Electronic Supplementary Information

Copper-catalyzed retro-aldol reaction of β-hydroxy ketones or nitrile with aldehydes: Chemo- and stereoselective access to (*E*)-enones and (*E*)-acrylonitriles

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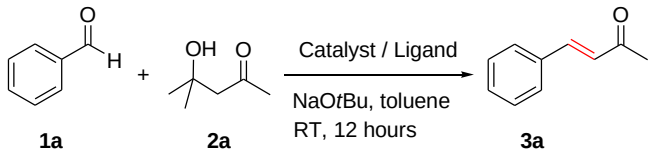
1. Additional results on catalyst/ligand effect

Table S1. Additional catalyst/ligand screening [a]

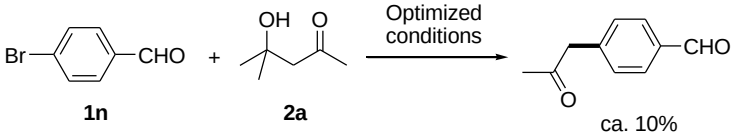


1a **2a** **3a**

Entry	*Catalyst*	*Ligand*	*Yield (%)* [b]
1	CuCl	DPPE	46
2	CuCl	Phen	53
3	CuCl	PPh_3	28
4	CuI	DPPE	48
5	CuI	Phen	35
6	$CuCl_2$	Phen	22

[a] Reaction conditions: **1a** (0.5 mmol)**, 2a** (2.0 mmol), Catalyst (6.0 mol%), Ligand (6.0 mol%), NaO*t*Bu (6.0 mol%), toluene (3 mL), 12 hours, room temperature. DPPE denotes 1, 2-bis(diphenylphosphino)ethane. Phen denotes 1,10-phenanthroline. [b] Isolated yields.

2. Side α-arylation reaction of *para*-bromobenzaldehyde with 2a

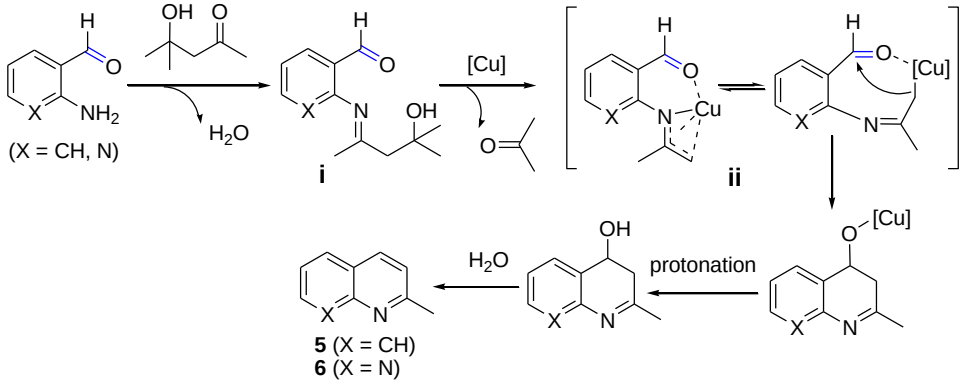


1n **2a** ca. 10% (S1)

3. Alternative mechanism for the formation of 5 and 6

For the mechanism of formation of **5** and **6**, aside from the mechanism proposed in Scheme 4b in the main text, another mechanism is also possible (Scheme S1). It involves initial amine-carbonyl condensation to form an *ortho*-imino nicotinaldehyde intermediate (**i**), This *ortho*-imino nicotinaldehyde intermediate then undergo copper-promoted retro-aldol C-C cleavage to generate a Cu imino-enolate intermediate (**ii)**. Intramolecular aldol condensation of **ii** would finally produce target **5** or **6**.

Scheme S1. Alternative mechanism



4. NMR spectra for all the products

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3a**

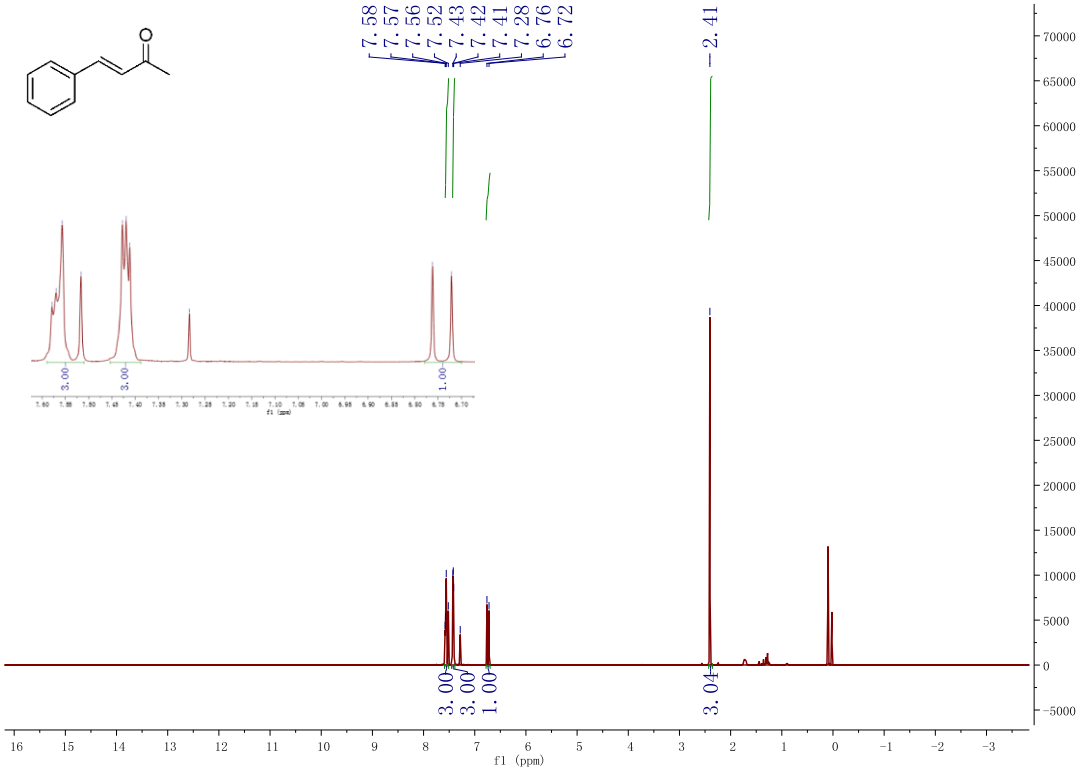


Figure S2. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3a**

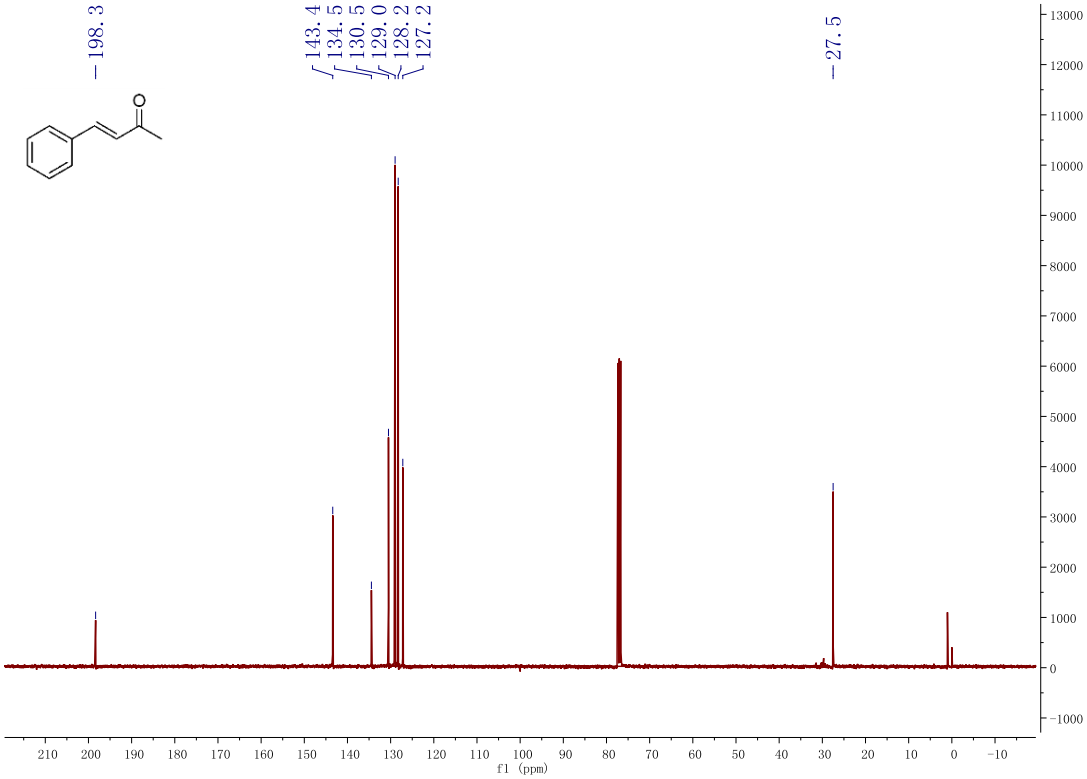


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3b**

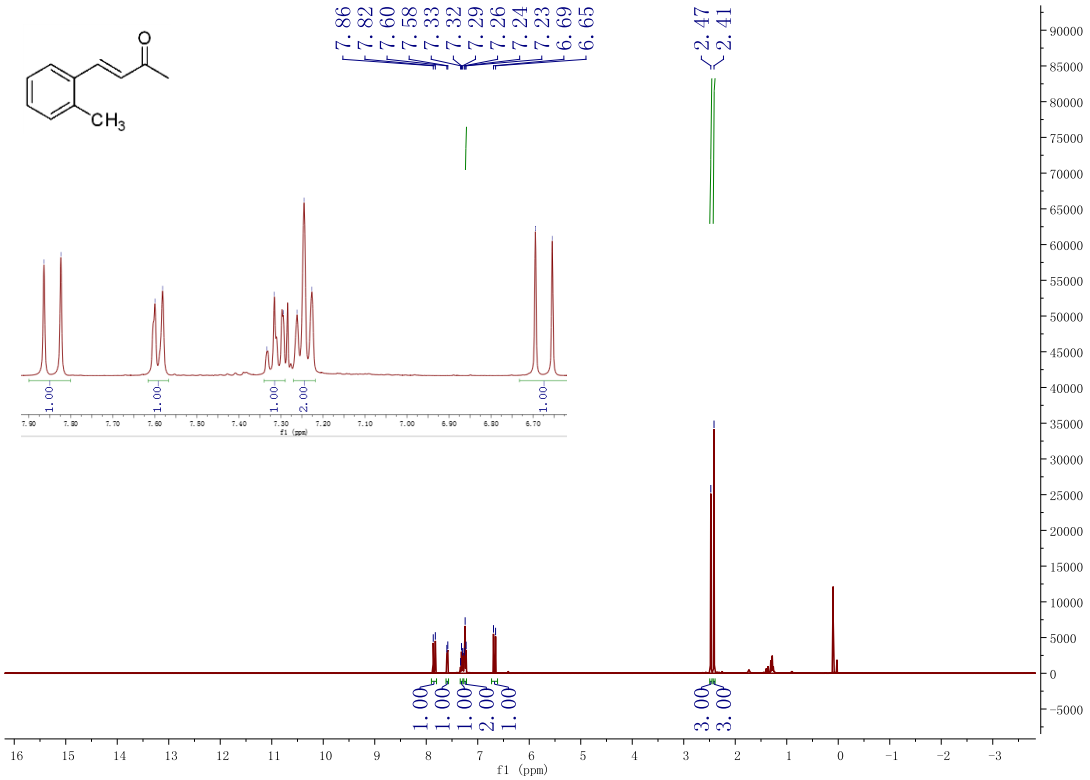


Figure S4. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3b**

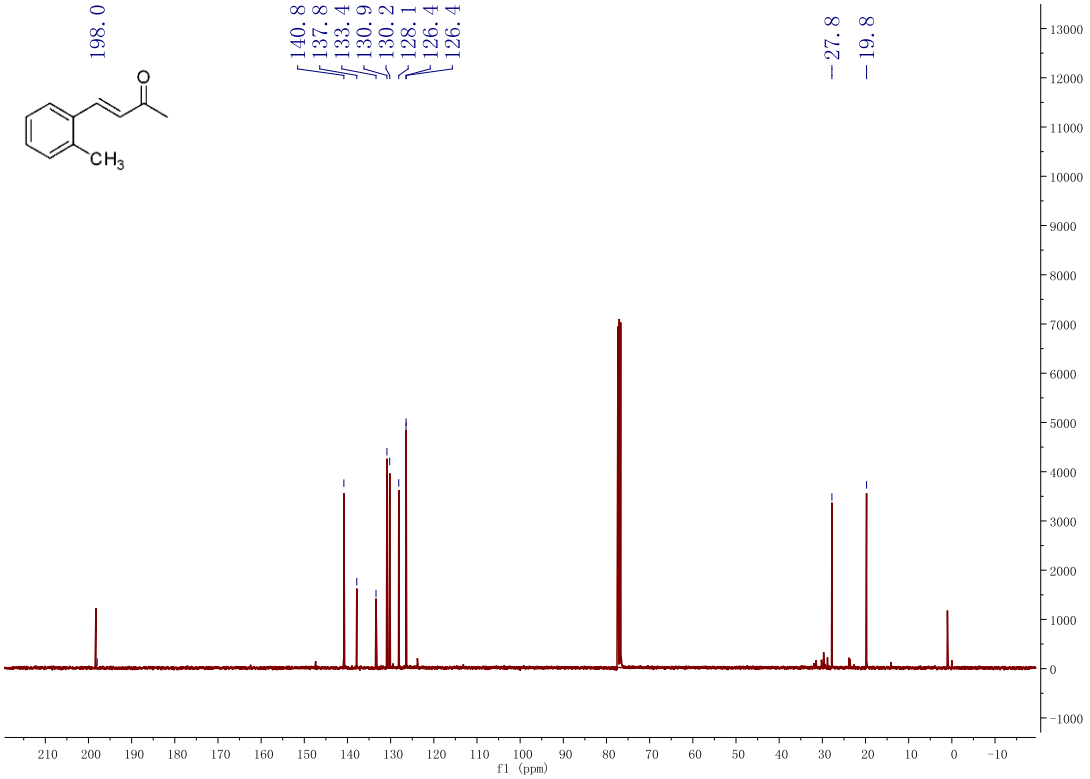


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3c**

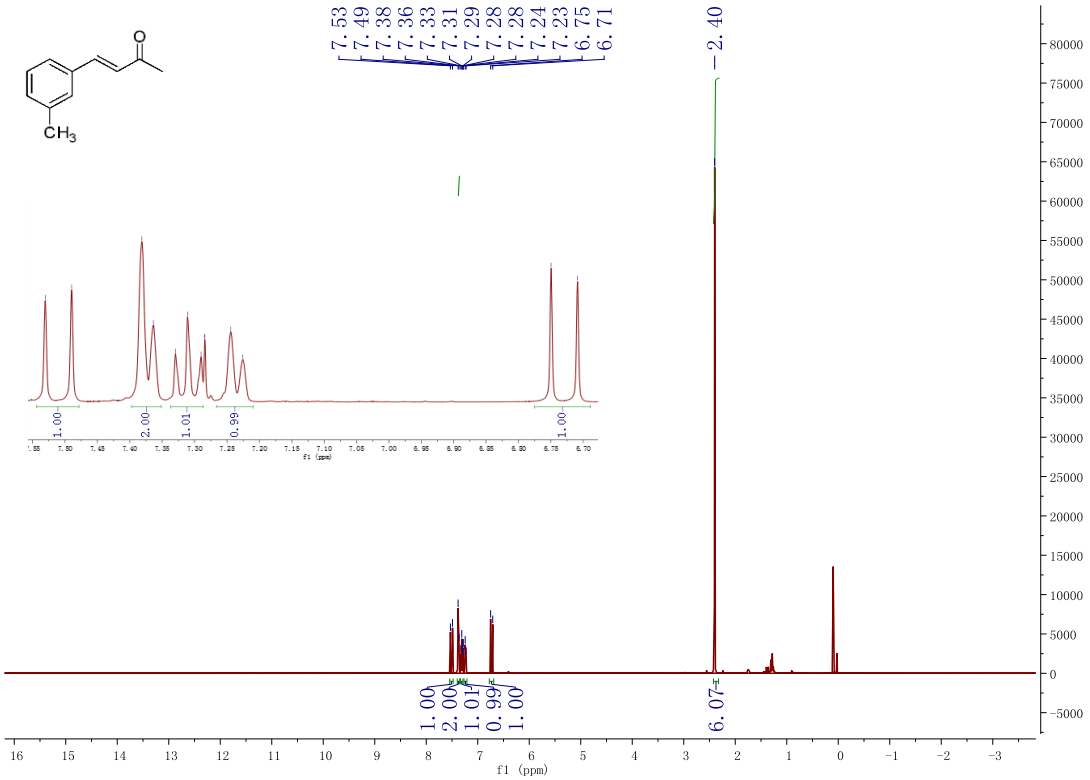


Figure S6. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3c**

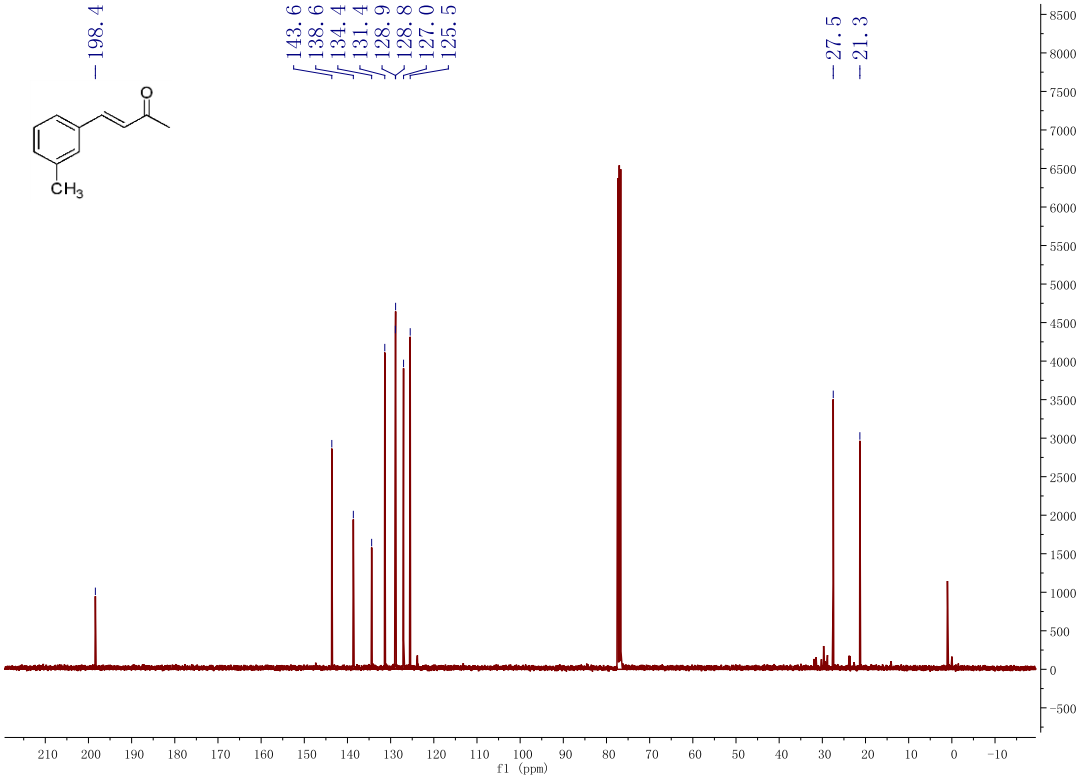


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3d**

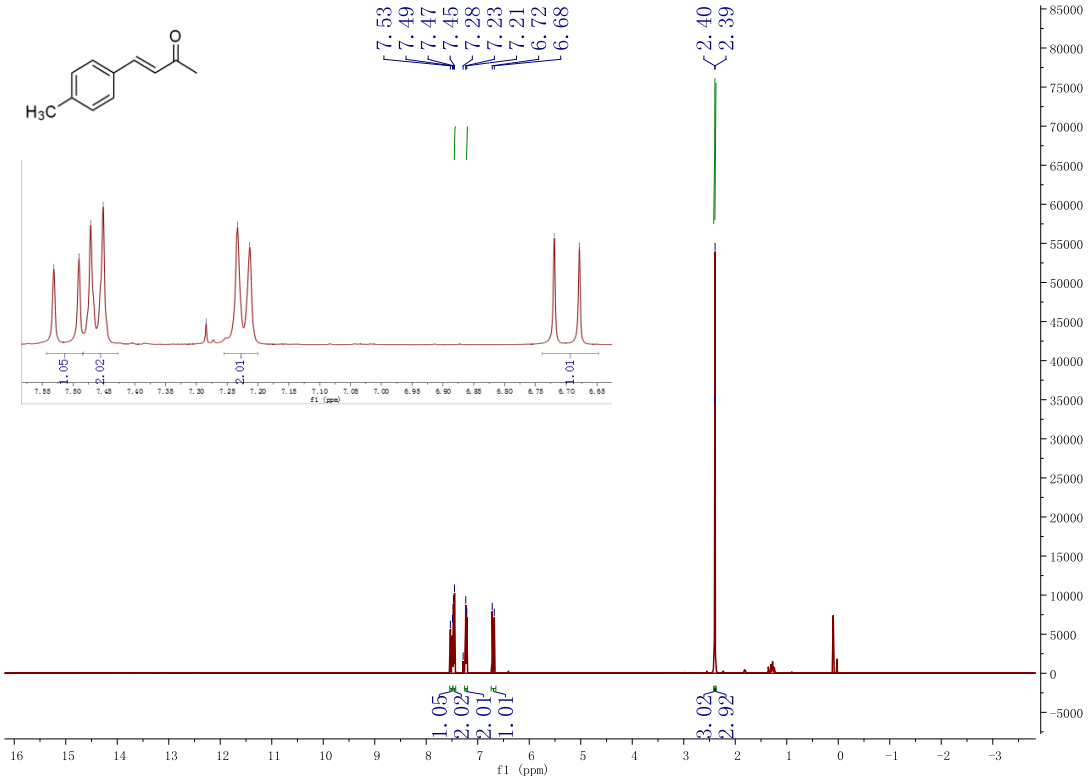


Figure S8. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3d**

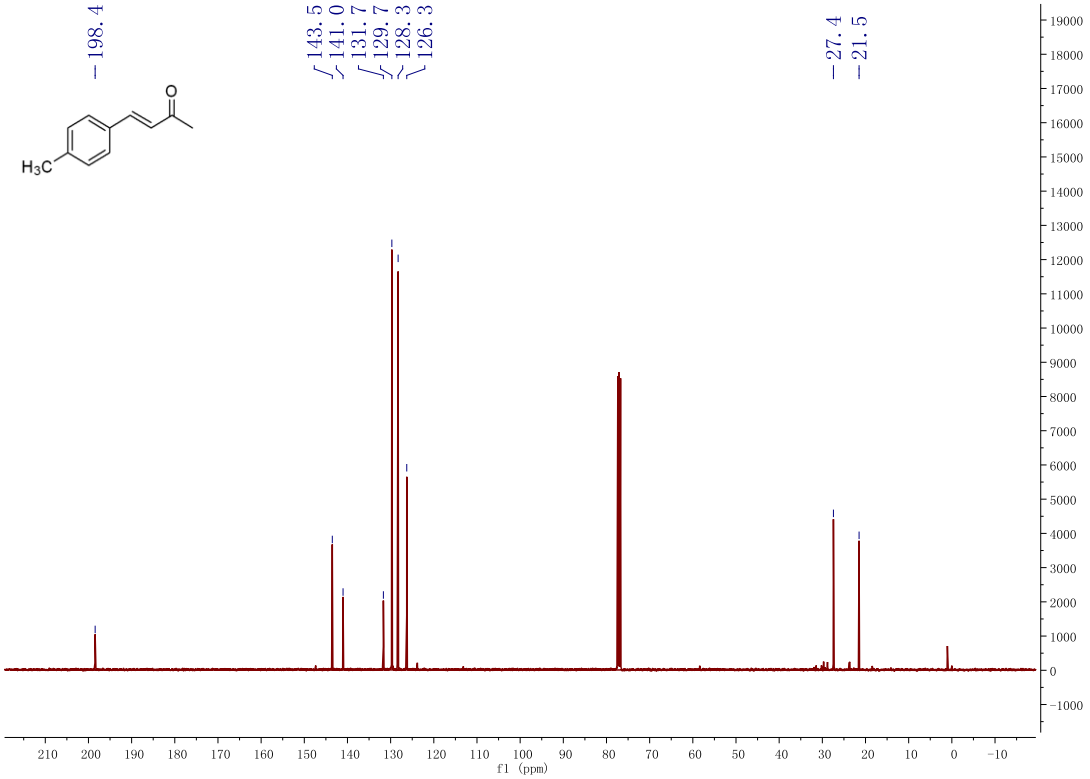


Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3e**

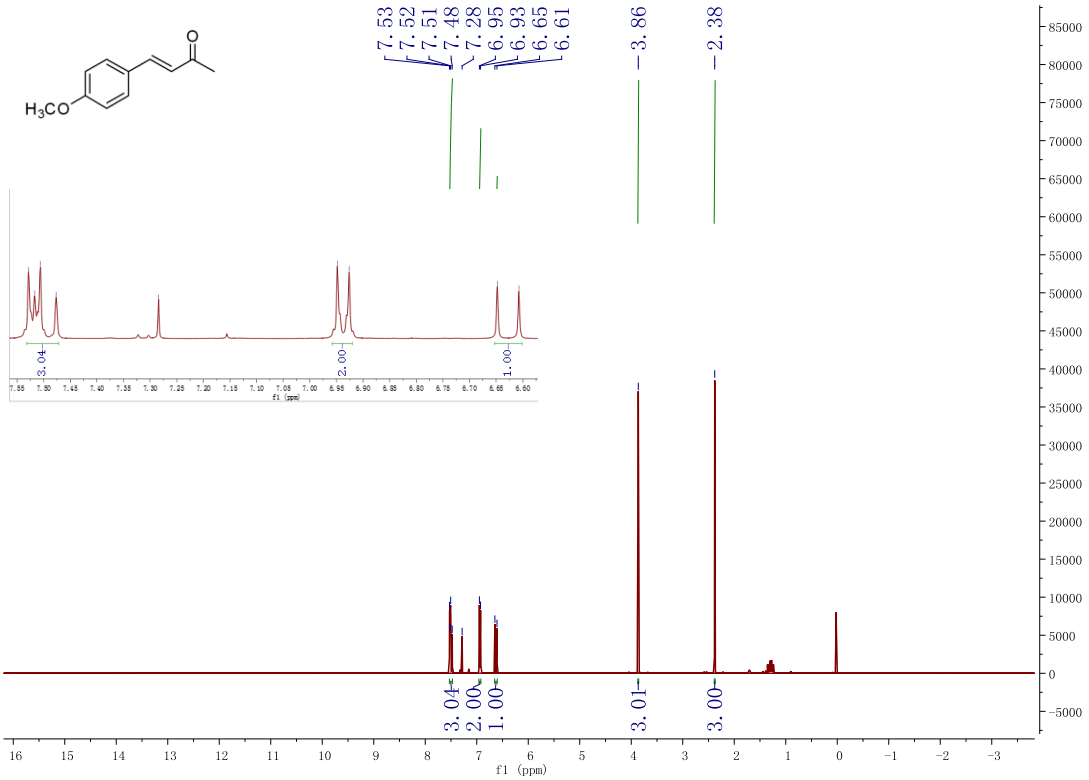


Figure S10. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3e**

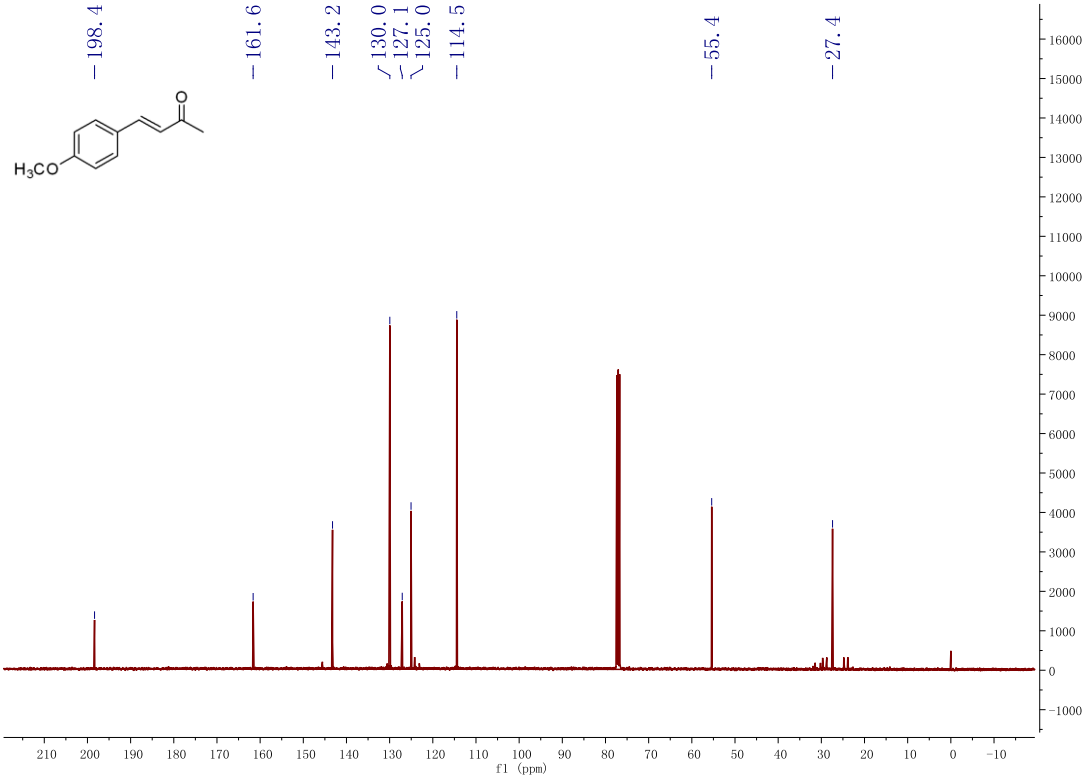


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3f** (trans:cis=3:1)

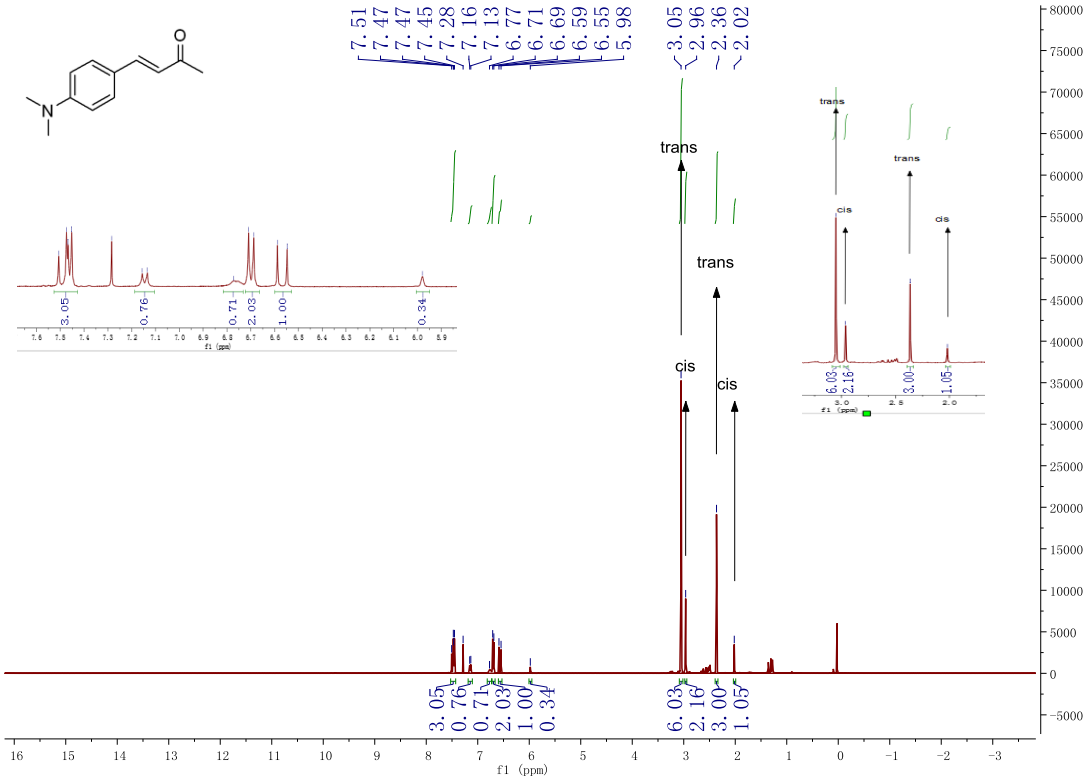


Figure S12. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3f**

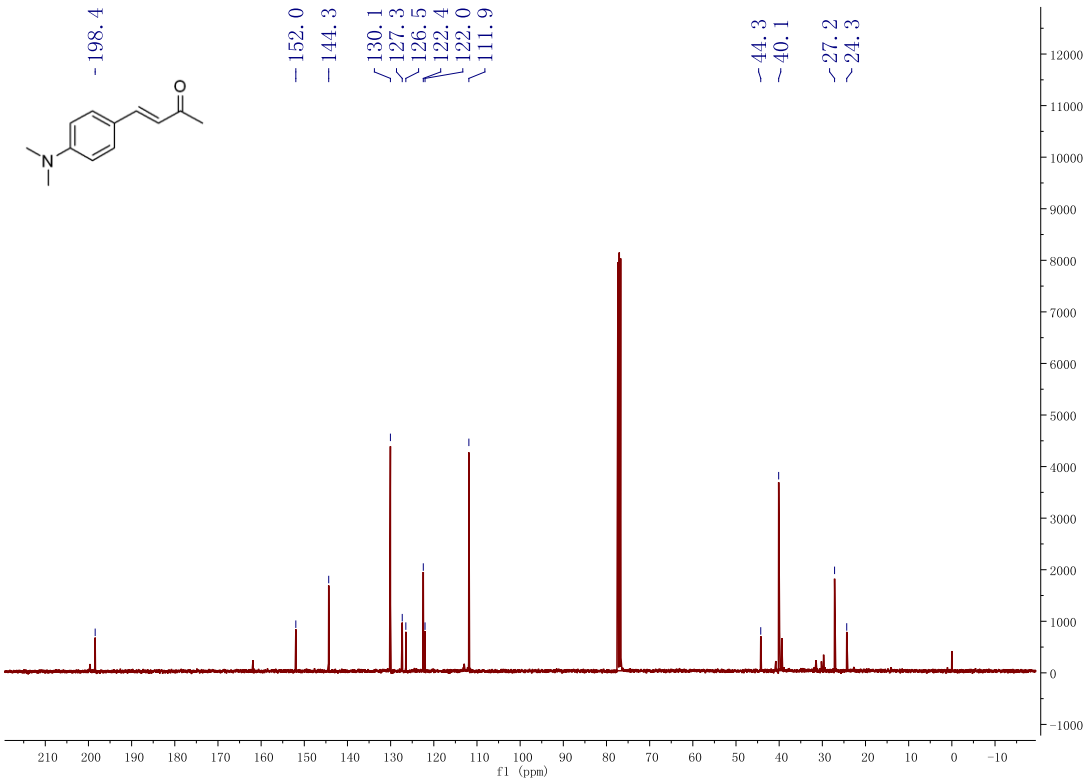


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3g**

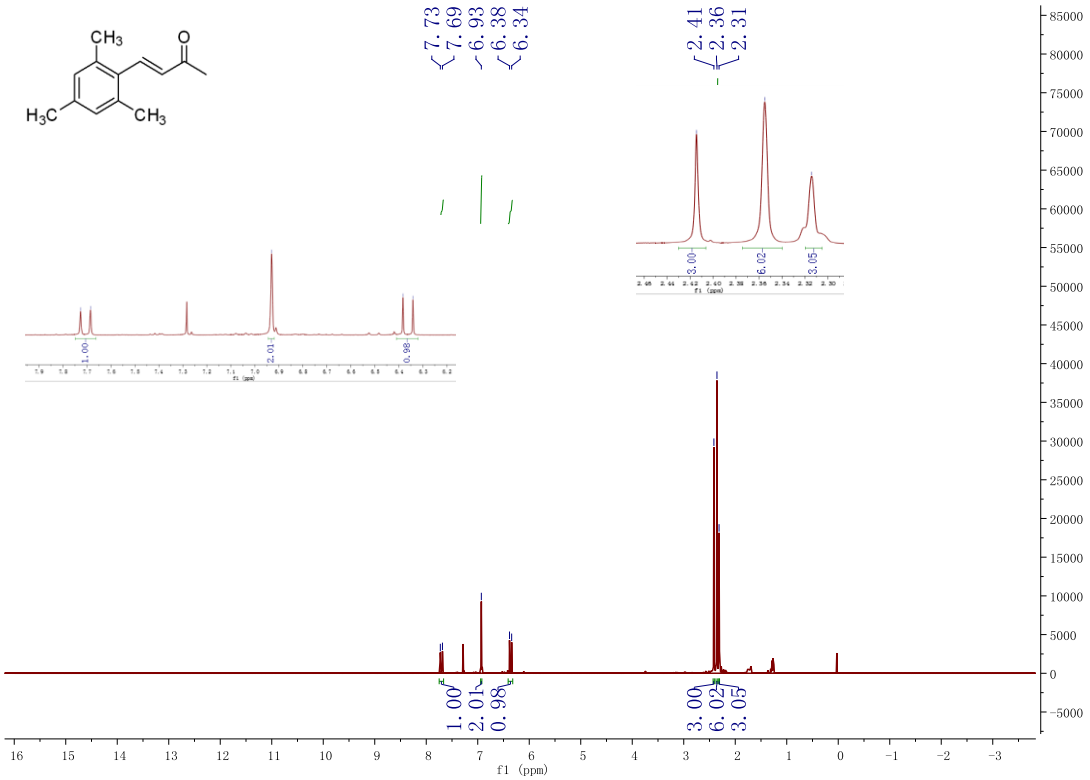


Figure S14. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3g**

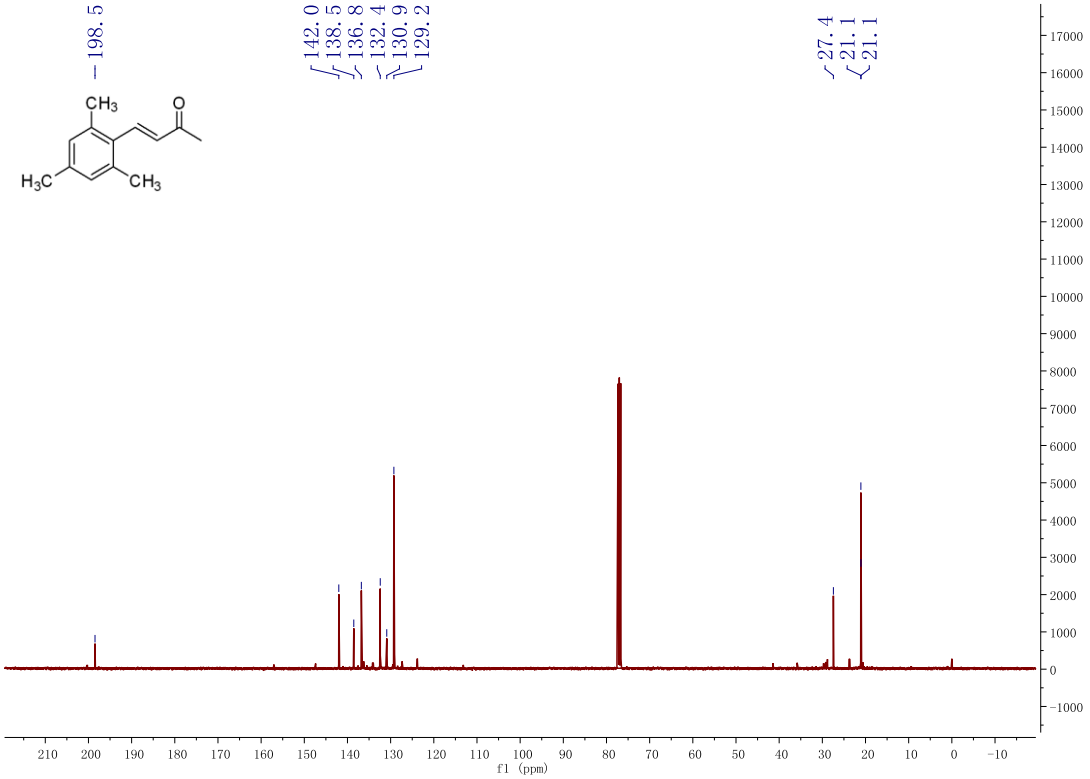


Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3h** (trans:cis=8:1)

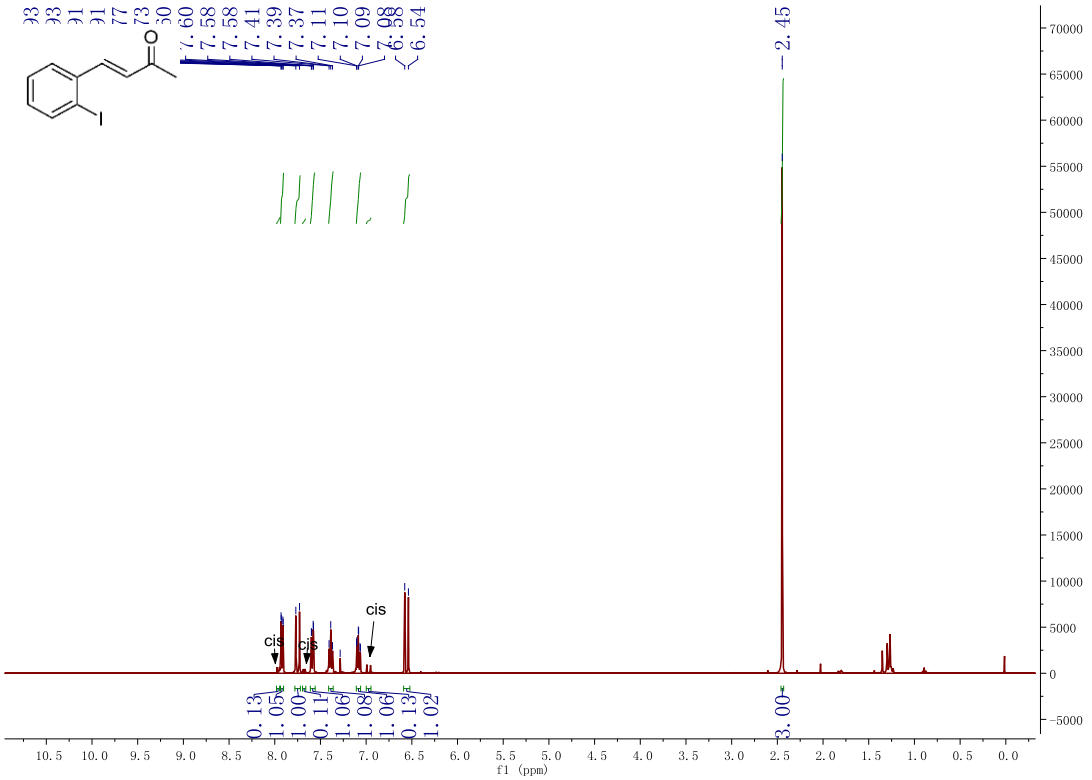


Figure S16. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3h**

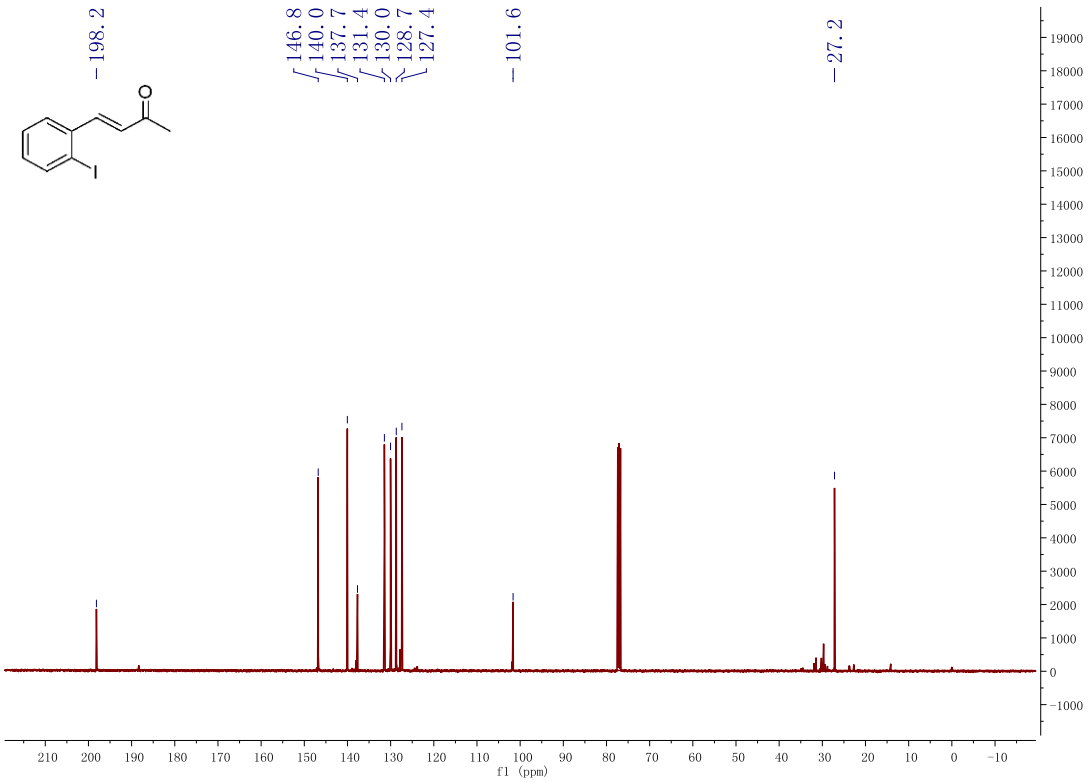


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3i** (trans:cis = 6:1)

