Rh-catalyzed C-H Alkylation Enabling Modular Synthesis of CF_3-substituted Benzannulated Macrocyclic Inhibitors of B cell responses

Tao Sun, [a]+ Shijun He,[b,c]+ Zhongliang Xu,[b] Jianping Zuo,[b,c] Yang Yu,*[a] and Weibo Yang*[b,c,d]

[a] Center for Supramolecular Chemistry and Catalysis and Department of Chemistry, Shanghai University, 99 Shang-Da Road, Shanghai 200444, China

[b] Chinese Academy of Sciences Key Laboratory of Receptor Research, Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, Shanghai, China

[c] University of Chinese Academy of Sciences, Beijing 100049, China

[d] School of Pharmaceutical Science and Technology, Hangzhou Institute for Advanced Study, University of Chinese Academy of Sciences, Hangzhou 310024, China.

Contents:

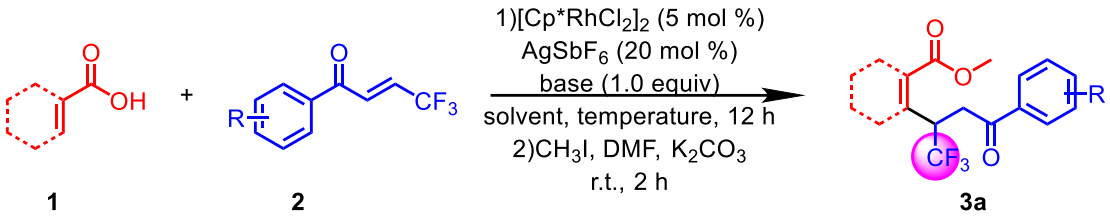
General comments:

NMR spectra were recorded at room temperature on the following spectrometers: Bruker Avance III 400 Spectrometer (400 MHz) and Bruker Avance III 500 (Cryo) Spectrometer (500 MHz). Chemical shifts are given in ppm and coupling constants in Hz. 1H spectra were calibrated in relation to the reference measurement of TMS (0.00 ppm). ^{13}C spectra were calibrated in relation to deuterated solvents. The following abbreviations were used for ^{1}H NMR spectra to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as combinations of them. For HRMS data, the ESI-positive method was applied on the Agilent G6520 Q-TOF. Chemicals were purchased from commercial suppliers. Unless stated otherwise, all the substrates and solvents were purified and dried according to standard methods prior to use. All the compounds as stock solution were dissolved with 100% dimethyl sulfoxide (DMSO, Sinopharm, China) and diluted with RPMI 1640 medium (Gibco, Grand Island, NY, USA) containing 10% fetal bovine serum (FBS) (Hyclone, South Logan, UT, USA). Thiazolyl Blue Tetrazolium Bromide (MTT) were obtained from Sigma-Aldrich (St.Louis.MO.USA); Concanavalin A (ConA) and lipopolysaccharide (LPS, Escherichia coli O55:B5) were purchased from Sigma (St. Louis, MO, USA), [^{3}H] thymidine was purchased from Perkin-Elmer (Waltham, MA, USA).

General procedure for the synthesis of *β*-trifluoromethyl-*α,β*-enones

β-trifluoromethyl-*α,β*-enones was synthesized according to literature procedure[1]. For example, pyrrolidine (1.8 mL, 21 mmol), trifluoroacetaldehyde hemiacetal (3.9 mL, 30 mmol) and the corresponding acetophenone (30 mmol) were dissolved in toluene. The mixture was heated at 120 °C until starting material was completely reacted (TLC). Then, the solvent was removed under reduced pressure and the resulting product was chromatographed on silica gel eluting with petroleum ether-EtOAc to afford the desired *β*-trifluoromethyl-*α,β*-enones 2**a-l**.

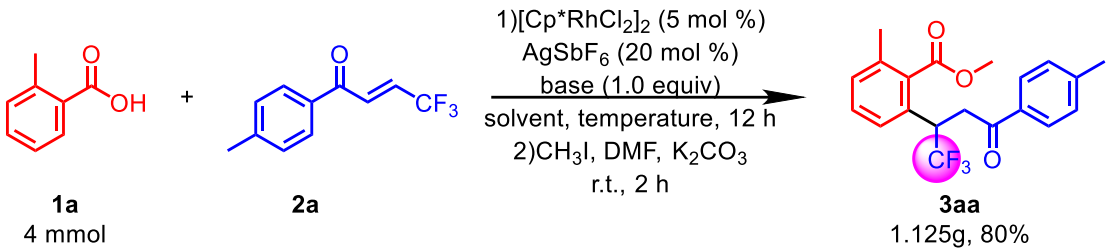
General procedure for C-H activation



1 **2** **3a**

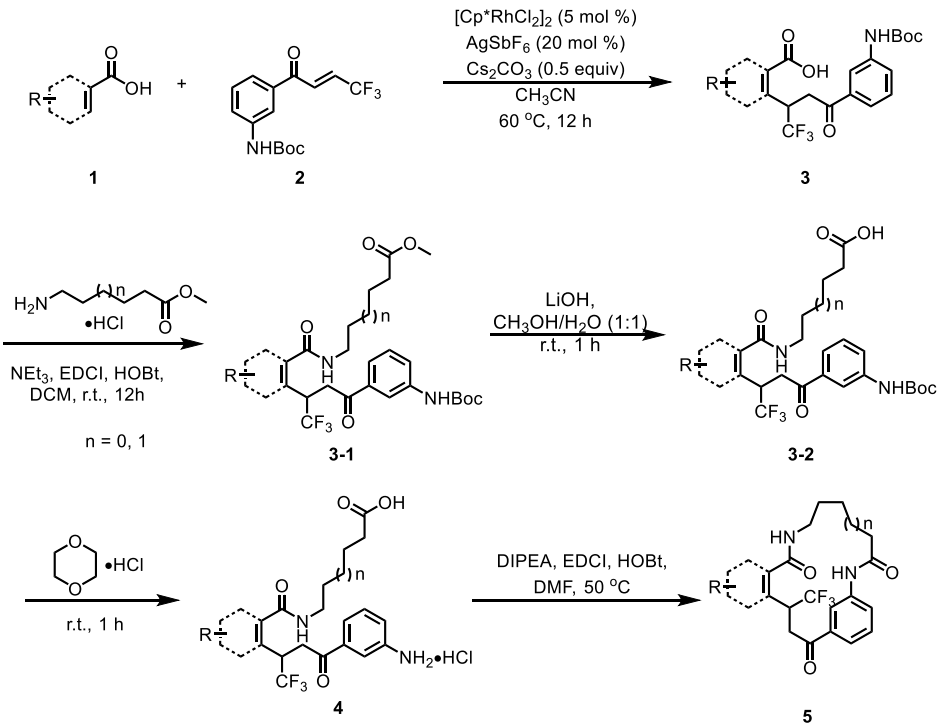
To the solution of the **1** (0.1 mmol, 1.0 equiv) in CH_3CN (0.6 mL), **2** (0.15 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), $AgSbF_6$ (20 mol %), Cs_2CO_3 (0.5 equiv) was added. The solution was stirred at 60 °C for 12 hours. The reaction progress was monitored by TLC. When the starting material disappeared, the solvent was removed under reduced pressure, CH_3I (3.0 equiv), K_2CO_3 (1.0 equiv) and DMF were added. The solution was stirred at room temperature for 2 hours. The reaction was quenched with water, and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography silica gel afford the corresponding **3a**.

Reaction in gram scale of 3aa



To the solution of the **1a** (4 mmol, 1.0 equiv) in CH_3CN (24 mL), **2a** (6 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), $AgSbF_6$ (20 mol %), Cs_2CO_3 (0.5 equiv) was added. The solution was stirred at 60 ^oC for 12 hours. The reaction progress was monitored by TLC. When the starting material disappeared, the solvent was removed under reduced pressure, CH_3I (3.0 equiv), K_2CO_3 (1.0 equiv) and DMF were added. The solution was stirred at room temperature for 2 hours. The reaction was quenched with water, and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography silica gel afford the 1.125 g (yield = 80%) **3aa**.

General procedure for the synthesis of construction of functional CF_3-supported benzannulated macrolactams



Reaction conditions: 1) **1** (0.1 mmol), **2** (0.15 mmol), $[Cp^*RhCl_2]_2$ (5 mol %), $AgSbF_6$ (20 mol %), Cs_2CO_3 (0.5 equiv), CH_3CN (0.6 mL) at 60 °C under air for 12 h; 2) **3** (0.3 mmol), amino acid esters (0.45 mmol), EDCI (1.2 equiv), HOBt (1.5 equiv), NEt_3 (4.5 equiv), DMF (3 mL) at r.t. under air for 12 h; 3) $CH_3OH/THF/H_2O$ (1 mL:1 mL:1 mL), LiOH (10 equiv); 4) hydrogen chloride-1,4-dioxane; 5) EDCI (1.2 equiv), HOBt (1.5 equiv), NEt_3 (4.5 equiv), DMF (60 mL) at 50 °C under air for 12 h.

To the solution of the **1** (0.1 mmol, 1.0 equiv) in CH_3CN (0.6 mL), **2** (0.15 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), $AgSbF_6$ (20 mol %), Cs_2CO_3 (0.5 equiv) was added. The solution was stirred at 60 °C for 12 hours. The reaction progress was monitored by TLC or HPLC/MS (some reactions are difficult to be monitored by TLC, so MS was used instead of TLC). When the starting material disappeared, the reaction was quenched with water, and extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography silica gel afford the corresponding **3**.

3 (0.3 mmol, 1.0 equiv), amino acid (0.45 mmol, 1.5 equiv), EDCI (0.36 mmol, 1.2 equiv), HOBt (0.45 mmol, 1.5 equiv), NEt_3 (1.35 mmol, 4.5 equiv) were dissolved in DMF (3 mL). The mixture was stirred at r.t. under air for 12 h. The reaction progress was monitored by TLC, when the starting material disappeared, the reaction was quenched with water, and extracted with EtOAc. The combined organic layers were washed with water and brine solution in turns, dried over Na_2SO_4. After being filtered, the organic phase was concentrated and purified by flash chromatography silica gel afford the desired product **3-1**.

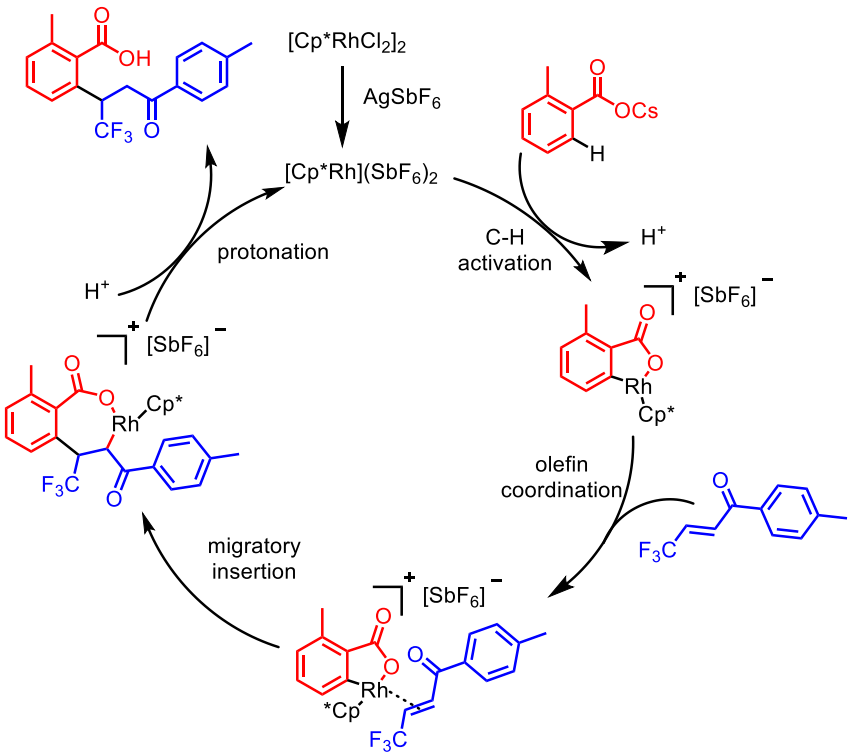
MeOH (0.7 mL) and THF (0.7 mL) was added to give a solution of **3-1**, then LiOH (10 equiv) in H_2O (0.7 mL) was added. The mixture was stirred at ambient temperature for 1 h. After removed solvent in vacuum, DCM was added and adjust pH = 3~4 by HCl (1 M). Hereafter, the resulting solution was concentrated under reduced pressure to afford crude product **3-2** without further purification.

The product **3-2** was dissolved in hydrogen chloride-1,4-dioxane (3 mL)， after stirred at ambient temperature for 1 h, the reaction was monitored by HPLC/MS,

when the starting material disappeared, the resulting solution was concentrated under reduced pressure to afford product **4** without further purification.

The resulting product **4** was dissolved in DMF (60 mL), then EDCI (1.2 equiv) and HOBt (1.5 equiv), NEt_3 (4.5 equiv) was added. After stirred overnight at 50 ^oC, the reaction progress was monitored by HPLC/MS, when the starting material disappeared, the reaction was quenched with water, and extracted with EtOAc. The combined organic layers were washed with water and brine solution in turns, dried over Na_2SO_4. After being filtered, the organic phase was concentrated and purified by flash chromatography silica gel afford the desired product **5**.

Plausible reaction mechanism



Biological assay

Animals

Inbred 6 to 8-week-old female BALB/c mice were purchased from Shanghai Jiesijie Experimental Animal Co., Ltd. (Certificate No. 2018-0004, China). The mice were housed under specific pathogen-free conditions with a controlled environment (12

hours of light/12 hours of dark cycle, 22±1 °C, 55±5% relative humidity). All mice were fed standard laboratory chow and water ad libitum and allowed to acclimatize in our facility for one week before any experiments started. All experiments were carried out according to the National Institutes of Health Guide for Care and Use of Laboratory Animals and were approved by the Bioethics Committee of the Shanghai Institute of Materia Medica (IACUC Protocol #2020-03-ZJP-120).

Splenocytes preparation

Mice were sacrificed and their spleens were isolated aseptically. The spleens were ground up, and a single cell suspension was prepared after cell debris and clumps were removed. Erythrocytes were depleted with ammonium chloride buffer solution. Cells were washed and suspended in RPMI 1640 media containing 10% FBS, penicillin (100 U/mL), and streptomycin (100 μg/mL). Cells were counted by trypan blue exclusion.

Cell viability assay

Splenocytes (8×10^5 /well) were seeded in the 96-well plates in triplicate with 1640 media containing 10% FBS, penicillin (100 U/mL), and streptomycin (100 μg/mL) in presence or absence of indicated concentrations of compounds, then the cells were cultured in a humidified, 37^{o}C, 5% CO_2-containing incubator for 48 hours. MTT solution was added to each well at a final concentration of 0.5mg/mL, and incubated for 4 hours before the end of culture. The quantity of formazan (presumably directly proportional to the number of viable cells) is measured at 570 nm with a microplate reader (Molecular Devices, Sunnyvale, CA, USA) and the cell viability was calculated.

Splenocytes proliferation assay

Splenocytes (5×10^5/well) were cultured in 96-well plates in triplicate with 1640 media containing 10% FBS, penicillin (100 U/mL), and streptomycin (100 μg/mL) in the presence or absence of indicated concentrations of compounds and stimulated

with 1 μg/mL of Con A or 10 μg/mL of LPS, respectively. Cells were maintained in a humidified, 37 ºC, 5% CO_2-containing incubator for 48 hours and pulsed with 0.5 μCi/well of [^{3}H] thymidine 8 h in advance of the end of culture. Cells were harvested onto glass fiber filters after freeze and thaw. The incorporated radioactivity was counted using a Beta Scintillation Counter (PerkinElmer Life Sciences, Boston, MA).

B cell purification and in vitro stimulation

After mononuclear cell suspension preparation, mouse splenic polyclonal $CD19^+$ B cells were isolated using PE-conjugated anti-CD19 Ab (BD Pharmingen, San Diego, CA, USA), anti-PE MicroBeads (Miltenyi Biotec GmbH, Bergisch Gladbach, Germany) and positively selected by a magnetic cell-sorting protocol (Miltenyi Biotec GmbH, Bergisch Gladbach, Germany). The purity of the resultant cell population was determined by flow cytometry analysis and was consistently 98%. Purified B cells were then cultured with medium alone or with the TLR4 ligand LPS (10 μg/ml) or anti-mouse IgM (10 μg/mL) plus anti-mouse CD40 (2.5 μg/mL). After incubation, for activation assays, cells were analyzed on flow cytometry at 24 h; For antibody secretion assays, cells were cultured for 6 days and the supernatants were collected for further determination.

Flow cytometry analysis

Cells were washed with phosphatebuffered saline and then were blocked with anti-mouse CD16/CD32 Ab (eBioscience) and stained with PerCp-Cy5.5-conjugated anti-mouse CD69 and BV421-conjugated anti-mouse MHC-II. All immunofluorescent mAbs used in this research were obtained from BD Biosciences (Franklin Lakes, NJ, USA). The data were analyzed using FlowJo software (Tree Star, Ashland, OR, USA).

Detection of antibodies

Supernatants were analyzed using a Luminex multiplex assay based suspension bead array (SBA) by a ProcartaPlex mouse antibody isotyping panel 7plex assay kit (EPX070-20815-901 (Invitrogen). Assay plates were read by Luminex 200

Instruments (Luminex, Austin, TX). The concentrations were calculated by the xPONENT software (LUMINEX, Austin, TX, USA). Heat maps were generated using GraphPad Prism 8.0 software.

Statistical analysis

The data from this research study were analyzed using GraphPad Prism 8.0 software. Statistical analysis was performed using oneway ANOVA, and data are presented as the mean ± SD. $P < 0.05$ was considered statistically significant.

Table S1. Inhibitory activity on Con A-induced T and LPS-induced B cell proliferation.

Compound	Cytotoxicity CC_{50} (μM)	Con A stimulation IC_{50} (μM)	LPS stimulation IC_{50} (μM)
5a	>200	42.35	5.50
5b	>200	51.44	12.95
5c	>200	29.23	3.90
5f	>200	97.9	2.24
5h	183.9	35.75	4.82
CsA*	8.38	0.05	0.32

* CsA, cyclosporin A, positive control, with much higher cytotoxicity

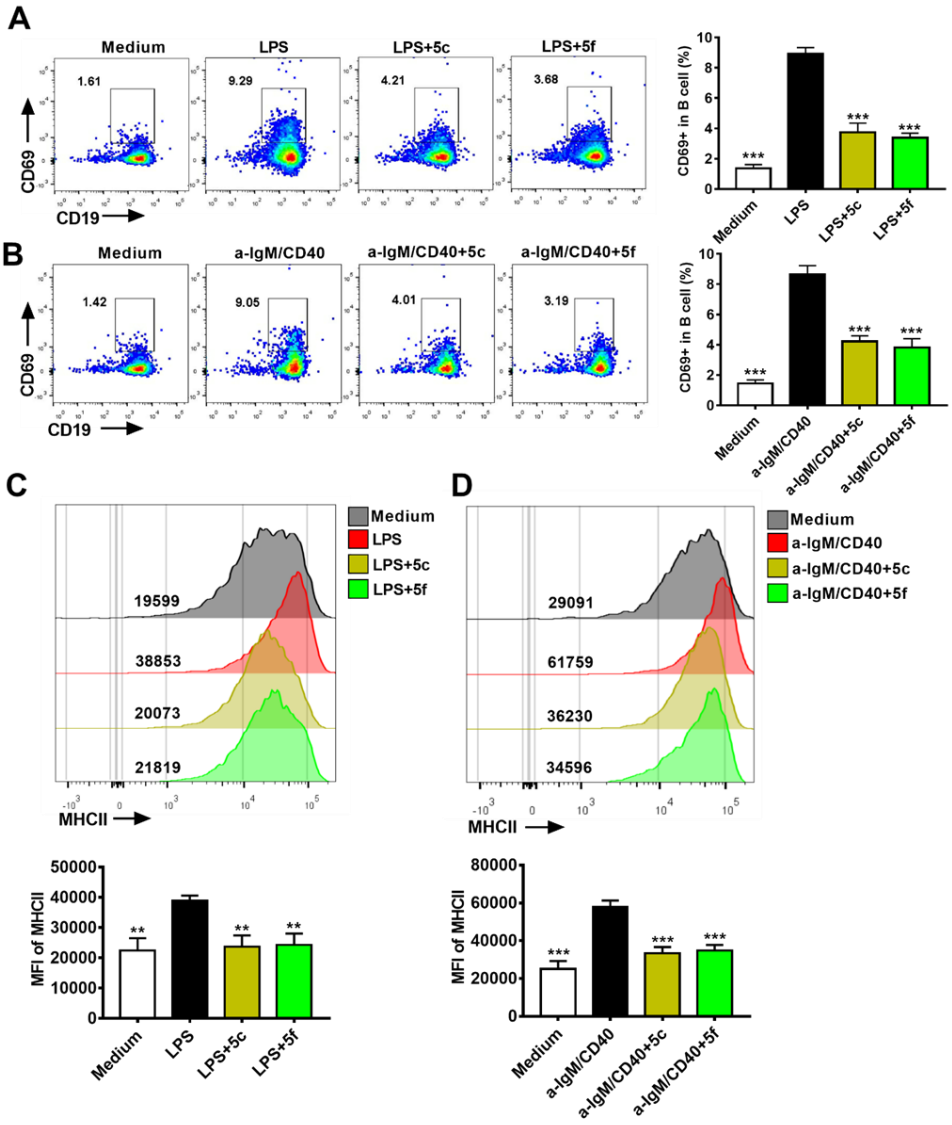


Figure S1. Compounds 5c and 5f impeded the activation and the upregulation of antigen-presenting molecule of LPS and anti-IgM/CD40-primed CD19+ B cells. Primary murine CD19+ B cells were cultured with LPS or anti-mouse IgM and purified hamster anti-mouse CD40 Ab in the absence or presence of compounds 5 μM in 96-well plates for 24 hours to determine B cell activation. Cells were collected and determined the expression of CD69 and MHC-II, and data were shown as the representative dot plots (A and B, left panel) or histograms displaying mean fluorescence intensity (MFI) (C and D, upper panel) and statistics analysis derived from 2 independent experiments with similar results (A and B, right panel for CD69; C and D, lower panel for MHC-II). Numbers inserted in C and D showing the MFI

value of MHCII molecule. Data were shown as mean ± SD, ** $P < 0.01$, ***$P < 0.001$ versus indicated stimuli-conditioned cells.

X-ray molecular structure and Crystallographic Data

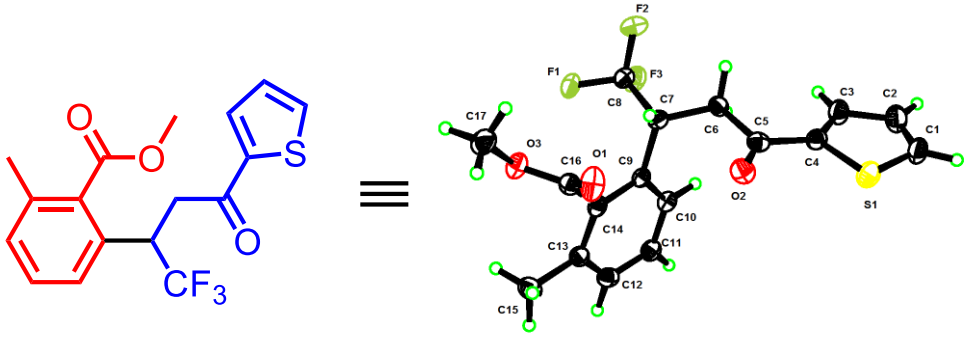


Table S2. Crystal data and structure refinement for 3ai	
Identification code	mo_22020163_0m
Empirical formula	$C_{17}H_{15}F_3O_3S$
Formula weight	356.35
Temperature/K	170.0
Crystal system	triclinic
Space group	P-1
a/Å	9.9842(4)
b/Å	10.3171(3)
c/Å	17.4171(7)
α/°	76.4580(10)
β/°	89.8730(10)
γ/°	70.4810(10)
Volume/Å^3	1638.32(11)
Z	4
ρ_{calcg}/cm^3	1.445
μ/mm^{-1}	0.241
F(000)	736.0
Crystal size/mm^3	0.16 × 0.09 × 0.04

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.324 to 52.846
Index ranges	-12 ⩽ h ⩽ 12, -12 ⩽ k ⩽ 12, -21 ⩽ l ⩽ 21
Reflections collected	18884
Independent reflections	6673 [R_{int} = 0.0465, R_{sigma} = 0.0586]
Data/restraints/parameters	6673/0/437
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0508, wR_2 = 0.1388
Final R indexes [all data]	R_1 = 0.0899, wR_2 = 0.1778
Largest diff. peak/hole / e Å^{-3}	0.22/-0.32

Table S3. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_22020163_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	*x*	*y*	*z*	U(eq)
S2	8527.3(8)	9832.8(8)	693.6(5)	42.9(2)
S1	-721.1(8)	6287.9(9)	8366.1(5)	45.4(2)
F6	5790.4(18)	5997.8(17)	3661.4(10)	44.5(4)
F3	4840.6(18)	8342.5(17)	6866.7(10)	46.5(5)
F4	5884.6(18)	6973.3(19)	4611.5(10)	46.8(5)
F5	4362.1(16)	8109.4(18)	3610.6(10)	46.6(5)
F1	6487.7(17)	6344.6(19)	6921.6(10)	50.8(5)
F2	4625(2)	7025(2)	6115.4(10)	53.9(5)
O3	7962(2)	3561.5(19)	7997.5(12)	38.2(5)
O6	7963(2)	9562(2)	2381.6(12)	38.5(5)
O2	2394(2)	5086.9(19)	8224.0(12)	39.3(5)
O1	6079(2)	2877(2)	8260.9(14)	48.4(6)
O4	7727(3)	8582(2)	4984.8(13)	47.6(6)
O5	8881(3)	9763(2)	4159.3(13)	52.6(6)
C9	4967(3)	6096(3)	8302.2(15)	25.7(6)
C14	6166(3)	4915(3)	8657.9(16)	27.8(6)
C20	9169(3)	7358(3)	4148.3(15)	28.7(6)
C16	6702(3)	3685(3)	8283.6(16)	30.1(6)
C10	4400(3)	7140(3)	8710.4(16)	29.7(6)

C11	5010(3)	7020(3)	9447.2(17)	32.8(6)
C21	8315(3)	6934(3)	3694.6(16)	28.3(6)
C12	6224(3)	5880(3)	9780.7(17)	33.3(6)
C7	4329(3)	6261(3)	7472.8(15)	28.4(6)
C25	10604(3)	6527(3)	4377.5(16)	34.4(6)
C30	7356(3)	8954(3)	2061.2(16)	28.3(6)
C13	6829(3)	4818(3)	9384.9(16)	30.0(6)
C5	1866(3)	6326(3)	7852.4(16)	29.7(6)
C27	6775(3)	7856(3)	3407.4(16)	29.3(6)
C29	6480(3)	8140(3)	2506.0(15)	30.6(6)
C6	2725(3)	7066(3)	7325.1(16)	29.4(6)
C31	7445(3)	9016(3)	1213.9(17)	33.4(6)
C28	5716(3)	7230(3)	3822.1(16)	34.2(6)
C19	8594(3)	8712(3)	4406.4(17)	35.1(7)
C4	360(3)	7134(3)	7864.5(16)	31.3(6)
C22	8917(3)	5667(3)	3471.3(17)	36.0(7)
C8	5069(3)	6989(3)	6849.0(17)	37.8(7)
C24	11149(3)	5258(3)	4155.1(17)	38.9(7)
C23	10329(3)	4829(3)	3703.1(18)	39.5(7)
C3	-399(3)	8526(3)	7504.2(19)	39.6(7)
C15	8142(3)	3579(3)	9764.8(18)	39.1(7)
C17	8556(3)	2405(3)	7627.6(19)	44.5(8)
C2	-1869(3)	8895(4)	7644(2)	49.0(8)
C26	11544(3)	6995(4)	4847(2)	51.7(9)
C1	-2162(3)	7777(4)	8097(2)	46.4(8)
C32	6742(4)	8550(4)	731(2)	63.2(11)
C34	8045(4)	9543(4)	-155(2)	56.3(9)
C18	7168(5)	9780(4)	5333(2)	69.5(12)
C33	7080(5)	8865(5)	-64(2)	79.6(14)

Table S4. Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_22020163_0m.

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S2	46.8(5)	46.0(5)	39.9(5)	-3.4(3)	7.4(4)	-25.9(4)
S1	43.6(5)	51.0(5)	46.9(5)	-5.0(4)	10.0(4)	-27.9(4)
F6	52.4(11)	42.1(10)	47.5(11)	-13.1(8)	12.6(9)	-25.9(8)
F3	47.2(10)	39.2(10)	52.1(12)	-4.2(8)	16.2(9)	-18.7(8)
F4	45.7(10)	64.7(12)	28.8(10)	-8.6(8)	8.4(8)	-19.6(9)
F5	29.7(9)	57.4(11)	44.8(11)	-8.0(8)	4.6(8)	-7.9(8)

F1	30.3(9)	64.6(12)	44.1(11)	-4.1(9)	13.7(8)	-5.5(8)
F2	56.5(11)	73.4(13)	27.3(10)	-8.5(9)	8.1(9)	-19.2(10)
O3	34.8(11)	35.3(11)	45.2(13)	-13.0(9)	13.7(9)	-11.1(9)
O6	47.6(12)	34.4(10)	37.6(12)	-9.8(9)	-1.4(9)	-18.8(9)
O2	41.0(11)	30.2(10)	43.8(12)	0.0(9)	-0.8(10)	-14.8(9)
O1	40.5(12)	37.2(11)	77.5(17)	-25.2(11)	13.9(11)	-18.9(10)
O4	71.4(15)	35.1(11)	43.9(13)	-19.0(9)	21.1(11)	-21.9(11)
O5	81.7(17)	41.1(12)	47.8(14)	-11.0(10)	8.5(12)	-37.6(12)
C9	25.3(13)	27.5(13)	26.4(14)	-5.3(11)	6.0(11)	-12.5(11)
C14	26.5(13)	27.2(13)	31.6(15)	-6.3(11)	7.9(11)	-12.1(11)
C20	34.9(14)	28.5(13)	23.8(14)	-1.9(11)	4.3(12)	-15.5(11)
C16	30.5(14)	24.4(13)	32.2(15)	-4.2(11)	2.1(12)	-7.4(11)
C10	29.8(14)	29.2(13)	32.1(16)	-9.5(11)	7.2(12)	-11.6(11)
C11	33.7(15)	33.5(14)	35.5(16)	-11.6(12)	7.4(13)	-15.2(12)
C21	30.9(14)	29.1(13)	26.0(14)	-8.3(11)	7.6(11)	-10.7(11)
C12	37.8(15)	38.0(15)	29.1(15)	-5.0(12)	2.7(12)	-21.6(13)
C7	30.9(14)	28.8(13)	25.4(14)	-7.6(11)	4.7(11)	-9.6(11)
C25	34.7(15)	40.7(16)	28.7(16)	-2.7(12)	5.5(12)	-17.9(13)
C30	31.0(14)	19.6(12)	29.6(15)	-3.8(10)	-1.2(12)	-4.2(11)
C13	28.1(13)	30.6(14)	30.4(15)	-0.4(11)	3.1(12)	-13.9(11)
C5	36.7(15)	30.1(14)	27.4(14)	-8.3(11)	-0.7(12)	-17.0(12)
C27	31.0(14)	27.9(13)	29.0(15)	-8.1(11)	2.9(12)	-9.5(11)
C29	30.8(14)	34.5(14)	25.9(15)	-5.8(11)	0.3(12)	-11.9(12)
C6	27.3(13)	29.3(13)	29.6(15)	-4.1(11)	-0.8(12)	-9.3(11)
C31	38.4(15)	27.4(13)	35.7(16)	-5.4(11)	6.7(13)	-14.6(12)
C28	32.6(15)	40.3(16)	24.0(15)	-8.2(12)	1.5(12)	-5.2(12)
C19	45.8(17)	36.3(16)	26.4(15)	-7.6(12)	-1.9(13)	-18.0(13)
C4	33.4(15)	36.1(15)	29.6(15)	-7.5(12)	4.3(12)	-19.0(12)
C22	38.0(16)	36.0(15)	36.5(17)	-14.2(13)	4.6(13)	-12.3(13)
C8	32.3(15)	44.2(17)	30.2(16)	-5.2(13)	6.1(13)	-7.3(13)
C24	28.5(14)	44.5(17)	35.4(17)	-0.3(13)	3.6(13)	-8.3(13)
C23	38.7(16)	33.0(15)	40.2(18)	-8.9(13)	8.8(14)	-4.2(13)
C3	31.3(15)	38.6(16)	47.0(19)	-4.3(13)	5.6(14)	-13.9(13)
C15	38.6(16)	36.2(15)	38.2(17)	-0.6(13)	-3.3(13)	-13.2(13)
C17	47.9(18)	35.8(16)	41.8(19)	-12.4(13)	12.0(15)	-2.2(14)
C2	33.5(16)	50.3(19)	58(2)	-7.8(16)	3.7(15)	-12.2(14)
C26	47.3(19)	56(2)	53(2)	-1.4(16)	-9.8(16)	-26.4(16)
C1	32.2(16)	68(2)	48(2)	-19.8(17)	12.0(14)	-25.2(15)
C32	104(3)	85(3)	39(2)	-23.0(18)	24(2)	-76(3)
C34	79(3)	67(2)	36.7(19)	-10.3(16)	20.3(18)	-44(2)
C18	113(3)	43.4(19)	58(2)	-28.7(18)	26(2)	-23(2)
C33	134(4)	119(4)	39(2)	-33(2)	28(2)	-102(3)

Table S5. Bond Lengths for mo_22020163_0m.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
S2	C31	1.717(3)		C20	C19	1.497(4)
S2	C34	1.677(4)		C10	C11	1.383(4)
S1	C4	1.720(3)		C11	C12	1.386(4)
S1	C1	1.685(3)		C21	C27	1.525(4)
F6	C28	1.343(3)		C21	C22	1.391(4)
F3	C8	1.346(3)		C12	C13	1.396(4)
F4	C28	1.338(3)		C7	C6	1.527(4)
F5	C28	1.346(3)		C7	C8	1.509(4)
F1	C8	1.340(3)		C25	C24	1.386(4)
F2	C8	1.341(3)		C25	C26	1.508(4)
O3	C16	1.329(3)		C30	C29	1.502(4)
O3	C17	1.441(3)		C30	C31	1.466(4)
O6	C30	1.222(3)		C13	C15	1.510(4)
O2	C5	1.223(3)		C5	C6	1.506(4)
O1	C16	1.202(3)		C5	C4	1.458(4)
O4	C19	1.339(4)		C27	C29	1.538(4)
O4	C18	1.447(4)		C27	C28	1.513(4)
O5	C19	1.196(3)		C31	C32	1.359(4)
C9	C14	1.406(4)		C4	C3	1.372(4)
C9	C10	1.391(4)		C22	C23	1.386(4)
C9	C7	1.529(4)		C24	C23	1.377(4)
C14	C16	1.502(4)		C3	C2	1.424(4)
C14	C13	1.397(4)		C2	C1	1.355(5)
C20	C21	1.398(4)		C32	C33	1.414(5)
C20	C25	1.403(4)		C34	C33	1.357(5)

Table S6. Bond Angles for mo_22020163_0m.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
C34	S2	C31	91.83(15)		C4	C5	C6	116.8(2)
C1	S1	C4	91.50(14)		C21	C27	C29	112.4(2)
C16	O3	C17	116.3(2)		C28	C27	C21	112.5(2)
C19	O4	C18	116.5(2)		C28	C27	C29	109.1(2)
C14	C9	C7	120.9(2)		C30	C29	C27	111.4(2)
C10	C9	C14	118.5(2)		C5	C6	C7	112.9(2)
C10	C9	C7	120.5(2)		C30	C31	S2	119.2(2)
C9	C14	C16	120.1(2)		C32	C31	S2	111.0(2)
C13	C14	C9	121.2(2)		C32	C31	C30	129.8(3)
C13	C14	C16	118.6(2)		F6	C28	F5	106.1(2)
C21	C20	C25	121.1(2)		F6	C28	C27	113.3(2)
C21	C20	C19	121.5(2)		F4	C28	F6	106.4(2)

C25	C20	C19	117.4(2)		F4	C28	F5	105.9(2)
O3	C16	C14	112.7(2)		F4	C28	C27	112.9(2)
O1	C16	O3	123.5(3)		F5	C28	C27	111.8(2)
O1	C16	C14	123.8(2)		O4	C19	C20	110.4(2)
C11	C10	C9	120.6(2)		O5	C19	O4	123.4(3)
C10	C11	C12	120.6(3)		O5	C19	C20	126.2(3)
C20	C21	C27	121.8(2)		C5	C4	S1	119.0(2)
C22	C21	C20	118.7(2)		C3	C4	S1	111.3(2)
C22	C21	C27	119.5(2)		C3	C4	C5	129.7(2)
C11	C12	C13	120.4(3)		C23	C22	C21	120.7(3)
C6	C7	C9	114.8(2)		F3	C8	C7	112.7(2)
C8	C7	C9	110.6(2)		F1	C8	F3	106.1(2)
C8	C7	C6	108.5(2)		F1	C8	F2	106.2(2)
C20	C25	C26	121.5(3)		F1	C8	C7	113.0(2)
C24	C25	C20	118.2(3)		F2	C8	F3	106.5(2)
C24	C25	C26	120.3(3)		F2	C8	C7	111.8(2)
O6	C30	C29	122.1(2)		C23	C24	C25	121.5(3)
O6	C30	C31	120.5(2)		C24	C23	C22	119.8(3)
C31	C30	C29	117.4(2)		C4	C3	C2	112.0(3)
C14	C13	C15	122.0(2)		C1	C2	C3	111.6(3)
C12	C13	C14	118.6(2)		C2	C1	S1	113.5(2)
C12	C13	C15	119.4(3)		C31	C32	C33	112.5(3)
O2	C5	C6	121.4(2)		C33	C34	S2	112.8(3)
O2	C5	C4	121.7(2)		C34	C33	C32	111.8(3)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for mo_22020163_0m.

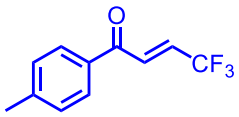
Atom	***x***	***y***	***z***	**U(eq)**
H10	3585.85	7942.94	8480.81	36
H11	4593.22	7724.68	9727.17	39
H12	6647.43	5820.21	10281.54	40
H7	4504.91	5287.16	7398.57	34
H27	6600.62	8793.02	3533.86	35
H29A	6703.91	7224.12	2358.72	37
H29B	5454.97	8685.12	2354.15	37
H6A	2521.38	8024.48	7413.76	35
H6B	2423.45	7182.54	6764.72	35
H22	8354.76	5371.93	3156.34	43
H24	12111.57	4670.23	4318.31	47
H23	10728.33	3961.55	3550.63	47
H3	8.77	9167.51	7197.74	48

H15A	7990.07	2689.37	9760.66	59
H15B	8324.67	3602.71	10312.94	59
H15C	8962.2	3638.76	9467.45	59
H17A	7888.72	2490.31	7191.57	67
H17B	8723.02	1501.85	8019.22	67
H17C	9461.3	2436.29	7420.42	67
H2	-2560.22	9811.85	7444.17	59
H26A	11851.94	7712.31	4492.28	78
H26B	12382.51	6176.01	5096.68	78
H26C	11009.81	7401.27	5257.45	78
H1	-3089.15	7827.94	8247.96	56
H32	6095.65	8067.11	908.68	76
H34	8408.46	9823.73	-646.87	68
H18A	6562.92	10604.71	4930.08	104
H18B	7960.18	10001.52	5534.44	104
H18C	6603	9544.43	5770.28	104
H33	6679.62	8629.65	-484.46	95

Characterization Data of Starting Materials

Note: All starting materials have been prepared according to the previously published procedure.[1]

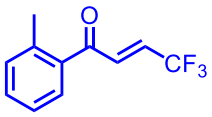
(*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one (2a).[1]



According to the general procedure, the product was isolated with 65%, 4.21 g.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.81 (m, 2 H), 7.53 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.36-7.29 (m, 2 H), 6.80 (dq, *J* = 15.5, 6.7 Hz, 1 H), 2.45 (s, 3 H).

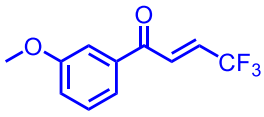
(*E*)-4,4,4-trifluoro-1-(*o*-tolyl)but-2-en-1-one (2b).[1]



According to the general procedure, the product was isolated with 33%, 142 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.0, 1.5 Hz, 1 H), 7.45 (td, *J* = 7.5, 1.4 Hz, 1 H), 7.31 (t, *J* = 7.1 Hz, 2 H), 7.25 (dq, *J* = 15.8, 2.0 Hz, 1 H), 6.63 (dq, *J* = 15.8, 6.6 Hz, 1 H), 2.50 (s, 3 H).

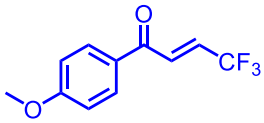
(*E*)-4,4,4-trifluoro-1-(3-methoxyphenyl)but-2-en-1-one (2c).[2]



According to the general procedure, the product was isolated with 49%, 226 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.48 (m, 3 H), 7.43 (t, *J* = 7.9 Hz, 1 H), 7.21-7.17 (m, 1 H), 6.82 (dq, *J* = 15.5, 6.6 Hz, 1 H), 3.88 (s, 3 H).

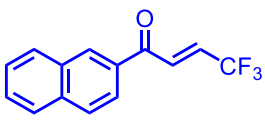
(*E*)-4,4,4-trifluoro-1-(4-methoxyphenyl)but-2-en-1-one (2d).[1]



According to the general procedure, the product was isolated with 39%, 360 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2 H), 7.53 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.03-6.97 (m, 2 H), 6.80 (dq, *J* = 15.5, 6.7 Hz, 1 H), 3.90 (s, 3 H).

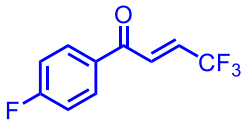
(*E*)-4,4,4-trifluoro-1-(naphthalen-2-yl)but-2-en-1-one (2e).[1]



According to the general procedure, the product was isolated with 64%, 322 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50-8.46 (m, 1 H), 8.05 (dd, *J* = 8.7, 1.8 Hz, 1 H), 8.03-8.00 (m, 1 H), 7.96 (d, *J* = 8.7 Hz, 1 H), 7.91 (d, *J* = 8.1 Hz, 1 H), 7.72 (dq, *J* = 15.5, 2.1 Hz, 1 H), 7.66 (ddd, *J* = 8.3, 7.0, 1.4 Hz, 1 H), 7.60 (ddd, *J* = 8.2, 6.9, 1.4 Hz, 1 H), 6.89 (dq, *J* = 15.5, 6.6 Hz, 1 H).

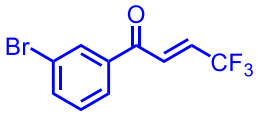
(*E*)-4,4,4-trifluoro-1-(4-fluorophenyl)but-2-en-1-one (2f).[3]



According to the general procedure, the product was isolated with 50%, 219 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06-7.99 (m, 2 H), 7.51 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.24-7.17 (m, 2 H), 6.83 (dq, *J* = 15.5, 6.6 Hz, 1 H).

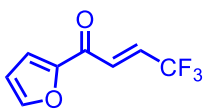
(*E*)-1-(3-bromophenyl)-4,4,4-trifluorobut-2-en-1-one (2g).[3]



According to the general procedure, the product was isolated with 42%, 235 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (t, *J* = 1.8 Hz, 1 H), 7.89 (ddd, *J* = 7.8, 1.7, 1.1 Hz, 1 H), 7.77 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1 H), 7.48 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.42 (t, *J* = 7.9 Hz, 1 H), 6.84 (dq, *J* = 15.5, 6.6 Hz, 1 H).

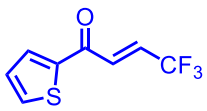
(*E*)-4,4,4-trifluoro-1-(furan-2-yl)but-2-en-1-one (2h).[3]



According to the general procedure, the product was isolated with 41%, 156 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 1.7, 0.7 Hz, 1 H), 7.44 (q, *J* = 15.6, 2.0 Hz, 1 H), 7.39-7.37 (m, 1 H), 6.90 (dq, *J* = 15.6, 6.7 Hz, 1 H), 6.64 (dd, *J* = 3.7, 1.7 Hz, 1 H).

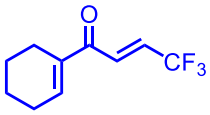
(*E*)-4,4,4-trifluoro-1-(thiophen-2-yl)but-2-en-1-one (2i).[1]



According to the general procedure, the product was isolated with 39%, 160 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 3.9, 1.1 Hz, 1 H), 7.79 (dd, *J* = 4.9, 1.1 Hz, 1 H), 7.40 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.22 (dd, *J* = 5.0, 3.9 Hz, 1 H), 6.87 (dq, *J* = 15.5, 6.7 Hz, 1 H).

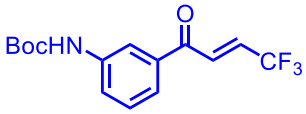
(*E*)-1-(cyclohex-1-en-1-yl)-4,4,4-trifluorobut-2-en-1-one (2j).



According to the general procedure, the product was isolated with 46%, 190 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (dq, *J* = 15.9, 2.2 Hz, 1 H), 7.02 (td, *J* = 3.9, 1.9 Hz, 1 H), 6.61 (dq, *J* = 15.5, 6.7 Hz, 1 H), 2.32 (dtp, *J* = 10.5, 4.4, 2.3 Hz, 4 H), 1.66 (dtdd, *J* = 11.2, 7.0, 4.9, 2.8 Hz, 4 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 188.40, 144.00, 139.89, 130.59 (q, *J* = 5.7 Hz), 128.34 (q, *J* = 34.7 Hz), 122.76 (q, *J* = 268.56 Hz), 26.45, 23.07, 21.65, 21.38; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{10}H_{12}F_3O$: 205.0835, Found: 205.0839.

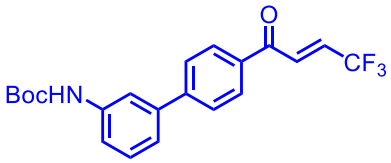
tert-butyl (*E*)-(3-(4,4,4-trifluorobut-2-enoyl)phenyl)carbamate (2k).



According to the general procedure, the product was isolated with 43%, 2.05 g.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (t, *J* = 2.0 Hz, 1 H), 7.74 (d, *J* = 8.1 Hz, 1 H), 7.61 (dt, *J* = 7.7, 1.3 Hz, 1 H), 7.50 (dq, *J* = 15.5, 2.0 Hz, 1 H), 7.44 (t, *J* = 7.9 Hz, 1 H), 6.81 (dq, *J* = 15.7, 6.7 Hz, 1 H), 6.77 (s, 1 H), 1.53(s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.79, 152.62, 139.45, 136.88, 130.99 (q, *J* = 5.5 Hz), 130.42 (q, *J* = 35.2 Hz), 129.68, 124.04, 123.30, 122.55 (d, *J* = 268.53 Hz), 118.34, 81.23, 28.30; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{15}H_{17}F_3NO_3$: 316.1155, Found: 316.1158.

tert-butyl (*E*)-(4'-(4,4,4-trifluorobut-2-enoyl)-[1,1'-biphenyl]-3-yl)carbamate (2l).

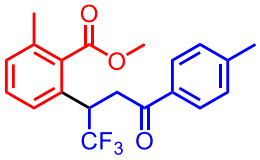


According to the general procedure, the product was isolated with 40%, 790 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-7.98 (m, 2 H), 7.78 (t, *J* = 2.0 Hz, 1 H), 7.76-7.72 (m, 2 H), 7.57 (dq, *J* = 15.6, 2.0 Hz, 1 H), 7.39 (t, *J* = 7.8 Hz, 1 H), 7.31 (ddt, *J* = 12.4, 7.6, 1.3 Hz, 2 H), 6.85 (dq, *J* = 15.5, 6.6 Hz, 1 H), 6.63 (s, 1 H), 1.54 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.49, 152.72, 146.64, 140.43, 139.14, 134.97, 131.04 (q, *J* = 5.6 Hz), 130.23 (q, *J* = 35.3 Hz), 129.63, 129.40, 127.71, 122.60 (q, *J* = 268.55 Hz), 121.98, 118.54, 117.33, 80.84, 28.35; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{21}H_{21}F_3NO_3$: 392.1468, Found: 392.1470.

Characterization Data of Desired Products

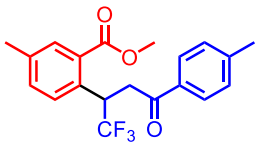
Methyl-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3aa).



According to the general procedure, the product was isolated with 82%, 28.7 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2 H,), 7.29-7.28 (m, 2 H,), 7.24 (d, *J* = 8.0 Hz, 1H), 7.16 (dd, *J* = 5.8, 2.7 Hz, 1 H), 4.52 (qdd, *J* = 9.3, 7.8, 5.0 Hz, 1 H), 3.98 (s, 3 H), 3.63 (dd, *J* = 17.7, 5.1 Hz, 1 H), 3.56 (dd, *J* = 17.7, 7.9 Hz, 1 H), 2.39 (s, 3 H), 2.35 (s, 3 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.40, 169.34, 144.38, 136.02, 135.39, 133.70, 132.41, 130.26, 129.72, 129.35, 128.25, 126.78 (q, *J* = 278.31 Hz), 124.84, 52.24, 41.09 (q, *J* = 27.8 Hz), 38.97, 21.65, 20.26; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_3$: 365.1359, Found: 365.1356.

