(*69 pages*)

Supporting Information For

Regioselective Synthesis of 2,3,4-Trisubstituted Pyrroles via Pd(II)-Catalyzed Three-Component Cascade Reactions of Amines, Alkyne Esters and Alkenes

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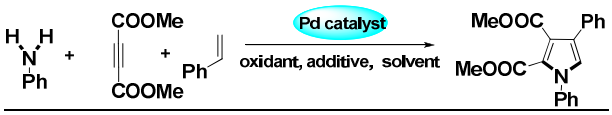
General Methods and Materials

$Pd(OAc)_2$, $K_2S_2O_8$ were purchased from Energy Chemical and used without further purification. Other chemicals were purchased from commercial suppliers, further dried and purified if necessary. The water used was re-distillated and ion-free. ^1H and ^{13}C NMR spectra were achieved on a Bruker AVANCE 400 MHz spectrometer (^1H 400 MHz; ^{13}C 100 MHz) in $CDCl_3$ or DMSO-d_6. Abbreviations for data quoted are s-singlet; brs-broad singlet; d-doublet; t-triplet; dd-doublet of doublets; m-multiplet. High-resolution mass spectra were measured on a Waters Micromass GCT facility. Thin-layer chromatographies were done on pre-coated silica gel 60F254 plates (Merck). Silica gel 60H (200-300 mesh) manufactured by Qingdao Haiyang Chemical Group Co. (China) was used for general chromatography.

Optimization of reaction conditions

Table S1[a]

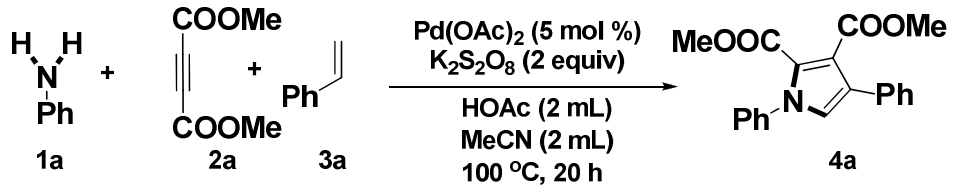


entry	catalyst	oxidant	additive	solvent	yield[b] (%)
1	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	Toluene	25
2	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	DMF	0
3	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	DMSO	0
4	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	MeOH	0
5	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	THF	<5
5	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	Dioxane	0
6	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	MeCN	73
7	$Pd(OAc)_2$	$K_2S_2O_8$	TsOH	MeCN	0
8	$Pd(OAc)_2$	$K_2S_2O_8$	TFA	MeCN	15
9	$Pd(OAc)_2$	$K_2S_2O_8$	TfOH	MeCN	<5
10	$Pd(OAc)_2$	BQ	HOAc	MeCN	0
11	$Pd(OAc)_2$	$Cu(OAc)_2$	HOAc	MeCN	0
12	$Pd(OAc)_2$	Ag_2CO_3	HOAc	MeCN	0
13	$Pd(TFA)_2$	$K_2S_2O_8$	HOAc	MeCN	0
14	$Pd(PPh_3)_2Cl_2$	$K_2S_2O_8$	HOAc	MeCN	0
15[c]	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	MeCN	89
16	---	$K_2S_2O_8$	HOAc	MeCN	0
17	$Pd(OAc)_2$	---	HOAc	MeCN	0
18	$Pd(OAc)_2$	$K_2S_2O_8$	---	MeCN	0
19[d]	$Pd(OAc)_2$	$K_2S_2O_8$	HOAc	MeCN	83

[a]Unless otherwise noted, reactions were carried out with **1a** (1.0 mmol), **2a** (1.0 mmol), **3a** (2.0 mmol), catalyst (5 mol %), oxidant (2.0 mmol), additive (2.0 mL) in 2.0 mL of solvent at 80 °C for 20 h. [b]All yields were isolated yields. [c]Reaction was carried out at at 100 °C. [d]10 mmol scale.

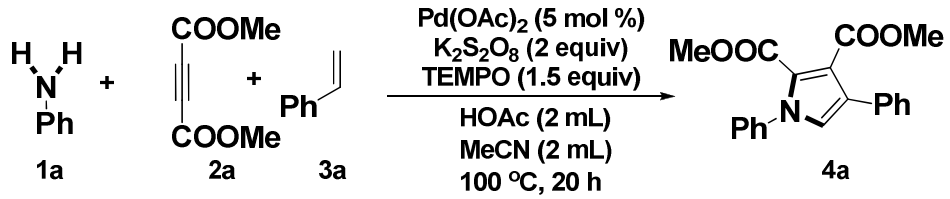
At the outset of this study, we chose $Pd(OAc)_2$ as the active Pd(II) catalyst and employed commercially available aniline (**1a**), dimethyl but-2-ynedioate (**2a**) and styrene (**3a**) as the model substrates for the reaction development of the three-component cascade reaction (Table 1). To our delight, the anticipated pyrrole **4a** was generated in 25% yield with excellent regio-/site-selectivity under the initial conditions (Table 1, entry 1), and its structure was confirmed by ^{1}H and ^{13}C NMR analysis and mass spectrometry. A survey of solvents revealed that MeCN was optimal (entries 1–6), affording pyrrole **3a** in 73% yield. The brief screening indicated HOAc and $K_2S_2O_8$ to be the best choice of additives and oxidants, respectively (entries 6–12). Changing the catalyst $Pd(OAc)_2$ to other two well known catalysts $Pd(TFA)_2$ and $Pd(PPh_3)_2Cl_2$ obviously inhibited the process (entries 13–14). Gratifyingly, an improved yield of product **4a** was obtained when the temperature was increased to 100 ^{o}C (entry 15). The control experiments indicated that no desired product was detected in the absence of the catalyst, the additive or the oxidant (entries 16–18). In summary, the optimal conditions for the three-component cascade reaction were identified as the following: 5 mol % $Pd(OAc)_2$, 2.0 equiv of $K_2S_2O_8$, and 2.0 mL of HOAc in MeCN at 100 ^{o}C for 20 h under an atmosphere of air. Finally, we were pleased to find that the reaction could be smoothly performed on a 10 mmol scale under the optimized conditions without a significant decrease in the product yield (83%, entry 19), which illustrated the remarkable robustness of this Pd(II)-catalyzed system.

General catalytic procedure for the synthesis of pyrroles



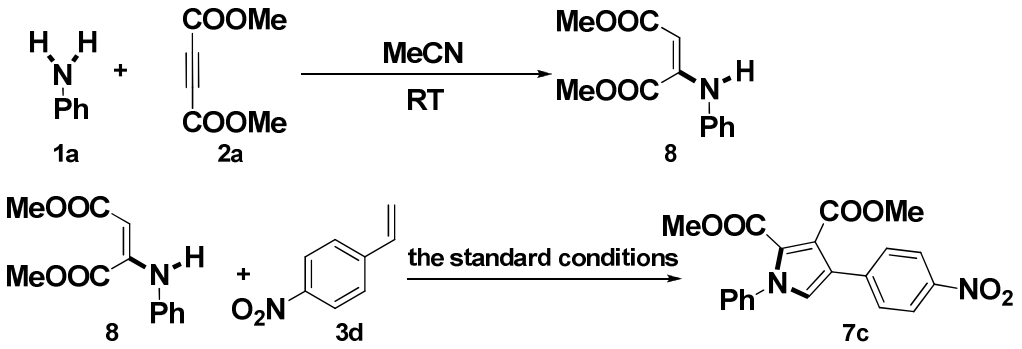
A reaction kettle (30 mL) was charged with aniline (**1a**, 1.0 mmol), and dimethyl acetylenedicarboxylate (**2a**, 1.0 mmol). The mixture was stirred at room temperature for 10 minutes, then styrene (**3a**, 2.0 mmol, 2.0 eq), potassium persulfate (2.0 eq, 0.54g), palladium acetate (11.2 mg), acetonitrile (2 mL), and acetic acid (2 mL) were added into the mixture, which was stirred at 100 ^{o}C for 20 hours. The obtained mixture was quenched by sat. aq. $NaHCO_3$, and diluted with 20 mL of dichloromethane and washed with 10 mL of H_2O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na_2SO_4. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 10 : 1) to afford pyrrole product **4a** in 89% yield. All other products are synthesized in a similar manner, with the yields listed in the main text calculated from the isolated, pure products.

The experimental procedure for radical capture experiment with TEMPO



A reaction kettle (30 mL) was charged with aniline (**1a**, 1.0 mmol), and dimethyl acetylenedicarboxylate (**2a**, 1.0 mmol). The mixture was stirred at room temperature for 10 minutes, then styrene (**3a**, 2.0 mmol, 2.0 eq), potassium persulfate (2.0 eq, 0.54g), palladium acetate (11.2 mg), acetonitrile (2 mL), TEMPO (234 mg, 1.5 mmol), and acetic acid (2 mL) was added in the mixture. The obtained mixture was stirred at 100 ^{o}C for 20 hours, and **4a** was not detected.

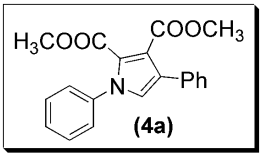
The experimental investigation for the Reaction Mechanism



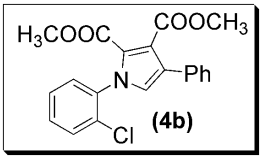
A reaction kettle (30 mL) was charged with aniline (**1a**, 1.0 mmol), and dimethyl acetylenedicarboxylate (**2a**, 1.0 mmol) in acetonitrile (2 mL). The mixture was stirred at room temperature for 10 minutes, then evaporated in vacuo. The obtained residue was purified by flash column chromatography using a mixture of PE and EA as eluent to afford the enamine **8** in 76% yield: **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 9.66 (s, 1H), 7.26 - 7.30 (m, 2H), 7.07 - 7.11 (t, 1H), 6.90 (d, J = 8.0 Hz, 2H), 3.74 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 169.9, 164.9, 148.0, 140.3, 129.2, 124.2, 120.7, 93.6, 52.7, 51.2; **HRMS (ESI-TOF)** m/z calcd for $C_{12}H_{14}NO_4$ $[M + H]^+$ 236.0917, found 236.0920.

A reaction kettle (30 mL) was charged with the enamine (**8**, 1.0 mmol), 4-nitrostyrene (**3d**, 2.0 mmol, 2.0 eq), potassium persulfate (2.0 eq, 0.54g), palladium acetate (11.2 mg), acetonitrile (2 mL), and acetic acid (2 mL) in the mixture. The mixture was stirred at 100 ^{o}C for 20 hours. The obtained mixture was quenched by sat. aq. $NaHCO_3$, and diluted with 20 mL of dichloromethane and washed with 10 mL of H_2O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na_2SO_4. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 10 : 1) to afford pyrrole product **7c** in 65% yield.

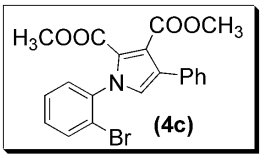
Characterization data for products



1,4-Diphenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4a): Obtained as a colorless oil (298.2 mg, 89% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.44 - 7.46 (m, 5H), 7.33 - 7.38 (m, 4H), 7.26 - 7.30 (t, 1H), 3.85 (s, 3H), 3.70 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.4, 139.5, 133.1, 129.0, 128.63, 128.56, 127.7, 127.2, 126.14, 125.97, 124.9, 123.2, 121.8, 52.4, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{18}NO_4$ $[M + H]^+$ 336.1230, found 336.1249.

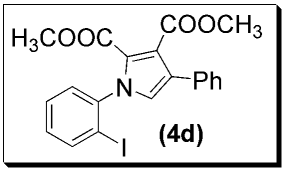


1-(2-Chloro-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4b): Obtained as a yellow oil (276.8 mg, 75% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.51 - 7.53 (m, 1H), 7.44 - 7.46 (m, 2H), 7.35 - 7.43 (m, 5H), 7.27 - 7.31 (m, 1H), 6.95 (s, 1H), 3.87 (s, 3H), 3.70 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.0, 159.8, 137.5, 133.0, 132.1, 130.1, 130.0, 128.9, 128.7, 127.5, 127.4, 127.2, 125.8, 124.9, 122.8, 122.3, 52.6, 51.9; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}NClO_4$ $[M + H]^+$ 370.0841, found 370.0849.

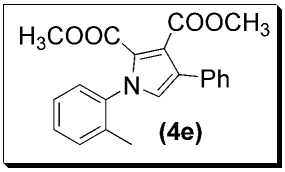


1-(2-Bromo-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4c): Obtained as a yellow oil (289.1 mg, 70% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.68 - 7.71 (m, 1H), 7.43 - 7.47 (m, 2H), 7.41 - 7.43 (m, 1H), 7.27 - 7.39 (m, 5H), 6.95 (s, 1H), 3.87 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.0, 159.8, 139.2, 133.1, 133.0, 130.4, 129.0, 128.7, 128.0, 127.5,

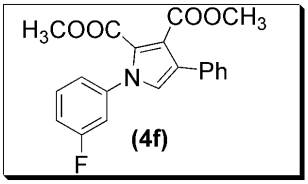
127.2, 125.7, 124.9, 122.7, 122.2, 122.1, 52.6, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}NBrO_4$ $[M + H]^+$ 414.0335, found 414.0344.



1-(2-Iodo-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4d): Obtained as a yellow oil (308.9 mg, 67% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.92 - 7.94 (m, 1H), 7.44 - 7.48 (m, 3H), 7.36 - 7.40 (m, 3H), 7.28 - 7.32 (m, 1H), 6.93 (s, 1H), 3.88 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.0, 159.7, 142.8, 139.3, 133.0, 130.4, 128.9, 128.7, 128.3, 127.5, 127.2, 125.6, 125.0, 122.4, 122.3, 97.5, 52.6, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}NIO_4$ $[M + H]^+$ 462.0197, found 462.0207.

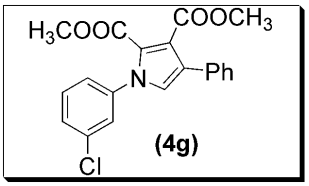


4-Phenyl-1-o-tolyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4e): Obtained as a pale yellow oil (289.6 mg, 83% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.46 (m, 2H), 7.35 - 7.39 (m, 3H), 7.26 - 7.32 (m, 3H), 7.21 - 7.24 (m, 1H), 6.92 (s, 1H), 3.87 (s, 3H), 3.67 (s, 3H), 2.11 (s, 3H),; **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.1, 150.0, 139.0, 135.4, 133.2, 130.6, 129.1, 128.7, 127.5, 127.3, 127.2, 126.5, 125.8, 124.7, 123.0, 121.6, 52.5, 51.9, 17.4; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_4$ $[M + H]^+$ 350.1387, found 350.1386.

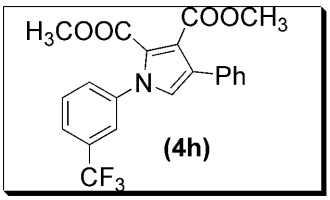


1-(3-Fluoro-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4f): Obtained as a pale orange viscous oil (268.3 mg, 76% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.92 - 7.94 (m, 1H), 7.44 - 7.48 (m, 3H), 7.36 - 7.40 (m, 3H), 7.28 - 7.32 (m, 1H), 6.93 (s, 1H), 3.88 (s, 3H), 3.69 (s, 3H); **^{13}C**

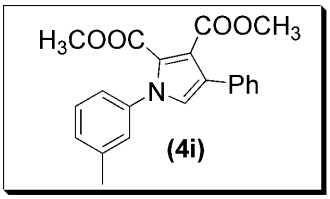
NMR (100 MHz, $CDCl_3$) δ ppm: 166.6, 150.2, 140.6, 132.9, 130.2, 130.1, 128.7, 127.7, 127.3, 125.8, 125.2, 123.0, 122.3, 122.0, 115.6, 114.0, 52.5, 52.1; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}FNO_4$ $[M + H]^+$ 354.1136, found 354.1173.



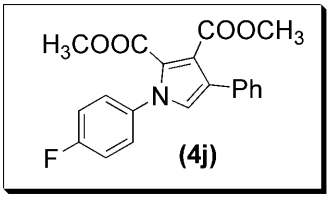
1-(3-Chloro-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4g): Obtained as a orange viscous oil (284.1 mg, 77% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.41 - 7.45 (m, 4H), 7.36 - 7.40 (m, 4H), 7.28 - 7.33 (m, 1H), 7.00 (s, 1H), 3.86 (s, 3H), 3.74 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.6, 160.1, 140.1, 134.5, 132.8, 129.9, 128.8, 128.7, 127.6, 127.3, 126.5, 125.9, 125.2, 124.6, 122.9, 122.4, 52.5, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}ClNO_4$ $[M + H]^+$ 370.0841, found 370.0461.



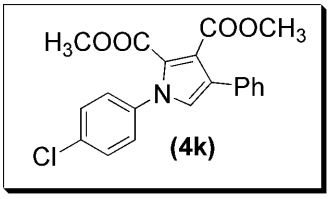
4-Phenyl-1-(3-trifluoromethyl-phenyl)-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4h): Obtained as a yellow viscous oil (290.2 mg, 72% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.72 (d, J = 7.6Hz, 1H), 7.56 - 7.64 (m, 3H), 7.44 - 7.46 (m, 2H), 7.37 - 7.40 (m, 2H), 7.30 - 7.34 (m, 1H), 7.03 (s, 1H), 3.88 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.6, 160.1, 139.9, 132.7, 131.7, 131.4, 129.8, 129.6, 128.7, 127.6, 127.4, 125.9, 125.4, 123.4, 122.9, 122.8, 52.5, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{17}F_3NO_4$ $[M + H]^+$ 404.1104, found 404.0739.



4-Phenyl-1-m-tolyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4i): Obtained as a pale yellow viscous oil (286.2 mg, 82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.46 (m, 2H), 7.30 - 7.39 (m, 4H), 7.14 - 7.19 (m, 3H), 6.99 (s, 1H), 3.84 (s, 3H), 3.72 (s, 3H), 2.41 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.8, 160.5, 139.4, 139.0, 133.2, 129.3, 128.71, 128.69, 128.59, 128.17, 127.7, 127.1, 126.6, 125.9, 123.2, 110.5, 52.4, 52.0, 21.3; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_4$ $[M + H]^+$ 350.1387, found 350.1376.

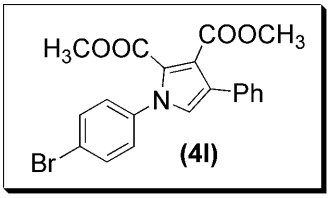


1-(4-Fluoro-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4j): Obtained as a yellow viscous oil (275.3 mg, 78% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.42 - 7.45 (m, 2H), 7.30 - 7.39 (m, 5H), 7.11 - 7.17 (m, 2H), 6.98 (s, 1H), 3.85 (s, 3H), 3.72 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.2, 135.5, 133.0, 128.7, 128.1, 128.0, 127.6, 127.3, 126.2, 124.9, 123.0, 122.2, 115.8, 52.5, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}FNO_4$ $[M + H]^+$ 354.1136, found 354.1178.

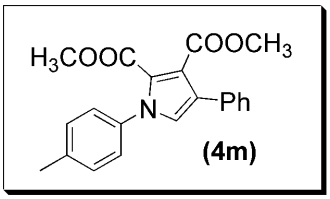


1-(4-Chloro-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4k): Obtained as a yellow viscous oil (287.8 mg, 78% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.42 - 7.45 (m, 4H), 7.36 - 7.41 (m, 2H), 7.27 - 7.32 (m, 3H), 6.98 (s, 1H), 3.86 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.2, 137.9, 134.5, 132.9, 129.2, 128.7, 127.60, 127.55, 127.3,

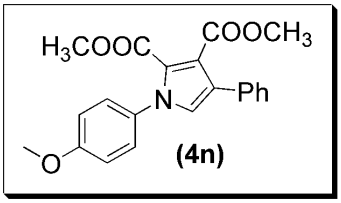
126.0, 124.4, 122.4, 110.0, 52.5, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}ClNO_4$ $[M + H]^+$ 370.0841, found 370.0838.



1-(4-Bromo-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4l): Obtained as a yellow viscous oil (313.9 mg, 76% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.57 - 7.61 (m, 2H), 7.36 - 7.44 (m, 4H), 7.29 - 7.33 (m, 1H), 7.22 - 7.26 (m, 2H), 6.98 (s, 1H), 3.86 (s, 3H), 3.72 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.6, 160.2, 138.4, 132.8, 132.1, 128.7, 127.9, 127.6, 127.3, 125.9, 125.1, 124.8, 122.5, 122.4, 52.5, 52.1; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}BrNO_4$ $[M + H]^+$ 414.0335, found 414.0313.

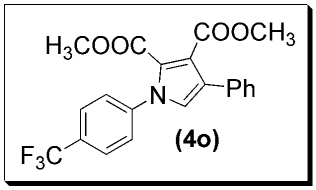


4-Phenyl-1-p-tolyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4m): Obtained as a yellow viscous oil (328.1 mg, 94% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.45 (m, 2H), 7.35 - 7.39 (m, 2H), 7.29 - 7.31 (m, 1H), 7.22 - 7.27 (m, 4H), 6.98 (s, 1H), 3.84 (s, 3H), 3.72 (s, 3H), 2.41 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.8, 160.5, 138.5, 136.9, 133.2, 129.6, 128.6, 127.7, 127.1, 126.0, 125.9, 124.7, 123.3, 121.6, 52.4, 51.9, 21.2; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_4$ $[M + H]^+$ 350.1387, found 350.1419.

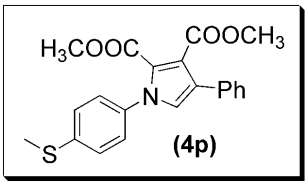


1-(4-Methoxy-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4n): Obtained as a yellow viscous oil (332.2 mg, 91%

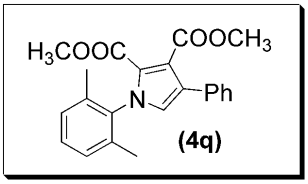
yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.45 (m, 2H), 7.35 - 7.39 (m, 2H), 7.26 - 7.31 (m, 3H), 6.95 - 6.97 (m, 2H), 6.94 (s, 1H), 3.85 (s, 6H), 3.72 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.8, 160.4, 159.5, 133.2, 132.3, 128.6, 127.7, 127.3, 127.1, 126.3, 124.6, 123.3, 121.5, 114.0, 55.5, 52.4, 51.9; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_5$ $[M + H]^+$ 366.1336, found 366.1343.



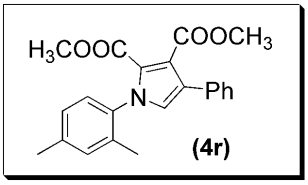
4-Phenyl-1-(4-trifluoromethyl-phenyl)-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4o): Obtained as a yellow viscous oil (298.2 mg, 74% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.74 (d, J = 8.4 Hz, 2H), 7.43 - 7.49 (m, 4H), 7.36 - 7.40 (t, 2H), 7.29 – 7.33 (m, 1H), 7.02 (s, 1H), 3.86 (s, 3H), 3.74 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.5, 160.1, 142.3, 132.7, 130.6, 128.7, 127.6, 127.4, 126.7, 126.2, 125.8, 125.4, 122.9, 117.0, 55.6, 52.1; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{17}FNO_4$ $[M + H]^+$ 404.1104, found 404.1103.



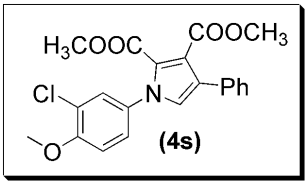
1-(4-Methylsulfanyl-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4p): Obtained as a yellow viscous oil (346.7 mg, 91% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.45 (m, 2H), 7.36 - 7.40 (m, 2H), 7.28 - 7.32 (m, 5H), 6.98 (s, 1H), 3.85 (s, 3H), 3.73 (s, 3H), 2.53 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.4, 139.6, 136.3, 133.1, 128.6, 127.7, 127.2, 126.5, 126.4, 126.0, 124.7, 123.0, 121.9, 52.4, 52.0, 15.6; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}SNO_4$ $[M + H]^+$ 382.1108, found 382.1153.



1-(2,6-Dimethyl-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4q): Obtained as a yellow viscous oil (265.1 mg, 73% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.46 (d, J = 7.6 Hz, 2H), 7.36 - 7.39 (m, 2H), 7.23 - 7.31 (m, 2H), 7.14 (d, J = 7.6 Hz, 2H), 6.85 (s, 1H), 3.86 (s, 3H), 3.67 (s, 3H), 2.05 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.4, 138.3, 135.6, 133.3, 128.8, 128.7, 128.0, 127.5, 127.1, 125.2, 124.7, 122.6, 121.3, 52.4, 51.9, 17.5; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{22}NO_4$ $[M + H]^+$ 364.1543, found 364.1547.

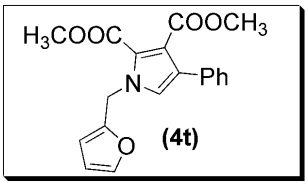


1-(2,4-Dimethyl-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4r): Obtained as a yellow viscous oil (297.7 mg, 82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.44 - 7.46 (t, 2H), 7.36 - 7.39 (m, 2H), 7.27 - 7.33 (m, 1H), 7.01 - 7.12 (m, 3H), 6.91 (s, 1H), 3.87 (s, 3H), 3.69 (s, 3H), 2.38 (s, 3H), 2.07 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.1, 160.0, 138.9, 136.4, 135.0, 133.3, 131.2, 128.7, 127.5, 127.1, 127.0, 125.9, 124.5, 123.0.6, 121.4, 52.5, 51.8, 21.2, 17.3; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{22}NO_4$ $[M + H]^+$ 364.1543, found 364.1589.

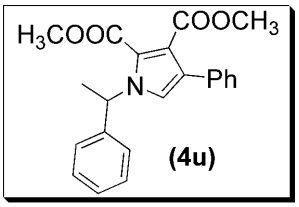


1-(3-Chloro-4-methoxy-phenyl)-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4s): Obtained as a yellow viscous oil (327.2 mg, 82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.34 - 7.43 (m, 5H), 7.29 (d, J = 7.2 Hz, 1H), 7.23 (d, J = 8.8 Hz, 1H), 6.96 (s, 1H), 3.93 (s, 3H), 3.84 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.2, 132.9, 132.5, 128.6, 128.5, 128.2, 127.7, 127.6, 127.2, 126.2, 125.8, 124.8, 122.4, 122.0, 111.5, 56.3, 52.4, 52.0; **HRMS**

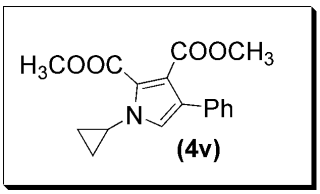
(ESI-TOF) m/z calcd for $C_{21}H_{19}ClNO_5$ $[M + H]^+$ 400.0946, found 400.0962.



1-Furan-2-ylmethyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4t): Obtained as a yellow viscous oil (294.9 mg, 87% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.31 - 7.38 (m, 5H), 7.23 - 7.27 (m, 1H), 6.99 (s, 1H), 6.37 (d, J = 3.2 Hz), 6.31 (q, 1H), 5.50 (s, 2H), 3.84 (s, 3H), 3.81 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.3, 160.7, 149.7, 142.9, 132.3, 128.6, 127.3, 127.0, 125.5, 123.9 122.4, 120.5, 110.6, 109.4, 52.4, 51.9, 45.0; **HRMS (ESI-TOF)** m/z calcd for $C_{19}H_{18}NO_5$ $[M + H]^+$ 340.1180, found 340.1183.

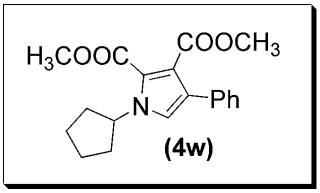


4-Phenyl-1-(1-phenyl-ethyl)-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4u): Obtained as a pale yellow viscous oil (304.9 mg, 84% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.31 - 7.38 (m, 6H), 7.21 - 7.28 (m, 4H), 7.02 (s, 1H), 6.48 (q, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 1.83 (d, J = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.4, 160.9, 141.7, 133.6, 128.8, 128.6, 127.8, 127.5, 127.0, 126.5, 124.1, 122.4, 122.0, 121.5, 56.0, 52.4, 51.9, 22.0; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{22}NO_4$ $[M + H]^+$ 364.1543, found 364.1552.

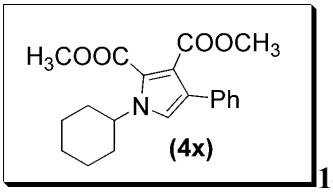


1-Cyclopropyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4v): Obtained as a orange viscous oil (203.3 mg, 68% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.31 - 7.37 (m, 4H), 7.24 - 7.27 (m, 1H), 6.93 (s, 1H), 3.87 (s, 3H), 3.81 (s, 3H), 3.68 - 3.74 (m, *1*H), 1.04 - 1.09 (m, *2*H), 0.96 - 1.02

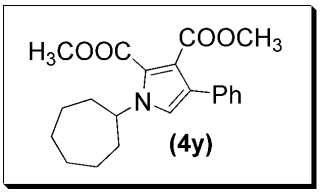
(m, *2*H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.9, 160.6, 133.5, 128.5, 127.5, 126.9, 124.1, 123.5, 123.3, 121.6, 52.3, 51.8, 31.5, 7.5; **HRMS (ESI-TOF)** m/z calcd for $C_{17}H_{18}NO_4$ $[M + H]^+$ 300.1230, found 300.1236.



1-Cyclopentyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4w): Obtained as a orange viscous oil (271.4 mg, 83% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.32 - 7.40 (m, 4H), 7.23 - 7.27 (m, 1H), 7.04 (s, 1H), 5.36 - 5.41 (m, *1*H), 3.83 (s, 3H), 3.80 (s, 3H), 2.18 - 2.22 (m, *2*H), 1.72 - 1.84 (m, *6*H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.3, 161.0, 133.7, 128.5, 127.5, 126.8, 123.9, 121.9, 121.4, 121.3, 58.8, 52.2, 51.8, 33.8, 24.0; **HRMS (ESI-TOF)** m/z calcd for $C_{19}H_{22}NO_4$ $[M + H]^+$ 328.1543, found 328.1528.

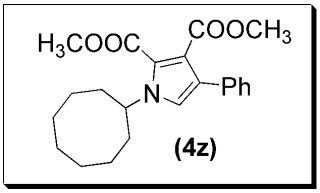


1-Cyclohexyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4x): Obtained as a orange viscous oil (296.7 mg, 87% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.32 - 7.40 (m, 4H), 7.24 - 7.27 (m, 1H), 7.08 (s, 1H), 4.87 - 4.92 (m, *1*H), 3.84 (s, 3H), 3.81 (s, 3H), 2.14 (d, J = 11.2 Hz, 2H), 1.90 (d, J = 12.8 Hz, 2H), 1.43 - 1.64 (m, *4*H), 1.17 - 1.26 (m, *2*H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.5, 160.9, 133.7, 128.6, 127.4, 126.8, 123.8, 121.40, 121.38, 120.9, 57.0, 52.3, 51.8, 34.7, 25.8, 25.5; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{24}NO_4$ $[M + H]^+$ 342.1700, found 342.1700.

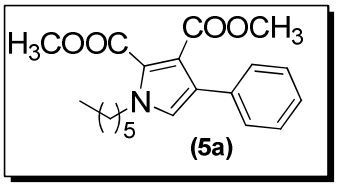


1-Cycloheptyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4y): Obtained as a orange viscous oil (269.8 mg, 76% yield); **^{1}H**

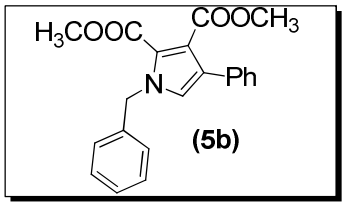
NMR (400 MHz, DMSO-d_6) δ ppm: 7.60 (s, 1H), 7.34 - 7.41 (m, 4H), 7.23 - 7.27 (m, 1H), 4.87 - 4.92 (m, *1*H), 3.77 (s, 3H), 3.75 (s, 3H), 1.90 - 2.02 (m, 4H), 1.73 - 1.78 (m, *2*H), 1.45 - 1.66 (m, *6*H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ ppm: 167.2, 160.8, 133.8, 129.0, 127.2, 127.0, 123.3, 123.0, 120.9, 120.7, 59.1, 52.5, 52.3, 36.2, 27.3, 24.6; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{26}NO_4$ $[M + H]^+$ 356.1856, found 356.1834.



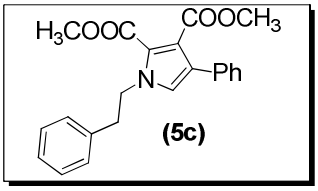
1-Cyclooctyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (4z): Obtained as a orange viscous oil (262.0 mg, 71% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.32 - 7.40 (m, 4H), 7.24 - 7.27 (m, 1H), 7.05 (s, 1H), 5.26 - 5.33 (m, *1*H), 3.84 (s, 3H), 3.81 (s, 3H), 1.91 - 2.07 (m, *4*H), 1.52 - 1.79 (m, *10*H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.6, 161.0, 133.8, 128.6, 127.4, 126.8, 124.0, 123.4, 122.0, 121.1, 120.6, 57.3, 52.3, 51.2, 34.8, 26.6, 26.2, 24.6; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{28}NO_4$ $[M + H]^+$ 370.2013, found 370.2012.



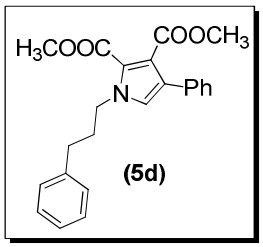
1-Hexyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (5a): Obtained as a yellow viscous oil (266.5 mg, 81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.32 - 7.39 (m, 4H), 7.25 - 7.27 (t, 1H), 6.91 (s, 1H), 4.25 - 4.29 (t, 2H), 3.83 (s, 3H), 3.81 (s, 3H), 1.76 - 1.80 (m, 2H), 1.24 - 1.36 (m, 6H), 0.87 - 0.90 (t, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.4, 160.7, 133.5, 128.6, 127.3, 126.8, 125.5, 123.5, 122.0, 120.6, 52.3, 51.7, 49.7, 31.5, 31.4, 26.3, 22.5, 14.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{26}NO_4$ $[M + H]^+$ 344.1856, found 344.1858.



1-Benzyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (5b): Obtained as a colorless oil (307.1 mg, 88% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.31 - 7.39 (m, 7H), 7.23 - 7.29 (m, 3H), 7.16 - 7.18 (m, 2H), 6.94 (s, 1H), 5.52 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.3, 160.7, 137.1, 133.3, 128.9, 128.7, 127.9, 127.4, 127.2, 127.0, 125.8, 124.0, 122.3, 121.2, 52.5, 51.9; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_4$ $[M + H]^+$ 350.1387, found 350.1396.

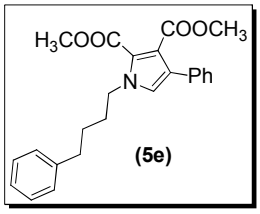


1-Phenethyl-4-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (5c): Obtained as a pale orange viscous oil (290.4 mg, 80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.23 - 7.34 (m, 8H), 7.15 - 7.17 (m, 2H), 6.69 (s, 1H), 4.47 - 4.51 (t, 2H), 3.85 (s, 3H), 3.82 (s, 3H), 3.05 - 3.09 (t, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.4, 160.7, 137.9, 133.4, 128.9, 128.7, 128.6, 127.3, 126.9, 126.8, 125.8, 123.4, 122.4, 120.3, 52.4, 51.8, 51.3, 38.2; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{22}NO_4$ $[M + H]^+$ 364.1543, found 364.1545.

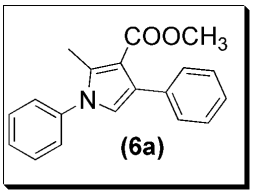


4-Phenyl-1-(3-phenyl-propyl)-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (5d): Obtained as a pale orange viscous oil (309.1 mg, 82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.33 - 7.38 (m, 4H), 7.24 - 7.31 (m, 3H), 7.16 - 7.21 (m, 3H), 6.86 (s, 1H), 4.26 - 4.29 (t, 2H), 3.81 (s, 2H), 3.80 (s, 3H), 2.63 -

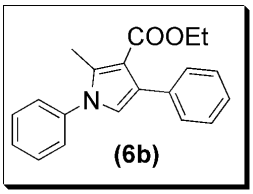
2.67 (t, 2H), 2.08 - 2.16 (q, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.5, 160.6, 140.9, 133.5, 128.7, 128.6, 128.4, 127.3, 127.0, 126.2, 125.6, 123.6, 122.3, 120.7, 52.4, 51.8, 49.1, 32.80, 32.77; **HRMS (ESI-TOF)** m/z calcd for $C_{23}H_{24}NO_4$ $[M + H]^+$ 378.1700, found 378.1714.



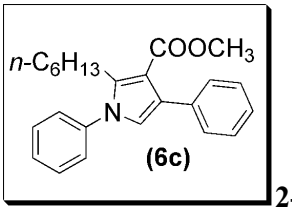
4-Phenyl-1-(4-phenyl-butyl)-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (5e): Obtained as a yellow viscous oil (316.7 mg, 81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.32 - 7.38 (m, 4H), 7.24 - 7.29 (m, 3H), 7.15 - 7.20 (m, 3H), 6.88 (s, 1H), 4.27 - 4.31 (t, 2H), 3.82 (s, 6H), 2.62 - 2.65 (t, 2H), 1.79 - 1.87 (m, 2H), 1.62 - 1.69 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 167.5, 160.6, 141.9, 133.5, 128.7, 128.5, 128.4, 127.3, 126.9, 126.0, 125.6, 123.5, 122.1, 120.6, 52.4, 51.8, 49.5, 35.5, 31.1, 28.5; **HRMS (ESI-TOF)** m/z calcd for $C_{24}H_{26}NO_4$ $[M + H]^+$ 392.1856, found 392.1914.



