Electronic Supplementary Material (ESI) for Green Chemistry.
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Supplementary Information

I. Experimental

Materials

Commercially available chemicals were purchased from commercial suppliers and used as received without further purification, unless otherwise noted. Guaiacol (99%), *p*-cresol (99%), 4'-hydroxyacetophenone (99%), 4-hydroxybiphenyl (99%), 1-naphthol (99%), 4-nitrophenol (99%), 4-(trifluoromethyl)phenol (98%), catechol (99%), isoeugenol (97%), diethylaminosulfur trifluoride (DAST, 95%), 1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate) (Selectfluor, 96%), acetonitrile-d_3, (99.8 atom% D), chloroform-d, (99.8 atom% D), 4-dimethylaminopyridine (DMAP, 99%) were purchased from J&K Scientific Ltd. Phenol (99%), 4-hydroxybenzonitrile (99%), 4-fluorophenol (99%), 4-ethylphenol (99%), 3',5'-dimethoxy-4'-hydroxyacetophenone and anhydrous potassium fluoride (99%) were obtained from Acros. Acetovanillone (98.5%) was provided by Amethyst. Benzoyl fluoride (98%) was obtained from TCI Shanghai Co., Ltd. Anhydrous copper fluoride (99.5%) and cerium fluoride (99.9%) were supplied by Alfa Aesar. Organic salts including sodium acetate (99%), sodium propionate (99%), sodium butyrate (99%) and sodium benzoate (99%) were purchased from Acros. Sodium acrylate (99%) was purchased from Beijing InnoChem Science & Technology Co., Ltd. Solvents including acetonitrile (A. R. grade), diethyl ether (A. R. grade), dichloromethane (A. R. grade), 1, 4-dioxane (A. R. grade), ethyl acetate (A. R. grade) and inorganic bases including potassium carbonate (99%) and sodium carbonate (99%) were supplied by Sinopharm Chemical Reagent Co., Ltd, China.

General reaction procedure

In an oven-dried round bottom flask equipped with a magnetic stirrer, acylating reagent sodium organic salt (1.1 mmol, 1.1 equiv.), DMAP (12.2 mg, 0.1 mmol, 0.1 equiv.) and the solvent acetonitrile (2 mL) were added under open air. Then, phenolic substrate (1.0 mmol, 1.0 equiv.) was added, followed by dropwise addition of DAST (1.1 mmol, 1.0 equiv.). The mixture was stirred at room temperature for desired time with a stirring speed of 600 r.p.m, and the reactions were monitored by TLC. After reaction, distilled water (3 mL) and diethyl ether (5 mL) was added. The organic matter was further extracted twice using diethyl ether, combined, washed with brine (5 mL) and condensed under reduced pressure (rotary evaporator) for qualitative and quantitative analysis. Control experiments were conducted in a similar manner under given conditions.

Characterization methods

The quantitative analysis of prodcuts was conducted using a gas chromatograph (GC, Agilent 7890B) equipped with a flame ionization detector (FID) and a HP-5 capillary column (0.32 mm in diameter, 30 m in length). Qualitative analysis of products was conducted using GC-MS (SHIMADZU GC-MS-QP2010) with HP-5MS capillary column (0.25mm in diameter, 30m in length) and by comparing the retention time with respective authentic standards in GC traces. The conversion and yields of reactions were calculated from the GC data using internal standard curves and integrated peak area.

In-situ NMR spectra of reaction mixtures were recorded on Bruker Avance Neo 700 MHz system equipped with a 5 mm BBO CryoProbe at 25˚C. A standard alignment operations: lock, tune, shim, loopadj, autogain and acquisition were performed for each sample. For all 1D spectra, a standard exponential multiplication was applied to the fid and then a Fourier transform was performed. All ^{1}H-^{13}C HSQC (Heteronuclear Single Quantum Coherence) experiments were performed using 2D $^{1}H/^{13}C$ correlation via double inept transfer with phase sensitive using Echo/Antiecho-TPPI gradient selection, using shaped pulses for all 180 degree pulses on ^{13}C and with decoupling during acquisition (pulse sequence: hsqcetgpsisp2.2). All ^{1}H-^{13}C HMBC (Heteronuclear Multiple Bond Correlation) experiments were performed using 2D $^{1}H/^{13}C$ correlation via heteronuclear zero and double quantum coherence, optimized on long range couplings with low-pass J-filter to suppress one-bond correlations (pulse sequence: hmbcgplpndqf). All DOSY (Diffusion-Ordered spectroscopy) experiments were performed using bipolar gradient pulses for diffusion with longitudinal eddy current delay (pulse sequence: ledbpgp2s).

Other liquid-state ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 400 HD NMR spectrometer equipped with 5 mm pulsed-field-gradient (PFG) probes. Characteristic resonance bands of deuterated solvents were used as internal reference. Spectra were all recorded at 25 ^{o}C.

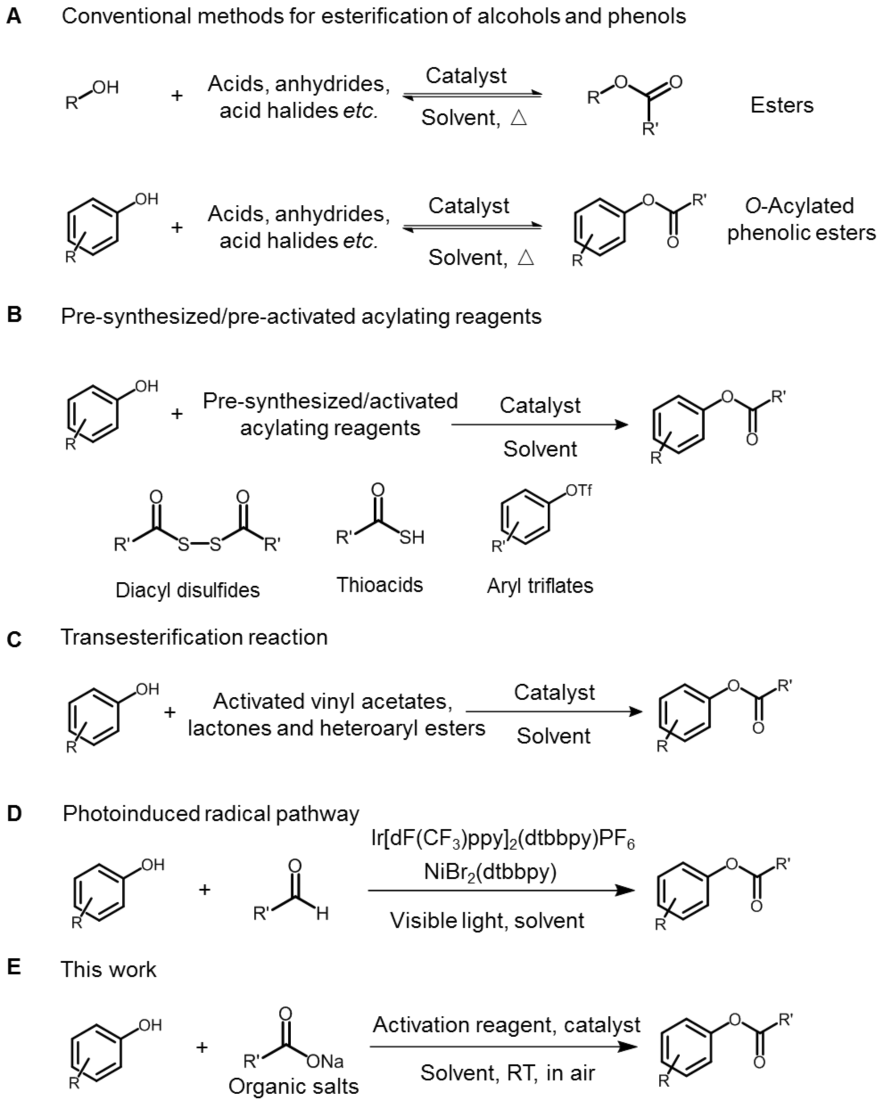
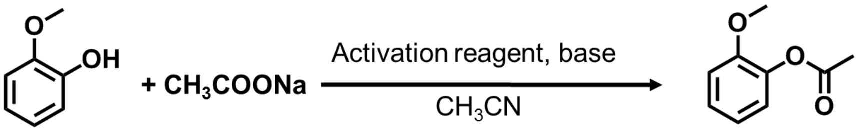


Fig. S1 Synthesis strategies for phenolic esters

Table S1. Additional reaction results for the esterification of guaiacol with sodium acetate



Entry	Activation reagent	Base	Solvent	Atmosphere	Yield (%)
1	KF	DMAP	Acetonitrile	Air	0
2	CsF_2	DMAP	Acetonitrile	Air	0
3	CuF_2	DMAP	Acetonitrile	Air	0
4	KF	DMAP	Acetonitrile	Argon	0
5	CsF_2	DMAP	Acetonitrile	Argon	0
6	CuF_2	DMAP	Acetonitrile	Argon	0

Reactions are performed at 1.0 mmol scale. Guaiacol 1mmol, sodium acetate 1.1 mmol, DMAP 0.1 mmol, activation reagent 1.1 mmol, 100 ^{o}C, 6 h.

Fig. S2 Chemical structures of **A** Selectfluor (1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate)) and **B** DAST (diethylaminosulfur trifluoride), both of them are industrially widely used reagents.

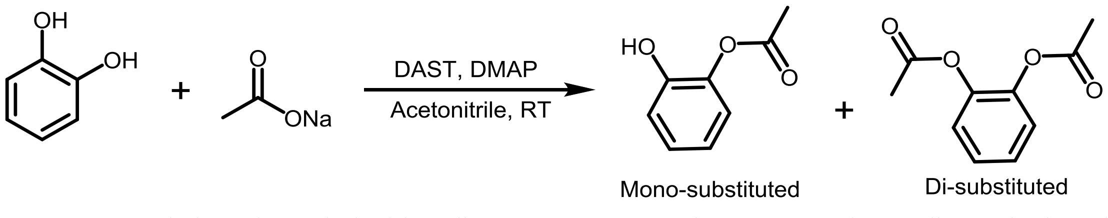


Fig. S3 *O*-Acylation of catechol with sodium acetate. Due to the presence of two adjacent hydroxyl groups in catechol, sodium acetate (2.1 mmol, 2.1 equiv.) was used. Under standard condition with 2.1 mmol sodium acetate, both mono- and di-substituted products were obtained with yields about 36% and 32%, respectively. By further increasing the amount of catalyst to 0.3 equiv. and reaction time to 24 h, the di-substituted product (1,2-diacetoxybenzene) was generated with yield of 96%.

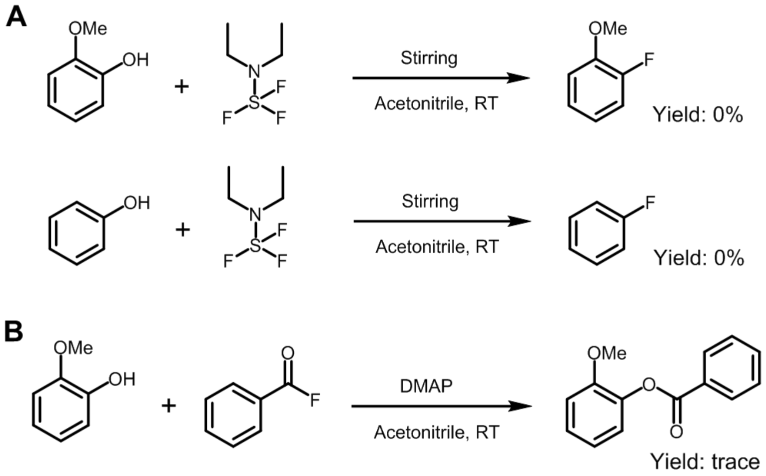


Fig. S4 Control experiments: (A) reaction between phenolic substrates and DAST. Reaction condition: guaiacol or phenol 1.0 mmol, DAST 1.1 mmol, acetonitrile 2 mL, RT, in air, 6 h. The reaction did not produce any deoxyfluorinated products such as 2-fluoroanisole and fluorobenzene, indicating that DAST cannot act as a fluorination reagent for phenolic compounds. (B) reaction between guaiacol and benzoyl fluoride with catalytic amount of DMAP. Reaction condition: guaiacol 1.0 mmol, benzoyl fluoride 1.1 mmol, DMAP 0.1 mmol, acetonitrile, 2 mL, RT, in air, 6 h. This reaction only produced trace amount of guaiacol benzoate, indicating the DAST-activation of phenolic substrate is of crucial importance for the selective acylation reaction to take place.

II. Study about the interaction between DAST and phenolic substrate

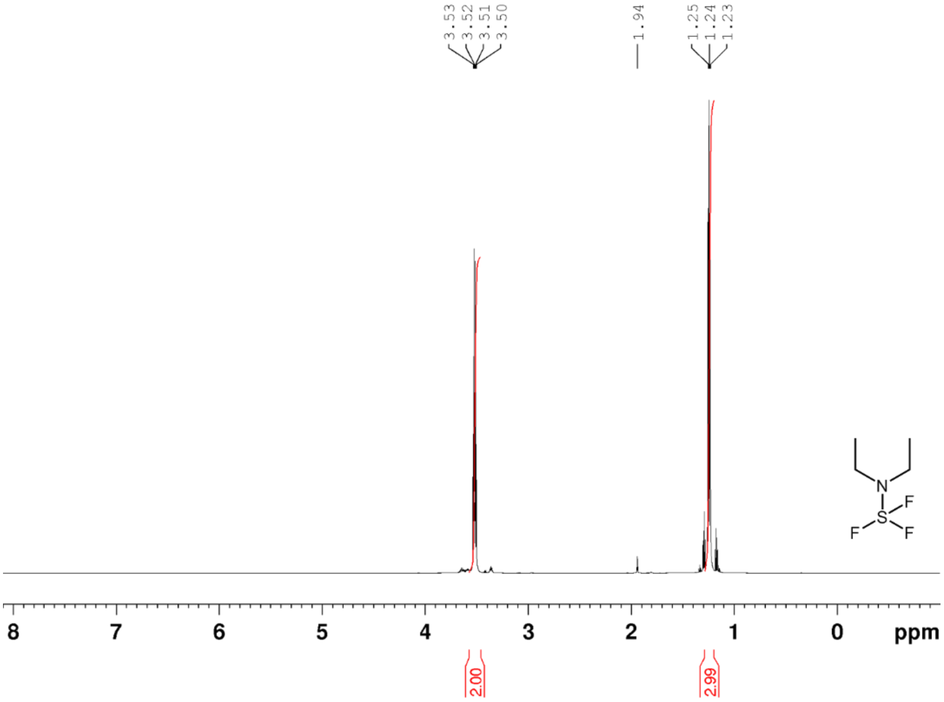


Fig. S5 ^{1}H NMR spectrum of DAST in acetonitrile-d_3. The spectrum used the resonance of acetonitrile-d_3 (δ_H, 1.94 ppm) as internal reference. The resonance bands of CH_3 and CH_2 are assigned to about 1.24 ppm and 3.52 ppm, respectively.

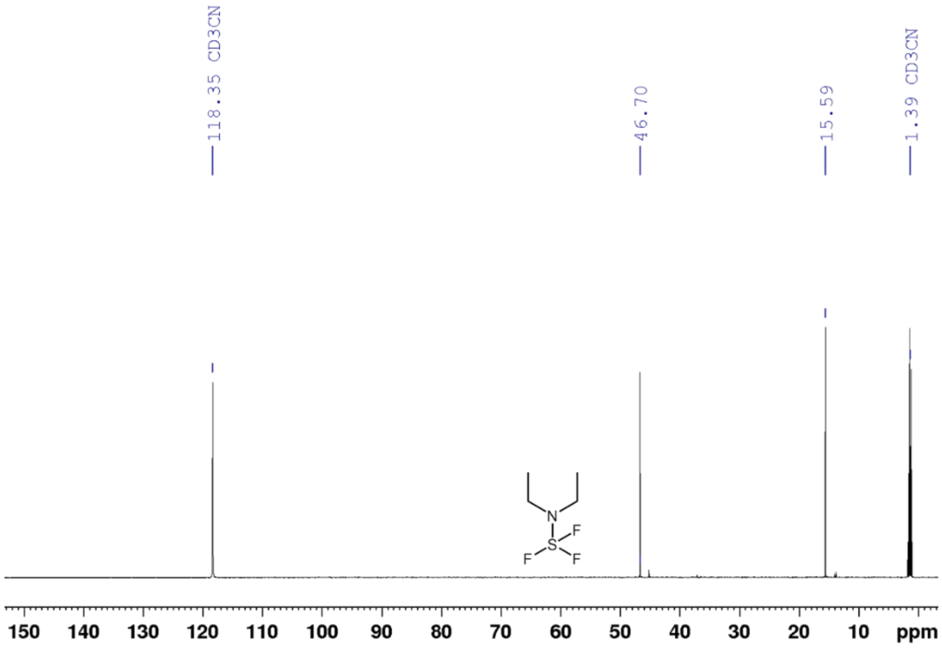


Fig. S6 ^{13}C NMR spectrum of DAST in acetonitrile-d_3. The spectrum used resonance signal of acetonitrile-d_3 (δ_C, 1.39 ppm) as internal reference. The ^{13}C resonance bands of CH_3 and CH_2 are assigned to about 15.6 ppm and 46.7 ppm, respectively.

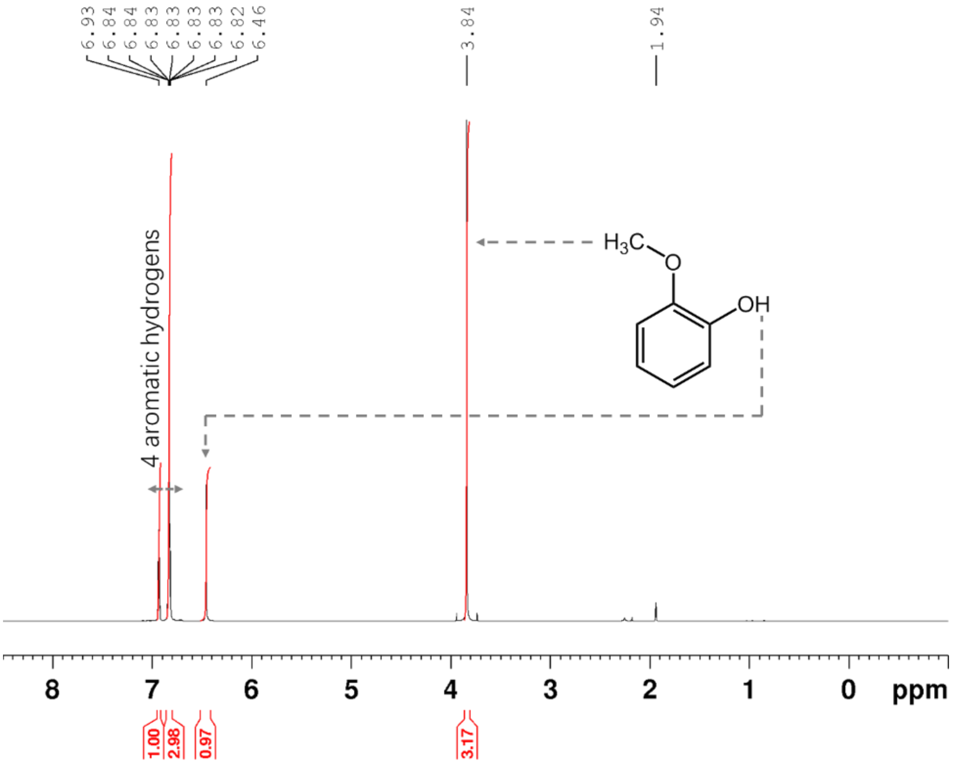


Fig. S7 ^{1}H NMR spectrum of guaiacol in acetonitrile-d_3, with assignation of resonance signals. The spectrum used the resonance of acetonitrile-d_3 (δ_H, 1.94 ppm) as internal reference.

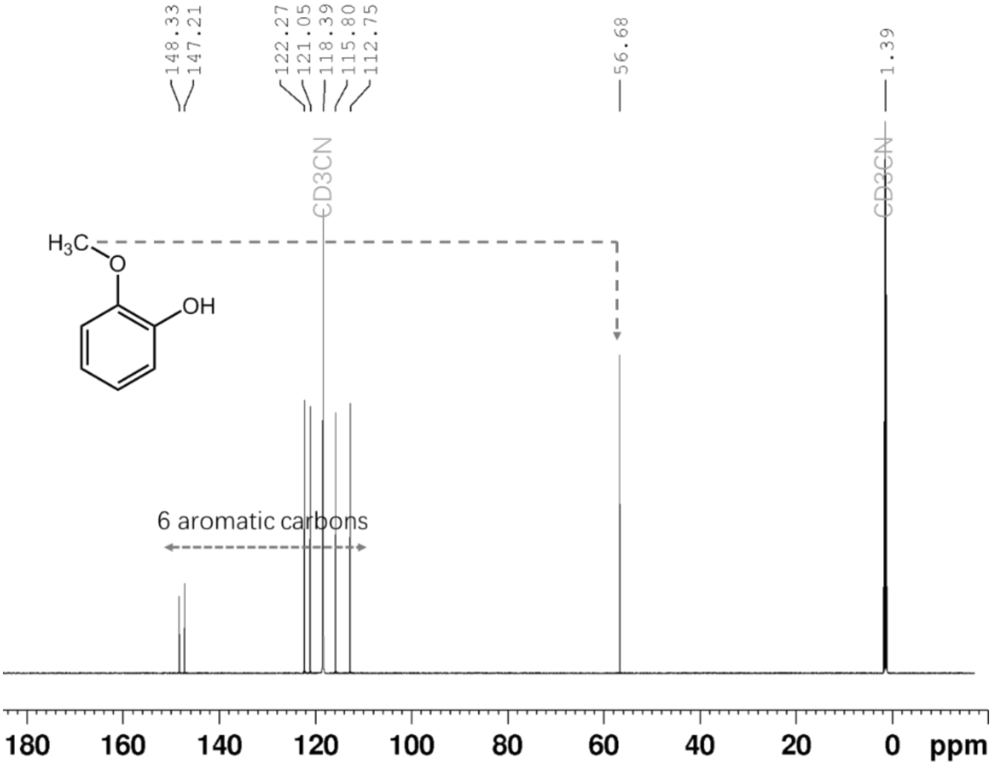


Fig. S8 ^{13}C NMR spectrum of guaiacol in acetonitrile-d_3, with assignation of resonance signals. The spectrum used resonance signal of acetonitrile-d_3 (δ_C, 1.39 ppm) as internal reference.

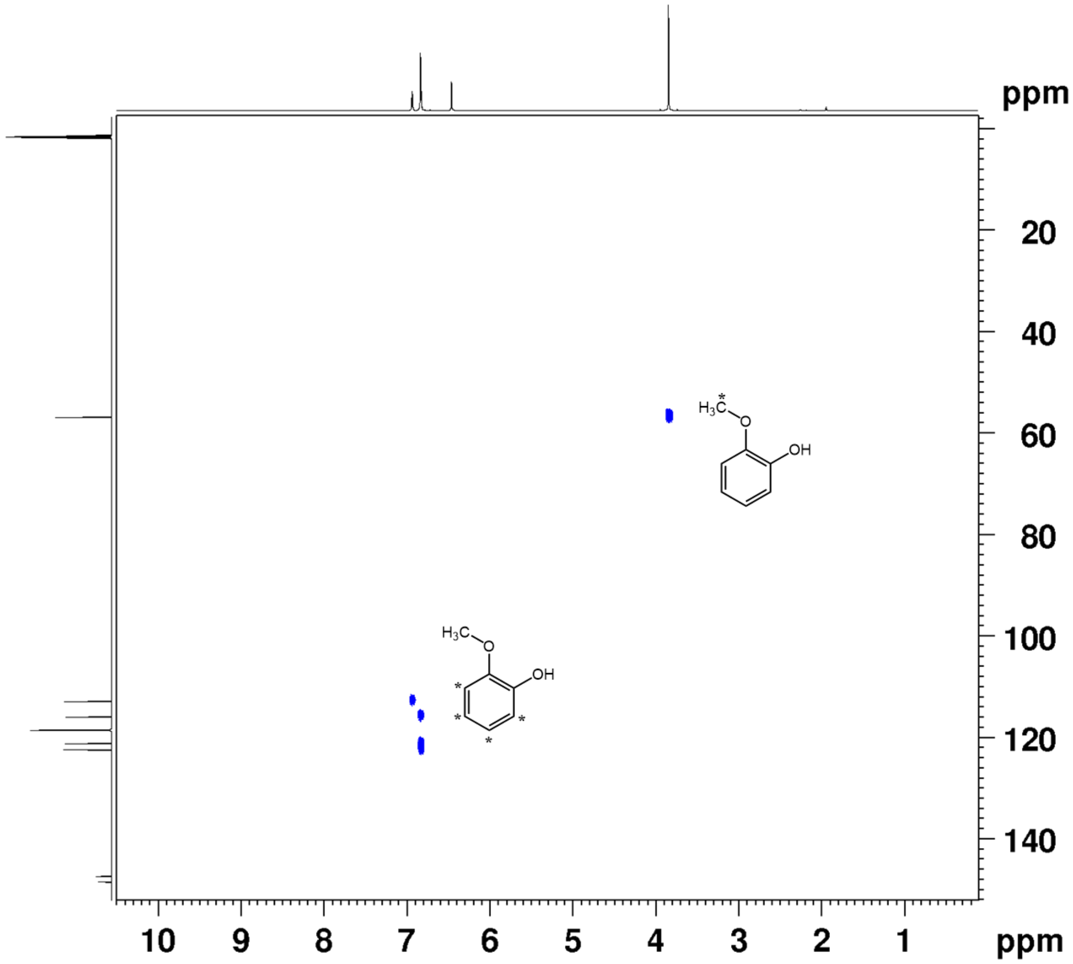


Fig. S9 Full 2D HSQC NMR spectrum of guaiacol in acetonitrile-d*3*, with assignation of resonance signals. Resonance signal of acetonitrile-d*3* (δ_H/δ_C, 1.94/1.39 ppm) is used as internal reference.