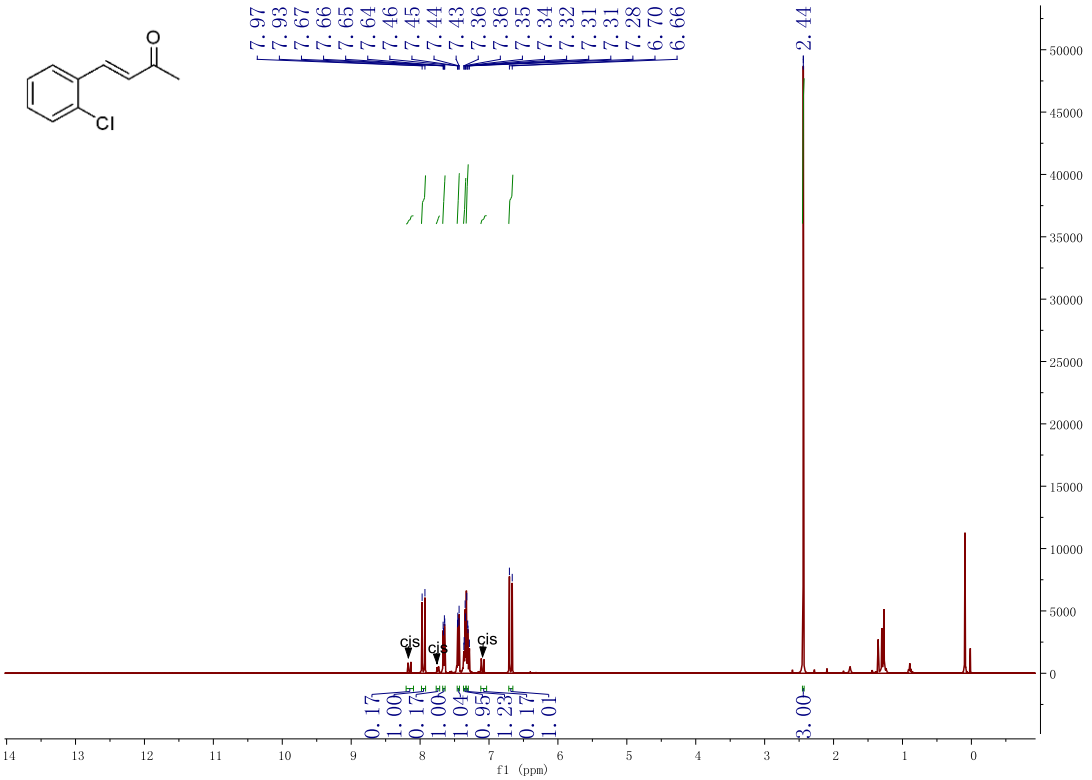


Figure S18. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3i**

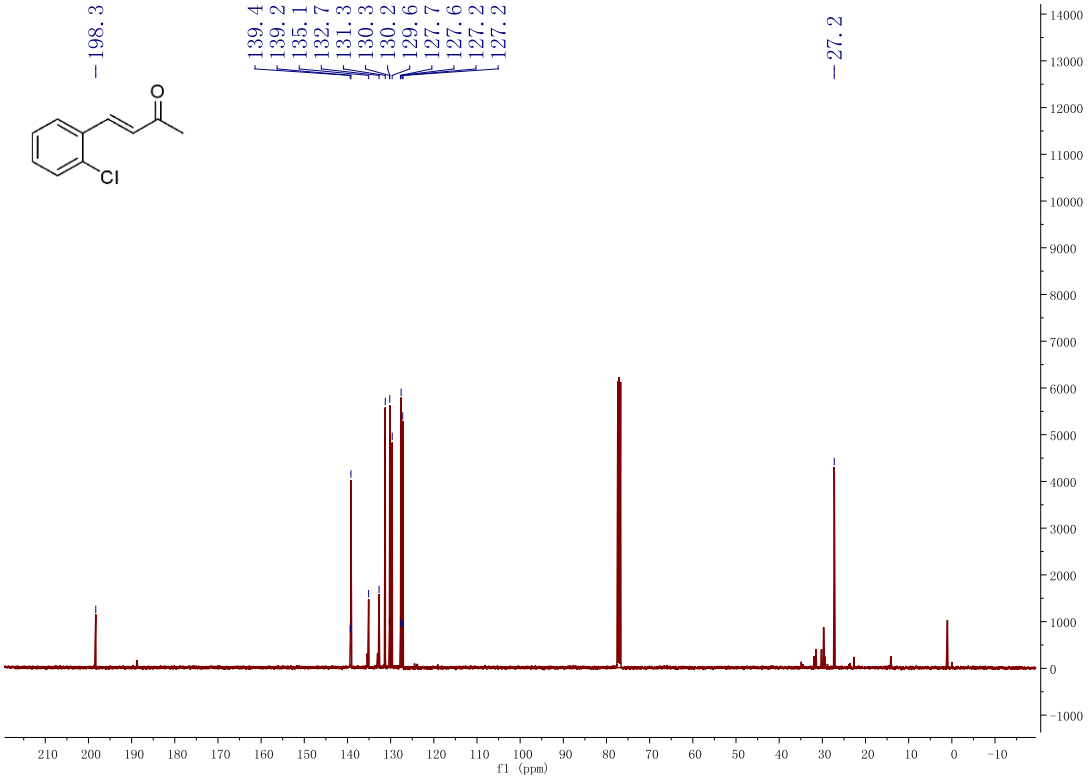


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3j**

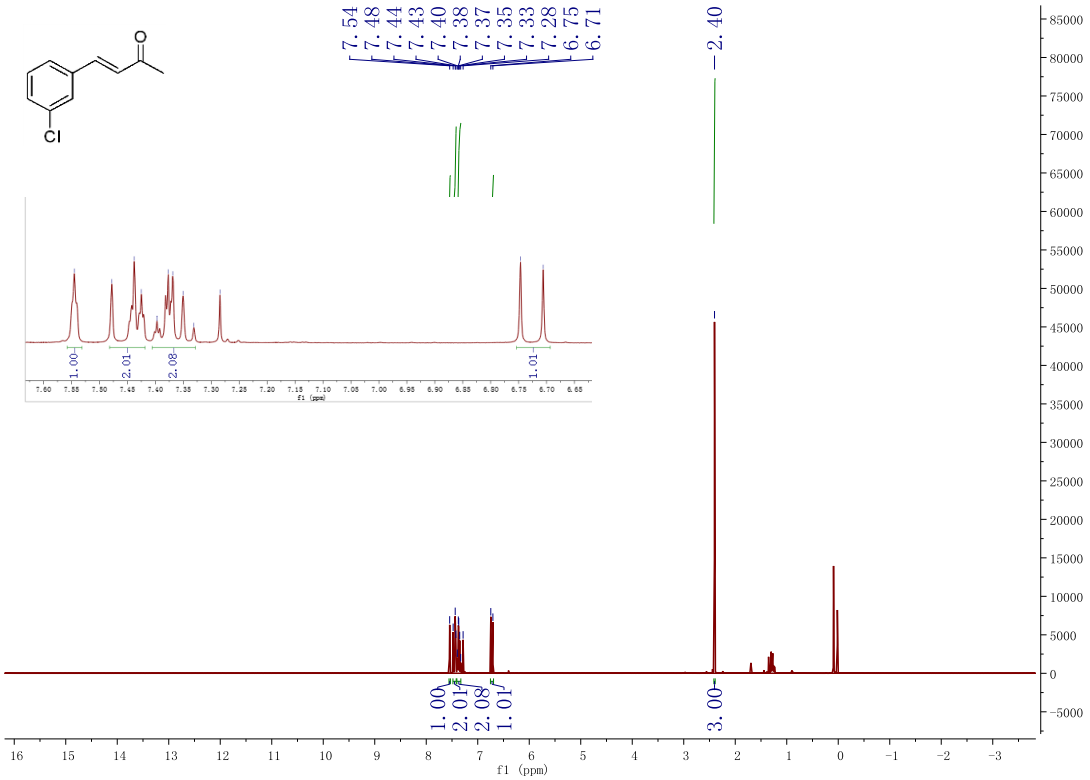


Figure S20. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3j**

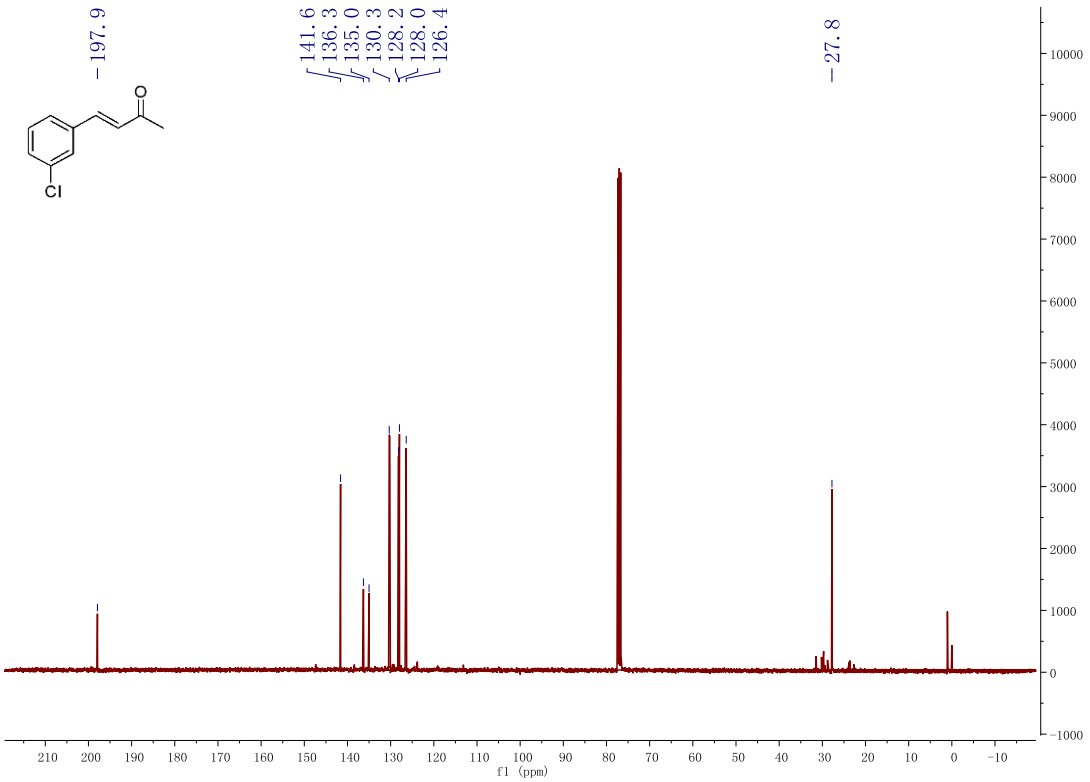


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3k**

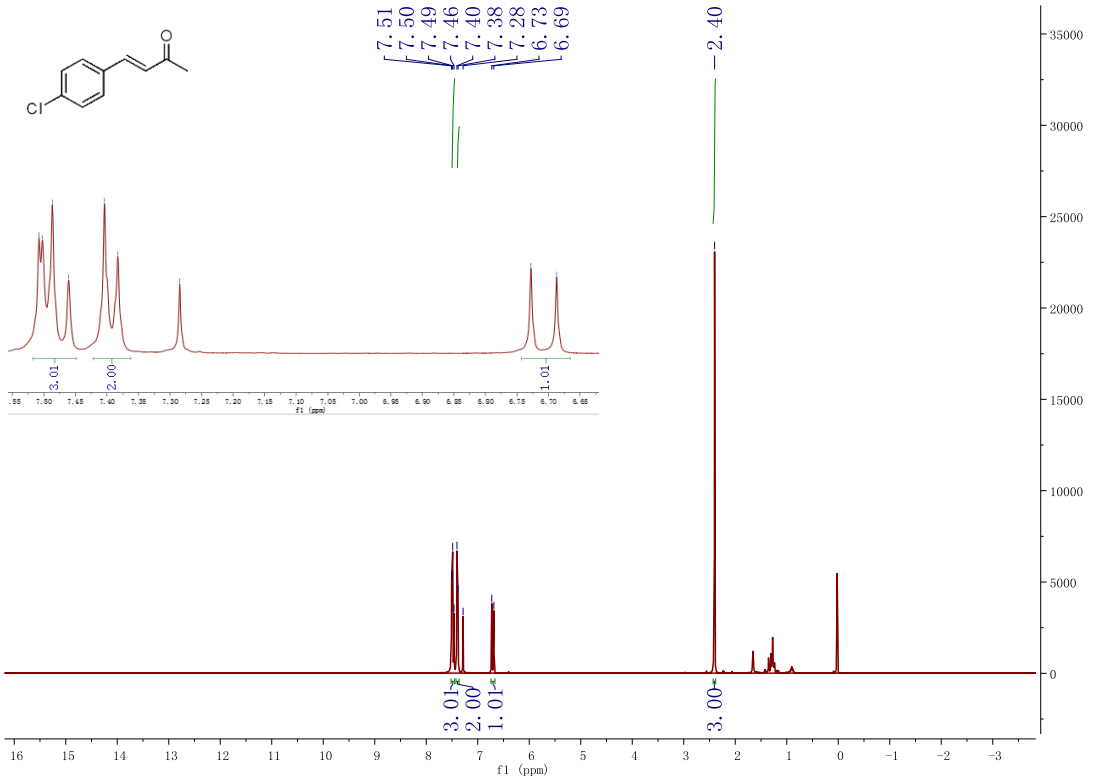


Figure S22. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3k**

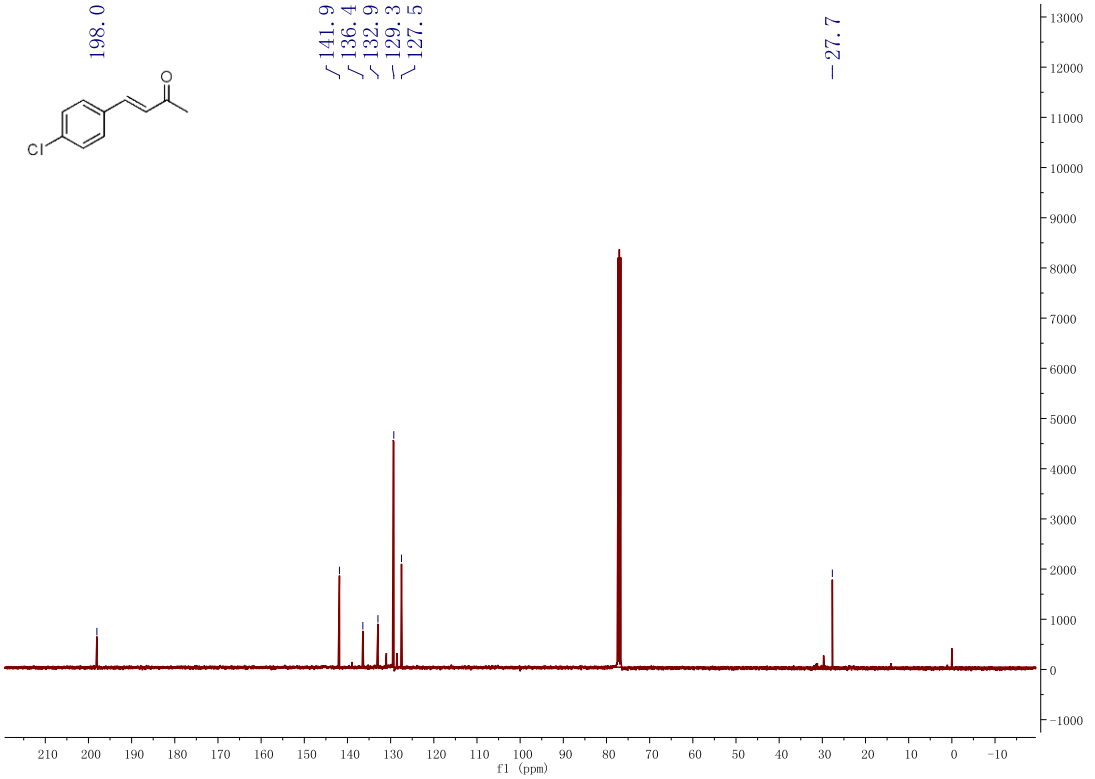


Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3l**

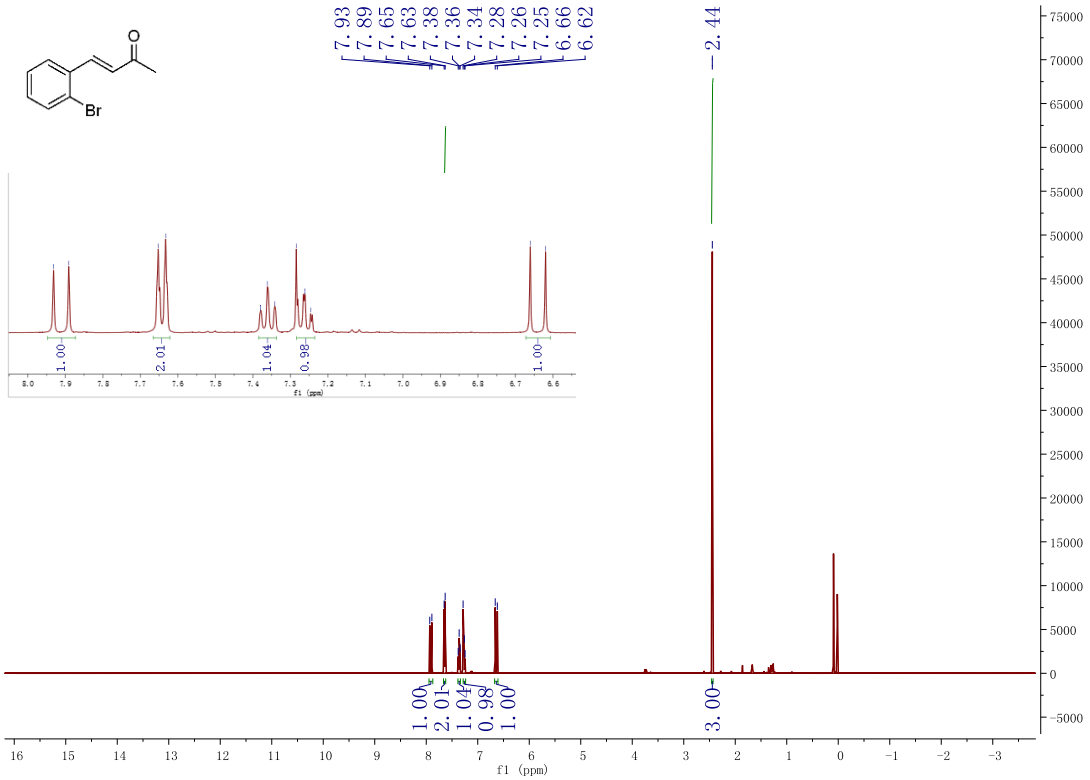


Figure S24. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3l**

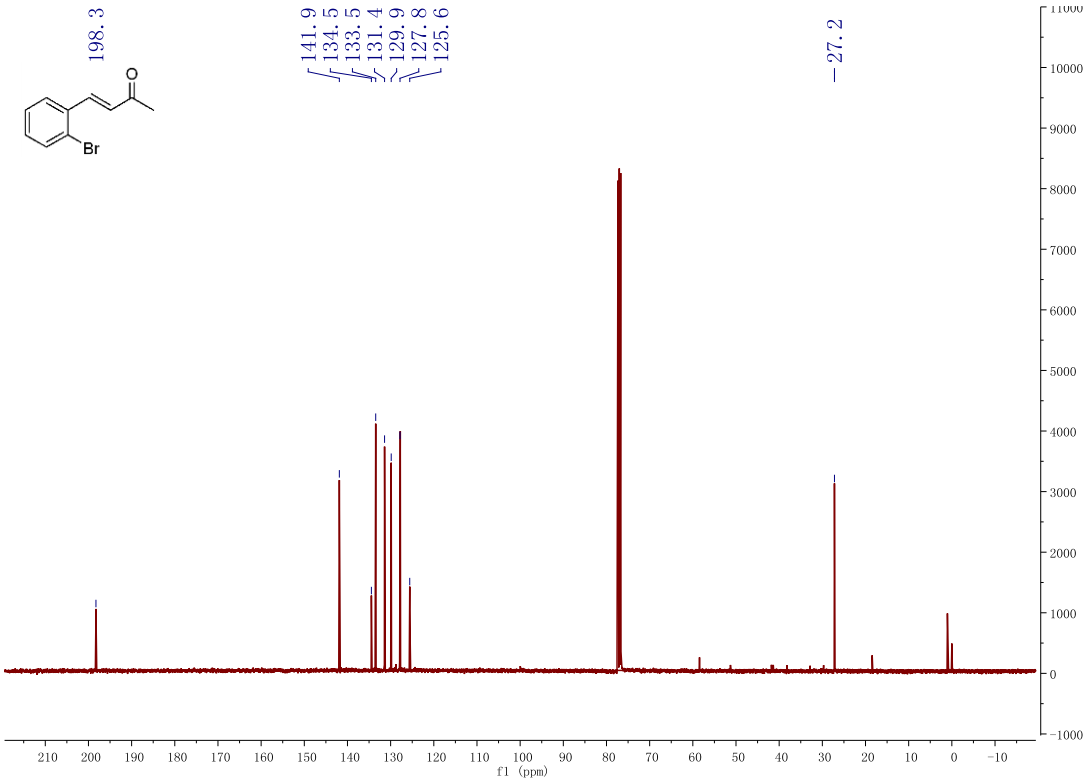


Figure S25. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3m** (E/Z ratio = 6:1)

