Supporting Information

Chemoselective Synthesis of Polycyclic Spiroindolines and Polysubstituted Pyrroles via the Domino Reaction of 2-Isocyanoethylindoles

Xiang Wang, [†,‡] Shun-Yi Wang, [*,†] and Shun-Jun Ji[*,†]

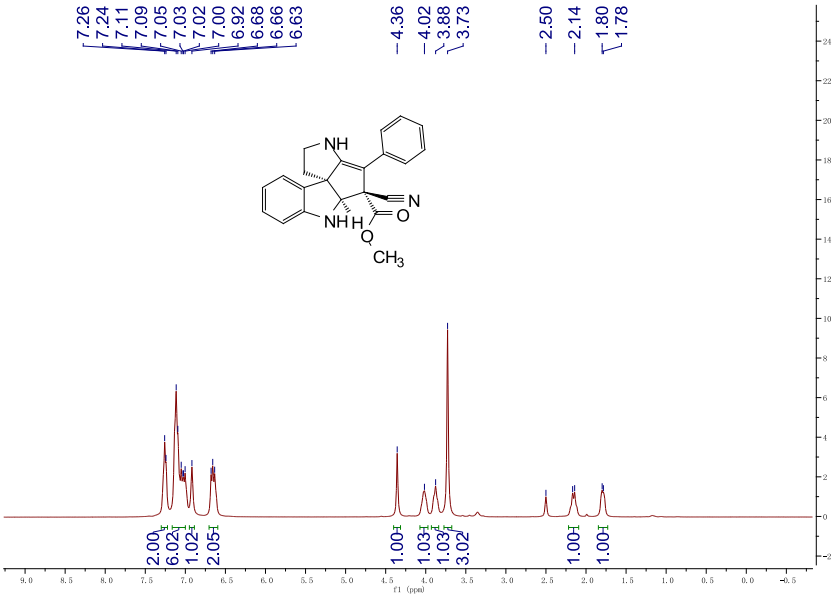
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[‡]*School of Chemistry and Chemical Engineering, Huaiyin Normal University, Huaian, 223300, China*

shunyi@suda.edu.cn; shunjun@suda.edu.cn

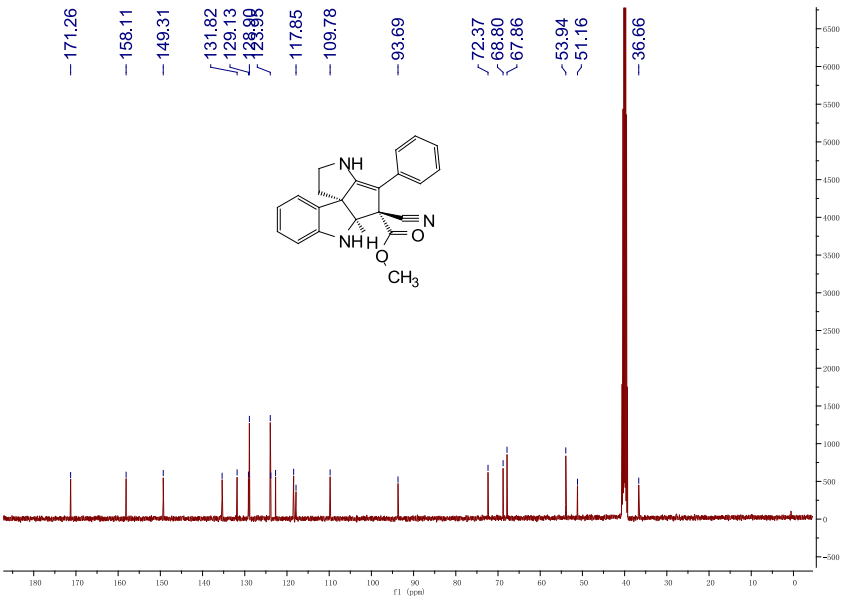
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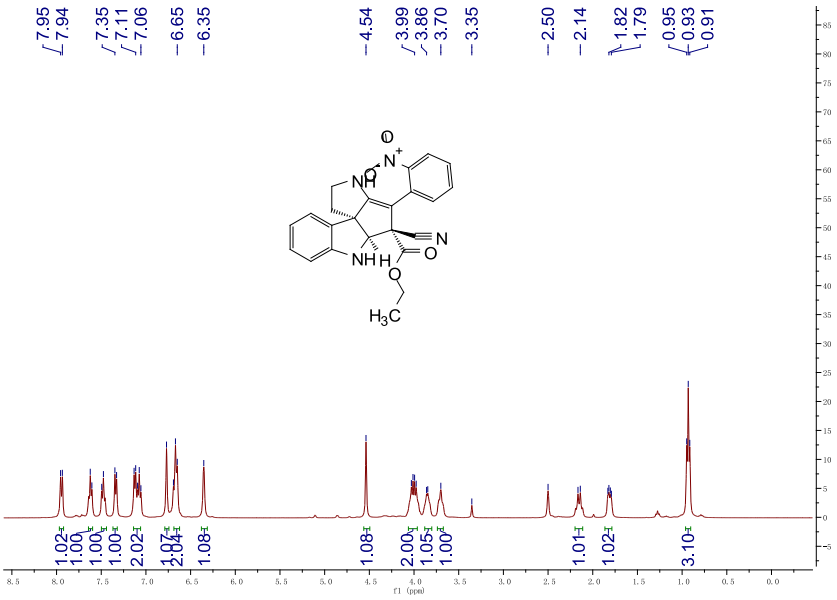
NMR spectrum of compounds 3 and 5