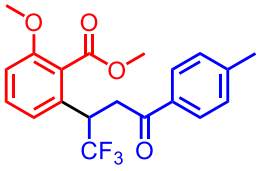
Methyl-5-methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl) benzoate (3ba).



According to the general procedure, the product was isolated with 77%, 28.0 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 1.9 Hz, 1 H), 7.82 (d, *J* = 1.7 Hz, 1 H), 7.76 (d, J = 2.0 Hz, 1 H), 7.40 (d, *J* = 8.1 Hz, 1 H), 7.31–7.28 (m, 1 H), 7.26 (d, *J* = 8.0 Hz, 2 H), 5.66 (pd, *J* = 9.6, 4.7 Hz, 1 H), 3.98 (s, 3 H), 3.69 (dd, *J* = 17.7, 9.3 Hz, 1 H), 3.62 (dd, *J* = 17.7, 4.7 Hz, 1 H), 2.42 (s, 3 H), 2.36 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.85, 167.98, 144.29, 137.73, 133.83, 132.73, 132.73, 131.71, 131.47, 129.32, 127.10 (q, *J* = 278.02 Hz), 128.17, 127.83, 52.34, 38.69 (q, *J* = 27.8 Hz), 38.67, 21.64, 20.90; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_3$: 365.1359, Found: 365.1359.

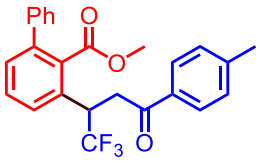
Methyl-2-methoxy-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3ca).



According to the general procedure, the product was isolated with 74%, 28.0 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88–7.77 (m, 2 H), 7.35 (t, *J* = 8.2 Hz, 1 H), 7.26 (d, *J* = 2.8 Hz, 2 H), 7.05 (dt, *J* = 8.1, 1.2 Hz, 1 H), 6.89 (dd, *J* = 8.4, 0.8 Hz, 1 H), 4.48–4.33 (m, 1 H), 3.97 (s, 3 H), 3.82 (s, 3 H), 3.61 (dd, *J* = 17.6, 5.2 Hz, 1 H), 3.54 (dd, *J* = 17.5, 7.8 Hz, 1 H), 2.40 (s, 3 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.23, 167.65, 156.75, 144.37, 133.70, 130.86, 129.36, 128.26, 126.63 (q, *J* = 278.51 Hz), 125.45, 119.46, 119.45, 110.98, 55.96, 52.52, 41.19 (q, *J* = 27.8 Hz), 38.78, 21.66; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_4$: 381.1308, Found: 381.1312.

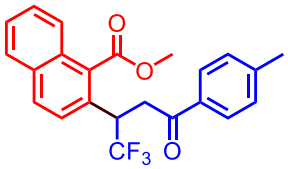
Methyl-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-[1,1'-biphenyl]-2-carboxylate (3da).



According to the general procedure, the product was isolated with 58%, 24.5 mg.

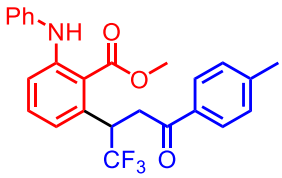
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87–7.79 (m, 2 H), 7.50–7.43 (m, 2 H), 7.41–7.32 (m, 6 H), 7.28–7.22 (m, 2 H), 4.78–4.64 (m, 1H), 3.68 (dd, *J* = 17.7, 5.2 Hz, 1 H), 3.62 (dd, *J* = 17.9, 8.0 Hz, 1 H), 3.57 (s, 3 H), 2.40 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.33, 169.27, 144.39, 141.29, 140.75, 134.72, 133.71, 133.04, 129.82, 129.37, 128.30, 128.27, 127.54, 126.78 (q, *J* = 278.65 Hz), 126.40, 52.13, 40.74 (q, *J* = 27.8 Hz)., 39.01, 21.67; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{25}H_{22}F_3O_3$: 427.1516, Found: 427.1527.

Methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1-naphthoate (3ea).



According to the general procedure, the product was isolated with 75%, 35.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 9.0 Hz, 1 H), 7.90–7.86 (m, 1 H), 7.83 (td, *J* = 6.6, 1.7 Hz, 3 H), 7.60–7.56 (m, 1 H), 7.55–7.48 (m, 2 H), 7.23 (d, *J* = 8.0 Hz, 2 H), 4.77 (qdd, *J* = 9.3, 7.8, 4.9 Hz, 1 H), 4.12 (s, 3 H), 3.73 (dd, *J* = 17.6, 5.0 Hz, 1 H), 3.64 (dd, *J* = 17.6, 7.8 Hz, 1 H), 2.39 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.28, 169.00, 144.47, 133.65, 133.09, 132.73, 130.61, 130.06, 129.98, 129.39, 128.26, 128.00, 127.50, 126.91, 126.83 (q, *J* = 278.59 Hz), 125.66, 123.90, 52.64, 41.61 (q, *J* = 27.6 Hz), 38.68, 21.65; **^{19}F NMR** (476 MHz, $CDCl_3$) δ -68.31 (CF_3); **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{23}H_{20}F_3O_3$: 401.1359, Found: 401.1370.

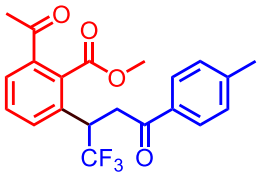
Methyl-2-(phenylamino)-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3fa).



According to the general procedure, the product was isolated with 64%, 28.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87–7.77 (m, 2 H), 7.67 (s, 1 H), 7.31–7.25 (m, 3 H), 7.24–7.18 (m, 3 H), 7.12–7.04 (m, 2 H), 7.02–6.97 (m, 1 H), 6.94 (dt, *J* = 7.4, 1.3 Hz, 1 H), 5.1–4.82 (m, 1 H), 4.00 (s, 3 H), 3.71–3.53 (m, 2 H), 2.40 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.82, 168.75, 144.45, 141.53, 135.68, 133.75, 131.42, 129.38, 128.24, 127.04 (q, *J* = 278.98 Hz), 122.53, 120.62, 120.51, 118.77, 115.90, 52.44,

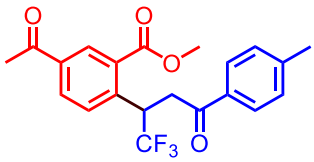
40.69 (q, *J* = 27.2 Hz), 39.29, 21.67; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{25}H_{23}F_3NO_3$: 442.1625, Found: 442.1635.

Methyl-2-acetyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3ga).



According to the general procedure, the product was isolated with 98%, 38.5 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87–7.81 (m, 2 H), 7.76 (dd, *J* = 7.8, 1.1 Hz, 1 H), 7.69 (dt, *J* = 8.0, 1.2 Hz, 1 H), 7.53 (t, *J* = 7.9 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 2 H), 4.63 (pd, *J* = 8.9, 5.0 Hz, 1 H), 3.96 (s, 3 H), 3.70 (dd, *J* = 17.6, 5.0 Hz, 1 H), 3.55 (dd, *J* = 17.5, 8.1 Hz, 1 H), 2.59 (s, 3 H), 2.42 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.44, 194.00, 168.79, 144.56, 137.55, 134.60, 133.86, 133.49, 131.33, 129.88, 129.41, 128.65, 128.25, 126.49 (q, *J* = 278.66 Hz), 52.84, 40.63 (q, *J* = 27.9 Hz), 38.85, 27.72, 21.66; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{21}H_{20}F_3O_4$: 393.1308, Found: 393.1314.

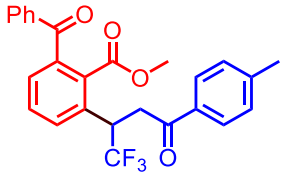
Methyl-5-acetyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3ha).



According to the general procedure, the product was isolated with 70%, 27.6 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 2.0 Hz, 1 H), 8.03 (dd, *J* = 8.3, 2.0 Hz, 1 H), 7.82–7.75 (m, 2 H), 7.62–7.52 (m, 1 H), 7.26–7.21 (m, 2 H), 5.76 (pd, *J* = 9.6, 4.4 Hz, 1 H), 4.02 (s, 3 H), 3.74 (dd, *J* = 17.9, 9.8 Hz, 1 H), 3.67 (dd, *J* = 18.0, 4.4 Hz, 1 H), 2.61 (s, 3 H), 2.39 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.66, 194.49, 167.07, 144.63, 140.84, 136.31, 133.52, 132.44, 131.23, 130.88, 129.41, 128.39,

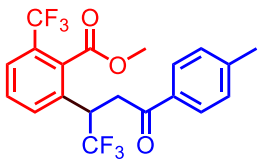
128.15, 126.71 (q, J = 278.46 Hz), 52.72, 39.12 (q, J = 27.7 Hz), 38.57, 26.60, 21.66; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{21}H_{20}F_3O_4$: 393.1308, Found: 393.1317.

Methyl-2-benzoyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzoate (3ia).



According to the general procedure, the product was isolated with 83%, 37.5 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85–7.80 (m, 2 H), 7.79–7.74 (m, 2 H), 7.67 (dd, J = 7.8, 1.6 Hz, 1 H), 7.61–7.56 (m, 1 H), 7.53 (t, J = 7.7 Hz, 1 H), 7.46 (ddd, J = 7.6, 4.6, 3.3 Hz, 3 H), 7.25 (d, J = 8.1 Hz, 2 H), 5.15–5.00 (m, 1 H), 3.71–3.60 (m, 2 H), 3.58 (s, 3 H), 2.40 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.06, 194.23, 167.41, 144.51, 140.06, 136.71, 134.73, 133.91, 133.61, 133.22, 130.31, 130.04, 129.78, 129.40, 128.86, 128.52, 128.22, 126.74 (q, J = 278.34 Hz),52.45, 39.88 (q, J = 27.8 Hz), 38.89, 21.67; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{26}H_{22}F_3O_4$: 455.1465, Found: 455.1477.

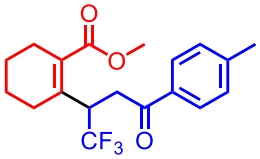
Methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-6-(trifluoromethyl)benzoat e (3ja).



According to the general procedure, the product was isolated with 25%, 10.4 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87–7.82 (m, 2 H), 7.71 (t, J = 7.8 Hz, 2 H), 7.58 (t, J = 7.9 Hz, 1 H), 7.28 (d, J = 7.9 Hz, 2 H), 4.60 (pd, J = 8.9, 4.8 Hz, 1 H), 4.03 (s, 3 H), 3.72 (dd, J = 17.7, 4.9 Hz, 1 H), 3.57 (dd, J = 17.7, 8.0 Hz, 1 H), 2.43 (s, 3 H).; **^{13}C**

NMR (126 MHz, $CDCl_3$) δ 193.77, 167.02, 144.68, 133.95 (q, *J* = 2.2 Hz), 133.45 (q, *J* = 2.2 Hz), 133.37, 131.08, 130.06, 129.44, 128.67(q, *J* =32.1 Hz), 128.22, 126.35 (q, *J* = 4.7 Hz), 126.34 (q, *J* = 278.51 Hz), 123.24 (q, *J* = 272.20 Hz), 53.11, 40.75 (q, *J* = 27.8 Hz), 38.81, 21.70; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{17}F_6O_3$: 419.1076, Found: 419.1089.

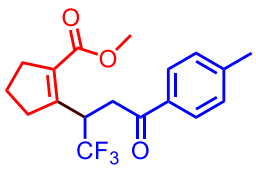
Methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)cyclohex-1-ene-1-carboxylate (3ka).



According to the general procedure, the product was isolated with 68%, 24.2 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88–7.74 (m, 2 H), 7.32–7.24 (m, 2 H), 5.07 (qdd, *J* = 10.1, 7.8, 5.9 Hz, 1 H), 3.71 (s, 3 H), 3.37–3.26 (m, 2 H), 2.42 (s, 3 H), 2.33 (dh, *J* = 8.4, 2.6 Hz, 2 H), 2.19 (m, 1 H), 2.12–2.03 (m, 1 H), 1.59 (m, 4 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.20, 168.96, 144.32, 137.42, 133.83, 132.25, 129.40, 128.24, 126.80 (q, *J* = 278.4 Hz), 51.63, 41.29 (q, *J* = 27.8 Hz), 35.18, 27.37, 25.81, 21.82, 21.67, 21.64. ; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{19}H_{22}F_3O_3$: 355.1516, Found: 355.1522.

Methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)cyclopent-1-ene-1-carboxylate (3la).

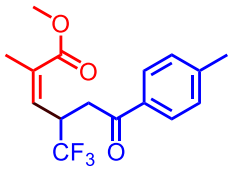


According to the general procedure, the product was isolated with 59%, 19.8 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90–7.83 (m, 2 H), 7.30 (d, *J* = 8.3 Hz, 2 H), 5.26 (pd,

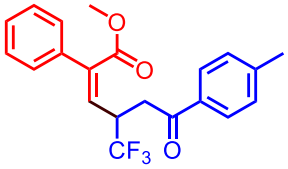
J = 9.8, 4.3 Hz, 1 H), 3.74 (s, 3 H), 3.41 (dd, *J* = 16.9, 4.4 Hz, 1 H), 3.32 (dd, *J* = 16.9, 9.8 Hz, 1 H), 2.66 (td, *J* = 7.6, 3.9 Hz, 2 H), 2.63–2.54 (m, 1 H), 2.52–2.46 (m, 1 H), 2.44 (s, 3 H), 1.9–1.77 (m, 2 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.07, 165.59, 148.07, 144.45, 134.39, 133.65, 129.44, 128.21, 126.47 (q, *J* = 280.7 Hz),51.38, 38.79 (q, *J* = 27.6 Hz), 35.70, 34.28, 33.61, 21.69, 21.39; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{18}H_{20}F_3O_3$: 341.1359, Found: 341.1366.

Methyl-(*Z*)-2-methyl-6-oxo-6-(*p*-tolyl)-4-(trifluoromethyl)hex-2-enoate (3ma).



According to the general procedure, the product was isolated with 95%, 29.8 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01–7.61 (m, 2 H), 7.26 (d, *J* = 8.0 Hz, 2 H), 5.77 (dq, *J* = 10.0, 1.6 Hz, 1 H), 4.84 (ddt, *J* = 13.5, 9.0, 4.6 Hz, 1 H), 3.75 (s, 3 H), 3.40 (dd, *J* = 17.1, 4.6 Hz, 1 H), 3.10 (dd, *J* = 17.1, 8.1 Hz, 1 H), 2.41 (s, 3 H), 1.95 (d, *J* = 1.6 Hz, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.83, 167.24, 144.34, 133.85, 133.39, 132.52, 132.50, 132.47, 129.38, 128.22, 126.70 (q, *J* = 278.07 Hz), 51.76, 39.01 (q, *J* = 27.6 Hz), 37.85, 21.63, 20.90; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -70.71 (CF_3); **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{16}H_{18}F_3O_3$: 315.1203, Found: 315.1209.

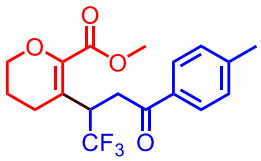
Methyl-(*Z*)-6-oxo-2-phenyl-6-(*p*-tolyl)-4-(trifluoromethyl)hex-2-enoate (3na).



According to the general procedure, the product was isolated with 91%, 34.4 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88–7.82 (m, 2 H), 7.35–7.22 (m, 7 H), 6.02 (d, *J* = 10.3 Hz, 1 H), 4.63 (ddd, *J* = 8.4, 4.8, 1.9 Hz, 1 H), 3.81 (s, 3 H), 3.47 (dd, *J* = 17.1, 4.7 Hz, 1 H), 3.22 (dd, *J* = 17.1, 7.9 Hz, 1 H), 2.41 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.58, 167.21, 144.48, 139.72, 136.96, 133.81, 131.16, 131.14, 129.45, 128.46, 128.36, 128.29, 127.66, 126.61 (q, *J* = 278.01 Hz), 52.21, 39.69 (q, *J* = 27.9 Hz), 37.84, 21.68; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -70.40 (CF_3); **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{21}H_{20}F_3O_3$: 377.1359, Found: 377.1370.

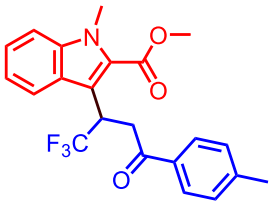
Methyl-5-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-3,4-dihydro-2H-pyran-6-carboxylate (3oa).



According to the general procedure, the product was isolated with 48%, 17.0 mg.

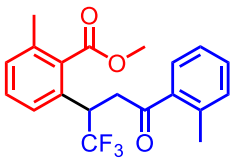
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92–7.83 (m, 2 H), 7.30 (d, *J* = 8.5 Hz, 2 H), 5.28 (ddt, *J* = 13.8, 9.8, 4.5 Hz, 1 H), 4.10 (dddd, *J* = 10.4, 6.9, 3.4, 1.0 Hz, 1 H), 4.00 (dddd, *J* = 10.8, 7.4, 3.4, 1.0 Hz, 1 H), 3.79 (s, 3 H), 3.35 (d, *J* = 1.6 Hz, 1 H), 3.34–3.28 (m, 1 H), 2.44 (s, 3 H), 2.25 (dt, *J* = 18.1, 6.3 Hz, 1 H), 2.15 (dt, *J* = 17.9, 6.5 Hz, 1 H), 1.90 (dq, *J* = 10.5, 3.3 Hz, 1 H), 1.83 (ddd, *J* = 13.8, 6.8, 3.3 Hz, 1 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.28, 163.35, 144.42, 143.93, 133.71, 129.45, 128.23, 126.91 (q, *J* = 279.47 Hz), 114.51, 65.98, 52.29, 39.30 (q, *J* = 27.4 Hz), 34.84, 21.69, 21.44, 21.28; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{18}H_{20}F_3O_4$: 357.1308, Found: 357.1315.

Methyl-1-methyl-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1H-indole-2-carboxylate (3pa).



According to the general procedure, the product was isolated with 45%, 18.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.93–7.86 (m, 1 H), 7.85–7.79 (m, 2 H), 7.47–7.33 (m, 2 H), 7.27–7.18 (m, 3 H), 5.74–5.56 (m, 1 H), 4.06 (s, 3 H), 4.00 (s, 3 H), 3.97–3.88 (m, 1 H), 3.80–3.72 (m, 1 H), 2.40 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.20, 162.67, 144.21, 138.75, 133.79, 130.00, 129.29, 129.14, 128.13, 127.97, 127.49 (q, *J* = 278.33 Hz), 125.72, 124.92, 121.99, 120.77, 114.84, 110.72, 52.12, 37.45, 36.57 (q, *J* = 29.1 Hz), 32.31, 21.63.; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{22}H_{21}F_3NO_3$: 404.1468, Found: 404.1476.

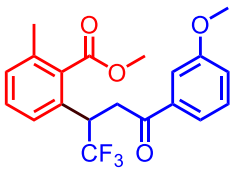
Methyl-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(*o*-tolyl)butan-2-yl)benzoate (3ab).



According to the general procedure, the product was isolated with 64%, 23.5 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.8, 1.4 Hz, 1 H), 7.37 (td, *J* = 7.5, 1.4 Hz, 1 H), 7.31 (d, *J* = 5.7 Hz, 2 H), 7.28–7.24 (m, 1 H), 7.22 (d, *J* = 8.0 Hz, 1 H), 7.20–7.16 (m, 1 H), 4.51 (qdd, *J* = 9.3, 7.5, 5.6 Hz, 1 H), 3.96 (s, 3 H), 3.57 (dd, *J* = 17.3, 5.6 Hz, 1 H), 3.43 (dd, *J* = 17.3, 7.5 Hz, 1 H), 2.35 (s, 3 H), 2.34 (s, 3 H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 198.69, 169.28, 138.50, 137.07, 135.99, 135.24, 132.18, 132.17, 132.03, 131.61, 130.28, 129.77, 128.12, 127.77, 126.66 (q, *J* = 278.35 Hz), 125.69, 125.07, 52.29, 41.15 (q, *J* = 27.8 Hz), 40.82, 20.93, 20.25.; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_3$: 365.1359, Found: 365.1353.

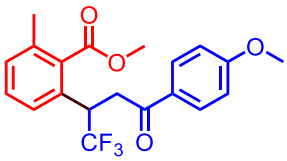
Methyl-2-methyl-6-(1,1,1-trifluoro-4-(3-methoxyphenyl)-4-oxobutan-2-yl)benzoa

te (3ac).



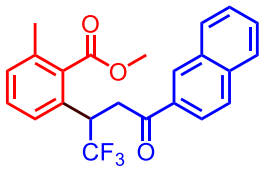
According to the general procedure, the product was isolated with 89%, 34.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (dt, *J* = 7.7, 1.2 Hz, 1 H), 7.44 (dd, *J* = 2.7, 1.6 Hz, 1 H), 7.36 (t, *J* = 8.0 Hz, 1 H), 7.29 (d, *J* = 4.7 Hz, 2 H), 7.18 (q, *J* = 4.4 Hz, 1 H), 7.11 (ddd, *J* = 8.3, 2.7, 0.9 Hz, 1 H), 4.57–4.41 (m, 1 H), 3.98 (s, 3 H), 3.82 (s, 3 H), 3.68–3.54 (m, 2 H), 2.36 (s, 3 H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.66, 169.33, 159.90, 137.48, 136.06, 135.39, 132.26, 130.32, 129.76, 129.66, 126.72 (q, *J* = 278.24 Hz), 124.79, 120.67, 120.15, 112.28, 55.47, 52.26, 41.12 (q, *J* = 27.8 Hz), 39.18, 20.27; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_4$: 381.1308, Found: 381.1318.

Methyl-2-methyl-6-(1,1,1-trifluoro-4-(4-methoxyphenyl)-4-oxobutan-2-yl)benzoa te (3ad).



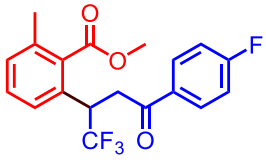
According to the general procedure, the product was isolated with 92%, 35.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97–7.83 (m, 2 H), 7.33–7.28 (m, 2 H), 7.16 (dd, *J* = 5.7, 3.1 Hz, 1 H), 6.95–6.85 (m, 2 H), 4.57–4.42 (m, 1 H), 3.98 (s, 3 H), 3.85 (s, 3 H), 3.64–3.57 (dd, *J* = 17.5, 5.7 Hz, 1 H), 3.53 (dd, *J* = 17.5, 7.9 Hz, 1 H), 2.35 (s, 3 H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.32, 169.34, 163.78, 136.01, 135.39, 132.42, 130.43, 130.24, 129.70, 129.26, 126.80 (q, *J* = 278.22 Hz), 124.84, 122.63, 113.82, 55.50, 52.24, 41.14 (q, *J* = 27.8 Hz), 38.70, 20.25; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{20}H_{20}F_3O_4$: 381.1308, Found:381.1312 .

Methyl-2-methyl-6-(1,1,1-trifluoro-4-(naphthalen-2-yl)-4-oxobutan-2-yl)benzoate (3ae).



According to the general procedure, the product was isolated with 78%, 31.0 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.49–8.40 (m, 1 H), 7.97 (ddd, *J* = 9.8, 8.4, 1.6 Hz, 2 H), 7.88–7.80 (m, 2 H), 7.57 (dddd, *J* = 19.3, 8.2, 6.9, 1.4 Hz, 2 H), 7.36 (d, *J* = 7.9 Hz, 1 H), 7.30 (t, *J* = 7.7 Hz, 1 H), 7.21–7.14 (m, 1 H), 4.58 (qdd, *J* = 9.3, 7.6, 5.2 Hz, 1 H), 3.98 (s, 3 H), 3.8–3.68 (m, 2 H), 2.36 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.79, 169.37, 136.10, 135.74, 135.42, 133.48, 132.43, 132.36, 130.34, 129.87, 129.79, 129.60, 128.73, 128.59, 127.80, 126.95, 126.81 (q, *J* = 278.98 Hz), 124.87, 123.76, 52.28, 41.26 (q, *J* = 27.7 Hz), 39.23, 20.29; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{23}H_{20}F_3O_3$: 401.1359, Found: 401.1361.

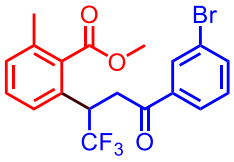
Methyl-2-methyl-6-(1,1,1-trifluoro-4-(4-fluorophenyl)-4-oxobutan-2-yl)benzoate (3af).



According to the general procedure, the product was isolated with 88%, 32.3 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00–7.91 (m, 2 H), 7.30 (d, *J* = 5.3 Hz, 2 H), 7.21–7.15 (m, 1 H), 7.14–7.08 (m, 2 H), 4.51 (qdd, *J* = 9.3, 7.8, 5.1 Hz, 1 H), 3.99 (s, 3 H), 3.62 (dd, *J* = 17.7, 5.1 Hz, 1 H), 3.56 (dd, *J* = 17.7, 7.8 Hz, 1 H), 2.35 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.28, 169.31, 165.96 (d, *J* = 255.6 Hz), 136.12,

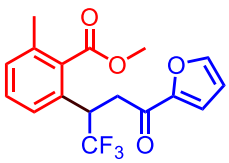
135.36, 132.58 (d, *J* = 3.1 Hz), 132.21, 130.86, 130.76, 130.37, 129.78, 126.68 (q, *J* = 278.32 Hz),124.77, 115.95, 115.73, 52.28, 41.07 (q, *J* = 28.0 Hz), 39.05, 20.28; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{19}H_{17}F_3O_3$: 369.1108, Found: 369.1109.

Methyl-2-(4-(3-bromophenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-methylbenzoate (3ag).



According to the general procedure, the product was isolated with 36%, 15.4 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 (t, *J* = 1.8 Hz, 1 H), 7.85 (ddd, *J* = 7.8, 1.7, 1.1 Hz, 1 H), 7.69 (ddd, *J* = 7.9, 2.0, 1.0 Hz, 1 H), 7.34 (t, *J* = 7.9 Hz, 1 H), 7.30 (d, *J* = 6.5 Hz, 2 H), 7.21–7.16 (m, 1 H), 4.50 (qdd, *J* = 9.2, 7.9, 5.0 Hz, 1 H), 3.99 (s, 3 H), 3.61 (dd, *J* = 17.8, 5.0 Hz, 1 H), 3.55 (dd, *J* = 17.8, 7.9 Hz, 1 H), 2.36 (s, 3 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.59, 169.30, 137.79, 136.38, 136.17, 135.34, 132.09, 131.20, 130.42, 130.29, 129.82, 126.62, 126.61 (q, *J* = 278.21 Hz), 124.75, 123.08, 77.28, 77.02, 76.77, 52.30, 40.98 (q, *J* = 27.9 Hz), 39.29, 20.29; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{19}H_{17}BrF_3O_3$: 429.0308, Found: 429.0311.

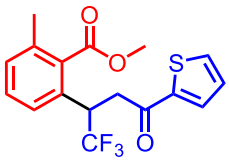
Methyl-2-methyl-6-(1,1,1-trifluoro-4-(furan-2-yl)-4-oxobutan-2-yl)benzoate (3ah).



According to the general procedure, the product was isolated with 88%, 30.0 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 1.7, 0.8 Hz, 1 H), 7.34–7.27 (m, 2 H), 7.19 (dd, *J* = 3.7, 0.8 Hz, 1 H), 7.16 (dd, *J* = 2.3, 1.7 Hz, 1 H), 6.52 (dd, *J* = 3.6, 1.7 Hz, 1 H), 4.53–4.35 (m, 1 H), 3.98 (s, 3 H), 3.52 (dd, *J* = 17.4, 5.3 Hz, 1 H), 3.44 (dd, *J* = 17.3, 8.1 Hz, 1 H), 2.34 (s, 3 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 184.15, 169.27, 152.16, 146.56, 136.02, 135.35, 131.98, 130.35, 129.74, 126.58 (q, *J* = 278.25 Hz), 117.46, 112.51, 52.29, 40.76 (q, *J* = 27.9 Hz), 38.90, 20.22; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{17}H_{16}F_3O_4$: 341.0995, Found: 341.1003.

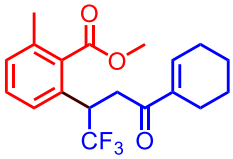
Methyl-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(thiophen-2-yl)butan-2-yl)benzoate (3ai).



According to the general procedure, the product was isolated with 81%, 28.8 mg.

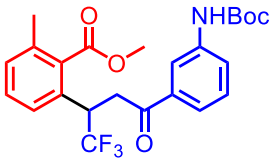
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 3.8, 1.2 Hz, 1 H), 7.64 (dd, *J* = 4.9, 1.1 Hz, 1 H), 7.33–7.29 (m, 2 H), 7.19–7.16 (m, 1 H), 7.12 (dd, *J* = 4.9, 3.8 Hz, 1 H), 4.46 (tdd, *J* = 9.2, 8.1, 5.0 Hz, 1 H), 3.97 (s, 3 H), 3.59 (dd, *J* = 17.2, 5.1 Hz, 1 H), 3.49 (dd, *J* = 17.1, 8.0 Hz, 1 H), 2.34 (s, 3 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.70, 169.28, 143.21, 136.09, 135.33, 134.25, 132.19, 131.97 (q, *J* = 1.6 Hz), 130.39, 129.78, 128.17, 126.58 (q, *J* = 278.45 Hz), 124.82, 52.29, 41.23 (q, *J* = 28.0 Hz), 39.68 (q, *J* = 1.9 Hz), 20.24; **^{19}F NMR** (471 MHz, $CDCl_3$) δ -68.91; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{17}H_{16}F_3O_3S$: 357.0767, Found: 357.0771.

Methyl-2-(4-(cyclohex-1-en-1-yl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-methylbenzoate (3aj).



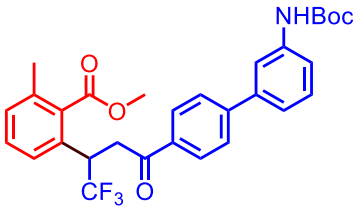
According to the general procedure, the product was isolated with 34%, 12.0 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.7 Hz, 1 H), 7.27 (d, *J* = 8.1 Hz, 1 H), 7.19 (dt, *J* = 7.5, 1.0 Hz, 1 H), 6.92 (tt, *J* = 4.0, 1.7 Hz, 1 H), 4.39 (qdd, *J* = 9.4, 7.9, 5.1 Hz, 1 H), 4.02 (s, 3 H), 3.33 (dd, *J* = 17.2, 5.1 Hz, 1 H), 3.25 (dd, *J* = 17.2, 7.9 Hz, 1 H), 2.37 (s, 3 H), 2.29–2.23 (m, 2 H), 2.20 (dddd, J = 6.6, 4.9, 3.5, 1.9 Hz, 2 H), 1.66–1.56 (m, 4 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.64, 169.33, 140.50, 139.01, 135.90, 135.35, 132.55, 130.13, 129.63, 126.78 (q, *J* = 278.31 Hz), 124.88, 123.45, 52.26, 41.20 (d, *J* = 27.8 Hz), 37.57, 26.08, 23.13, 21.78, 21.43, 20.22; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{19}H_{22}F_3O_3$: 355.1516, Found: 355.1523.

Methyl-2-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-methylbenzoate (3ak).



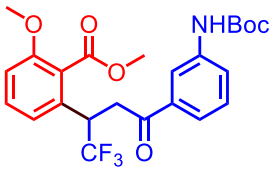
According to the general procedure, the product was isolated with 80%, 37.3 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (t, *J* = 2.0 Hz, 1 H), 7.69–7.61 (m, 1 H), 7.57 (ddd, *J* = 7.8, 1.7, 1.0 Hz, 1 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 7.31–7.27 (m, 2 H), 7.20–7.12 (m, 1 H), 6.71 (s, 1 H), 4.58–4.42 (m, 1 H), 3.97 (s, 3 H), 3.63 (dd, *J* = 17.8, 5.0 Hz, 1 H), 3.56 (dd, *J* = 17.7, 7.8 Hz, 1 H), 2.34 (s, 3 H), 1.52 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.59, 169.38, 152.64, 139.05, 136.82, 136.02, 135.33, 132.31, 130.29, 129.78, 129.35, 126.72 (q, *J* = 278.38 Hz), 124.89, 123.40, 122.59, 117.85, 81.01, 52.26, 41.07 (q, *J* = 27.8 Hz), 39.23, 28.29, 20.26; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{24}H_{27}F_3NO_5$:466.1836, Found: 466.1840.

Methyl-2-(4-(3'-((tert-butoxycarbonyl)amino)-[1,1'-biphenyl]-4-yl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-methylbenzoate (3al).



According to the general procedure, the product was isolated with 82%, 44.4 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03– 7.96 (m, 2 H), 7.74–7.71 (m, 1 H), 7.69–7.61 (m, 2 H), 7.37 (t, *J* = 7.8 Hz, 1 H), 7.34 –7.30 (m, 3 H), 7.28 (t, *J* = 1.5 Hz, 1 H), 7.20–7.16 (m, 1 H), 6.60 (s, 1 H), 4.61–4.48 (m, 1 H), 3.99 (s, 3 H), 3.67 (dd, *J* = 17.7, 5.0 Hz, 1 H), 3.61 (dd, *J* = 17.6, 8.0 Hz, 1 H), 2.36 (s, 3 H), 1.53 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 94.41, 169.34, 152.70, 145.89, 140.61, 139.05, 136.07, 135.39, 134.94, 132.31, 130.32, 129.77, 129.55, 128.67, 127.38, 126.75 (q, *J* = 278.29 Hz), 124.83, 121.93, 118.34, 117.28, 80.78, 52.28, 41.14 (q, *J* = 27.7 Hz), 39.12; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{30}H_{31}F_3NO_5$: 542.2149, Found: 542.2160.

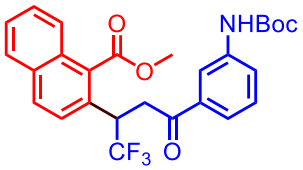
Methyl-2-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-methoxybenzoate (3ck).



According to the general procedure, the product was isolated with 77%, 37.0 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.87 (t, *J* = 2.0 Hz, 1 H), 7.72–7.68 (m, 1 H), 7.61 (dt, *J* = 7.8, 1.3 Hz, 1 H), 7.38 (q, *J* = 7.9 Hz, 2 H), 7.08 (d, *J* = 8.0 Hz, 1 H), 6.91 (dd, *J* =

8.4, 0.8 Hz, 1 H), 6.69 (s, 1 H), 4.48–4.38 (m, 1 H), 3.99 (s, 3 H), 3.84 (s, 3 H), 3.64 (dd, *J* = 17.6, 5.2 Hz, 1 H), 3.57 (dd, *J* = 17.6, 7.7 Hz, 1 H), 1.55 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.42, 167.71, 156.75, 152.61, 139.03, 136.81, 133.57, 130.93, 129.38, 126.57 (q, *J* = 278.06 Hz), 125.39, 123.38, 122.61, 119.50, 117.85, 111.03, 81.01, 55.97, 52.54, 41.19 (q, *J* = 28.2 Hz), 39.06, 28.30; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{24}H_{27}F_3NO_6$: 482.1785, Found: 482.1796.

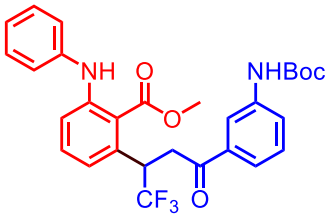
Methyl-2-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-1-naphthoate (3ek).



According to the general procedure, the product was isolated with 80%, 40.1 mg.

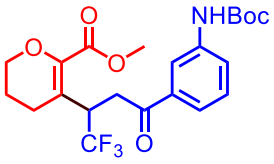
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 1H), 7.88–7.84 (m, 2 H), 7.83–7.79 (m, 1 H), 7.64 (d, *J* = 8.1 Hz, 1 H), 7.59–7.55 (m, 2 H), 7.54–7.48 (m, 2 H), 7.34 (t, *J* = 7.9 Hz, 1 H), 6.64 (s, 1 H), 4.78–4.69 (m, 1 H), 4.10 (s, 3 H), 3.72 (dd, *J* = 17.7, 5.0 Hz, 1 H), 3.63 (dd, *J* = 17.6, 7.8 Hz, 1 H), 1.51 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.44, 169.02, 152.59, 139.05, 136.79, 133.05, 132.74, 130.66, 129.96, 129.39, 128.01, 127.51, 127.03 (q, *J* = 278.60 Hz), 126.92, 125.64, 123.91, 123.41, 122.60, 117.81, 81.03, 52.65, 41.60 (q, *J* = 28.0 Hz), 38.94, 28.30; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{27}H_{27}F_3NO_5$:502.1836, Found: 502.1838.

Methyl-2-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-6-(phenylamino)benzoate (3fk).



According to the general procedure, the product was isolated with 86%, 46.6 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (t, *J* = 2.0 Hz, 1 H), 7.66 (s, 1 H), 7.64 (d, *J* = 8.6 Hz, 1 H), 7.59 (dt, *J* = 8.0, 1.2 Hz, 1 H), 7.37 (t, *J* = 7.9 Hz, 1 H), 7.31–7.26 (m, 2 H), 7.25–7.23 (m, 1 H), 7.23–7.19 (m, 1 H), 7.13–7.08 (m, 2 H), 7.00 (tt, *J* = 7.4, 1.2 Hz, 1 H), 6.94 (d, *J* = 7.3 Hz, 1 H), 6.59 (s, 1 H), 4.99 (dqd, *J* = 12.9, 9.4, 6.4 Hz, 1 H), 4.00 (s, 3 H), 3.65–3.61 (m, 1 H), 3.60–3.56 (m, 1 H), 1.53 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.95, 168.73, 152.57, 144.48, 141.53, 139.02, 136.93, 135.58, 131.47, 129.39, 126.97 (q, *J* = 278.33 Hz), 123.39, 122.62, 122.55, 120.54, 118.82, 117.80, 115.94, 81.07, 52.45, 40.67 (q, *J* = 27.5 Hz), 39.55, 28.31; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{29}H_{30}F_3N_2O_5$: 543.2101, Found: 543.2102.

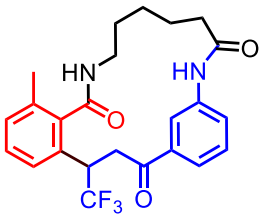
Methyl-5-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1,1,1-trifluoro-4-oxobutan-2-yl)-3,4-dihydro-2H-pyran-6-carboxylate (3ok).



According to the general procedure, the product was isolated with 46%, 21.0 mg. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (t, *J* = 2.0 Hz, 1 H), 7.73 (d, *J* = 8.0 Hz, 1 H), 7.63 (dt, *J* = 7.8, 1.2 Hz, 1 H), 7.43 (t, *J* = 7.9 Hz, 1 H), 6.63 (s, 1 H), 5.34–5.22 (m, 1 H), 4.13–4.08 (m, 1 H), 4.05–3.99 (m, 1 H), 3.81 (s, 3 H), 3.3–3.32 (m, 2 H), 2.26 (dt, *J* = 18.2, 6.4 Hz, 1 H), 2.16 (dt, *J* = 18.0, 6.5 Hz, 1 H), 1.92 (ddq, *J* = 13.5, 6.5, 3.4 Hz, 1 H), 1.85 (dqd, *J* = 13.5, 6.7, 3.4 Hz, 1 H), 1.56 (s, 9 H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.38, 163.38, 152.55, 150.79, 139.07, 136.95, 129.48, 126.63 (q, *J* =

278.46 Hz), 123.36, 122.60, 117.75, 114.37, 81.04, 66.00, 52.30, 39.34 (q, *J* = 28.6 Hz), 35.17, 28.31, 21.45, 21.31; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{22}H_{27}F_3NO_6$: 458.1785, Found: 458.1782.

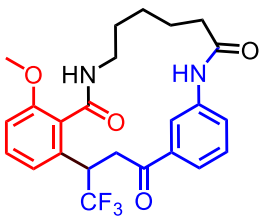
1^3-methyl-2-(trifluoromethyl)-6,13-diaza-1(1,2),5(1,3)-dibenzenacyclotetradecaphane-4,7,14-trione (5a).



According to the general procedure, the product was obtained with 22.0 mg.

^{1}H NMR (500 MHz, DMSO) δ 10.07 (s, 1 H), 8.39 (s, 1 H), 8.27 (s, 1 H), 7.49 (d, *J* = 5.5 Hz, 1 H), 7.45 (d, *J* = 4.9 Hz, 2 H), 7.41 (d, *J* = 8.0 Hz, 1 H), 7.36 (t, *J* = 7.7 Hz, 1 H), 7.24 (d, *J* = 7.4 Hz, 1 H), 4.13–4.01 (m, 1 H), 3.52–3.36 (m, 2 H), 3.27–3.15 (m, 1 H), 2.87 (s, 1 H), 2.35 (s, 1 H), 2.32–2.25 (m, 1 H), 2.17 (s, 3 H), 1.77 (s, 2 H), 1.65 (s, 1 H), 1.45 (s, 3 H); **^{13}C NMR** (126 MHz, DMSO) δ 196.41, 172.43, 167.48, 139.68, 139.29, 135.59, 134.34, 130.03, 129.52, 129.35, 128.48, 126.17 (q, *J* = 280.02 Hz), 124.93, 124.74, 122.50, 120.72, 44.02 (q, *J* = 28.0 Hz), 40.72, 36.85, 28.04, 25.96, 24.49, 19.06; **^{19}F NMR** (471 MHz, DMSO) δ -66.88; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{24}H_{25}F_3N_2O_3$: 447.1890, Found: 447.1900.

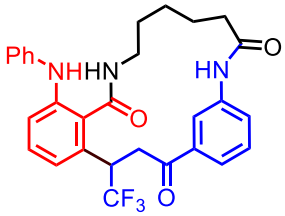
1^3-methoxy-2-(trifluoromethyl)-6,13-diaza-1(1,2),5(1,3)-dibenzenacyclotetradecaphane-4,7,14-trione (5b).



According to the general procedure, the product was obtained with 21.9 mg.

^{1}H NMR (500 MHz, DMSO) δ 10.06 (s, 1 H), 8.35 (s, 1 H), 8.13 (t, *J* = 5.3 Hz, 1 H), 7.53–7.37 (m, 4 H), 7.14 (d, *J* = 7.9 Hz, 1 H), 7.06 (d, *J* = 8.3 Hz, 1 H), 4.10 (q, *J* = 8.2 Hz, 1 H), 3.73 (s, 3 H), 3.52–3.37 (m, 2 H), 3.20–3.09 (m, 1 H), 2.88 (td, *J* = 11.1, 10.4, 5.0 Hz, 1H), 2.41–2.24 (m, 2 H), 1.76 (s, 2 H), 1.62 (s, 1 H), 1.43 (s, 3 H).; **^{13}C NMR** (126 MHz, DMSO) δ 196.29, 172.32, 165.09, 155.71, 139.17, 135.53, 131.18, 129.71, 129.41, 129.24, 128.79, 126.05 (q, *J* = 280.56 Hz), 124.68, 122.70, 122.43, 120.69, 119.41, 111.41, 55.59, 43.53 (q, *J* = 28.0 Hz), 40.55, 36.75, 28.08, 27.97, 25.98, 24.43.; **^{19}F NMR** (471 MHz, DMSO) δ -66.70; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{24}H_{26}F_3N_2O_4$: 463.1839, Found: 463.1838.

1^{3}-(phenylamino)-2-(trifluoromethyl)-6,13-diaza-1(1,2),5(1,3)-dibenzenacyclotetradecaphane-4,7,14-trione (5c).

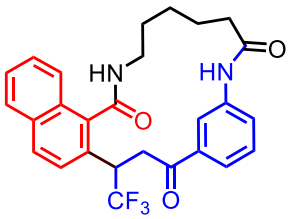


According to the general procedure, the product was obtained with 17.0 mg.

^{1}H NMR (500 MHz, DMSO) δ 10.07 (s, 1 H), 8.35 (s, 1 H), 8.20 (t, *J* = 5.3 Hz, 1 H), 7.52 (s, 1 H), 7.47 (d, *J* = 5.9 Hz, 2 H), 7.33 (t, *J* = 8.0 Hz, 1 H), 7.23–7.17 (m, 3 H), 7.14 (d, *J* = 7.8 Hz, 1 H), 7.03 (s, 1 H), 7.00–6.97 (m, 2 H), 6.84 (tt, *J* = 7.2, 1.1 Hz, 1 H), 4.14 (dt, *J* = 15.5, 7.8 Hz, 1 H), 3.56–3.42 (m, 2 H), 3.17 (d, *J* = 5.2 Hz, 1 H), 2.87 (ddd, *J* = 14.3, 9.9, 5.0 Hz, 1 H), 2.41–2.32 (m, 1 H), 2.31–2.21 (m, 1 H), 1.75 (s, 2 H), 1.57 (s, 1 H), 1.41 (d, *J* = 9.0 Hz, 3 H) ; **^{13}C NMR** (126 MHz, DMSO) δ 197.15, 172.93, 166.62, 143.92, 141.12, 139.75, 136.25, 131.86, 131.39, 129.92, 129.81, 129.47, 126.05 (q, *J* = 280.56 Hz), 125.30, 123.20, 121.20, 120.85, 120.71, 118.95, 118.49, 49.07, 44.19 (q, *J* = 28.03 Hz), 41.25, 37.28, 28.27, 26.44, 24.87; **^{19}F**

NMR (471 MHz, DMSO) δ -66.52; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{29}H_{28}F_3N_3O_3$: 524.2156, Found: 524.2152.

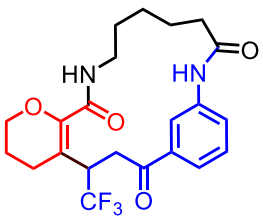
2-(trifluoromethyl)-6,13-diaza-1(2,1)-naphthalena-5(1,3)-benzenacyclotetradecaphane-4,7,14-trione (5d).



According to the general procedure, the product was obtained with 26.2 mg.

^{1}H NMR (500 MHz, DMSO) δ 10.09 (s, 1 H), 8.82 (s, 1 H), 8.54 (s, 0.5 H), 8.01 (s, 2.5 H), 7.89–7.42 (m, 7 H), 4.27 (m, 1 H), 3.76 (m, 1 H), 3.44 (m, 1 H), 2.72 (s, 0.5 H), 2.42–2.04 (m, 2.5 H), 1.79 (m, 3 H), 1.48 (m, 2 H), 1.43–1.14 (m, 1 H); **^{13}C NMR** (126 MHz, DMSO) δ 205.47, 172.99, 167.34, 132.94, 129.59, 128.34, 127.42, 126.01, 125.57, 124.76, 122.48, 41.06, 37.61, 30.04, 26.72, 25.44; **^{19}F NMR** (471 MHz, DMSO) δ -65.44, -67.45; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{27}H_{25}F_3N_2O_3$: 483.1890, Found: 483.1884.

2-(trifluoromethyl)-13,14-dihydro-12H-6,13-diaza-1(5,6)-pyrana-5(1,3)-benzenacyclotetradecaphane-4,7,14-trione (5e).

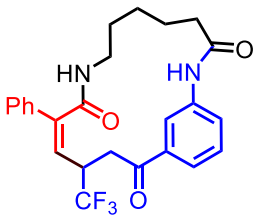


According to the general procedure, the product was obtained with 26.3 mg.

^{1}H NMR (500 MHz, DMSO) δ 9.99 (s, 1 H), 8.08 (dd, *J* = 8.8, 4.1 Hz, 1 H), 7.92 (s,

1 H), 7.72 (d, *J* = 7.9 Hz, 1 H), 7.51 (d, *J* = 7.8 Hz, 1 H), 7.44 (t, *J* = 7.8 Hz, 1 H), 6.13–5.96 (m, 1 H), 4.00 (dp, *J* = 8.2, 4.8 Hz, 2 H), 3.43–3.35 (m, 1 H), 3.25 (dd, *J* = 13.5, 4.5 Hz, 1 H), 3.04–2.96 (m, 1 H), 2.70 (dq, *J* = 14.1, 4.8 Hz, 1 H), 2.32 (ddd, *J* = 18.3, 9.4, 4.6 Hz, 2 H), 2.20 (ddd, *J* = 13.2, 8.9, 4.6 Hz, 1 H), 2.06 (dt, *J* = 18.0, 6.4 Hz, 1 H), 1.86–1.76 (m, 2 H), 1.65 (t, *J* = 7.4 Hz, 1 H), 1.57 (dq, *J* = 13.3, 6.1, 5.5 Hz, 1 H), 1.40 (dh, *J* = 13.2, 7.4 Hz, 2 H), 1.31 (q, *J* = 7.4 Hz, 2 H); **^{13}C NMR** (126 MHz, DMSO) δ 198.86, 171.98, 162.61, 143.86, 139.54, 136.18, 129.56, 127.45 (q, *J* = 280.63 Hz), 124.57, 122.51, 121.72, 112.84, 66.00, 39.00, 38.33, 36.74, 29.77, 25.75, 25.35, 21.50, 21.13 ; **^{19}F NMR** (471 MHz, DMSO) δ -65.13; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{22}H_{25}F_3N_2O_4$: 439.1839, Found:439.1840.