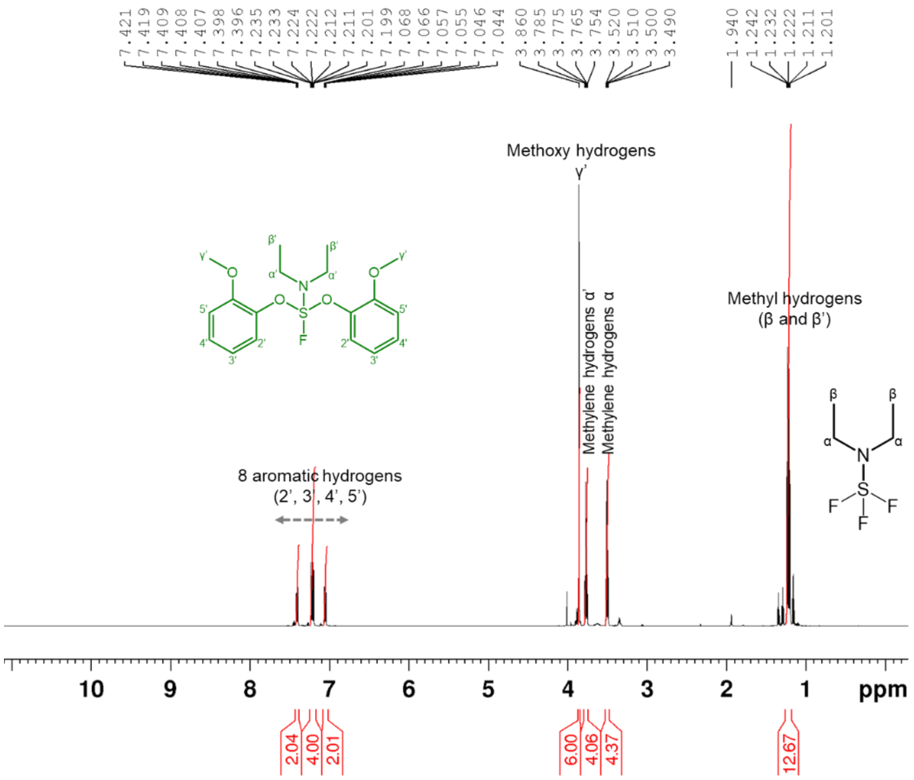


Fig. S10 ^{1}H NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with the same molar ratio (1:1.1) of standard condition in acetonitrile-d_3, with assignation of resonance signals. The spectrum was recorded immediately after mixing at RT, and the resonance of acetonitrile-d_3 (δ_H, 1.94 ppm) is used as internal reference.

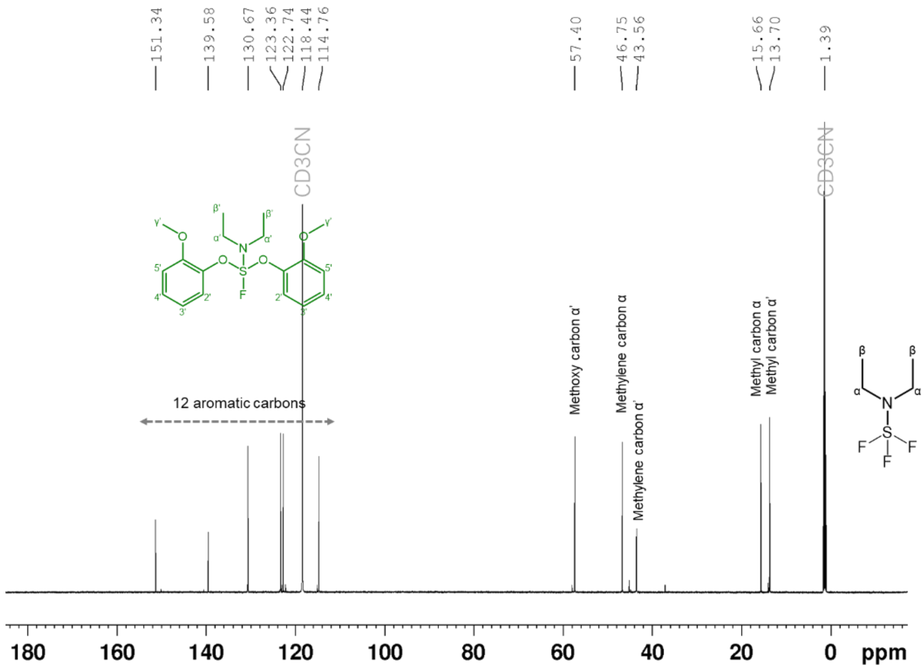


Fig. S11 ^{13}C NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with the same molar ratio (1:1.1) of standard condition in acetonitrile-d_3, with assignation of resonance signals. The spectrum was recorded immediately after mixing at RT, and the resonance of acetonitrile-d_3 (δ_C, 1.39 ppm) is used as internal reference.

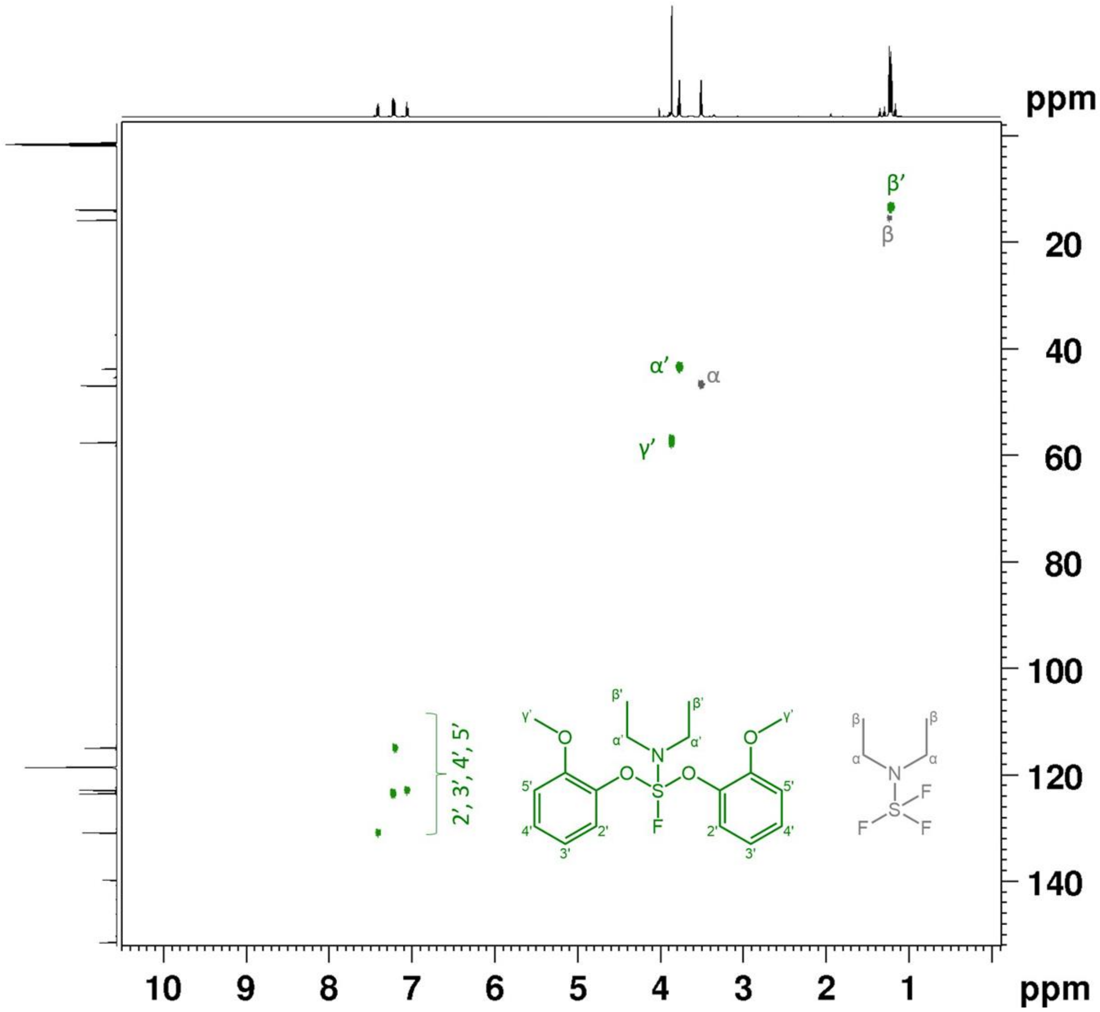


Fig. S12 Full 2D HSQC NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with the same molar ratio (1:1.1) of standard condition in acetonitrile-d*3*, with assignation of resonance signals. Contours are coded to corresponding structures. The spectrum was recorded immediately after mixing at RT, and the resonance of acetonitrile-d*3* (δ_H/δ_C, 1.94/1.39 ppm) is used as internal reference.

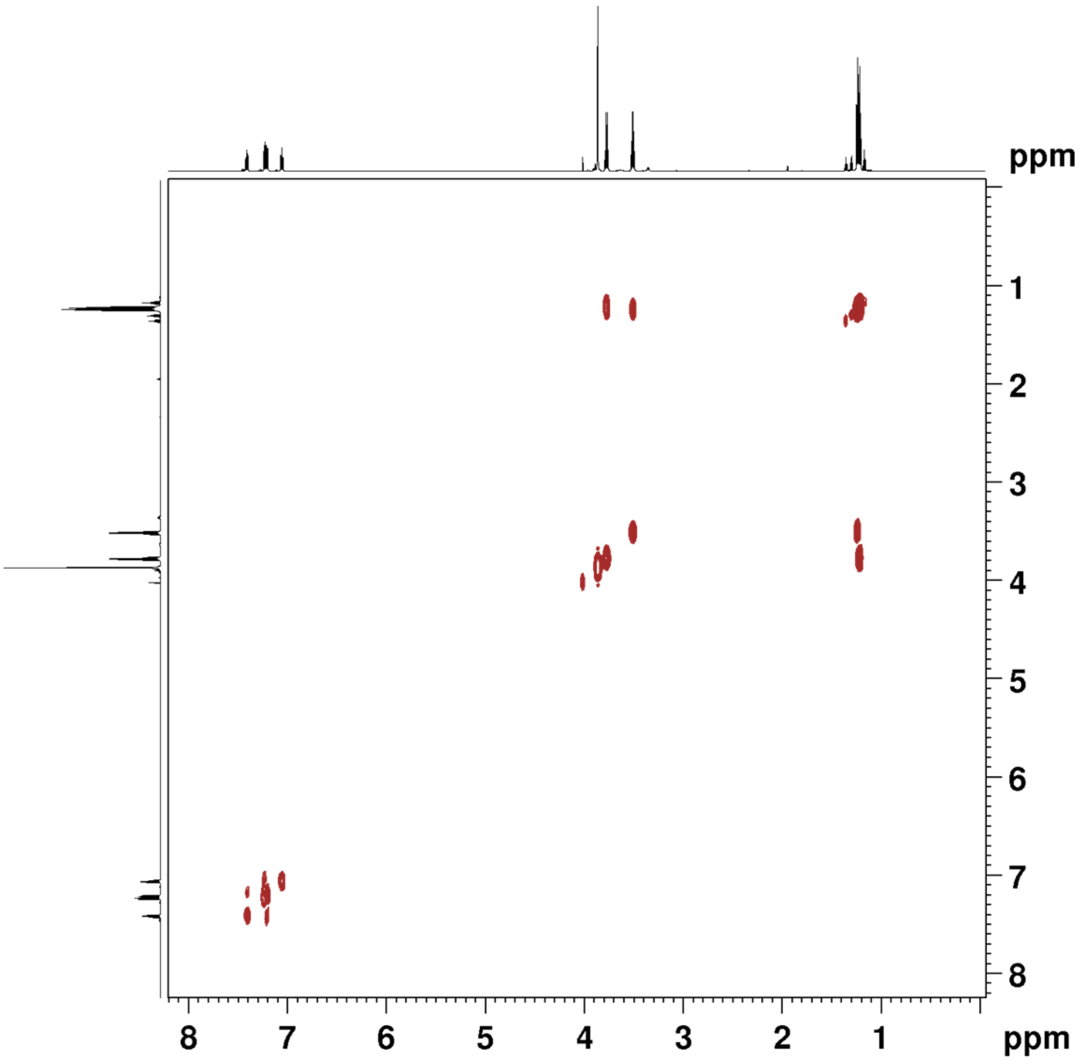


Fig. S13 2D COSY NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with the same molar ratio (1:1.1) of standard condition in acetonitrile-d_3, with assignation of resonance signals. Contours are coded to corresponding structures. The spectrum was recorded immediately after mixing at RT, and the resonance of acetonitrile-d_3 (δ_H, 1.94 ppm) is used as internal reference.

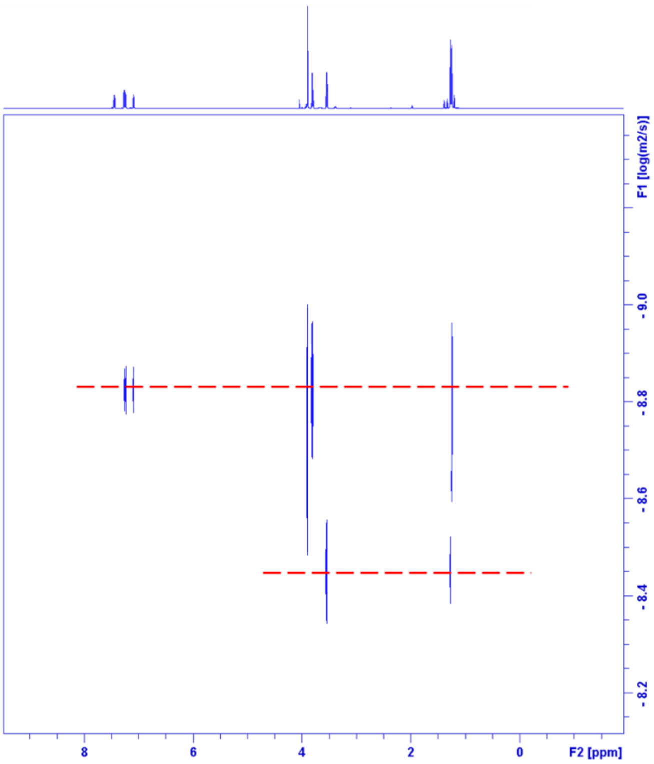


Fig. S14 DOSY NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with the same molar ratio (1:1.1) of standard condition in acetonitrile-d_3. The spectrum was calibrated by the characteristic resonance of acetonitrile-d_3 (δ_H, 1.94 ppm).

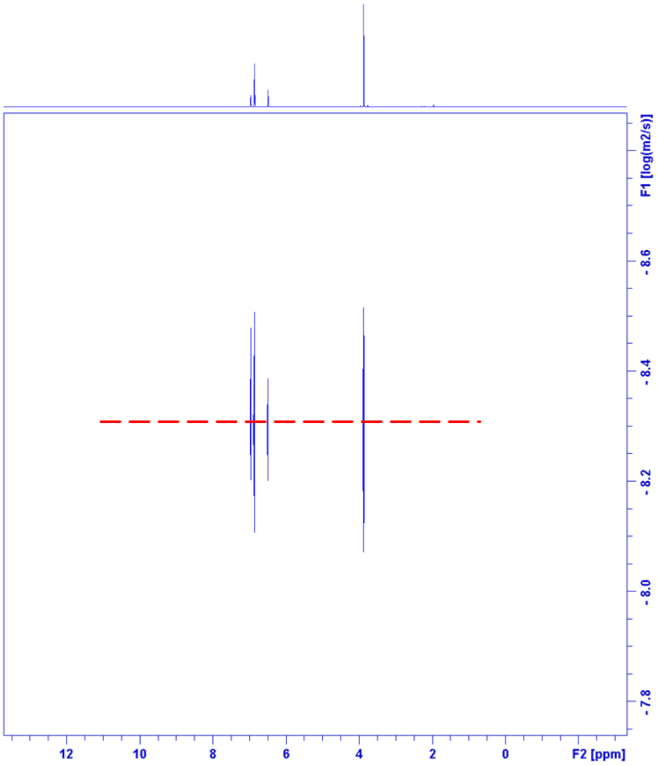


Fig. S15 DOSY NMR spectrum of guaiacol in acetonitrile-d_3. The spectrum was calibrated by the characteristic resonance of acetonitrile-d_3 (δ_H, 1.94 ppm).

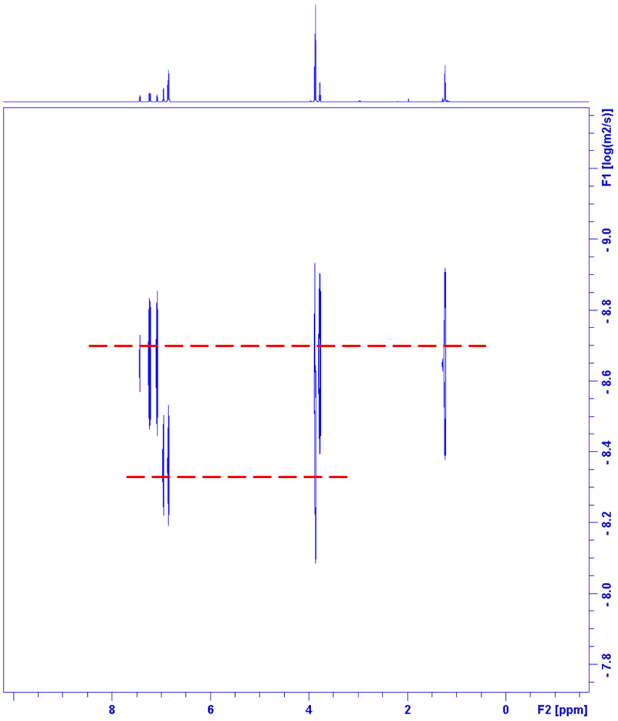


Fig. S16 DOSY NMR spectrum of the crude mixture obtained by mixing guaiacol and DAST with molar ratio 1:0.2 in acetonitrile-d*3*. Guaiacol is in excessive amount in this experiment. The spectrum was calibrated by the characteristic resonance of acetonitrile-d*3* (δ_H, 1.94 ppm).

The interaction between guaiacol and DAST and formation of the activated intermediate was verified by DOSY (diffusion-ordered spectroscopy) experiments. From the DOSY NMR spectra of mixture of guaiacol and DAST with molar ratio of 1:1.1 (Fig. S13), 1:0.2 (Fig. S15) and guaiacol (Fig. S14) in acetonitrile-d*3*, it is obvious that there are primarily two species with different diffusion coefficients present in the two crude mixtures, respectively. As diffusion coefficients decrease with the increasing of molecular weight for both linear and globular molecules, a new specie with higher molecular weight than guaiacol and DAST was found in both mixtures, which is attributed to the generation of the activated intermediate. These results are in consistency with the ^{1}H, ^{13}C, 2D HSQC, HMBC and COSY NMR characterization results.

III. Study about the interaction between DAST and organic salt

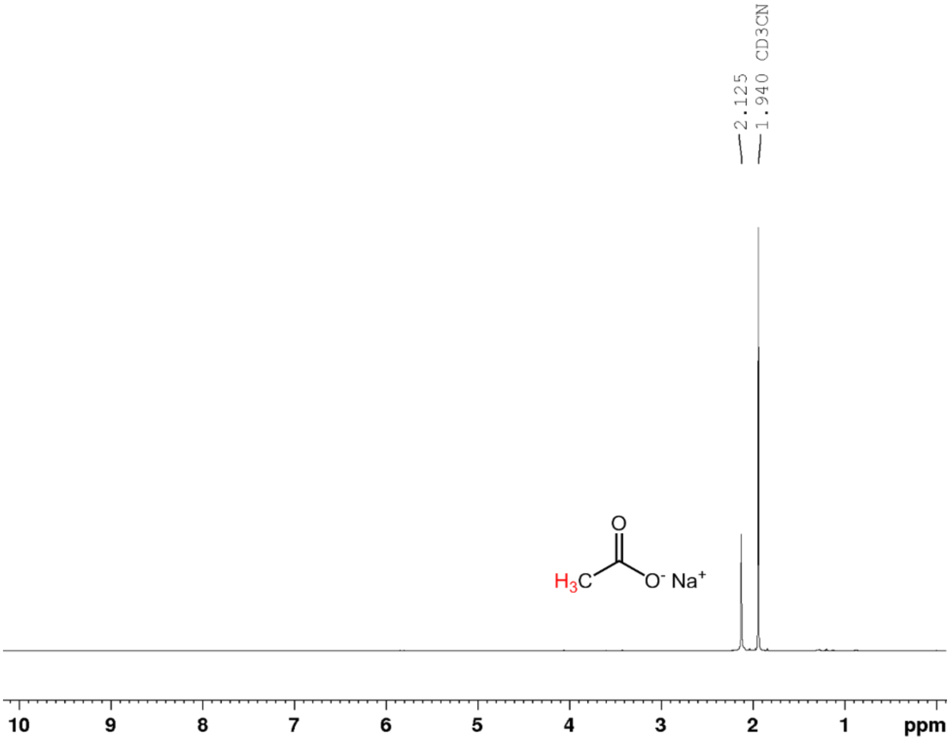


Fig. S17 ^{1}H NMR spectrum of sodium acetate in acetonitrile-d_3. The spectrum used the resonance of acetonitrile-d_3 (δ_H, 1.94 ppm) as internal reference. The resonance band of the methyl group is assigned to ca. 2.13 ppm.

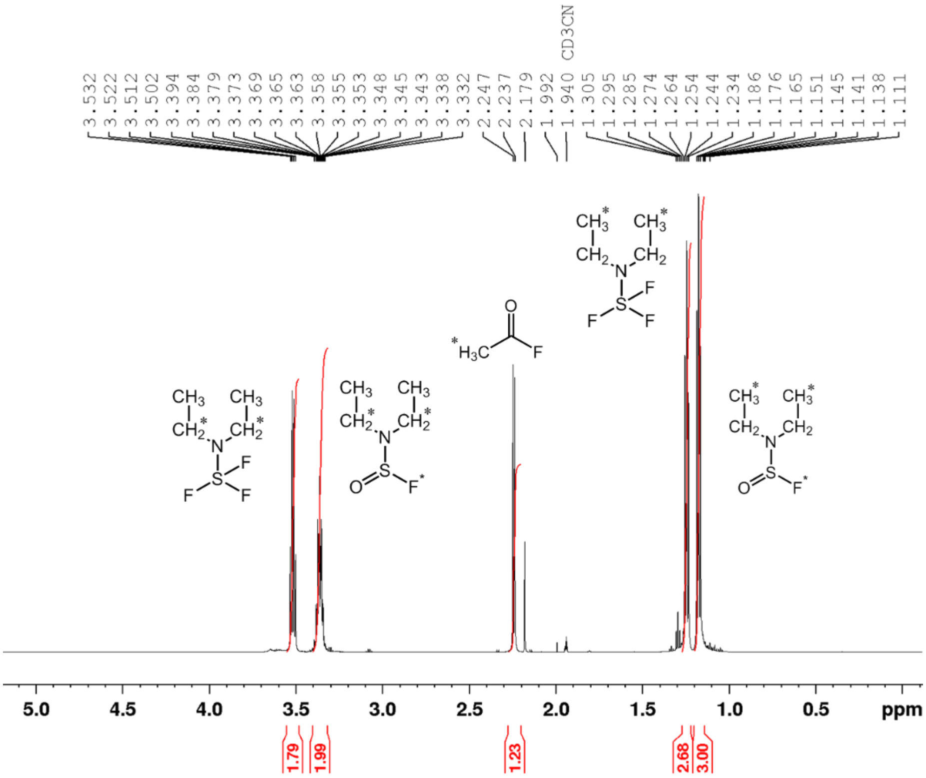


Fig. S18 ^{1}H NMR spectrum of the crude reaction mixture obtained by mixing DAST and sodium acetate with the same molar ratio (1:1) of standard condition in acetonitrile-d$_3$, with assignation of resonance signals. The spectrum was recorded immediately after mixing for about 15 min at RT, and the resonance of acetonitrile-d$_3$ (δ_H, 1.94 ppm) is used as internal reference.