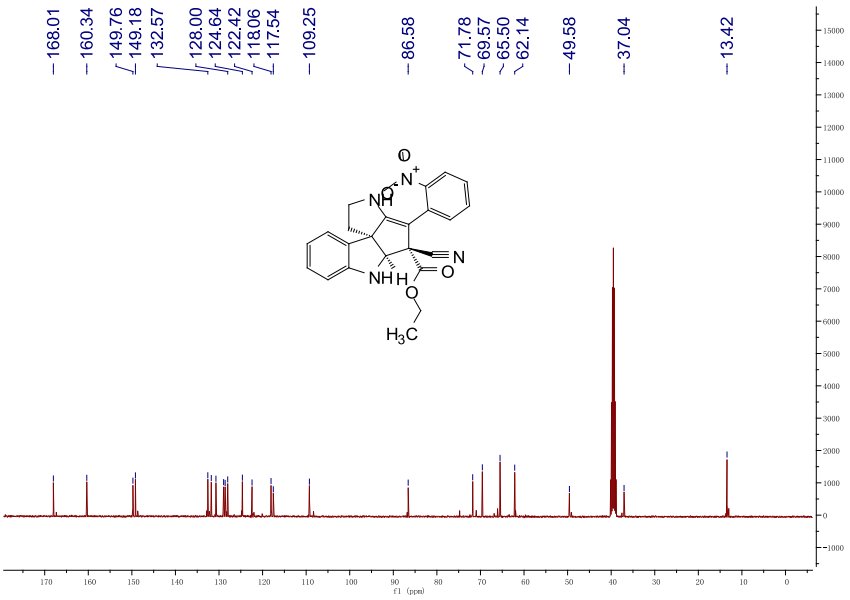
^{1}H NMR spectrum of compound 3a



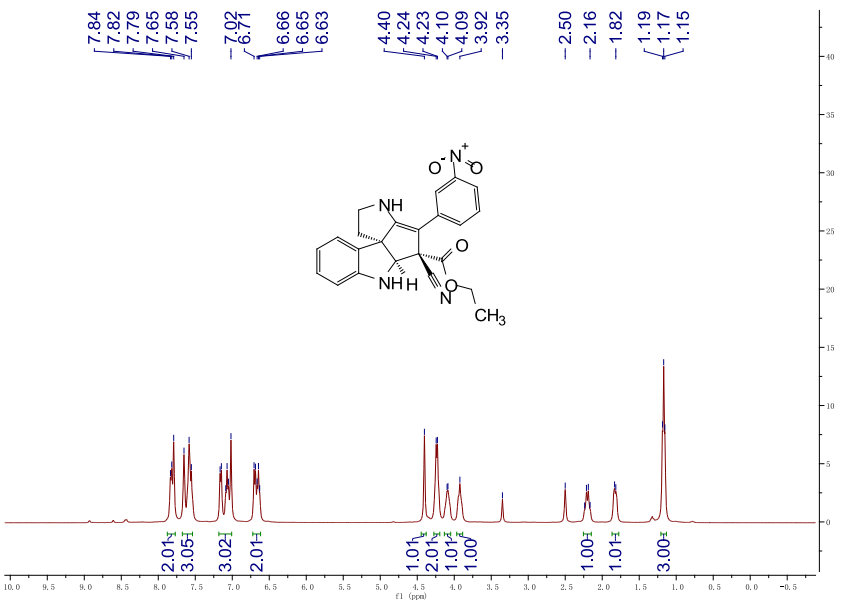
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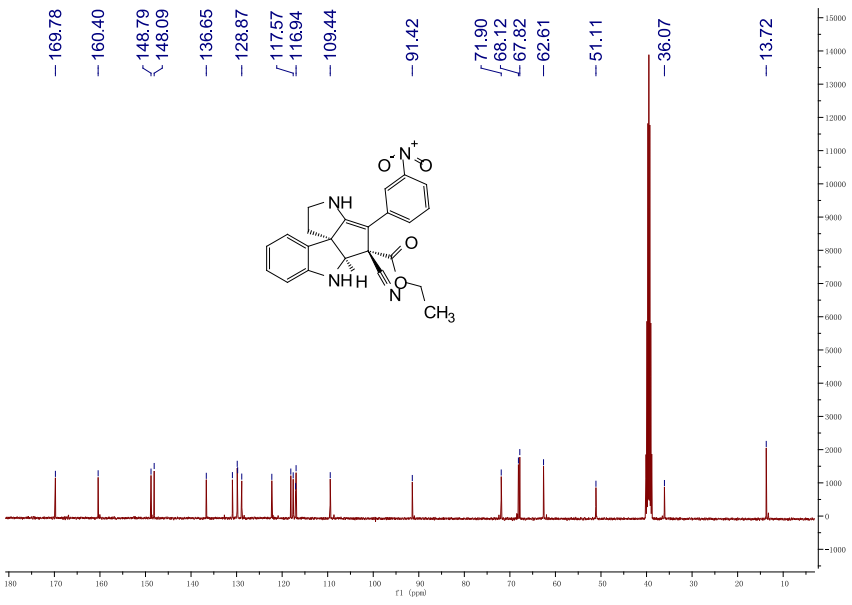
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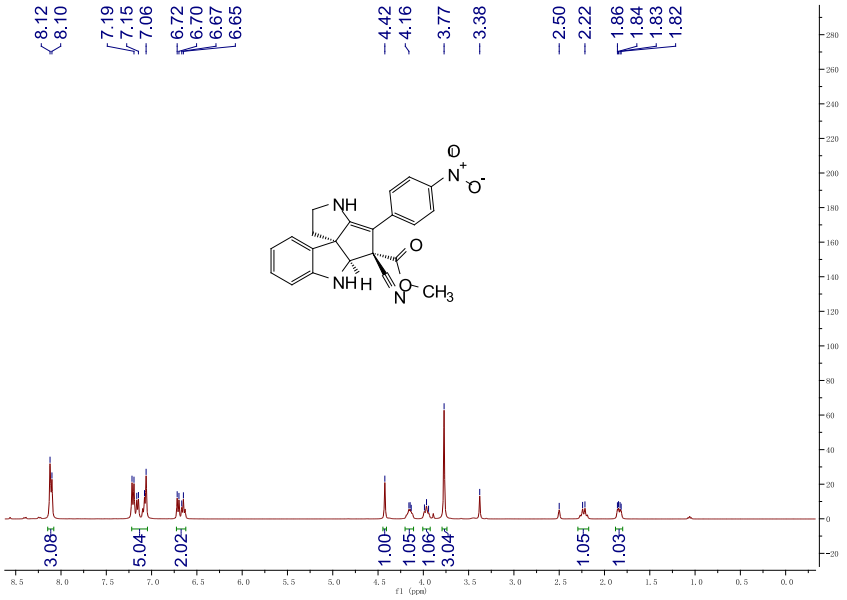
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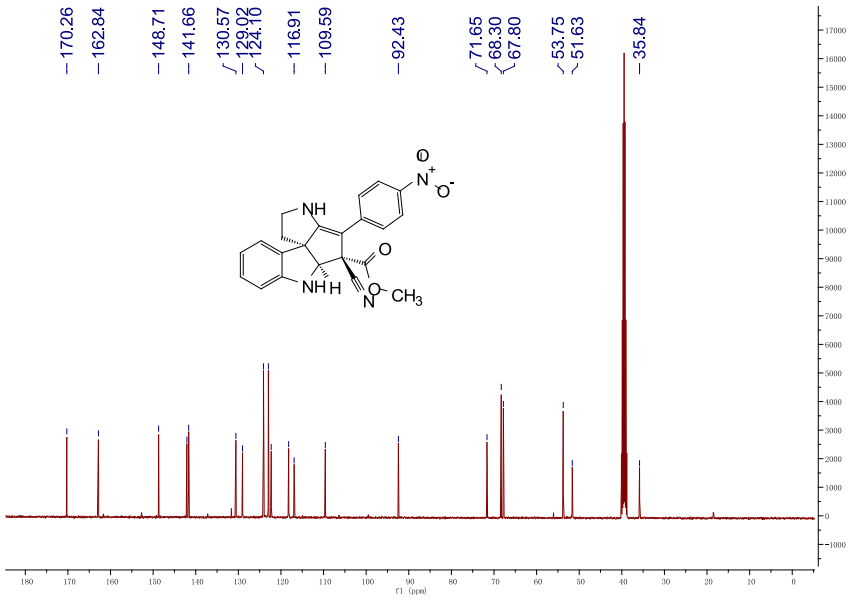
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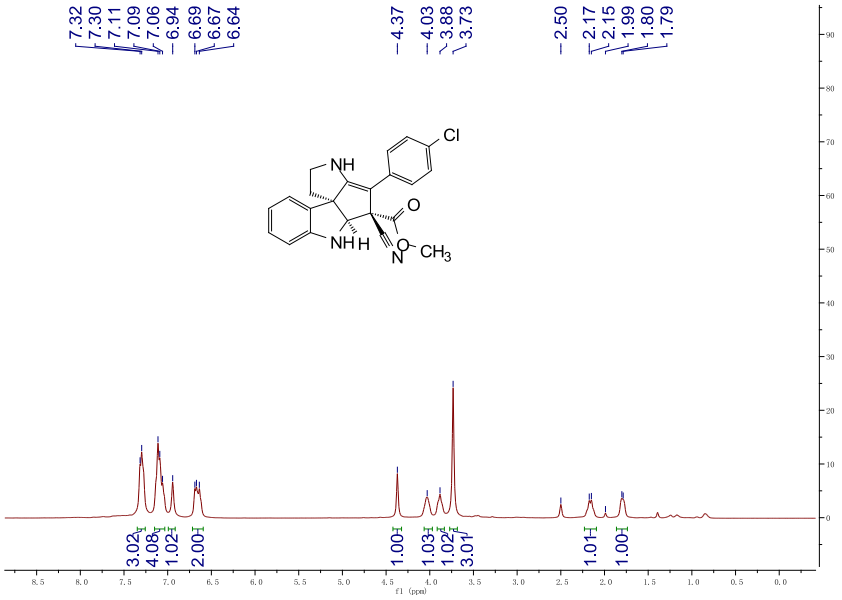
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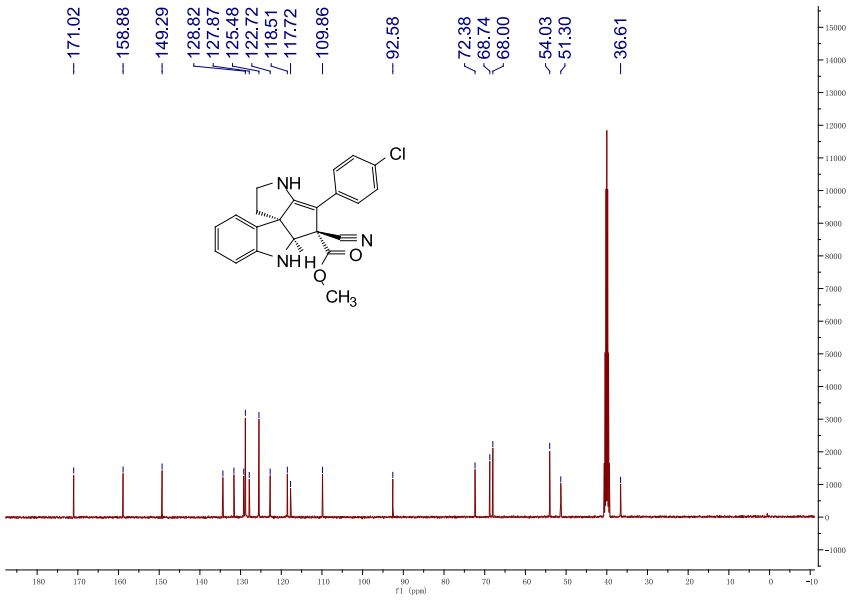
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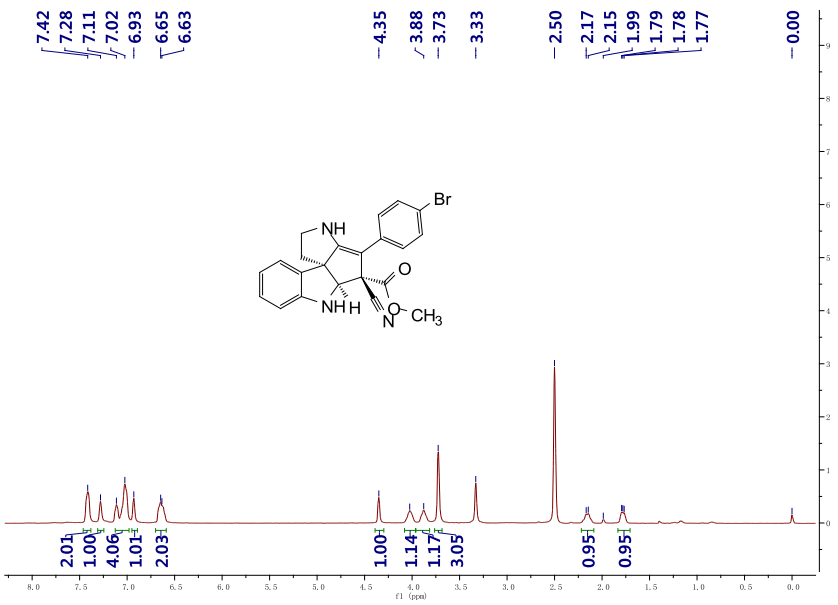
