

NMR Spectroscopic and Computational analysis of *E/Z* Isomerism in Imines

Derived from Isatin

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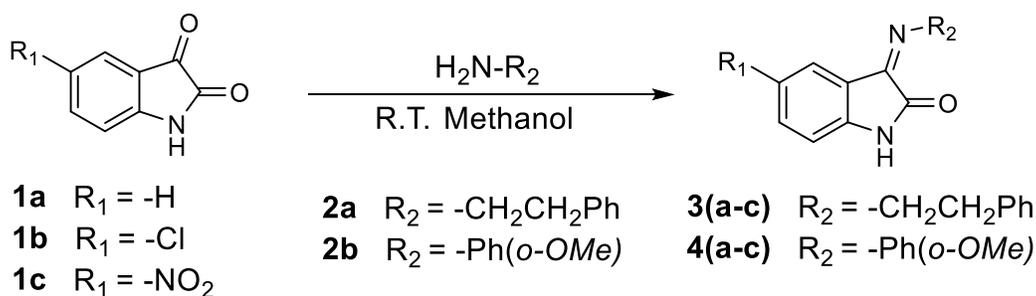
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Keywords: Isatin, Isomerization, Isomers, Schiff base.

Supplementary information

Spectroscopic data

An equimolar amount of Isatin (1a-c) was added to an amine (2a-b) solution (500 mg, 4 mmol) in methanol (10 mL). The mixture was stirred at room temperature (RT) for 24 h. The resulting precipitate was filtered and washed with cold methanol. The resulting product was characterized by melting point, ¹H- and ¹³C-NMR spectroscopy and mass spectrometry (ESI-MS)



¹H-NMR (CDCl₃)
3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3a)

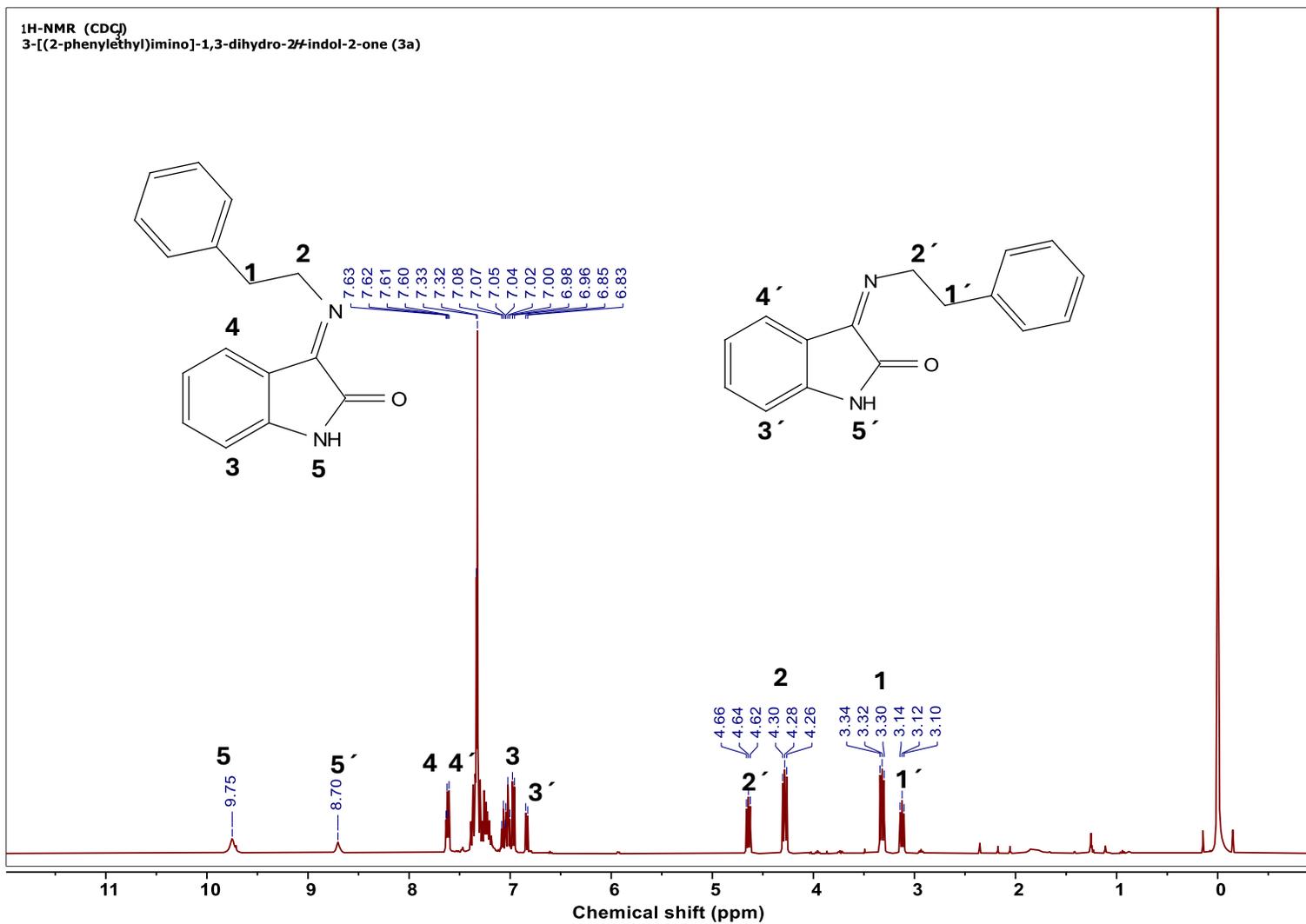


Figure S1: ¹H-NMR of 3a in CDCl₃

¹³C-NMR (CDCl₃)
3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3a)