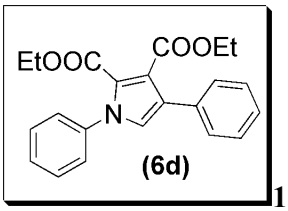
2-Methyl-1,4-diphenyl-1H-pyrrole-3-carboxylic acid methyl ester (6a): Obtained as a yellow viscous oil (224.1 mg, 77% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.47 - 7.51 (m, 2H), 7.39 - 7.43 (m, 3H), 7.32 - 7.37 (m, 4H), 7.25 - 7.29 (m, 1H), 6.72 (s, 1H), 3.70 (s, 3H), 2.46 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.3, 139.0, 136.8, 135.5, 129.4, 129.2, 128.7, 128.2, 127.7, 126.8, 126.6, 126.4, 121.0, 50.7, 12.8; **HRMS (ESI-TOF)** m/z calcd for $C_{19}H_{18}NO_2$ $[M + H]^+$ 292.1332, found 292.1367.



2-Methyl-1,4-diphenyl-1H-pyrrole-3-carboxylic acid ethyl ester (6b): Obtained as a yellow viscous oil (219.6 mg, 72% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.47 - 7.51 (m, 2H), 7.42 - 7.44 (m, 3H), 7.32 - 7.38 (m, 4H), 7.25 - 7.29 (m, 1H), 6.72 (s, 1H), 4.16 - 4.21 (m, 2H), 2.46 (s, 3H), 1.13 - 1.16 (t, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 165.9, 139.0, 136.6, 135.6, 129.4, 129.3, 129.1, 128.1, 127.6, 126.4, 126.3, 120.9, 111.8, 59.5, 14.1, 12.7; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{20}NO_2$ $[M + H]^+$ 306.1489, found 306.1530.

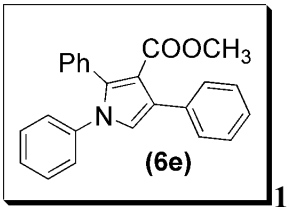


2-Hexyl-1,4-diphenyl-1H-pyrrole-3-carboxylic acid methyl ester (6c): Obtained as a yellow viscous oil (227.4 mg, 63% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.40 - 7.48 (m, 5H), 7.30 - 7.35 (m, 4H), 7.23 - 7.26 (m, 1H), 6.65 (s, 1H), 3.68 (s, 3H), 2.81 - 2.85 (t, 2H), 1.45 - 1.50 (m, 2H), 1.17 - 1.22 (m, 6H), 0.79 - 0.83 (t, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.2, 142.0, 139.1, 135.7, 129.3, 129.1, 128.4, 127.7, 126.9, 126.5, 126.3, 122.4, 110.6, 50.7, 31.3, 30.1, 29.2, 25.8, 22.6, 14.1; **HRMS (ESI-TOF)** m/z calcd for $C_{24}H_{28}NO_2$ $[M + H]^+$ 362.2115, found 362.2113.

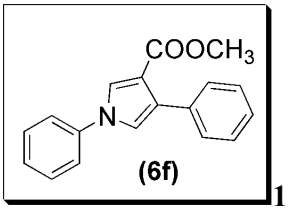


1,4-Diphenyl-1H-pyrrole-2,3-dicarboxylic acid diethyl ester (6d): Obtained as a yellow viscous oil (323.1 mg, 89% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.47 (m, 4H), 7.34 - 7.38 (m, 4H), 7.25 - 7.30 (m, 2H), 6.99 (s, 1H), 4.29 - 4.35 (m, 2H), 4.13 - 4.19 (m, 2H), 1.27 - 1.30 (t, 3H), 1.13 - 1.67 (t, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.3, 159.9, 139.6, 133.3, 128.9, 128.52,

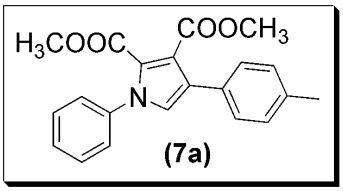
128.48, 127.8, 127.1, 126.3, 1253.7, 124.8, 122.7, 120.1, 61.4, 60.8, 14.1, 13.9; **HRMS (ESI-TOF)** m/z calcd for $C_{22}H_{22}NO_4$ $[M + H]^+$ 364.1543, found 364.1517.



1,2,4-Triphenyl-1H-pyrrole-3-carboxylic acid methyl ester (6e): Obtained as a pale orange solid (335.4 mg, 95% yield), mp 98 - 100 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.50 (d, J = 7.2Hz, 2H), 7.35 - 7.41 (m, 3H), 7.22 - 7.32 (m, 9H), 7.09 (d, J = 6.8Hz, 1H), 6.96 (s, 1H), 3.55 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 165.3, 138.6, 137.2, 134.4, 130.7, 130.4, 128.4, 128.2, 127.4, 127.3, 127.0, 126.7, 126.2, 126.0, 125.4, 121.5, 112.8, 50.3; **HRMS (ESI-TOF)** m/z calcd for $C_{24}H_{20}NO_2$ $[M + H]^+$ 354.1489, found 354.1488.

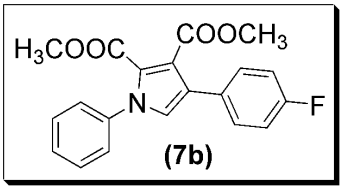


1,4-Diphenyl-1H-pyrrole-3-carboxylic acid methyl ester (6f): Obtained as a yellow viscous oil (188.4 mg, 68% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.77 (d, J = 2.8Hz, 1H), 7.54 (d, J = 7.6Hz, 2H), 7.43 - 7.49 (m, 4H), 7.28 - 7.40 (m, 4H), 7.07 (d, J = 6.4Hz, 1H), 3.76 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 164.9, 139.6, 134.3, 129.9, 129.3, 128.5, 127.9, 120, 126.9, 126.1, 120.8, 119.8, 115.1, 51.1; **HRMS (ESI-TOF)** m/z calcd for $C_{18}H_{16}NO_2$ $[M + H]^+$ 278.1176, found 278.1177.

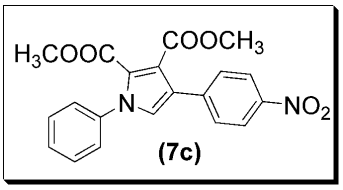


1-Phenyl-4-p-tolyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7a): Obtained as a yellow viscous oil (321.1 mg, 92% yield); **^{1}H**

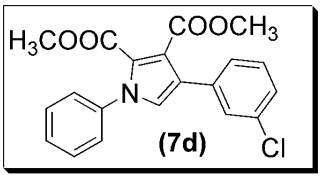
NMR (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.47 (m, 4H), 7.33 - 7.36 (m, 4H), 7.17 - 7.19 (m, 2H), 6.99 (s, 1H), 3.85 (s, 3H), 3.71 (s, 3H), 2.36 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.8, 160.4, 139.5, 136.9, 130.2, 129.4, 128.5, 127.6, 126.2, 125.8, 124.9, 122.9, 121.8, 52.4, 51.9, 21.2; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_4$ $[M + H]^+$ 350.1387, found 350.1385.



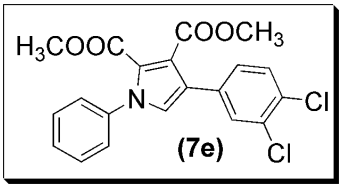
4-(4-Fluoro-phenyl)-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7b): Obtained as a yellow solid (268.3 mg, 76% yield), mp 74 - 76 ^oC; **^{1}H NMR** (400 MHz, dmso-d_6) δ ppm: 7.57 (s, 1H), 7.46 - 7.52 (m, 6H), 7.34 - 7.37 (m, 1H), 7.21 - 7.26 (m, 3H), 3.77 (s, 3H), 3.65 (s, 3H); **^{13}C NMR** (100 MHz, dmso-d_6) δ ppm: 166.1, 160.4, 139.2, 132.8, 129.8, 129.5, 129.2, 128.8, 128.7, 126.9, 126.1, 123.0, 121.0, 52.7, 52.5; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}FNO_4$ $[M + H]^+$ 354.1136, found 354.1144.



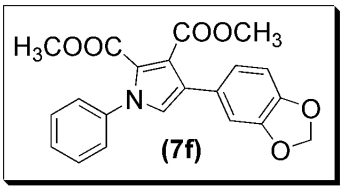
4-(4-Nitro-phenyl)-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7c): Obtained as a yellow solid (243.2 mg, 64% yield), mp 82 - 84 ^oC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.66 (d, J = 8.0Hz, 2H), 7.66 (d, J = 8.4Hz, 2H), 7.47 - 7.50 (m, 3H), 7.34 - 7.36 (m, 3H), 7.07 (s, 1H), 3.86 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.0, 160.4, 139.0, 138.0, 132.4, 129.1, 128.9, 128.3, 126.0, 125.9, 123.2, 120.8, 118.9, 110.6, 52.5, 52.2; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}N_2O_6$ $[M + H]^+$ 381.1081, found 381.1085.



4-(3-Chloro-phenyl)-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester: Obtained as a yellow viscous oil (273.1 mg, 74% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.42 - 7.45 (m, 4H), 7.36 - 7.41 (m, 2H), 7.27 - 7.32 (m, 3H), 6.98 (s, 1H), 3.86 (s, 3H), 3.73 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.7, 160.2, 137.9, 134.5, 132.9, 129.2, 128.7, 127.60, 127.55, 127.3, 126.0, 124.4, 122.4, 110.0, 52.5, 52.0; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{17}ClNO_4$ $[M + H]^+$ 370.0841, found 370.0838.

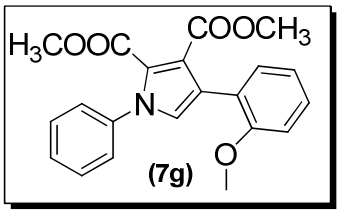


4-(3,4-Dichloro-phenyl)-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7e): Obtained as a yellow viscous oil (274.1 mg, 68% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.54 (d, J = 2.0Hz, 2H), 7.45 - 7.49 (m, *3*H), 7.43 (s, 1H), 7.33 - 7.36 (m, 2H), 7.29 - 7.31 (m, 1H), 7.00 (s, 1H), 3.86 (s, 3H), 3.72 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.0, 160.4, 139.1, 133.3, 132.5, 131.2, 130.4, 129.7, 129.1, 128.8, 127.2, 125.9, 125.7, 123.3, 122.8, 120.8, 52.5, 52.2; **HRMS (ESI-TOF)** m/z calcd for $C_{20}H_{16}Cl_2NO_4$ $[M + H]^+$ 404.0451, found 404.0497.



4-Benzo[1,3]dioxol-5-yl-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7f): Obtained as a yellow solid (337.3 mg, 89% yield), mp 58 - 60 ^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.43 - 7.49 (m, 3H), 7.38 - 7.40 (m, 2H), 7.24 - 7.28 (m, 4H), 7.03 - 7.08 (m, 1H), 6.96 (s, 1H), 3.76 (s, 3H), 3.70 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 164.2, 161.7, 139.0, 135.4, 129.3, 129.1, 128.6, 126.8, 126.1, 125.4, 125.10, 125.06, 119.6, 115.7, 114.0, 113.7, 52.4, 51.8;

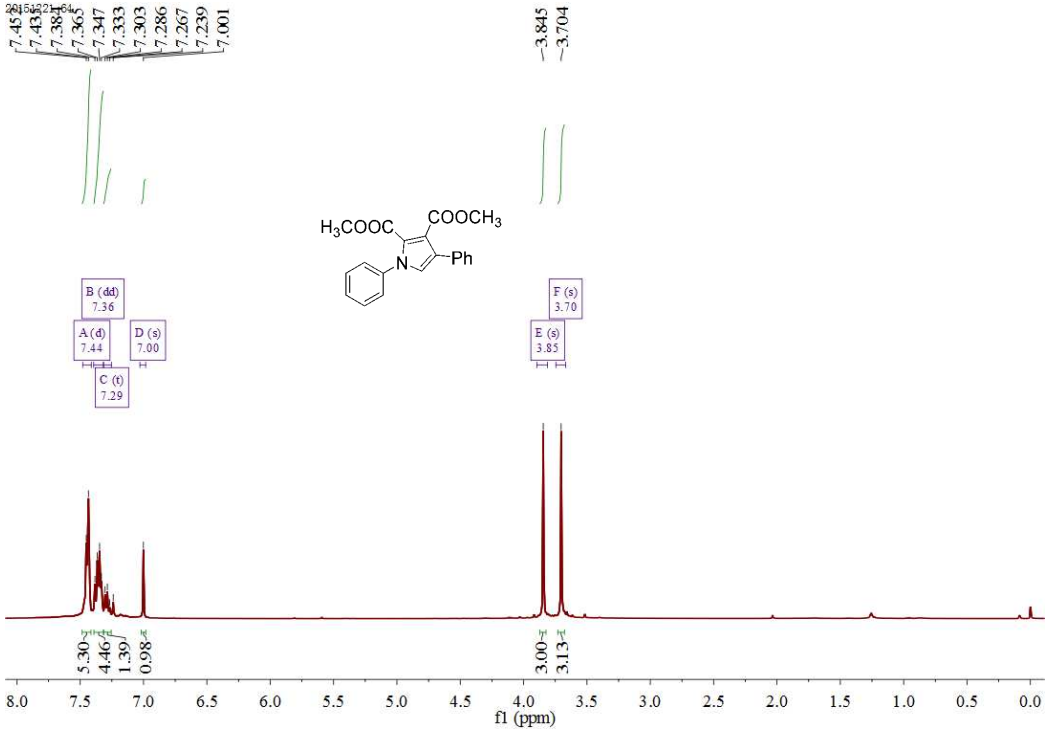
HRMS (ESI-TOF) m/z calcd for $C_{21}H_{18}NO_6$ $[M + H]^+$ 380.1129, found 380.1131. 7.

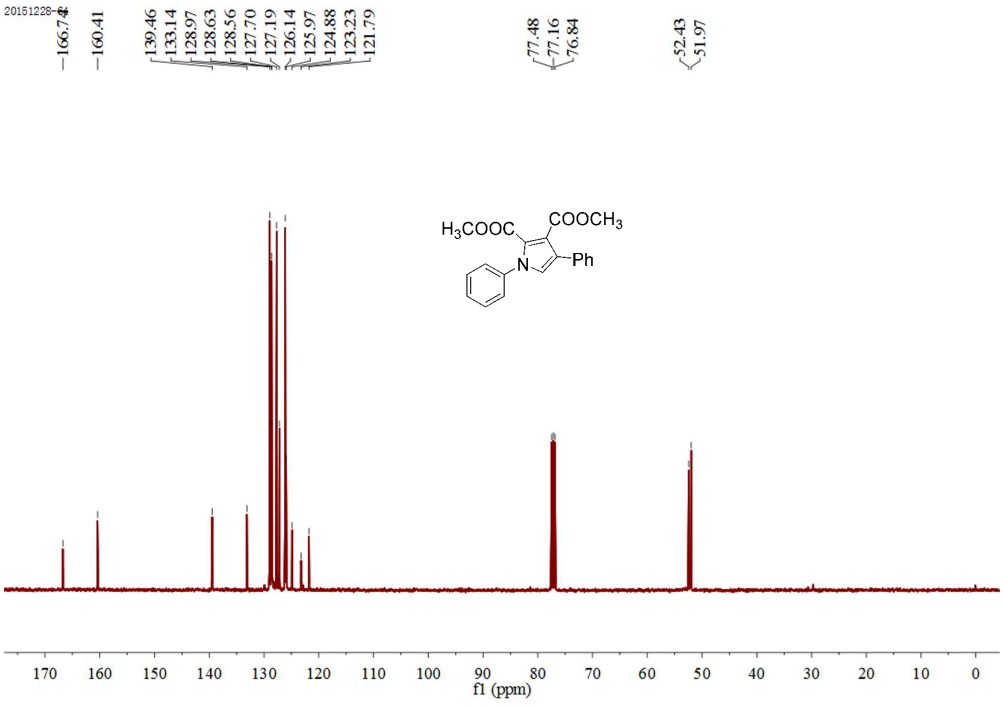


4-(2-Methoxy-phenyl)-1-phenyl-1H-pyrrole-2,3-dicarboxylic acid dimethyl ester (7g): Obtained as a yellow viscous oil (295.7 mg, 81% yield); **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.41 - 7.46 (m, 3H), 7.32 - 7.36 (m, 3H), 7.26 - 7.30 (m, 1H), 7.02 (s, 1H), 6.91 - 6.99 (m, 2H), 3.79 (s, 3H), 3.78 (s, 3H), 3.70 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 166.3, 160.7, 156.4, 139.7, 130.1, 128.9, 128.6, 128.3, 127.0, 126.0, 123.3, 122.6, 122.2, 121.3, 120.7, 110.7, 55.2, 51.93, 51.88; **HRMS (ESI-TOF)** m/z calcd for $C_{21}H_{20}NO_5$ $[M + H]^+$ 366.1336, found 366.1339.

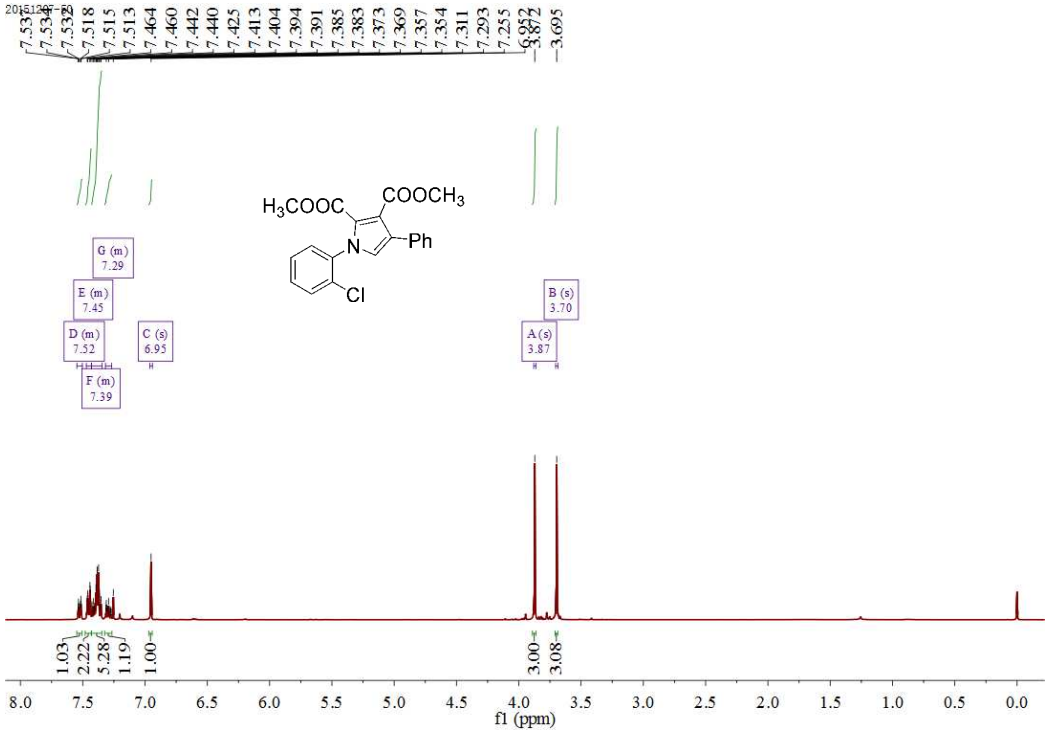
Copies of ^{1}H and ^{13}C NMR spectra of products

Product 4a





Product 4b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Cl
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D (m) 7.52
F (m) 7.39
C (s) 6.95
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1.00
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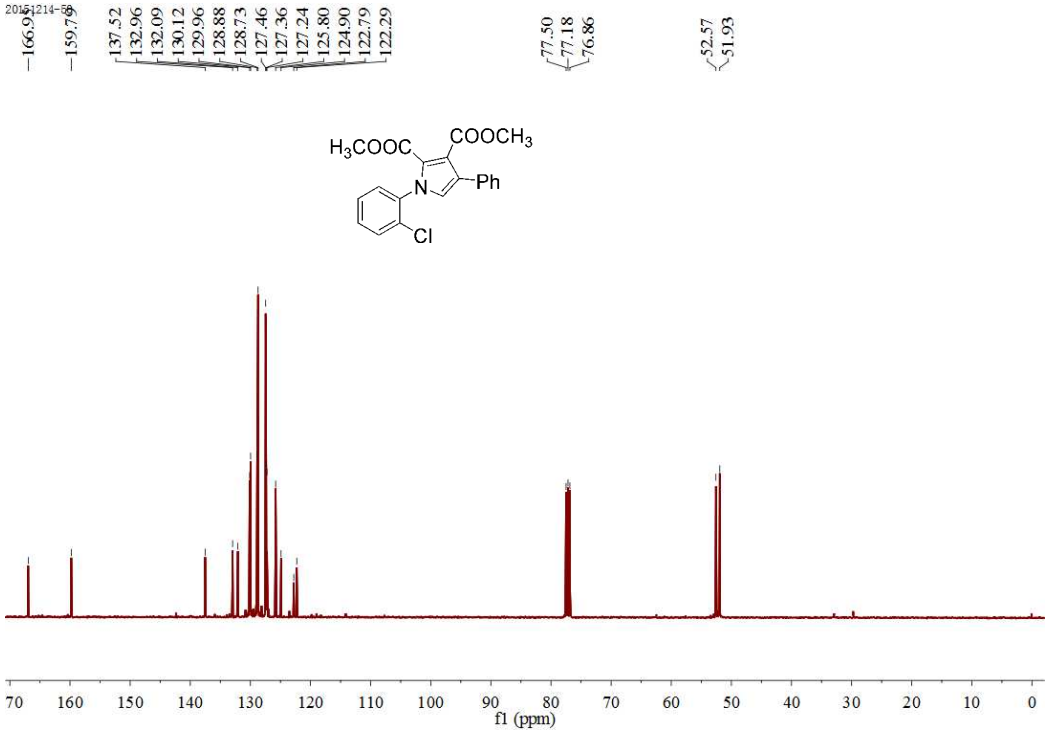
3.08
f1 (ppm)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COOCH3
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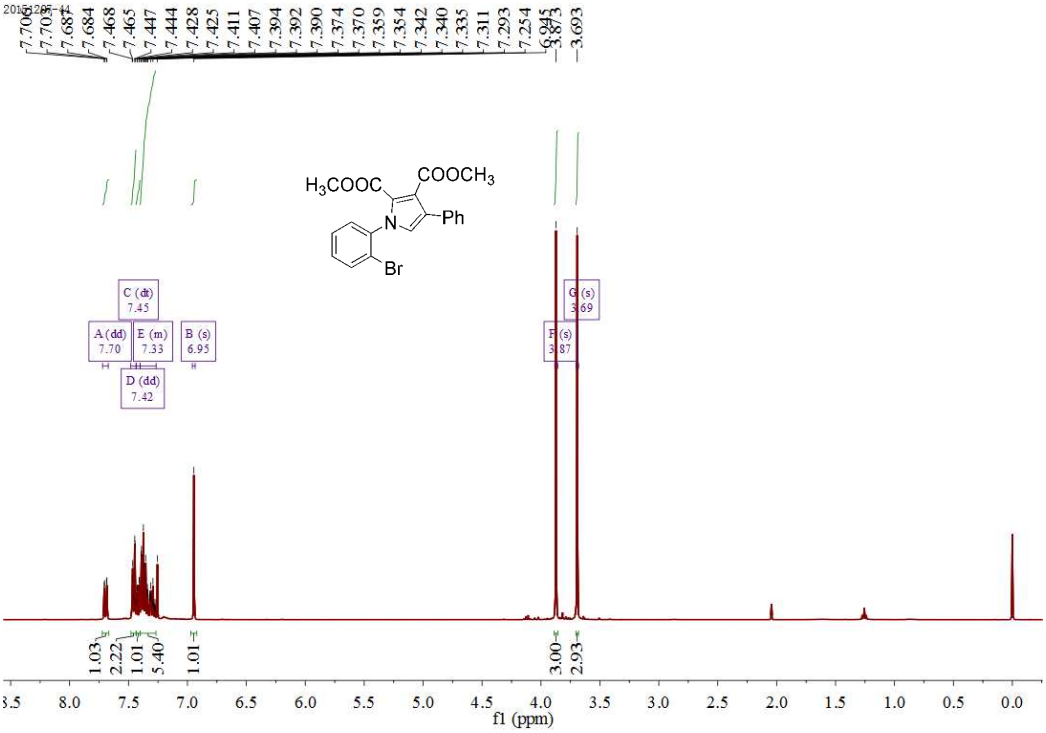
Cl
f1 (ppm)

Product 4c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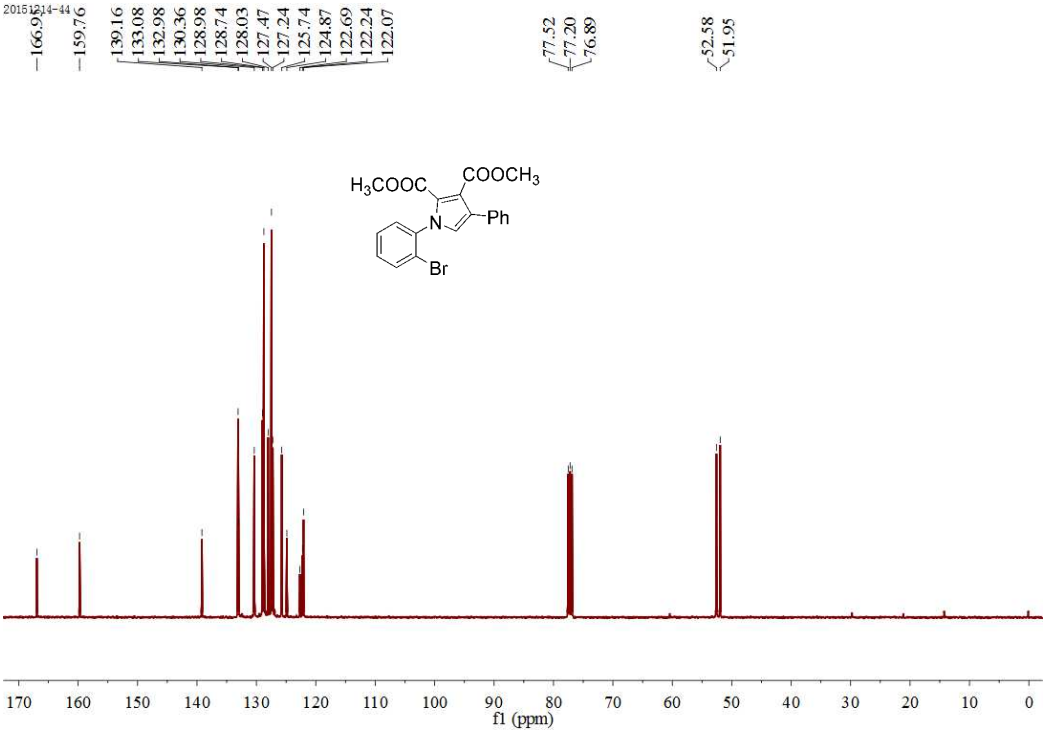
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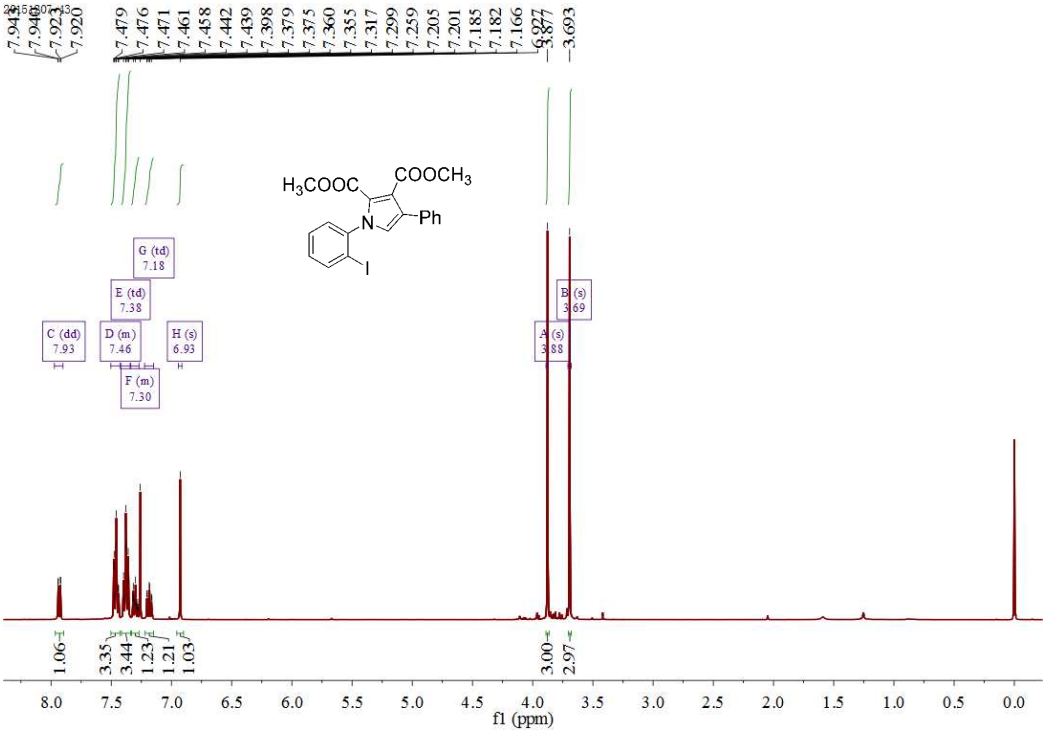
Ph
Br
f1 (ppm)

Product 4d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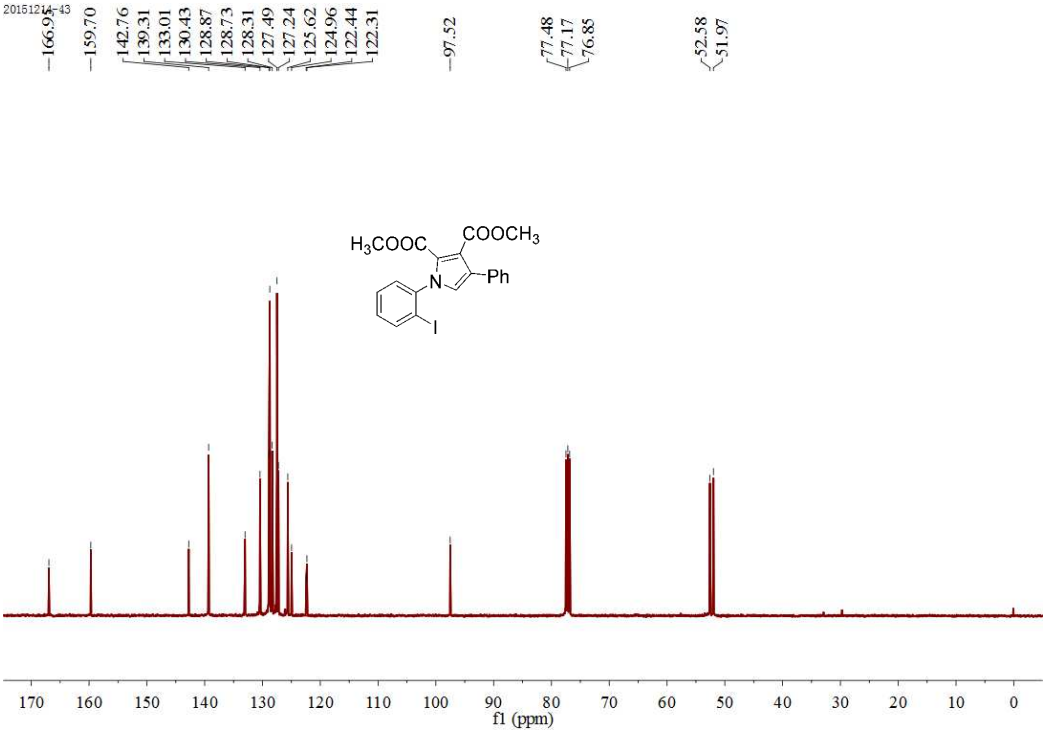
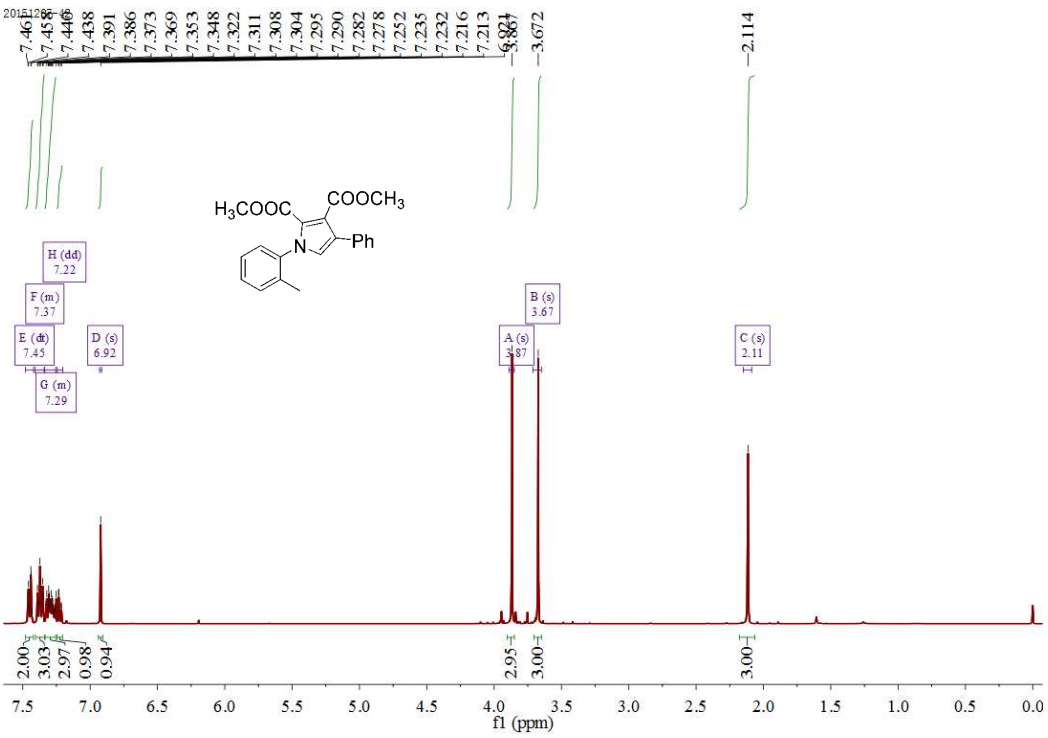
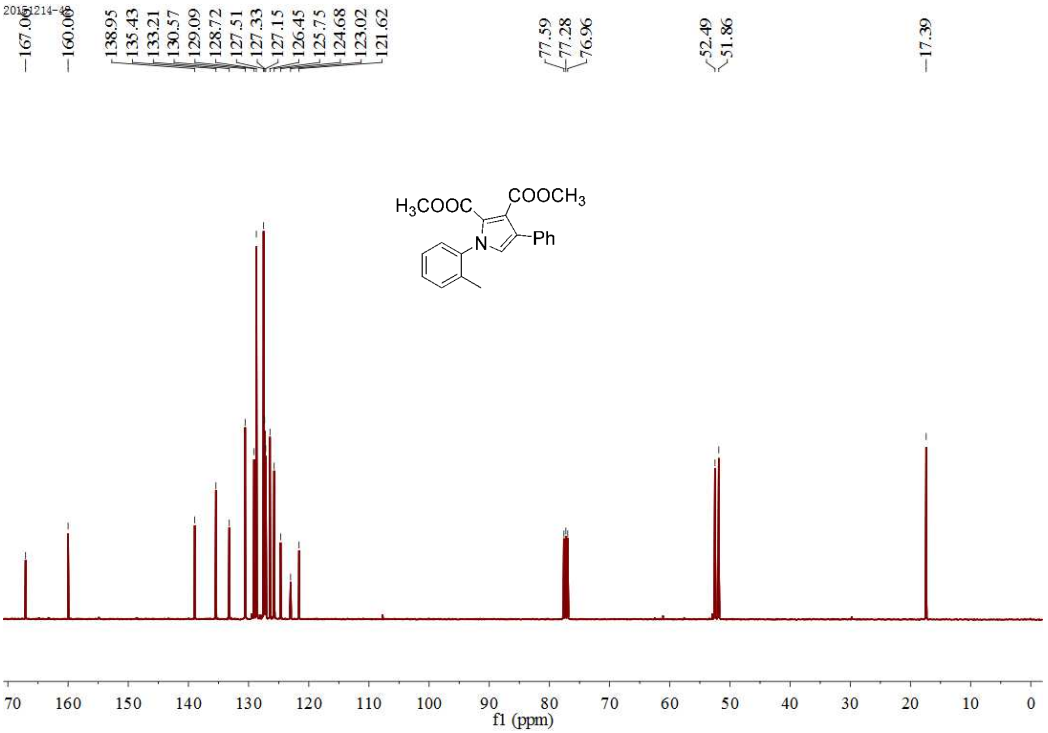
H (s) 6.93
F (m) 7.30
B (s) 3.69
A (s) 3.88
1.06
3.35
3.44
1.23
1.21
1.03
3.00
2.97
f1 (ppm)