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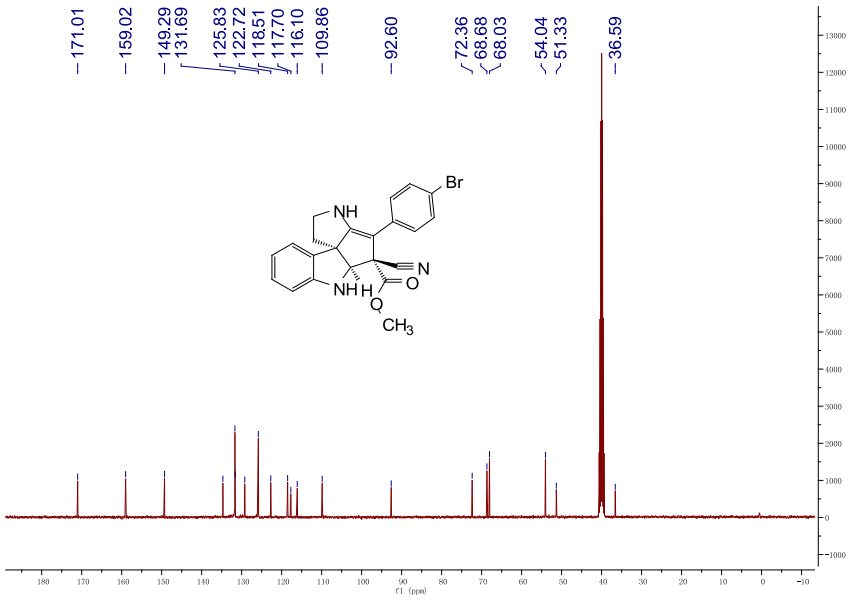
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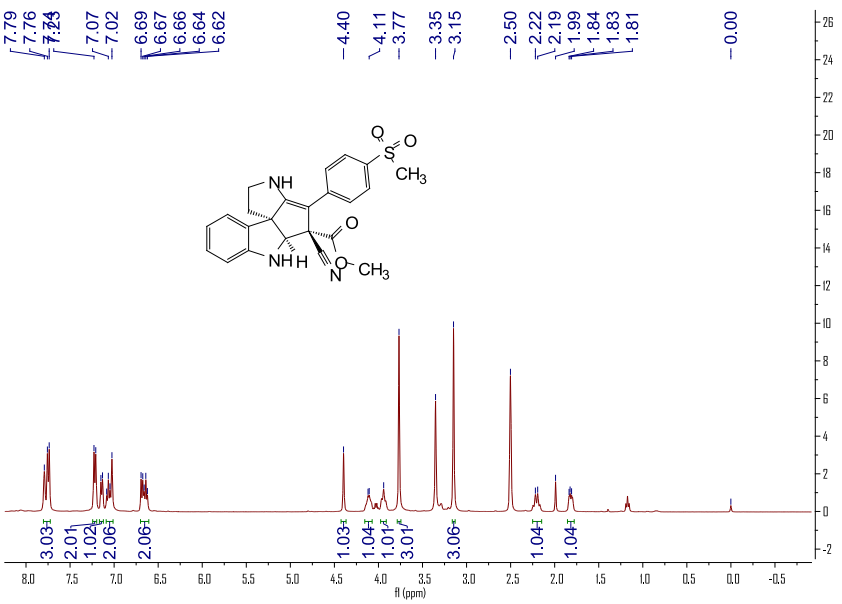
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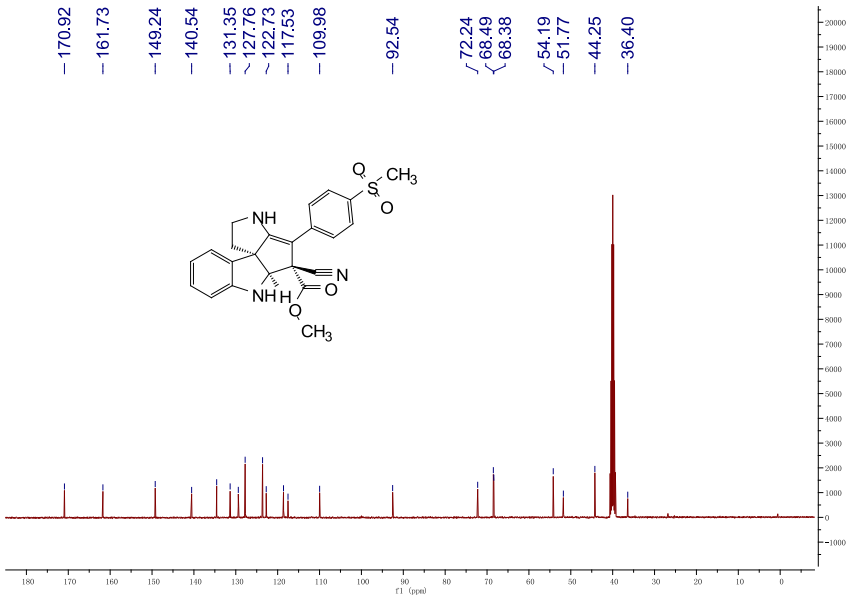
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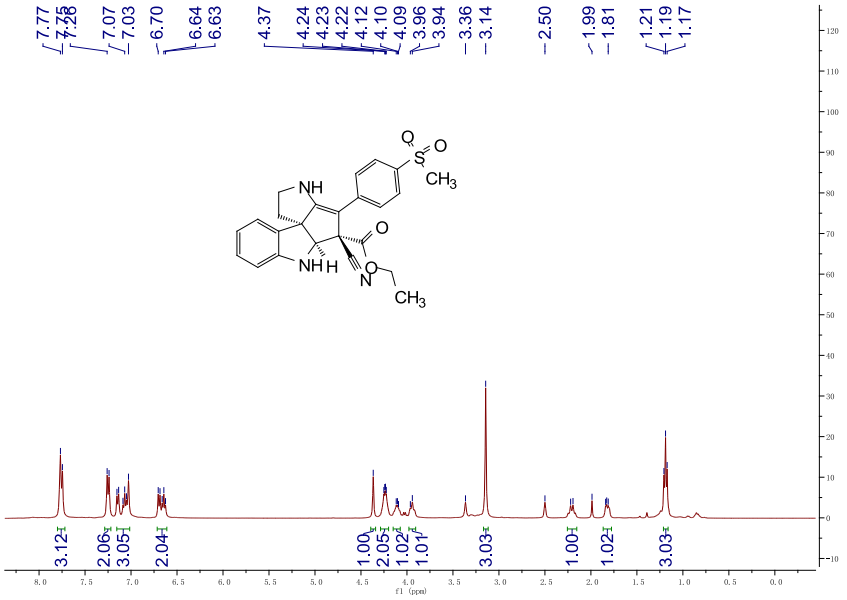
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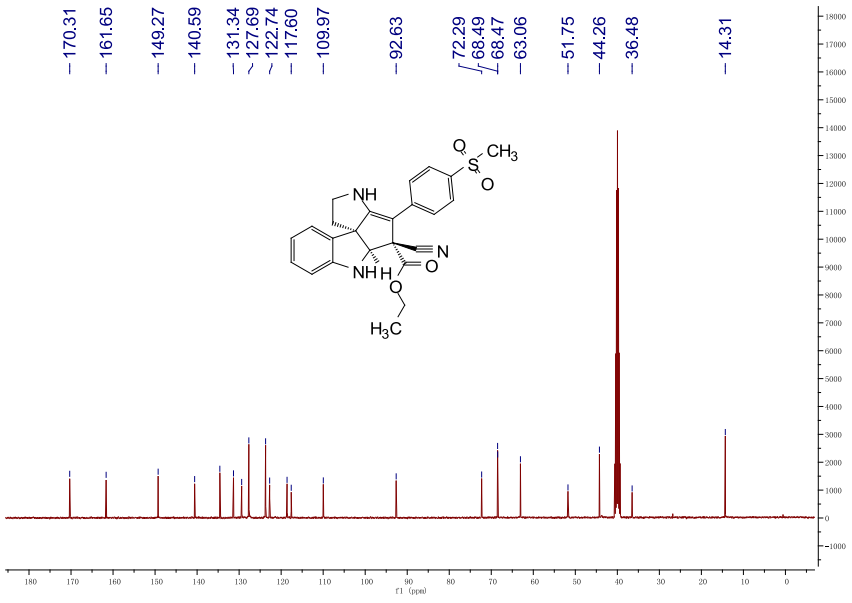
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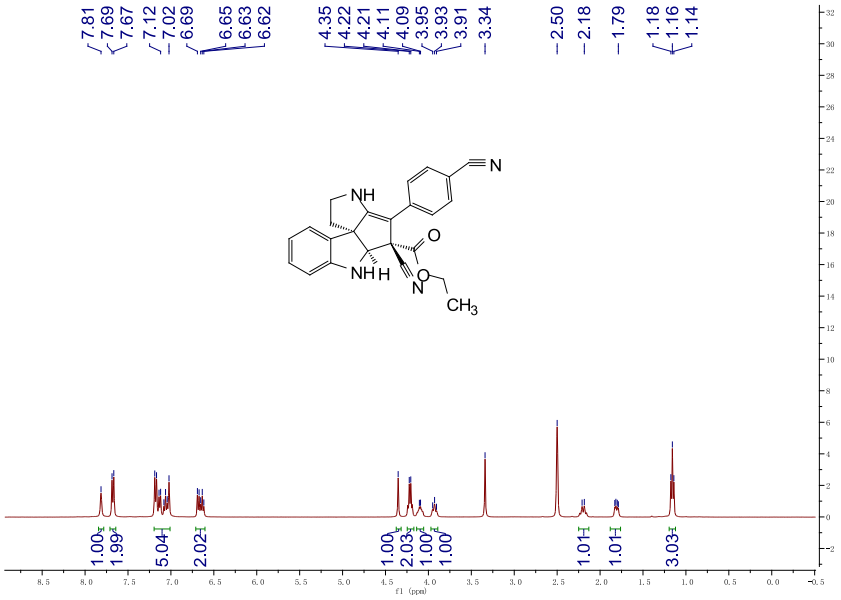
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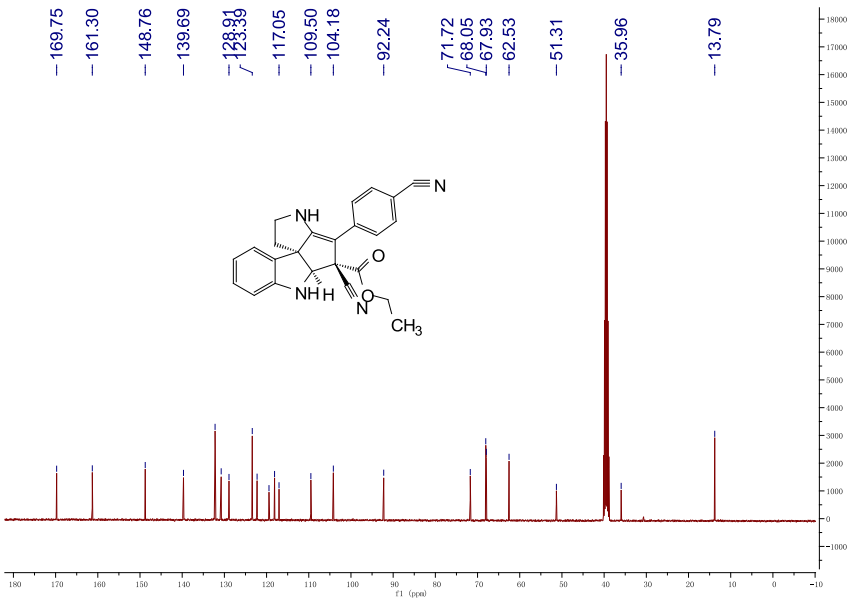
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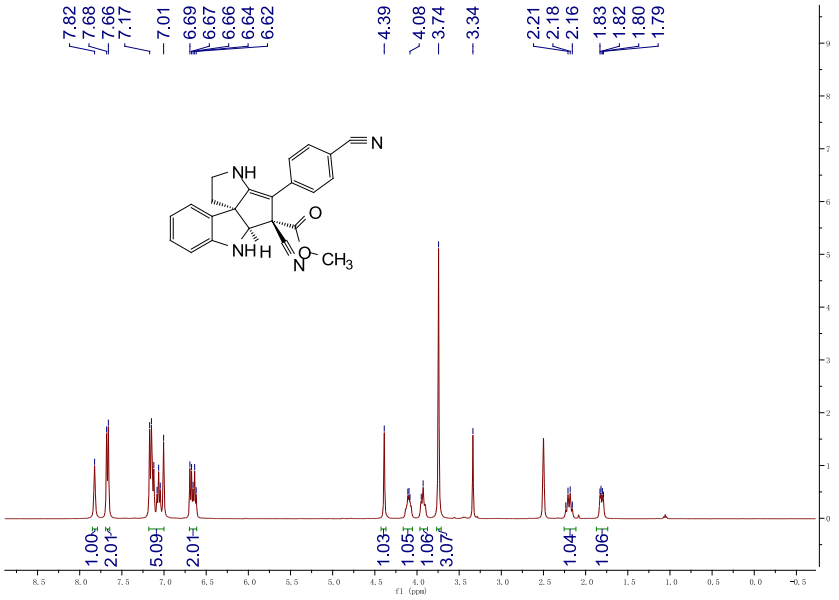