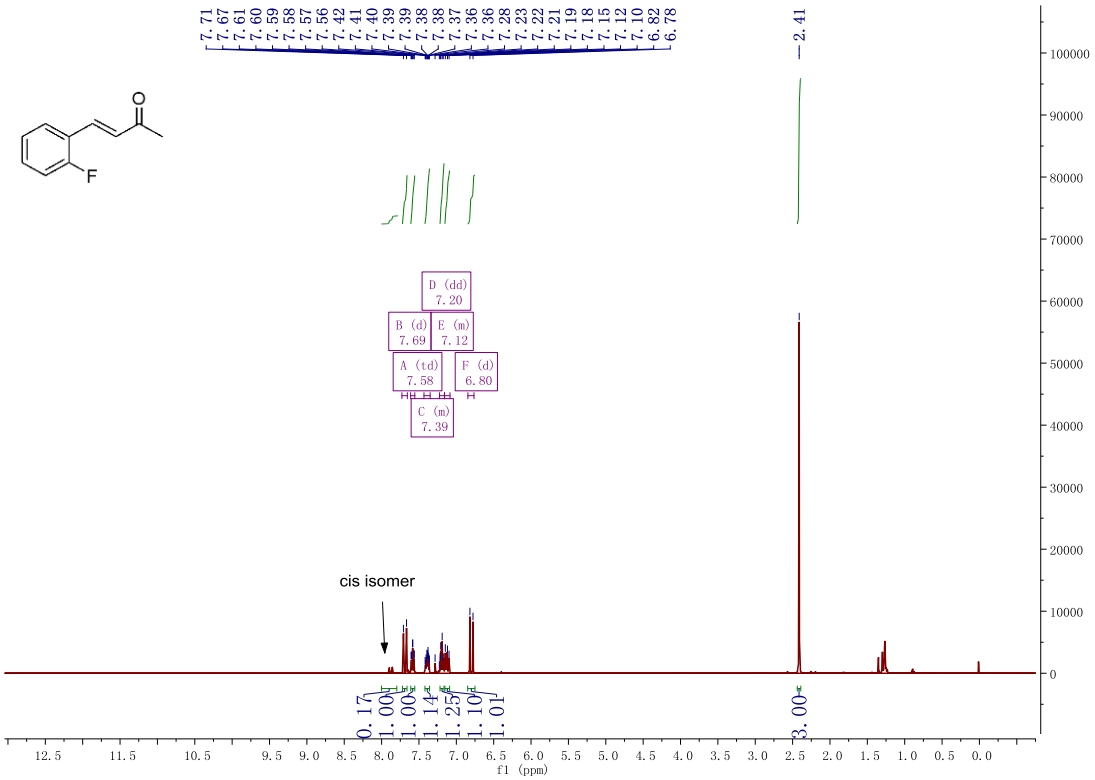


Figure S26. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3m**

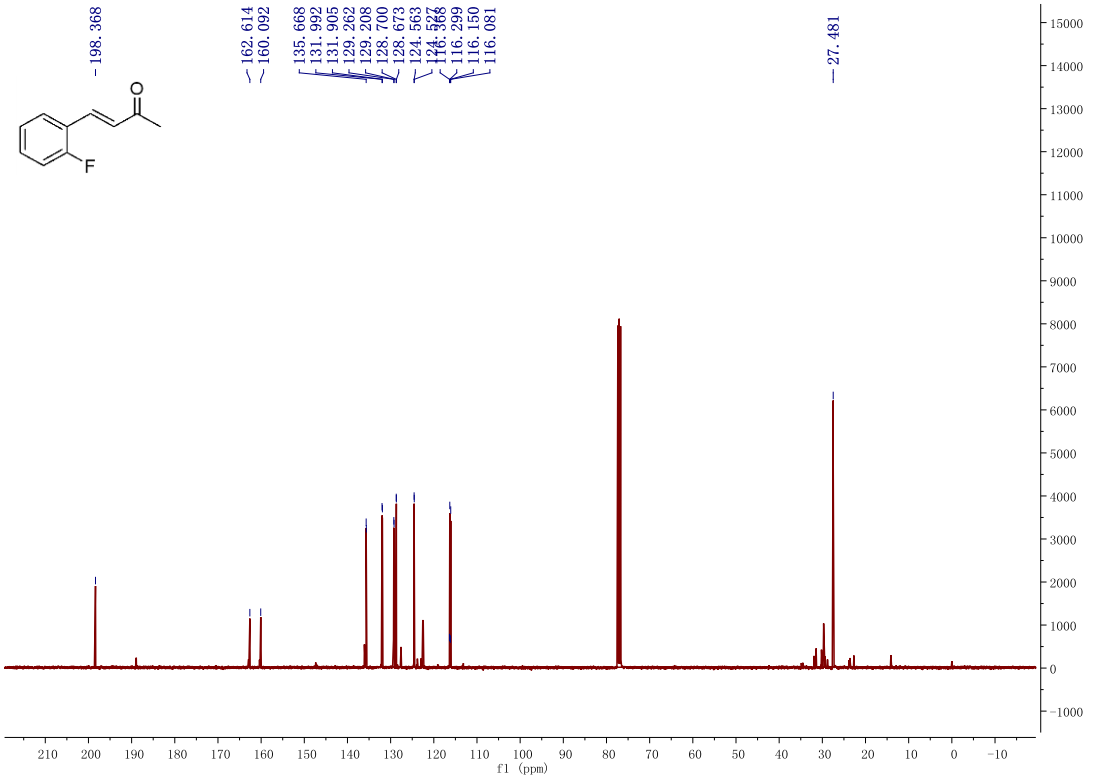


Figure S27. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3m**

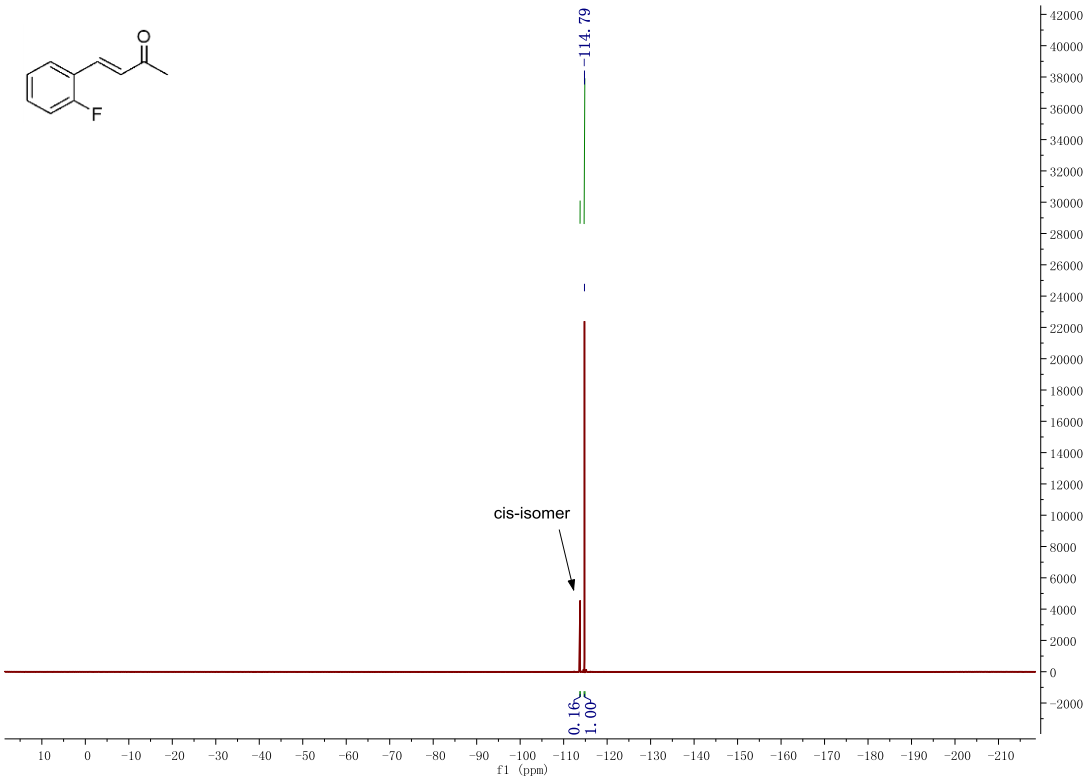


Figure S28. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3n**

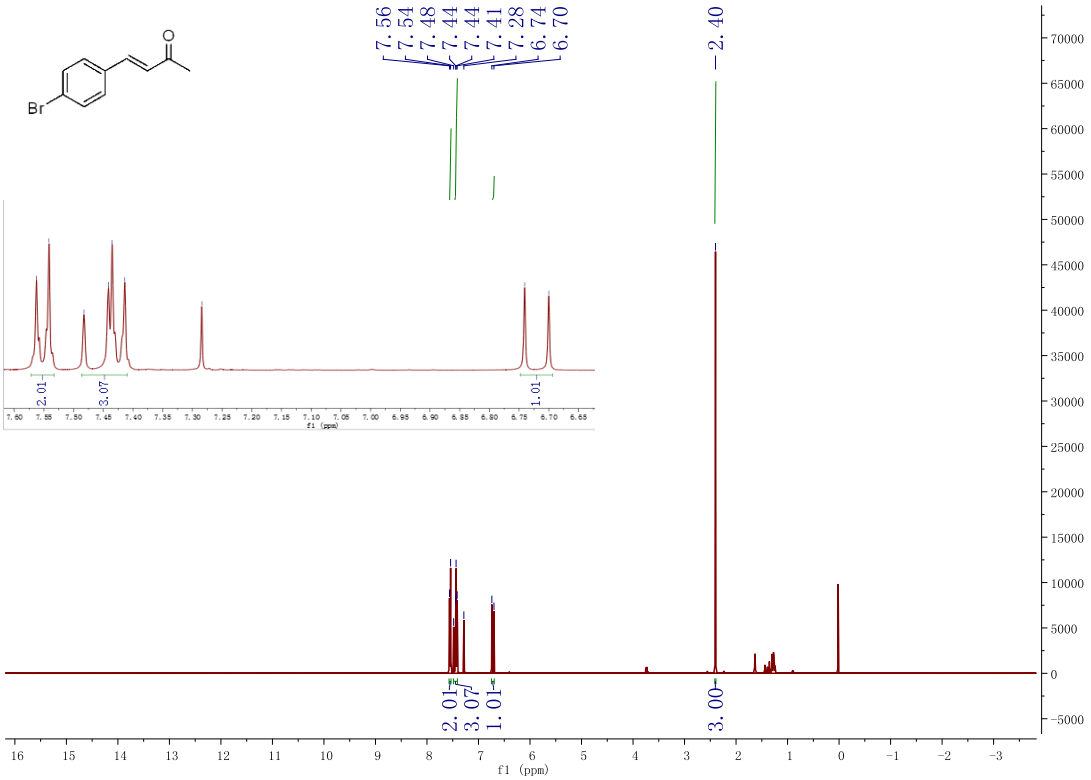


Figure S29. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3n**

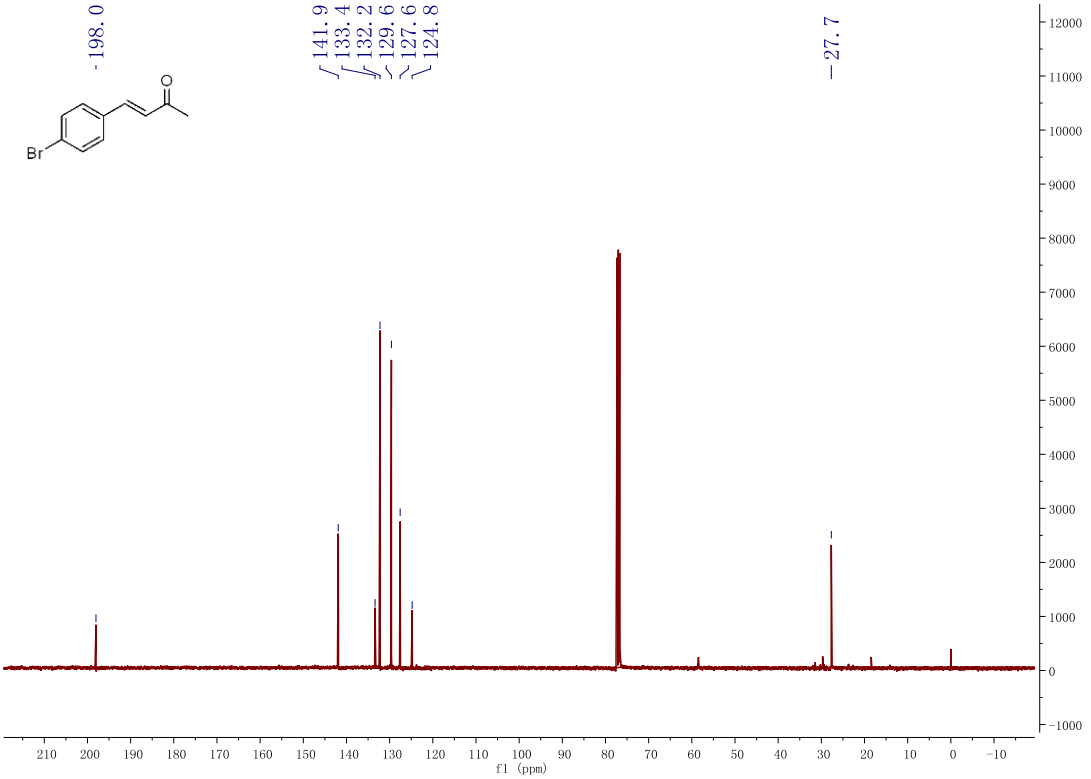


Figure S30. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3o**

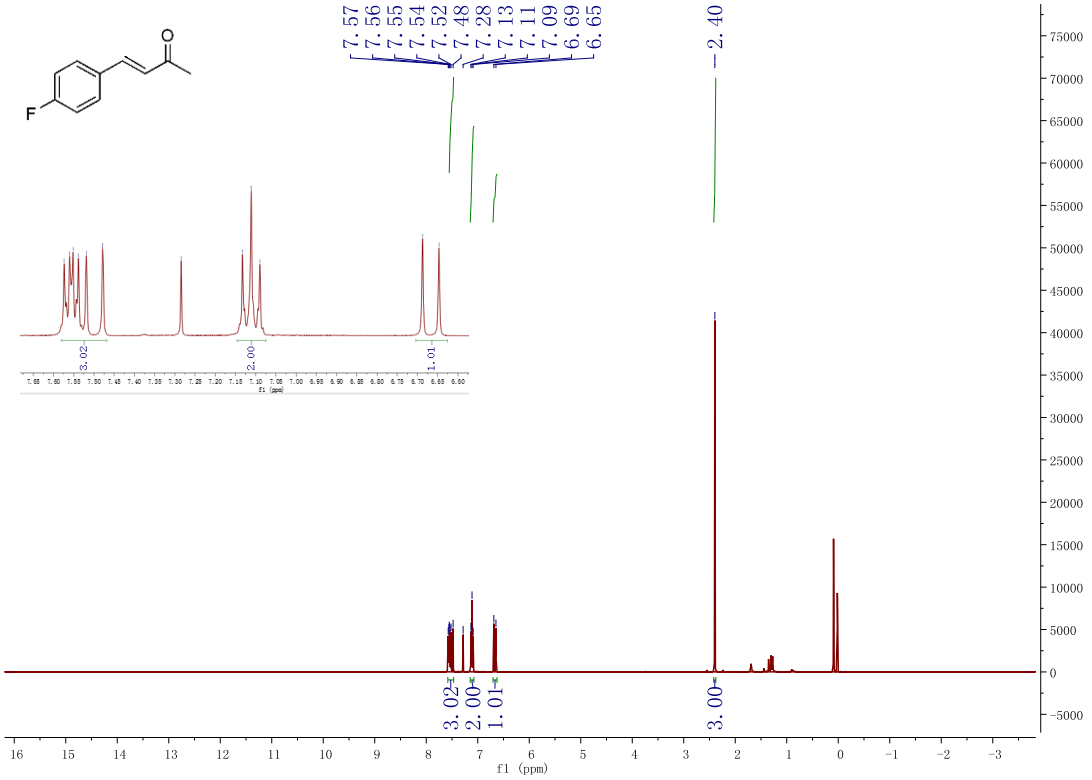


Figure S31. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3o**

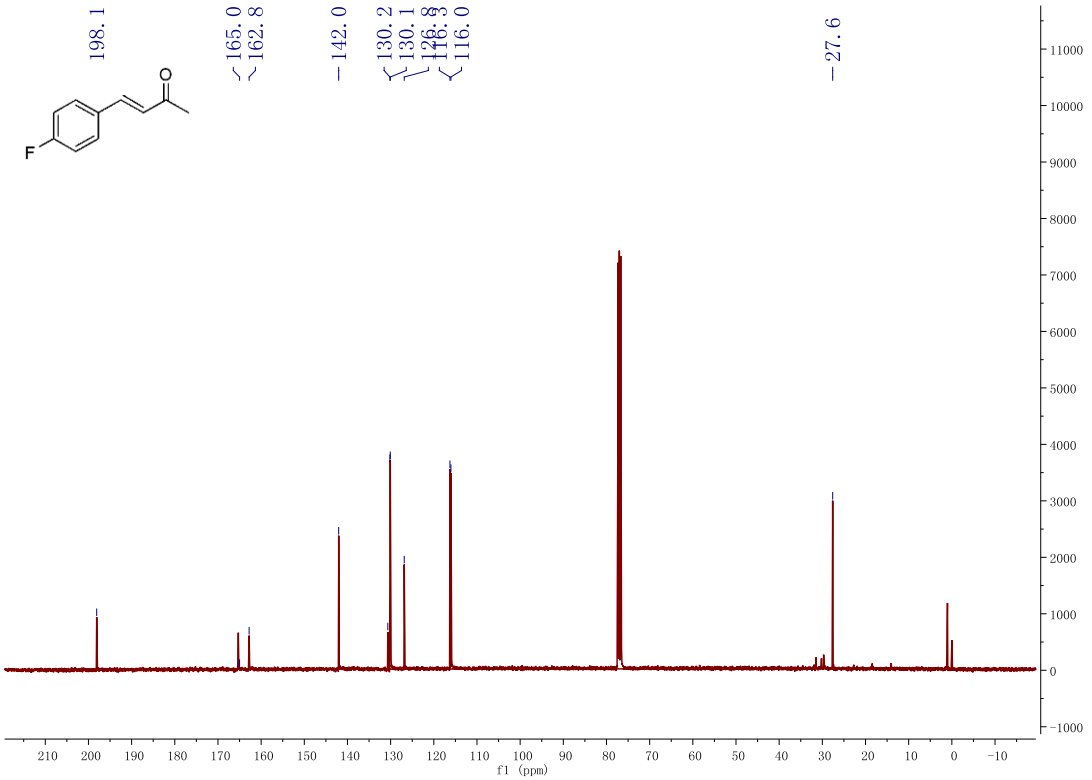


Figure S32. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3o**

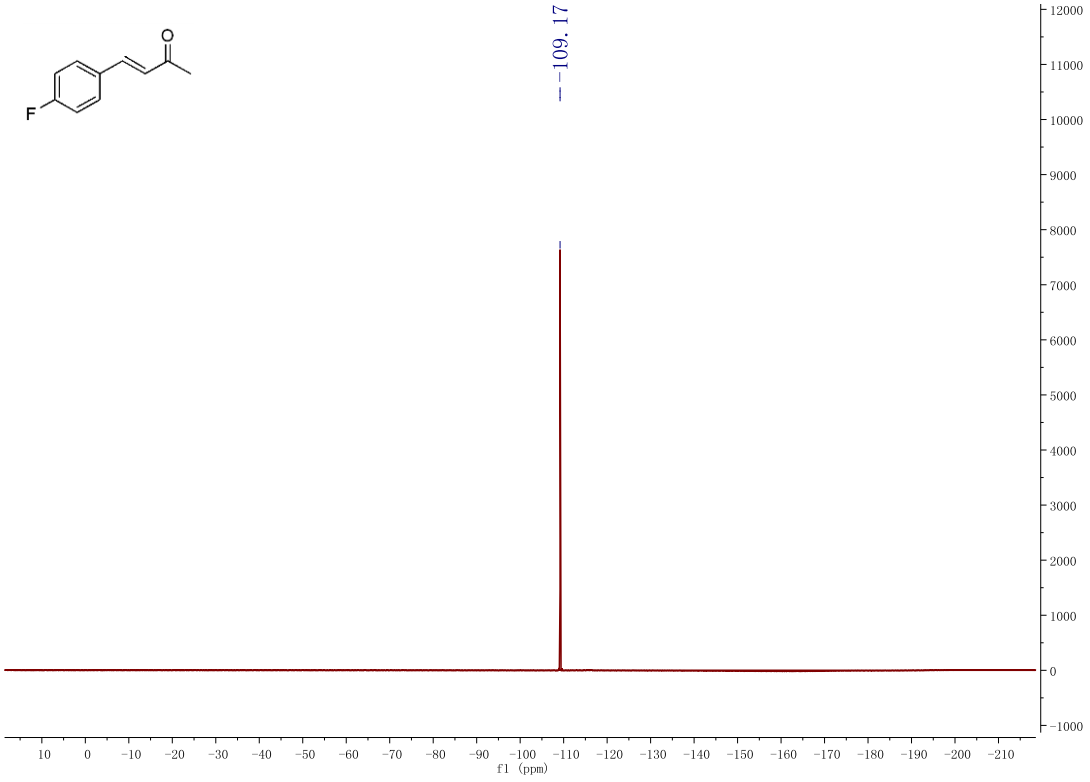


Figure S33. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3p**

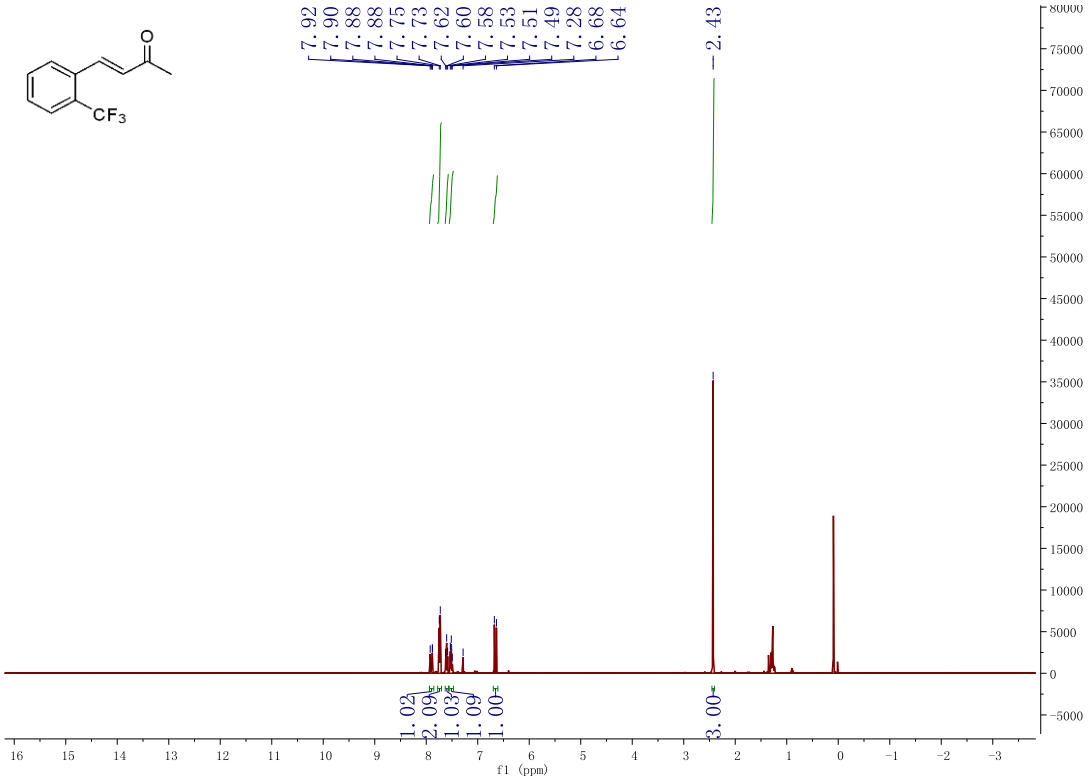


Figure S34. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3p**

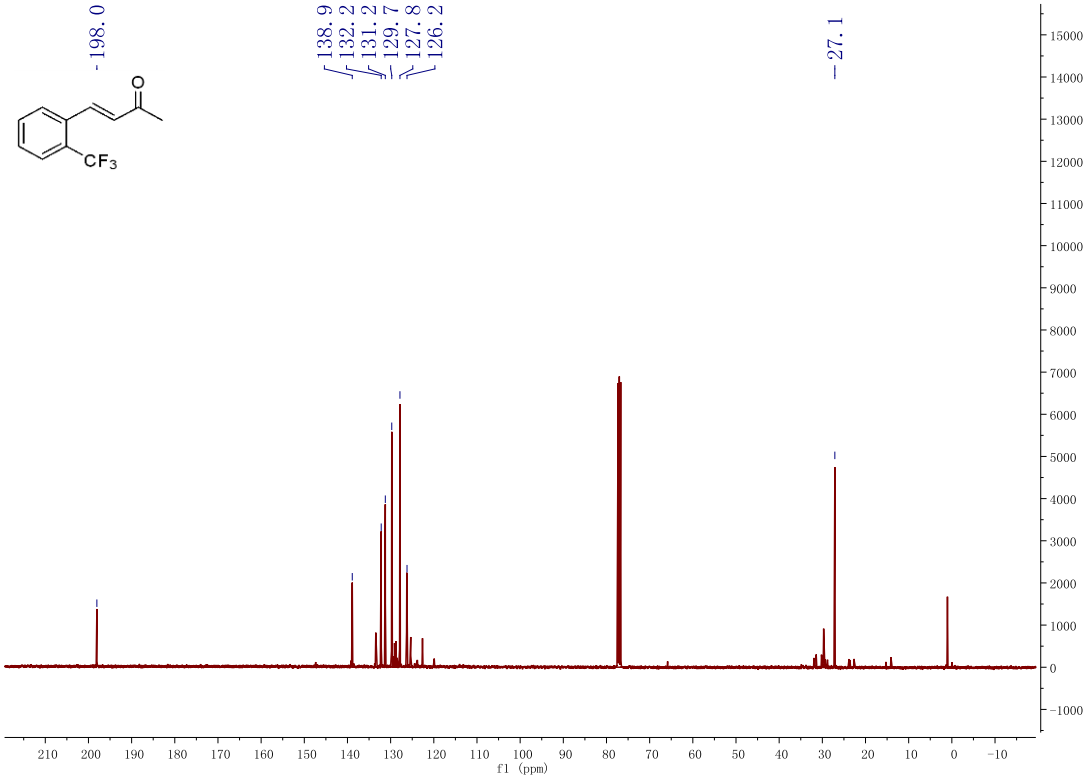


Figure S35. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3p**

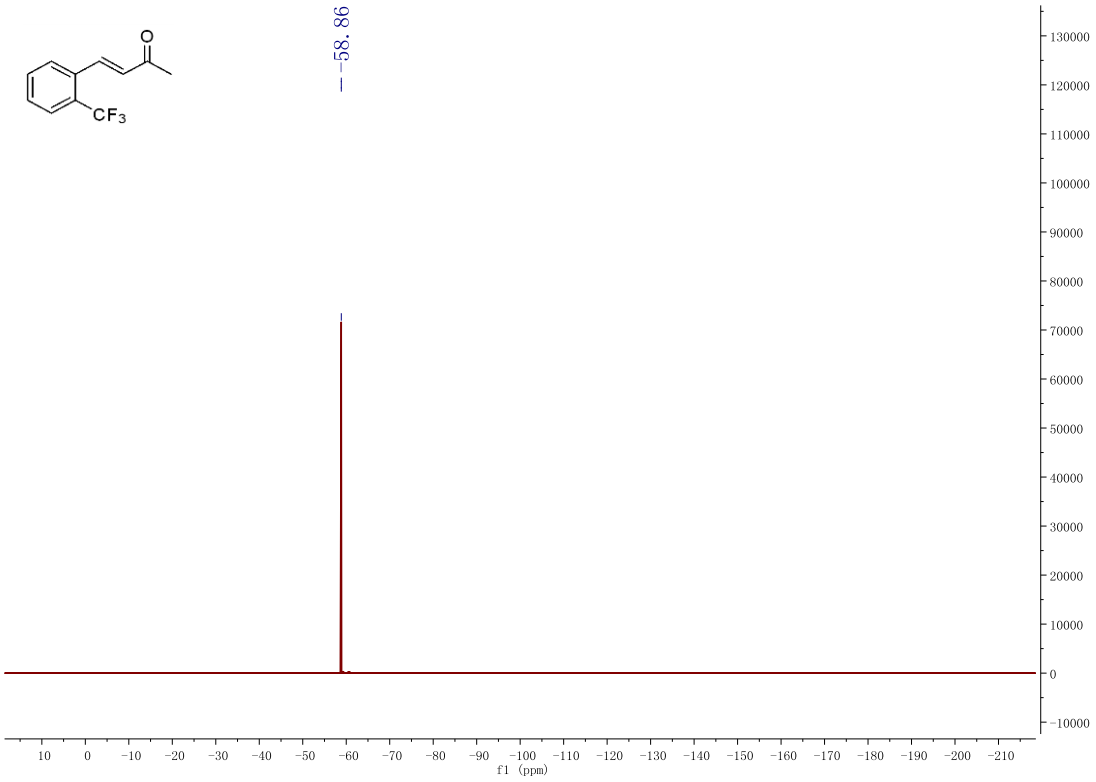


Figure S36. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3q**

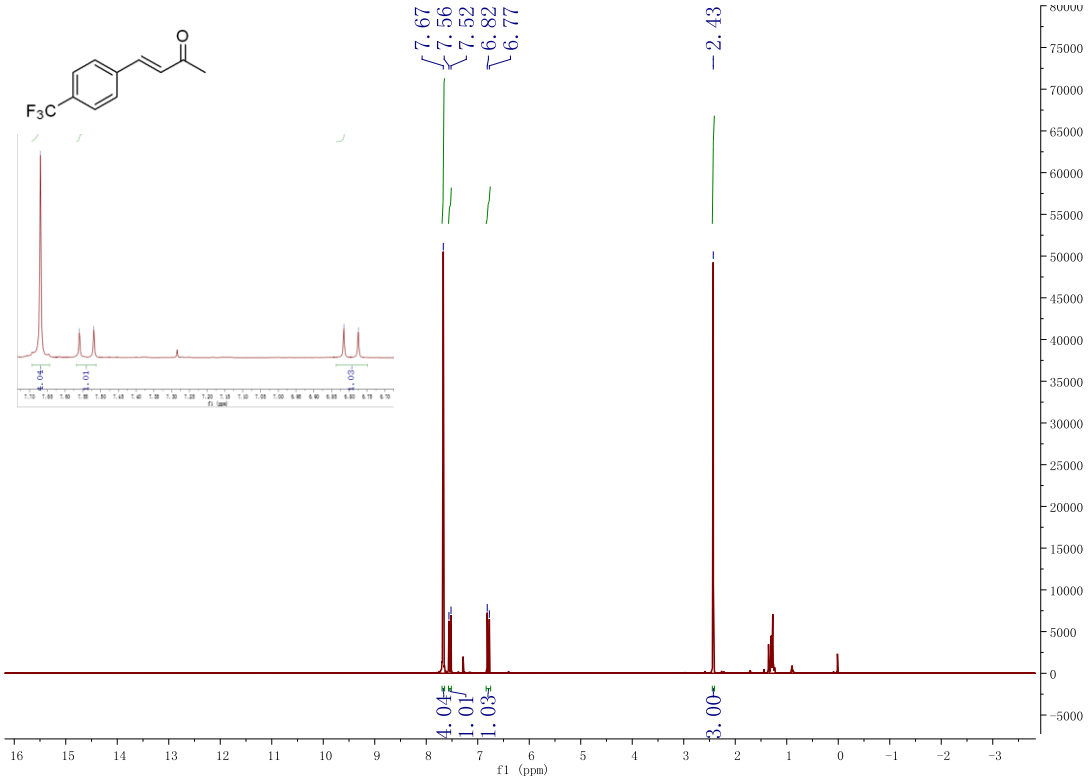


Figure S37. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3q**

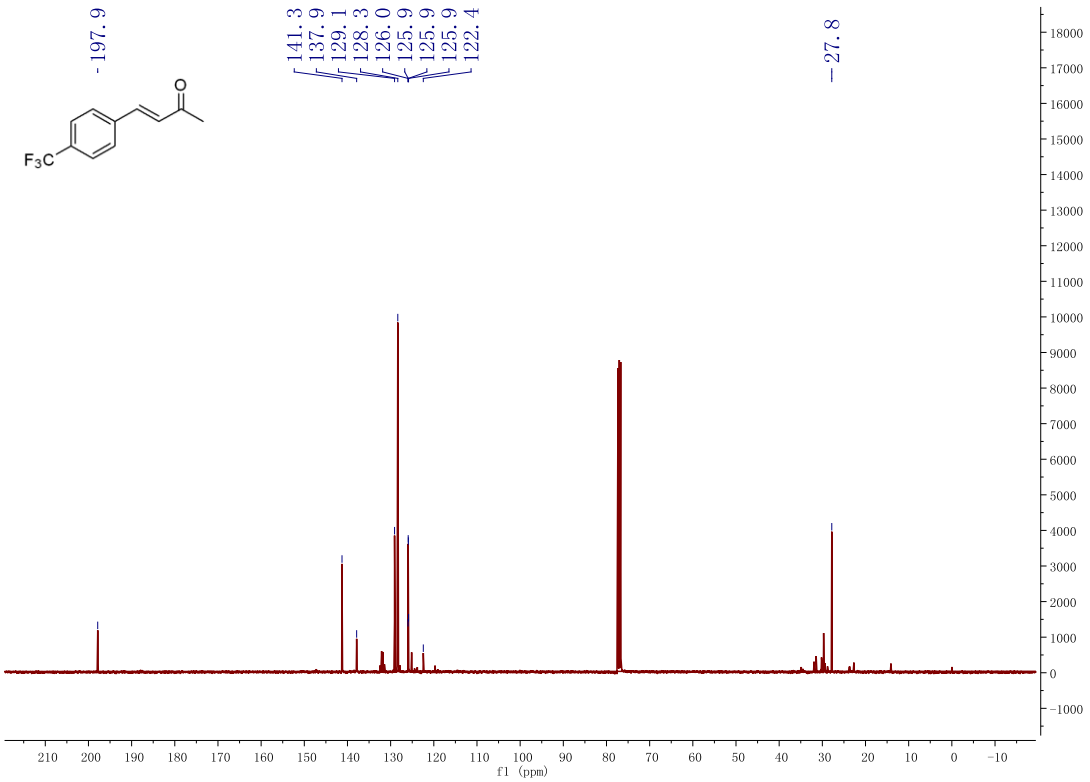


Figure S38. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3q**

Figure S39. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3r**

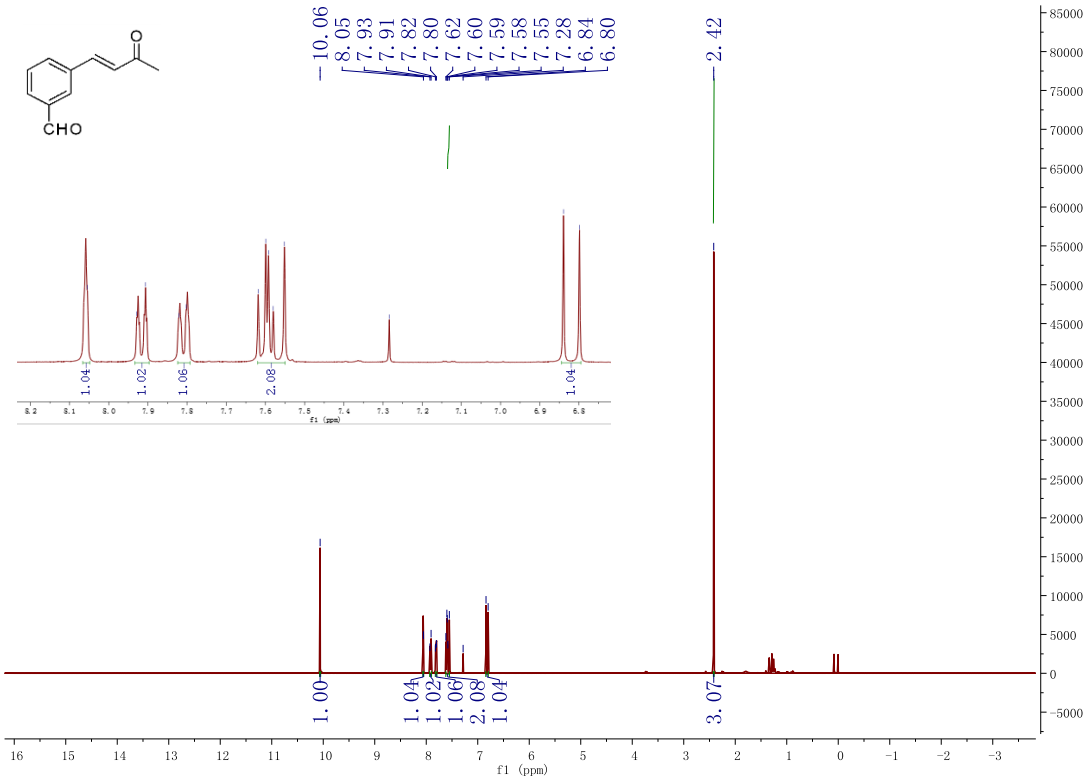


Figure S40. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3r**

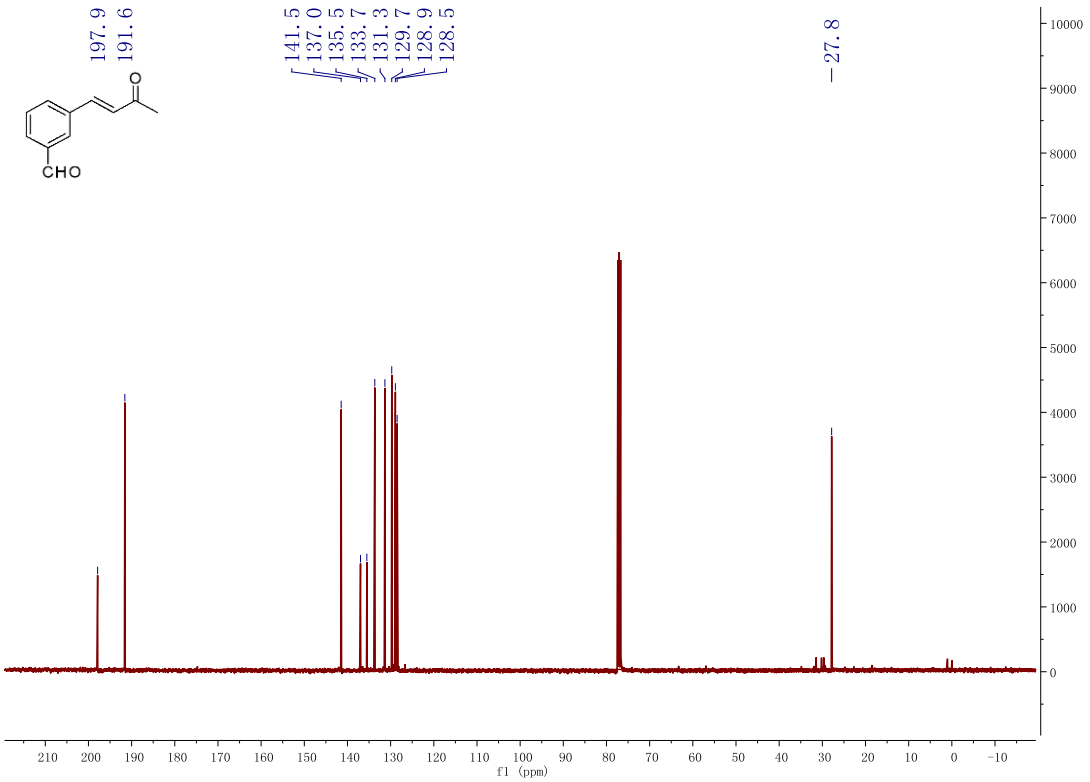


Figure S41. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3s**

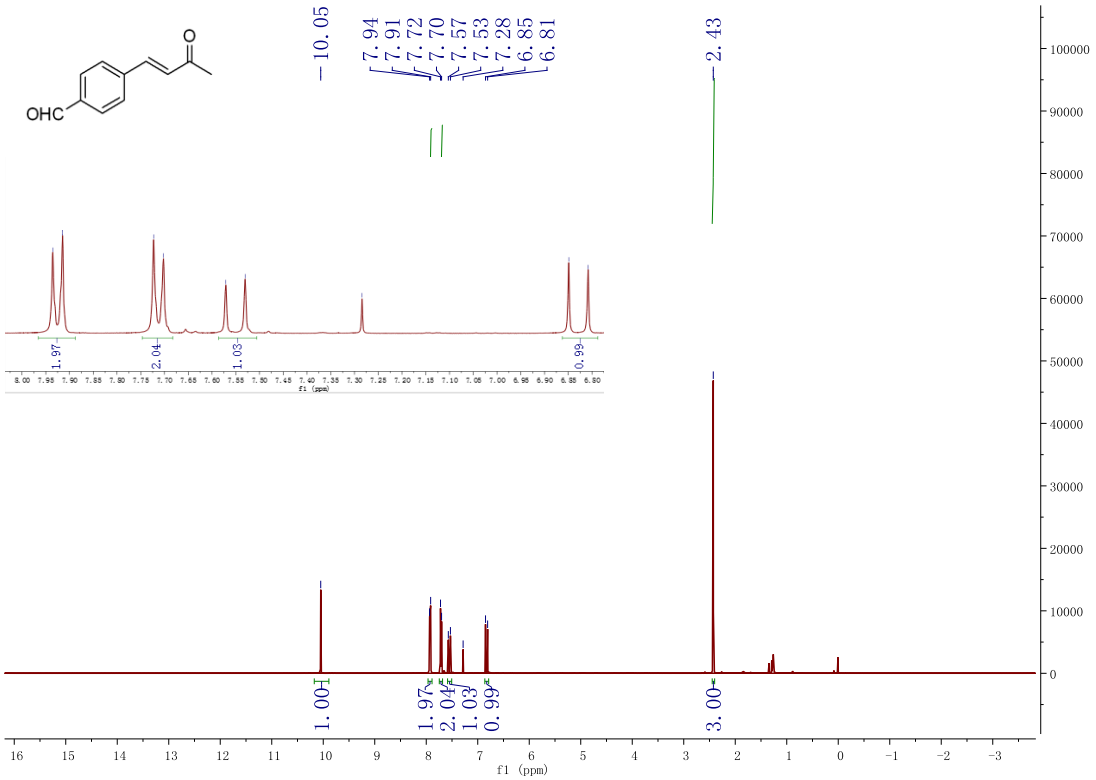


Figure S42. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3s**

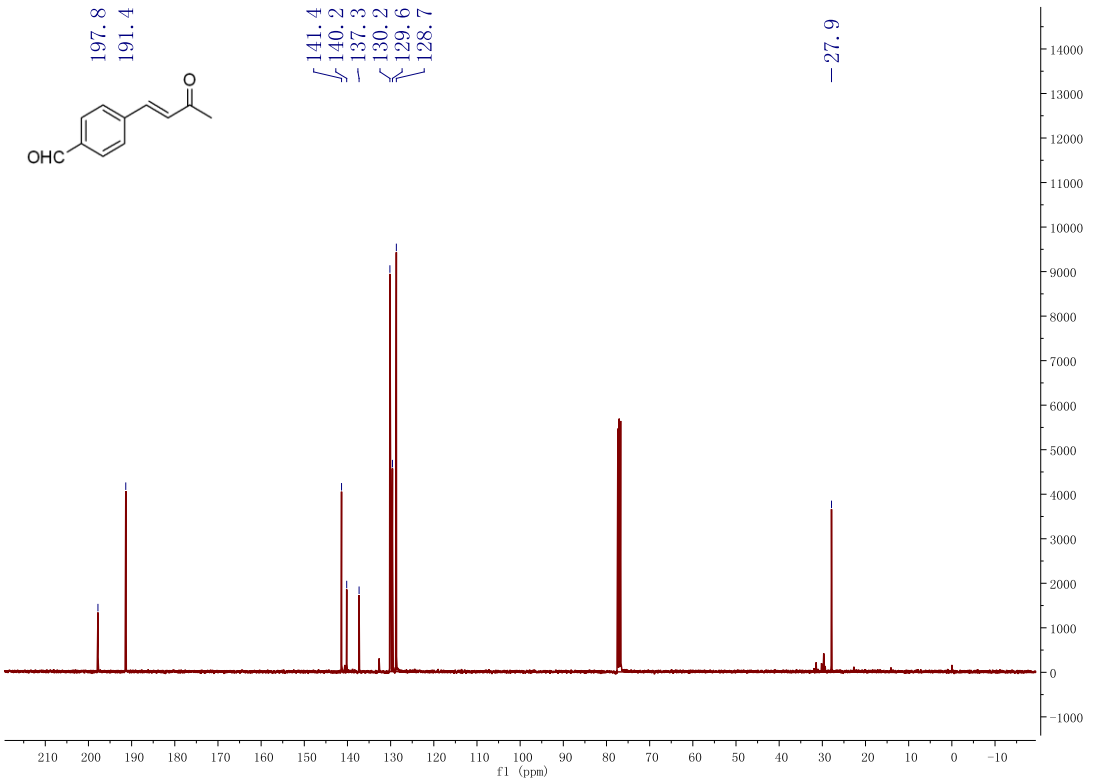