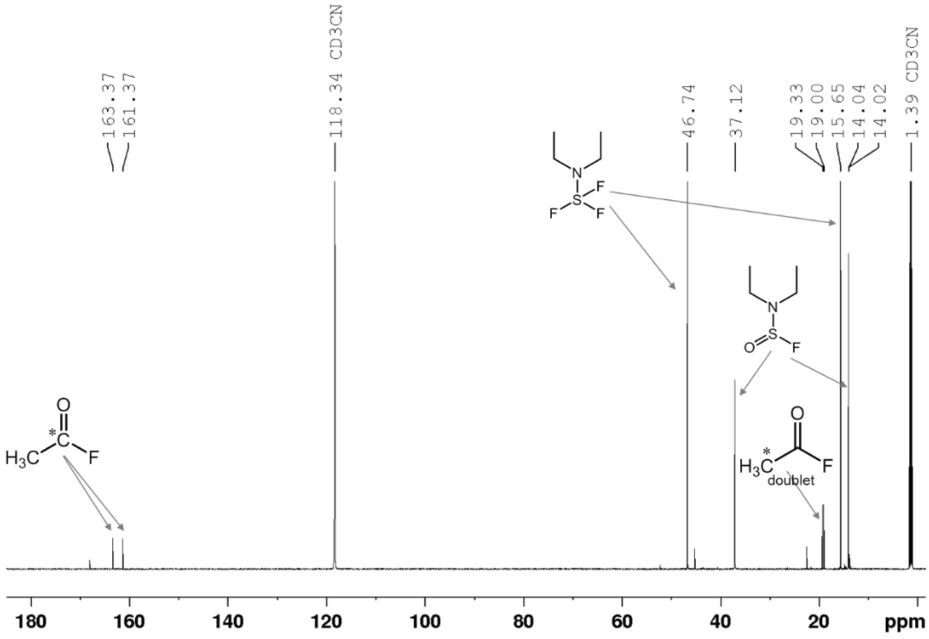


Fig. S19 ^{13}C NMR spectrum of the crude reaction mixture obtained by mixing DAST and sodium acetate with the same molar ratio (1:1) of standard condition in acetonitrile-d$_3$, with assignation of resonance signals. The spectrum was recorded immediately after mixing for about 15 min at RT, and the resonance of acetonitrile-d$_3$ (δ_C, 1.39 ppm) is used as internal reference.

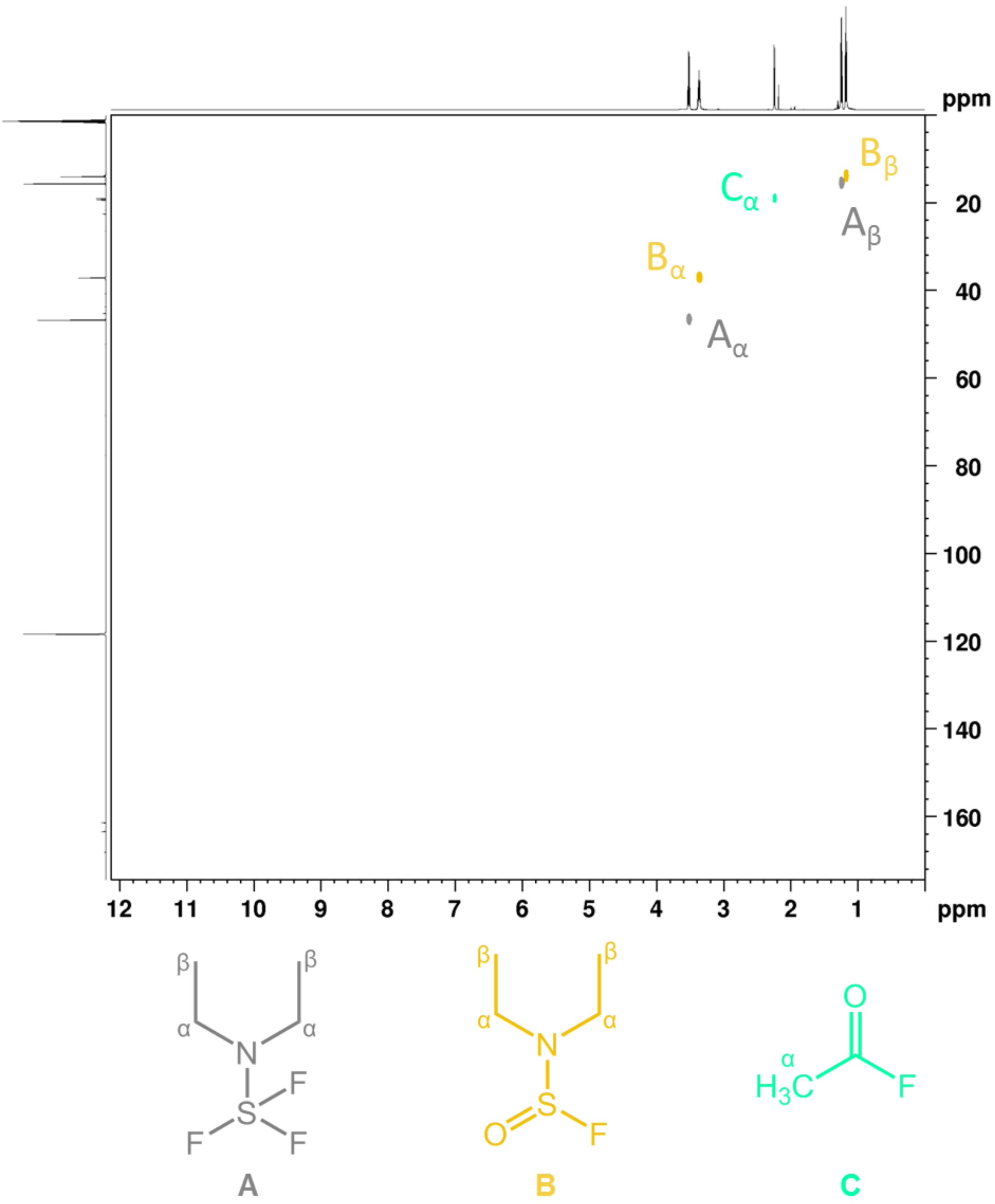


Fig. S20 Full 2D HSQC NMR spectrum of the crude reaction mixture obtained by mixing DAST and sodium acetate with the same molar ratio (1:1) of standard condition in acetonitrile-d_3, with assignation of resonance signals. Contours are coded to corresponding structures. The spectrum was recorded immediately after mixing for about 15 min at RT, and the resonance of acetonitrile-d_3 (δ_H/δ_C, 1.94/1.39 ppm) is used as internal reference.

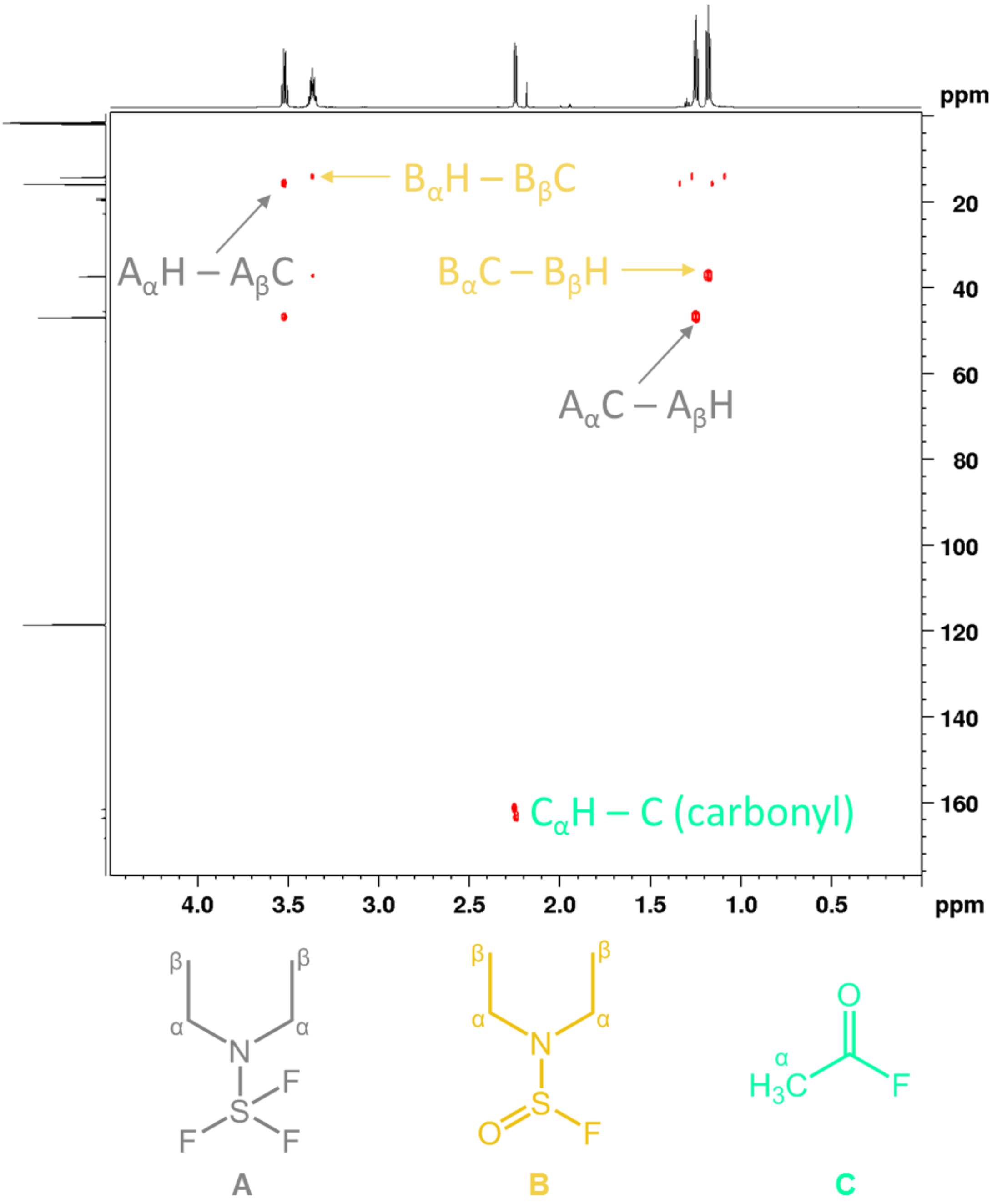


Fig. S21 Full 2D HMBC NMR spectrum of the crude reaction mixture obtained by mixing DAST and sodium acetate with the same molar ratio (1:1) of standard condition in acetonitrile-d_3, with assignation of resonance signals. The spectrum was recorded immediately after mixing for about 15 min at RT. The spectrum was calibrated using characteristic resonance signals in HSQC NMR spectrum.

IV. NMR characterization of standard reaction

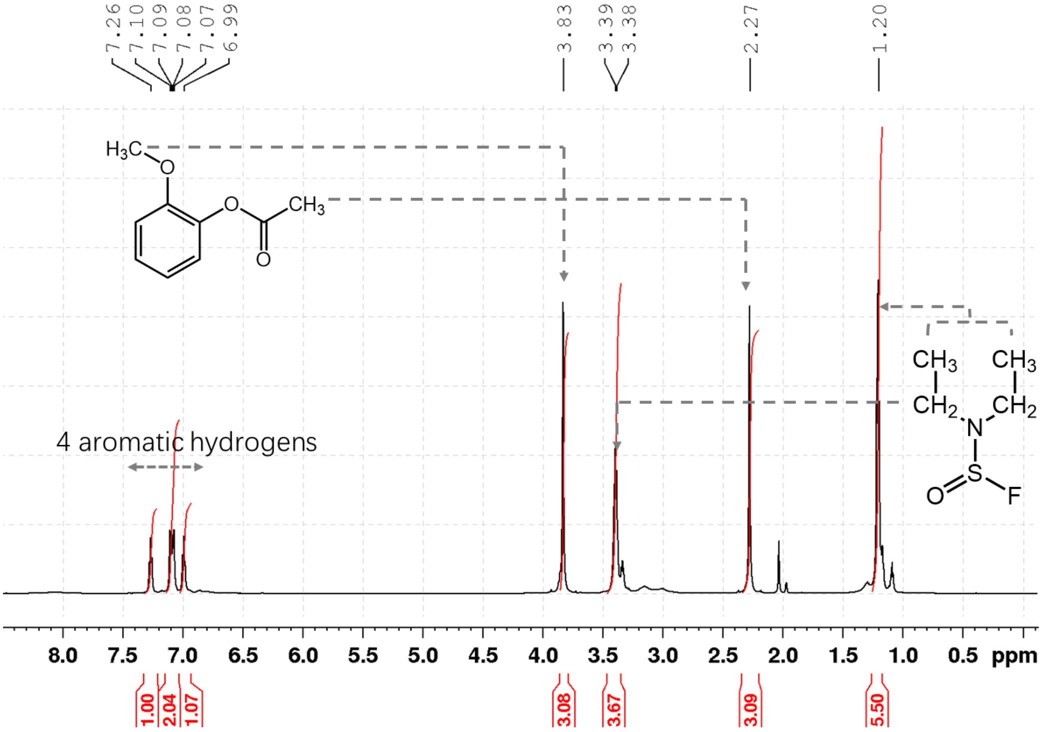


Fig. S22 ^{1}H NMR spectrum of the post-reaction crude standard reaction mixture in acetonitrile-d*3*, with assignation of resonance signals. The spectrum was recorded after 6 h reaction at RT, and the resonance of acetonitrile-d*3* (δ_H, 1.94 ppm) is used as internal reference.

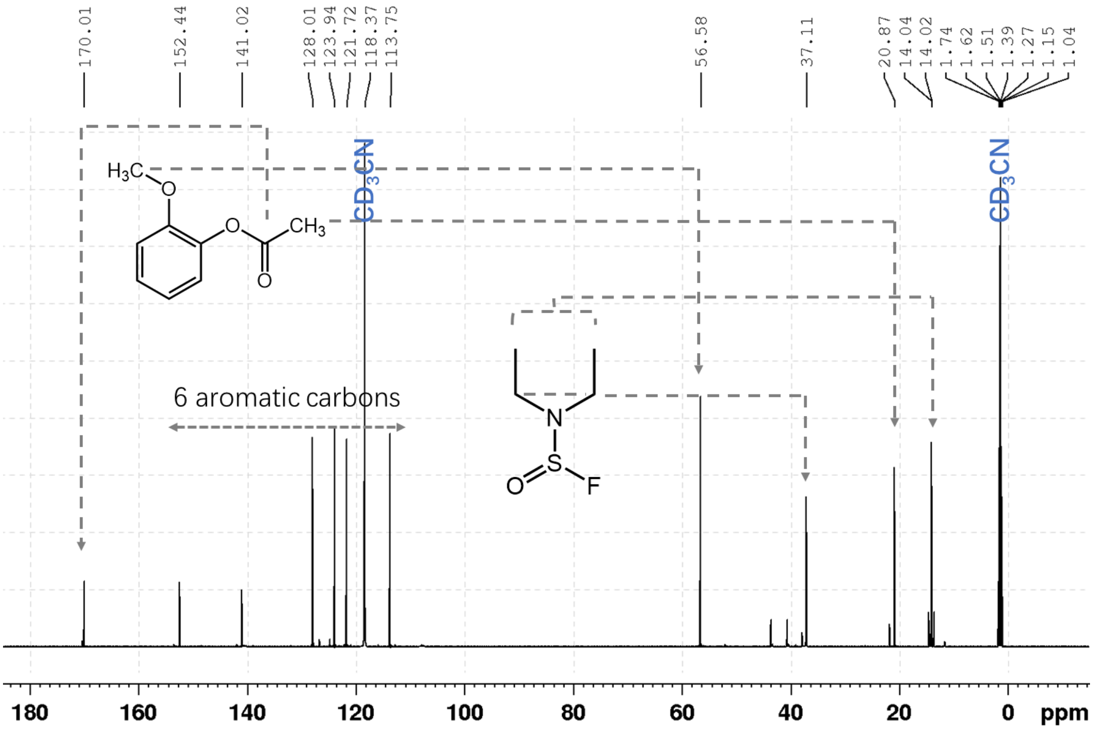


Fig. S23 ^{13}C NMR spectrum of the post-reaction crude standard reaction mixture in acetonitrile-d*3*, with assignation of resonance signals. The spectrum was recorded after 6 h reaction at RT, and the resonance of acetonitrile-d*3* (δ_C, 1.39 ppm) is used as internal reference.

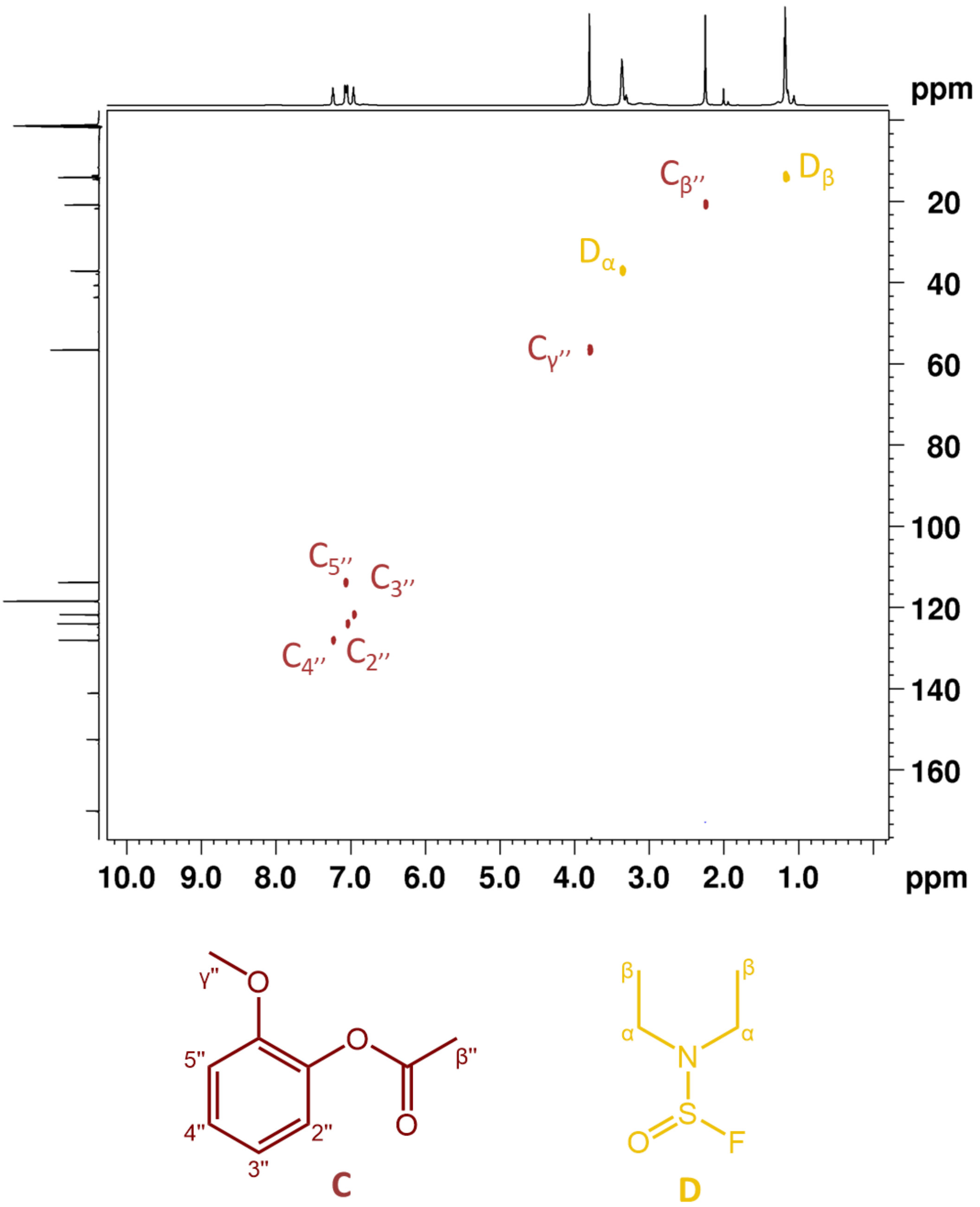


Fig. S24 Full 2D HSQC NMR spectrum of the post-reaction crude standard reaction mixture in acetonitrile-d$_3$, with assignation of resonance signals. Contours are coded to corresponding structures. The spectrum was recorded after 6 h reaction at RT, and the resonance of acetonitrile-d$_3$ (δ_H/δ_C, 1.94/1.39 ppm) is used as internal reference.

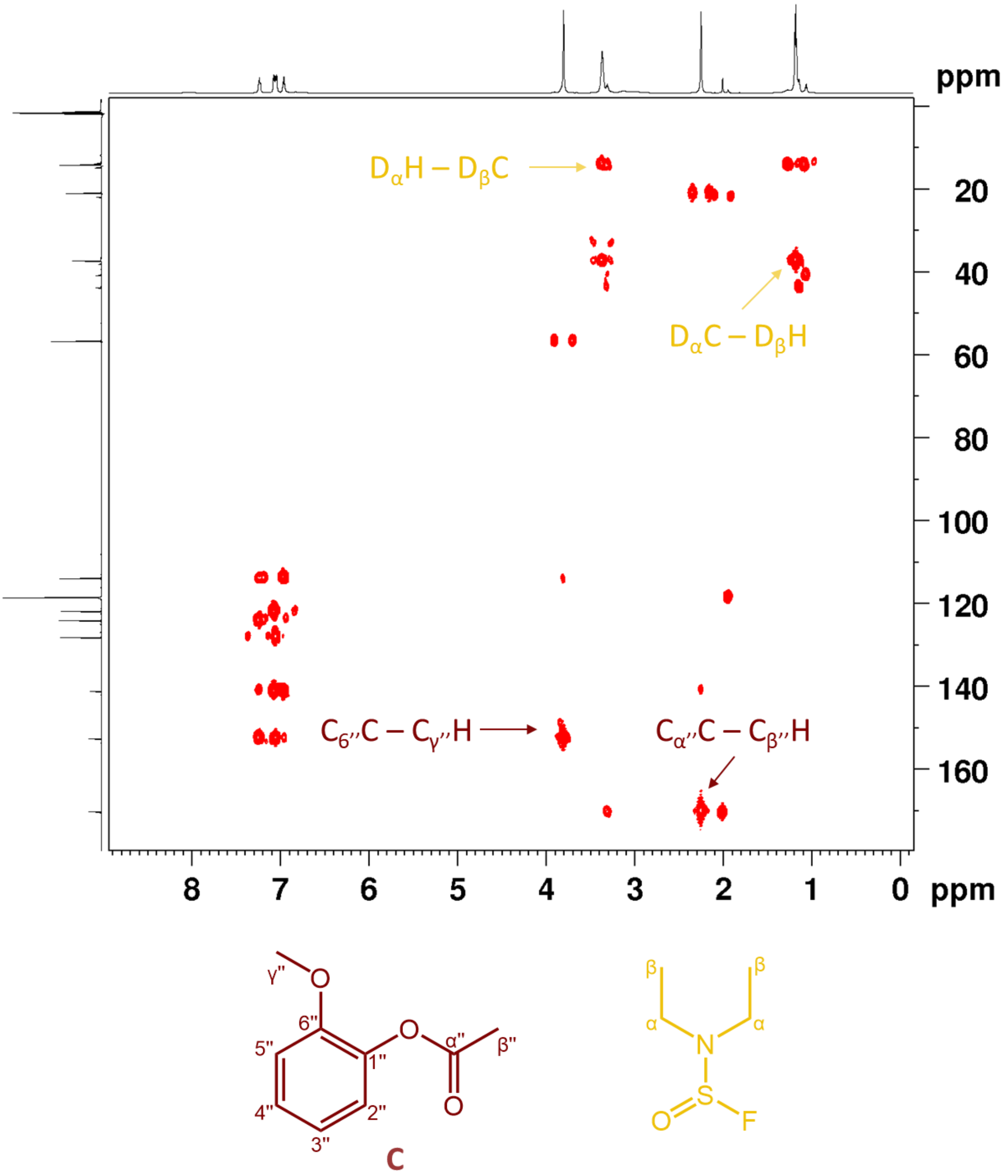
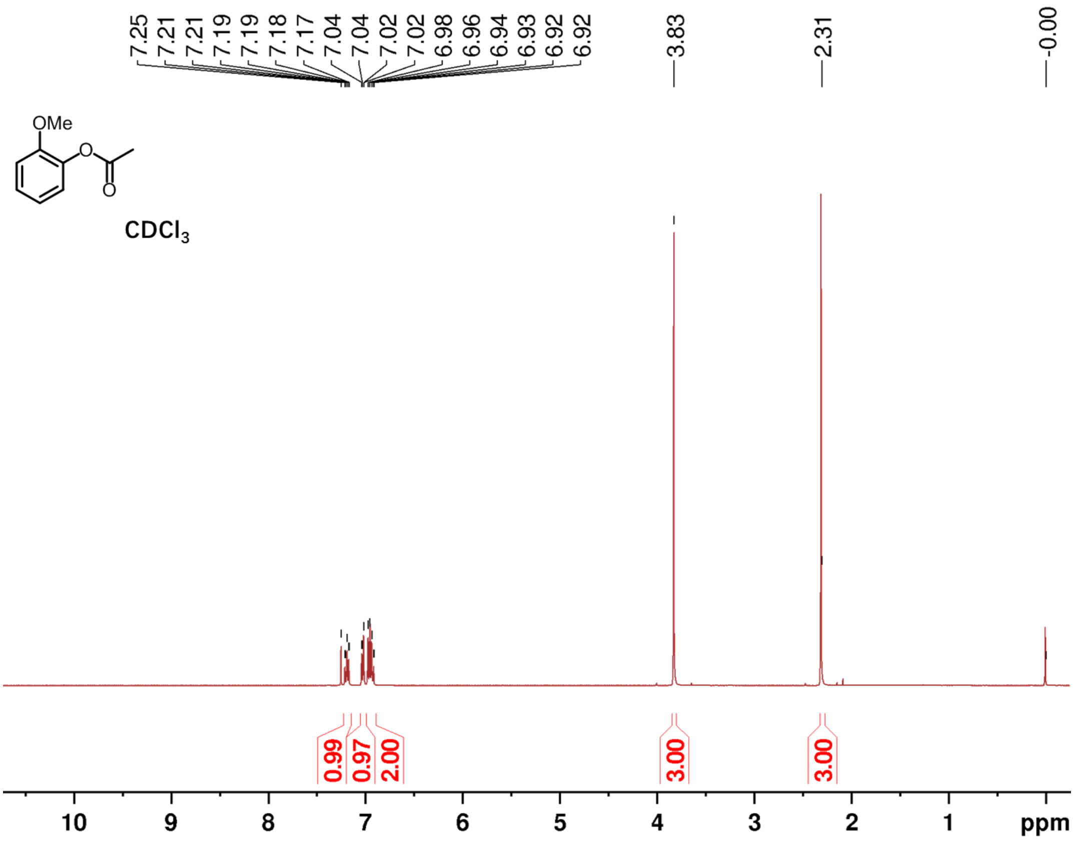


Fig. S25 Full 2D HMBC NMR spectrum of the post-reaction crude standard reaction mixture in acetonitrile-d_3, with assignation of resonance signals. Contours are coded to corresponding structures. The spectrum was recorded after 6 h reaction at RT. The spectrum was calibrated using characteristic resonance signals in HSQC NMR spectrum.