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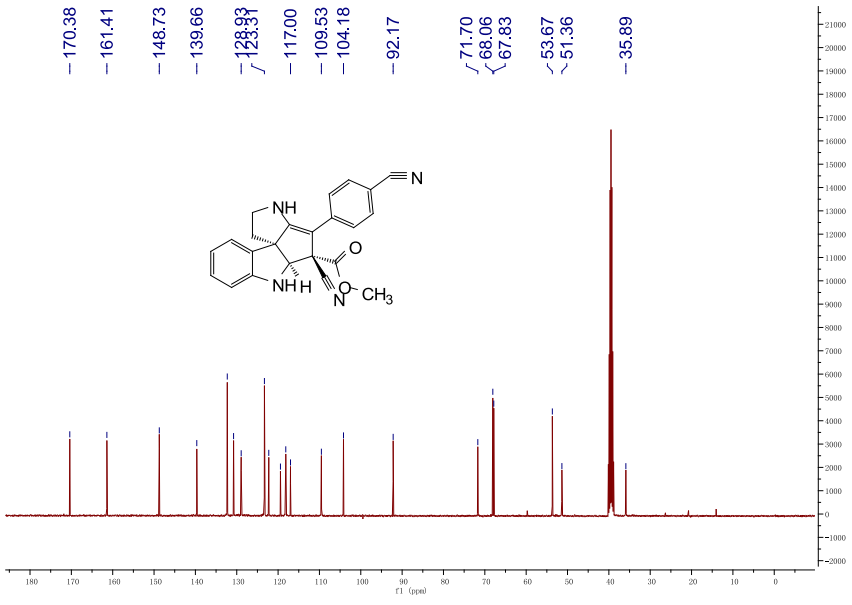
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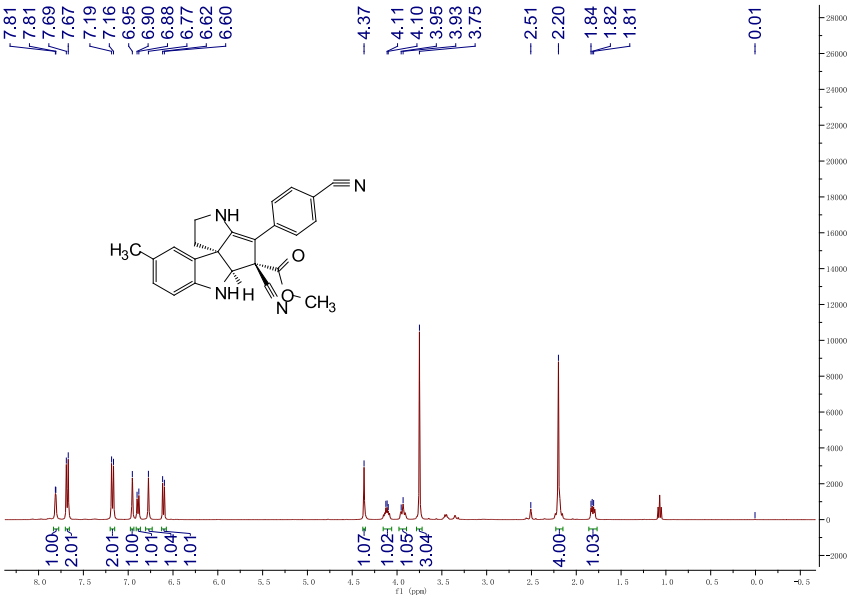
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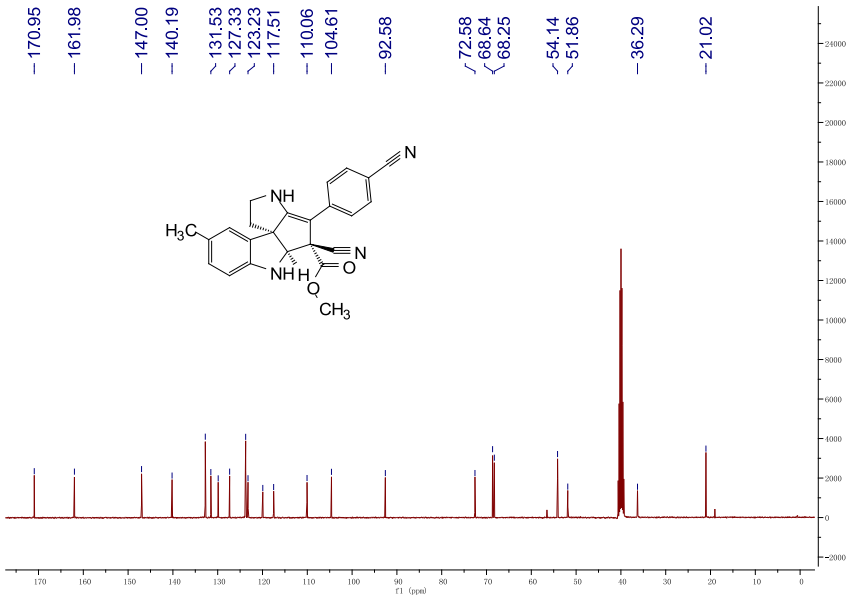
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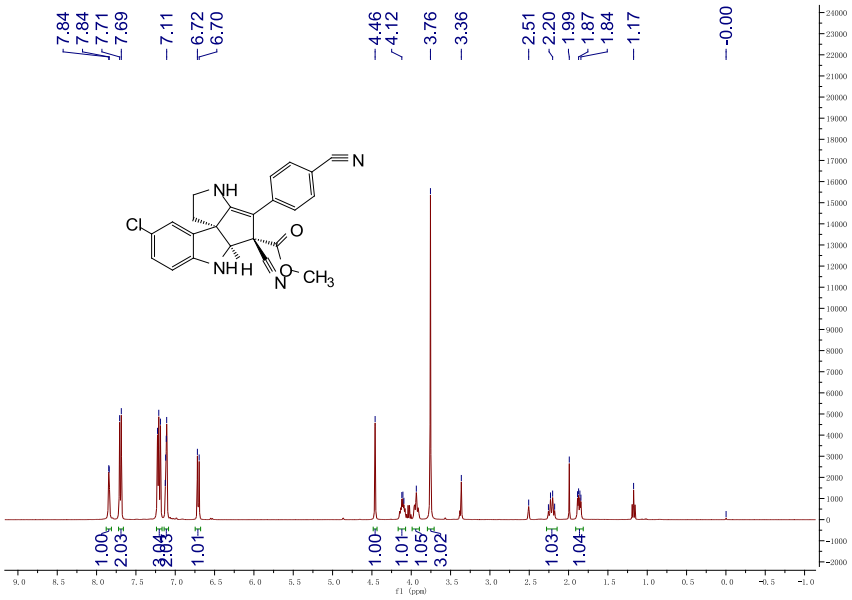
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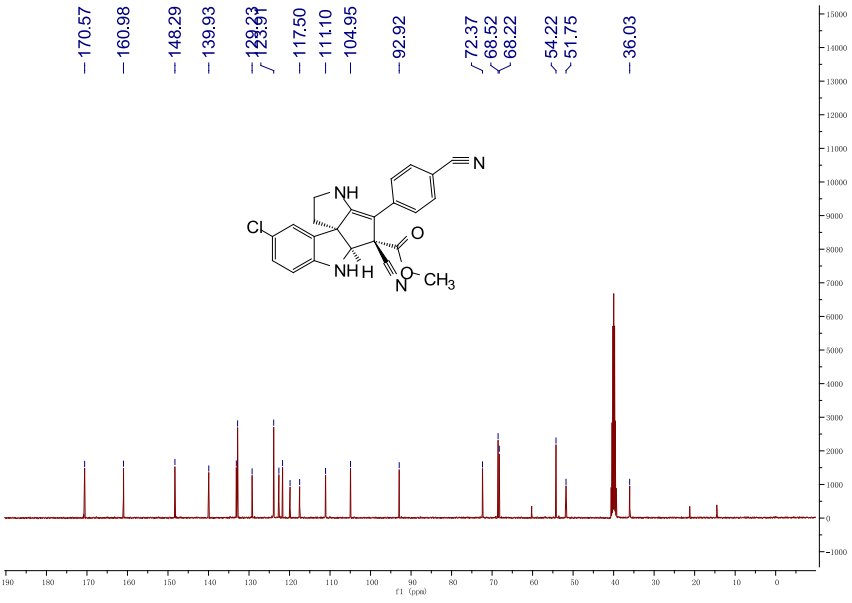
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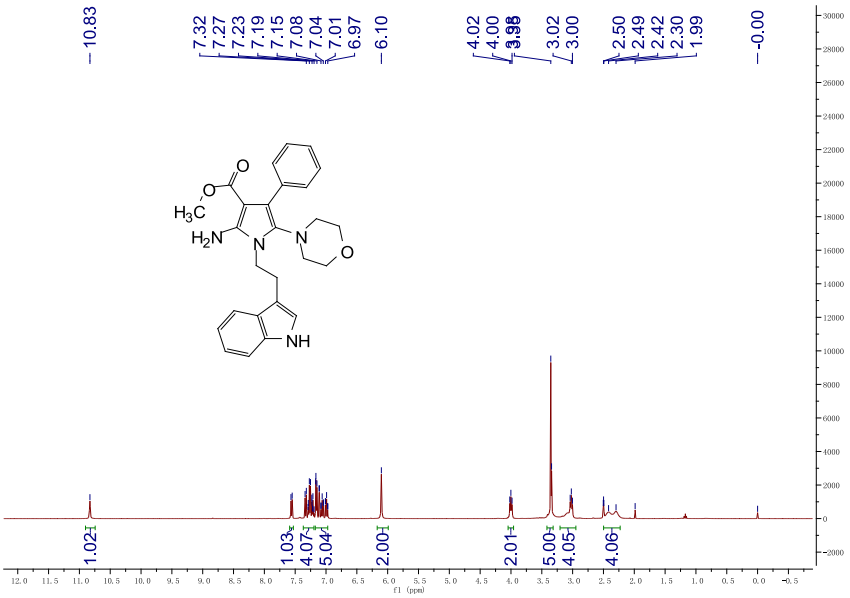
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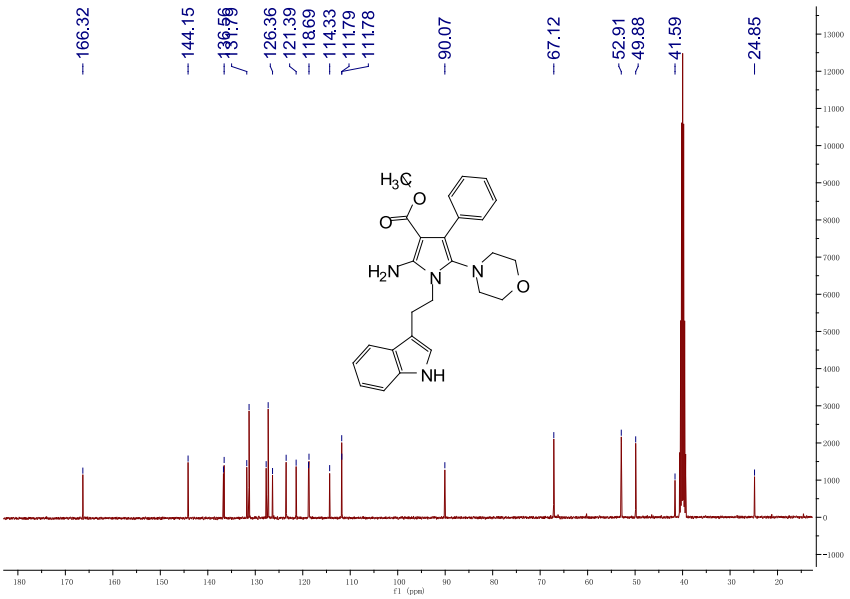
