Supporting Information

Direct synthesis of 3-acylbenzothiophenes via the radical cyclization of 2-alkynylthioanisoles with α-oxocarboxylic acids

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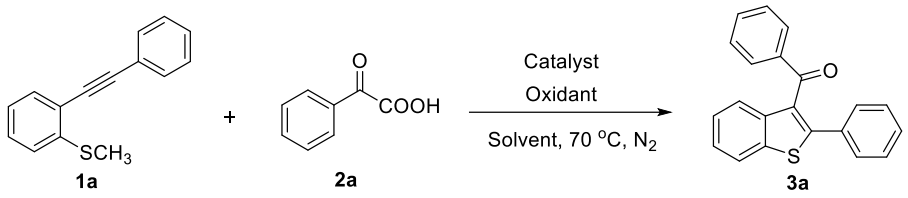
1. General Information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvents were treated according to general methods. Melting points are uncorrected and recorded on Digital Melting Point Apparatus WRS-1B. ^{1}H NMR and ^{13}C NMR spectra were measured on a 500 MHz Bruker spectrometer (500 MHz for ^{1}H and 125 MHz for ^{13}C) using DMSO-d_6 or Acetone-d_6 or $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. High-resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Column chromatography was performed using EM silica gel 60 (300-400 mesh).

2. Optimization of the Reaction Conditions

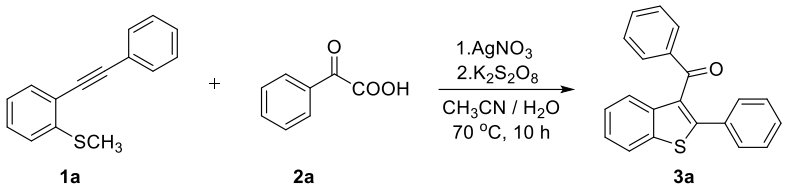


entry	catalyst	oxidant	solvent (v/v)	yield %[b]
1	$AgNO_3$	$K_2S_2O_8$	Actone/H_2O(1/1)	20
2	$AgNO_3$	$K_2S_2O_8$	DMSO/H_2O (1/1)	0
3	$AgNO_3$	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	81
4	$AgNO_3$	$K_2S_2O_8$	CH_3CN	0
5	$AgNO_3$	$K_2S_2O_8$	H_2O	0
6	$AgNO_3$	$K_2S_2O_8$	CH_3CN/H_2O (3/1)	42
7	$AgNO_3$	$K_2S_2O_8$	CH_3CN/H_2O (1/3)	15
8	---	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	18
9	$AgNO_3$	---	CH_3CN/H_2O (1/1)	0
10	Ag_2O	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	0
11	Ag_2CO_3	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	65
12	AgOAc	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	40
13	$AgNO_3$	$Na_2S_2O_8$	DMSO	69
14	$AgNO_3$	$(NH_4)_2S_2O_8$	DMSO	20
15	$AgNO_3$	O_2	DMSO	0
[c]16	$AgNO_3$	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	61
[d]17	$AgNO_3$	$K_2S_2O_8$	CH_3CN/H_2O (1/1)	76

Table S1 [a]Reaction conditions unless specified otherwise: **1a** (0.2 mmol), **2a** (0.6 mmol), [Ag] (0.02 mmol), $K_2S_2O_8$ (0.6 mmol), solvent (2 mL), 70 °C, under N_2, 10 h. [b]Isolated yield. [c]Under air. [d]At 80 °C.

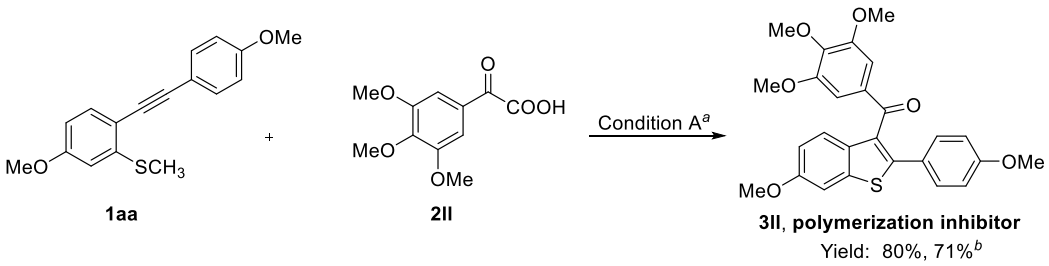
3. Experimental Procedure

General Procedure for the preparation of 3a



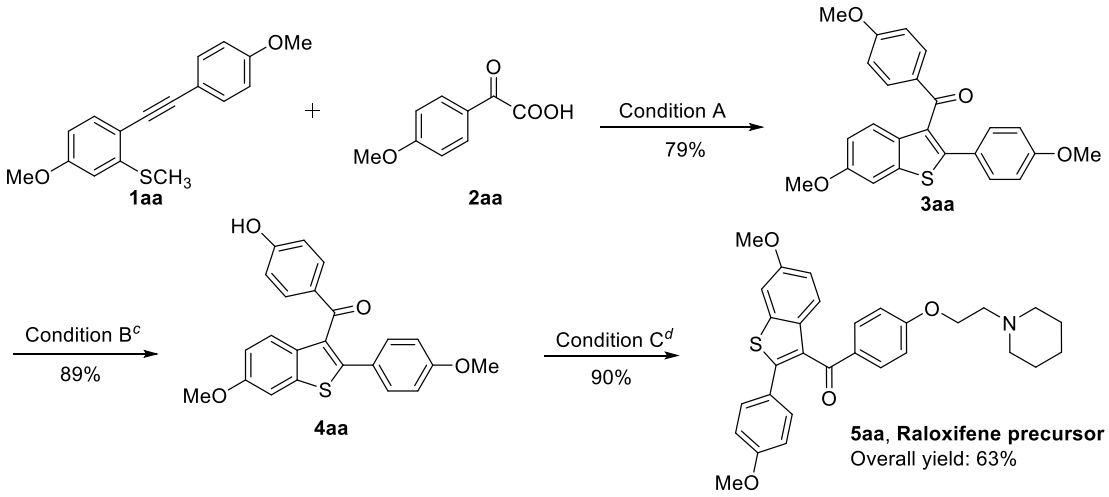
To the mixture of phenylglyoxylic acid (0.6 mmol), alkynyl thioanisoles (0.2 mmol), in a schlenk flask was added $AgNO_3$ (0.02 mmol) and $K_2S_2O_8$ (0.6 mmol) in CH_3CN /H_2O (v/v=1/1, 2 mL) under nitrogen atmosphere. The reaction was stirred at 70 ^oC for 10 h. Upon completion, the reaction mixture was concentrated under vacuum. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt (20:1-2:1) to afford the corresponding products.

The following preparation of 3ll (polymerization inhibitor)



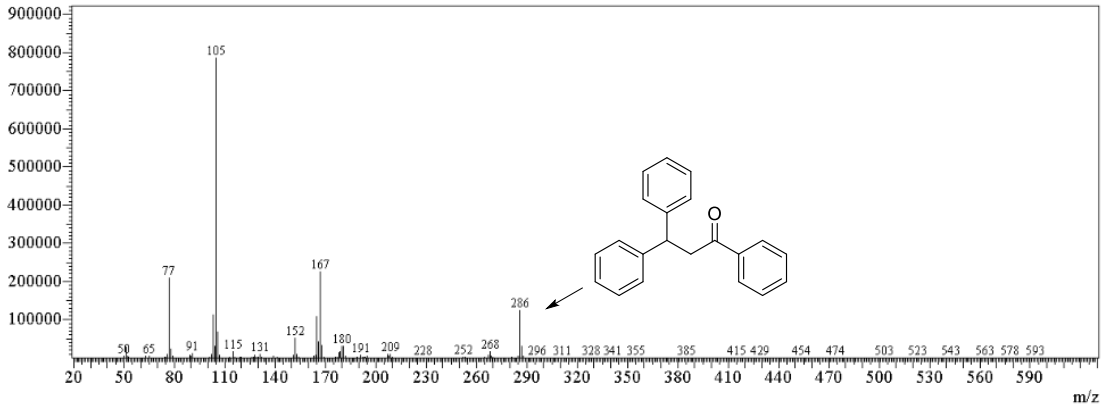
[a]Condition A: to the mixture of 1a (0.2 mmol), 2ll (0.6 mmol) in a schlenk flask was added $AgNO_3$ (0.02 mmol) and $K_2S_2O_8$ (0.6 mmol) in CH_3CN /H_2O (v/v=1/1, 2 mL) under nitrogen atmosphere. The reaction was stirred at 70 ^oC for 10 h. Upon completion, the reaction mixture was concentrated under vacuum. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt (5:1) to afford **3ll**. [b]The reaction was conducted in 10 mmol under **condition A**.

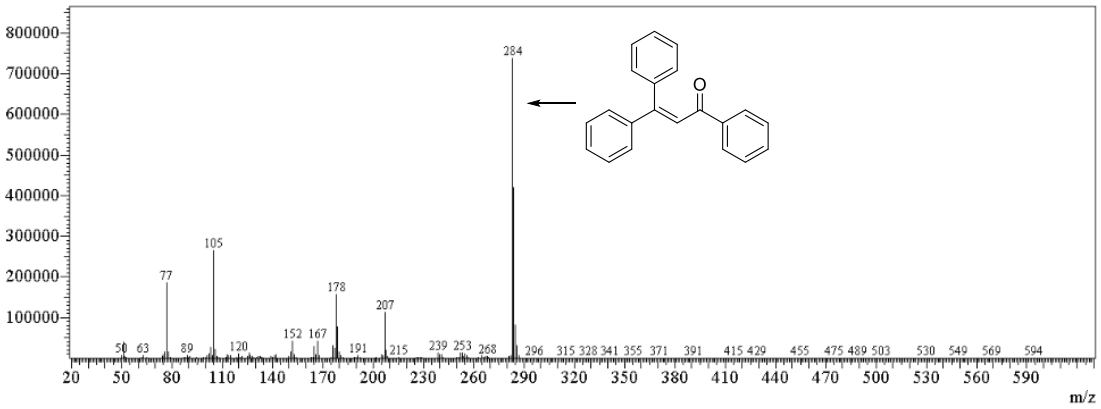
The following preparation of 5aa (Raloxifene precursor)

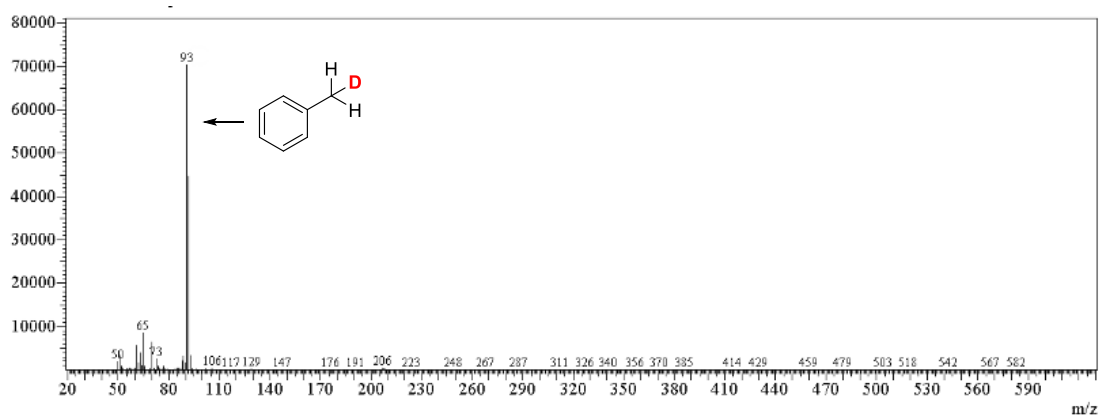


[a]**Condition A**: to the mixture of 1aa (0.2 mmol), 2aa (0.6 mmol) in a schlenk flask was added $AgNO_3$ (0.02 mmol) and $K_2S_2O_8$ (0.6 mmol) in CH_3CN/H_2O (v/v=1/1, 2 mL) under nitrogen atmosphere. The reaction was stirred at 70 ^oC for 10 h. Upon completion, the reaction mixture was concentrated under vacuum. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt (10:1) to afford **3aa**; [c]**Condition B**: A solution of compound **3aa** (1.0 mmol) in dry DMF (2 mL) was added to a solution of sodium ethanethioate (1.5 mmol in 3 mL of DMF). The reaction mixture was heated at 80 ℃ for 4 h and then cooled to room temperature. Ethyl acetate (10 mL) and water (10 mL) were added to the mixture. After neutralization with 1 M HCl, the reaction mixture was extracted with ethyl acetate (30 mL). The organic layer was removed, washed with brine, and dried over Na_2SO_4. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt (2:1) to afford **4aa**; [d]**Condition C**: to a solution of **4aa** (1.0 mmol), 1-(2-chloroethyl)-piperidine monohydrochloride (1.1 mmol), cesium carbonate (2.1 mmol) in DMF (8 mL) was stirred at 25 ^oC for 14 h. The light brown suspension was then heated for 30 min at 50 ^oC. The aqueous phase was separated and extracted with methylene chloride (twice the volume of the reaction solvent X 2), and the combined organic extracts were dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt/triethylamine (2:1/0.1,) to afford **5aa**.

4. The GC-MS data







5. Computational Studies

5.1. Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of computational programs.[1] The geometries of all stationary points were optimized using the uM06 hybrid functional at the basis set level of 6-31g*. Frequencies were analytically computed at the same level of theory to obtain the free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). The solvent effect of toluene was evaluated by using the SMD polarizable continuum model by carrying out single point calculations at the uM06/6-311+G(d,P) level. All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. All the energies given in the text are relative free energies corrected with solvation effects.

According to the calculated results in Figure 1, the addition of acyl radical **E** to **1a** could go through **TS1** and **TS1'** with almost the same energies, indicating both intermediates F anf F' are possible in the first step. However, the energies for the cyclizations from **F** and **F'** are quite different. The **TS2'** is much higher than that of **TS2**, making the formation of a four-membered ring product difficult. All these are in good agreement with the experimental observations.

[1] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

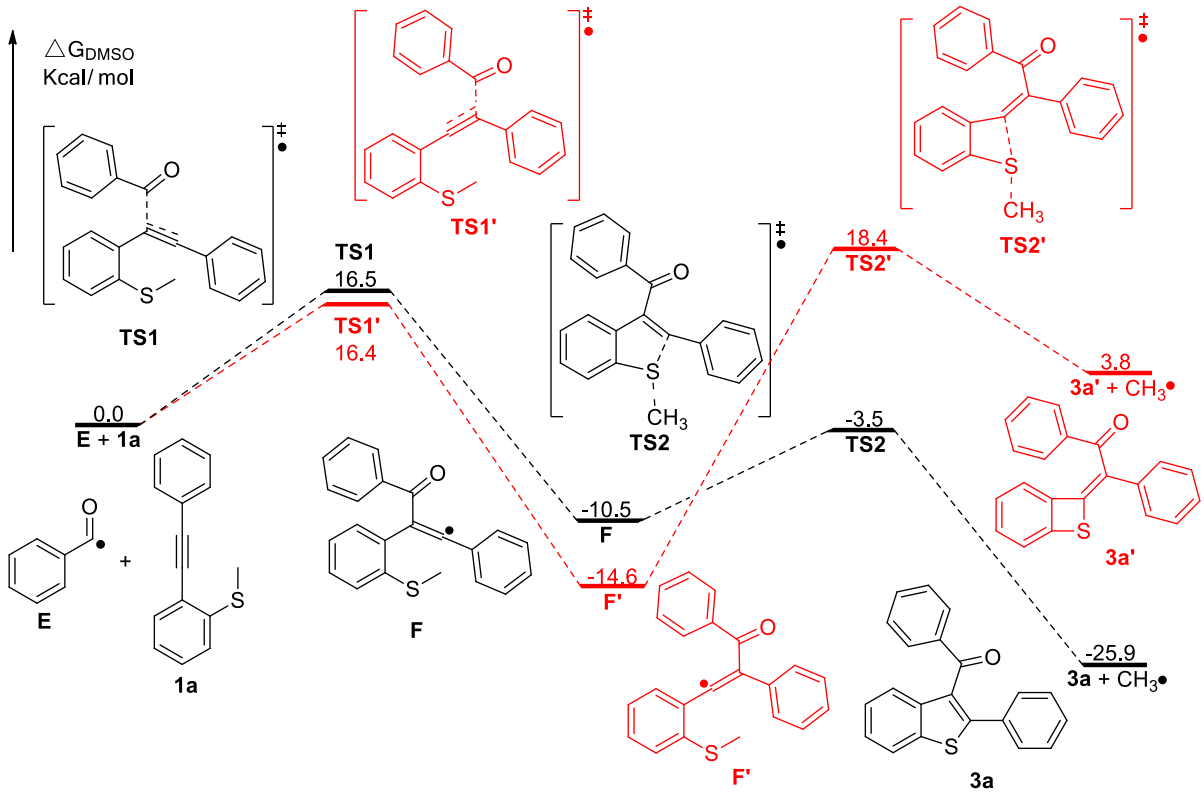


Figure S1. Calculated Potential Energy Surface.

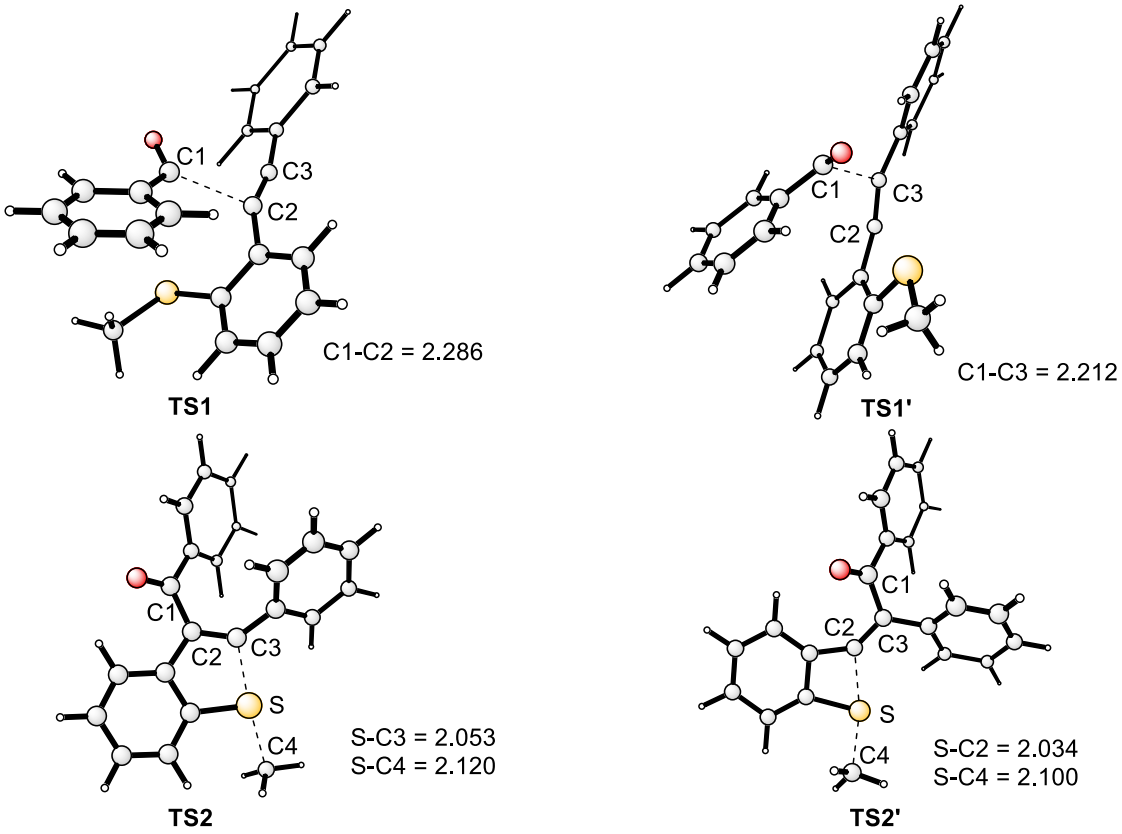


Figure S2. Geometries for Key Transition State

5.2. Calculated Energy Values

Table S2. Energies (in Hartree) calculated at SMD-uM06/6-311+G(d,P)//uM06/6-31g* level

Species	G_{298}[a]	E[b]	G_{Sol}[c]
E	-344.606074	-344.6721989	-344.7659264
1a	-976.293183	-976.4698109	-976.6428956
TS1	-1320.875579	-1321.141796	-1321.406036
TS1'	-1320.876989	-1321.144494	-1321.40744
F	-1320.927396	-1321.192836	-1321.448213
F'	-1320.928657	-1321.192824	-1321.453564
TS2	-1320.913365	-1321.184319	-1321.442531
TS2'	-1320.881159	-1321.145928	-1321.401551
CH_3·	-39.786364	-39.7954112	-39.80755457
3a	-1281.166454	-1281.404511	-1281.646972
3a'	-1281.118573	-1281.354271	-1281.597252

[a] Sum of electronic and thermal free energies

[b] Electronic energies

[c] Single point energies in solution

5.3. Cartesian Coordinates for All Species

E

C	-0.34927800	0.49615900	0.00004200
C	1.03934300	0.50902300	0.00057100
C	1.72183900	1.72543400	0.00011500
C	1.01573900	2.93425700	-0.00092700
C	-0.37030100	2.91741800	-0.00149500
C	-1.04997300	1.69918700	-0.00099200
H	-0.88807800	-0.44921100	0.00042000
H	1.61554900	-0.41544300	0.00134900
H	1.57506100	3.86847300	-0.00129400
H	-0.92885000	3.85176600	-0.00231000
H	-2.13861700	1.68936300	-0.00142900
C	3.19749300	1.72772100	0.00070500
O	3.92942300	2.66838900	0.00048000

1a

C	0.58322900	-2.64647500	3.37457400
C	1.44290000	-1.66192700	2.88833600
C	0.92225300	-0.65290800	2.04503200
C	-0.43776000	-0.66645400	1.71632600
C	-1.28280300	-1.65161400	2.20631400
C	-0.76601800	-2.63918600	3.03656400
H	0.95753200	-3.43243800	4.02585900
H	-0.81703100	0.11870300	1.06467700
H	-2.33798100	-1.64784500	1.94169000

H	-1.41687600	-3.41821500	3.43024900
C	1.76767700	0.37399500	1.53411400
C	2.49363700	1.24789000	1.10587800
C	3.34448100	2.27761100	0.60547500
C	3.93021000	2.16264800	-0.66297100
C	3.60673100	3.41778000	1.37794400
C	4.75860400	3.16660700	-1.14445400
H	3.72524600	1.27571800	-1.25959200
C	4.43569700	4.41776400	0.88961700
H	3.15217600	3.50370900	2.36316200
C	5.01350200	4.29541500	-0.37090800
H	5.20962300	3.06683800	-2.13026800
H	4.63486700	5.29867000	1.49737900
C	4.75860400	3.16660700	-1.14445400
H	3.72524600	1.27571800	-1.25959200
C	4.43569700	4.41776400	0.88961700
H	3.15217600	3.50370900	2.36316200
C	5.01350200	4.29541500	-0.37090800
H	5.20962300	3.06683800	-2.13026800
H	4.63486700	5.29867000	1.49737900
H	5.66479600	5.08066200	-0.75070400
S	3.17363500	-1.57912900	3.25715800
C	3.40176400	-3.02585900	4.32249300
H	3.16433400	-3.95909700	3.79923400
H	4.46383400	-3.03475200	4.58607400
H	2.81440900	-2.95241500	5.24476300

TS1

C	-0.77592300	-0.35731500	-1.41962900
C	0.16876800	0.23498200	-0.59010900
C	1.44346600	0.51679200	-1.08320000
C	1.76963000	0.20275300	-2.40882500
C	0.82653300	-0.40030200	-3.22802900
C	-0.44663600	-0.68057700	-2.73296000
H	-1.77157200	-0.57184600	-1.03585000
H	-0.07785600	0.48077000	0.44099000
H	2.76905400	0.43802600	-2.77164700
H	1.07785200	-0.64752100	-4.25820500
H	-1.18636100	-1.15275100	-3.37744400
C	2.50269800	1.09504100	-0.23026700
O	3.45560700	1.71536600	-0.57338100
C	0.75060400	-2.53049100	1.76913700
C	1.74006000	-1.56077800	1.60829100
C	1.59641800	-0.30948200	2.24110500
C	0.47218000	-0.08275400	3.04795700
C	-0.51010900	-1.05077100	3.19455100
C	-0.37384100	-2.27416900	2.54381500
H	0.85960000	-3.50136000	1.28966200
H	0.37790000	0.88611500	3.53599900
H	-1.38148900	-0.85104500	3.81518400
H	-1.13864500	-3.04139200	2.65164700
C	2.53887900	0.75659300	2.03000000
C	3.35759200	1.59547900	2.43226600
C	4.33841200	2.59081100	2.60444600
C	5.67702200	2.33163400	2.24769600
C	4.01153500	3.85034800	3.14324300
C	6.64853800	3.30221000	2.42558300
H	5.92410500	1.36134100	1.82059800
C	4.99214000	4.81447100	3.31235200
H	2.97848300	4.05387500	3.41994500
C	6.31313800	4.54644100	2.95816600
H	7.67851100	3.09062300	2.14295200
H	4.72603000	5.78592800	3.72597900
H	7.07999500	5.30683400	3.09503200
S	3.20268900	-1.83308200	0.64033000
C	2.58328800	-3.00079800	-0.60596700
H	1.63982500	-2.63572500	-1.03042700
H	3.33903000	-3.03525200	-1.39725600
H	2.45305500	-4.01216400	-0.20566600

TS1’

C	0.84990700	2.27623900	-1.45147200

C	1.00474200	1.12779800	-0.68767100
C	2.19132300	0.39921000	-0.76299300
C	3.22999400	0.82594600	-1.59396700
C	3.07969700	1.98713600	-2.34028300
C	1.88955300	2.70742500	-2.27281100
H	-0.07770300	2.84357900	-1.40254000
H	0.21825300	0.78416000	-0.01590300
H	4.15059200	0.24430400	-1.62188000
H	3.89141000	2.33420800	-2.97733900
H	1.77312700	3.61633500	-2.86083000
C	2.37075500	-0.82128700	0.05165800
O	3.17171800	-1.69382100	-0.10781800
C	0.91609800	-3.71863800	3.12828500
C	1.60693200	-2.70389700	2.47983000
C	1.34583300	-1.36575900	2.79918900
C	0.37899400	-1.06847300	3.76974500
C	-0.31062200	-2.08957600	4.40873400
C	-0.04317500	-3.41794500	4.09111500
H	1.13036200	-4.75658300	2.87883400
H	0.18186900	-0.02587800	4.01463000
H	-1.05959500	-1.84698700	5.16079200
H	-0.58125500	-4.21918200	4.59488100
C	2.05882400	-0.28064300	2.17407900
C	2.64633900	0.80919000	2.15806400
C	3.32640200	2.00112400	1.82961100
C	4.71266800	1.98969200	1.52174700
C	2.62077200	3.21425100	1.76316900
C	5.33536100	3.18315100	1.16379500
C	3.25504600	4.39152300	1.40246600
H	1.55774400	3.20298200	1.99920700
C	4.61375700	4.37205000	1.10348300
H	6.39501600	3.19987200	0.92052500
H	2.69246300	5.32155400	1.35393800
H	5.12503100	5.29046000	0.81968900
S	5.52860500	0.41978300	1.59051100
C	7.24022300	0.87075900	1.20742900
H	7.33978100	1.28120400	0.19605300
H	7.64798600	1.57638200	1.94024500
H	7.81173400	-0.06066000	1.26268300
H	2.35473000	-2.93073600	1.72298700