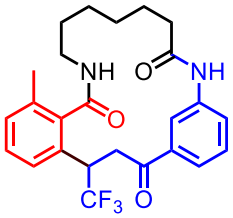
(*Z*)-11-phenyl-13-(trifluoromethyl)-2,9-diaza-1(1,3)-benzenacyclopentadecaphan-11-ene-3,10,15-trione (5f).



According to the general procedure, the product was obtained with 19.0 mg.

^{1}H NMR (500 MHz, DMSO) δ 10.09 (s, 1 H), 8.13 (s, 1 H), 8.07 (t, *J* = 5.4 Hz, 1 H), 7.55–7.46 (m, 3 H), 7.43–7.31 (m, 5 H), 5.89 (d, *J* = 10.1 Hz, 1 H), 4.06–3.93 (m, 1 H), 3.44 (dd, *J* = 13.8, 6.2 Hz, 1 H), 3.16 (dq, *J* = 13.4, 6.3, 5.6 Hz, 1 H), 3.12–3.01 (m, 2 H), 2.42–2.33 (m, 1 H), 2.29 (q, *J* = 8.6, 8.1 Hz, 1 H), 1.75 (s, 2 H), 1.58 (s, 2 H), 1.48–1.38 (m, 2 H); **^{13}C NMR** (126 MHz, DMSO) δ 197.41, 172.30, 166.34, 143.21, 138.90, 136.35, 129.44, 128.62, 128.52, 126.72, 126.19 (q, *J* = 279.14 Hz), 125.94, 122.99, 122.47, 121.75, 42.30 (q, *J* = 30.02 Hz), 36.56, 28.22, 26.09, 24.32; **^{19}F NMR** (471 MHz, DMSO) δ -67.76; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{25}H_{25}F_3N_2O_3$: 459.1890, Found: 459.1886.

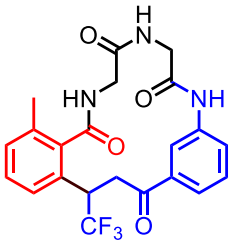
1^{3}-methyl-2-(trifluoromethyl)-6,14-diaza-1(1,2),5(1,3)-dibenzenacyclopentadecaphane-4,7,15-trione (5g).



According to the general procedure, the product was obtained with 39.2 mg.

^{1}H NMR (500 MHz, DMSO) δ 9.85 (s, 1 H), 8.54 (s, 1 H), 8.21 (s, 1 H), 7.97 (s, 1 H), 7.49 (d, *J* = 6.3 Hz, 2 H), 7.43–7.36 (m, 2 H), 7.32–7.26 (m, 1 H), 3.98 (s, 1 H), 3.47 (dd, *J* = 13.8, 5.0 Hz, 1 H), 3.42–3.34 (m, 1 H), 3.00 (d, *J* = 52.4 Hz, 2 H), 2.53 (d, *J* = 12.8 Hz, 1 H), 2.28 (s, 3 H), 2.21 (ddd, *J* = 13.1, 9.1, 3.7 Hz, 1 H), 1.88 (s, 1 H), 1.66 (s, 2 H), 1.49–1.30 (m, 5 H).; **^{13}C NMR** (126 MHz, DMSO) δ 197.48, 172.25, 168.31, 139.77, 139.60, 135.80, 134.77, 131.19, 130.62, 130.00, 129.31, 126.80 (q, *J* = 279.63 Hz), 125.40, 124.41, 122.65, 120.91, 44.20 (q, *J* = 27.0 Hz), 41.51, 37.52, 27.82, 25.66, 24.44, 24.36, 19.61; **^{19}F NMR** (471 MHz, DMSO) δ -66.40; **HRMS** [ESI] Calcd for $[M+H]^{+}$ $C_{25}H_{27}F_3N_2O_3$: 461.2047, Found: 461.2056.

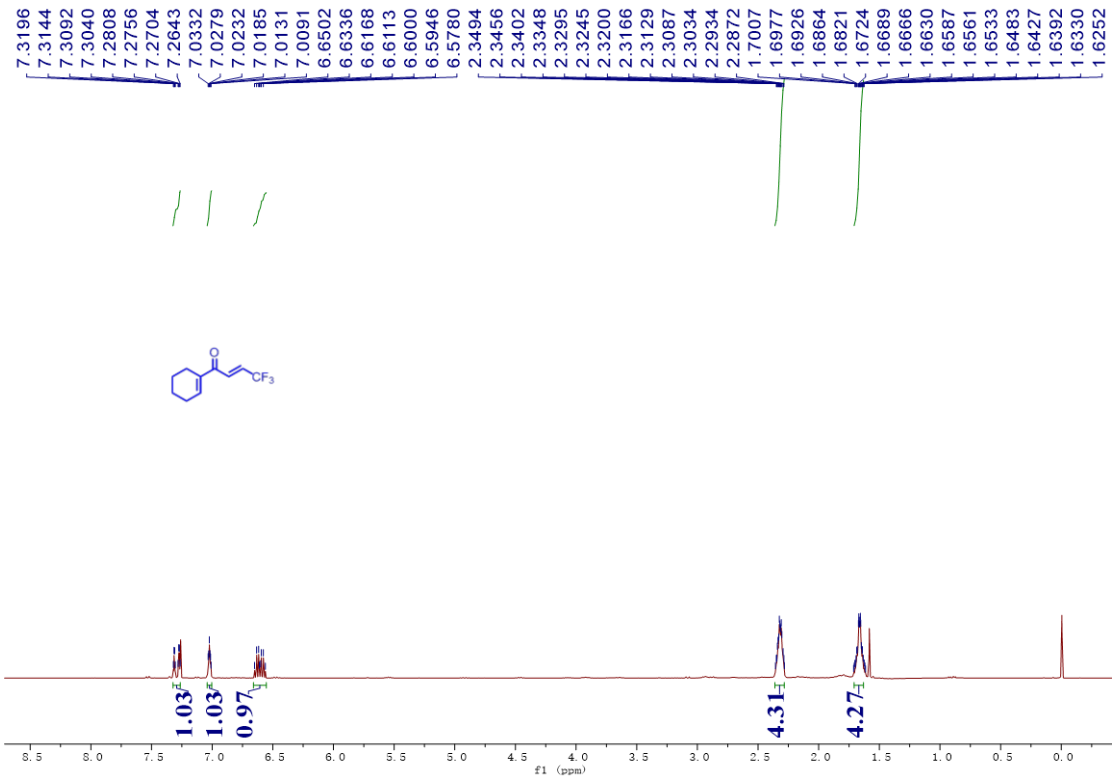
1^{3}-methyl-2-(trifluoromethyl)-6,9,12-triaza-1(1,2),5(1,3)-dibenzenacyclotridecaphane-4,7,10,13-tetraone (5h).

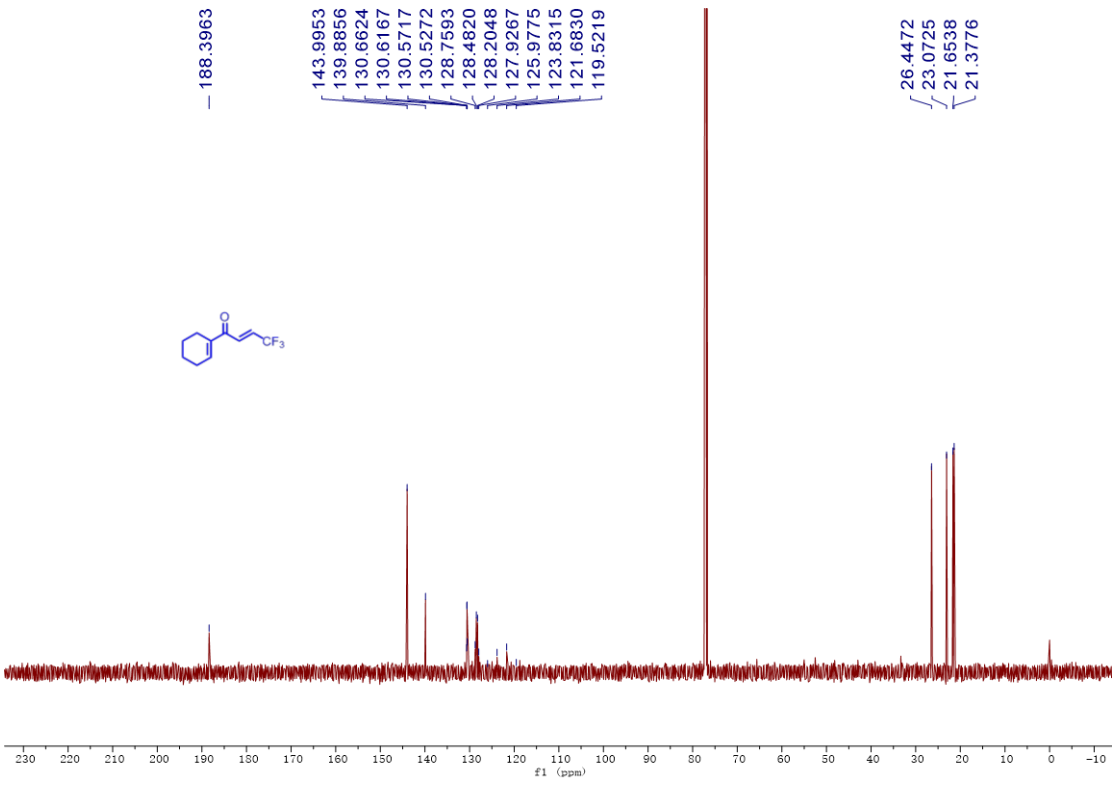


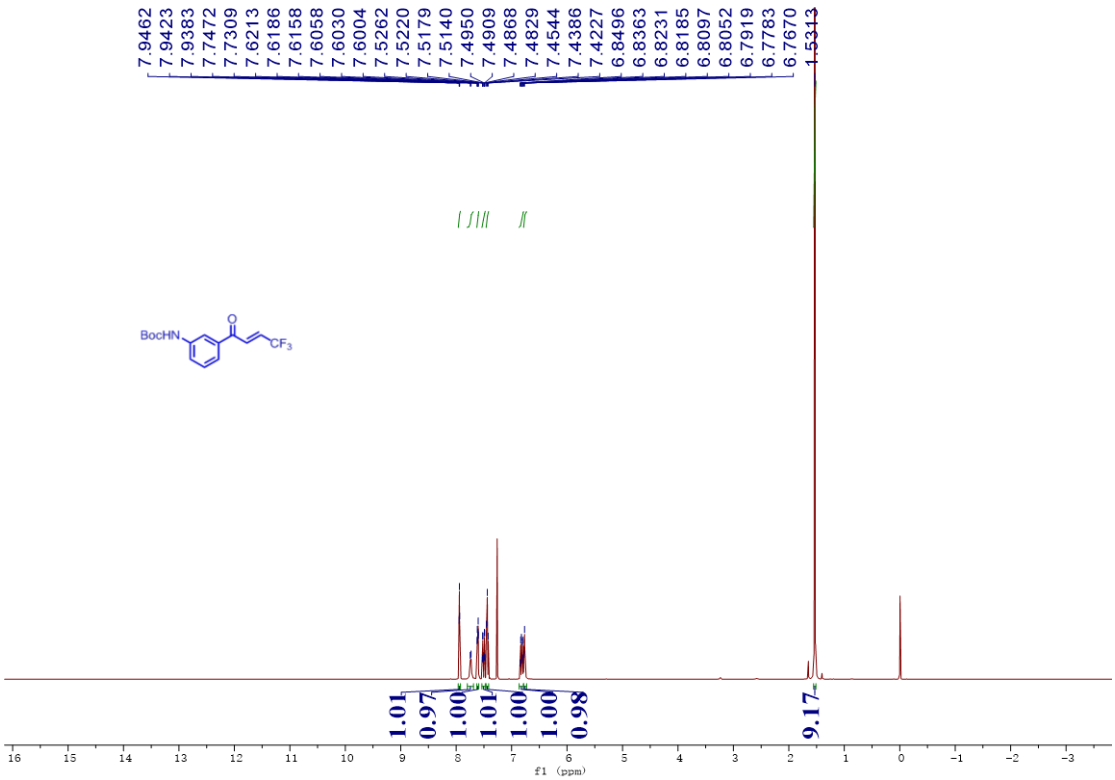
According to the general procedure, the product was obtained with 28.0 mg.

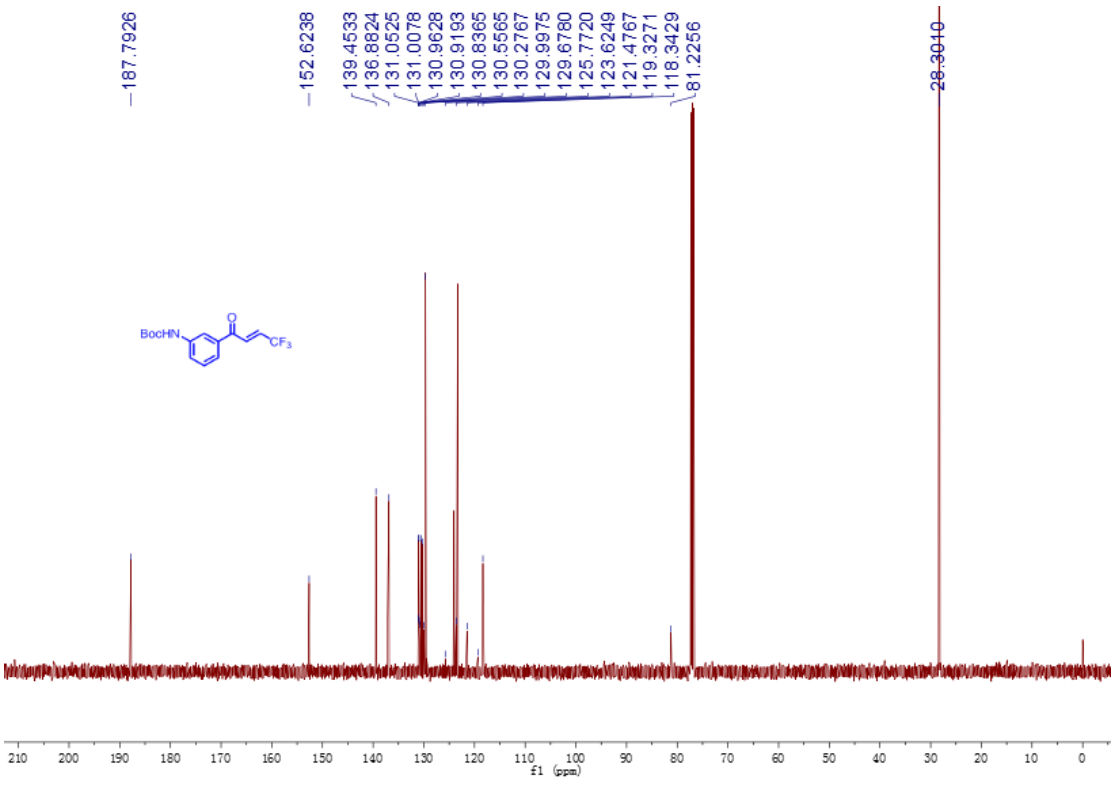
^{1}H NMR (500 MHz, DMSO) δ 9.34 (s, 1 H), 9.28 (s, 1 H), 8.62 (s, 1 H), 8.32 (d, *J* = 7.5 Hz, 1 H), 8.04 (s, 1 H), 7.60 (d, *J* = 7.6 Hz, 1 H), 7.54 (d, *J* = 7.8 Hz, 2 H), 7.46 (d,

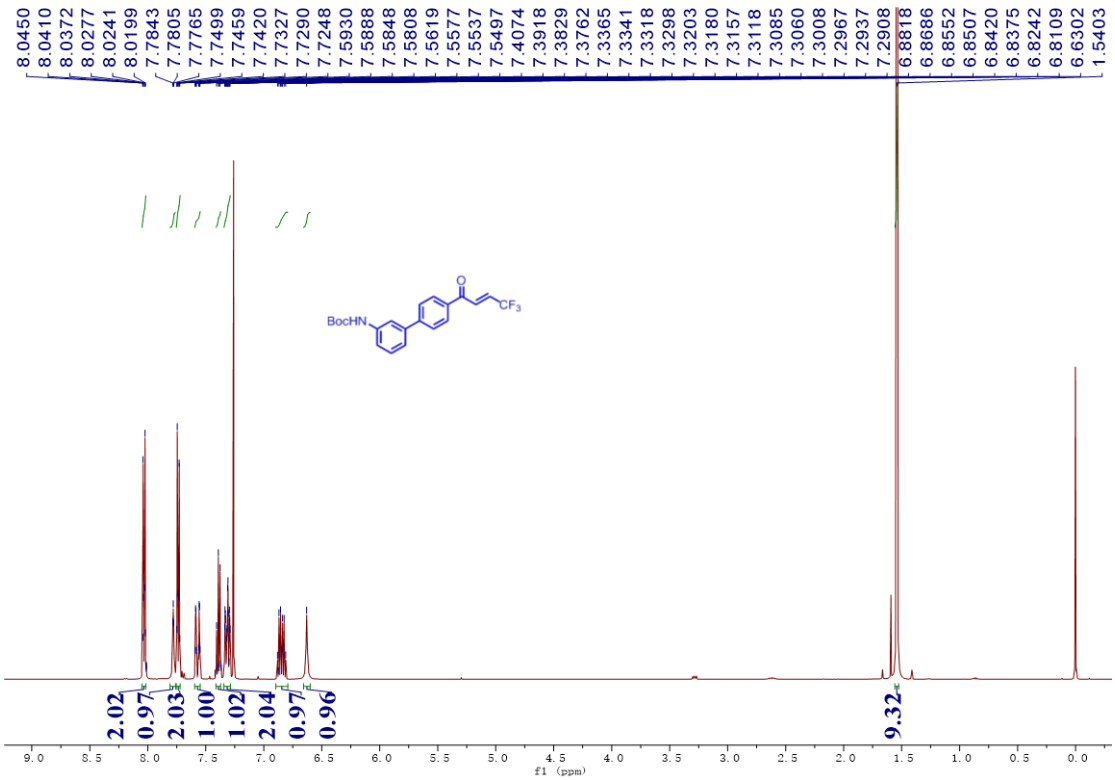
J = 9.3 Hz, 2 H), 7.35 (d, *J* = 7.0 Hz, 1 H), 4.23 (s, 1 H), 4.10 (d, *J* = 14.7 Hz, 1 H), 3.89–3.74 (m, 2 H), 3.73–3.61 (m, 2 H), 2.88 (t, *J* = 13.5 Hz, 1 H), 2.36 (s, 3 H); **^{13}C NMR** (126 MHz, DMSO) δ 196.04, 171.09, 170.64, 169.12, 139.17, 136.74, 136.53, 135.14, 133.16, 131.22, 130.51, 130.19, 127.07 (q, *J* = 279.53 Hz), 125.03, 124.00, 122.35, 121.82, 46.21 (q, *J* = 27.2 Hz), 45.18, 45.04, 44.32, 20.86; **^{19}F NMR** (471 MHz, DMSO) δ -64.28; **HRMS** [ESI] Calcd for $[M+H]^+$ $C_{22}H_{20}F_3N_3O_4$: 448.1479, Found: 448.1491.

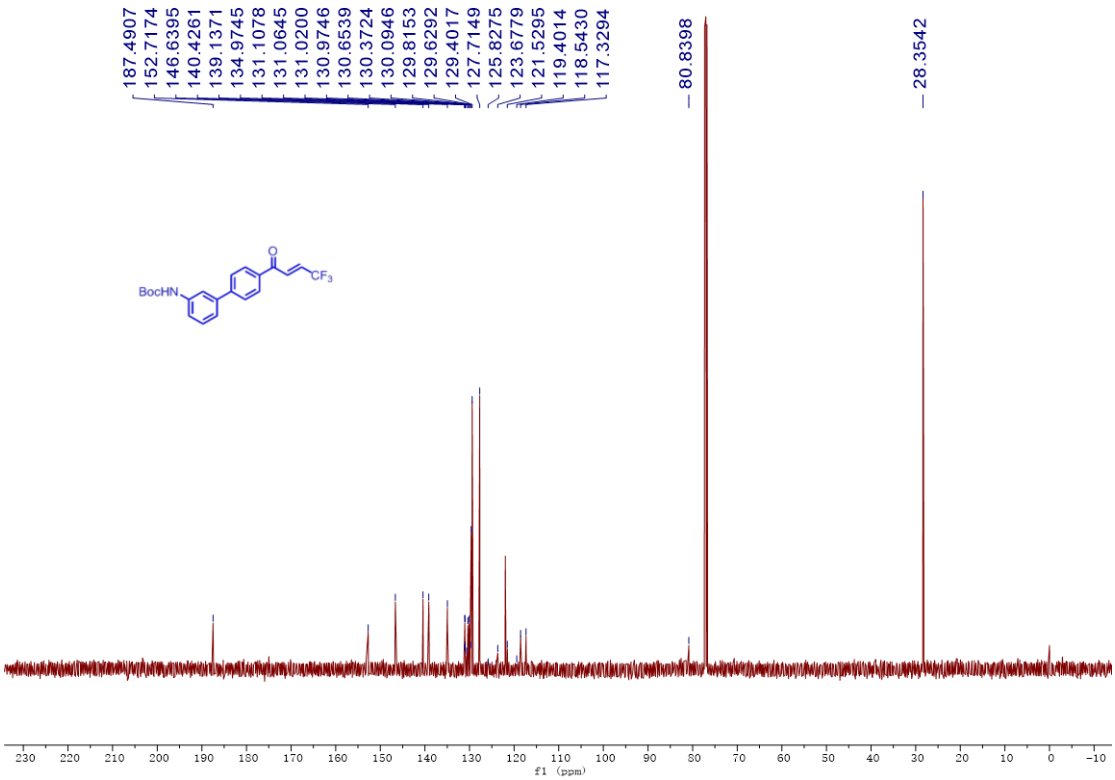

7.3196
7.3144
7.3092
7.3040
7.2808
7.2756
7.2704
7.2643
7.0332
7.0279
7.0232
7.0185
7.0131
7.0091
6.6502
6.6336
6.6168
6.6113
6.6000
6.5946
6.5780
2.3494
2.3456
2.3402
2.3348
2.3295
2.3245
2.3200
2.3166
2.3129
2.3087
2.3034
2.2934
2.2872
1.7007
1.6977
1.6926
1.6864
1.6821
1.6724
1.6689
1.6666
1.6630
1.6587
1.6561
1.6533
1.6483
1.6427
1.6392
1.6330
1.6252
O
CF3
1.03
1.03
0.97
4.31
4.27
f1 (ppm)

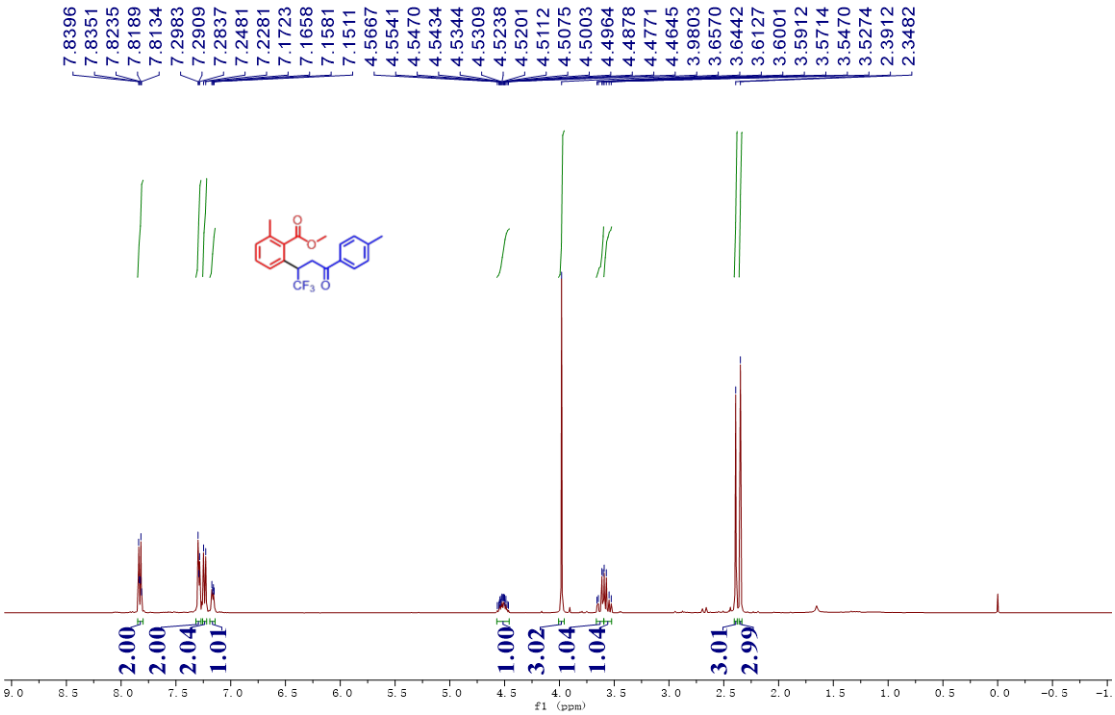

188.3963
143.9953
139.8856
130.6624
130.6167
130.5717
130.5272
128.7593
128.4820
128.2048
127.9267
125.9775
123.8315
121.6830
119.5219
26.4472
23.0725
21.6538
21.3776
O
CF3
f1 (ppm)

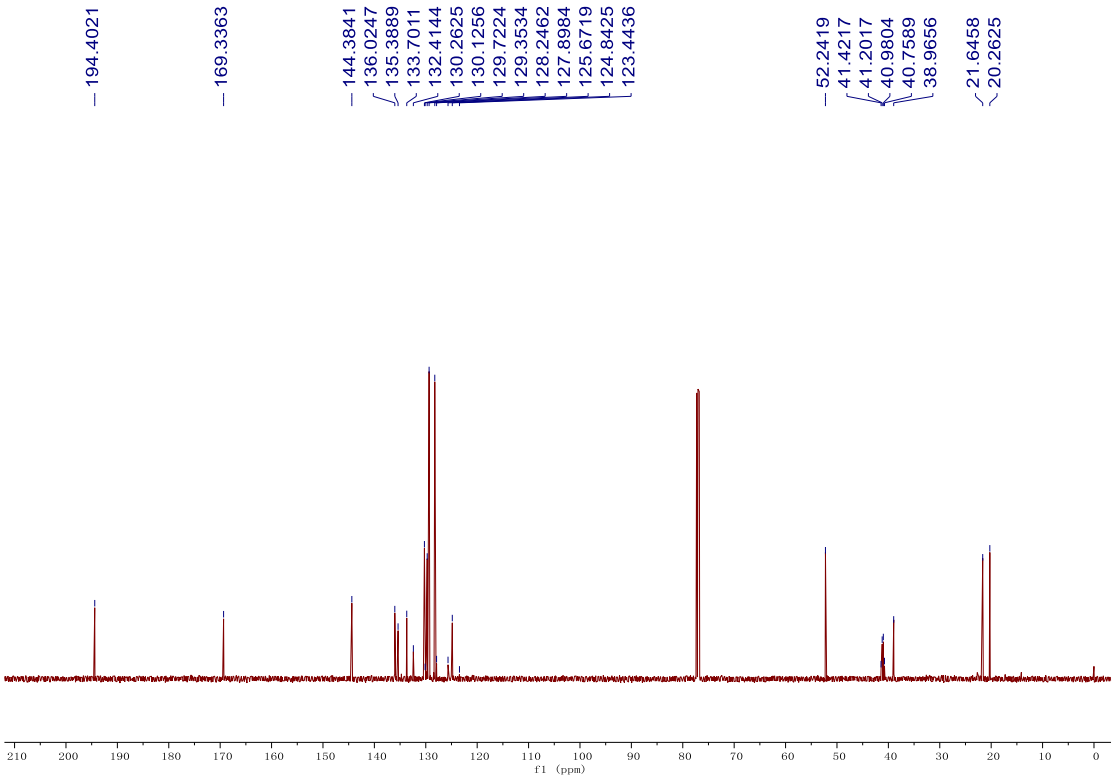

7.9462
7.9423
7.9383
7.7472
7.7309
7.6213
7.6186
7.6158
7.6058
7.6030
7.6004
7.5262
7.5220
7.5179
7.5140
7.4950
7.4909
7.4868
7.4829
7.4544
7.4386
7.4227
6.8496
6.8363
6.8231
6.8185
6.8097
6.8052
6.7919
6.7783
6.7670
1.5313
BocHN
CF3
1.01
0.97
1.00
1.01
1.00
1.00
0.98
9.17
f1 (ppm)

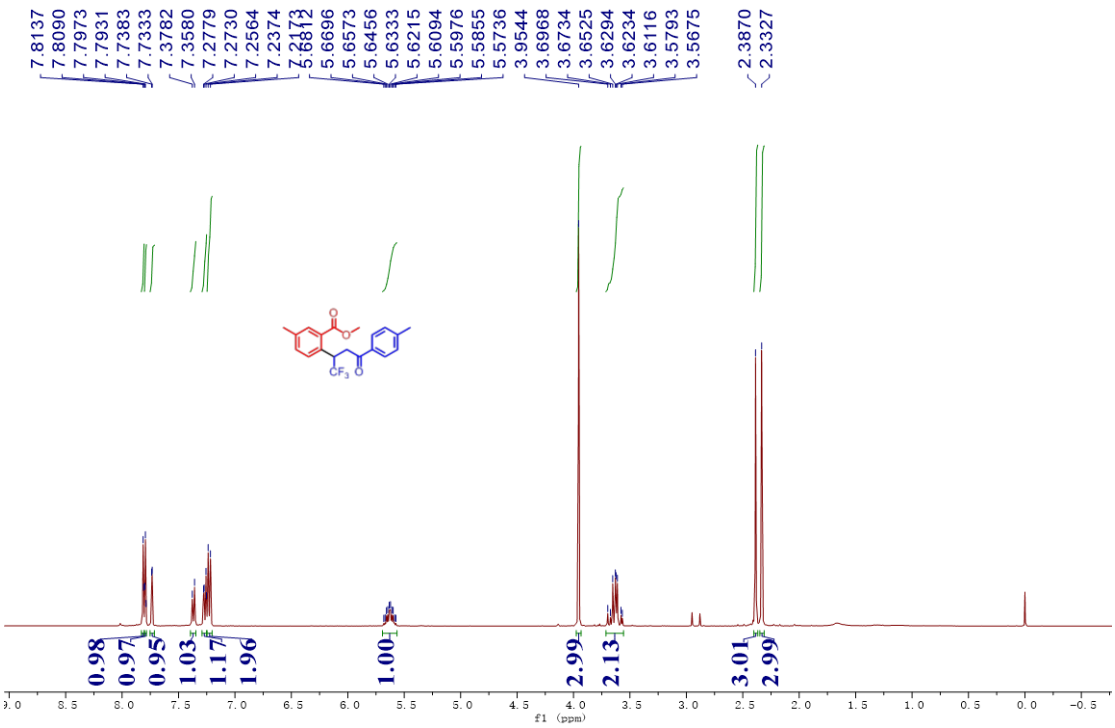

187.7926
152.6238
139.4533
136.8824
131.0525
131.0078
130.9628
130.9193
130.8365
130.5565
130.2767
129.9975
129.6780
125.7720
123.6249
121.4767
119.3271
118.3429
81.2256
28.3010
BocHN
CF3
f1 (ppm)

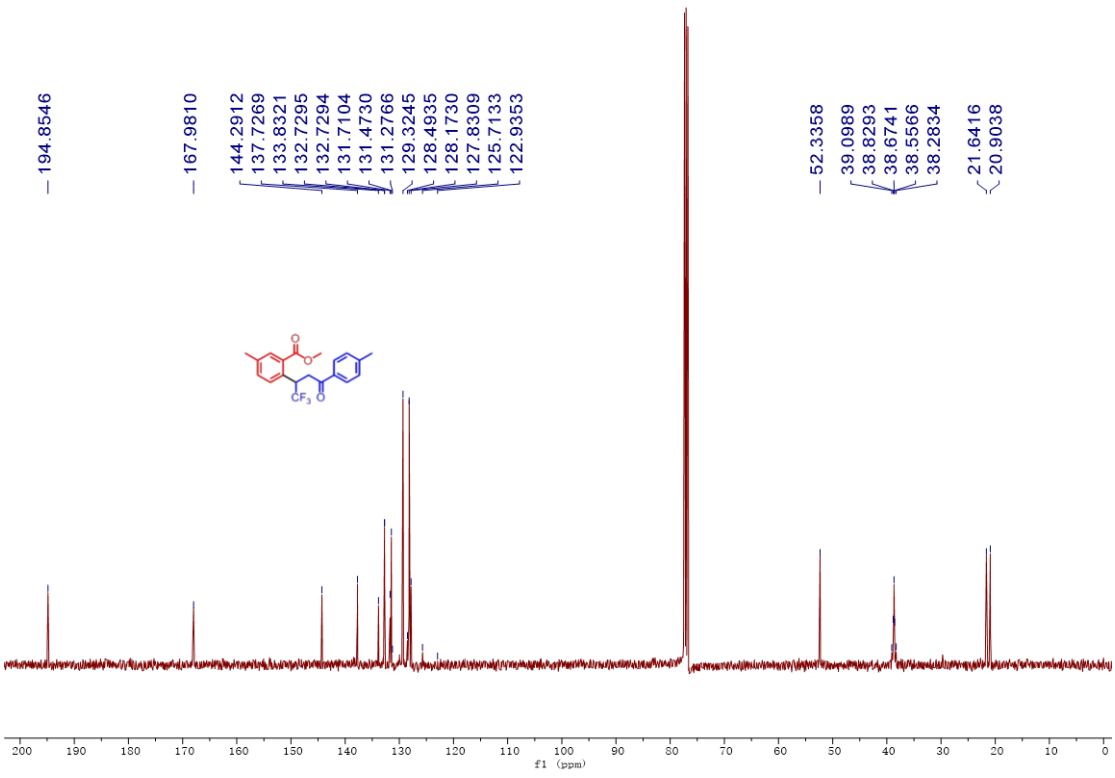

8.0450
8.0410
8.0372
8.0277
8.0241
8.0199
7.7843
7.7805
7.7765
7.7499
7.7459
7.7420
7.7327
7.7290
7.7248
7.5930
7.5888
7.5848
7.5808
7.5619
7.5577
7.5537
7.5497
7.4074
7.3918
7.3829
7.3762
7.3365
7.3341
7.3318
7.3298
7.3203
7.3180
7.3157
7.3118
7.3085
7.3060
7.3008
7.2967
7.2937
7.2908
6.8818
6.8686
6.8552
6.8507
6.8420
6.8375
6.8242
6.8109
6.6302
1.5403
BocHN
O
CF3
2.02
0.97
2.03
1.00
1.02
2.04
0.97
0.96
9.32
f1 (ppm)

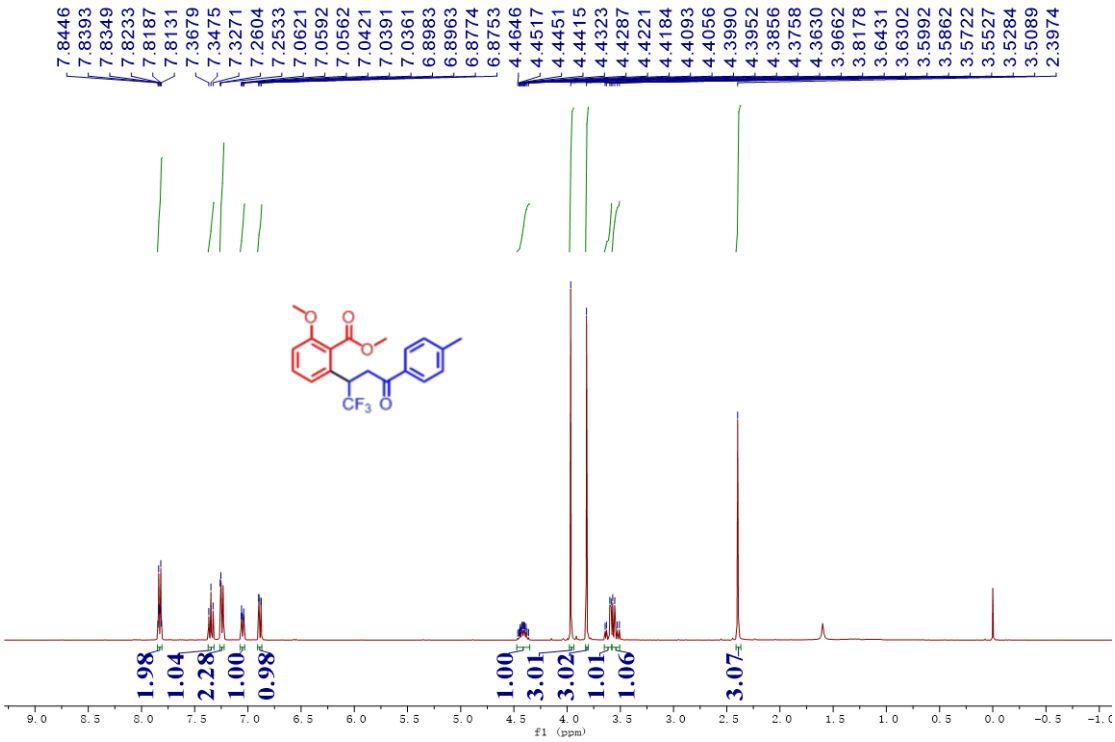

187.4907
152.7174
146.6395
140.4261
139.1371
134.9745
131.1078
131.0645
131.0200
130.9746
130.6539
130.3724
130.0946
129.8153
129.6292
129.4017
127.7149
125.8275
123.6779
121.5295
119.4014
118.5430
117.3294
80.8398
28.3542
BocHN
O
CF3
f1 (ppm)

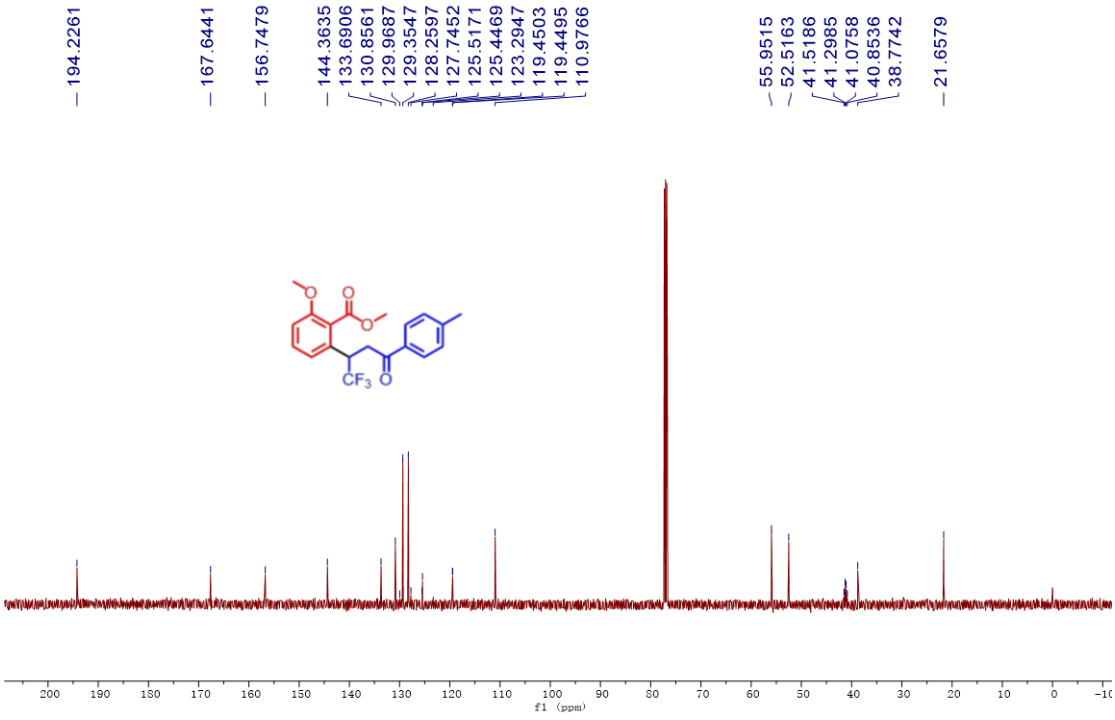

7.8396
7.8351
7.8235
7.8189
7.8134
7.2983
7.2909
7.2837
7.2481
7.2281
7.1723
7.1658
7.1581
7.1511
4.5667
4.5541
4.5470
4.5434
4.5344
4.5309
4.5238
4.5201
4.5112
4.5075
4.5003
4.4964
4.4878
4.4771
4.4645
3.9803
3.6570
3.6442
3.6127
3.6001
3.5912
3.5714
3.5470
3.5274
2.3912
2.3482
2.00
2.00
2.04
1.01
1.00
3.02
1.04
1.04
3.01
2.99
f1 (ppm)

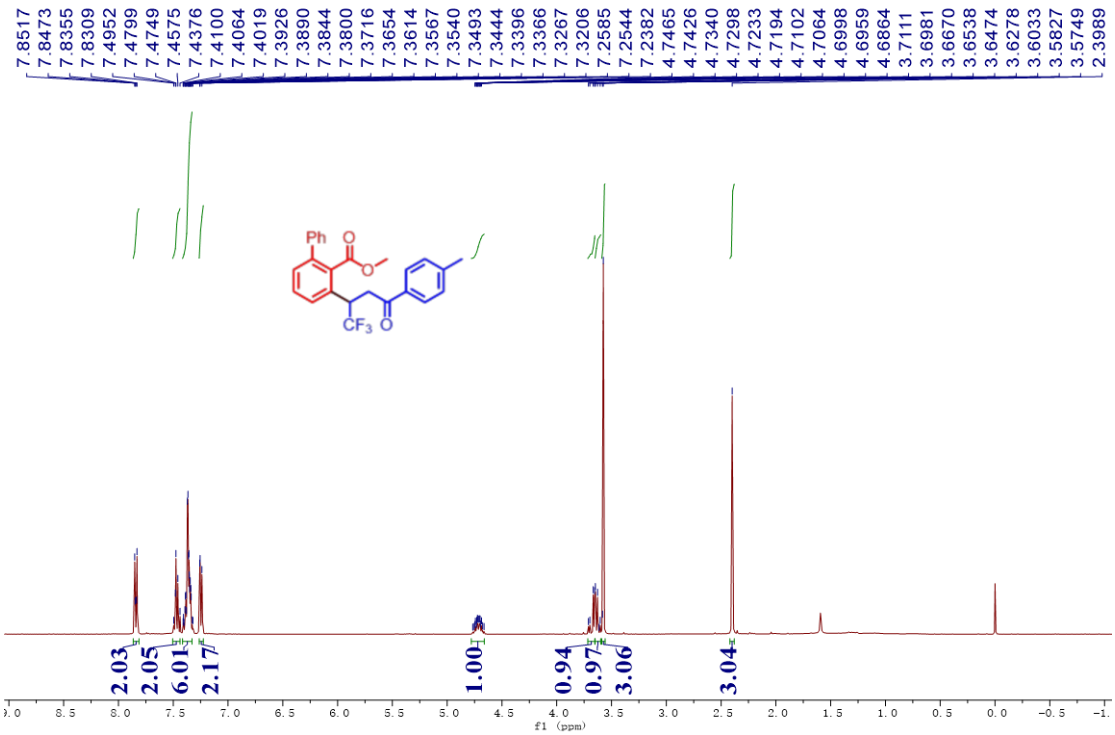

194.4021
169.3363
144.3841
136.0247
135.3889
133.7011
132.4144
130.2625
130.1256
129.7224
129.3534
128.2462
127.8984
125.6719
124.8425
123.4436
52.2419
41.4217
41.2017
40.9804
40.7589
38.9656
21.6458
20.2625
f1 (ppm)

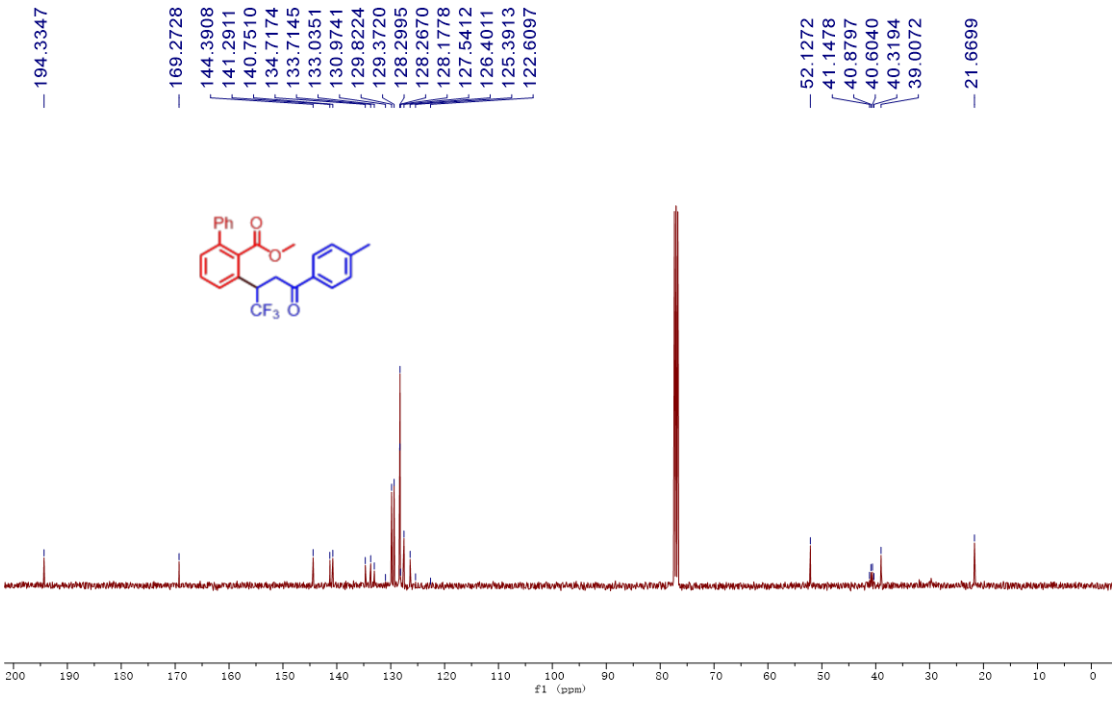

7.8137
7.8090
7.7973
7.7931
7.7383
7.7333
7.3782
7.3580
7.2779
7.2730
7.2564
7.2374
7.2173
5.6812
5.6696
5.6573
5.6456
5.6333
5.6215
5.6094
5.5976
5.5855
5.5736
3.9544
3.6968
3.6734
3.6525
3.6294
3.6234
3.6116
3.5793
3.5675
2.3870
2.3327
0.98
0.97
0.95
1.03
1.17
1.96
1.00
2.99
2.13
3.01
2.99
f1 (ppm)

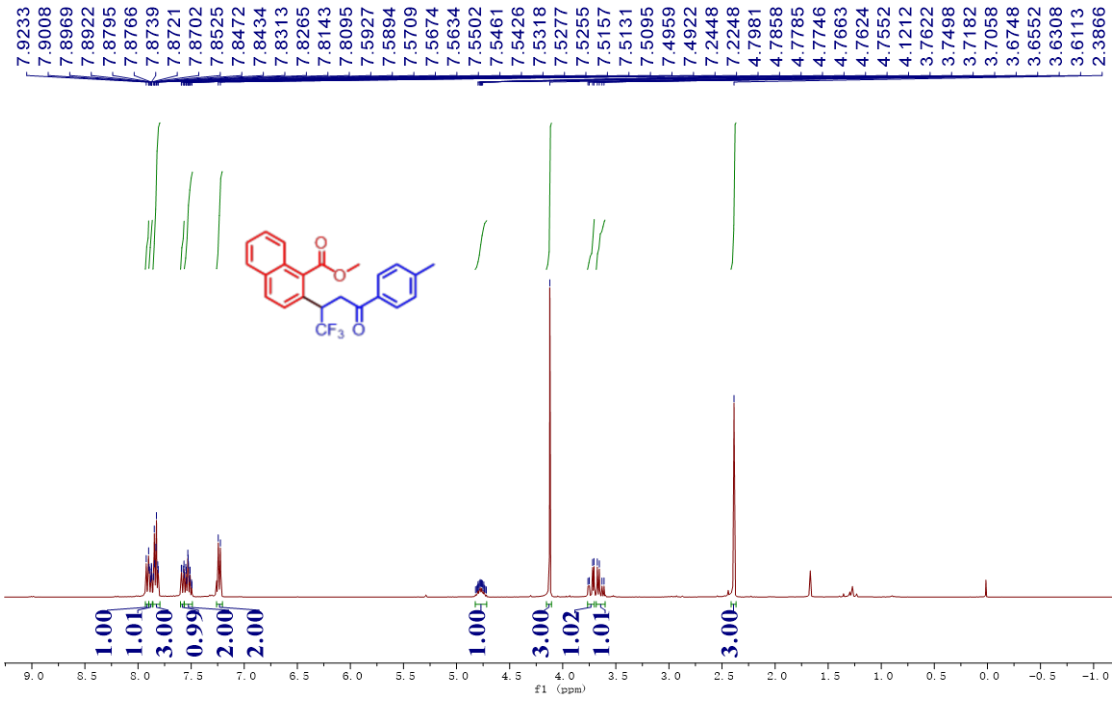

194.8546
167.9810
144.2912
137.7269
133.8321
132.7295
132.7294
131.7104
131.4730
131.2766
129.3245
128.4935
128.1730
127.8309
125.7133
122.9353
52.3358
39.0989
38.8293
38.6741
38.5566
38.2834
21.6416
20.9038
f1 (ppm)