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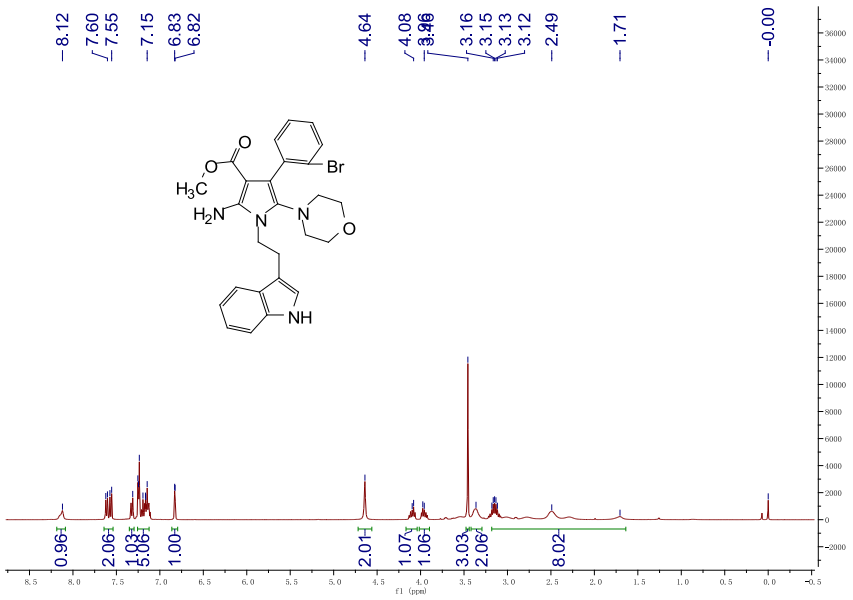
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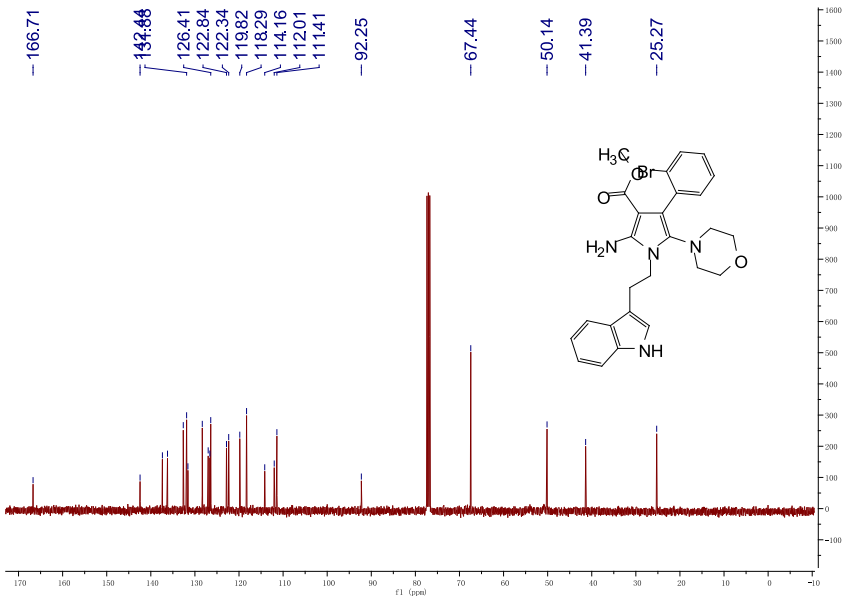
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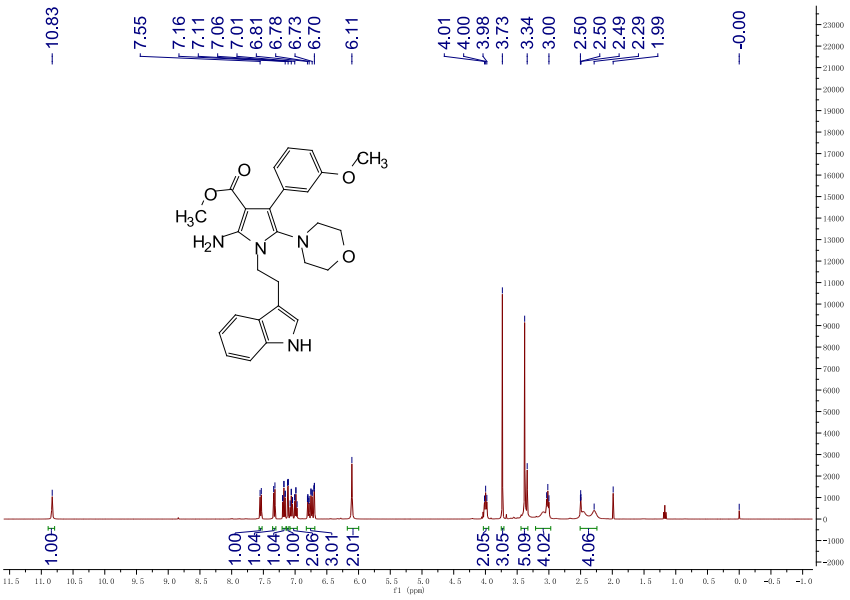
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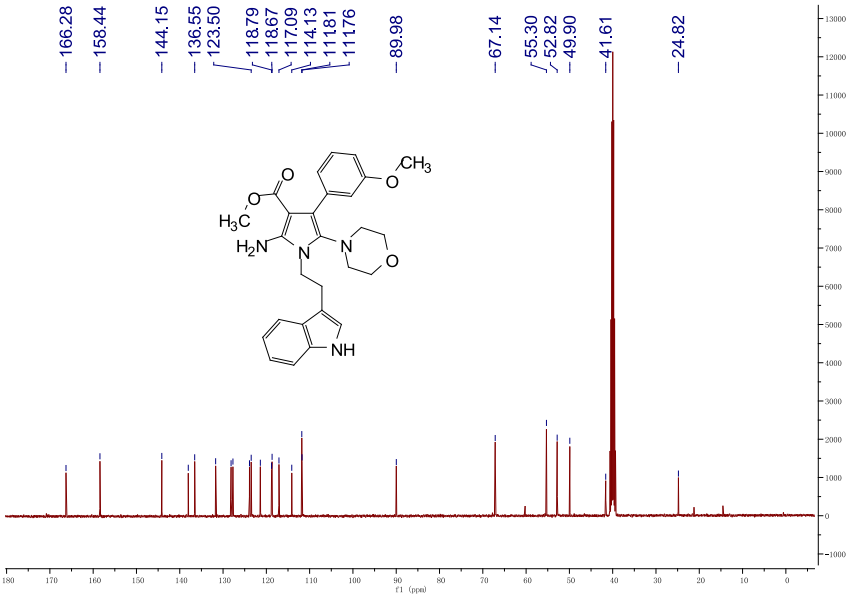
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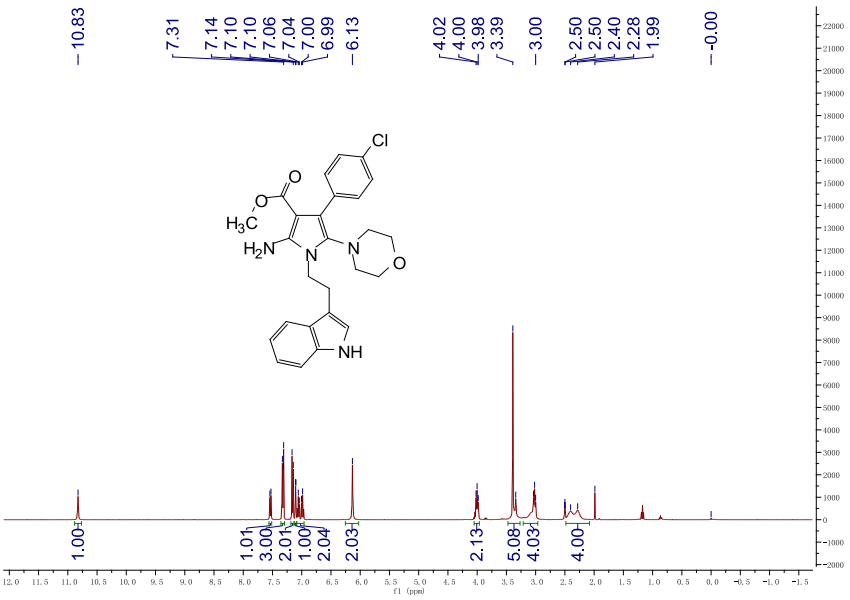
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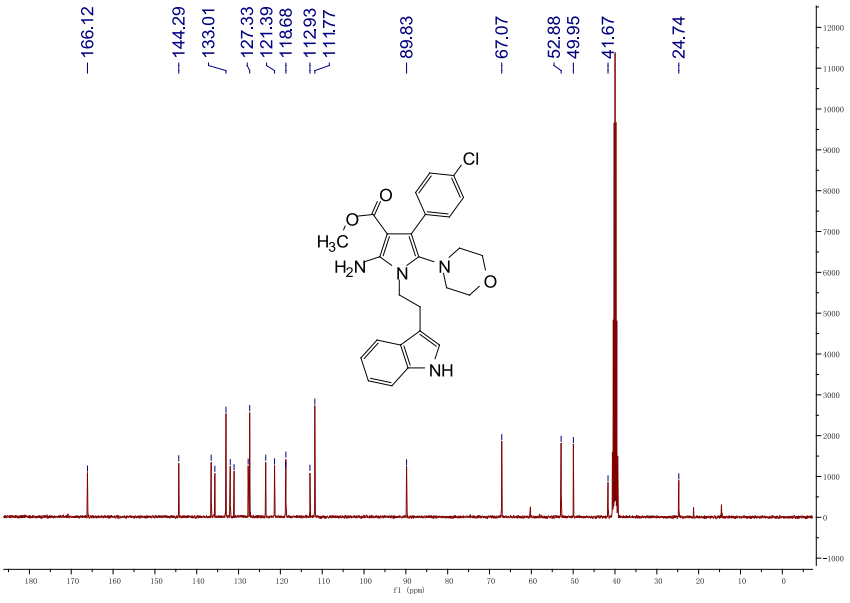
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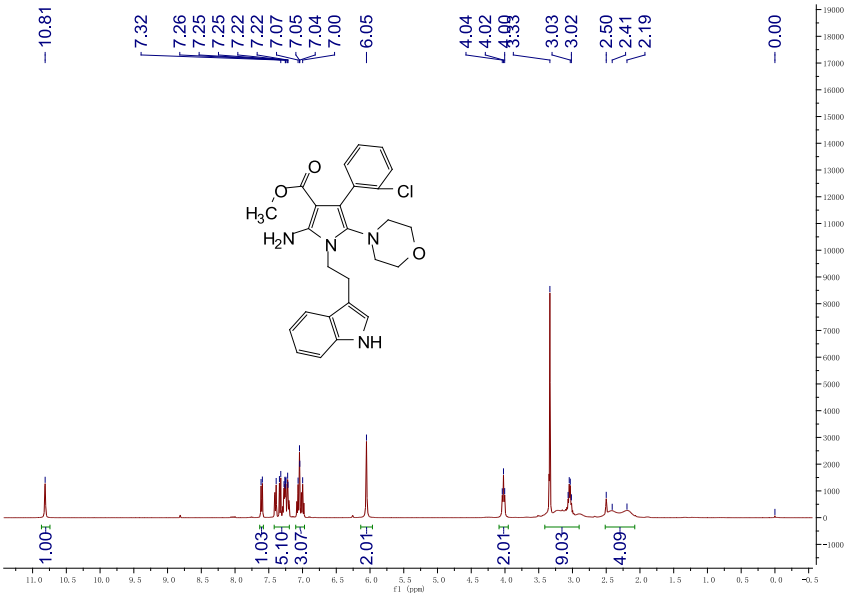
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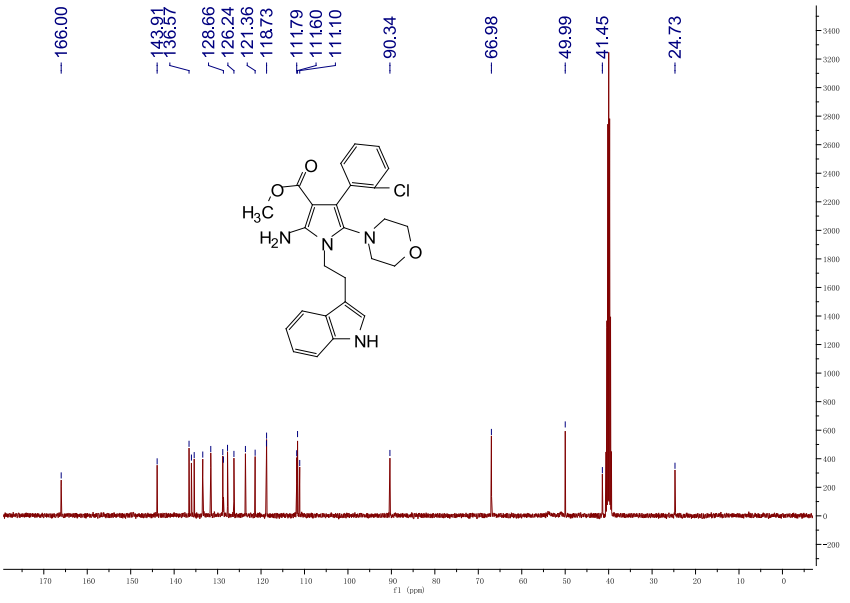