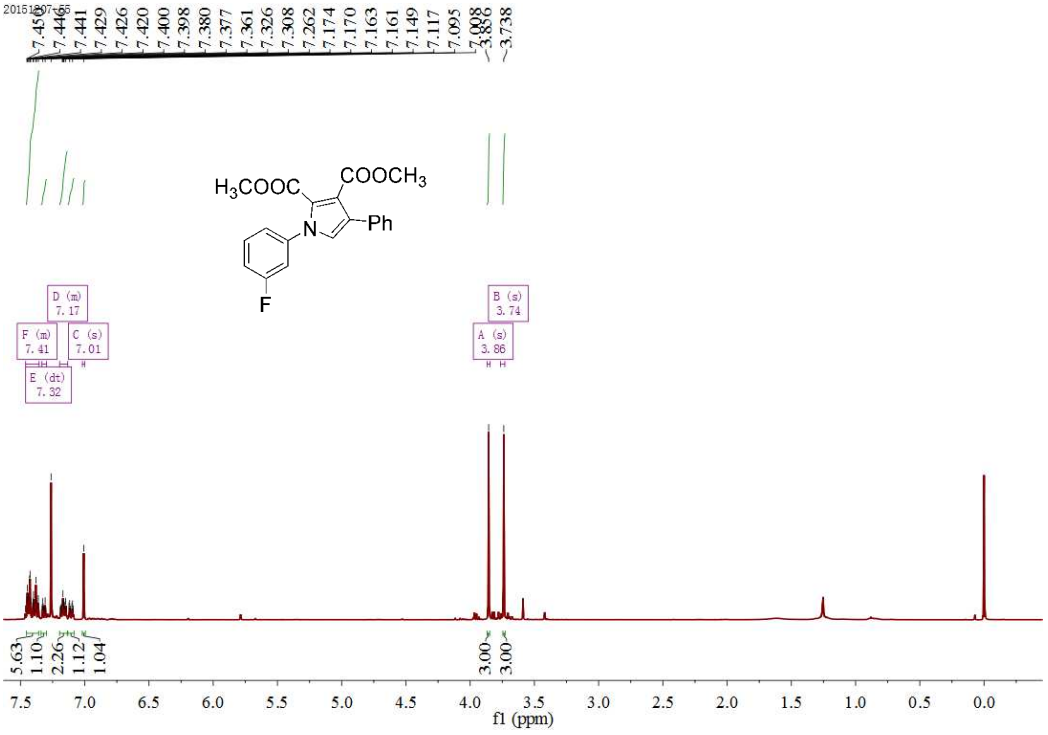

166.95
159.70
142.76
139.31
133.01
130.43
128.87
128.73
128.31
127.49
127.24
125.62
124.96
122.44
122.31
97.52
77.48
77.17
76.85
52.58
51.97
H3COOC
COOCH3
N
Ph
I
f1 (ppm)

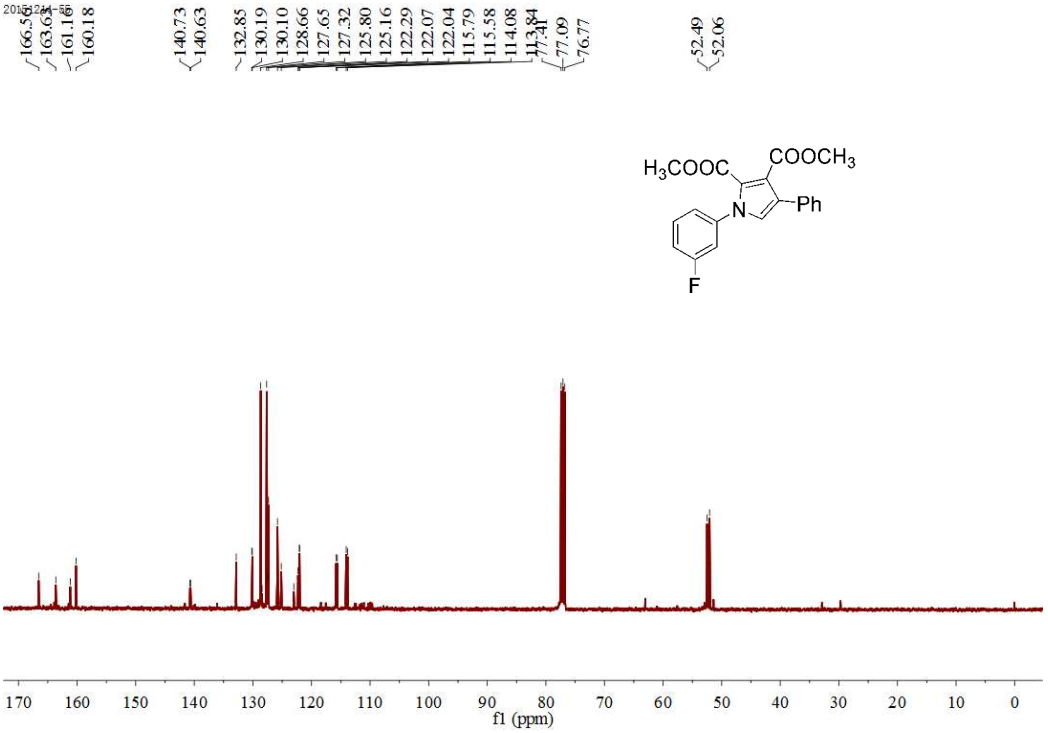
Product 4e


7.461
7.458
7.446
7.438
7.391
7.386
7.373
7.369
7.353
7.348
7.322
7.311
7.308
7.304
7.295
7.290
7.282
7.278
7.252
7.235
7.232
7.216
7.213
6.921
3.867
3.672
2.114
H3COOC
COOCH3
N
Ph
H (dd) 7.22
F (m) 7.37
E (dt) 7.45
G (m) 7.29
D (s) 6.92
A (s) 3.87
B (s) 3.67
C (s) 2.11
2.00
3.03
2.97
0.98
0.94
2.95
3.00
3.00
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
f1 (ppm)

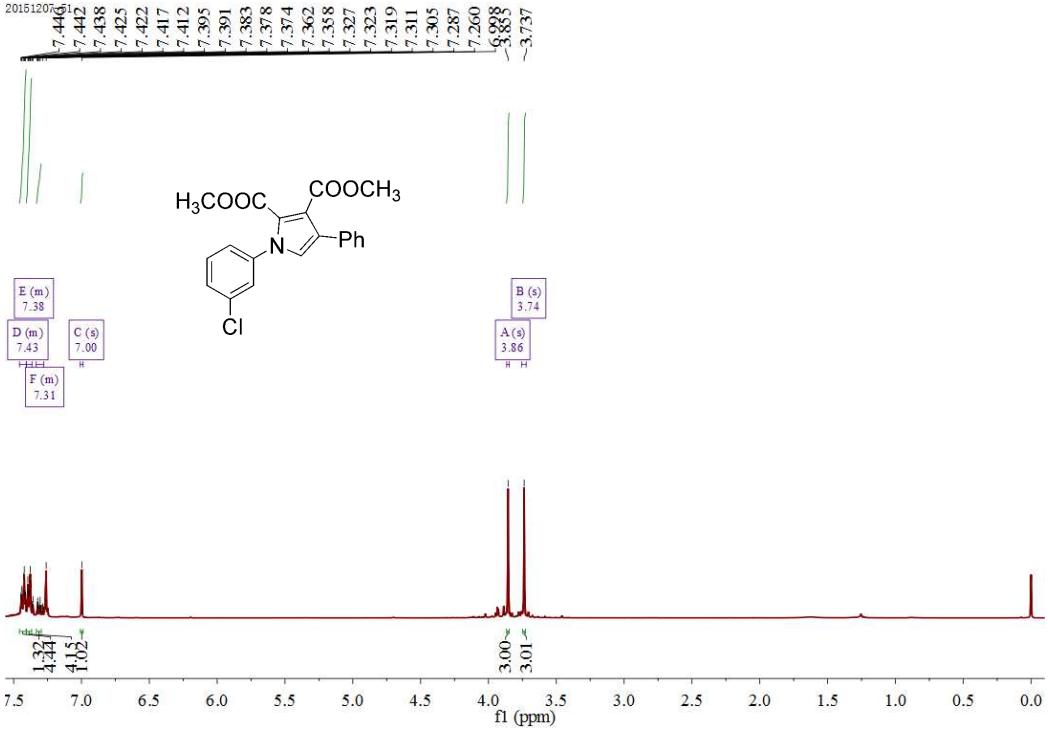

167.06
160.06
138.95
135.43
133.21
130.57
129.09
128.72
127.51
127.33
127.15
126.45
125.75
124.68
123.02
121.62
77.59
77.28
76.96
52.49
51.86
17.39
H3COOC
COOCH3
N
Ph
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

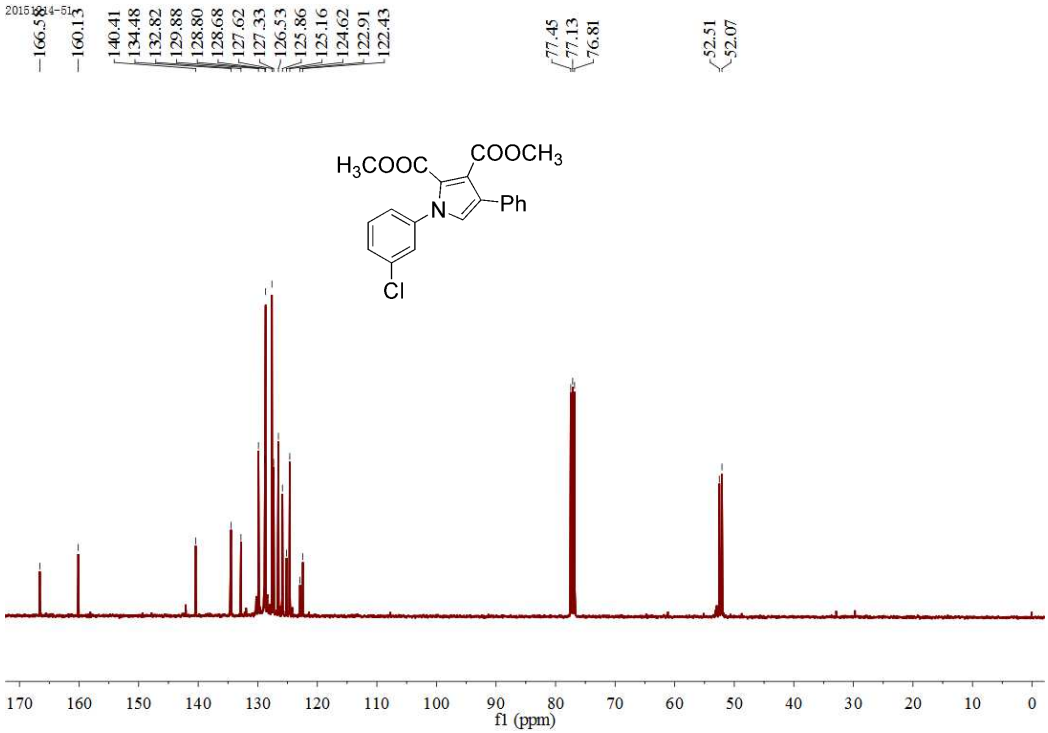
Product 4f


7.456
7.446
7.441
7.429
7.426
7.420
7.400
7.398
7.380
7.377
7.361
7.326
7.308
7.262
7.174
7.170
7.163
7.161
7.149
7.117
7.095
7.008
3.886
3.738
H3COOC
COOCH3
N
Ph
F
D (m) 7.17
F (m) 7.41
C (s) 7.01
E (dt) 7.32
B (s) 3.74
A (s) 3.86
5.63
1.10
2.26
1.12
1.04
3.00
3.00
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
f1 (ppm)

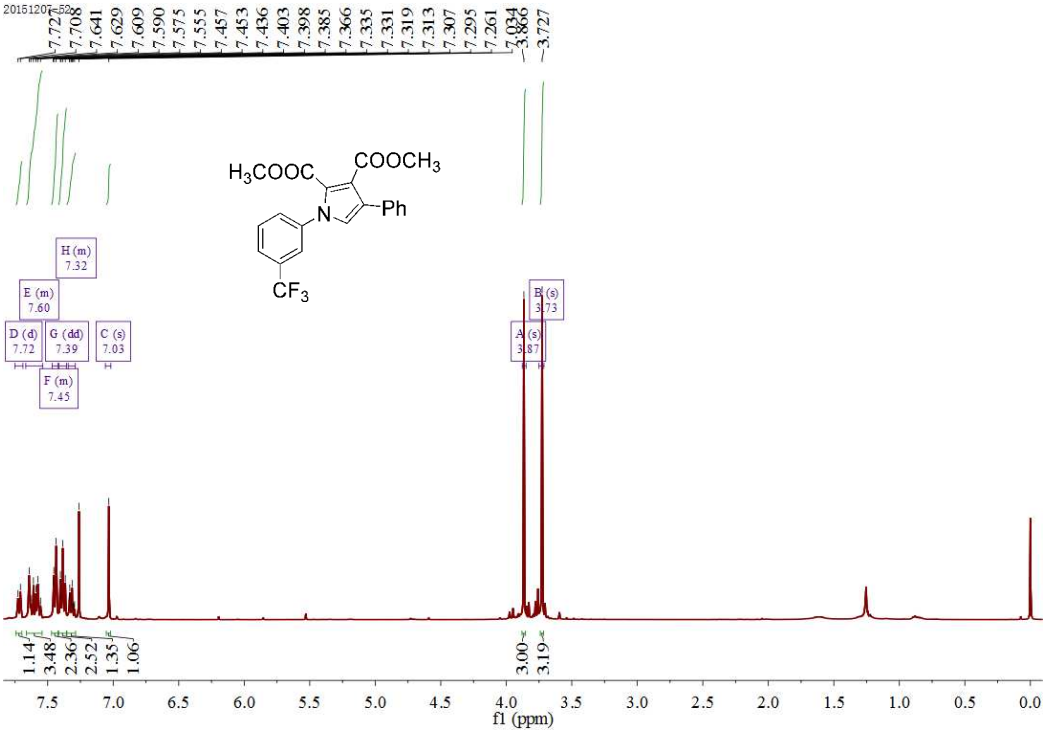

166.56
163.63
161.16
160.18
140.73
140.63
132.85
130.19
130.10
128.66
127.65
127.32
125.80
125.16
122.29
122.07
122.04
115.79
115.58
114.08
113.84
77.41
77.09
76.77
52.49
52.06
H3COOC
COOCH3
N
Ph
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

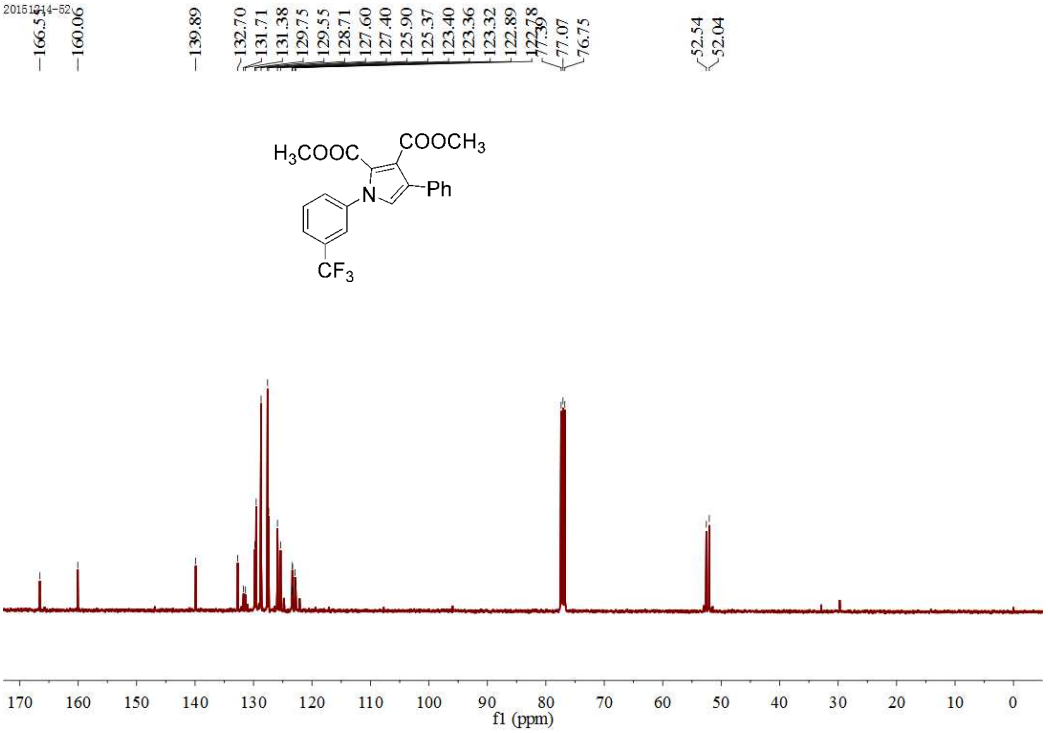
Product 4g


7.442
7.438
7.425
7.422
7.417
7.412
7.395
7.391
7.383
7.378
7.374
7.362
7.358
7.327
7.323
7.319
7.311
7.305
7.287
7.260
6.998
3.885
3.737
H3COOC
COOCH3
N
Ph
Cl
E (m) 7.38
D (m) 7.43
C (s) 7.00
F (m) 7.31
B (s) 3.74
A (s) 3.86
1.32
4.44
4.15
1.02
3.00
3.01
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
f1 (ppm)

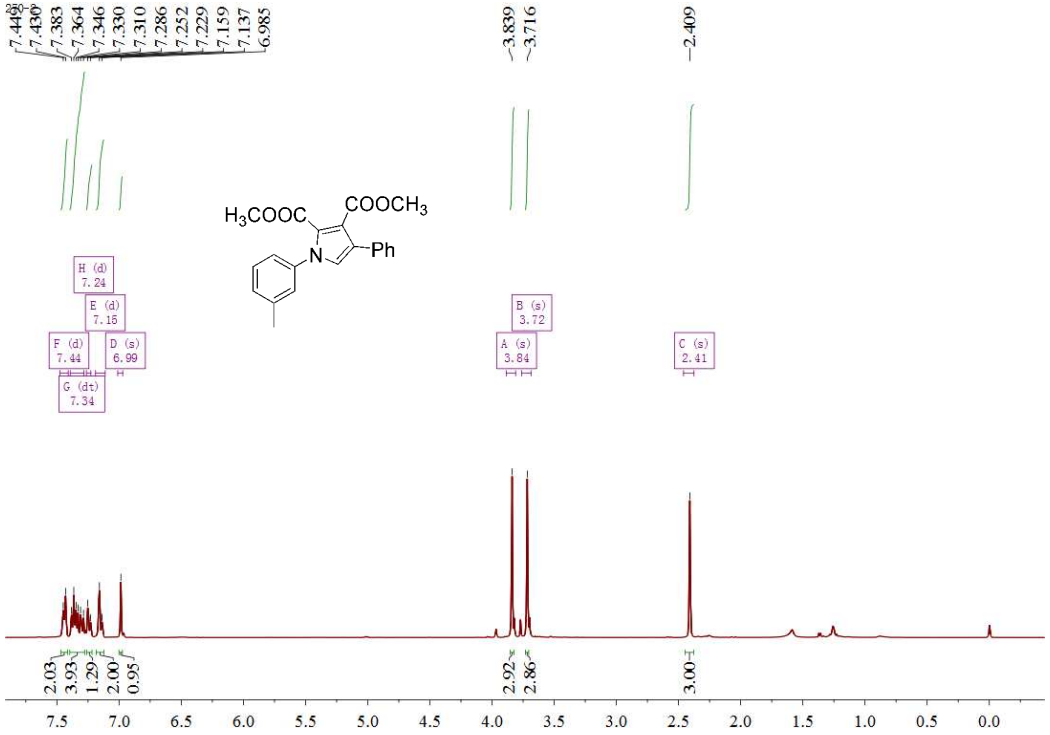

166.58
160.13
140.41
134.48
132.82
129.88
128.80
128.68
127.62
127.33
126.53
125.86
125.16
124.62
122.91
122.43
77.45
77.13
76.81
52.51
52.07
H3COOC
COOCH3
N
Ph
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

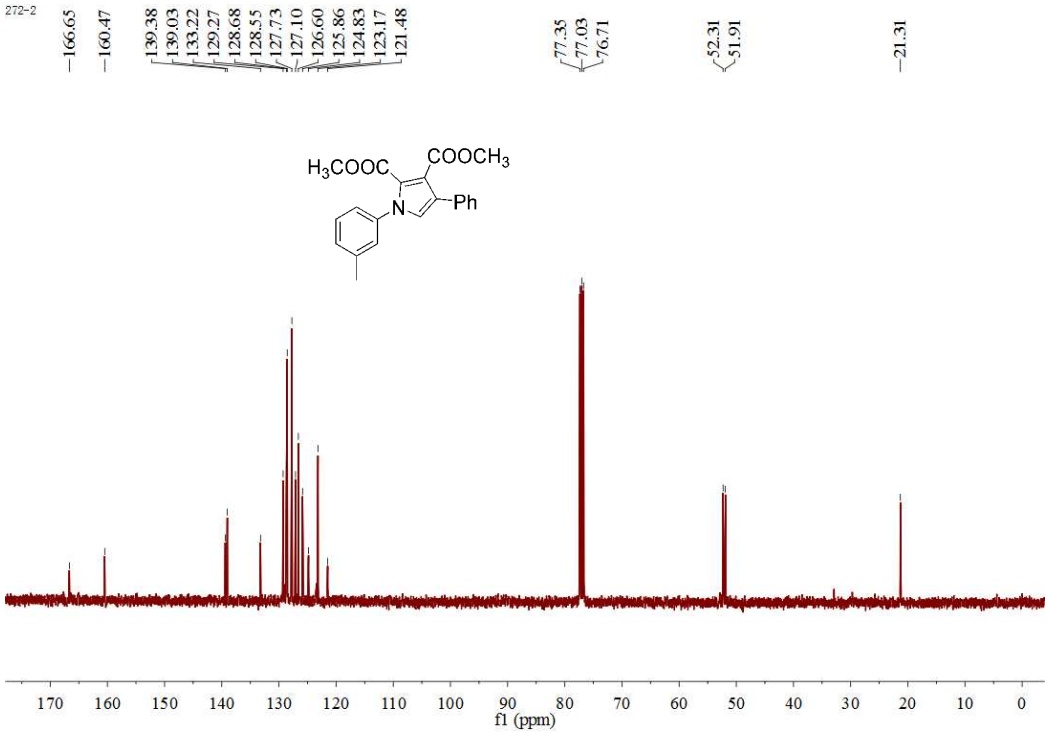
Product 4h


20151207-52
7.722
7.708
7.641
7.629
7.609
7.590
7.575
7.555
7.457
7.453
7.436
7.403
7.398
7.385
7.366
7.335
7.331
7.319
7.313
7.307
7.295
7.261
7.034
3.866
3.727
H (m) 7.32
E (m) 7.60
D (d) 7.72
G (dd) 7.39
C (s) 7.03
F (m) 7.45
B (s) 3.73
A (s) 3.87
1.14
3.48
2.36
2.52
1.35
1.06
3.00
3.19
f1 (ppm)

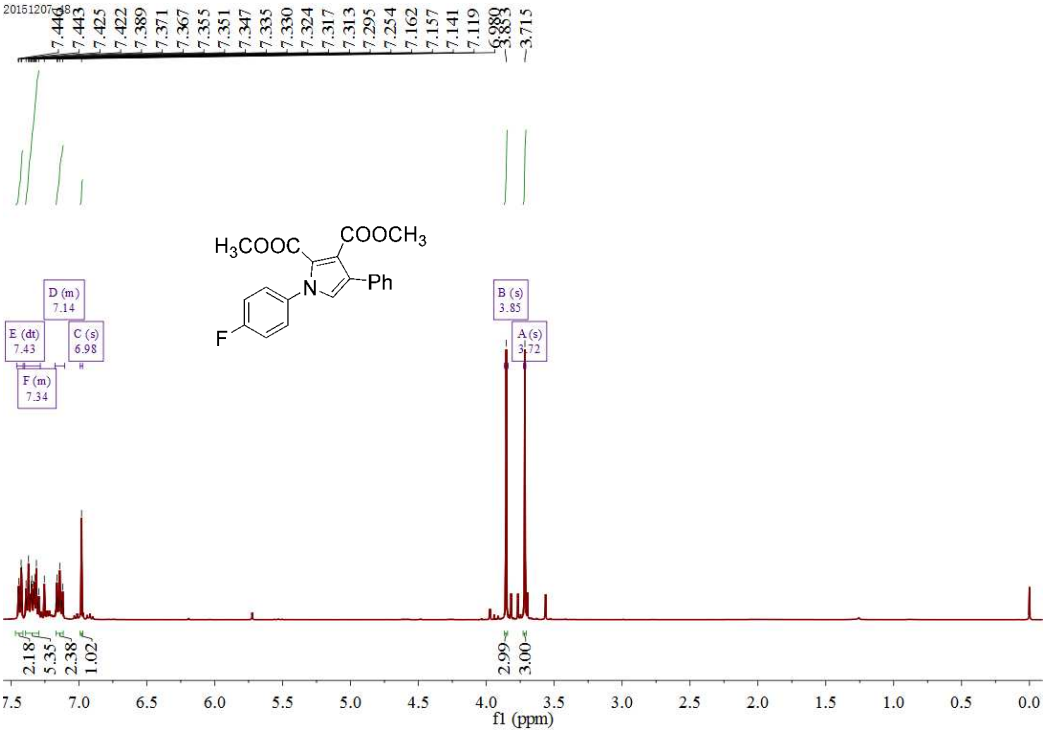

20151214-52
166.51
160.06
139.89
132.70
131.71
131.38
129.75
129.55
128.71
127.60
127.40
125.90
125.37
123.40
123.36
123.32
122.89
122.78
77.39
77.07
76.75
52.54
52.04
f1 (ppm)

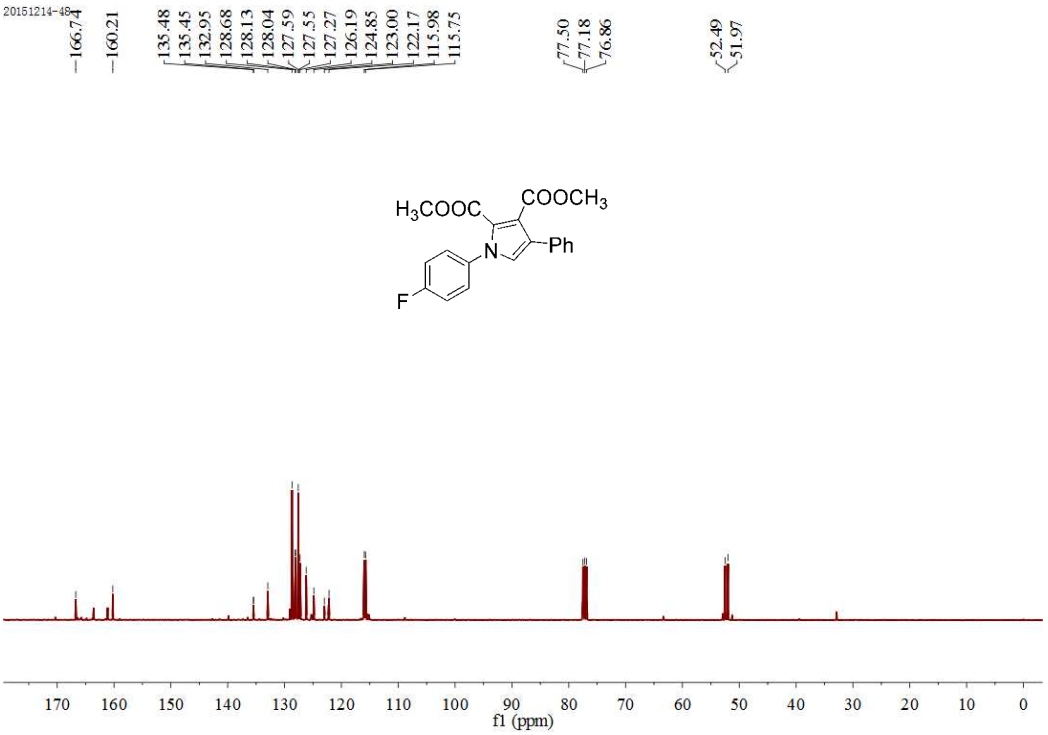
Product 4i


7.443
7.430
7.383
7.364
7.346
7.330
7.310
7.286
7.252
7.229
7.159
7.137
6.985
3.839
3.716
2.409
H3COOC
COOCH3
N
Ph
H (d) 7.24
E (d) 7.15
F (d) 7.44
D (s) 6.99
G (dt) 7.34
B (s) 3.72
A (s) 3.84
C (s) 2.41
2.03
3.93
1.29
2.00
0.95
2.92
2.86
3.00
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

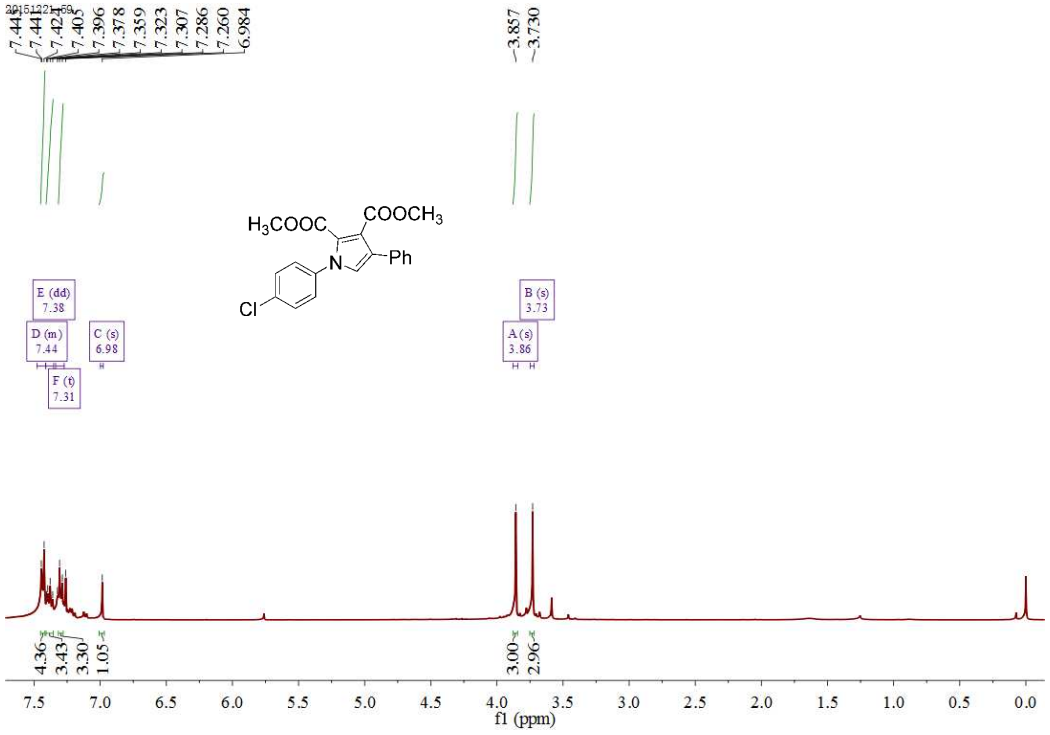

272-2
166.65
160.47
139.38
139.03
133.22
129.27
128.68
128.55
127.73
127.10
126.60
125.86
124.83
123.17
121.48
77.35
77.03
76.71
52.31
51.91
21.31
H3COOC
COOCH3
N
Ph
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

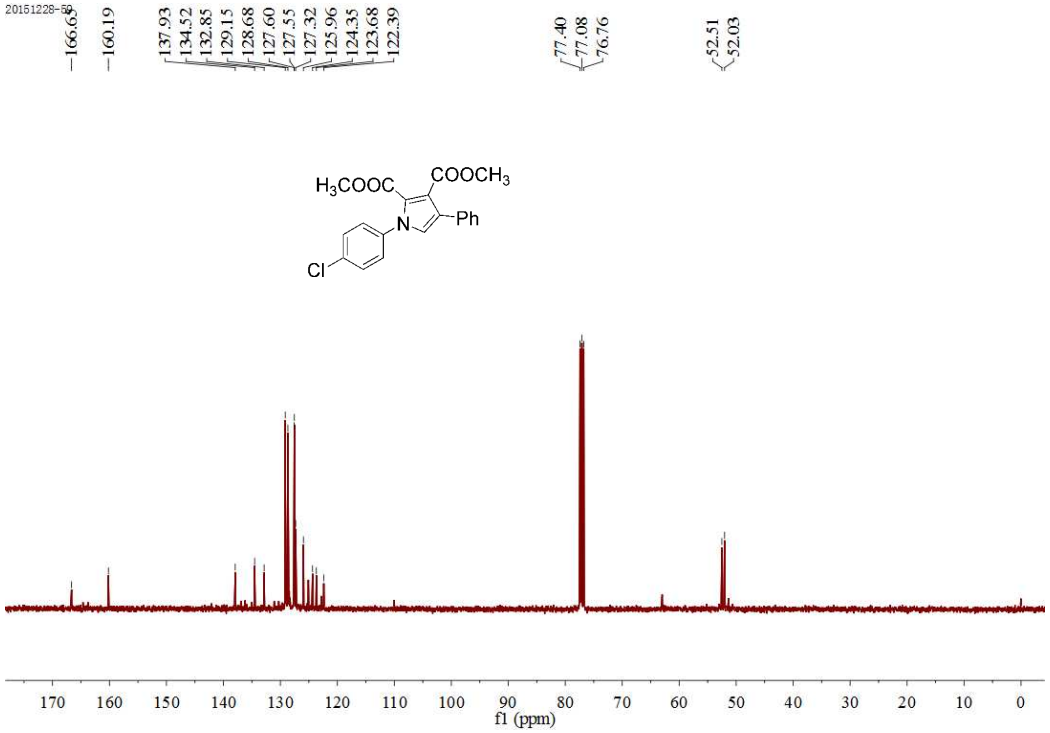
Product 4j


20151207-48
7.446
7.443
7.425
7.422
7.389
7.371
7.367
7.355
7.351
7.347
7.335
7.330
7.324
7.317
7.313
7.295
7.254
7.162
7.157
7.141
7.119
6.980
3.853
3.715
H3COOC
COOCH3
N
Ph
F
D (m) 7.14
E (dt) 7.43
C (s) 6.98
F (m) 7.34
B (s) 3.85
A (s) 3.72
2.18
5.35
2.38
1.02
2.99
3.00
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
f1 (ppm)

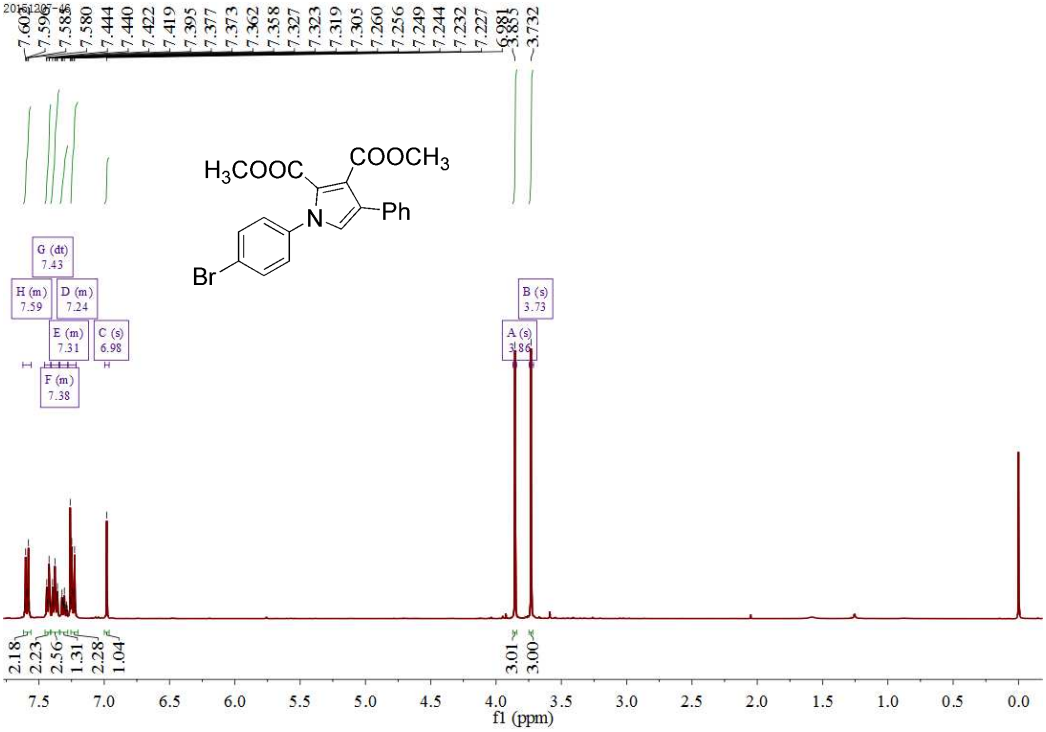

20151214-48
166.74
160.21
135.48
135.45
132.95
128.68
128.13
128.04
127.59
127.55
127.27
126.19
124.85
123.00
122.17
115.98
115.75
77.50
77.18
76.86
52.49
51.97
H3COOC
COOCH3
N
Ph
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

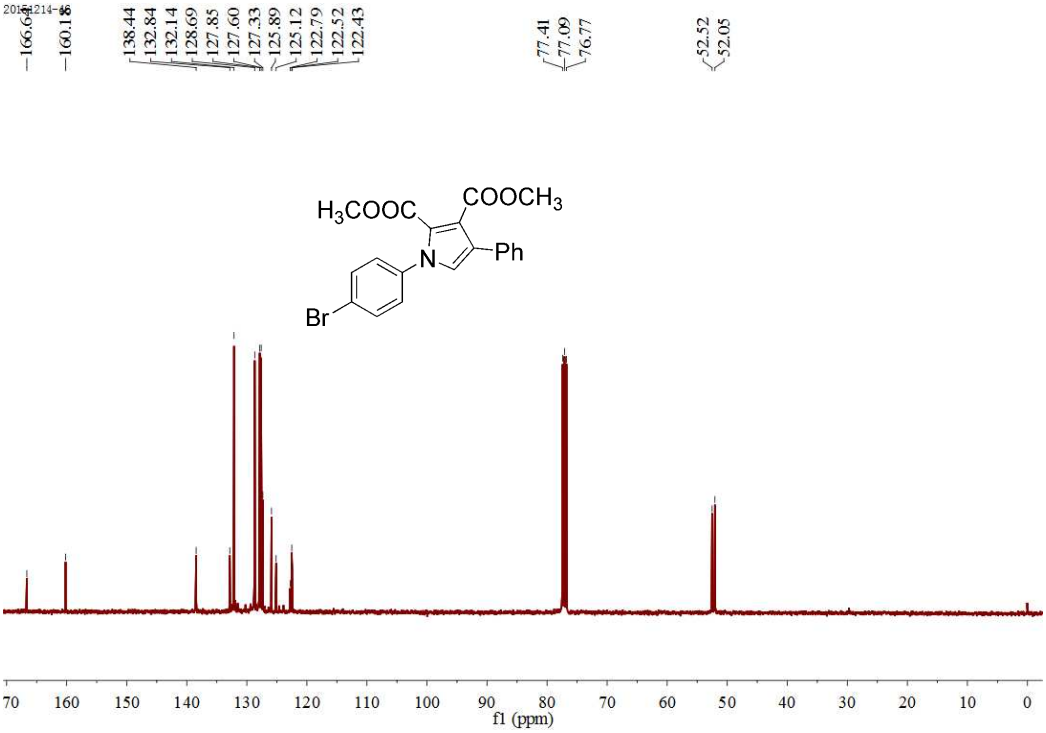
Product 4k


7.445
7.441
7.422
7.405
7.396
7.378
7.359
7.323
7.307
7.286
7.260
6.984
3.857
3.730
H3COOC
COOCH3
Ph
N
Cl
E (dd) 7.38
D (m) 7.44
C (s) 6.98
F (t) 7.31
B (s) 3.73
A (s) 3.86
4.36
3.43
3.30
1.05
3.00
2.96
f1 (ppm)