F

C	-0.57615300	0.19594800	-1.57480000
C	0.42411800	0.40607500	-0.63055600
C	1.76634700	0.39117100	-1.01482800
C	2.09377600	0.17243900	-2.35662000
C	1.09714700	-0.05097300	-3.29446200
C	-0.24134600	-0.03889000	-2.90416300
H	-1.62092800	0.21757700	-1.27004300
H	0.15596800	0.59416600	0.40778600
H	3.14633600	0.18069000	-2.63428300
H	1.35930900	-0.23051700	-4.33580900
H	-1.02462800	-0.20859000	-3.64129900
C	2.88759100	0.65018900	-0.06419800
O	3.96968100	1.02887600	-0.46904700
C	1.05995200	-2.84314200	2.24092300
C	1.86890400	-1.88619400	1.62402100
C	1.80120900	-0.54343400	2.03289000
C	0.92317100	-0.20924300	3.07330300
C	0.11502200	-1.16221200	3.67301500
C	0.17598900	-2.48710900	3.24920500
H	1.14548300	-3.88496200	1.93417300
H	0.87604800	0.83268200	3.38945100
H	-0.56530800	-0.87129900	4.47138600
H	-0.45164800	-3.24462900	3.71507700
C	2.63507900	0.52771600	1.43043300
C	3.18103100	1.46677500	2.17800900
C	4.02456800	2.55037700	2.39860300
C	5.42814500	2.38416200	2.27353300
C	3.52405500	3.81308600	2.80368900
C	6.27987900	3.43805600	2.54437200
H	5.80390300	1.42374800	1.92705400

C	4.39208900	4.85774200	3.06125900
H	2.44785000	3.94474900	2.90419700
C	5.77169600	4.67732500	2.94057600
H	7.35443700	3.30230100	2.43416600
H	3.99527300	5.82504700	3.36490100
H	6.44944200	5.50256200	3.15076900
S	3.04144400	-2.39492200	0.37474900
C	1.89605800	-3.11340200	-0.84724300
H	1.09034900	-2.40544500	-1.07297500
H	2.47644900	-3.29478800	-1.75796400
H	1.47551800	-4.06375000	-0.50128600

F’

C	1.49001600	4.14393400	-2.11630400
C	1.13991700	3.99745400	-0.78305200
C	1.60349300	2.90011000	-0.05114500
C	2.41416000	1.94554700	-0.67153900
C	2.76034100	2.09251400	-2.00884700
C	2.30232000	3.19139800	-2.72913700
H	1.13117300	5.00063800	-2.68396400
H	0.50198100	4.72061000	-0.27878900
H	2.76263000	1.08106800	-0.10694700
H	3.38883600	1.34631500	-2.49112900
H	2.57745900	3.30610100	-3.77647700
C	1.19554400	2.78202000	1.37253200
O	0.37194400	3.52004600	1.87741200
C	-1.58888100	-1.87471200	1.84008300
C	-0.39051900	-1.18327700	1.72982000
C	-0.16933100	-0.02661600	2.54475900
C	-1.18483600	0.37103800	3.45335500
C	-2.36641800	-0.33634200	3.54692000
C	-2.56951800	-1.45948700	2.74252100
H	-1.77897700	-2.75138800	1.22547800
H	-1.00523900	1.26182800	4.05247100
H	-3.14020200	-0.01202800	4.23974900
H	-3.49942600	-2.02092600	2.81233300
C	1.02547700	0.66728200	2.48683300
C	1.82561000	1.66457700	2.19063400
C	3.24819900	1.75396100	2.56933800
C	3.95050300	0.60130500	2.93908800
C	3.91643800	2.98151800	2.55713200
C	5.28732500	0.67829100	3.29898900
H	3.42842300	-0.35658400	2.92927800
C	5.25727900	3.05541400	2.91616500
H	3.37805200	3.88769700	2.27805900
C	5.94624200	1.90614700	3.28772600
H	5.82382900	-0.22570600	3.58279400
H	5.76492200	4.01844200	2.90717200
H	6.99703500	1.96468300	3.56601300
S	0.93097700	-1.61363700	0.63420500
C	0.29230900	-3.11129500	-0.15858000
H	-0.61617500	-2.90654900	-0.73582800
H	1.07554800	-3.44716500	-0.84469600
H	0.10336800	-3.90383300	0.57421200

TS2

C	2.48124600	1.39870000	-2.36241000
C	1.90697700	0.90408000	-1.19918800
C	1.07028000	1.71395600	-0.42899700
C	0.78508100	3.01192100	-0.85912600
C	1.37166800	3.51192200	-2.01290300
C	2.22594600	2.70714000	-2.76227600
H	3.13453600	0.76310100	-2.95756100
H	2.11626500	-0.11575800	-0.87913500
H	0.11088600	3.61946600	-0.25774100
H	1.16357700	4.53211000	-2.33087800
H	2.68840900	3.09909900	-3.66682400
C	0.45378100	1.25742900	0.84988300
O	-0.61310000	1.72617500	1.21952800
C	0.76285900	-2.72931000	3.86342600
C	1.31339500	-1.68136300	3.12671500
C	0.48667600	-0.72881800	2.49999900

C	-0.90232100	-0.85264200	2.63168900
C	-1.44471300	-1.89665900	3.36324600
C	-0.61588000	-2.83549200	3.97711400
H	1.40362100	-3.45694500	4.35738500
H	-1.54078800	-0.10924900	2.16296400
H	-2.52549700	-1.97930900	3.46183300
H	-1.04580900	-3.65147300	4.55528600
C	1.18661300	0.27157900	1.69863400
C	2.52978500	0.27251900	1.81662900
C	3.63240900	1.06187600	1.35396700
C	4.77023200	0.45581800	0.79613300
C	3.58934200	2.46583400	1.43724100
C	5.81142900	1.22963400	0.30387400
H	4.80962900	-0.63115200	0.72353000
C	4.62642600	3.23149300	0.93032400
H	2.72142400	2.94250900	1.89135700
C	5.74134800	2.61856700	0.36054600
H	6.68123300	0.74520500	-0.13694400
H	4.56881100	4.31714900	0.98514600
H	6.55534600	3.22383300	-0.03400500
S	3.05681100	-1.41683000	2.93898000
C	3.63508900	-3.24044000	3.03743500
H	2.99428700	-3.86825900	2.41216700
H	4.66209300	-3.23802100	2.66200000
H	3.62645200	-3.57033600	4.08174800

TS2’

C	1.81739500	5.55036100	-0.80396500
C	1.29888900	4.71369800	0.17311500
C	1.65527200	3.36204500	0.20972000
C	2.51985700	2.85464300	-0.76387000
C	3.02434700	3.68950600	-1.75292000
C	2.68142500	5.03792000	-1.76885200
H	1.54457800	6.60404800	-0.81922600
H	0.60555700	5.08486200	0.92545200
H	2.79301700	1.80103800	-0.75572200
H	3.69144500	3.28636800	-2.51257300
H	3.08646900	5.69283400	-2.53868200
C	1.02638600	2.50703600	1.25825200
O	0.01150100	2.87816400	1.82571800
C	-1.71415400	-2.30392000	2.07893400
C	-0.58062700	-1.52446000	2.01024200
C	-0.60489600	-0.16918500	1.65979300
C	-1.80224800	0.46594300	1.36382500
C	-2.96249800	-0.31027500	1.42056600
C	-2.91981800	-1.65889100	1.77106700
H	-1.69451300	-3.35715500	2.35155700
H	-1.83931800	1.52430000	1.12100200
H	-3.92355300	0.15084700	1.20047100
H	-3.84795700	-2.22730100	1.81113400
C	0.82115300	0.12797000	1.73338200
C	1.64643300	1.17357400	1.57545100
C	3.10924900	1.07755200	1.74874900
C	3.84036800	-0.01858600	1.27520800
C	3.79583900	2.10911600	2.40057700
C	5.21520400	-0.08702300	1.46528800
H	3.32437400	-0.81001600	0.73225700
C	5.16947600	2.03975900	2.58866200
H	3.23928700	2.96971100	2.77258800
C	5.88416500	0.93985900	2.12342300
H	5.76850200	-0.94508800	1.08712500
H	5.68483900	2.84910200	3.10300900
H	6.96174800	0.88648000	2.26794100
S	1.18669700	-1.69753700	2.23638400
C	1.01683400	-3.58464100	3.47693800
H	0.68946800	-4.30544500	2.72758200
H	2.03358600	-3.72235700	3.83748500
H	0.28394800	-3.32796300	4.24015000

CH_3.

C	4.03288700	-3.17589000	4.50780100
H	3.71870400	-3.92656400	3.79277400

H	5.00909300	-2.71522400	4.41616400
H	3.37076900	-2.88600600	5.31468500

3a

C	0.78557000	0.72621400	-2.47296400
C	1.26859300	0.72272700	-1.17049300
C	1.20611700	1.88362400	-0.39517900
C	0.65952600	3.04908900	-0.94229400
C	0.16943800	3.04876200	-2.23914400
C	0.23271000	1.88684000	-3.00571400
H	0.84023200	-0.17904400	-3.07454600
H	1.70411600	-0.18347400	-0.75202900
H	0.63565600	3.94545400	-0.32572500
H	-0.26035500	3.95662700	-2.65871000
H	-0.14897700	1.88772500	-4.02543000
C	1.75176400	1.94679500	0.98891100
O	1.91802700	3.02107900	1.54294000
C	0.81688100	-2.59048400	2.88351900
C	1.61146900	-1.49753300	2.53963900
C	1.07262000	-0.35081900	1.92308400
C	-0.30588900	-0.31503100	1.65846200
C	-1.09503600	-1.39814500	1.99776500
C	-0.53831300	-2.53212500	2.60595300
H	1.25379000	-3.46617300	3.36034200
H	-0.74806700	0.56228000	1.18792100
H	-2.16338300	-1.36906300	1.79236700
H	-1.17664800	-3.37417300	2.86675100
C	2.07502700	0.65621600	1.67039200
C	3.32559700	0.28556300	2.09019100
C	4.61251400	0.98690700	2.00162900
C	5.76287000	0.29377200	1.59902900
C	4.72637700	2.33910500	2.34896200
C	6.99024700	0.93814800	1.52880900
H	5.68483600	-0.75656700	1.31822500
C	5.95699400	2.97923400	2.27247900
H	3.84126600	2.87656700	2.67811100
C	7.09051500	2.28507300	1.86335500
H	7.87137900	0.38579500	1.20692800
H	6.02954100	4.03057400	2.54521100
H	8.05274900	2.79130300	1.80759500
S	3.32791300	-1.32554600	2.79991400

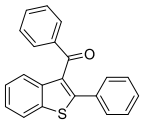
3a'

C	2.26805400	5.34439800	-0.78869600
C	1.66513500	4.56786400	0.18913500
C	1.99226800	3.21442300	0.31878300
C	2.91687700	2.64512900	-0.56115600
C	3.50551100	3.41930100	-1.55294300
C	3.18776100	4.76958200	-1.66291900
H	2.01721700	6.39996200	-0.87692000
H	0.92626700	4.98633600	0.86985500
H	3.16971200	1.58948900	-0.47714400
H	4.21679200	2.96778600	-2.24193400
H	3.65702000	5.37664100	-2.43541700
C	1.25880700	2.42177900	1.34681300
O	0.20490600	2.83786100	1.80289500
C	-1.68232000	-2.23231200	2.20529100
C	-0.53637000	-1.47369200	2.18712600
C	-0.50909100	-0.12174200	1.82501900
C	-1.67250200	0.54392300	1.47597300
C	-2.85056100	-0.21058200	1.47970500
C	-2.85559700	-1.55838300	1.83451300
H	-1.69662900	-3.28218100	2.48777700
H	-1.67128900	1.60194600	1.22872000
H	-3.78942600	0.26950500	1.21037400
H	-3.79790700	-2.10435800	1.83222900
C	0.93546000	0.09760800	1.97754600
C	1.81367400	1.09880700	1.78355400
C	3.26053700	0.96102600	2.04358100
C	3.98372000	-0.16790800	1.64095300
C	3.93901400	1.98801600	2.71116300
C	5.34247800	-0.27189600	1.91363600
H	3.48027700	-0.95920300	1.08583000

C	5.29608100	1.88258100	2.98290000	H	5.80502300	2.68878400	3.50830800
H	3.38772900	2.87374000	3.02790600	H	7.06712700	0.66886600	2.79771700
C	6.00244200	0.75072100	2.58666100	S	1.22759200	-1.61678100	2.50934200
H	5.89023400	-1.15535100	1.59016900				

6. Analytical Data for All Products

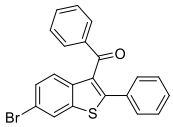
phenyl(2-phenylbenzo[b]thiophen-3-yl)methanone[1]



3a

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow soild (81% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 (d, *J* = 7.0 Hz, 1H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.55-7.52 (m, 1H), 7.49-7.35 (m, 7H), 7.31 (d, *J* = 7.5 Hz, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.5, 145.2, 138.9, 138.1, 136.8, 133.7, 132.5., 131.0, 129.3, 129.0, 128.8, 128.7, 128.7, 125.4, 125.4, 122.9, 122.6.

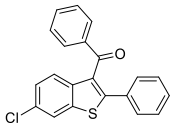
(6-bromo-2-phenylbenzo[b]thiophen-3-yl)(phenyl)methanone



3b

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (70% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.45-8.44 (m, 1H), 7.68 (d, *J* = 7.0 Hz, 2H), 7.60-7.57 (m, 1H), 7.54-7.51 (m, 2H), 7.40-7.34 (m, 4H), 7.32-7.29 (m, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.0, 146.3, 139.8, 137.9, 136.6, 133.8, 132.1, 130.5, 129.4, 129.3, 128.9, 128.8, 128.7, 128.6, 125.1, 124.5, 118.3. **HRMS** (ESI) calcd for $C_{21}H_{13}BrOS$ $[M+H]^+$: 414.9768, found: 414.9766.

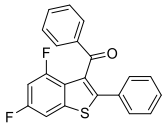
(6-chloro-2-phenylbenzo[b]thiophen-3-yl)(phenyl)methanone



3c

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (67% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.19 (d, J = 8.5 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 7.64-7.63 (m, 1H), 7.53-7.49 (m, 2H), 7.39-7.29 (m, 7H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.1, 146.4, 139.4, 137.7, 136.6, 133.8, 132.2, 130.5, 130.1, 129.4, 129.3, 128.9, 128.8, 128.7, 126.0, 124.2, 122.2. **HRMS** (ESI) calcd for $C_{21}H_{13}ClOS$ $[M+H]^+$: 349.0449, found: 349.0454.

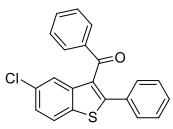
(4,6-difluoro-2-phenylbenzo[b]thiophen-3-yl)(phenyl)methanone



3d

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (58% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.00 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.63-.761 (m, 1H), 7.48-7.43 (m, 4H), 7.39-7.33 (m, 4H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.1, 159.9 (dd, $J_{C\text{-}F}$ = 243.8 Hz, $J_{C\text{-}F}$ = 245.0 Hz), 142.6 (d, $J_{C\text{-}F}$ = 3.8 Hz), 140.8 (q, $J_{C\text{-}F}$ = 12.5 Hz), 136.4 (d, $J_{C\text{-}F}$ = 2.5 Hz), 134.2, 131.6, 129.5 (d, $J_{C\text{-}F}$ = 8.8 Hz), 129.4, 129.0 (d, $J_{C\text{-}F}$ = 1.3 Hz), 128.4, 128.1 (d, $J_{C\text{-}F}$ = 3.8 Hz), 105.6 (dd, $J_{C\text{-}F}$ = 26.3 Hz, $J_{C\text{-}F}$ = 26.2 Hz), 101.6 (dd, $J_{C\text{-}F}$ = 27.5 Hz, $J_{C\text{-}F}$ = 28.8 Hz). **HRMS** (ESI) calcd for $C_{21}H_{12}F_2OS$ $[M+H]^+$: 351.0650, found: 351.0647.

(5-chloro-2-phenylbenzo[b]thiophen-3-yl)(phenyl)methanone

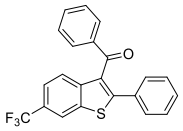


3e

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to

afford yellow oil (50% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.19 (d, J = 7.5 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 7.64 (s, 1H), 7.53-7.49 (m, 2H), 7.38-7.37 (m, 2H), 7.35-7.32 (m, 2H), 7.30-7.29 (m, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.8, 148.2, 140.1, 136.7, 136.6, 133.7, 132.2, 130.6, 130.1, 129.4, 128.9, 128.8, 128.6, 125.5, 124.4, 122.1. **HRMS** (ESI) calcd for $C_{21}H_{13}ClOS$ $[M+H]^+$: 349.0449, found: 349.0456.

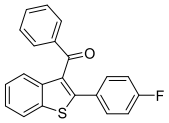
phenyl(2-phenyl-6-(trifluoromethyl)benzo[b]thiophen-3-yl)methanone



3f

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (71% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.69 (s, 1H), 7.80 (d, J = 8.5 Hz, 1H), 7.74 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 7.5 Hz, 2H), 7.55-7.52 (m, 1H), 7.43-7.42 (m, 2H), 7.38-7.32 (m, 5H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.9, 149.4, 141.5, 138.2, 136.6, 133.8, 132.0, 130.6, 129.6, 129.4, 128.9, 128.9, 128.7, 125.4, 124.5 (d, J_{C-F} = 302.5 Hz), 123.8, 121.9 (d, J_{C-F} = 3.75 Hz), 120.5 (d, J_{C-F} = 3.75 Hz). **HRMS** (ESI) calcd for $C_{22}H_{13}F_3OS$ $[M+Na]^+$: 405.0537, found: 405.0546.

(2-(4-fluorophenyl)benzo[b]thiophen-3-yl)(phenyl)methanone

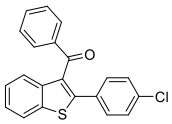


3h

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (78% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 2H), 7.61 (d, J = 8.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.49-7.42 (m, 4H), 7.39-7.36 (m, 2H), 7.18-7.14 (m, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.3, 163.3, 161.3, 144.4, 138.9, 138.1, 136.8, 133.7, 131.1 (d, J_{C-F} = 8.8 Hz), 129.4, 128.7, 125.5, 125.5, 123.0, 122.6, 115.9 (d, J_{C-F} = 22.5 Hz). **HRMS** (ESI) calcd for

$C_{21}H_{13}FOS$ $[M+Na]^+$: 355.0569, found: 355.0571.

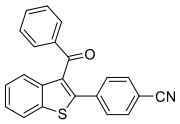
(2-(4-chlorophenyl)benzo[b]thiophen-3-yl)(phenyl)methanone



3i

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (71% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 (d, *J* = 7.5 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 2H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.46-7.38 (m, 6H), 7.32-7.31 (m, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.3, 143.9, 138.9, 138.2, 136.8, 133.9, 133.8, 131.6, 131.5, 130.5, 129.4, 128.9, 128.8, 125.6, 125.6, 123.1, 122.7. **HRMS** (ESI) calcd for $C_{21}H_{13}ClOS$ $[M+H]^+$: 349.0449, found: 349.0463.

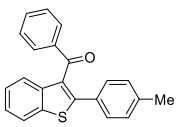
4-(3-benzoylbenzo[b]thiophen-2-yl)benzonitrile



3j

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford white soild (24% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.45-7.43 (m, 2H), 7.33-7.32 (m, 2H), 7.22-7.18 (m, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.5, 149.3, 141.2, 139.6, 139.3, 133.2, 132.2, 130.3, 129.8, 129.6, 129.0, 125.9, 125.8, 124.0, 122.3, 118.2, 116.2.

phenyl(2-(p-tolyl)benzo[b]thiophen-3-yl)methanone

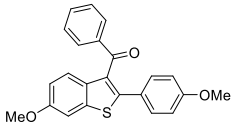


3m

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to

afford yellow oil (86% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.10 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 7.0 Hz, 2H), 7.54-7.30 (m, 2H), 7.46-7.36 (m, 4H), 7.29 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.0 Hz, 2H), 2.22 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.7, 145.1, 139.1, 138.8, 138.0, 136.8, 133.8, 130.6, 129.7, 129.5, 129.3, 128.8, 128.6, 125.4, 125.3, 122.8, 122.6, 20.7. **HRMS** (ESI) calcd for $C_{22}H_{16}OS$ $[M+Na]^+$: 351.0820, found: 351.0825.

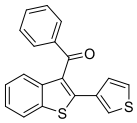
(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(phenyl)methanone



3n

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow oil (79% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.69-7.65 (m, 3H), 7.53-7.65 (m, 1H), 7.43 (d, J = 9.0 Hz, 1H), 7.37-7.34 (m, 2H), 7.28 (d, J = 8.5 Hz, 2H), 7.02-7.00 (m, 1H), 6.83 (d, J = 8.5 Hz, 2H), 3.84 (s, 3H), 3.68 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.7, 159.6, 157.4, 142.7, 139.4, 136.9, 133.6, 133.1, 129.9, 129.7, 129.3, 128.6, 125.1, 123.4, 115.1, 114.3, 105.1, 55.5, 55.1. **HRMS** (ESI) calcd for $C_{23}H_{18}O_3S$ $[M+Na]^+$: 397.0875, found: 397.0869.

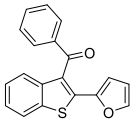
phenyl(2-(thiophen-3-yl)benzo[b]thiophen-3-yl)methanone



3o

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (65% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.09 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 7.5 Hz, 2H), 7.65-7.64 (m, 1H), 7.61-7.58 (m, 1H), 7.54-7.52 (m, 1H), 7.50 (s, 1H), 7.46-7.38 (m, 4H), 7.08-7.07 (m, 1H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 194.2, 139.7, 139.3, 138.1, 137.2, 134.4, 133.3, 131.0, 129.8, 129.3, 128.3, 127.8, 126.3, 125.9, 125.8, 123.2, 123.0. **HRMS** (ESI) calcd for $C_{19}H_{12}OS_2$ $[M+H]^+$: 321.0408, found: 321.0411.

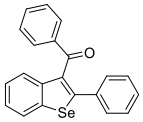
(2-(furan-2-yl)benzo[b]thiophen-3-yl)(phenyl)methanone



3p

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (53% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.02 (m, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.76-7.74 (m, 3H), 7.62 (s, 1H), 7.48-7.45 (m, 2H), 7.41-7.38 (m, 1H), 7.31 (d, *J* = 3.5 Hz, 1H), 6.64-6.63 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 182.0, 152.9, 149.0, 147.1, 144.1, 139.4, 134.0, 133.3, 129.3, 129.2, 126.9, 125.8, 124.6, 123.6, 120.4, 119.4, 112.4.

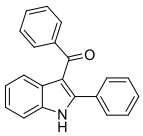
phenyl(2-phenylbenzo[b]selenophen-3-yl)methanone



3q

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (62% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.55-7.52 (m, 1H), 7.49-7.35 (m, 7H), 7.31 (d, *J* = 7.5 Hz, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 194.9, 148.3, 141.3, 140.4, 136.6, 134.6, 134.4, 133.9, 129.2, 128.9, 128.8, 128.8, 128.6, 125.9, 125.4, 125.3, 124.6. **HRMS** (ESI) calcd for $C_{21}H_{14}OSe$ $[M+Na]^+$: 385.0108, found: 385.0109.

phenyl(2-phenyl-1H-indol-3-yl)methanone[4]

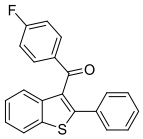


3r

Following the general procedure, using petroleum ether/AcOEt (4:1) as the eluant to

afford white soild (50% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.22 (s, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.53-7.52 (m, 3H), 7.39-7.34 (m, 3H), 7.26-7.14 (m, 7H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.1, 144.0, 139.8, 135.8, 131.5, 131.2, 129.5, 129.0, 128.4, 128.1, 127.9, 127.7, 122.8, 121.3, 120.5, 112.1, 111.8.

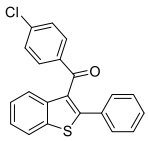
(4-fluorophenyl)(2-phenylbenzo[b]thiophen-3-yl)methanone



3w

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (72% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13 (d, J = 8.0 Hz, 1H), 7.78-7.75 (m, 2H), 7.63 (d, J = 7.5 Hz, 1H), 7.49-7.43 (m, 2H) , 7.40-7.38 (m, 2H), 7.34-7.31 (m, 3H), 7.20-7.16 (m, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 191.9, 166.07, 164.05, 145.6, 138.8, 138.2, 133.6, 132.5, 132.4 (d, $J_{C\text{-}F}$ = 8.8 Hz), 130.7, 129.1, 128.9, 128.8, 125.5, 125.4, 122.9, 122.6, 115.8 (d, $J_{C\text{-}F}$ = 22.5 Hz). **HRMS** (ESI) calcd for $C_{21}H_{13}FOS$ $[M+Na]^+$: 355.0569, found: 355.0574.

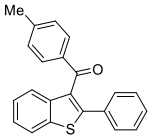
(4-chlorophenyl)(2-phenylbenzo[b]thiophen-3-yl)methanone[1]



3x

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (69% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.14 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 8.5 Hz, 2H), 8.10 (d, J = 8.0 Hz, 1H), 7.50-7.45 (m, 2H), 7.42-7.38 (m, 4H), 7.33-7.31 (m, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.2, 146.1, 138.8, 138.5, 138.2, 135.6, 132.4, 131.2, 130.5, 129.2, 128.9, 128.8, 120.5, 120.5, 123.0, 122.6.

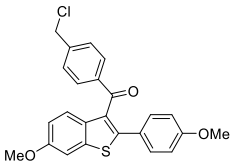
(2-phenylbenzo[b]thiophen-3-yl)(p-tolyl)methanone[1]



3y

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (89% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.07 (d, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.41-7.37 (m, 4H), 7.29 (d, *J* = 6.5 Hz, 3H), 7.14 (d, *J* = 7.0 Hz, 2H), 2.23 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.2, 144.4, 144.2, 139.0, 138.1, 134.2, 132.6, 131.4, 129.5, 129.3, 129.0, 128.9, 128.6, 125.3, 125.3, 122.8, 122.5, 21.1.

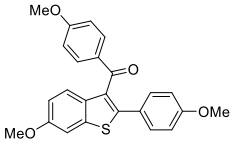
(4-(chloromethyl)phenyl)(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)methanone



3z

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow oil (68% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.70 (d, *J* = 8.0 Hz, 2H), 7.65 (s, 1H), 7.44-7.41 (m, 3H), 7.28 (d, *J* = 9.0 Hz, 2H), 7.03-7.00 (m, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 4.73 (s, 2H), 3.84 (s, 3H), 3.68 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.1, 159.6, 157.4, 143.0, 142.8, 139.4, 136.6, 133.0, 129.9, 129.7, 129.6, 128.9, 125.0, 123.4, 115.1, 114.3, 105.1, 55.5, 55.1, 45.0. **HRMS** (ESI) calcd for $C_{24}H_{19}ClO_3S$ $[M+H]^+$: 423.0816, found: 423.0812.