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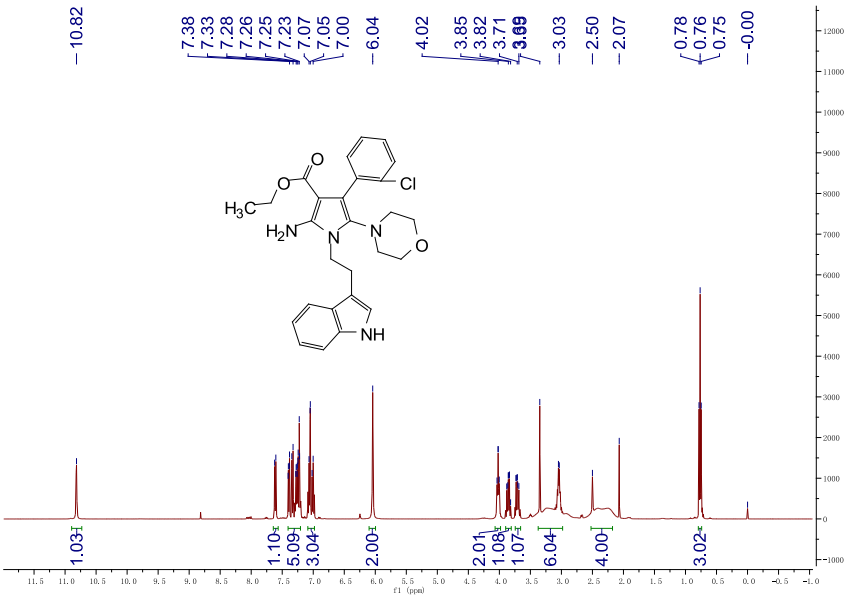
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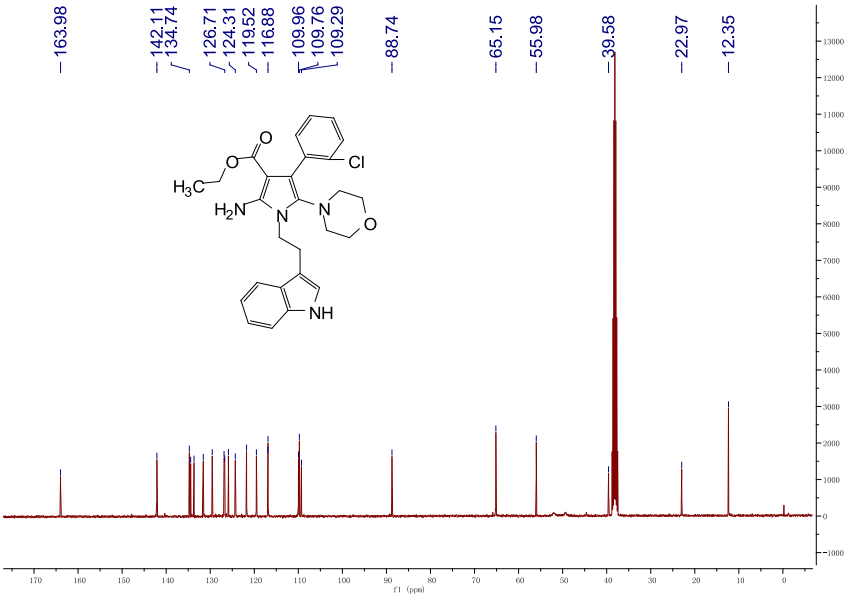
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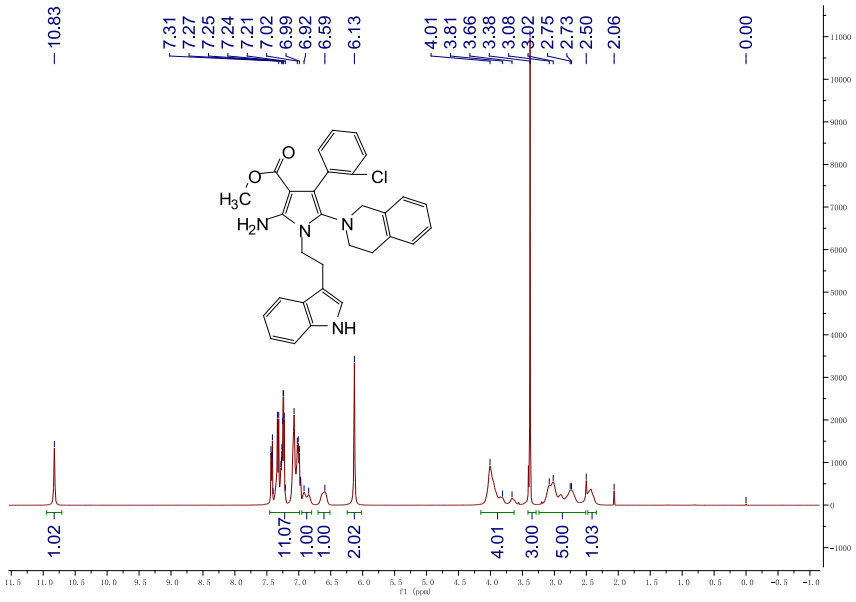
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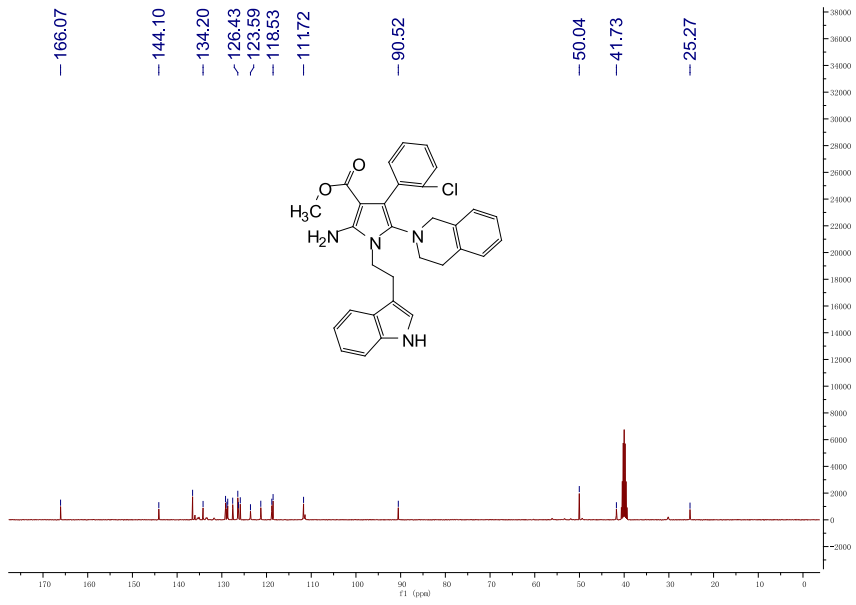
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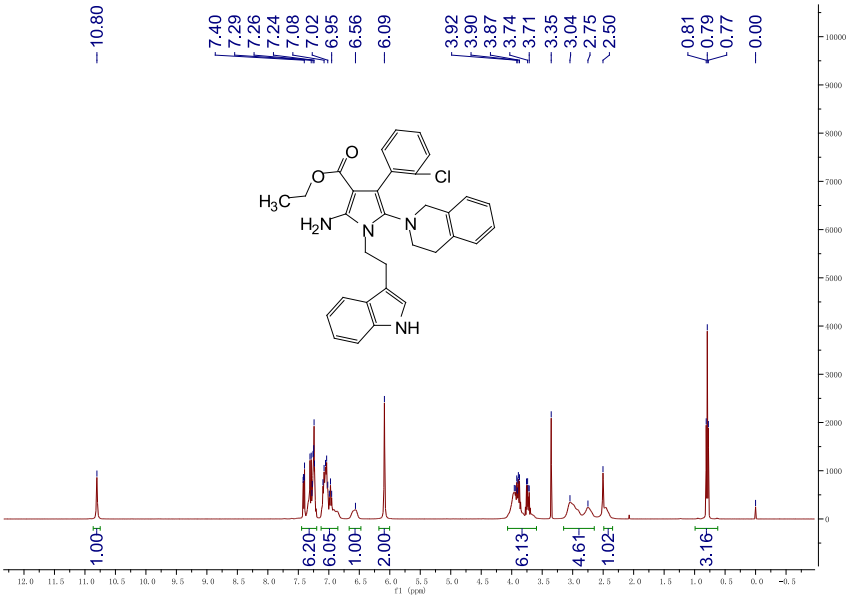
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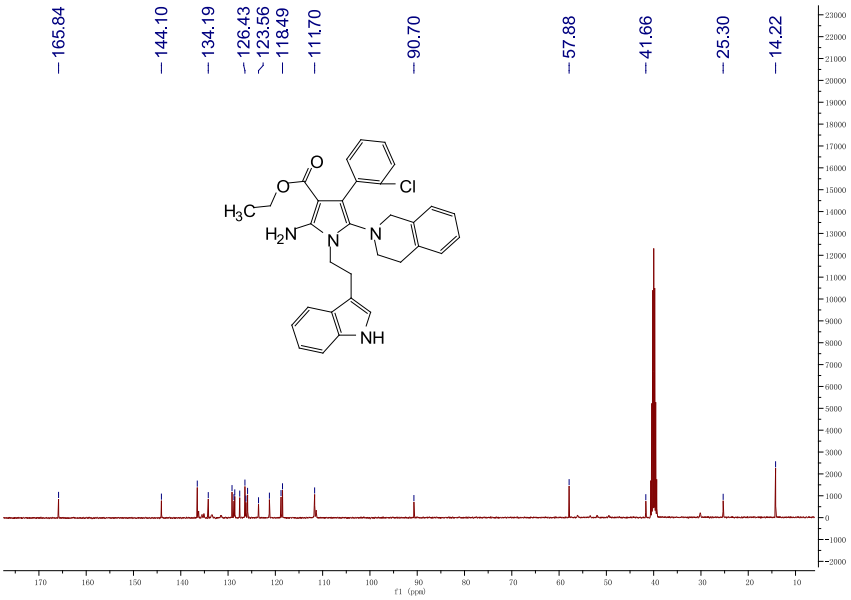
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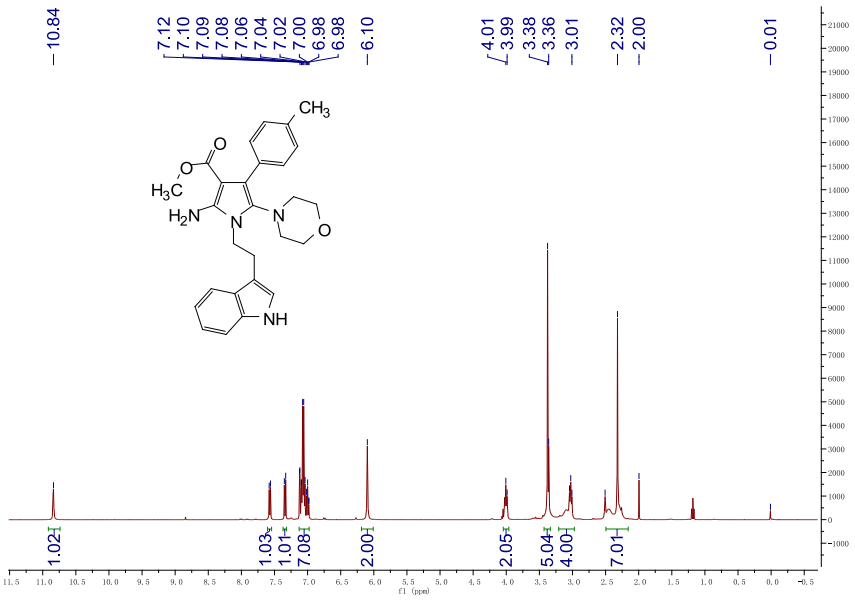