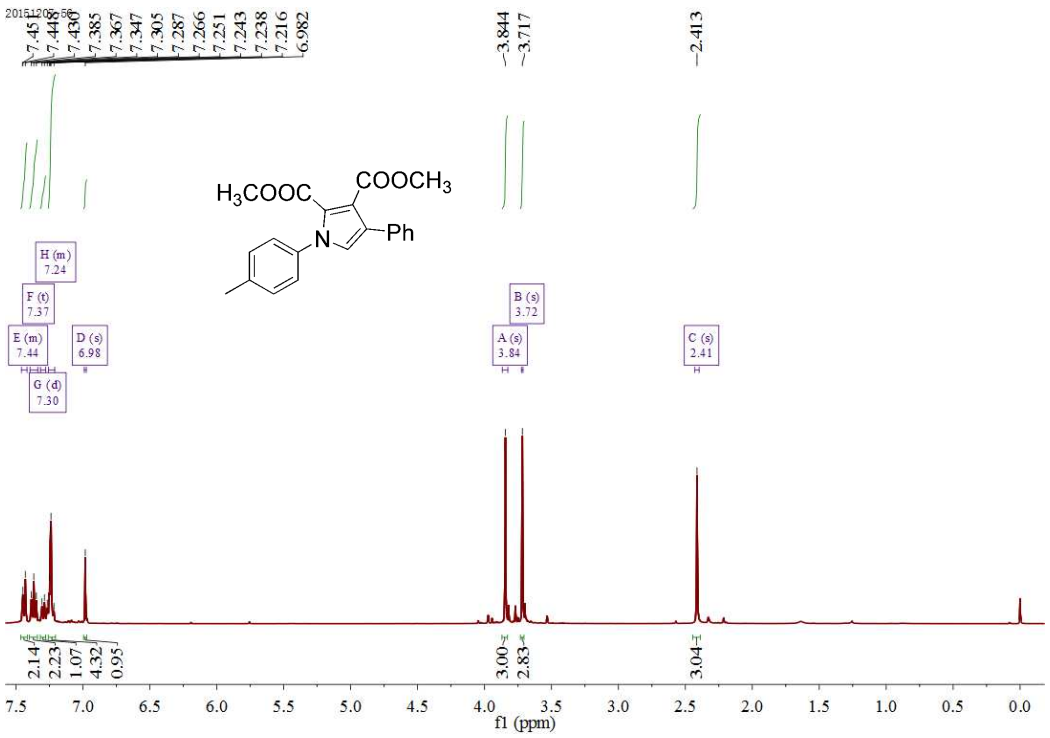

166.63
160.19
137.93
134.52
132.85
129.15
128.68
127.60
127.55
127.32
125.96
124.35
123.68
122.39
77.40
77.08
76.76
52.51
52.03
H3COOC
COOCH3
Ph
N
Cl
f1 (ppm)

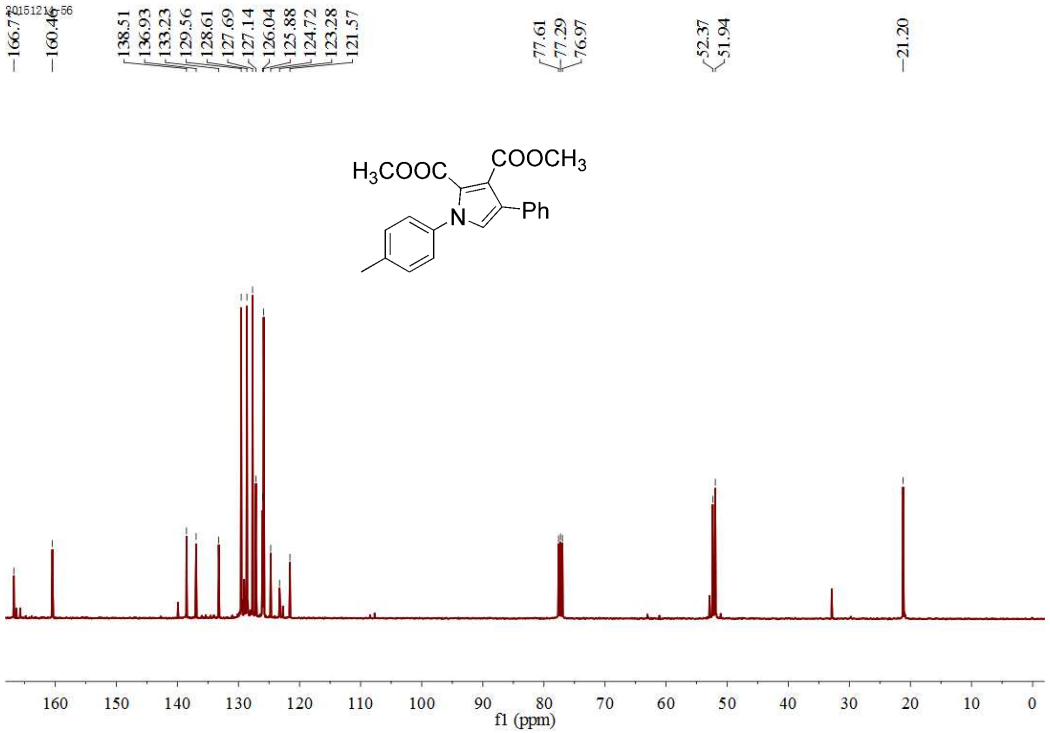
Product 4l


7.602
7.596
7.585
7.580
7.444
7.440
7.422
7.419
7.395
7.377
7.373
7.362
7.358
7.327
7.323
7.319
7.305
7.260
7.256
7.249
7.244
7.232
7.227
6.981
3.885
3.732
H3COOC
COOCH3
N
Ph
Br
G (dt) 7.43
H (m) 7.59
D (m) 7.24
E (m) 7.31
C (s) 6.98
F (m) 7.38
B (s) 3.73
A (s) 3.86
2.18
2.23
2.56
1.31
2.28
1.04
3.01
3.00
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
f1 (ppm)

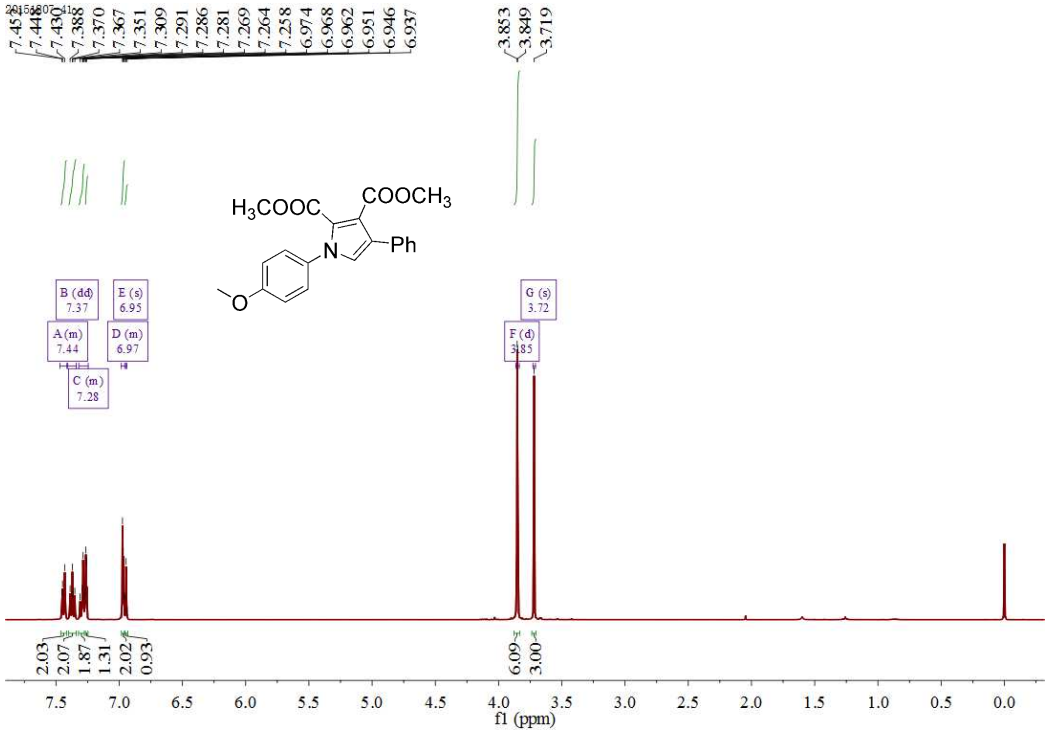

166.64
160.18
138.44
132.84
132.14
128.69
127.85
127.60
127.33
125.89
125.12
122.79
122.52
122.43
77.41
77.09
76.77
52.52
52.05
H3COOC
COOCH3
N
Ph
Br
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

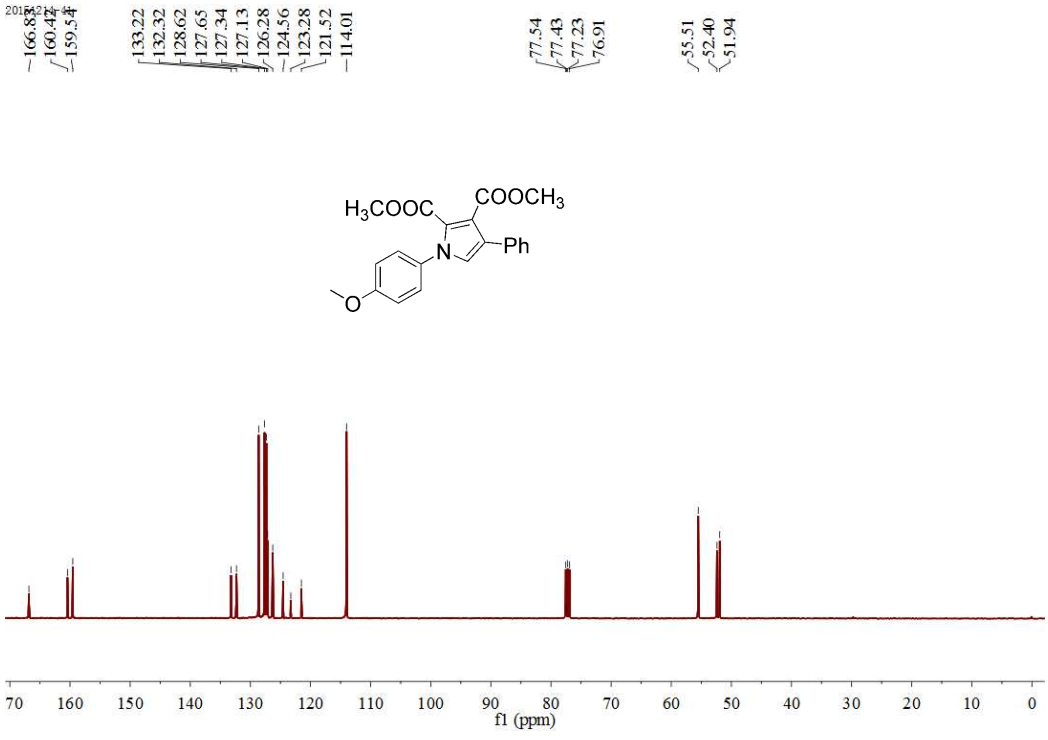
Product 4m


7.451
7.448
7.430
7.385
7.367
7.347
7.305
7.287
7.266
7.251
7.243
7.238
7.216
6.982
3.844
3.717
2.413
H3COOC
COOCH3
N
Ph
H (m) 7.24
F (t) 7.37
E (m) 7.44
D (s) 6.98
G (d) 7.30
B (s) 3.72
A (s) 3.84
C (s) 2.41
2.14
2.23
1.07
4.32
0.95
3.00
2.83
3.04
f1 (ppm)

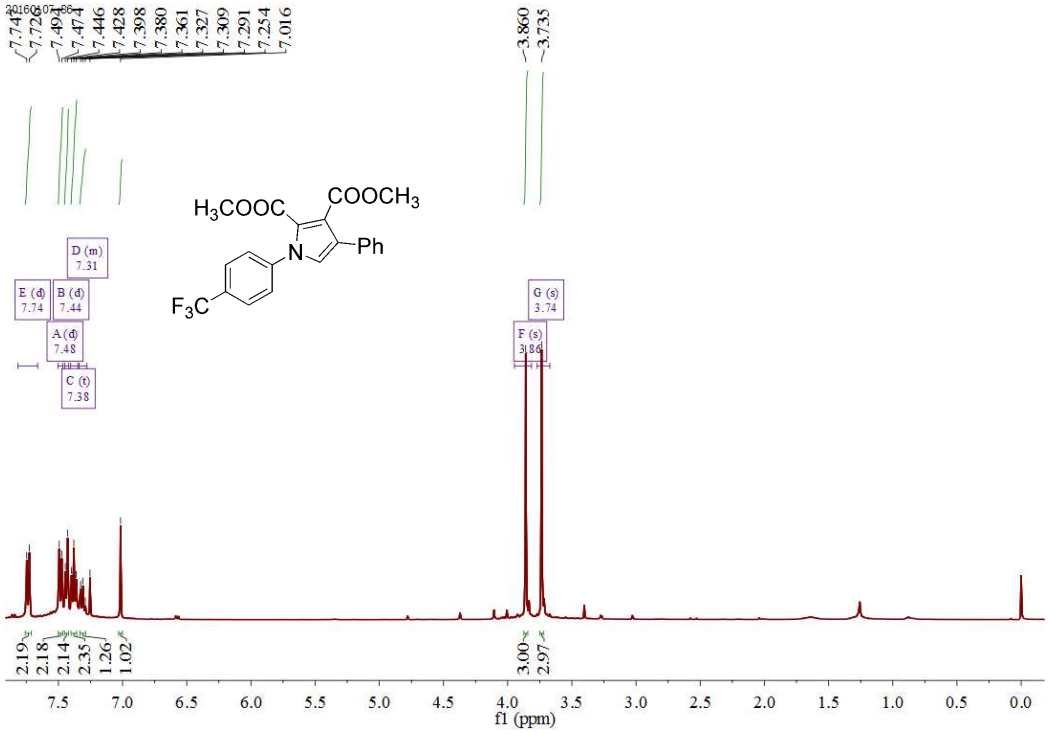

166.72
160.46
138.51
136.93
133.23
129.56
128.61
127.69
127.14
126.04
125.88
124.72
123.28
121.57
77.61
77.29
76.97
52.37
51.94
21.20
H3COOC
COOCH3
N
Ph
f1 (ppm)

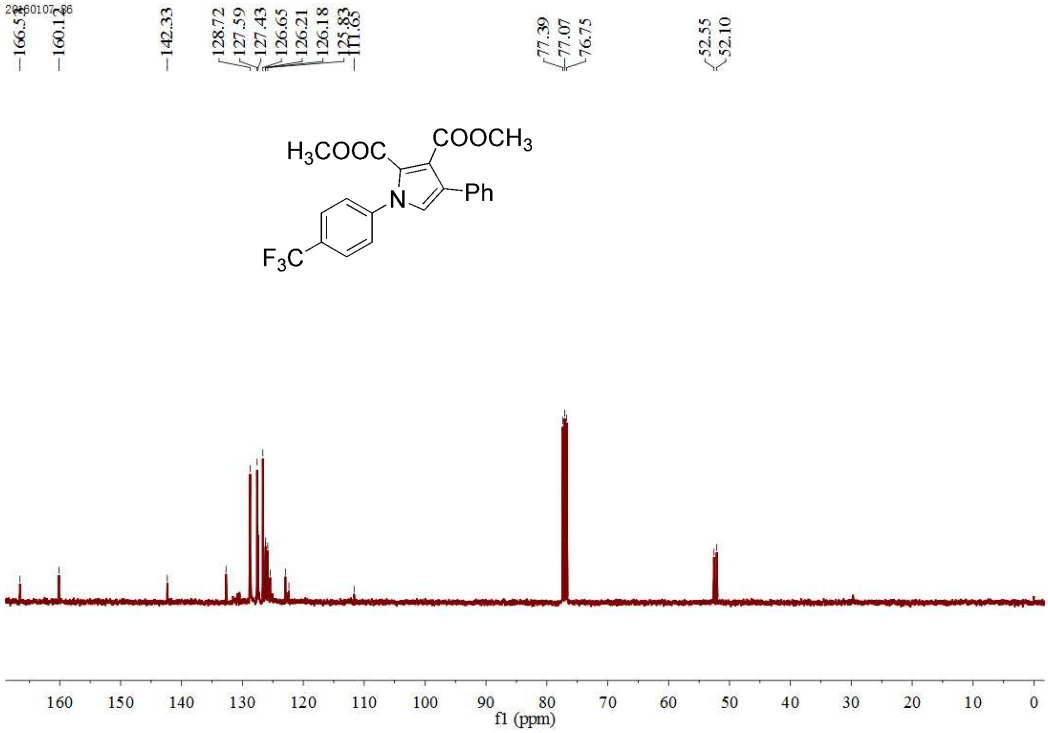
Product 4n


7.453
7.448
7.430
7.388
7.370
7.367
7.351
7.309
7.291
7.286
7.281
7.269
7.264
7.258
6.974
6.968
6.962
6.951
6.946
6.937
3.853
3.849
3.719
H3COOC
COOCH3
N
Ph
O
B (dd) 7.37
E (s) 6.95
A (m) 7.44
D (m) 6.97
C (m) 7.28
G (s) 3.72
F (d) 3.85
2.03
2.07
1.87
1.31
2.02
0.93
6.09
3.00
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
f1 (ppm)

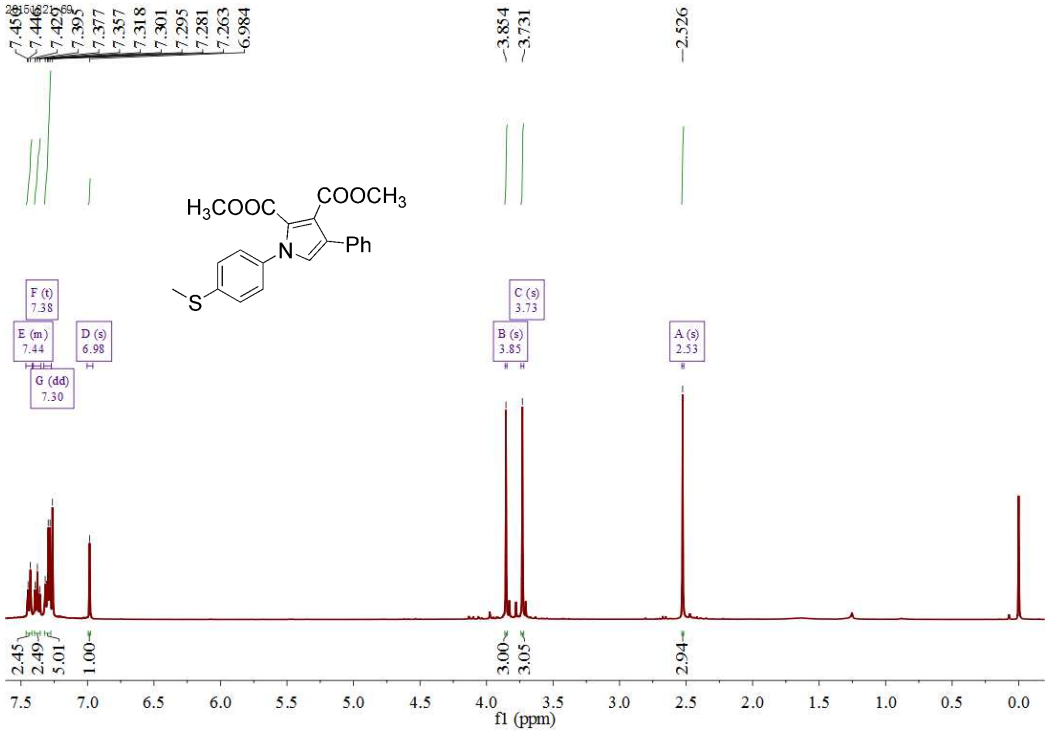

166.83
160.42
159.54
133.22
132.32
128.62
127.65
127.34
127.13
126.28
124.56
123.28
121.52
114.01
77.54
77.43
77.23
76.91
55.51
52.40
51.94
H3COOC
COOCH3
N
Ph
O
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

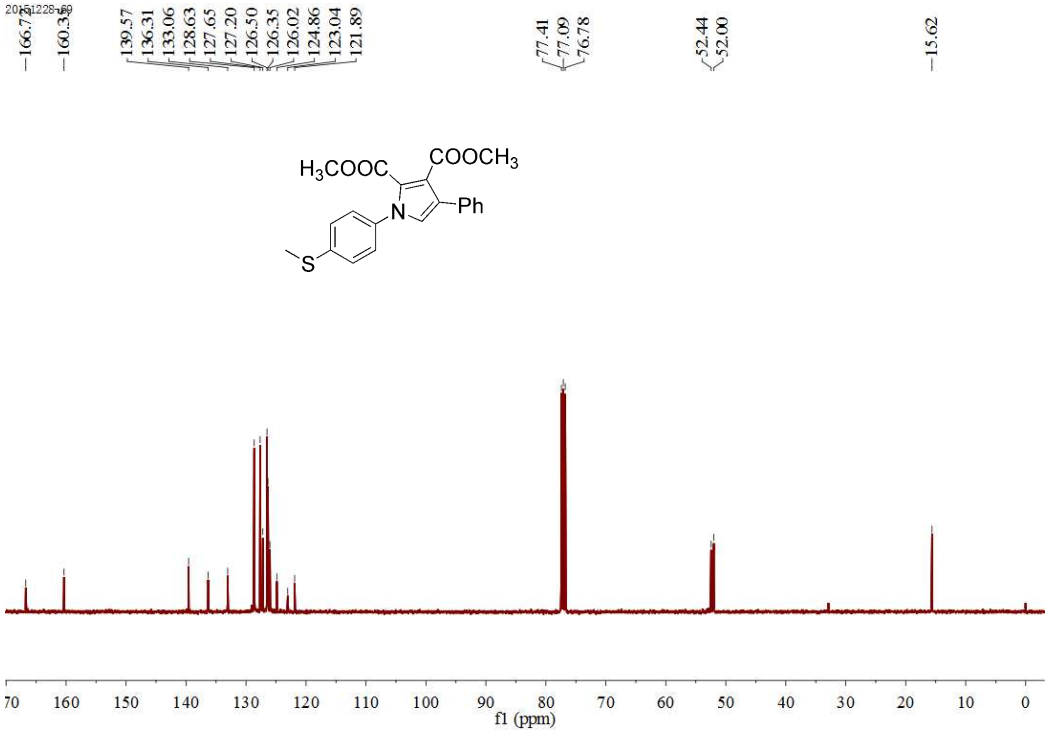
Product 4o


7.744
7.726
7.494
7.474
7.446
7.428
7.398
7.380
7.361
7.327
7.309
7.291
7.254
7.016
3.860
3.735
H3COOC
COOCH3
Ph
N
F3C
D (m) 7.31
E (d) 7.74
B (d) 7.44
A (d) 7.48
C (t) 7.38
G (s) 3.74
F (s) 3.86
2.19
2.18
2.14
2.35
1.26
1.02
3.00
2.97
f1 (ppm)

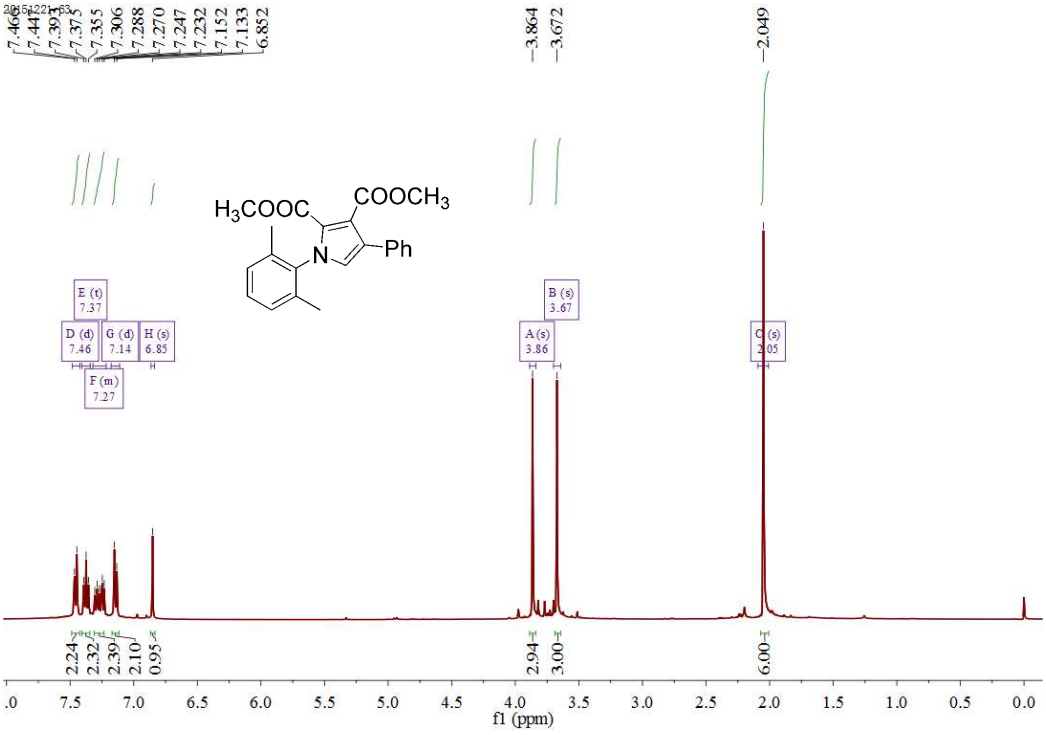

166.5
160.1
142.33
128.72
127.59
127.43
126.65
126.21
126.18
77.39
77.07
76.75
52.55
52.10
H3COOC
COOCH3
Ph
N
F3C
f1 (ppm)

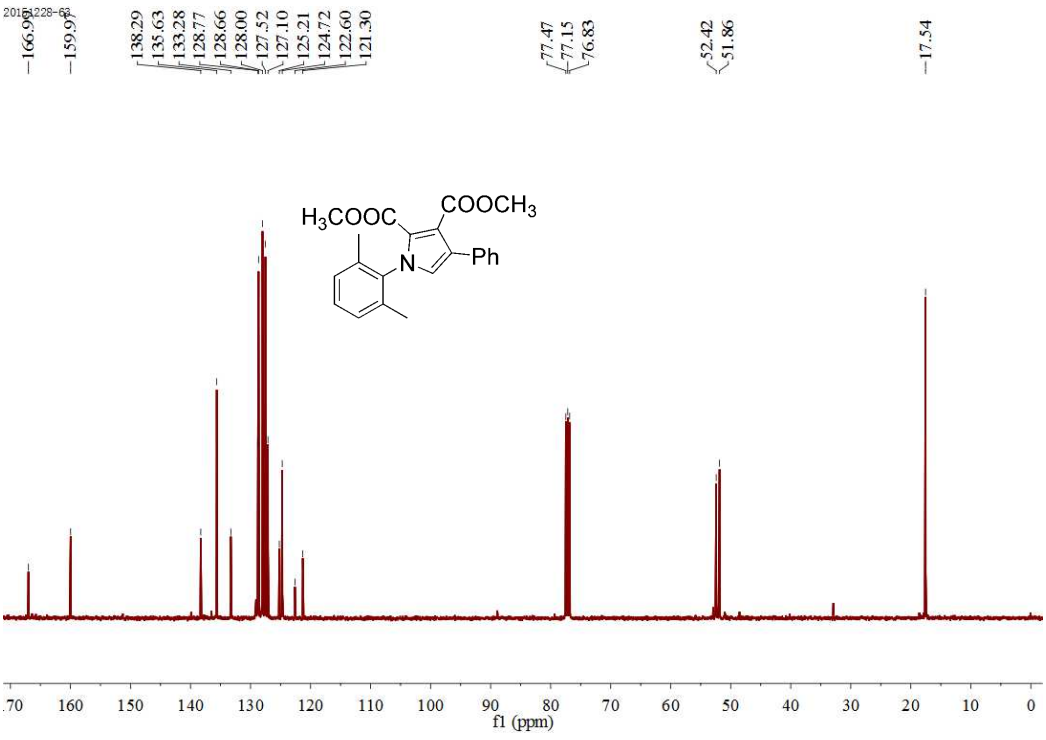
Product 4p


7.456
7.446
7.429
7.395
7.377
7.357
7.318
7.301
7.295
7.281
7.263
6.984
3.854
3.731
2.526
H3COOC
COOCH3
Ph
N
S
F (t) 7.38
E (m) 7.44
D (s) 6.98
G (dd) 7.30
C (s) 3.73
B (s) 3.85
A (s) 2.53
2.45
2.49
5.01
1.00
3.00
3.05
2.94
f1 (ppm)

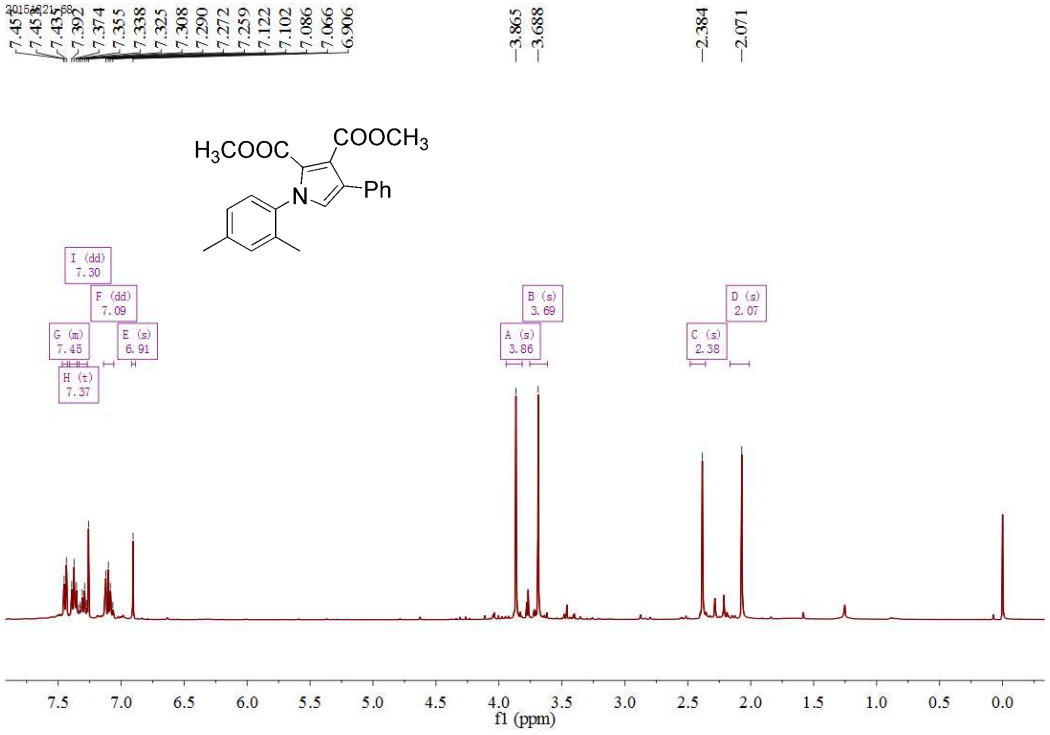

166.72
160.31
139.57
136.31
133.06
128.63
127.65
127.20
126.50
126.35
126.02
124.86
123.04
121.89
77.41
77.09
76.78
52.44
52.00
15.62
H3COOC
COOCH3
Ph
N
S
f1 (ppm)

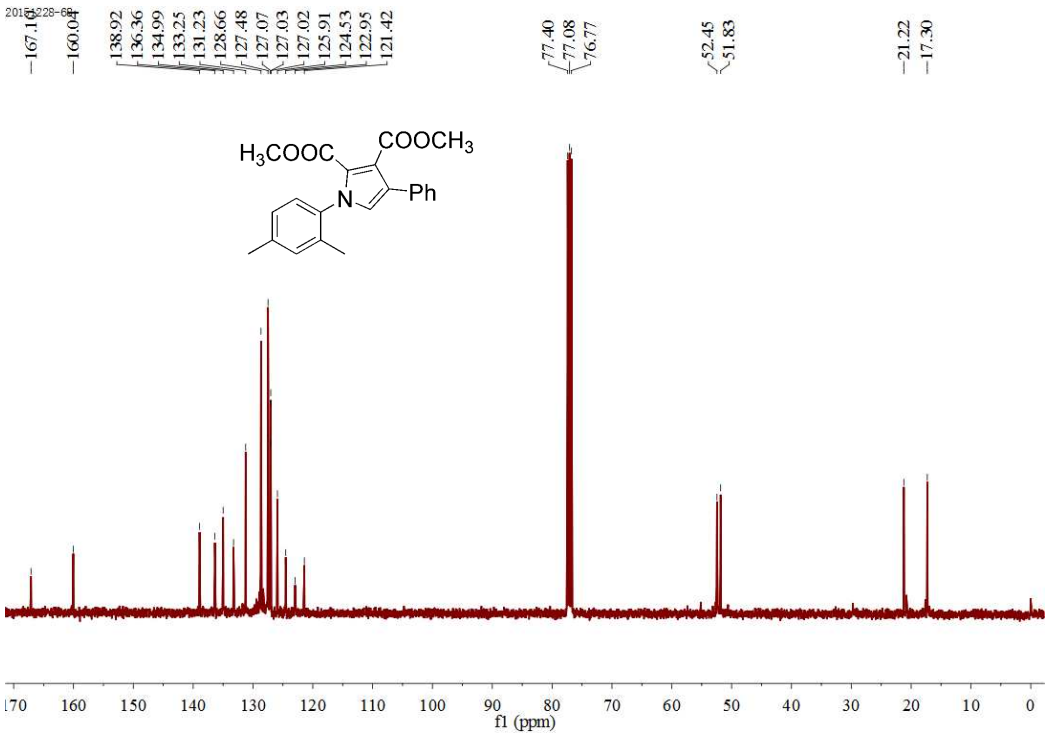
Product 4q


7.466
7.447
7.393
7.375
7.355
7.306
7.288
7.270
7.247
7.232
7.152
7.133
6.852
3.864
3.672
2.049
H3COOC
COOCH3
N
Ph
E (t) 7.37
D (d) 7.46
G (d) 7.14
H (s) 6.85
F (m) 7.27
B (s) 3.67
A (s) 3.86
C (s) 2.05
2.24
2.32
2.39
2.10
0.95
2.94
3.00
6.00
f1 (ppm)

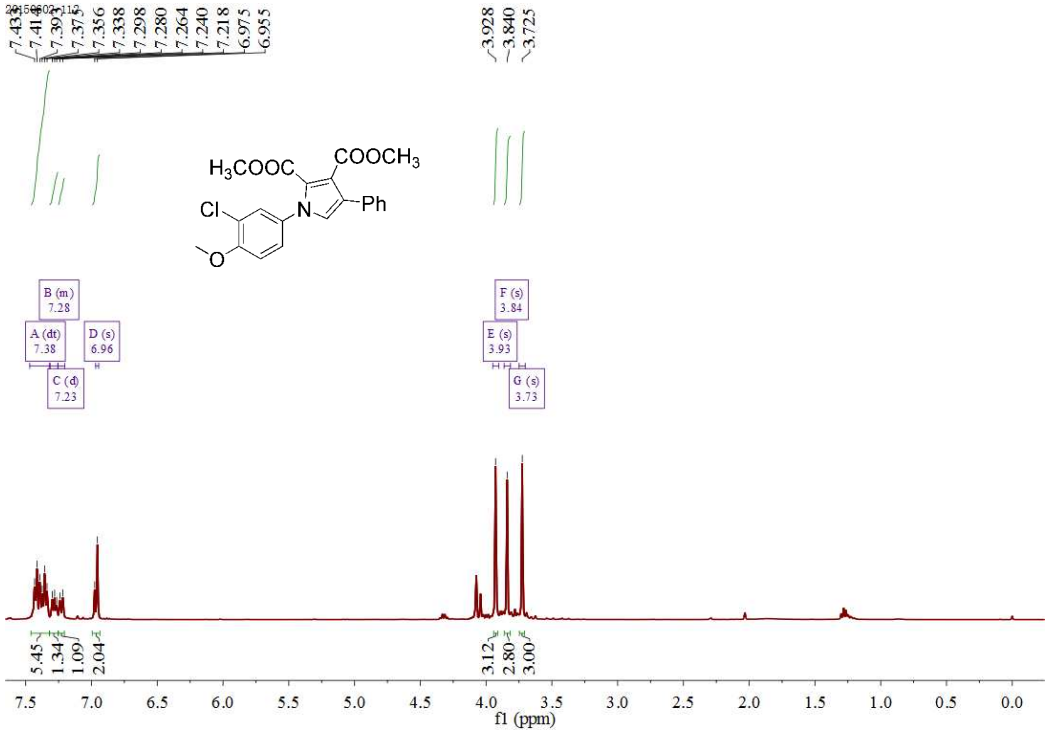

166.99
159.97
138.29
135.63
133.28
128.77
128.66
128.00
127.52
127.10
125.21
124.72
122.60
121.30
77.47
77.15
76.83
52.42
51.86
17.54
H3COOC
COOCH3
N
Ph
f1 (ppm)