Figure S43. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3t**

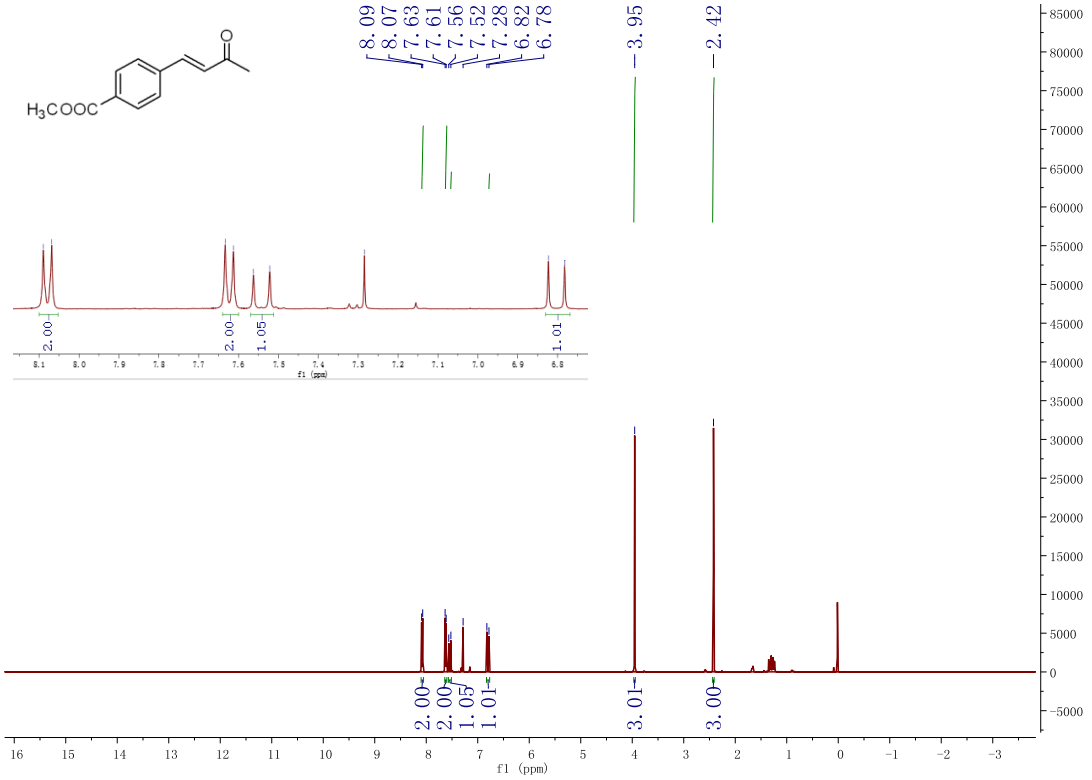


Figure S44. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3t**

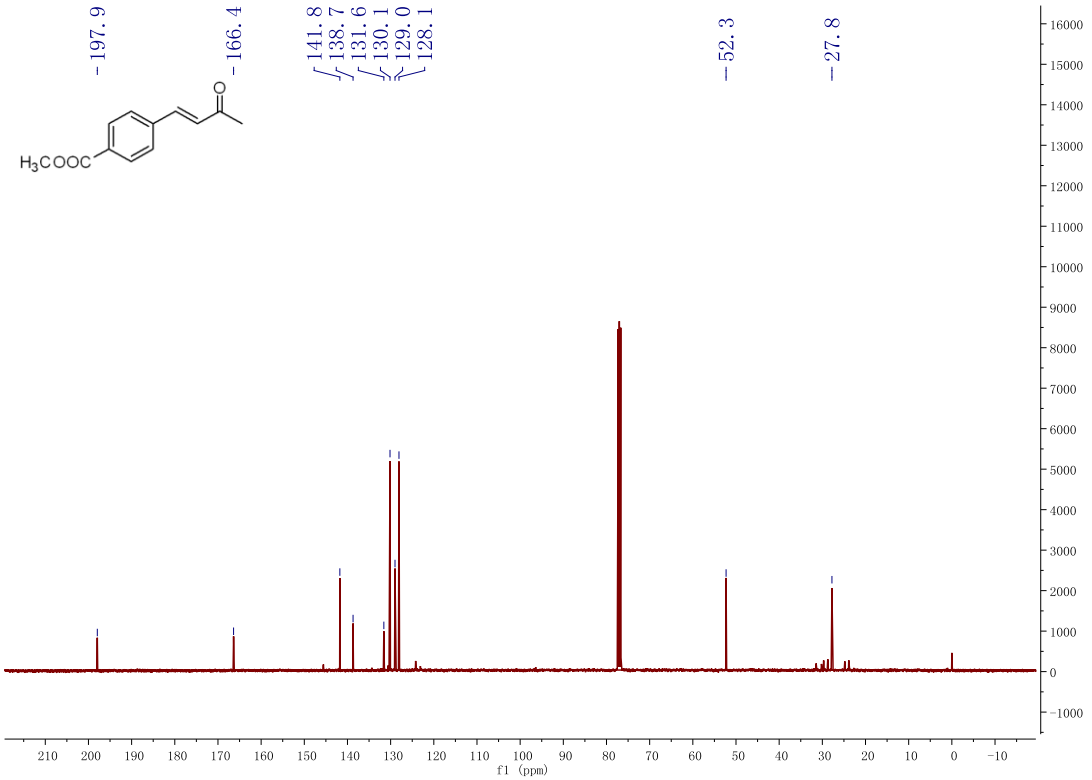


Figure S45. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3u**

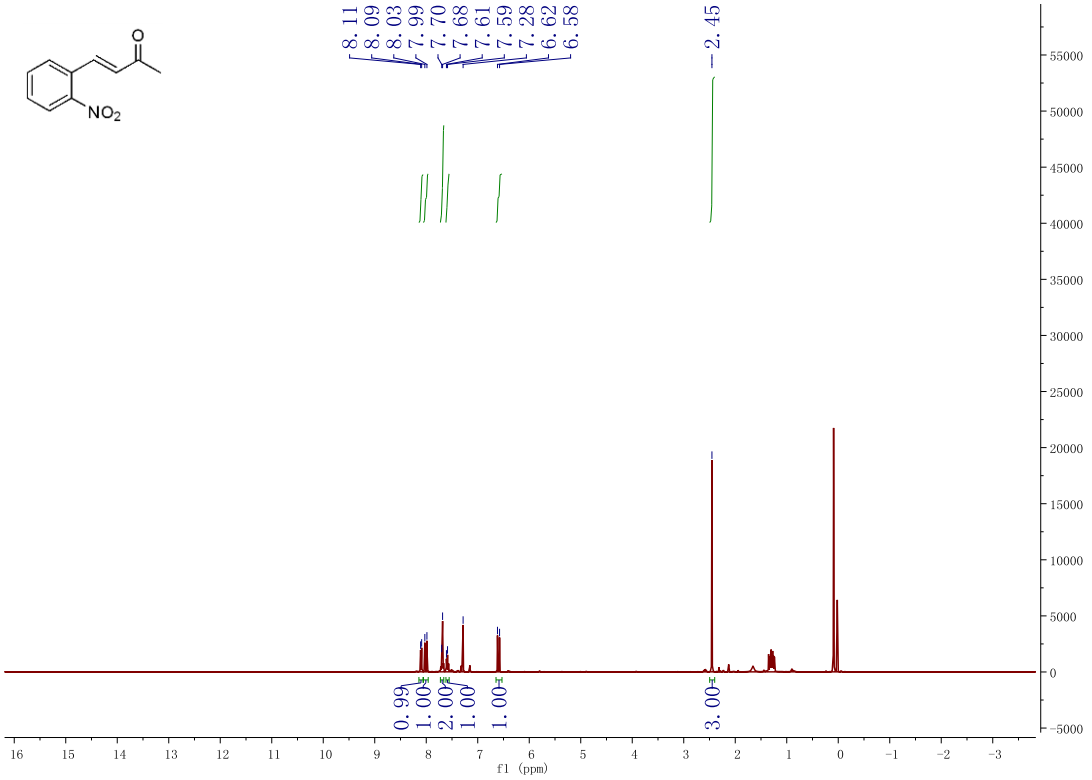


Figure S46. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3u**

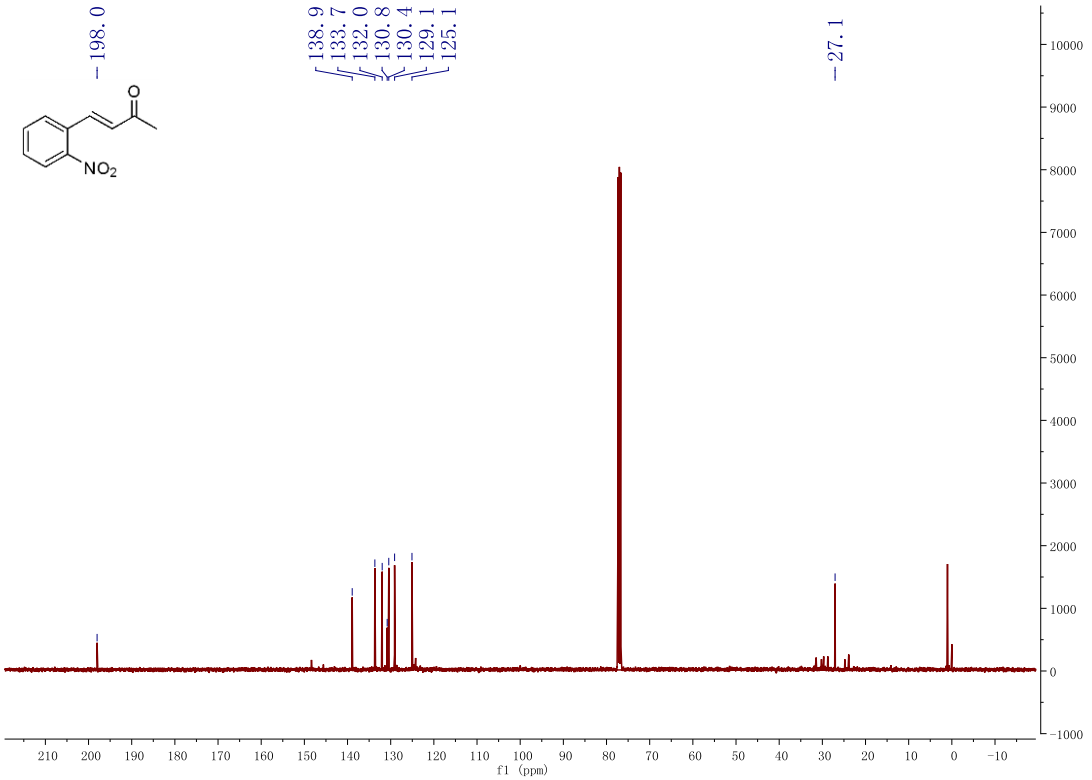


Figure S47. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3v**

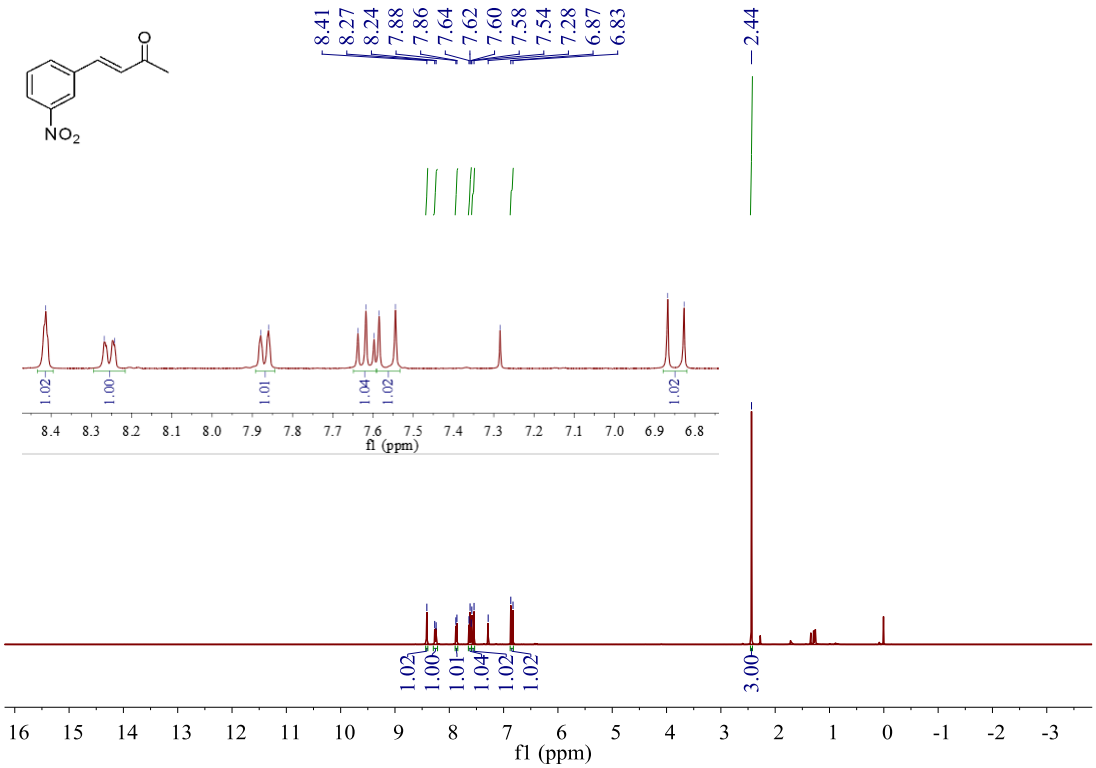


Figure S48. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3v**

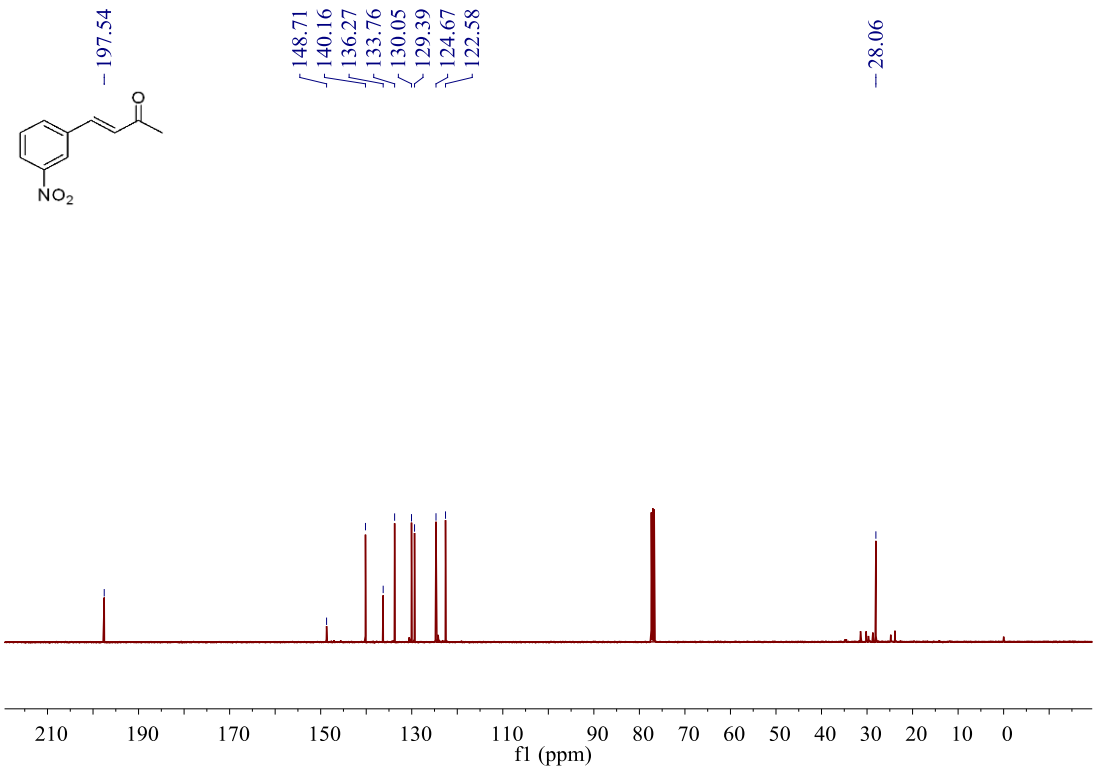


Figure S49. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3w**

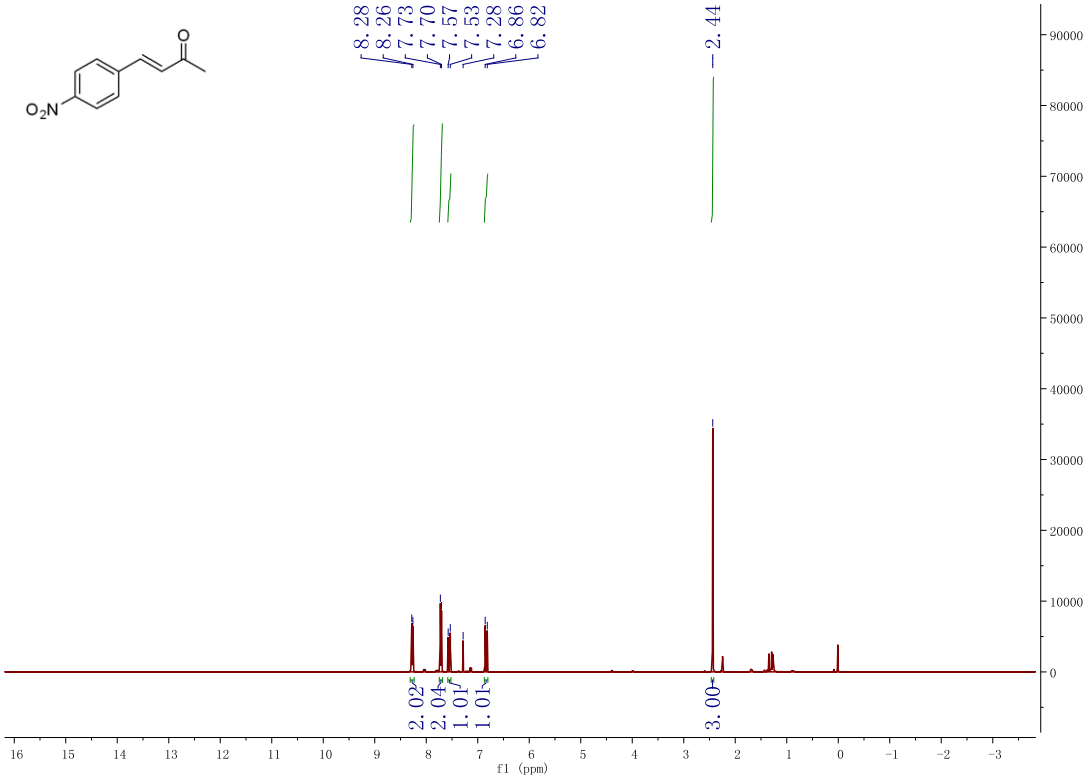


Figure S50. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3w**

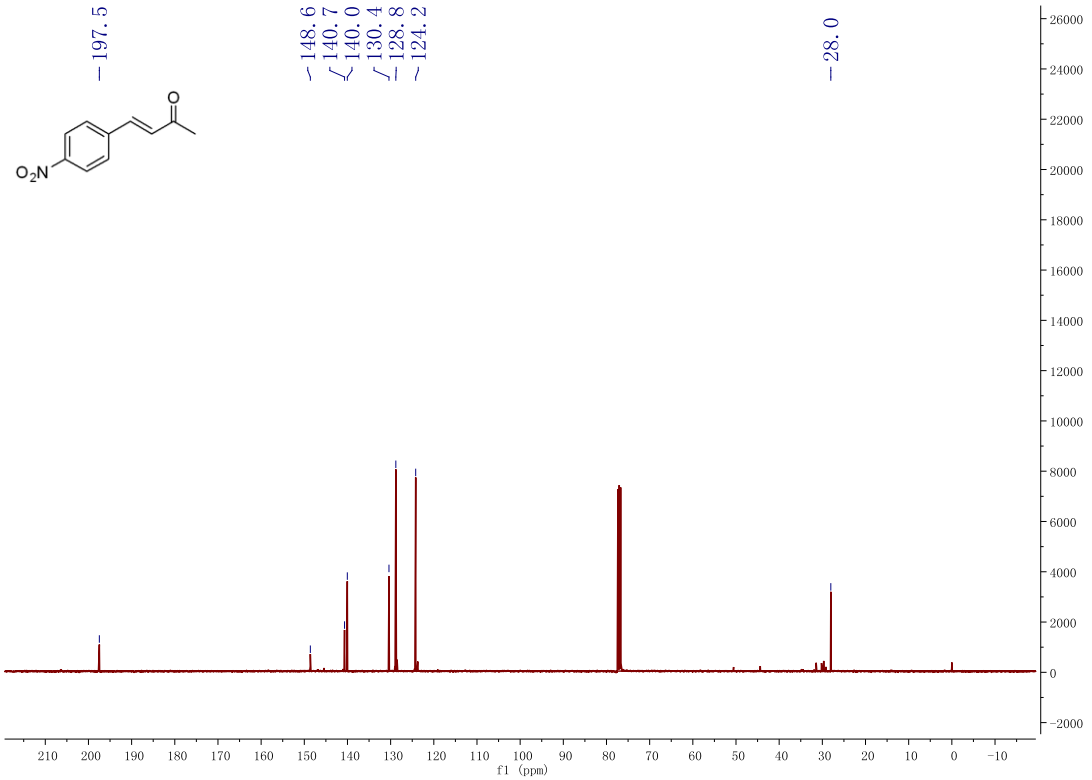


Figure S51. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3x**

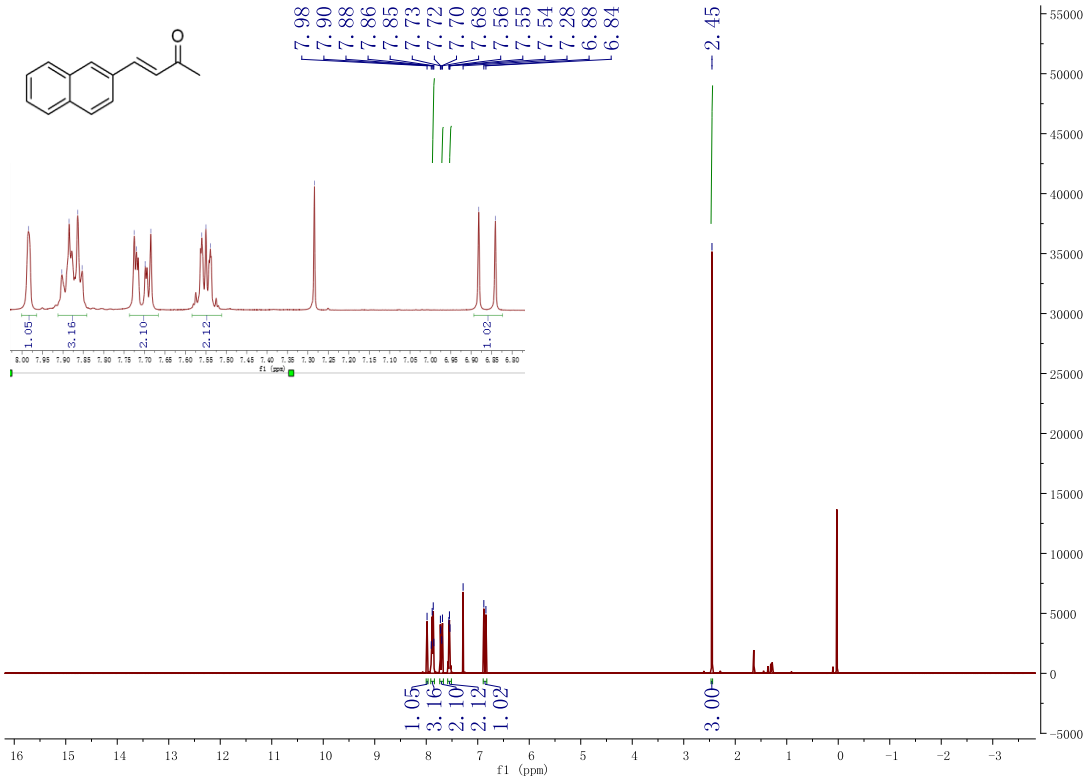


Figure S52. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3x**

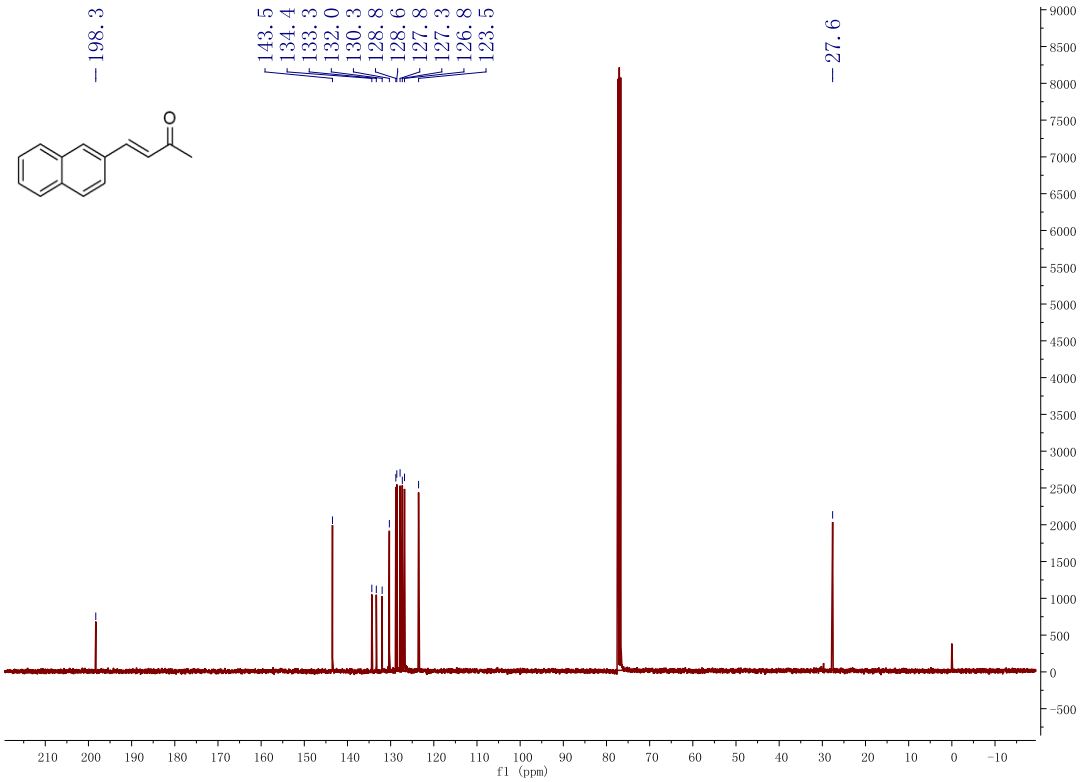


Figure S53. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3y**

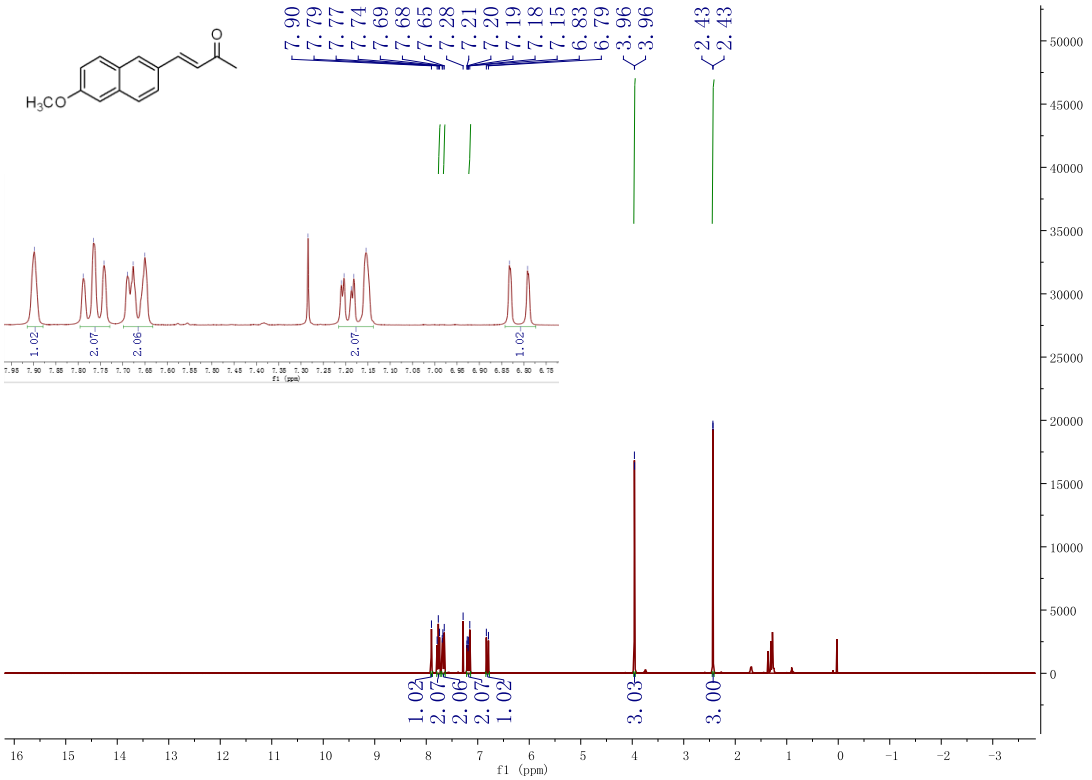


Figure S54. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **3y**

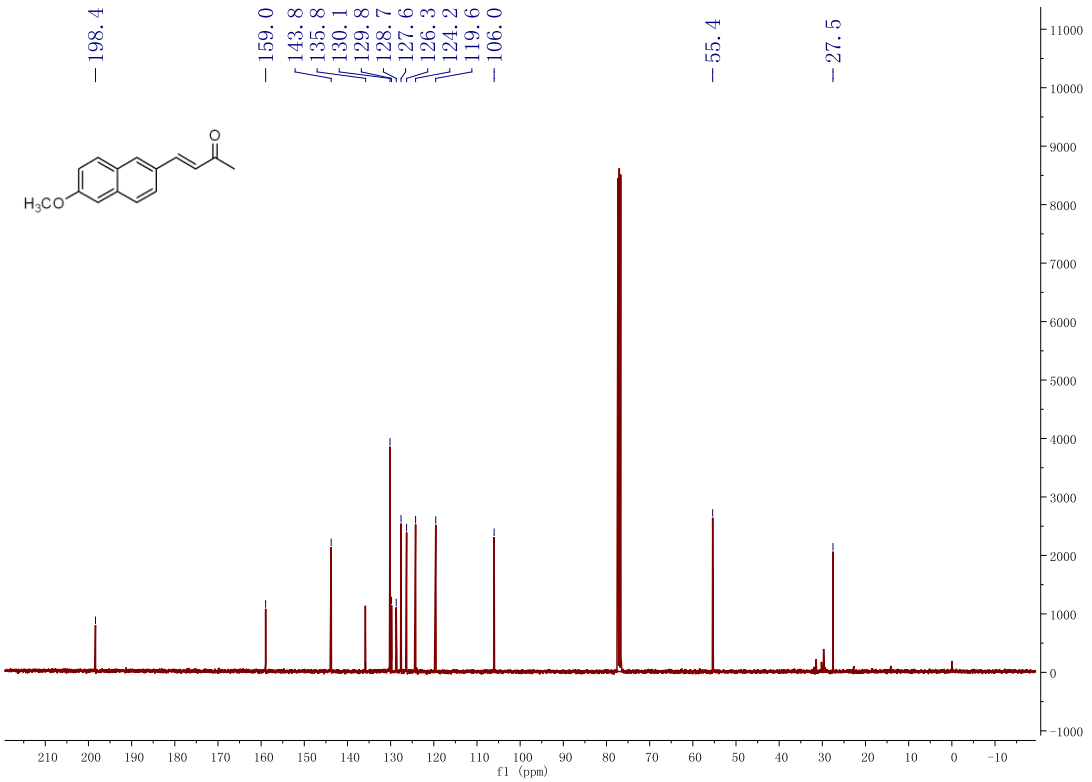


Figure S55. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4a** (trans:cis=5:1)

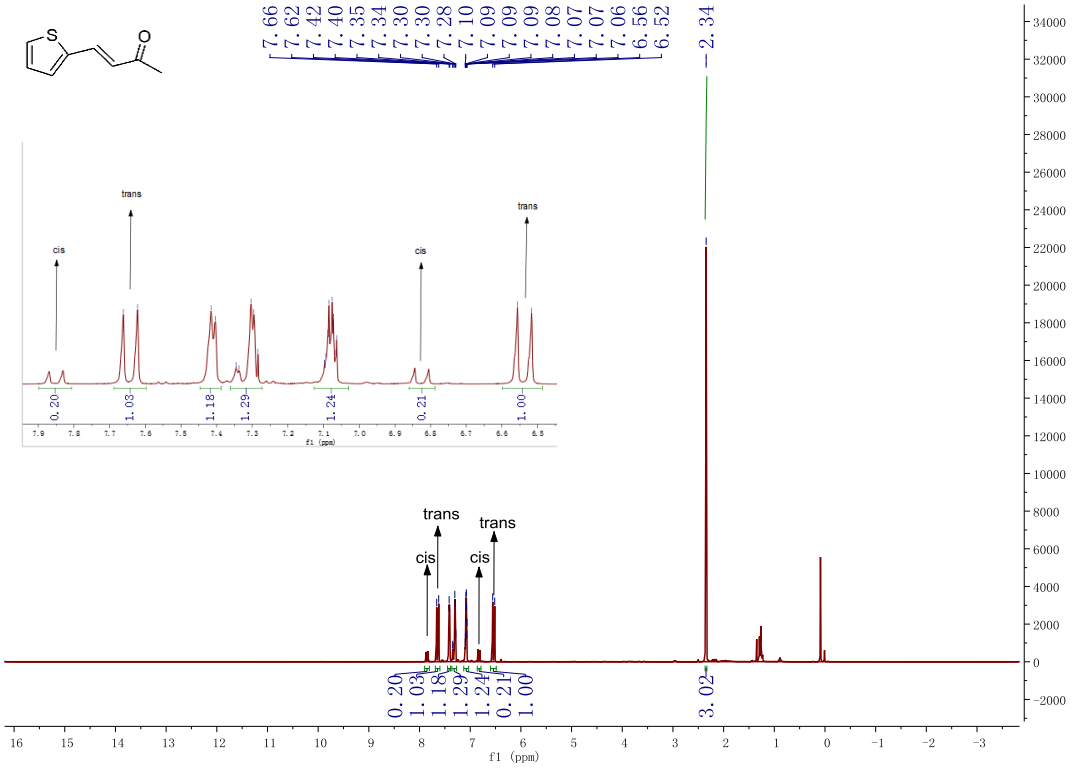


Figure S56. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4a**

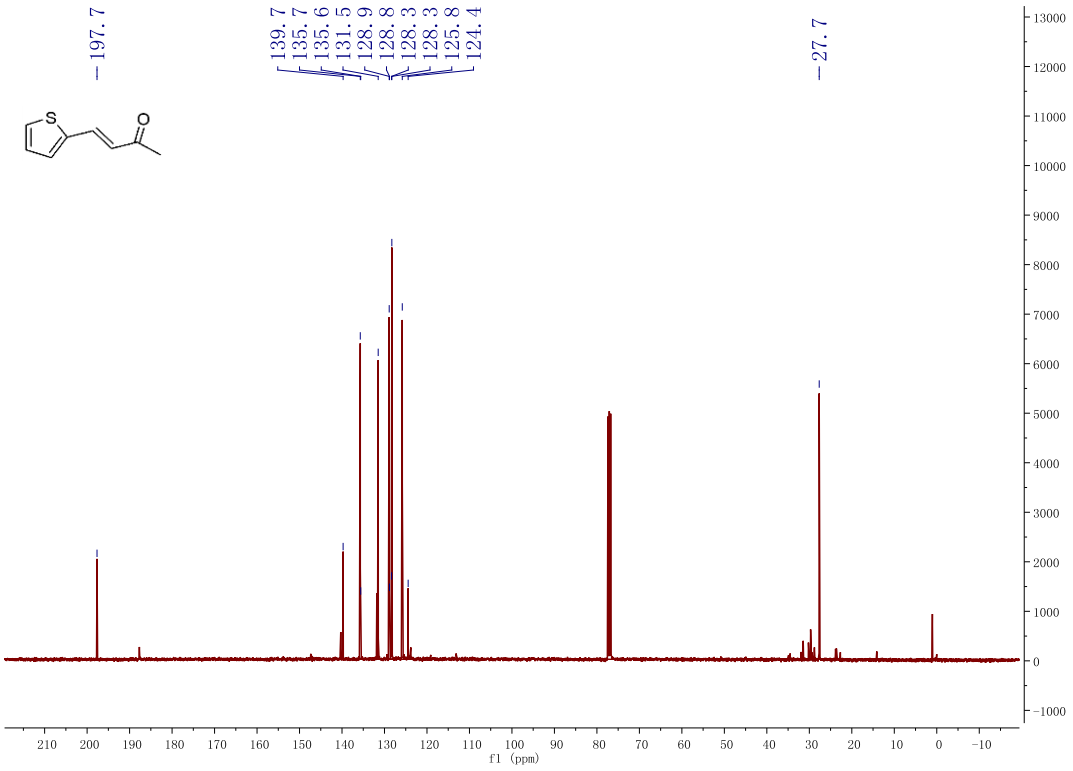


Figure S57. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4b**

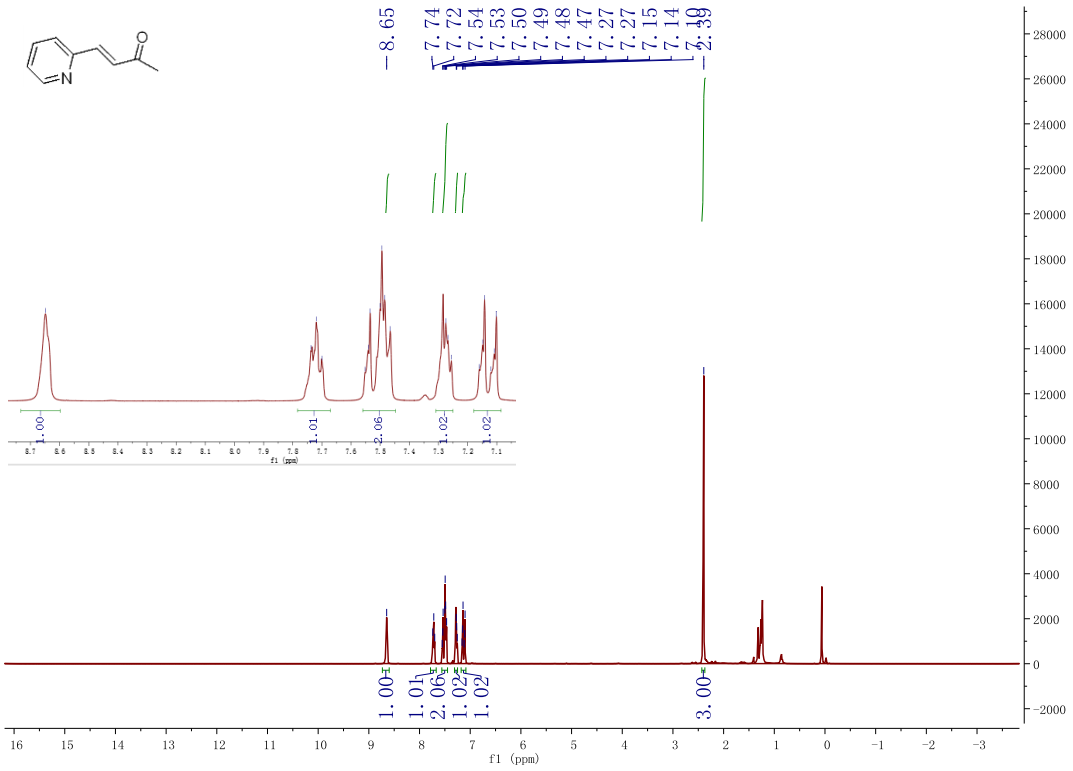


Figure S58. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4b**

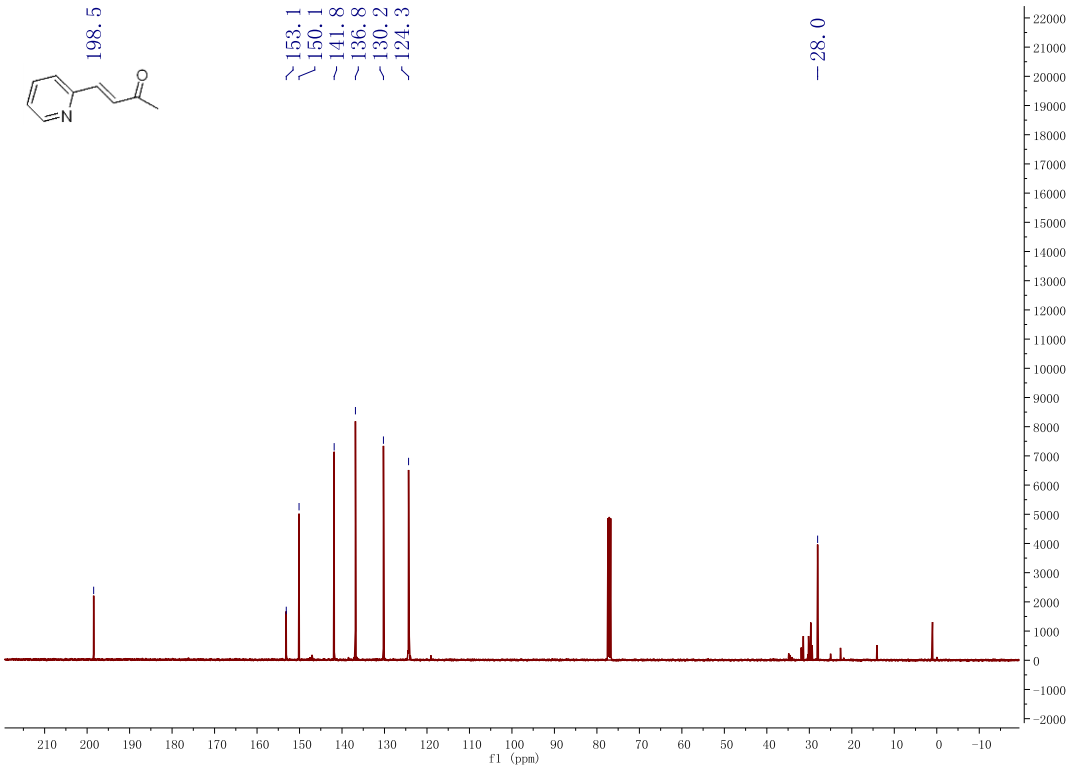


Figure S59. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4c** (trans:cis=3:1)

