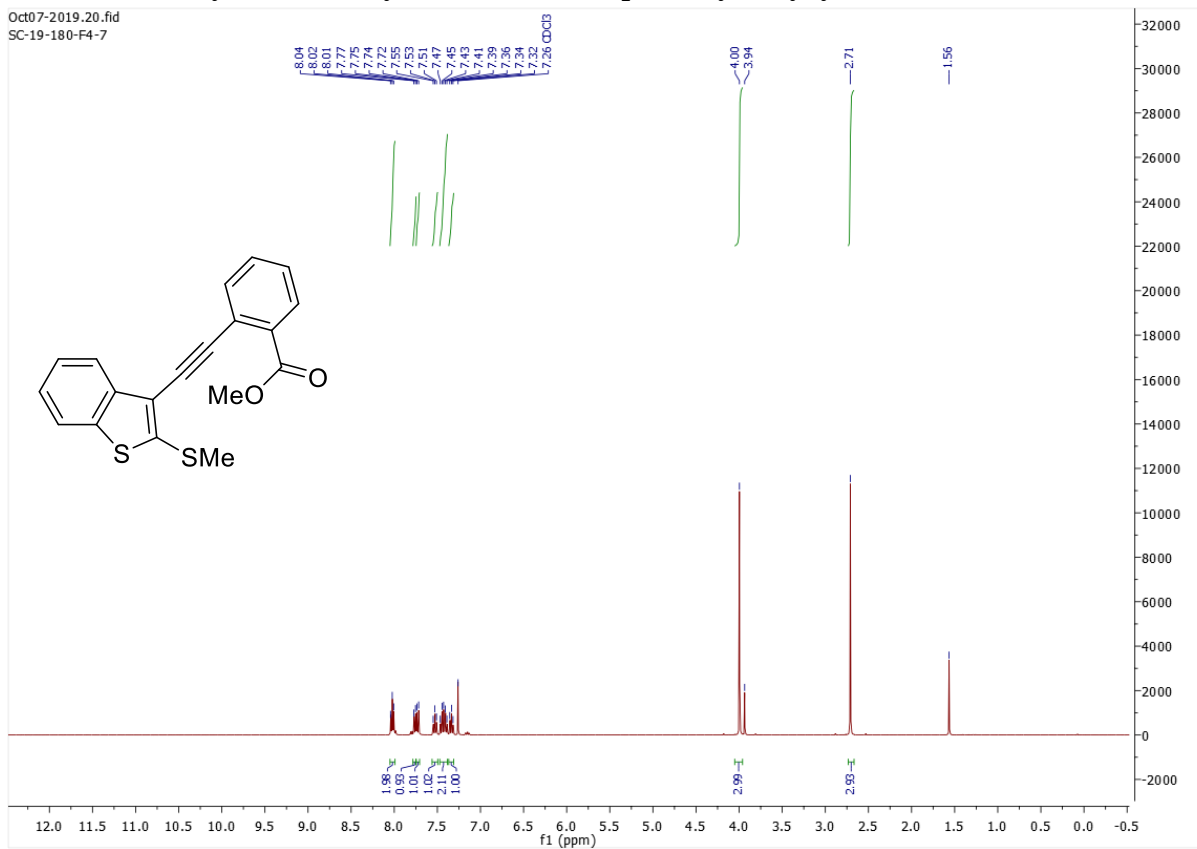
¹H NMR of methyl 3-iodobenzo[*b*]thieno[3,2-*d*]thiophene-2-carboxylate (26):



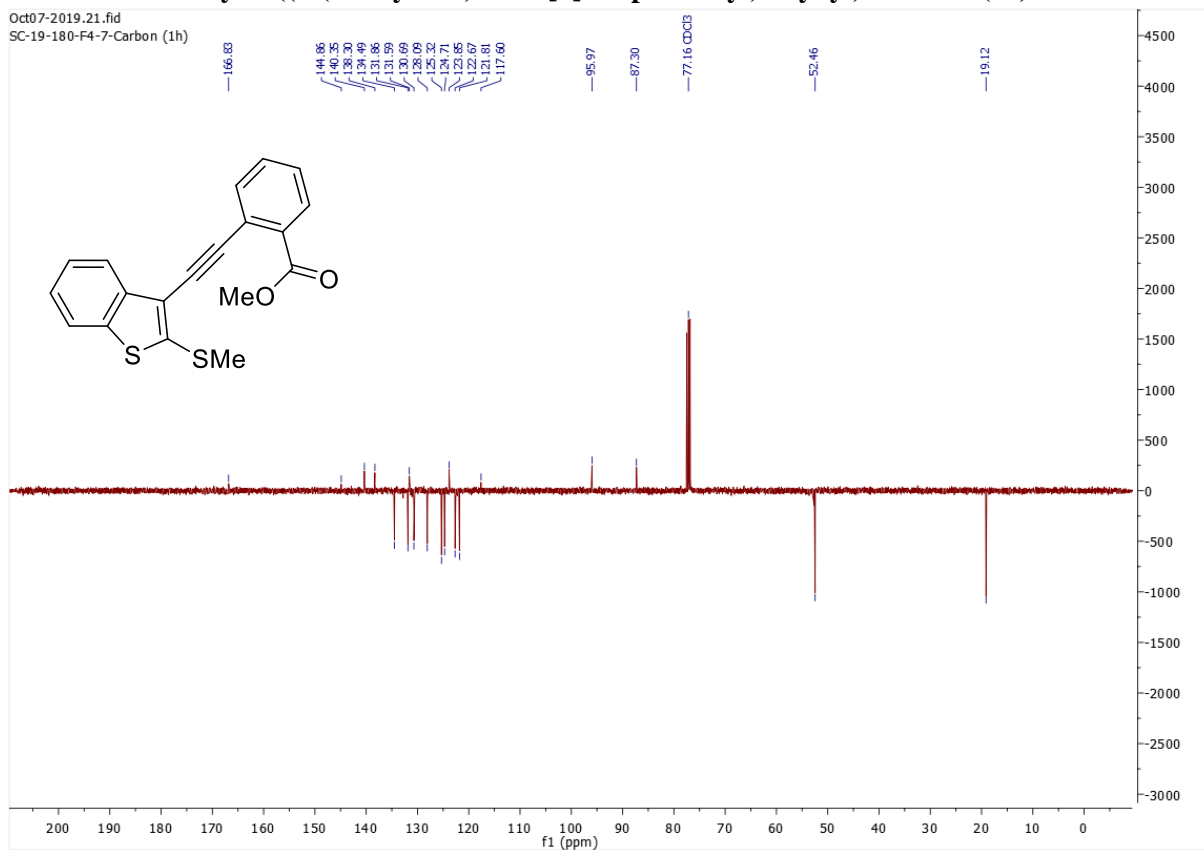
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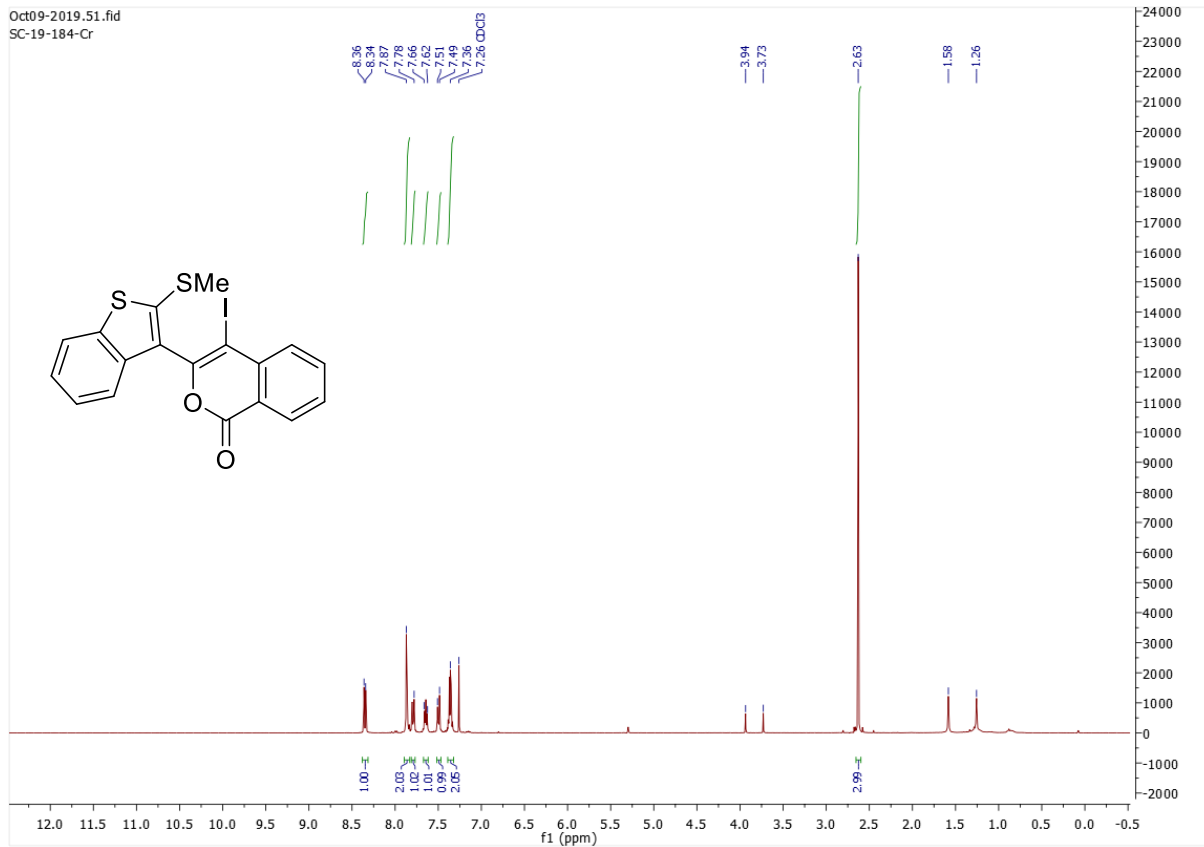
¹H NMR of methyl 2-((2-(methylthio)benzo[*b*]thiophen-3-yl)ethynyl)benzoate (27):