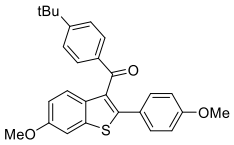
(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(4-methoxyphenyl)methanone[2]



3aa

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow soild (79% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.69 (d, J = 9.0 Hz, 2H), 7.63 (s, 1H), 7.34-7.30 (m, 3H), 7.00-6.98 (m, 1H), 6.91- 6.86 (m, 4H), 3.83 (s, 3H), 3.75 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.3, 163.6, 159.5, 157.4, 140.8, 139.4, 133.2, 131.8, 130.2, 129.6, 125.2, 123.3, 115.0, 114.3, 114.0, 105.1, 55.5, 55.5, 55.1.

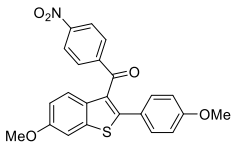
(4-(tert-butyl)phenyl)(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)methanone



3bb

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow oil (71% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.64-7.60 (m, 3H), 7.38-7.35 (m, 3H), 7.28-7.27 (m, 2H), 6.98 (d, J = 8.5 Hz, 1H), 6.82-6.81 (m, 2H), 3.82 (s, 3H), 3.67 (s, 3H), 1.18 (s, 9H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.5, 159.5, 157.4, 156.7, 141.9, 139.3, 134.3, 133.1, 130.0, 129.8, 129.3, 125.4, 125.1, 123.4, 115.0, 114.2, 105.1, 55.5, 55.1, 39.0, 30.6. **HRMS** (ESI) calcd for $C_{27}H_{26}O_3S$ $[M+H]^+$: 431.1676, found: 431.1668.

(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(4-nitrophenyl)methanone

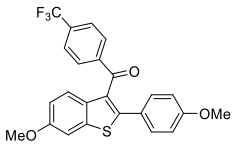


3cc

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow soild (31% yield), mp: 172-173 °C. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.12 (d, J = 8.5 Hz, 2H), 7.85 (d, J = 9.0 Hz, 2H), 7.71-7.70 (m, 1H), 7.65 (d, J = 9.0

Hz, 1H), 7.25 (d, *J* = 9.0 Hz, 2H), 7.09-7.07 (m, 1H), 6.81 (d, *J* = 7.5 Hz, 2H), 3.86 (s, 3H), 3.66 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 191.8, 159.9, 157.6, 149.6, 146.2, 142.1, 139.5, 132.6, 130.6, 130.5, 128.7, 124.7, 123.7, 123.5, 115.4, 114.2, 105.2, 55.6, 55.2. **HRMS** (ESI) calcd for $C_{23}H_{17}NO_5S$ $[M+H]^+$: 442.0725, found 447.0726.

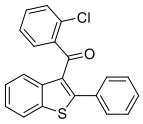
(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(4-(trifluoromethyl)phenyl)methanone



3dd

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow oil (46% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.80 (d, *J* = 8.5 Hz, 2H), 7.69-7.65 (m, 3H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.23 (d, *J* = 9.0 Hz, 2H), 7.07-7.05 (m, 1H), 6.80 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 3.66 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.3, 159.8, 157.5, 145.5, 140.4, 139.5, 132.2 (q, J_{C-F} = 31.3 Hz), 130.4, 130.0, 128.9, 125.4 (d, J_{C-F} = 3.8 Hz), 124.8, 123.7, 123.5 (d, J_{C-F} = 271.3 Hz), 115.3, 114.2, 105.1, 55.5, 55.1. **HRMS** (ESI) calcd for $C_{24}H_{17}F_3O_3S$ $[M+H]^+$: 443.0923, found: 443.0926.

(2-chlorophenyl)(2-phenylbenzo[b]thiophen-3-yl)methanone

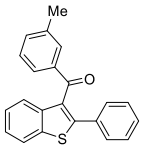


3ee

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (70% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.13-8.08 (m, 2H), 7.55-7.49 (m, 2H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.33-7.32 (m, 2H), 7.27-7.22 (m, 5H), 7.16-7.14 (m, 1H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 190.6, 151.7, 138.3, 138.2, 138.0, 132.4, 132.2, 131.0, 131.0, 130.8, 129.9, 129.3, 129.1, 128.2, 126.8, 125.9,

125.6, 123.6, 122.4. **HRMS** (ESI) calcd for $C_{21}H_{13}ClOS$ $[M+Na]^+$: 371.0274, found: 371.0276.

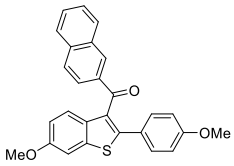
(2-phenylbenzo[b]thiophen-3-yl)(m-tolyl)methanone



3ff

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (84% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.12 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.54 (s, 1H), 7.48-7.39 (m, 5H), 7.35-7.29 (m, 4H), 7.26-7.23 (m, 1H), 2.22 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.5, 145.2, 139.0, 138.2, 138.1, 136.8, 134.4, 132.7, 131.2, 129.6, 129.1, 128.8, 128.7, 128.6, 126.8, 125.4, 125.4, 122.9, 122.6, 20.6. **HRMS** (ESI) calcd for $C_{22}H_{16}OS$ $[M+Na]^+$: 351.0820, found: 351.0824.

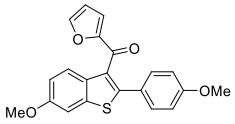
(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(naphthalen-2-yl)methanone



3gg

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow soild (57% yield), mp: 161-162 ^{o}C. **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.24 (s, 1H), 7.93-7.91 (m, 3H), 7.78-7.86 (d, J = 8.5 Hz, 1H), 7.69 (s, 1H), 7.62-7.59 (m, 1H), 7.52-7.46 (m, 2H), 7.33 (d, J = 8.5 Hz, 2H), 7.02-7.00 (m, 1H), 6.78 (d, J = 8.5 Hz, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.6, 159.5, 157.4, 142.8, 139.5, 135.1, 134.3, 133.2, 131.9, 129.9, 129.9, 129.6, 128.9, 128.4, 127.5, 126.9, 125.2, 124.3, 123.5, 115.1, 114.3, 105.2, 55.5, 55.1. **HRMS** (ESI) calcd for $C_{27}H_{20}O_3S$ $[M+H]^+$: 425.1206, found: 425.1210.

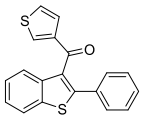
furan-2-yl(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)methanone



3hh

Following the general procedure, using petroleum ether/AcOEt (10:1) as the eluant to afford yellow oil (41% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.88 (s, 1H), 7.65 (s, 1H), 7.55-7.53 (m, 1H), 7.34-7.32 (m, 2H), 7.05-7.04 (m, 1H), 6.97-6.92 (m, 3H), 6.52 (s, 1H), 3.84 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 179.8, 159.6, 157.4, 152.0, 148.6, 143.3, 139.4, 132.8, 129.8, 129.0, 125.3, 123.2, 121.4, 115.1, 114.4, 112.7, 105.1, 55.5, 55.2. **HRMS** (ESI) calcd for $C_{21}H_{16}O_4S$ $[M+H]^+$: 365.0842, found: 365.0834.

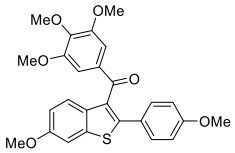
(2-phenylbenzo[b]thiophen-3-yl)(thiophen-3-yl)methanone[1]



3ii

Following the general procedure, using petroleum ether/AcOEt (20:1) as the eluant to afford yellow oil (45% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.09 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 7.0 Hz, 2H), 7.65-7.64 (m, 1H), 7.61-7.58 (m, 1H), 7.54-7.51 (m, 1H), 7.50 (s, 1H), 7.46-7.43 (m, 4H), 7.08-7.07 (m, 1H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 193.8, 139.3, 138.8, 137.6, 136.7, 133.9, 132.8, 130.5, 129.3, 128.9, 127.8, 127.3, 125.8, 125.5, 125.4, 122.7, 122.5.

(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(3,4,5-trimethoxyphenyl)methanone[2]

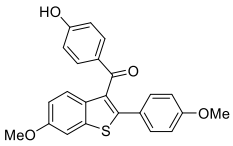


3ll

Following the general procedure, using petroleum ether/AcOEt (5:1) as the eluant to

afford yellow soild (80% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.66 (s, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.06-7.04 (m, 1H),6.99 (s, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 3.85 (s, 3H), 3.70 (s, 3H), 3.65 (s, 9H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 192.0, 159.6, 157.4, 152.5, 143.4, 142.1, 139.5, 133.2, 131.9, 130.1, 129.4, 125.4, 123.7, 115.1, 114.2, 107.1, 105.1, 60.1, 55.9, 55.5, 55.2.

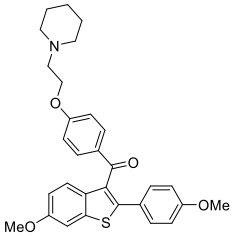
(4-hydroxyphenyl)(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)methanone[3]



4aa

Following the general procedure, using petroleum ether/AcOEt (2:1) as the eluant to afford yellow soild (89% yield). **^{1}H NMR** (500 MHz, Acetone-d_6) δ 7.68 (d, *J* = 9.0 Hz, 2H), 7.53-7.52 (m, 1H), 7.45 (d, *J* = 9.0 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.01-6.98 (m, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.79 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (125 MHz, Acetone-d_6) δ 193.2, 163.4, 160.9, 158.8, 141.9, 140.8, 134.8, 133.1, 131.9, 130.8, 130.3, 126.8, 124.5, 116.1, 115.7, 115.0, 105.5, 56.0, 55.6.

(6-methoxy-2-(4-methoxyphenyl)benzo[b]thiophen-3-yl)(4-(2-(piperidin-1-yl)ethoxy)phenyl)methanone [3]

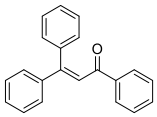


5aa

Following the general procedure, using petroleum ether/AcOEt/triethylamine (2:1:0.1) as the eluant to afford yellow soild (90% yield). **^{1}H NMR** (500 MHz, Acetone-d_6) δ 7.73 (d, *J* = 9.0 Hz, 2H), 7.56-7.55 (m, 1H), 7.45 (d, *J* = 9.0 Hz, 1H), 7.37 (d, *J* = 9.0 Hz, 2H), 7.01-6.99 (m, 1H), 6.90-6.85 (m, 4H), 4.11 (t, *J* = 7.0 Hz, 2H), 3.89 (s, 3H),

3.75 (s, 3H), 2.66 (t, *J* = 7.0 Hz, 2H), 2.43 (s, 4H), 1.53-1.48 (m, 4H), 1.40-1.38 (m, 2H); **^{13}C NMR** (125 MHz, Acetone-d_6) δ 193.2, 164.2, 160.9, 158.9, 142.2, 140.9, 134.7, 132.8, 131.8, 131.2, 130.9, 126.8, 124.6, 115.8, 115.2, 115.0, 105.6, 67.3, 58.4, 56.0, 55.6, 26.8, 25.0.

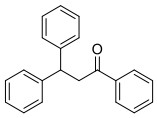
1,3,3-triphenylprop-2-en-1-one[5]



4a

Following the general procedure, using petroleum ether as the eluant to afford yellow soild (52% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 7.91 (d, *J* = 7.5 Hz, 2H), 7.56-7.54 (m, 1H), 7.45-7.40 (m, 7H), 7.31 (s, 1H), 7.28-7.27 (m, 3H), 7.09-7.08 (m, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 191.9, 152.5, 140.6, 138.8, 137.6, 132.8, 129.2, 129.2, 128.4, 128.4, 128.4, 128.1, 127.9, 124.4.

1,3,3-triphenylpropan-1-one[6]



4b

Following the general procedure, using petroleum ether as the eluant to afford white soild (37% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.64-7.61 (m, 1H), 7.52-7.49 (m, 2H), 7.38 (d, *J* = 7.5 Hz, 2H), 7.26-7.23 (m, 4H), 7.15-7.12 (m, 2H), 4.66 (t, *J* = 7.5 Hz, 1H), 3.90 (d, *J* = 7.5 Hz, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 198.0, 144.6, 136.7, 133.1, 128.6, 128.3, 128.0, 127.6, 126.0, 45.8, 43.3.

Reference

[1] F. Gao, J. T. Wang, L. L. Liu, N. Ma, C. Yang, Y. Gao and W. J. Xia, *Chem. Commun*., 2017, **53**, 8533.

[2] A. Acharya, S. V. Kumar and H. Ila, *Chem*. - *Eur*. *J*., 2015, **21**, 17116.

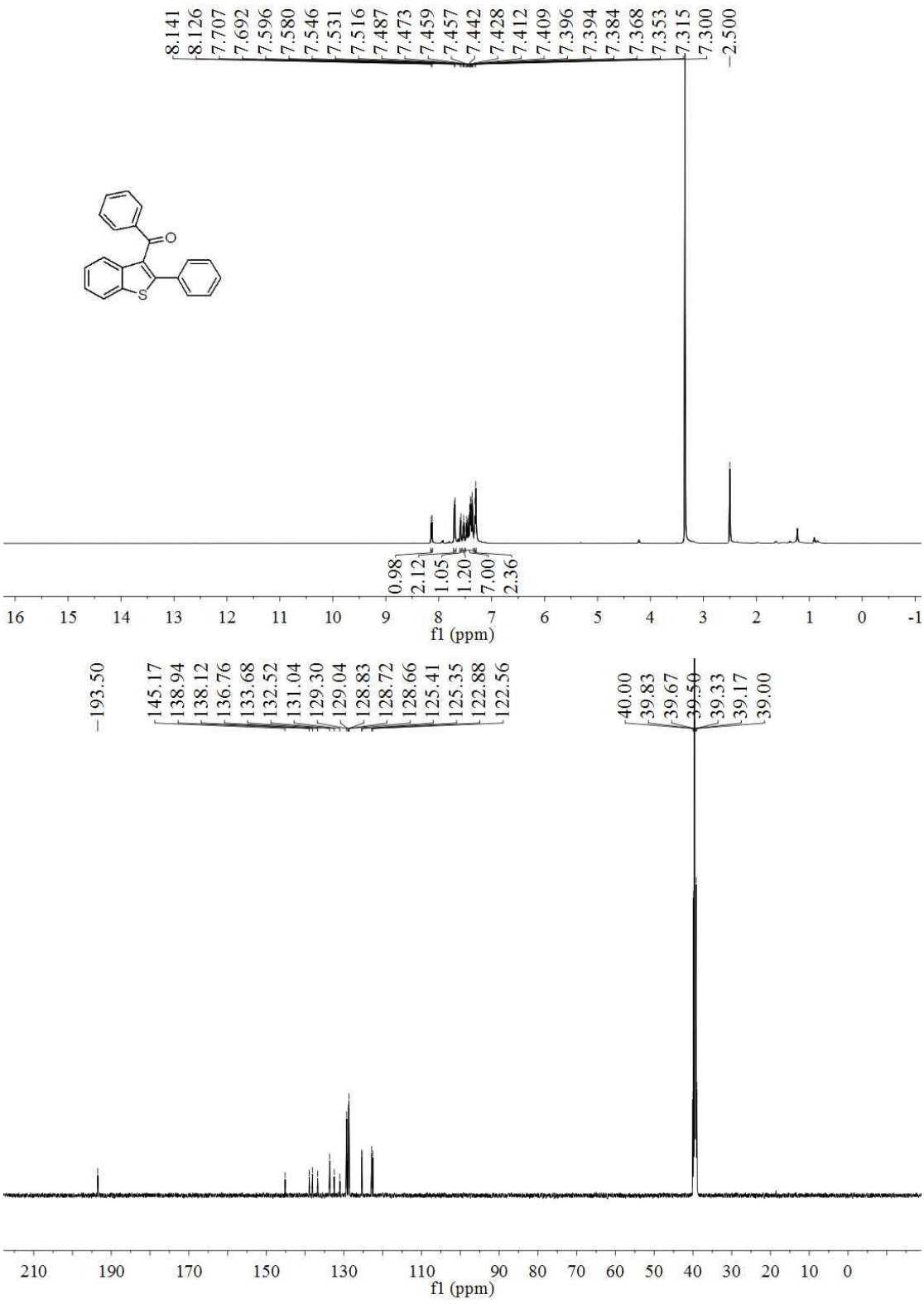
[3] J. Liu, Q. Li, X. F. Yang, R. B. van Breemen, J. L. Bolton and G. R. Thatcher, *Chem*. *Res*. *Toxicol*., 2005*,* **18***,* 1485.

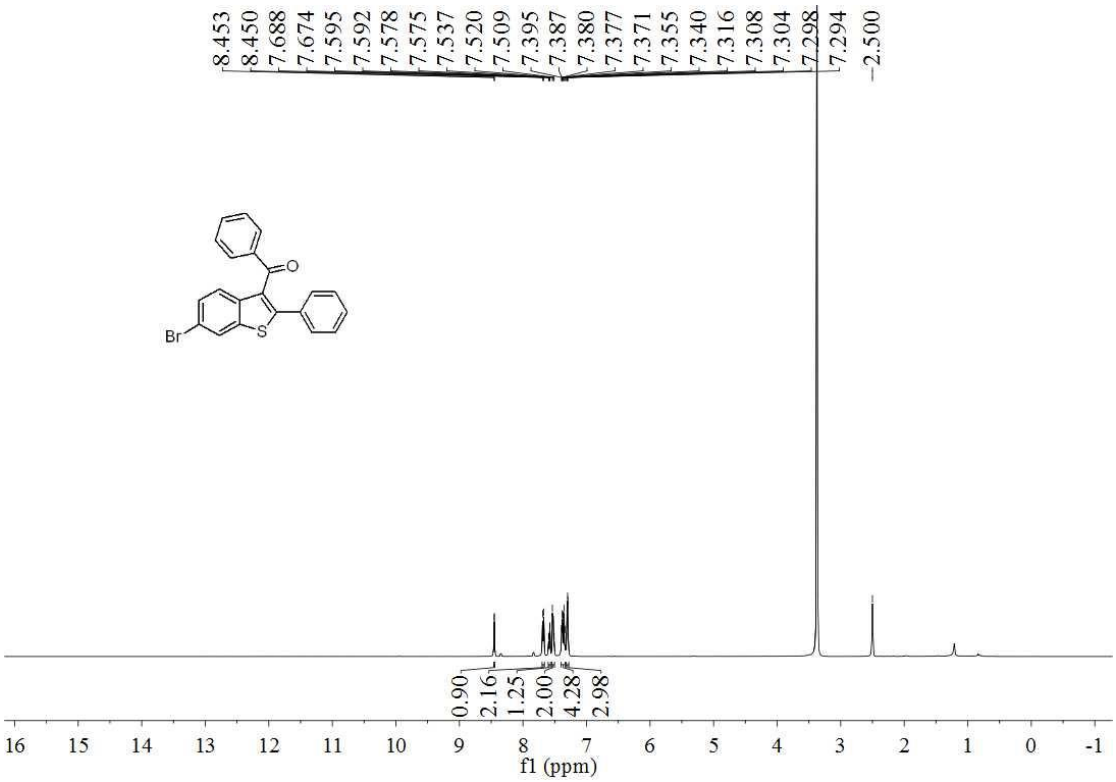
[4] S. Tang, X. L. Gao and A. W. Lei, *Chem. Commun*., 2017, **53**, 3354.

[5] R. C. Jones, M. Galezowski and D. F. O'Shea, *J. Org. Chem*., 2013, **78**, 8044.

[6] A. Devineau, G. Pousse, C. Taillier, J. Blanchet, J. Rouden and V. Dalla, *Adv. Synth. Catal*., 2010, **352**, 2881.