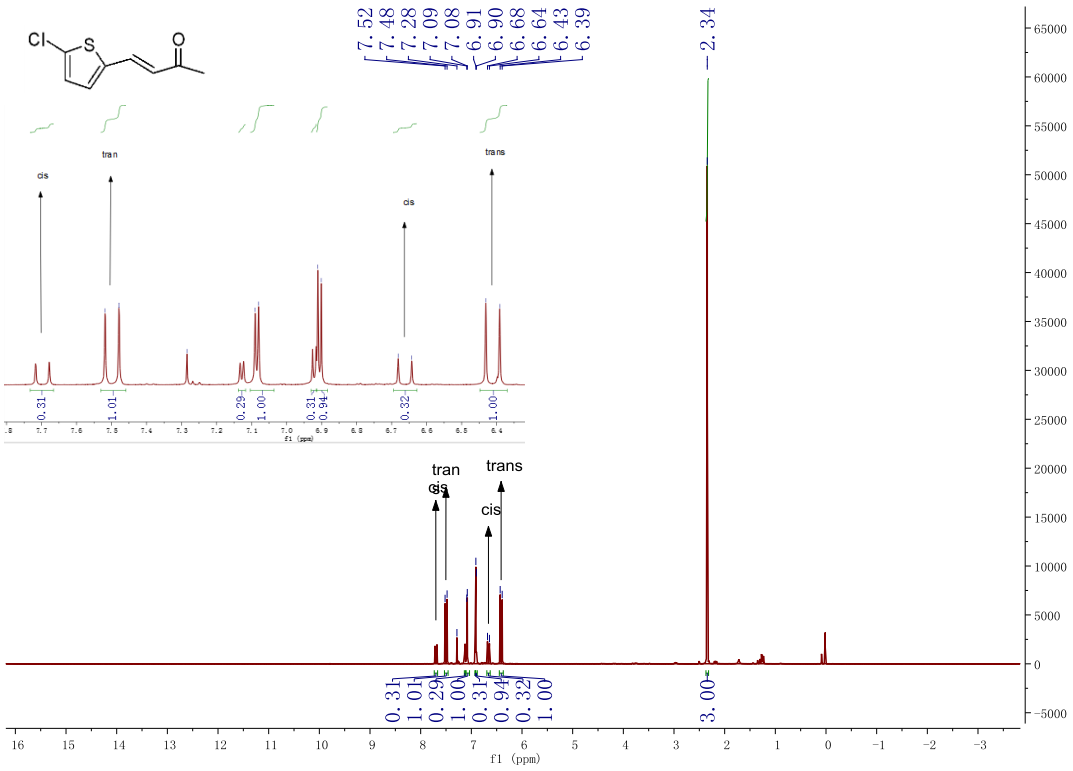


Figure S60. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4c**

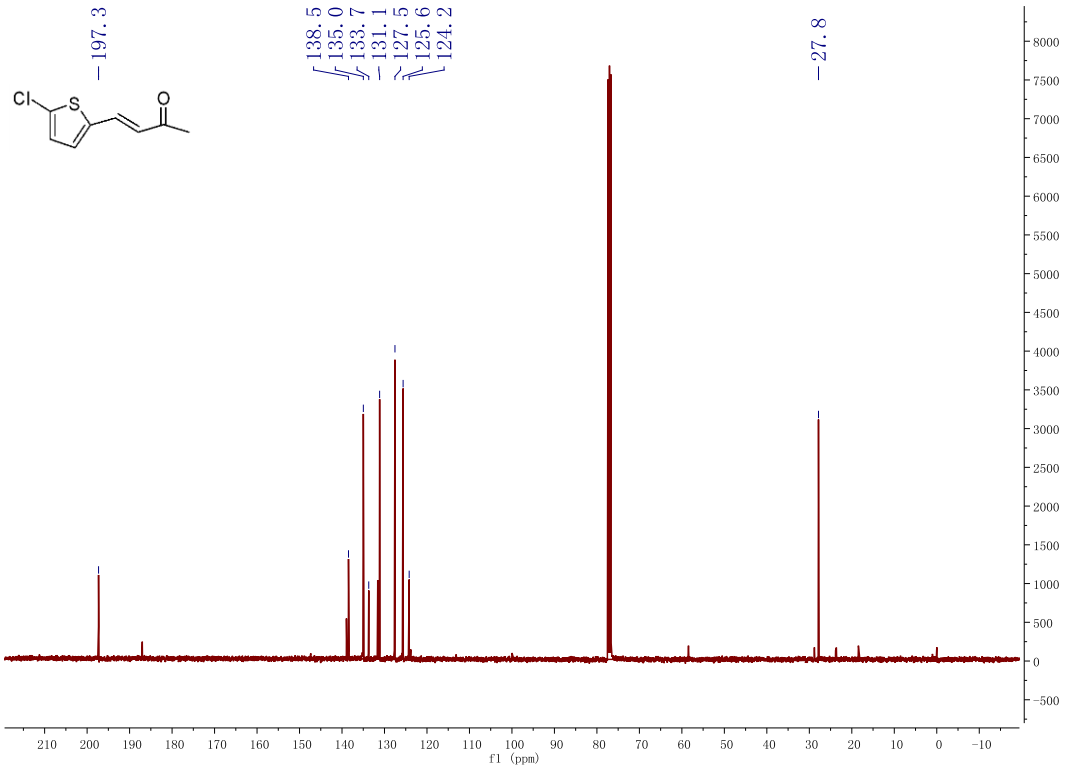


Figure S61. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4d**

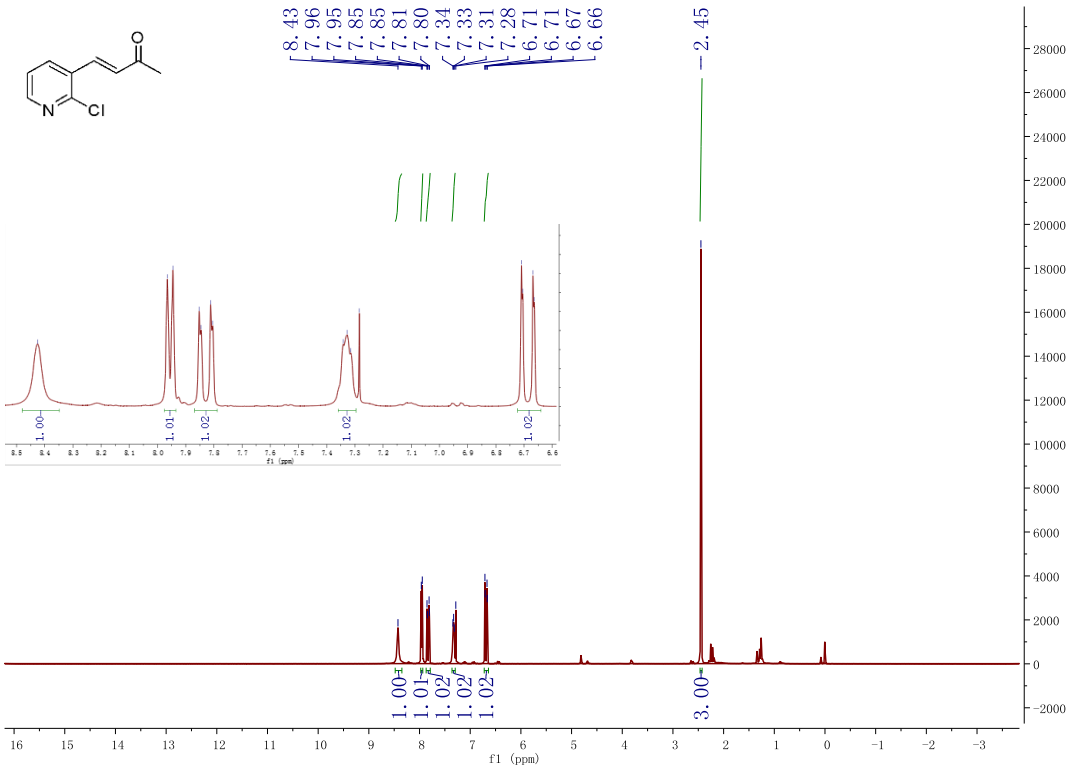


Figure S62. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4d**

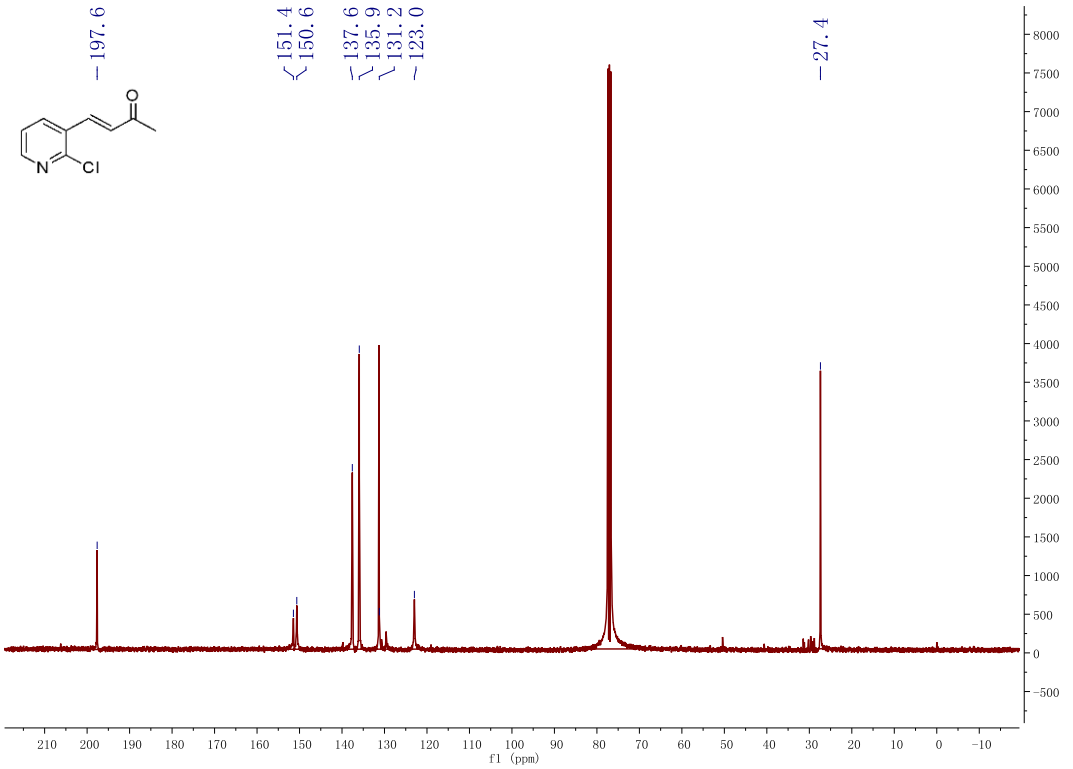


Figure S63. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4e**

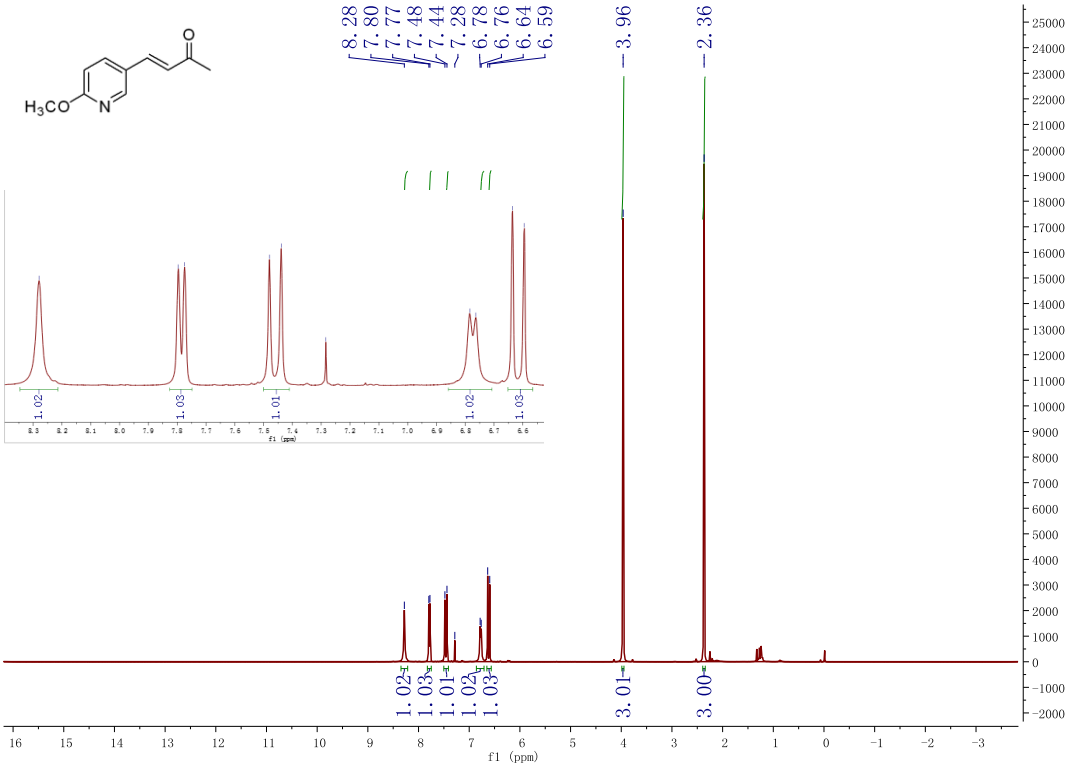


Figure S64. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4e**

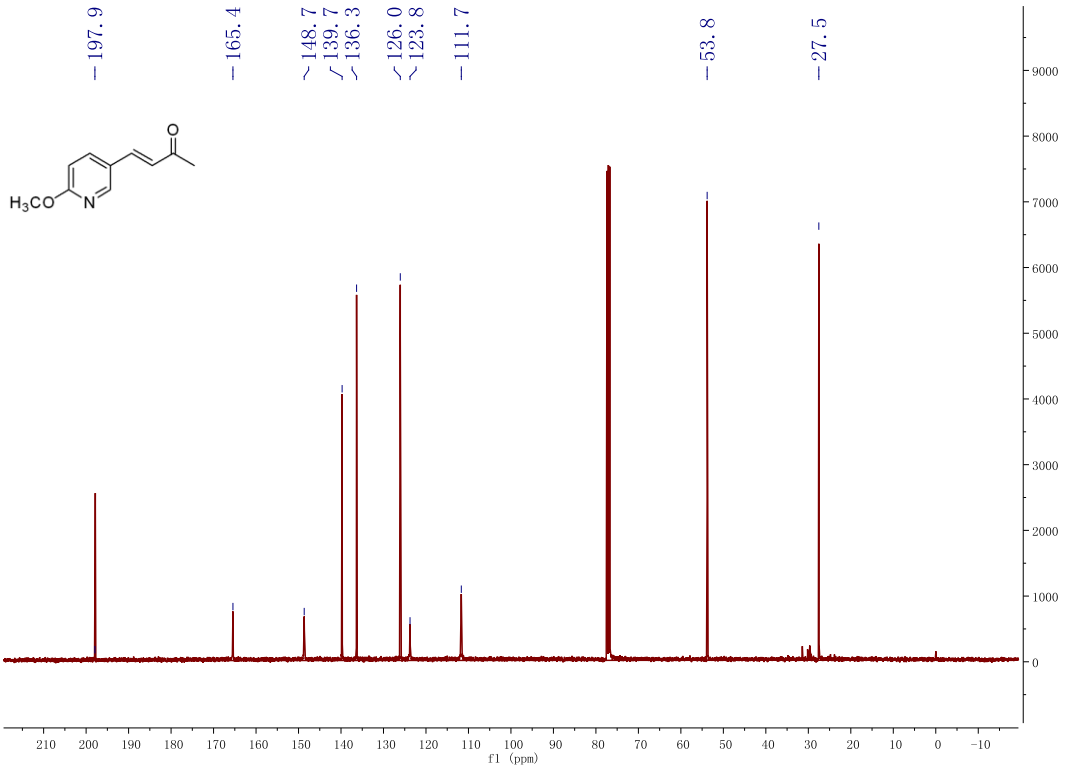


Figure S65. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4f**

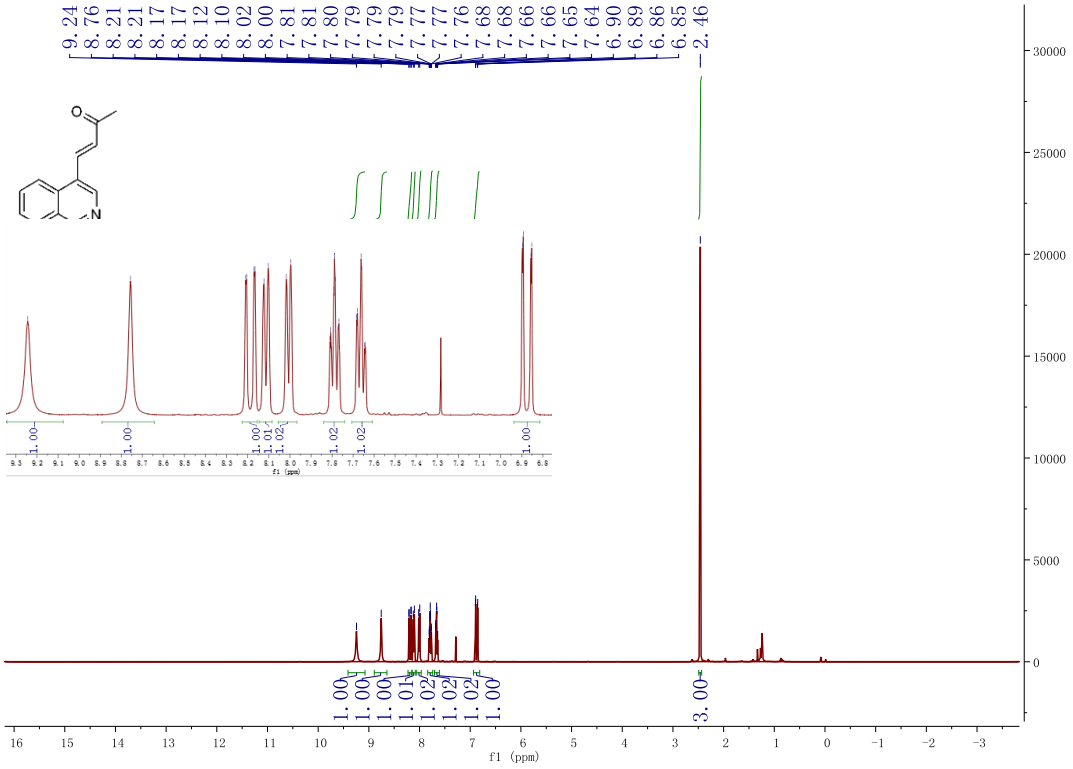


Figure S66. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4f**

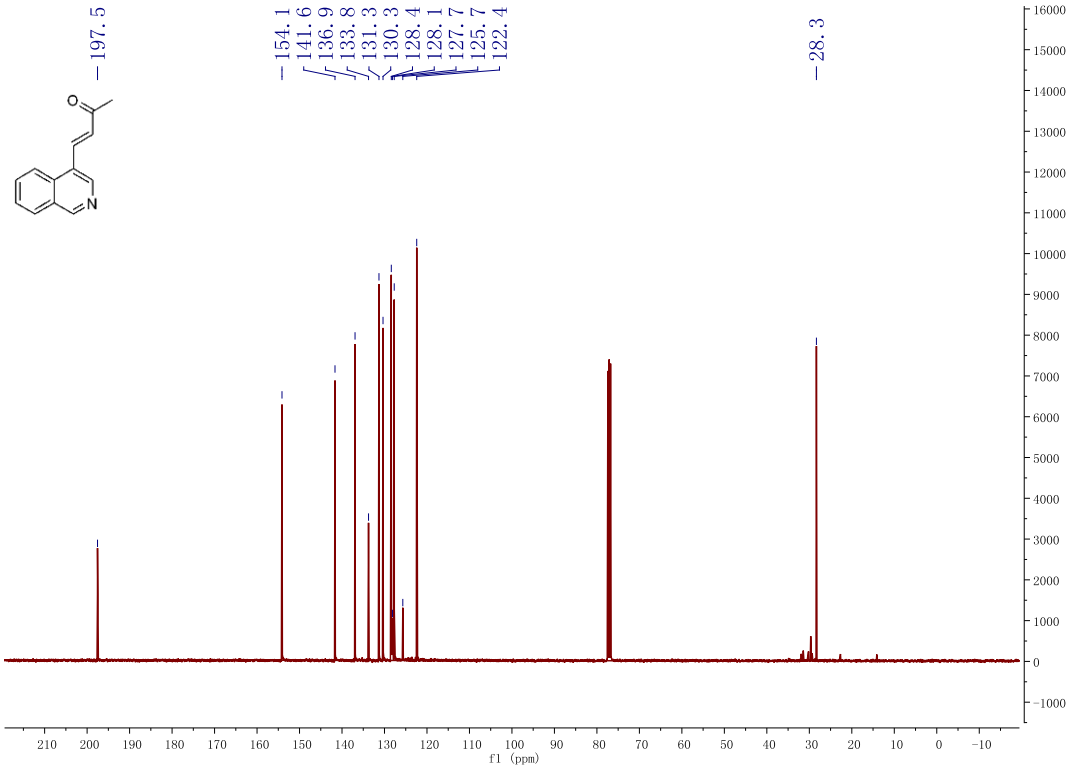


Figure S67. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5a**

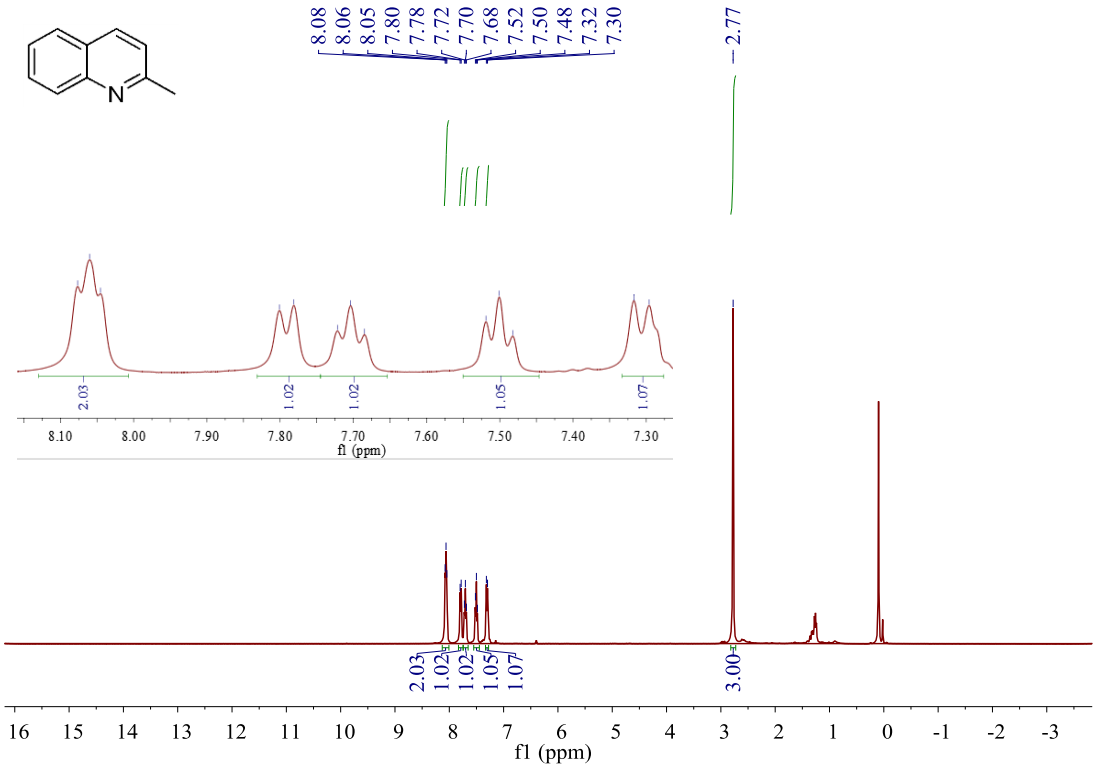


Figure S68. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **5a**

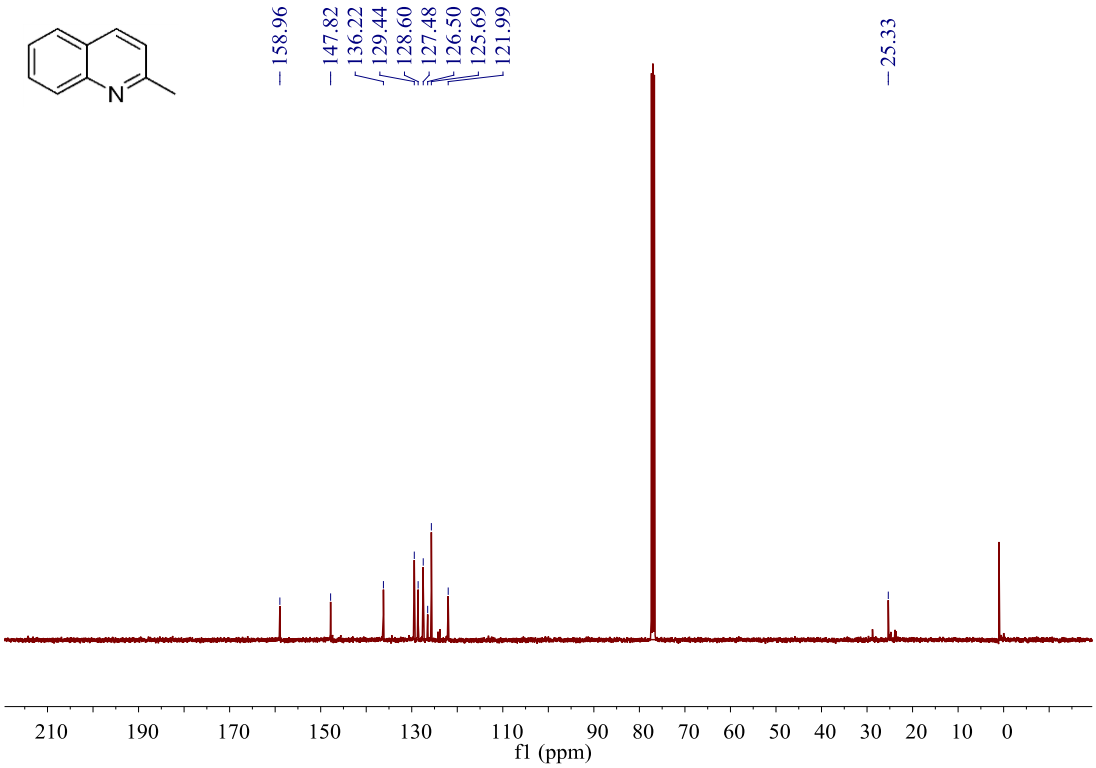


Figure S69. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**

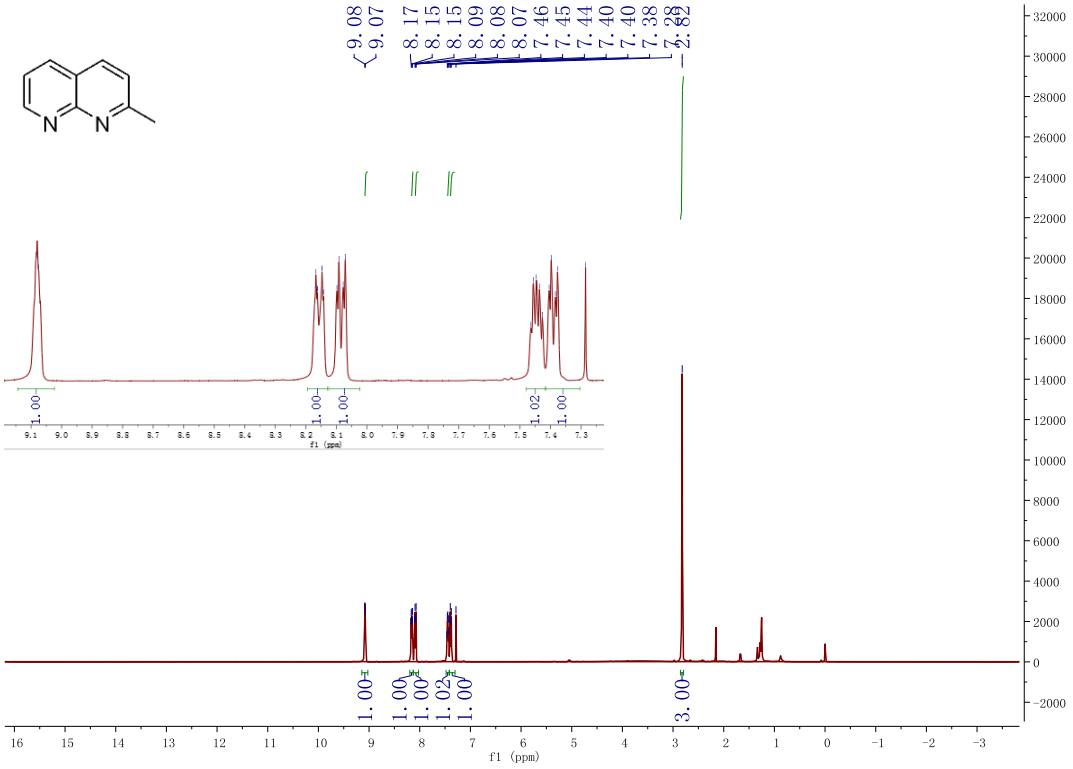


Figure S70. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **6**

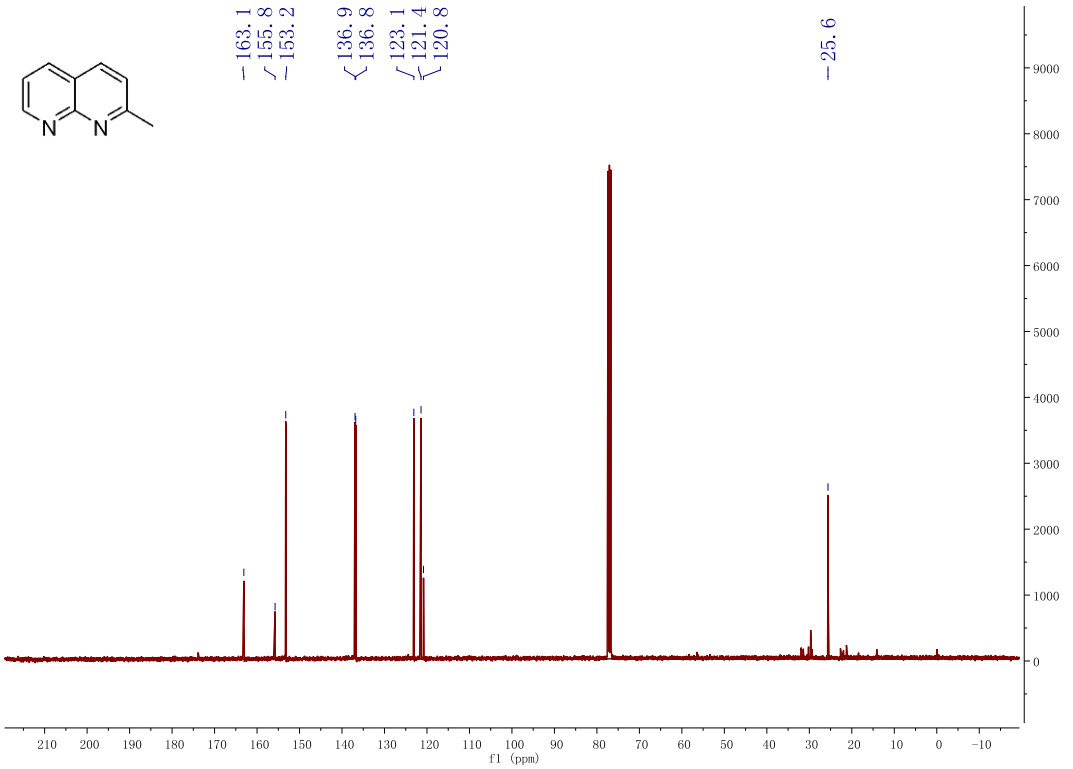


Figure S71. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7a**

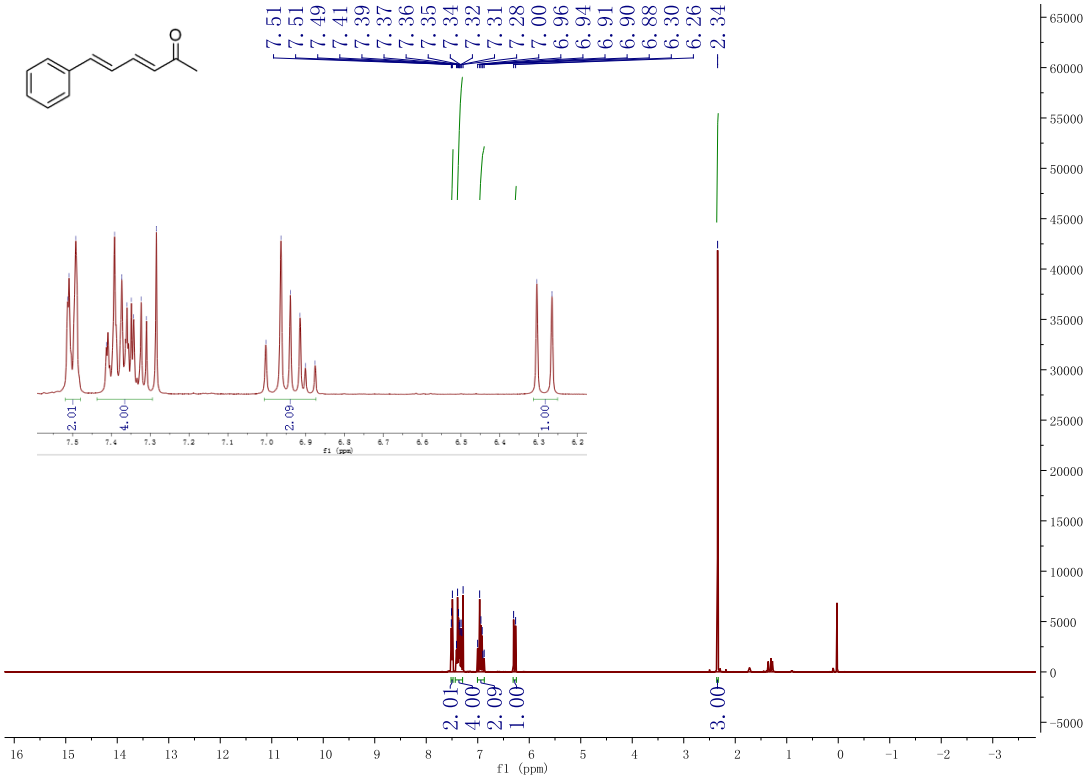


Figure S72. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **7a**

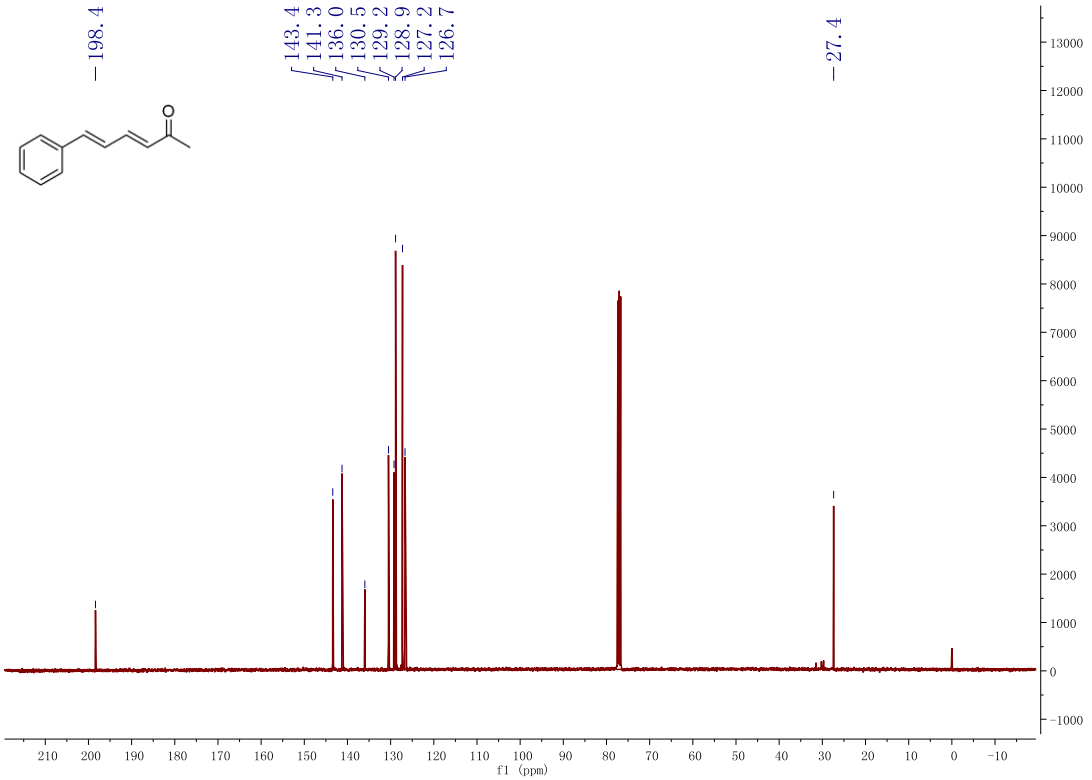


Figure S73. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7b**

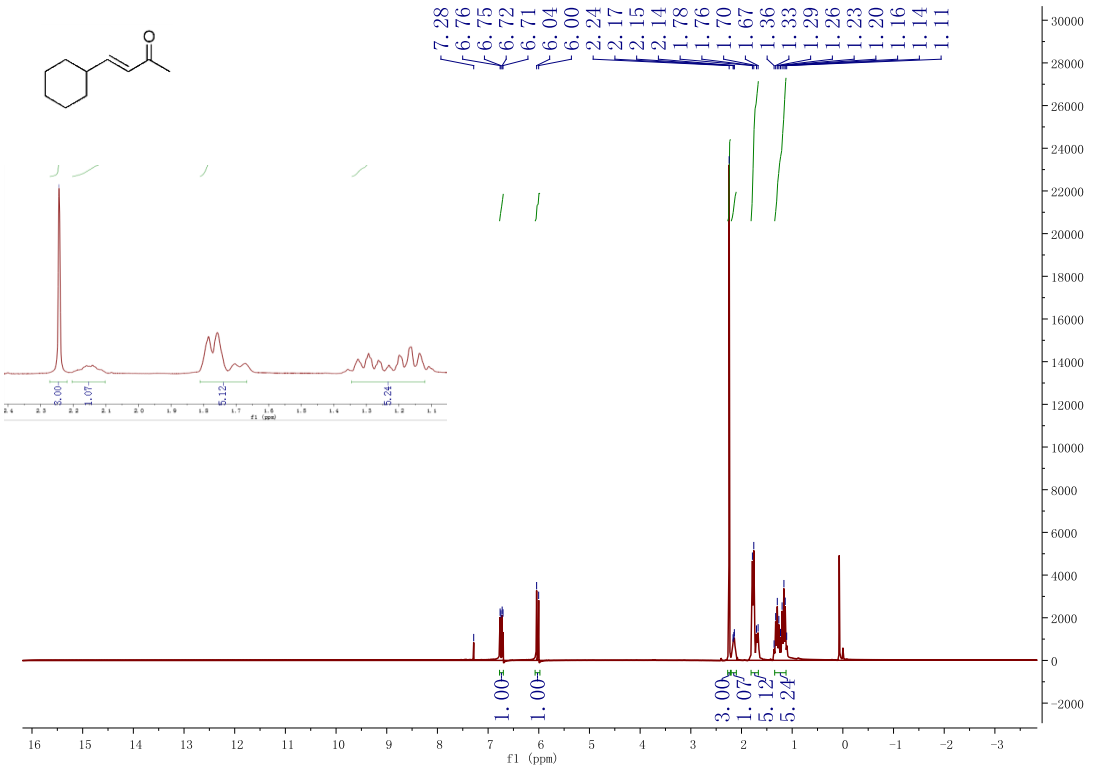


Figure S74. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **7b**

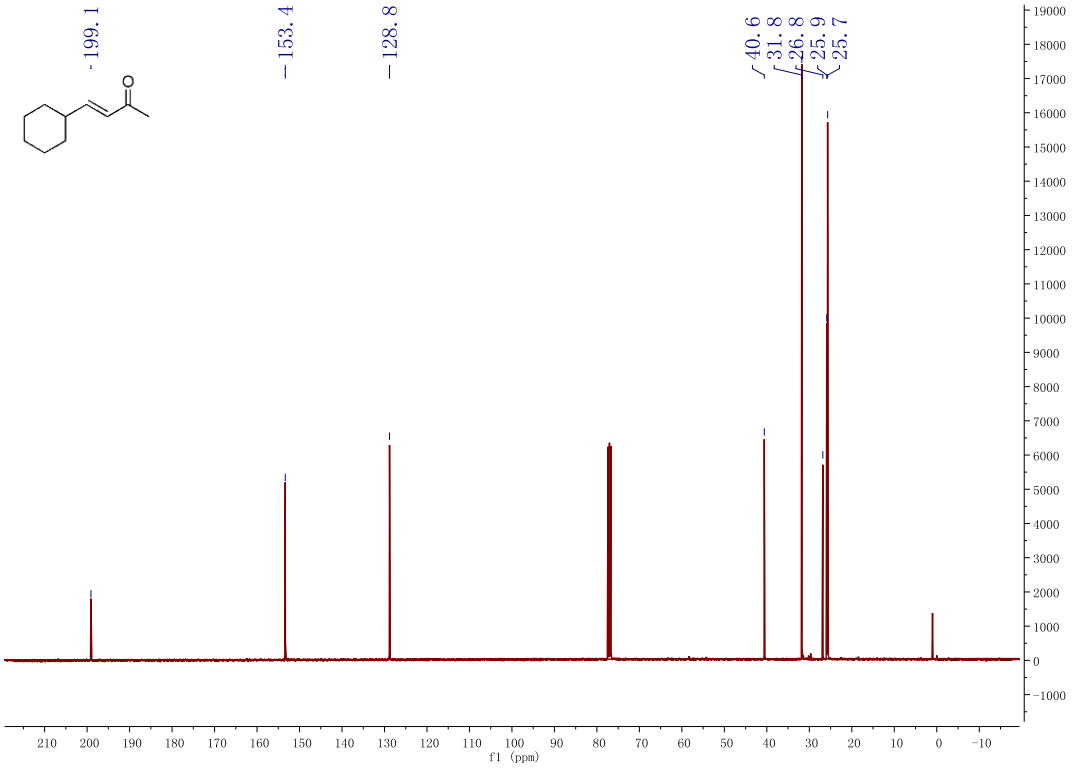


Figure S75. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*E*)-chalcone (mixed with acetophenone in a ratio of 2:1)

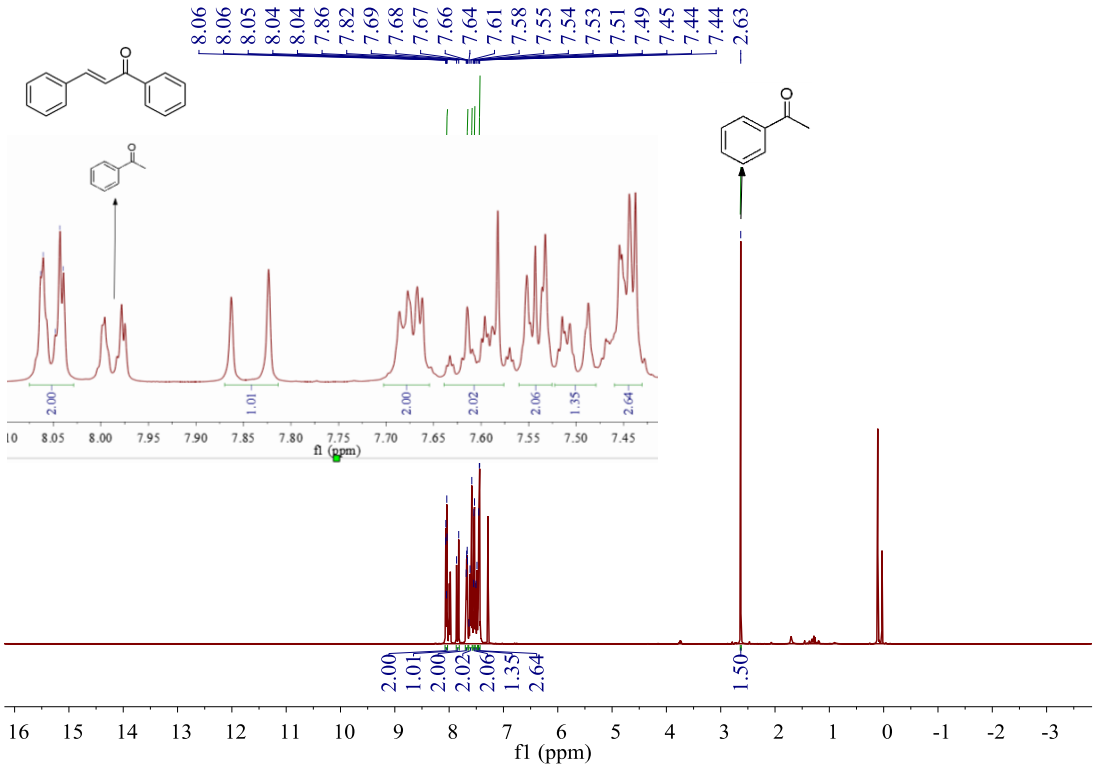


Figure S76. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of (*E*)-chalcone

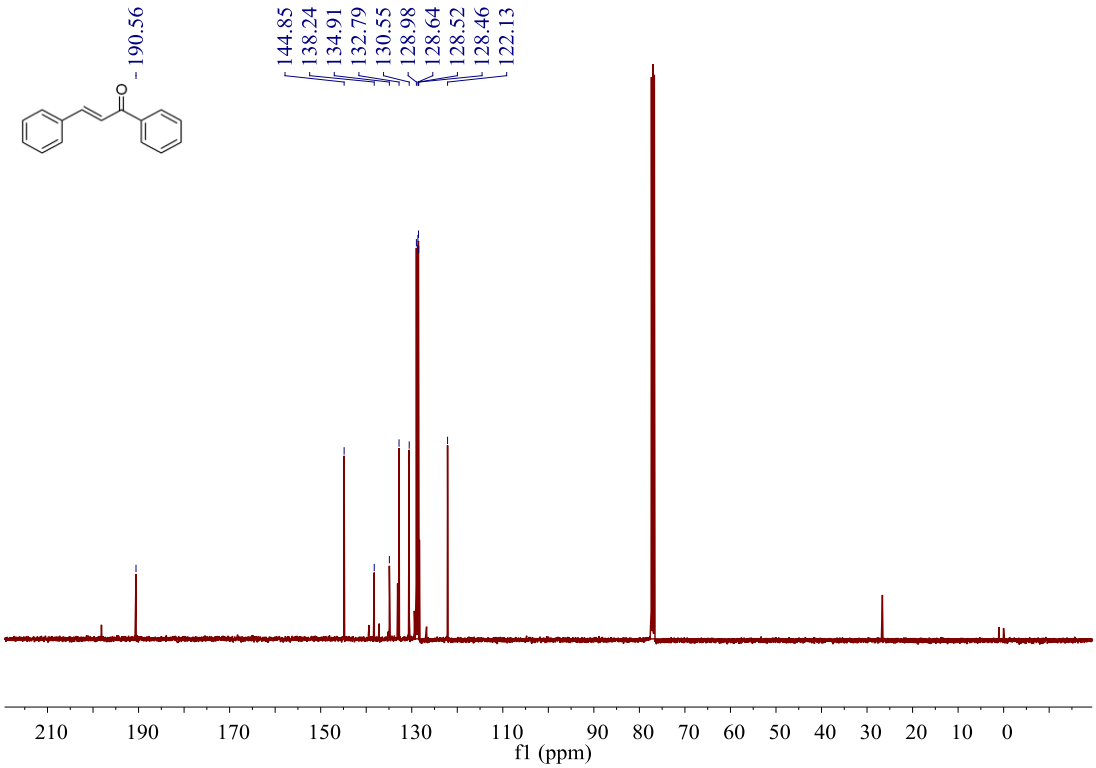


Figure S77. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of acetophenone

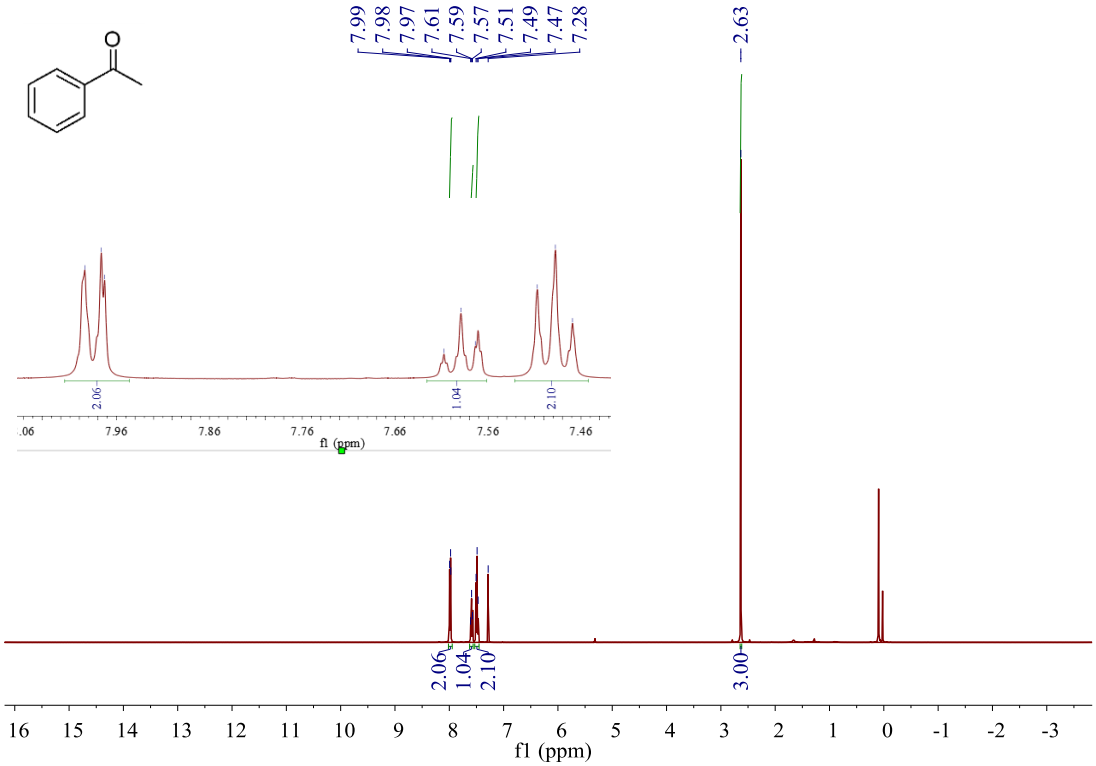


Figure S78. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of acetophenone

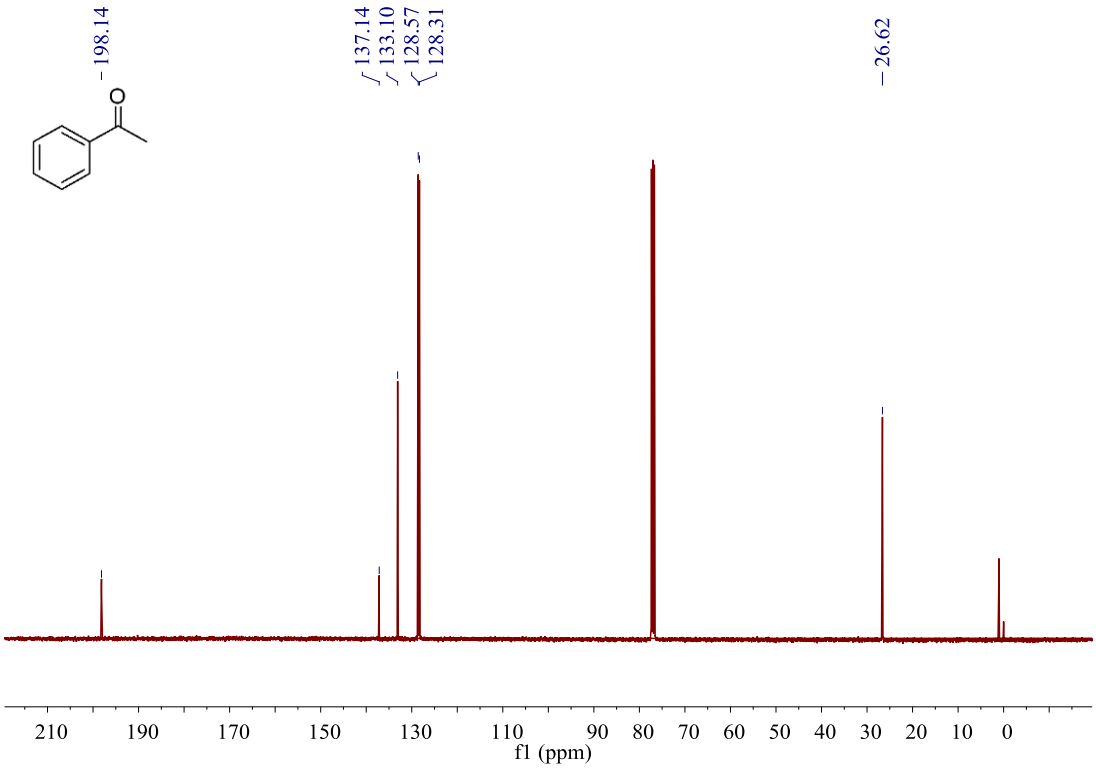


Figure S79. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of benzophenone

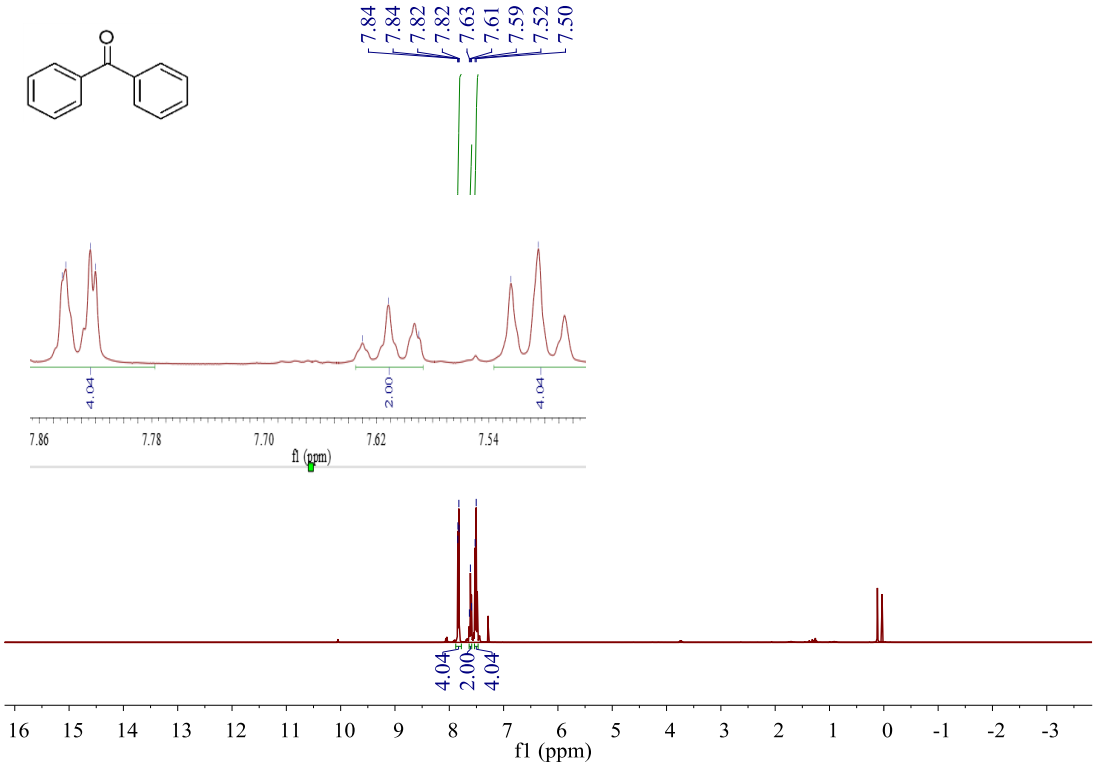


Figure S80. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of benzophenone

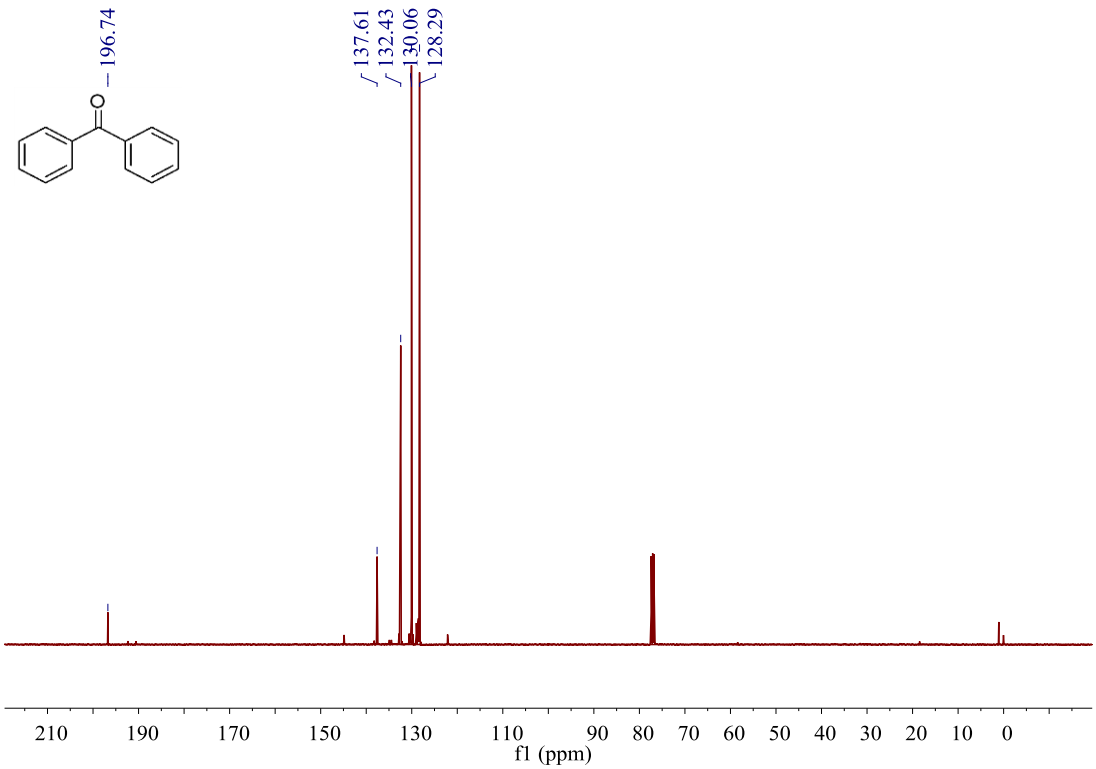


Figure S81. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8a** (trans:cis =9:1)

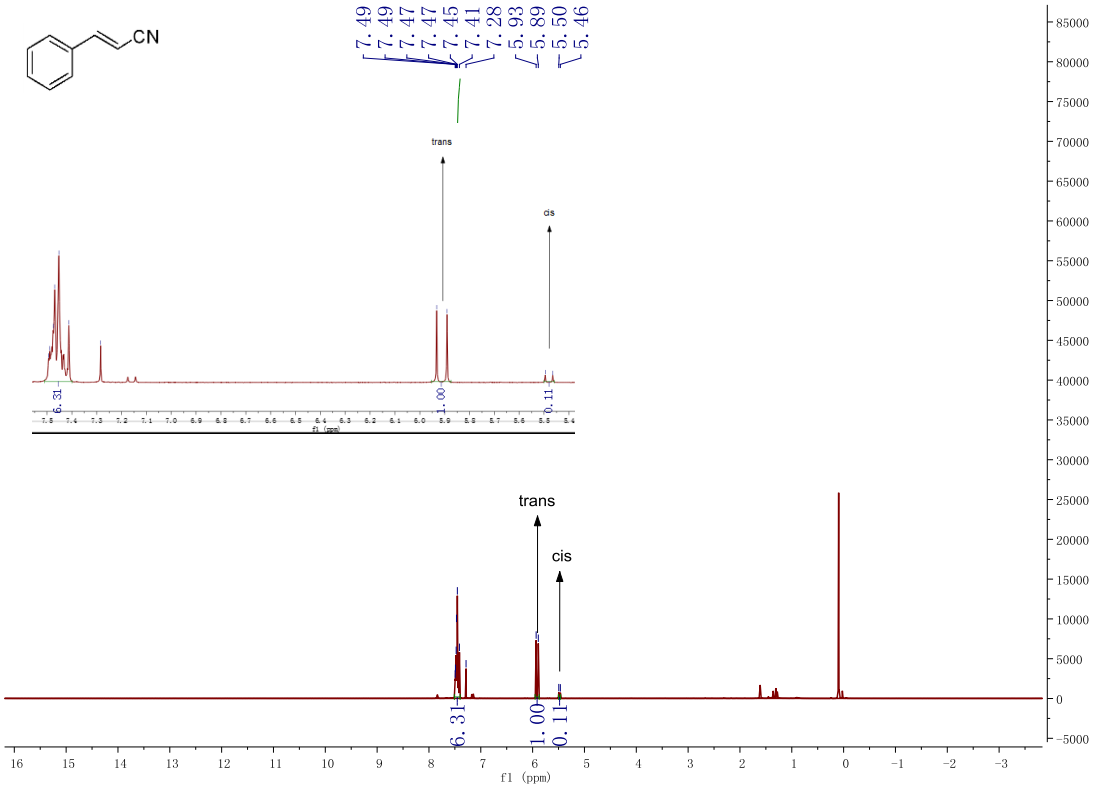


Figure S82. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8a**

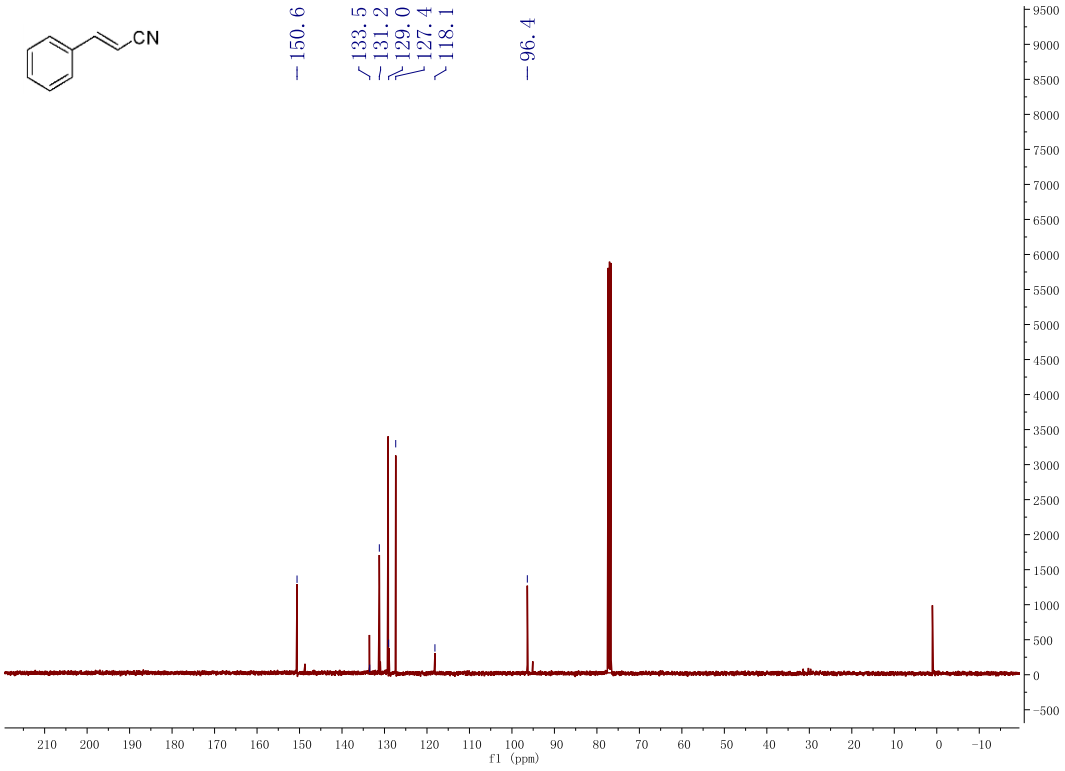


Figure S83. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8b** (trans :cis =6:1)