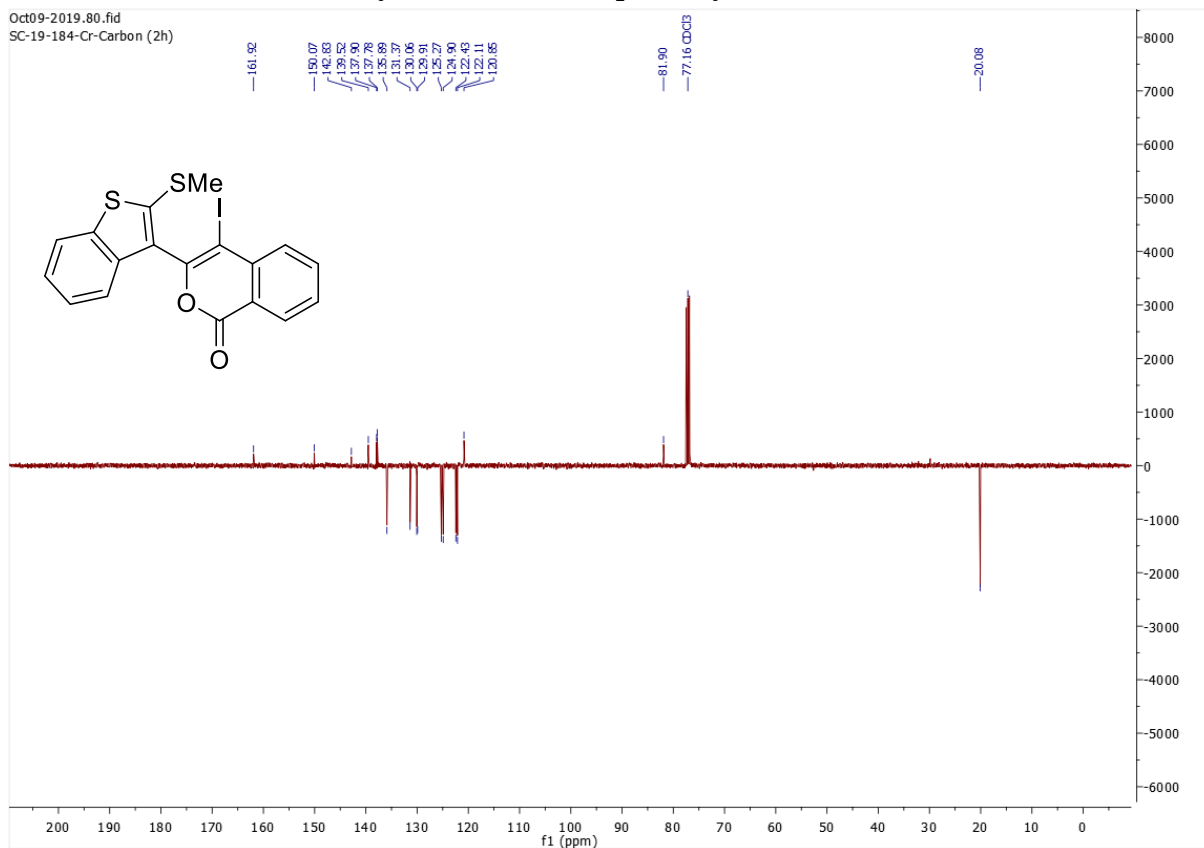
¹³C NMR of methyl 2-((2-(methylthio)benzo[*b*]thiophen-3-yl)ethynyl)benzoate (27):



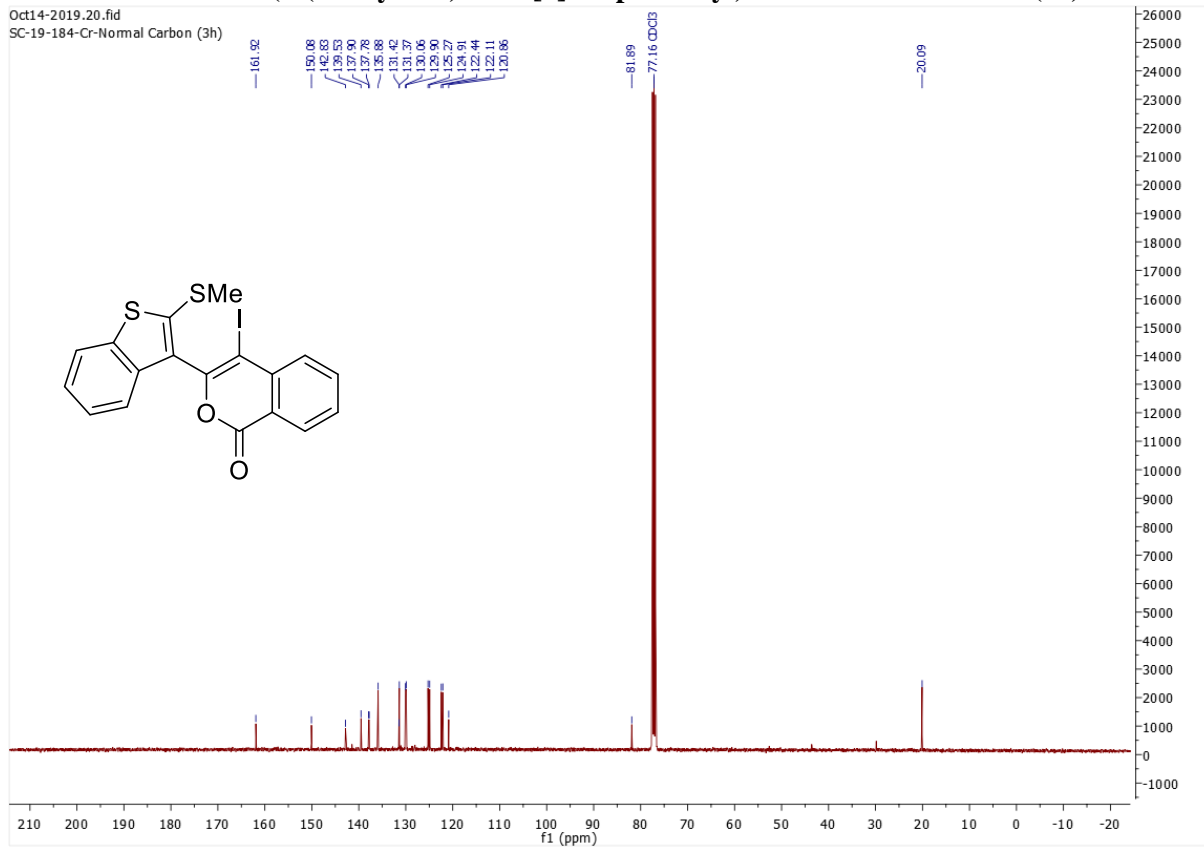
¹H NMR of 4-iodo-3-(2-(methylthio)benzo[*b*]thiophen-3-yl)-1*H*-isochromen-1-one (28):