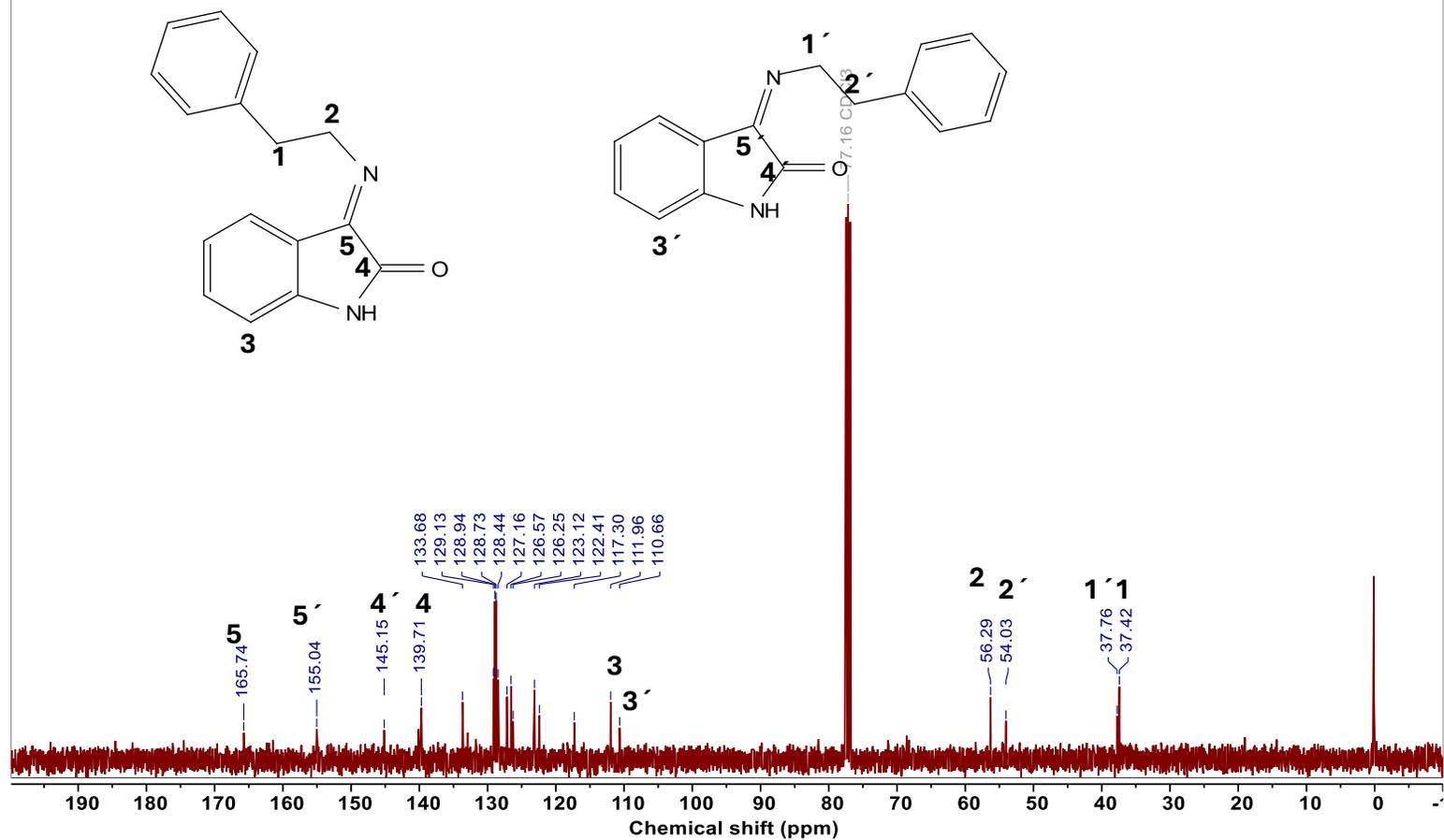


Figure S2: ¹³C-NMR of 3a in CDCl₃

¹H-NMR (d₆-DMSO)
3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3a)