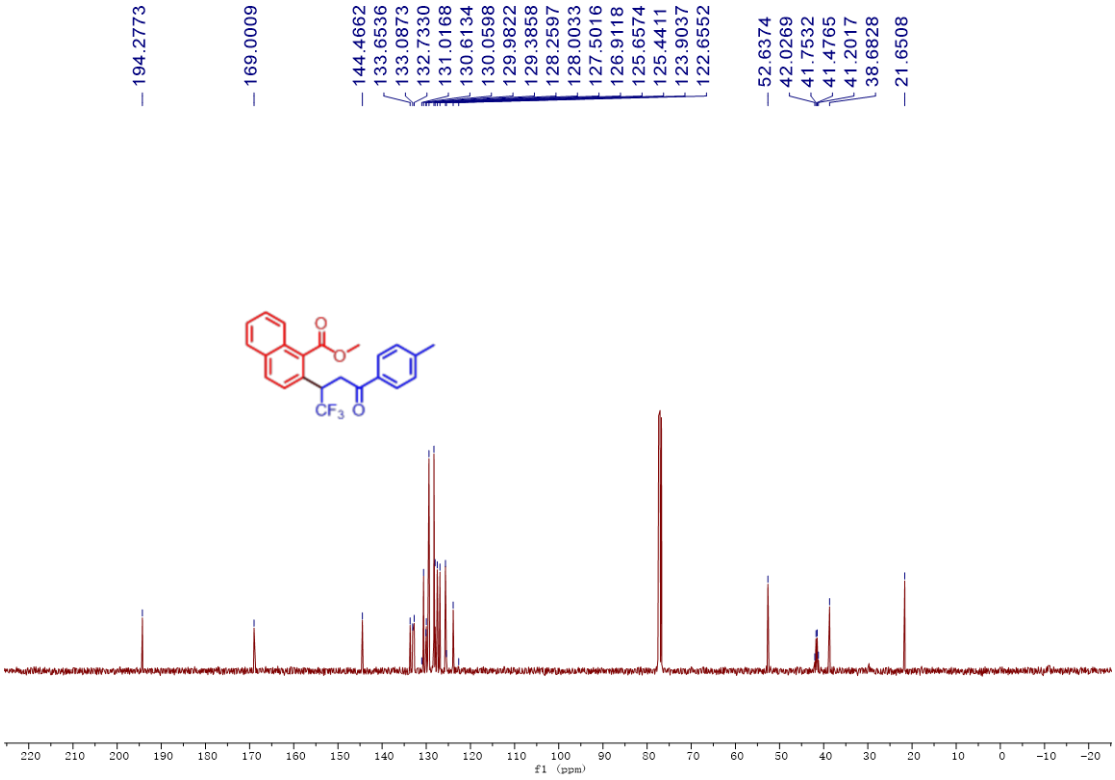

7.8446
7.8393
7.8349
7.8233
7.8187
7.8131
7.3679
7.3475
7.3271
7.2604
7.2533
7.0621
7.0592
7.0562
7.0421
7.0391
7.0361
6.8983
6.8963
6.8774
6.8753
4.4646
4.4517
4.4451
4.4415
4.4323
4.4287
4.4221
4.4184
4.4093
4.4056
4.3990
4.3952
4.3856
4.3758
4.3630
3.9662
3.8178
3.6431
3.6302
3.5992
3.5862
3.5722
3.5527
3.5284
3.5089
2.3974
1.98
1.04
2.28
1.00
0.98
1.00
3.01
3.02
1.01
1.06
3.07
f1 (ppm)

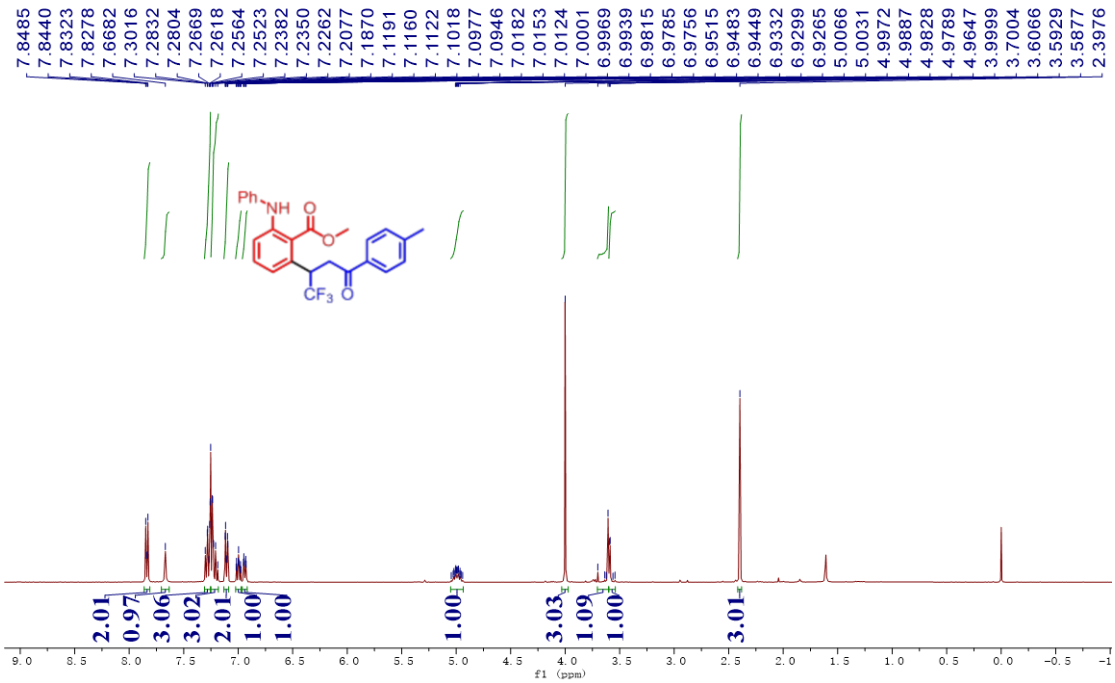

194.2261
167.6441
156.7479
144.3635
133.6906
130.8561
129.9687
129.3547
128.2597
127.7452
125.5171
125.4469
123.2947
119.4503
119.4495
110.9766
55.9515
52.5163
41.5186
41.2985
41.0758
40.8536
38.7742
21.6579
f1 (ppm)

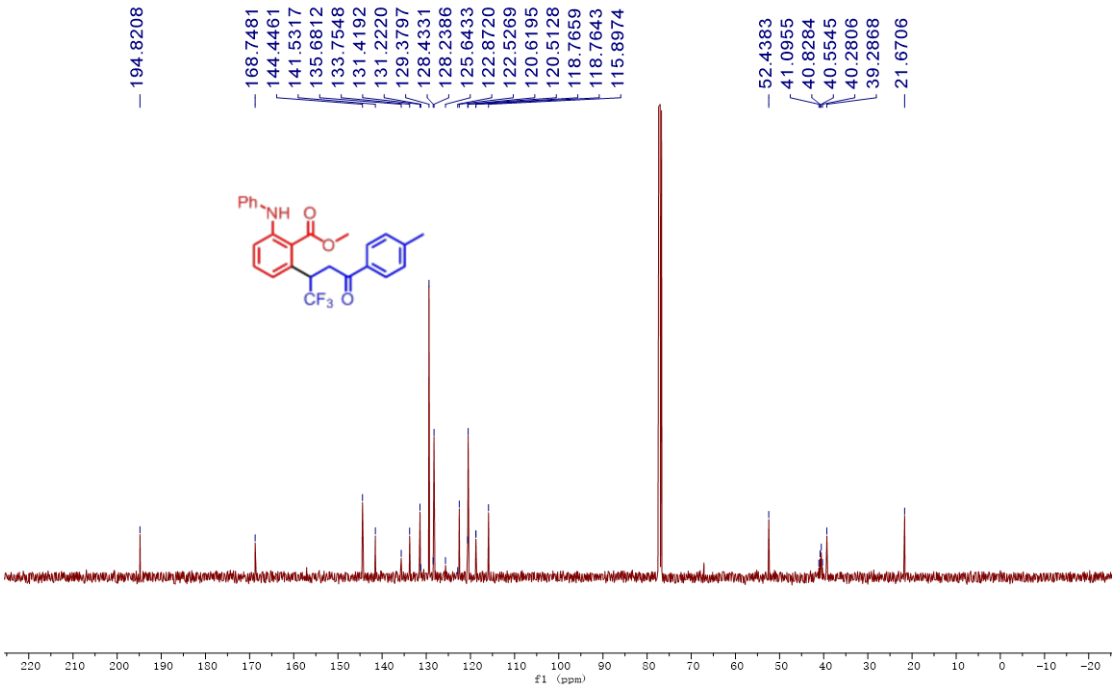

7.8517
7.8473
7.8355
7.8309
7.4952
7.4799
7.4749
7.4575
7.4376
7.4100
7.4064
7.4019
7.3926
7.3890
7.3844
7.3800
7.3716
7.3654
7.3614
7.3567
7.3540
7.3493
7.3444
7.3396
7.3366
7.3267
7.3206
7.2585
7.2544
7.2382
4.7465
4.7426
4.7340
4.7298
4.7233
4.7194
4.7102
4.7064
4.6998
4.6959
4.6864
3.7111
3.6981
3.6670
3.6538
3.6474
3.6278
3.6033
3.5827
3.5749
2.3989
Ph
O
O
CF3
O
2.03
2.05
6.01
2.17
1.00
0.94
0.97
3.06
3.04
f1 (ppm)

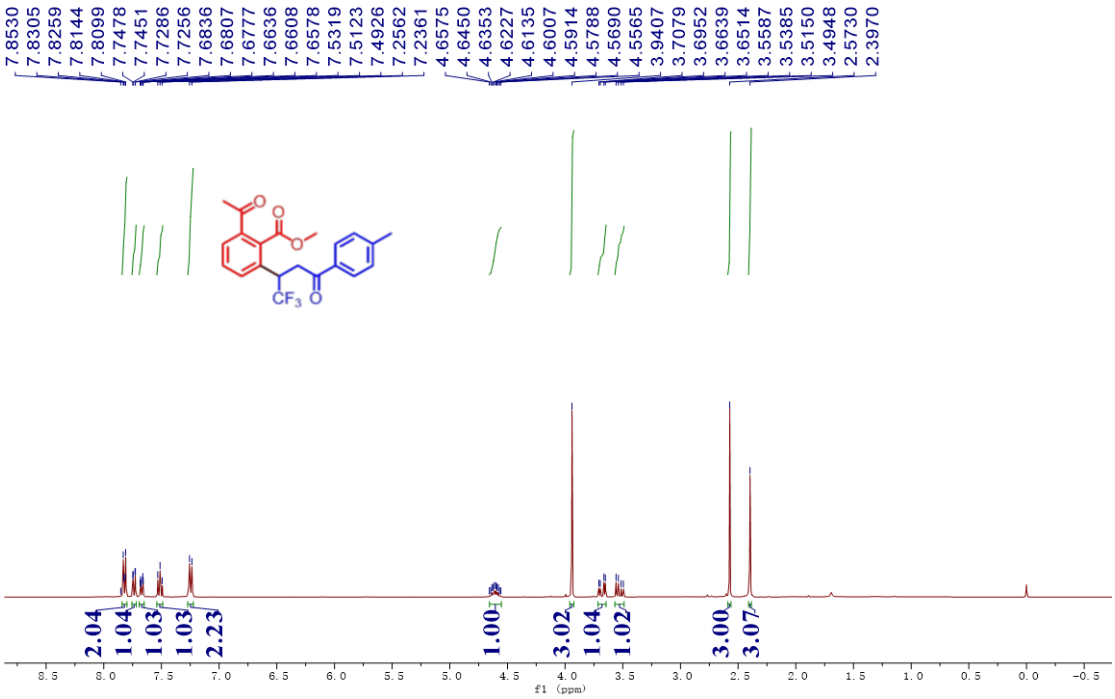

194.3347
169.2728
144.3908
141.2911
140.7510
134.7174
133.7145
133.0351
130.9741
129.8224
129.3720
128.2995
128.2670
128.1778
127.5412
126.4011
125.3913
122.6097
52.1272
41.1478
40.8797
40.6040
40.3194
39.0072
21.6699
Ph
O
O
CF3
O
f1 (ppm)

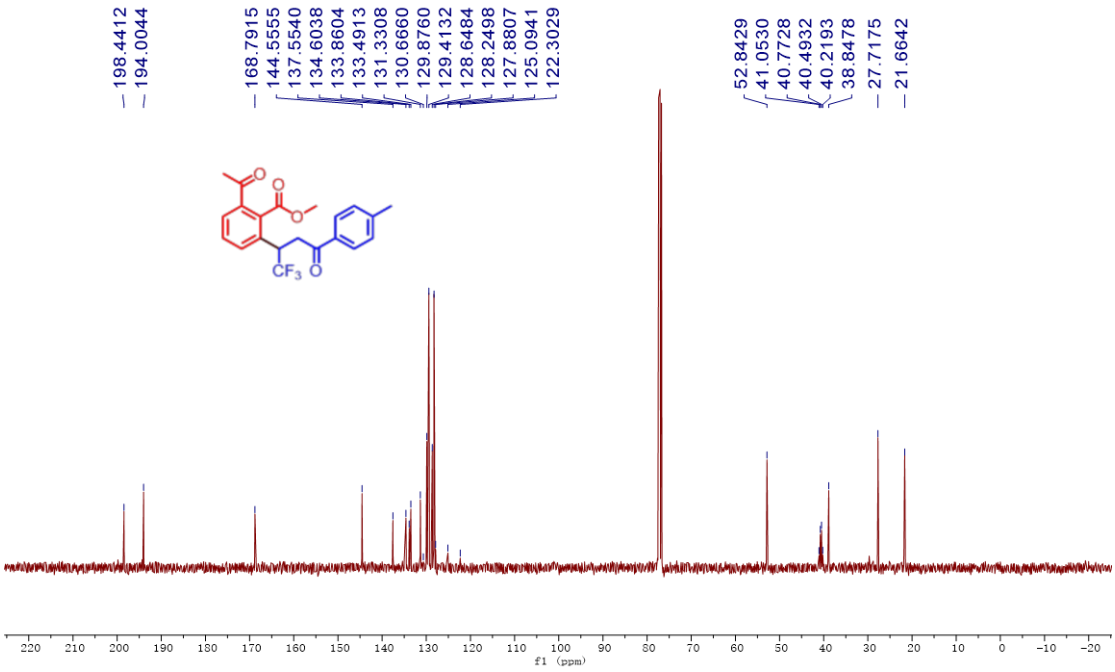

7.9233
7.9008
7.8969
7.8922
7.8795
7.8766
7.8739
7.8721
7.8702
7.8525
7.8472
7.8434
7.8313
7.8265
7.8143
7.8095
7.5927
7.5894
7.5709
7.5674
7.5634
7.5502
7.5461
7.5426
7.5318
7.5277
7.5255
7.5157
7.5131
7.5095
7.4959
7.4922
7.2448
7.2248
4.7981
4.7858
4.7785
4.7746
4.7663
4.7624
4.7552
4.1212
3.7622
3.7498
3.7182
3.7058
3.6748
3.6552
3.6308
3.6113
2.3866
1.00
1.01
3.00
0.99
2.00
2.00
1.00
3.00
1.02
1.01
3.00
f1 (ppm)

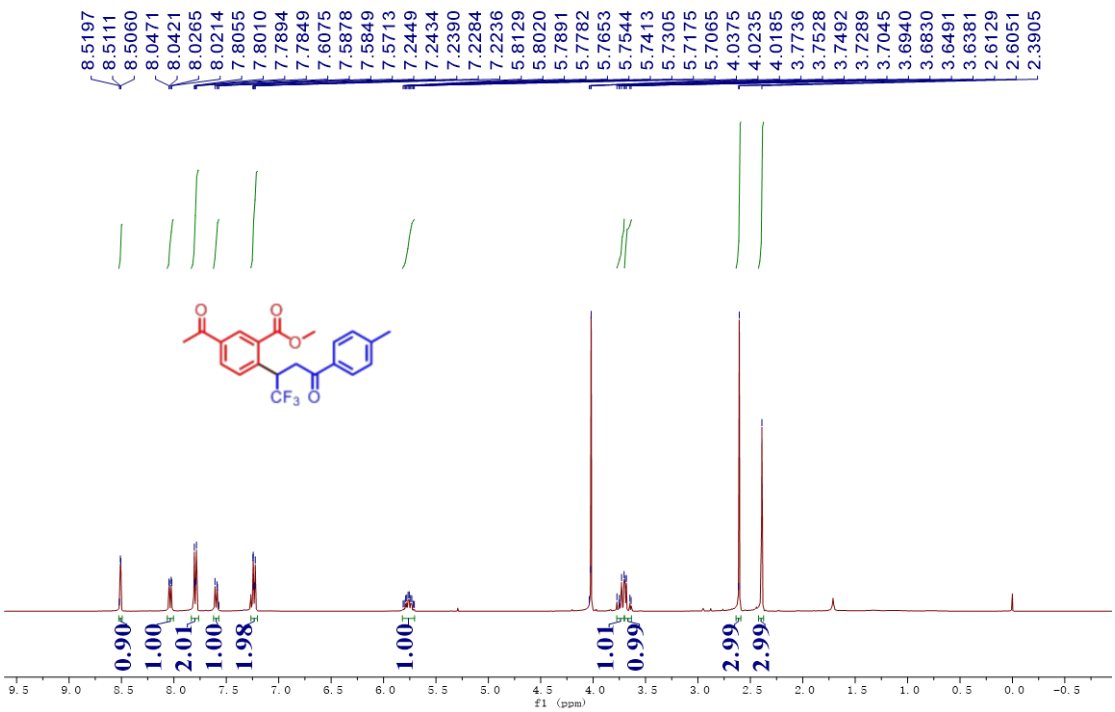

194.2773
169.0009
144.4662
133.6536
133.0873
132.7330
131.0168
130.6134
130.0598
129.9822
129.3858
128.2597
128.0033
127.5016
126.9118
125.6574
125.4411
123.9037
122.6552
52.6374
42.0269
41.7532
41.4765
41.2017
38.6828
21.6508
f1 (ppm)

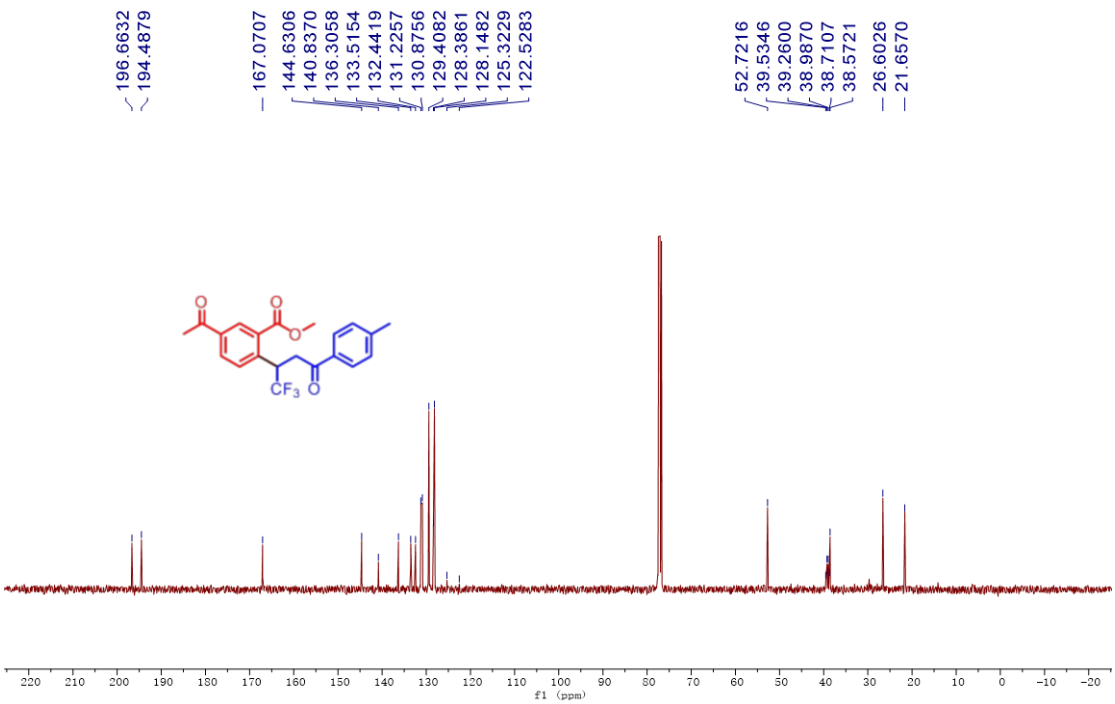

7.8485
7.8440
7.8323
7.8278
7.6682
7.3016
7.2832
7.2804
7.2669
7.2618
7.2564
7.2523
7.2382
7.2350
7.2262
7.2077
7.1870
7.1191
7.1160
7.1122
7.1018
7.0977
7.0946
7.0182
7.0153
7.0124
7.0001
6.9969
6.9939
6.9815
6.9785
6.9756
6.9515
6.9483
6.9449
6.9332
6.9299
6.9265
5.0066
5.0031
4.9972
4.9887
4.9828
4.9789
4.9647
3.9999
3.7004
3.6066
3.5929
3.5877
2.3976
Ph
NH
O
O
CF3
O
2.01
0.97
3.06
3.02
2.01
1.00
1.00
1.00
3.03
1.09
1.00
3.01
f1 (ppm)

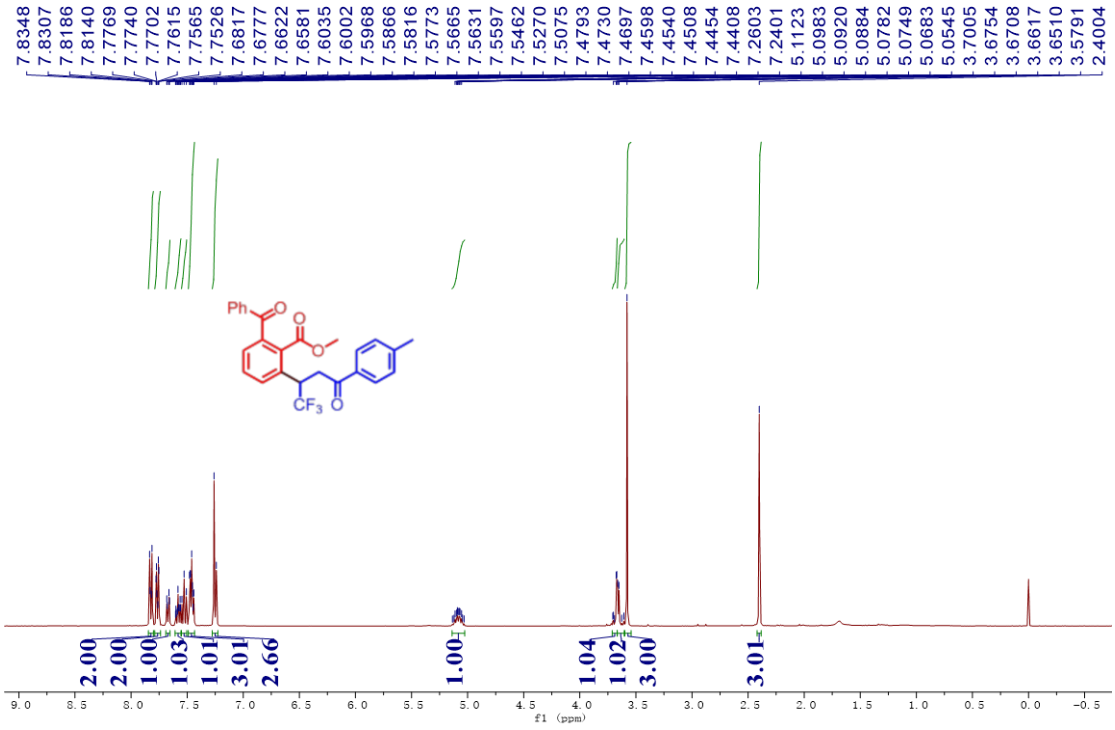

194.8208
168.7481
144.4461
141.5317
135.6812
133.7548
131.4192
131.2220
129.3797
128.4331
128.2386
125.6433
122.8720
122.5269
120.6195
120.5128
118.7659
118.7643
115.8974
52.4383
41.0955
40.8284
40.5545
40.2806
39.2868
21.6706
Ph
NH
O
O
CF3
O
f1 (ppm)

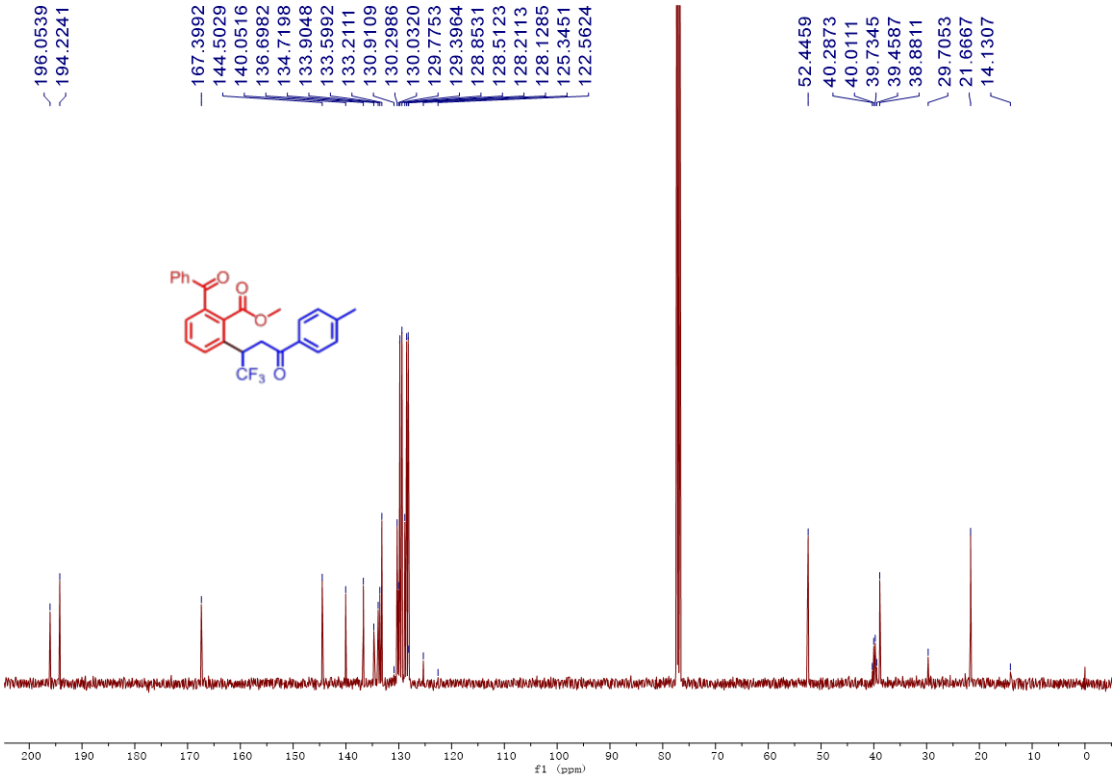

7.8530
7.8305
7.8259
7.8144
7.8099
7.7478
7.7451
7.7286
7.7256
7.6836
7.6807
7.6777
7.6636
7.6608
7.6578
7.5319
7.5123
7.4926
7.2562
7.2361
4.6575
4.6450
4.6353
4.6227
4.6135
4.6007
4.5914
4.5788
4.5690
4.5565
3.9407
3.7079
3.6952
3.6639
3.6514
3.5587
3.5385
3.5150
3.4948
2.5730
2.3970
2.04
1.04
1.03
1.03
2.23
1.00
3.02
1.04
1.02
3.00
3.07
f1 (ppm)

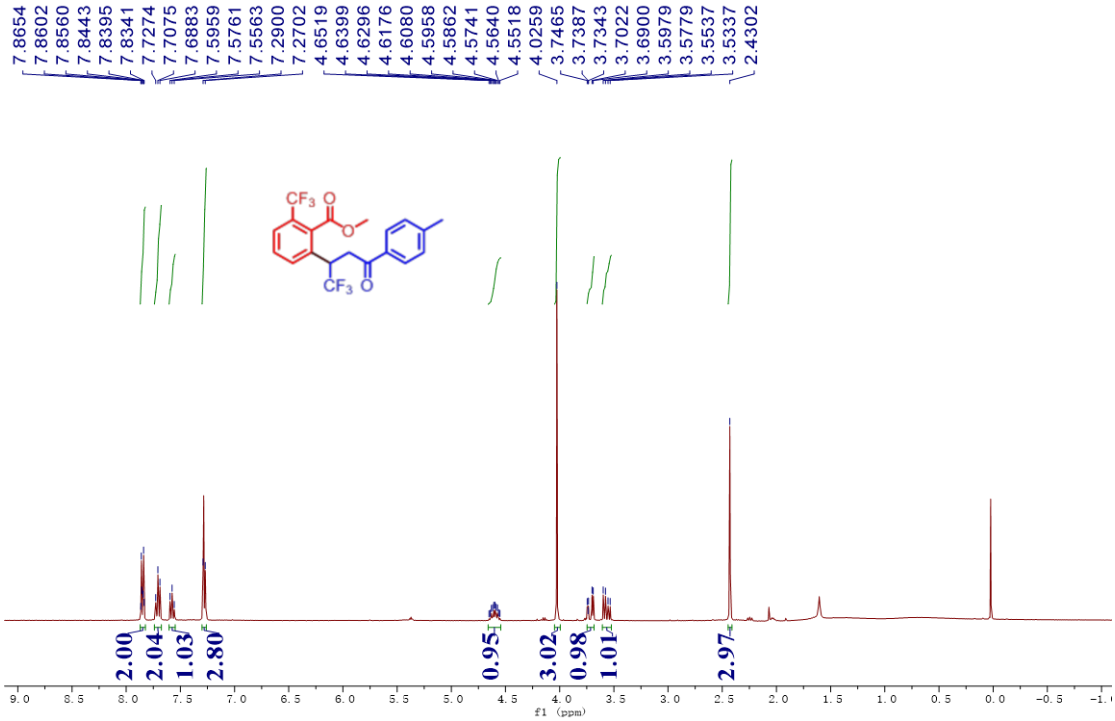

198.4412
194.0044
168.7915
144.5555
137.5540
134.6038
133.8604
133.4913
131.3308
130.6660
129.8760
129.4132
128.6484
128.2498
127.8807
125.0941
122.3029
52.8429
41.0530
40.7728
40.4932
40.2193
38.8478
27.7175
21.6642
f1 (ppm)

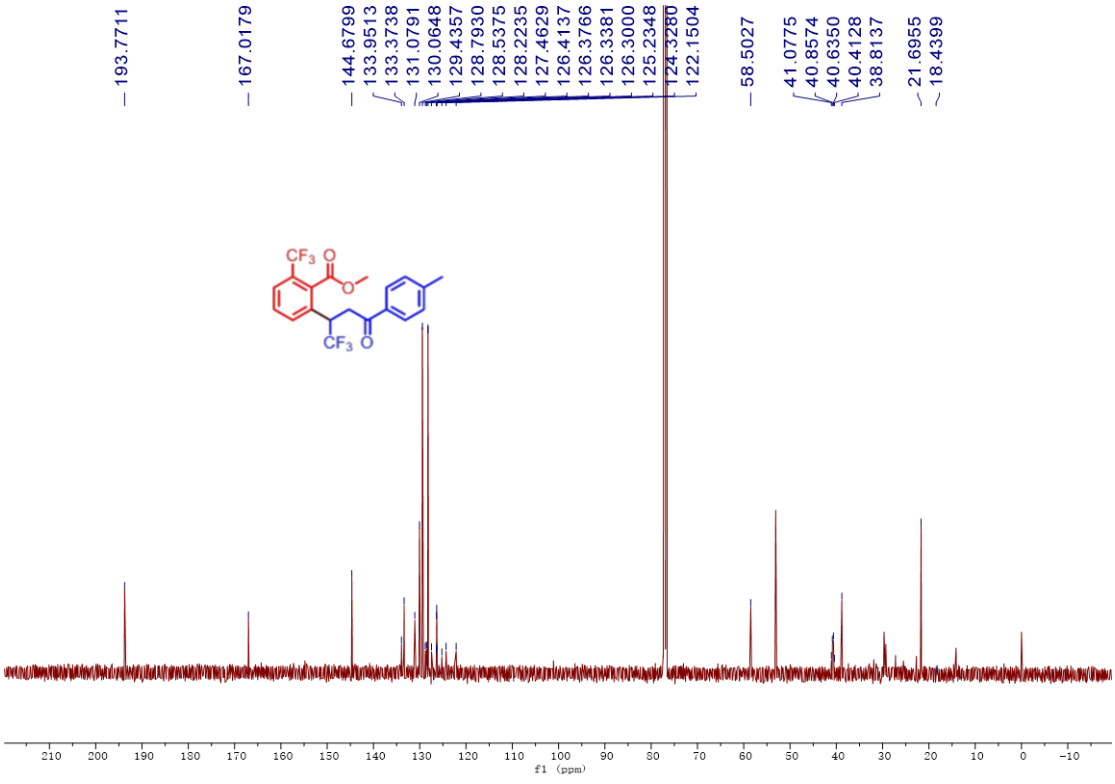

8.5197
8.5111
8.5060
8.0471
8.0421
8.0265
8.0214
7.8055
7.8010
7.7894
7.7849
7.6075
7.5878
7.5849
7.5713
7.2449
7.2434
7.2390
7.2284
7.2236
5.8129
5.8020
5.7891
5.7782
5.7653
5.7544
5.7413
5.7305
5.7175
5.7065
4.0375
4.0235
4.0185
3.7736
3.7528
3.7492
3.7289
3.7045
3.6940
3.6830
3.6491
3.6381
2.6129
2.6051
2.3905
0.90
1.00
2.01
1.00
1.98
1.00
1.01
0.99
2.99
2.99
f1 (ppm)

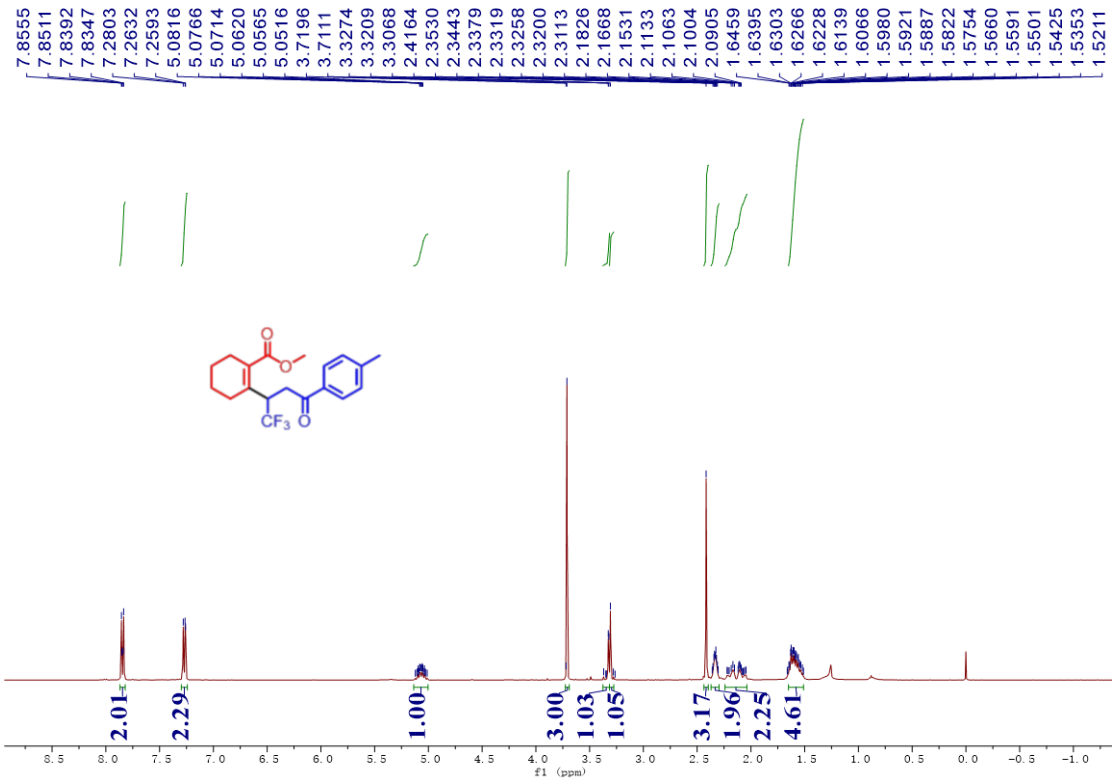

196.6632
194.4879
167.0707
144.6306
140.8370
136.3058
133.5154
132.4419
131.2257
130.8756
129.4082
128.3861
128.1482
125.3229
122.5283
52.7216
39.5346
39.2600
38.9870
38.7107
38.5721
26.6026
21.6570
f1 (ppm)

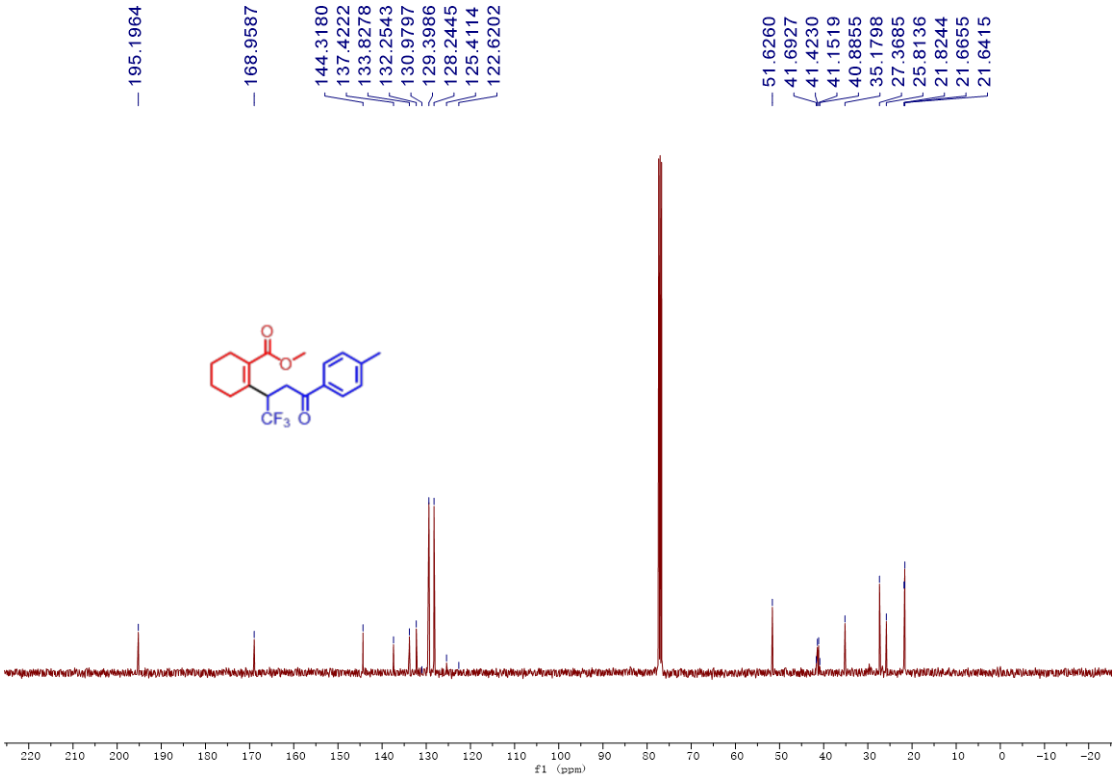

7.8348
7.8307
7.8186
7.8140
7.7769
7.7740
7.7702
7.7615
7.7565
7.7526
7.6817
7.6777
7.6622
7.6581
7.6035
7.6002
7.5968
7.5866
7.5816
7.5773
7.5665
7.5631
7.5597
7.5462
7.5270
7.5075
7.4793
7.4730
7.4697
7.4598
7.4540
7.4508
7.4454
7.4408
7.2603
7.2401
5.1123
5.0983
5.0920
5.0884
5.0782
5.0749
5.0683
5.0545
3.7005
3.6754
3.6708
3.6617
3.6510
3.5791
2.4004
Ph
O
O
O
CF3
2.00
2.00
1.00
1.03
1.01
3.01
2.66
1.00
1.04
1.02
3.00
3.01
f1 (ppm)

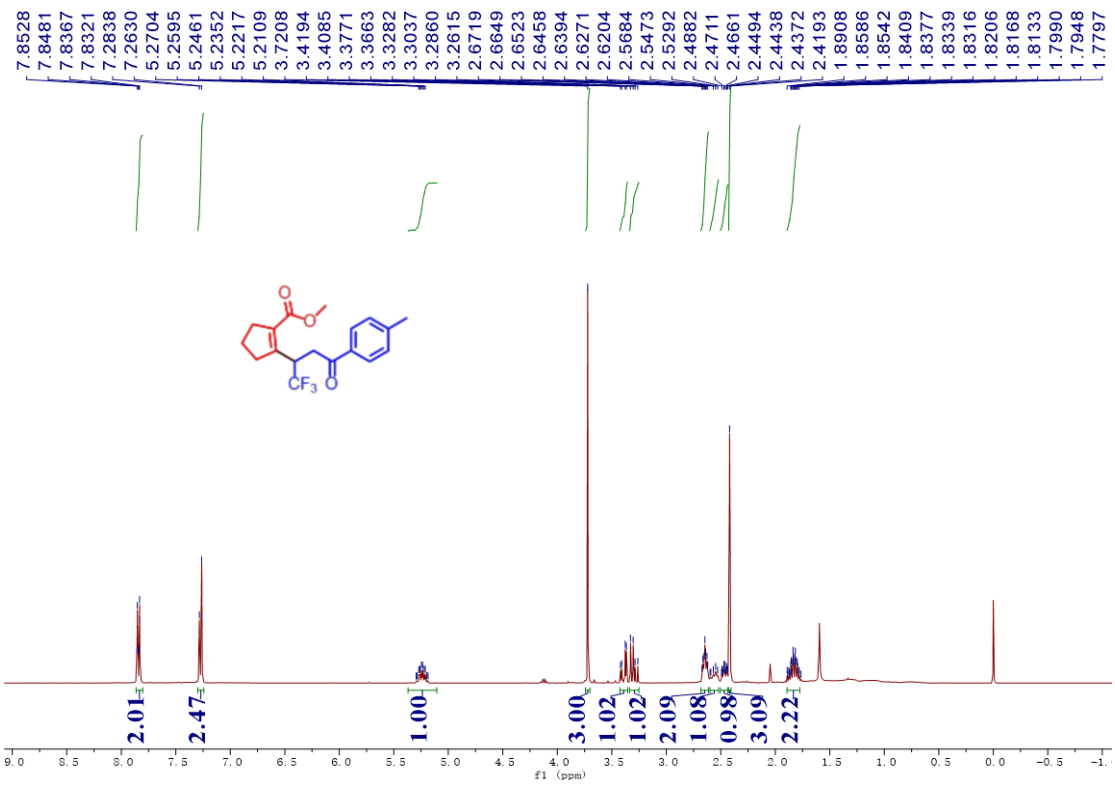

196.0539
194.2241
167.3992
144.5029
140.0516
136.6982
134.7198
133.9048
133.5992
133.2111
130.9109
130.2986
130.0320
129.7753
129.3964
128.8531
128.5123
128.2113
128.1285
125.3451
122.5624
52.4459
40.2873
40.0111
39.7345
39.4587
38.8811
29.7053
21.6667
14.1307
Ph
O
O
O
CF3
f1 (ppm)

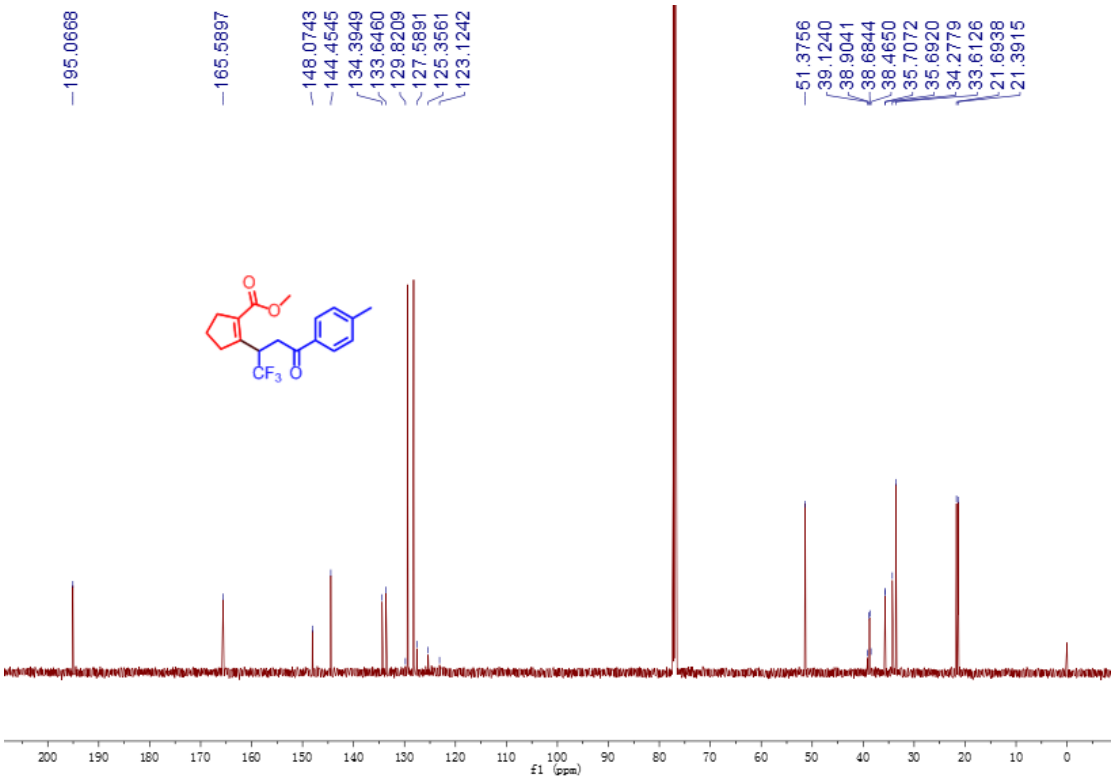

7.8654
7.8602
7.8560
7.8443
7.8395
7.8341
7.7274
7.7075
7.6883
7.5959
7.5761
7.5563
7.2900
7.2702
4.6519
4.6399
4.6296
4.6176
4.6080
4.5958
4.5862
4.5741
4.5640
4.5518
4.0259
3.7465
3.7387
3.7343
3.7022
3.6900
3.5979
3.5779
3.5537
3.5337
2.4302
CF3
O
O
CF3
O
2.00
2.04
1.03
2.80
0.95
3.02
0.98
1.01
2.97
f1 (ppm)

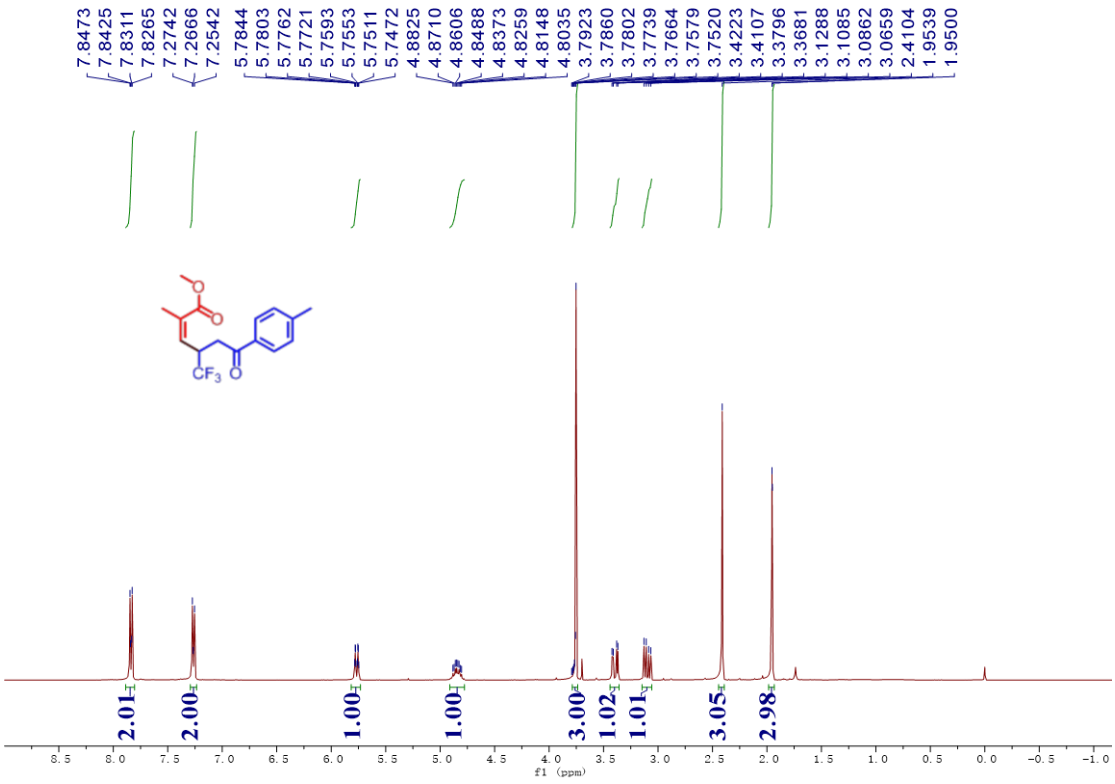

193.7711
167.0179
144.6799
133.9513
133.3738
131.0791
130.0648
129.4357
128.7930
128.5375
128.2235
127.4629
126.4137
126.3766
126.3381
126.3000
125.2348
124.3280
122.1504
58.5027
41.0775
40.8574
40.6350
40.4128
38.8137
21.6955
18.4399
CF3
O
O
CF3
O
f1 (ppm)