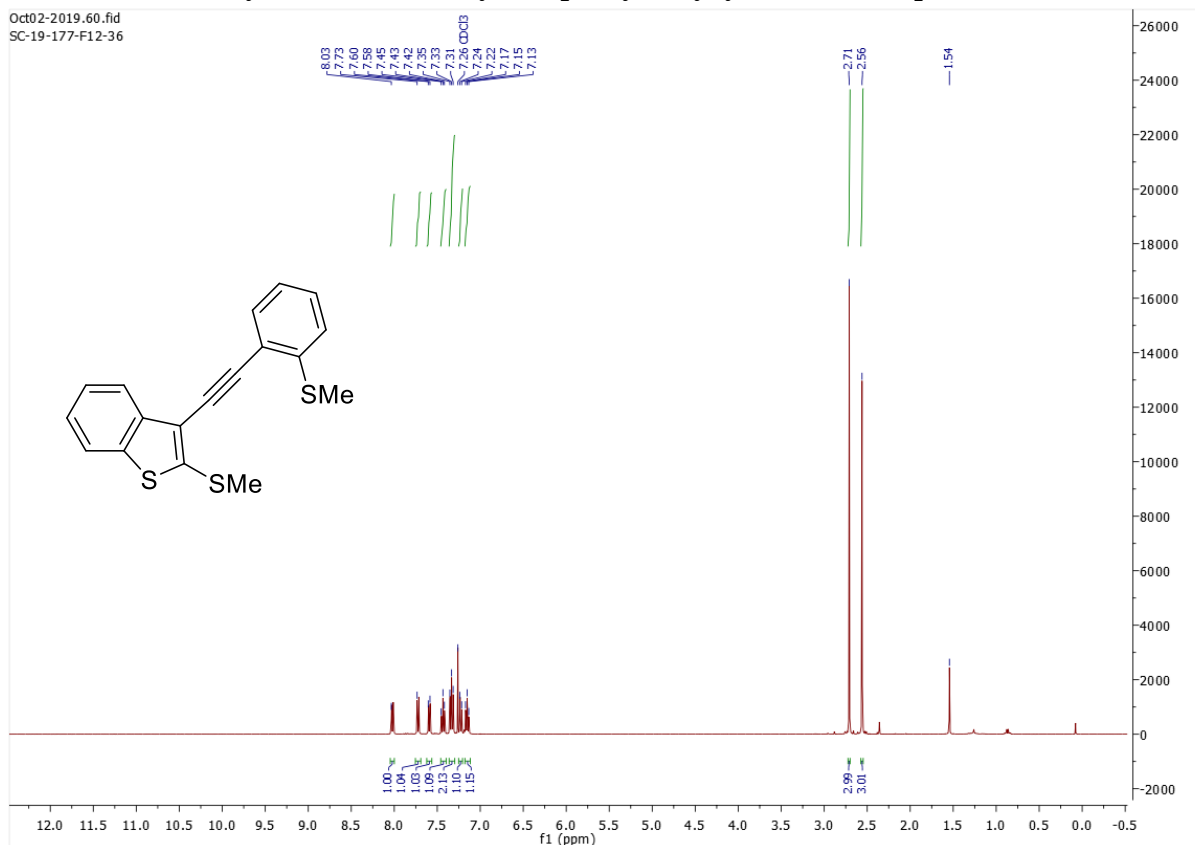
¹³C NMR of 4-iodo-3-(2-(methylthio)benzo[*b*]thiophen-3-yl)-1*H*-isochromen-1-one (28):



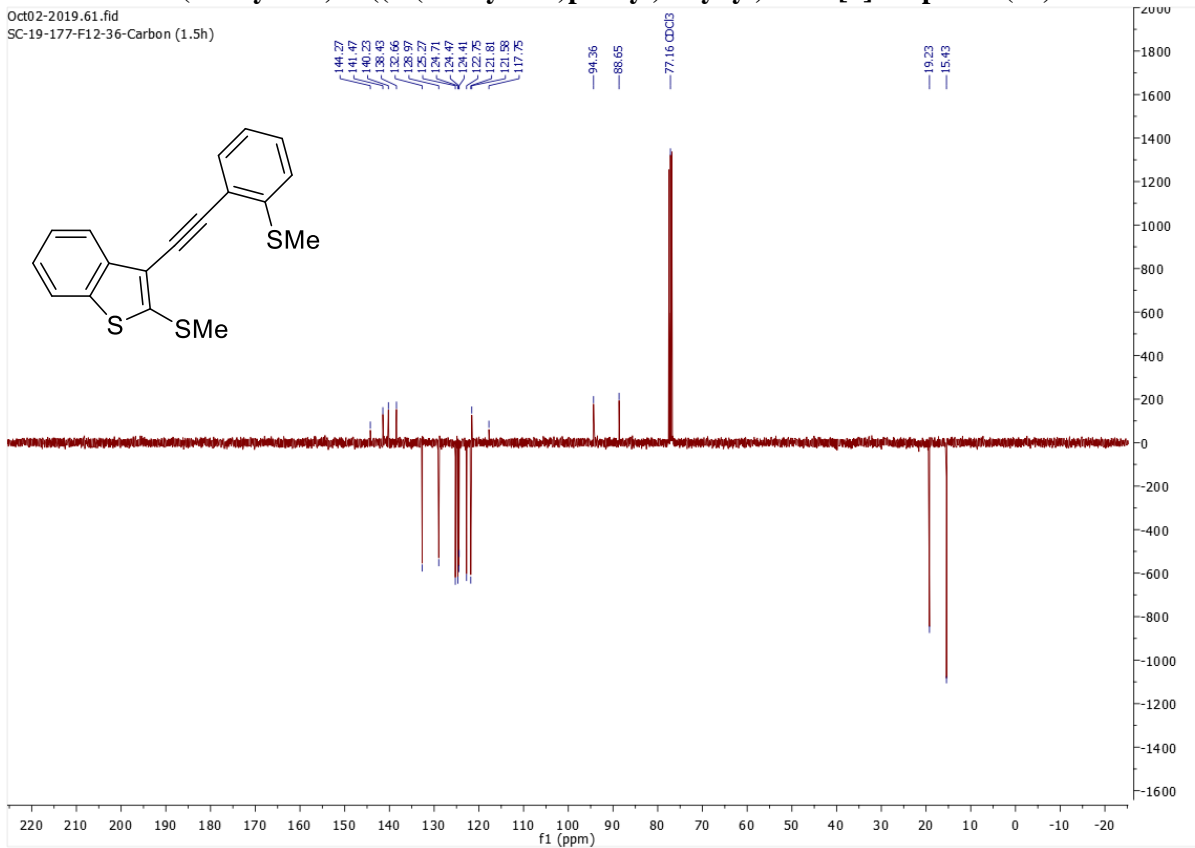
¹³C NMR of 4-iodo-3-(2-(methylthio)benzo[*b*]thiophen-3-yl)-1*H*-isochromen-1-one (28):



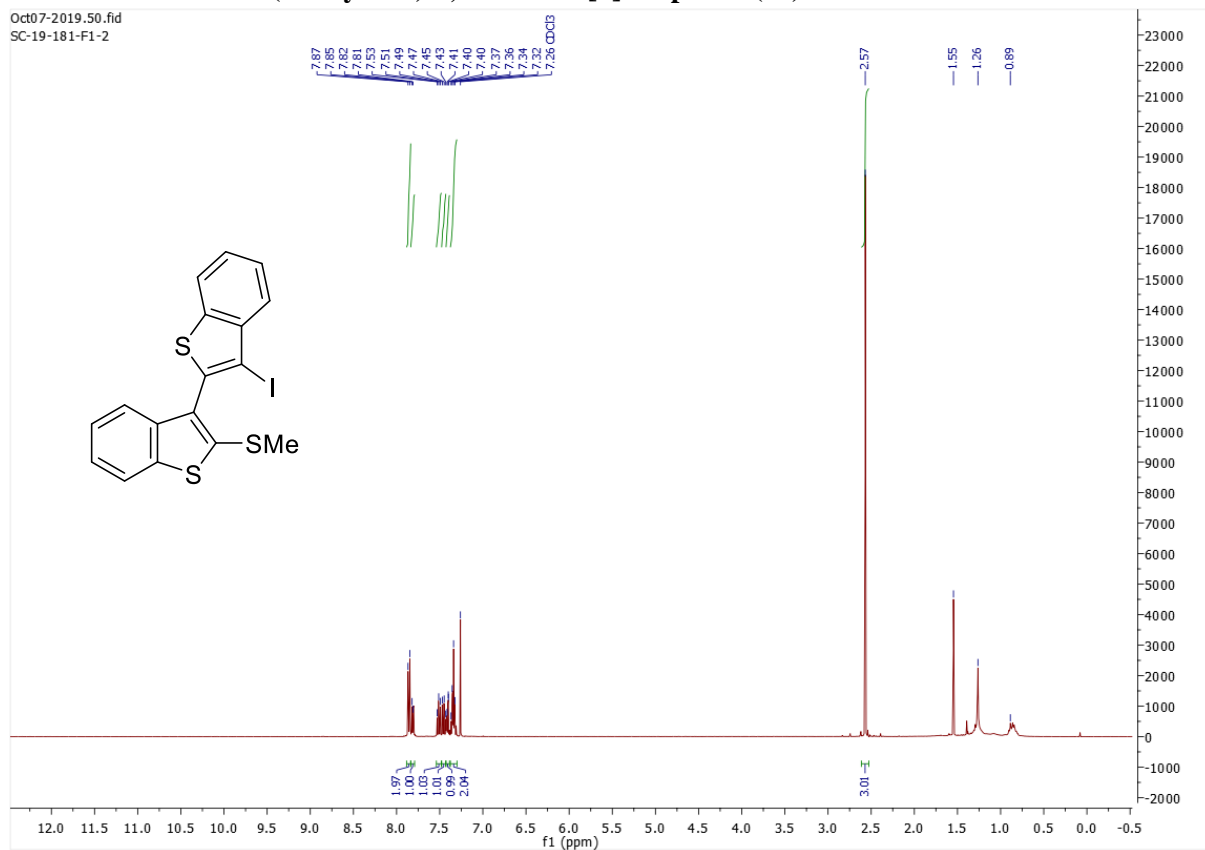
¹H NMR of 2-(methylthio)-3-((2-(methylthio)phenyl)ethynyl)benzo[*b*]thiophene (29):



