Supplementary Materials: Oxidative Radical Cyclization-Cyclization Reaction Leading to 1*H*-benzo[*f*]isoindole Derivatives

Eito Yoshioka and Hideto Miyabe

1. Calculation Study

Calculation studies were performed on Density Functional B3LYP 6-311 + G** by using Spartan'14 (WAVEFUNCTION, INC, Irvine, CA, USA).

Table S1. Gibbs free energy, enthalpy, and entropy at 298.15 K.

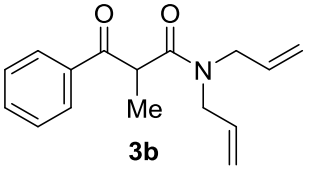
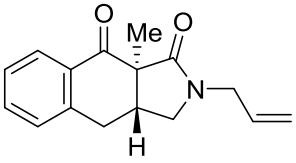
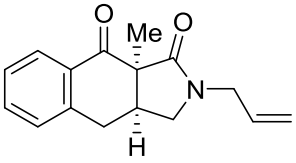
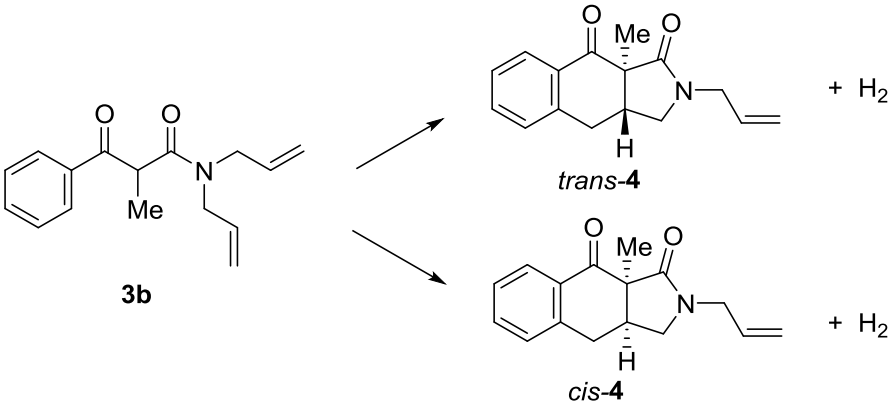
Structure	G (kJ/mol)	H (kJ/mol)	S (kJ/mol·K)
 **3b**	−2169377.66	−2169196.34	608.16
 *trans*-**4**	−2166314.41	−2166151.45	546.56
 *cis*-**4**	−2166337.05	−2166172.33	552.46
H_2	−3100.70741	−3061.86143	130.29

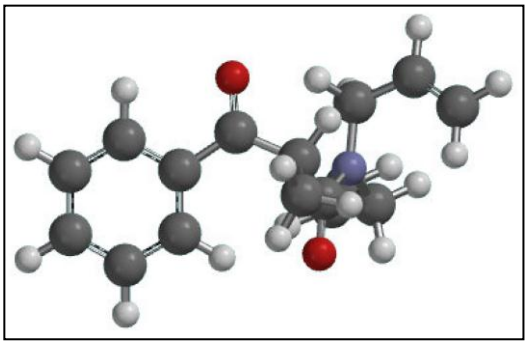
Table S2. Change in Gibbs free energy, enthalpy, and entropy.



Change	**(*trans*-4 + H_2) – 3b**	**(*cis*-4 + H_2) – 3b**
ΔG (kJ/mol)	−37.46	−60.10
ΔH (kJ/mol)	−16.97	−37.85
ΔS (kJ/mol·K)	68.69	74.59

Coordinates of All Stationary Points

(1) Coordinates of 3b (Angstroms)

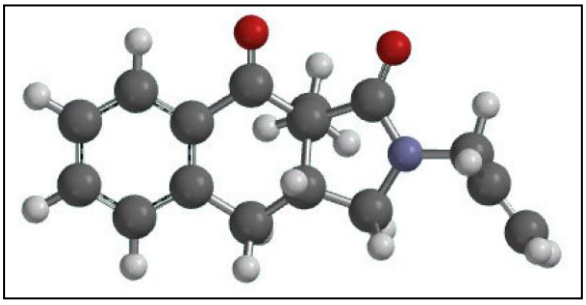


ATOM	X	Y	Z
1 H	-1.2646558040	1.6356614303	1.3559097959
2 C	-0.8020116420	2.5211260567	0.9397501531
3 C	0.3482697654	4.8139480586	-0.1681960521
4 C	0.4706209251	2.4486168004	0.3551764100
5 C	-1.4941169350	3.7307303497	0.9557172657
6 C	-0.9213389801	4.8772041499	0.4100076776
7 C	1.0347933216	3.6079825070	-0.2021090228
8 H	-2.4831657247	3.7750374682	1.3975809015
9 H	-1.4610260968	5.8176016274	0.4326602714
10 H	2.0144068234	3.5391214373	-0.6585366249
11 H	0.7974104940	5.7044522356	-0.5934764719
12 C	1.2666932382	1.1841894992	0.2554900913
13 C	0.9683968236	-0.0488054846	1.1410507481
14 C	-0.3227347042	-0.7901454590	0.7242249101
15 N	-0.2392115084	-1.6611464021	-0.3274857857
16 C	-1.4494905710	-2.4081996198	-0.7174740277
17 H	-2.1193358541	-2.4051980586	0.1431810652
18 H	-1.1616827142	-3.4410593269	-0.9310459928
19 C	0.9643210328	-1.9256674551	-1.1170901038
20 H	0.6409495082	-2.0971367616	-2.1501816778
21 H	1.5962824852	-1.0369151606	-1.1609365010
22 C	-2.1348881561	-1.7953164624	-1.9091039657
23 H	-2.4682204482	-0.7679673770	-1.7822183380
24 C	-2.3469776607	-2.4279170688	-3.0607322695
25 H	-2.8584859305	-1.9487454836	-3.8879681719
26 H	-2.0258170392	-3.4545158948	-3.2127331962
27 C	1.7853316711	-3.1038129807	-0.6534463707
28 H	2.6274384373	-3.3391987901	-1.3018261682
29 C	1.5767535018	-3.8330963676	0.4388964667
30 H	2.2301278929	-4.6588017055	0.6950099583
31 H	0.7497670287	-3.6346995409	1.1129350231
32 O	-1.3741339055	-0.6096136262	1.3298224903
33 O	2.2106442248	1.1195824040	-0.5150095680
34 H	1.8170302750	-0.7056309657	0.9503671725
35 C	0.9529741256	0.2775165081	2.6436306387
36 H	0.9560589485	-0.6508482225	3.2194578437
37 H	0.0724686615	0.8457257716	2.9353268349
38 H	1.8465544901	0.8459419102	2.9133745905

Point Group: c1 Number of degrees of freedom: 108

Energy is -826.535677253

(2) Coordinates of *trans*-4 (Angstroms)