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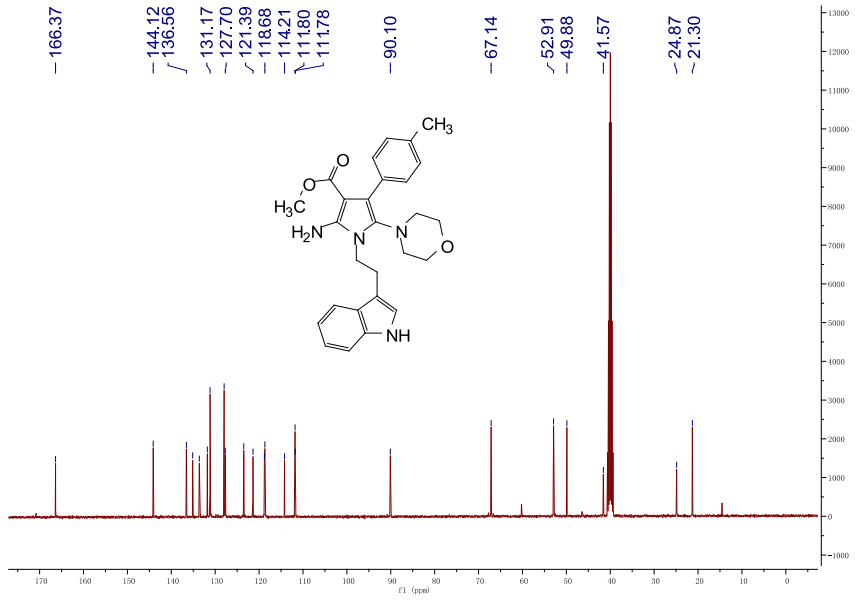
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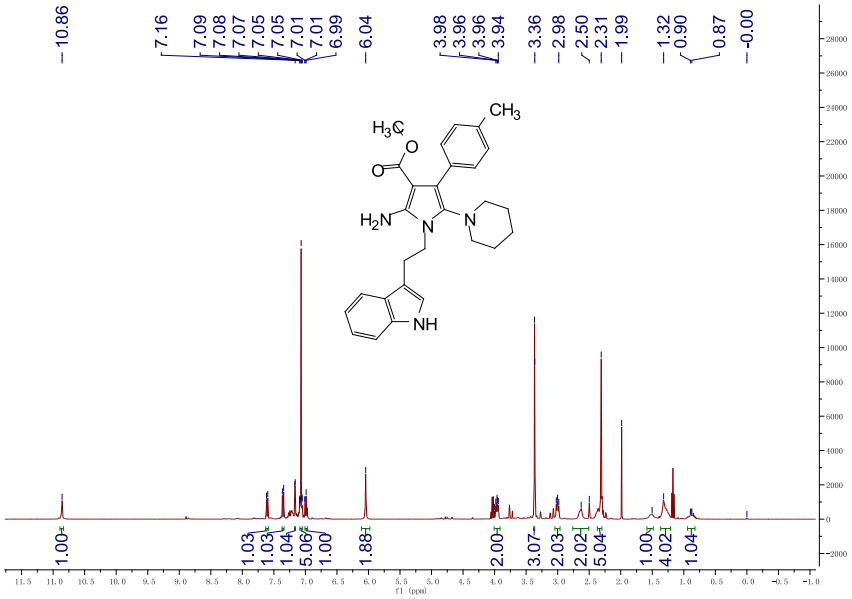
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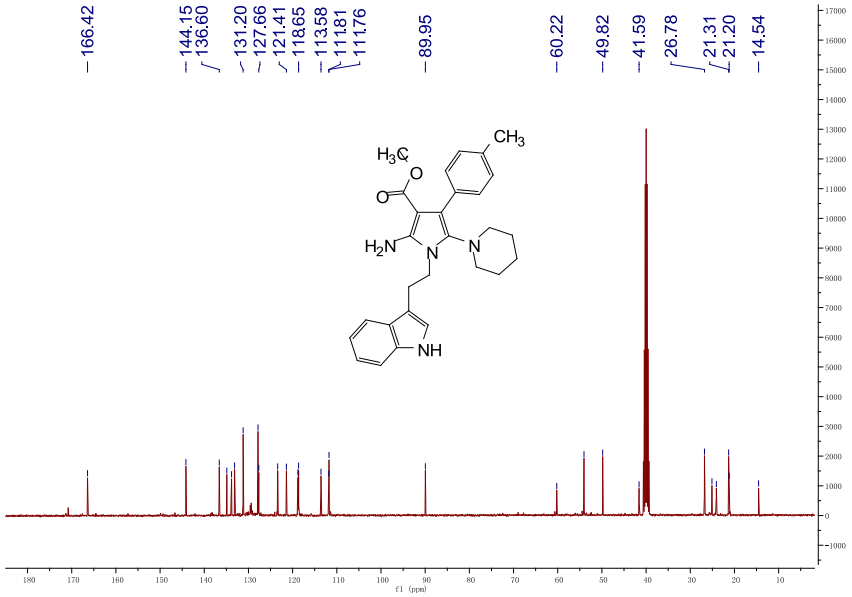
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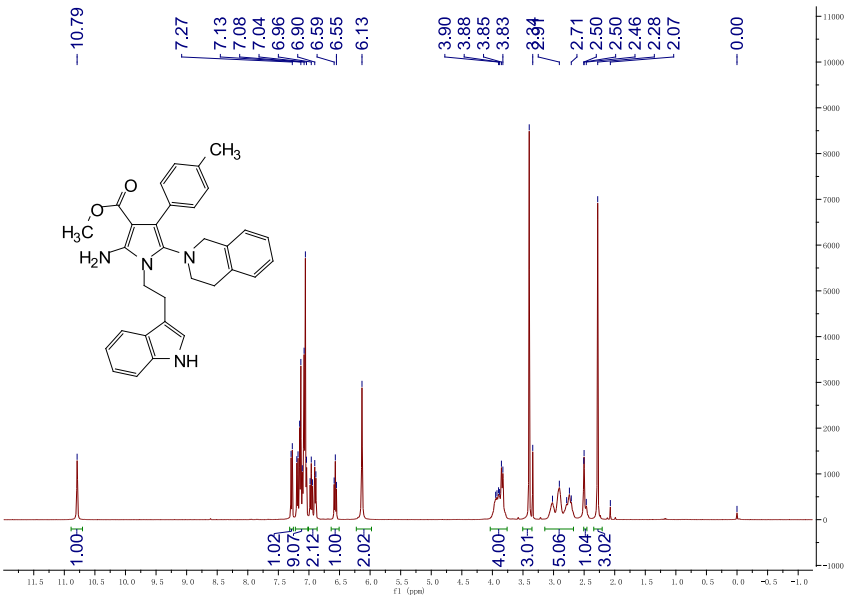
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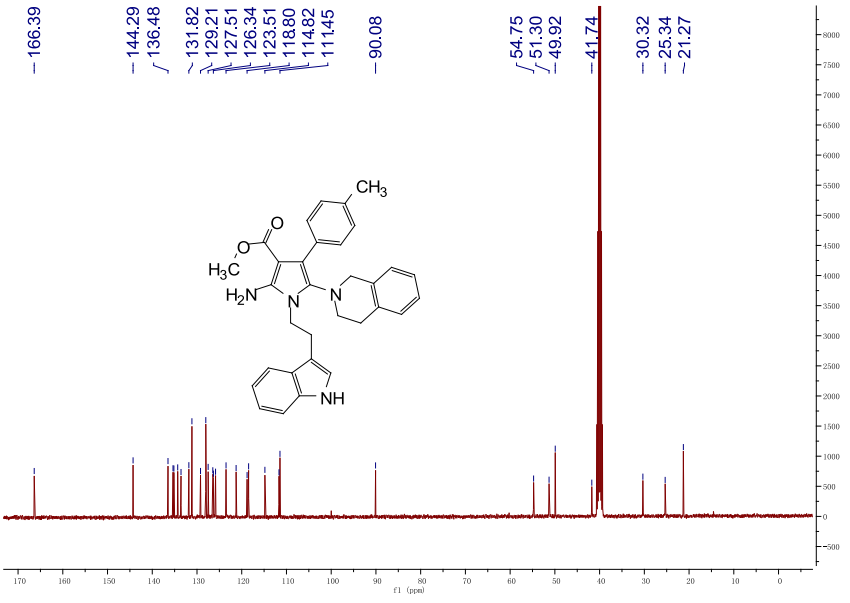
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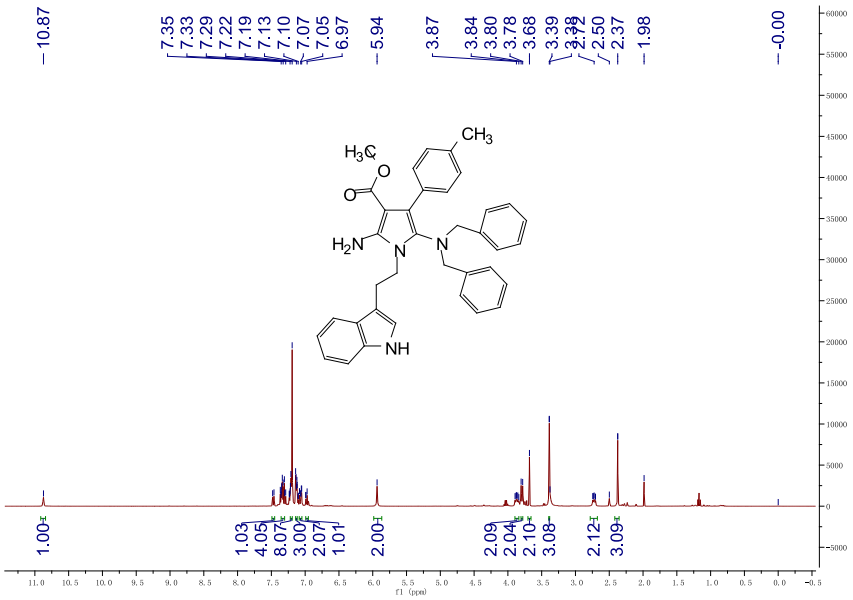
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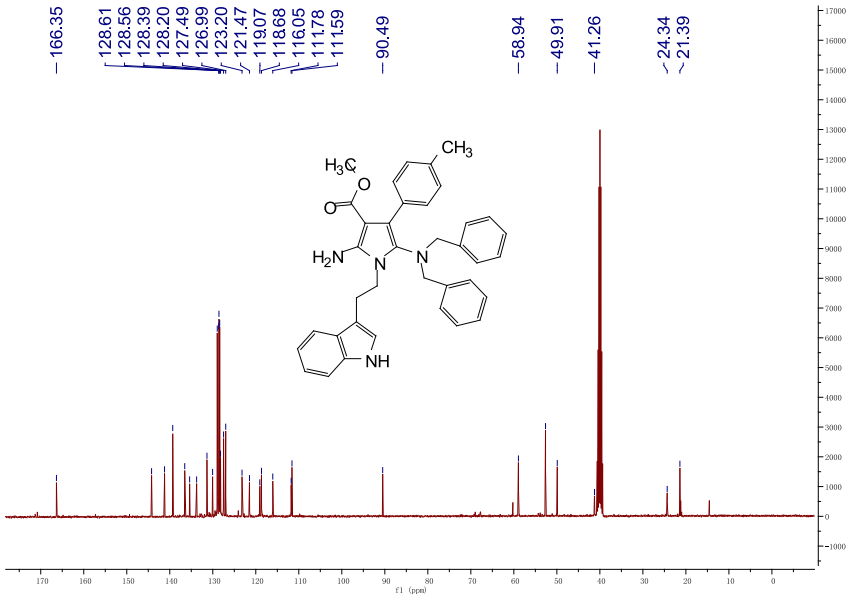
^{1}H NMR spectrum of compound 5k