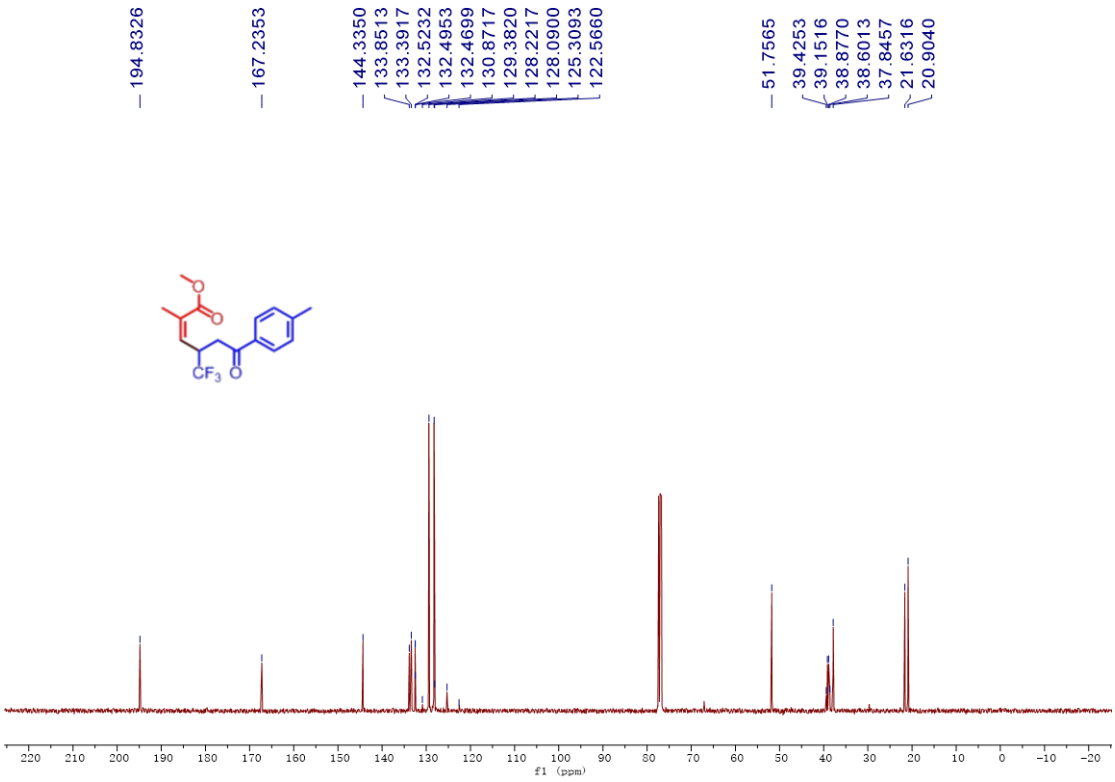

7.8555
7.8511
7.8392
7.8347
7.2803
7.2632
7.2593
5.0816
5.0766
5.0714
5.0620
5.0565
5.0516
3.7196
3.7111
3.3274
3.3209
3.3068
2.4164
2.3530
2.3443
2.3379
2.3319
2.3258
2.3200
2.3113
2.1826
2.1668
2.1531
2.1133
2.1063
2.1004
2.0905
1.6459
1.6395
1.6303
1.6266
1.6228
1.6139
1.6066
1.5980
1.5921
1.5887
1.5822
1.5754
1.5660
1.5591
1.5501
1.5425
1.5353
1.5211
CF3
O
2.01
2.29
1.00
3.00
1.03
1.05
3.17
1.96
2.25
4.61
f1 (ppm)

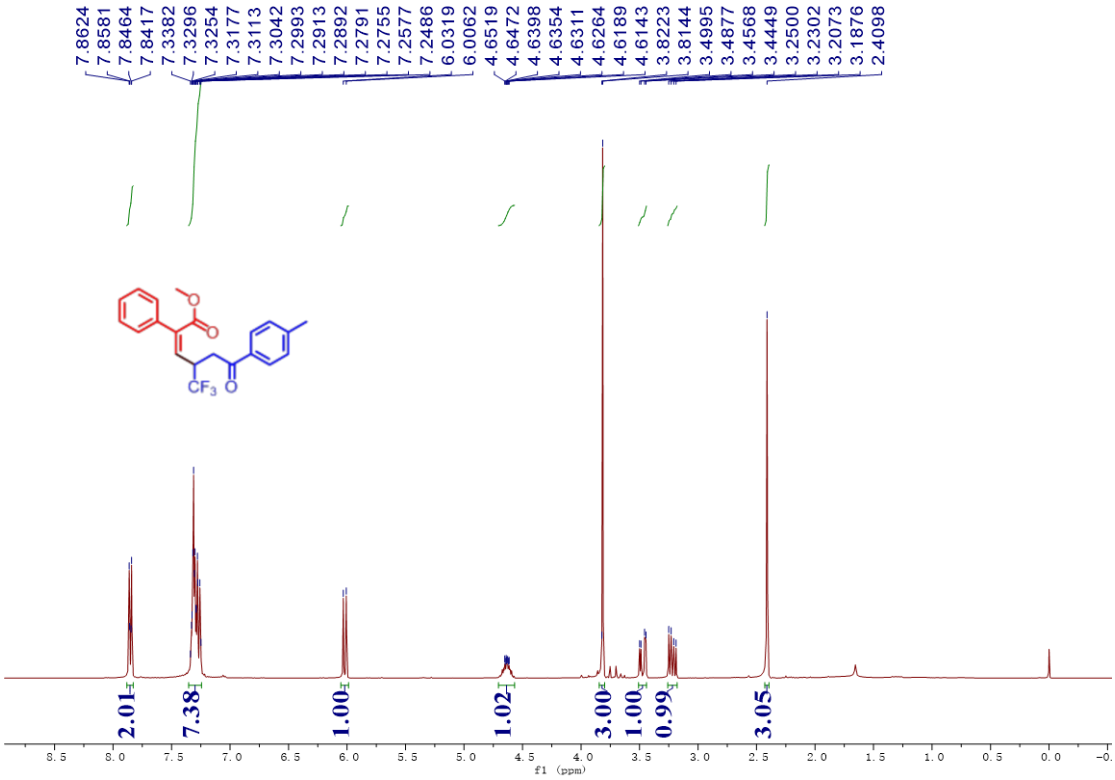

195.1964
168.9587
144.3180
137.4222
133.8278
132.2543
130.9797
129.3986
128.2445
125.4114
122.6202
51.6260
41.6927
41.4230
41.1519
40.8855
35.1798
27.3685
25.8136
21.8244
21.6655
21.6415
CF3
O
f1 (ppm)

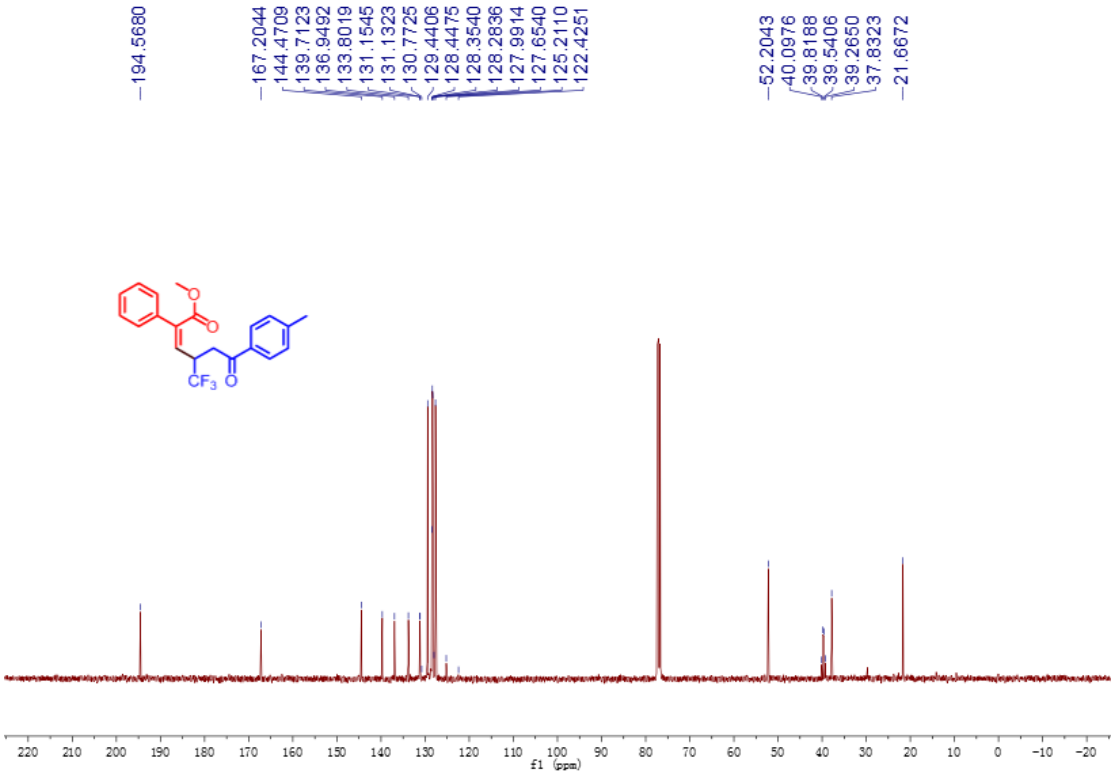

7.8528
7.8481
7.8367
7.8321
7.2838
7.2630
5.2704
5.2595
5.2461
5.2352
5.2217
5.2109
3.7208
3.4194
3.4085
3.3771
3.3663
3.3282
3.3037
3.2860
3.2615
2.6719
2.6649
2.6523
2.6458
2.6394
2.6271
2.6204
2.5684
2.5473
2.5292
2.4882
2.4711
2.4661
2.4494
2.4438
2.4372
2.4193
1.8908
1.8586
1.8542
1.8409
1.8377
1.8339
1.8316
1.8206
1.8168
1.8133
1.7990
1.7948
1.7797
CF3
O
2.01
2.47
1.00
3.00
1.02
1.02
2.09
1.08
0.98
3.09
2.22
f1 (ppm)

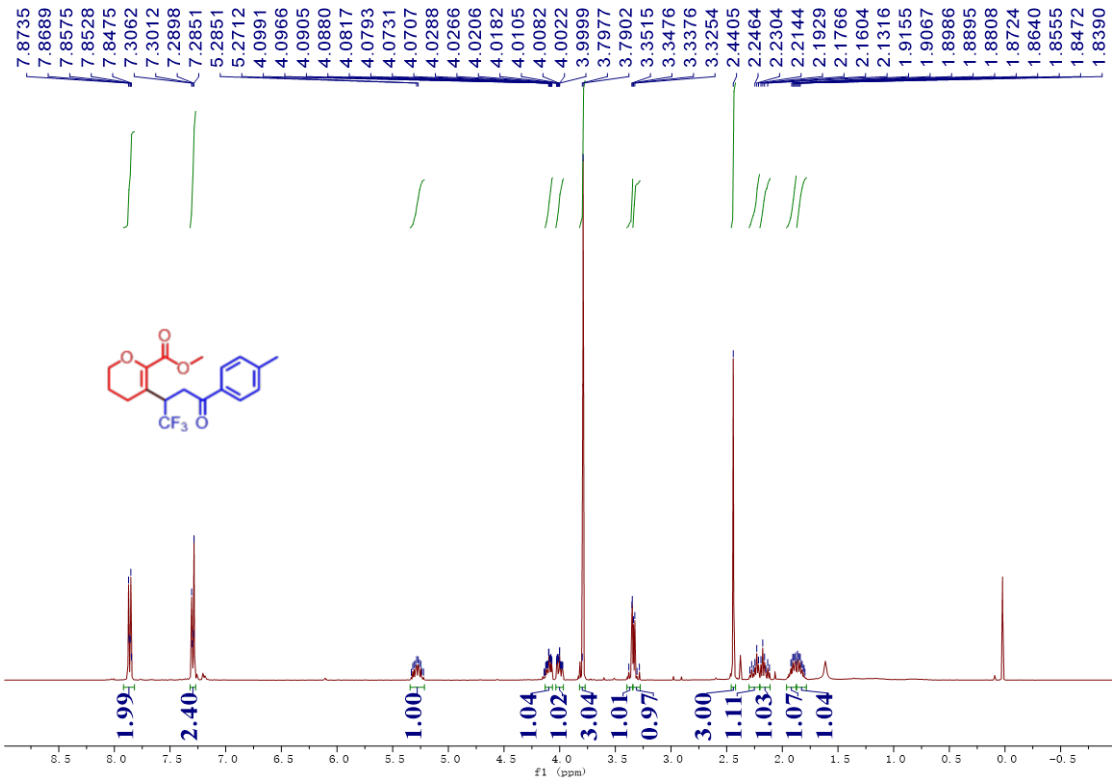

195.0668
165.5897
148.0743
144.4545
134.3949
133.6460
129.8209
127.5891
125.3561
123.1242
51.3756
39.1240
38.9041
38.6844
38.4650
35.7072
35.6920
34.2779
33.6126
21.6938
21.3915
CF3
O
f1 (ppm)

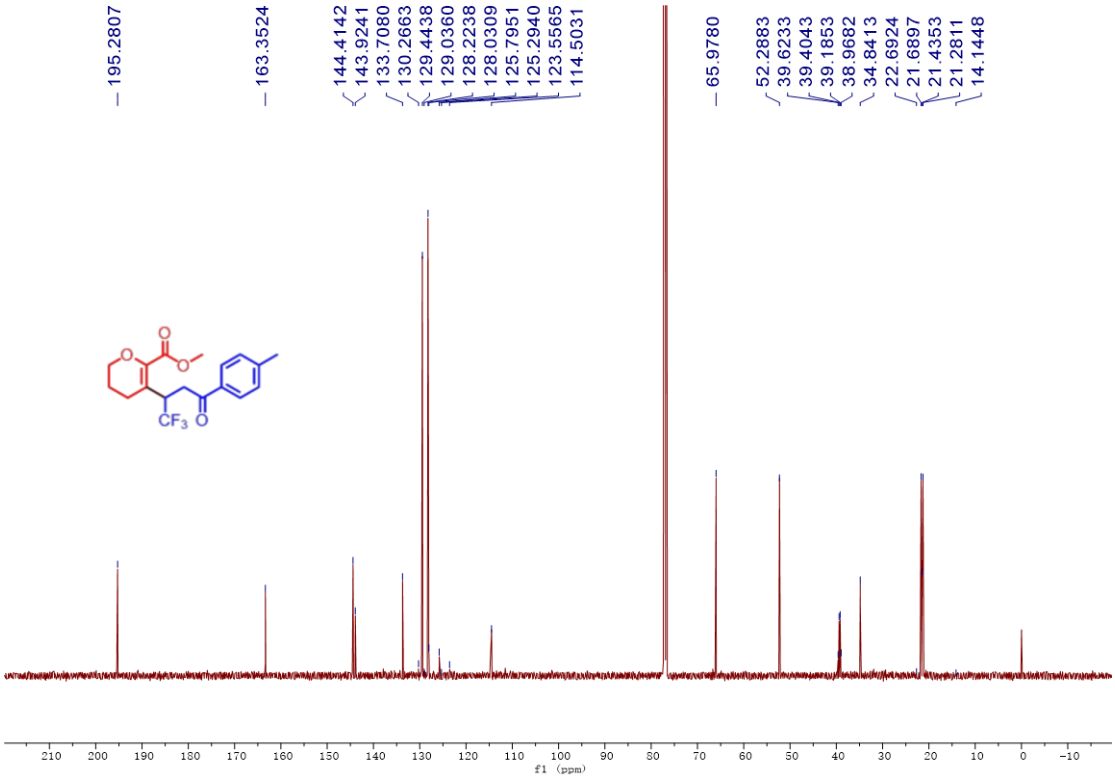

7.8473
7.8425
7.8311
7.8265
7.2742
7.2666
7.2542
5.7844
5.7803
5.7762
5.7721
5.7593
5.7553
5.7511
5.7472
4.8825
4.8710
4.8606
4.8488
4.8373
4.8259
4.8148
4.8035
3.7923
3.7860
3.7802
3.7739
3.7664
3.7579
3.7520
3.4223
3.4107
3.3796
3.3681
3.1288
3.1085
3.0862
3.0659
2.4104
1.9539
1.9500
2.01
2.00
1.00
1.00
3.00
1.02
1.01
3.05
2.98
f1 (ppm)

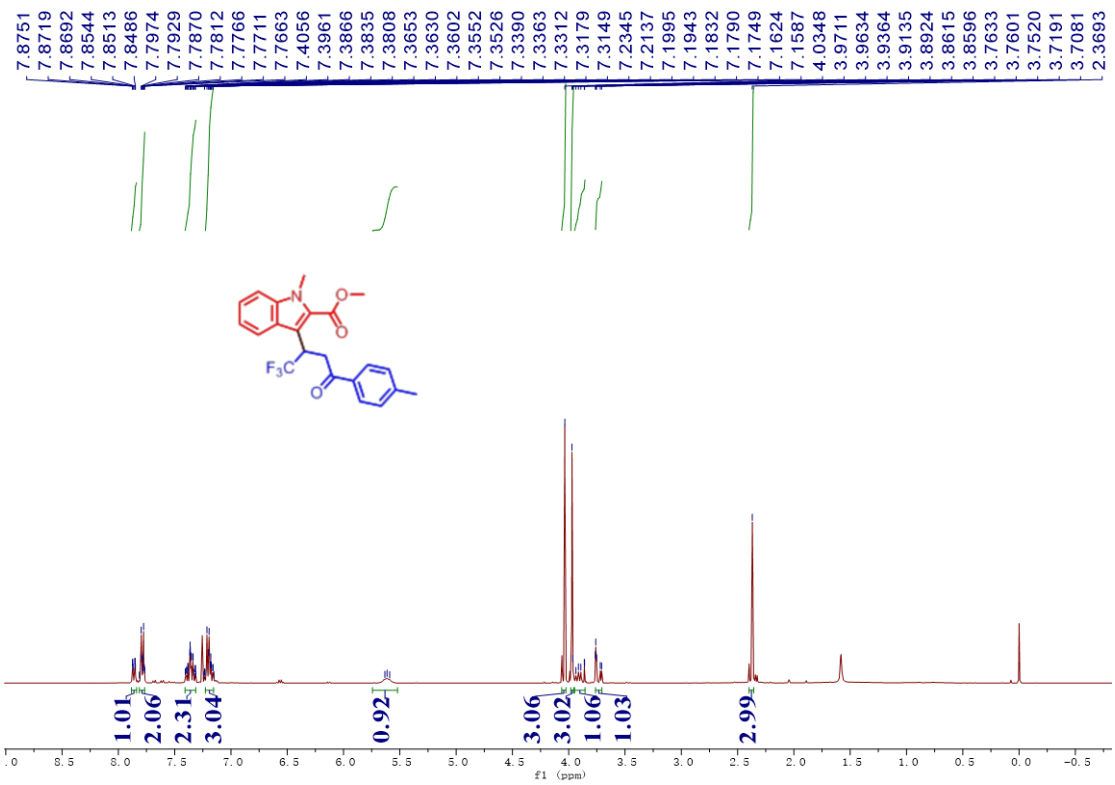

194.8326
167.2353
144.3350
133.8513
133.3917
132.5232
132.4953
132.4699
130.8717
129.3820
128.2217
128.0900
125.3093
122.5660
51.7565
39.4253
39.1516
38.8770
38.6013
37.8457
21.6316
20.9040
f1 (ppm)

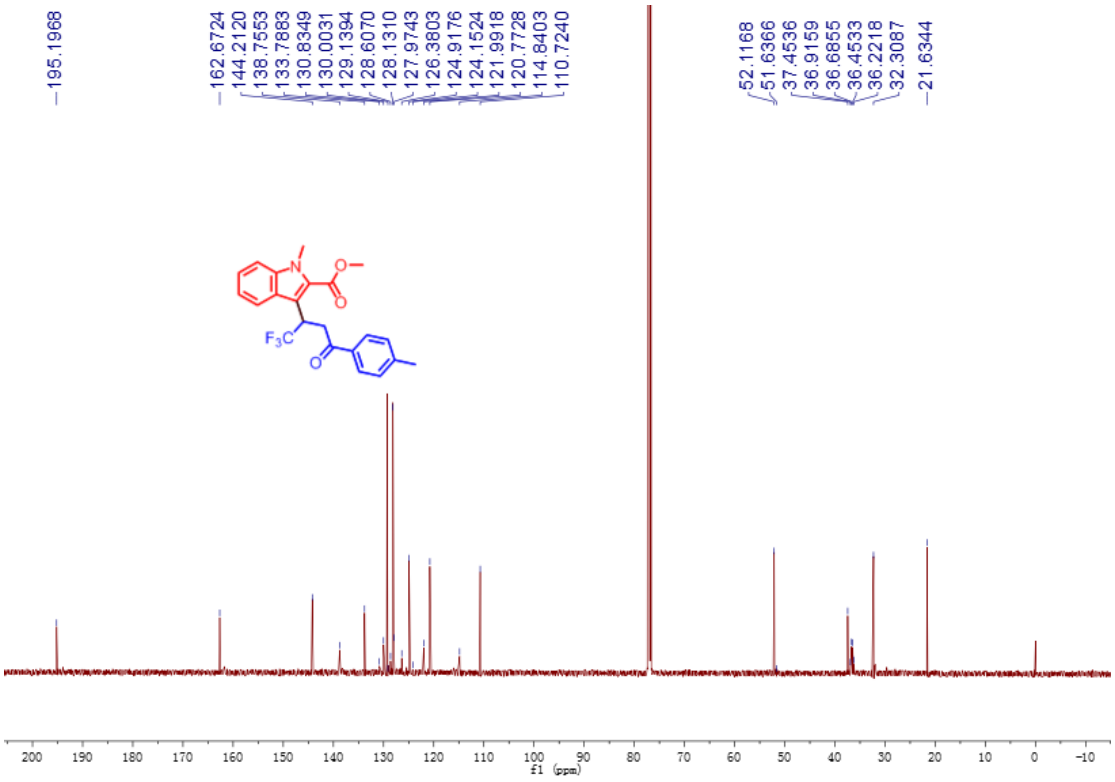

7.8624
7.8581
7.8464
7.8417
7.3382
7.3296
7.3254
7.3177
7.3113
7.3042
7.2993
7.2913
7.2892
7.2791
7.2755
7.2577
7.2486
6.0319
6.0062
4.6519
4.6472
4.6398
4.6354
4.6311
4.6264
4.6189
4.6143
3.8223
3.8144
3.4995
3.4877
3.4568
3.4449
3.2500
3.2302
3.2073
3.1876
2.4098
2.01
7.38
1.00
1.02
3.00
1.00
0.99
3.05
f1 (ppm)

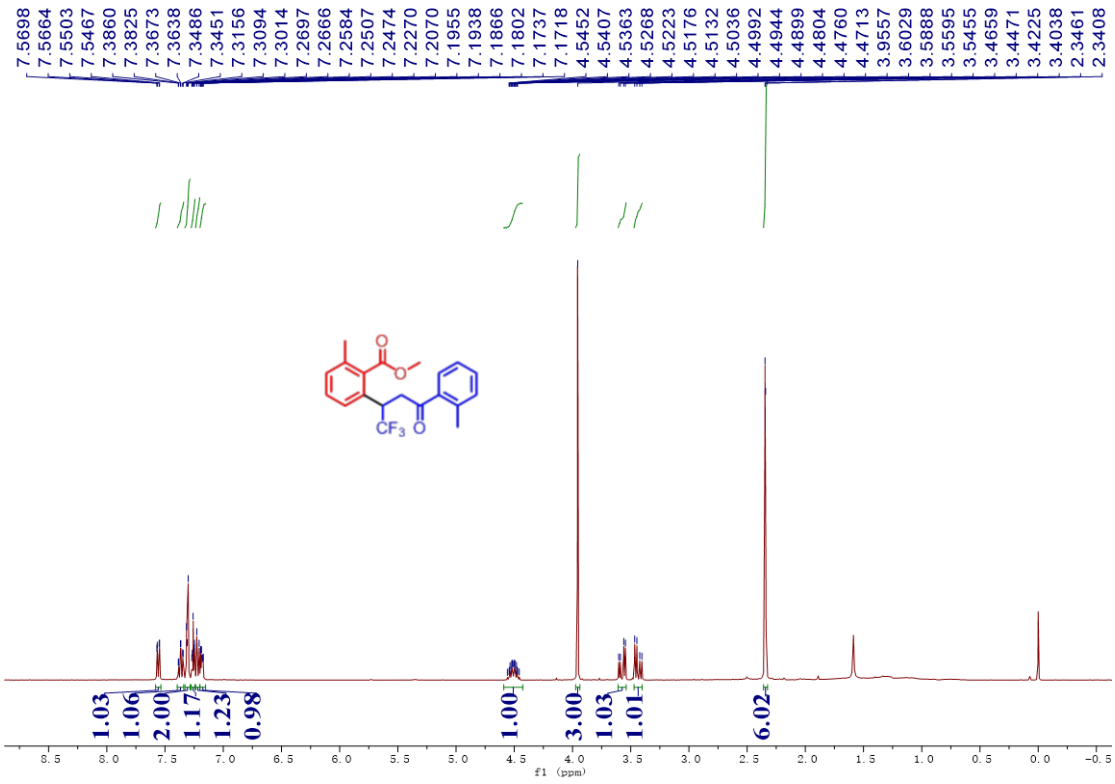

194.5680
167.2044
144.4709
139.7123
136.9492
133.8019
131.1545
131.1323
130.7725
129.4406
128.4475
128.3540
128.2836
127.9914
127.6540
125.2110
122.4251
52.2043
40.0976
39.8188
39.5406
39.2650
37.8323
21.6672
f1 (ppm)

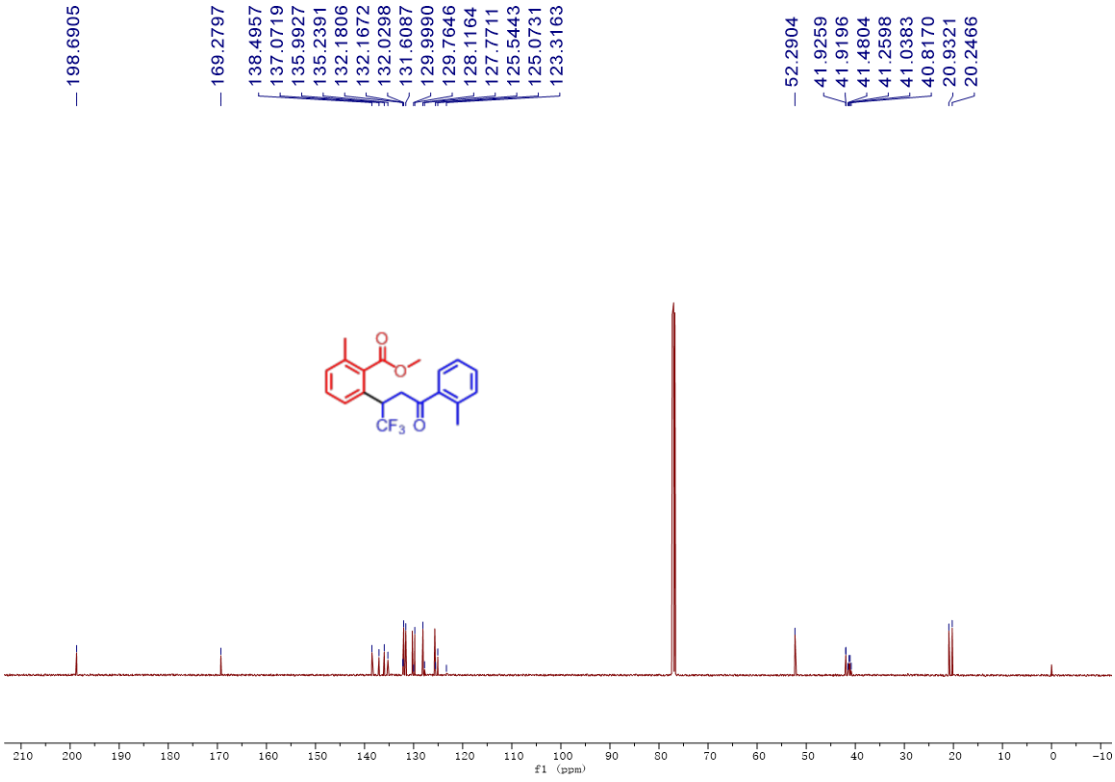

7.8735
7.8689
7.8575
7.8528
7.8475
7.3062
7.3012
7.2898
7.2851
5.2851
5.2712
4.0991
4.0966
4.0905
4.0880
4.0817
4.0793
4.0731
4.0707
4.0288
4.0266
4.0206
4.0182
4.0105
4.0082
4.0022
3.9999
3.7977
3.7902
3.3515
3.3476
3.3376
3.3254
2.4405
2.2464
2.2304
2.2144
2.1929
2.1766
2.1604
2.1316
1.9155
1.9067
1.8986
1.8895
1.8808
1.8724
1.8640
1.8555
1.8472
1.8390
1.99
2.40
1.00
1.04
1.02
3.04
1.01
0.97
3.00
1.11
1.03
1.07
1.04
f1 (ppm)

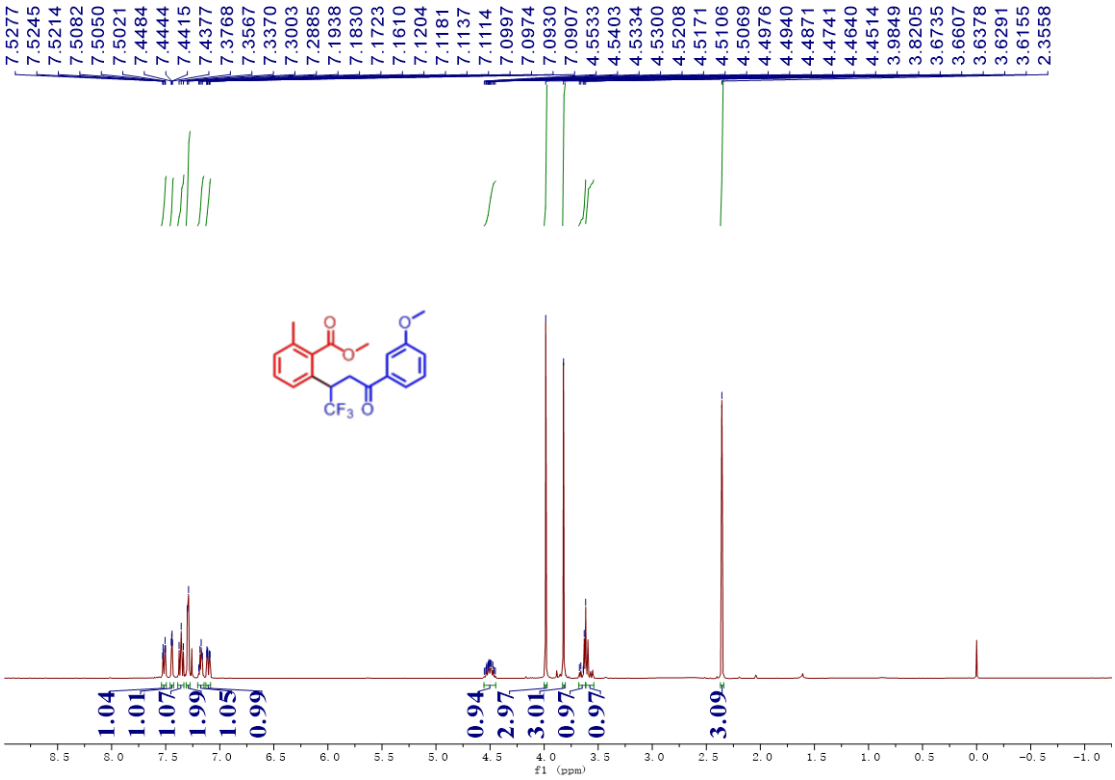

195.2807
163.3524
144.4142
143.9241
133.7080
130.2663
129.4438
129.0360
128.2238
128.0309
125.7951
125.2940
123.5565
114.5031
65.9780
52.2883
39.6233
39.4043
39.1853
38.9682
34.8413
22.6924
21.6897
21.4353
21.2811
14.1448
f1 (ppm)

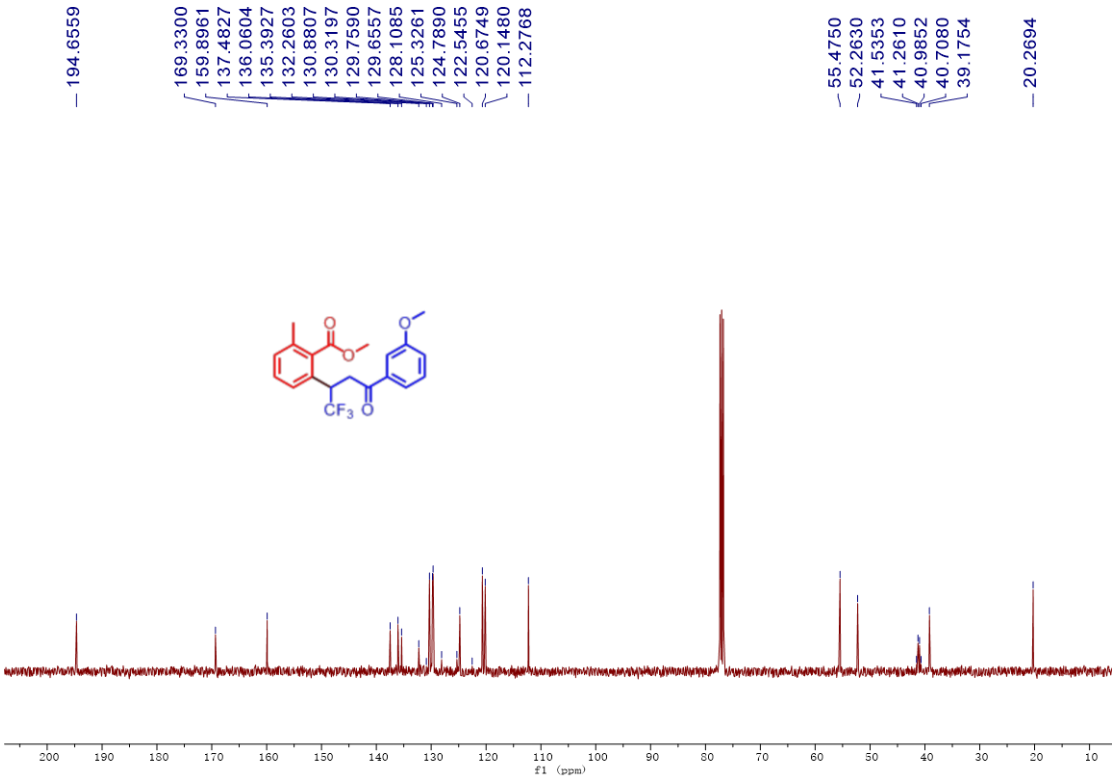

7.8751
7.8719
7.8692
7.8544
7.8513
7.8486
7.7974
7.7929
7.7870
7.7812
7.7766
7.7711
7.7663
7.4056
7.3961
7.3866
7.3835
7.3808
7.3653
7.3630
7.3602
7.3552
7.3526
7.3390
7.3363
7.3312
7.3179
7.3149
7.2345
7.2137
7.1995
7.1943
7.1832
7.1790
7.1749
7.1624
7.1587
4.0348
3.9711
3.9634
3.9364
3.9135
3.8924
3.8615
3.8596
3.7633
3.7601
3.7520
3.7191
3.7081
2.3693
1.01
2.06
2.31
3.04
0.92
3.06
3.02
1.06
1.03
2.99
f1 (ppm)

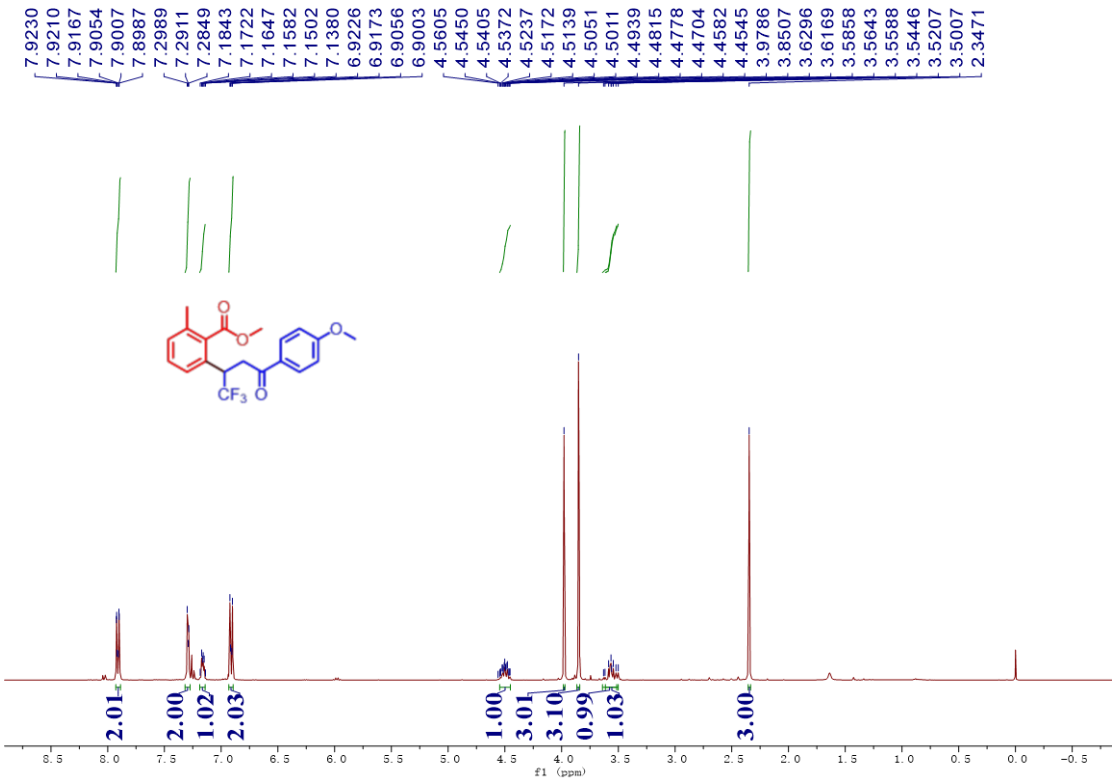

195.1968
162.6724
144.2120
138.7553
133.7883
130.8349
130.0031
129.1394
128.6070
128.1310
127.9743
126.3803
124.9176
124.1524
121.9918
120.7728
114.8403
110.7240
52.1168
51.6366
37.4536
36.9159
36.6855
36.4533
36.2218
32.3087
21.6344
f1 (ppm)

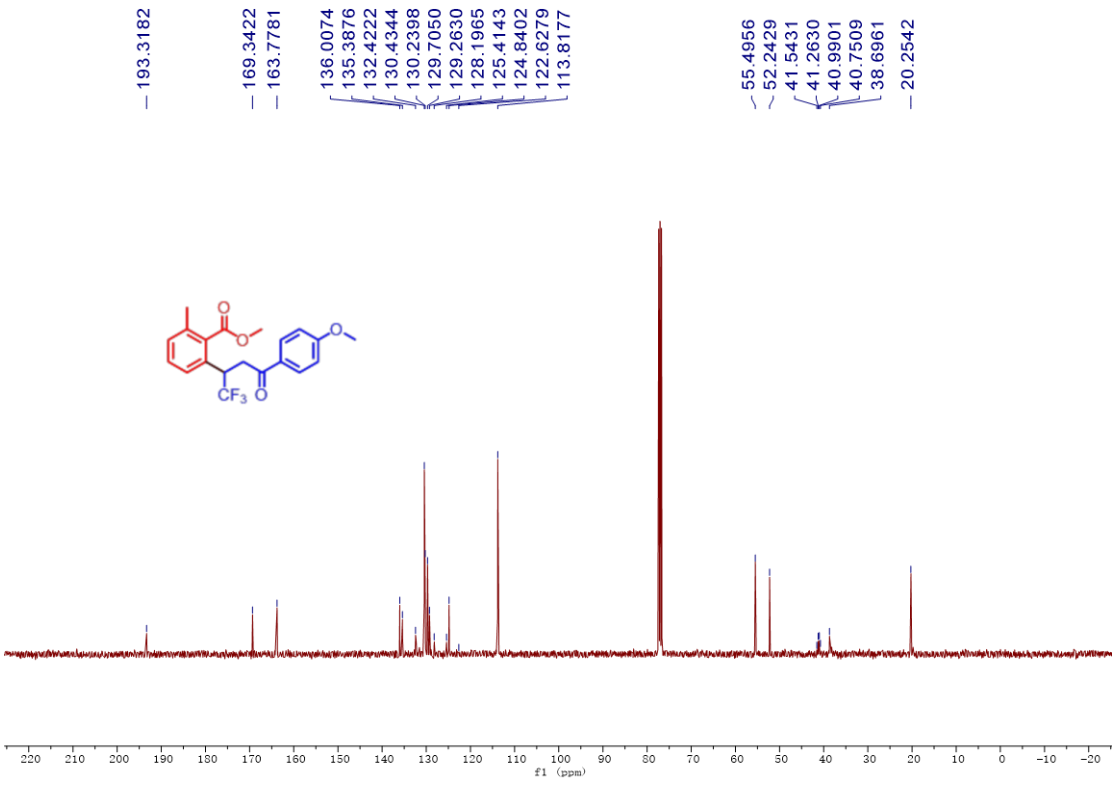

7.5698
7.5664
7.5503
7.5467
7.3860
7.3825
7.3673
7.3638
7.3486
7.3451
7.3156
7.3094
7.3014
7.2697
7.2666
7.2584
7.2507
7.2474
7.2270
7.2070
7.1955
7.1938
7.1866
7.1802
7.1737
7.1718
4.5452
4.5407
4.5363
4.5268
4.5223
4.5176
4.5132
4.5036
4.4992
4.4944
4.4899
4.4804
4.4760
4.4713
3.9557
3.6029
3.5888
3.5595
3.5455
3.4659
3.4471
3.4225
3.4038
2.3461
2.3408
CF3
O
1.03
1.06
2.00
1.17
1.23
0.98
1.00
3.00
1.03
1.01
6.02
f1 (ppm)

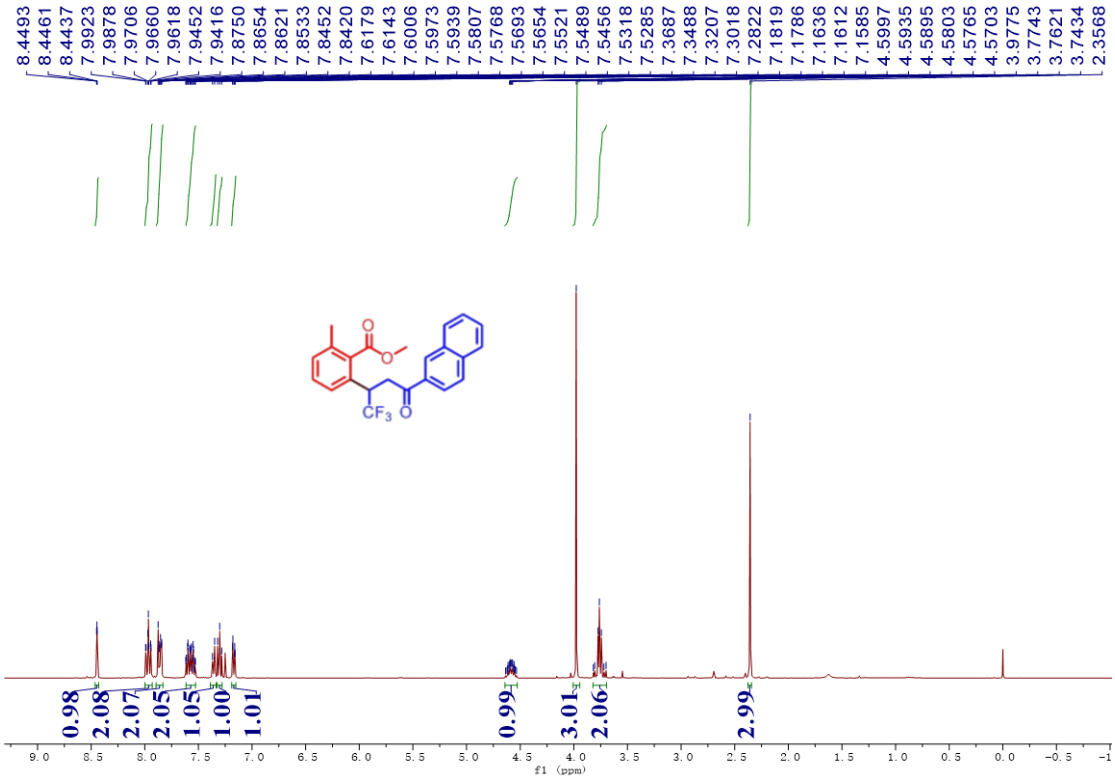

198.6905
169.2797
138.4957
137.0719
135.9927
135.2391
132.1806
132.1672
132.0298
131.6087
129.9990
129.7646
128.1164
127.7711
125.5443
125.0731
123.3163
52.2904
41.9259
41.9196
41.4804
41.2598
41.0383
40.8170
20.9321
20.2466
CF3
O
f1 (ppm)

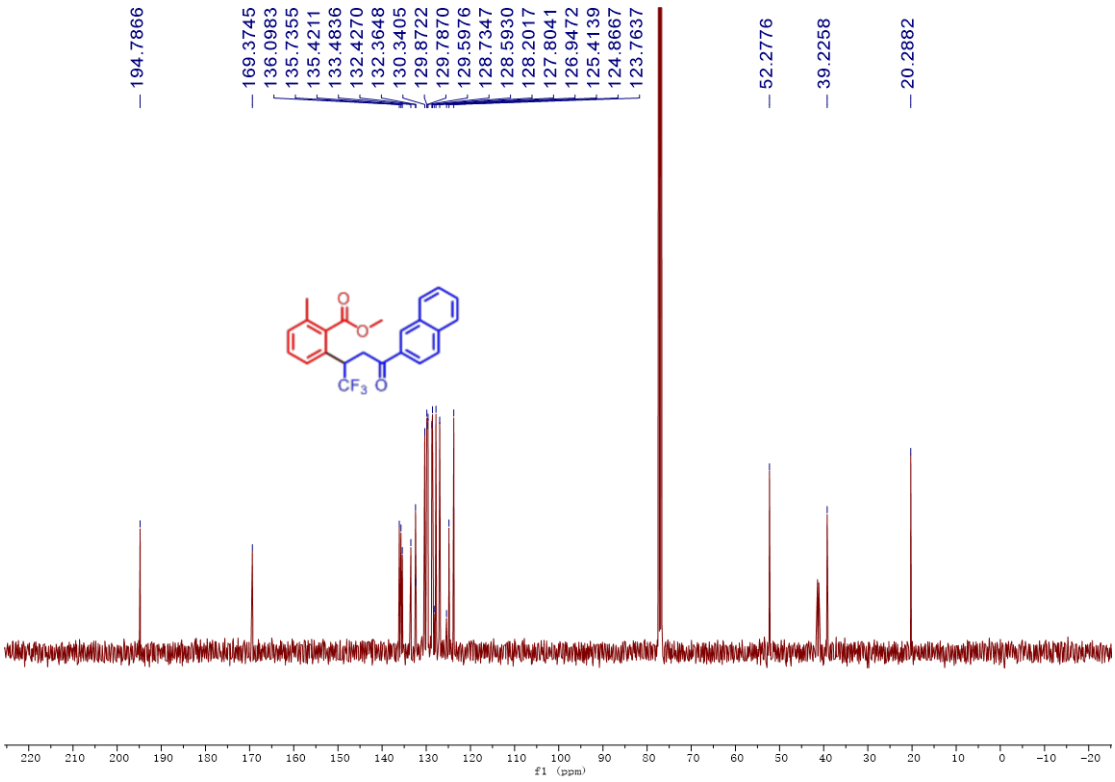

7.5277
7.5245
7.5214
7.5082
7.5050
7.5021
7.4484
7.4444
7.4415
7.4377
7.3768
7.3567
7.3370
7.3003
7.2885
7.1938
7.1830
7.1723
7.1610
7.1204
7.1181
7.1137
7.1114
7.0997
7.0974
7.0930
7.0907
4.5533
4.5403
4.5334
4.5300
4.5208
4.5171
4.5106
4.5069
4.4976
4.4940
4.4871
4.4741
4.4640
4.4514
3.9849
3.8205
3.6735
3.6607
3.6378
3.6291
3.6155
2.3558
1.04
1.01
1.07
1.99
1.05
0.99
0.94
2.97
3.01
0.97
0.97
3.09
f1 (ppm)