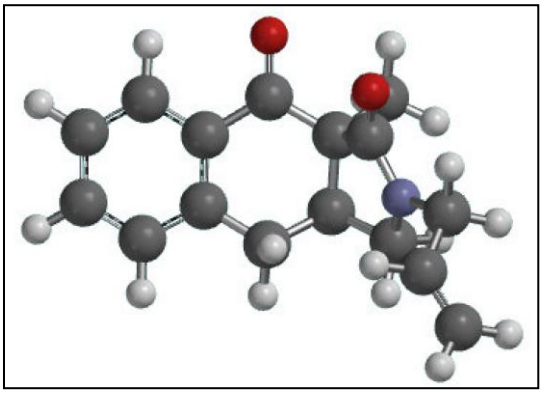


ATOM	X	Y	Z
1 H	-0.8824200811	2.4672710192	-3.5500661472
2 C	-1.5747875847	2.3230850727	-2.7292822539
3 C	-3.2931463973	1.9075394458	-0.5874992310
4 C	-1.2082111353	1.4311027915	-1.7112385234
5 C	-2.7882438496	2.9939423546	-2.6846146451
6 C	-3.6510663250	2.7832248095	-1.6071383777
7 C	-2.0779484958	1.2160265332	-0.6205001700
8 H	-3.0633523920	3.6778405414	-3.4793227191
9 H	-4.5990663246	3.3076850269	-1.5587368513
10 H	-3.9622868198	1.7621884694	0.2546862565
11 C	0.1202802325	0.7221832849	-1.8515738220
12 C	0.3055132742	-0.4297884898	-0.8654531802
13 C	1.7298454577	-0.9085141959	-0.5201392522
14 N	1.7377873597	-1.1536044744	0.8394121543
15 C	0.4555517638	-0.9061151830	1.4963541358
16 C	-0.2075408199	0.0544901175	0.5090202708
17 H	0.6014429549	-0.4611080354	2.4837669937
18 H	-0.1109190713	-1.8403777876	1.6268701622
19 H	0.2656737854	1.0310844533	0.6781427151
20 C	-1.7089730683	0.2776585168	0.5166144991
21 H	-2.2464777951	-0.6721491384	0.4061284221
22 H	-2.0389012729	0.7091586540	1.4672237944
23 C	-0.4343305600	-1.6656848344	-1.4456846736
24 H	0.0927389929	-1.9980640940	-2.3417110354
25 H	-1.4656870228	-1.4346749933	-1.7201052396
26 H	-0.4455513004	-2.4941187861	-0.7326700928
27 O	2.6500257346	-1.1320234060	-1.2775499185
28 O	0.9210566201	1.0345262912	-2.7029284475
29 C	2.8322148819	-1.8565947484	1.4960145542
30 H	3.5685431651	-2.0573845791	0.7127844966
31 H	2.4758435882	-2.8204403842	1.8822261960
32 C	3.4548248041	-1.0537062280	2.6067334958
33 H	3.8644583310	-0.0889233898	2.3151812746
34 C	3.5351128289	-1.4571760150	3.8722969468
35 H	4.0139102232	-0.8525656709	4.6341844699
36 H	3.1340863172	-2.4159929483	4.1885737427

Point Group: c1 Number of degrees of freedom: 102

Energy is -825.355043536

(3) Coordinates of *cis*-4 (Angstroms)



ATOM	X	Y	Z
1 H	-0.7519288141	3.0558244154	-3.1447452655
2 C	-1.1456453246	3.0085477489	-2.1365814294
3 C	-2.1313858829	2.8100182868	0.4563917627
4 C	-0.8859140999	1.8579941807	-1.3772235910
5 C	-1.8906691795	4.0501666907	-1.6043703378
6 C	-2.3888404149	3.9471079119	-0.3030136586

7 C	-1.3746265932	1.7566331763	-0.0655863167
8 H	-2.0889683123	4.9367976383	-2.1958050513
9 H	-2.9791549159	4.7537688323	0.1178039684
10 H	-2.5171014046	2.7381447014	1.4683920486
11 C	-0.1162880410	0.7489523959	-2.0123412694
12 C	-0.0164406953	-0.6003031324	-1.2837197783
13 C	1.4085464750	-0.8555698126	-0.7121635049
14 N	1.2480237753	-1.5385243366	0.4669658291
15 C	-0.1438415540	-1.8024966072	0.8090606559
16 C	-0.9046590867	-0.7514458605	-0.0253524174
17 H	-0.3098984869	-1.6765333482	1.8826446472
18 H	-0.4273626586	-2.8300310699	0.5447970482
19 H	-1.9011828681	-1.1085334970	-0.2982035839
20 C	-1.0292772137	0.5560199484	0.7759314953
21 H	-1.7729178302	0.4294797922	1.5682167155
22 H	-0.0742925098	0.7512739331	1.2817685854
23 O	0.3810949508	0.8807284336	-3.1124806762
24 O	2.4689222631	-0.5610429302	-1.2216305308
25 C	2.3689875554	-2.1371812093	1.1815410828
26 H	3.2552025383	-1.9285165884	0.5751514087
27 H	2.2389430895	-3.2255483014	1.2289783558
28 C	2.5437403265	-1.5725455291	2.5659038440
29 H	2.7056594582	-0.4976486810	2.6150739996
30 C	2.5287103859	-2.2943532640	3.6834841936
31 H	2.6852185547	-1.8410526772	4.6557932895
32 H	2.3721810656	-3.3692057490	3.6645322433
33 C	-0.2868812277	-1.7194828736	-2.3186187899
34 H	0.4151858660	-1.6306403877	-3.1464986179
35 H	-1.3028333238	-1.6299295604	-2.7133115837
36 H	-0.1803058668	-2.7108726702	-1.8707847708