7. NMR Spectra for All Products

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7.592
7.578
7.575
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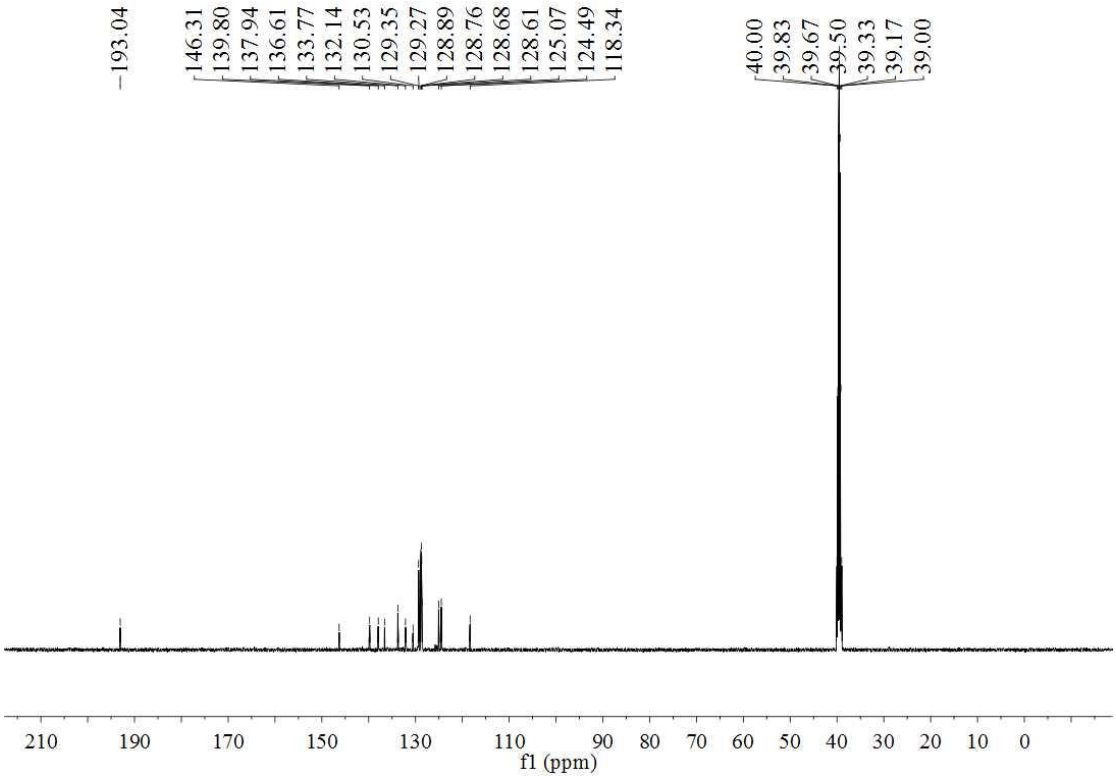
7.520
7.509
7.395
7.387
7.380
7.377
7.371
7.355
7.340
7.316
7.308
7.304
7.298
7.294
2.500
O
Br
S
0.90
2.16
1.25
2.00
4.28
2.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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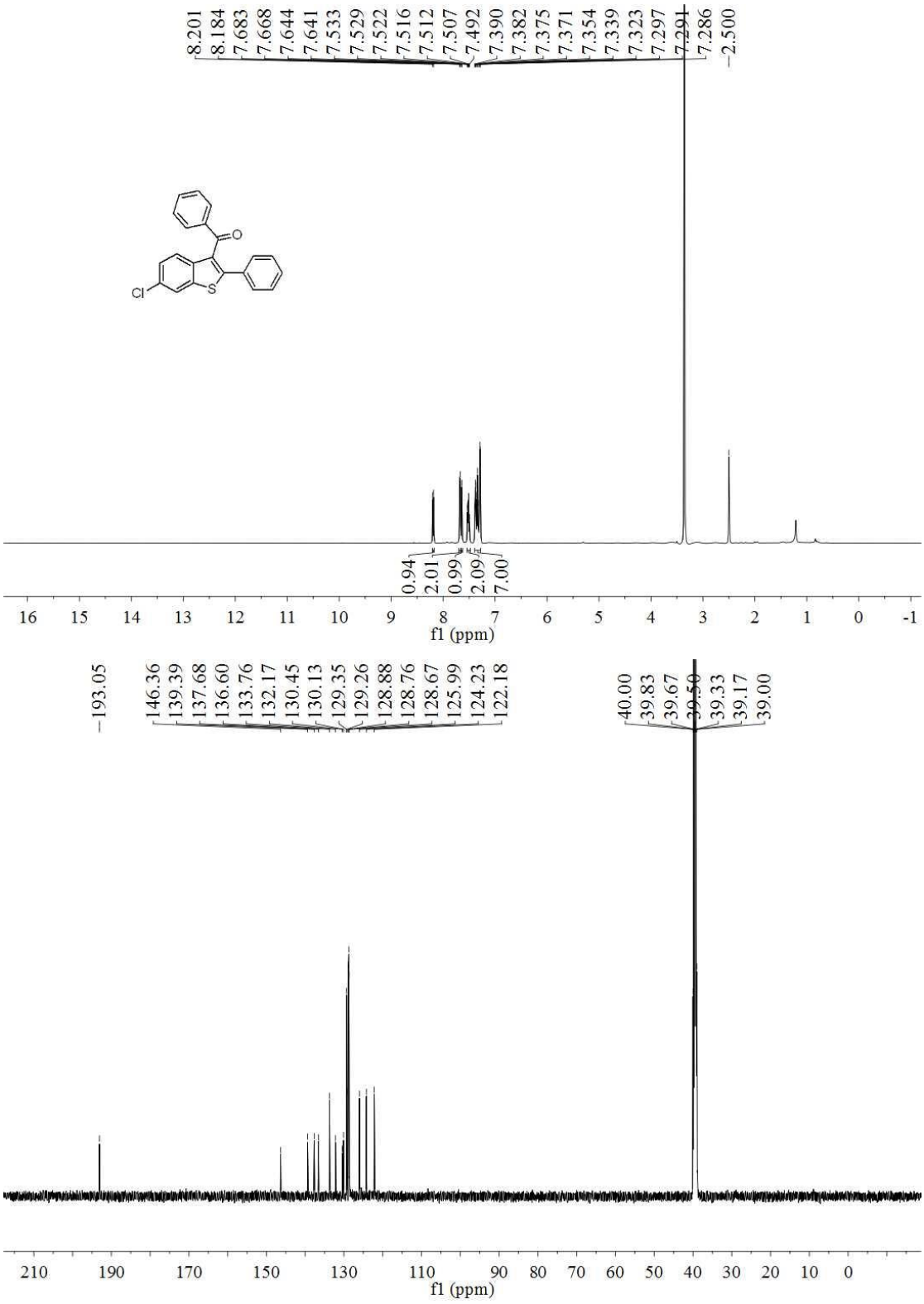
139.80
137.94
136.61
133.77
132.14
130.53
129.35
129.27
128.89
128.76
128.68
128.61
125.07
124.49
118.34
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.644
7.641
7.533
7.529
7.522
7.516
7.512
7.507
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7.390
7.382
7.375
7.371
7.354
7.339
7.323
7.297
7.291
7.286
2.500
O
Cl
S
0.94
2.01
0.99
2.09
7.00
f1 (ppm)
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146.36
139.39
137.68
136.60
133.76
132.17
130.45
130.13
129.35
129.26
128.88
128.76
128.67
125.99
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122.18
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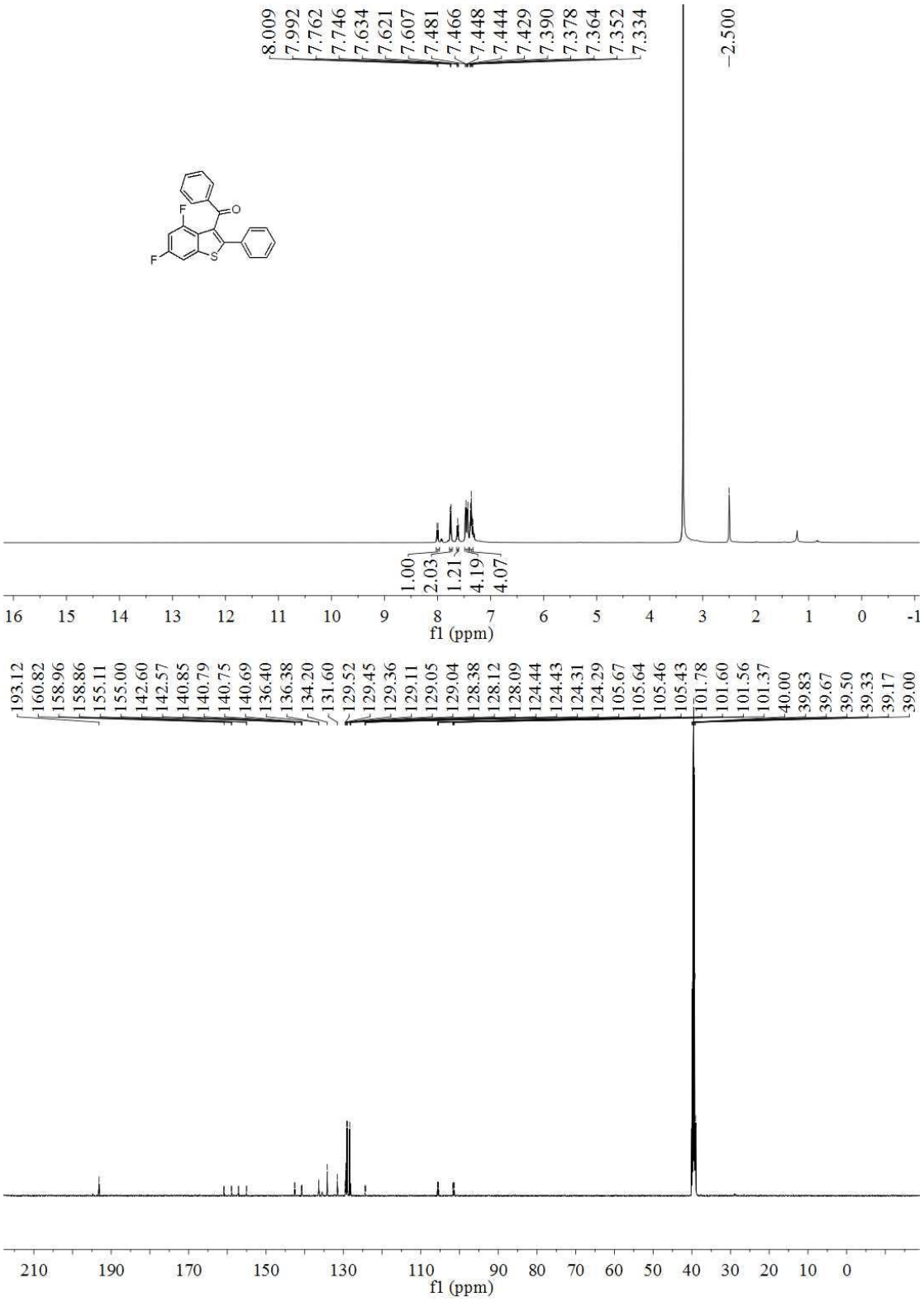
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)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7.466
7.448
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7.429
7.390
7.378
7.364
7.352
7.334
2.500
F
O
F
S
1.00
2.03
1.21
4.19
4.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
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160.82
158.96
158.86
155.11
155.00
142.60
142.57
140.85
140.79
140.75
140.69
136.40
136.38
134.20
131.60
129.52
129.45
129.36
129.11
129.05
129.04
128.38
128.12
128.09
124.44
124.43
124.31
124.29
105.67
105.64
105.46
105.43
101.78
101.60
101.56
101.37
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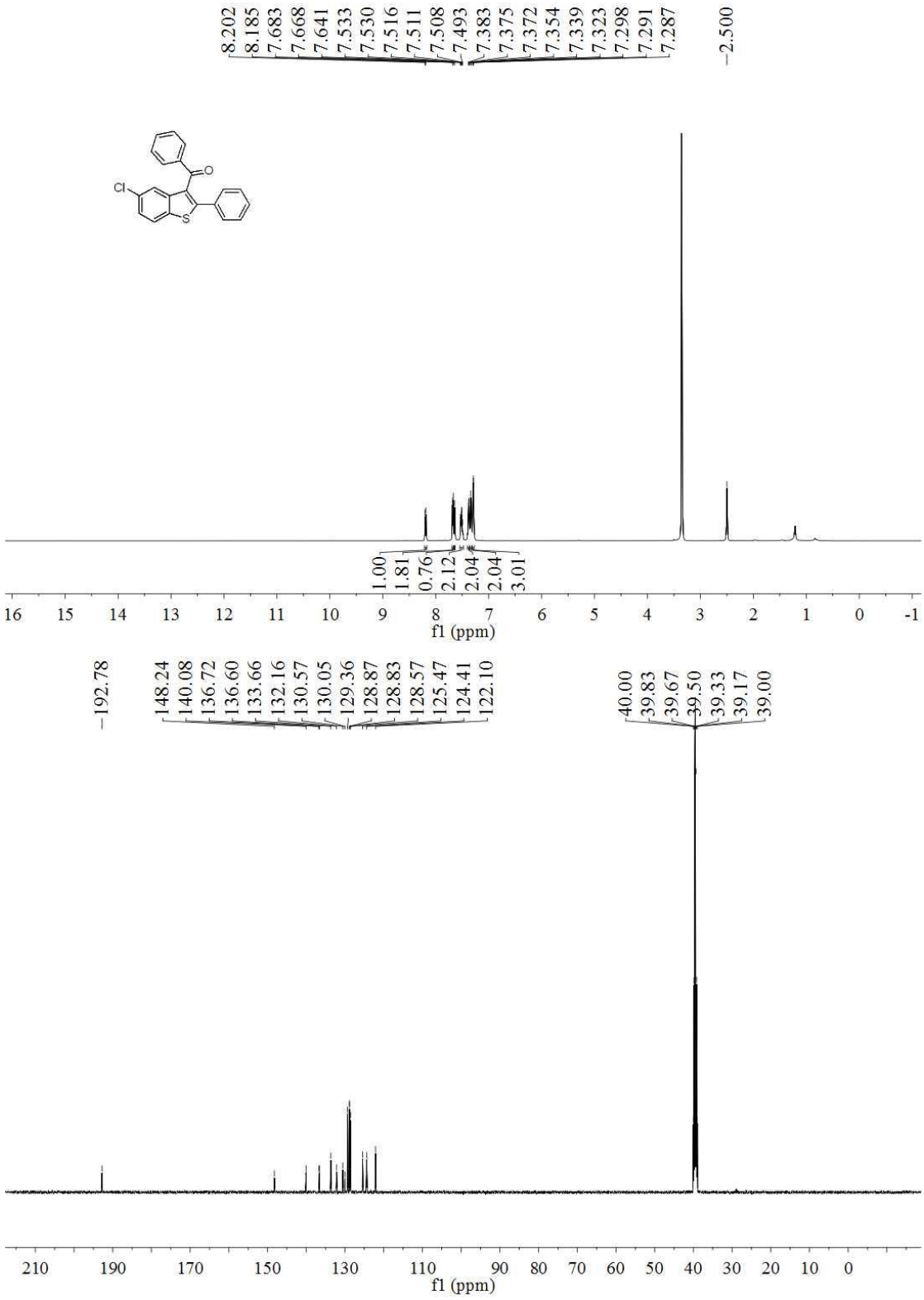
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.516
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7.508
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7.375
7.372
7.354
7.339
7.323
7.298
7.291
7.287
2.500
Cl
O
S
1.00
1.81
0.76
2.12
2.04
2.04
3.01
f1 (ppm)
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148.24
140.08
136.72
136.60
133.66
132.16
130.57
130.05
129.36
128.87
128.83
128.57
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122.10
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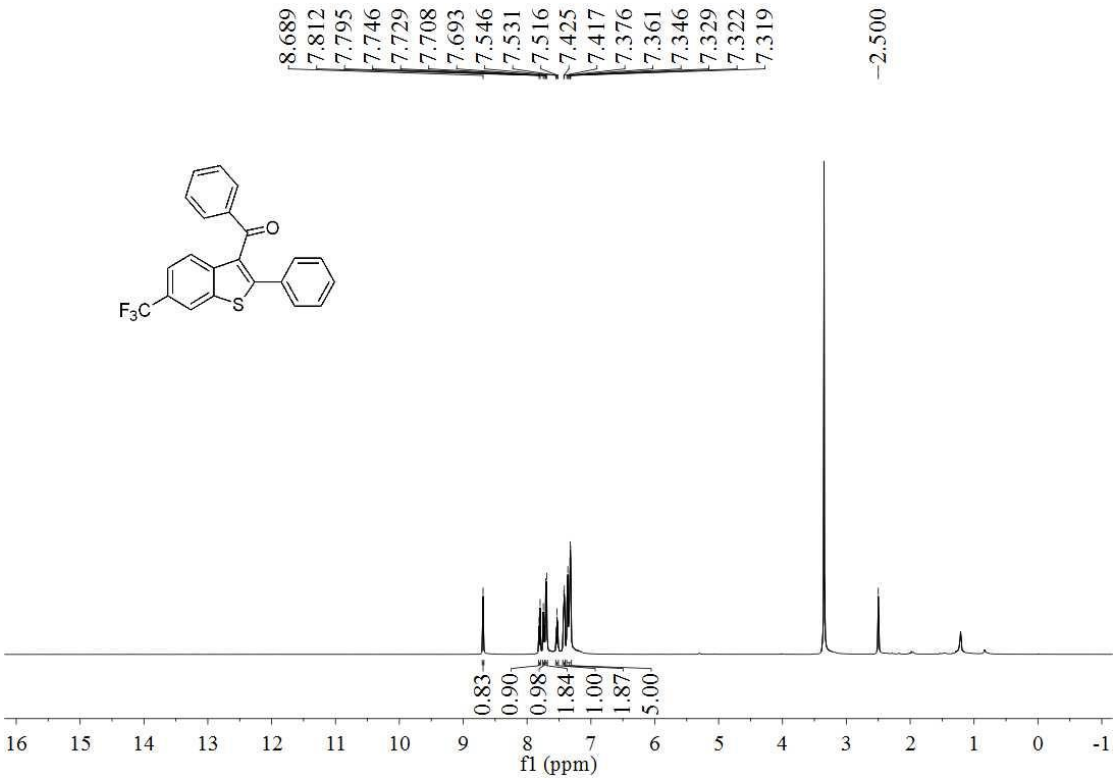
39.00
f1 (ppm)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7.516
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7.417
7.376
7.361
7.346
7.329
7.322
7.319
2.500
O
F3C
S
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0.90
0.98
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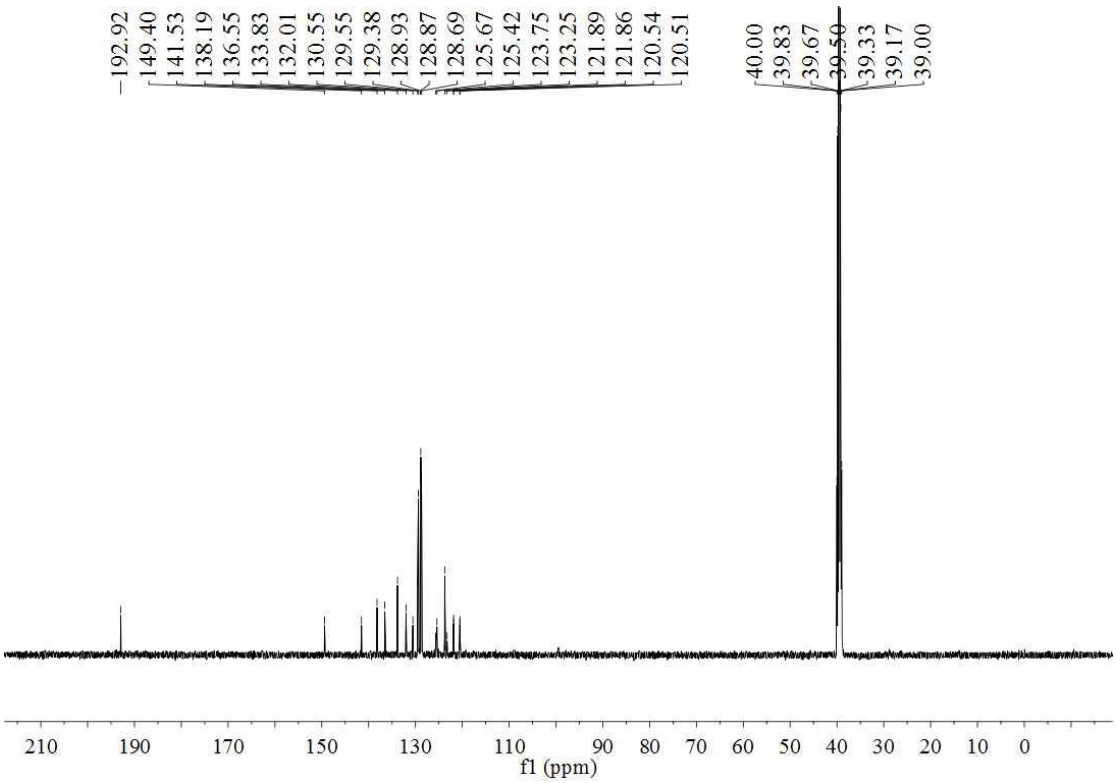
1.00
1.87
5.00
f1 (ppm)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133.83
132.01
130.55
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129.38
128.93
128.87
128.69
125.67
125.42
123.75
123.25
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39.50
39.33
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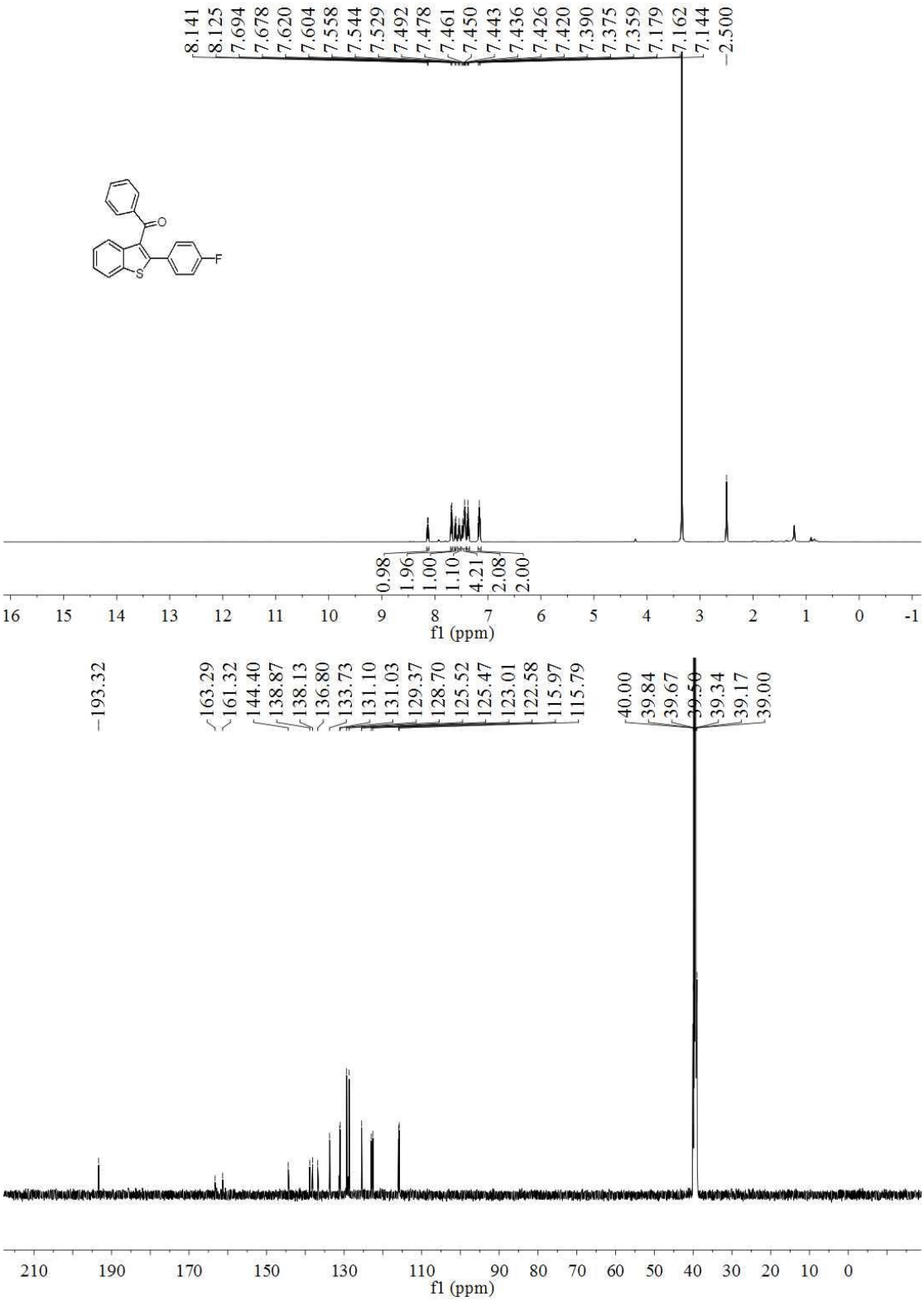
39.00
f1 (ppm)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7.436
7.426
7.420
7.390
7.375
7.359
7.179
7.162
7.144
2.500
O
S
F
0.98
1.96
1.00
1.10
4.21
2.08
2.00
f1 (ppm)
193.32
163.29
161.32
144.40
138.87
138.13
136.80
133.73
131.10
131.03
129.37
128.70
125.52
125.47
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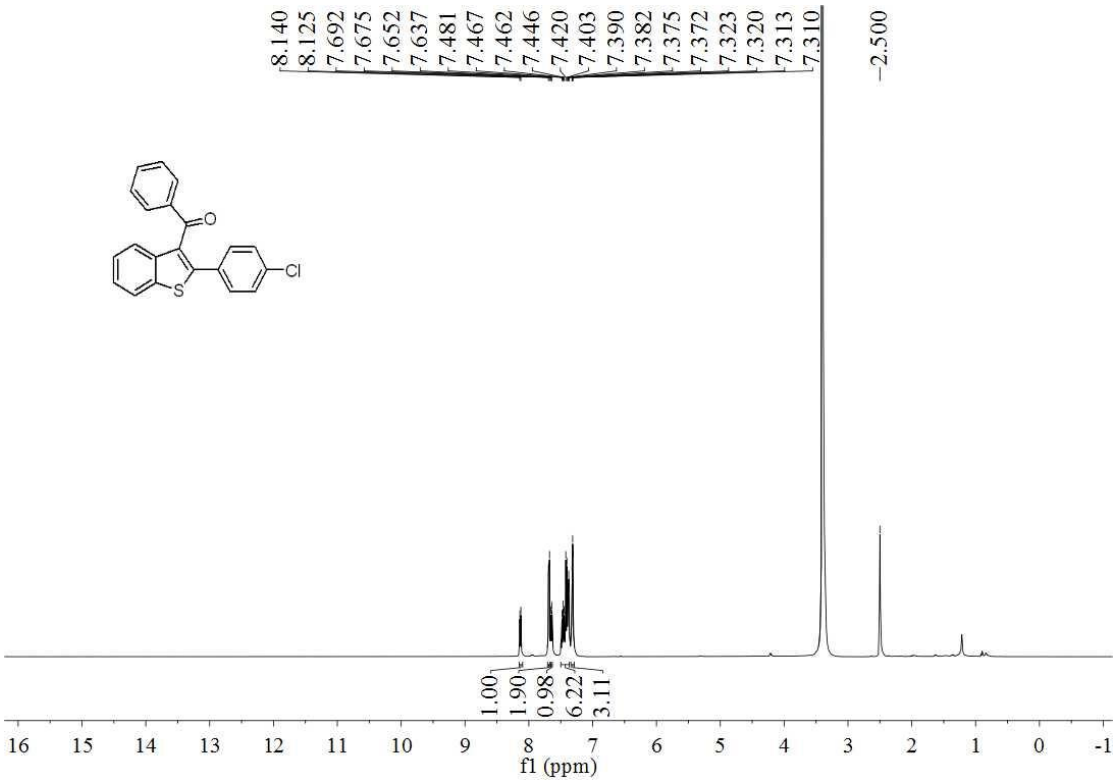
f1 (ppm)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7.375
7.372
7.323
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Cl
S
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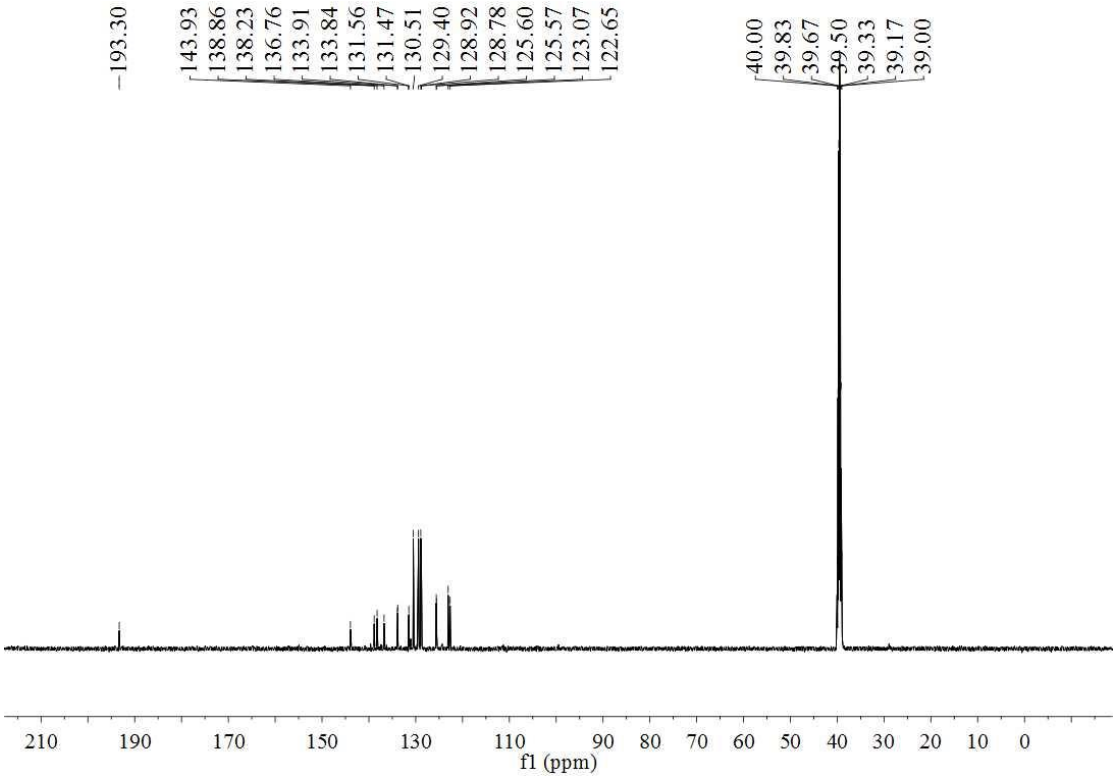
3.11
f1 (ppm)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133.91
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131.56
131.47
130.51
129.40
128.92
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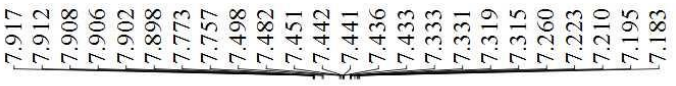
39.50
39.33
39.17
39.00
f1 (ppm)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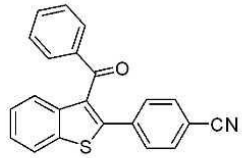
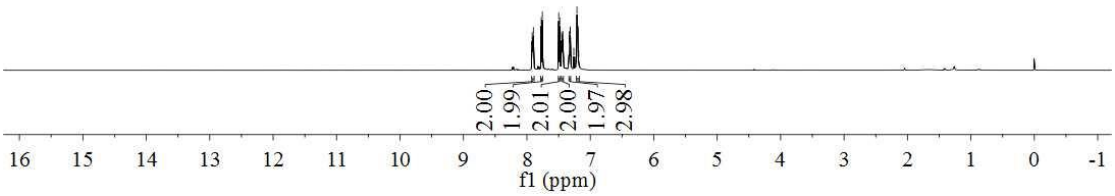
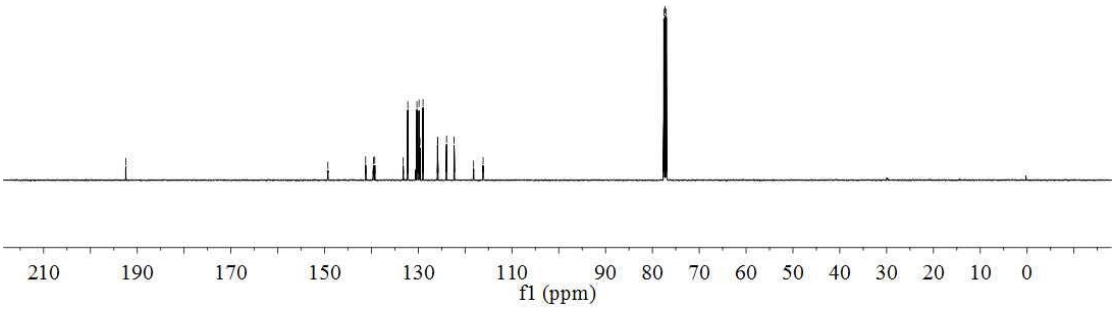
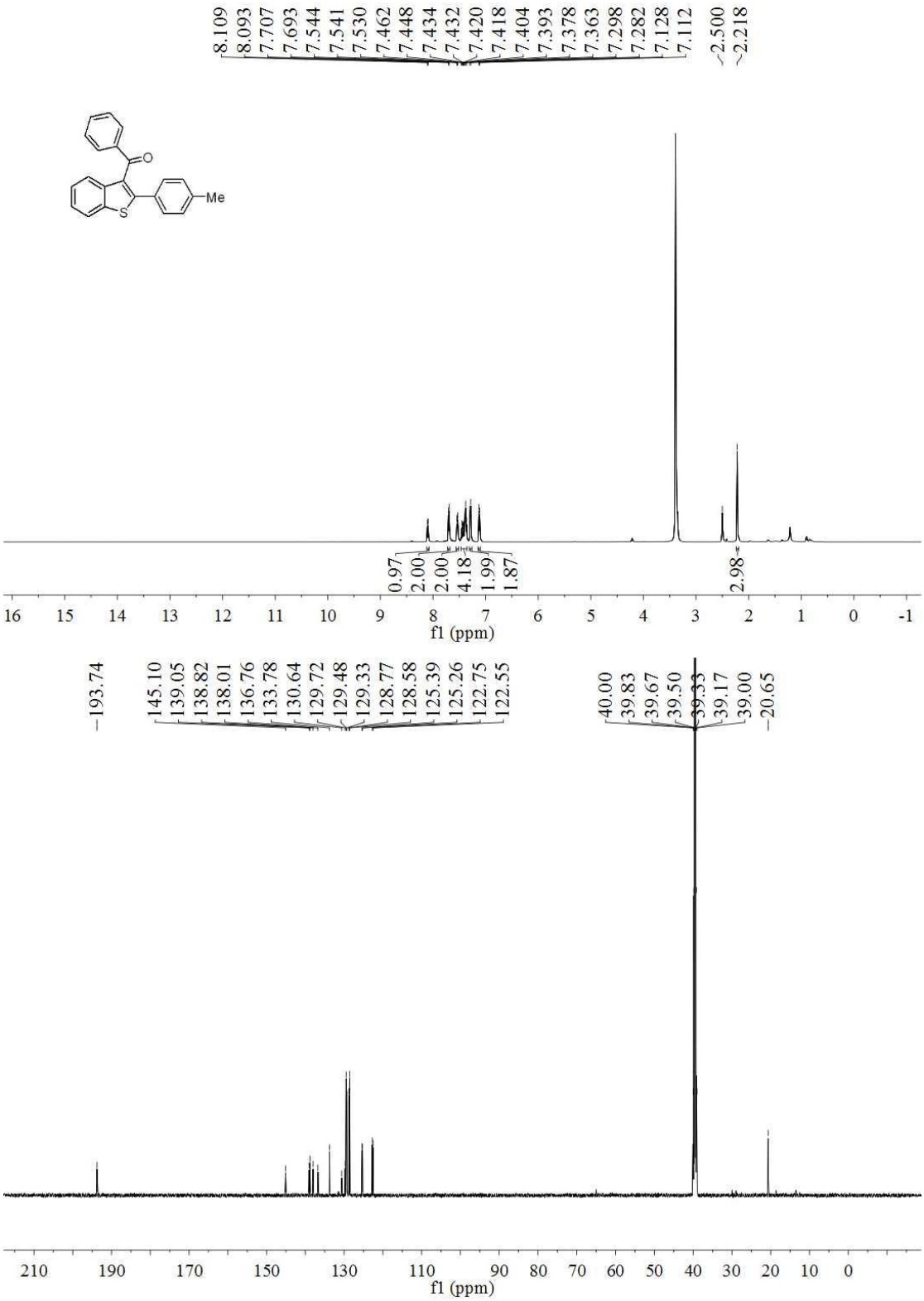
7.436
7.433
7.333
7.331
7.319
7.315
7.260
7.223
7.210
7.195
7.183