NMR spectra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7.18
7.17
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6.94
6.93
6.92
6.92
3.83
2.31
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OMe
O
O
CDCl$_3$
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3
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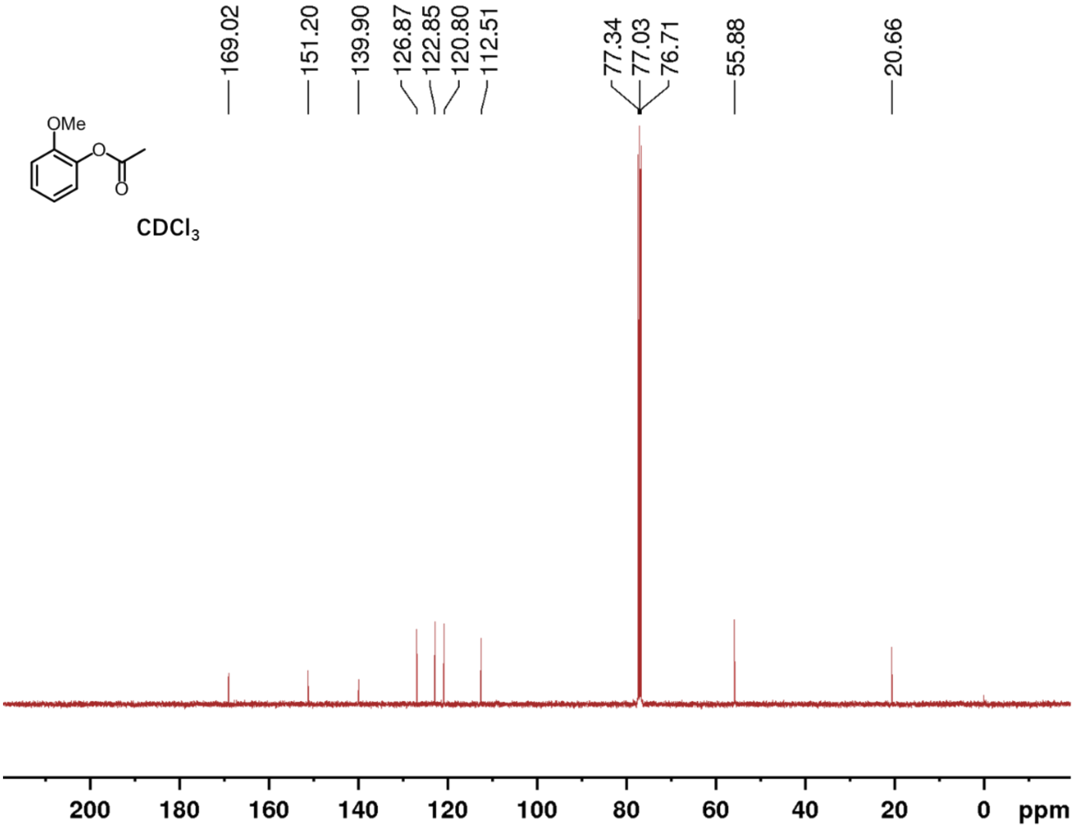
ppm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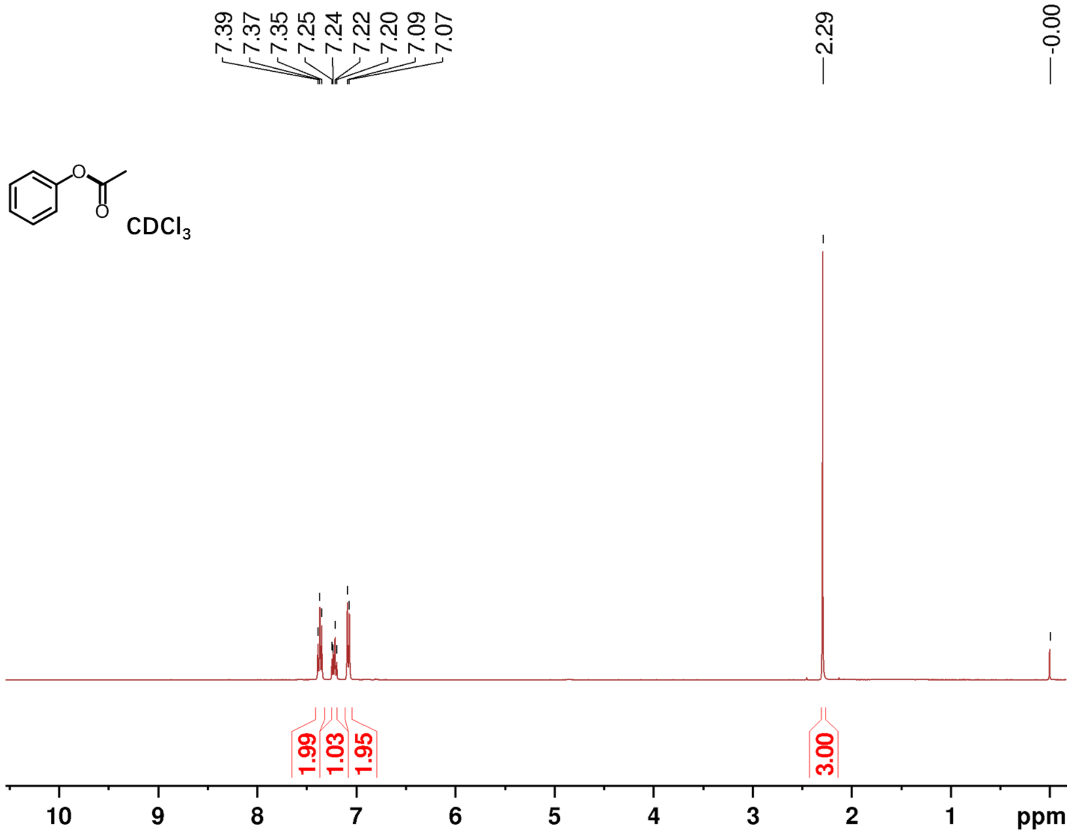
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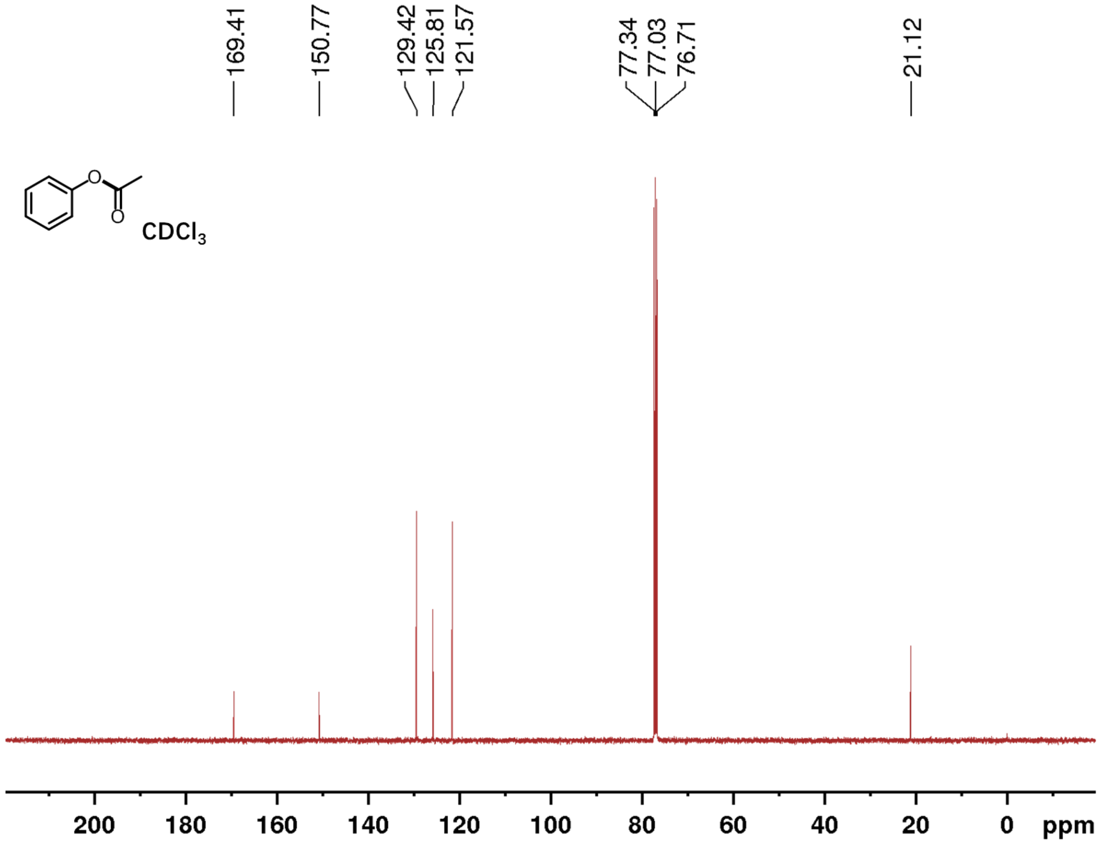
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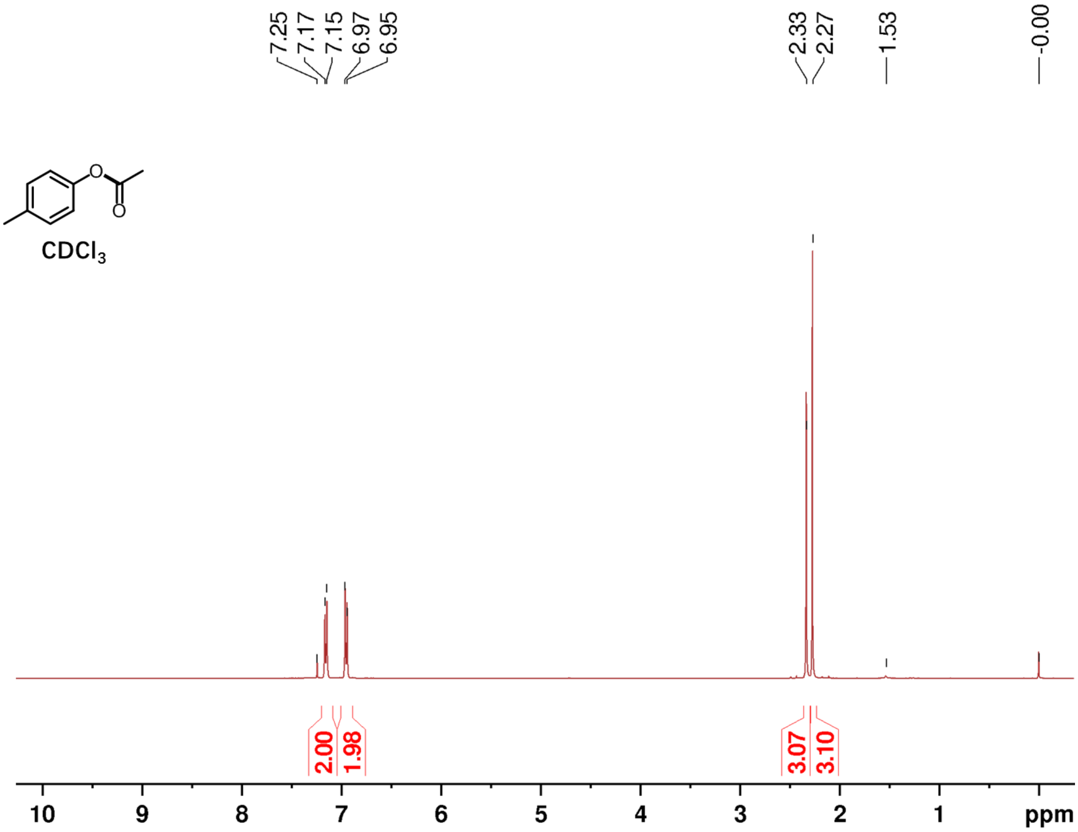
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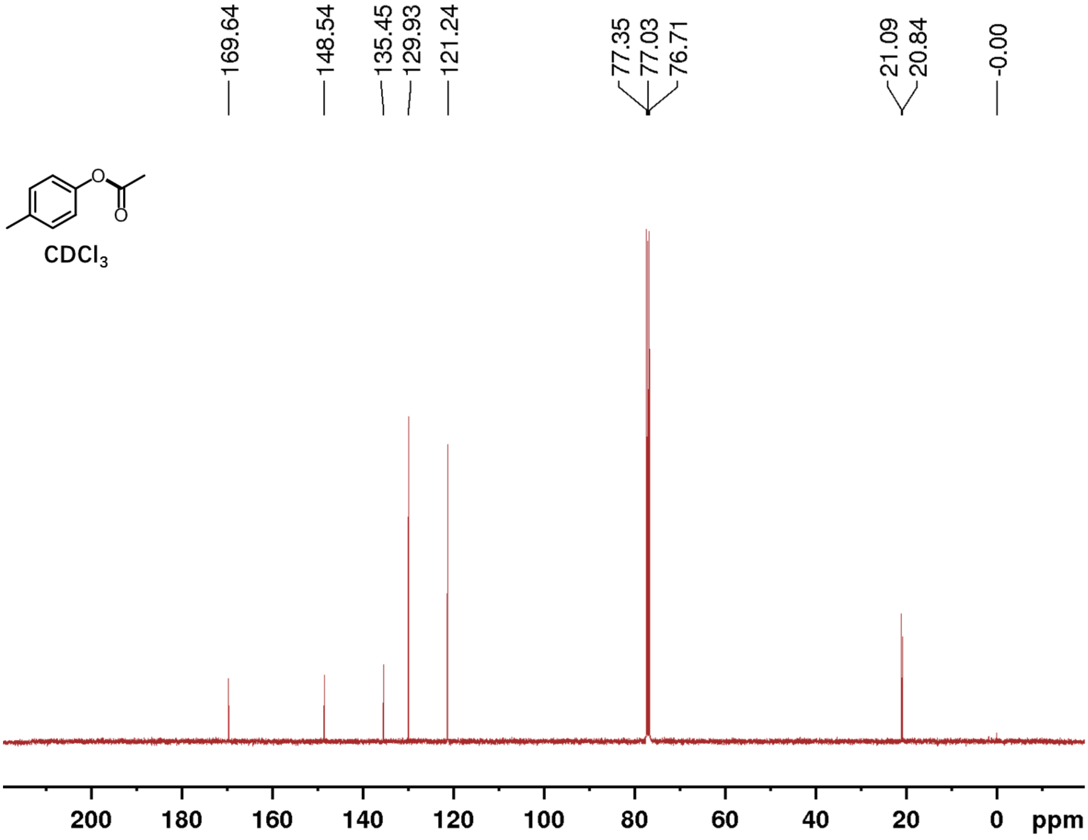
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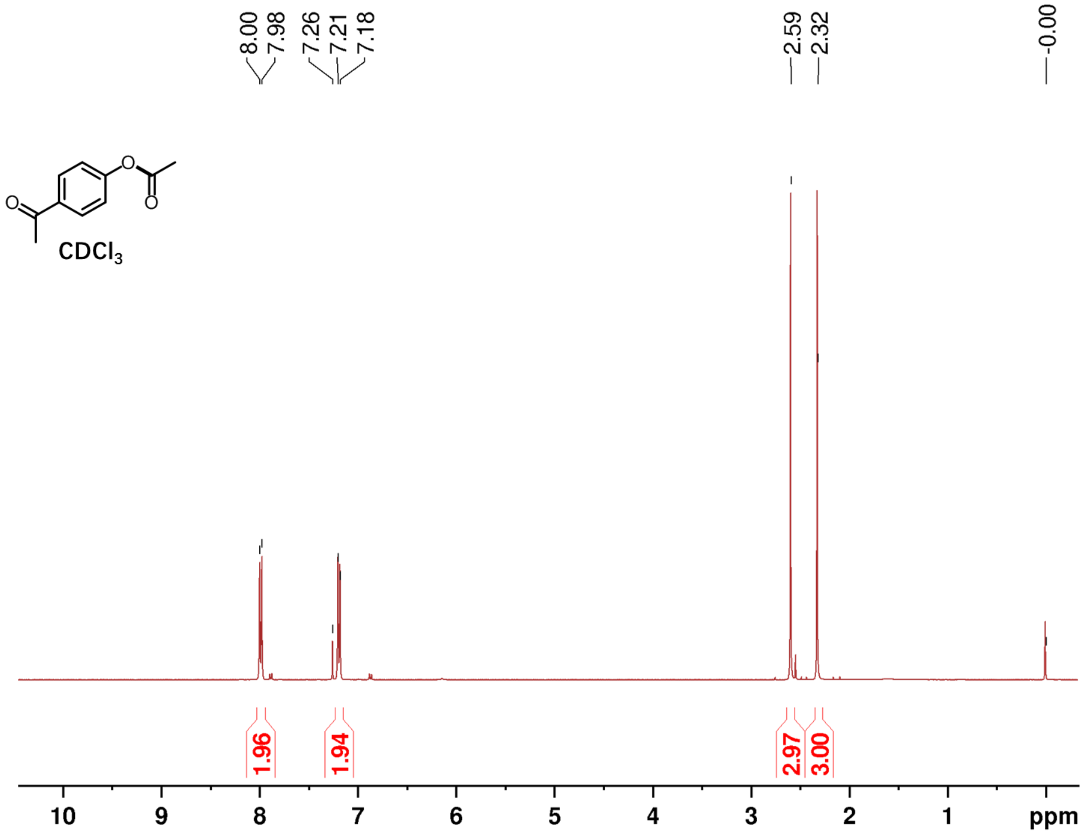
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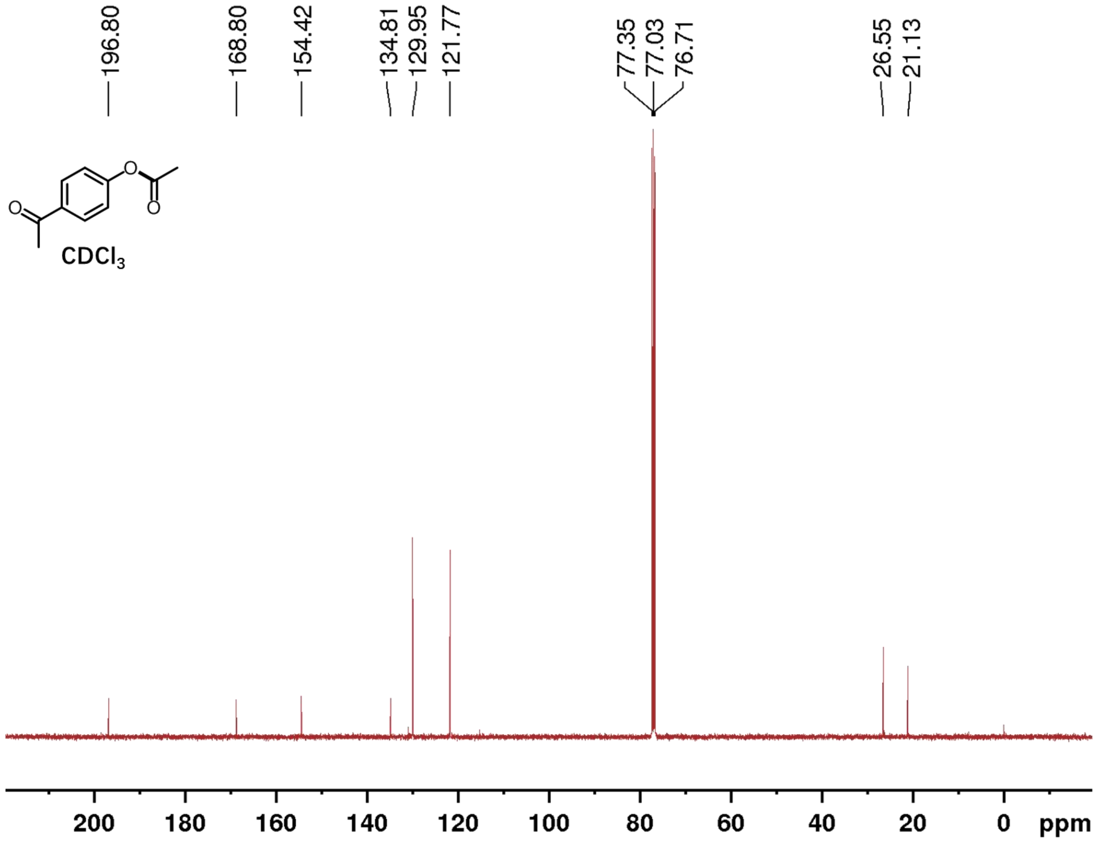