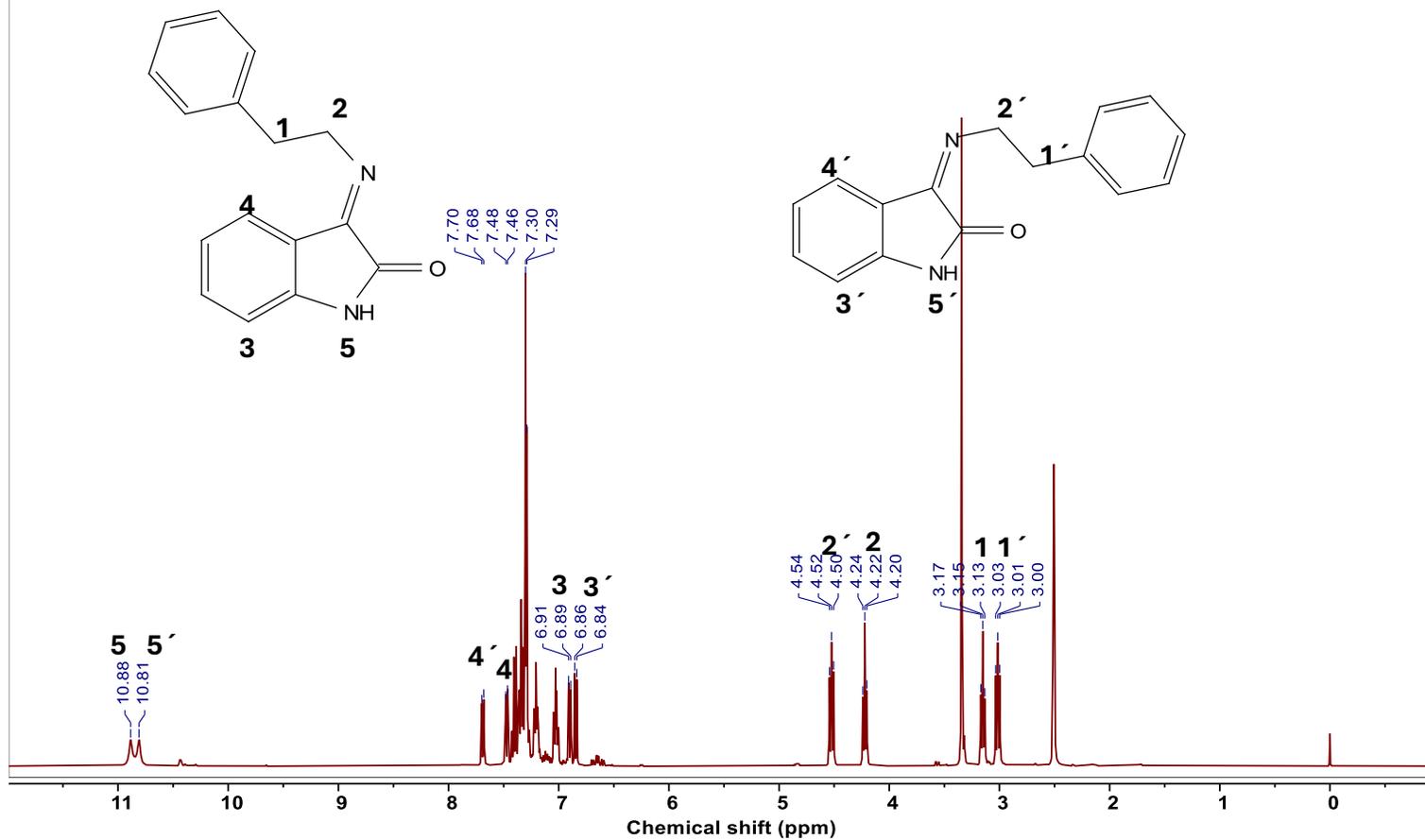


Figure S3: ¹H-NMR of 3a in d₆-DMSO

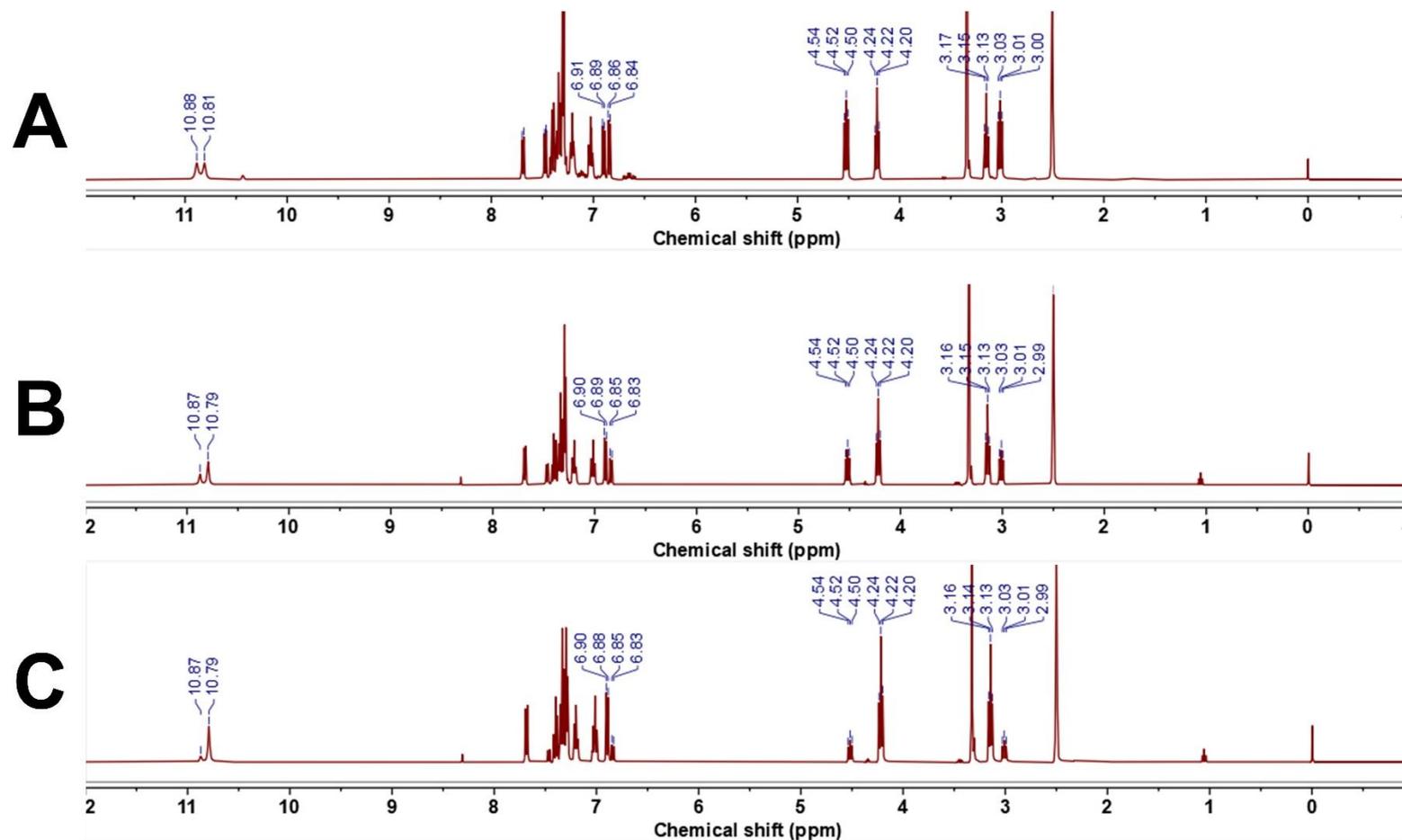


Figure S4: $^1\text{H-NMR}$ of **3a** in $\text{d}_6\text{-DMSO}$ at different time after dissolving the sample: 24h (A), 4h (B) and 30 min (C)

¹³C-NMR (d₆-DMSO)
3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3a)

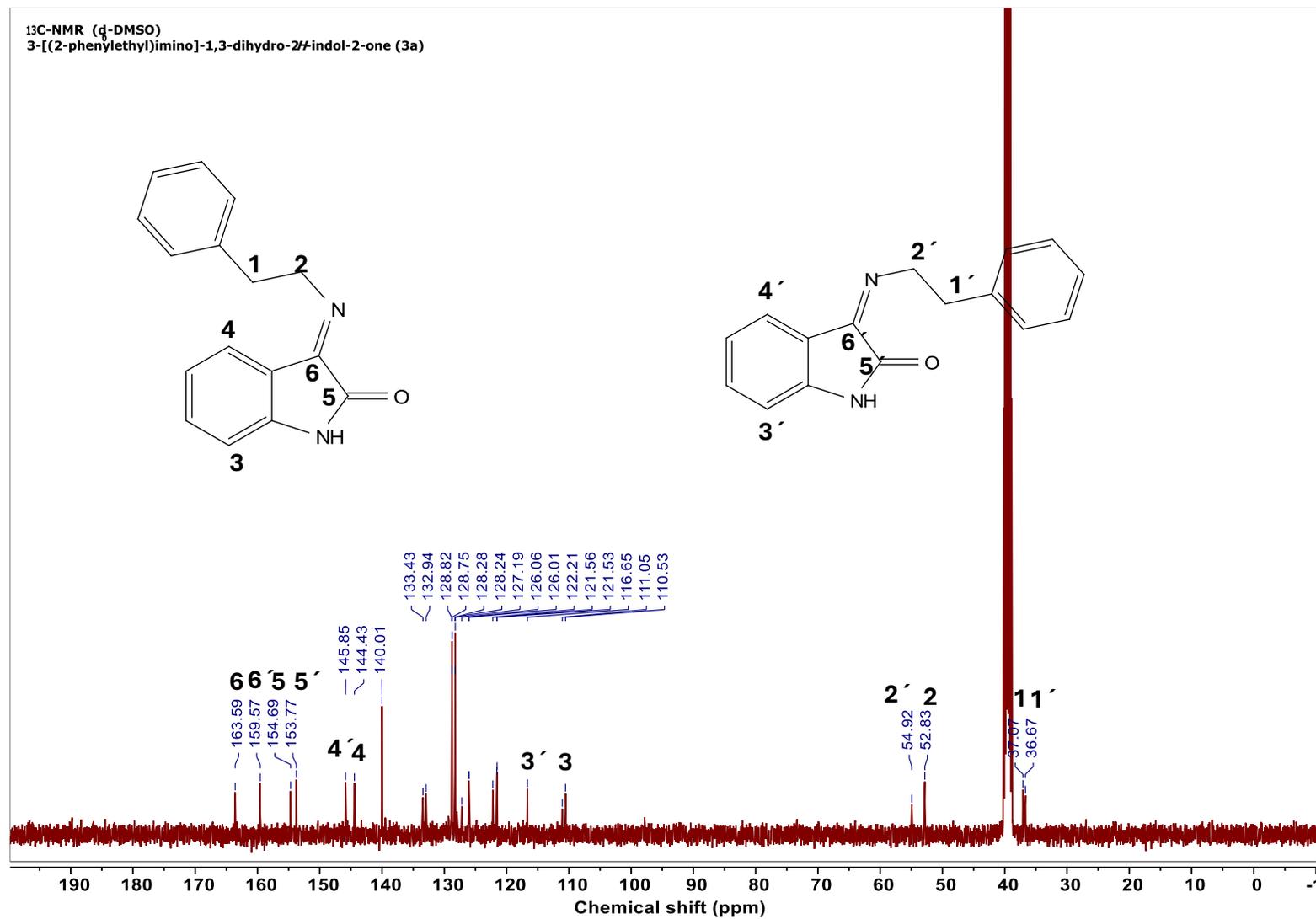


Figure S5: ¹³C-NMR of 3a in d₆-DMSO

NOESY (d-DMSO)
3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3a)