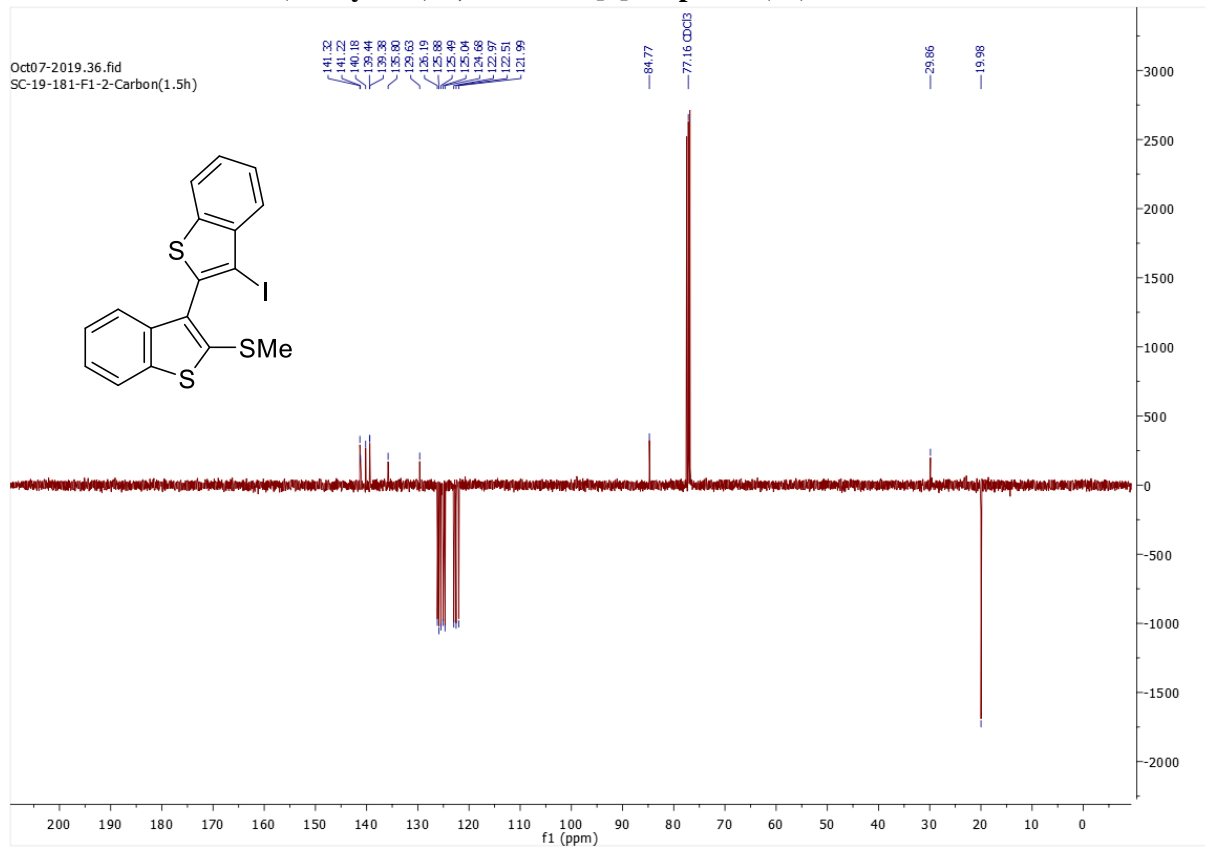
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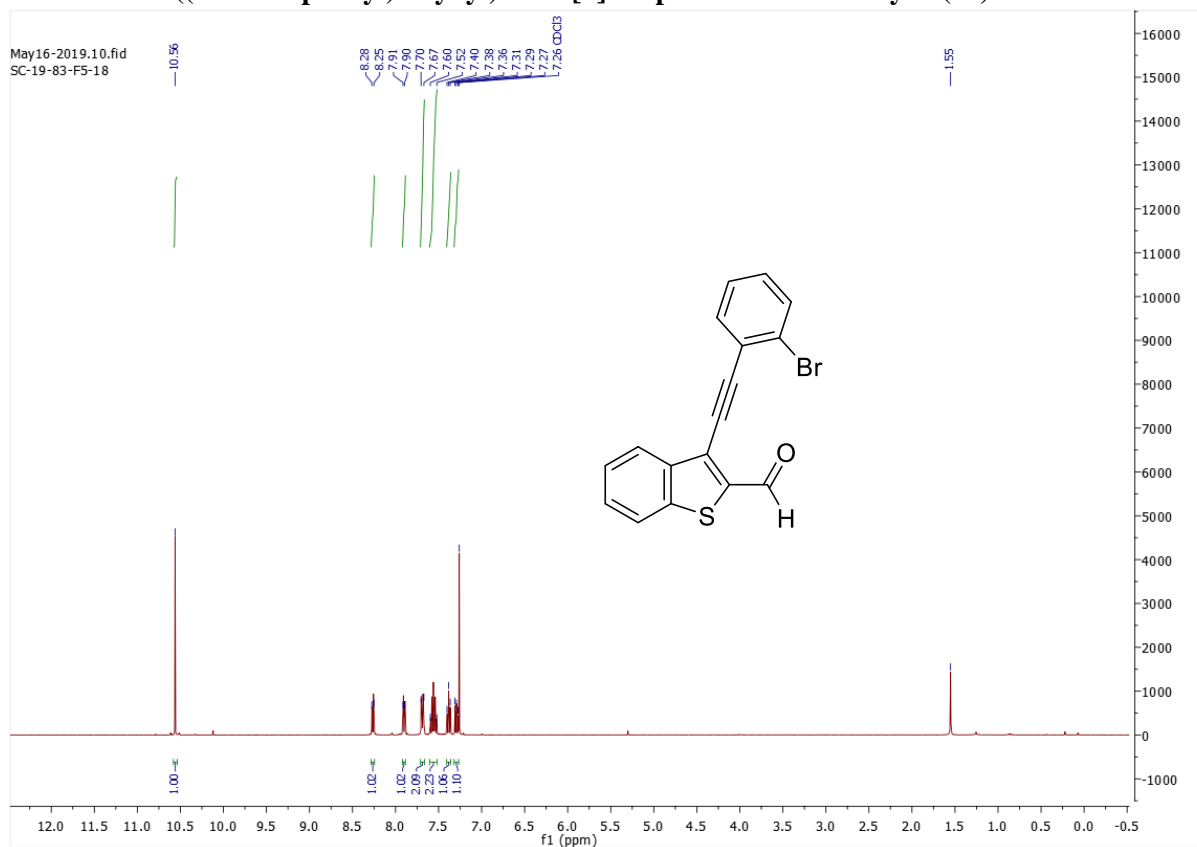
¹H NMR of 3-iodo-2'-(methylthio)-2,3'-bibenzo[*b*]thiophene (30):