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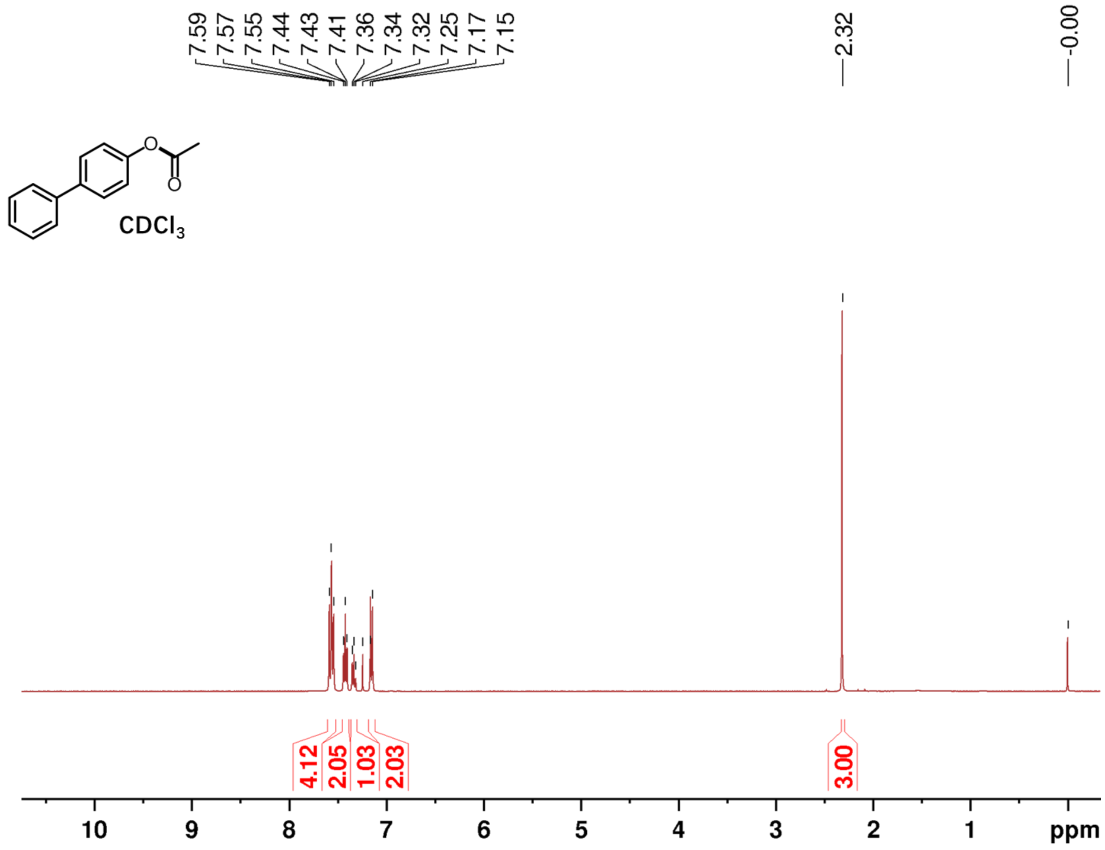
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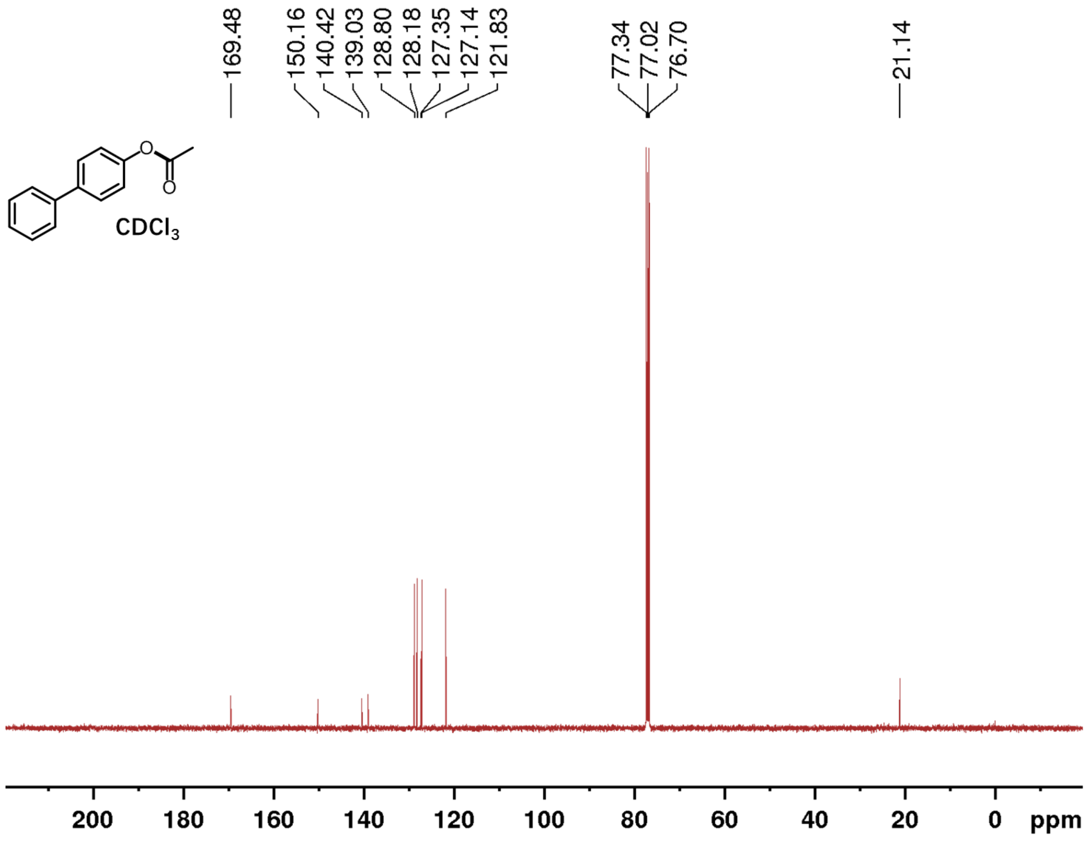
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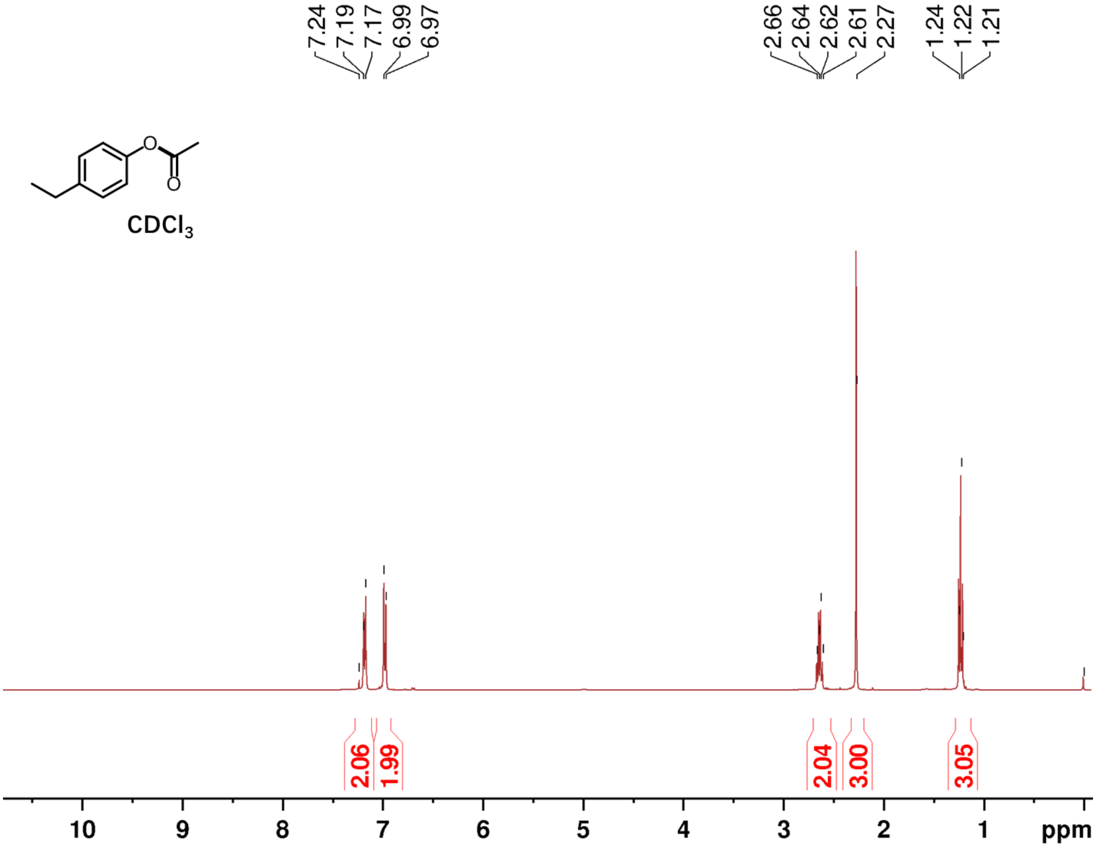
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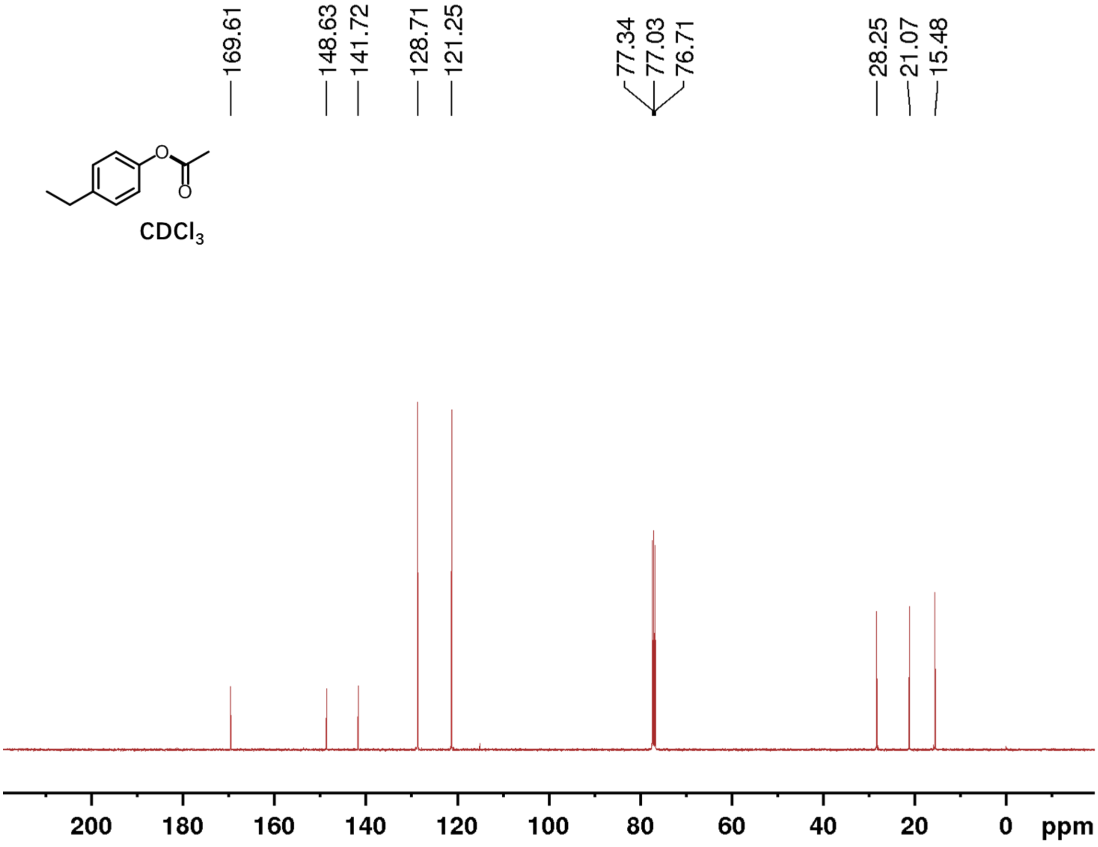
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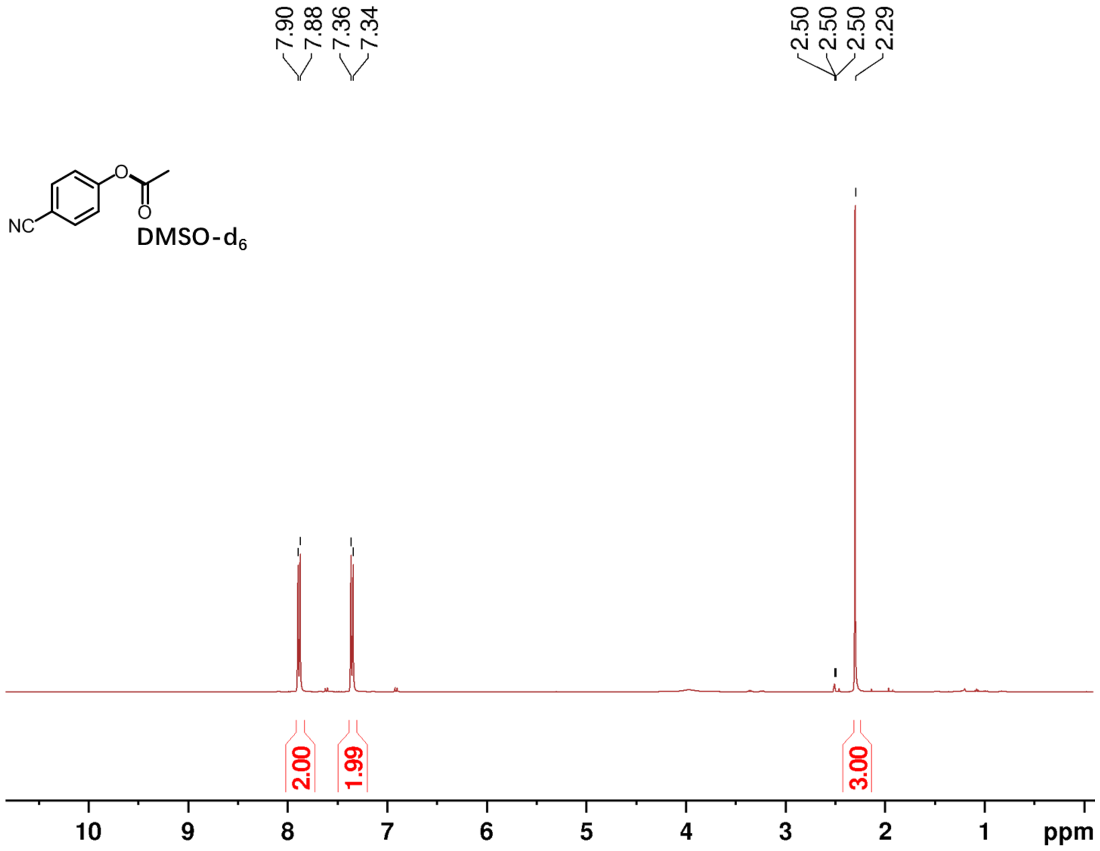
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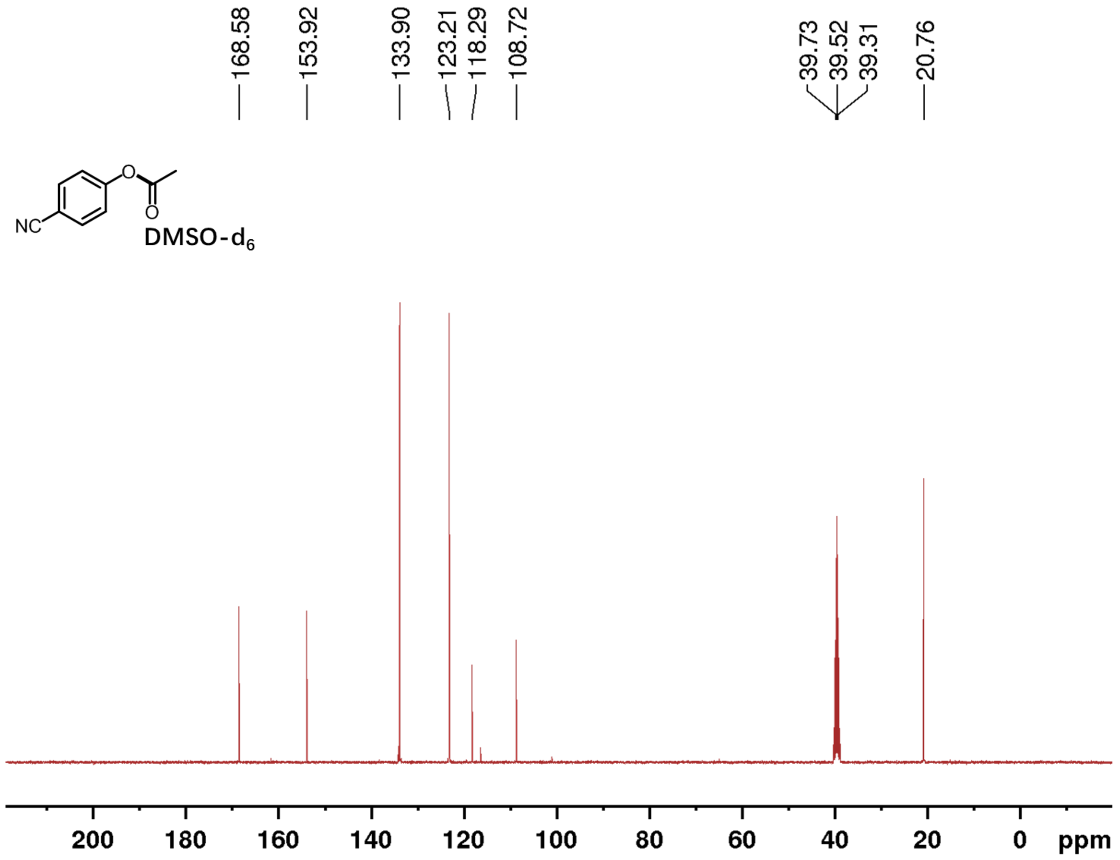
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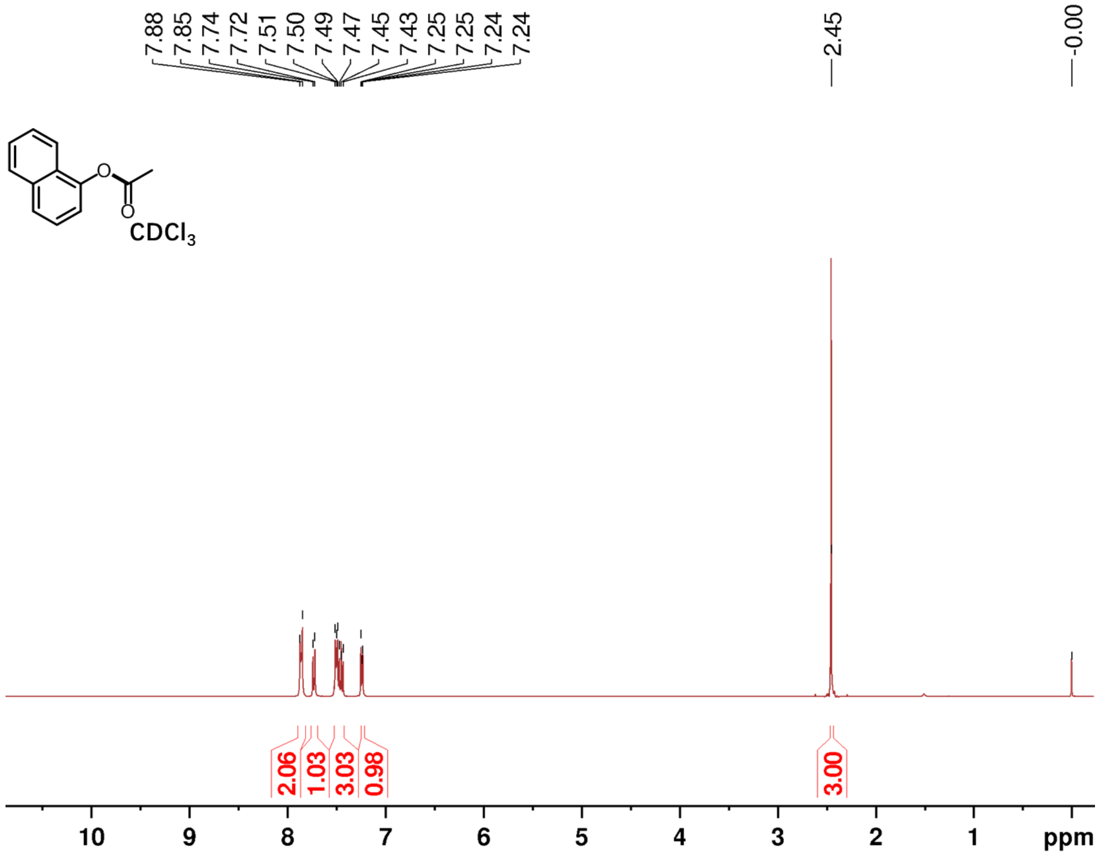
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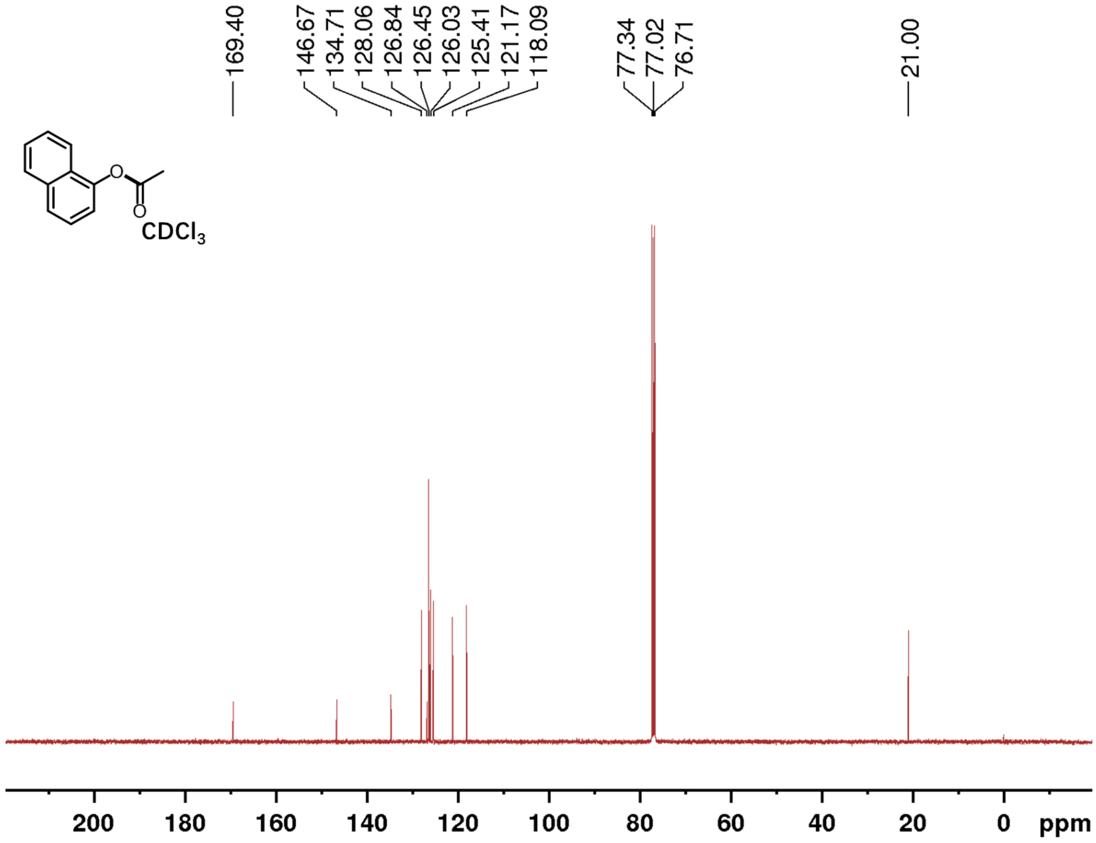
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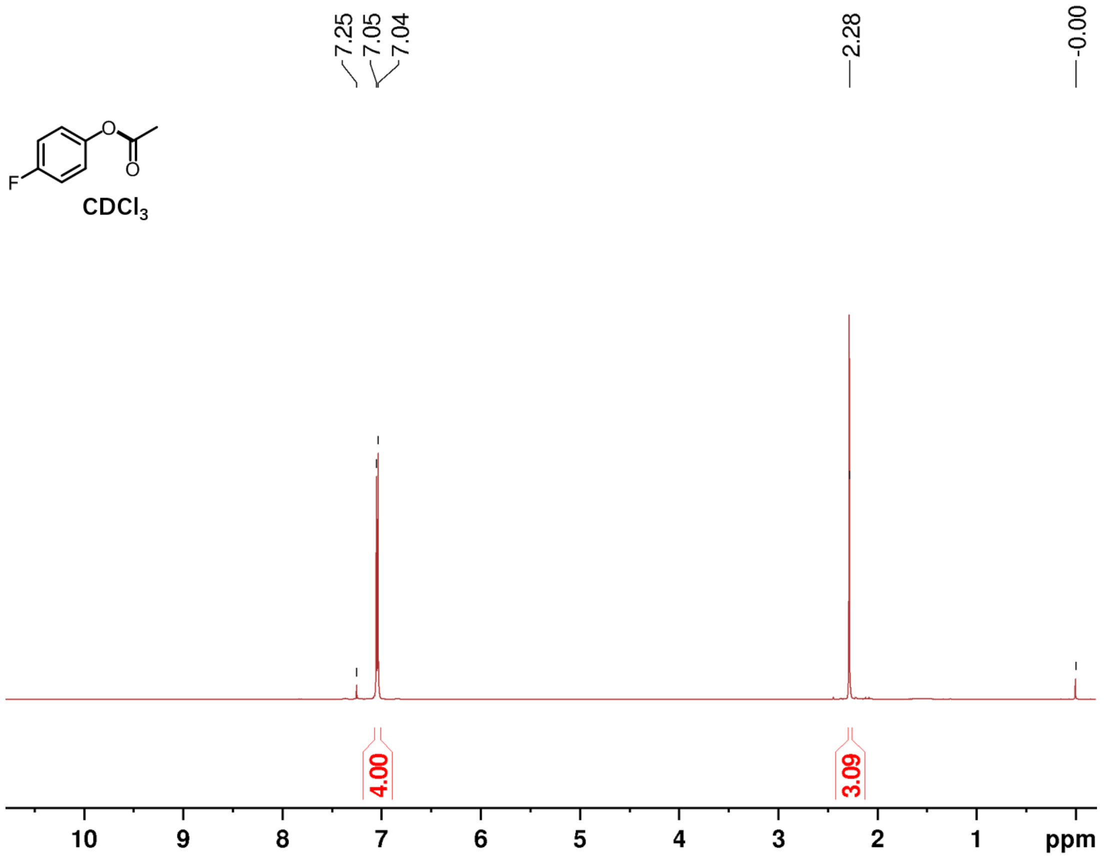
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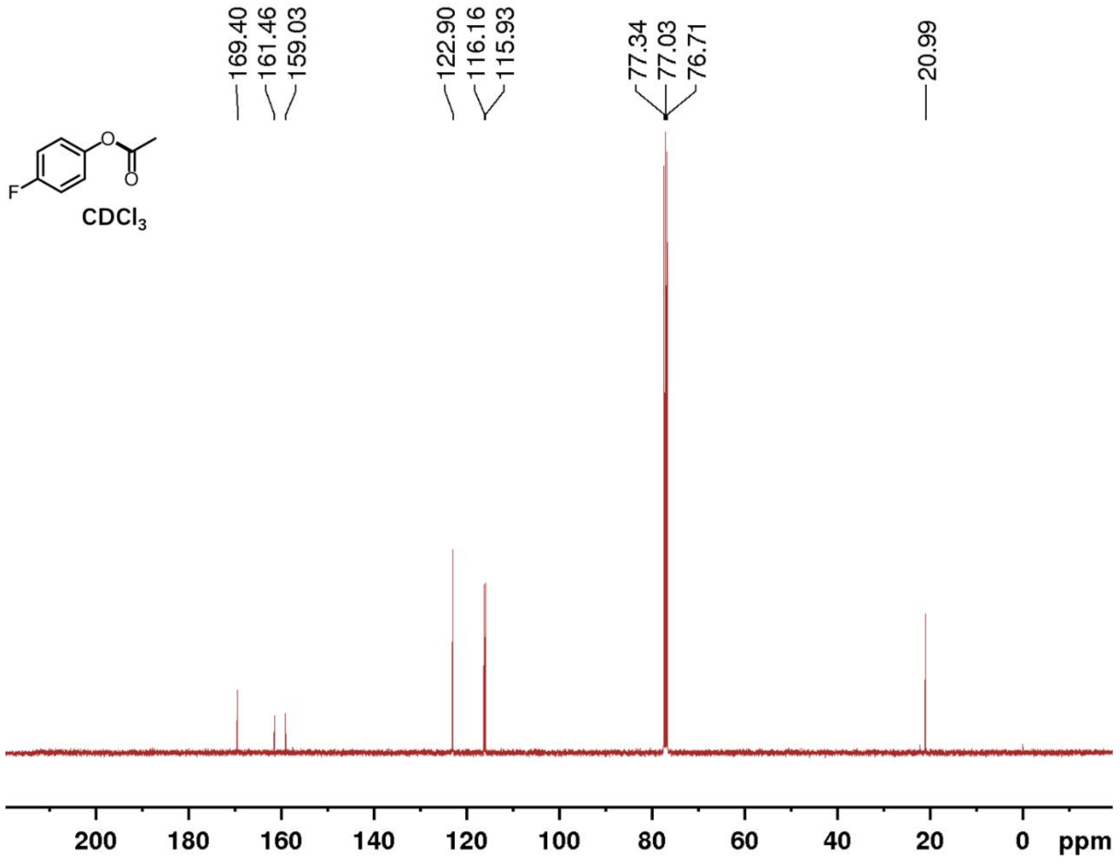
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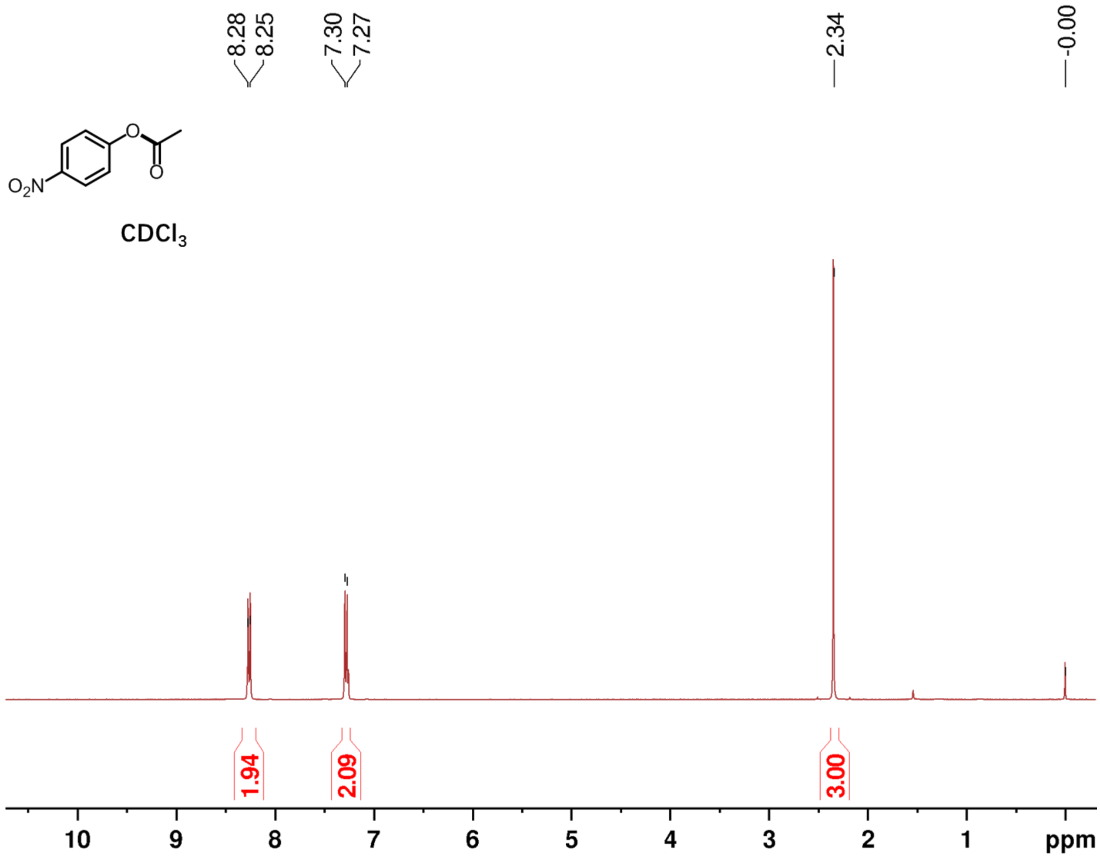