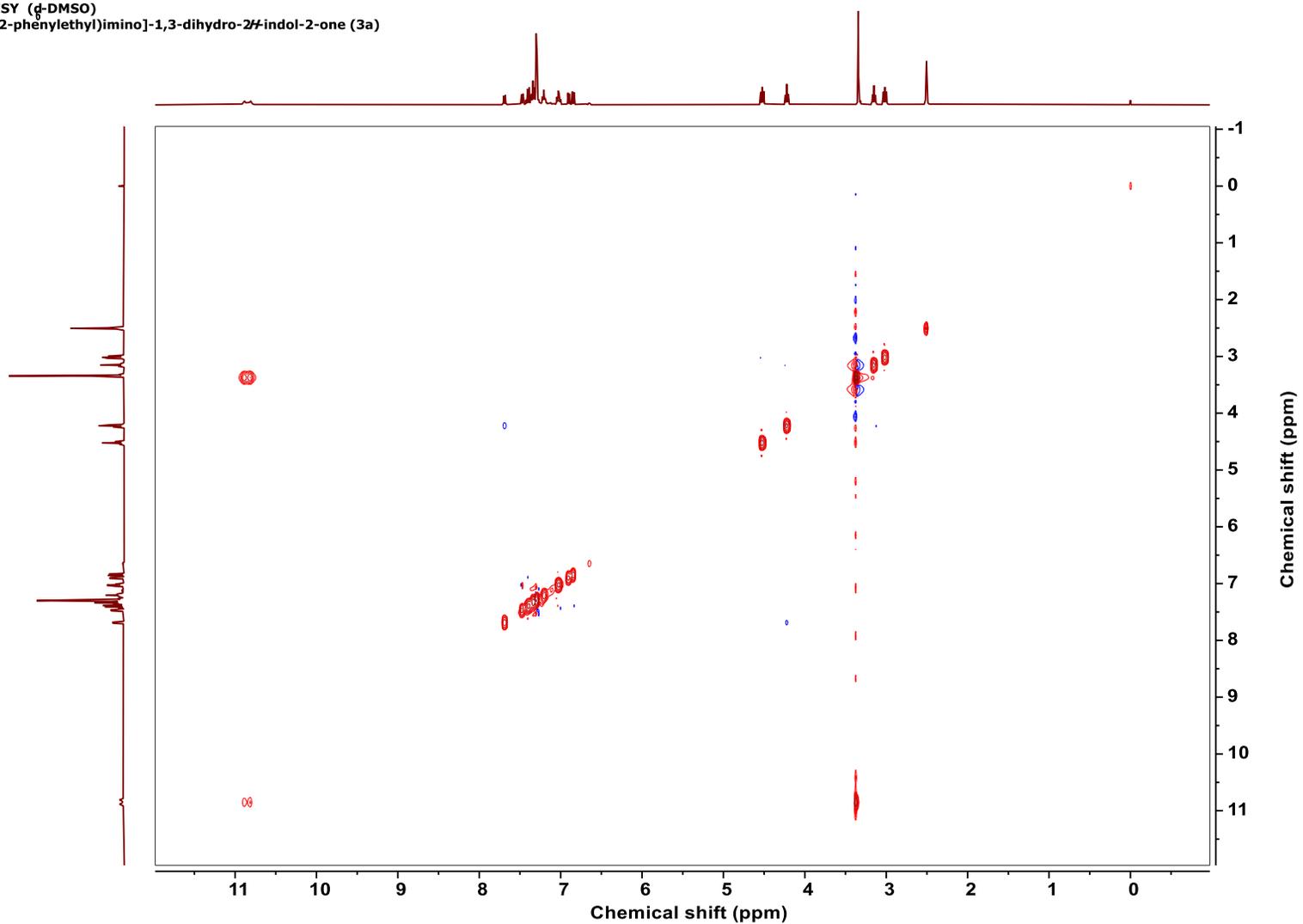


Figure S6: NOESY of 3a in d₆-DMSO

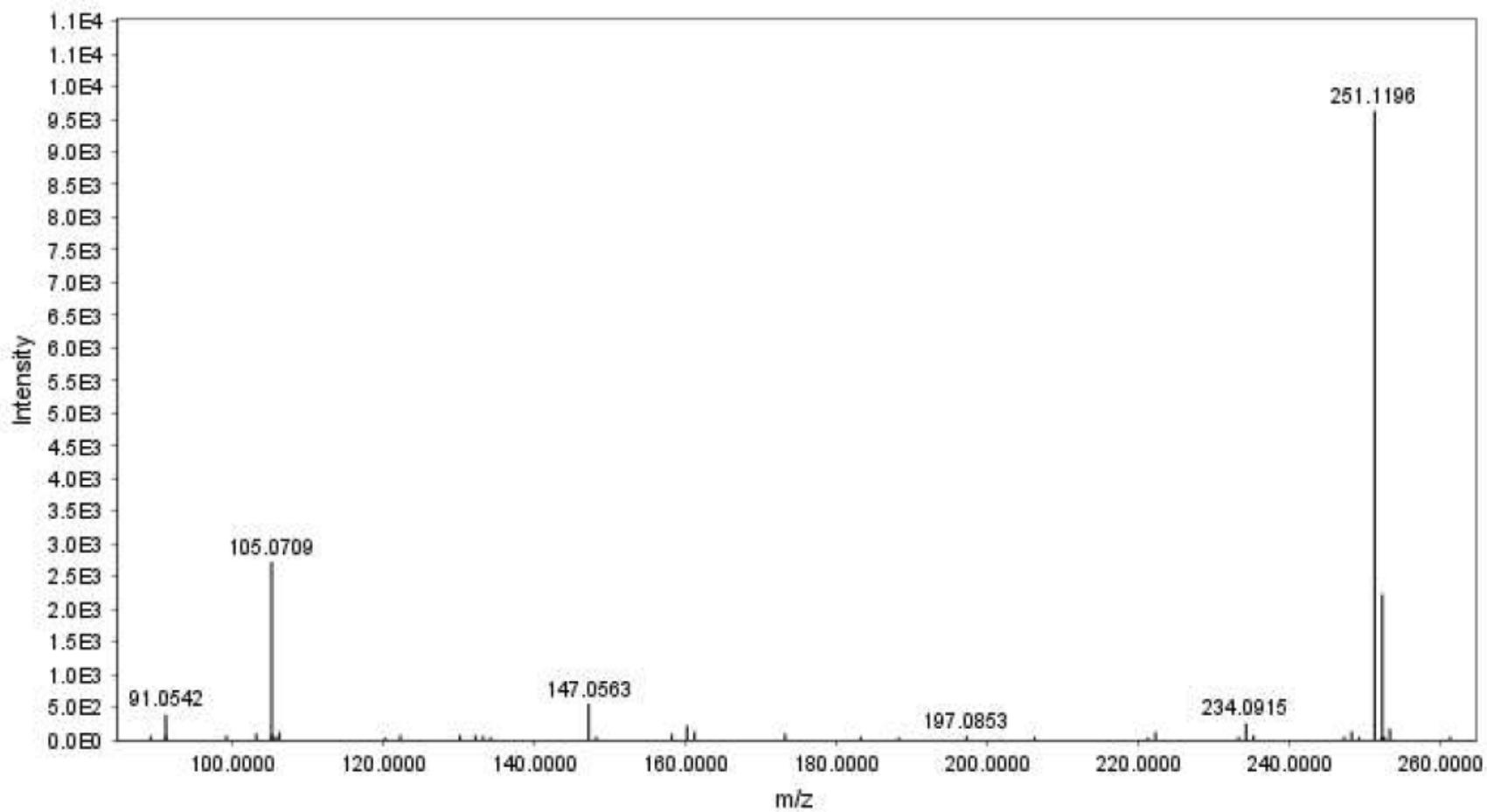


Figure S7: Mass spectra (ESI-MS) of **3a**

¹H-NMR (d₆-DMSO)
5-chloro-3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3b)