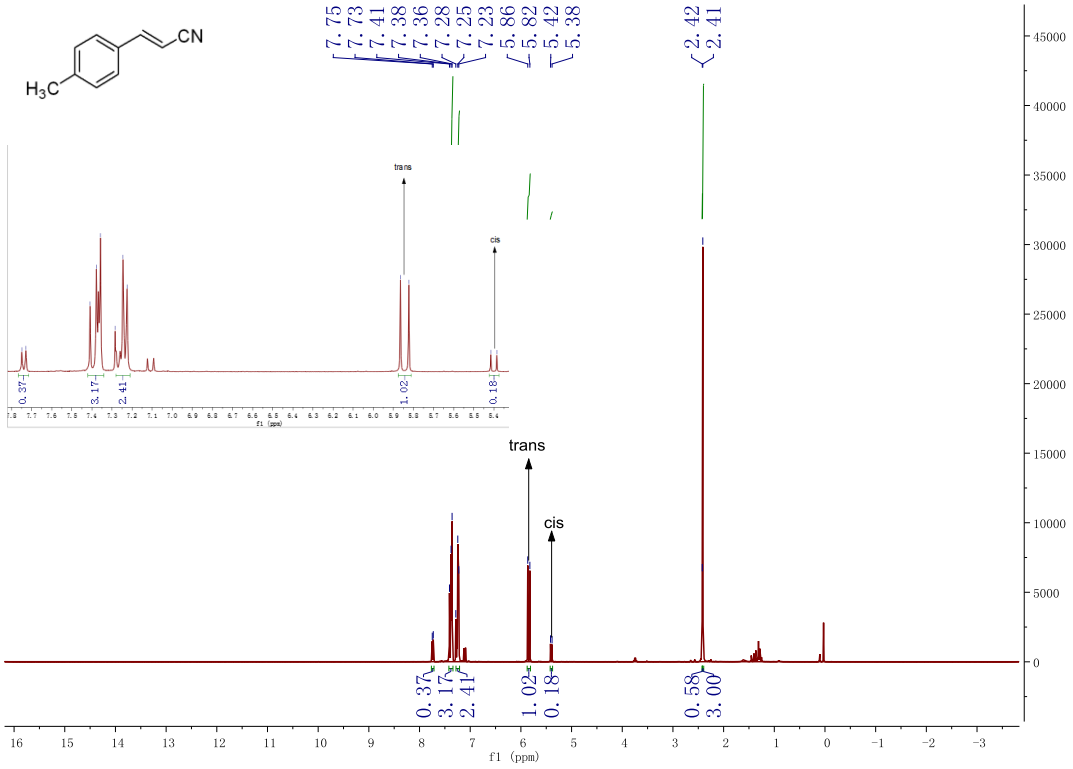


Figure S84. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8b**

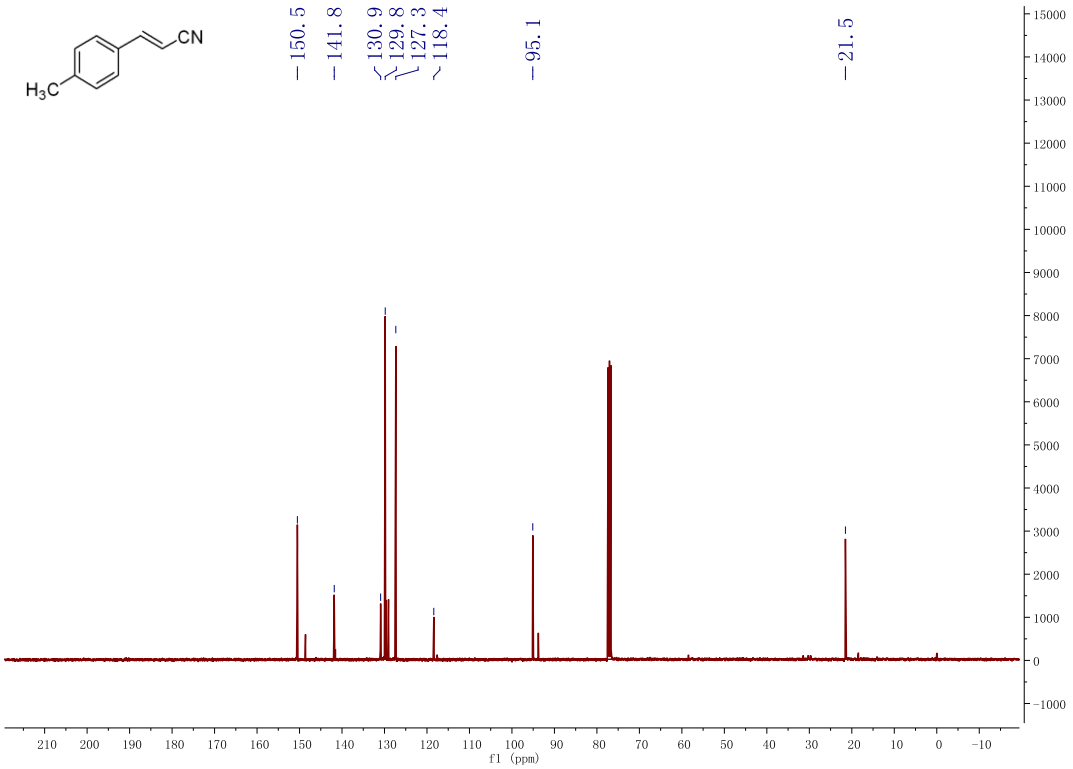


Figure S85. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8c** (trans :cis =5:1)

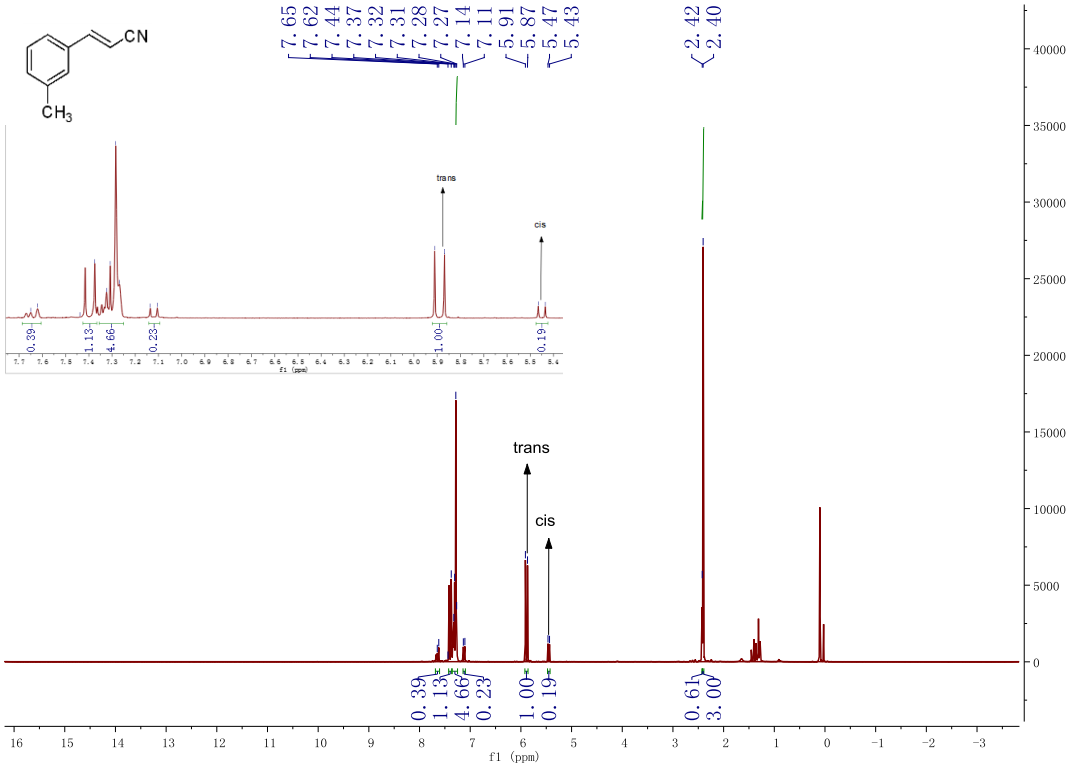


Figure S86. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8c**

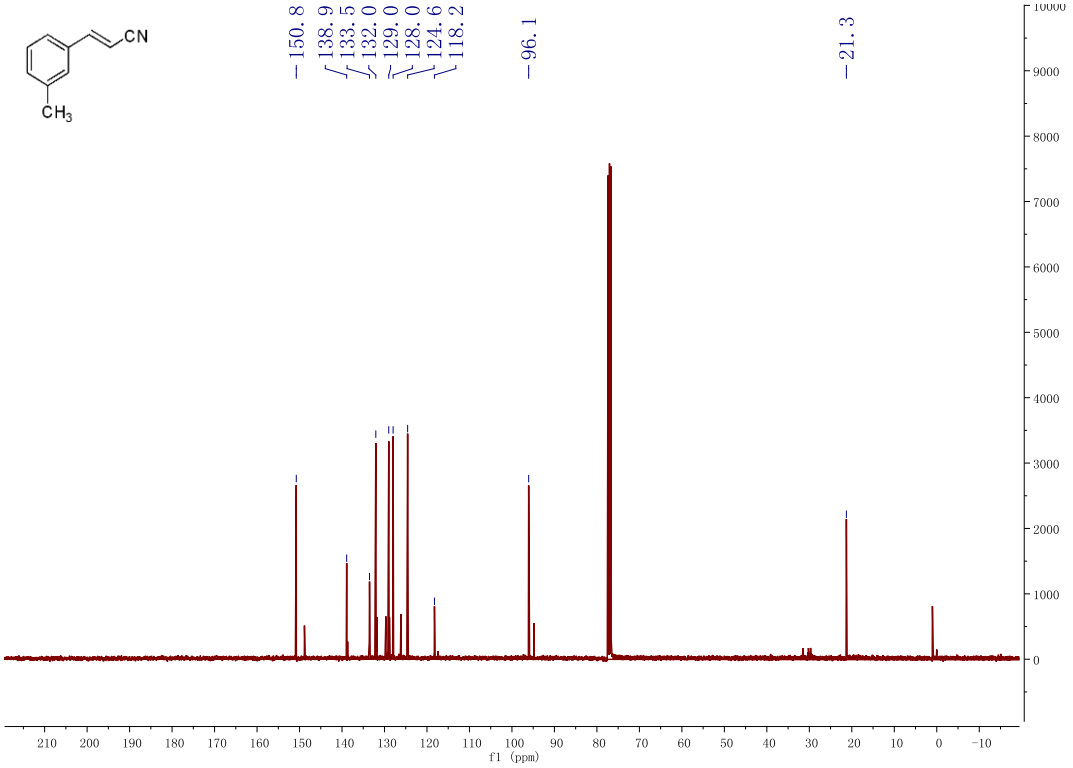


Figure S87. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8d**

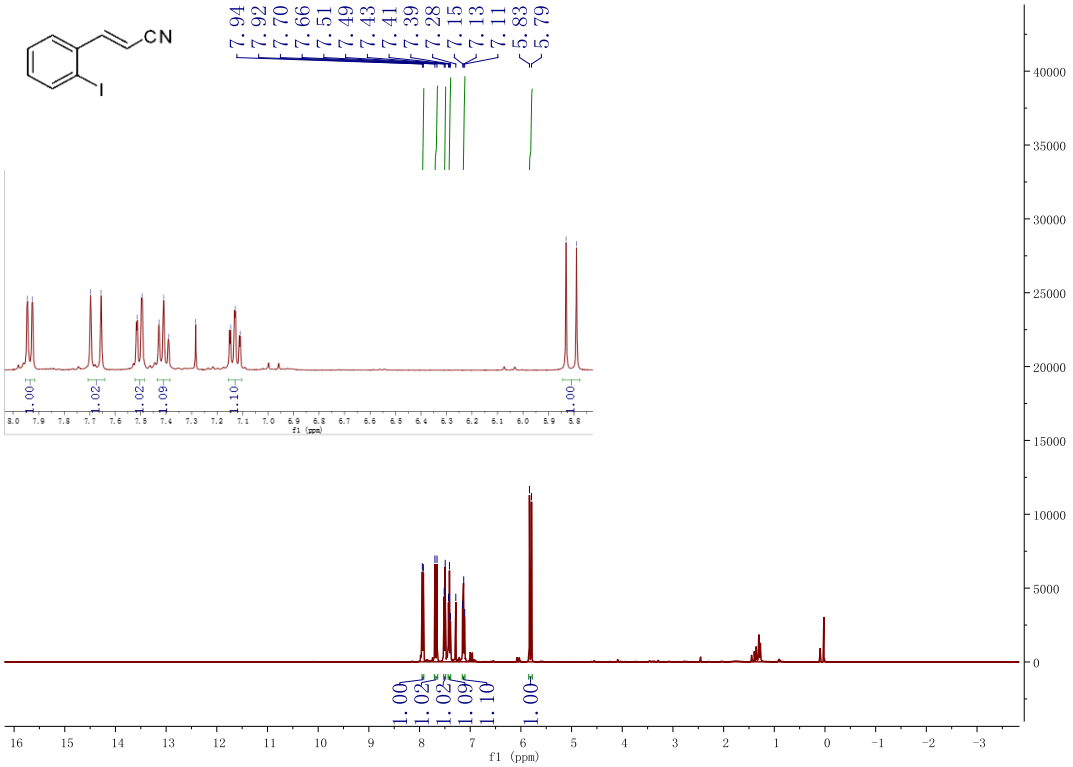


Figure S88. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8d**

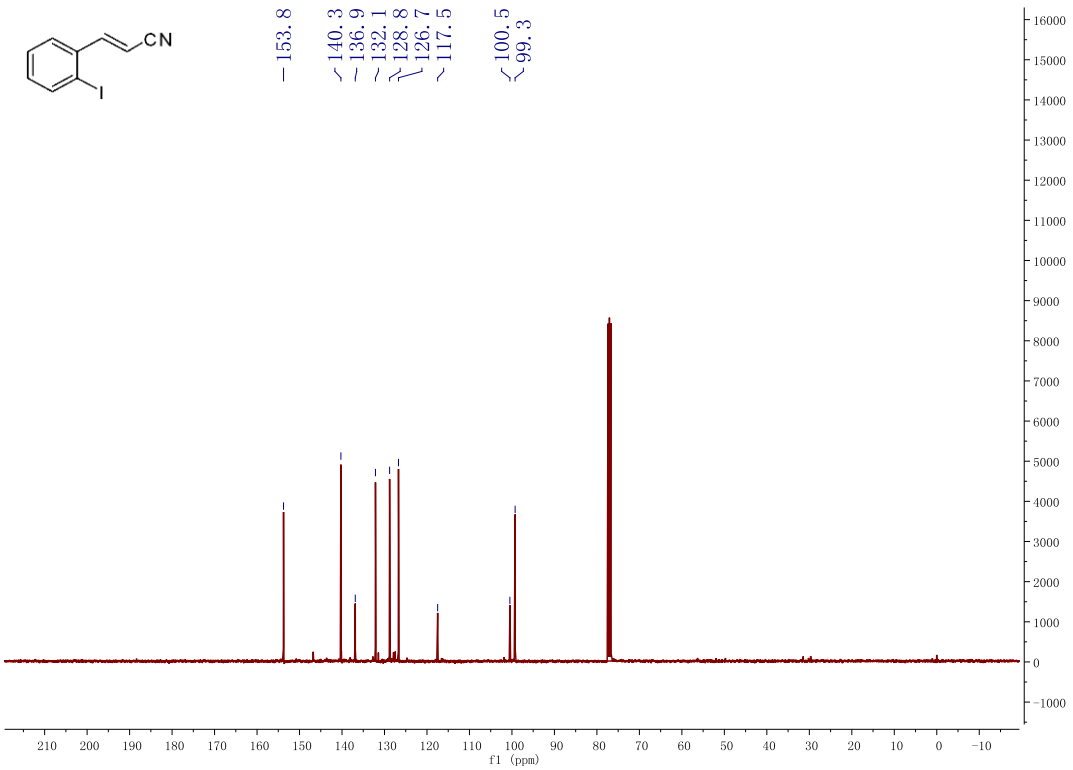


Figure S89. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8e**

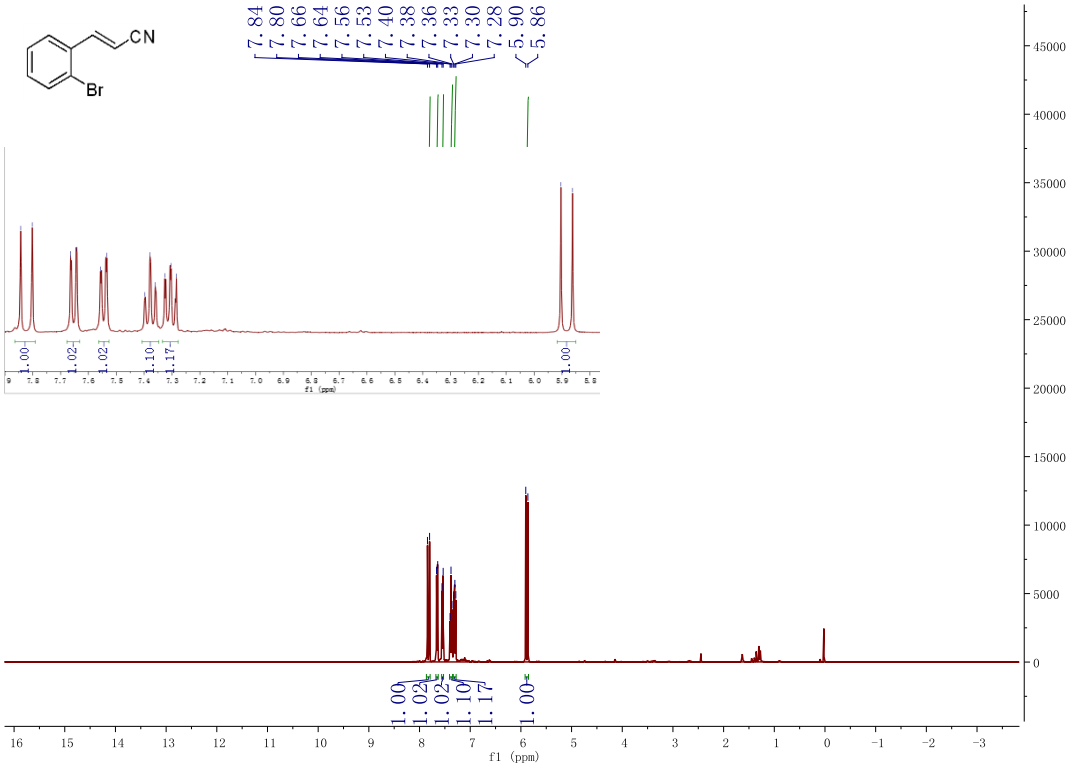


Figure S90. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8e**

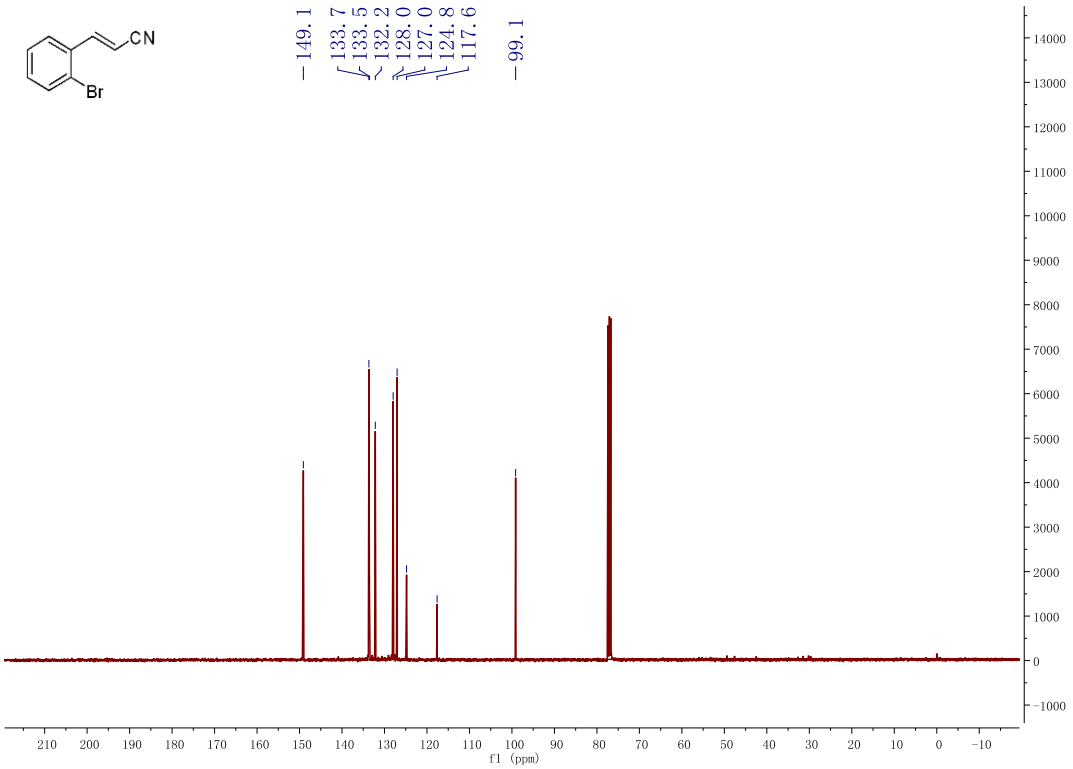


Figure S91. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8f** (trans:cis =6:1)

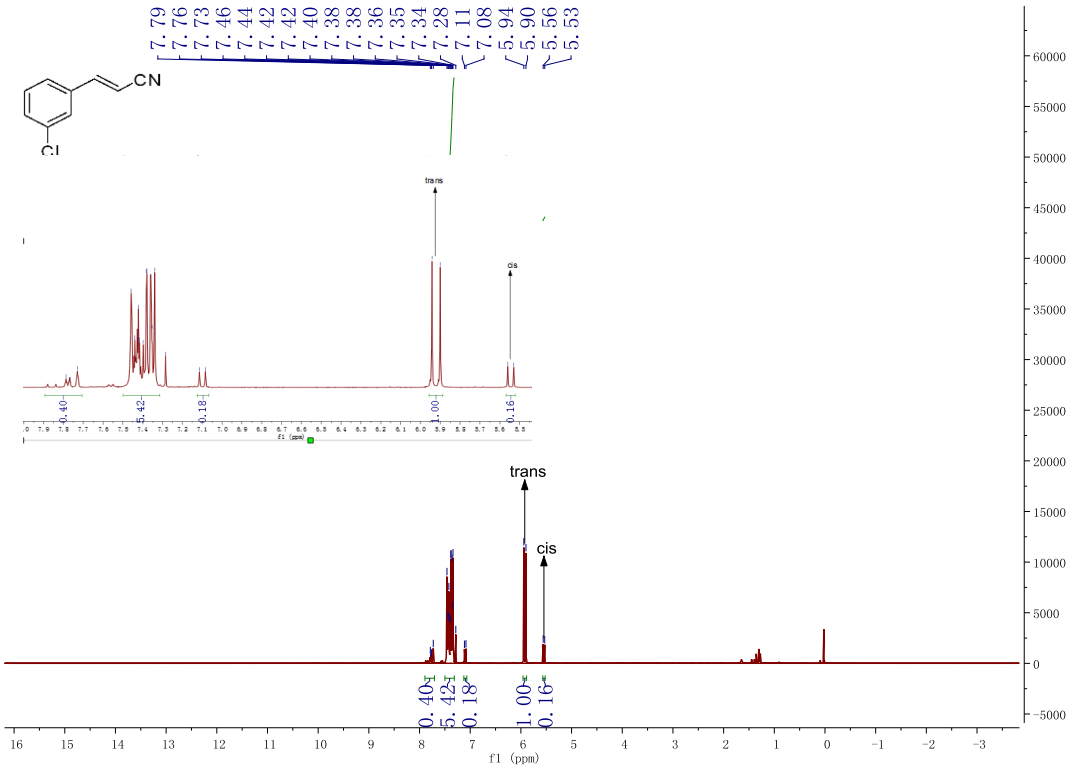


Figure S92. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8f**

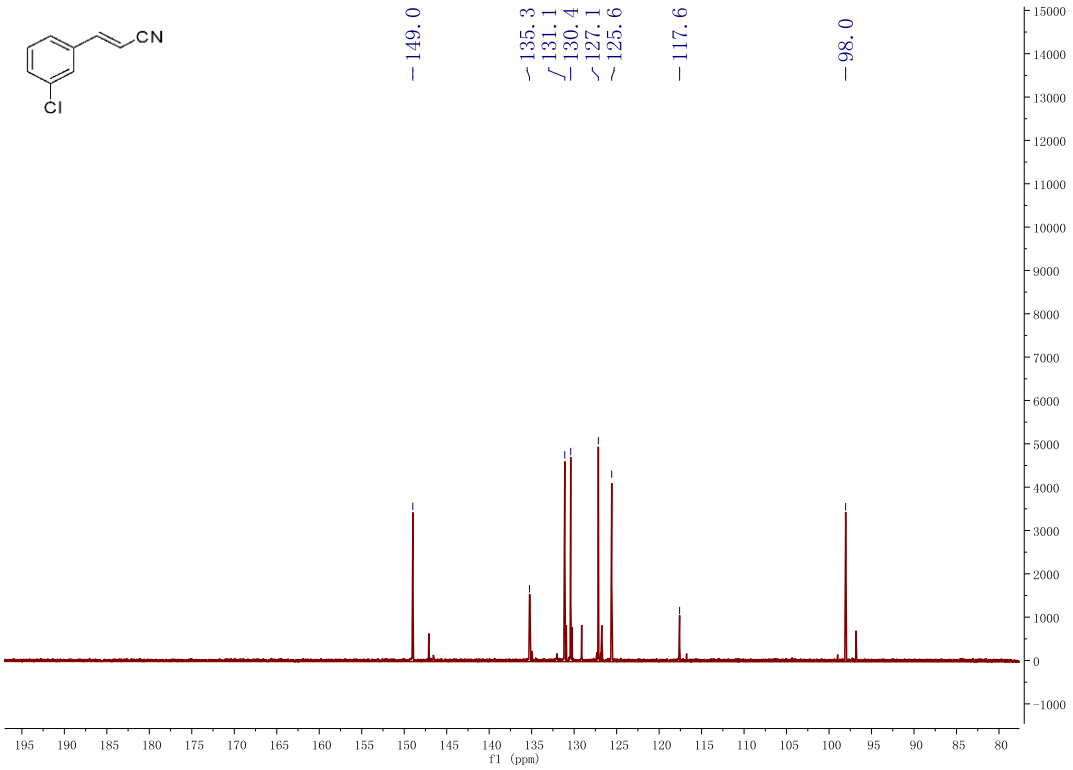


Figure S93. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8g** (trans :cis =7:1)

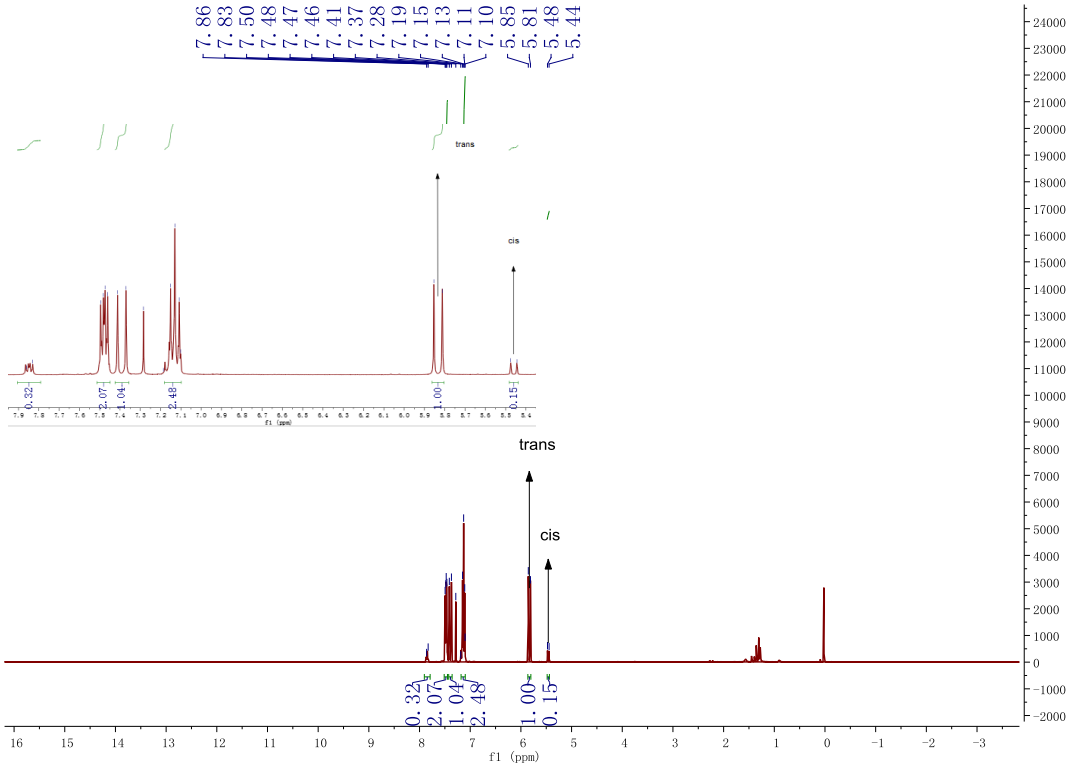


Figure S94. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8g**

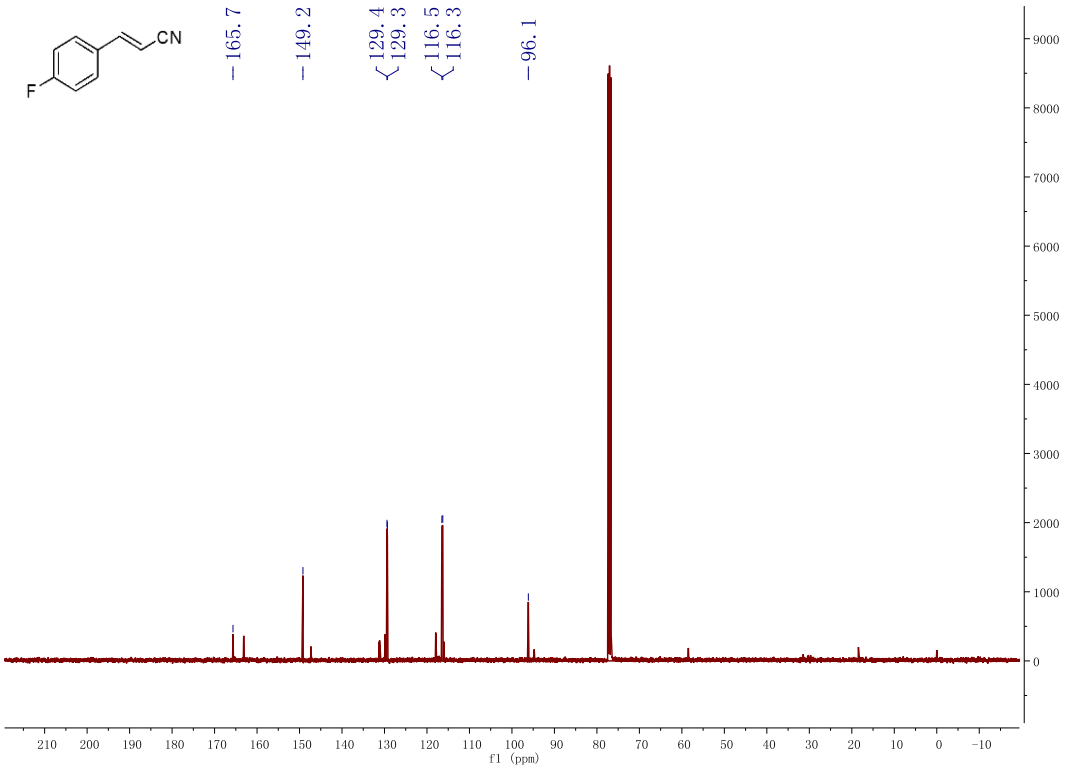


Figure S95. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **8g**

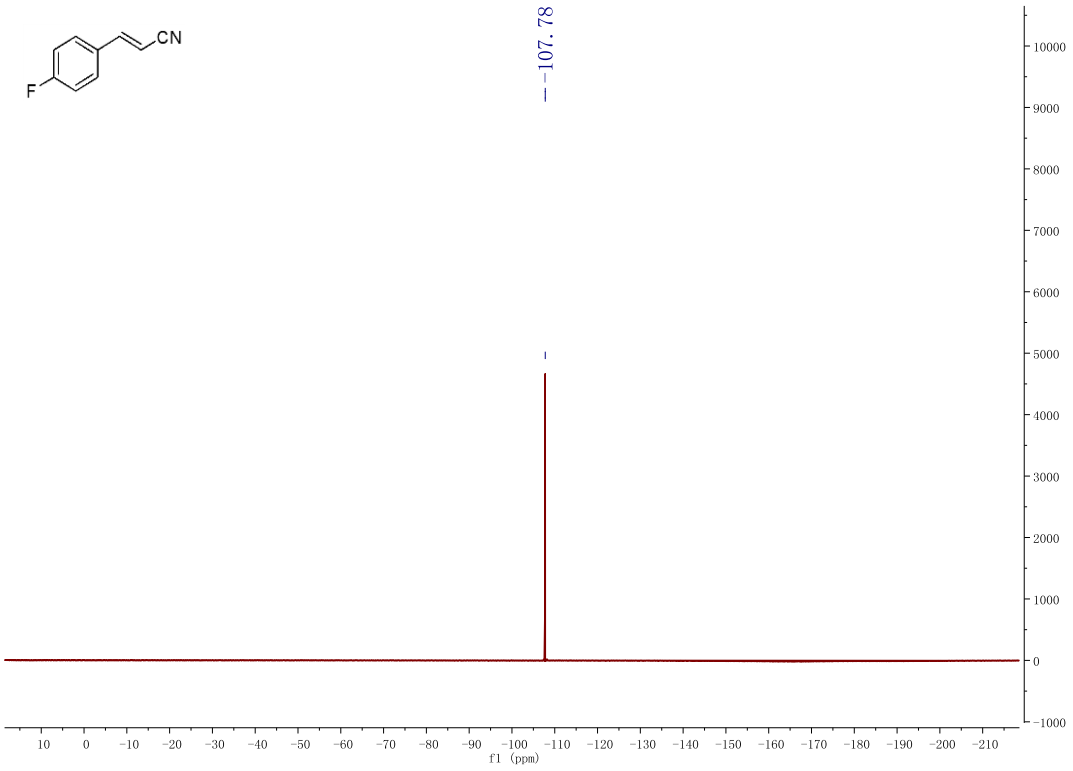


Figure S96. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8i** (trans:cis = 7:1)

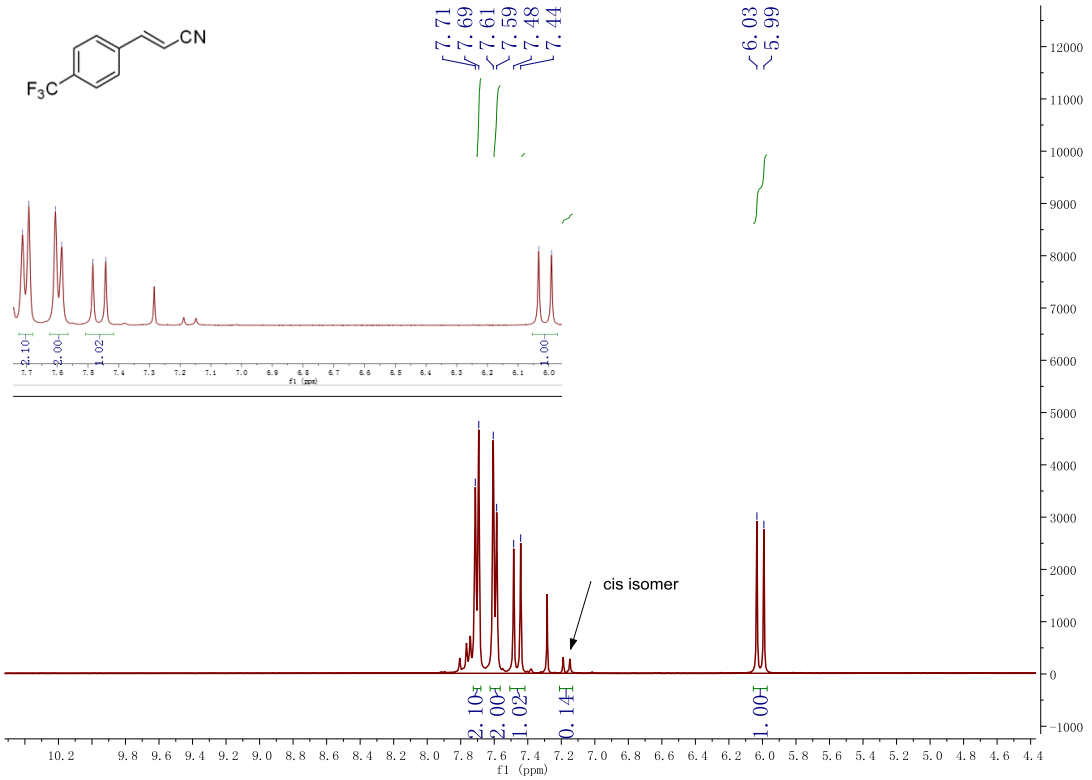


Figure S97. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8i**

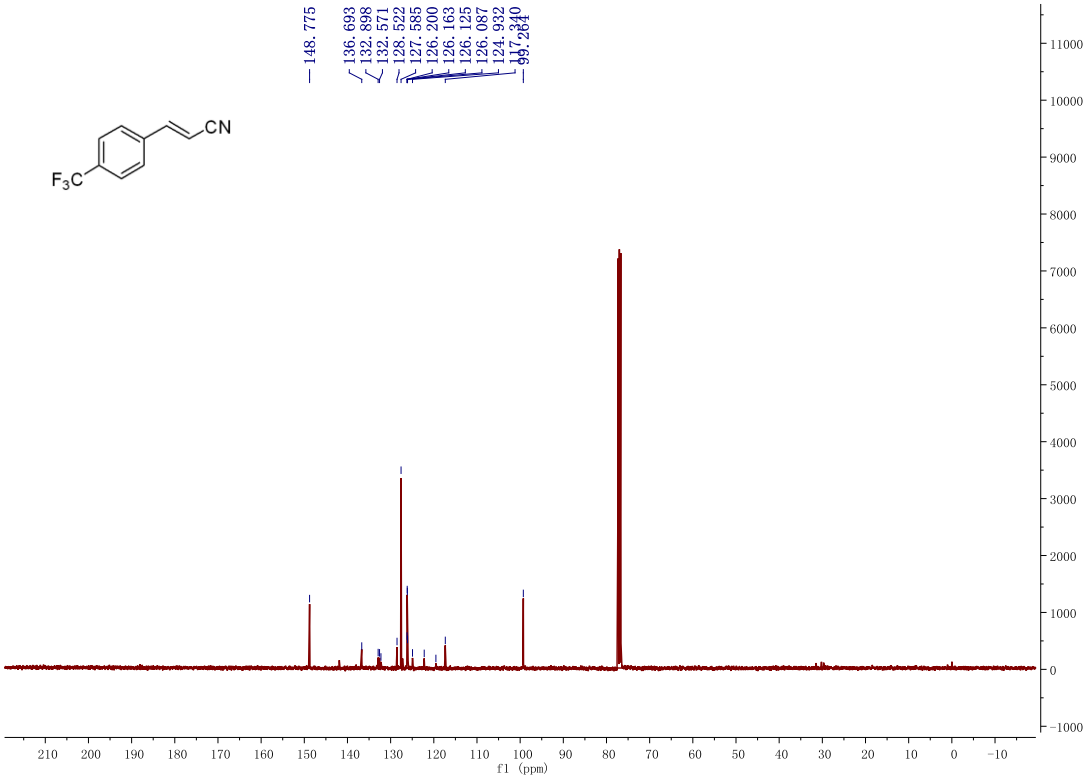


Figure S98. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **8i**

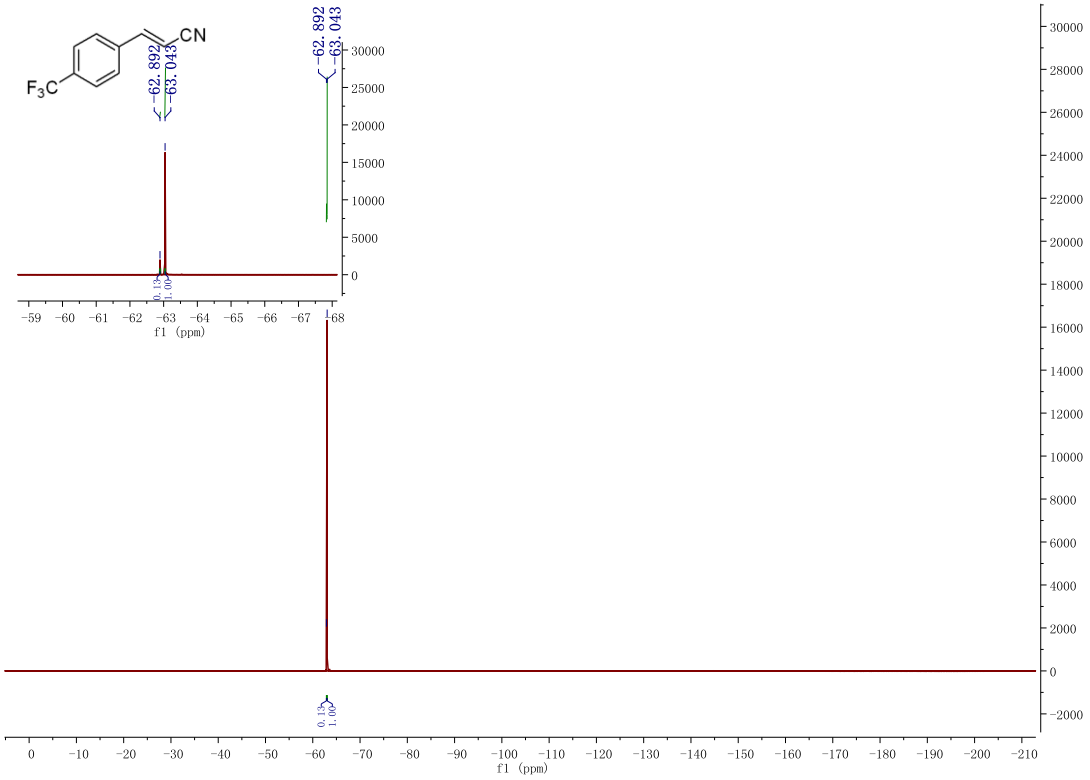


Figure S99. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8k** (trans :cis =7:1)

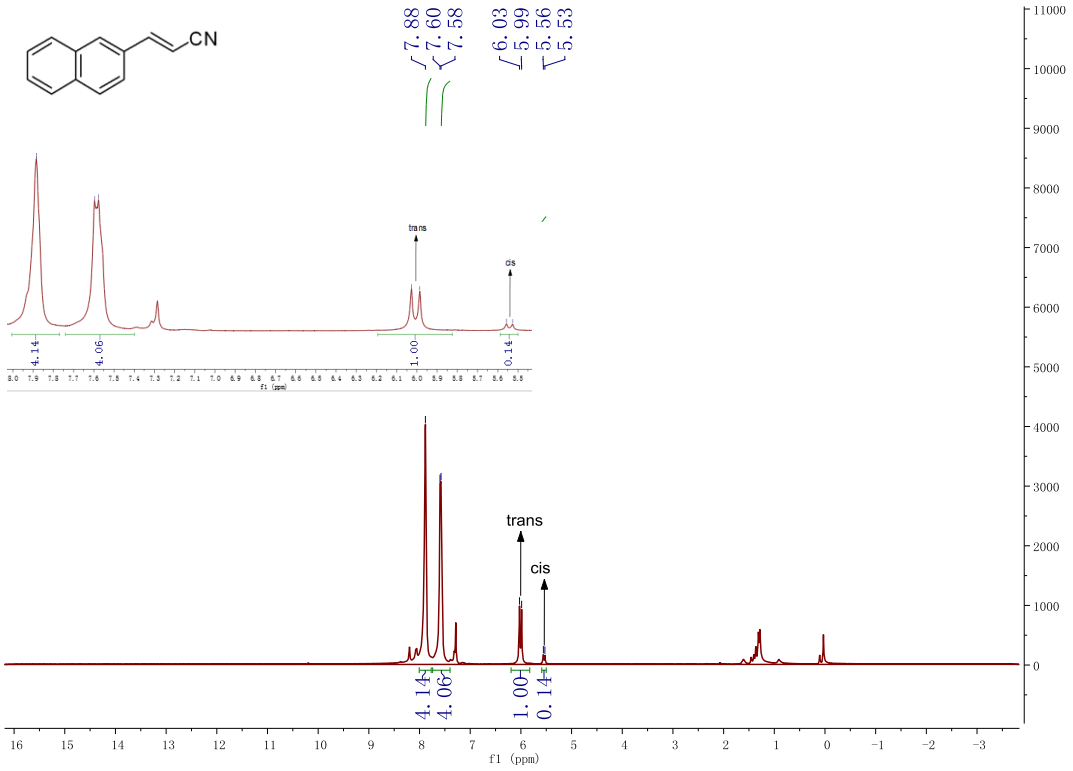


Figure S100. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8k**

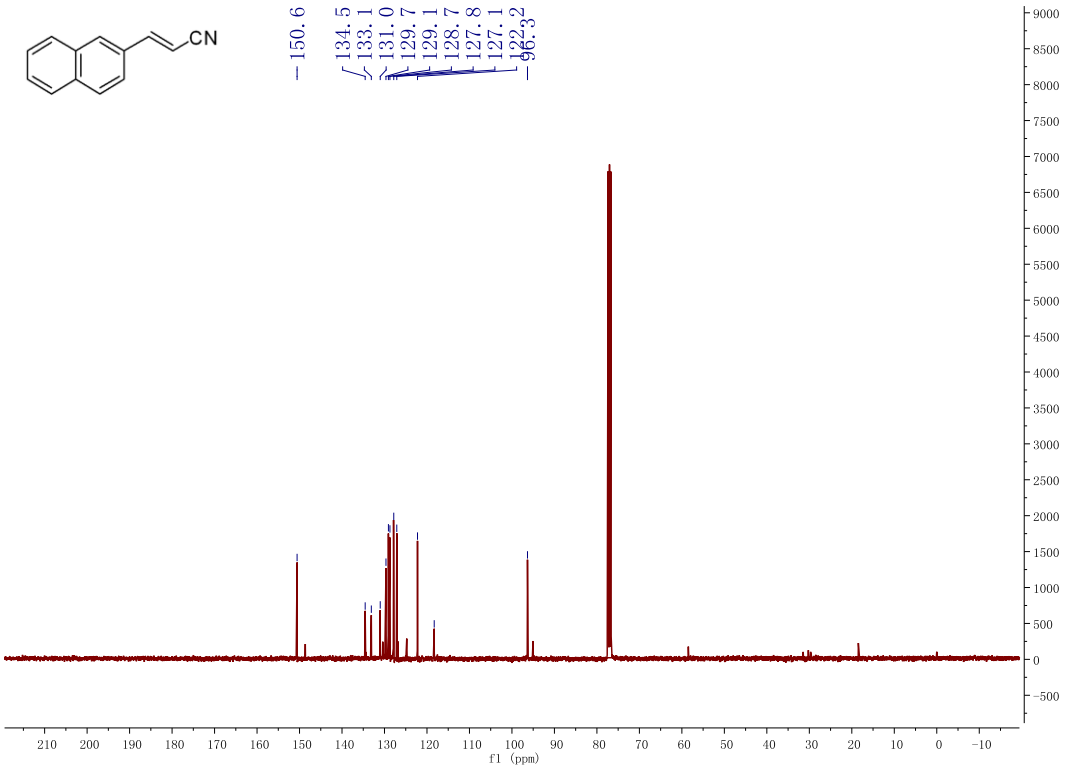


Figure S101. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **8l** (trans :cis =8:1)