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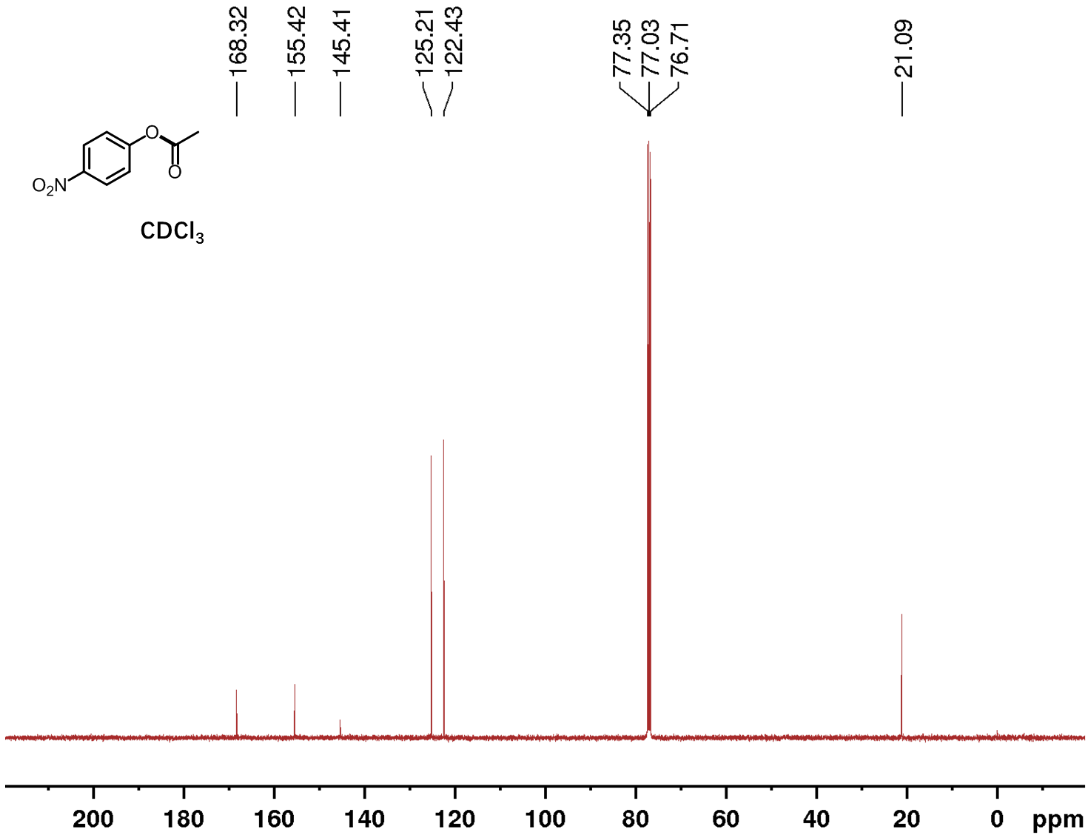
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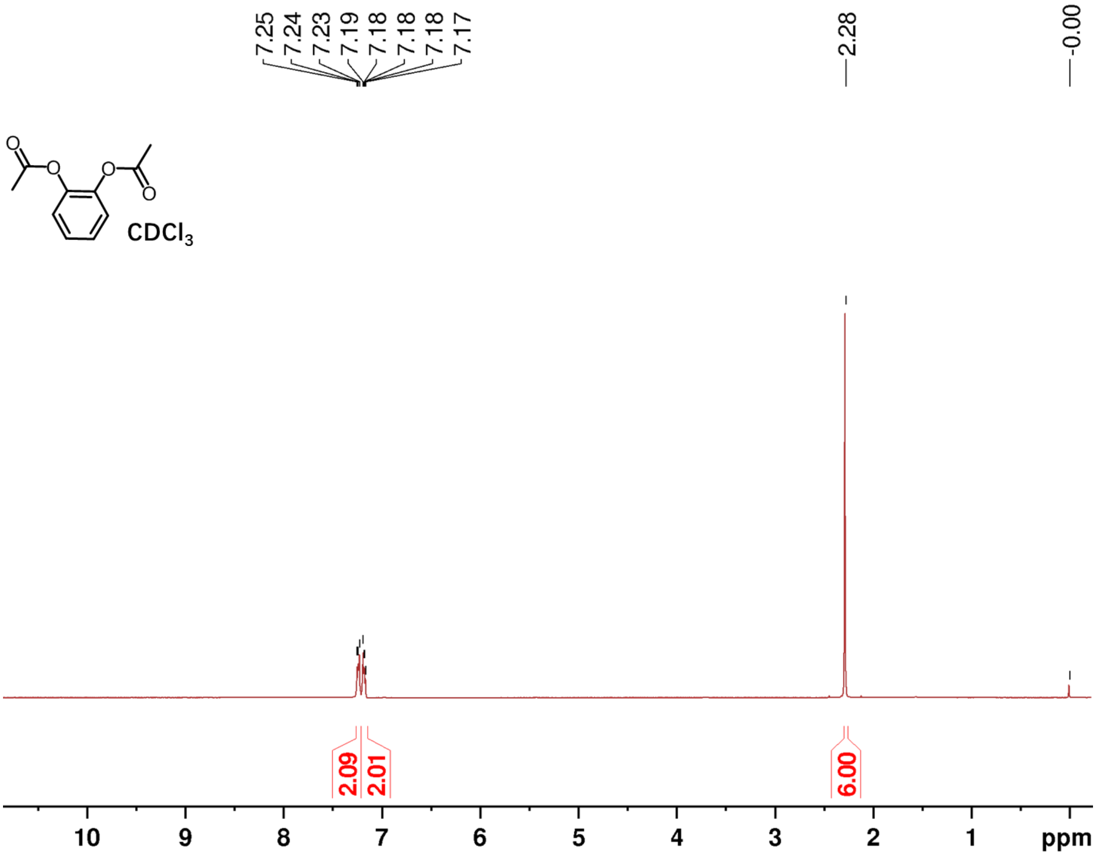
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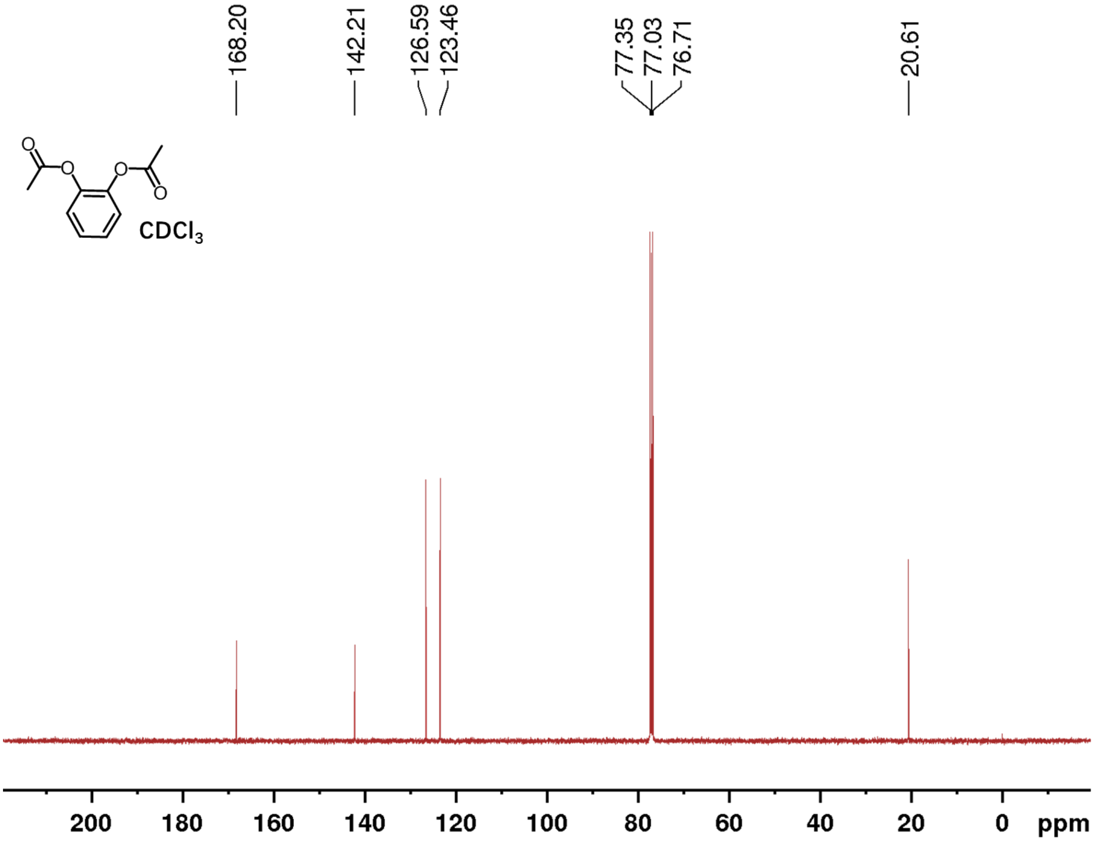
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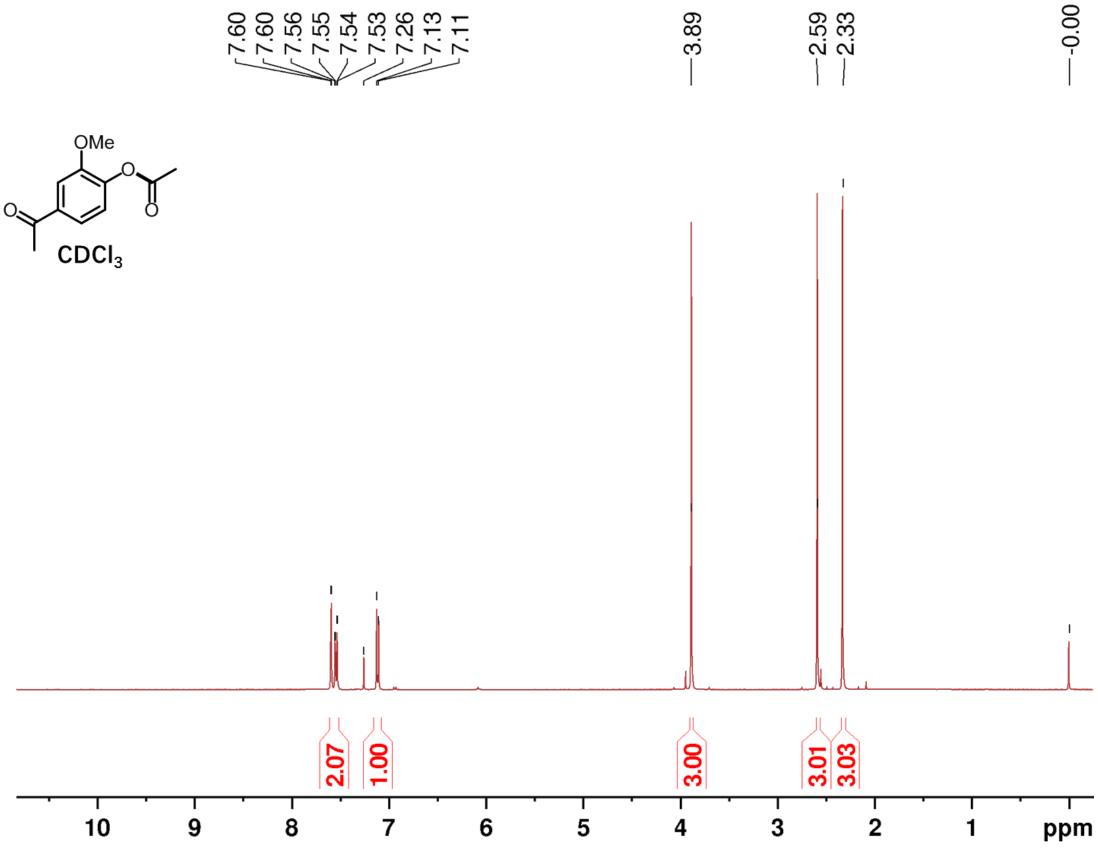
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OMe
O
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O
CDCl$_3$
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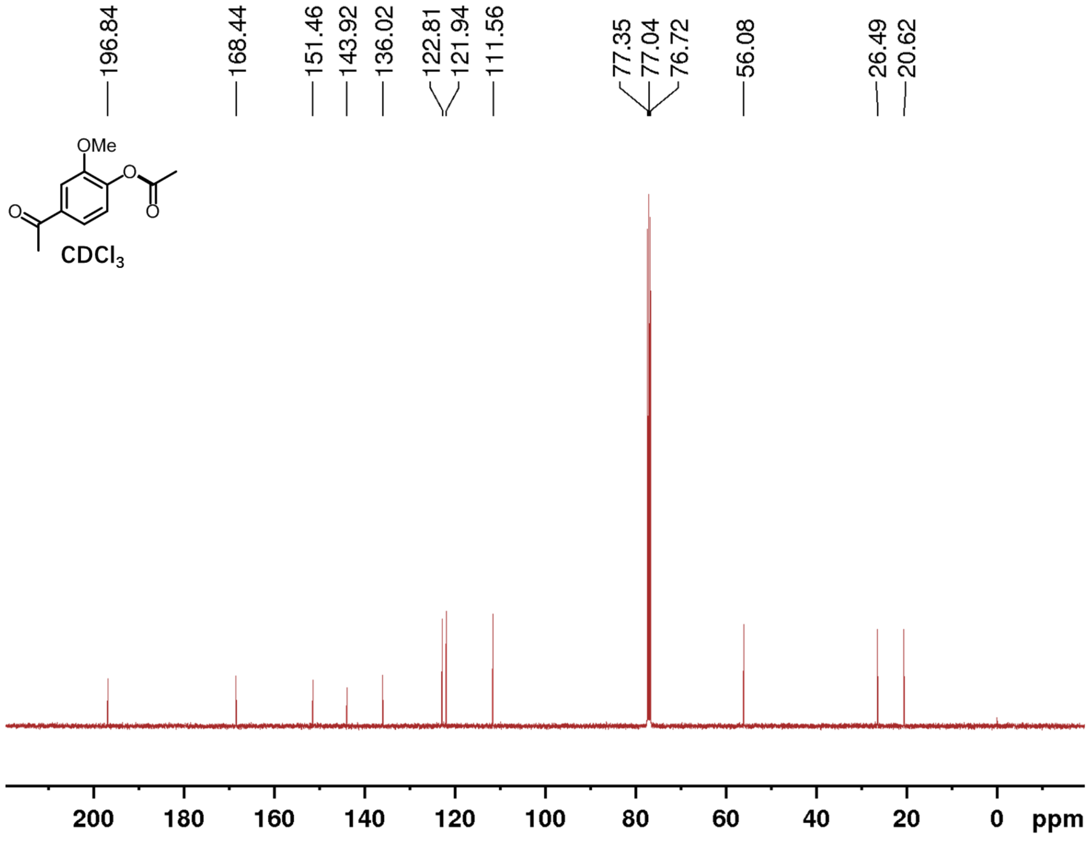
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56.08
26.49
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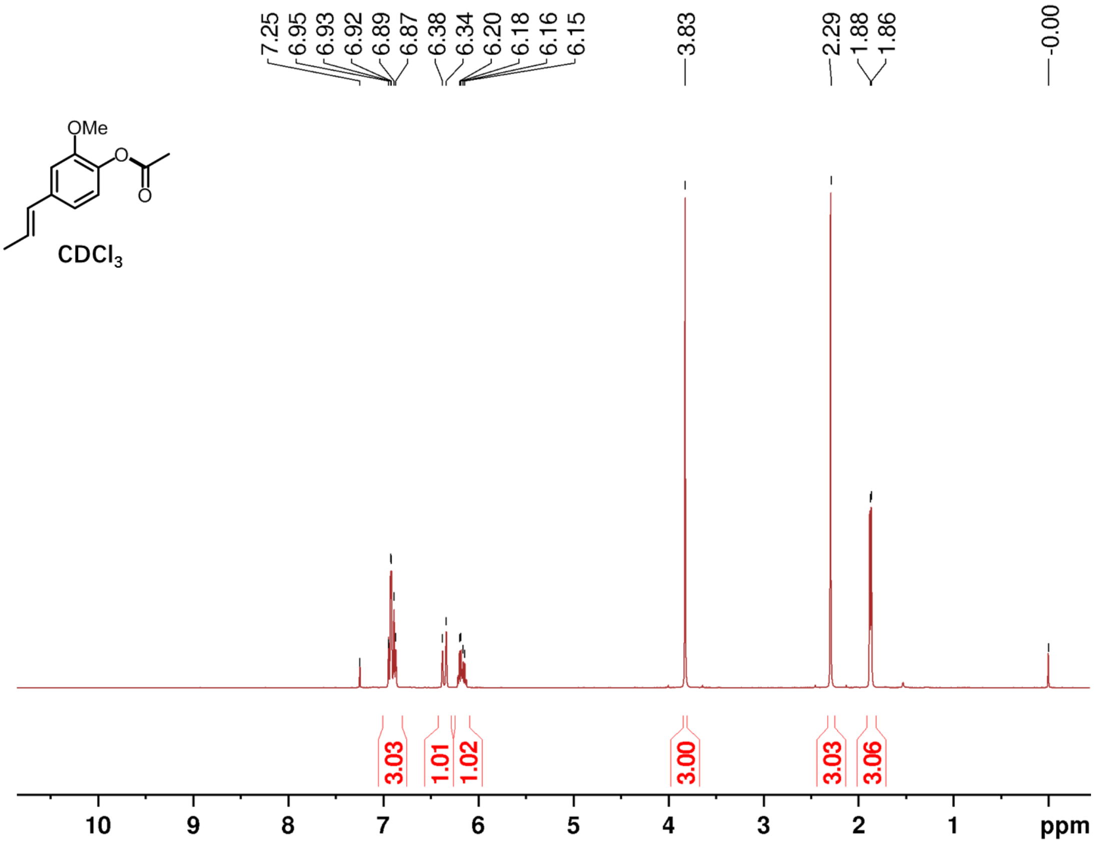
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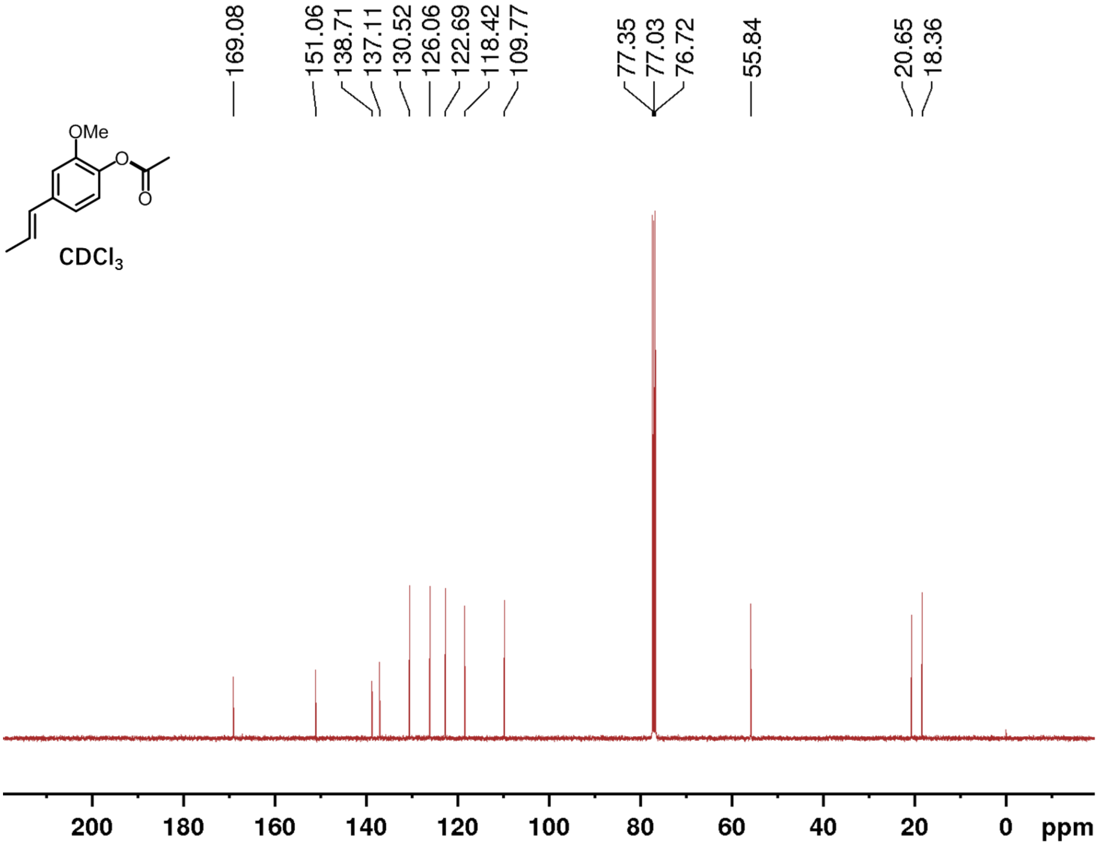
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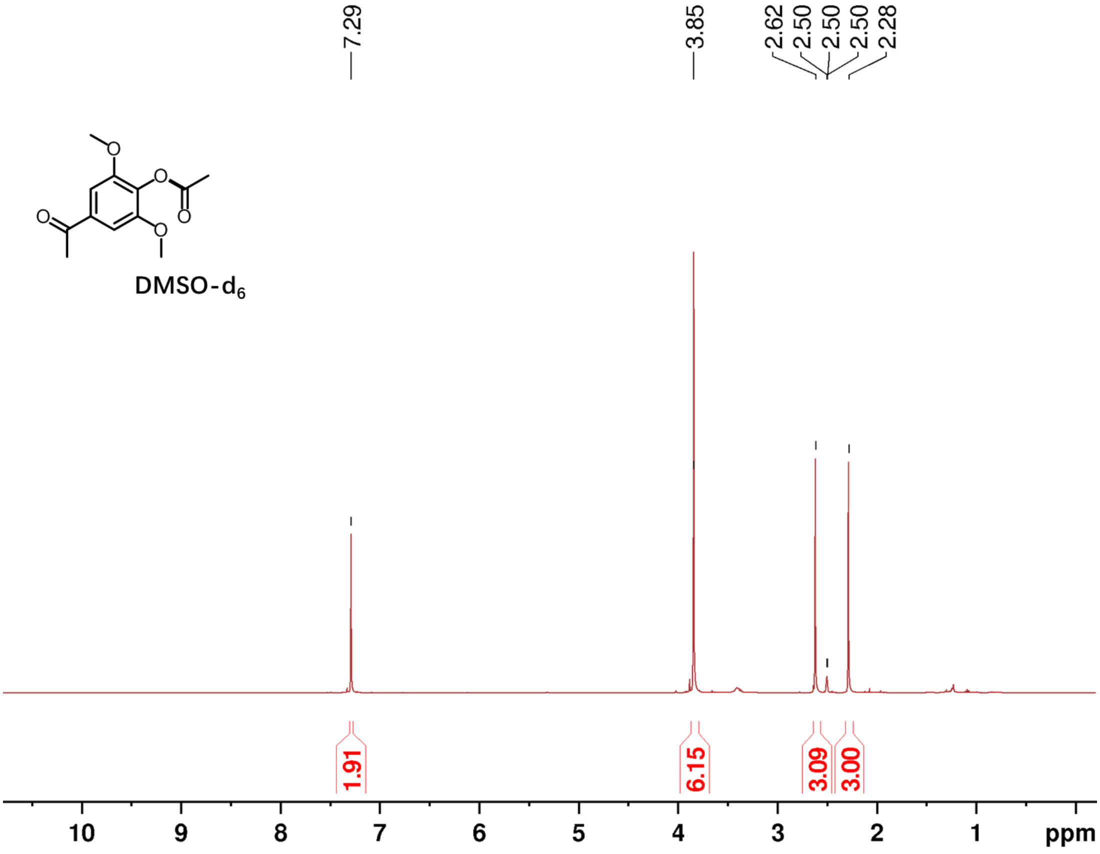
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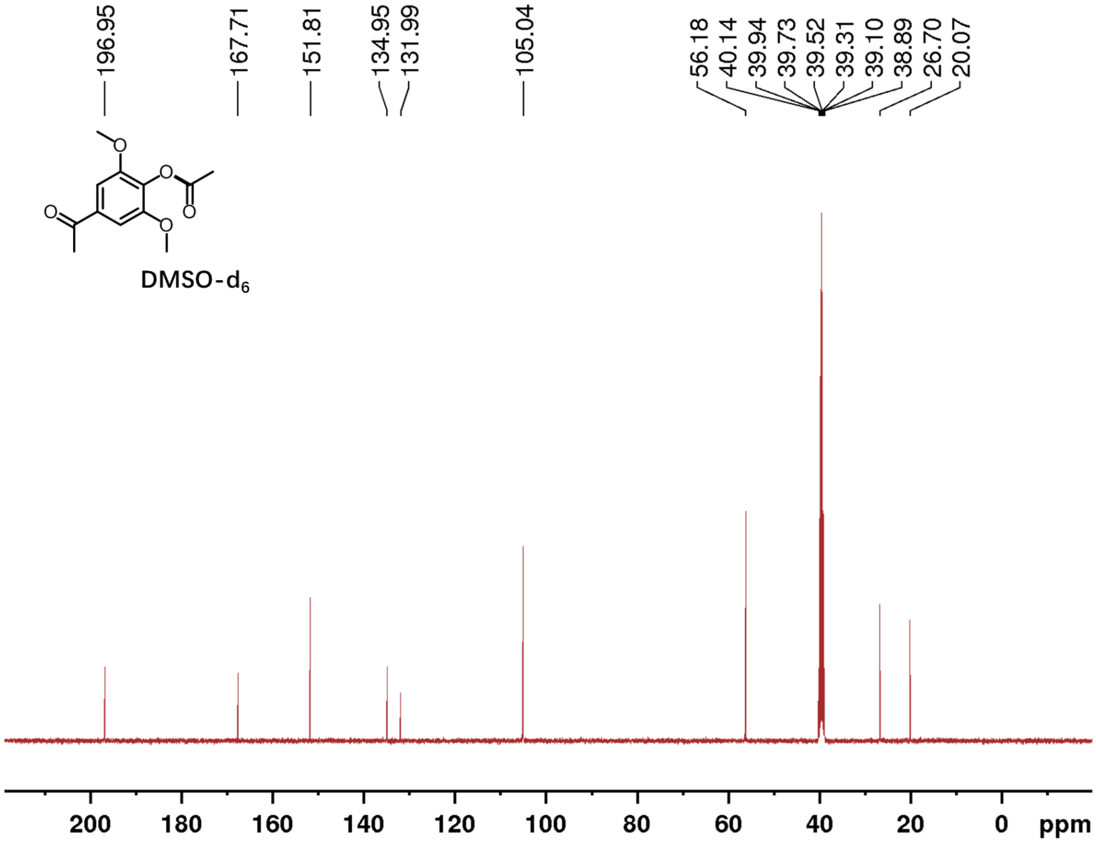