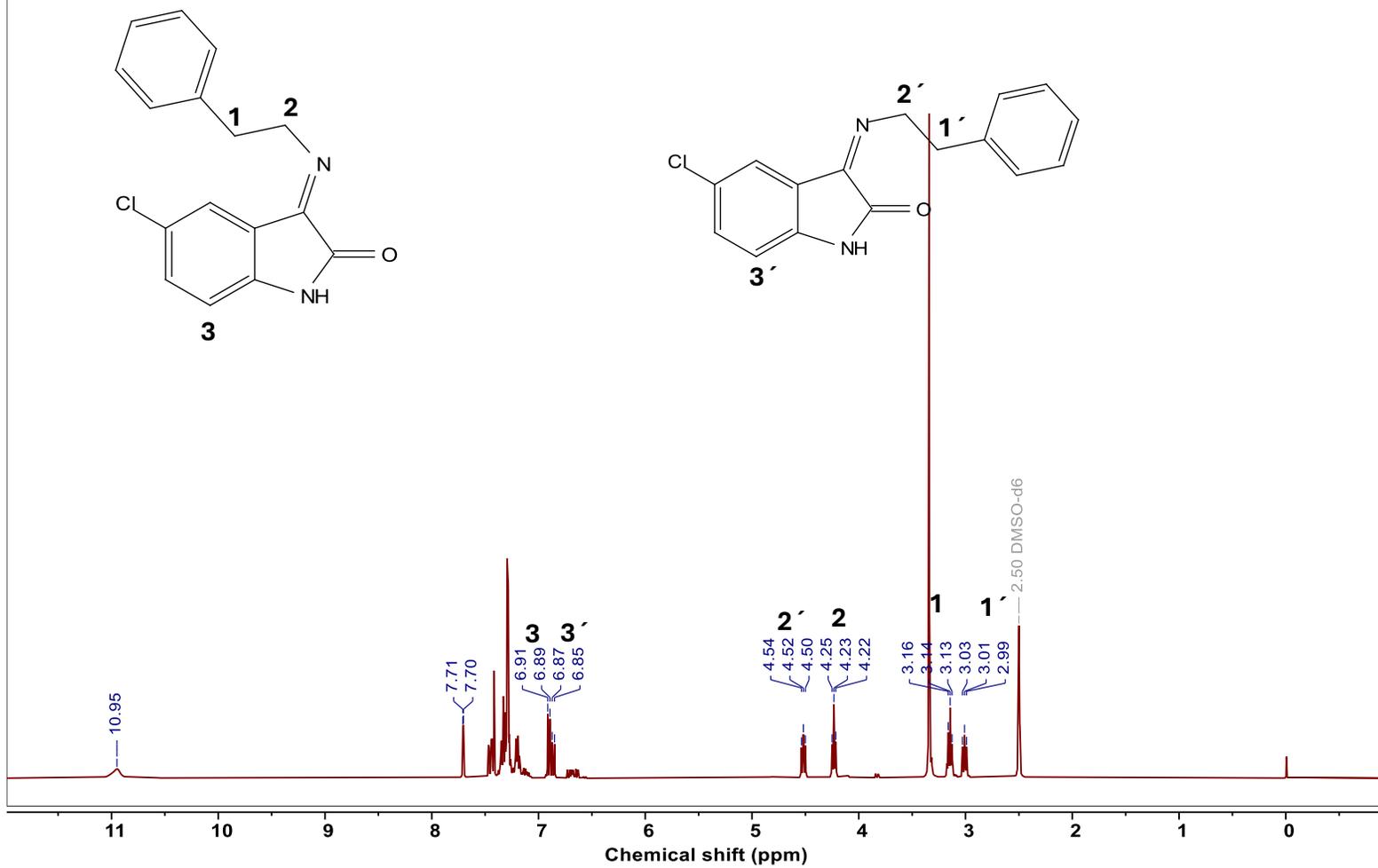


Figure S8: ¹H-NMR of 3b in d₆-DMSO

¹³C-NMR (d₆-DMSO)
5-chloro-3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3b)