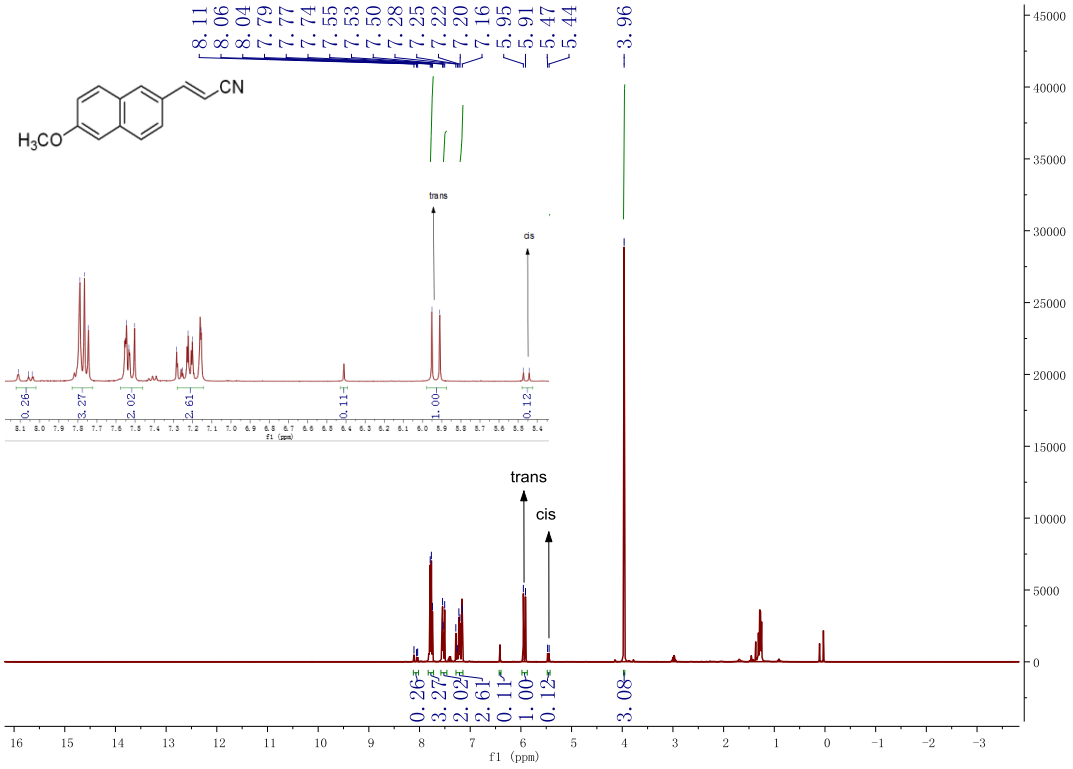


Figure S102. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8l**

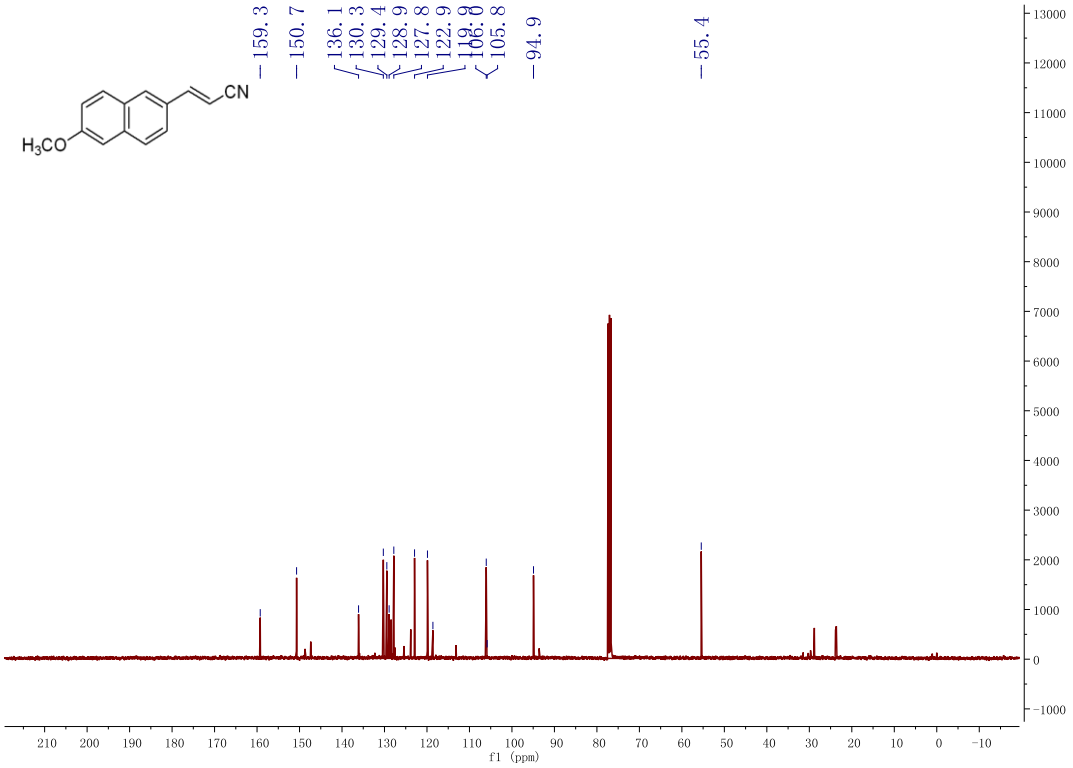


Figure S103. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2h**

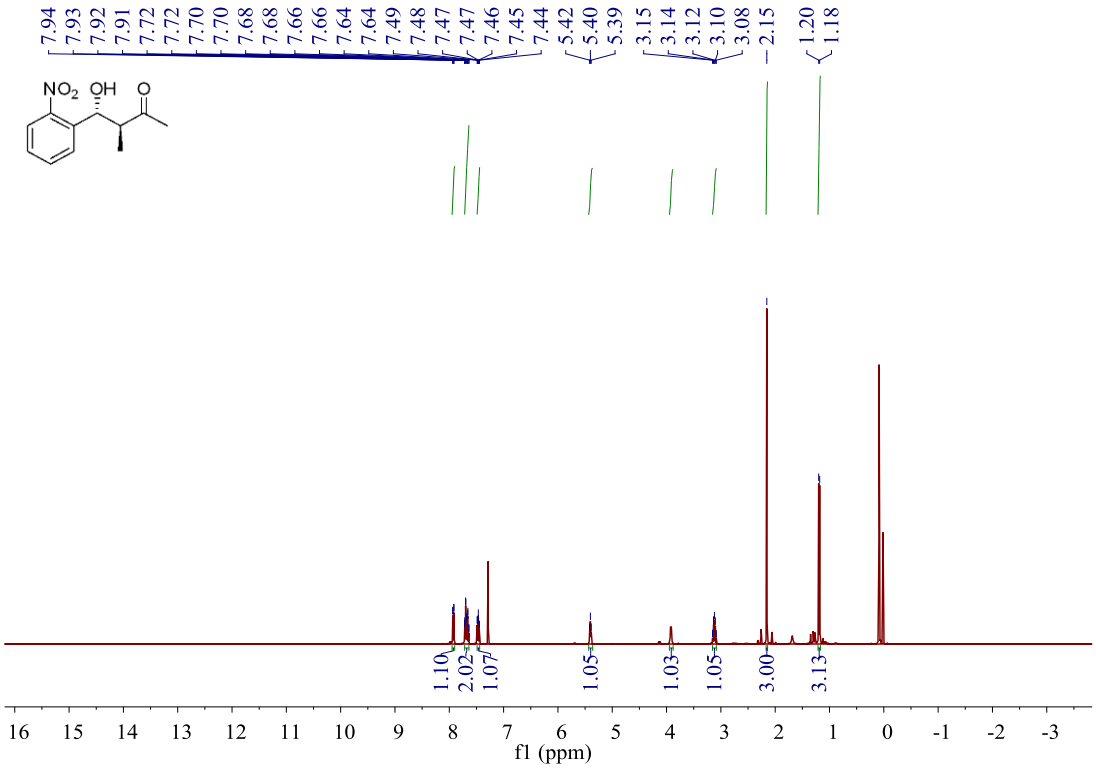


Figure S104. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **2h**

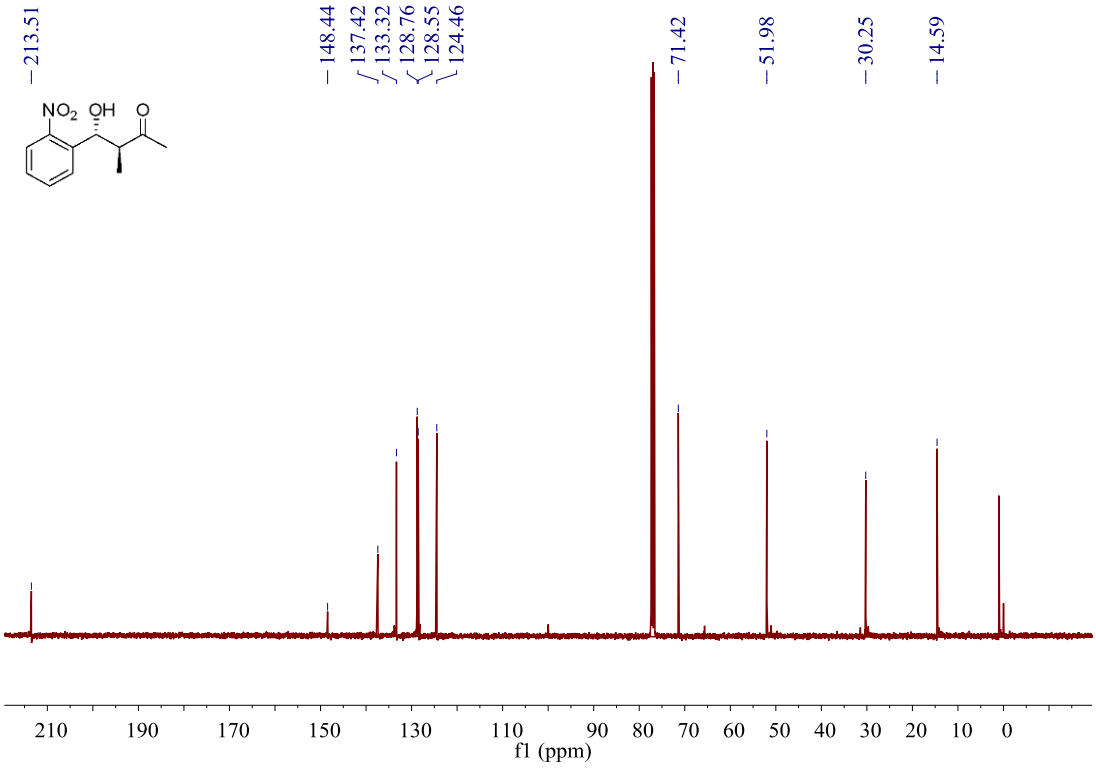


Figure S105. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5b**

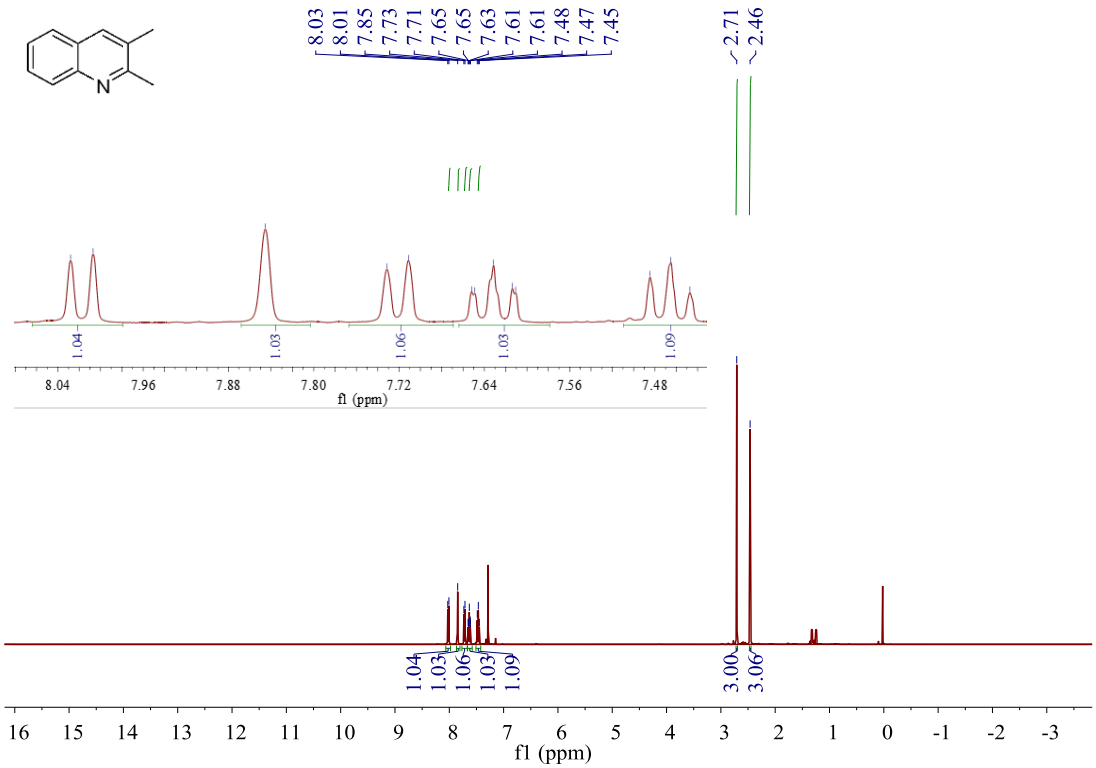
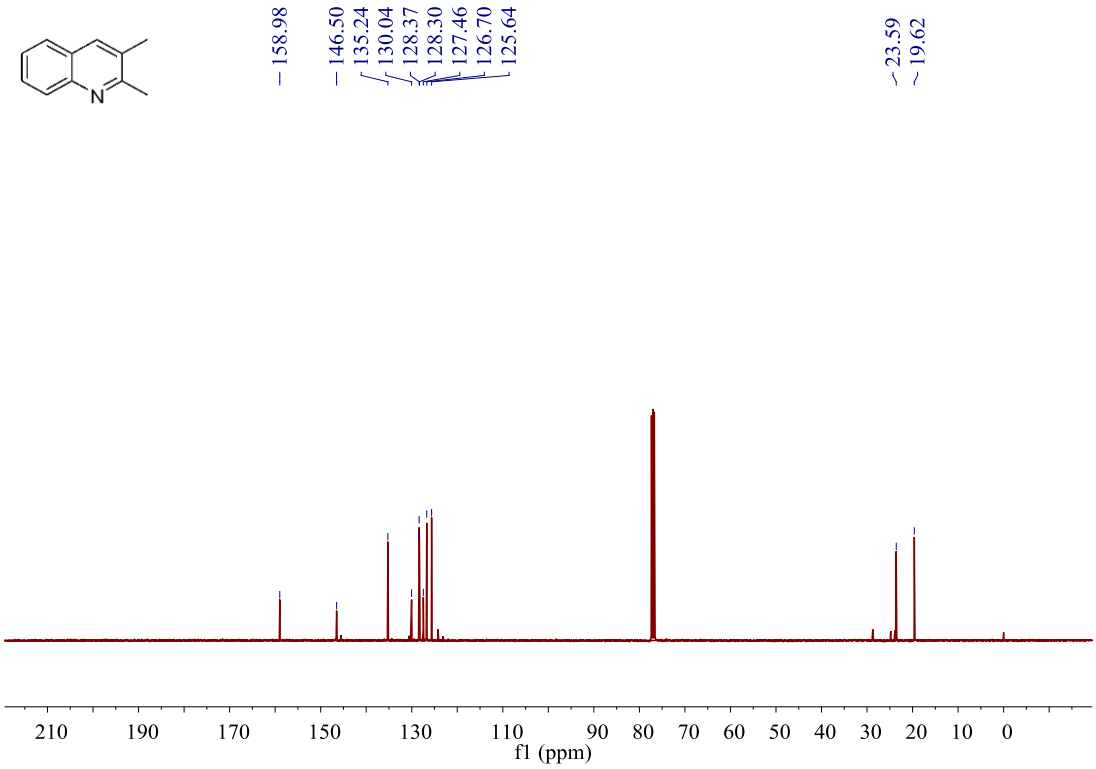


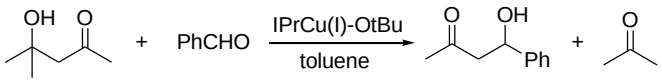
Figure S106. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **5b**



5. DFT computational studies

5.1 Computational methods and model reaction

All calculations were performed with Gaussian 09.[1] Geometry optimization calculations were done using B3LYP method with LANL2DZ for Cu, and 6-31G(d) for C, H, O, N atoms.[2,3] Frequency analyses were conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to get the thermodynamic energy corrections. For each saddle point, the intrinsic reaction coordinate (IRC) analysis[4] was carried out to confirm that it connected the correct reactant and product on the potential energy surface. Solution-phase single-point energy calculations were performed on the gas-phase stationary points by using M06[5] with a larger basis set (i.e. SDD[6] for Cu and 6-311+G(d, p) for the other elements). Solvent effect (solvent = toluene) was considered by using self-consistent reaction field (SCRF) method[7] with SMD solvation model.[8] For each stationary point, its energy was calculated by the solution-phase single-point electronic energy corrected by Gibbs free energy correction item. For complexes with several possible isomers, the most stable ones were discussed. Eq S2 shows the model reaction studied in DFT calculations.



2a **1a** **PD** (S2)

References:

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5.2 Cartesian coordinates of stationary points in Figure 1

IPrCu(I)-OtBu (A)

Electronic energy = -1589.31812931 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.288526	-0.779849	-1.053410
2	6	0	2.664299	-0.704582	0.207619
3	6	0	3.267374	-0.085345	1.320415
4	6	0	4.540212	0.469236	1.137997
5	6	0	5.182068	0.408781	-0.095677
6	6	0	4.560643	-0.208189	-1.177802
7	7	0	1.351335	-1.287513	0.366371
8	6	0	0.177903	-0.615030	0.164731
9	7	0	-0.783796	-1.550467	0.427396
10	6	0	-0.222020	-2.771851	0.784531
11	6	0	1.124037	-2.606099	0.745758
12	29	0	-0.036404	1.205987	-0.360981
13	8	0	-0.021789	2.941151	-0.849007
14	6	0	-1.036071	3.874674	-1.070287
15	6	0	-0.368965	5.172670	-1.576515
16	6	0	-2.205028	-1.303553	0.353492
17	6	0	-2.874025	-0.861244	1.511874
18	6	0	-4.250262	-0.622962	1.410078
19	6	0	-4.928457	-0.820322	0.210379
20	6	0	-4.241937	-1.265817	-0.915994
21	6	0	-2.865670	-1.520812	-0.871977
22	6	0	-2.158158	-0.623137	2.837932
23	6	0	-2.755920	-1.479878	3.970971
24	6	0	-2.138970	-1.992484	-2.127990
25	6	0	-2.098668	-0.880722	-3.194813
26	6	0	2.577266	0.025983	2.676205
27	6	0	3.428430	-0.579236	3.809034
28	6	0	2.622392	-1.421395	-2.266459
29	6	0	3.484069	-2.547603	-2.869094
30	6	0	-1.799333	4.173220	0.239614
31	6	0	-2.154819	0.872958	3.207541
32	6	0	-2.750765	-3.289055	-2.692711
33	6	0	2.196931	1.489276	2.979276
34	6	0	2.267683	-0.357608	-3.324626
35	1	0	-2.570513	4.944878	0.109728
36	1	0	-2.287459	3.260182	0.604170
37	1	0	-1.096029	4.513040	1.009092
38	1	0	-1.100840	5.966716	-1.776204
39	1	0	0.345918	5.537063	-0.830003
40	1	0	0.184296	4.968521	-2.500394
41	1	0	-0.828884	-3.630300	1.026088
42	1	0	1.933706	-3.289726	0.947451
43	1	0	-4.795683	-0.272662	2.281670
44	1	0	-5.995923	-0.625105	0.152529
45	1	0	-4.781409	-1.413292	-1.847094
46	1	0	5.030472	0.962742	1.972064
47	1	0	6.167925	0.849818	-0.216115
48	1	0	5.067663	-0.240301	-2.137827
49	1	0	-1.102655	-2.217144	-1.857471

50	1	0	-1.113596	-0.927394	2.720727
51	1	0	1.682360	-1.875443	-1.938282
52	1	0	1.645654	-0.546763	2.632356
53	1	0	-1.537425	-1.217478	-4.074776
54	1	0	-3.108001	-0.607800	-3.524627
55	1	0	-1.616351	0.020954	-2.803904
56	1	0	-2.172454	-3.633887	-3.557797
57	1	0	-2.754176	-4.090246	-1.944699
58	1	0	-3.784087	-3.139761	-3.026115
59	1	0	-1.610056	1.032082	4.145954
60	1	0	-1.672749	1.468379	2.425500
61	1	0	-3.173717	1.254402	3.343411
62	1	0	-2.187317	-1.333386	4.896701
63	1	0	-3.797873	-1.209610	4.177632
64	1	0	-2.731821	-2.547071	3.721993
65	1	0	1.748558	-0.821395	-4.172103
66	1	0	1.616213	0.414474	-2.901947
67	1	0	3.167623	0.135023	-3.710988
68	1	0	2.947892	-3.035705	-3.691375
69	1	0	4.428066	-2.164761	-3.273641
70	1	0	3.727123	-3.311081	-2.121124
71	1	0	1.669104	1.554804	3.938427
72	1	0	3.086409	2.127304	3.040925
73	1	0	1.545217	1.895297	2.198405
74	1	0	2.876504	-0.545710	4.755601
75	1	0	3.687051	-1.624219	3.602622
76	1	0	4.363695	-0.026606	3.954146
77	6	0	-2.034211	3.368472	-2.135845
78	1	0	-2.815395	4.106954	-2.362394
79	1	0	-1.498692	3.136382	-3.064313
80	1	0	-2.522397	2.449870	-1.785346

2a

Electronic energy = -386.301685569 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351407	-0.114399	0.776181
2	6	0	-1.044833	-0.022465	-0.025867
3	6	0	-1.076625	1.176574	-0.976489
4	8	0	-0.922589	-1.177679	-0.873275
5	6	0	0.159876	0.053158	0.960791
6	6	0	1.517949	0.191310	0.274316
7	6	0	2.203696	-1.083910	-0.174983
8	8	0	2.007481	1.289976	0.083369
9	1	0	2.391021	-1.743273	0.682614
10	1	0	1.539007	-1.621796	-0.860835
11	1	0	3.148777	-0.847449	-0.668311
12	1	0	0.031205	0.924400	1.611404
13	1	0	0.142782	-0.848228	1.589626
14	1	0	-1.133026	2.114899	-0.416047
15	1	0	-0.178521	1.208018	-1.598670
16	1	0	-1.949148	1.102648	-1.633376
17	1	0	-2.508564	0.777843	1.391980
18	1	0	-3.200997	-0.219264	0.093205
19	1	0	-2.340241	-0.983685	1.447675

20	1	0	-1.073360	-1.964099	-0.323713

CP1

Electronic energy = -1975.64293549 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.035905	-2.587128	-1.578350
2	6	0	-1.841612	-2.364883	-0.200704
3	6	0	-2.913089	-2.278980	0.712925
4	6	0	-4.209742	-2.412452	0.202153
5	6	0	-4.432432	-2.617545	-1.156389
6	6	0	-3.355588	-2.704375	-2.033488
7	7	0	-0.494430	-2.273970	0.315215
8	6	0	0.321249	-1.175459	0.246451
9	7	0	1.442031	-1.565185	0.930841
10	6	0	1.325754	-2.865421	1.408738
11	6	0	0.109870	-3.314715	1.013890
12	6	0	2.604141	-0.735669	1.156764
13	6	0	3.745818	-0.944008	0.355230
14	6	0	4.870673	-0.152012	0.616002
15	6	0	4.856223	0.807160	1.624764
16	6	0	3.716434	0.987152	2.403161
17	6	0	2.563995	0.219120	2.194434
18	6	0	3.799914	-2.005865	-0.740508
19	6	0	4.295551	-1.443349	-2.085752
20	6	0	1.360828	0.381008	3.120297
21	6	0	0.951200	1.849006	3.335635
22	29	0	0.117816	0.523695	-0.648439
23	8	0	0.249308	2.125345	-1.628685
24	6	0	1.280729	2.437951	-2.541272
25	6	0	0.920525	3.762133	-3.246421
26	6	0	-2.712224	-2.079502	2.213737
27	6	0	-3.476823	-0.853156	2.744885
28	6	0	-0.882868	-2.753189	-2.563312
29	6	0	-0.767891	-4.219694	-3.027321
30	8	0	-0.283782	3.587561	0.525735
31	6	0	-1.493287	4.291230	0.325163
32	6	0	-2.113345	4.497980	1.714592
33	8	0	-2.341912	1.258381	0.243147
34	6	0	-3.029553	2.235626	-0.022522
35	6	0	-4.525244	2.228491	0.247150
36	6	0	-1.208675	5.661440	-0.323778
37	6	0	-2.448818	3.494927	-0.629851
38	6	0	-3.097183	-3.351884	2.996152
39	6	0	-1.004797	-1.797785	-3.764318
40	6	0	1.636270	-0.320156	4.468096
41	6	0	4.667168	-3.204386	-0.302016
42	6	0	2.623899	2.605916	-1.801251
43	6	0	1.405047	1.328772	-3.603910
44	1	0	-4.794626	3.058756	0.912233
45	1	0	-5.071191	2.387092	-0.692014
46	1	0	-4.834408	1.280506	0.691682
47	1	0	-3.258995	4.154823	-0.961455
48	1	0	-1.849363	3.197353	-1.498903
49	1	0	-3.066087	5.038809	1.658460

50	1	0	-2.275989	3.535068	2.210081
51	1	0	-1.425829	5.079430	2.338154
52	1	0	-2.114604	6.276790	-0.397296
53	1	0	-0.470263	6.199923	0.279845
54	1	0	-0.798685	5.535440	-1.331150
55	1	0	-0.383099	-4.261955	1.164143
56	1	0	2.110798	-3.338772	1.976557
57	1	0	-5.056434	-2.351796	0.879855
58	1	0	-5.447693	-2.715521	-1.531958
59	1	0	-3.539658	-2.875038	-3.090055
60	1	0	3.720361	1.734668	3.190151
61	1	0	5.737934	1.416039	1.806161
62	1	0	5.767205	-0.284888	0.017708
63	1	0	0.046707	-2.498479	-2.047057
64	1	0	-1.650268	-1.890837	2.394629
65	1	0	2.783160	-2.376848	-0.903129
66	1	0	0.505950	-0.119016	2.656494
67	1	0	-0.127721	-1.895855	-4.414516
68	1	0	-1.891323	-2.016233	-4.371287
69	1	0	-1.064360	-0.756913	-3.431818
70	1	0	0.088040	-4.341336	-3.701826
71	1	0	-0.630137	-4.898764	-2.177918
72	1	0	-1.667702	-4.539085	-3.566531
73	1	0	-3.246486	-0.698595	3.805994
74	1	0	-3.191574	0.042021	2.186722
75	1	0	-4.562609	-0.985071	2.661740
76	1	0	-2.911559	-3.212897	4.067765
77	1	0	-4.160117	-3.588850	2.868624
78	1	0	-2.522641	-4.224167	2.663231
79	1	0	4.242281	-2.219823	-2.858067
80	1	0	3.687045	-0.594648	-2.411893
81	1	0	5.337979	-1.109303	-2.029674
82	1	0	4.670035	-3.980785	-1.076273
83	1	0	5.705440	-2.896798	-0.129994
84	1	0	4.297227	-3.653875	0.626533
85	1	0	0.064663	1.886399	3.980562
86	1	0	1.737985	2.424583	3.838133
87	1	0	0.700088	2.347941	2.394441
88	1	0	0.759842	-0.247136	5.122992
89	1	0	1.870873	-1.382669	4.332647
90	1	0	2.483293	0.144509	4.987294
91	1	0	-0.012506	3.134314	-0.327617
92	1	0	3.438048	2.888422	-2.482332
93	1	0	2.533391	3.382266	-1.032706
94	1	0	2.903313	1.671521	-1.300519
95	1	0	2.192576	1.545959	-4.337775
96	1	0	1.636234	0.370247	-3.122681
97	1	0	0.455461	1.214569	-4.139451
98	1	0	1.669298	4.040921	-3.998921
99	1	0	-0.051431	3.670324	-3.745429
100	1	0	0.856077	4.576109	-2.516173

TS^{deprotonation}

Electronic energy = -1975.63003295 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.531465	-1.543181	0.084913
2	6	0	2.501298	-1.189812	0.983778
3	6	0	2.725382	-0.366828	2.106084
4	6	0	4.024719	0.120340	2.298935
5	6	0	5.057677	-0.207292	1.426667
6	6	0	4.812048	-1.035583	0.335142
7	7	0	1.185906	-1.750659	0.776475
8	6	0	0.109852	-1.097884	0.226354
9	7	0	-0.869602	-2.060176	0.223529
10	6	0	-0.414661	-3.262781	0.755789
11	6	0	0.876578	-3.065479	1.111399
12	29	0	-0.017659	0.753213	-0.363374
13	8	0	0.144763	2.857219	0.593203
14	6	0	-0.862398	3.807035	0.770316
15	6	0	-0.252668	5.226518	0.733540
16	6	0	-2.229393	-1.892041	-0.233275
17	6	0	-3.243145	-1.729320	0.732333
18	6	0	-4.564007	-1.637324	0.277976
19	6	0	-4.862772	-1.689641	-1.080953
20	6	0	-3.840417	-1.840186	-2.012703
21	6	0	-2.502777	-1.951794	-1.613469
22	6	0	-2.954453	-1.654994	2.229648
23	6	0	-3.515109	-2.882955	2.974568
24	6	0	-1.418074	-2.141169	-2.668294
25	6	0	-1.339266	-0.929027	-3.616730
26	6	0	1.642647	-0.051821	3.134231
27	6	0	1.887053	-0.857281	4.428034
28	6	0	3.306022	-2.474457	-1.104889
29	6	0	3.877297	-3.879755	-0.820490
30	8	0	-2.257612	1.360985	-0.581181
31	6	0	-2.750303	2.469690	-0.389011
32	6	0	-1.925206	3.731518	-0.399204
33	6	0	-4.238278	2.598637	-0.123087
34	6	0	-1.542627	3.584600	2.133974
35	6	0	-3.484778	-0.347197	2.846709
36	6	0	-1.618640	-3.453507	-3.452140
37	6	0	1.525339	1.455057	3.426567
38	6	0	3.892928	-1.918578	-2.415529
39	1	0	-4.410283	3.124549	0.824599
40	1	0	-4.704318	3.206429	-0.909743
41	1	0	-4.706062	1.612224	-0.095486
42	1	0	-2.582332	4.608098	-0.362545
43	1	0	-1.358390	3.753275	-1.336416
44	1	0	-2.370841	4.285583	2.303273
45	1	0	-1.924580	2.560757	2.211182
46	1	0	-0.809638	3.722852	2.935761
47	1	0	-0.998672	6.007973	0.929305
48	1	0	0.533754	5.297551	1.492785
49	1	0	0.202221	5.422972	-0.244021
50	1	0	-1.051460	-4.130033	0.829251
51	1	0	1.598752	-3.723844	1.566835
52	1	0	-5.368519	-1.520111	0.998744
53	1	0	-5.894890	-1.615483	-1.413917
54	1	0	-4.082819	-1.878391	-3.070892
55	1	0	4.229073	0.759732	3.152185
56	1	0	6.058052	0.180818	1.599232
57	1	0	5.626547	-1.289137	-0.336671

58	1	0	-0.453880	-2.212363	-2.157296
59	1	0	-1.869506	-1.654558	2.368551
60	1	0	2.226519	-2.577567	-1.253963
61	1	0	0.680120	-0.370096	2.724433
62	1	0	-0.526206	-1.066634	-4.339599
63	1	0	-2.270339	-0.802486	-4.182489
64	1	0	-1.149476	-0.005940	-3.060535
65	1	0	-0.800570	-3.597106	-4.167975
66	1	0	-1.640609	-4.321118	-2.782411
67	1	0	-2.557044	-3.446366	-4.019033
68	1	0	-3.196314	-0.281798	3.902493
69	1	0	-3.075537	0.522151	2.323655
70	1	0	-4.578567	-0.288847	2.798647
71	1	0	-3.269889	-2.828808	4.041911
72	1	0	-4.606352	-2.940050	2.884670
73	1	0	-3.100944	-3.817789	2.579541
74	1	0	3.616272	-2.568690	-3.253895
75	1	0	3.519684	-0.912667	-2.626226
76	1	0	4.987797	-1.873885	-2.386487
77	1	0	3.680659	-4.552638	-1.663694
78	1	0	4.962560	-3.836963	-0.669610
79	1	0	3.436063	-4.326135	0.077249
80	1	0	0.716548	1.625131	4.148214
81	1	0	2.444386	1.856964	3.870529
82	1	0	1.291244	2.017218	2.516514
83	1	0	1.087781	-0.664838	5.153679
84	1	0	1.916903	-1.936049	4.233454
85	1	0	2.838603	-0.576569	4.895493
86	8	0	0.646302	2.283805	-1.647672
87	1	0	0.530061	2.792501	-0.599679
88	6	0	1.869968	2.519882	-2.331757
89	6	0	3.065743	2.281586	-1.392373
90	6	0	1.924226	1.563462	-3.531562
91	6	0	1.878854	3.977735	-2.832005
92	1	0	4.021972	2.473610	-1.895889
93	1	0	2.998800	2.941076	-0.519526
94	1	0	3.068436	1.248277	-1.029069
95	1	0	2.853954	1.681707	-4.102330
96	1	0	1.854279	0.525831	-3.187059
97	1	0	1.078900	1.751281	-4.203331
98	1	0	2.782991	4.201854	-3.412348
99	1	0	1.005394	4.161856	-3.467758
100	1	0	1.839321	4.674263	-1.986177

CP2

Electronic energy = -1975.64631131 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.863740	-0.335358	-0.767320
2	6	0	-3.024417	-0.837831	0.248590
3	6	0	-3.293633	-0.651587	1.620319
4	6	0	-4.429781	0.094767	1.957496
5	6	0	-5.267433	0.618080	0.976513
6	6	0	-4.989383	0.396748	-0.369652
7	7	0	-1.857582	-1.596868	-0.135133

8	6	0	-0.575850	-1.116594	-0.123483
9	7	0	0.169604	-2.171911	-0.569538
10	6	0	-0.628927	-3.275408	-0.854677
11	6	0	-1.905064	-2.915607	-0.574148
12	6	0	1.609057	-2.204318	-0.702855
13	6	0	2.207219	-1.612634	-1.833799
14	6	0	3.591916	-1.767040	-1.979683
15	6	0	4.346778	-2.462331	-1.038928
16	6	0	3.732586	-3.005335	0.086160
17	6	0	2.351315	-2.887395	0.282887
18	6	0	1.410638	-0.846944	-2.885790
19	6	0	2.070618	0.497063	-3.249197
20	6	0	1.717574	-3.465343	1.545964
21	6	0	2.235725	-2.743708	2.806176
22	29	0	-0.005487	0.639797	0.399778
23	8	0	3.017138	2.209736	-0.123220
24	6	0	4.210271	2.026489	0.639149
25	6	0	4.554471	3.316910	1.406461
26	6	0	-2.437100	-1.262643	2.726114
27	6	0	-1.874364	-0.197790	3.686289
28	6	0	-3.610690	-0.586064	-2.252355
29	6	0	-4.691559	-1.515880	-2.841541
30	8	0	0.638992	2.208850	1.198384
31	6	0	0.032272	3.462363	1.124373
32	6	0	-1.454449	3.392521	1.535050
33	8	0	-0.690304	2.262380	-1.648568
34	6	0	-0.733509	3.454192	-1.359529
35	6	0	-1.738661	4.375520	-2.030314
36	6	0	0.764529	4.422088	2.087697
37	6	0	0.178585	4.073826	-0.327048
38	6	0	-3.226322	-2.342647	3.494266
39	6	0	-3.505430	0.722649	-3.057390
40	6	0	1.928397	-4.988230	1.651053
41	6	0	1.178644	-1.716544	-4.138455
42	6	0	4.032286	0.856805	1.622393
43	6	0	5.313547	1.714139	-0.379353
44	1	0	-2.388861	4.834113	-1.273958
45	1	0	-1.215130	5.197896	-2.534534
46	1	0	-2.346157	3.829407	-2.755072
47	1	0	0.008191	5.156654	-0.294356
48	1	0	1.218183	3.898051	-0.626722
49	1	0	-1.948814	4.371919	1.473806
50	1	0	-2.003481	2.684536	0.903285
51	1	0	-1.529035	3.040704	2.569982
52	1	0	0.286209	5.408929	2.132747
53	1	0	0.764389	3.987952	3.093691
54	1	0	1.804330	4.558010	1.774791
55	1	0	-2.832805	-3.460583	-0.647048
56	1	0	-0.211638	-4.200125	-1.220647
57	1	0	-4.663456	0.262278	3.004890
58	1	0	-6.143927	1.193683	1.262247
59	1	0	-5.655034	0.800330	-1.127030
60	1	0	4.333790	-3.524565	0.827056
61	1	0	5.419513	-2.569156	-1.176281
62	1	0	4.084733	-1.331033	-2.842907
63	1	0	-2.648738	-1.096635	-2.354488
64	1	0	-1.579617	-1.756121	2.260440
65	1	0	0.432234	-0.606646	-2.462274

66	1	0	0.638515	-3.291164	1.499938
67	1	0	-3.318521	0.494687	-4.113927
68	1	0	-4.432672	1.306216	-3.006398
69	1	0	-2.679711	1.337994	-2.688403
70	1	0	-4.471169	-1.739274	-3.891979
71	1	0	-4.749902	-2.466170	-2.297533
72	1	0	-5.683402	-1.050406	-2.799923
73	1	0	-1.244363	-0.674848	4.446644
74	1	0	-1.263378	0.534842	3.149564
75	1	0	-2.674381	0.339351	4.209815
76	1	0	-2.586071	-2.817342	4.247118
77	1	0	-4.090942	-1.914176	4.014688
78	1	0	-3.596761	-3.124156	2.820772
79	1	0	1.385263	1.083164	-3.871684
80	1	0	2.306090	1.079850	-2.352988
81	1	0	2.995290	0.354827	-3.822580
82	1	0	0.587912	-1.165851	-4.880085
83	1	0	2.130084	-1.996277	-4.607204
84	1	0	0.641292	-2.641372	-3.896075
85	1	0	1.732239	-3.131750	3.699939
86	1	0	3.313613	-2.891802	2.939757
87	1	0	2.050331	-1.666234	2.747504
88	1	0	1.422980	-5.382432	2.540503
89	1	0	1.528455	-5.510444	0.774205
90	1	0	2.991075	-5.244142	1.733139
91	1	0	2.219209	2.219560	0.473714
92	1	0	4.937758	0.692208	2.220309
93	1	0	3.201561	1.064110	2.307548
94	1	0	3.805118	-0.065053	1.076862
95	1	0	6.283765	1.580772	0.113990
96	1	0	5.071761	0.798542	-0.929130
97	1	0	5.401795	2.533199	-1.102081
98	1	0	5.514208	3.229252	1.931680
99	1	0	4.616786	4.161731	0.711295
100	1	0	3.782963	3.541022	2.151142

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tBuOH

Electronic energy = -233.666739553 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.490490	-0.030589	-0.356413
2	6	0	-0.005379	-0.000176	0.014443
3	6	0	0.663209	1.280981	-0.508079
4	8	0	0.014711	-0.002285	1.451925
5	6	0	0.717068	-1.249705	-0.512674
6	1	0	0.679901	-1.305481	-1.606985
7	1	0	1.775020	-1.240741	-0.217638
8	1	0	0.257042	-2.154630	-0.102090
9	1	0	-1.622394	-0.028872	-1.443735
10	1	0	-1.964963	-0.929014	0.051970
11	1	0	-2.002490	0.843518	0.059380
12	1	0	0.625090	1.338182	-1.602301
13	1	0	0.163713	2.163856	-0.095604
14	1	0	1.719964	1.316989	-0.211114
15	1	0	0.944982	0.011411	1.729055

IPrCu(I)-alkoxide (B)

Electronic energy = -1741.96148208 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.878134	-0.767246	1.665110
2	6	0	-2.313564	-1.381787	0.529054
3	6	0	-3.055295	-1.649610	-0.639095
4	6	0	-4.409408	-1.292842	-0.640547
5	6	0	-4.996253	-0.690260	0.468773
6	6	0	-4.236187	-0.429728	1.605531
7	7	0	-0.916481	-1.746388	0.556246
8	6	0	0.101055	-0.877631	0.281385
9	7	0	1.227587	-1.638413	0.419964
10	6	0	0.918185	-2.946945	0.778783
11	6	0	-0.434635	-3.015009	0.864816
12	29	0	0.007498	1.012012	0.006259
13	8	0	0.051272	2.804203	0.518191
14	6	0	-0.110995	3.956628	-0.205989
15	6	0	0.810273	5.055188	0.375969
16	6	0	2.565587	-1.136609	0.209831
17	6	0	3.163468	-1.329093	-1.052215
18	6	0	4.461329	-0.836528	-1.234303
19	6	0	5.131814	-0.178593	-0.206511
20	6	0	4.512450	0.005176	1.026394
21	6	0	3.215182	-0.466058	1.265598
22	6	0	2.438349	-2.006277	-2.211486
23	6	0	3.229851	-3.206265	-2.765945
24	6	0	2.570480	-0.242371	2.630222
25	6	0	2.429394	1.258478	2.957562
26	6	0	-2.439940	-2.287029	-1.881676
27	6	0	-3.107792	-3.636238	-2.212872
28	6	0	-2.081326	-0.467104	2.931374
29	6	0	-2.637259	-1.251189	4.137180
30	8	0	-0.409212	1.583961	-2.295566
31	6	0	-0.517587	2.798225	-2.480339
32	6	0	0.333060	3.781787	-1.732691
33	6	0	-1.549112	3.332167	-3.456218
34	6	0	-1.580699	4.440130	-0.136767
35	6	0	2.107584	-0.988964	-3.322337
36	6	0	3.343461	-0.986220	3.737848
37	6	0	-2.484840	-1.328150	-3.088112
38	6	0	-2.023642	1.045775	3.227108
39	1	0	-2.156815	4.116340	-2.990664
40	1	0	-1.038611	3.792425	-4.312813
41	1	0	-2.190836	2.523235	-3.812778
42	1	0	0.319881	4.756419	-2.234580
43	1	0	1.361981	3.408430	-1.701262
44	1	0	-1.759841	5.359136	-0.712328
45	1	0	-2.260069	3.658873	-0.497889
46	1	0	-1.838576	4.637365	0.909572
47	1	0	0.704711	6.017894	-0.141766
48	1	0	0.564075	5.198803	1.433817
49	1	0	1.856327	4.734403	0.314855
50	1	0	1.680798	-3.694146	0.933084