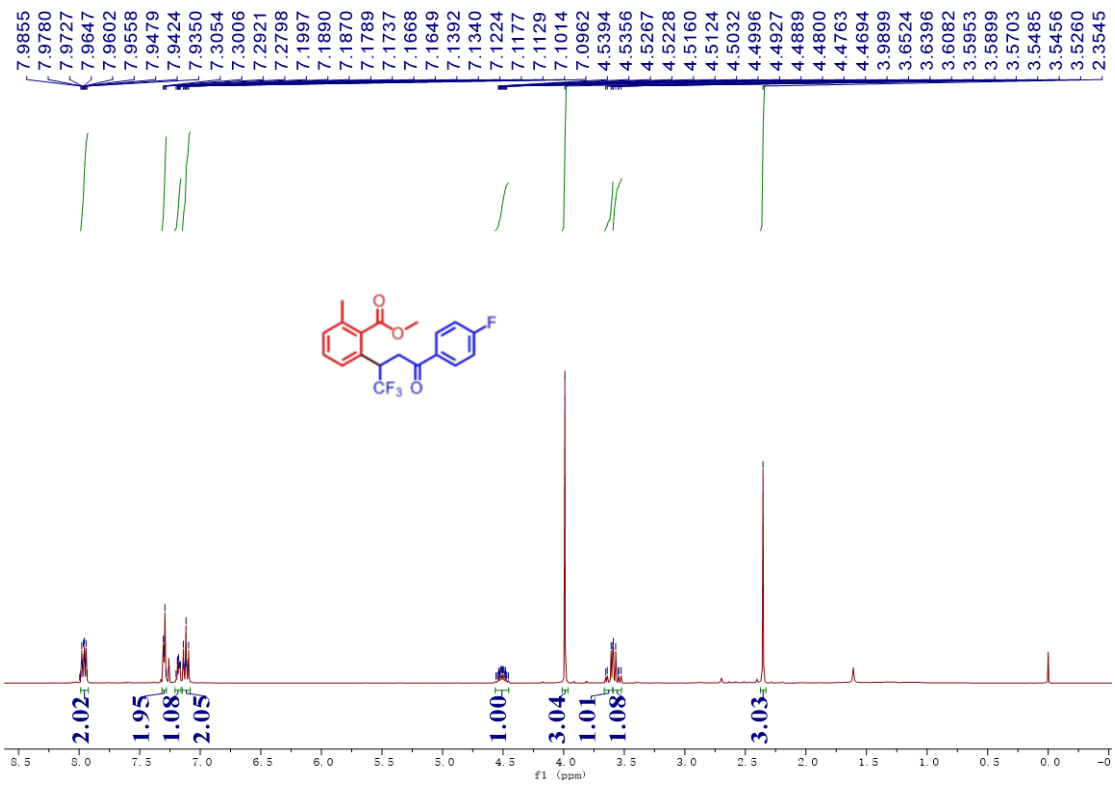

194.6559
169.3300
159.8961
137.4827
136.0604
135.3927
132.2603
130.8807
130.3197
129.7590
129.6557
128.1085
125.3261
124.7890
122.5455
120.6749
120.1480
112.2768
55.4750
52.2630
41.5353
41.2610
40.9852
40.7080
39.1754
20.2694
f1 (ppm)

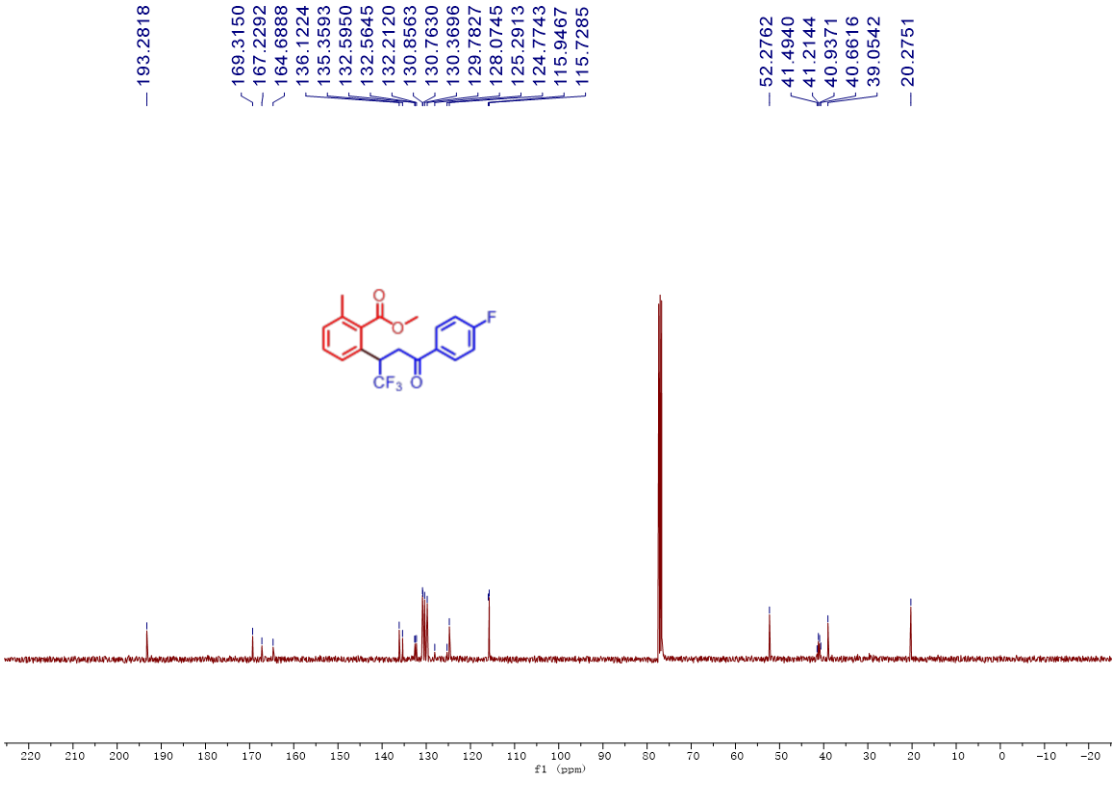

7.9230
7.9210
7.9167
7.9054
7.9007
7.8987
7.2989
7.2911
7.2849
7.1843
7.1722
7.1647
7.1582
7.1502
7.1380
6.9226
6.9173
6.9056
6.9003
4.5605
4.5450
4.5405
4.5372
4.5237
4.5172
4.5139
4.5051
4.5011
4.4939
4.4815
4.4778
4.4704
4.4582
4.4545
3.9786
3.8507
3.6296
3.6169
3.5858
3.5643
3.5588
3.5446
3.5207
3.5007
2.3471
O
O
O
CF3
2.01
2.00
1.02
2.03
1.00
3.01
3.10
0.99
1.03
3.00
f1 (ppm)

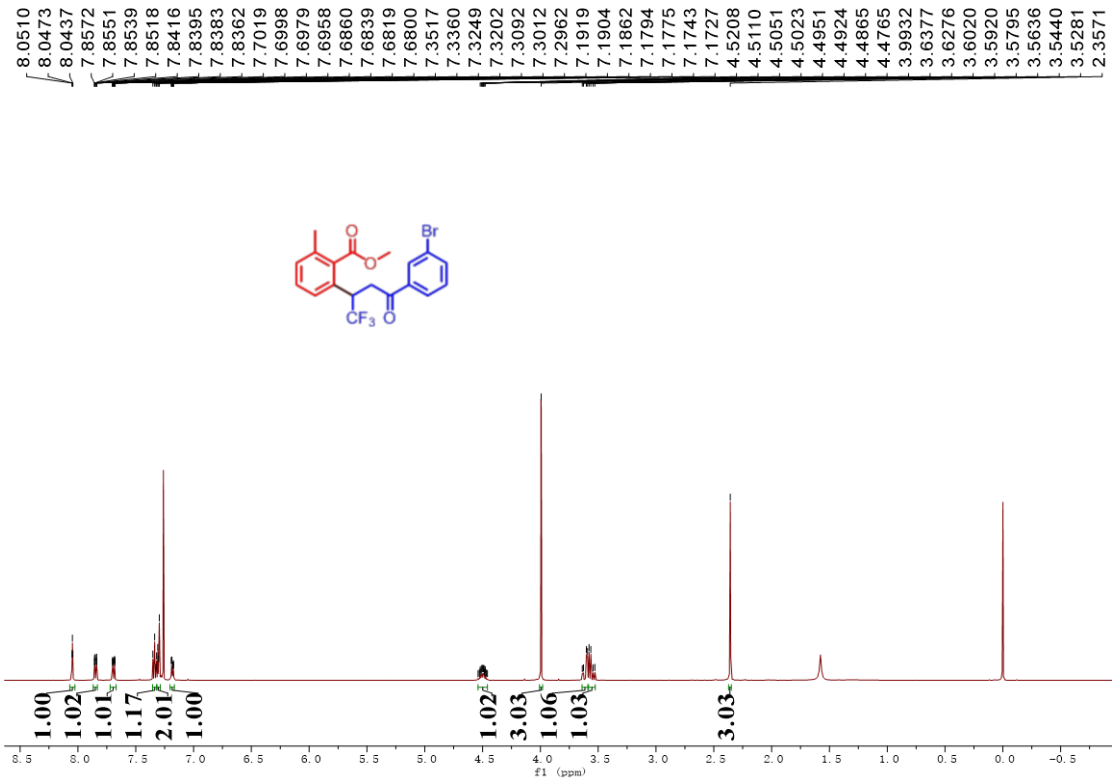

193.3182
169.3422
163.7781
136.0074
135.3876
132.4222
130.4344
130.2398
129.7050
129.2630
128.1965
125.4143
124.8402
122.6279
113.8177
55.4956
52.2429
41.5431
41.2630
40.9901
40.7509
38.6961
20.2542
O
O
O
CF3
f1 (ppm)

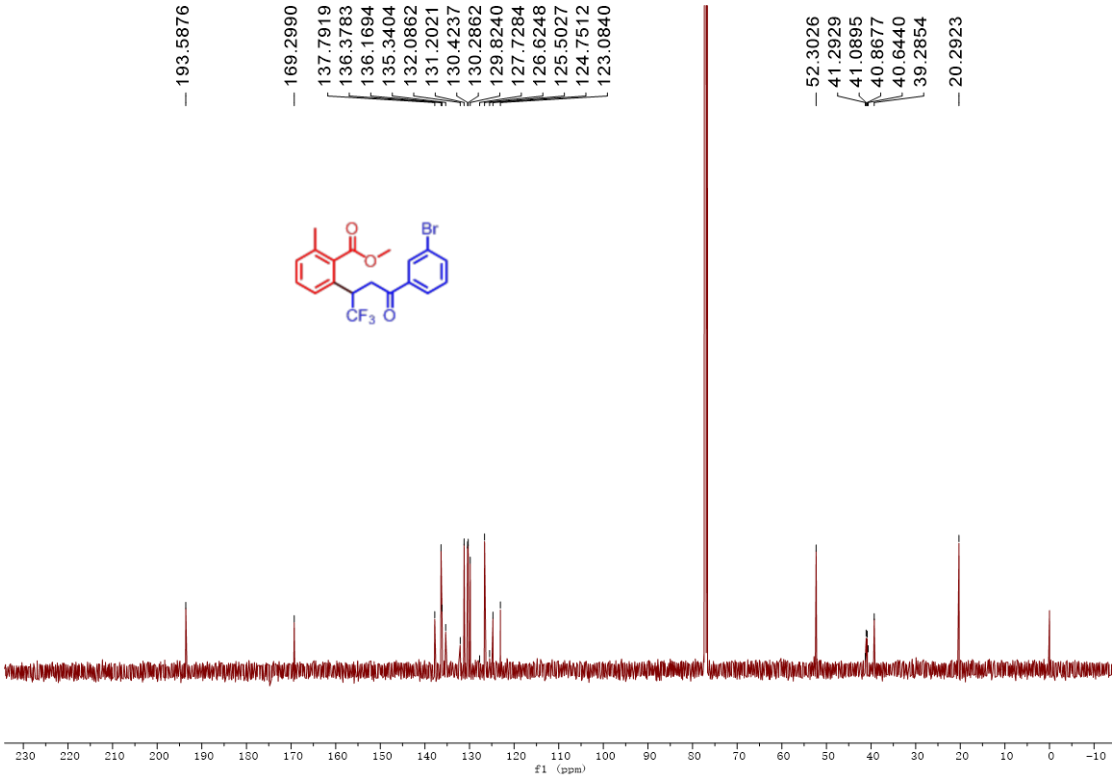

8.4493
8.4461
8.4437
7.9923
7.9878
7.9706
7.9660
7.9618
7.9452
7.9416
7.8750
7.8654
7.8621
7.8533
7.8452
7.8420
7.6179
7.6143
7.6006
7.5973
7.5939
7.5807
7.5768
7.5693
7.5654
7.5521
7.5489
7.5456
7.5318
7.5285
7.3687
7.3488
7.3207
7.3018
7.2822
7.1819
7.1786
7.1636
7.1612
7.1585
4.5997
4.5935
4.5895
4.5803
4.5765
4.5703
3.9775
3.7743
3.7621
3.7434
2.3568
0.98
2.08
2.07
2.05
1.05
1.00
1.01
0.99
3.01
2.06
2.99
f1 (ppm)

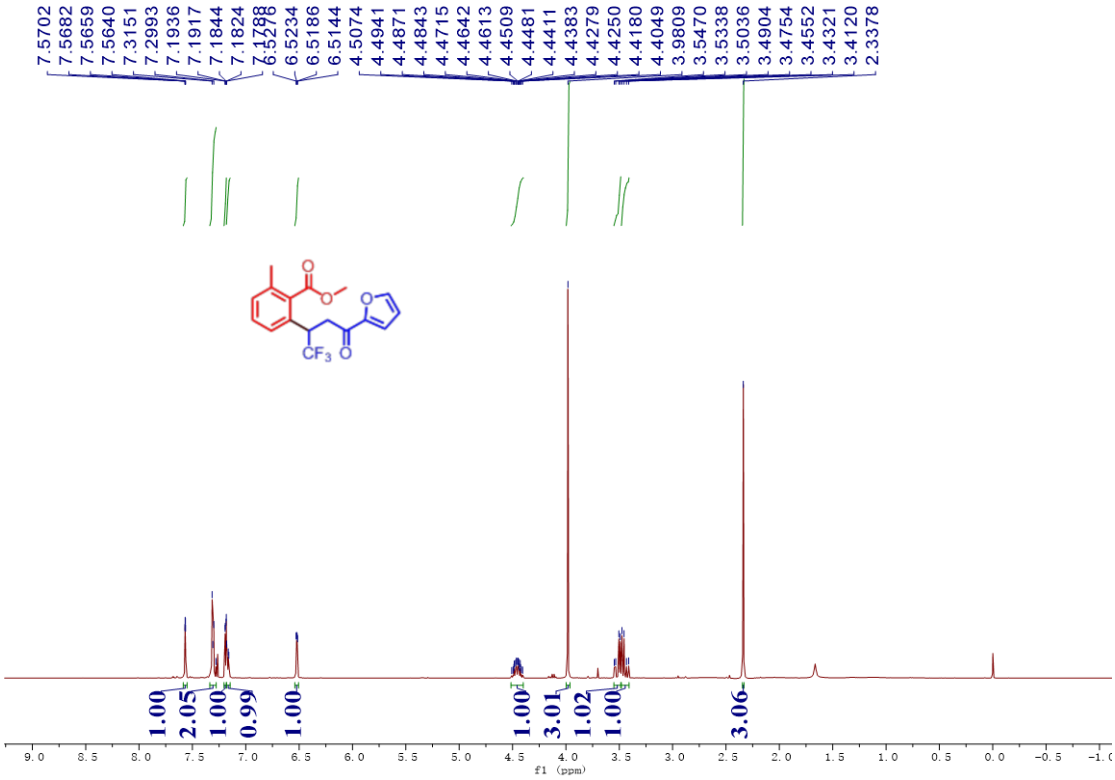

194.7866
169.3745
136.0983
135.7355
135.4211
133.4836
132.4270
132.3648
130.3405
129.8722
129.7870
129.5976
128.7347
128.5930
128.2017
127.8041
126.9472
125.4139
124.8667
123.7637
52.2776
39.2258
20.2882
f1 (ppm)

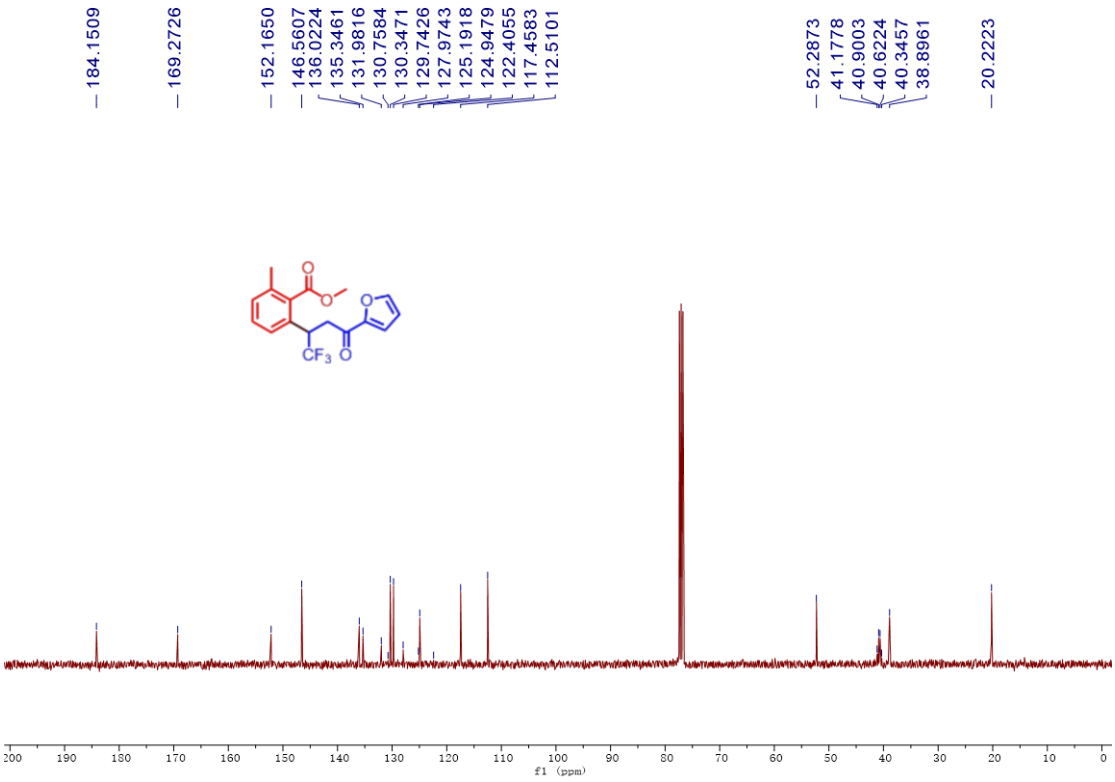

7.9855
7.9780
7.9727
7.9647
7.9602
7.9558
7.9479
7.9424
7.9350
7.3054
7.3006
7.2921
7.2798
7.1997
7.1890
7.1870
7.1789
7.1737
7.1668
7.1649
7.1392
7.1340
7.1224
7.1177
7.1129
7.1014
7.0962
4.5394
4.5356
4.5267
4.5228
4.5160
4.5124
4.5032
4.4996
4.4927
4.4889
4.4800
4.4763
4.4694
3.9899
3.6524
3.6396
3.6082
3.5953
3.5899
3.5703
3.5485
3.5456
3.5260
2.3545
F
O
O
CF3
2.02
1.95
1.08
2.05
1.00
3.04
1.01
1.08
3.03
f1 (ppm)

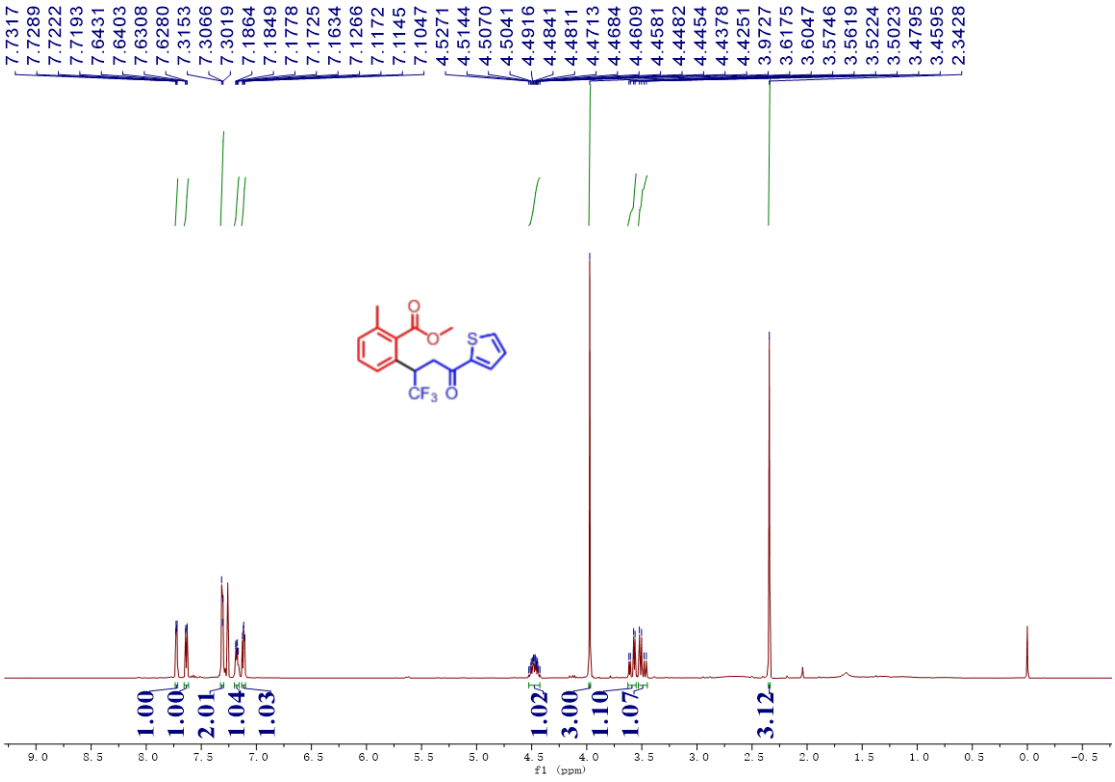

193.2818
169.3150
167.2292
164.6888
136.1224
135.3593
132.5950
132.5645
132.2120
130.8563
130.7630
130.3696
129.7827
128.0745
125.2913
124.7743
115.9467
115.7285
52.2762
41.4940
41.2144
40.9371
40.6616
39.0542
20.2751
F
O
O
CF3
f1 (ppm)

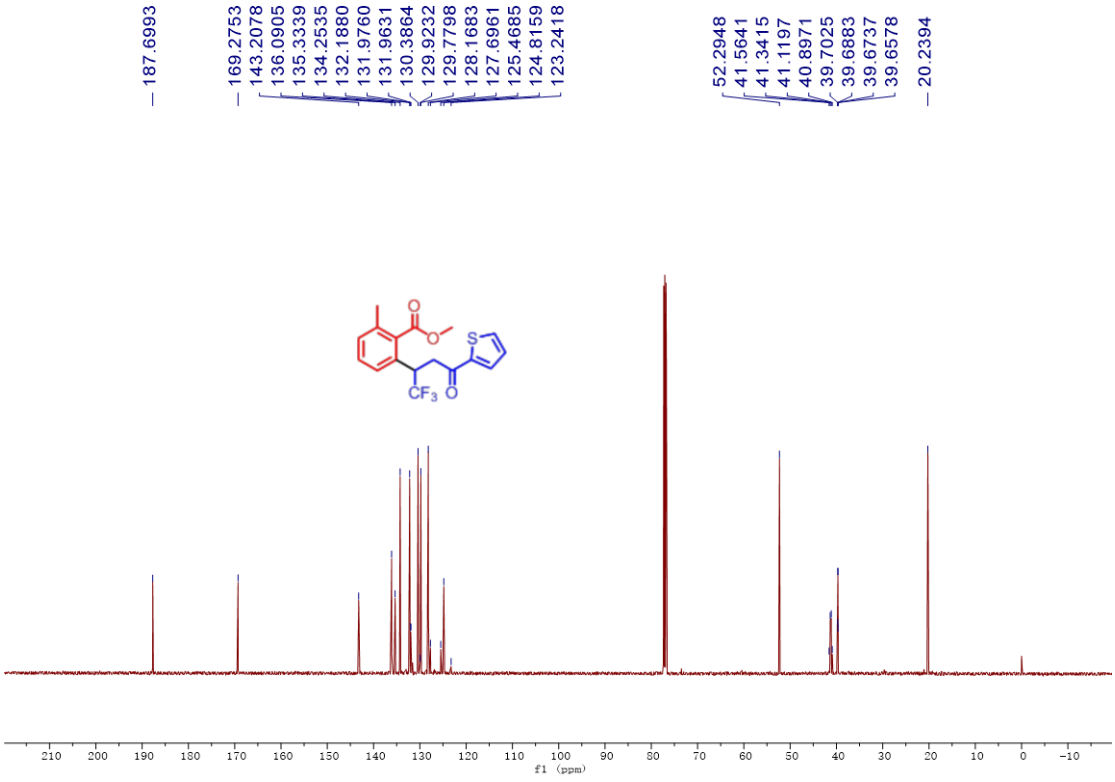

8.0510
8.0473
8.0437
7.8572
7.8551
7.8539
7.8518
7.8416
7.8395
7.8383
7.8362
7.7019
7.6998
7.6979
7.6958
7.6860
7.6839
7.6819
7.6800
7.3517
7.3360
7.3249
7.3202
7.3092
7.3012
7.2962
7.1919
7.1904
7.1862
7.1794
7.1775
7.1743
7.1727
4.5208
4.5110
4.5051
4.5023
4.4951
4.4924
4.4865
4.4765
3.9932
3.6377
3.6276
3.6020
3.5920
3.5795
3.5636
3.5440
3.5281
2.3571
Br
O
O
CF3
1.00
1.02
1.01
1.17
2.01
1.00
1.02
3.03
1.06
1.03
3.03
f1 (ppm)

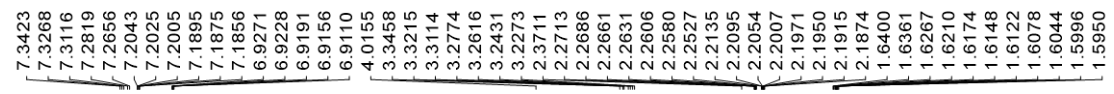

193.5876
169.2990
137.7919
136.3783
136.1694
135.3404
132.0862
131.2021
130.4237
130.2862
129.8240
127.7284
126.6248
125.5027
124.7512
123.0840
52.3026
41.2929
41.0895
40.8677
40.6440
39.2854
20.2923
Br
O
O
CF3
f1 (ppm)


7.5702
7.5682
7.5659
7.5640
7.3151
7.2993
7.1936
7.1917
7.1844
7.1824
6.5234
6.5186
6.5144
4.5074
4.4941
4.4871
4.4843
4.4715
4.4642
4.4613
4.4509
4.4481
4.4411
4.4383
4.4279
4.4250
4.4180
4.4049
3.9809
3.5470
3.5338
3.5036
3.4904
3.4754
3.4552
3.4321
3.4120
2.3378
1.00
2.05
1.00
0.99
1.00
1.00
3.01
1.02
1.00
3.06
f1 (ppm)

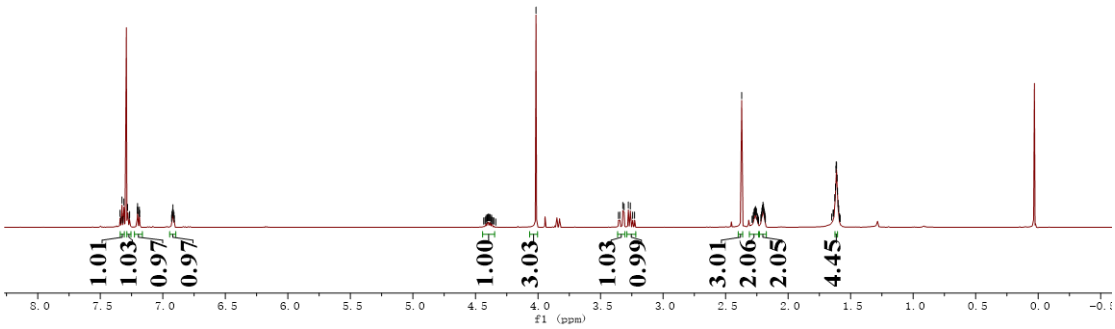

184.1509
169.2726
152.1650
146.5607
136.0224
135.3461
131.9816
130.7584
130.3471
129.7426
127.9743
125.1918
124.9479
122.4055
117.4583
112.5101
52.2873
41.1778
40.9003
40.6224
40.3457
38.8961
20.2223
f1 (ppm)

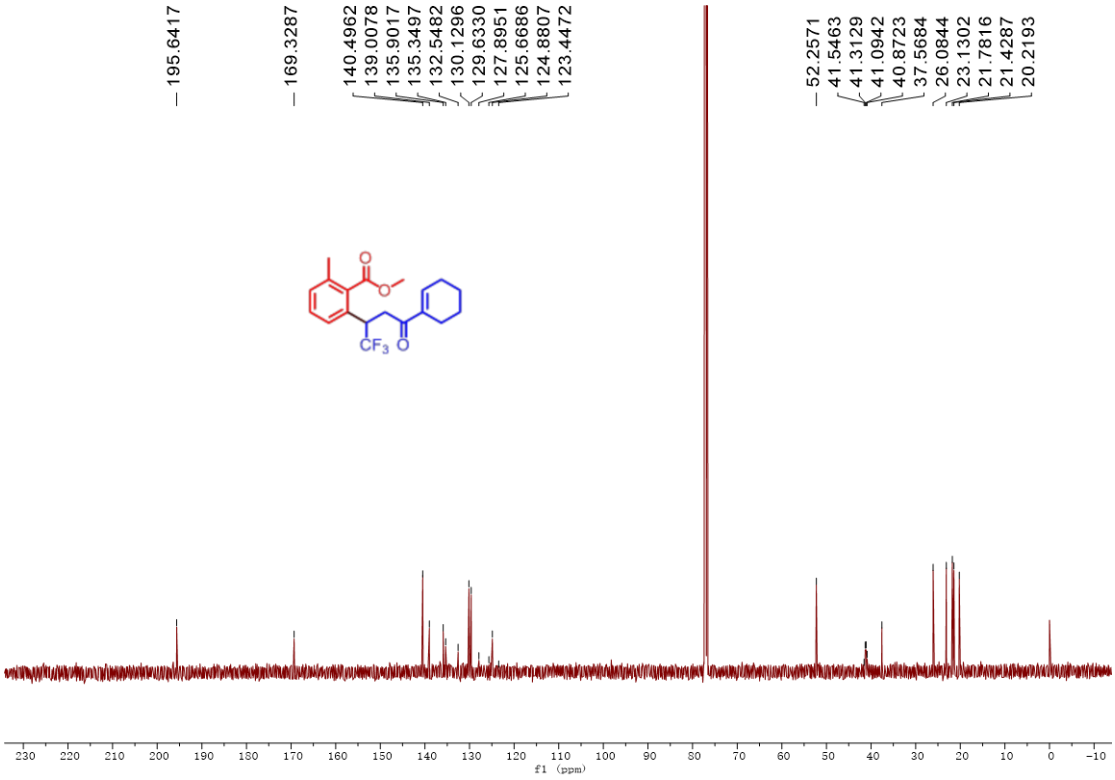

7.7317
7.7289
7.7222
7.7193
7.6431
7.6403
7.6308
7.6280
7.3153
7.3066
7.3019
7.1864
7.1849
7.1778
7.1725
7.1634
7.1266
7.1172
7.1145
7.1047
4.5271
4.5144
4.5070
4.5041
4.4916
4.4841
4.4811
4.4713
4.4684
4.4609
4.4581
4.4482
4.4454
4.4378
4.4251
3.9727
3.6175
3.6047
3.5746
3.5619
3.5224
3.5023
3.4795
3.4595
2.3428
1.00
1.00
2.01
1.04
1.03
1.02
3.00
1.10
1.07
3.12
f1 (ppm)


187.6993
169.2753
143.2078
136.0905
135.3339
134.2535
132.1880
131.9760
131.9631
130.3864
129.9232
129.7798
128.1683
127.6961
125.4685
124.8159
123.2418
52.2948
41.5641
41.3415
41.1197
40.8971
39.7025
39.6883
39.6737
39.6578
20.2394
f1 (ppm)

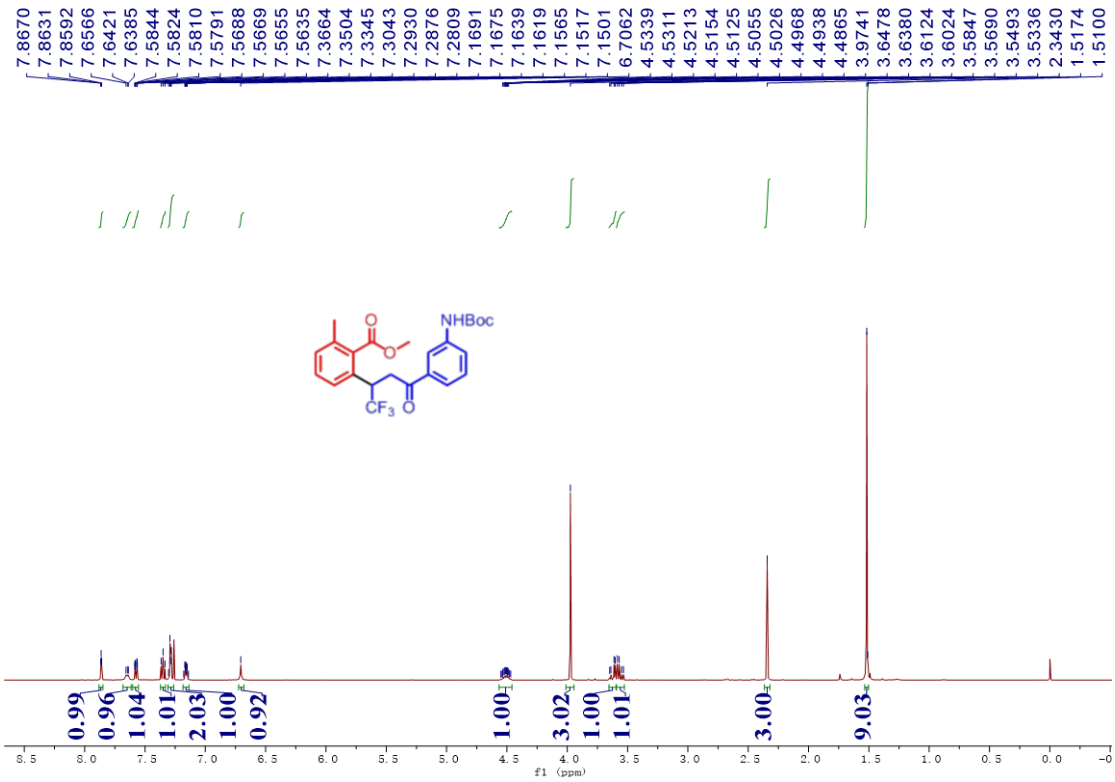

7.3423
7.3268
7.3116
7.2819
7.2656
7.2043
7.2025
7.2005
7.1895
7.1875
7.1856
6.9271
6.9228
6.9191
6.9156
6.9110
4.0155
3.3458
3.3215
3.3114
3.2774
3.2616
3.2431
3.2273
3.2711
2.2713
2.2686
2.2661
2.2631
2.2606
2.2580
2.2527
2.2135
2.2095
2.2054
2.2007
2.1971
2.1950
2.1915
2.1874
1.6400
1.6361
1.6267
1.6210
1.6174
1.6148
1.6122
1.6078
1.6044
1.5996
1.5950

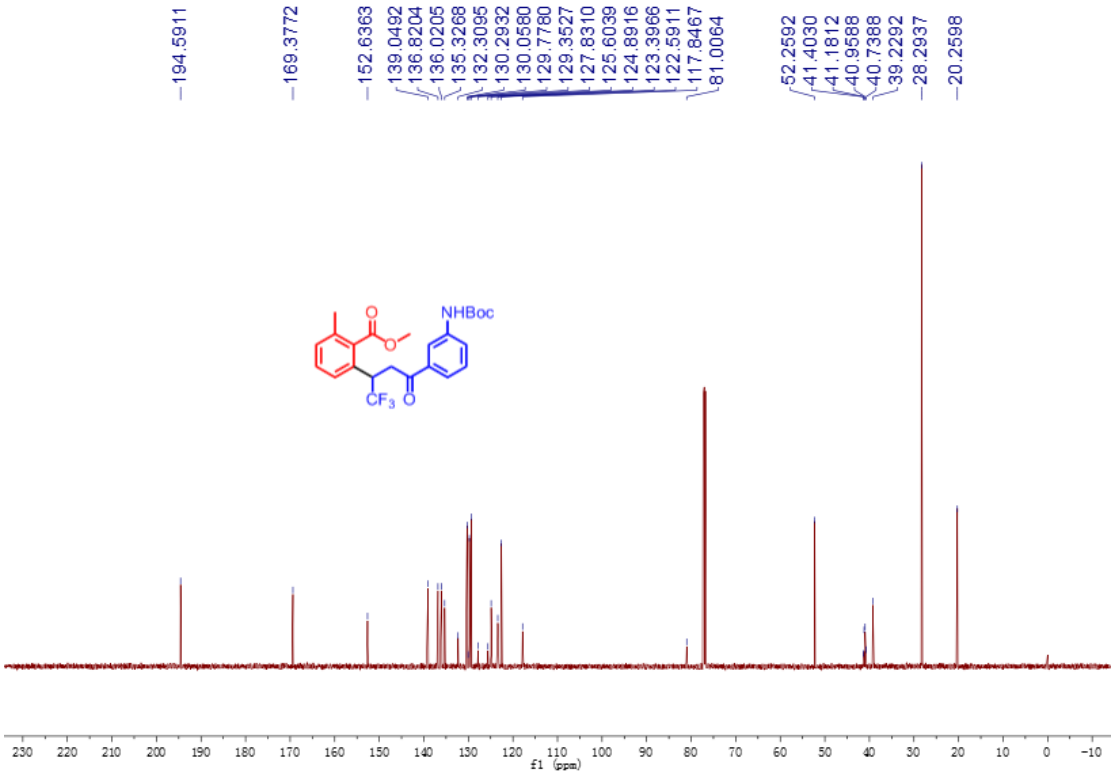

O
O
CF3
O

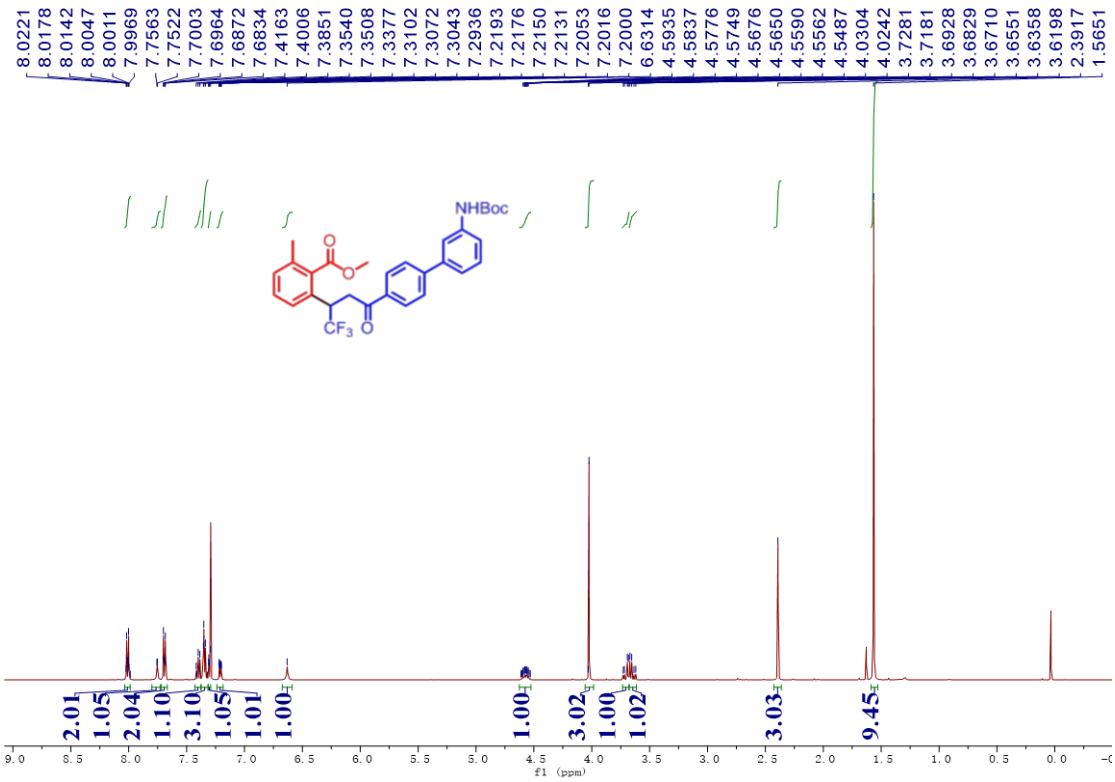

1.01
1.03
0.97
0.97
1.00
3.03
1.03
0.99
3.01
2.06
2.05
4.45
f1 (ppm)

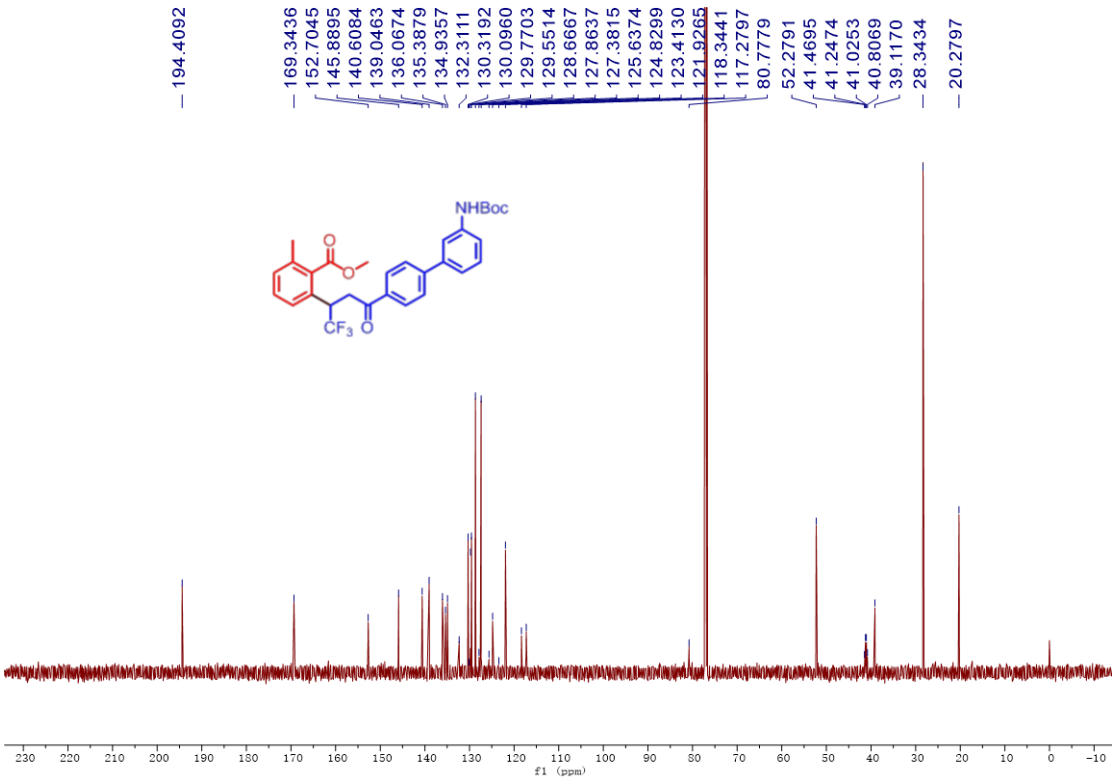

195.6417
169.3287
140.4962
139.0078
135.9017
135.3497
132.5482
130.1296
129.6330
127.8951
125.6686
124.8807
123.4472
52.2571
41.5463
41.3129
41.0942
40.8723
37.5684
26.0844
23.1302
21.7816
21.4287
20.2193
f1 (ppm)

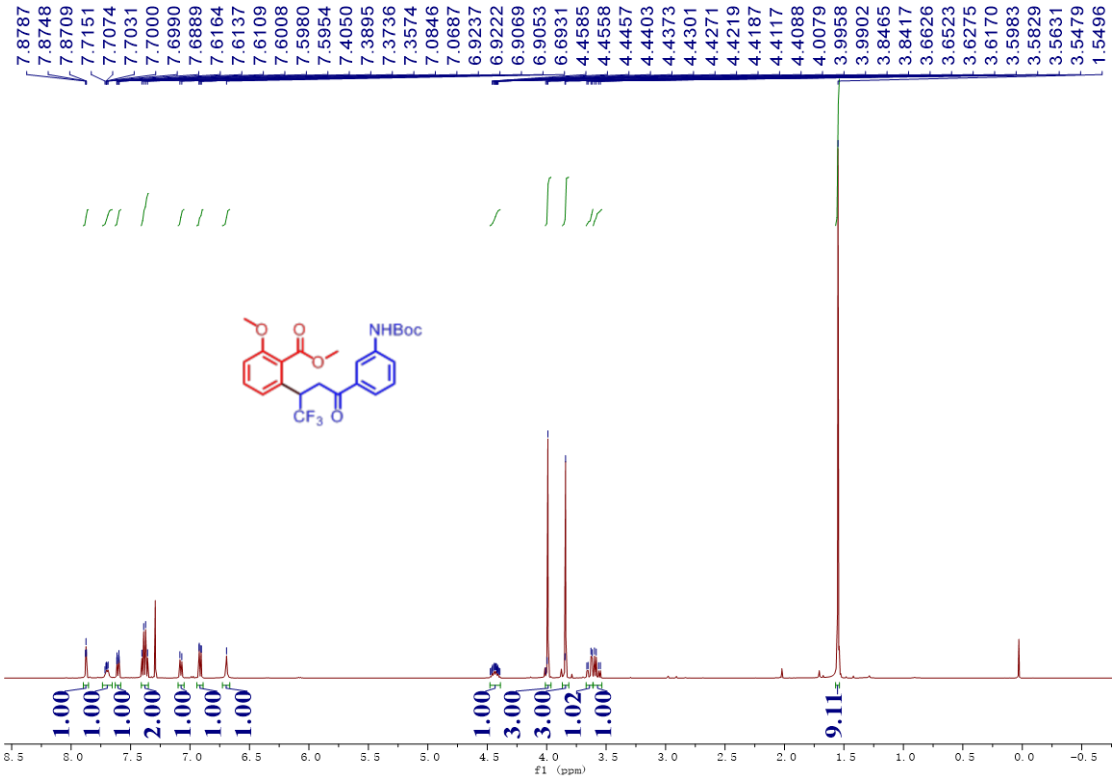
O
O
CF3
O

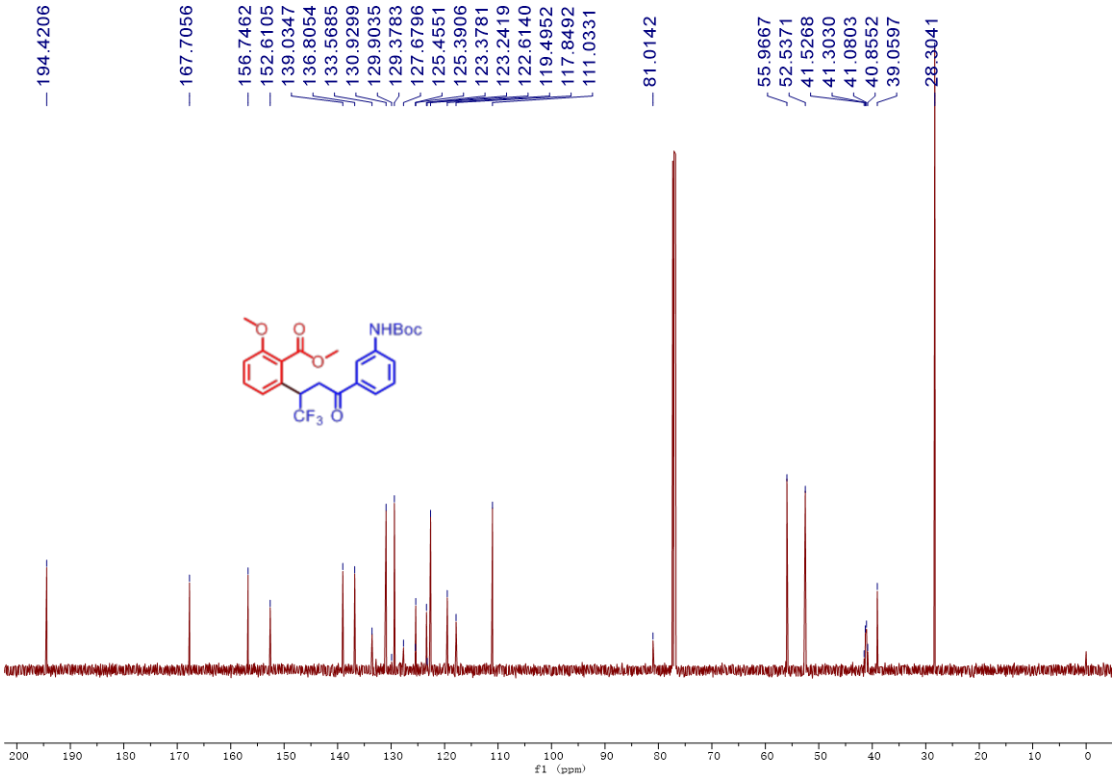

7.8670
7.8631
7.8592
7.6566
7.6421
7.6385
7.5844
7.5824
7.5810
7.5791
7.5688
7.5669
7.5655
7.5635
7.3664
7.3504
7.3345
7.3043
7.2930
7.2876
7.2809
7.1691
7.1675
7.1639
7.1619
7.1565
7.1517
7.1501
6.7062
4.5339
4.5311
4.5213
4.5154
4.5125
4.5055
4.5026
4.4968
4.4938
4.4865
3.9741
3.6478
3.6380
3.6124
3.6024
3.5847
3.5690
3.5493
3.5336
2.3430
1.5174
1.5100
NHBoc
CF3
O
0.99
0.96
1.04
1.01
2.03
1.00
0.92
1.00
3.02
1.00
1.01
3.00
9.03
f1 (ppm)