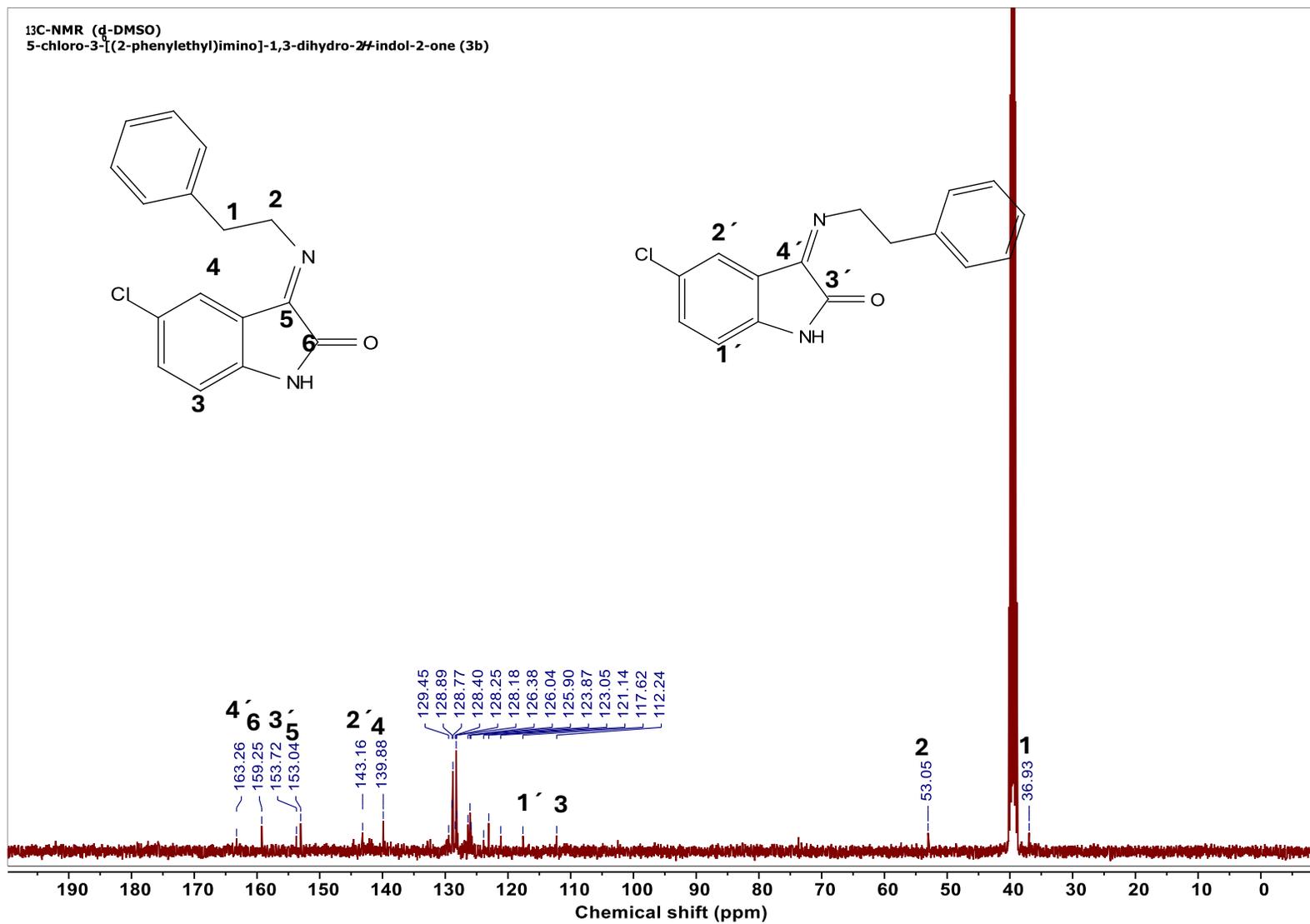
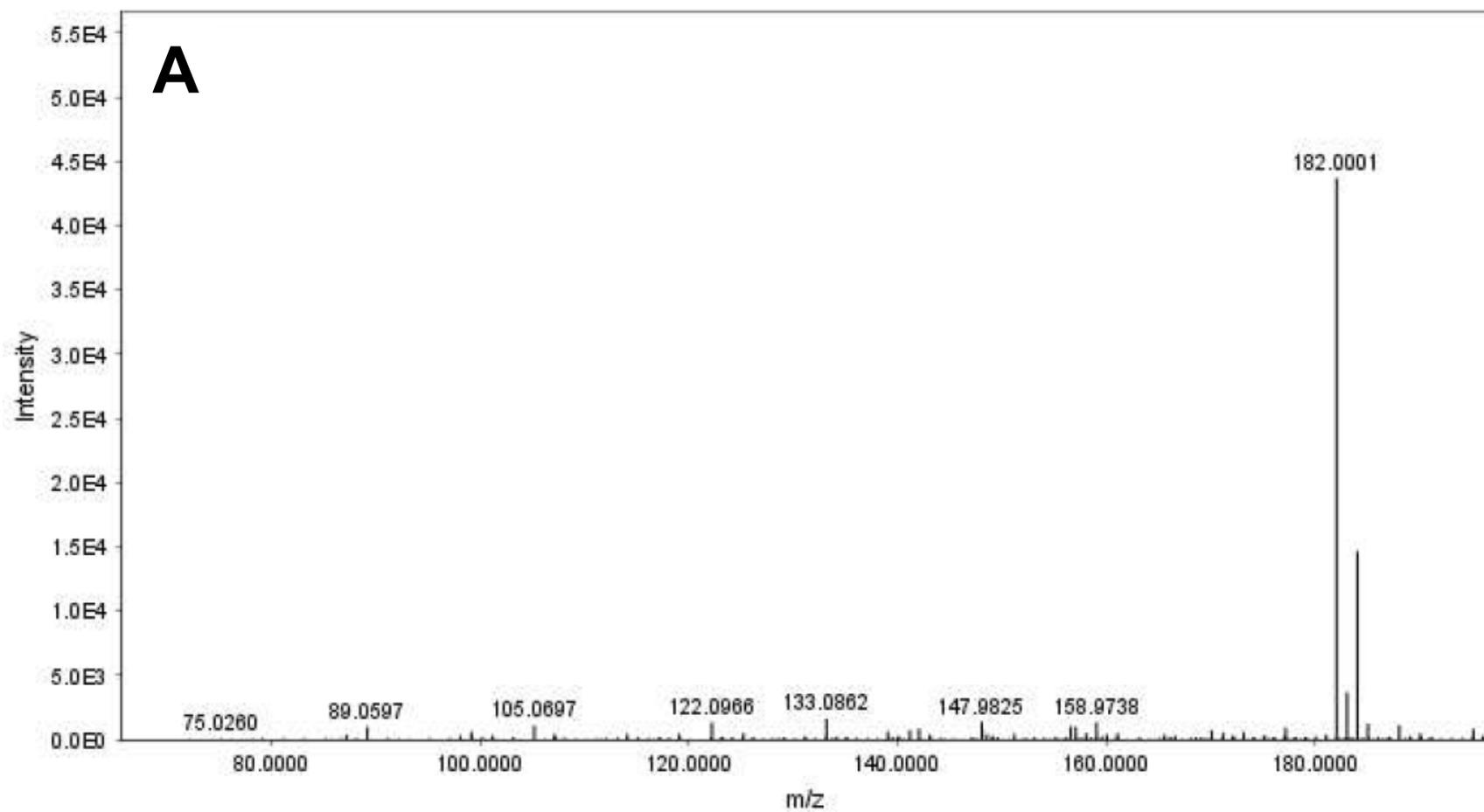