Point Group: c1 Number of degrees of freedom: 102

Energy is -825.363056225

2. HMQC, HMBC and NOESY Experiments

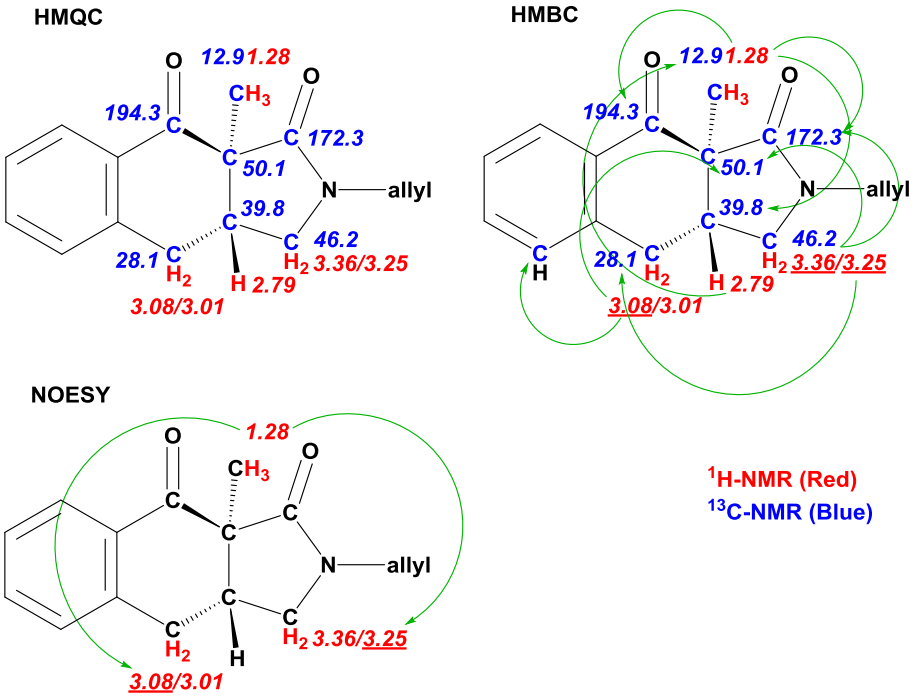


Figure S1. HMQC, HMBC and NOESY of *trans*-**4.**

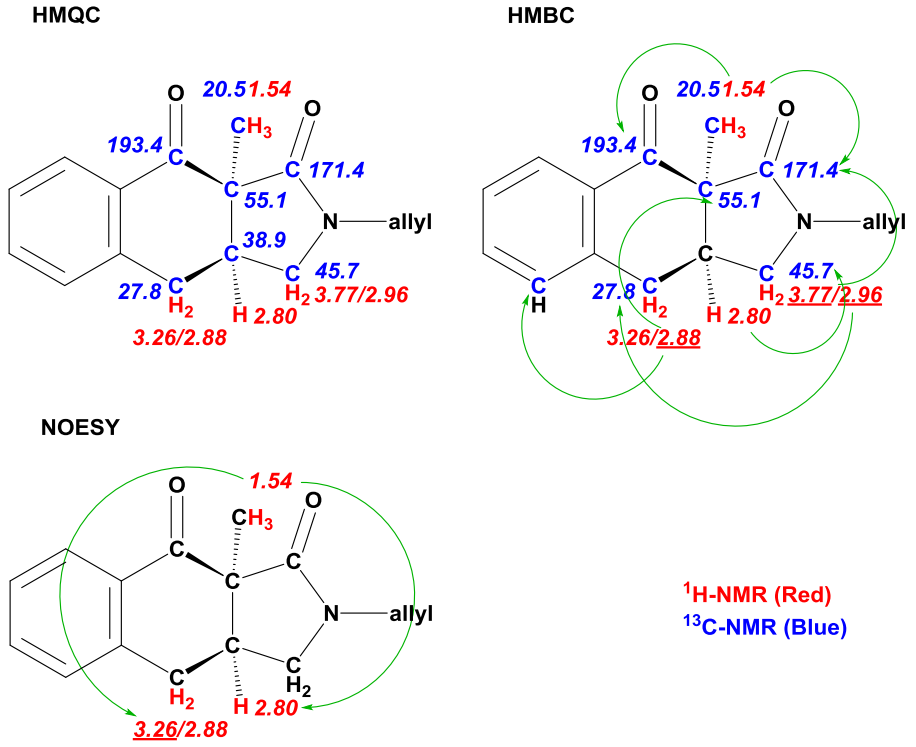