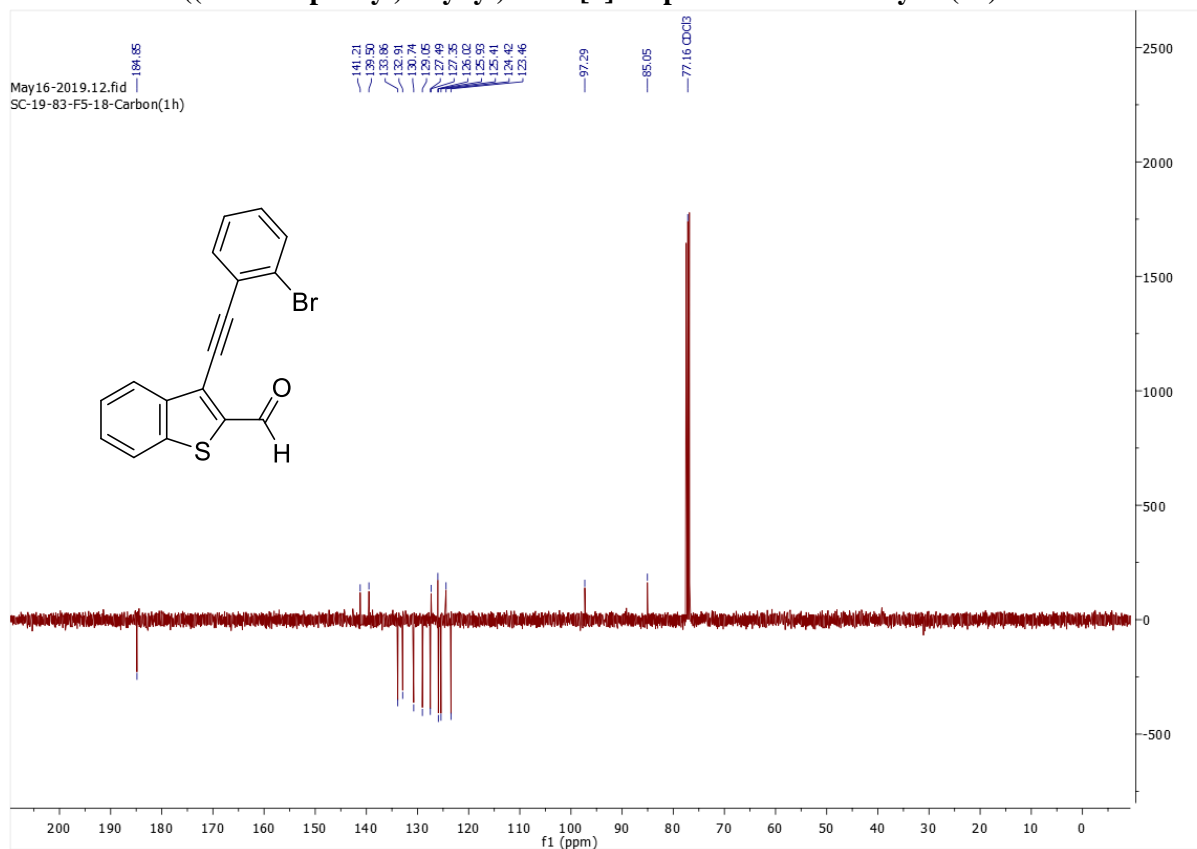
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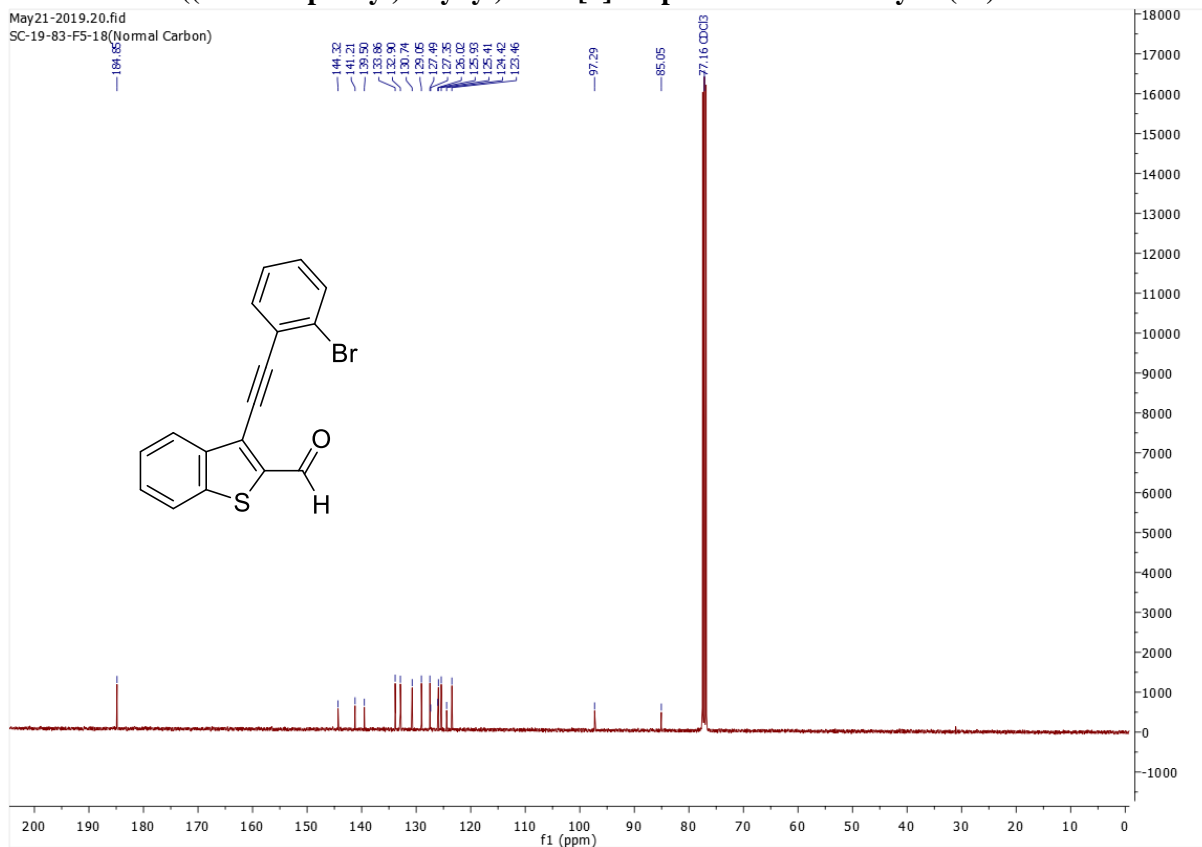
¹H NMR of 3-((2-bromophenyl)ethynyl)benzo[*b*]thiophene-2-carbaldehyde (33):



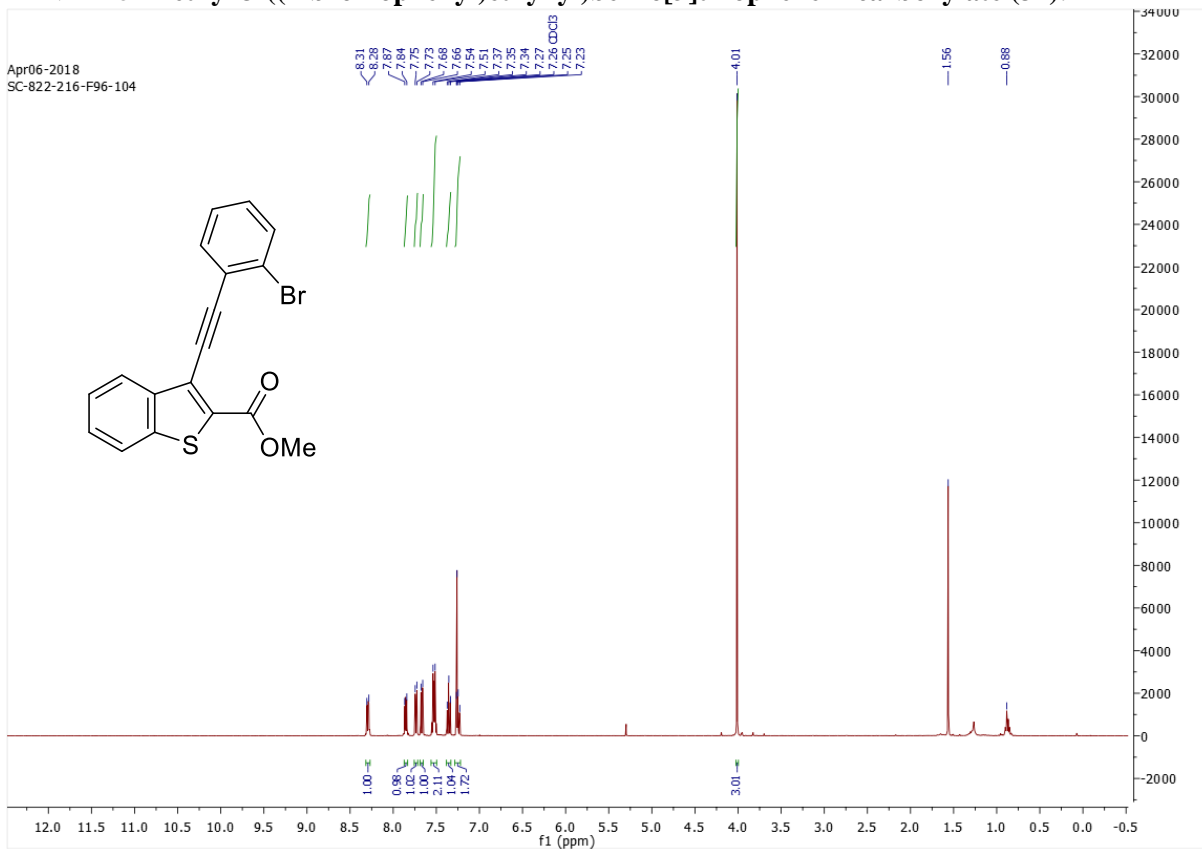
¹³C NMR of 3-((2-bromophenyl)ethynyl)benzo[*b*]thiophene-2-carbaldehyde (33):