51	1	0	-1.092908	-3.833578	1.110280
52	1	0	4.949413	-0.962750	-2.196618
53	1	0	6.138606	0.197254	-0.369159
54	1	0	5.041605	0.527727	1.817971
55	1	0	-5.008693	-1.483370	-1.526369
56	1	0	-6.048440	-0.418757	0.445838
57	1	0	-4.702190	0.047337	2.462792
58	1	0	1.560556	-0.661507	2.601768
59	1	0	1.486156	-2.394403	-1.837900
60	1	0	-1.052325	-0.802930	2.773766
61	1	0	-1.384930	-2.489208	-1.674818
62	1	0	1.941354	1.380391	3.932446
63	1	0	3.409644	1.747056	3.017601
64	1	0	1.827645	1.784916	2.208419
65	1	0	2.841222	-0.856889	4.703785
66	1	0	3.409976	-2.060713	3.530080
67	1	0	4.365467	-0.603086	3.841365
68	1	0	1.558864	-1.480264	-4.135182
69	1	0	1.489084	-0.171273	-2.938679
70	1	0	3.021538	-0.557810	-3.748719
71	1	0	2.654476	-3.708880	-3.552289
72	1	0	4.185157	-2.896215	-3.205002
73	1	0	3.447197	-3.940774	-1.981734
74	1	0	-1.435069	1.224086	4.135460
75	1	0	-1.556923	1.603039	2.407375
76	1	0	-3.025911	1.457644	3.397715
77	1	0	-2.021431	-1.067506	5.025417
78	1	0	-3.663335	-0.948369	4.377033
79	1	0	-2.644939	-2.330672	3.945840
80	1	0	-2.017638	-1.801702	-3.960499
81	1	0	-3.517356	-1.078211	-3.361136
82	1	0	-1.948303	-0.397875	-2.875549
83	1	0	-2.618284	-4.101754	-3.076464
84	1	0	-3.044804	-4.334141	-1.369656
85	1	0	-4.168291	-3.510850	-2.461036

TS$^{\text{retro-aldol}}$

Electronic energy = -1741.94334625 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.245419	3.834539	-3.024686
2	6	0	-0.153932	3.212683	-2.168796
3	6	0	0.762714	4.017975	-1.501633
4	8	0	-0.194607	1.931122	-2.057678
5	29	0	-0.033414	0.946361	-0.348882
6	8	0	-0.030811	2.602340	0.886416
7	6	0	-0.117963	3.837619	0.631465
8	6	0	-1.499104	4.439049	0.422132
9	6	0	0.927314	4.764246	1.237906
10	1	0	-1.200369	4.927673	-3.043283
11	1	0	-1.153473	3.463593	-4.052686
12	1	0	-2.231981	3.521243	-2.660938
13	1	0	0.816441	5.077334	-1.736205
14	1	0	1.665678	3.559502	-1.111924
15	1	0	-1.462577	5.423016	-0.053307

16	1	0	-2.122851	3.764907	-0.170022
17	1	0	-1.975640	4.553863	1.408093
18	1	0	0.952683	5.745413	0.756484
19	1	0	0.673072	4.912047	2.299002
20	1	0	1.917726	4.305321	1.193270
21	6	0	0.056369	-0.905647	0.183145
22	7	0	-0.981282	-1.761414	0.426031
23	7	0	1.166250	-1.686869	0.343252
24	6	0	-0.527940	-3.042786	0.727463
25	6	0	-2.370555	-1.373430	0.367223
26	6	0	0.827157	-2.995649	0.675530
27	6	0	2.516565	-1.204877	0.173559
28	1	0	1.573852	-3.756397	0.841308
29	1	0	-1.205080	-3.853135	0.947816
30	6	0	3.092682	-1.246073	-1.112201
31	6	0	4.403472	-0.771494	-1.246269
32	6	0	5.107007	-0.276653	-0.151623
33	6	0	4.509458	-0.241691	1.105309
34	6	0	3.200720	-0.701691	1.298207
35	6	0	2.347733	-1.766237	-2.337866
36	1	0	4.875713	-0.783858	-2.224452
37	1	0	6.122875	0.087924	-0.279748
38	1	0	5.063608	0.155900	1.950788
39	6	0	2.567175	-0.624124	2.683929
40	6	0	-3.045171	-1.457937	-0.867502
41	6	0	-4.393184	-1.078391	-0.892802
42	6	0	-5.038308	-0.632022	0.257257
43	6	0	-4.343878	-0.551025	1.461256
44	6	0	-2.994825	-0.917187	1.545616
45	6	0	-2.367361	-1.930235	-2.150130
46	1	0	-4.941931	-1.129098	-1.828866
47	1	0	-6.084755	-0.341378	0.214109
48	1	0	-4.854152	-0.191470	2.350283
49	6	0	-2.256125	-0.788750	2.874384
50	1	0	1.565348	-1.059986	2.625335
51	6	0	3.361732	-1.445330	3.718211
52	6	0	2.398469	0.839694	3.138884
53	6	0	2.130970	-0.651864	-3.381954
54	6	0	3.063301	-2.983030	-2.957335
55	1	0	1.357199	-2.102050	-2.017292
56	1	0	-1.240779	-1.172539	2.737812
57	6	0	-2.129122	0.688249	3.299660
58	6	0	-2.917203	-1.635488	3.979417
59	6	0	-2.318345	-0.810897	-3.210146
60	1	0	-1.332458	-2.191897	-1.910849
61	6	0	-3.041295	-3.200107	-2.707138
62	1	0	1.918101	0.873628	4.124573
63	1	0	3.369478	1.342303	3.225751
64	1	0	1.779052	1.407292	2.436620
65	1	0	2.857526	-1.419525	4.691415
66	1	0	3.456197	-2.493684	3.411829
67	1	0	4.373498	-1.047607	3.859597
68	1	0	1.581608	-1.050085	-4.243949
69	1	0	1.553800	0.180983	-2.966719
70	1	0	3.086511	-0.259638	-3.750884
71	1	0	2.482396	-3.374841	-3.800469
72	1	0	4.057608	-2.717991	-3.335500
73	1	0	3.189404	-3.790499	-2.226542

74	1	0	-1.572062	0.761704	4.241818
75	1	0	-1.600483	1.276866	2.542715
76	1	0	-3.115530	1.140175	3.460609
77	1	0	-2.333048	-1.572471	4.905039
78	1	0	-3.931673	-1.286865	4.205644
79	1	0	-2.984334	-2.690966	3.690936
80	1	0	-1.811317	-1.174898	-4.112357
81	1	0	-3.327657	-0.496668	-3.503228
82	1	0	-1.775377	0.068123	-2.846880
83	1	0	-2.505223	-3.554551	-3.595305
84	1	0	-3.047671	-4.009605	-1.967803
85	1	0	-4.080042	-3.009925	-3.001760

CP3

Electronic energy = -1741.95242004 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.315059	-1.331327	0.197075
2	6	0	-2.563567	-0.693347	-0.811231
3	6	0	-3.070612	0.373790	-1.580686
4	6	0	-4.377868	0.797140	-1.310066
5	6	0	-5.145057	0.185002	-0.323014
6	6	0	-4.617672	-0.867778	0.419285
7	7	0	-1.220875	-1.164285	-1.068022
8	6	0	-0.090066	-0.580179	-0.572137
9	7	0	0.922196	-1.367066	-1.040497
10	6	0	0.433137	-2.412218	-1.816319
11	6	0	-0.917881	-2.284242	-1.833940
12	29	0	0.022796	1.083172	0.359402
13	8	0	-0.198323	0.093471	3.380013
14	6	0	-0.125621	1.234058	3.819381
15	6	0	1.200614	1.836117	4.231001
16	6	0	2.323139	-1.155553	-0.752647
17	6	0	3.052941	-0.254843	-1.555304
18	6	0	4.409714	-0.082048	-1.255502
19	6	0	5.010054	-0.772538	-0.205971
20	6	0	4.263703	-1.657004	0.567150
21	6	0	2.902685	-1.870829	0.314552
22	6	0	2.432875	0.485670	-2.737147
23	6	0	2.879688	-0.150675	-4.069835
24	6	0	2.122548	-2.865999	1.169865
25	6	0	2.129922	-2.482238	2.662275
26	6	0	-2.271135	1.057138	-2.686066
27	6	0	-2.902830	0.795852	-4.068368
28	6	0	-2.774818	-2.491328	1.029225
29	6	0	-3.552808	-3.790563	0.736419
30	8	0	-0.042430	2.820941	1.002011
31	6	0	0.941130	3.714858	0.973864
32	6	0	2.268830	3.441066	0.916681
33	6	0	0.442909	5.146263	1.040933
34	6	0	-1.344652	2.127423	3.896044
35	6	0	2.734940	1.995868	-2.715572
36	6	0	2.650311	-4.300182	0.960327
37	6	0	-2.106860	2.567581	-2.425456
38	6	0	-2.774506	-2.168454	2.535997

39	1	0	1.260973	5.873215	1.039391
40	1	0	-0.216120	5.354746	0.188233
41	1	0	-0.157963	5.295368	1.947470
42	1	0	3.007044	4.236227	0.909375
43	1	0	2.632571	2.416879	0.877696
44	1	0	-1.341888	2.758452	4.791272
45	1	0	-1.304698	2.777395	3.011218
46	1	0	-2.257478	1.527838	3.855969
47	1	0	1.521888	2.537108	3.446688
48	1	0	1.116252	2.399550	5.167169
49	1	0	1.955262	1.052207	4.330542
50	1	0	1.086193	-3.140309	-2.271030
51	1	0	-1.684779	-2.876745	-2.307298
52	1	0	5.002506	0.604959	-1.851494
53	1	0	6.064058	-0.619594	0.010259
54	1	0	4.742331	-2.189860	1.383606
55	1	0	-4.798775	1.618561	-1.882460
56	1	0	-6.157354	0.530650	-0.130831
57	1	0	-5.223695	-1.336299	1.189268
58	1	0	1.078156	-2.853298	0.843898
59	1	0	1.346148	0.378290	-2.671235
60	1	0	-1.733516	-2.663820	0.741247
61	1	0	-1.267677	0.622061	-2.700594
62	1	0	1.584226	-3.236954	3.241595
63	1	0	3.150291	-2.435194	3.061387
64	1	0	1.641462	-1.517727	2.831025
65	1	0	2.046601	-5.014902	1.531763
66	1	0	2.615492	-4.593482	-0.095652
67	1	0	3.689082	-4.397930	1.297241
68	1	0	2.190216	2.493367	-3.527007
69	1	0	2.435087	2.455064	-1.767125
70	1	0	3.801389	2.199970	-2.868261
71	1	0	2.407609	0.362328	-4.916170
72	1	0	3.966491	-0.078351	-4.196949
73	1	0	2.608153	-1.211544	-4.121482
74	1	0	-2.380856	-3.023956	3.098281
75	1	0	-2.144208	-1.302069	2.758927
76	1	0	-3.788018	-1.970980	2.905831
77	1	0	-3.122129	-4.626982	1.299242
78	1	0	-4.605926	-3.700735	1.027745
79	1	0	-3.524690	-4.047710	-0.329175
80	1	0	-1.479410	3.015412	-3.205456
81	1	0	-3.073293	3.085511	-2.441685
82	1	0	-1.634414	2.758657	-1.455988
83	1	0	-2.293966	1.252246	-4.857712
84	1	0	-2.981441	-0.277406	-4.277136
85	1	0	-3.910248	1.223084	-4.135701

Acetone

Electronic energy = -193.152122818 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.293235	-0.614964	-0.000203
2	6	0	0.000002	0.185562	-0.000028
3	6	0	-1.293241	-0.614960	0.000196

4	8	0	0.000005	1.401220	0.000004
5	1	0	-1.336700	-1.276737	0.874542
6	1	0	-2.148882	0.063164	0.011346
7	1	0	-1.346379	-1.258200	-0.887455
8	1	0	1.346411	-1.257974	0.887624
9	1	0	1.336648	-1.276989	-0.874358
10	1	0	2.148884	0.063146	-0.011527

IPrCu(I)-enolate (C)

Electronic energy = -1548.78573988 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.902335	1.693757	-0.374978
2	6	0	-2.265328	0.580620	-0.959347
3	6	0	-2.951131	-0.605997	-1.285525
4	6	0	-4.325560	-0.648285	-1.019376
5	6	0	-4.983561	0.438043	-0.450278
6	6	0	-4.276871	1.593765	-0.128890
7	7	0	-0.850437	0.668610	-1.246274
8	6	0	0.141093	0.260672	-0.400720
9	7	0	1.292329	0.544548	-1.078993
10	6	0	1.022631	1.114023	-2.318618
11	6	0	-0.328248	1.191047	-2.424229
12	6	0	2.623673	0.280390	-0.581143
13	6	0	3.274538	1.280938	0.167938
14	6	0	4.567863	1.003302	0.626864
15	6	0	5.184151	-0.214332	0.351666
16	6	0	4.514441	-1.185587	-0.387014
17	6	0	3.219180	-0.963458	-0.870650
18	6	0	2.613744	2.610906	0.516728
19	6	0	2.302622	2.687460	2.025299
20	6	0	2.502019	-2.061193	-1.650271
21	6	0	2.215185	-3.280070	-0.750067
22	29	0	-0.048460	-0.594021	1.291721
23	8	0	-0.100387	-1.482365	2.882027
24	6	0	-1.143533	-2.088832	3.443258
25	6	0	-0.751270	-2.917022	4.651729
26	6	0	-2.259216	-1.823760	-1.889012
27	6	0	-2.386513	-3.053826	-0.967996
28	6	0	-2.146869	2.955377	0.031417
29	6	0	-2.761671	4.227323	-0.582484
30	6	0	-2.786285	-2.128598	-3.305245
31	6	0	-2.054851	3.061872	1.567286
32	6	0	3.282156	-2.471578	-2.914063
33	6	0	3.457865	3.815284	0.057933
34	6	0	-2.432832	-2.016079	3.035389
35	1	0	-1.611075	-3.411368	5.114806
36	1	0	-0.017537	-3.680694	4.362561
37	1	0	-0.265201	-2.278936	5.400890
38	1	0	-3.219220	-2.546541	3.562205
39	1	0	-2.723709	-1.407767	2.181641
40	1	0	-0.962408	1.564164	-3.212928
41	1	0	1.809266	1.405524	-2.996661
42	1	0	-4.884418	-1.549638	-1.252893
43	1	0	-6.049598	0.380700	-0.247735

44	1	0	-4.798399	2.428833	0.329496
45	1	0	5.000646	-2.136008	-0.586395
46	1	0	6.187755	-0.409403	0.719883
47	1	0	5.095964	1.748932	1.213971
48	1	0	-1.123329	2.877890	-0.348369
49	1	0	-1.192586	-1.598075	-1.981213
50	1	0	1.658284	2.665578	-0.013786
51	1	0	1.535092	-1.669222	-1.980282
52	1	0	-1.469571	3.943669	1.854980
53	1	0	-3.049090	3.155448	2.019481
54	1	0	-1.574901	2.175007	1.994541
55	1	0	-2.155884	5.103105	-0.322242
56	1	0	-2.812364	4.161529	-1.675417
57	1	0	-3.776760	4.408820	-0.211622
58	1	0	-1.801662	-3.888772	-1.372109
59	1	0	-2.029745	-2.838291	0.044872
60	1	0	-3.427825	-3.387360	-0.888254
61	1	0	-2.248116	-2.980960	-3.736376
62	1	0	-3.852583	-2.382806	-3.290136
63	1	0	-2.657524	-1.271108	-3.976064
64	1	0	1.787542	3.626182	2.261845
65	1	0	1.662091	1.856001	2.338494
66	1	0	3.220998	2.647914	2.622651
67	1	0	2.927473	4.750948	0.269672
68	1	0	4.421206	3.858466	0.578693
69	1	0	3.661741	3.775988	-1.018266
70	1	0	1.656908	-4.041037	-1.308336
71	1	0	3.144317	-3.740532	-0.394293
72	1	0	1.624018	-2.994295	0.126476
73	1	0	2.715959	-3.218730	-3.482255
74	1	0	3.465411	-1.612671	-3.569895
75	1	0	4.253473	-2.914042	-2.664496

PhCHO

Electronic energy = -345.566490799 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.325977	-1.331748	0.000044
2	6	0	0.045736	-1.101006	0.000070
3	6	0	0.534021	0.215024	0.000051
4	6	0	-0.361463	1.292624	0.000118
5	6	0	-1.736576	1.060526	-0.000076
6	6	0	-2.217128	-0.251327	-0.000102
7	6	0	1.992584	0.468995	-0.000013
8	8	0	2.847630	-0.396042	-0.000095
9	1	0	2.274432	1.546010	-0.000019
10	1	0	0.024202	2.310200	0.000270
11	1	0	-2.431245	1.895792	-0.000127
12	1	0	-3.288444	-0.434252	-0.000148
13	1	0	-1.707205	-2.349192	0.000136
14	1	0	0.760043	-1.918751	0.000101

TS^{aldol}

Electronic energy = -1894.36086368 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.963012	-3.444697	-3.156993
2	6	0	-1.347620	-2.053821	-2.680449
3	6	0	-2.678307	-1.710972	-2.528708
4	8	0	-0.363156	-1.278166	-2.360069
5	29	0	-0.078491	-0.475475	-0.602216
6	8	0	-1.803544	-1.275248	0.305059
7	6	0	-2.650253	-2.087416	-0.141956
8	1	0	-2.360208	-3.133596	-0.327224
9	6	0	-4.111735	-1.861015	-0.010171
10	1	0	-1.829881	-4.051406	-3.436960
11	1	0	-0.294679	-3.365046	-4.022402
12	1	0	-0.401977	-3.966087	-2.369859
13	1	0	-3.465253	-2.361964	-2.894697
14	1	0	-2.944434	-0.680394	-2.318523
15	6	0	1.212358	0.644006	0.299172
16	7	0	2.436771	0.271985	0.778590
17	7	0	1.169527	1.990758	0.526769
18	6	0	3.138804	1.360170	1.288727
19	6	0	2.932191	-1.083939	0.748627
20	6	0	2.339216	2.444898	1.129631
21	6	0	0.042294	2.826313	0.186959
22	1	0	2.486230	3.482711	1.384701
23	1	0	4.125870	1.257591	1.711684
24	6	0	-0.040254	3.358015	-1.115742
25	6	0	-1.153449	4.153036	-1.417298
26	6	0	-2.136835	4.407919	-0.465606
27	6	0	-2.027619	3.869859	0.814025
28	6	0	-0.937784	3.066335	1.171090
29	6	0	1.016337	3.098086	-2.185376
30	1	0	-1.251984	4.573284	-2.414049
31	1	0	-2.993063	5.025972	-0.722806
32	1	0	-2.803587	4.071189	1.547172
33	6	0	-0.857529	2.476461	2.576095
34	6	0	3.639472	-1.521390	-0.389154
35	6	0	4.113403	-2.839347	-0.385828
36	6	0	3.886477	-3.684493	0.696810
37	6	0	3.176106	-3.227343	1.803645
38	6	0	2.683127	-1.917764	1.857407
39	6	0	3.893659	-0.628408	-1.599558
40	1	0	4.661657	-3.208518	-1.247796
41	1	0	4.260600	-4.704748	0.676196
42	1	0	2.996164	-3.898301	2.638677
43	6	0	1.889272	-1.454726	3.075266
44	1	0	0.081427	1.921087	2.658543
45	6	0	-0.829714	3.577911	3.653806
46	6	0	-1.999537	1.472351	2.829118
47	6	0	0.439585	2.297098	-3.370083
48	6	0	1.666934	4.412110	-2.662241
49	1	0	1.808530	2.488892	-1.740106
50	1	0	1.671074	-0.389470	2.954074
51	6	0	0.534729	-2.186489	3.166900
52	6	0	2.698561	-1.606218	4.377979
53	6	0	3.240032	-1.201498	-2.873517
54	1	0	3.428373	0.342972	-1.408401

55	6	0	5.401478	-0.380774	-1.804777
56	1	0	-1.902415	1.035082	3.830451
57	1	0	-2.979446	1.962481	2.776685
58	1	0	-1.983147	0.658568	2.096988
59	1	0	-0.715229	3.132092	4.648827
60	1	0	0.002105	4.274171	3.495452
61	1	0	-1.756588	4.163275	3.658977
62	1	0	1.221937	2.120389	-4.118328
63	1	0	0.053976	1.323837	-3.048915
64	1	0	-0.373429	2.843497	-3.863391
65	1	0	2.465259	4.199556	-3.382839
66	1	0	0.940344	5.066567	-3.157701
67	1	0	2.103413	4.971423	-1.826441
68	1	0	-0.030289	-1.828295	4.036140
69	1	0	-0.071987	-2.013179	2.271998
70	1	0	0.674643	-3.268137	3.283182
71	1	0	2.129573	-1.206497	5.225536
72	1	0	2.922553	-2.656450	4.598095
73	1	0	3.651401	-1.066885	4.323860
74	1	0	3.412440	-0.522463	-3.717688
75	1	0	3.673057	-2.173597	-3.139489
76	1	0	2.159100	-1.327536	-2.750518
77	1	0	5.562937	0.303903	-2.645703
78	1	0	5.861903	0.061095	-0.913184
79	1	0	5.935286	-1.311978	-2.028358
80	6	0	-5.002556	-2.929546	-0.192364
81	6	0	-6.373423	-2.746967	-0.021331
82	6	0	-6.871287	-1.490203	0.334162
83	6	0	-5.988933	-0.421189	0.521175
84	6	0	-4.618013	-0.604151	0.355412
85	1	0	-4.612451	-3.906280	-0.471761
86	1	0	-7.053897	-3.582528	-0.163880
87	1	0	-7.940220	-1.345167	0.467130
88	1	0	-6.373913	0.556520	0.800311
89	1	0	-3.923079	0.216062	0.504041

D

Electronic energy = -1894.37920902 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.805690	-0.298174	0.293198
2	6	0	-4.397807	-1.540633	-0.202471
3	6	0	-5.369185	-2.520507	-0.441786
4	6	0	-6.720606	-2.264440	-0.203820
5	6	0	-7.119862	-1.016790	0.281617
6	6	0	-6.156490	-0.036345	0.530646
7	6	0	-2.913547	-1.807531	-0.488883
8	8	0	-2.092353	-1.016694	0.253521
9	29	0	-0.400815	-0.315924	-0.040803
10	6	0	1.266766	0.560577	0.284518
11	7	0	2.456844	0.001603	0.654668
12	6	0	3.409116	0.975382	0.938879
13	6	0	2.808755	2.175733	0.737574
14	7	0	1.504233	1.904206	0.337773
15	6	0	2.693946	-1.421168	0.736300

16	6	0	3.355917	-2.053842	-0.335454
17	6	0	3.586849	-3.430892	-0.228617
18	6	0	3.169297	-4.146860	0.889877
19	6	0	2.511501	-3.496057	1.929707
20	6	0	2.259448	-2.119013	1.881890
21	6	0	0.517174	2.911071	0.023247
22	6	0	0.452625	3.402134	-1.296069
23	6	0	-0.511412	4.379293	-1.573379
24	6	0	-1.372799	4.843617	-0.583042
25	6	0	-1.288536	4.336040	0.710460
26	6	0	-0.343186	3.358761	1.045681
27	6	0	1.362573	2.896534	-2.411537
28	6	0	2.173117	4.041563	-3.049591
29	6	0	-0.290581	2.814152	2.469895
30	6	0	-1.585032	2.056832	2.829618
31	6	0	3.813059	-1.306447	-1.585378
32	6	0	5.348168	-1.332695	-1.724364
33	6	0	1.555192	-1.442329	3.054454
34	6	0	2.406706	-1.531722	4.337211
35	8	0	-0.369644	-1.272697	-2.388853
36	6	0	-1.325614	-2.046003	-2.456897
37	6	0	-2.707242	-1.622940	-2.061323
38	6	0	-1.124026	-3.495564	-2.857208
39	6	0	0.560504	2.116687	-3.473193
40	6	0	0.005963	3.930270	3.491160
41	6	0	3.126132	-1.849294	-2.853922
42	6	0	0.140886	-2.013104	3.282717
43	1	0	-2.745784	-2.890289	-0.291274
44	1	0	-1.563939	-4.162517	-2.104663
45	1	0	-1.641695	-3.699627	-3.803458
46	1	0	-0.060621	-3.716729	-2.970350
47	1	0	-3.463161	-2.210308	-2.594171
48	1	0	-2.848665	-0.559517	-2.276509
49	1	0	3.179033	3.184004	0.837105
50	1	0	4.410320	0.722645	1.250751
51	1	0	-0.591775	4.775487	-2.581495
52	1	0	-2.115576	5.600291	-0.821515
53	1	0	-1.970938	4.698553	1.473701
54	1	0	4.094104	-3.949146	-1.037360
55	1	0	3.355658	-5.215917	0.950654
56	1	0	2.187186	-4.064478	2.796517
57	1	0	0.531817	2.094950	2.529189
58	1	0	2.081779	2.197152	-1.974693
59	1	0	1.438855	-0.380985	2.816948
60	1	0	3.512726	-0.259157	-1.486367
61	1	0	-1.510699	1.644722	3.843311
62	1	0	-2.455624	2.723248	2.805737
63	1	0	-1.771936	1.228829	2.137615
64	1	0	0.094339	3.508359	4.499153
65	1	0	0.941699	4.451122	3.256994
66	1	0	-0.794824	4.678396	3.514958
67	1	0	1.231172	1.756809	-4.262994
68	1	0	0.059274	1.248086	-3.034576
69	1	0	-0.198577	2.753276	-3.943674
70	1	0	2.867137	3.642315	-3.798405
71	1	0	1.524075	4.765700	-3.555610
72	1	0	2.758597	4.586457	-2.299817
73	1	0	-0.338969	-1.495072	4.121905

74	1	0	-0.494797	-1.884819	2.399774
75	1	0	0.175132	-3.080811	3.530903
76	1	0	1.915011	-0.994781	5.156902
77	1	0	2.545024	-2.571100	4.657318
78	1	0	3.400790	-1.093222	4.190917
79	1	0	3.448598	-1.272408	-3.729518
80	1	0	3.390582	-2.898290	-3.035726
81	1	0	2.037129	-1.773080	-2.774263
82	1	0	5.661578	-0.749363	-2.598158
83	1	0	5.841029	-0.911511	-0.840171
84	1	0	5.721414	-2.355094	-1.856209
85	1	0	-5.063919	-3.499189	-0.810495
86	1	0	-7.460356	-3.039707	-0.390131
87	1	0	-8.171106	-0.814414	0.471681
88	1	0	-6.458673	0.934581	0.917315
89	1	0	-4.042820	0.445043	0.500827

CP4

Electronic energy = -2128.06808127 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.822603	0.456293	-2.387026
2	6	0	3.995660	0.124509	-1.303008
3	6	0	4.461189	0.380558	-0.009419
4	6	0	5.727553	0.934452	0.199778
5	6	0	6.546647	1.249061	-0.884902
6	6	0	6.085755	1.011232	-2.183147
7	6	0	2.607154	-0.478917	-1.531294
8	6	0	2.709929	-1.851723	-2.249060
9	6	0	1.323311	-2.350522	-2.645383
10	6	0	0.931069	-3.736732	-2.189338
11	8	0	1.887848	-0.623020	-0.338104
12	29	0	0.172883	0.036901	-0.128410
13	8	0	1.631587	-2.949827	1.054312
14	6	0	2.632308	-3.263302	2.026892
15	6	0	2.196616	-4.590707	2.658277
16	6	0	-1.568615	0.758156	0.190587
17	7	0	-2.790627	0.151187	0.140266
18	6	0	-3.806809	1.036963	0.479132
19	6	0	-3.215565	2.229859	0.742290
20	7	0	-1.850942	2.042324	0.561255
21	6	0	-3.027846	-1.234586	-0.206790
22	6	0	-2.973826	-2.203368	0.815117
23	6	0	-3.267315	-3.526566	0.462428
24	6	0	-3.597870	-3.866380	-0.845888
25	6	0	-3.635864	-2.887916	-1.835862
26	6	0	-3.349857	-1.548833	-1.543490
27	6	0	-2.645975	-1.858473	2.264713
28	6	0	-1.539628	-2.760264	2.843325
29	6	0	-3.425277	-0.491222	-2.641413
30	6	0	-4.889517	-0.080519	-2.905885
31	6	0	-0.857202	3.076693	0.741787
32	6	0	-0.290484	3.252796	2.019745
33	6	0	0.677911	4.254153	2.161966
34	6	0	1.059217	5.046007	1.082297

35	6	0	0.474674	4.854578	-0.166491
36	6	0	-0.498349	3.867722	-0.367703
37	6	0	-0.671812	2.388859	3.217922
38	6	0	-1.166400	3.238334	4.404660
39	6	0	-1.103967	3.669744	-1.753900
40	6	0	-1.761853	4.959325	-2.281843
41	6	0	0.496648	1.473485	3.633366
42	6	0	-0.053453	3.131463	-2.745316
43	6	0	4.003974	-3.425154	1.347774
44	6	0	2.689128	-2.154081	3.092310
45	6	0	-2.741304	-0.937816	-3.946984
46	6	0	-3.916540	-1.907265	3.138276
47	8	0	0.574221	-1.639323	-3.298879
48	1	0	2.081310	0.183425	-2.238966
49	1	0	1.640255	-4.475911	-2.586526
50	1	0	1.003022	-3.784101	-1.094286
51	1	0	-0.081414	-3.979004	-2.521100
52	1	0	3.302650	-1.756279	-3.168597
53	1	0	3.216144	-2.569575	-1.595858
54	1	0	-4.841585	0.734624	0.500899
55	1	0	-3.627767	3.182137	1.036725
56	1	0	-3.886833	-3.167799	-2.853992
57	1	0	-3.822574	-4.899648	-1.096965
58	1	0	-3.233396	-4.299419	1.224202
59	1	0	0.783974	5.476162	-1.001749
60	1	0	1.816390	5.814180	1.214116
61	1	0	1.143489	4.411072	3.130563
62	1	0	-2.267077	-0.832220	2.292388
63	1	0	-2.889774	0.396001	-2.287600
64	1	0	-1.501186	1.739460	2.920843
65	1	0	-1.892803	2.915077	-1.677542
66	1	0	-1.272575	-2.415897	3.850099
67	1	0	-1.873291	-3.800852	2.935743
68	1	0	-0.638134	-2.746695	2.221840
69	1	0	-3.681563	-1.628075	4.172291
70	1	0	-4.688107	-1.221734	2.768528
71	1	0	-4.346481	-2.915879	3.152365
72	1	0	-2.711521	-0.097217	-4.650566
73	1	0	-1.716194	-1.276540	-3.770920
74	1	0	-3.295233	-1.746827	-4.438814
75	1	0	-4.934880	0.698532	-3.676116
76	1	0	-5.476928	-0.936668	-3.258801
77	1	0	-5.375879	0.307961	-2.003754
78	1	0	0.196361	0.824576	4.464764
79	1	0	0.813954	0.837481	2.800391
80	1	0	1.364346	2.058443	3.960339
81	1	0	-1.495192	2.588451	5.223864
82	1	0	-0.375801	3.888287	4.796899
83	1	0	-2.010028	3.876235	4.117069
84	1	0	-0.509952	2.953325	-3.725966
85	1	0	0.769413	3.843059	-2.880128
86	1	0	0.373023	2.186569	-2.392395
87	1	0	-2.241648	4.769600	-3.248975
88	1	0	-2.526124	5.332085	-1.590197
89	1	0	-1.027135	5.759067	-2.429919
90	1	0	1.858776	-2.102538	0.584119
91	1	0	3.437411	-2.372937	3.864327
92	1	0	2.948205	-1.194340	2.630686

93	1	0	1.713108	-2.045040	3.578058
94	1	0	2.912411	-4.919413	3.420656
95	1	0	1.212739	-4.486649	3.128564
96	1	0	2.125626	-5.368785	1.890235
97	1	0	4.776273	-3.714860	2.071311
98	1	0	3.952097	-4.200083	0.574401
99	1	0	4.320184	-2.488421	0.875512
100	1	0	3.805167	0.150937	0.822592
101	1	0	6.072139	1.123053	1.214129
102	1	0	7.531520	1.680350	-0.723796
103	1	0	6.710349	1.261183	-3.037656
104	1	0	4.472759	0.285331	-3.403706

TS^{protonation}

Electronic energy = -2128.04976822 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.088866	-2.476374	0.528848
2	6	0	-2.404083	-2.128834	-0.651857
3	6	0	-1.813938	-3.087903	-1.498030
4	6	0	-1.936350	-4.433573	-1.133464
5	6	0	-2.605788	-4.806950	0.028166
6	6	0	-3.170723	-3.836703	0.850704
7	7	0	-2.353254	-0.738687	-1.044454
8	6	0	-1.453573	0.193442	-0.600094
9	7	0	-1.828410	1.337149	-1.256831
10	6	0	-2.921956	1.117278	-2.087625
11	6	0	-3.254990	-0.188871	-1.950466
12	6	0	-1.196575	2.627467	-1.105427
13	6	0	-1.789779	3.567172	-0.235514
14	6	0	-1.178585	4.821927	-0.125300
15	6	0	-0.028732	5.127816	-0.848557
16	6	0	0.528374	4.184676	-1.706649
17	6	0	-0.041659	2.914171	-1.860945
18	6	0	-3.074308	3.277783	0.538009
19	6	0	-2.954860	3.614596	2.035826
20	6	0	0.561598	1.929629	-2.858179
21	6	0	2.071278	1.722023	-2.638982
22	29	0	0.053290	-0.000265	0.591357
23	8	0	1.051141	0.086183	2.424739
24	6	0	1.109110	1.130618	3.395558
25	6	0	2.328623	0.880821	4.302186
26	6	0	-1.060117	-2.711787	-2.769452
27	6	0	0.385429	-3.244321	-2.747474
28	6	0	-3.741644	-1.443976	1.442279
29	6	0	-5.269082	-1.639869	1.512693
30	8	0	2.291682	0.089883	0.420571
31	6	0	3.067179	-1.019131	0.067959
32	1	0	2.640081	-1.499246	-0.828507
33	8	0	0.786867	-2.645759	0.679161
34	6	0	1.706482	-2.688555	1.484166
35	6	0	1.531035	-3.344875	2.837815
36	6	0	4.511635	-0.637184	-0.269724
37	6	0	3.072440	-2.089664	1.186501
38	6	0	-1.811444	-3.184251	-4.029818

39	6	0	-3.111094	-1.455904	2.847758
40	6	0	0.258583	2.376898	-4.303456
41	6	0	-4.270954	4.022211	-0.090476
42	6	0	1.243102	2.497222	2.699870
43	6	0	-0.181792	1.072836	4.222552
44	1	0	2.425544	-3.897612	3.146678
45	1	0	1.366628	-2.538853	3.564001
46	1	0	0.658123	-4.001971	2.831006
47	1	0	3.732756	-2.927092	0.912250
48	1	0	3.493914	-1.669642	2.108962
49	1	0	-4.036547	-0.778333	-2.403094
50	1	0	-3.350246	1.904037	-2.688051
51	1	0	-1.492452	-5.198074	-1.764593
52	1	0	-2.686128	-5.857748	0.294325
53	1	0	-3.689930	-4.138453	1.756060
54	1	0	1.420793	4.437275	-2.271038
55	1	0	0.431951	6.106806	-0.745767
56	1	0	-1.608723	5.569161	0.534961
57	1	0	-3.560362	-0.451637	1.018942
58	1	0	-0.996437	-1.620413	-2.814820
59	1	0	-3.280794	2.205395	0.466466
60	1	0	0.082279	0.957936	-2.707846
61	1	0	-3.563799	-0.676900	3.473104
62	1	0	-3.266927	-2.417737	3.350958
63	1	0	-2.033833	-1.269955	2.795242
64	1	0	-5.725412	-0.858833	2.132515
65	1	0	-5.724950	-1.593081	0.516919
66	1	0	-5.531281	-2.608832	1.953556
67	1	0	0.939276	-2.866637	-3.615463
68	1	0	0.895921	-2.926702	-1.834095
69	1	0	0.412783	-4.339939	-2.790113
70	1	0	-1.269434	-2.882815	-4.934005
71	1	0	-1.910909	-4.276077	-4.047997
72	1	0	-2.820367	-2.758338	-4.081941
73	1	0	-3.869644	3.315202	2.560797
74	1	0	-2.110878	3.092103	2.496288
75	1	0	-2.818798	4.689008	2.204360
76	1	0	-5.196947	3.784532	0.446603
77	1	0	-4.125832	5.108174	-0.047696
78	1	0	-4.410016	3.747505	-1.142168
79	1	0	2.445163	0.965197	-3.339225
80	1	0	2.640566	2.641272	-2.822551
81	1	0	2.276511	1.378304	-1.620328
82	1	0	0.658245	1.648754	-5.019138
83	1	0	-0.819541	2.470978	-4.480540
84	1	0	0.718376	3.348252	-4.521925
85	1	0	1.886308	0.130693	1.608755
86	1	0	1.315806	3.315349	3.427440
87	1	0	2.137627	2.517254	2.067379
88	1	0	0.376940	2.685567	2.055364
89	1	0	-0.201560	1.853770	4.992784
90	1	0	-1.053240	1.205326	3.571455
91	1	0	-0.275120	0.098590	4.715875
92	1	0	2.412992	1.643717	5.086138
93	1	0	2.247819	-0.099589	4.785537
94	1	0	3.253458	0.896244	3.713513
95	6	0	5.049553	0.583376	0.150072
96	6	0	6.376297	0.914717	-0.136229

97	6	0	7.185222	0.030734	-0.852372
98	6	0	6.654775	-1.187519	-1.285521
99	6	0	5.329562	-1.514004	-0.996449
100	1	0	4.405378	1.272782	0.685726
101	1	0	6.777609	1.869211	0.197043
102	1	0	8.216625	0.289913	-1.078158
103	1	0	7.271568	-1.879695	-1.854081
104	1	0	4.921459	-2.461115	-1.347403

CP5

Electronic energy = -2128.06497218 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.812439	-1.105028	-1.062517
2	6	0	5.158287	-0.203574	-0.211638
3	6	0	5.878511	0.880771	0.300369
4	6	0	7.226423	1.053158	-0.023082
5	6	0	7.872974	0.145070	-0.863595
6	6	0	7.159265	-0.937049	-1.385018
7	6	0	3.699041	-0.426473	0.159992
8	6	0	3.574411	-1.509149	1.253515
9	6	0	2.181989	-2.118179	1.377855
10	6	0	1.821249	-2.733189	2.711910
11	8	0	3.126381	0.795796	0.573265
12	29	0	-0.335342	0.153126	0.822357
13	8	0	0.980584	0.415024	2.121353
14	6	0	0.952474	1.419721	3.121096
15	6	0	-0.273133	1.218120	4.031853
16	6	0	-1.674987	0.011793	-0.543660
17	7	0	-2.395137	-1.063212	-0.985279
18	6	0	-3.284959	-0.698653	-1.989797
19	6	0	-3.118857	0.631848	-2.194398
20	7	0	-2.137235	1.050178	-1.304333
21	6	0	-2.259421	-2.419062	-0.501123
22	6	0	-2.907192	-2.780118	0.696763
23	6	0	-2.775340	-4.106805	1.126098
24	6	0	-2.043054	-5.033213	0.389522
25	6	0	-1.423795	-4.649668	-0.796600
26	6	0	-1.511981	-3.335186	-1.269375
27	6	0	-3.753993	-1.806627	1.511368
28	6	0	-3.215361	-1.641057	2.945001
29	6	0	-0.838736	-2.955807	-2.586054
30	6	0	-1.596105	-3.566442	-3.783671
31	6	0	-1.674751	2.416825	-1.204309
32	6	0	-2.428522	3.325771	-0.434029
33	6	0	-1.982062	4.651939	-0.381053
34	6	0	-0.834633	5.051572	-1.060287
35	6	0	-0.109680	4.130936	-1.811813
36	6	0	-0.510037	2.792179	-1.905421
37	6	0	-3.699789	2.922721	0.308806
38	6	0	-4.948497	3.533365	-0.359842
39	6	0	0.272025	1.820464	-2.784873
40	6	0	-0.066511	2.057310	-4.272154
41	6	0	-3.643691	3.292057	1.803280
42	6	0	1.792299	1.882806	-2.548557

43	6	0	2.241218	1.288309	3.958537
44	6	0	0.902286	2.822006	2.480703
45	6	0	0.650561	-3.346970	-2.620032
46	6	0	-5.236357	-2.231540	1.518374
47	8	0	1.399355	-2.135228	0.439018
48	1	0	3.175944	-0.813327	-0.729623
49	1	0	2.683750	-3.199229	3.201308
50	1	0	1.468429	-1.909230	3.343498
51	1	0	1.011892	-3.457164	2.588227
52	1	0	4.251055	-2.348292	1.029786
53	1	0	3.899459	-1.103170	2.218774
54	1	0	-3.941658	-1.414828	-2.457503
55	1	0	-3.598690	1.313732	-2.878421
56	1	0	-0.855392	-5.380973	-1.363250
57	1	0	-1.957098	-6.058601	0.739507
58	1	0	-3.259852	-4.417822	2.047248
59	1	0	0.783793	4.455344	-2.335791
60	1	0	-0.502989	6.084863	-1.003002
61	1	0	-2.539032	5.379302	0.202333
62	1	0	-3.699463	-0.823961	1.034188
63	1	0	-0.883003	-1.867217	-2.688647
64	1	0	-3.797161	1.834204	0.251856
65	1	0	-0.047072	0.804836	-2.533020
66	1	0	-3.818627	-0.908012	3.493778
67	1	0	-3.252381	-2.584661	3.501822
68	1	0	-2.178193	-1.290685	2.936983
69	1	0	-5.840547	-1.498860	2.066442
70	1	0	-5.635412	-2.308098	0.500380
71	1	0	-5.373001	-3.205262	2.003193
72	1	0	1.105940	-2.988011	-3.550986
73	1	0	1.185823	-2.909356	-1.773708
74	1	0	0.784947	-4.434858	-2.590342
75	1	0	-1.131680	-3.258210	-4.727771
76	1	0	-1.579298	-4.662107	-3.743674
77	1	0	-2.646366	-3.252684	-3.804863
78	1	0	-4.540520	2.924250	2.315698
79	1	0	-2.767383	2.851209	2.289005
80	1	0	-3.600858	4.376732	1.953511
81	1	0	-5.859088	3.205913	0.155736
82	1	0	-4.919685	4.628860	-0.326794
83	1	0	-5.028578	3.235365	-1.411561
84	1	0	2.287819	1.120468	-3.161549
85	1	0	2.211998	2.852215	-2.842768
86	1	0	2.057111	1.697674	-1.502169
87	1	0	0.464187	1.335433	-4.904024
88	1	0	-1.140735	1.951977	-4.465180
89	1	0	0.231687	3.064104	-4.588729
90	1	0	2.314953	0.625212	1.137827
91	1	0	0.902428	3.618113	3.237112
92	1	0	1.767856	2.968458	1.825377
93	1	0	-0.003390	2.929394	1.871094
94	1	0	-0.311487	1.958953	4.841244
95	1	0	-1.197935	1.302650	3.446688
96	1	0	-0.250434	0.217988	4.481131
97	1	0	2.297900	2.054231	4.742140
98	1	0	2.283715	0.304358	4.441270
99	1	0	3.117970	1.390021	3.310399
100	1	0	5.363285	1.589699	0.939045

101	1	0	7.772416	1.902486	0.380963
102	1	0	8.921416	0.281796	-1.116459
103	1	0	7.649323	-1.645037	-2.049154
104	1	0	5.258826	-1.944045	-1.481571

PD

Electronic energy = -538.716767448 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.989863	-1.188075	-0.155111
2	6	0	1.629097	-1.115435	0.144811
3	6	0	0.984788	0.126506	0.224443
4	6	0	1.728179	1.291775	0.002326
5	6	0	3.088355	1.220694	-0.303502
6	6	0	3.722784	-0.020722	-0.382575
7	6	0	-0.503859	0.202180	0.524424
8	6	0	-1.353186	-0.012132	-0.736839
9	6	0	-2.867388	-0.027624	-0.509413
10	6	0	-3.455939	0.987783	0.454104
11	8	0	-0.921776	-0.800032	1.452487
12	8	0	-3.568825	-0.816174	-1.112177
13	1	0	-0.722036	1.203182	0.931159
14	1	0	-3.145235	0.737577	1.475308
15	1	0	-3.095674	2.001600	0.238296
16	1	0	-4.545495	0.960663	0.389217
17	1	0	-1.126680	0.795176	-1.448090
18	1	0	-1.083374	-0.956990	-1.217659
19	1	0	1.240300	2.262171	0.073227
20	1	0	3.653213	2.133891	-0.471439
21	1	0	4.782658	-0.077905	-0.615455
22	1	0	3.478690	-2.157183	-0.211772
23	1	0	1.056431	-2.020112	0.328207
24	1	0	-0.344153	-0.742121	2.230512