O
CN
S

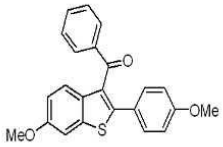

2.00
1.99
2.01
2.00
1.97
2.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

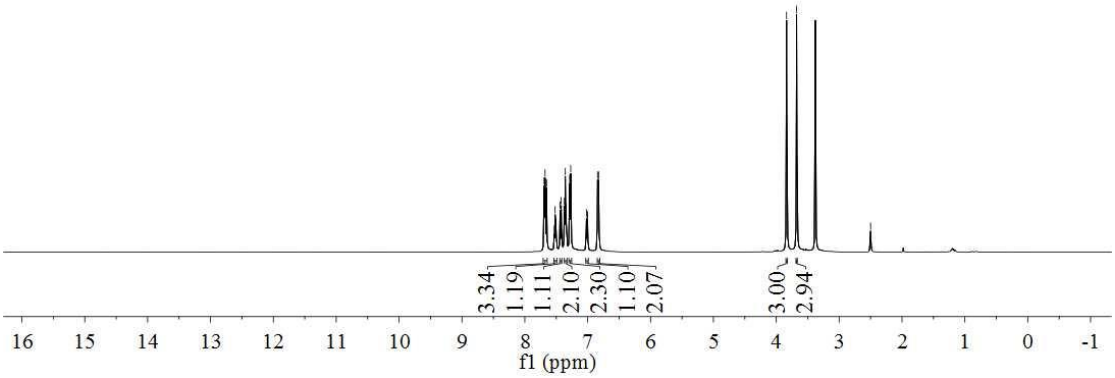

192.46
149.29
141.24
139.55
139.28
133.22
132.23
130.28
129.84
129.63
128.98
125.88
125.81
123.95
122.34
118.18
116.16
77.55
77.30
77.05

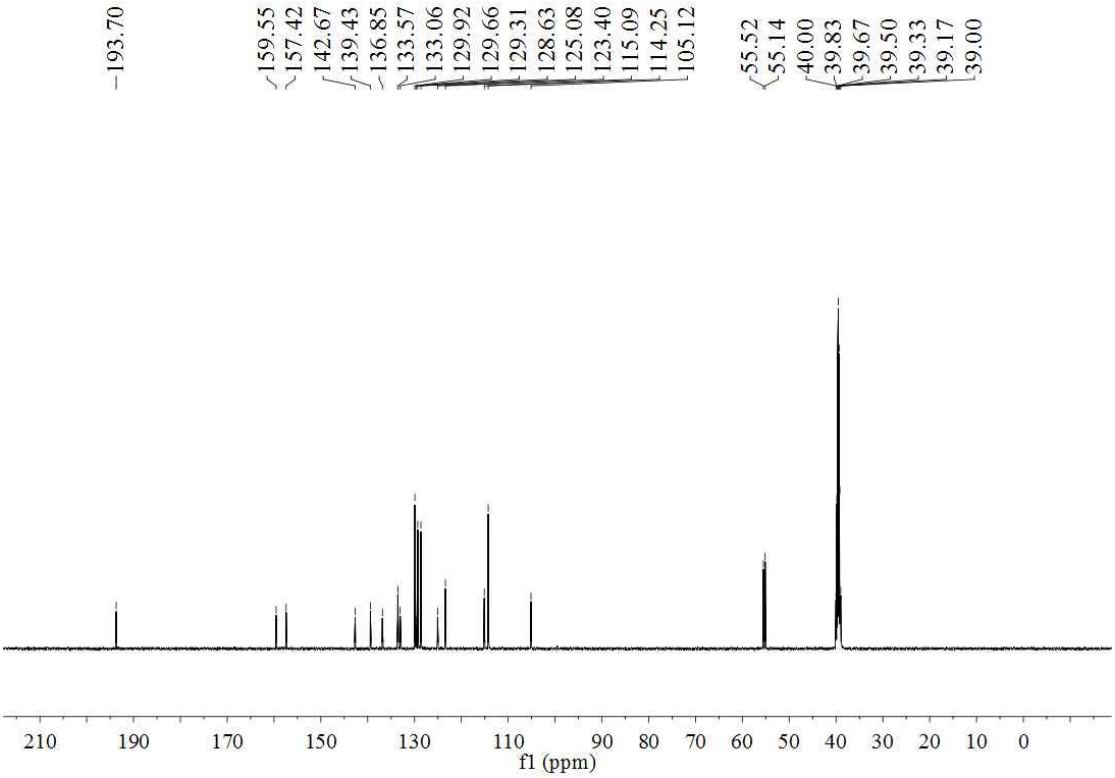

210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

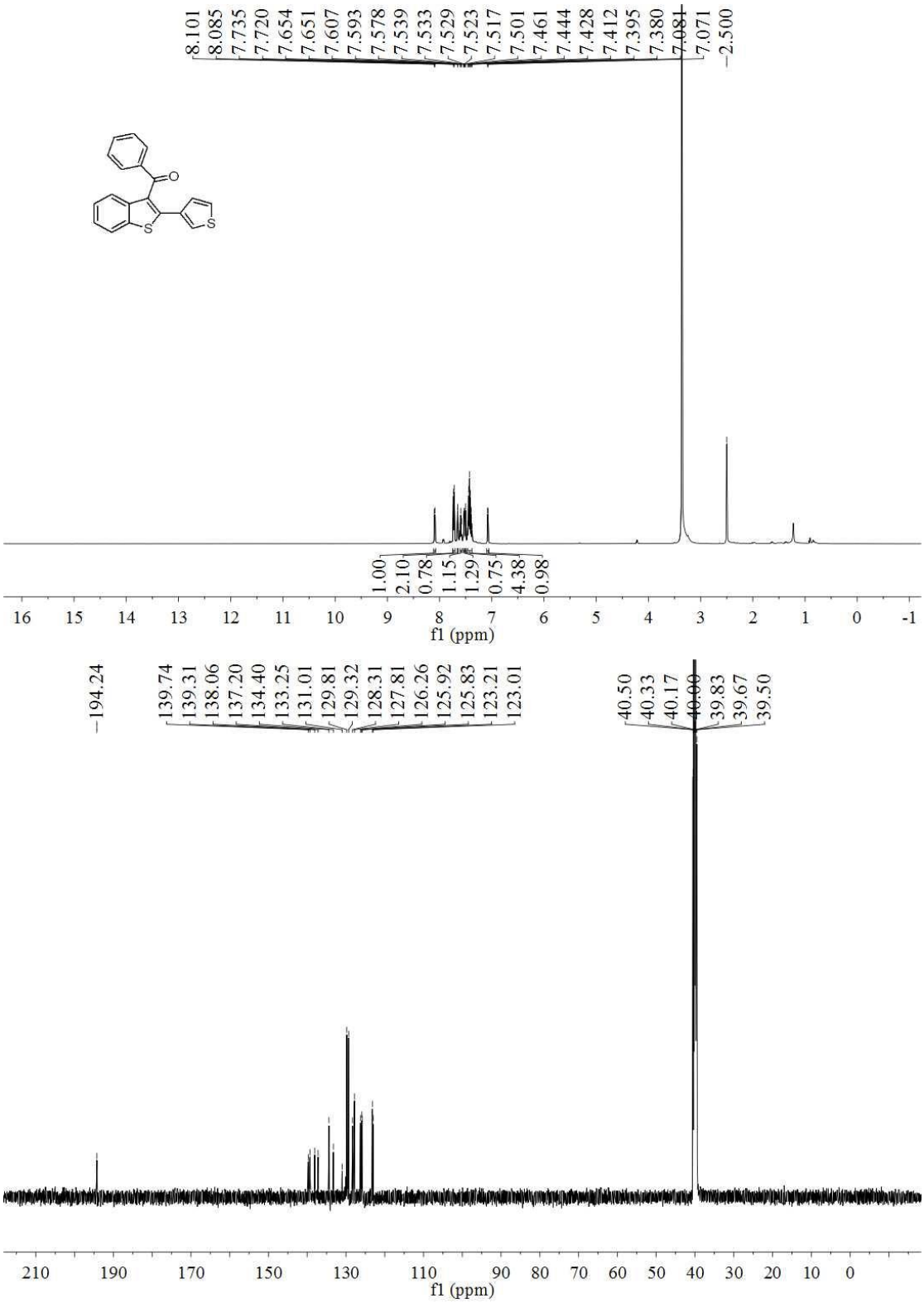

8.109
8.093
7.707
7.693
7.544
7.541
7.530
7.462
7.448
7.434
7.432
7.420
7.418
7.404
7.393
7.378
7.363
7.298
7.282
7.128
7.112
2.500
2.218
O
Me
S
0.97
2.00
2.00
4.18
1.99
1.87
2.98
f1 (ppm)
193.74
145.10
139.05
138.82
138.01
136.76
133.78
130.64
129.72
129.48
129.33
128.77
128.58
125.39
125.26
122.75
122.55
40.00
39.83
39.67
39.50
39.33
39.17
39.00
20.65
f1 (ppm)

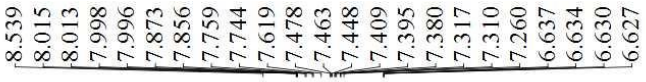

7.693
7.678
7.654
7.532
7.518
7.503
7.439
7.421
7.371
7.356
7.341
7.287
7.270
7.020
7.006
7.002
6.843
6.826
3.836
3.676
2.500

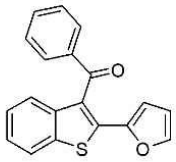

O
OMe
MeO
S

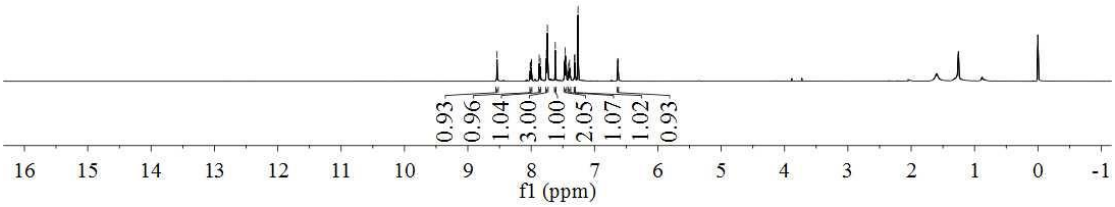

3.34
1.19
1.11
2.10
2.30
1.10
2.07
3.00
2.94
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

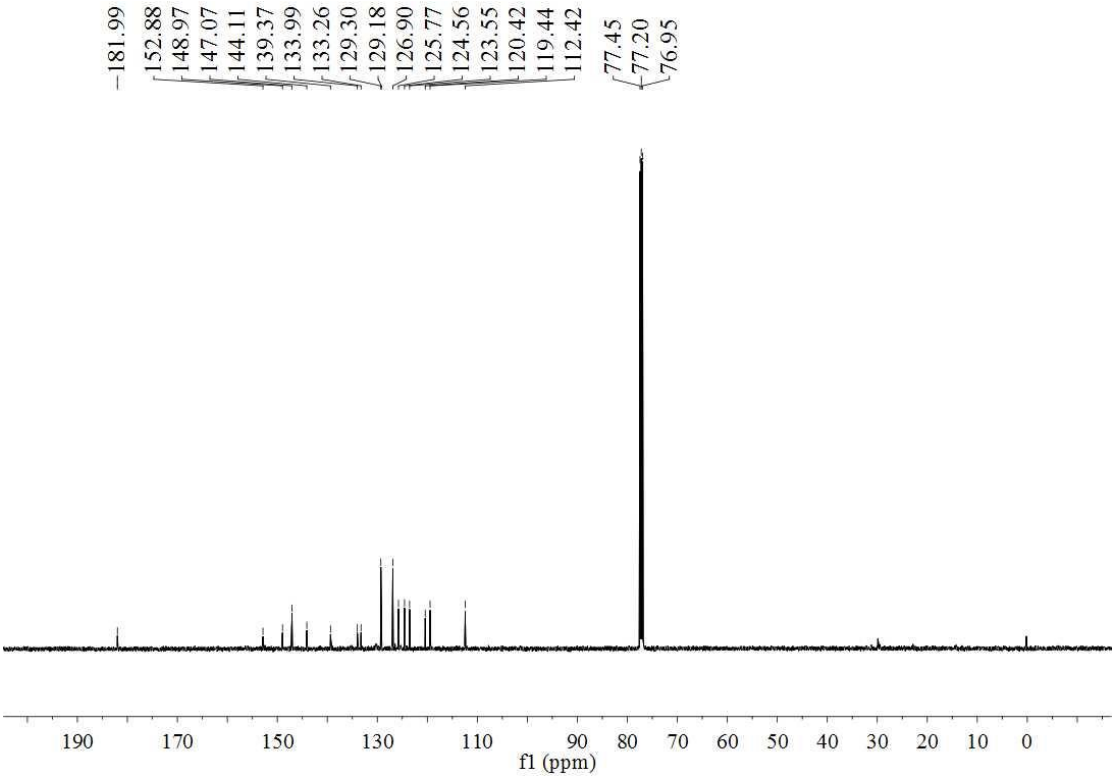

193.70
159.55
157.42
142.67
139.43
136.85
133.57
133.06
129.92
129.66
129.31
128.63
125.08
123.40
115.09
114.25
105.12
55.52
55.14
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

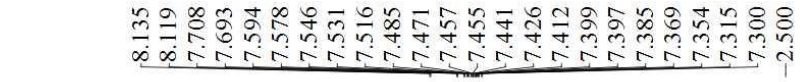

8.101
8.085
7.735
7.720
7.654
7.651
7.607
7.593
7.578
7.539
7.533
7.529
7.523
7.517
7.501
7.461
7.444
7.428
7.412
7.395
7.380
7.081
7.071
2.500
1.00
2.10
0.78
1.15
1.29
0.75
4.38
0.98
f1 (ppm)
194.24
139.74
139.31
138.06
137.20
134.40
133.25
131.01
129.81
129.32
128.31
127.81
126.26
125.92
125.83
123.21
123.01
40.50
40.33
40.17
40.00
39.83
39.67
39.50
f1 (ppm)

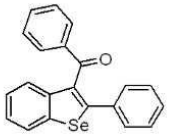

8.539
8.015
8.013
7.998
7.996
7.873
7.856
7.759
7.744
7.619
7.478
7.463
7.448
7.409
7.395
7.380
7.317
7.310
7.260
6.637
6.634
6.630
6.627

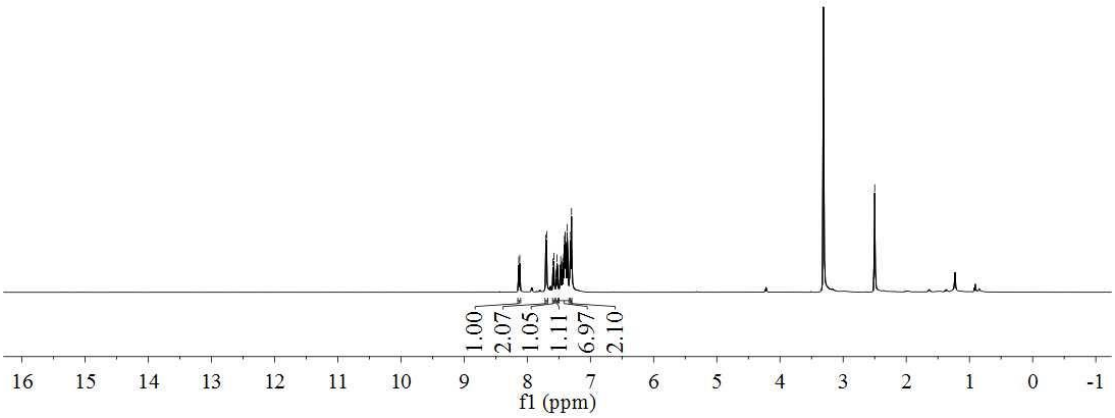

O
S
O

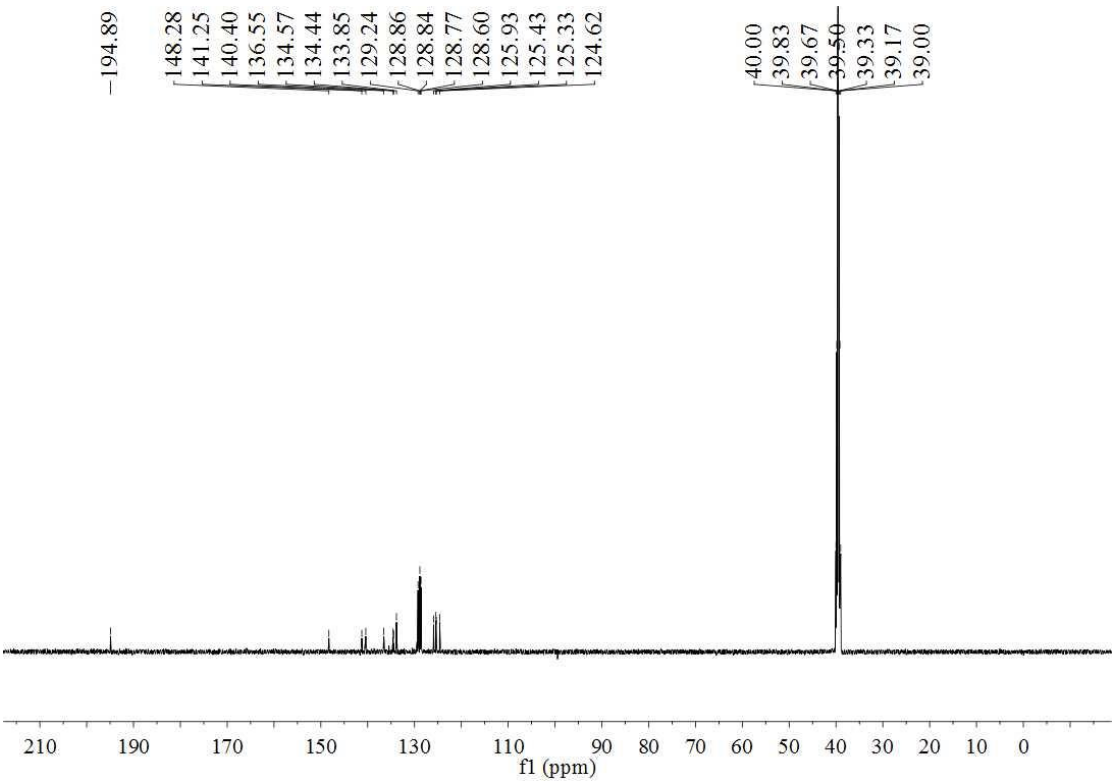

0.93
0.96
1.04
3.00
1.00
2.05
1.07
1.02
0.93
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

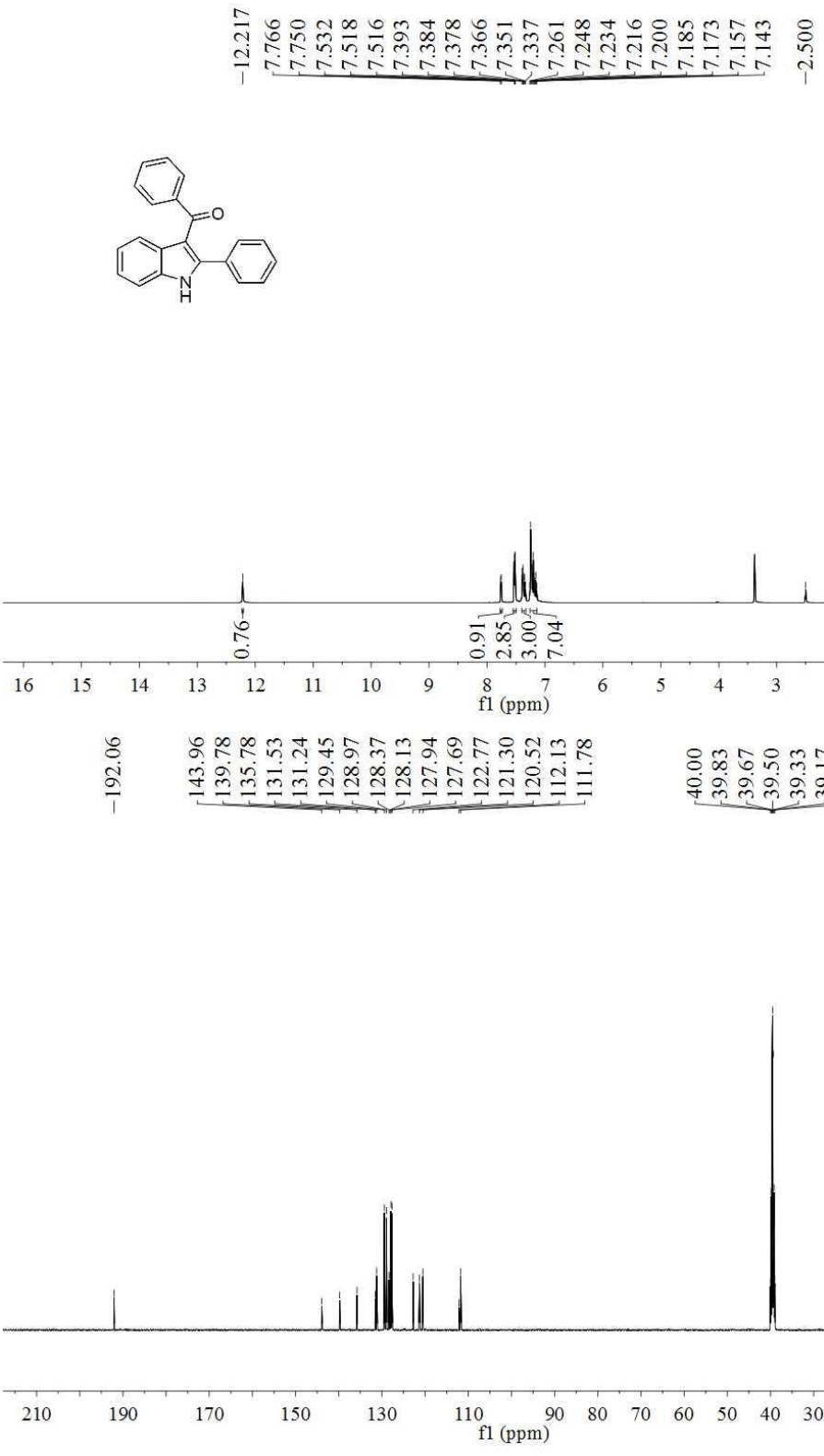

181.99
152.88
148.97
147.07
144.11
139.37
133.99
133.26
129.30
129.18
126.90
125.77
124.56
123.55
120.42
119.44
112.42
77.45
77.20
76.95
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

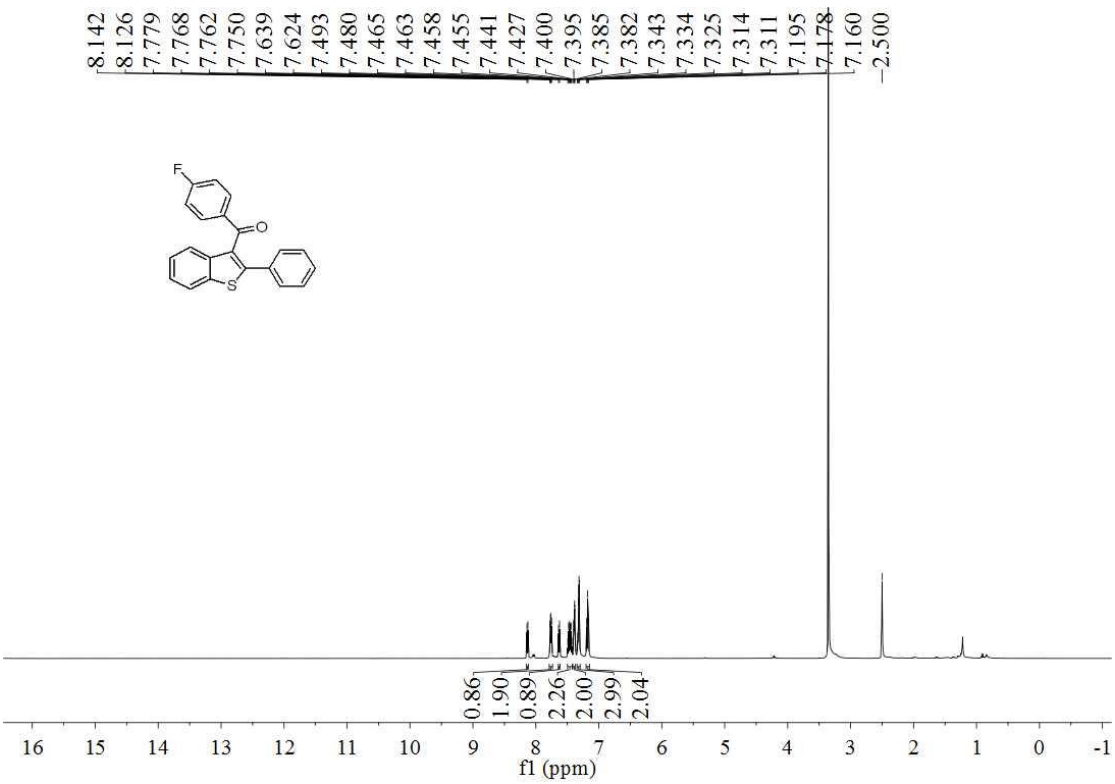

8.135
8.119
7.708
7.693
7.594
7.578
7.546
7.531
7.516
7.485
7.471
7.457
7.455
7.441
7.426
7.412
7.399
7.397
7.385
7.369
7.354
7.315
7.300
2.500