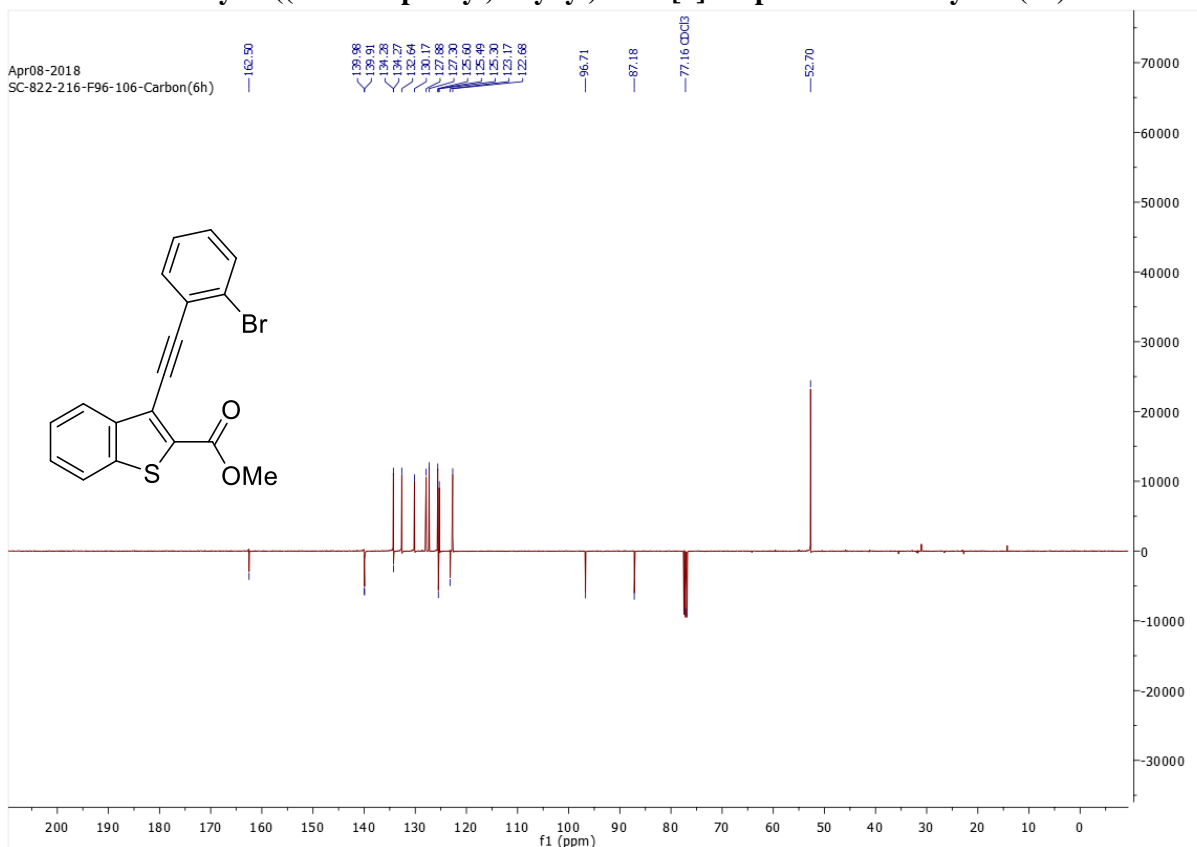
¹³C NMR of 3-((2-bromophenyl)ethynyl)benzo[*b*]thiophene-2-carbaldehyde (33):



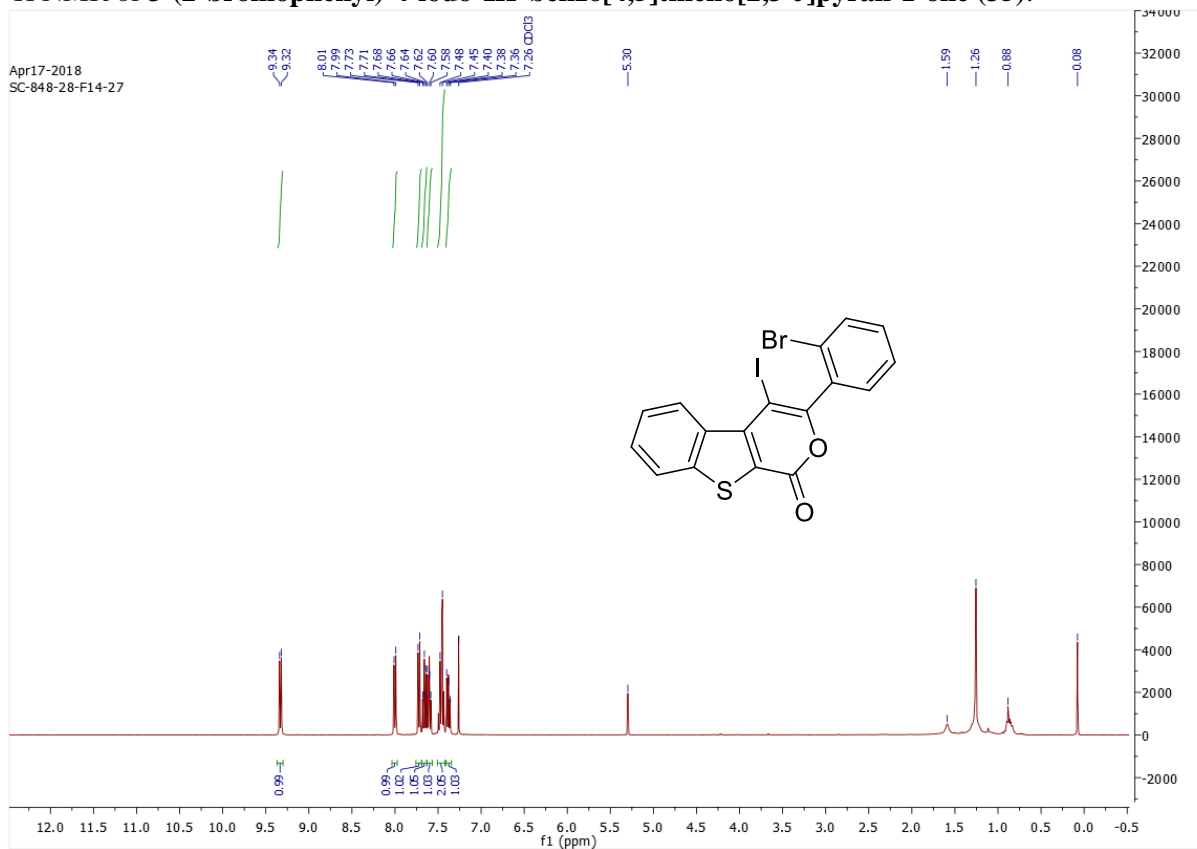
¹H NMR of methyl 3-((2-bromophenyl)ethynyl)benzo[*b*]thiophene-2-carboxylate (34):



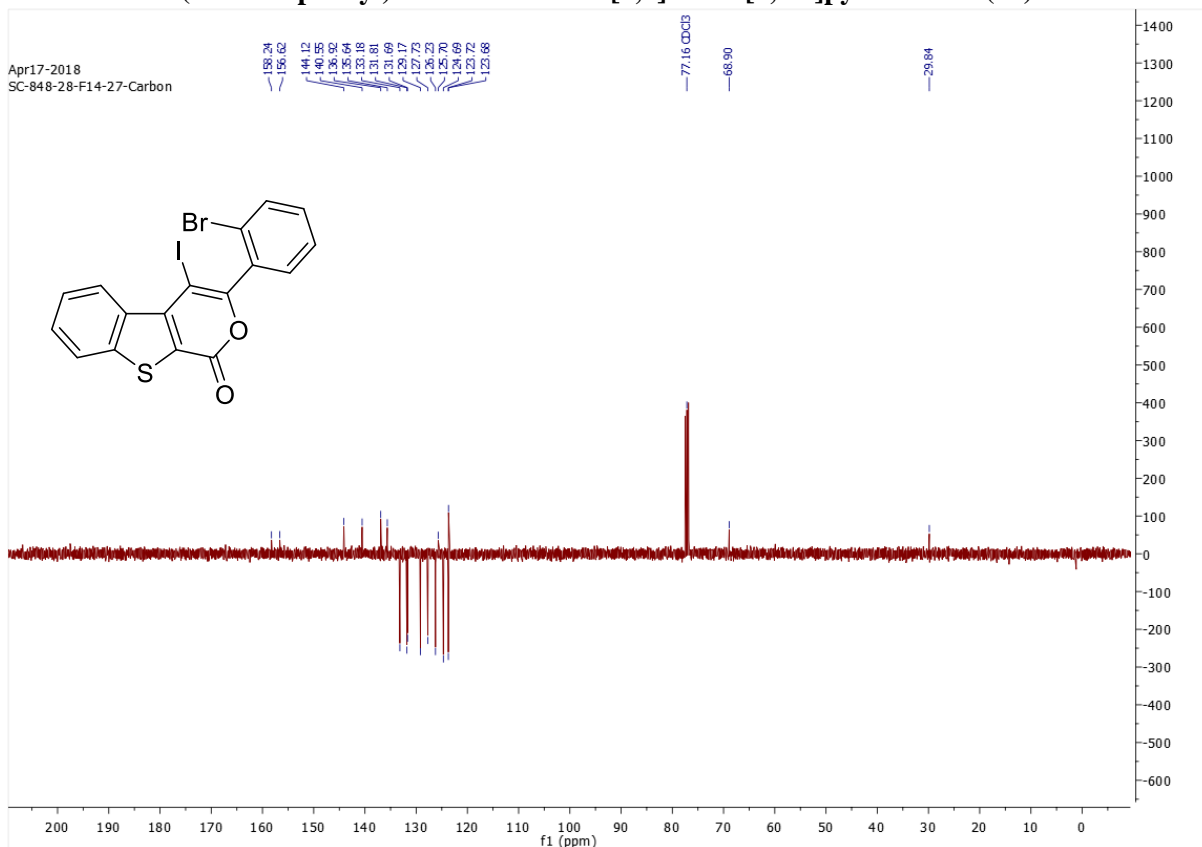
¹³C NMR of methyl 3-((2-bromophenyl)ethynyl)benzo[*b*]thiophene-2-carboxylate (34):