Figure S9: ¹³C-NMR of 3b in d₆-DMSO



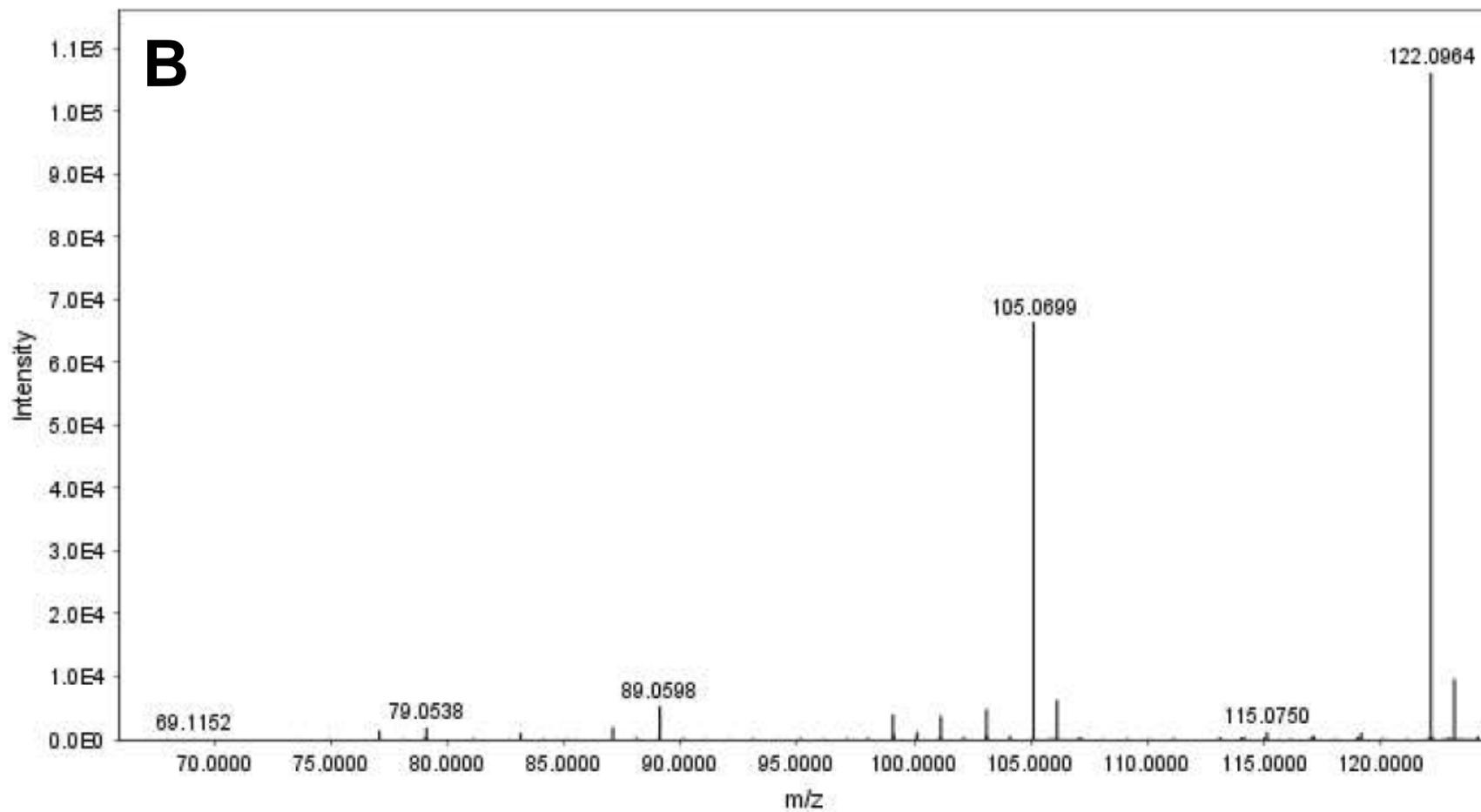


Figure S10: Mass spectra (ESI-MS) of the precursors of **3b**. 5-chloroisatin **1b** (A) and phenylethylamine **2a** (B)

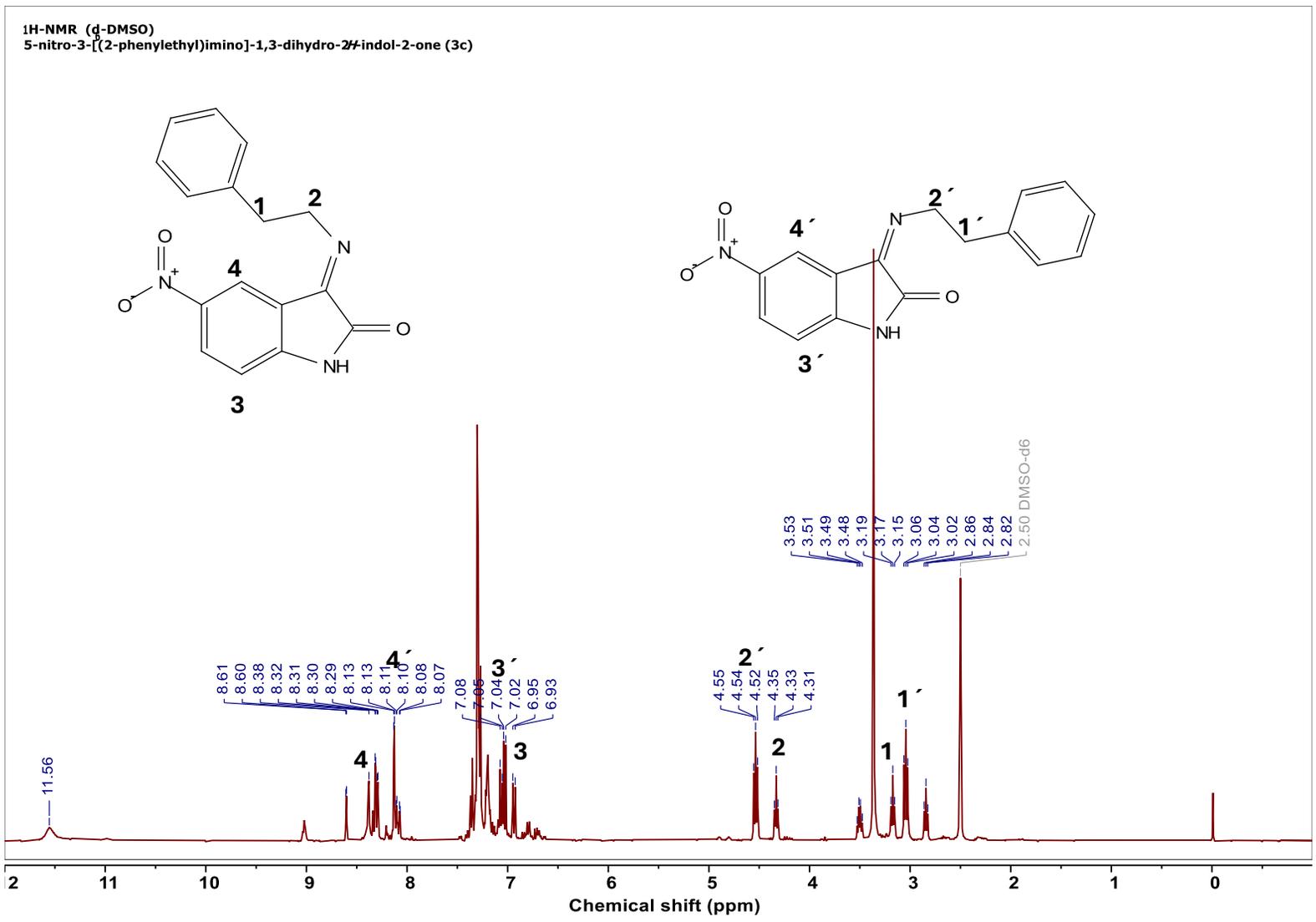


Figure S11: ¹H-NMR of **3c** and partial hydrolysis in solution of d₆-DMSO

¹³C-NMR (d₆-DMSO)
5-nitro-3-[(2-phenylethyl)imino]-1,3-dihydro-2H-indol-2-one (3c)