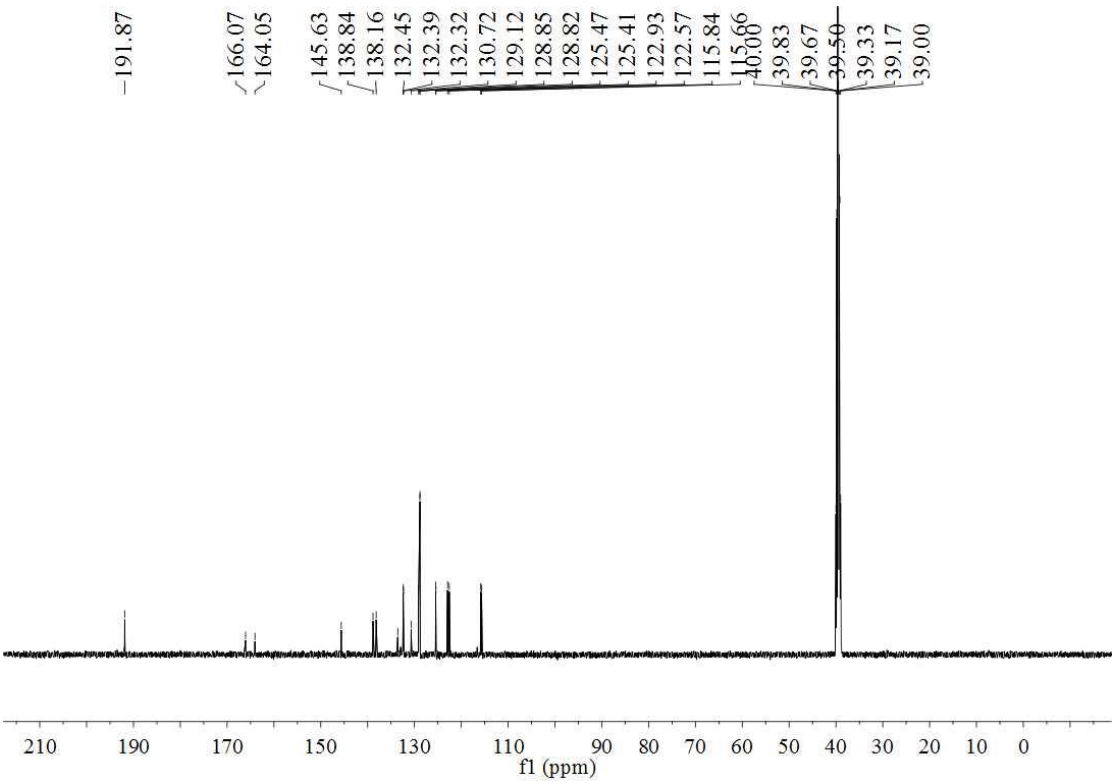

O
Se

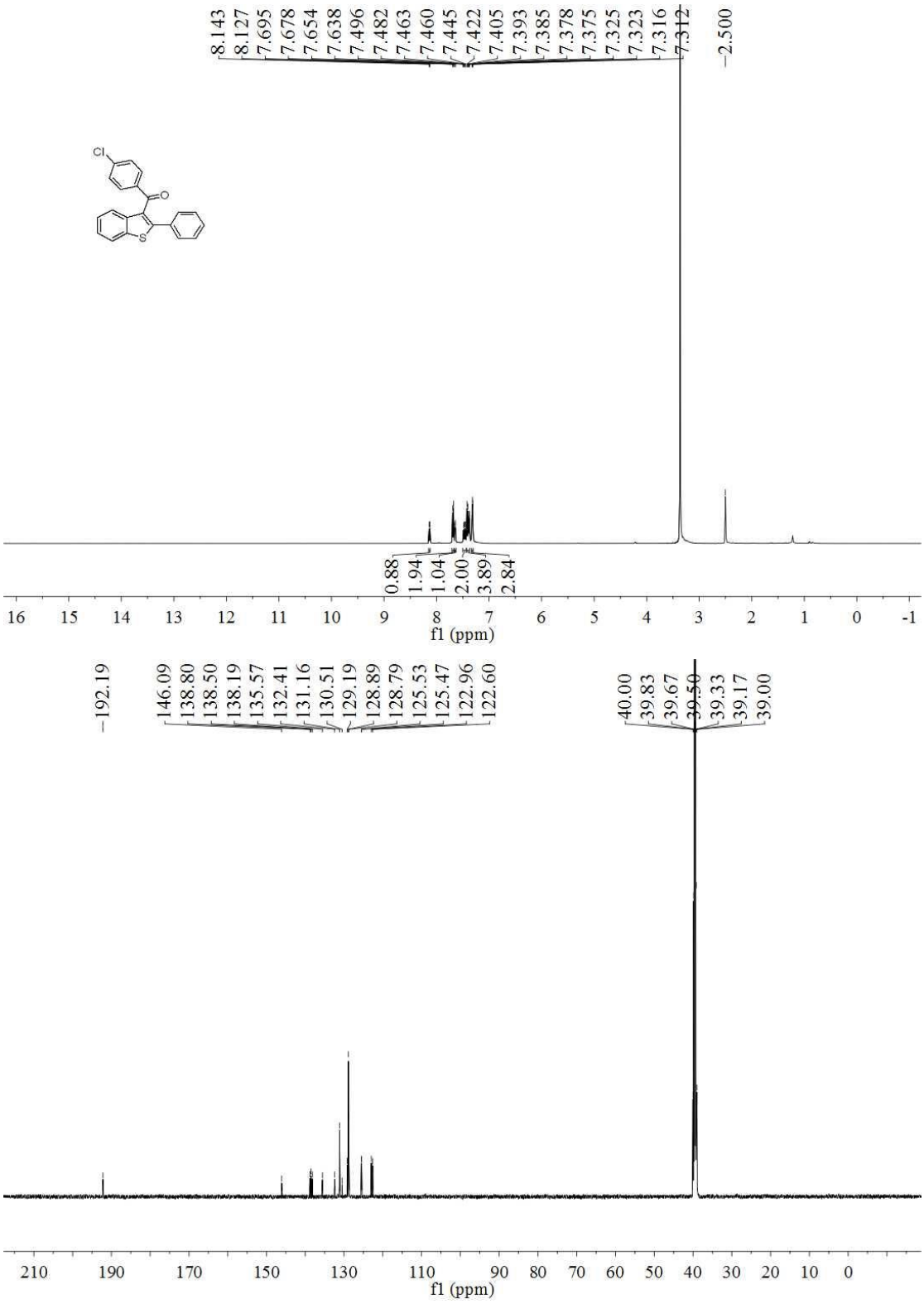

1.00
2.07
1.05
1.11
6.97
2.10
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

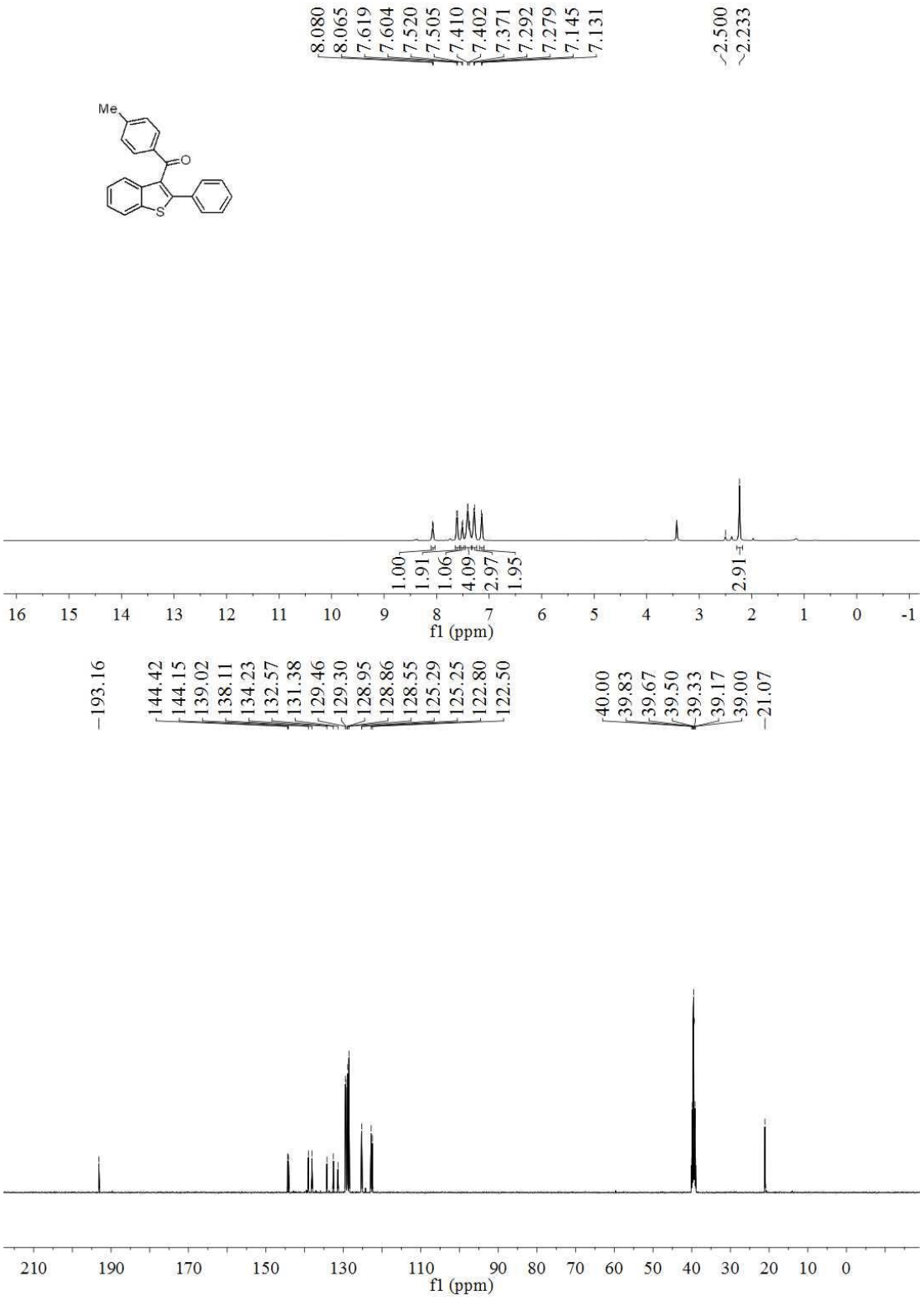

194.89
148.28
141.25
140.40
136.55
134.57
134.44
133.85
129.24
128.86
128.84
128.77
128.60
125.93
125.43
125.33
124.62
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

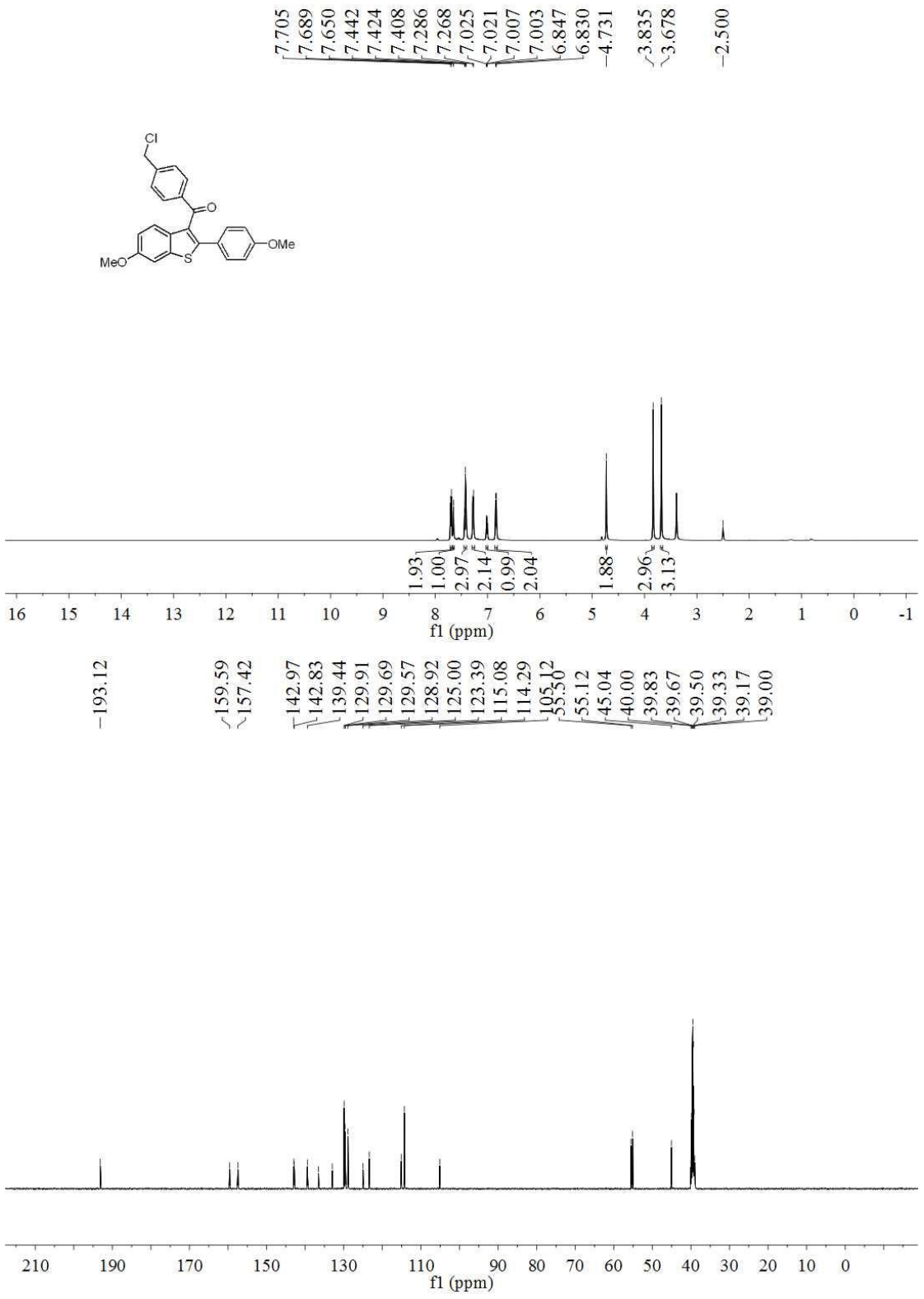

12.217
7.766
7.750
7.532
7.518
7.516
7.393
7.384
7.378
7.366
7.351
7.337
7.261
7.248
7.234
7.216
7.200
7.185
7.173
7.157
7.143
2.500
O
N
H
0.76
0.91
2.85
3.00
7.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
192.06
143.96
139.78
135.78
131.53
131.24
129.45
128.97
128.37
128.13
127.94
127.69
122.77
121.30
120.52
112.13
111.78
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

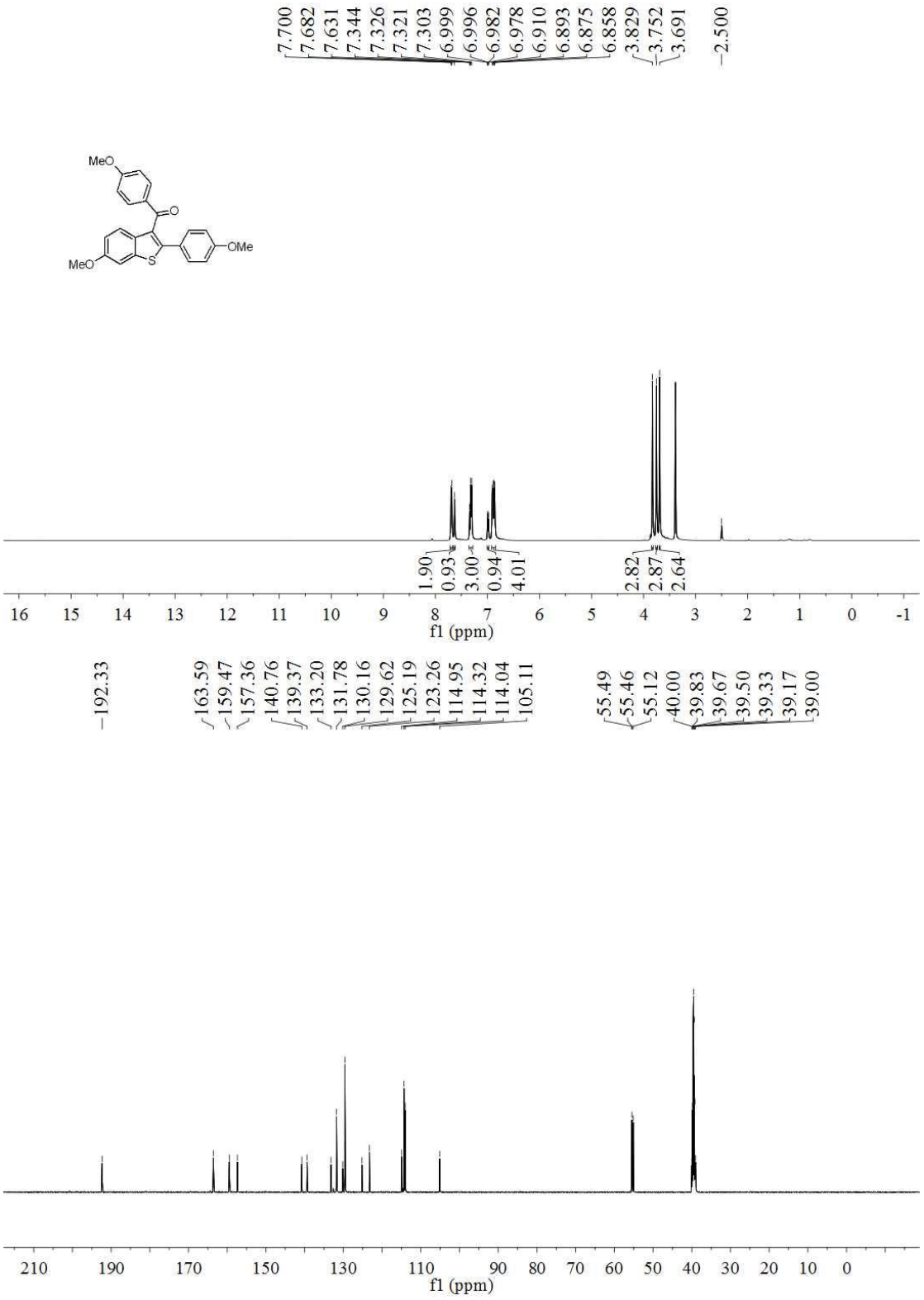

8.142
8.126
7.779
7.768
7.762
7.750
7.639
7.624
7.493
7.480
7.465
7.463
7.458
7.455
7.441
7.427
7.400
7.395
7.385
7.382
7.343
7.334
7.325
7.314
7.311
7.195
7.178
7.160
2.500
F
O
S
0.86
1.90
0.89
2.26
2.00
2.99
2.04
f1 (ppm)

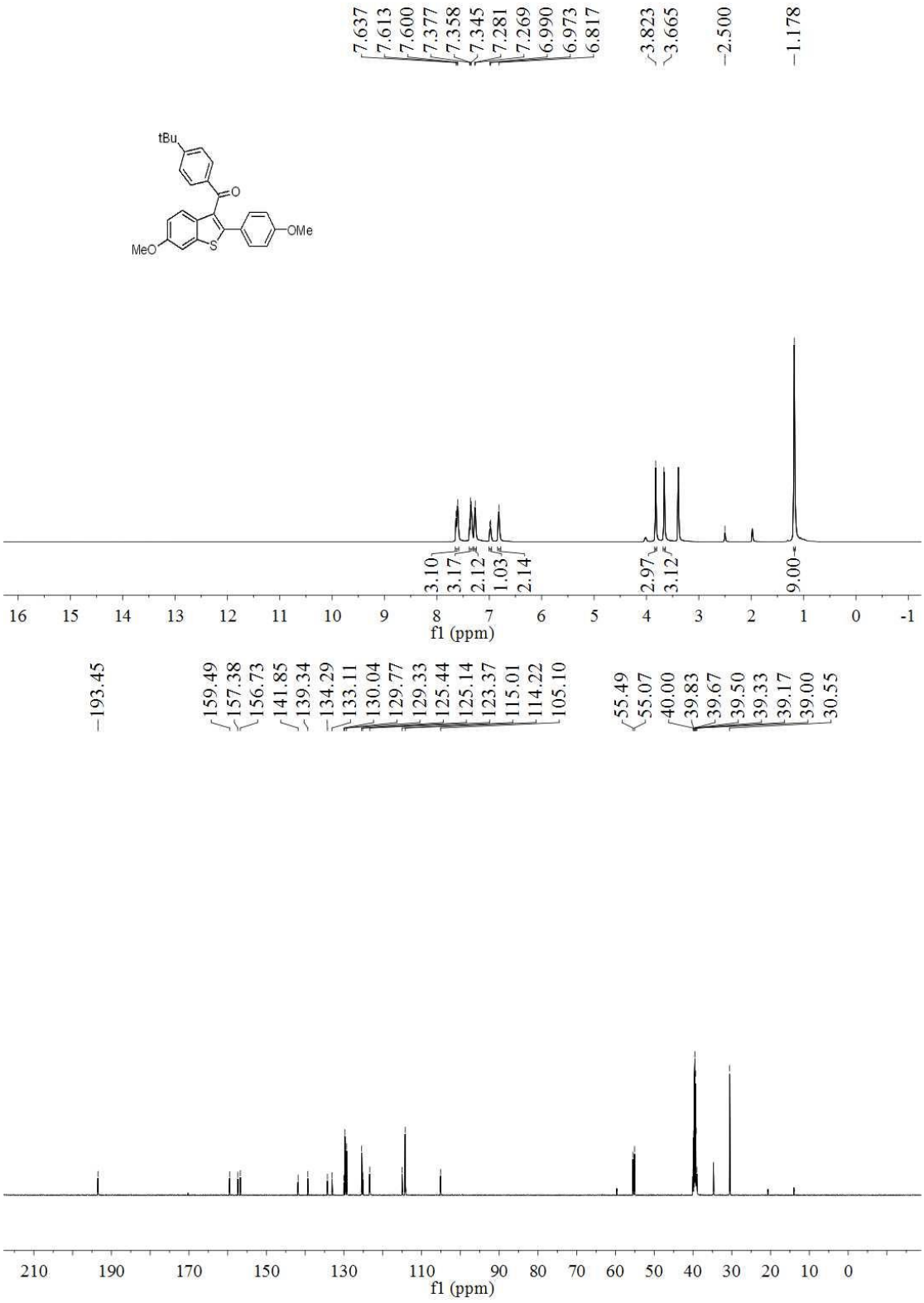

191.87
166.07
164.05
145.63
138.84
138.16
132.45
132.39
132.32
130.72
129.12
128.85
128.82
125.47
125.41
122.93
122.57
115.84
115.66
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

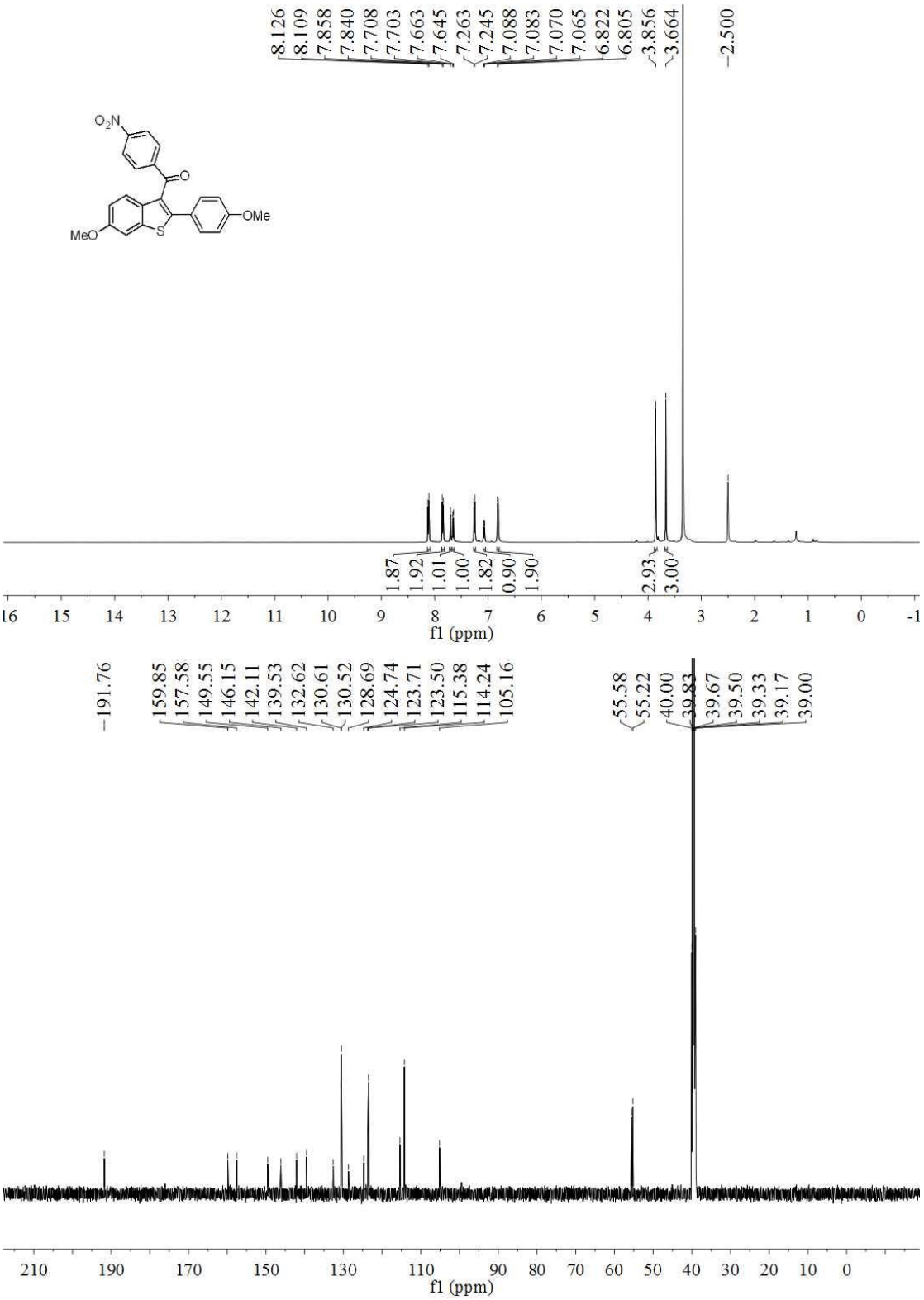

8.143
8.127
7.695
7.678
7.654
7.638
7.496
7.482
7.463
7.460
7.445
7.422
7.405
7.393
7.385
7.378
7.375
7.325
7.323
7.316
7.312
2.500
Cl
O
S
0.88
1.94
1.04
2.00
3.89
2.84
f1 (ppm)
192.19
146.09
138.80
138.50
138.19
135.57
132.41
131.16
130.51
129.19
128.89
128.79
125.53
125.47
122.96
122.60
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