Figure S2. HMQC, HMBC and NOESY of *cis*-**4.**

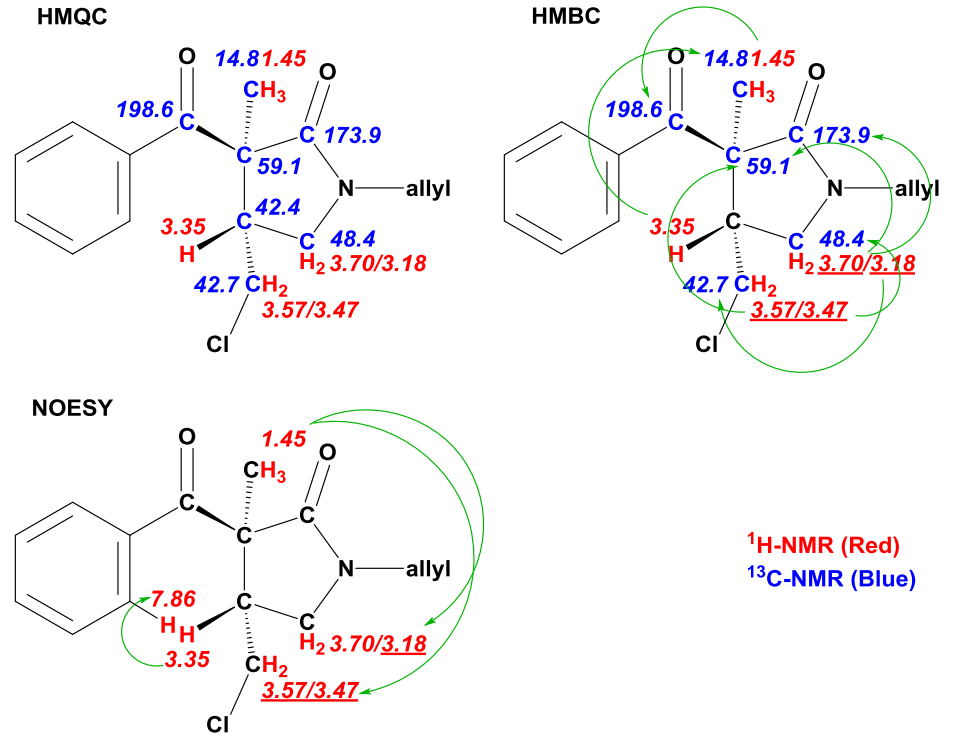


Figure S3. HMQC, HMBC and NOESY of *trans*-**5.**

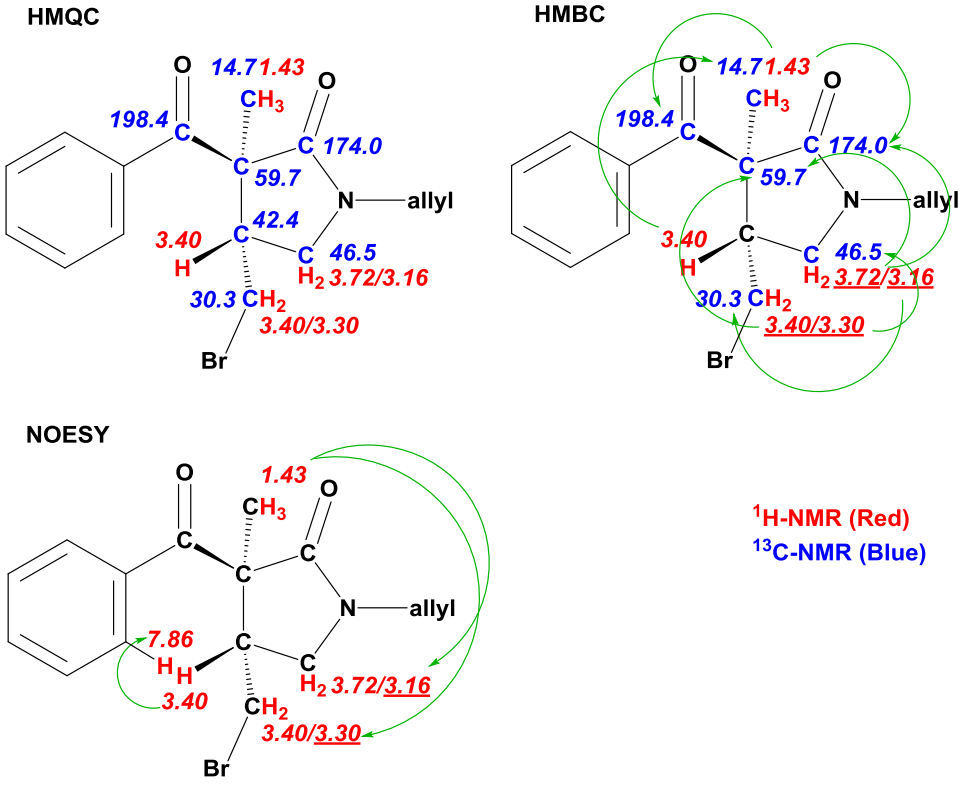


Figure S4. HMQC, HMBC and NOESY of *trans*-**6.**

3. ^{1}H and ^{13}C-NMR Spectra

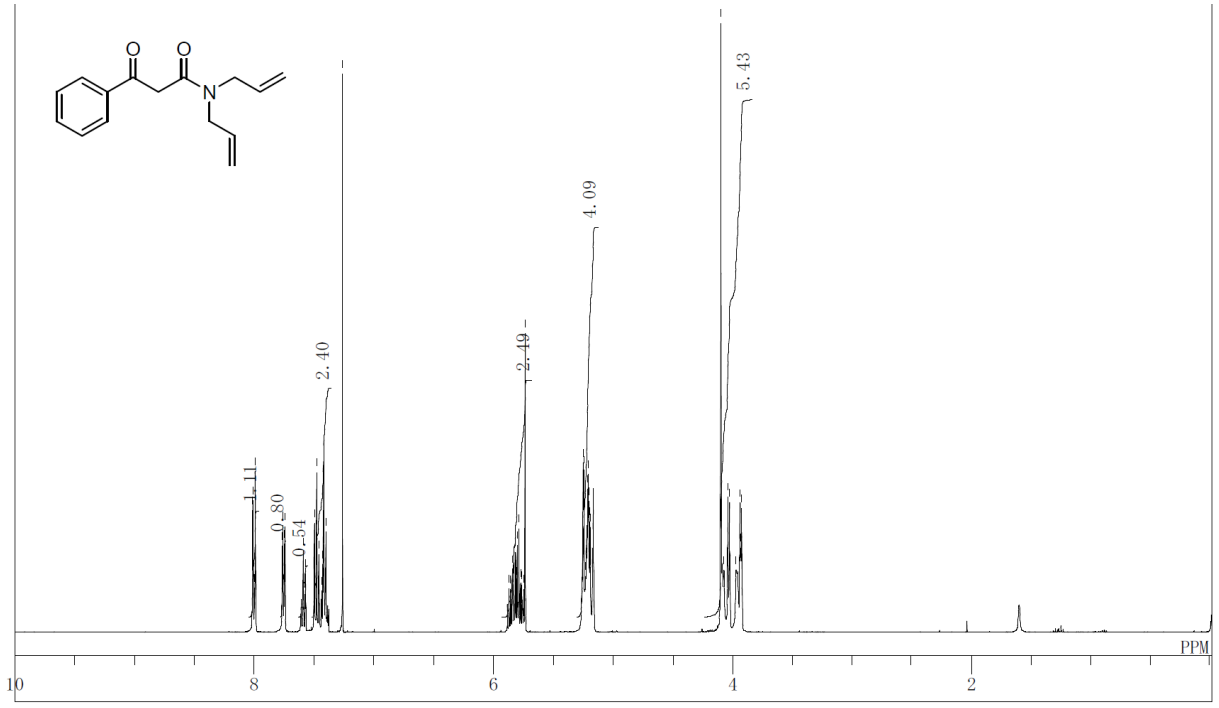