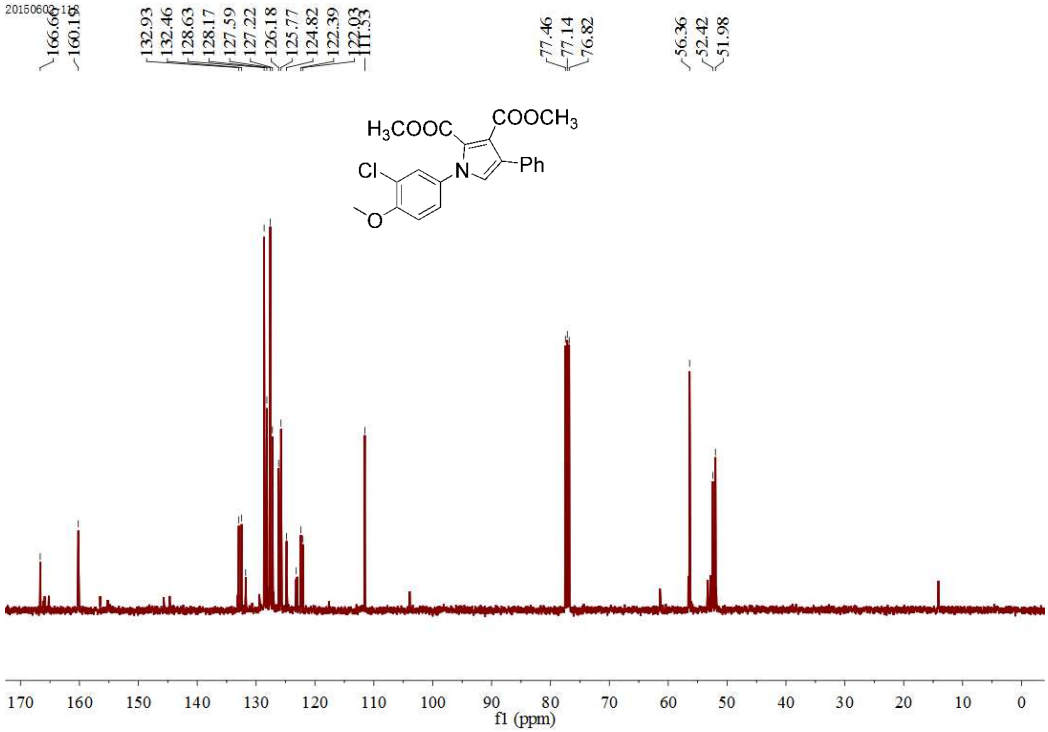
Product 4r


7.455
7.451
7.435
7.392
7.374
7.355
7.338
7.325
7.308
7.290
7.272
7.259
7.122
7.102
7.086
7.066
6.906
3.865
3.688
2.384
2.071
H3COOC
COOCH3
N
Ph
I (dd) 7.30
F (dd) 7.09
G (m) 7.45
E (s) 6.91
H (t) 7.37
B (s) 3.69
A (s) 3.86
D (s) 2.07
C (s) 2.38
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
f1 (ppm)

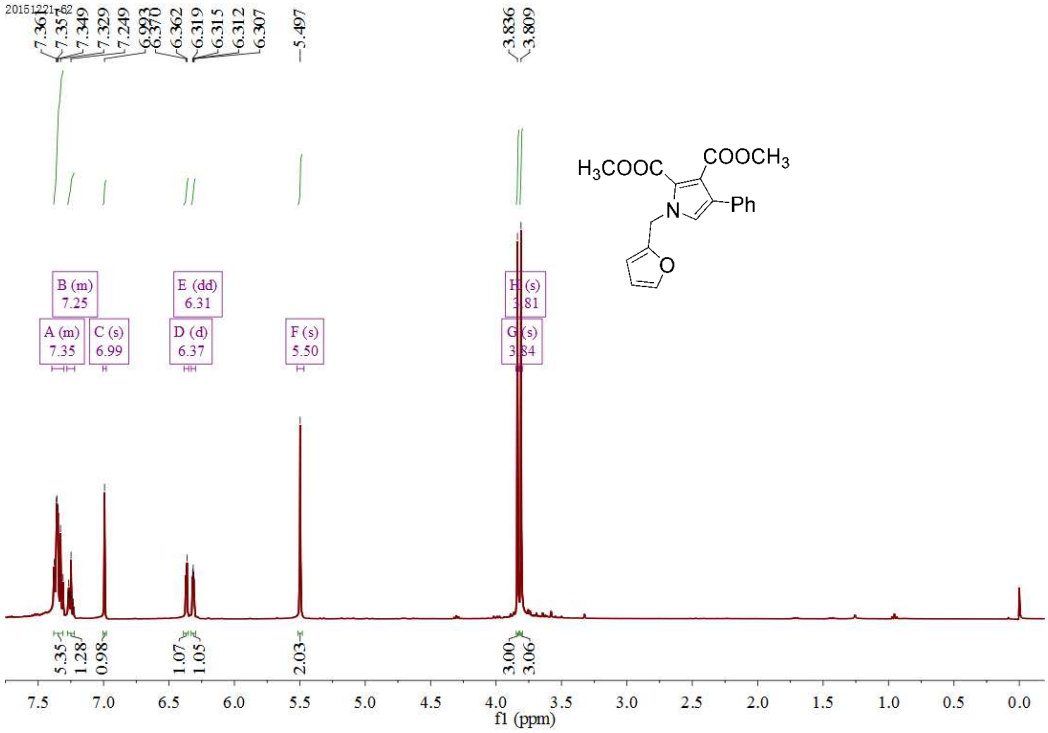

167.19
160.04
138.92
136.36
134.99
133.25
131.23
128.66
127.48
127.07
127.03
127.02
125.91
124.53
122.95
121.42
77.40
77.08
76.77
52.45
51.83
21.22
17.30
H3COOC
COOCH3
N
Ph
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

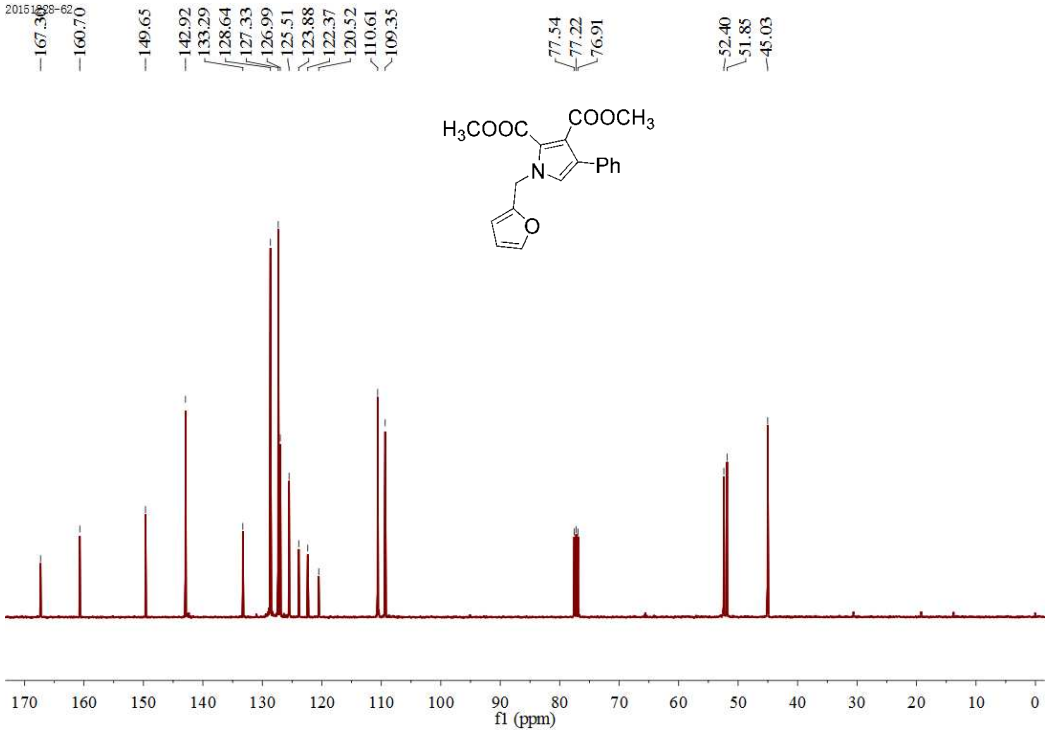
Product 4s


7.433
7.414
7.393
7.375
7.356
7.338
7.298
7.280
7.264
7.240
7.218
6.975
6.955
3.928
3.840
3.725
H3COOC
COOCH3
Cl
N
Ph
O
B (m) 7.28
A (dt) 7.38
D (s) 6.96
C (d) 7.23
F (s) 3.84
E (s) 3.93
G (s) 3.73
5.45
1.34
1.09
2.04
3.12
2.80
3.00
f1 (ppm)

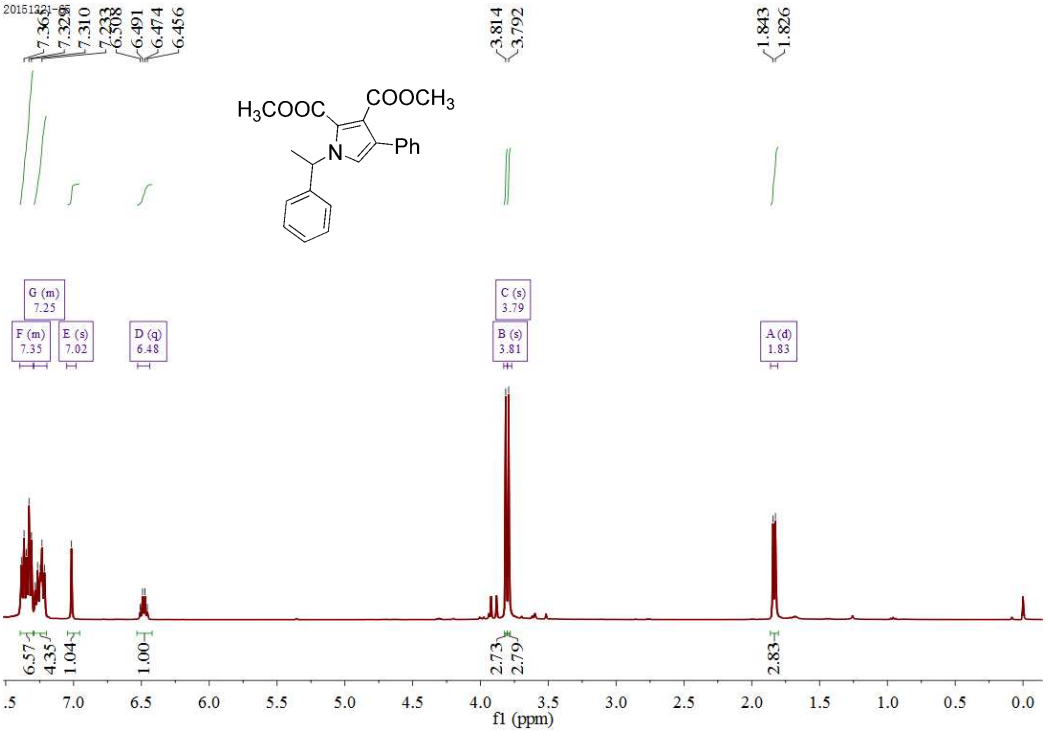

166.60
160.15
132.93
132.46
128.63
128.17
127.59
127.22
126.18
125.77
124.82
122.39
122.03
111.33
77.46
77.14
76.82
56.36
52.42
51.98
H3COOC
COOCH3
Cl
N
Ph
O
f1 (ppm)

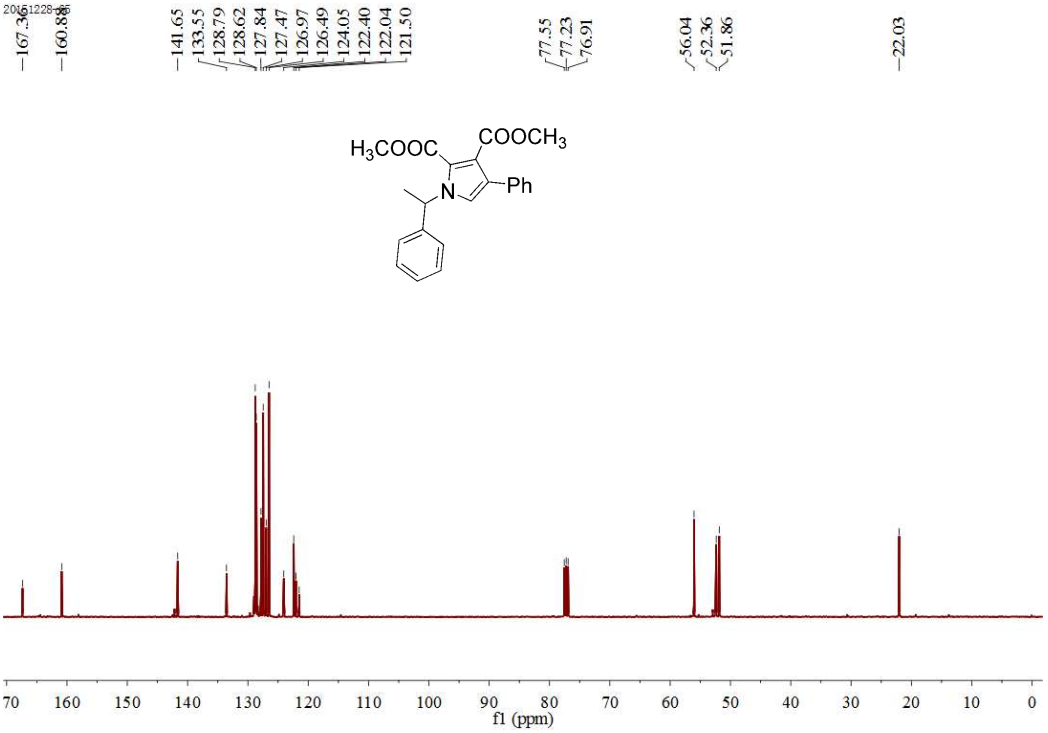
Product 4t


20151221-62
7.361
7.357
7.349
7.329
7.249
6.993
6.370
6.362
6.319
6.315
6.312
6.307
5.497
3.836
3.809
B (m) 7.25
E (dd) 6.31
H (s) 3.81
A (m) 7.35
C (s) 6.99
D (d) 6.37
F (s) 5.50
G (s) 3.84
5.35
1.28
0.98
1.07
1.05
2.03
3.00
3.06
f1 (ppm)

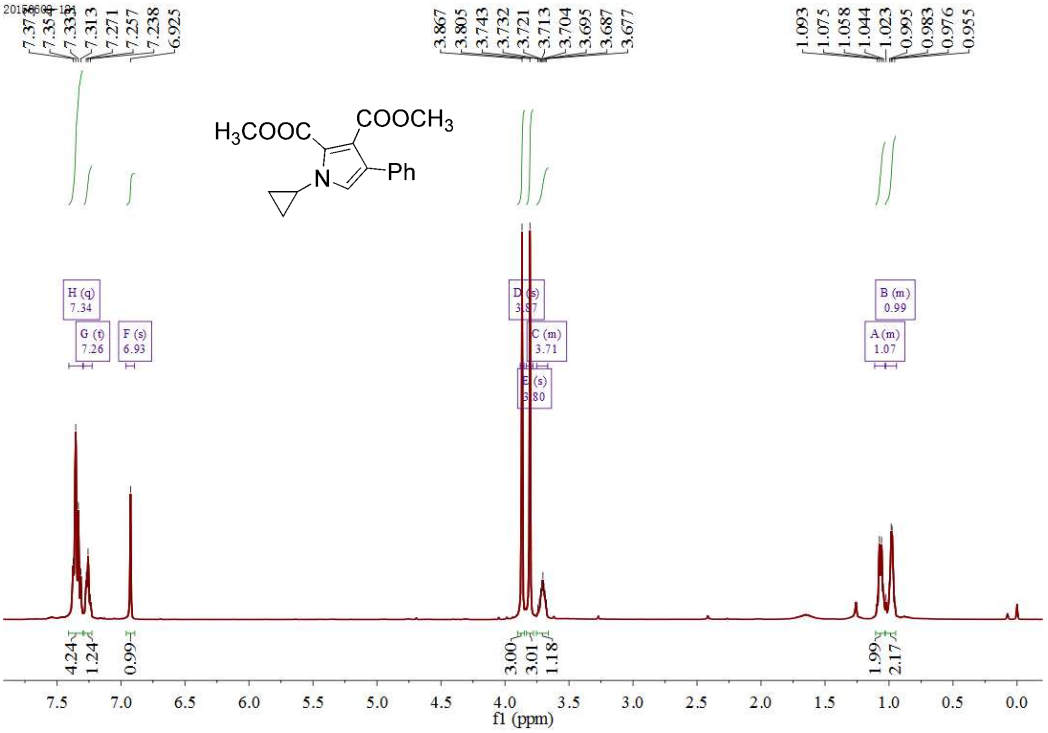

20151228-62
167.30
160.70
149.65
142.92
133.29
128.64
127.33
126.99
125.51
123.88
122.37
120.52
110.61
109.35
77.54
77.22
76.91
52.40
51.85
45.03
f1 (ppm)

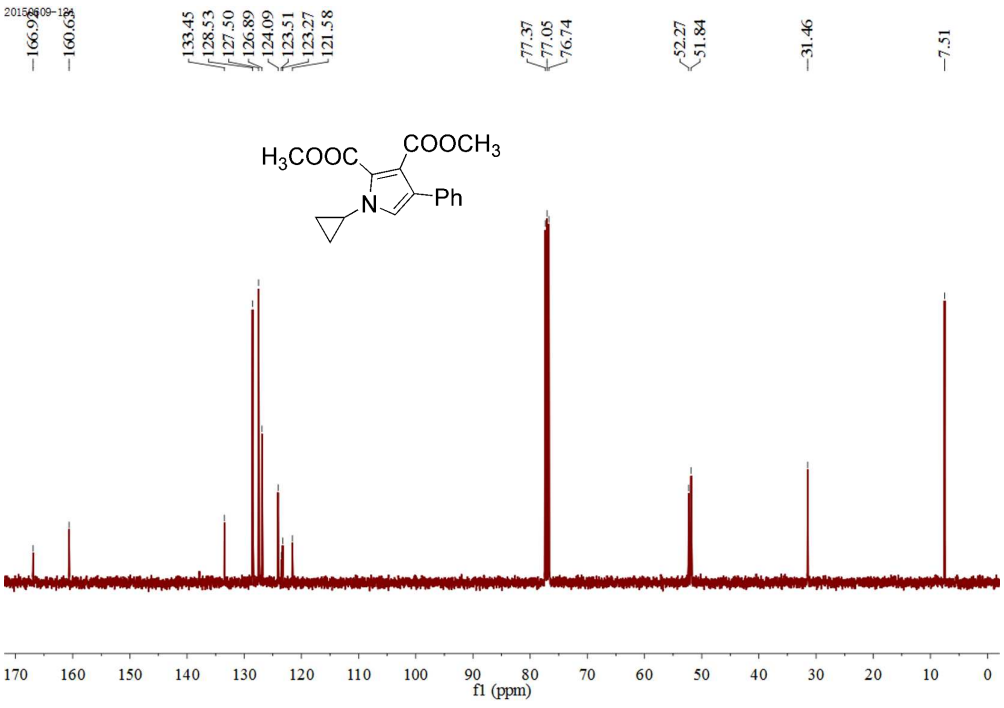
Product 4u


7.368
7.329
7.310
7.233
6.508
6.491
6.474
6.456
3.814
3.792
1.843
1.826
H3COOC
COOCH3
N
Ph
G (m) 7.25
F (m) 7.35
E (s) 7.02
D (q) 6.48
C (s) 3.79
B (s) 3.81
A (d) 1.83
6.57
4.35
1.04
1.00
2.73
2.79
2.83
f1 (ppm)

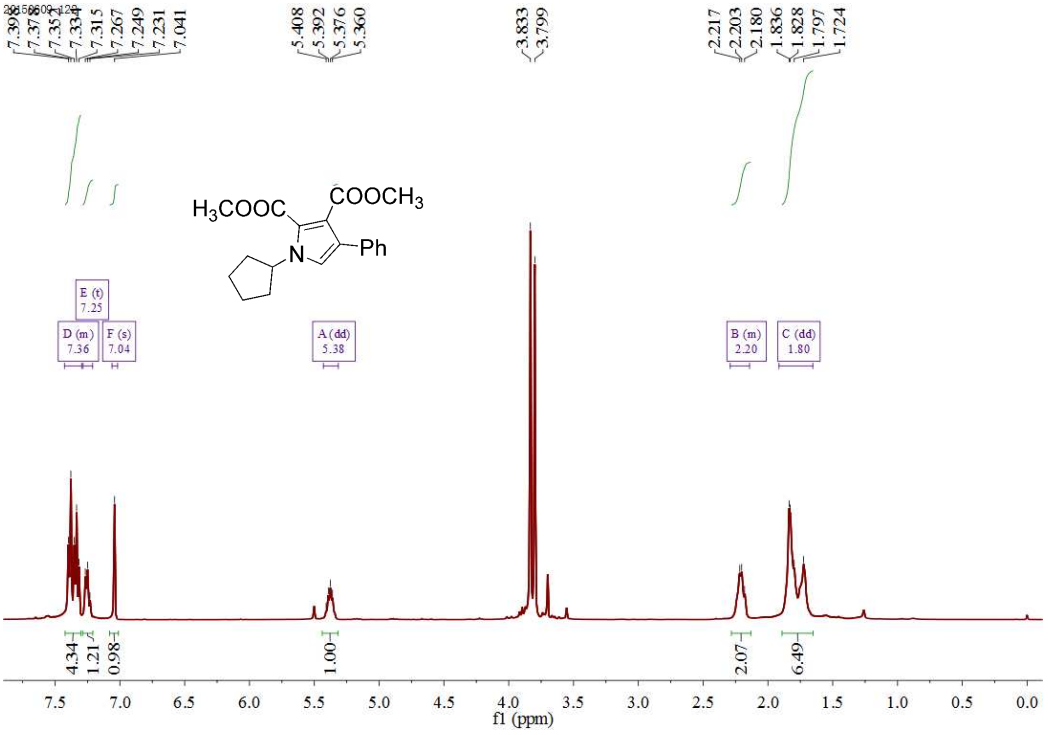

167.36
160.88
141.65
133.55
128.79
128.62
127.84
127.47
126.97
126.49
124.05
122.40
122.04
121.50
77.55
77.23
76.91
56.04
52.36
51.86
22.03
H3COOC
COOCH3
N
Ph
f1 (ppm)

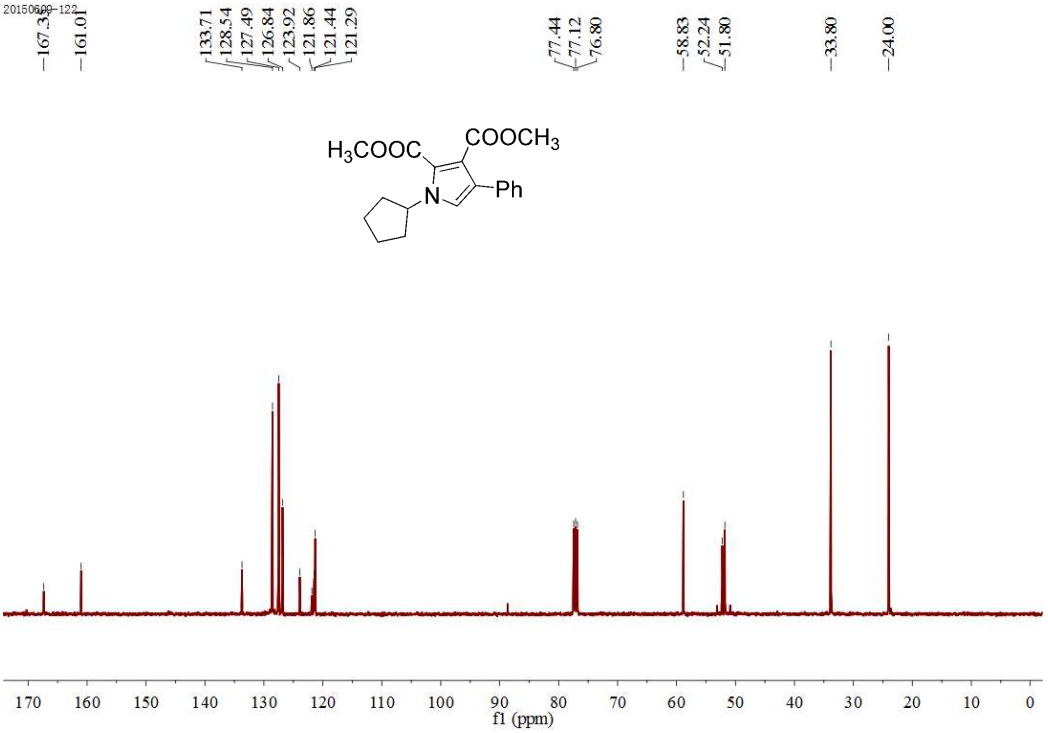
Product 4v


7.373
7.354
7.335
7.313
7.271
7.257
7.238
6.925
3.867
3.805
3.743
3.732
3.721
3.713
3.704
3.695
3.687
3.677
1.093
1.075
1.058
1.044
1.023
0.995
0.983
0.976
0.955
H3COOC
COOCH3
N
Ph
H (q) 7.34
G (t) 7.26
F (s) 6.93
D (s) 3.87
C (m) 3.71
E (s) 3.80
B (m) 0.99
A (m) 1.07
4.24
1.24
0.99
3.00
3.01
1.18
1.99
2.17
f1 (ppm)

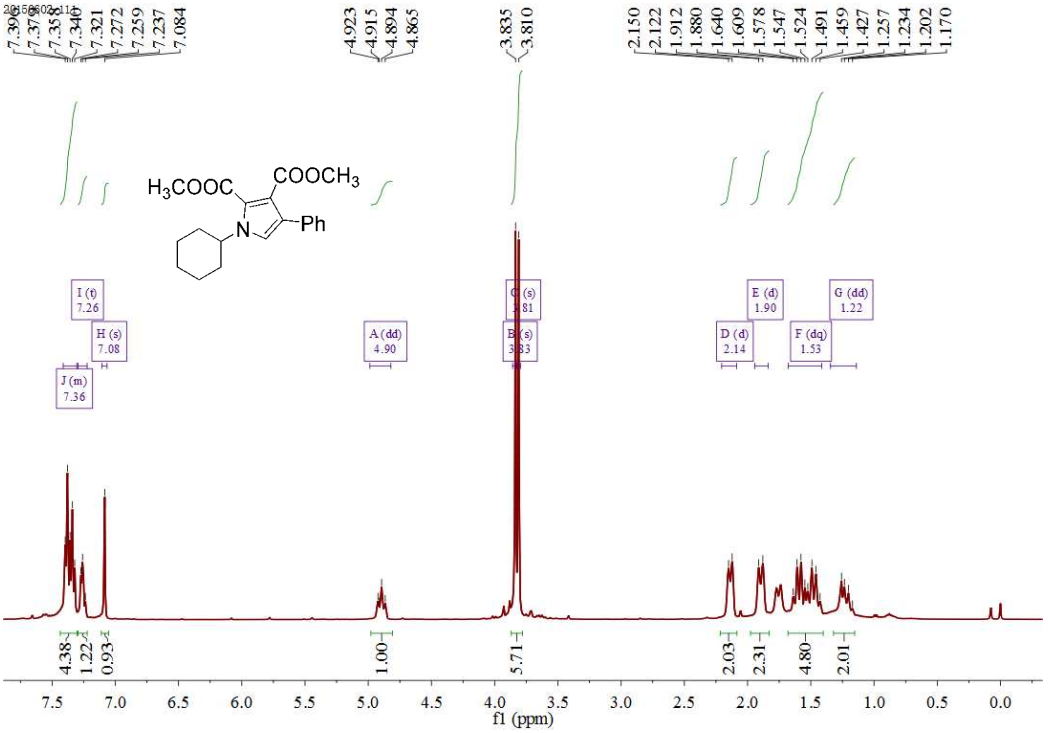

166.90
160.63
133.45
128.53
127.50
126.89
124.09
123.51
123.27
121.58
77.37
77.05
76.74
52.27
51.84
31.46
7.51
H3COOC
COOCH3
N
Ph
f1 (ppm)

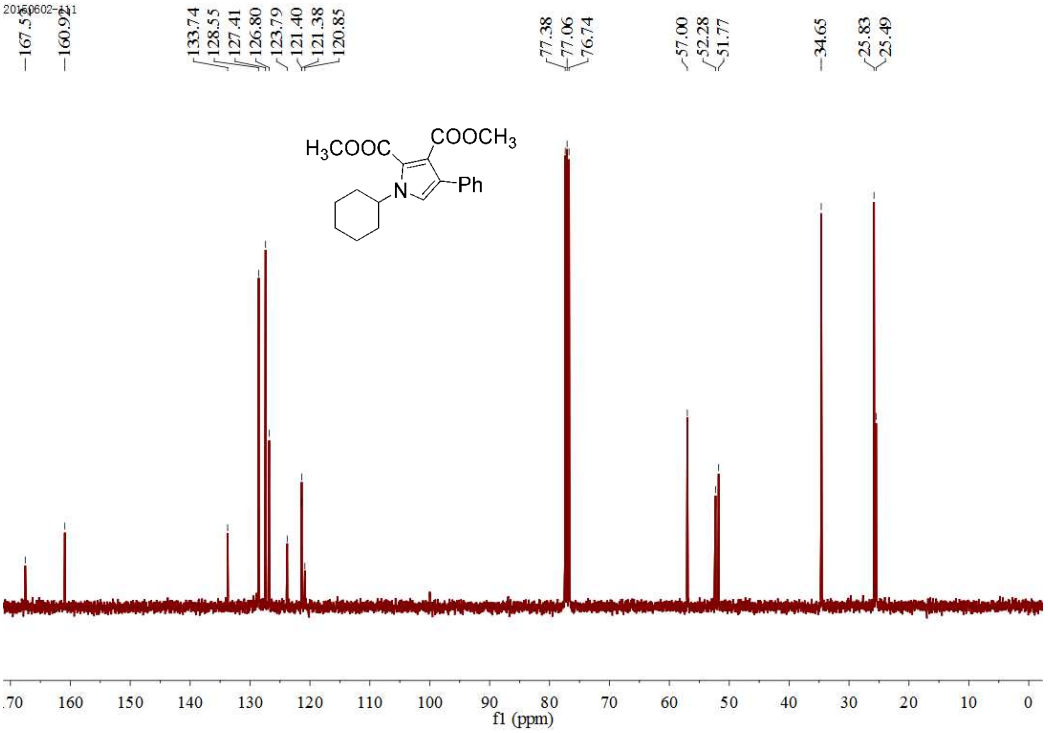
Product 4w


7.398
7.378
7.353
7.334
7.315
7.267
7.249
7.231
7.041
5.408
5.392
5.376
5.360
3.833
3.799
2.217
2.203
2.180
1.836
1.828
1.797
1.724
H3COOC
COOCH3
N
Ph
E (t) 7.25
D (m) 7.36
F (s) 7.04
A (dd) 5.38
B (m) 2.20
C (dd) 1.80
4.34
1.21
0.98
1.00
2.07
6.49
f1 (ppm)

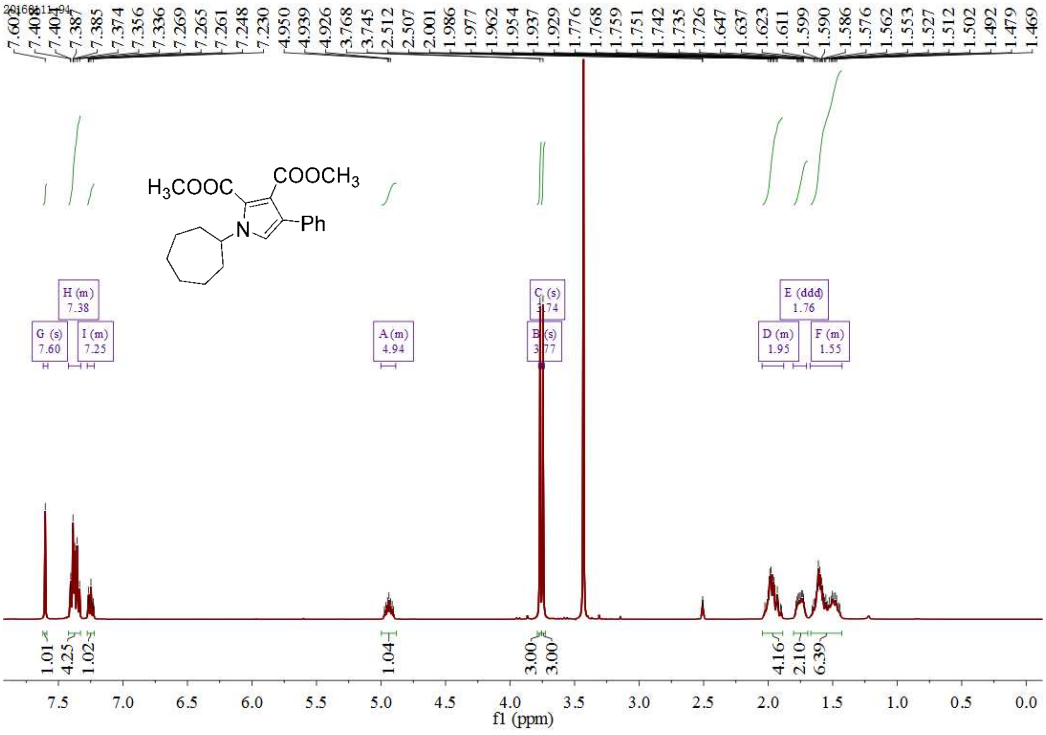

167.32
161.01
133.71
128.54
127.49
126.84
123.92
121.86
121.44
121.29
77.44
77.12
76.80
58.83
52.24
51.80
33.80
24.00
H3COOC
COOCH3
N
Ph
f1 (ppm)

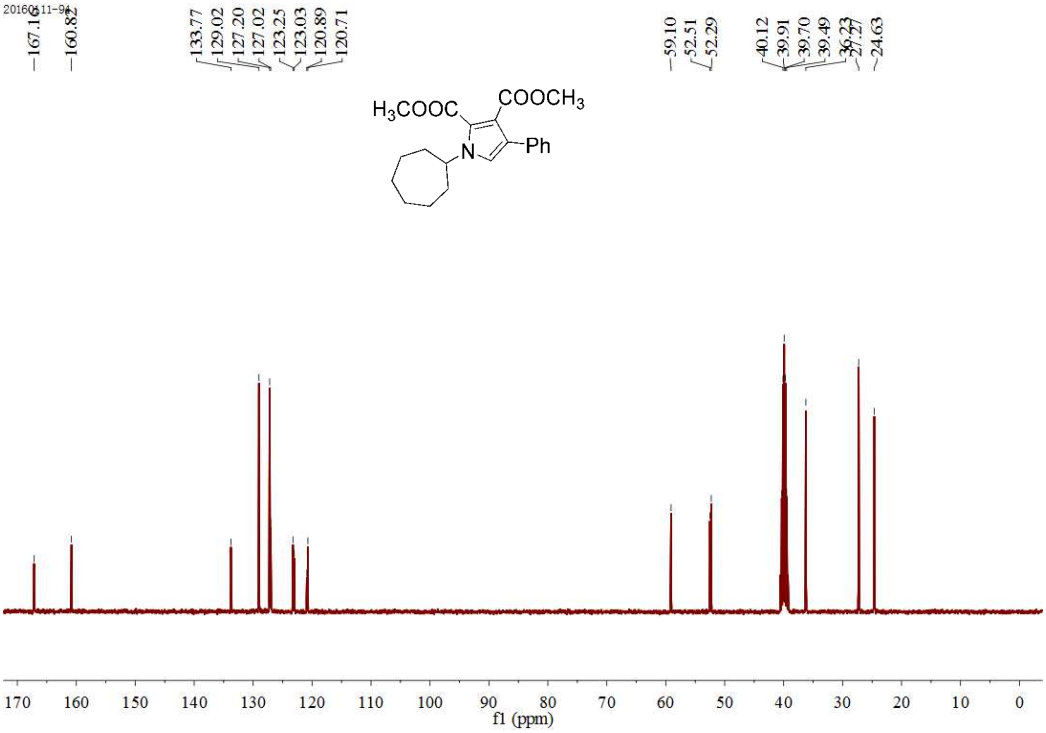
Product 4x


7.396
7.379
7.358
7.346
7.321
7.272
7.259
7.237
7.084
4.923
4.915
4.894
4.865
3.835
3.810
2.150
2.122
1.912
1.880
1.640
1.609
1.578
1.547
1.524
1.491
1.459
1.427
1.257
1.234
1.202
1.170
H3COOC
COOCH3
N
Ph
I (t) 7.26
H (s) 7.08
J (m) 7.36
A (dd) 4.90
C (s) 3.81
B (s) 3.83
E (d) 1.90
G (dd) 1.22
D (d) 2.14
F (dq) 1.53
4.38
1.22
0.93
1.00
5.71
2.03
2.31
4.80
2.01
f1 (ppm)