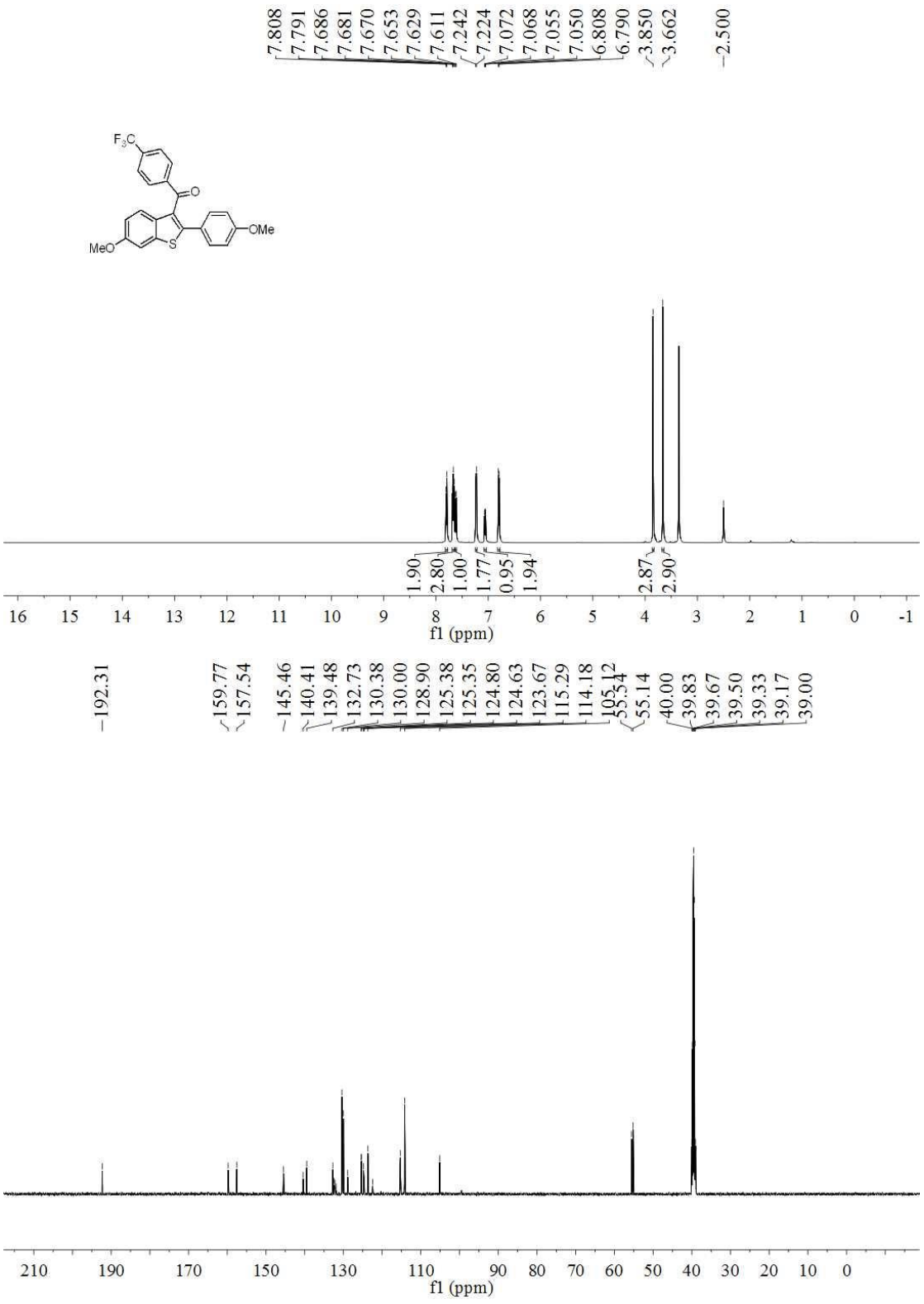

8.080
8.065
7.619
7.604
7.520
7.505
7.410
7.402
7.371
7.292
7.279
7.145
7.131
2.500
2.233
Me
O
S
1.00
1.91
1.06
4.09
2.97
1.95
2.91
f1 (ppm)
193.16
144.42
144.15
139.02
138.11
134.23
132.57
131.38
129.46
129.30
128.95
128.86
128.55
125.29
125.25
122.80
122.50
40.00
39.83
39.67
39.50
39.33
39.17
39.00
21.07
f1 (ppm)

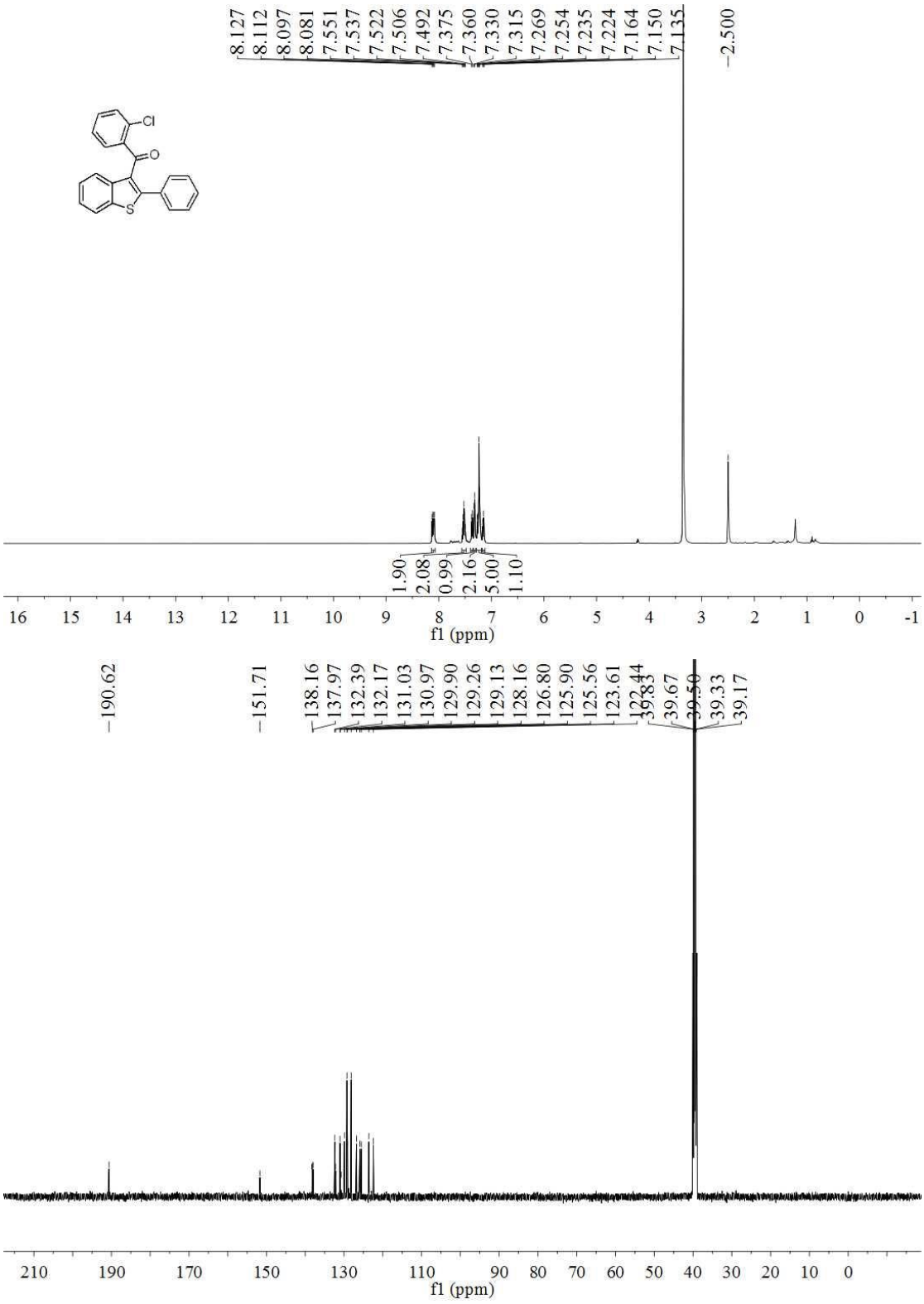

7.705
7.689
7.650
7.442
7.424
7.408
7.286
7.268
7.025
7.021
7.007
7.003
6.847
6.830
4.731
3.835
3.678
2.500
Cl
O
OMe
MeO
S
1.93
1.00
2.97
2.14
0.99
2.04
1.88
2.96
3.13
f1 (ppm)
193.12
159.59
157.42
142.97
142.83
139.44
129.91
129.69
129.57
128.92
125.00
123.39
115.08
114.29
105.12
55.50
55.12
45.04
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

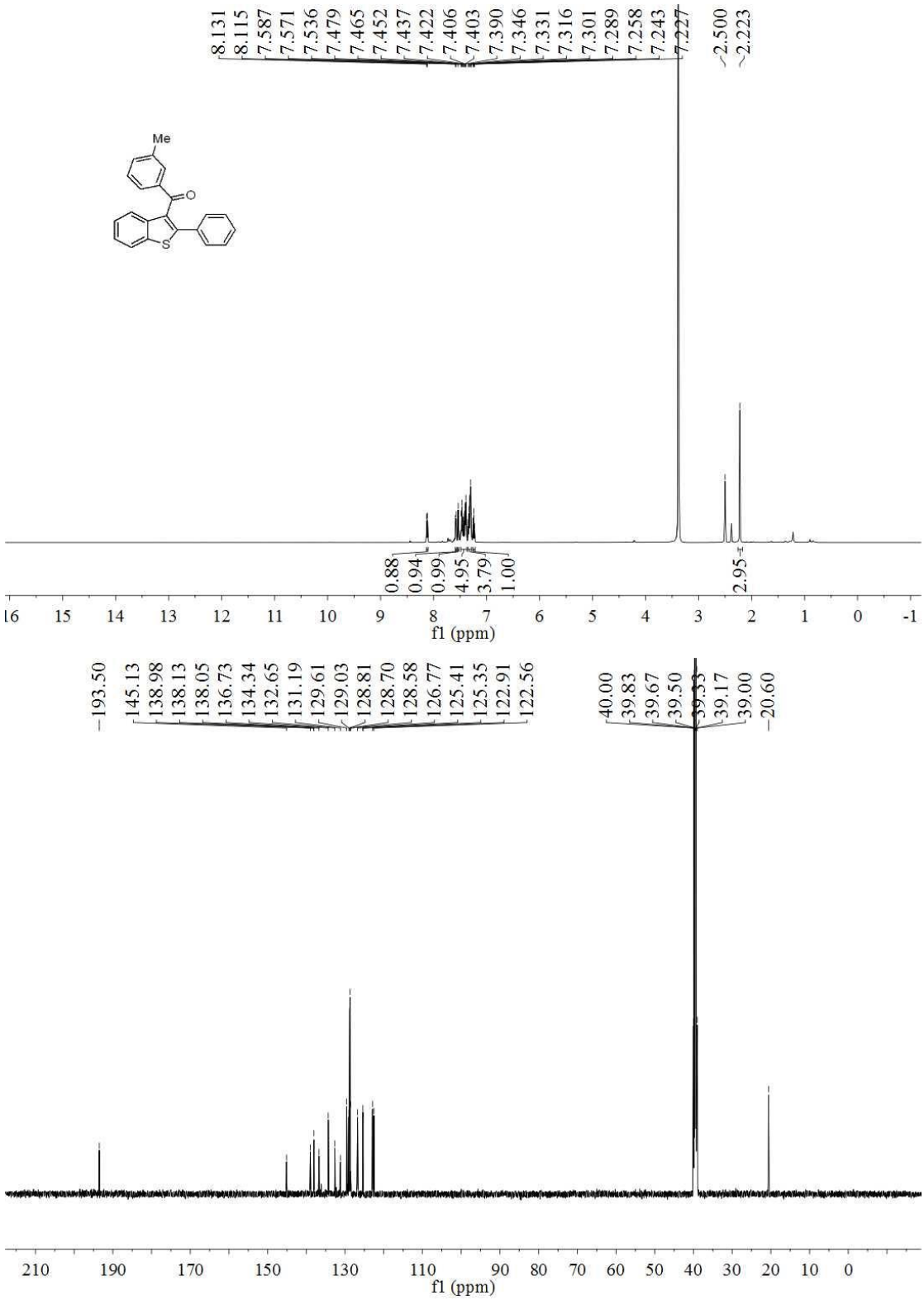

7.700
7.682
7.631
7.344
7.326
7.321
7.303
6.999
6.996
6.982
6.978
6.910
6.893
6.875
6.858
3.829
3.752
3.691
2.500
MeO
O
OMe
MeO
S
1.90
0.93
3.00
0.94
4.01
2.82
2.87
2.64
f1 (ppm)
192.33
163.59
159.47
157.36
140.76
139.37
133.20
131.78
130.16
129.62
125.19
123.26
114.95
114.32
114.04
105.11
55.49
55.46
55.12
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

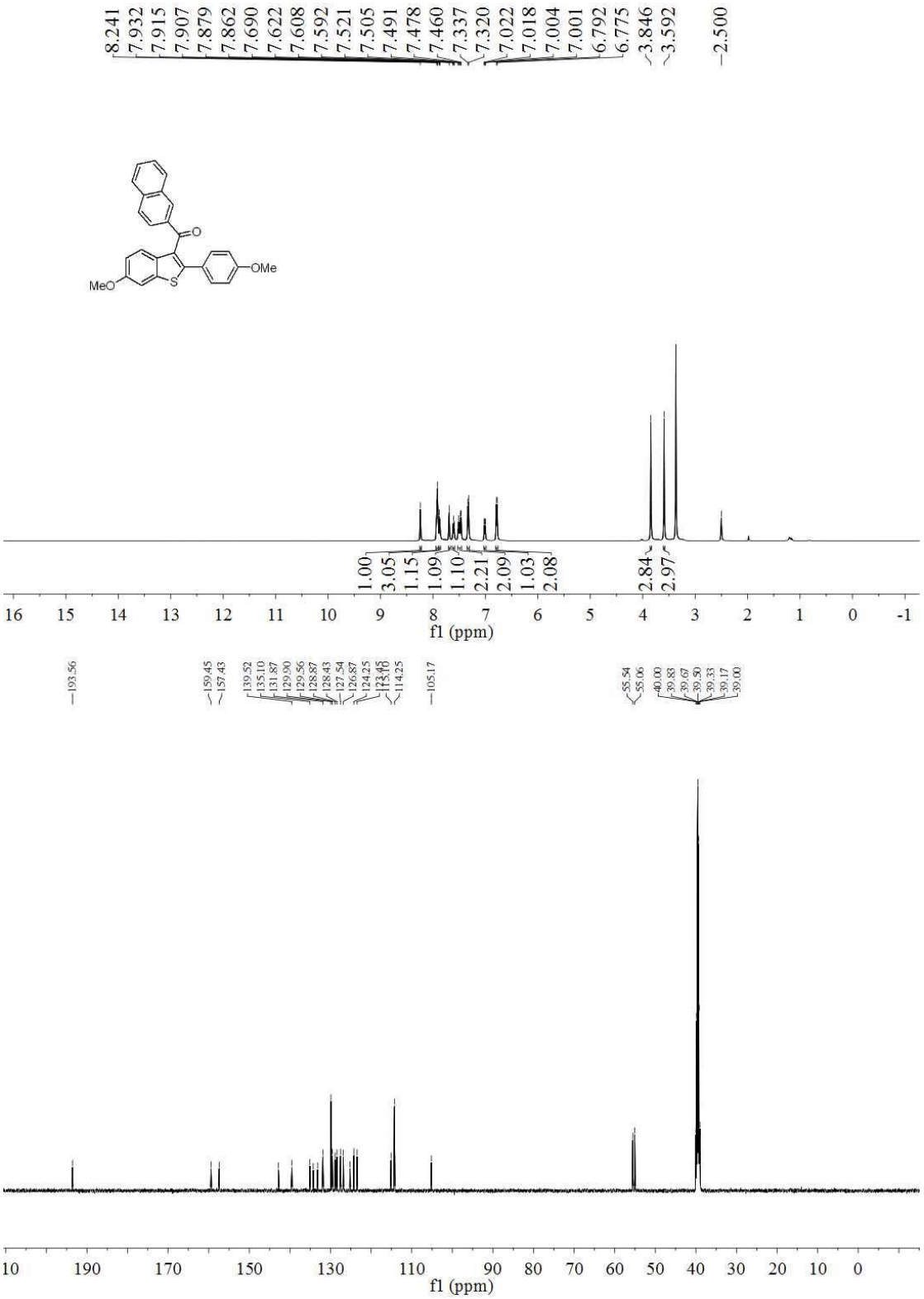

7.637
7.613
7.600
7.377
7.358
7.345
7.281
7.269
6.990
6.973
6.817
3.823
3.665
2.500
1.178
tBu
O
MeO
S
OMe
3.10
3.17
2.12
1.03
2.14
2.97
3.12
9.00
f1 (ppm)
193.45
159.49
157.38
156.73
141.85
139.34
134.29
133.11
130.04
129.77
129.33
125.44
125.14
123.37
115.01
114.22
105.10
55.49
55.07
40.00
39.83
39.67
39.50
39.33
39.17
39.00
30.55
f1 (ppm)


8.126
8.109
7.858
7.840
7.708
7.703
7.663
7.645
7.263
7.245
7.088
7.083
7.070
7.065
6.822
6.805
3.856
3.664
2.500
O2N
O
OMe
MeO
S
1.87
1.92
1.01
1.00
1.82
0.90
1.90
2.93
3.00
f1 (ppm)
191.76
159.85
157.58
149.55
146.15
142.11
139.53
132.62
130.61
130.52
128.69
124.74
123.71
123.50
115.38
114.24
105.16
55.58
55.22
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)


7.808
7.791
7.686
7.681
7.670
7.653
7.629
7.611
7.242
7.224
7.072
7.068
7.055
7.050
6.808
6.790
3.850
3.662
2.500
F3C
O
MeO
S
OMe
1.90
2.80
1.00
1.77
0.95
1.94
2.87
2.90
f1 (ppm)
192.31
159.77
157.54
145.46
140.41
139.48
132.73
130.38
130.00
128.90
125.38
125.35
124.80
124.63
123.67
115.29
114.18
105.12
55.54
55.14
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)


8.127
8.112
8.097
8.081
7.551
7.537
7.522
7.506
7.492
7.375
7.360
7.330
7.315
7.269
7.254
7.235
7.224
7.164
7.150
7.135
2.500
Cl
O
S
1.90
2.08
0.99
2.16
5.00
1.10
f1 (ppm)
190.62
151.71
138.16
137.97
132.39
132.17
131.03
130.97
129.90
129.26
129.13
128.16
126.80
125.90
125.56
123.61
122.44
39.83
39.67
39.50
39.33
39.17
f1 (ppm)


8.131
8.115
7.587
7.571
7.536
7.479
7.465
7.452
7.437
7.422
7.406
7.403
7.390
7.346
7.331
7.316
7.301
7.289
7.258
7.243
7.227
2.500
2.223
Me
O
S
0.88
0.94
0.99
4.95
3.79
1.00
2.95
f1 (ppm)
193.50
145.13
138.98
138.13
138.05
136.73
134.34
132.65
131.19
129.61
129.03
128.81
128.70
128.58
126.77
125.41
125.35
122.91
122.56
40.00
39.83
39.67
39.50
39.33
39.17
39.00
20.60
f1 (ppm)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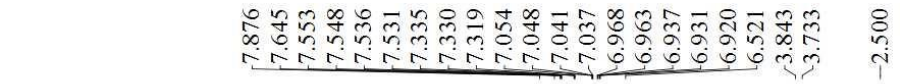
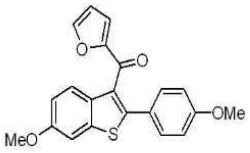
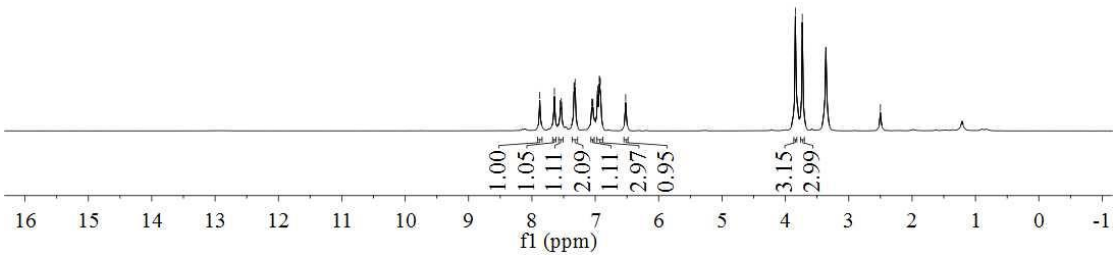
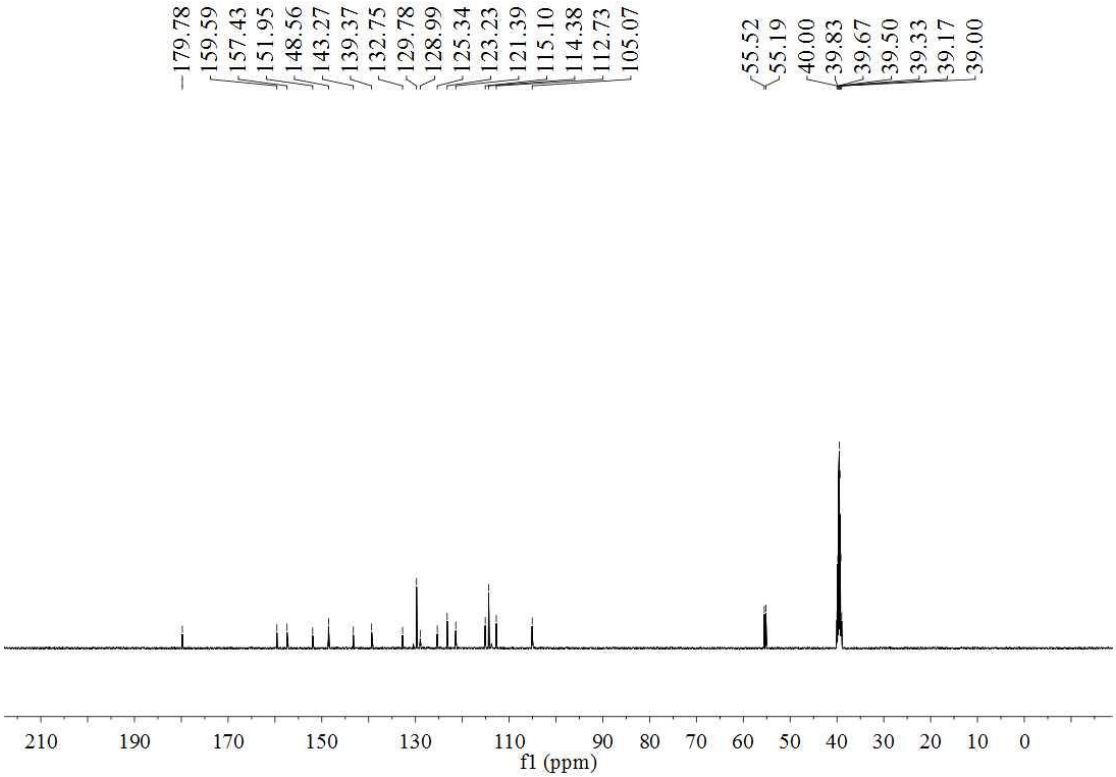
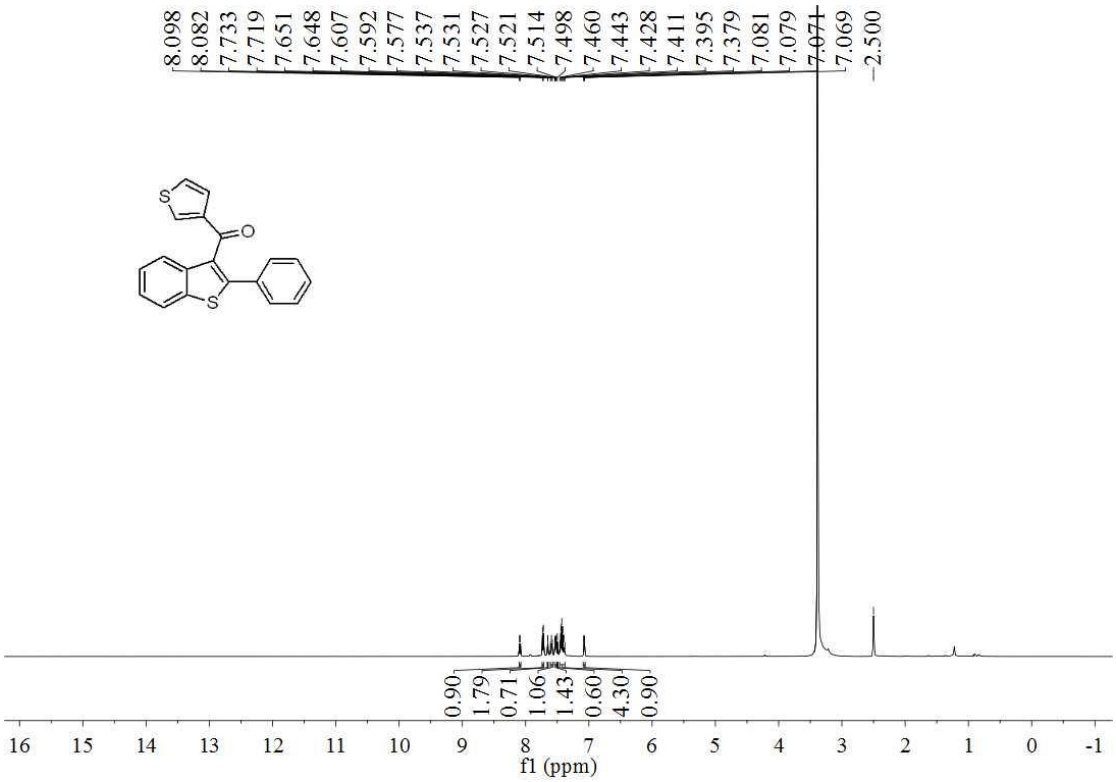
7.932
7.915
7.907
7.879
7.862
7.690
7.622
7.608
7.592
7.521
7.505
7.491
7.478
7.460
7.337
7.320
7.022
7.018
7.004
7.001
6.792
6.775
3.846
3.592
2.500
O
OMe
MeO
S
1.00
3.05
1.15
1.09
1.10
2.21
2.09
1.03
2.08
2.84
2.97
f1 (ppm)
193.56
159.45
157.43
139.52
135.10
131.87
129.90
129.56
128.87
128.43
127.54
126.87
124.25
123.45
123.10
114.25
105.17
55.54
55.06
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