Figure S5. ^{1}H-NMR ($CDCl_3$) of **3a.**

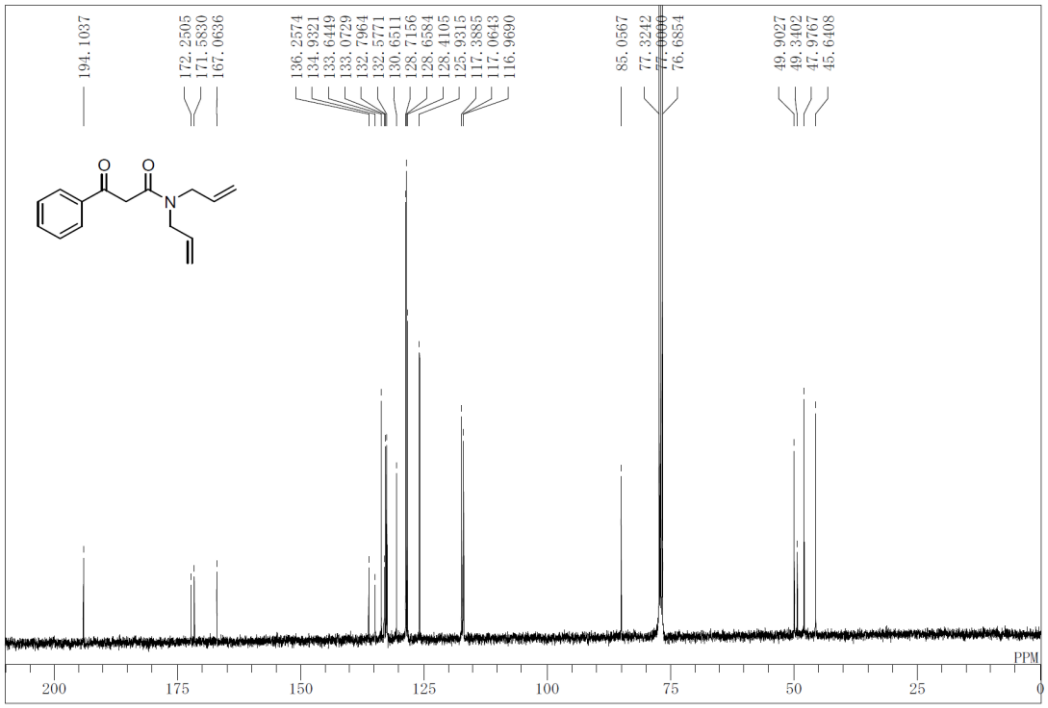


Figure S6. ^{13}C-NMR ($CDCl_3$) of **3a.**

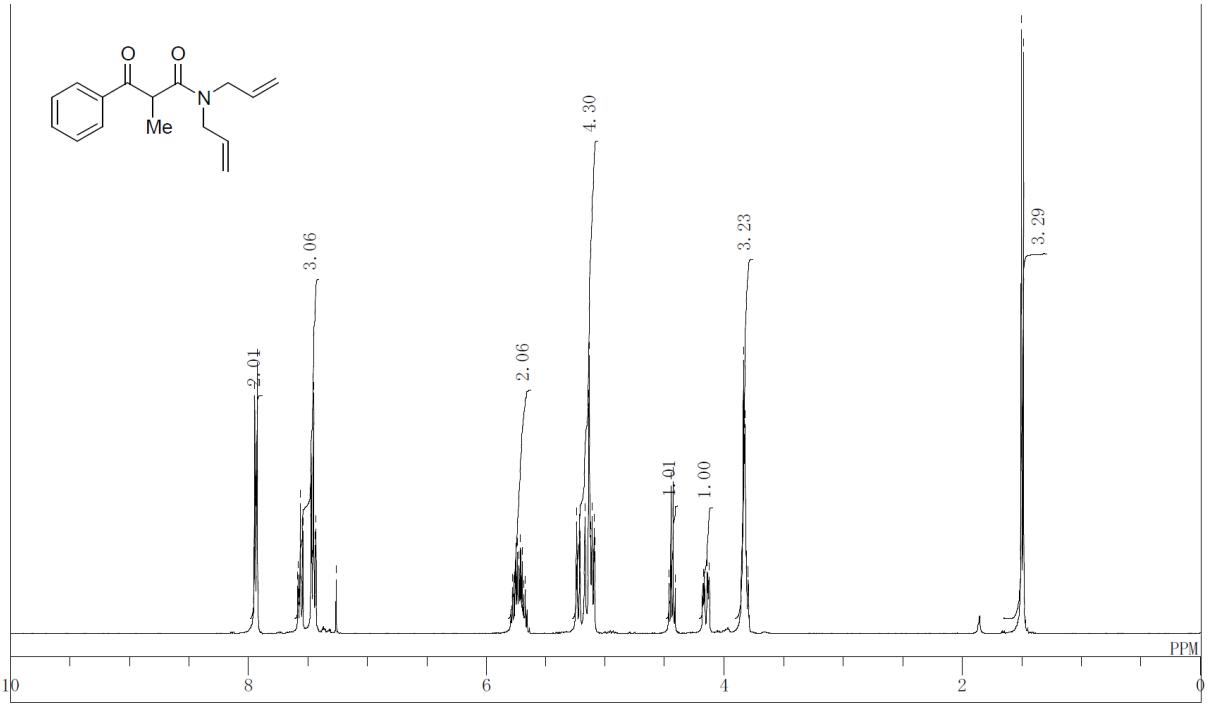


Figure S7. ^{1}H-NMR ($CDCl_3$) of **3b.**

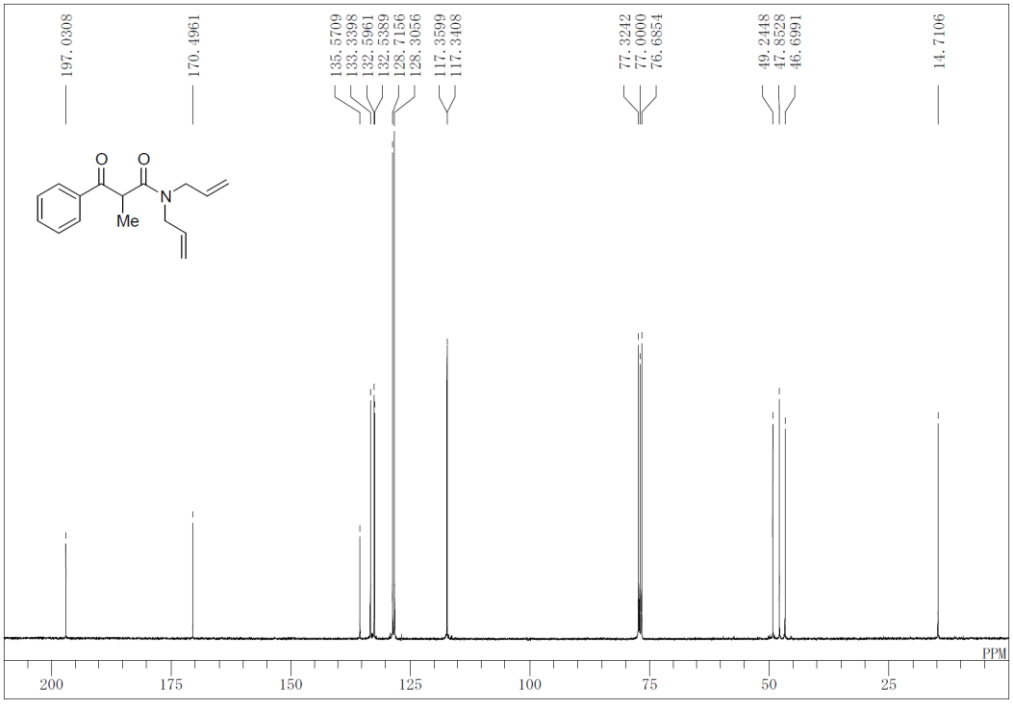