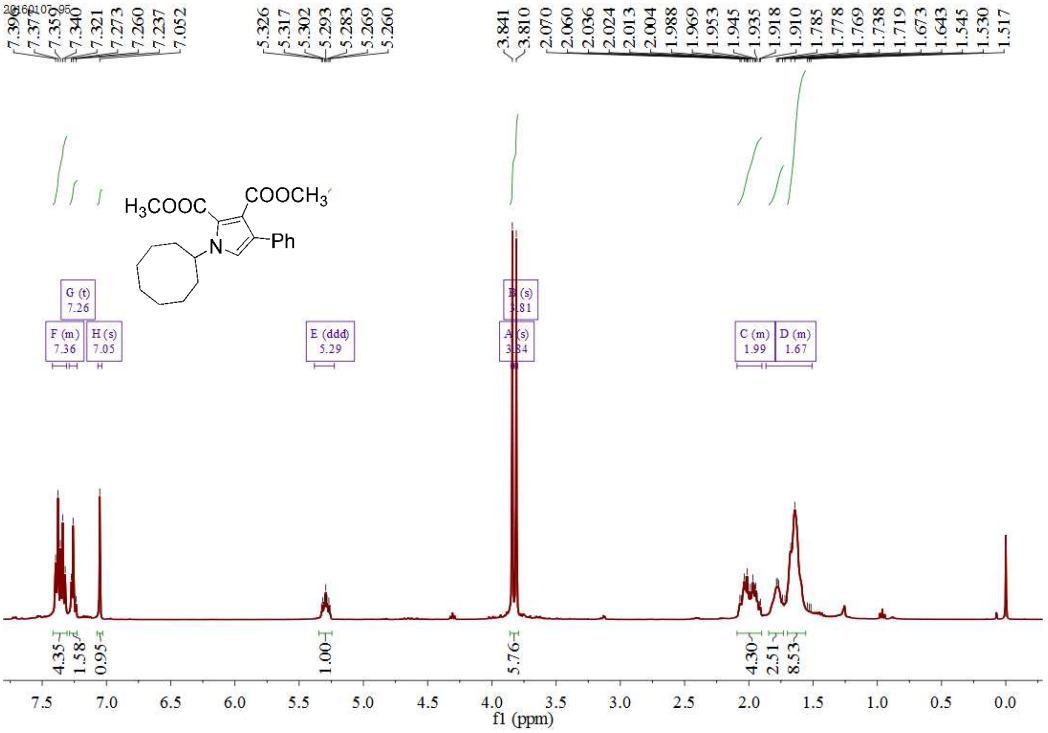

167.5
160.92
133.74
128.55
127.41
126.80
123.79
121.40
121.38
120.85
77.38
77.06
76.74
57.00
52.28
51.77
34.65
25.83
25.49
H3COOC
COOCH3
N
Ph
f1 (ppm)

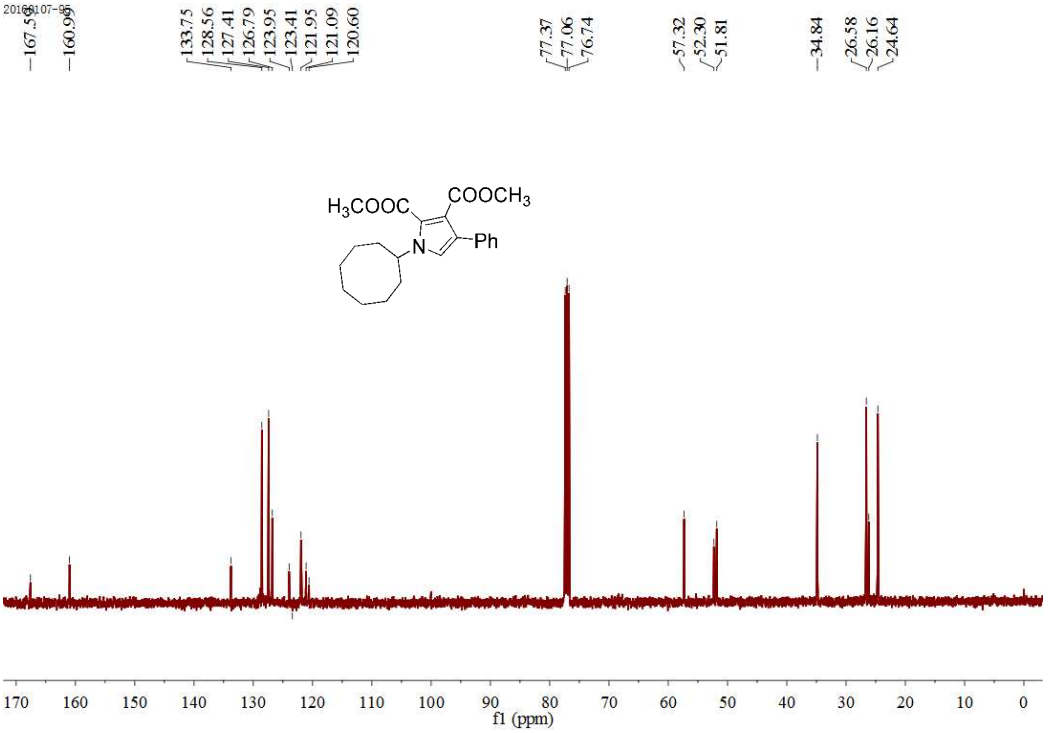
Product 4y


H3COOC
COOCH3
N
Ph
H (m) 7.38
G (s) 7.60
I (m) 7.25
A (m) 4.94
C (s) 3.74
B (s) 3.77
E (ddd) 1.76
D (m) 1.95
F (m) 1.55
1.01
4.25
1.02
1.04
3.00
3.00
4.16
2.10
6.39
f1 (ppm)

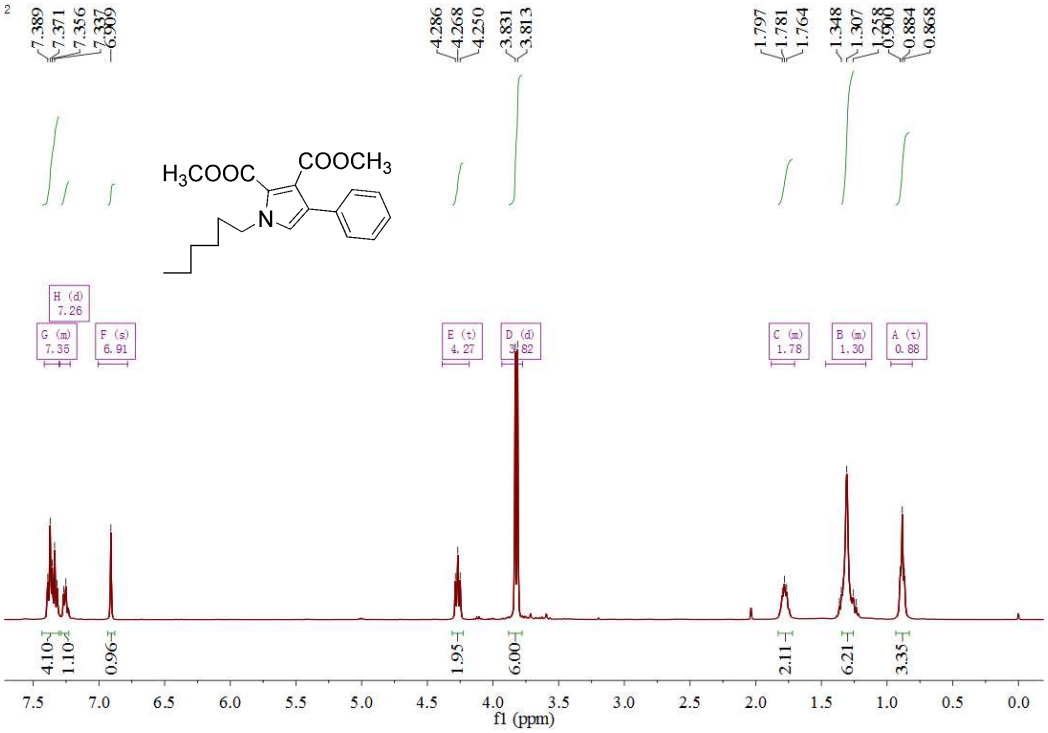

H3COOC
COOCH3
N
Ph
f1 (ppm)

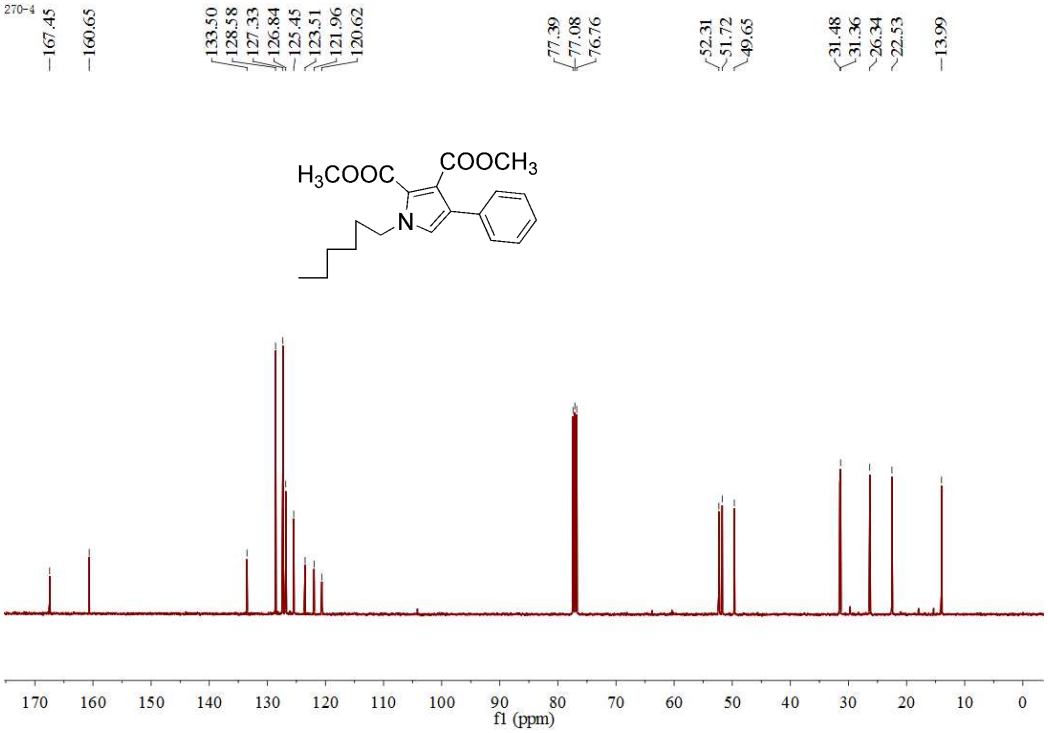
Product 4z


20160107-95
7.396
7.375
7.359
7.340
7.321
7.273
7.260
7.237
7.052
5.326
5.317
5.302
5.293
5.283
5.269
5.260
3.841
3.810
2.070
2.060
2.036
2.024
2.013
2.004
1.988
1.969
1.953
1.945
1.935
1.918
1.910
1.785
1.778
1.769
1.738
1.719
1.673
1.643
1.545
1.530
1.517
H3COOC
COOCH3
N
Ph
G (t) 7.26
F (m) 7.36
H (s) 7.05
E (ddd) 5.29
B (s) 3.81
A (s) 3.84
C (m) 1.99
D (m) 1.67
4.35
1.58
0.95
1.00
5.76
4.30
2.51
8.53
f1 (ppm)

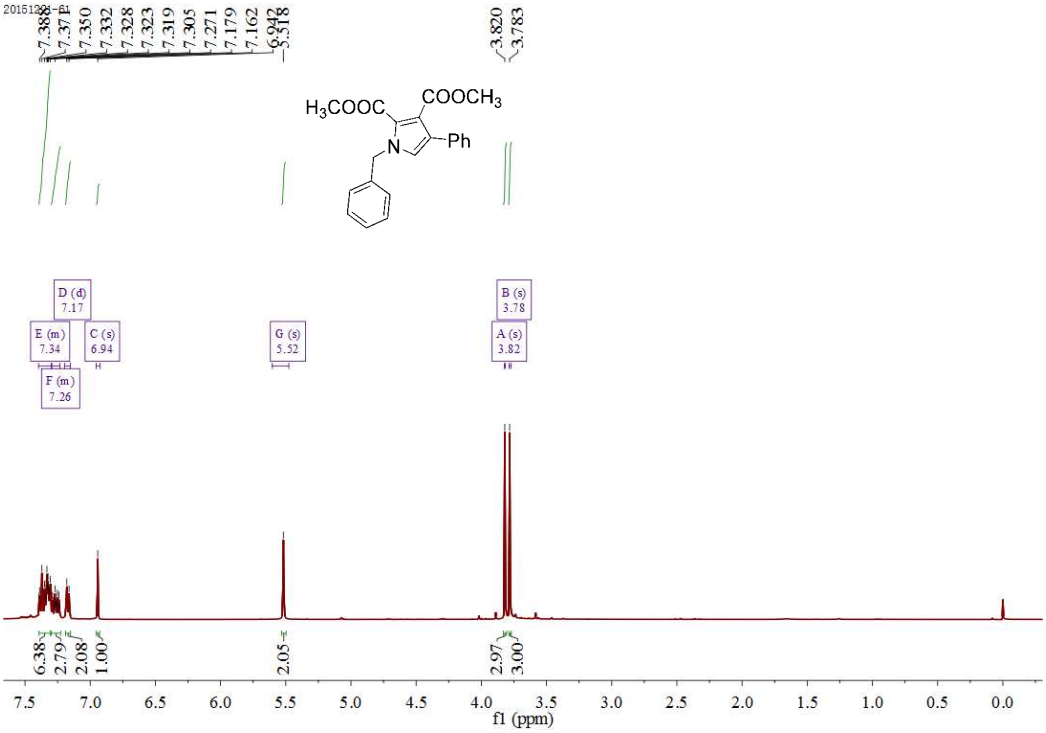

20160107-95
167.56
160.99
133.75
128.56
127.41
126.79
123.95
123.41
121.95
121.09
120.60
77.37
77.06
76.74
57.32
52.30
51.81
34.84
26.58
26.16
24.64
H3COOC
COOCH3
N
Ph
f1 (ppm)

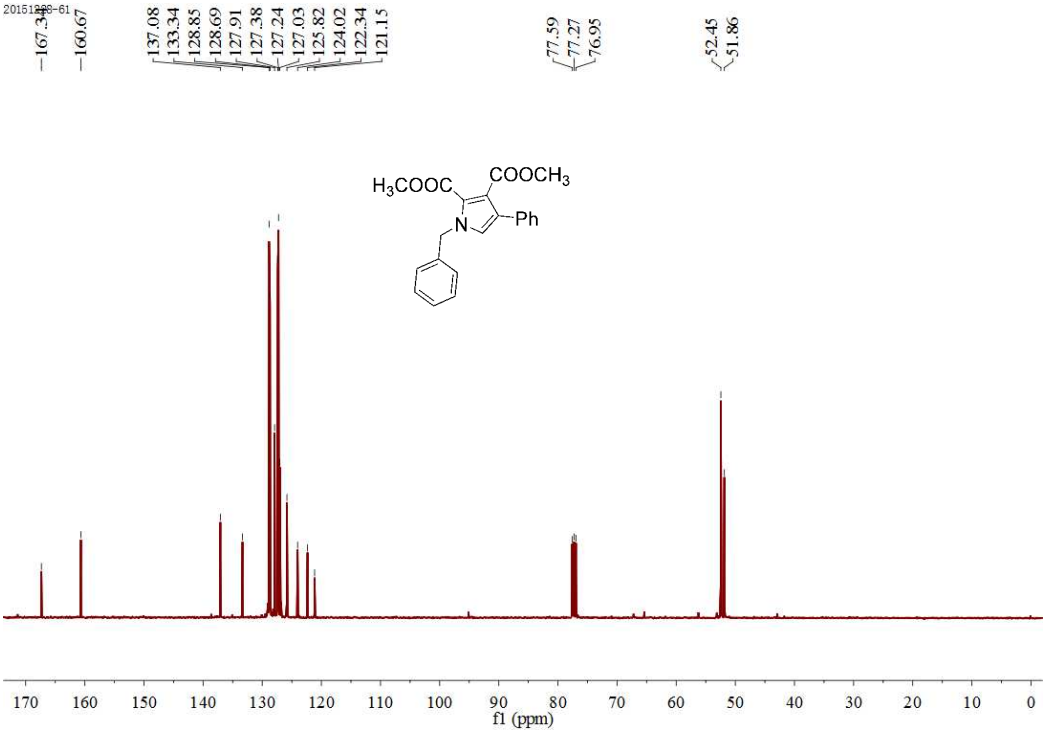
Product 5a


7.389
7.371
7.356
7.337
6.906
4.286
4.268
4.250
3.831
3.813
1.797
1.781
1.764
1.348
1.307
1.258
0.900
0.884
0.868
H3COOC
COOCH3
N
H (d) 7.26
G (m) 7.36
F (s) 6.91
E (t) 4.27
D (d) 3.82
C (m) 1.78
B (m) 1.30
A (t) 0.88
4.10
1.10
0.96
1.95
6.00
2.11
6.21
3.35
f1 (ppm)

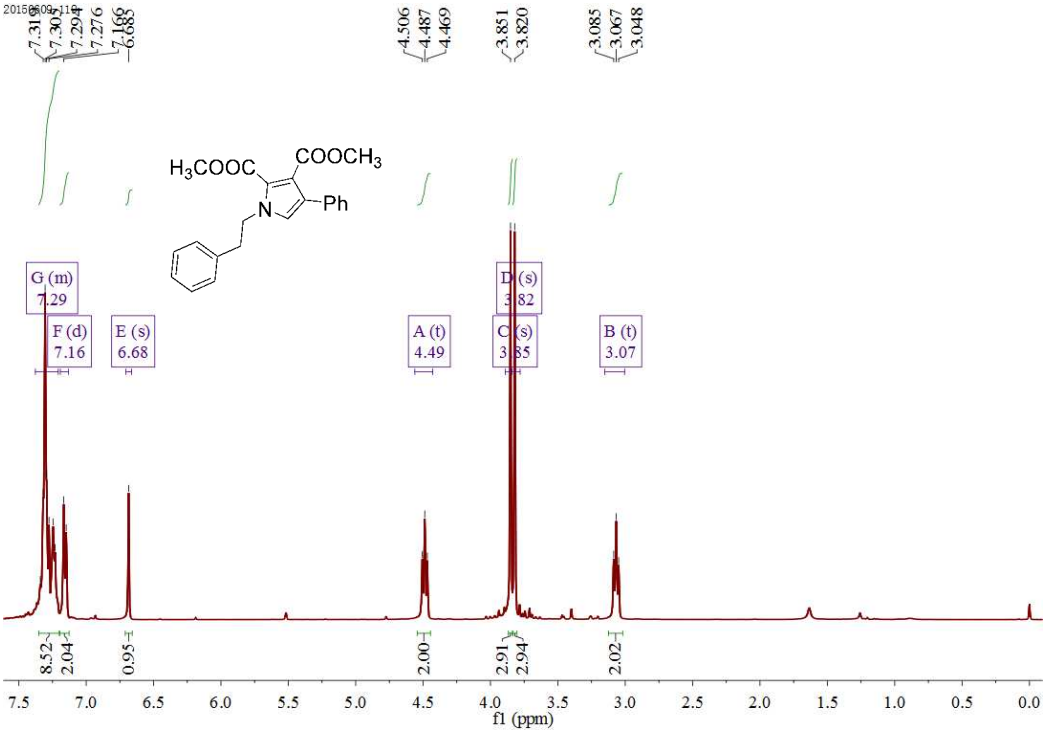

167.45
160.65
133.50
128.58
127.33
126.84
125.45
123.51
121.96
120.62
77.39
77.08
76.76
52.31
51.72
49.65
31.48
31.36
26.34
22.53
13.99
H3COOC
COOCH3
N
f1 (ppm)

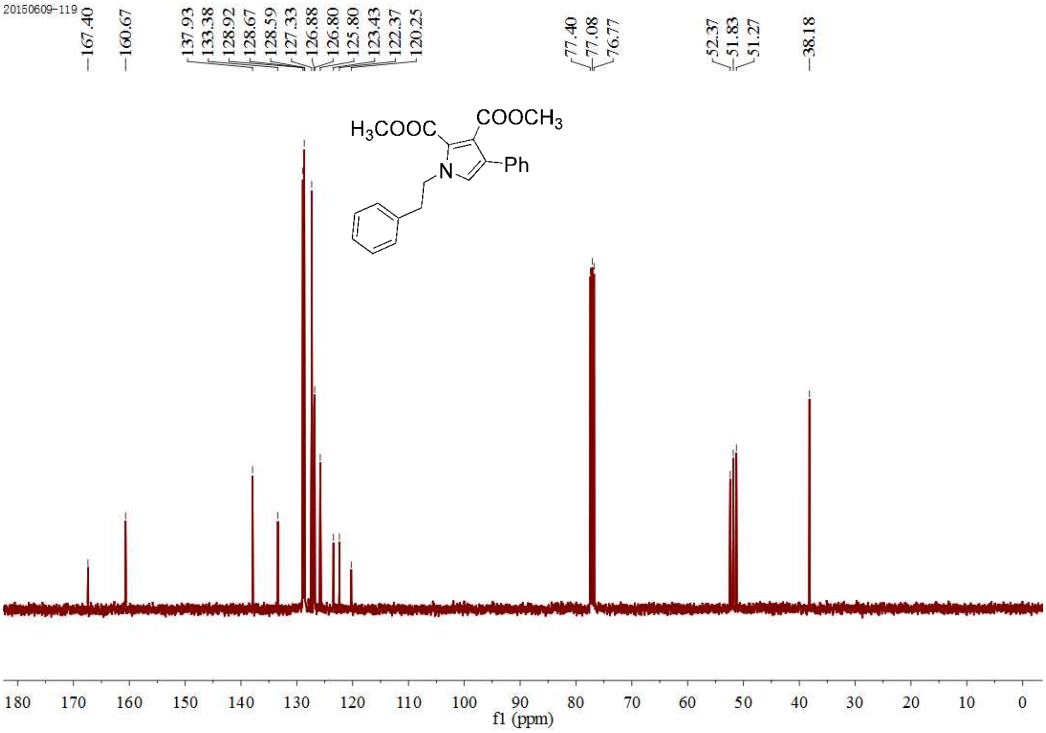
Product 5b


7.388
7.371
7.350
7.332
7.328
7.323
7.319
7.305
7.271
7.179
7.162
6.942
5.518
3.820
3.783
H3COOC
COOCH3
N
Ph
D (d) 7.17
E (m) 7.34
C (s) 6.94
F (m) 7.26
G (s) 5.52
B (s) 3.78
A (s) 3.82
6.38
2.79
2.08
1.00
2.05
2.97
3.00
f1 (ppm)

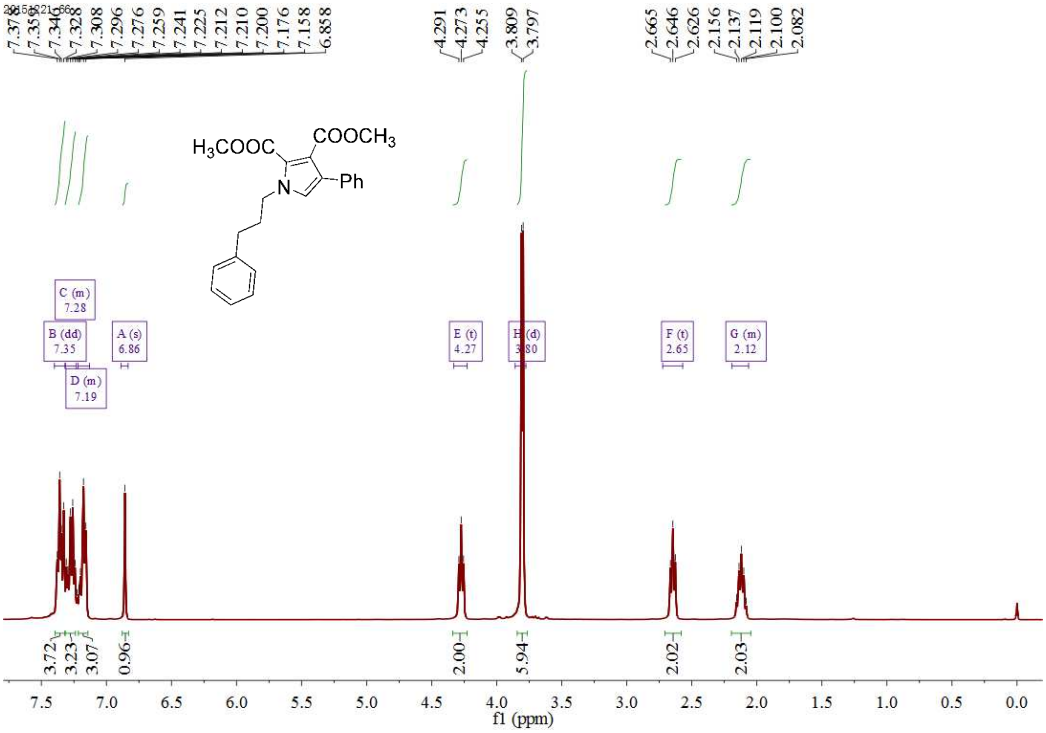

167.34
160.67
137.08
133.34
128.85
128.69
127.91
127.38
127.24
127.03
125.82
124.02
122.34
121.15
77.59
77.27
76.95
52.45
51.86
H3COOC
COOCH3
N
Ph
f1 (ppm)

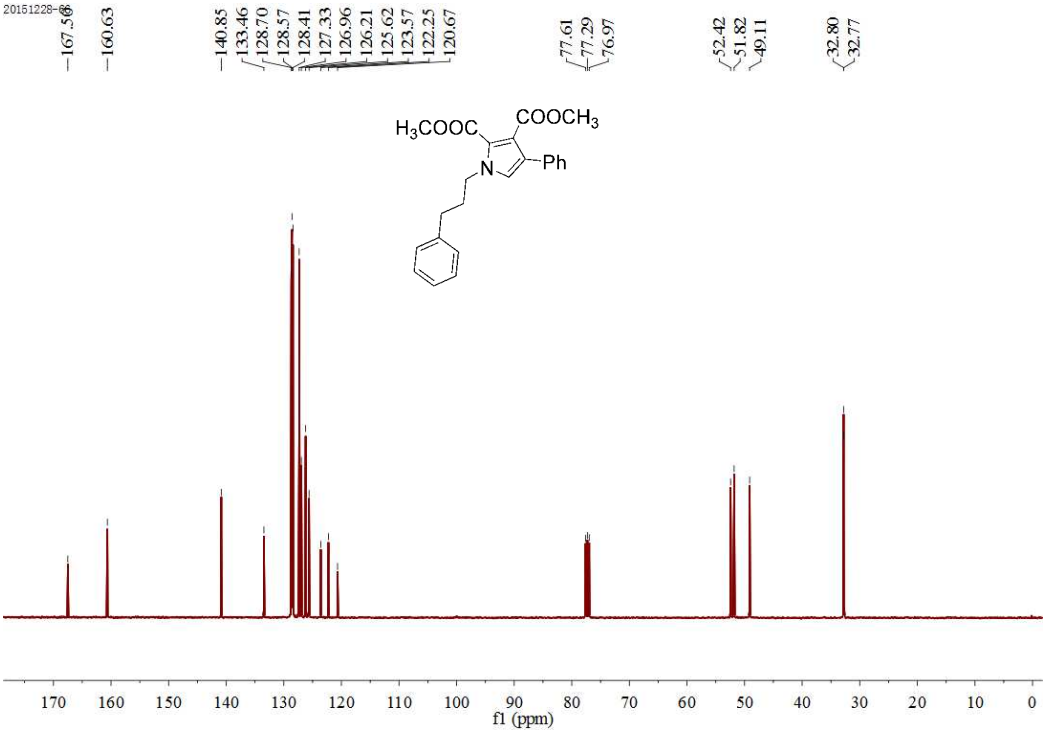
Product 5c


7.316
7.305
7.294
7.276
7.166
6.685
4.506
4.487
4.469
3.851
3.820
3.085
3.067
3.048
H3COOC
COOCH3
N
Ph
G (m)
7.29
F (d)
7.16
E (s)
6.68
A (t)
4.49
D (s)
3.82
C (s)
3.85
B (t)
3.07
8.52
2.04
0.95
2.00
2.91
2.94
2.02
f1 (ppm)

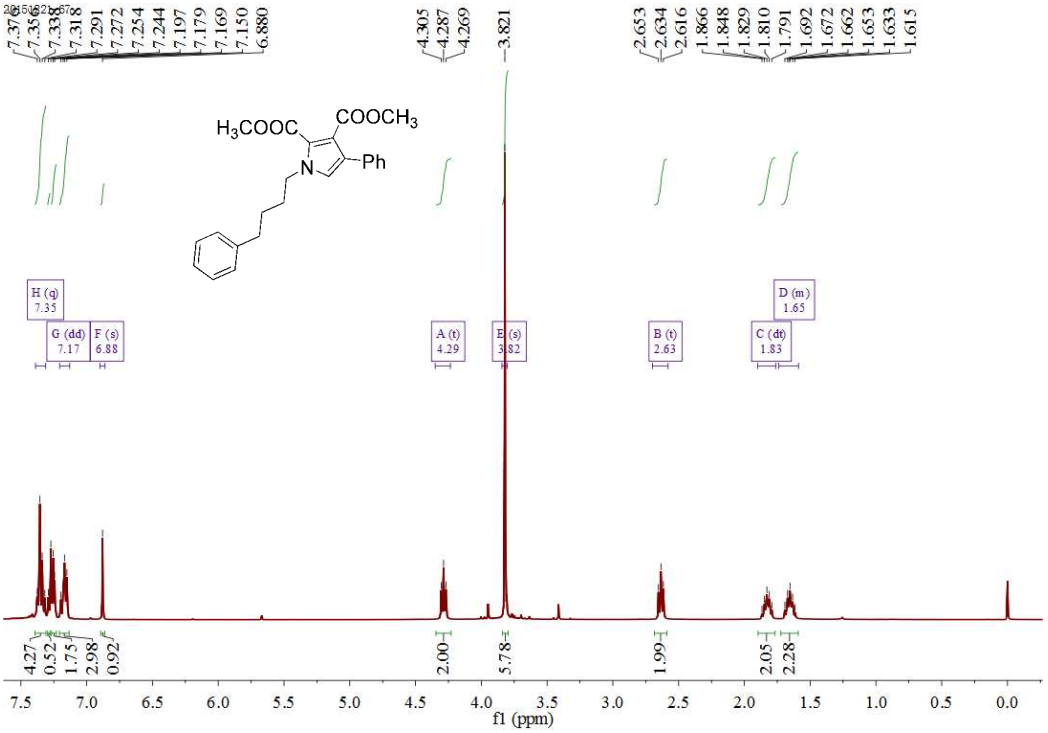

20150609-119
167.40
160.67
137.93
133.38
128.92
128.67
128.59
127.33
126.88
126.80
125.80
123.43
122.37
120.25
77.40
77.08
76.77
52.37
51.83
51.27
38.18
H3COOC
COOCH3
N
Ph
f1 (ppm)

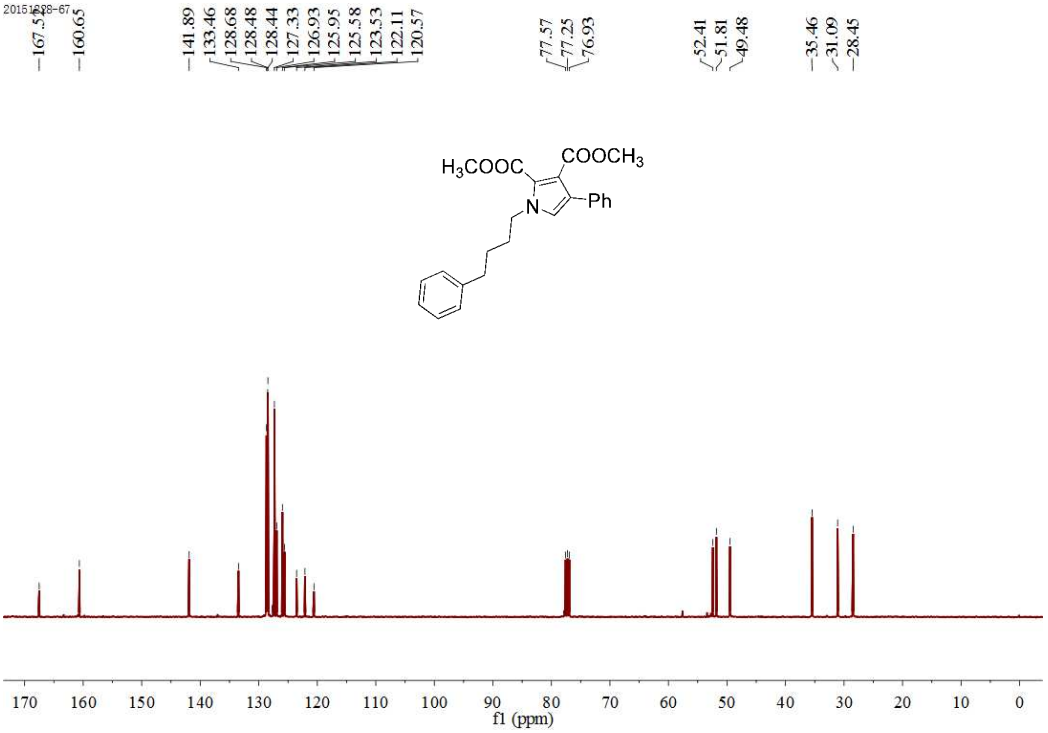
Product 5d


7.378
7.359
7.346
7.328
7.308
7.296
7.276
7.259
7.241
7.225
7.212
7.210
7.200
7.176
7.158
6.858
4.291
4.273
4.255
3.809
3.797
2.665
2.646
2.626
2.156
2.137
2.119
2.100
2.082
H3COOC
COOCH3
N
Ph
C (m) 7.28
B (dd) 7.35
A (s) 6.86
D (m) 7.19
E (t) 4.27
H (d) 3.80
F (t) 2.65
G (m) 2.12
3.72
3.23
3.07
0.96
2.00
5.94
2.02
2.03
f1 (ppm)

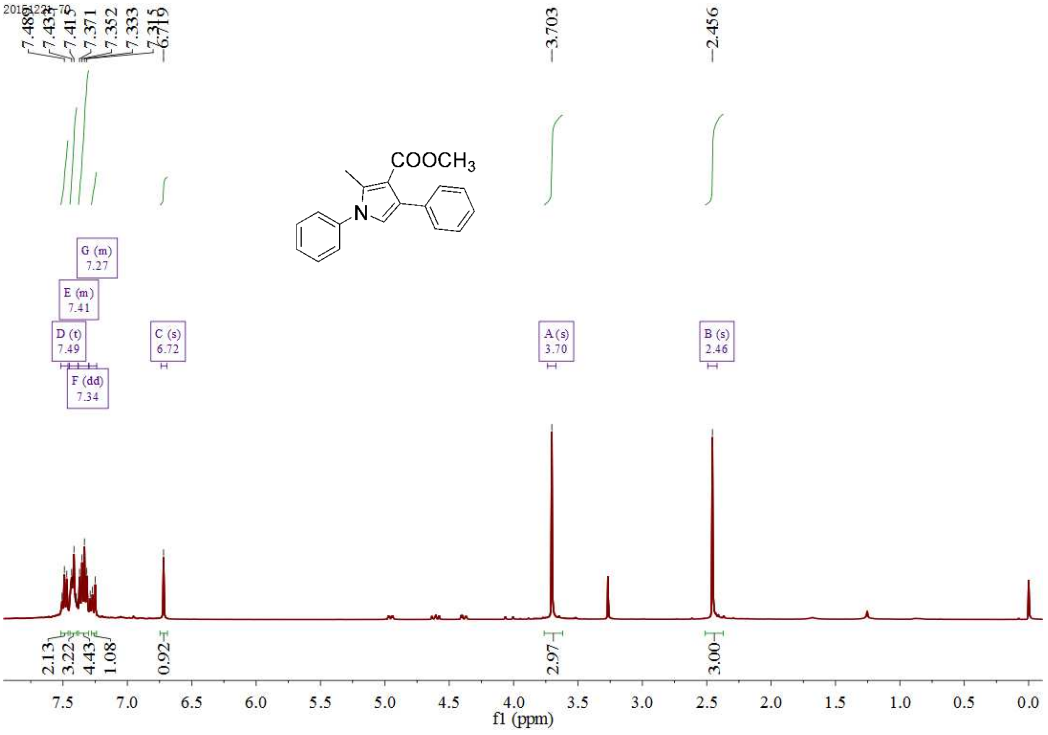

167.56
160.63
140.85
133.46
128.70
128.57
128.41
127.33
126.96
126.21
125.62
123.57
122.25
120.67
77.61
77.29
76.97
52.42
51.82
49.11
32.80
32.77
H3COOC
COOCH3
N
Ph
f1 (ppm)

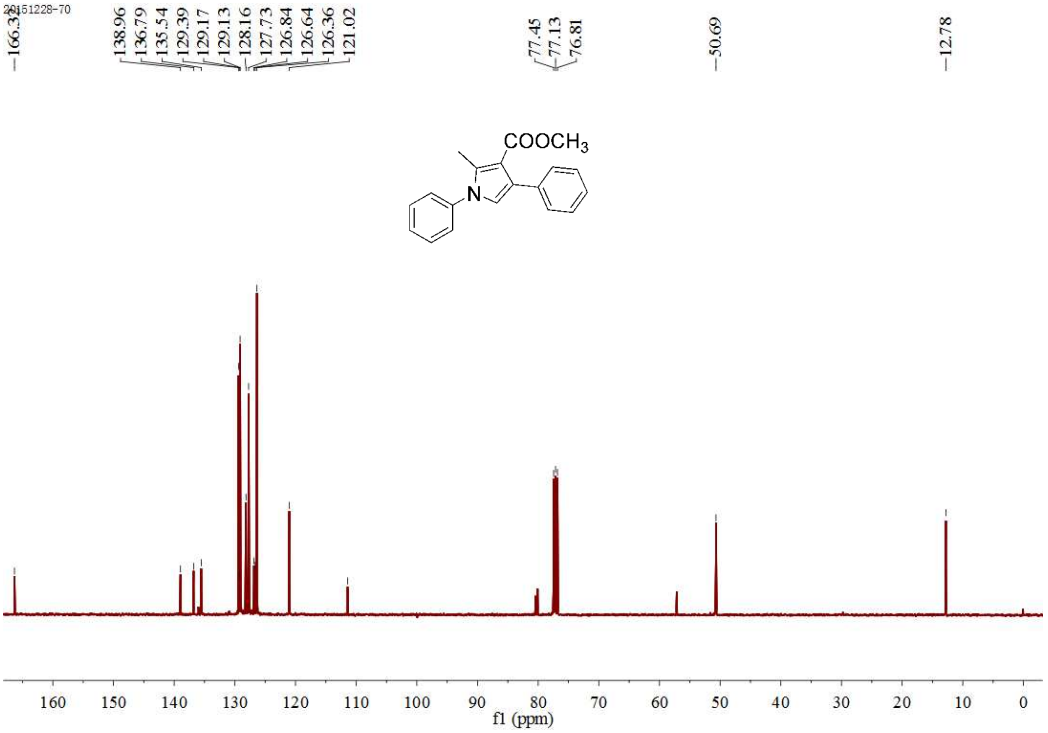
Product 5e


7.376
7.356
7.338
7.318
7.291
7.272
7.254
7.244
7.197
7.179
7.169
7.150
6.880
4.305
4.287
4.269
3.821
2.653
2.634
2.616
1.866
1.848
1.829
1.810
1.791
1.692
1.672
1.662
1.653
1.633
1.615
H3COOC
COOCH3
N
Ph
H (q) 7.35
G (dd) 7.17
F (s) 6.88
A (t) 4.29
E (s) 3.82
B (t) 2.63
D (m) 1.65
C (dt) 1.83
4.27
0.52
1.75
2.98
0.92
2.00
5.78
1.99
2.05
2.28
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
f1 (ppm)