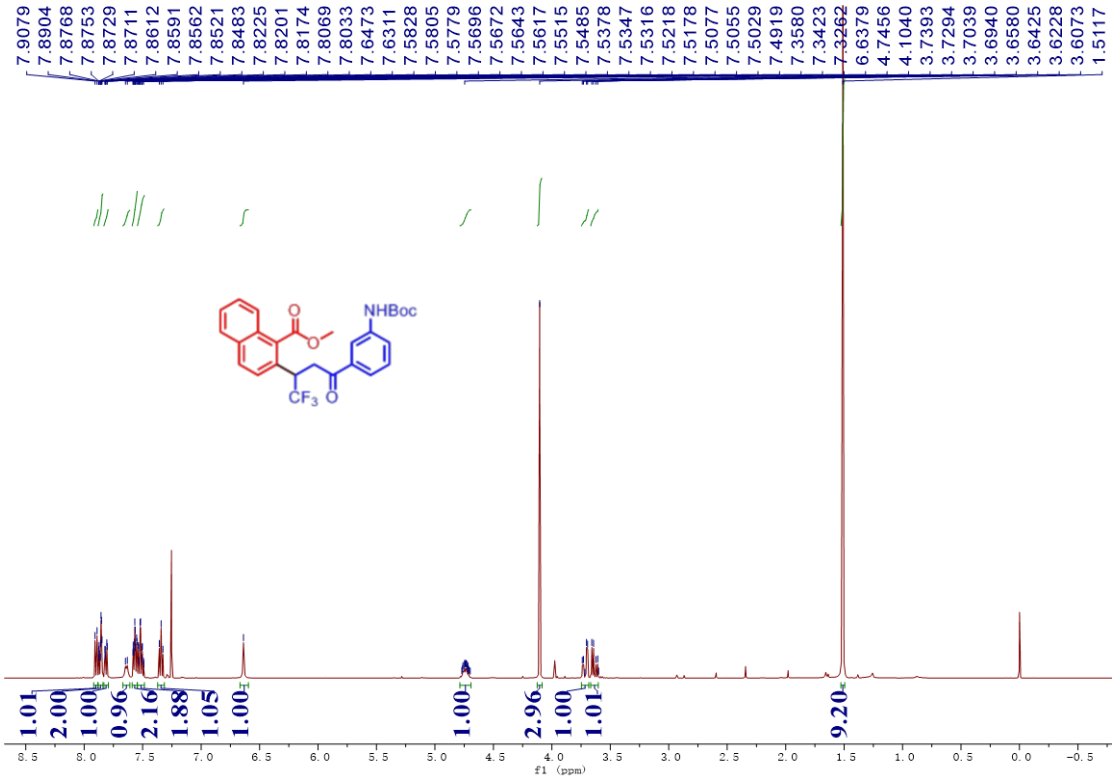

194.5911
169.3772
152.6363
139.0492
136.8204
136.0205
135.3268
132.3095
130.2932
130.0580
129.7780
129.3527
127.8310
125.6039
124.8916
123.3966
122.5911
117.8467
81.0064
52.2592
41.4030
41.1812
40.9588
40.7388
39.2292
28.2937
20.2598
NHBoc
CF3
O
f1 (ppm)

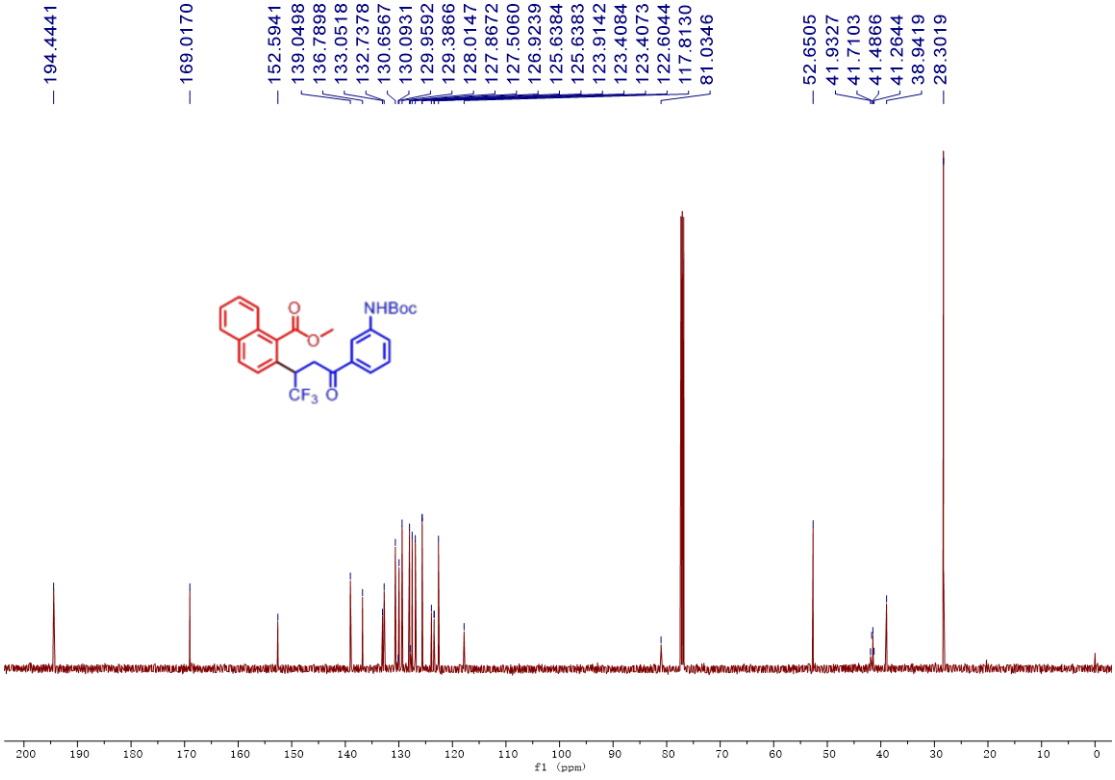

8.0221
8.0178
8.0142
8.0047
8.0011
7.9969
7.7563
7.7522
7.7003
7.6964
7.6872
7.6834
7.4163
7.4006
7.3851
7.3540
7.3508
7.3377
7.3102
7.3072
7.3043
7.2936
7.2193
7.2176
7.2150
7.2131
7.2053
7.2016
7.2000
6.6314
4.5935
4.5837
4.5776
4.5749
4.5676
4.5650
4.5590
4.5562
4.5487
4.0304
4.0242
3.7281
3.7181
3.6928
3.6829
3.6710
3.6551
3.6358
3.6198
2.3917
1.5651
NHBoc
O
O
CF3
O
2.01
1.05
2.04
1.10
3.10
1.05
1.01
1.00
1.00
3.02
1.00
1.02
3.03
9.45
f1 (ppm)

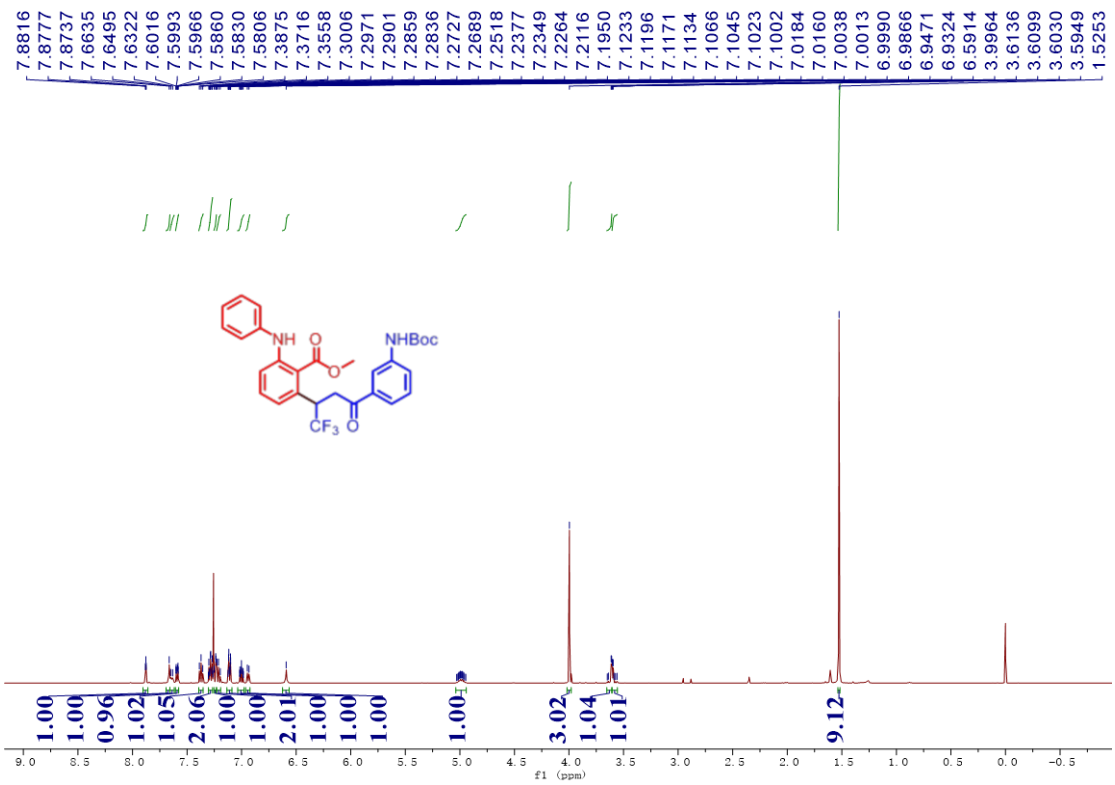

194.4092
169.3436
152.7045
145.8895
140.6084
139.0463
136.0674
135.3879
134.9357
132.3111
130.3192
130.0960
129.7703
129.5514
128.6667
127.8637
127.3815
125.6374
124.8299
123.4130
121.9265
118.3441
117.2797
80.7779
52.2791
41.4695
41.2474
41.0253
40.8069
39.1170
28.3434
20.2797
NHBoc
O
O
CF3
O
f1 (ppm)

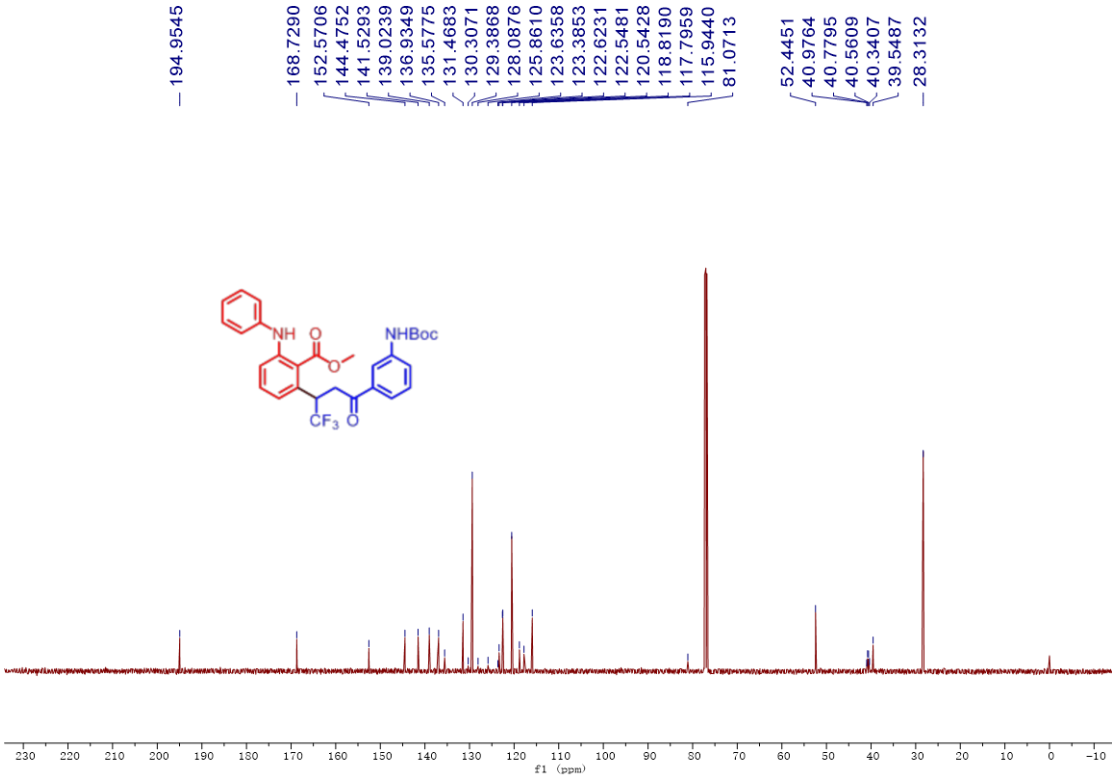

7.8787
7.8748
7.8709
7.7151
7.7074
7.7031
7.7000
7.6990
7.6889
7.6164
7.6137
7.6109
7.6008
7.5980
7.5954
7.4050
7.3895
7.3736
7.3574
7.0846
7.0687
6.9237
6.9222
6.9069
6.9053
6.6931
4.4585
4.4558
4.4457
4.4403
4.4373
4.4301
4.4271
4.4219
4.4187
4.4117
4.4088
4.0079
3.9958
3.9902
3.8465
3.8417
3.6626
3.6523
3.6275
3.6170
3.5983
3.5829
3.5631
3.5479
1.5496
NHBoc
CF3
O
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
1.02
1.00
9.11
f1 (ppm)

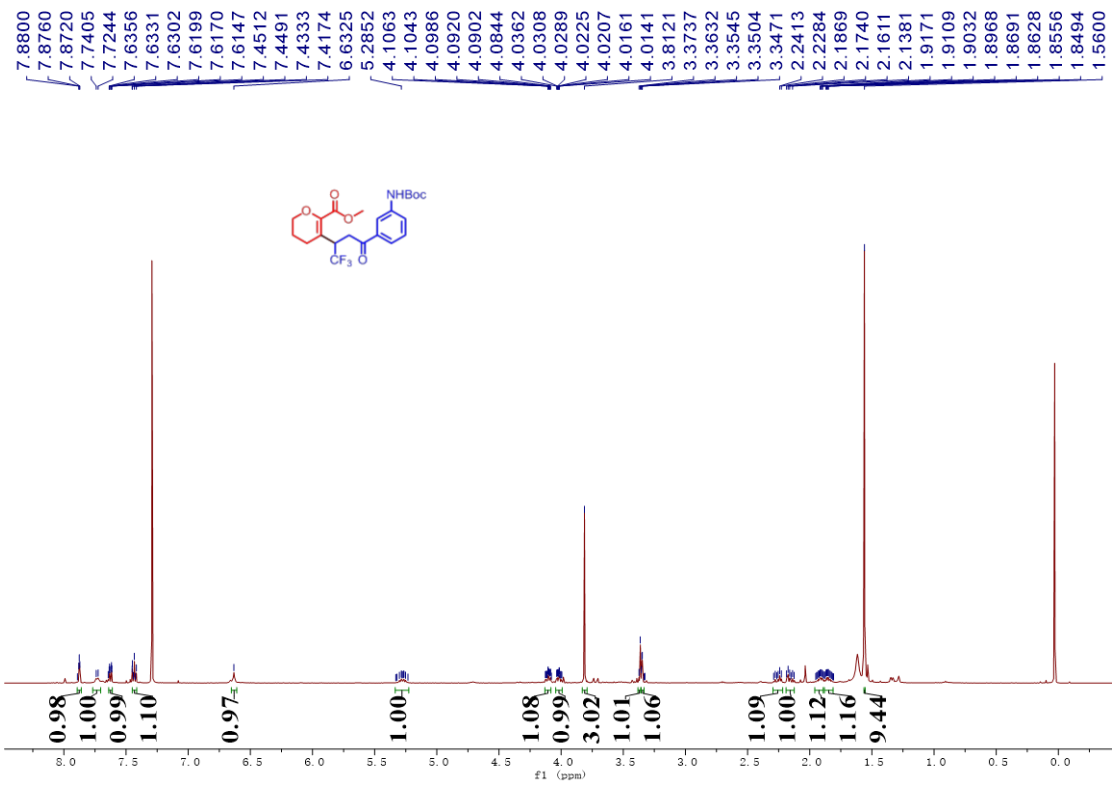

194.4206
167.7056
156.7462
152.6105
139.0347
136.8054
133.5685
130.9299
129.9035
129.3783
127.6796
125.4551
125.3906
123.3781
123.2419
122.6140
119.4952
117.8492
111.0331
81.0142
55.9667
52.5371
41.5268
41.3030
41.0803
40.8552
39.0597
28.3041
NHBoc
CF3
O
f1 (ppm)

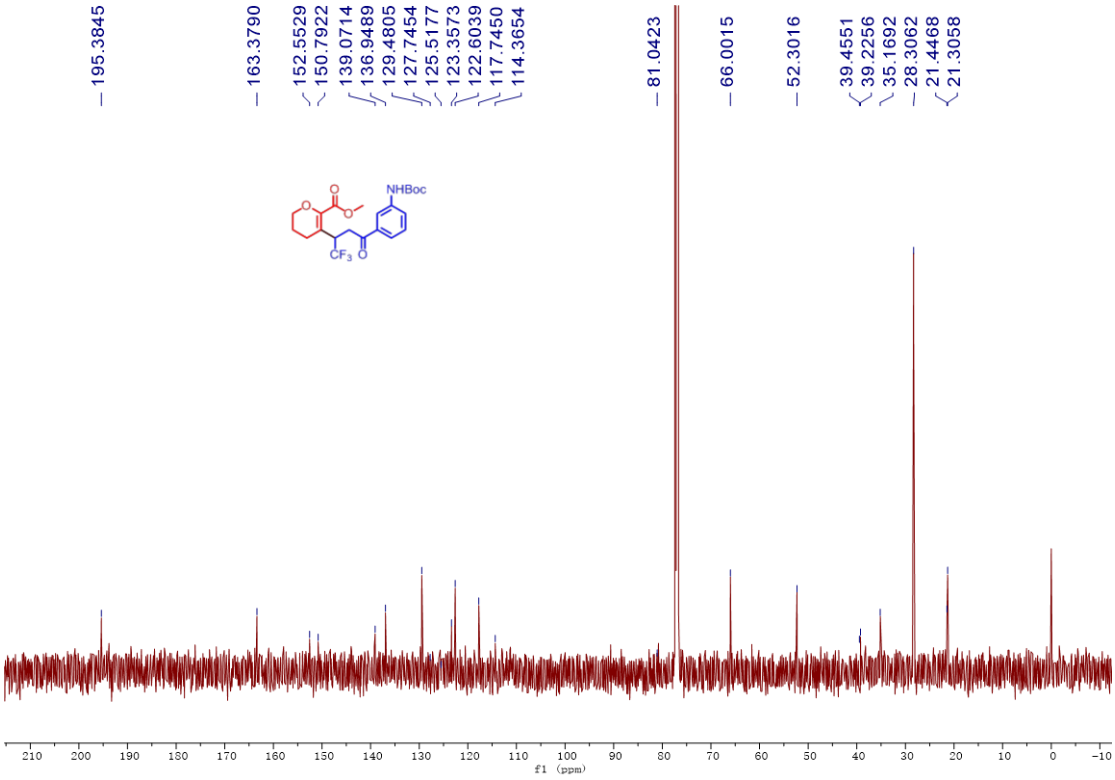

7.9079
7.8904
7.8768
7.8753
7.8729
7.8711
7.8612
7.8591
7.8562
7.8521
7.8483
7.8225
7.8201
7.8174
7.8069
7.8033
7.6473
7.6311
7.5828
7.5805
7.5779
7.5696
7.5672
7.5643
7.5617
7.5515
7.5485
7.5378
7.5347
7.5316
7.5218
7.5178
7.5077
7.5055
7.5029
7.4919
7.3580
7.3423
7.3262
6.6379
4.7456
4.1040
3.7393
3.7294
3.7039
3.6940
3.6580
3.6425
3.6228
3.6073
1.5117
NHBoc
O
O
CF3
O
1.01
2.00
1.00
0.96
2.16
1.88
1.05
1.00
1.00
2.96
1.00
1.01
9.20
f1 (ppm)

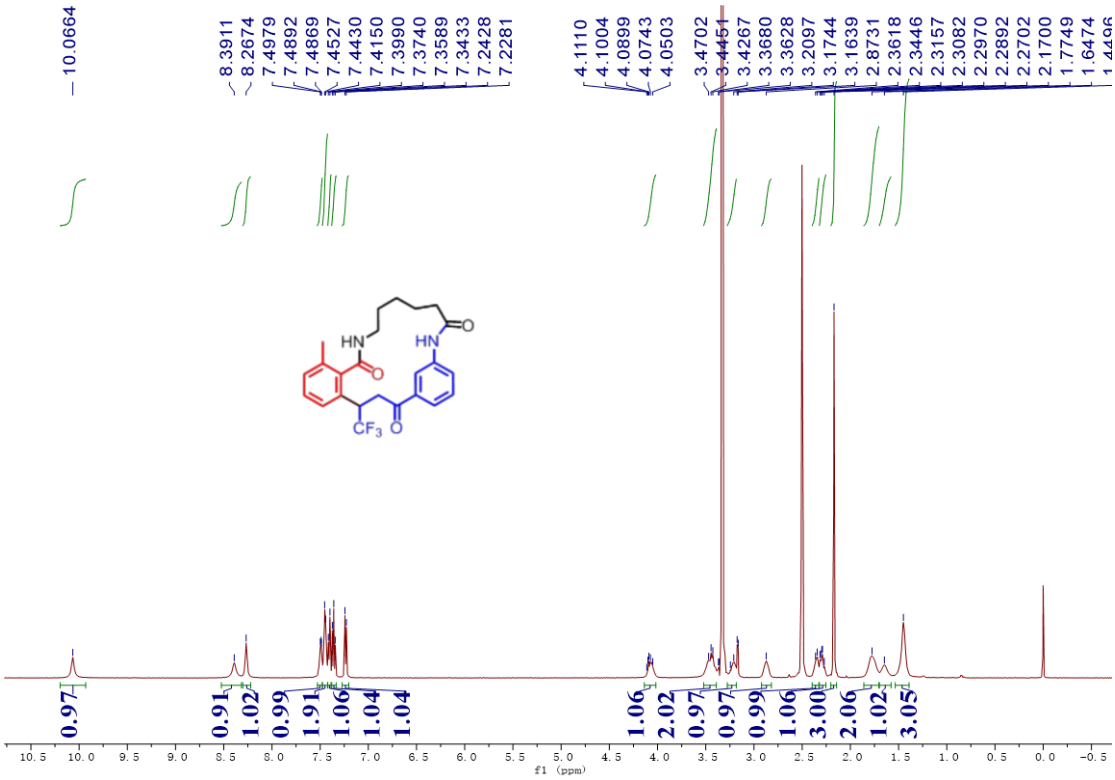

194.4441
169.0170
152.5941
139.0498
136.7898
133.0518
132.7378
130.6567
130.0931
129.9592
129.3866
128.0147
127.8672
127.5060
126.9239
125.6384
125.6383
123.9142
123.4084
123.4073
122.6044
117.8130
81.0346
52.6505
41.9327
41.7103
41.4866
41.2644
38.9419
28.3019
NHBoc
O
O
CF3
O
f1 (ppm)

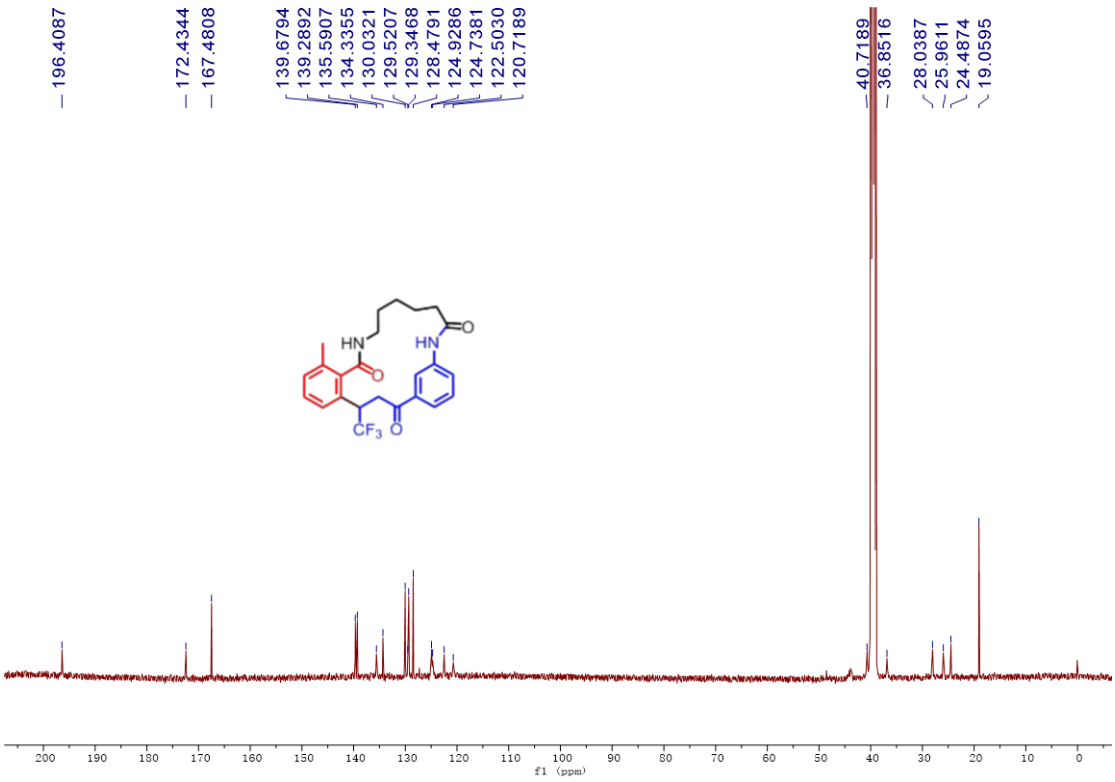

7.8816
7.8777
7.8737
7.6635
7.6495
7.6322
7.6016
7.5993
7.5966
7.5860
7.5830
7.5806
7.3875
7.3716
7.3558
7.3006
7.2971
7.2901
7.2859
7.2836
7.2727
7.2689
7.2518
7.2377
7.2349
7.2264
7.2116
7.1950
7.1233
7.1196
7.1171
7.1134
7.1066
7.1045
7.1023
7.1002
7.0184
7.0160
7.0038
7.0013
6.9990
6.9866
6.9471
6.9324
6.5914
3.9964
3.6136
3.6099
3.6030
3.5949
1.5253
NH
O
O
NHBoc
CF3
O
1.00
1.00
0.96
1.02
1.05
2.06
1.00
1.00
2.01
1.00
1.00
1.00
1.00
3.02
1.04
1.01
9.12
f1 (ppm)

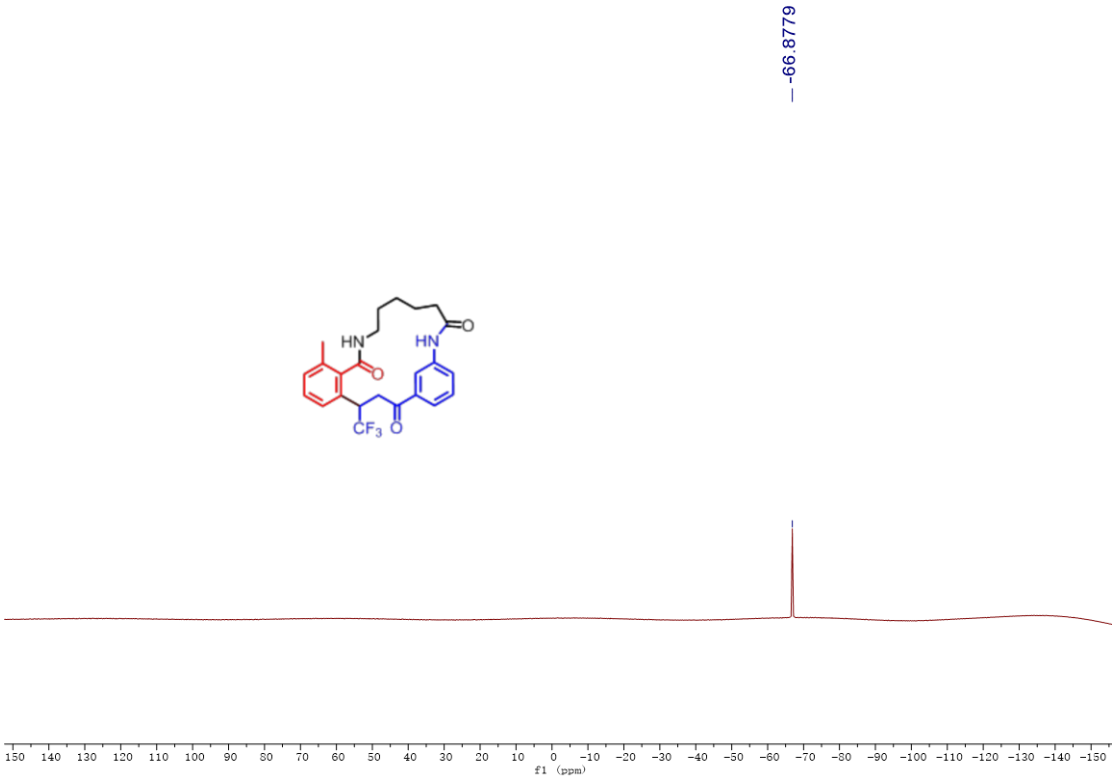

194.9545
168.7290
152.5706
144.4752
141.5293
139.0239
136.9349
135.5775
131.4683
130.3071
129.3868
128.0876
125.8610
123.6358
123.3853
122.6231
122.5481
120.5428
118.8190
117.7959
115.9440
81.0713
52.4451
40.9764
40.7795
40.5609
40.3407
39.5487
28.3132
NH
O
O
NHBoc
CF3
O
f1 (ppm)

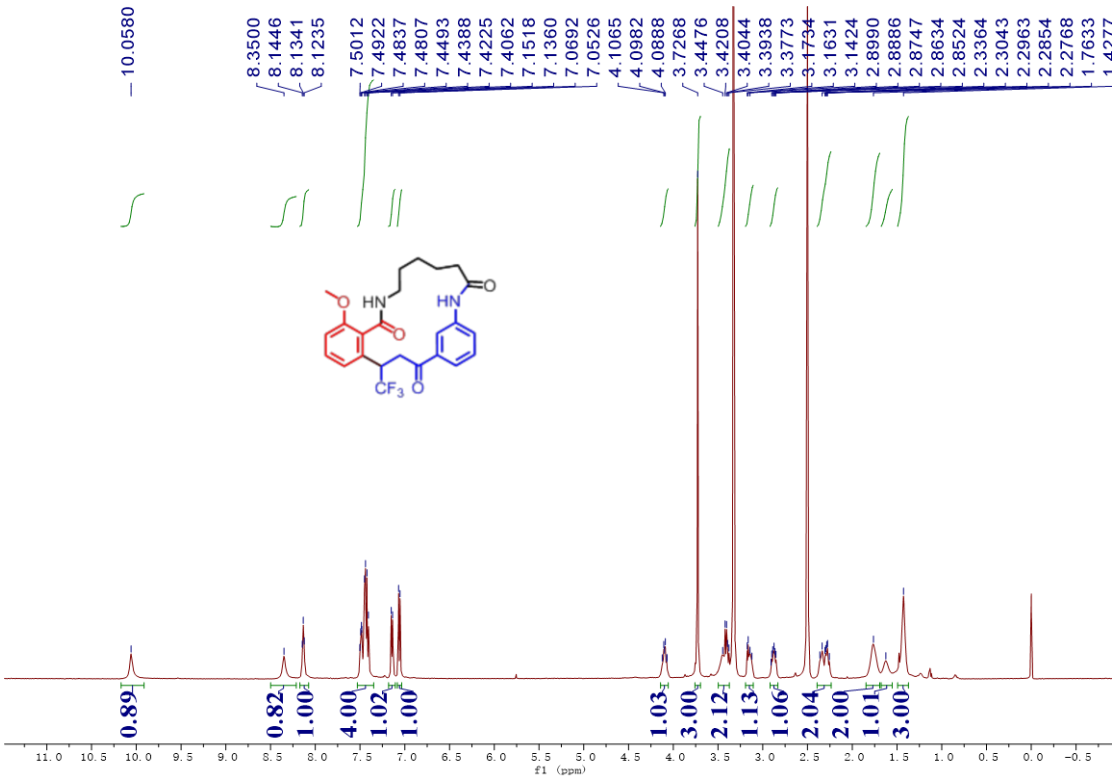

7.8800
7.8760
7.8720
7.7405
7.7244
7.6356
7.6331
7.6302
7.6199
7.6170
7.6147
7.4512
7.4491
7.4333
7.4174
6.6325
5.2852
4.1063
4.1043
4.0986
4.0920
4.0902
4.0844
4.0362
4.0308
4.0289
4.0225
4.0207
4.0161
4.0141
3.8121
3.3737
3.3632
3.3545
3.3504
3.3471
2.2413
2.2284
2.1869
2.1740
2.1611
2.1381
1.9171
1.9109
1.9032
1.8968
1.8691
1.8628
1.8556
1.8494
1.5600
NHBoc
CF3
O
0.98
1.00
0.99
1.10
0.97
1.00
1.08
0.99
3.02
1.01
1.06
1.09
1.00
1.12
1.16
9.44
f1 (ppm)

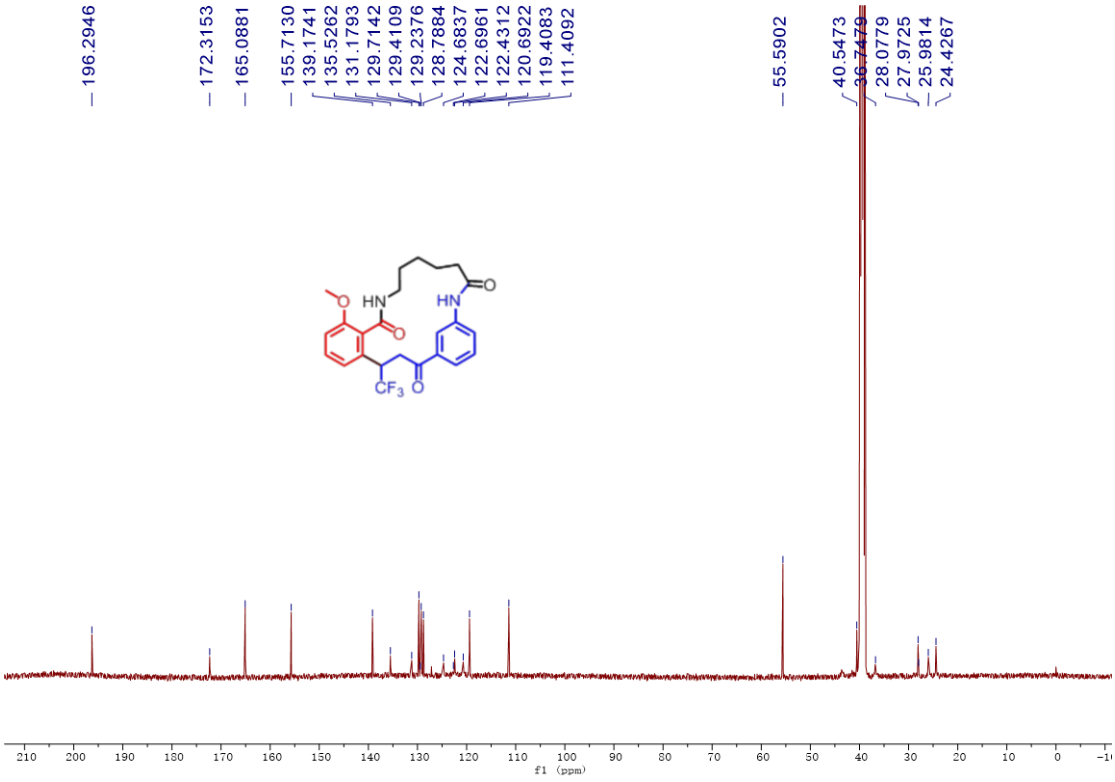

195.3845
163.3790
152.5529
150.7922
139.0714
136.9489
129.4805
127.7454
125.5177
123.3573
122.6039
117.7450
114.3654
81.0423
66.0015
52.3016
39.4551
39.2256
35.1692
28.3062
21.4468
21.3058
NHBoc
CF3
O
f1 (ppm)

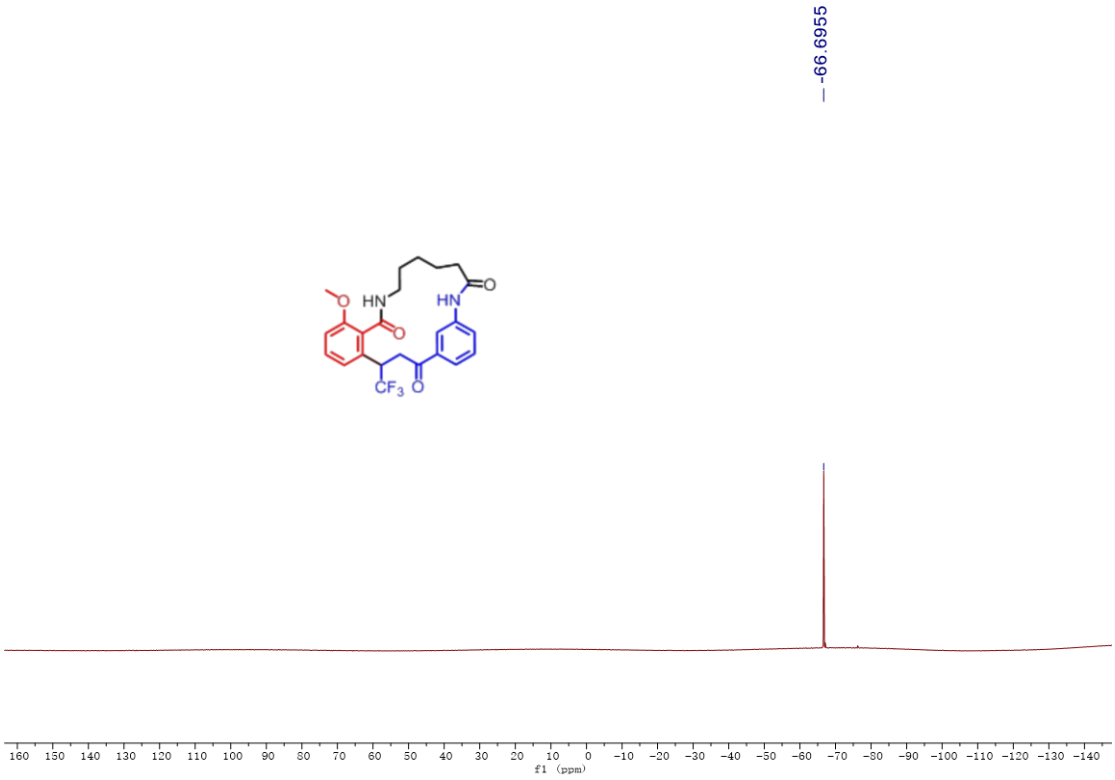

10.0664
8.3911
8.2674
7.4979
7.4892
7.4869
7.4527
7.4430
7.4150
7.3990
7.3740
7.3589
7.3433
7.2428
7.2281
4.1110
4.1004
4.0899
4.0743
4.0503
3.4702
3.4451
3.4267
3.3680
3.3628
3.2097
3.1744
3.1639
2.8731
2.3618
2.3446
2.3157
2.3082
2.2970
2.2892
2.2702
2.1700
1.7749
1.6474
0.97
0.91
1.02
0.99
1.91
1.06
1.04
1.04
1.06
2.02
0.97
0.97
0.99
1.06
3.00
2.06
1.02
3.05
f1 (ppm)

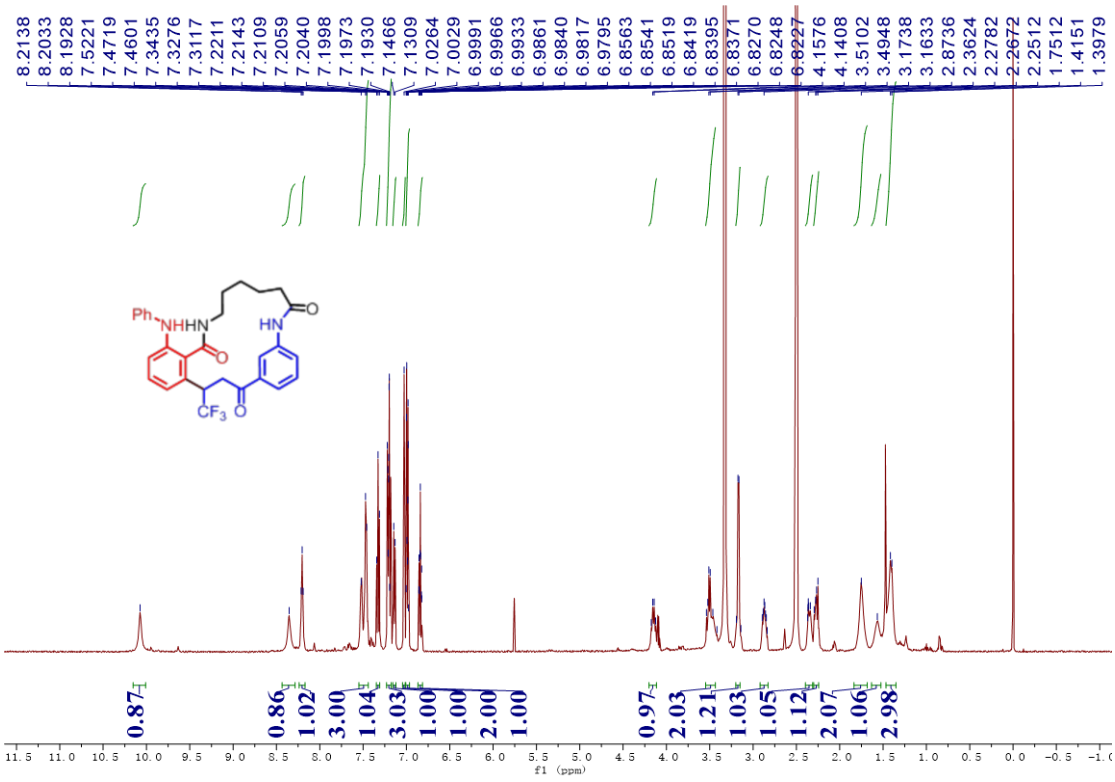

196.4087
172.4344
167.4808
139.6794
139.2892
135.5907
134.3355
130.0321
129.5207
129.3468
128.4791
124.9286
124.7381
122.5030
120.7189
40.7189
36.8516
28.0387
25.9611
24.4874
19.0595
f1 (ppm)

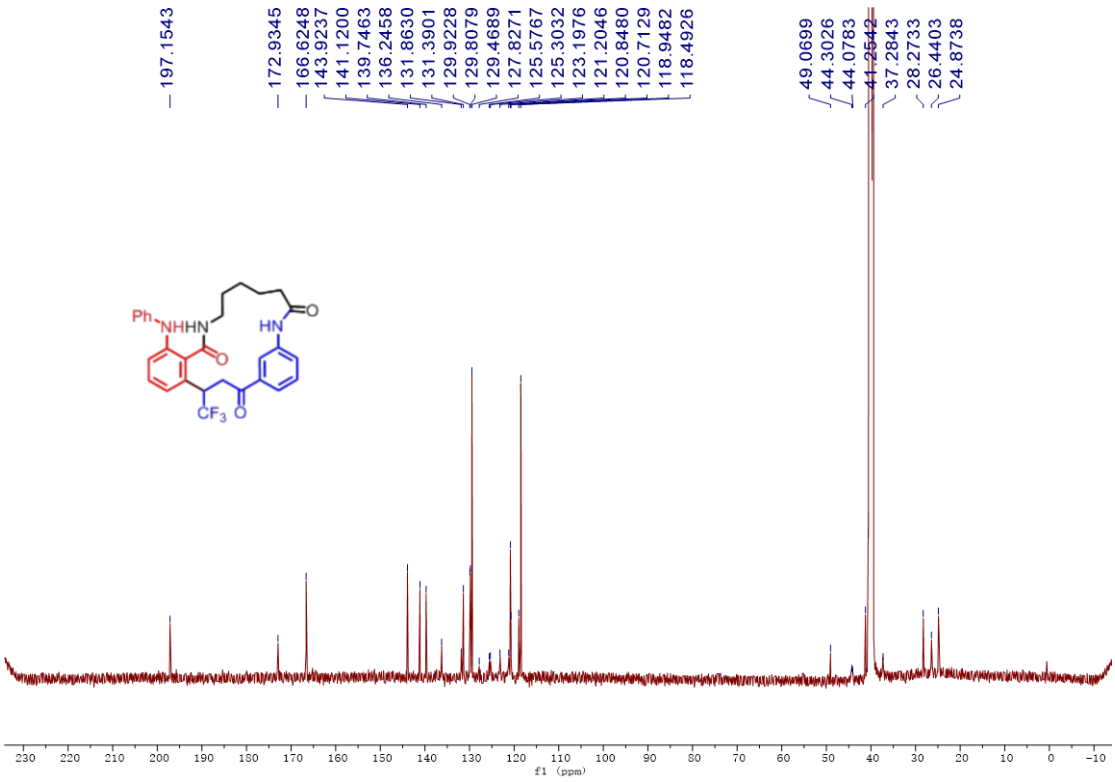

-66.8779
HN
HN
O
O
CF3
O
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

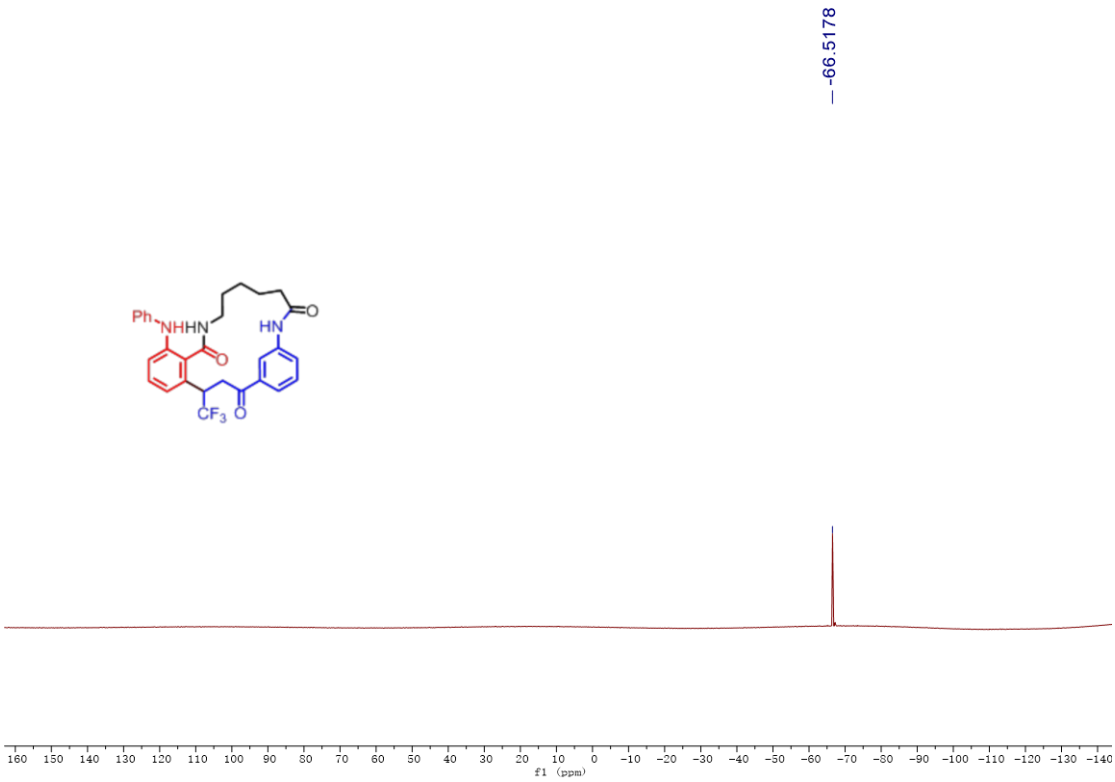

10.0580
8.3500
8.1446
8.1341
8.1235
7.5012
7.4922
7.4837
7.4807
7.4493
7.4388
7.4225
7.4062
7.1518
7.1360
7.0692
7.0526
4.1065
4.0982
4.0888
3.7268
3.4476
3.4208
3.4044
3.3938
3.3773
3.1734
3.1631
3.1424
2.8990
2.8886
2.8747
2.8634
2.8524
2.3364
2.3043
2.2963
2.2854
2.2768
1.7633
O
HN
HN
O
O
CF3
O
0.89
0.82
1.00
4.00
1.02
1.00
1.03
3.00
2.12
1.13
1.06
2.04
2.00
1.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