Figure S8. ^{13}C-NMR ($CDCl_3$) of **3b.**

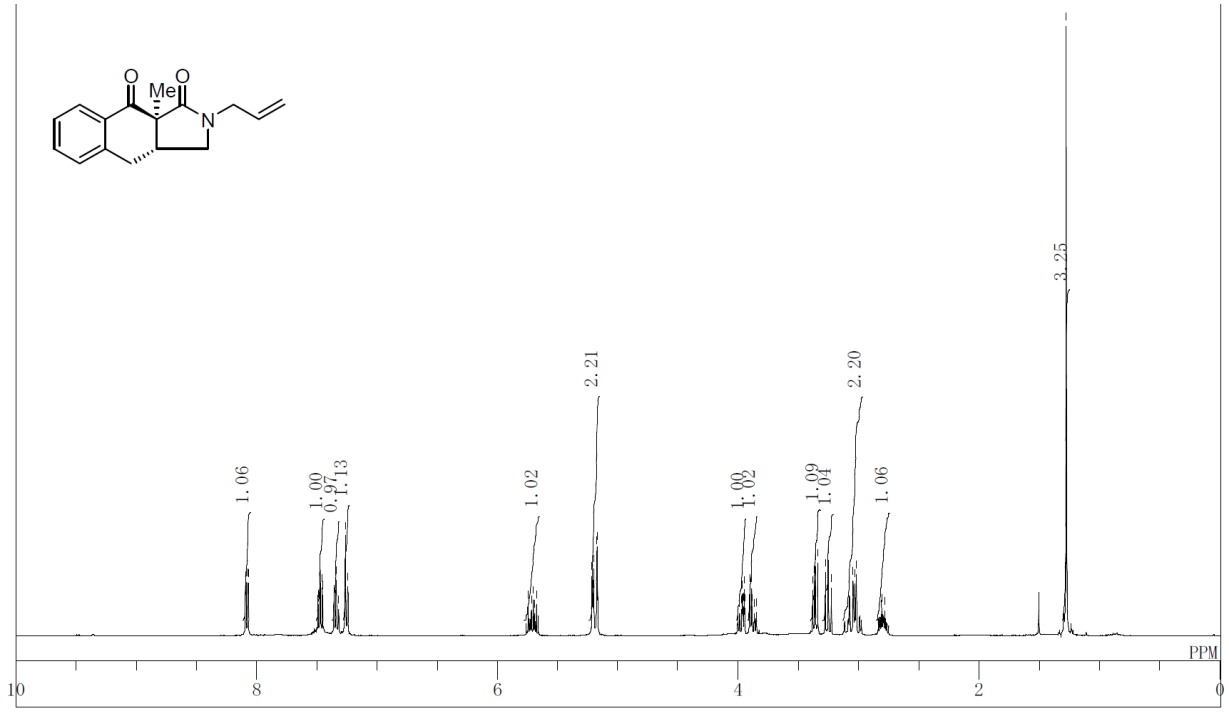


Figure S9. ^{1}H-NMR ($CDCl_3$) of ***trans*-4.**

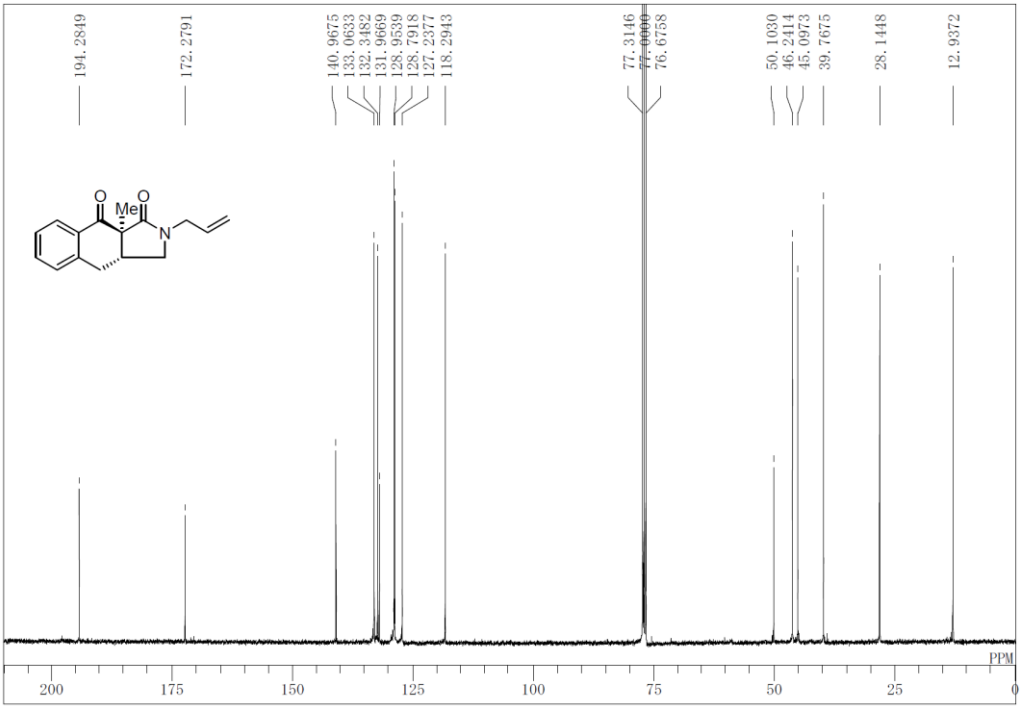


Figure S10. ^{13}C-NMR ($CDCl_3$) of ***trans*-4.**

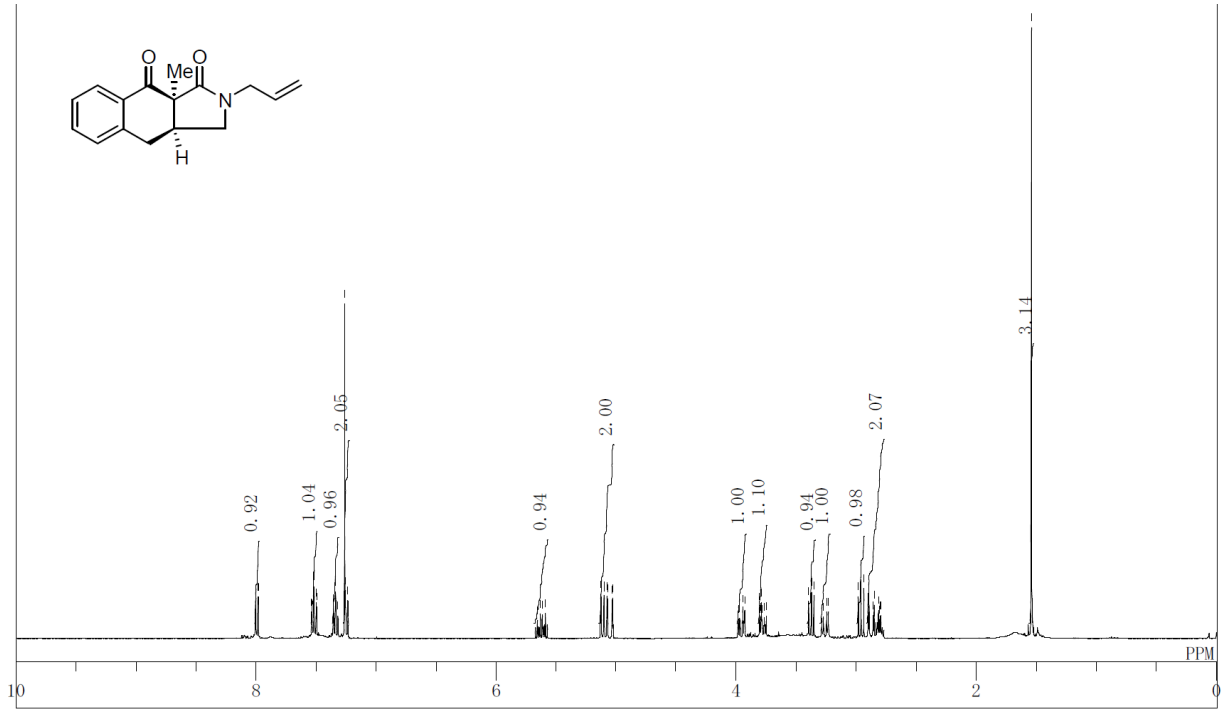