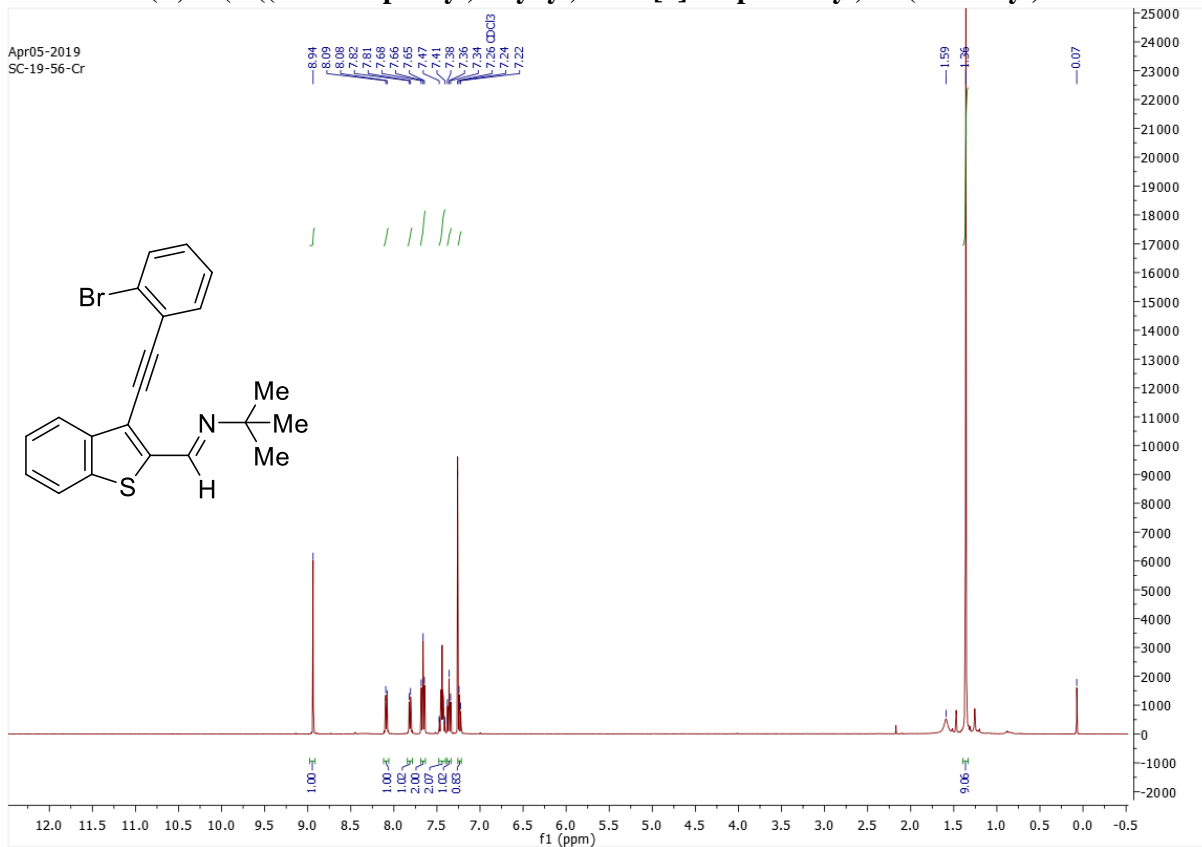
¹H NMR of 3-(2-bromophenyl)-4-iodo-1*H*-benzo[4,5]thieno[2,3-*c*]pyran-1-one (35):



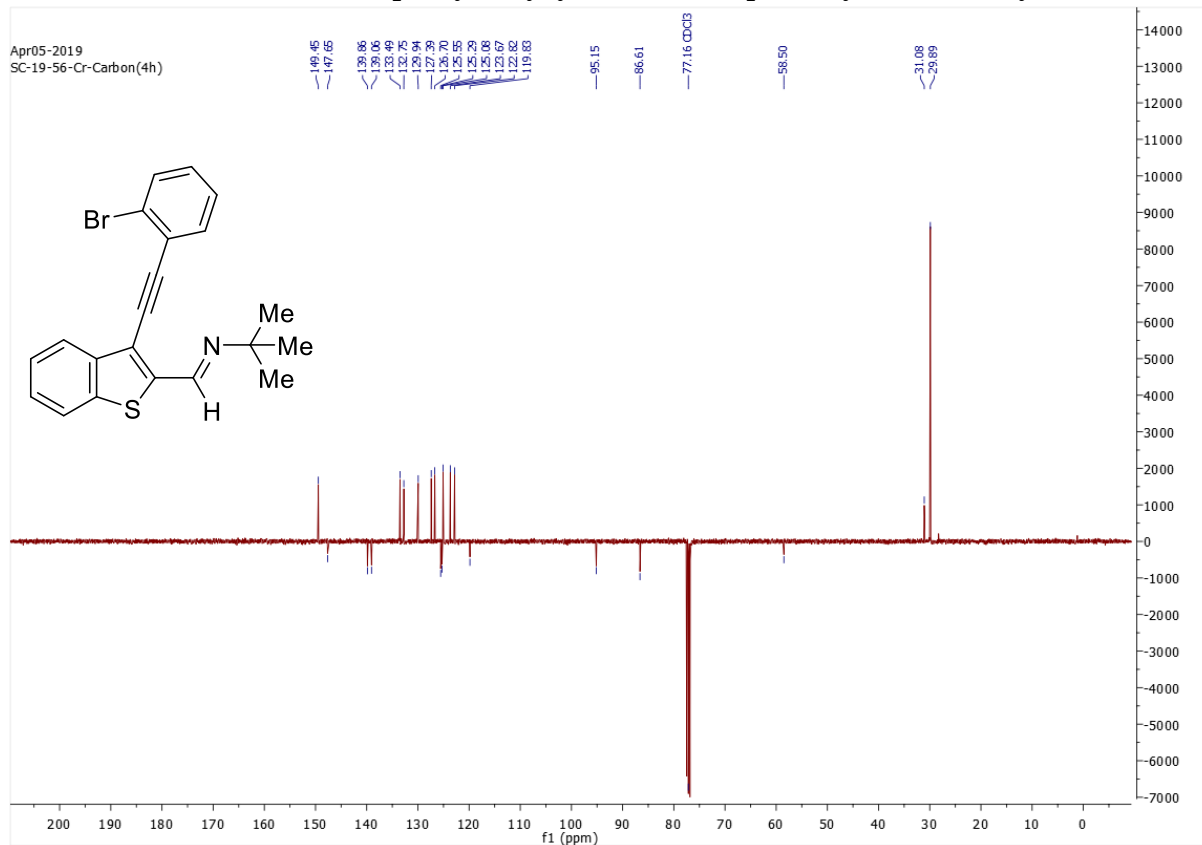
¹³C NMR of 3-(2-bromophenyl)-4-iodo-1H-benzo[4,5]thieno[2,3-c]pyran-1-one (35):



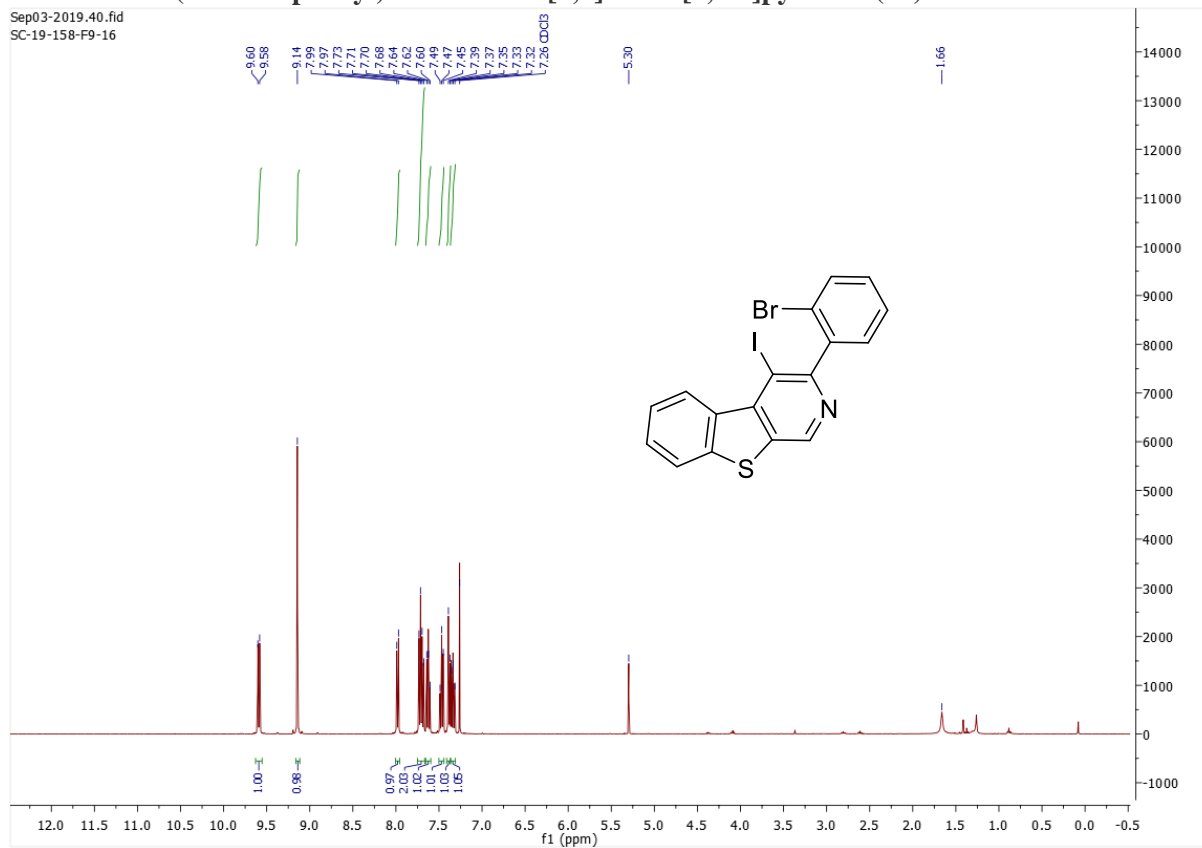
¹H NMR of (E)-1-(3-((2-bromophenyl)ethynyl)benzo[b]thiophen-2-yl)-N-(tert-butyl)methanimine (36):