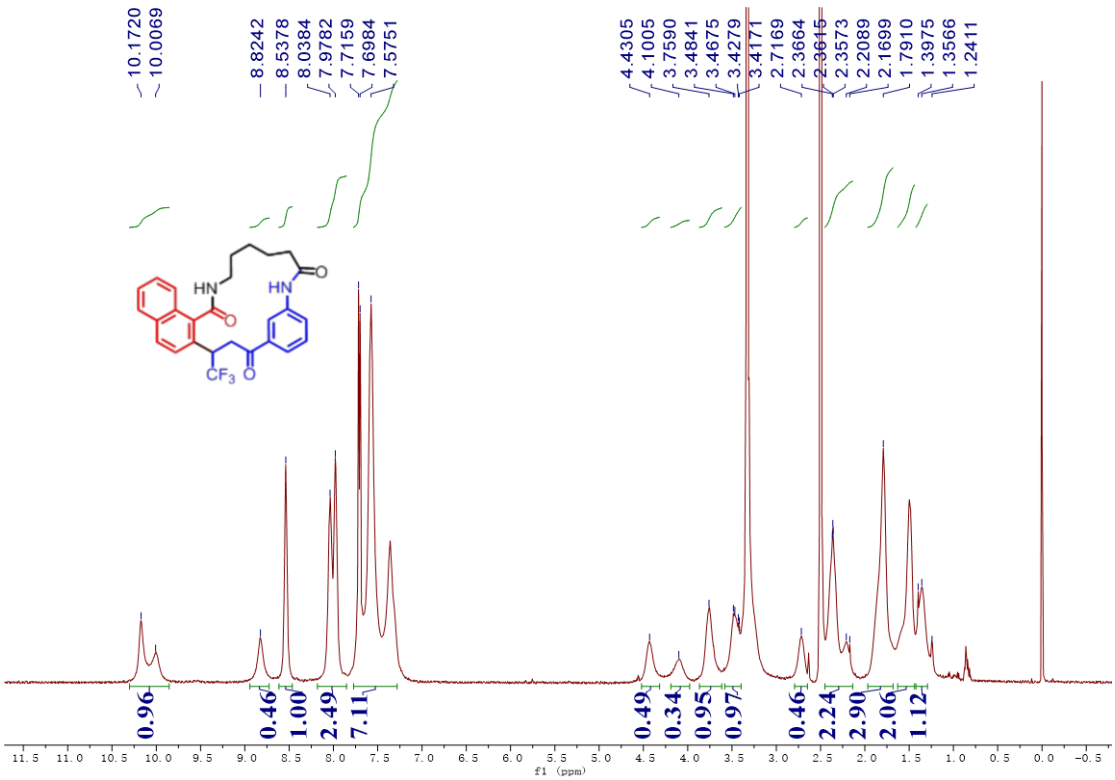

196.2946
172.3153
165.0881
155.7130
139.1741
135.5262
131.1793
129.7142
129.4109
129.2376
128.7884
124.6837
122.6961
122.4312
120.6922
119.4083
111.4092
55.5902
40.5473
36.7479
28.0779
27.9725
25.9814
24.4267
HN
HN
O
O
O
CF3
O
f1 (ppm)

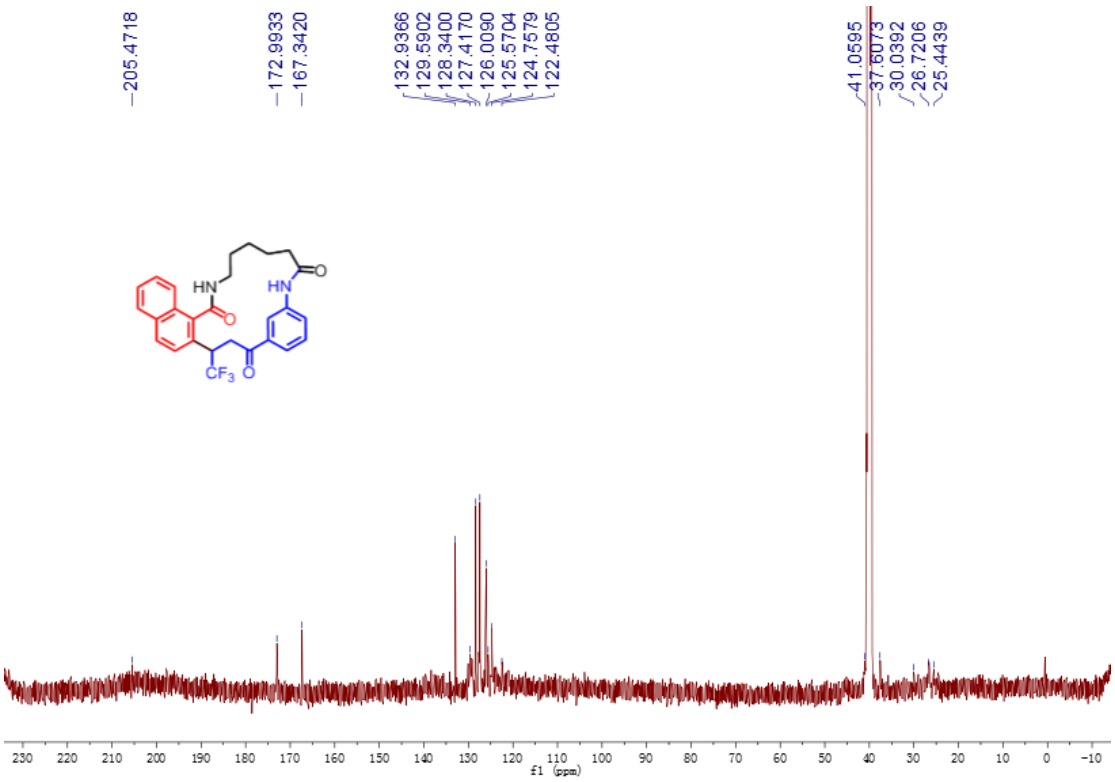

-66.6955
HN
HN
O
O
O
CF3
O
f1 (ppm)

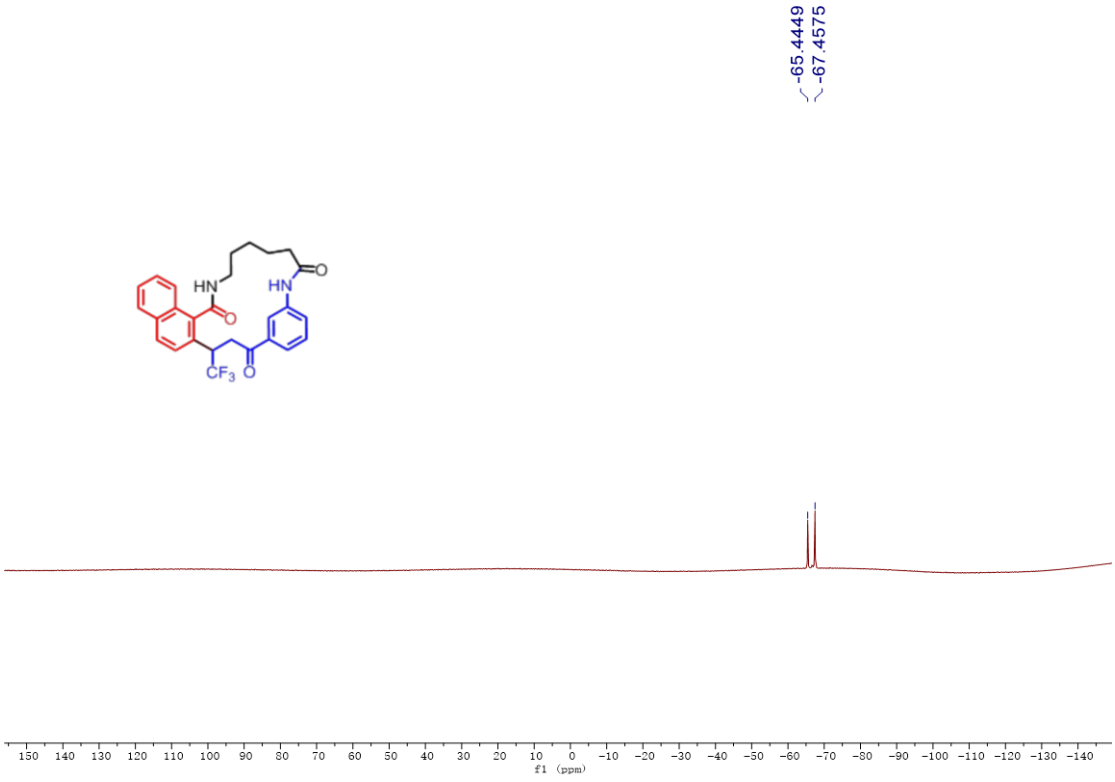

8.2138
8.2033
8.1928
7.5221
7.4719
7.4601
7.3435
7.3276
7.3117
7.2211
7.2143
7.2109
7.2059
7.2040
7.1998
7.1973
7.1930
7.1466
7.1309
7.0264
7.0029
6.9991
6.9966
6.9933
6.9861
6.9840
6.9817
6.9795
6.8563
6.8541
6.8519
6.8419
6.8395
6.8371
6.8270
6.8248
6.8227
4.1576
4.1408
3.5102
3.4948
3.1738
3.1633
2.8736
2.3624
2.2782
2.2672
2.2512
1.7512
1.4151
1.3979
Ph
NH
HN
HN
O
O
CF3
O
0.87
0.86
1.02
3.00
1.04
3.03
1.00
1.00
2.00
1.00
0.97
2.03
1.21
1.03
1.05
1.12
2.07
1.06
2.98
f1 (ppm)

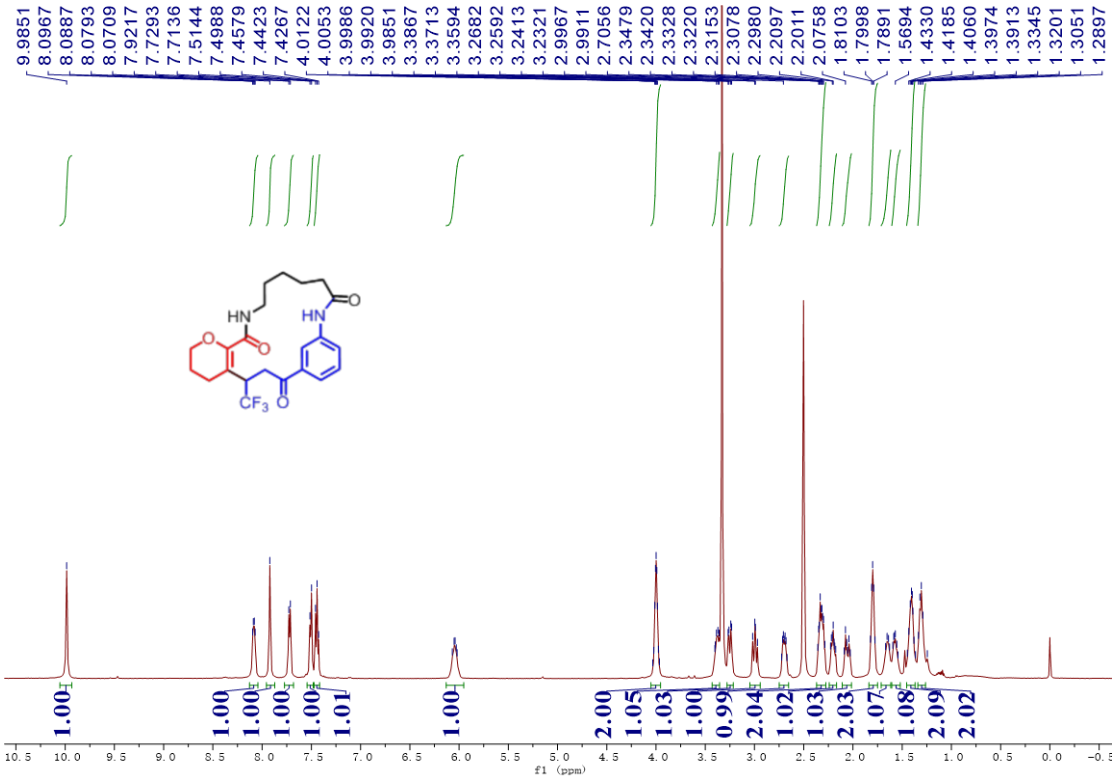

197.1543
172.9345
166.6248
143.9237
141.1200
139.7463
136.2458
131.8630
131.3901
129.9228
129.8079
129.4689
127.8271
125.5767
125.3032
123.1976
121.2046
120.8480
120.7129
118.9482
118.4926
49.0699
44.3026
44.0783
41.2542
37.2843
28.2733
26.4403
24.8738
Ph
NH
HN
HN
O
O
CF3
O
f1 (ppm)

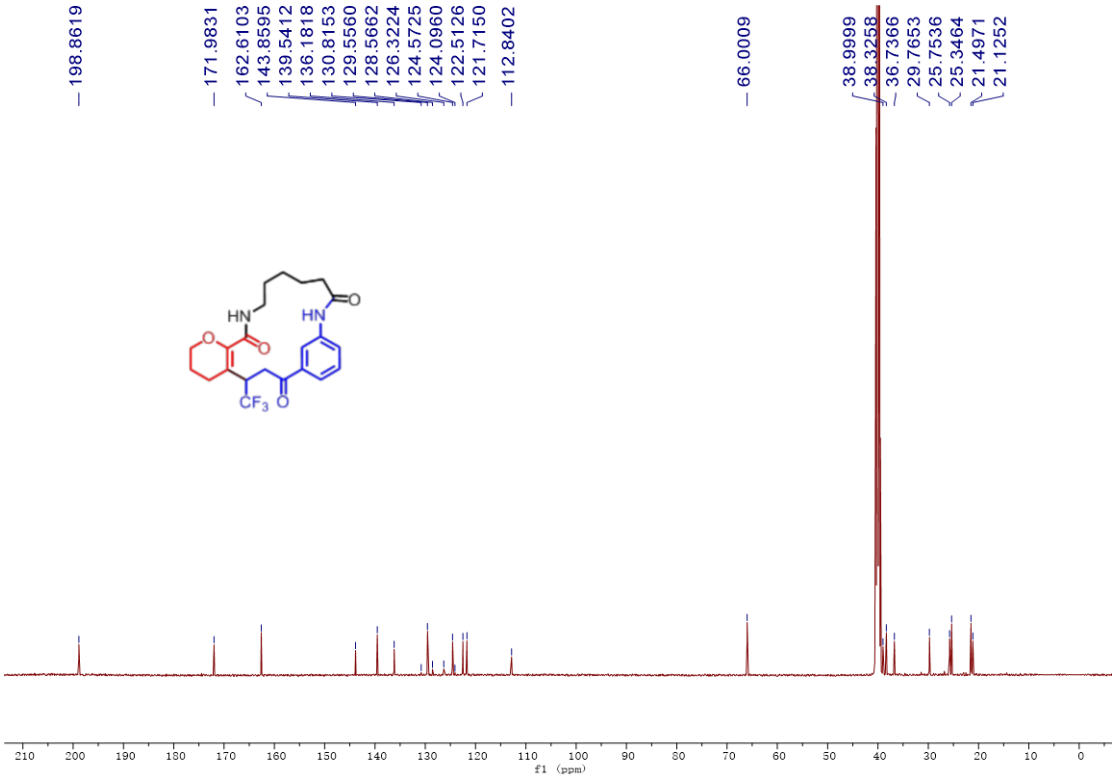

-66.5178
Ph
NH
HN
HN
O
O
CF3
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140
f1 (ppm)

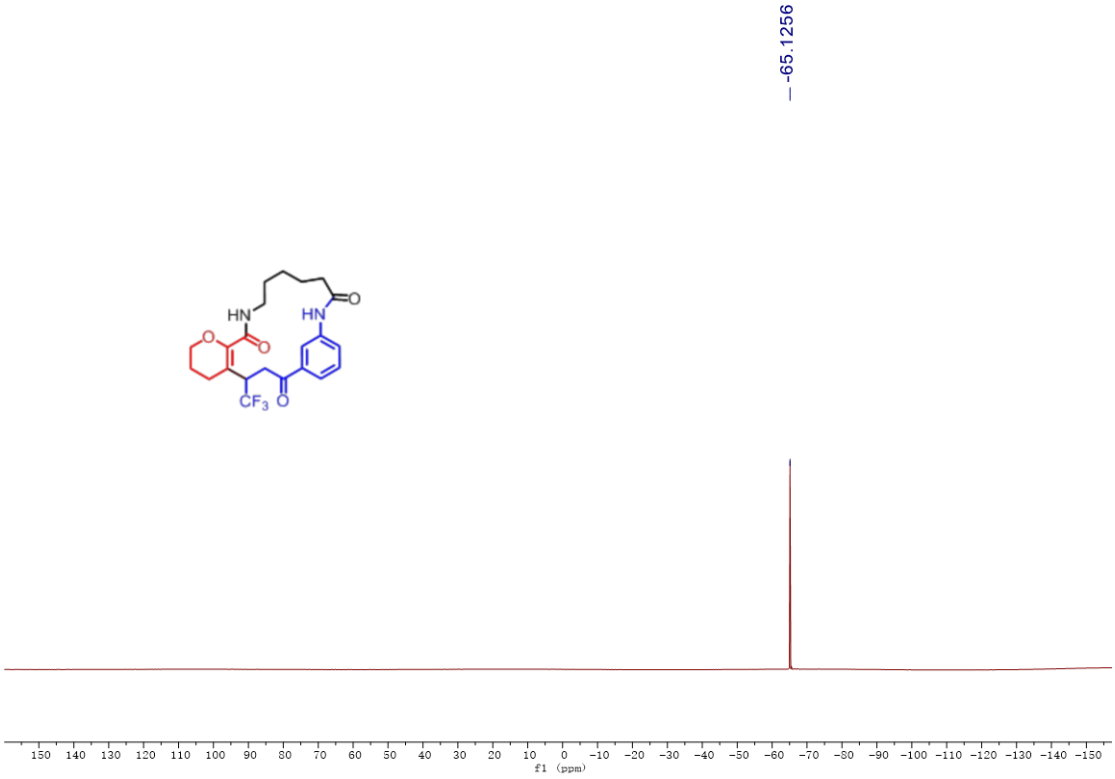

10.1720
10.0069
8.8242
8.5378
8.0384
7.9782
7.7159
7.6984
7.5751
4.4305
4.1005
3.7590
3.4841
3.4675
3.4279
3.4171
2.7169
2.3664
2.3615
2.3573
2.2089
2.1699
1.7910
1.3975
1.3566
1.2411
HN
HN
O
O
CF3
O
0.96
0.46
1.00
2.49
7.11
0.49
0.34
0.95
0.97
0.46
2.24
2.90
2.06
1.12
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

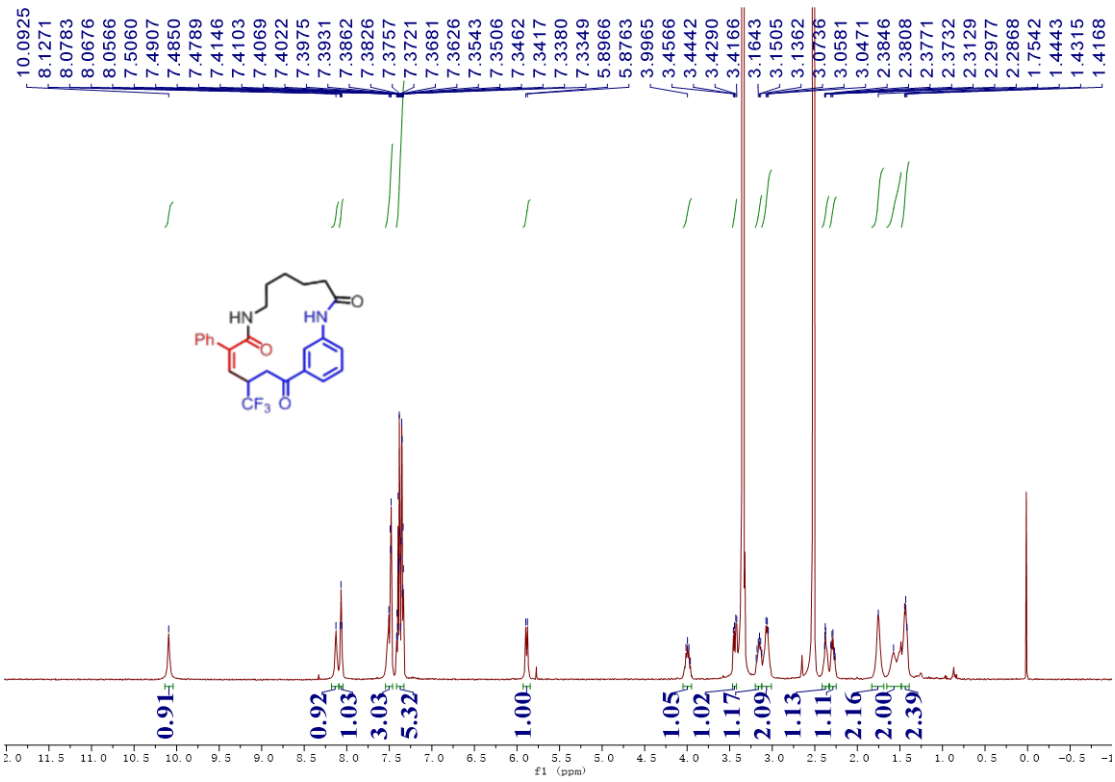

205.4718
172.9933
167.3420
132.9366
129.5902
128.3400
127.4170
126.0090
125.5704
124.7579
122.4805
41.0595
37.6073
30.0392
26.7206
25.4439
HN
HN
O
O
CF3
O
f1 (ppm)

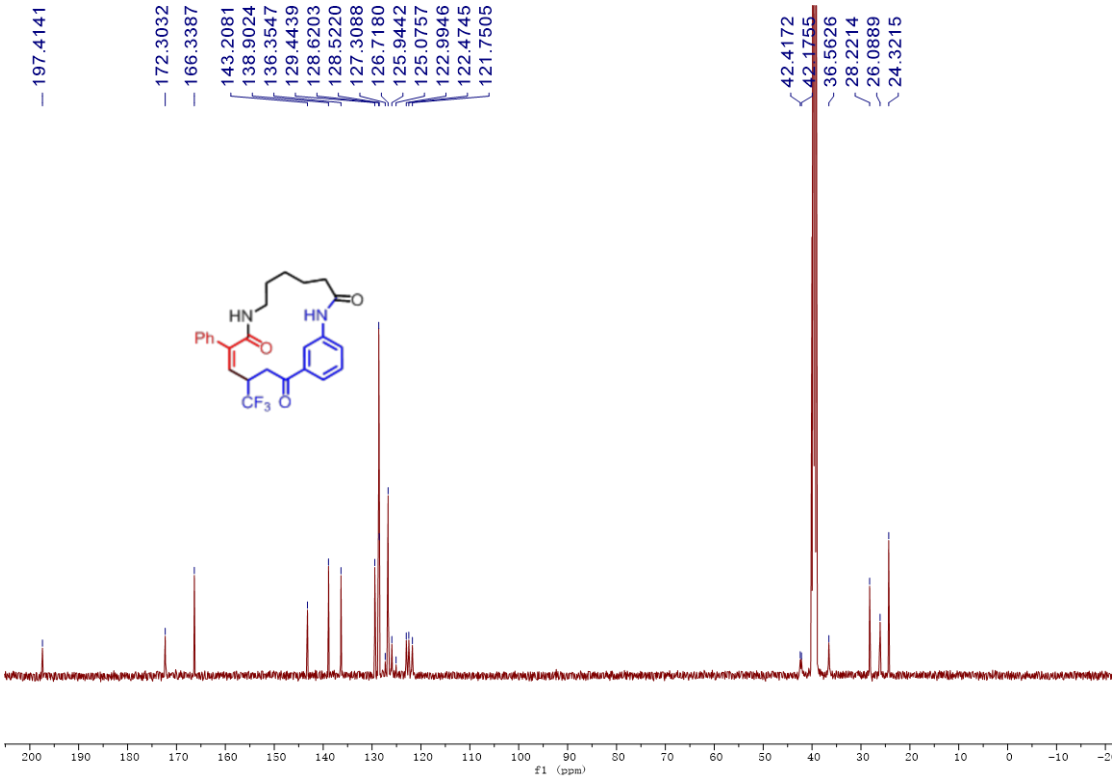

-65.4449
-67.4575
HN
HN
O
O
CF3
O
f1 (ppm)

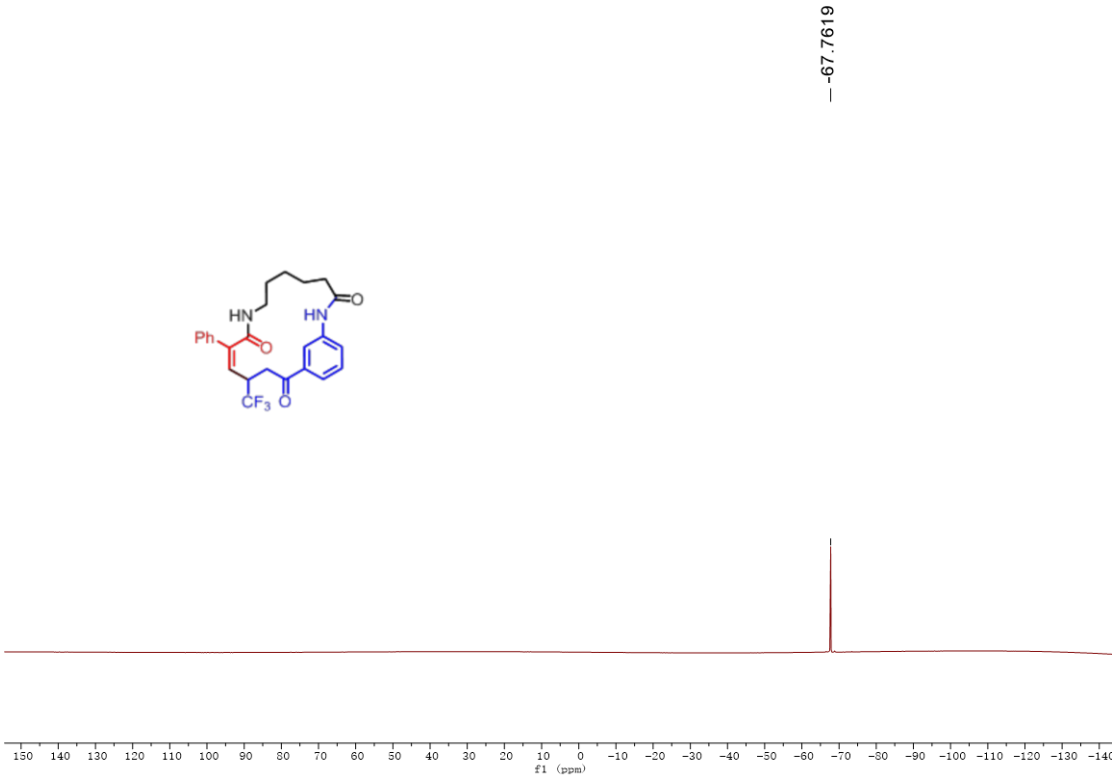

9.9851
8.0967
8.0887
8.0793
8.0709
7.9217
7.7293
7.7136
7.5144
7.4988
7.4579
7.4423
7.4267
4.0122
4.0053
3.9986
3.9920
3.9851
3.3867
3.3713
3.3594
3.2682
3.2592
3.2413
3.2321
2.9967
2.9911
2.7056
2.3479
2.3420
2.3328
2.3220
2.3153
2.3078
2.2980
2.2097
2.2011
2.0758
1.8103
1.7998
1.7891
1.5694
1.4330
1.4185
1.4060
1.3974
1.3913
1.3345
1.3201
1.3051
1.2897
HN
HN
O
O
O
CF3
1.00
1.00
1.00
1.00
1.01
1.00
2.00
1.05
1.03
1.00
0.99
2.04
1.02
1.03
2.03
1.07
1.08
2.09
2.02
f1 (ppm)

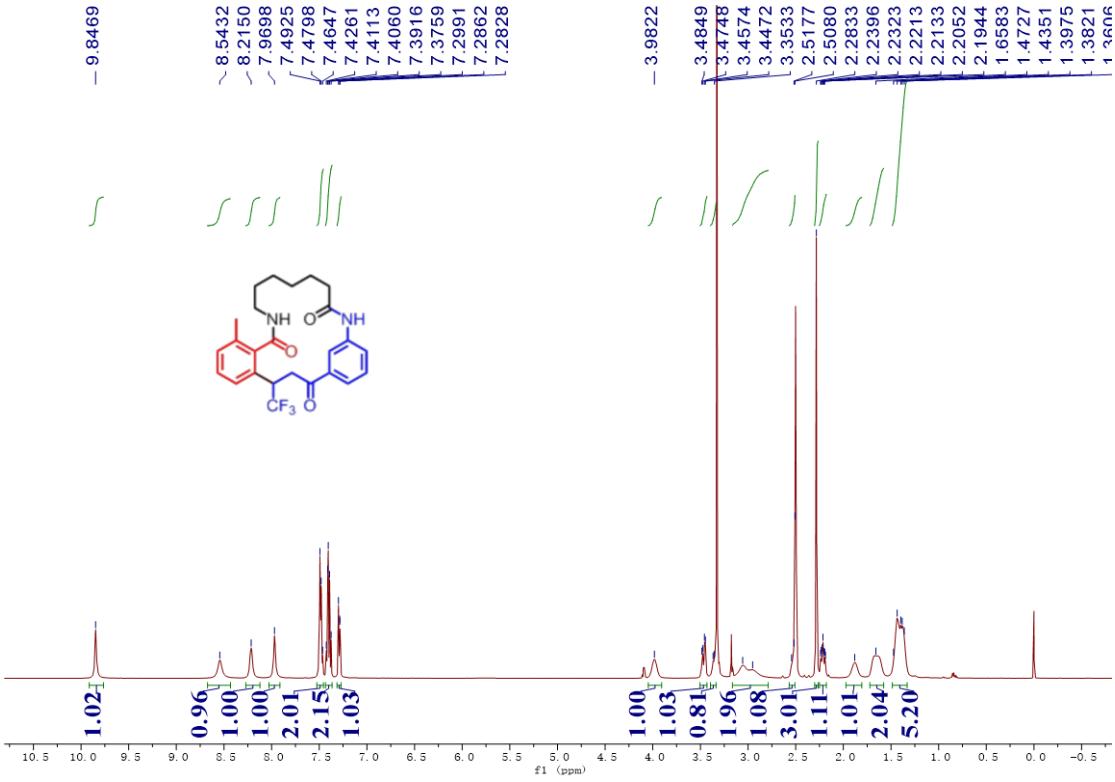

198.8619
171.9831
162.6103
143.8595
139.5412
136.1818
130.8153
129.5560
128.5662
126.3224
124.5725
124.0960
122.5126
121.7150
112.8402
66.0009
38.9999
38.3258
36.7366
29.7653
25.7536
25.3464
21.4971
21.1252
HN
HN
O
O
O
CF3
f1 (ppm)

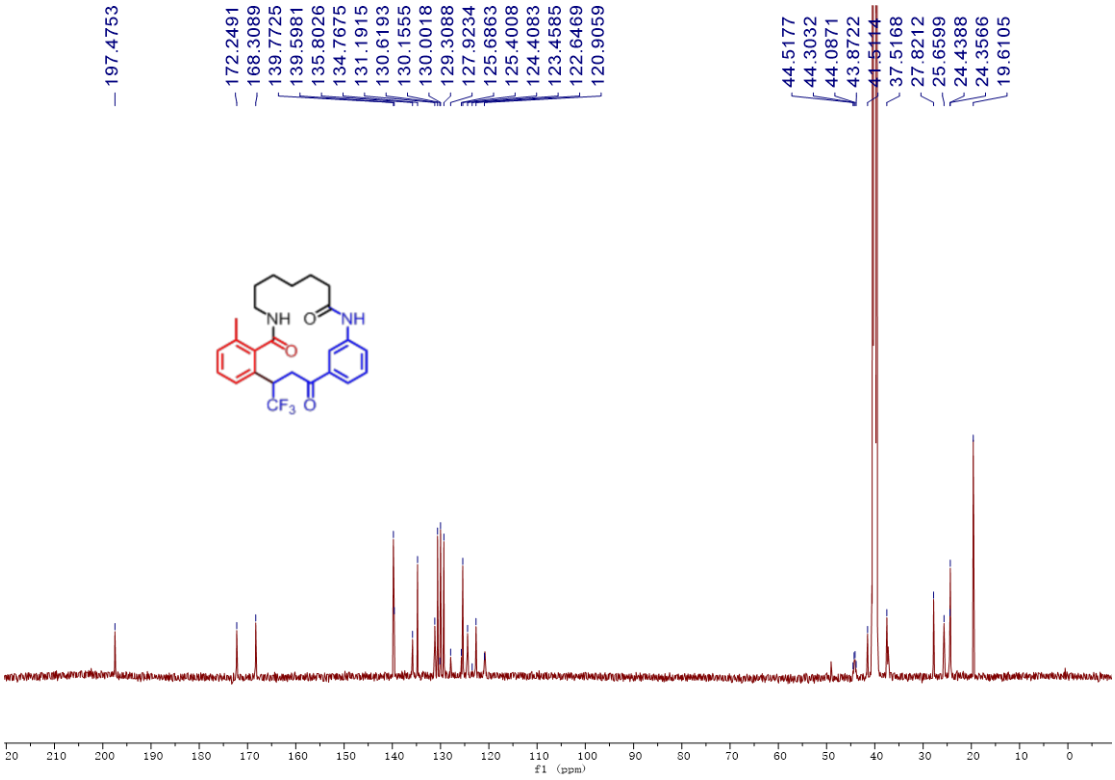

-65.1256
HN
HN
O
O
O
CF3
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

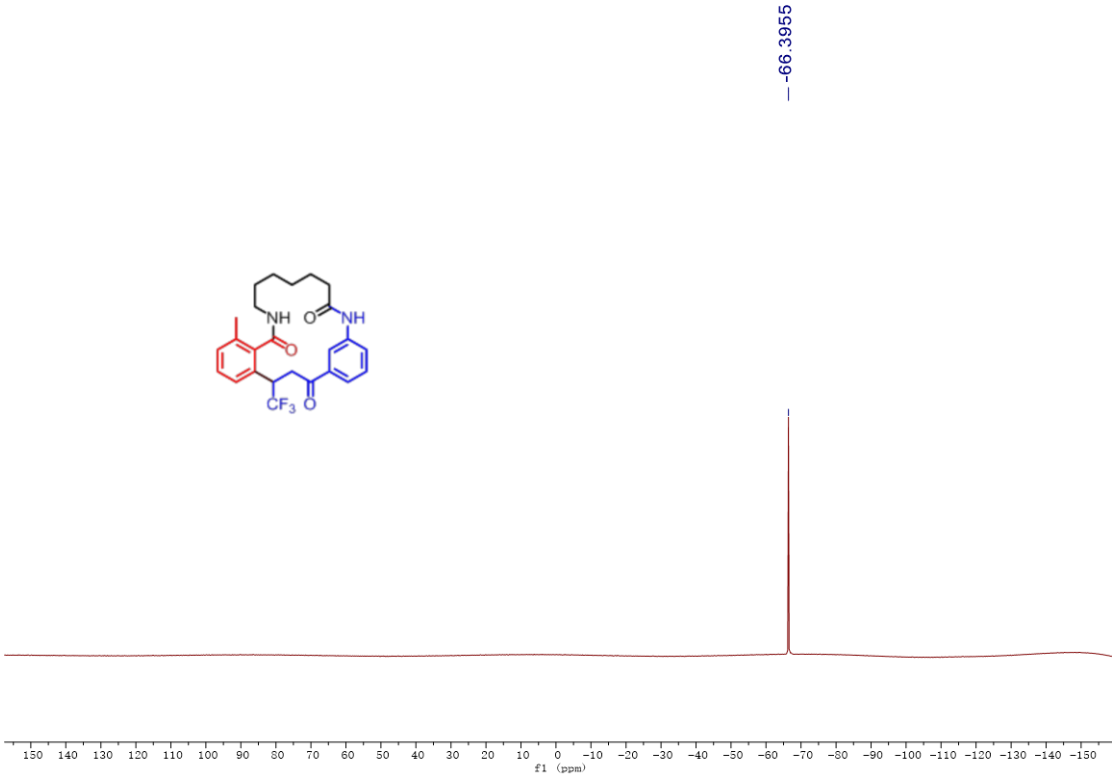

10.0925
8.1271
8.0783
8.0676
8.0566
7.5060
7.4907
7.4850
7.4789
7.4146
7.4103
7.4069
7.4022
7.3975
7.3931
7.3862
7.3826
7.3757
7.3721
7.3681
7.3626
7.3543
7.3506
7.3462
7.3417
7.3380
7.3349
5.8966
5.8763
3.9965
3.4566
3.4442
3.4290
3.4166
3.1643
3.1505
3.1362
3.0736
3.0581
3.0471
2.3846
2.3808
2.3771
2.3732
2.3129
2.2977
2.2868
1.7542
1.4443
1.4315
1.4168
HN
HN
Ph
O
O
CF3
0.91
0.92
1.03
3.03
5.32
1.00
1.05
1.02
1.17
2.09
1.13
1.11
2.16
2.00
2.39
f1 (ppm)

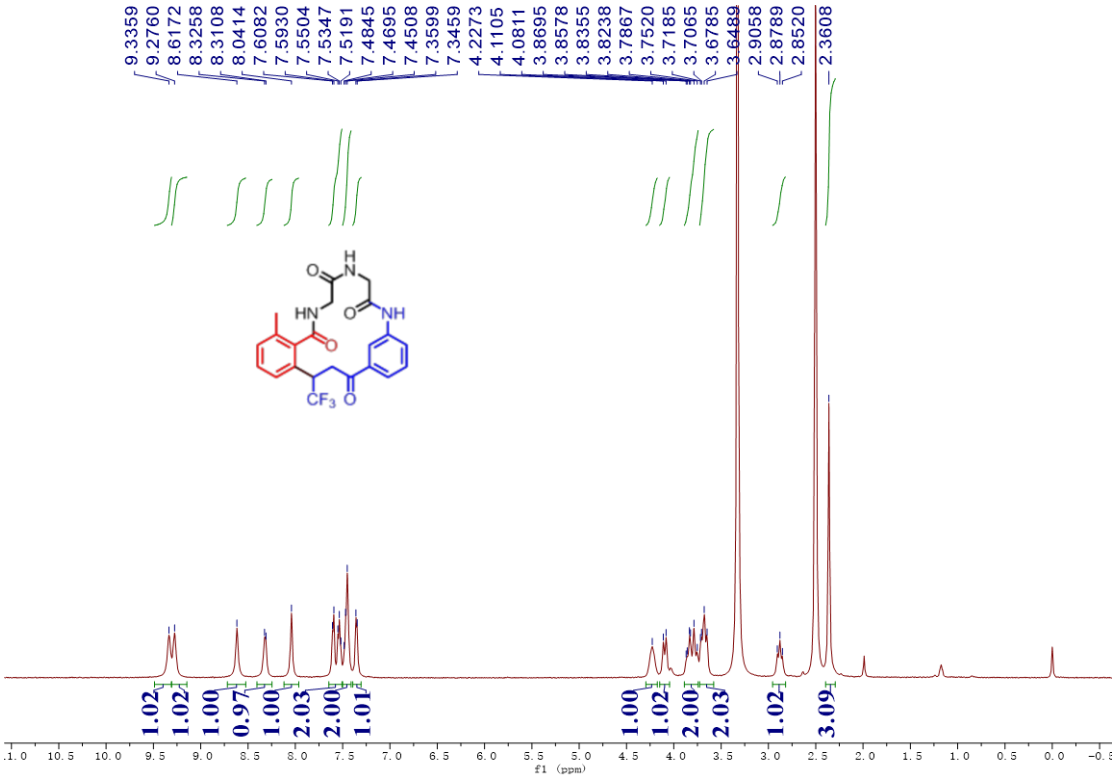

197.4141
172.3032
166.3387
143.2081
138.9024
136.3547
129.4439
128.6203
128.5220
127.3088
126.7180
125.9442
125.0757
122.9946
122.4745
121.7505
42.4172
42.1755
36.5626
28.2214
26.0889
24.3215
HN
HN
Ph
O
O
CF3
f1 (ppm)

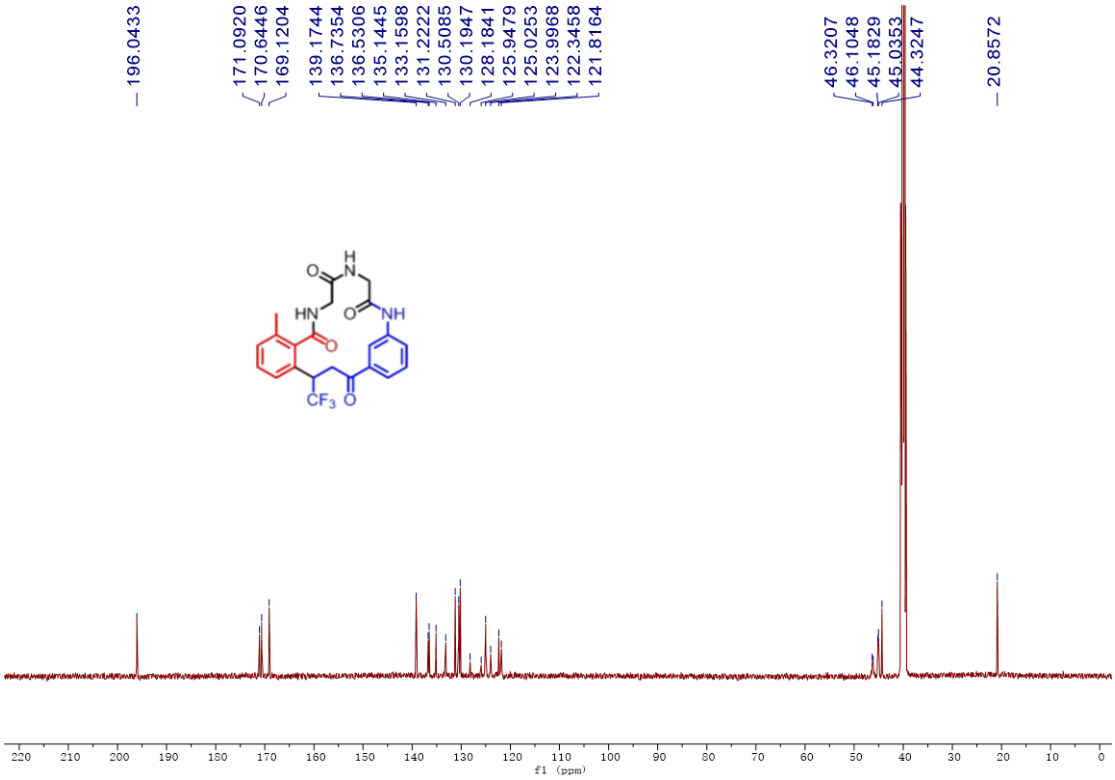

-67.7619
HN
HN
Ph
O
O
CF3
f1 (ppm)

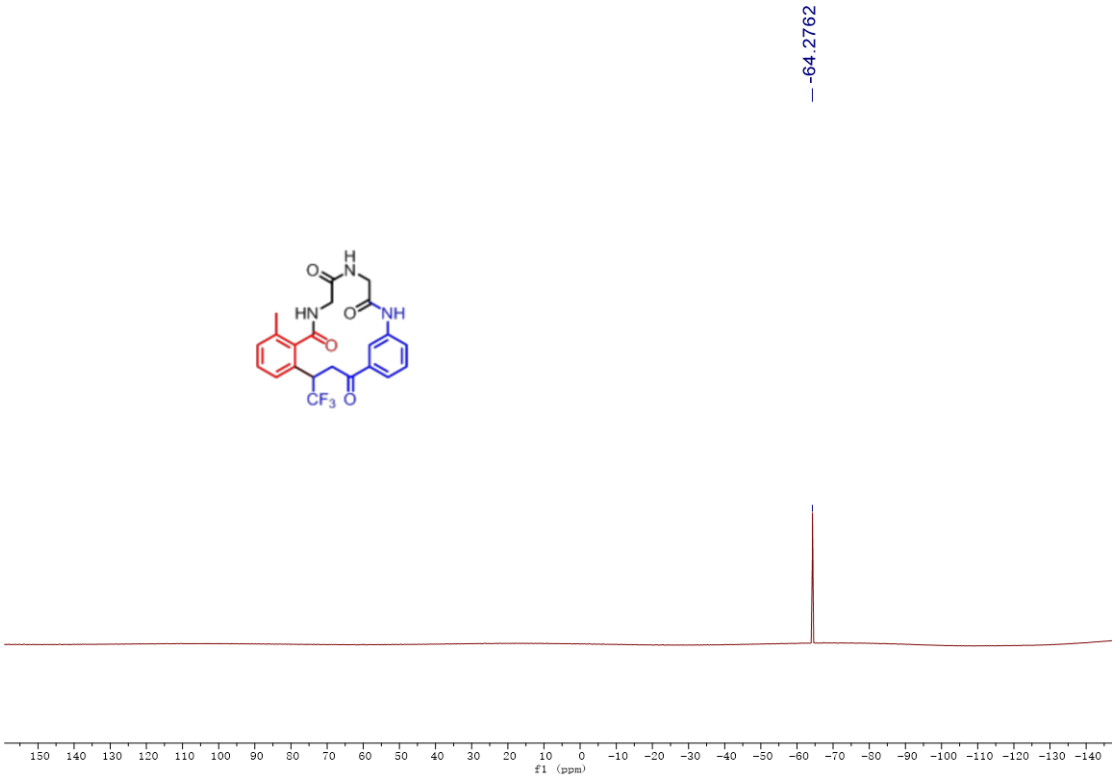

9.8469
8.5432
8.2150
7.9698
7.4925
7.4798
7.4647
7.4261
7.4113
7.4060
7.3916
7.3759
7.2991
7.2862
7.2828
3.9822
3.4849
3.4748
3.4574
3.4472
3.3533
2.5177
2.5080
2.2833
2.2396
2.2323
2.2213
2.2133
2.2052
2.1944
1.6583
1.4727
1.4351
1.3975
1.3821
1.02
0.96
1.00
1.00
2.01
2.15
1.03
1.00
1.03
0.81
1.96
1.08
3.01
1.11
1.01
2.04
5.20
NH
O
NH
O
CF3
O
f1 (ppm)


197.4753
172.2491
168.3089
139.7725
139.5981
135.8026
134.7675
131.1915
130.6193
130.1555
130.0018
129.3088
127.9234
125.6863
125.4008
124.4083
123.4585
122.6469
120.9059
44.5177
44.3032
44.0871
43.8722
41.5114
37.5168
27.8212
25.6599
24.4388
24.3566
19.6105
NH
O
NH
O
CF3
O
f1 (ppm)


-66.3955
NH
O
NH
O
CF3
O
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)


9.3359
9.2760
8.6172
8.3258
8.3108
8.0414
7.6082
7.5930
7.5504
7.5347
7.5191
7.4845
7.4695
7.4508
7.3599
7.3459
4.2273
4.1105
4.0811
3.8695
3.8578
3.8355
3.8238
3.7867
3.7520
3.7185
3.7065
3.6785
3.6489
2.9058
2.8789
2.8520
2.3608
H
N
O
HN
O
NH
O
CF3
O
1.02
1.02
1.00
0.97
1.00
2.03
2.00
1.01
1.00
1.02
2.00
2.03
1.02
3.09
f1 (ppm)


196.0433
171.0920
170.6446
169.1204
139.1744
136.7354
136.5306
135.1445
133.1598
131.2222
130.5085
130.1947
128.1841
125.9479
125.0253
123.9968
122.3458
121.8164
46.3207
46.1048
45.1829
45.0353
44.3247
20.8572
HN
O
NH
CF3
f1 (ppm)


-64.2762
HN
O
NH
CF3
f1 (ppm)

References

1) G. Blay, I. Fernández, M. C. Muñoz, J. R. Pedro, C. Vila, *Chem. Eur. J.*, 2010, **16**, 9117-9122.

2) Q. Jiang, T. Guo, K. Wu, Z. Yu, *Chem. Commun.*, 2016, **52**, 2913-2915.

3) D. G. Stark, L. C. Morrill, P.-P. Yeh, A. M. Z. Slawin, T. J. C. O'Riordan, A. D. Smith, *Angew. Chem. Int. Ed.*, 2013, **52**, 11642-11646.