Figure S11. ^{1}H-NMR ($CDCl_3$) of ***cis*-4.**

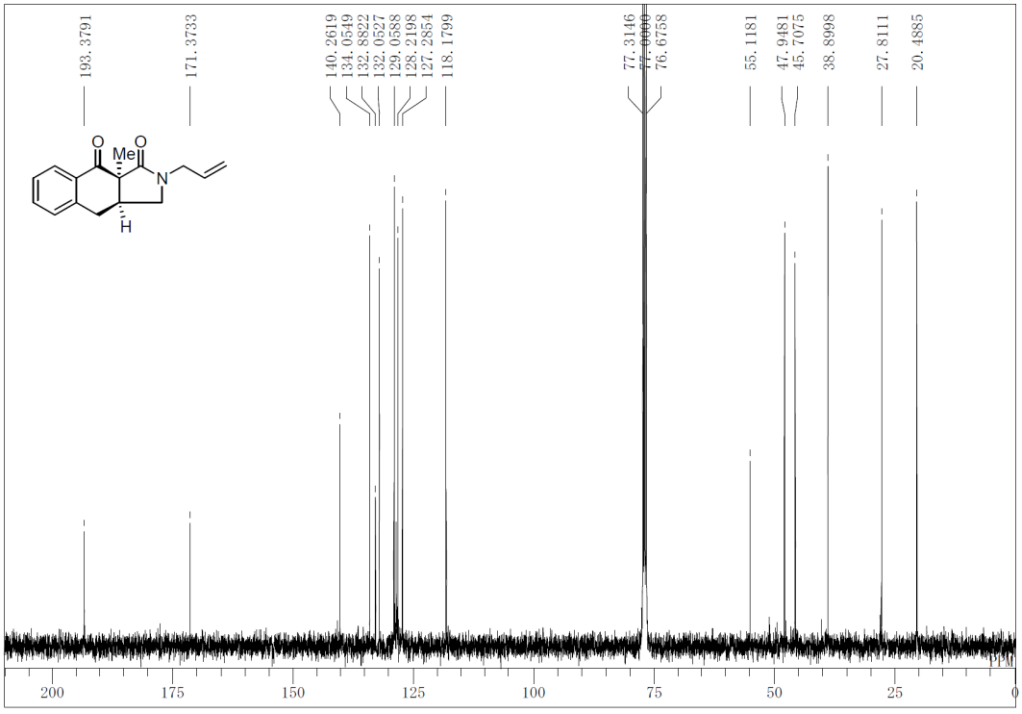


Figure S12. ^{13}C-NMR ($CDCl_3$) of ***cis*-4.**

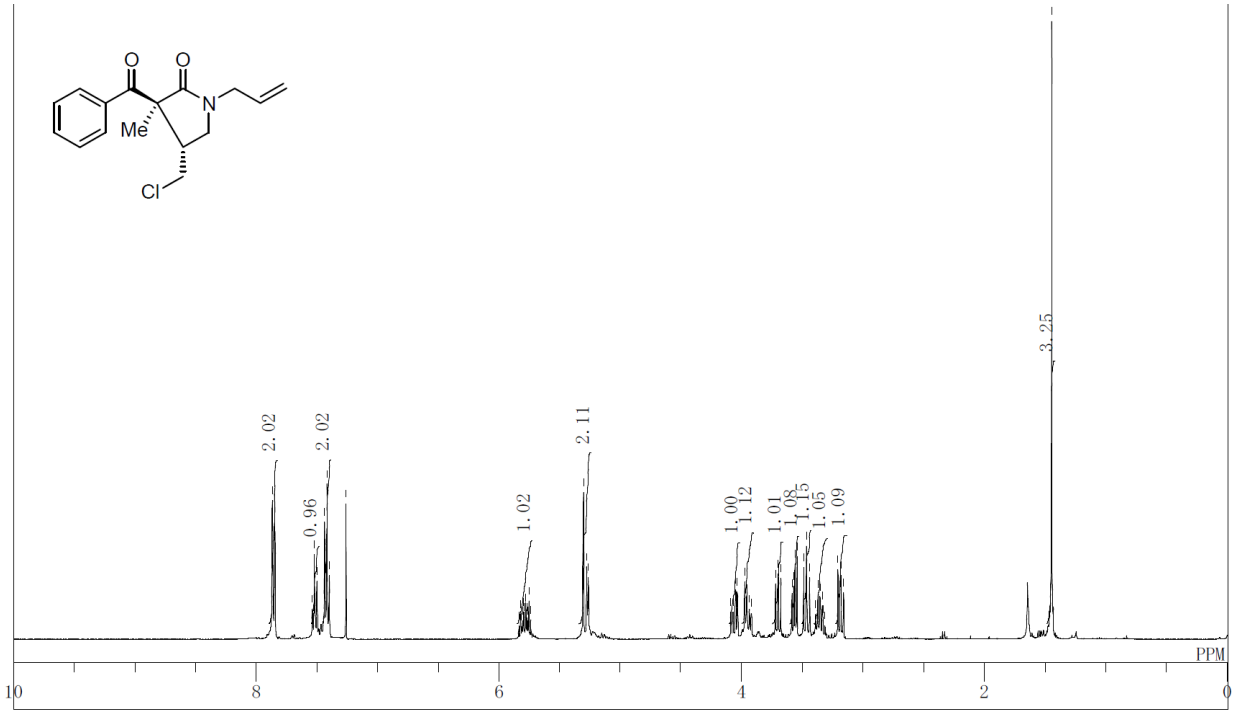


Figure S13. ^{1}H-NMR ($CDCl_3$) of ***trans*-5.**