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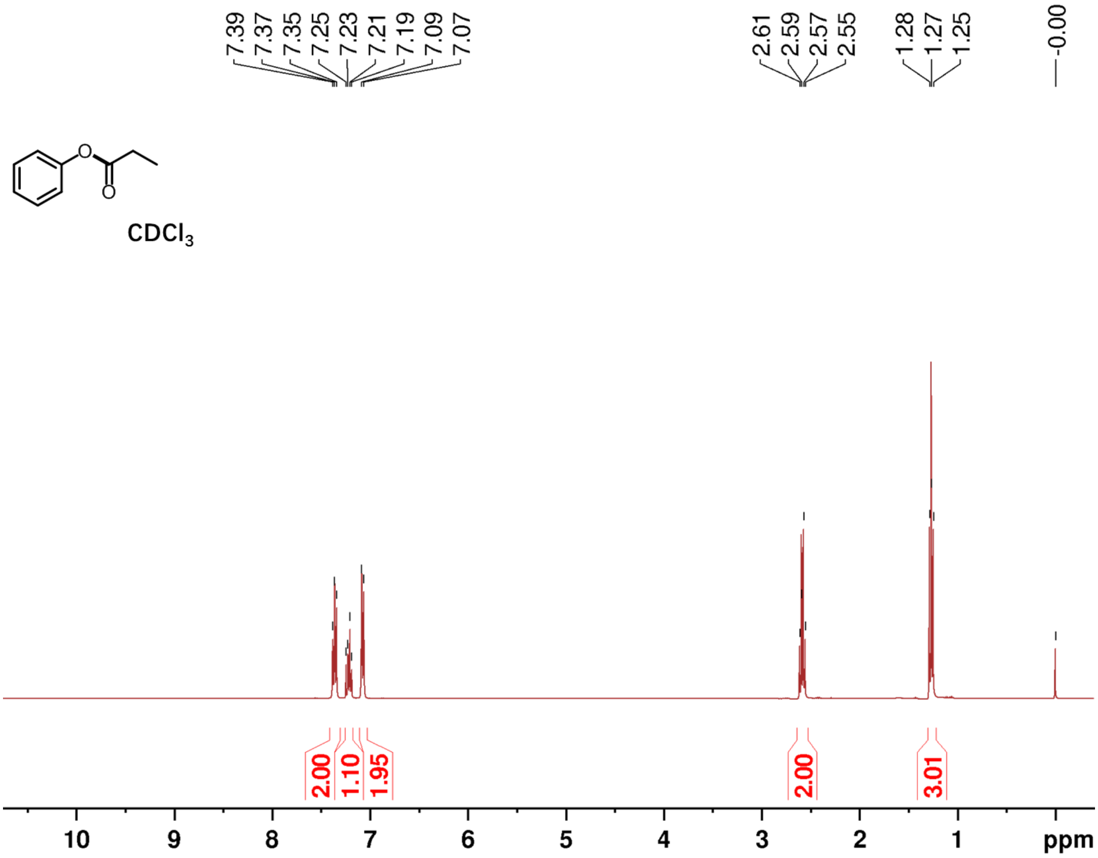
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CDCl$_3$
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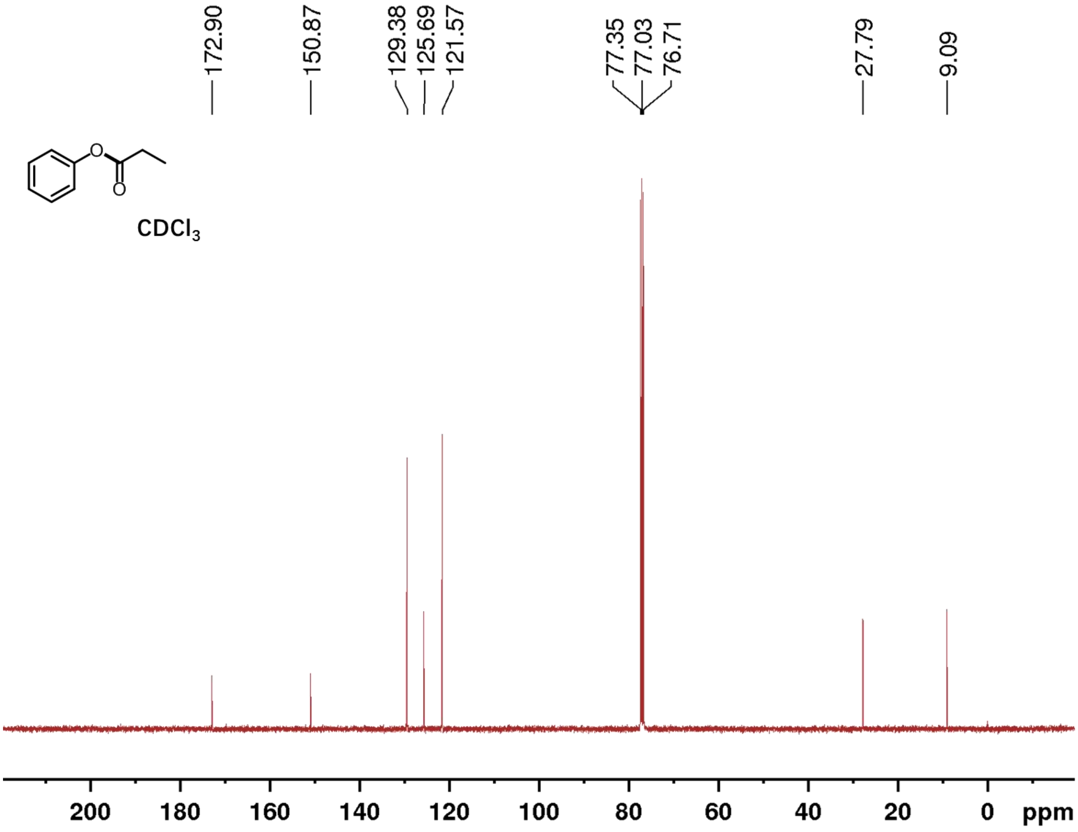
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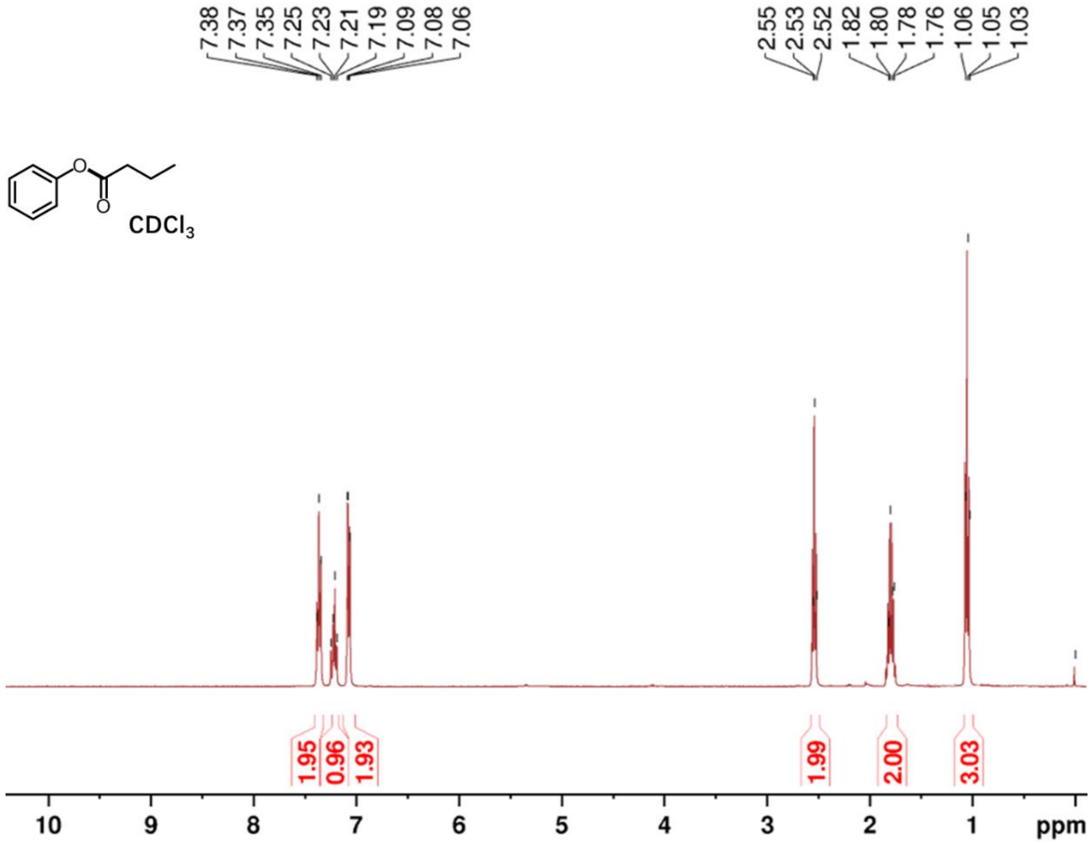
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O
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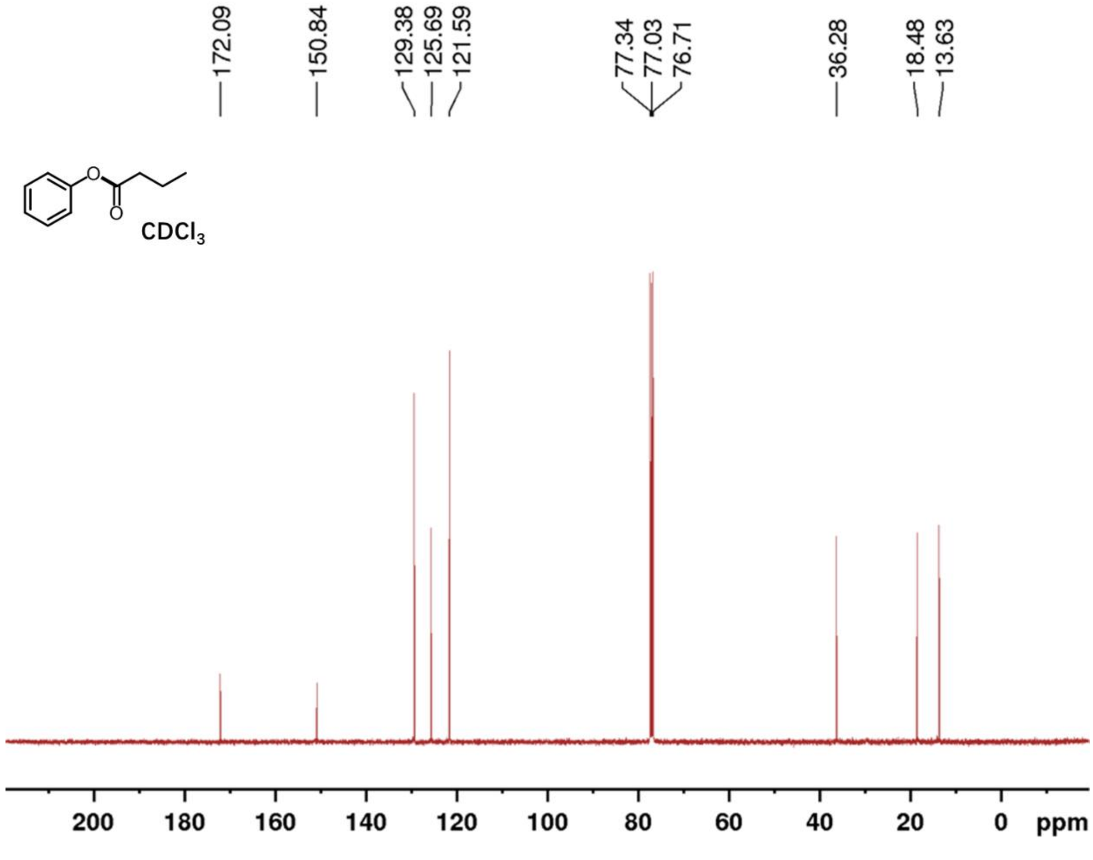
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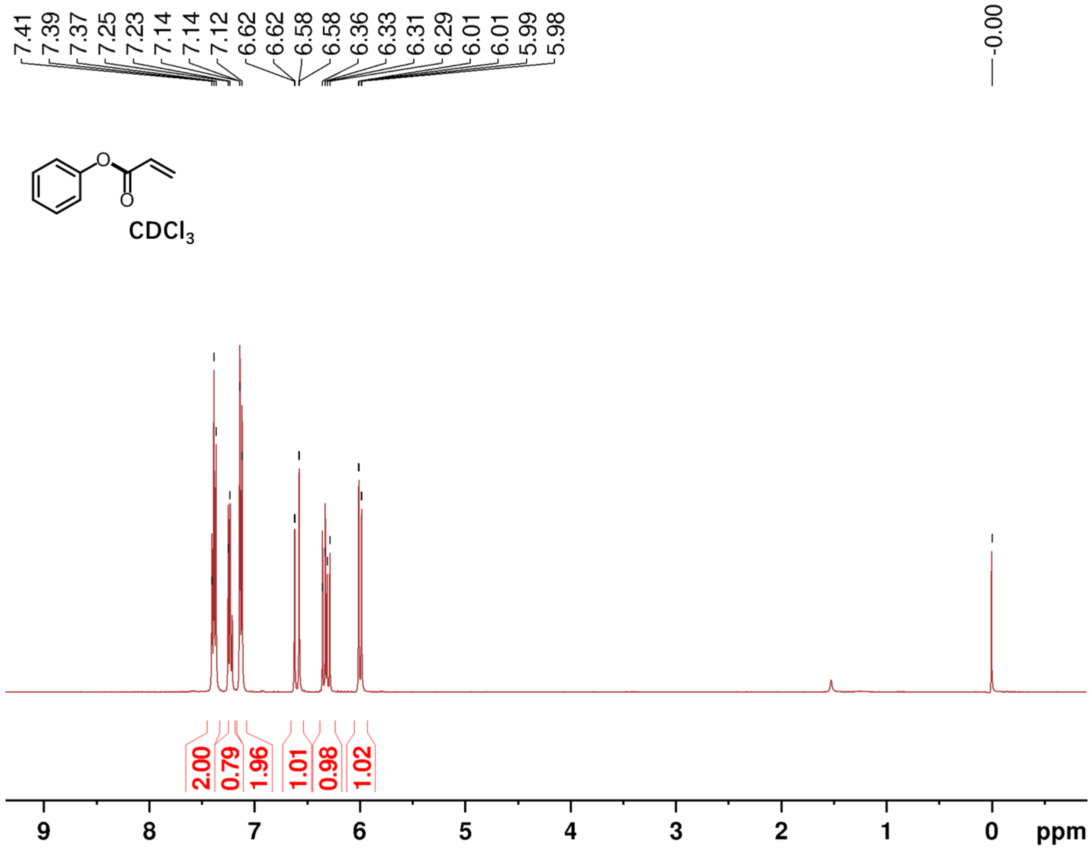
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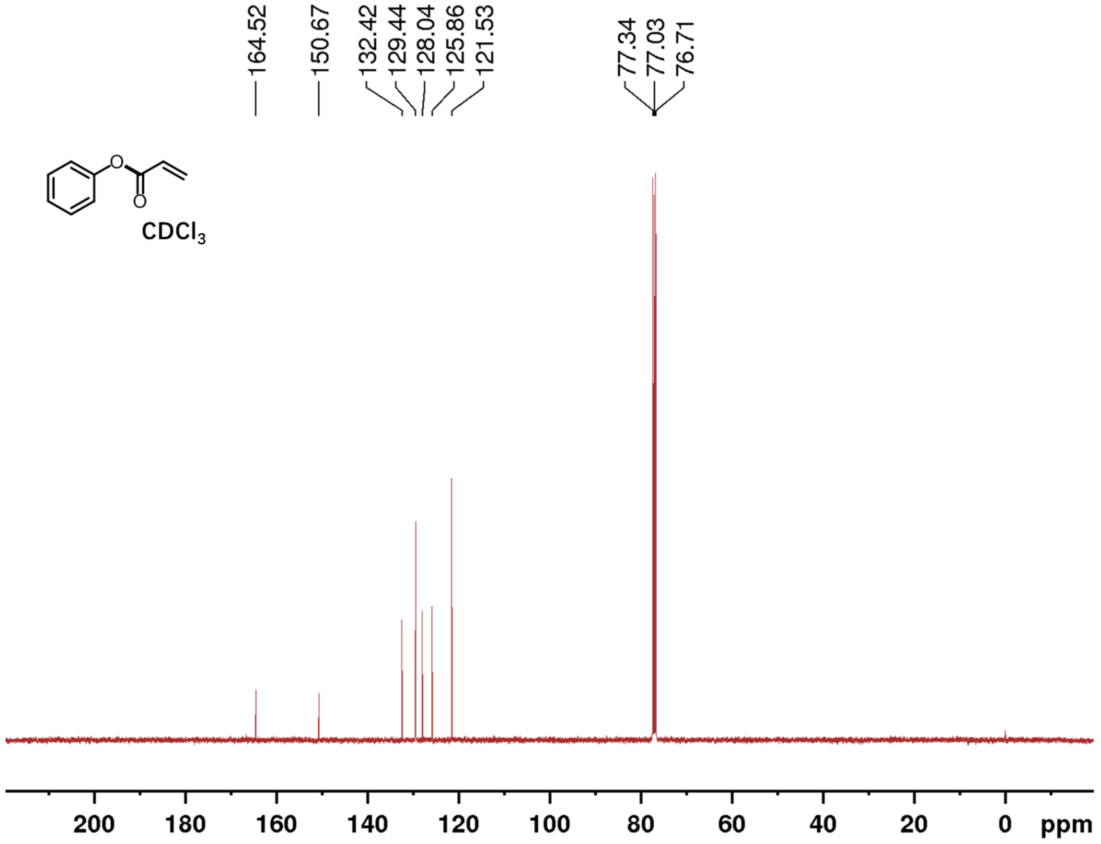
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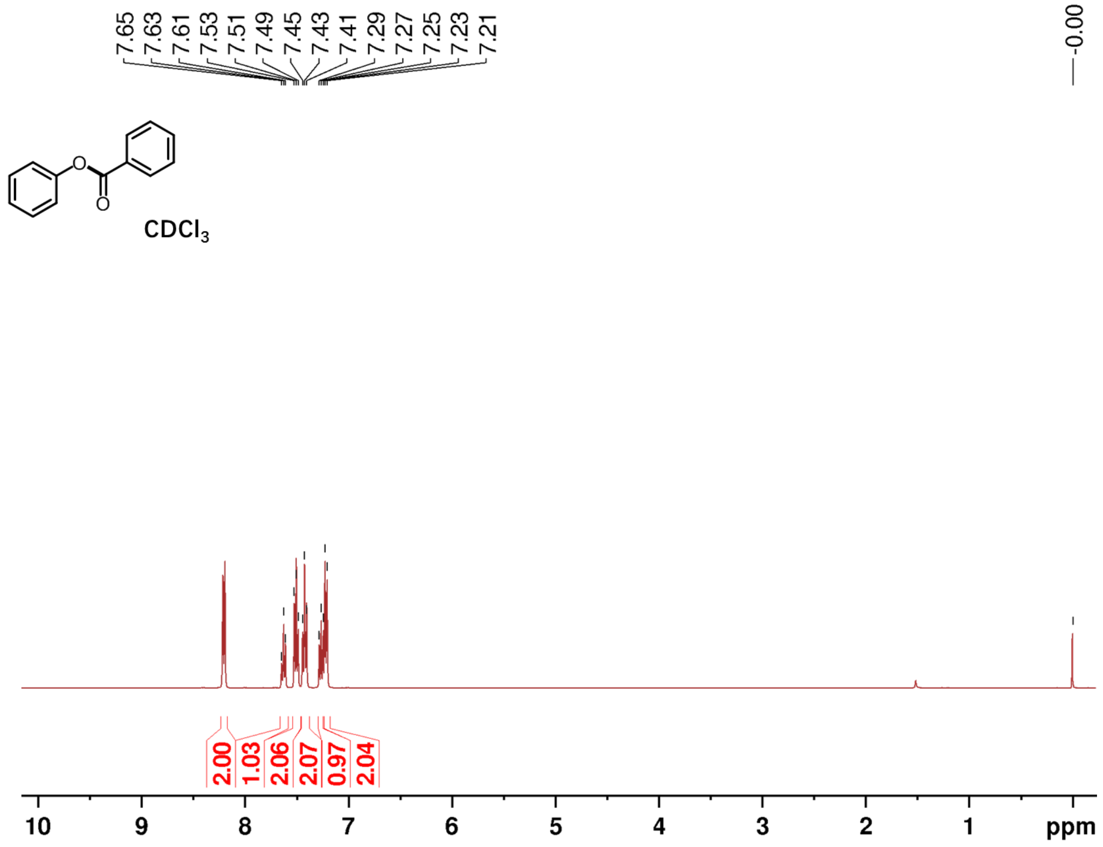
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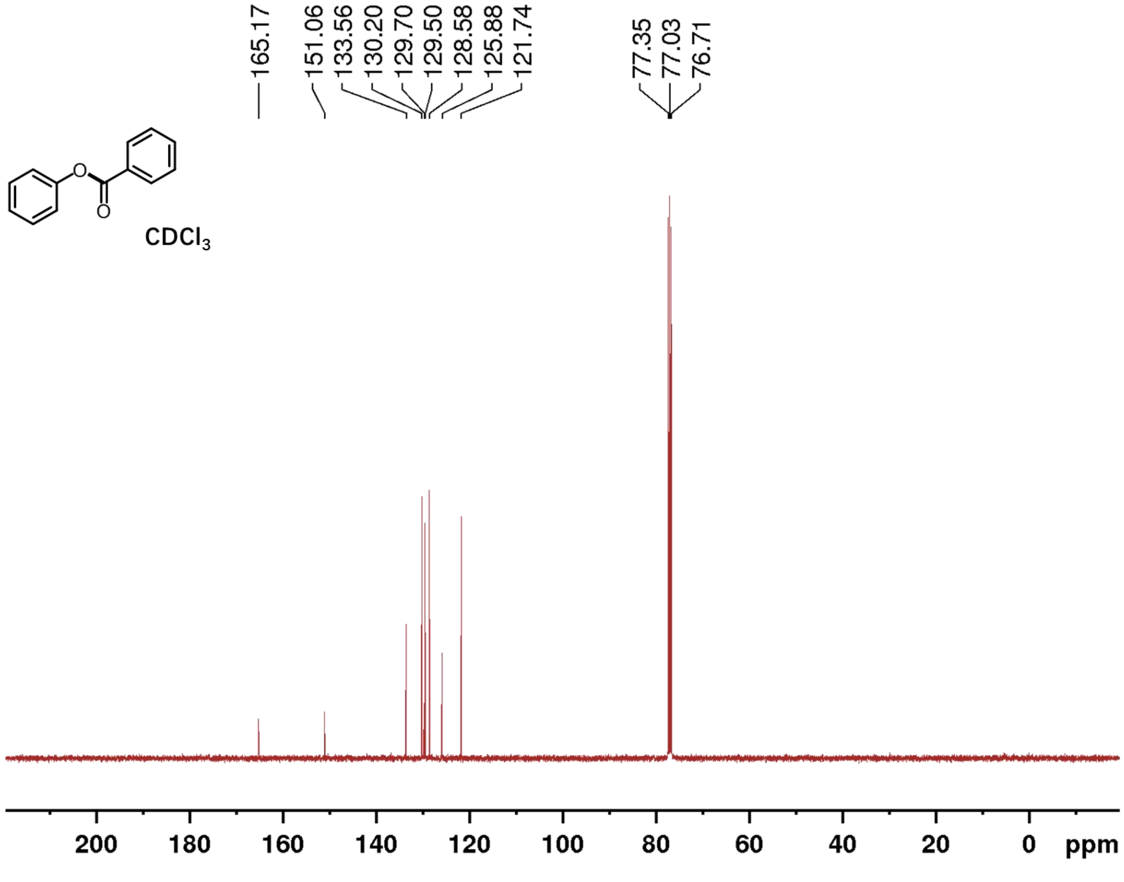
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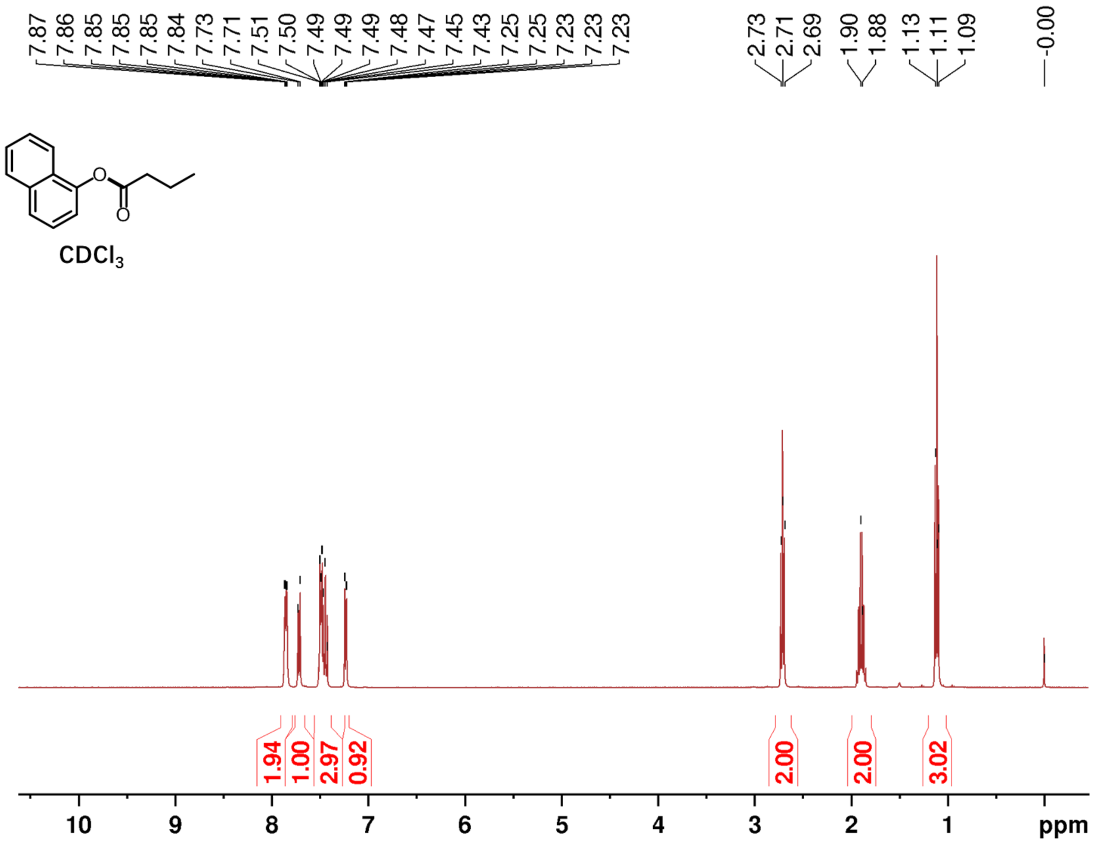