^{13}C NMR spectrum of compound 5k

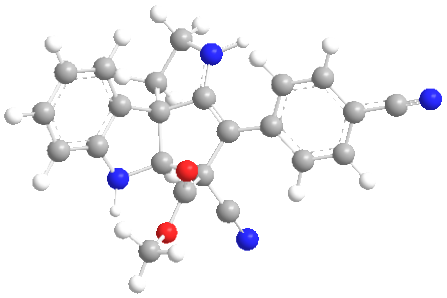


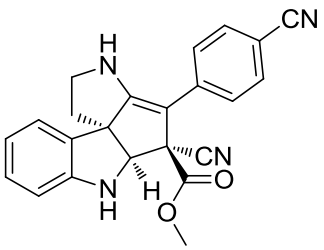
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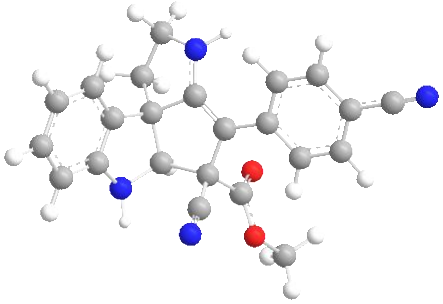
Density functional theory calculations of the possible configurations of product **3j'** and **3j** at the B3LYP/6-31G(d) level of theory.

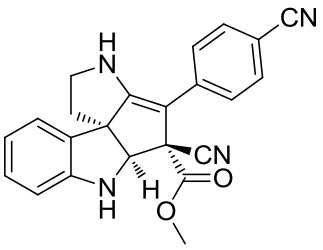




3j'

E= -1256.6954495 Hartree





3j

E= -1256.6970321 Hartree

XYZ Coordinates (3j')

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
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2	6	-0.000000412	0.000009664	0.000002180
3	6	0.000004144	0.000001230	-0.000004590
4	6	-0.000001483	-0.000013538	0.000004460
5	6	-0.000003667	0.000020676	0.000014230
6	6	0.000009705	-0.000003048	-0.000002752
7	7	-0.000005817	-0.000001058	-0.000003714
8	6	-0.000010203	0.000021658	-0.000006350
9	6	0.000007014	-0.000021194	-0.000017462

10	6	-0.000014855	0.000003680	0.000012700
11	6	0.000008886	-0.000001388	-0.000003028
12	6	-0.000001186	0.000007203	0.000004240
13	7	-0.000015077	-0.000014797	0.000002226
14	6	0.000006377	0.000019097	0.000009444
15	6	0.000006934	-0.000004325	0.000003195
16	6	-0.000004362	-0.000000159	-0.000003139
17	6	0.000007915	0.000004483	-0.000003516
18	8	0.000000320	-0.000003523	-0.000002019
19	8	0.000001488	-0.000000498	0.000005600
20	6	0.000000947	-0.000001653	-0.000008498
21	6	0.000002298	0.000000610	-0.000010155
22	7	-0.000002872	-0.000003818	-0.000002454
23	6	-0.000006277	-0.000000771	0.000000448
24	6	0.000002376	-0.000001888	-0.000003687
25	6	-0.000004127	-0.000000626	-0.000000251
26	6	0.000006473	0.000000158	-0.000001640
27	6	-0.000000907	-0.000007132	-0.000000709
28	6	0.000001371	-0.000001587	-0.000004144
29	7	0.000001779	-0.000002604	-0.000002755
30	1	0.000002681	0.000002032	0.000002691
31	1	0.000003405	-0.000000957	0.000003193
32	1	0.000000427	-0.000000086	0.000002120
33	1	-0.000000329	0.000002209	0.000003066
34	1	-0.000001071	-0.000001060	0.000000002
35	1	-0.000002011	-0.000000246	0.000001307
36	1	0.000002360	0.000003972	-0.000000737
37	1	-0.000002605	0.000001308	0.000002756
38	1	-0.000002552	0.000002001	0.000004394
39	1	-0.000000137	0.000004831	0.000003908
40	1	-0.000004498	0.000001921	0.000000795
41	1	0.000000692	-0.000003932	-0.000001210
42	1	0.000000735	-0.000002622	-0.000002266
43	1	0.000001203	-0.000003183	-0.000003749
44	1	0.000001099	-0.000001751	-0.000002225
45	1	-0.000000683	-0.000002092	-0.000003604
46	1	0.000001294	-0.000001010	0.000000692
47	1	0.000001181	0.000001959	0.000001878

E(b3lyp/6-31g) (d) = -1256.6954495

Zero-point correction= 0.367735 (Hartree/Particle)

Thermal correction to Energy= 0.391933

Thermal correction to Enthalpy= 0.392877

Thermal correction to Gibbs Free Energy= 0.313163

Sum of electronic and zero-point Energies=	-1256.327714
Sum of electronic and thermal Energies=	-1256.303517
Sum of electronic and thermal Enthalpies=	-1256.302573
Sum of electronic and thermal Free Energies=	-1256.382287

XYZ Coordinates (3j)

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001152	0.000006848	-0.000004825
2	6	0.000003671	-0.000006928	-0.000000301
3	6	-0.000002678	0.000003056	0.000007857
4	6	-0.000000281	-0.000002986	-0.000008863
5	6	0.000004981	-0.000004108	-0.000009150
6	6	-0.000001407	-0.000000787	0.000009911
7	7	-0.000001232	0.000008839	0.000010681
8	6	0.000025176	-0.000013041	-0.000002782
9	6	-0.000011953	0.000006380	0.000009178
10	6	-0.000020657	0.000001093	0.000005675
11	6	0.000007038	-0.000000044	0.000000220
12	6	-0.000001028	-0.000001900	0.000001493
13	7	0.000000176	0.000003464	-0.000006426
14	6	0.000001948	0.000001767	-0.000001042
15	6	-0.000004009	0.000001772	-0.000001059
16	6	-0.000001846	-0.000000370	-0.000004109
17	6	0.000008460	0.000001092	-0.000005028
18	7	-0.000005196	-0.000002221	0.000001327
19	6	0.000017021	-0.000003717	0.000002992
20	8	-0.000007399	0.000000884	-0.000003562
21	8	-0.000007962	0.000007274	0.000001146
22	6	-0.000001896	-0.000005428	-0.000005274
23	6	-0.000000228	-0.000001027	-0.000001823
24	6	0.000000237	-0.000000928	-0.000000097
25	6	-0.000000530	-0.000001385	-0.000000216
26	6	0.000002947	-0.000001025	-0.000000055
27	6	0.000001542	-0.000000539	0.000001045
28	6	0.000001310	-0.000001067	-0.000002321
29	7	0.000001105	-0.000002807	-0.000000131
30	1	0.000000959	0.000000673	0.000001600
31	1	0.000000078	0.000001715	0.000000966

32	1	0.000000545	-0.000000039	-0.000000879
33	1	0.000000717	0.000001469	0.000000847
34	1	-0.000005719	0.000001976	-0.000001623
35	1	-0.000006764	-0.000000673	-0.000000965
36	1	0.000001150	0.000001034	0.000001736
37	1	-0.000000195	0.000003289	0.000002014
38	1	0.000000545	0.000000380	0.000002170
39	1	0.000000196	0.000001632	0.000001013
40	1	0.000002938	0.000002414	0.000001187
41	1	-0.000002637	-0.000001452	-0.000000785
42	1	0.000000528	-0.000000268	0.000000056
43	1	-0.000002751	0.000001747	-0.000001472
44	1	-0.000000101	-0.000003095	0.000000209
45	1	0.000000447	-0.000002087	-0.000001593
46	1	0.000001372	-0.000000507	0.000000242
47	1	0.000000231	-0.000000370	0.000000816

E(b3lyp/6-31g) (d)= -1256.6970321
Zero-point correction= 0.367839 (Hartree/Particle)
Thermal correction to Energy= 0.392041
Thermal correction to Enthalpy= 0.392985
Thermal correction to Gibbs Free Energy= 0.313432
Sum of electronic and zero-point Energies= -1256.329193
Sum of electronic and thermal Energies= -1256.304991
Sum of electronic and thermal Enthalpies= -1256.304047
Sum of electronic and thermal Free Energies= -1256.383600

We found that the most stable configuration of **3j** was 4.15 kJ/mol lower in energy than the most stable configuration of isomers **3j'**. This result suggests that intermediate **C** could be easily transformed to more stable product **3j**.

X-ray structure of compound **3d** (Solvent has been omitted for clarity)