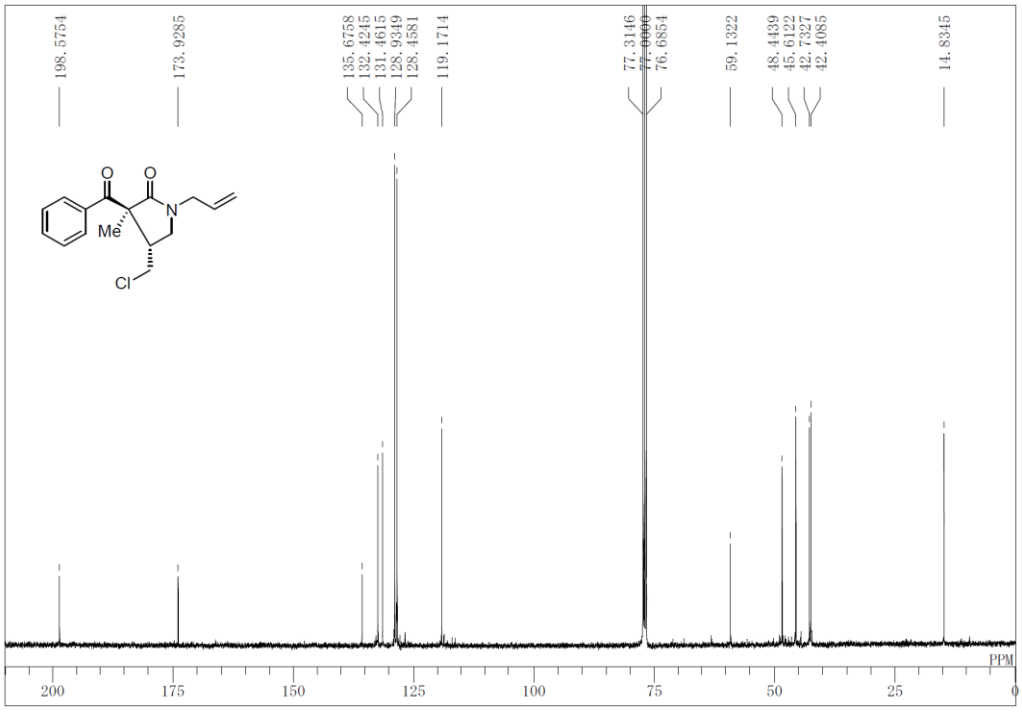


Figure S14. ^{13}C-NMR ($CDCl_3$) of ***trans*-5.**

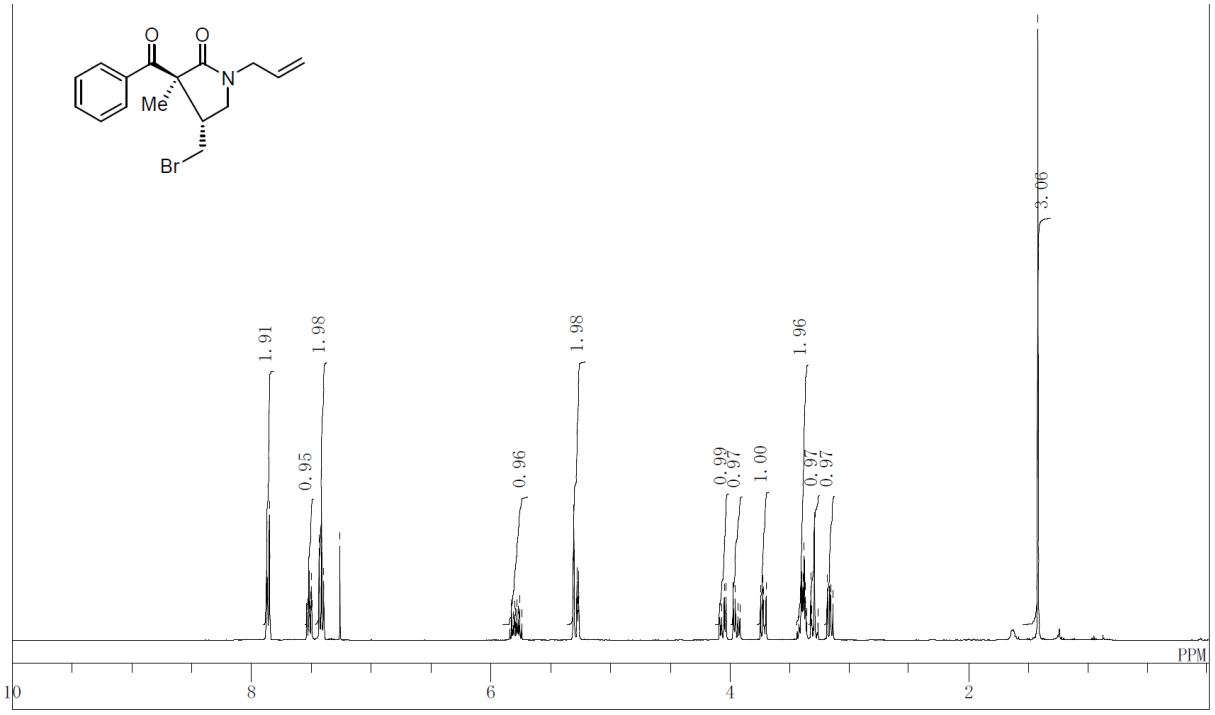


Figure S15. ^{1}H-NMR ($CDCl_3$) of ***trans*-6.**

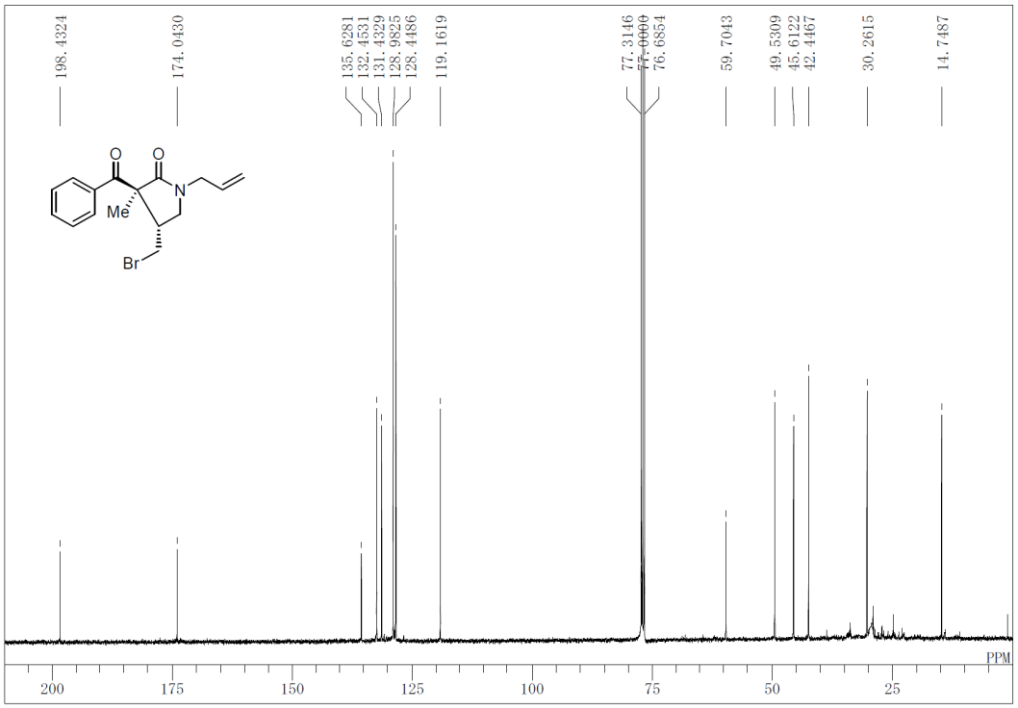


Figure S16. ^{13}C-NMR ($CDCl_3$) of ***trans*-6.**