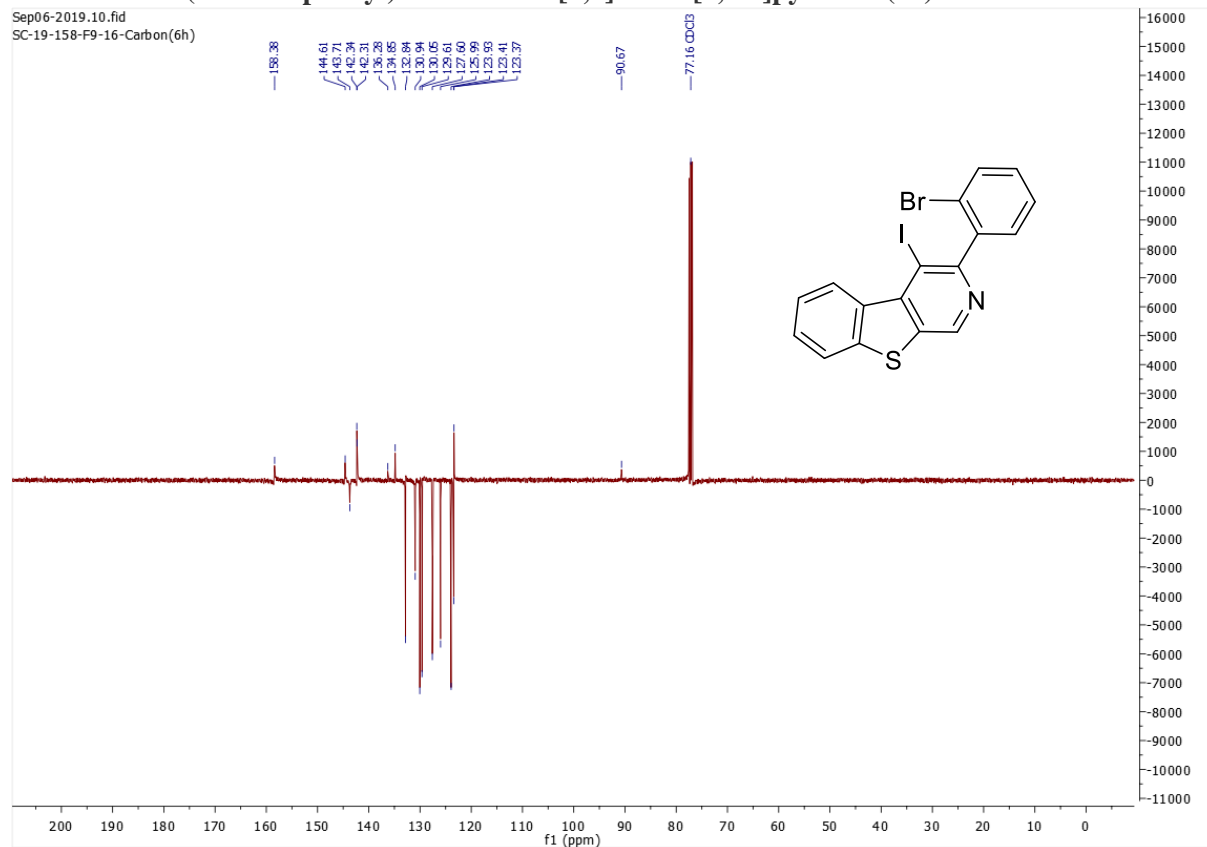
¹³C NMR of (*E*)-1-(3-((2-bromophenyl)ethynyl)benzo[*b*]thiophen-2-yl)-*N*-(*tert*-butyl)methanimine (36):



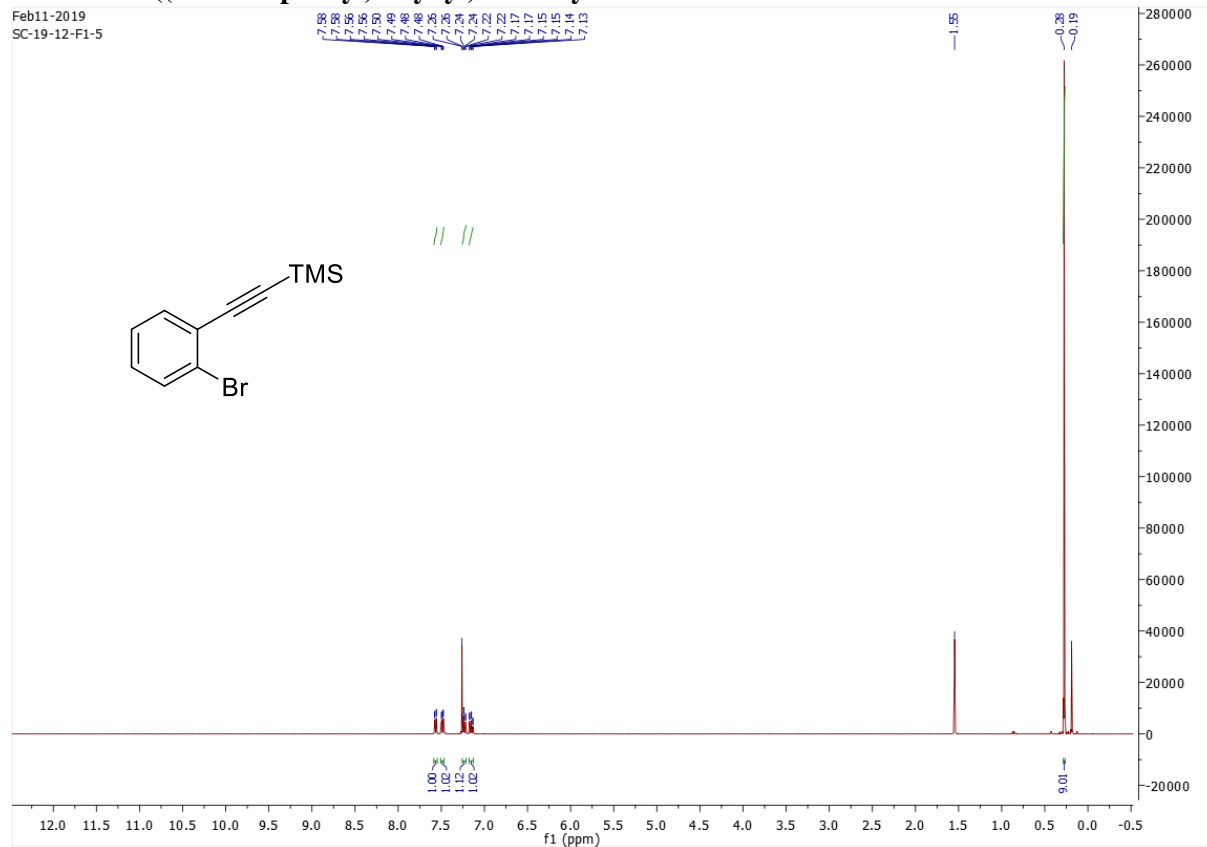
¹H NMR of 3-(2-bromophenyl)-4-iodobenzo[4,5]thieno[2,3-*c*]pyridine (37):



¹³C NMR of 3-(2-bromophenyl)-4-iodobenzo[4,5]thieno[2,3-c]pyridine (37):



¹H NMR of ((2-bromophenyl)ethynyl)trimethylsilane:



¹H NMR of 1-bromo-2-ethynylbenzene (39):

Feb12-2019
SC-19-14-Crude