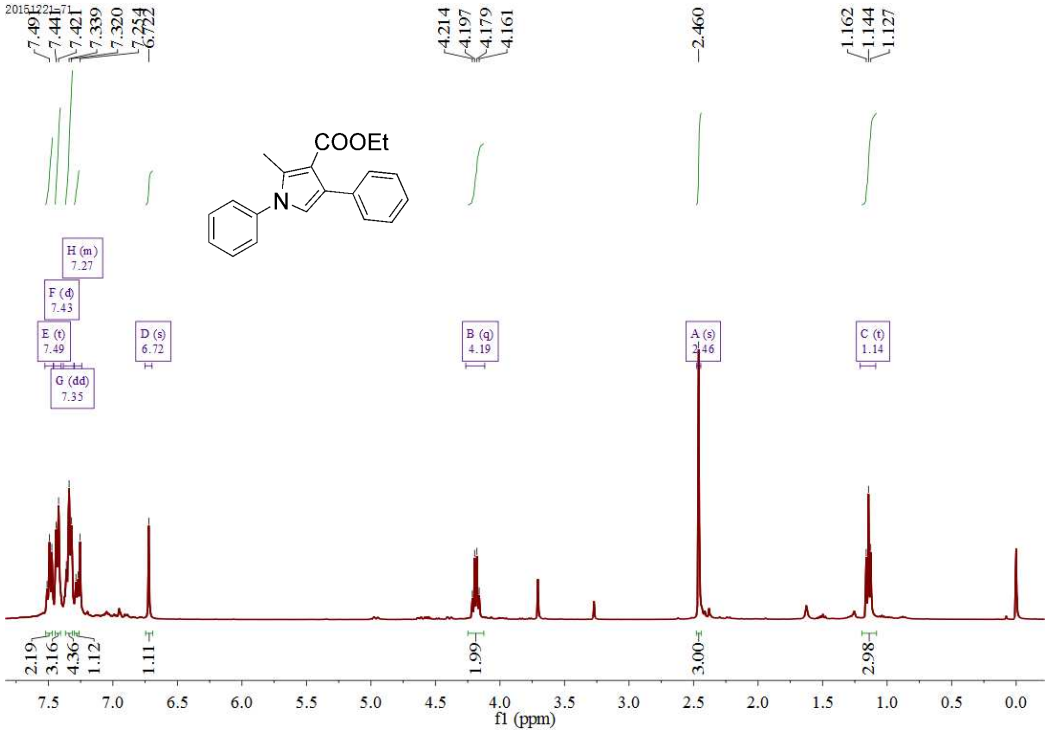

167.51
160.65
141.89
133.46
128.68
128.48
128.44
127.33
126.93
125.95
125.58
123.53
122.11
120.57
77.57
77.25
76.93
52.41
51.81
49.48
35.46
31.09
28.45
H3COOC
COOCH3
N
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

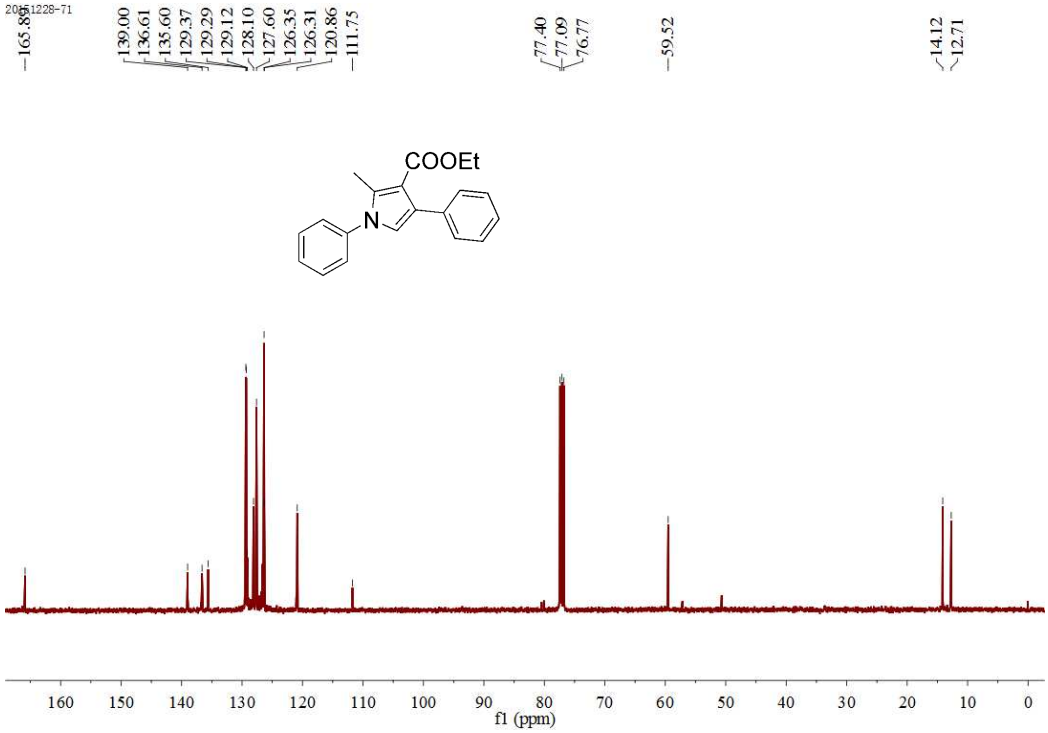
Product 6a


7.489
7.433
7.415
7.371
7.352
7.333
7.315
6.716
3.703
2.456
COOCH3
N
G (m) 7.27
E (m) 7.41
D (t) 7.49
F (dd) 7.34
C (s) 6.72
A (s) 3.70
B (s) 2.46
2.13
3.22
4.43
1.08
0.92
2.97
3.00
f1 (ppm)

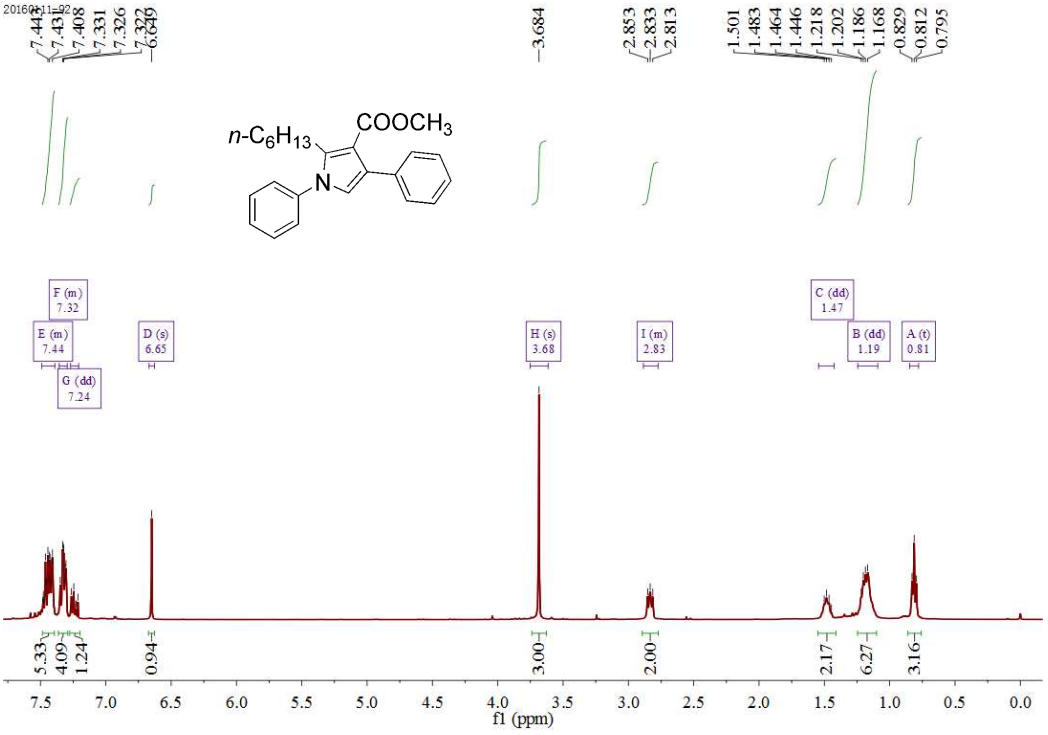

166.30
138.96
136.79
135.54
129.39
129.17
129.13
128.16
127.73
126.84
126.64
126.36
121.02
77.45
77.13
76.81
50.69
12.78
COOCH3
N
f1 (ppm)

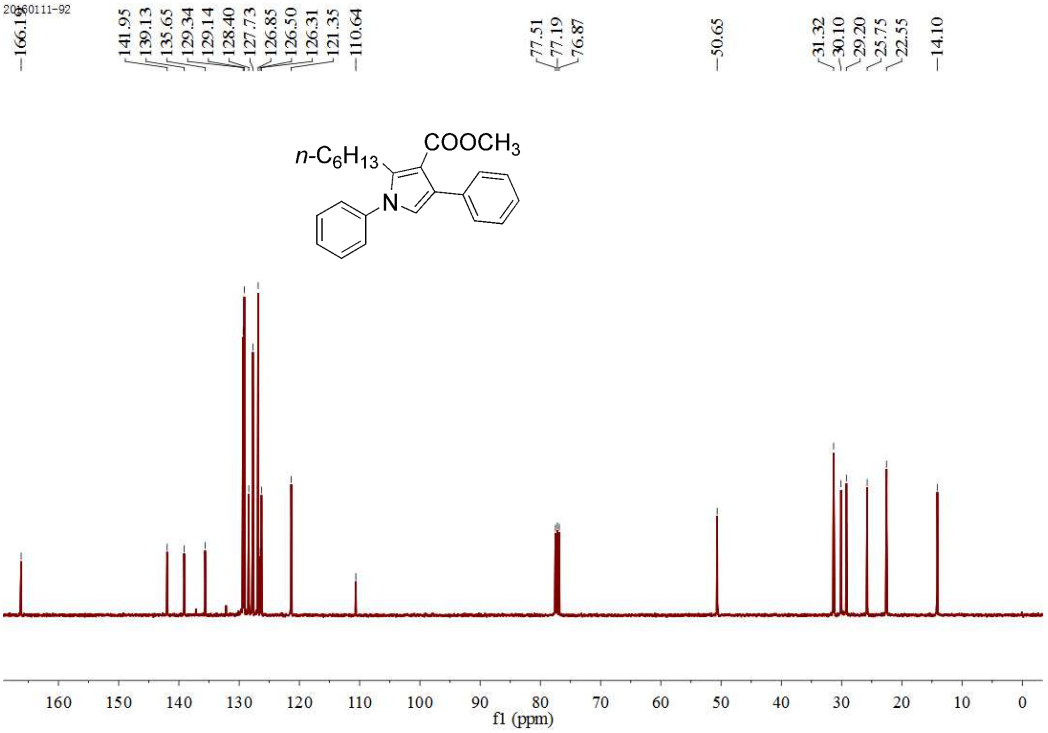
Product 6b


20151221-71
7.491
7.441
7.421
7.339
7.320
7.254
6.722
4.214
4.197
4.179
4.161
2.460
1.162
1.144
1.127
COOEt
N
H (m) 7.27
F (d) 7.43
E (t) 7.49
G (dd) 7.35
D (s) 6.72
B (q) 4.19
A (s) 2.46
C (t) 1.14
2.19
3.16
4.36
1.12
1.11
1.99
3.00
2.98
f1 (ppm)

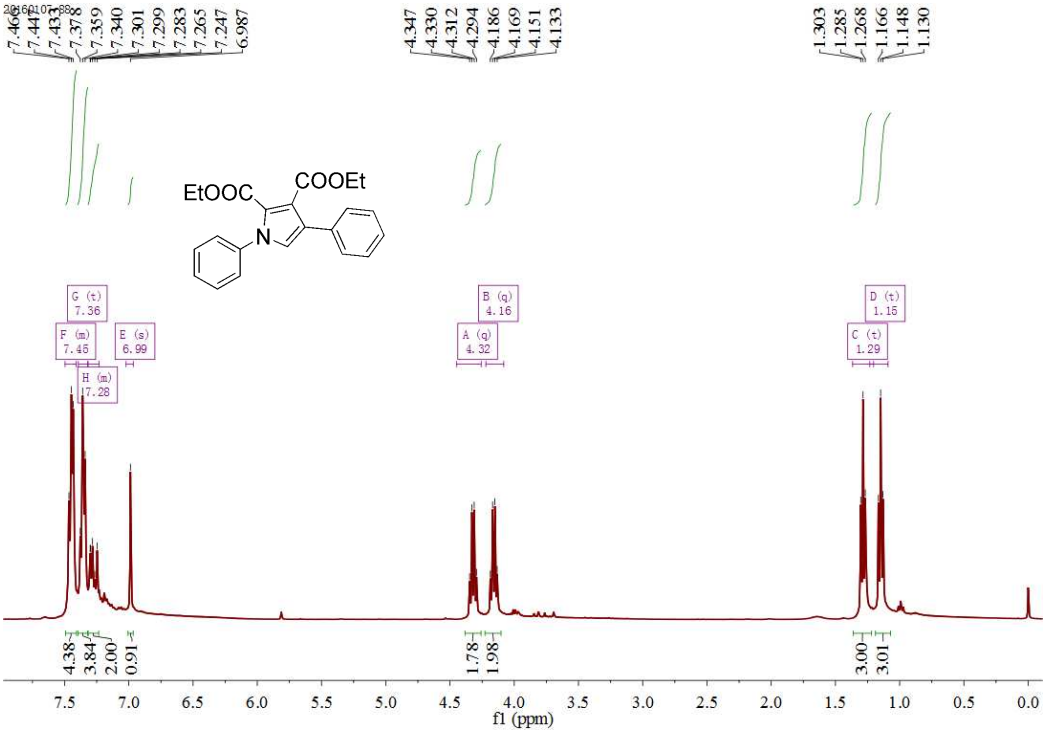

20151228-71
165.88
139.00
136.61
135.60
129.37
129.29
129.12
128.10
127.60
126.35
126.31
120.86
111.75
77.40
77.09
76.77
59.52
14.12
12.71
COOEt
N
f1 (ppm)

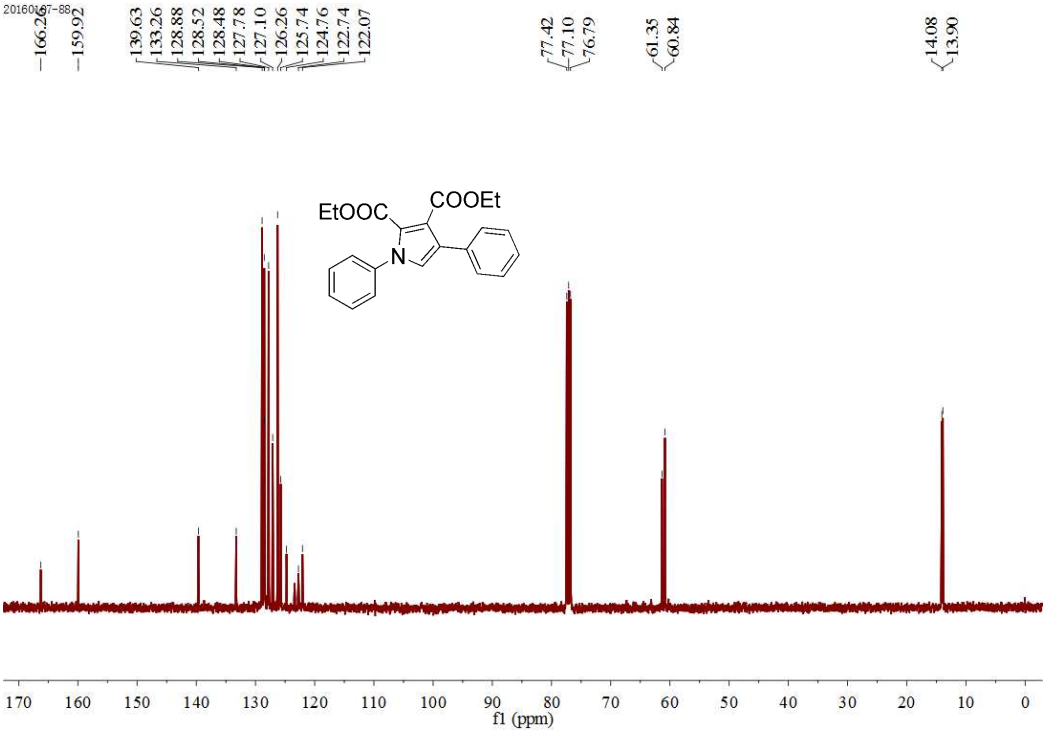
Product 6c


7.445
7.431
7.408
7.331
7.326
7.322
6.649
3.684
2.853
2.833
2.813
1.501
1.483
1.464
1.446
1.218
1.202
1.186
1.168
0.829
0.812
0.795
n-C6H13
COOCH3
N
F (m) 7.32
E (m) 7.44
G (dd) 7.24
D (s) 6.65
H (s) 3.68
I (m) 2.83
C (dd) 1.47
B (dd) 1.19
A (t) 0.81
5.33
4.09
1.24
0.94
3.00
2.00
2.17
6.27
3.16
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
f1 (ppm)

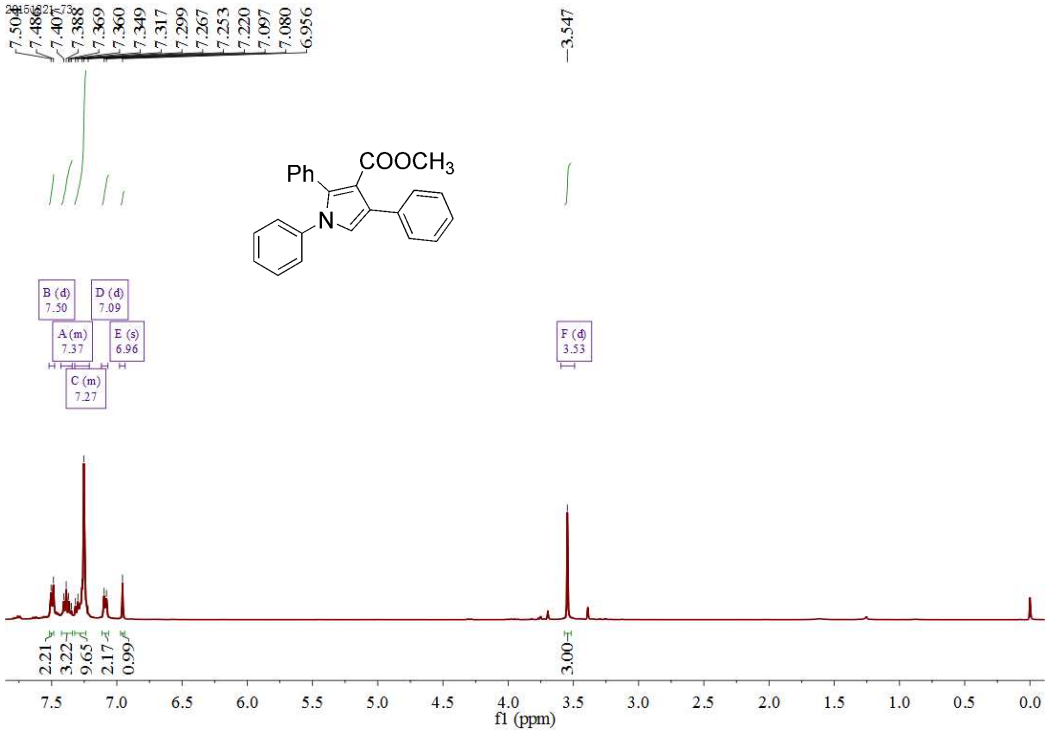

20160111-92
166.15
141.95
139.13
135.65
129.34
129.14
128.40
127.73
126.85
126.50
126.31
121.35
110.64
77.51
77.19
76.87
50.65
31.32
30.10
29.20
25.75
22.55
14.10
n-C6H13
COOCH3
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

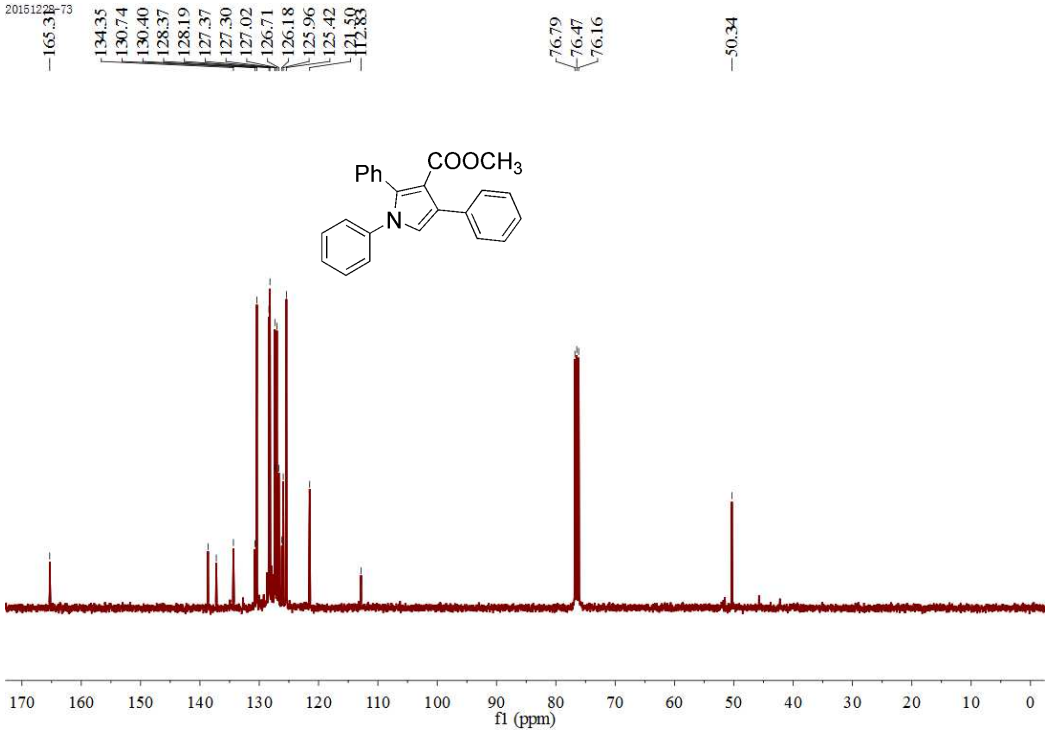
Product 6d


7.466
7.447
7.433
7.378
7.359
7.340
7.301
7.299
7.283
7.265
7.247
6.987
4.347
4.330
4.312
4.294
4.186
4.169
4.151
4.133
1.303
1.285
1.268
1.166
1.148
1.130
EtOOC
COOEt
N
G (t) 7.36
F (m) 7.48
E (s) 6.99
H (m) 7.28
B (q) 4.16
A (q) 4.32
D (t) 1.15
C (t) 1.29
4.38
3.84
2.00
0.91
1.78
1.98
3.00
3.01
f1 (ppm)

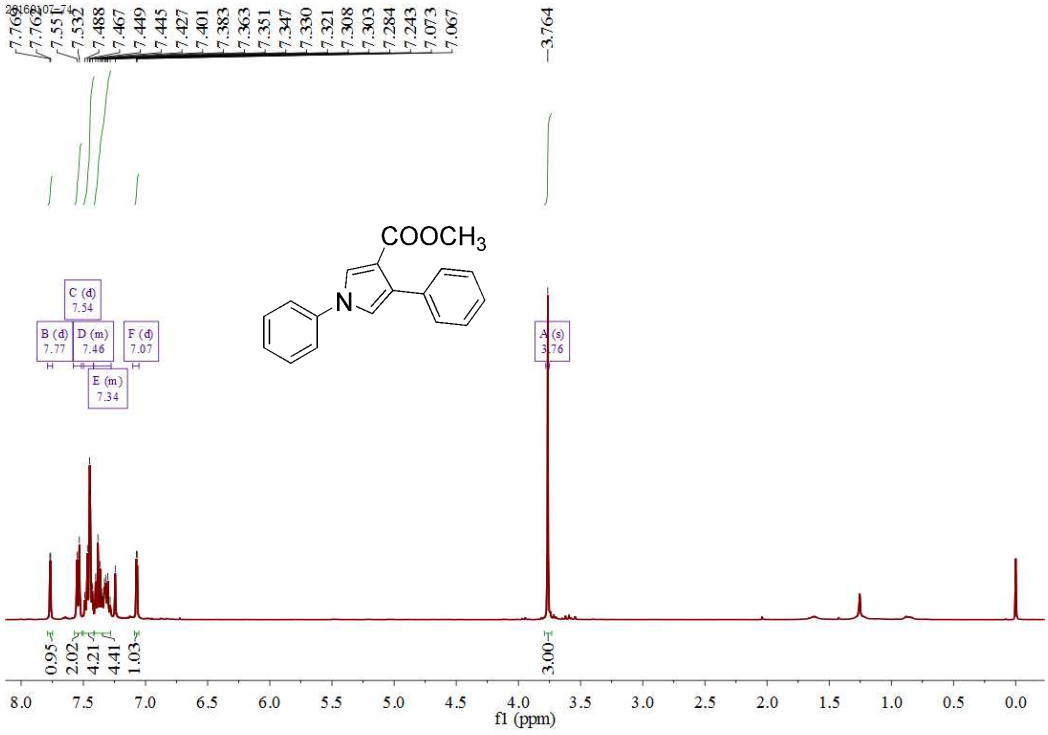

166.26
159.92
139.63
133.26
128.88
128.52
128.48
127.78
127.10
126.26
125.74
124.76
122.74
122.07
77.42
77.10
76.79
61.35
60.84
14.08
13.90
EtOOC
COOEt
N
f1 (ppm)

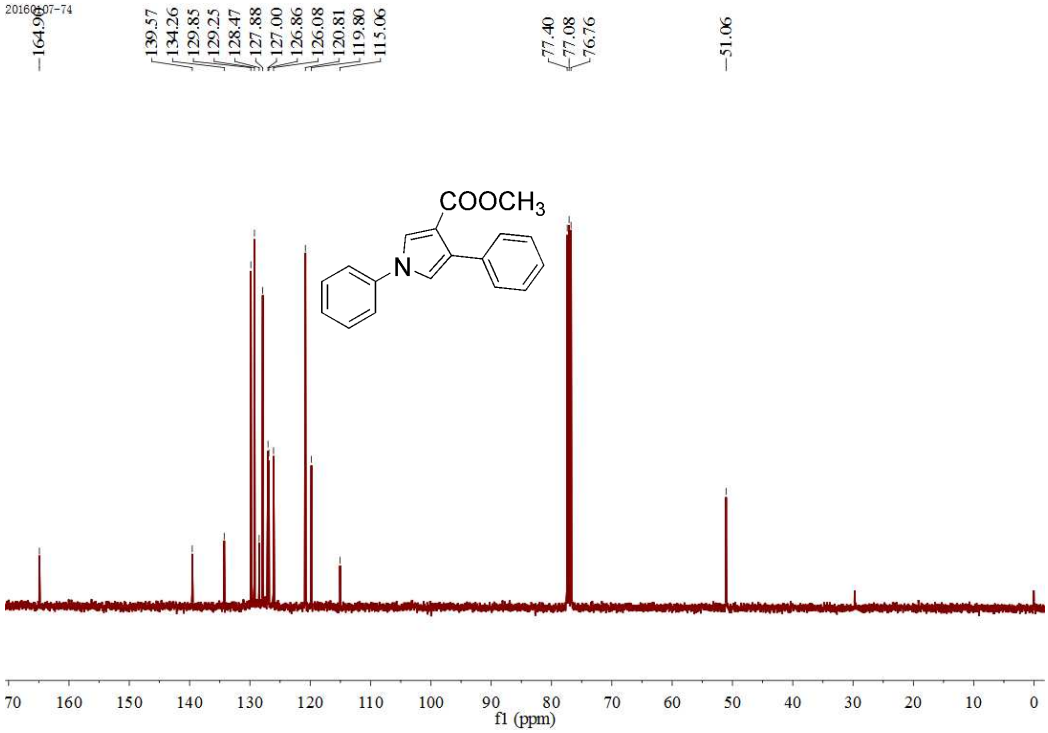
Product 6e


7.504
7.486
7.407
7.388
7.369
7.360
7.349
7.317
7.299
7.267
7.253
7.220
7.097
7.080
6.956
3.547
Ph
COOCH3
N
B (d) 7.50
D (d) 7.09
A (m) 7.37
E (s) 6.96
C (m) 7.27
F (d) 3.53
2.21
3.22
9.65
2.17
0.99
3.00
f1 (ppm)

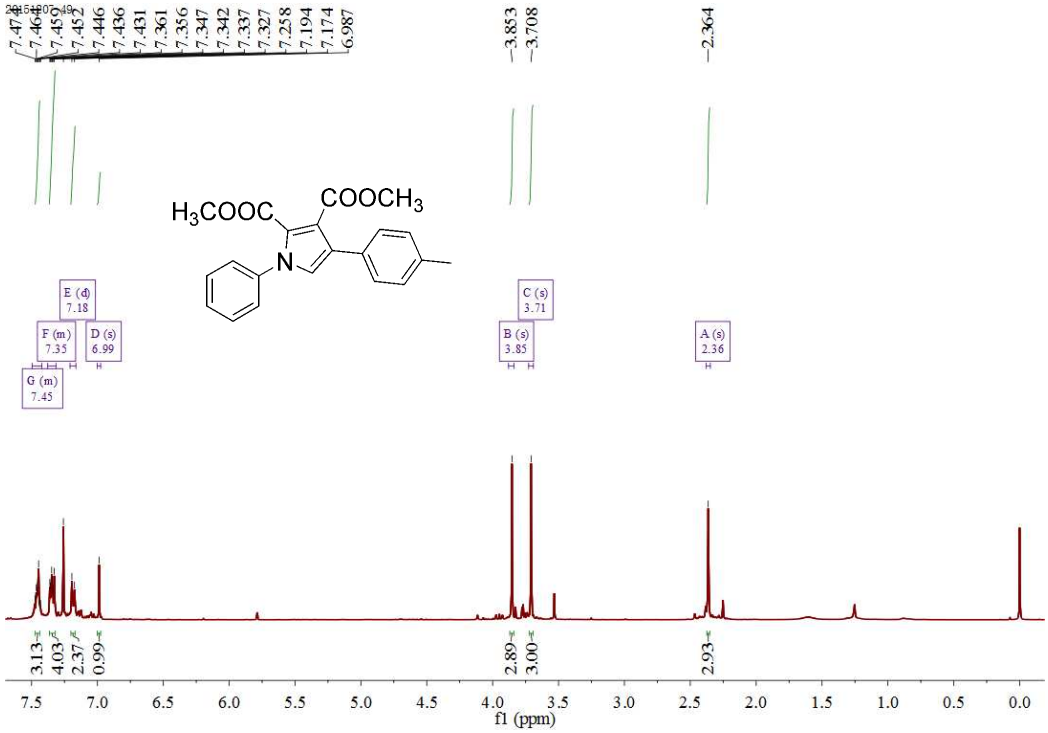

20151228-73
165.31
134.35
130.74
130.40
128.37
128.19
127.37
127.30
127.02
126.71
126.18
125.96
125.42
121.50
112.83
76.79
76.47
76.16
50.34
Ph
COOCH3
N
f1 (ppm)

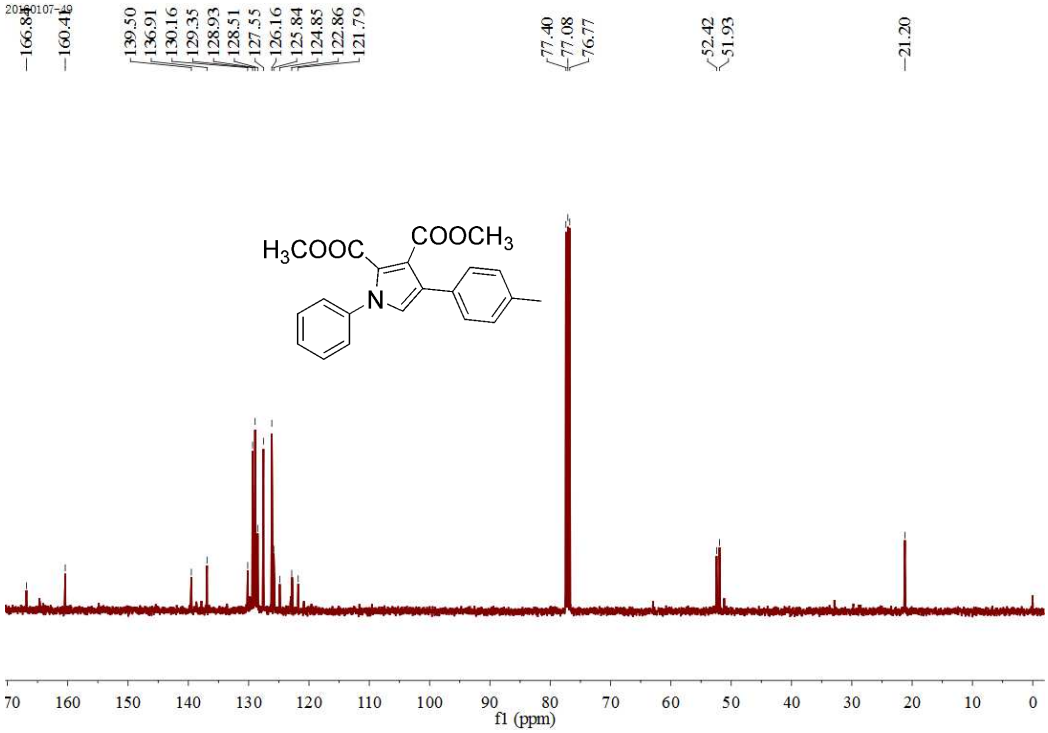
Product 6f


20160107-74
7.769
7.762
7.551
7.532
7.488
7.467
7.449
7.445
7.427
7.401
7.383
7.363
7.351
7.347
7.330
7.321
7.308
7.303
7.284
7.243
7.073
7.067
3.764
COOCH3
N
C (d) 7.54
B (d) 7.77
D (m) 7.46
F (d) 7.07
E (m) 7.34
A (s) 3.76
0.95
2.02
4.21
4.41
1.03
3.00
f1 (ppm)

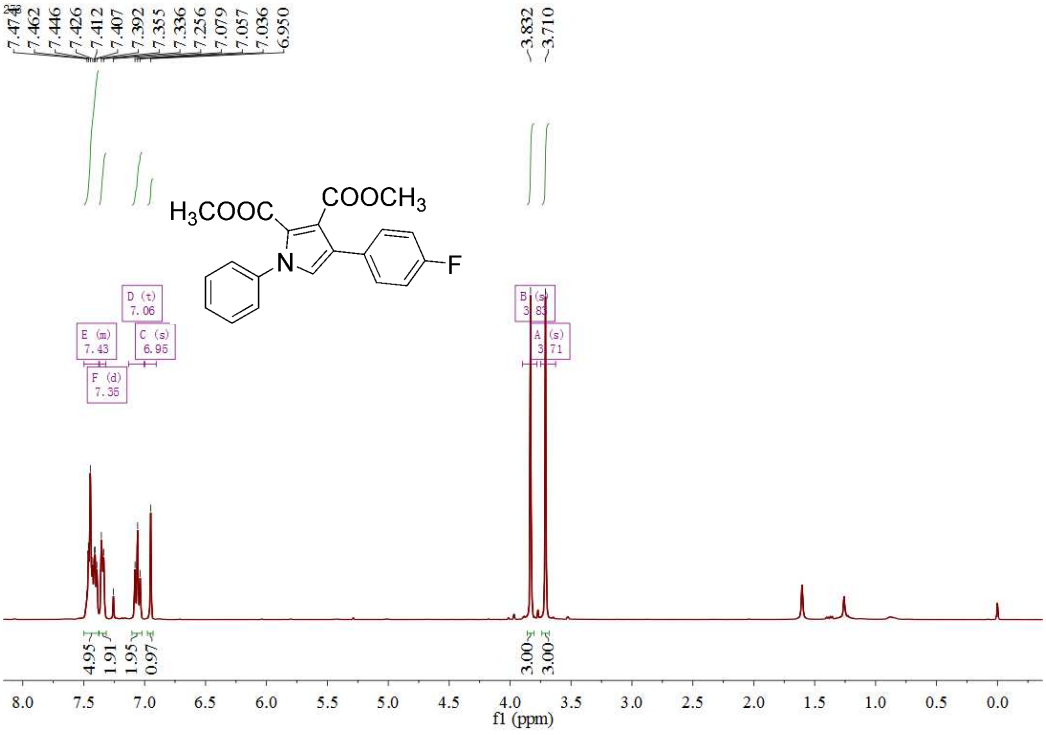

20160107-74
164.90
139.57
134.26
129.85
129.25
128.47
127.88
127.00
126.86
126.08
120.81
119.80
115.06
77.40
77.08
76.76
51.06
COOCH3
N
f1 (ppm)