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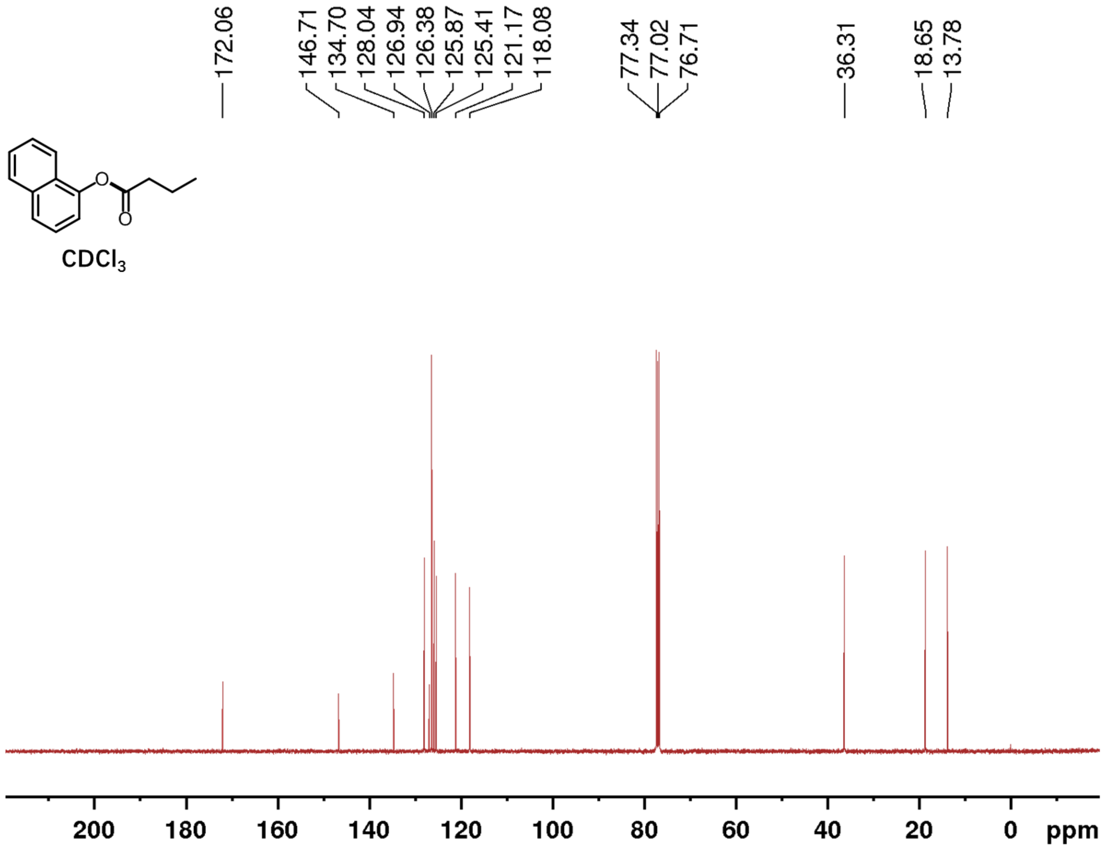
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76.71
36.31
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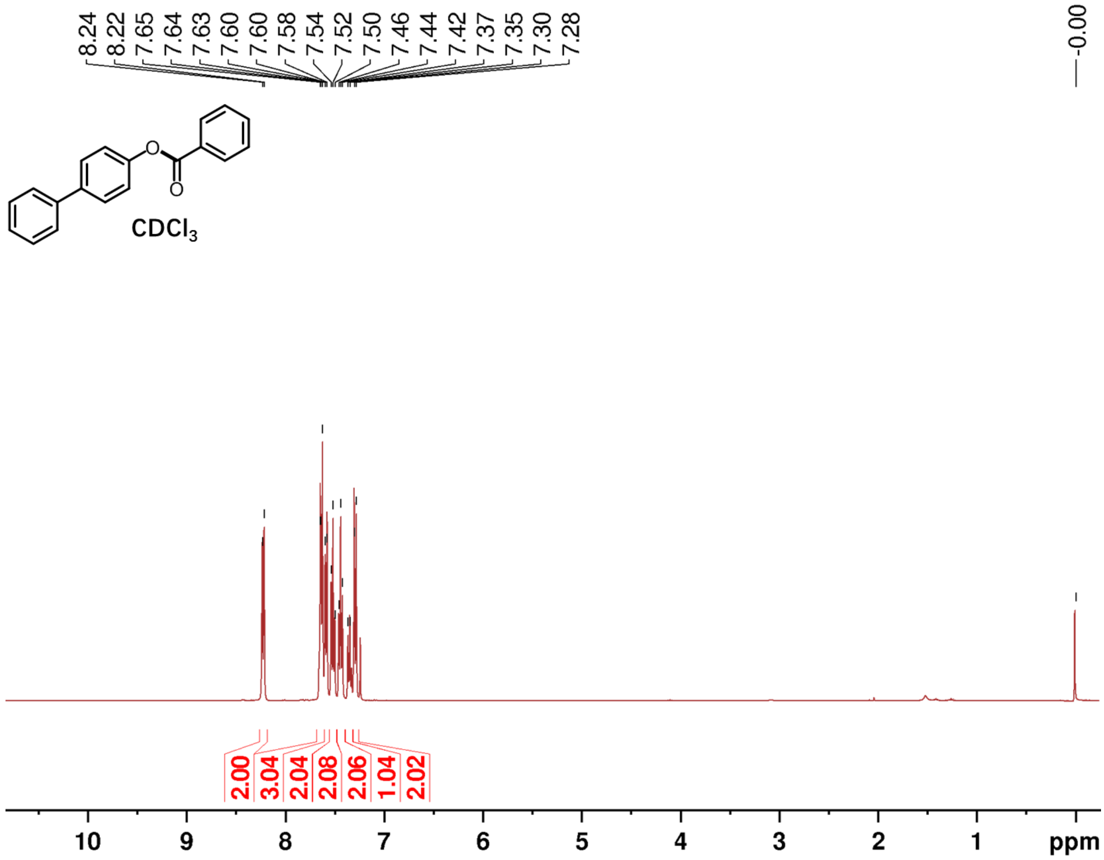
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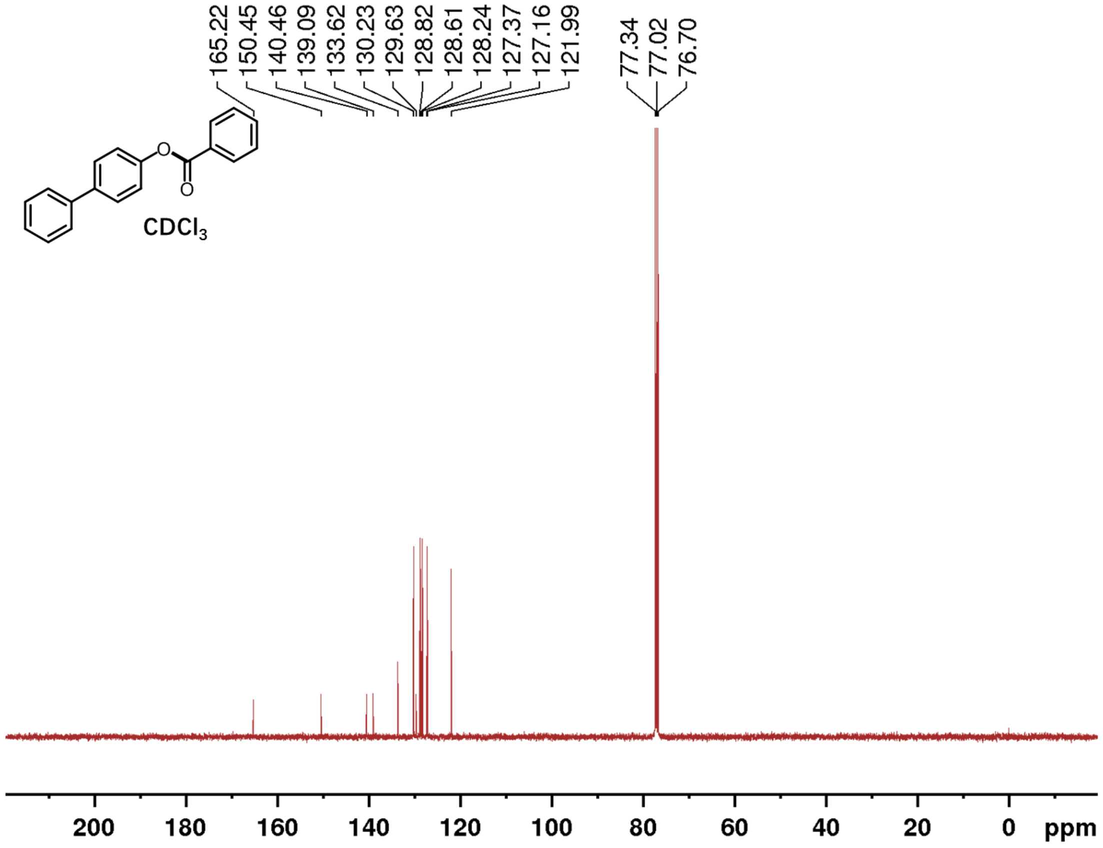
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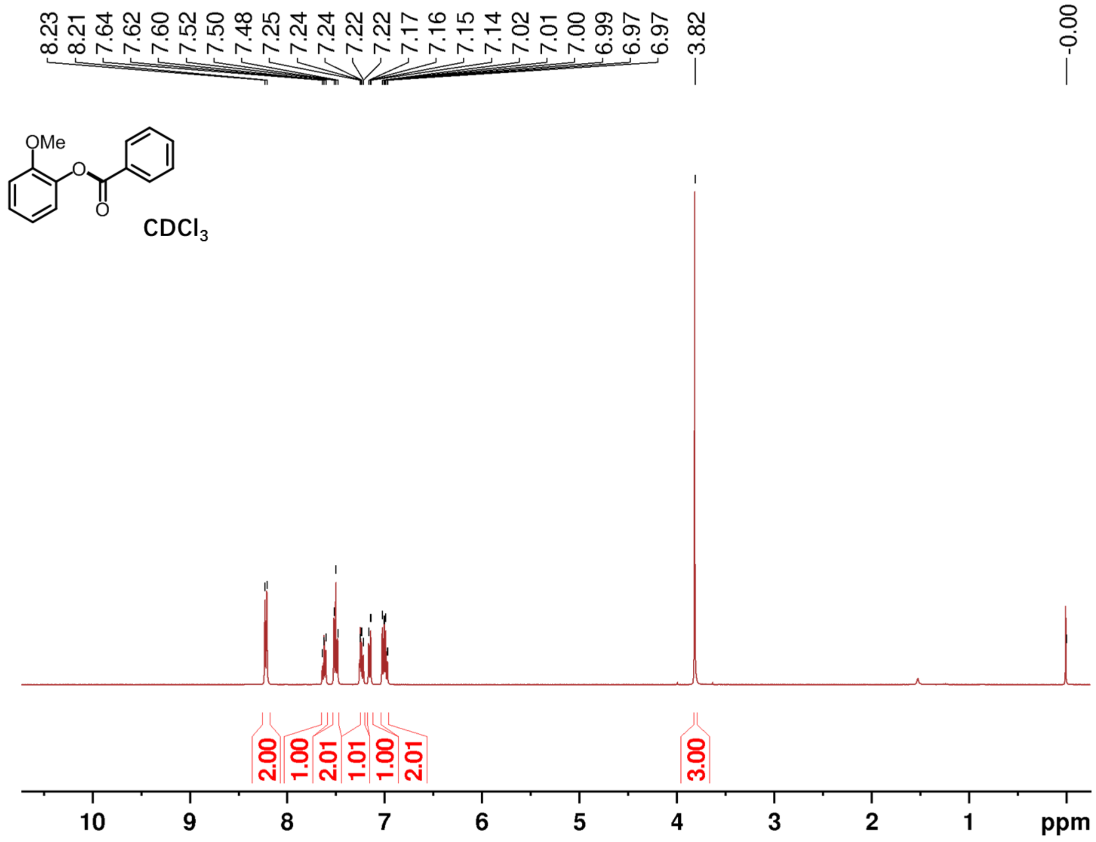
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7.14
7.02
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6.97
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OMe
O
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CDCl$_3$
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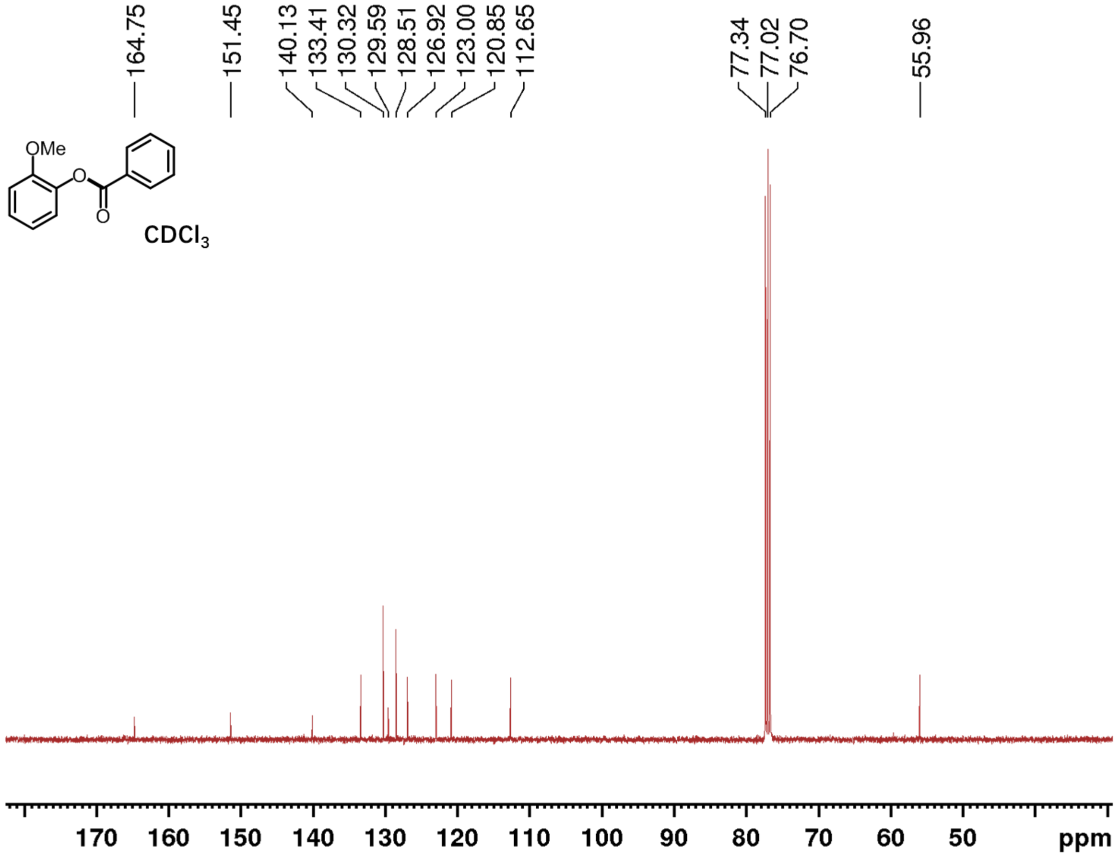
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77.02
76.70
55.96
OMe
O
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CDCl$_3$
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ppm