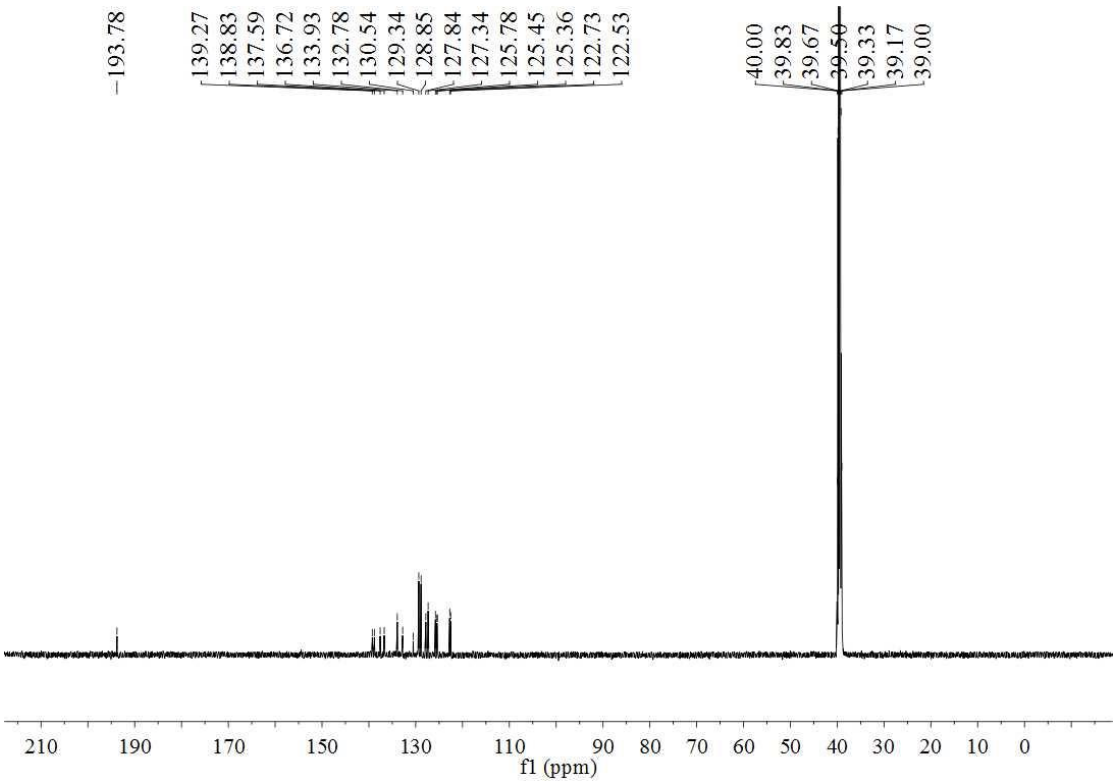

7.876
7.645
7.553
7.548
7.536
7.531
7.335
7.330
7.319
7.054
7.048
7.041
7.037
6.968
6.963
6.937
6.931
6.920
6.521
3.843
3.733
2.500

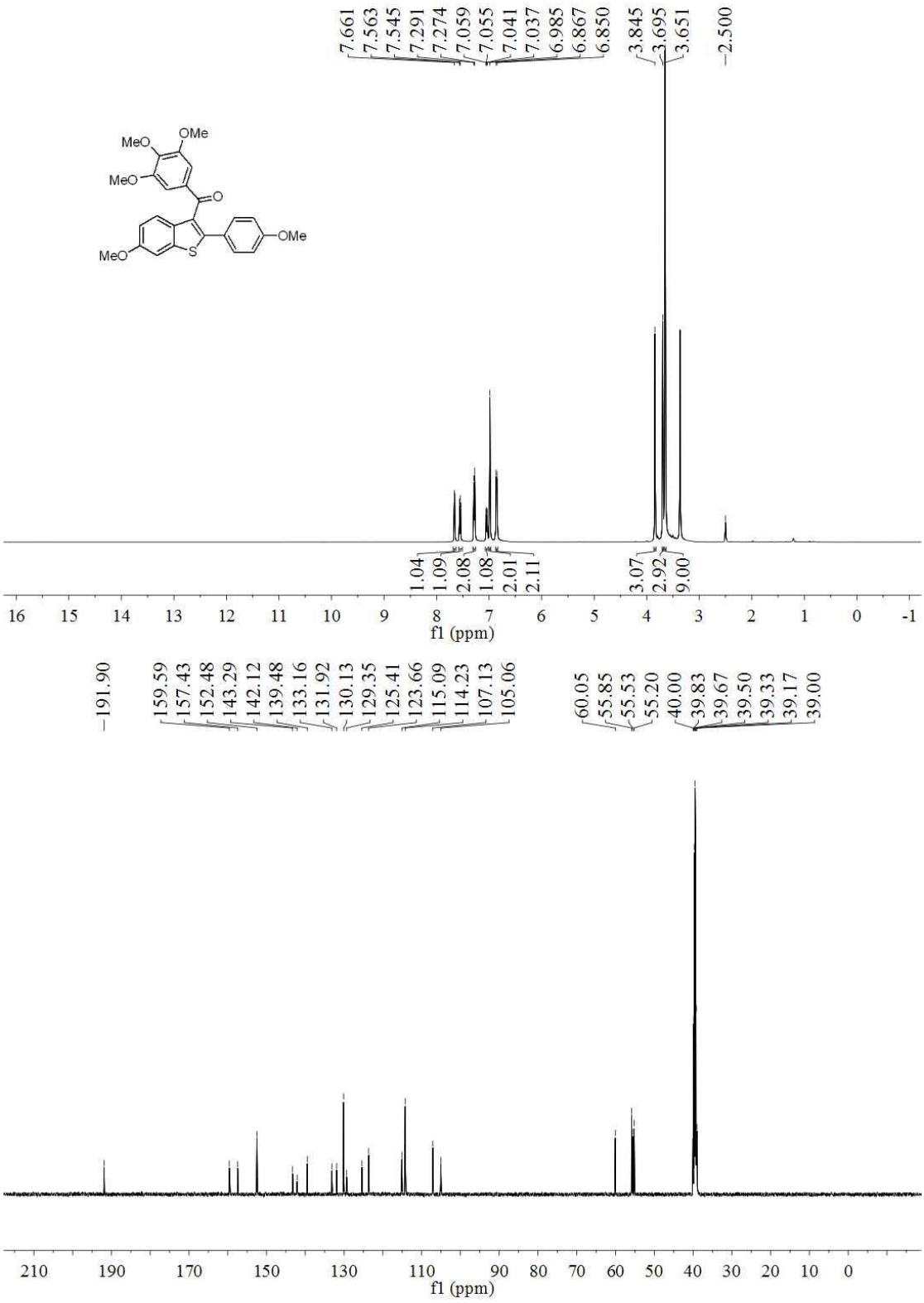

O
O
OMe
MeO
S

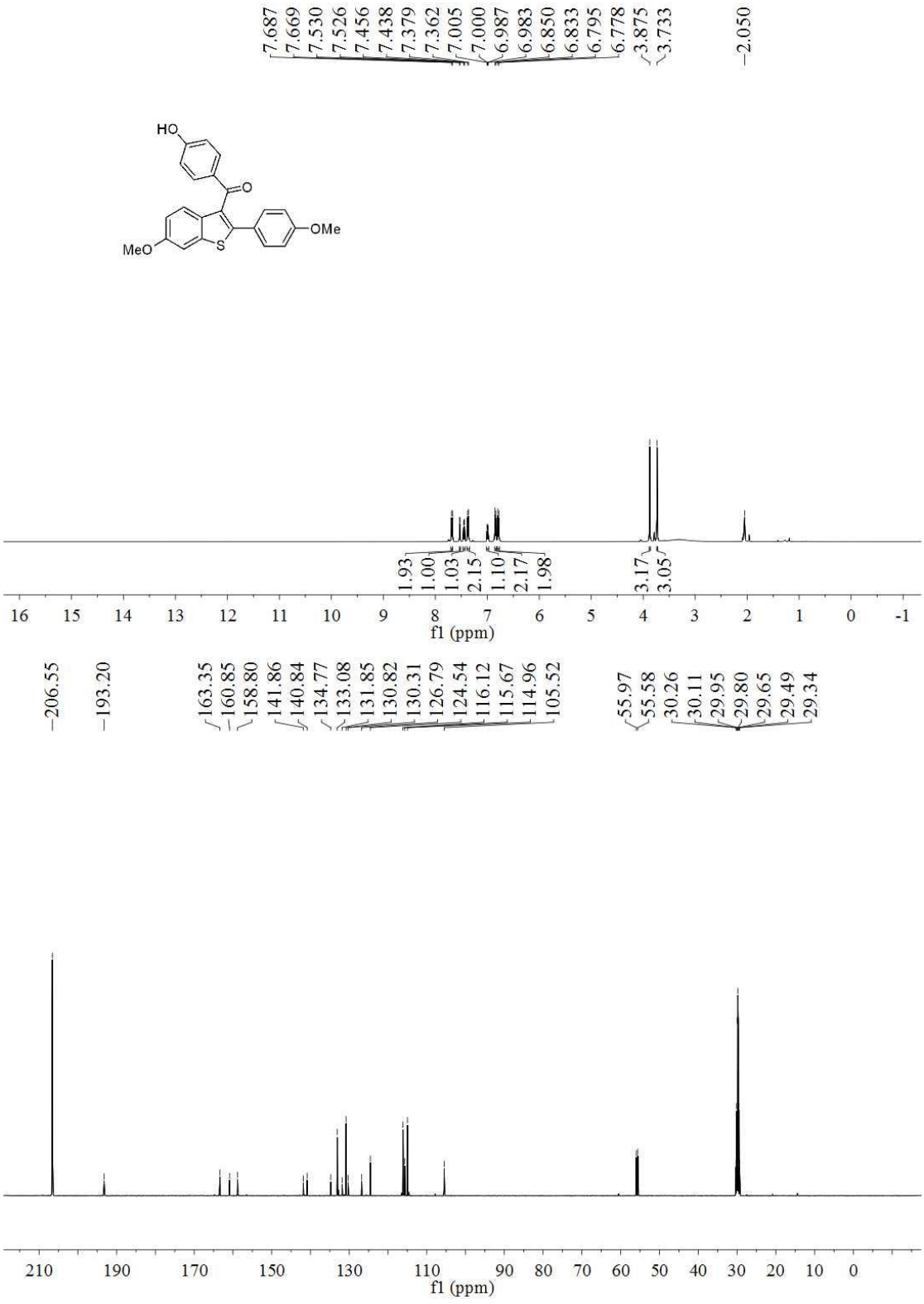

1.00
1.05
1.11
2.09
1.11
2.97
0.95
3.15
2.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

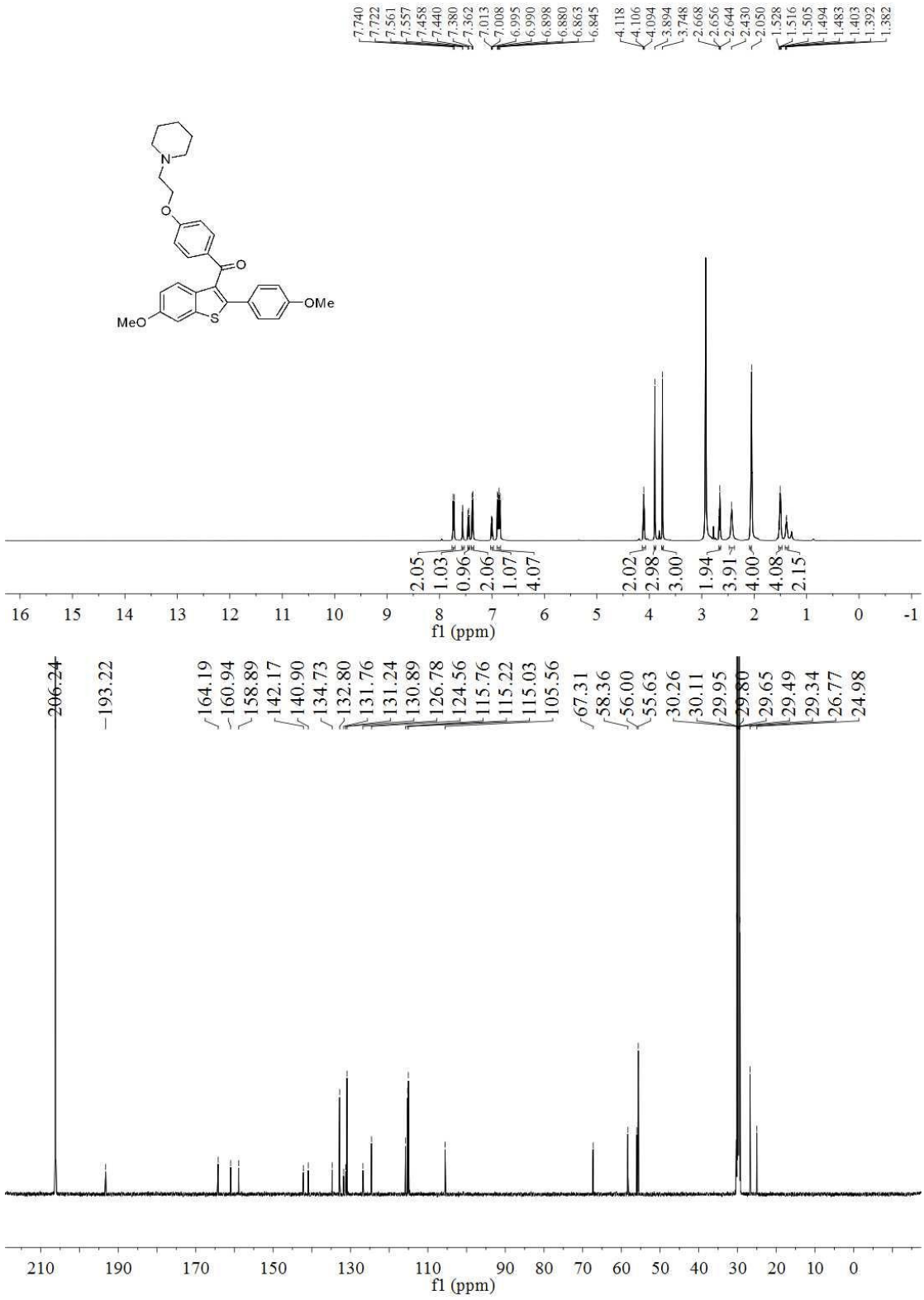

179.78
159.59
157.43
151.95
148.56
143.27
139.37
132.75
129.78
128.99
125.34
123.23
121.39
115.10
114.38
112.73
105.07
55.52
55.19
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

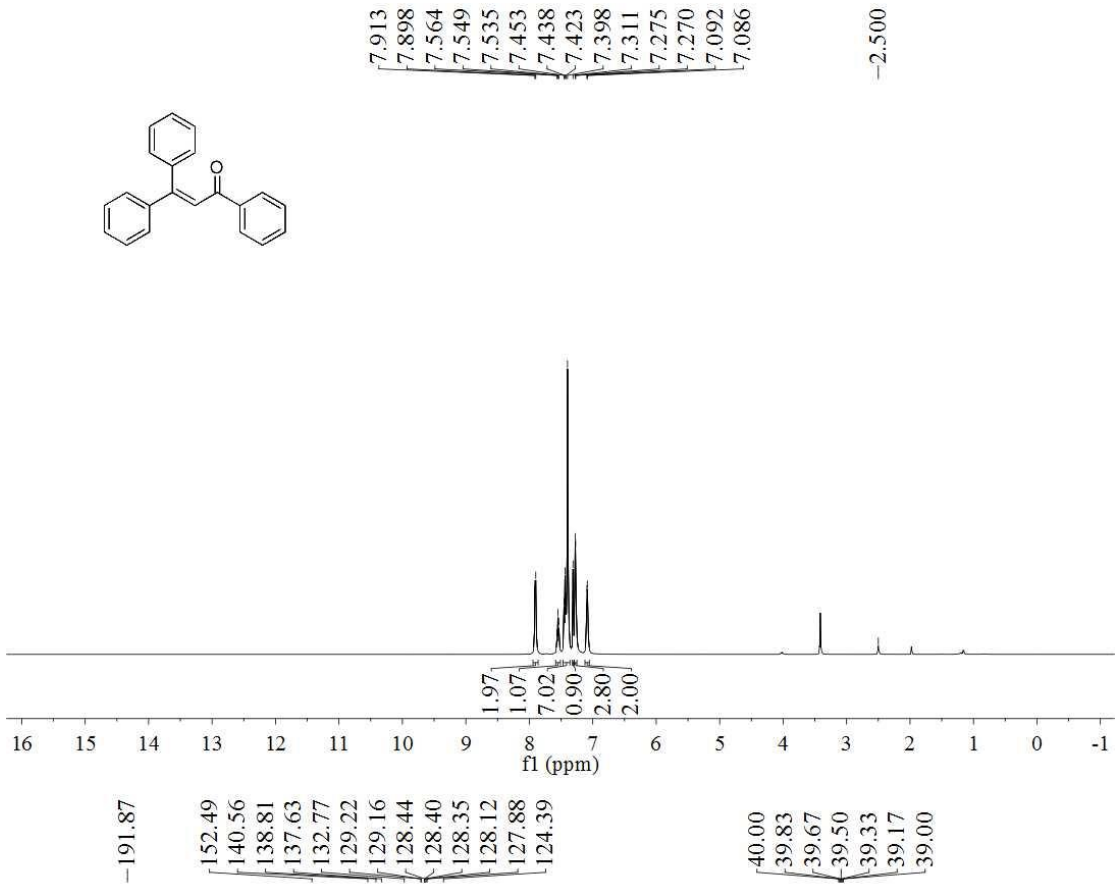

8.098
8.082
7.733
7.719
7.651
7.648
7.607
7.592
7.577
7.537
7.531
7.527
7.521
7.514
7.498
7.460
7.443
7.428
7.411
7.395
7.379
7.081
7.079
7.071
7.069
2.500
O
S
S
0.90
1.79
0.71
1.06
1.43
0.60
4.30
0.90
f1 (ppm)

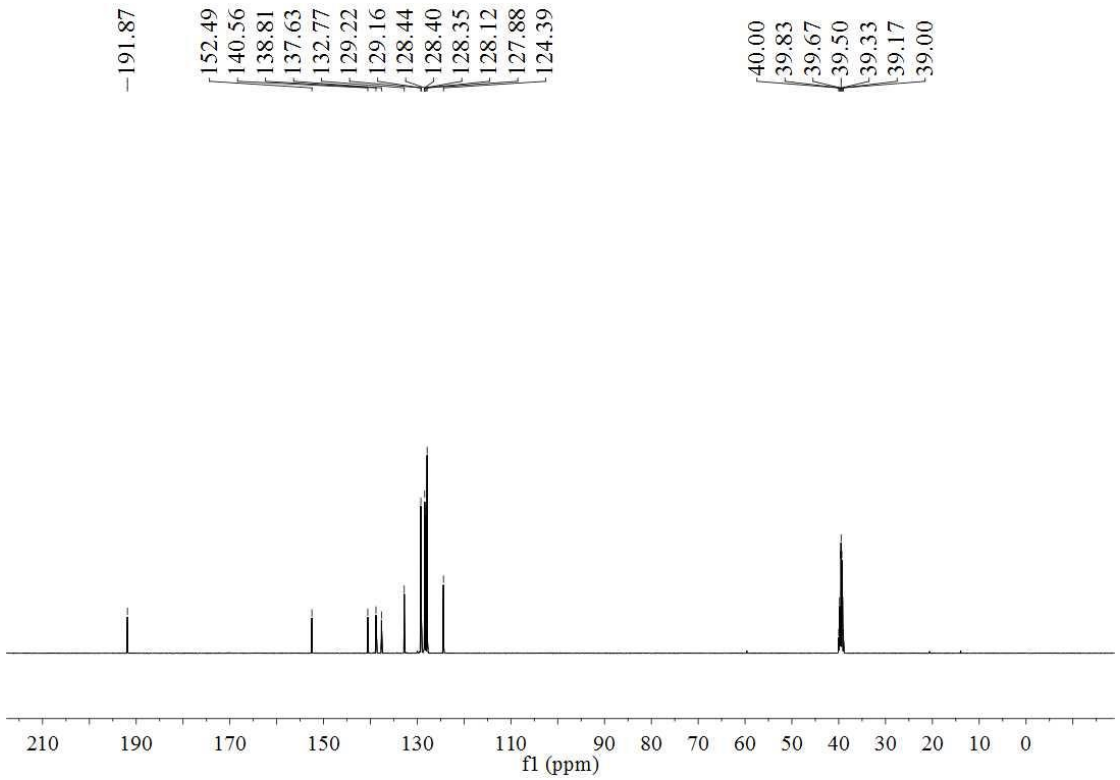

193.78
139.27
138.83
137.59
136.72
133.93
132.78
130.54
129.34
128.85
127.84
127.34
125.78
125.45
125.36
122.73
122.53
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)

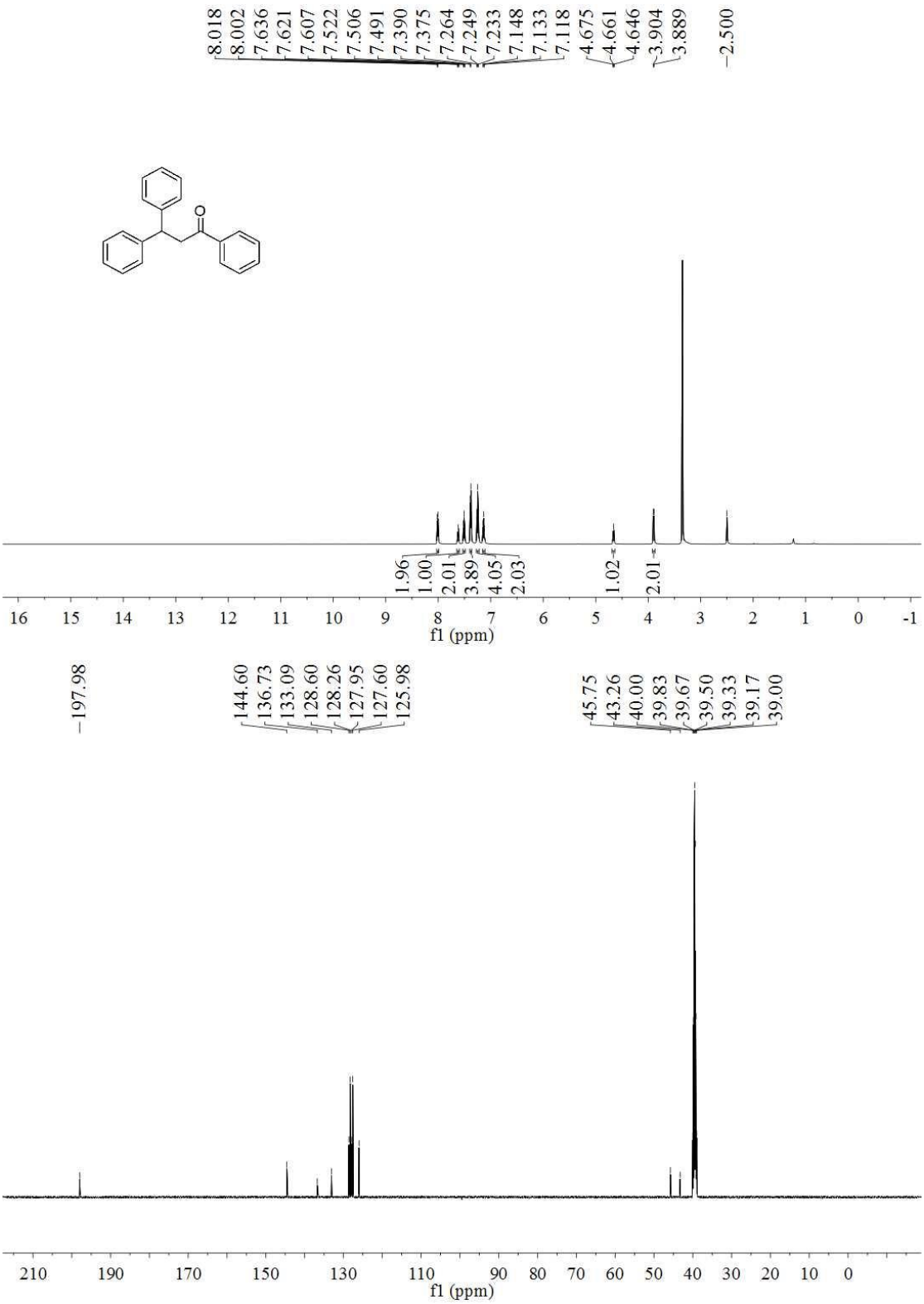

7.661
7.563
7.545
7.291
7.274
7.059
7.055
7.041
7.037
6.985
6.867
6.850
3.845
3.695
3.651
2.500
MeO
OMe
MeO
O
OMe
MeO
S
1.04
1.09
2.08
1.08
2.01
2.11
3.07
2.92
9.00
f1 (ppm)
191.90
159.59
157.43
152.48
143.29
142.12
139.48
133.16
131.92
130.13
129.35
125.41
123.66
115.09
114.23
107.13
105.06
60.05
55.85
55.53
55.20
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)


7.687
7.669
7.530
7.526
7.456
7.438
7.379
7.362
7.005
7.000
6.987
6.983
6.850
6.833
6.795
6.778
3.875
3.733
2.050
HO
O
OMe
MeO
S
1.93
1.00
1.03
2.15
1.10
2.17
1.98
3.17
3.05
f1 (ppm)
206.55
193.20
163.35
160.85
158.80
141.86
140.84
134.77
133.08
131.85
130.82
130.31
126.79
124.54
116.12
115.67
114.96
105.52
55.97
55.58
30.26
30.11
29.95
29.80
29.65
29.49
29.34
f1 (ppm)


7.740
7.722
7.561
7.557
7.458
7.440
7.380
7.362
7.013
7.008
6.995
6.990
6.898
6.880
6.863
6.845
4.118
4.106
4.094
3.894
3.748
2.668
2.656
2.644
2.430
2.050
1.528
1.516
1.505
1.494
1.483
1.403
1.392
1.382
O
N
O
O
S
MeO
OMe
2.05
1.03
0.96
2.06
1.07
4.07
2.02
2.98
3.00
1.94
3.91
4.00
4.08
2.15
f1 (ppm)
206.24
193.22
164.19
160.94
158.89
142.17
140.90
134.73
132.80
131.76
131.24
130.89
126.78
124.56
115.76
115.22
115.03
105.56
67.31
58.36
56.00
55.63
30.26
30.11
29.95
29.80
29.65
29.49
29.34
26.77
24.98
f1 (ppm)


7.913
7.898
7.564
7.549
7.535
7.453
7.438
7.423
7.398
7.311
7.275
7.270
7.092
7.086
2.500
1.97
1.07
7.02
0.90
2.80
2.00
f1 (ppm)


191.87
152.49
140.56
138.81
137.63
132.77
129.22
129.16
128.44
128.40
128.35
128.12
127.88
124.39
40.00
39.83
39.67
39.50
39.33
39.17
39.00
f1 (ppm)


8.018
8.002
7.636
7.621
7.607
7.522
7.506
7.491
7.390
7.375
7.264
7.249
7.233
7.148
7.133
7.118
4.675
4.661
4.646
3.904
3.889
2.500
O
1.96
1.00
2.01
3.89
4.05
2.03
1.02
2.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
197.98
144.60
136.73
133.09
128.60
128.26
127.95
127.60
125.98
45.75
43.26
40.00
39.83
39.67
39.50
39.33
39.17
39.00
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)