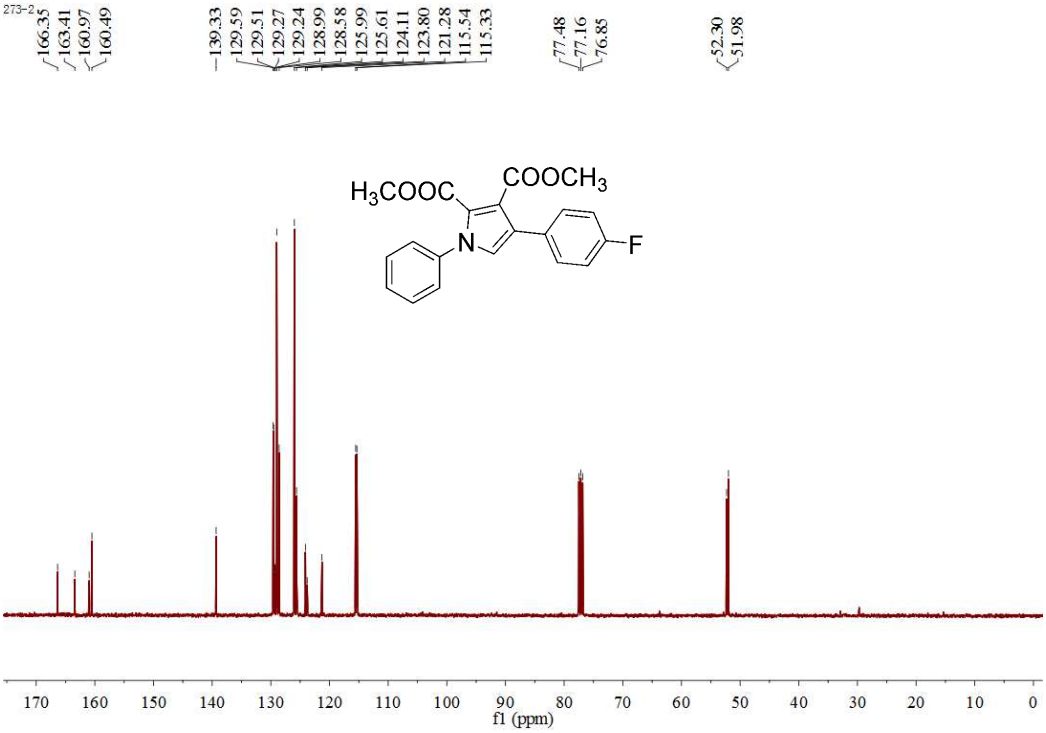
Product 7a


7.474
7.464
7.459
7.452
7.446
7.436
7.431
7.361
7.356
7.347
7.342
7.337
7.327
7.258
7.194
7.174
6.987
3.853
3.708
2.364
H3COOC
COOCH3
N
E (d) 7.18
F (m) 7.35
D (s) 6.99
G (m) 7.45
C (s) 3.71
B (s) 3.85
A (s) 2.36
3.13
4.03
2.37
0.99
2.89
3.00
2.93
f1 (ppm)

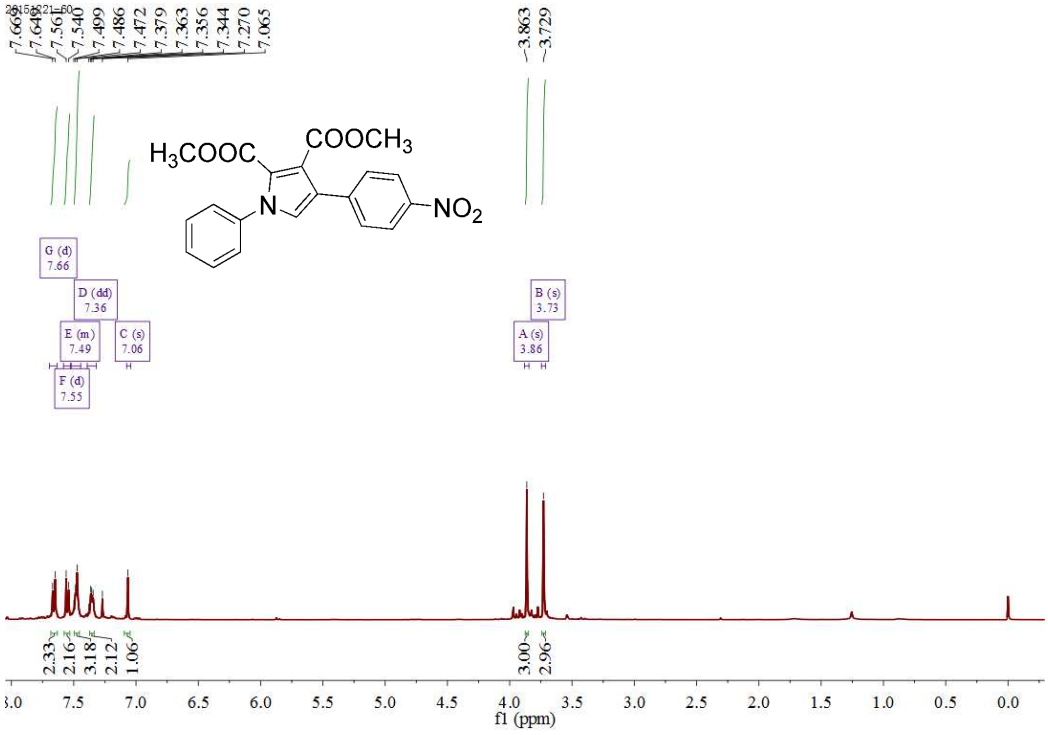

166.84
160.41
139.50
136.91
130.16
129.35
128.93
128.51
127.55
126.16
125.84
124.85
122.86
121.79
77.40
77.08
76.77
52.42
51.93
21.20
H3COOC
COOCH3
N
f1 (ppm)

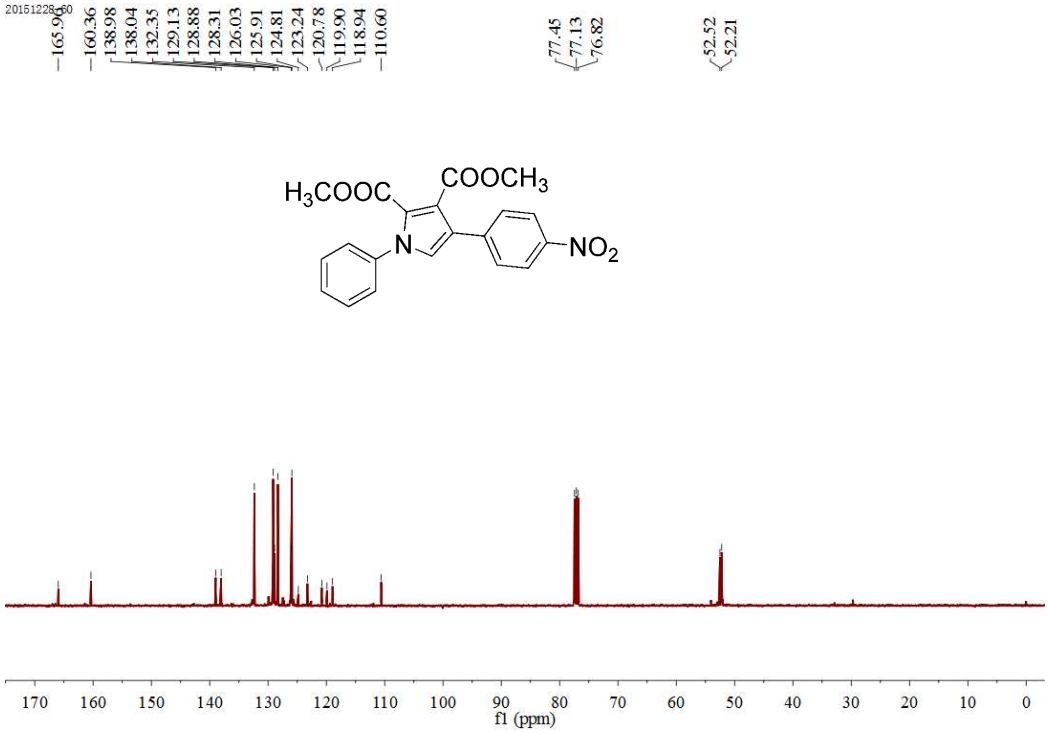
Product 7b


7.474
7.462
7.446
7.426
7.412
7.407
7.392
7.355
7.336
7.256
7.079
7.057
7.036
6.950
3.832
3.710
H3COOC
COOCH3
N
F
D (t) 7.06
E (m) 7.43
C (s) 6.96
F (d) 7.36
B (s) 3.83
A (s) 3.71
4.95
1.91
1.95
0.97
3.00
3.00
f1 (ppm)

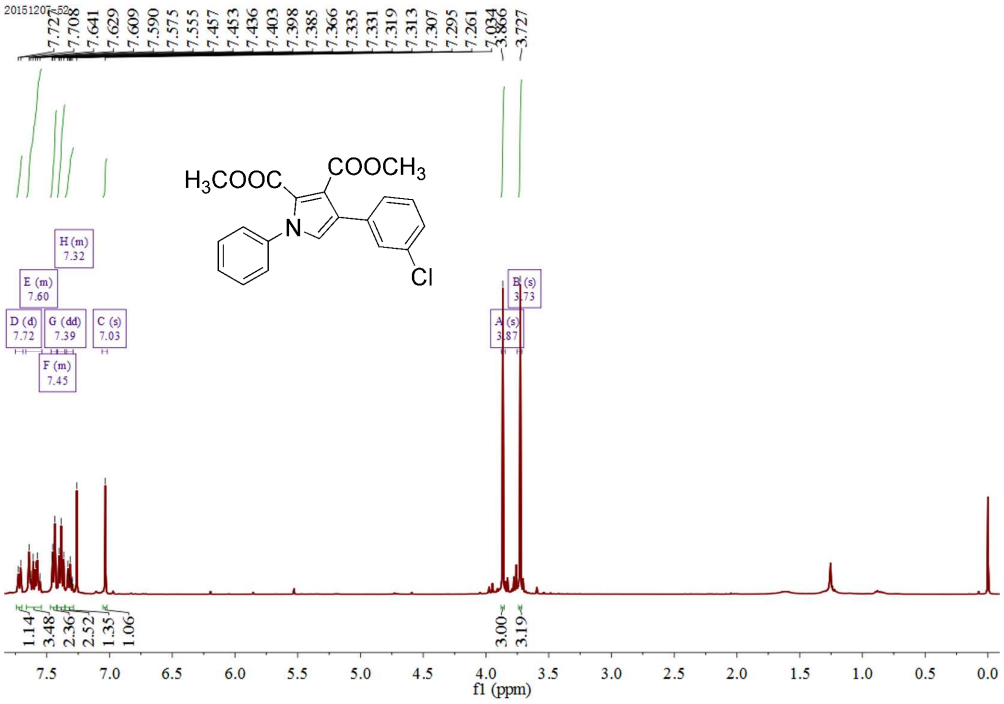

273-2
166.35
163.41
160.97
160.49
139.33
129.59
129.51
129.27
129.24
128.99
128.58
125.99
125.61
124.11
123.80
121.28
115.54
115.33
77.48
77.16
76.85
52.30
51.98
H3COOC
COOCH3
N
F
f1 (ppm)

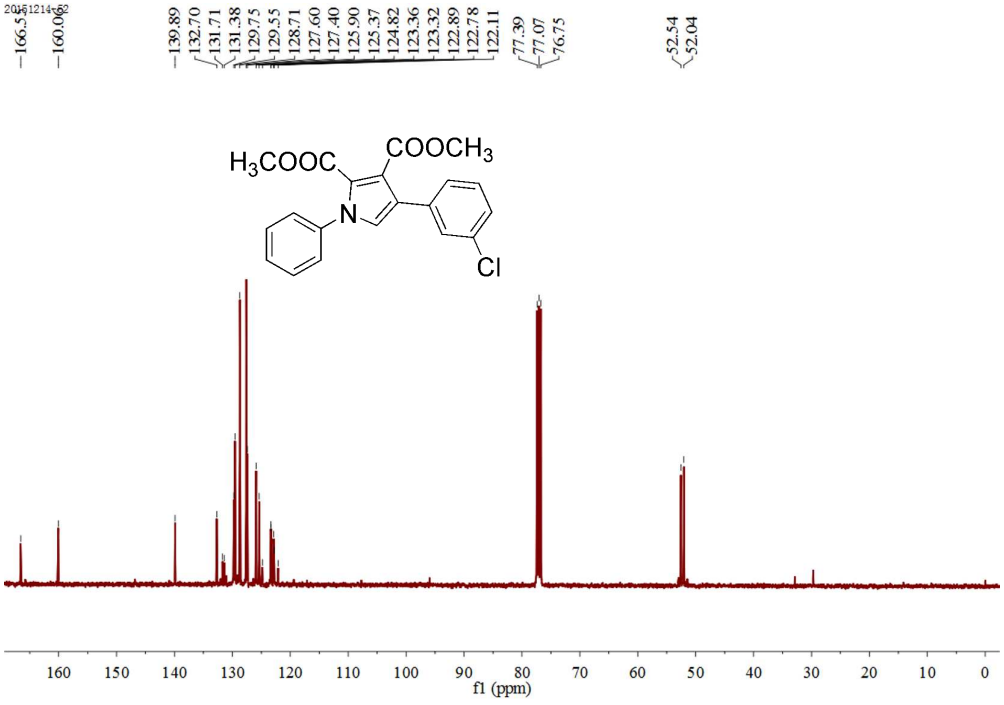
Product 7c


7.669
7.649
7.561
7.540
7.499
7.486
7.472
7.379
7.363
7.356
7.344
7.270
7.065
3.863
3.729
H3COOC
COOCH3
N
NO2
G (d) 7.66
D (dd) 7.36
E (m) 7.49
C (s) 7.06
F (d) 7.55
B (s) 3.73
A (s) 3.86
2.33
2.16
3.18
2.12
1.06
3.00
2.96
f1 (ppm)

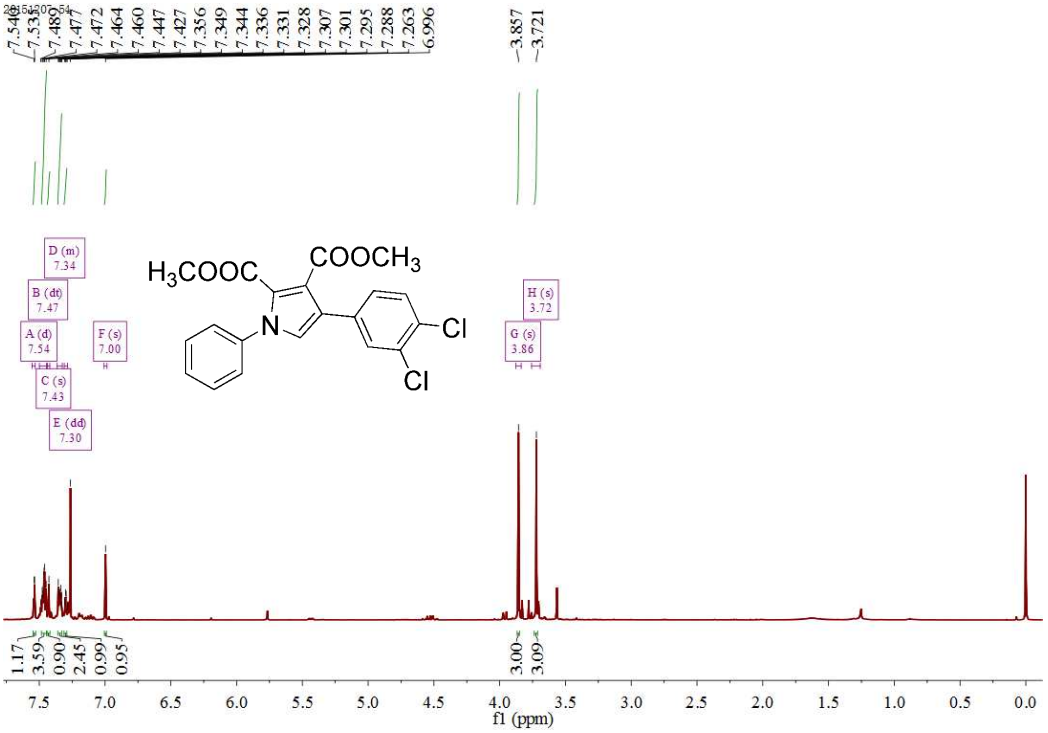

165.90
160.36
138.98
138.04
132.35
129.13
128.88
128.31
126.03
125.91
124.81
123.24
120.78
119.90
118.94
110.60
77.45
77.13
76.82
52.52
52.21
H3COOC
COOCH3
N
NO2
f1 (ppm)

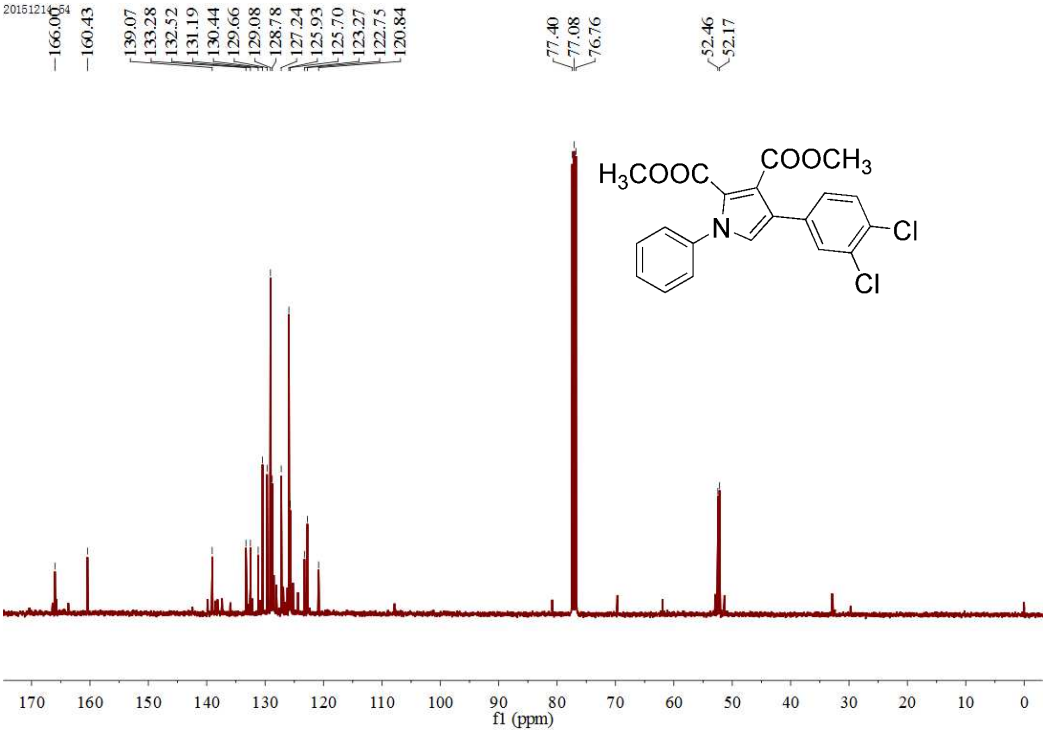
Product 7d


7.727
7.708
7.641
7.629
7.609
7.590
7.575
7.555
7.457
7.453
7.436
7.403
7.398
7.385
7.366
7.335
7.331
7.319
7.313
7.307
7.295
7.261
7.034
3.866
3.727
H (m) 7.32
E (m) 7.60
D (d) 7.72
G (dd) 7.39
C (s) 7.03
F (m) 7.45
E (s) 3.73
A (s) 3.87
1.14
3.48
2.36
2.52
1.35
1.06
3.00
3.19
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
f1 (ppm)

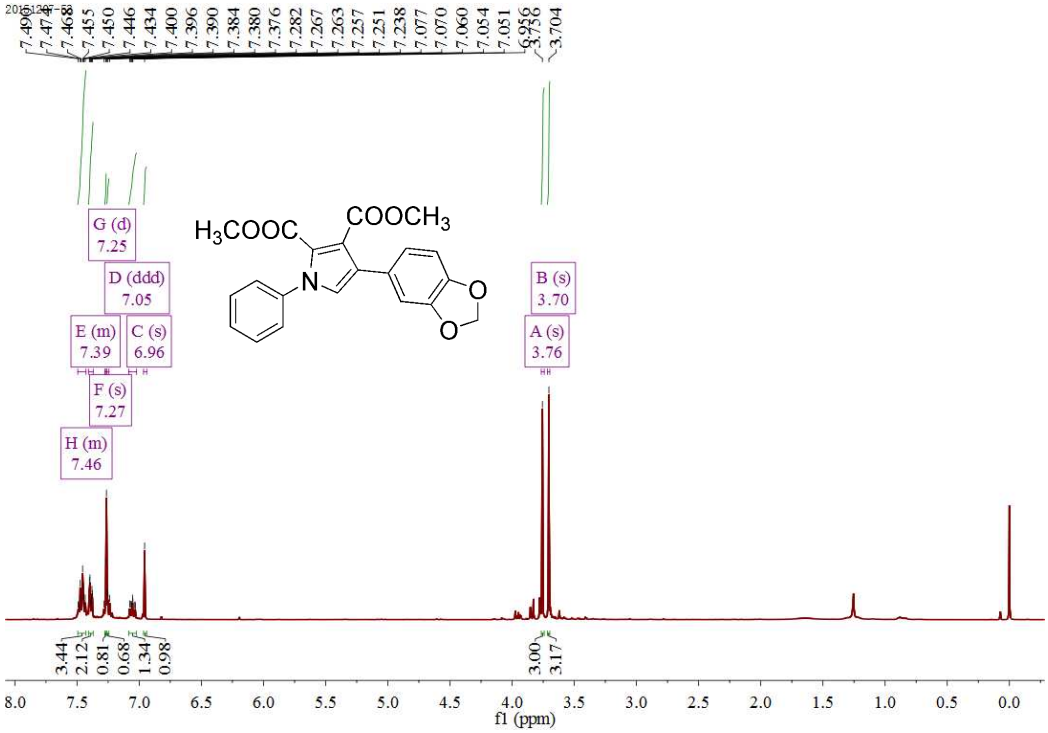

166.53
160.06
139.89
132.70
131.71
131.38
129.75
129.55
128.71
127.60
127.40
125.90
125.37
124.82
123.36
123.32
122.89
122.78
122.11
77.39
77.07
76.75
52.54
52.04
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

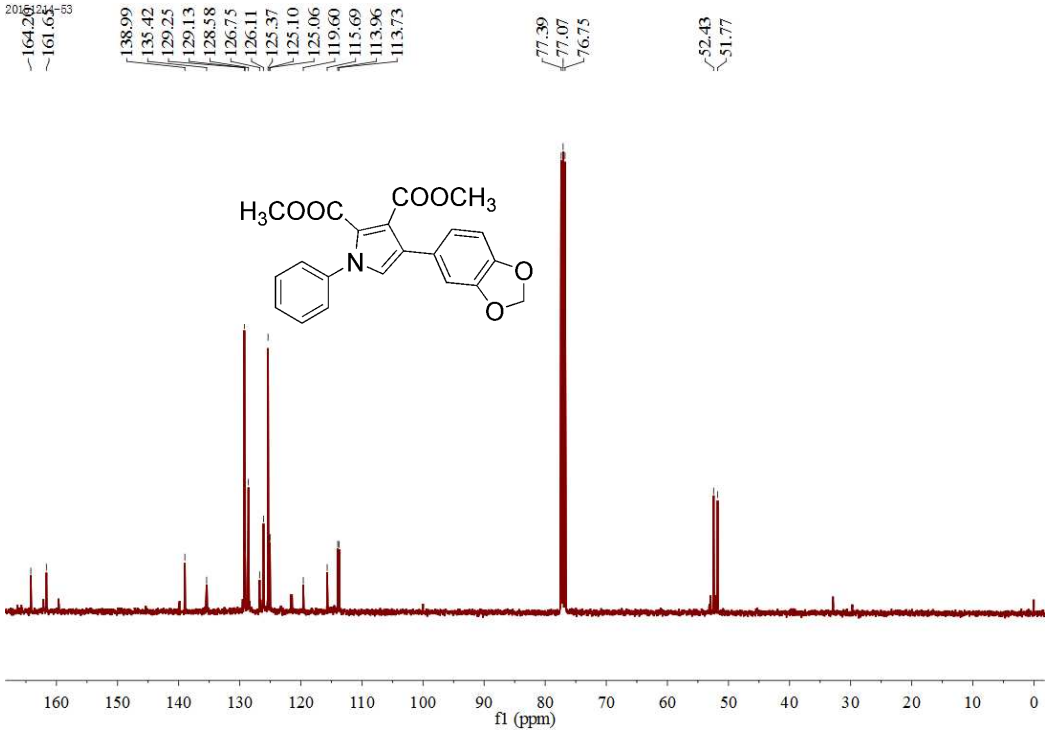
Product 7e


7.546
7.533
7.489
7.477
7.472
7.464
7.460
7.447
7.427
7.356
7.349
7.344
7.336
7.331
7.328
7.307
7.301
7.295
7.288
7.263
6.996
3.857
3.721
D (m) 7.34
B (dt) 7.47
A (d) 7.54
C (s) 7.43
E (dd) 7.30
F (s) 7.00
H (s) 3.72
G (s) 3.86
H3COOC
COOCH3
N
Cl
Cl
1.17
3.59
0.90
2.45
0.99
0.95
3.00
3.09
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
f1 (ppm)

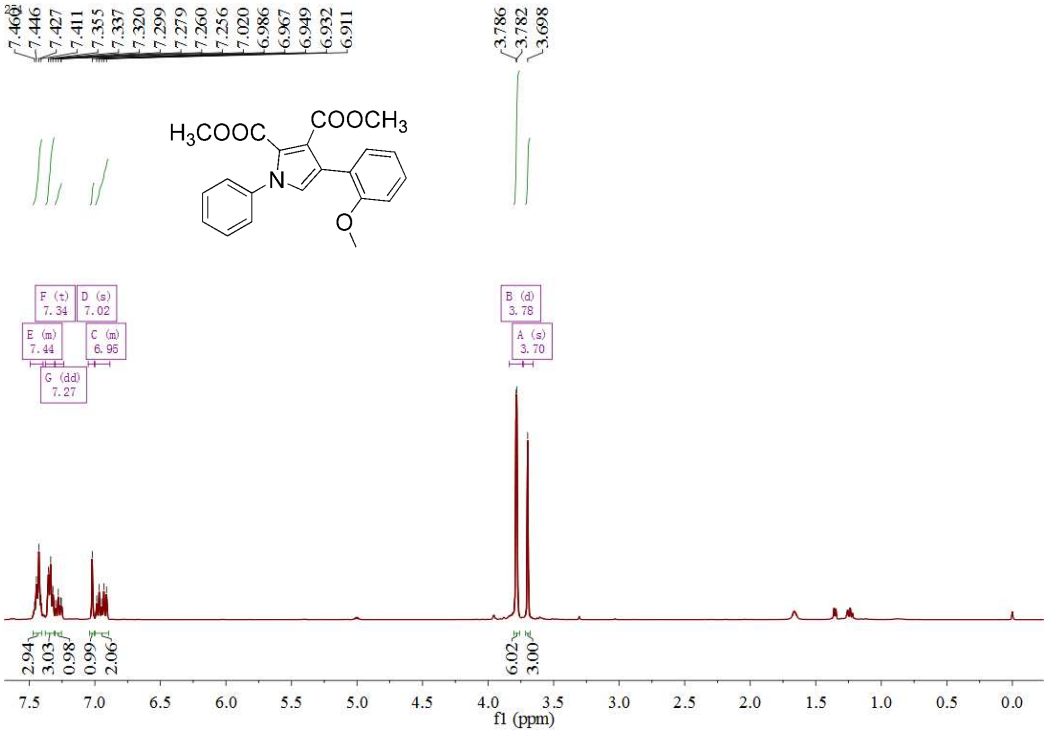

166.06
160.43
139.07
133.28
132.52
131.19
130.44
129.66
129.08
128.78
127.24
125.93
125.70
123.27
122.75
120.84
77.40
77.08
76.76
52.46
52.17
H3COOC
COOCH3
N
Cl
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

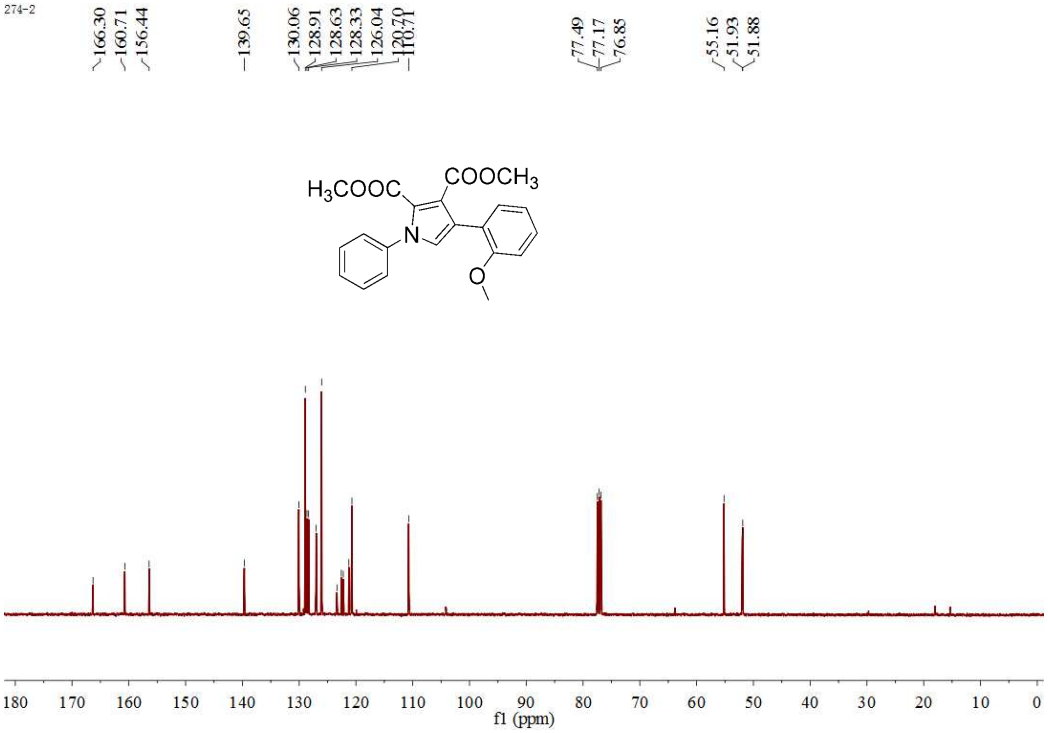
Product 7f


7.496
7.474
7.468
7.455
7.450
7.446
7.434
7.400
7.396
7.390
7.384
7.380
7.376
7.282
7.267
7.263
7.257
7.251
7.238
7.077
7.070
7.060
7.054
7.051
6.956
3.736
3.704
H3COOC
COOCH3
N
O
O
G (d) 7.25
D (ddd) 7.05
E (m) 7.39
C (s) 6.96
F (s) 7.27
H (m) 7.46
B (s) 3.70
A (s) 3.76
3.44
2.12
0.81
0.68
1.34
0.98
3.00
3.17
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
f1 (ppm)

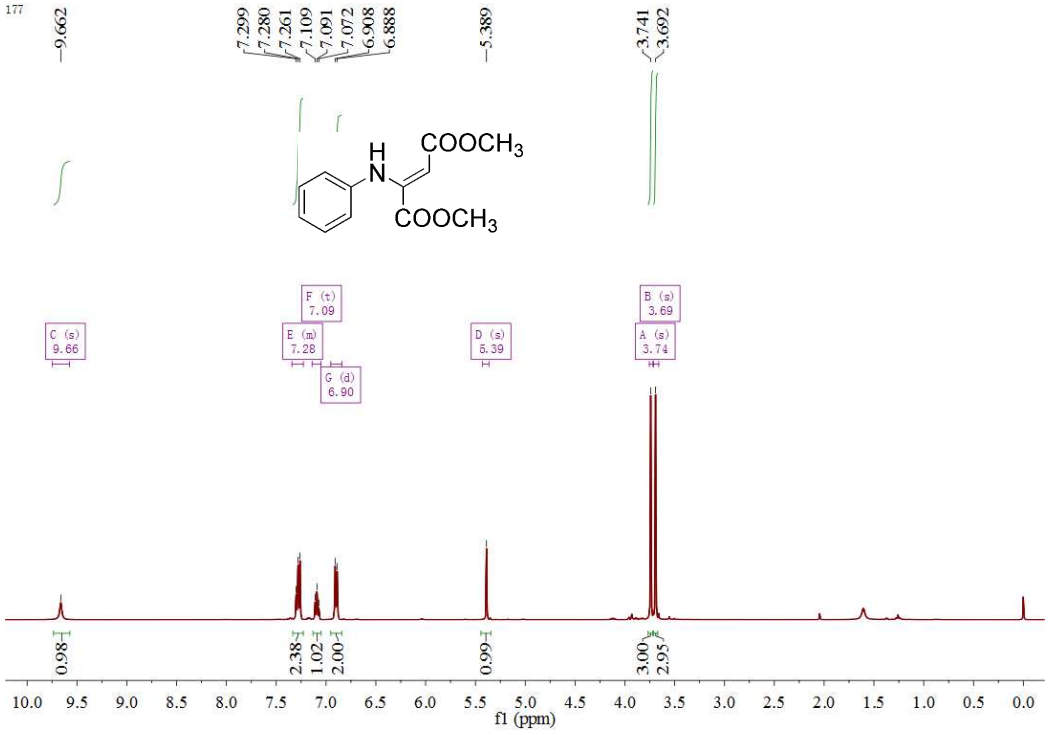

164.20
161.63
138.99
135.42
129.25
129.13
128.58
126.75
126.11
125.37
125.10
125.06
119.60
115.69
113.96
113.73
77.39
77.07
76.75
52.43
51.77
H3COOC
COOCH3
N
O
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

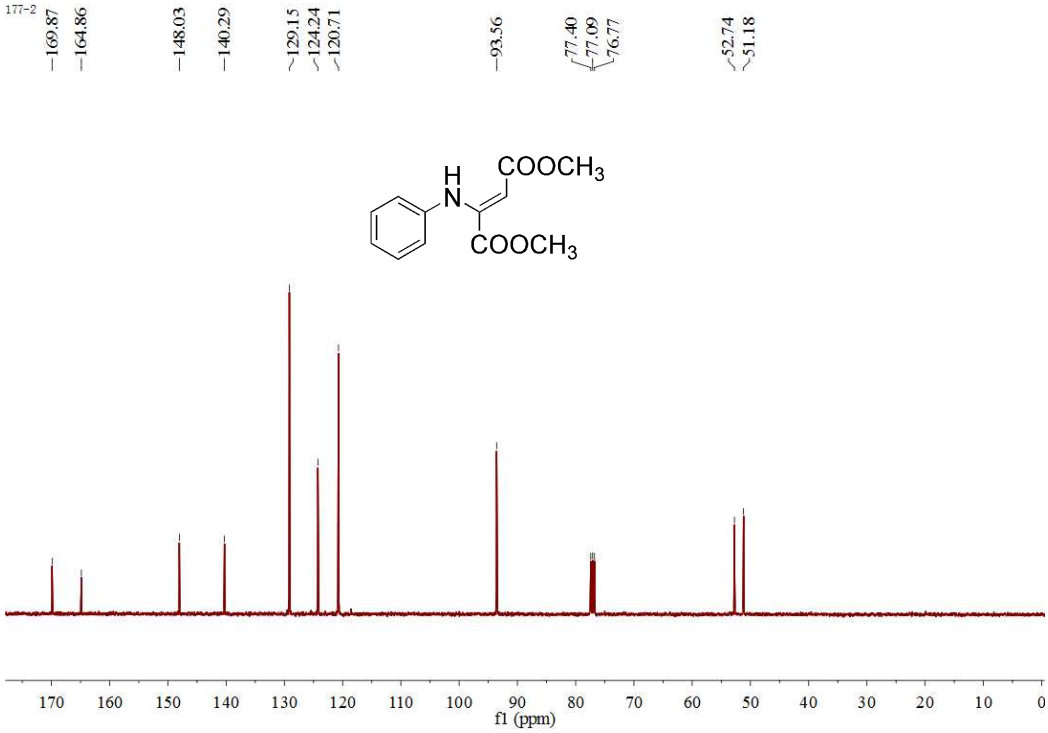
Product 7g


7.462
7.446
7.427
7.411
7.355
7.337
7.320
7.299
7.279
7.260
7.256
7.020
6.986
6.967
6.949
6.932
6.911
3.786
3.782
3.698
H3COOC
COOCH3
N
O
F (t) 7.34
D (s) 7.02
E (m) 7.44
C (m) 6.96
G (dd) 7.27
B (d) 3.78
A (s) 3.70
2.94
3.03
0.98
0.99
2.06
6.02
3.00
f1 (ppm)


274-2
166.30
160.71
156.44
139.65
130.06
128.91
128.63
128.33
126.04
120.70
110.71
77.49
77.17
76.85
55.16
51.93
51.88
H3COOC
COOCH3
N
O
f1 (ppm)

Compound 8


177
9.662
7.299
7.280
7.261
7.109
7.091
7.072
6.908
6.888
5.389
3.741
3.692
COOCH3
H
N
COOCH3
C (s) 9.66
F (t) 7.09
E (m) 7.28
G (d) 6.90
D (s) 5.39
B (s) 3.69
A (s) 3.74
0.98
2.38
1.02
2.00
0.99
3.00
2.95
f1 (ppm)


177-2
169.87
164.86
148.03
140.29
129.15
124.24
120.71
93.56
77.40
77.09
76.77
52.74
51.18
COOCH3
H
N
COOCH3
f1 (ppm)