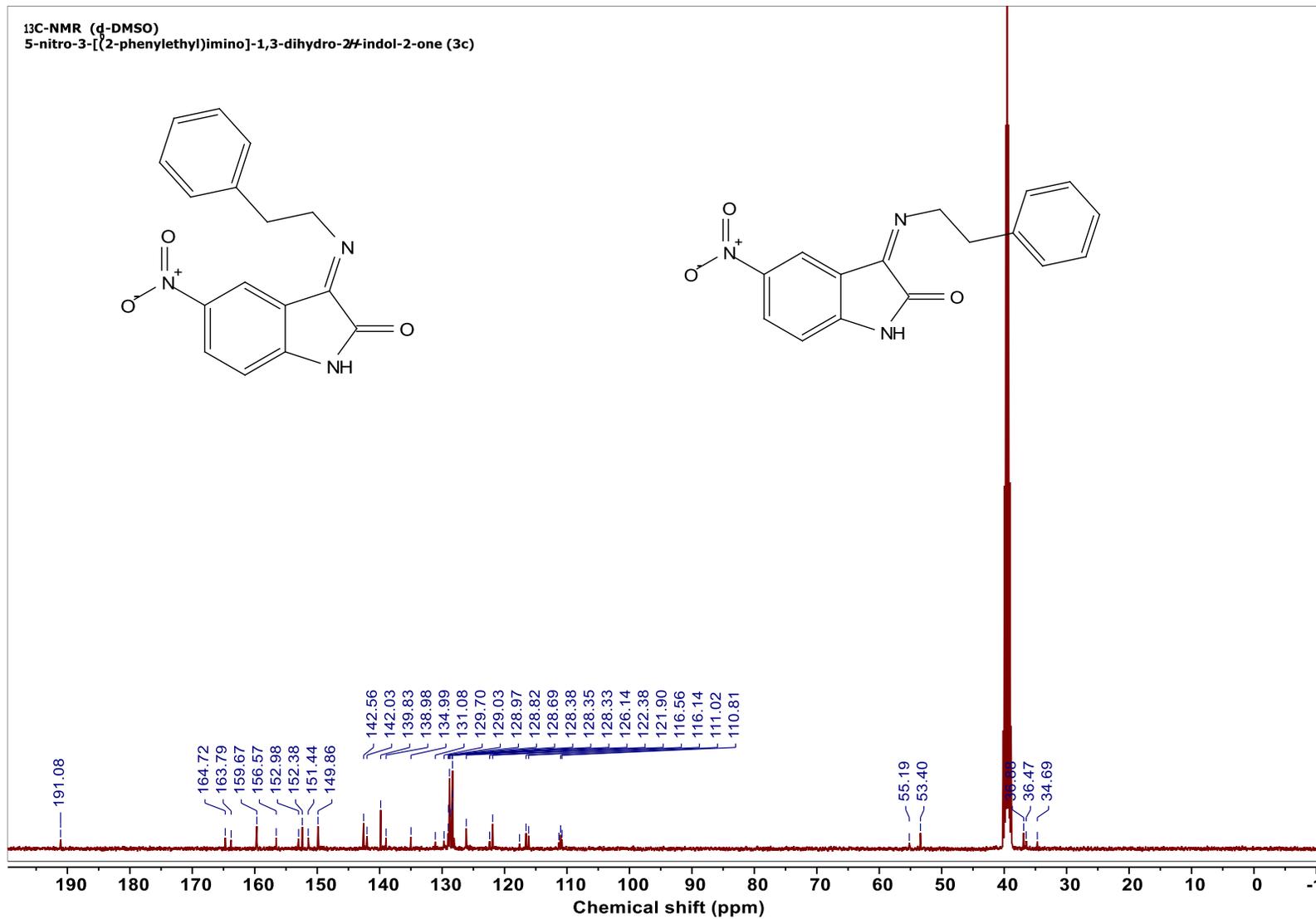


Figure S12: ¹³C-NMR of 3c and partial hydrolysis in solution of d₆-DMSO

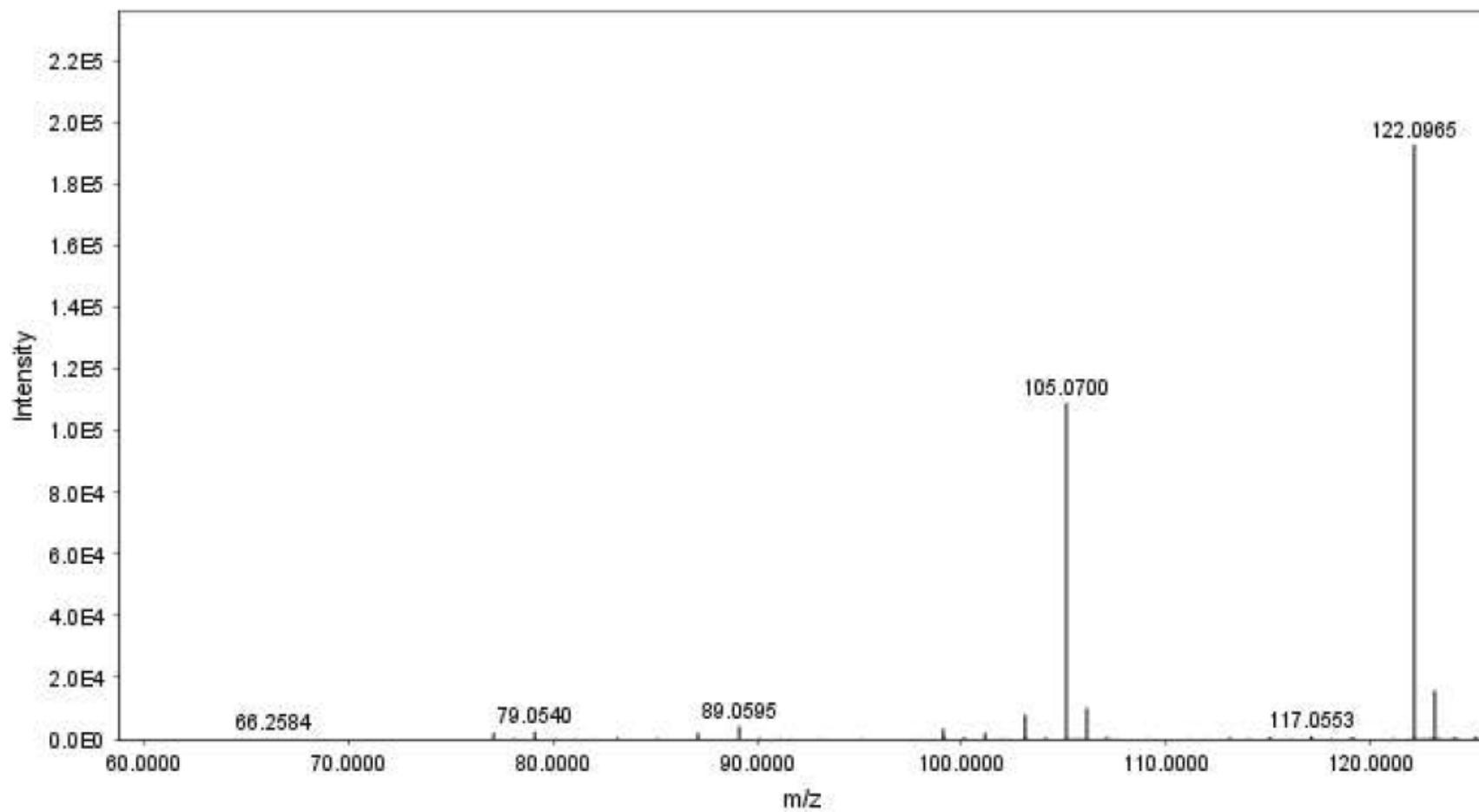


Figure S13: Mass spectra (ESI-MS) of the precursors of **3c**, phenylethylamine **2a**.

¹H-NMR (d₆-DMSO)
3-[(*p*-methoxyphenyl)imino]-1,3-dihydro-2*H*-indol-2-one (4a)

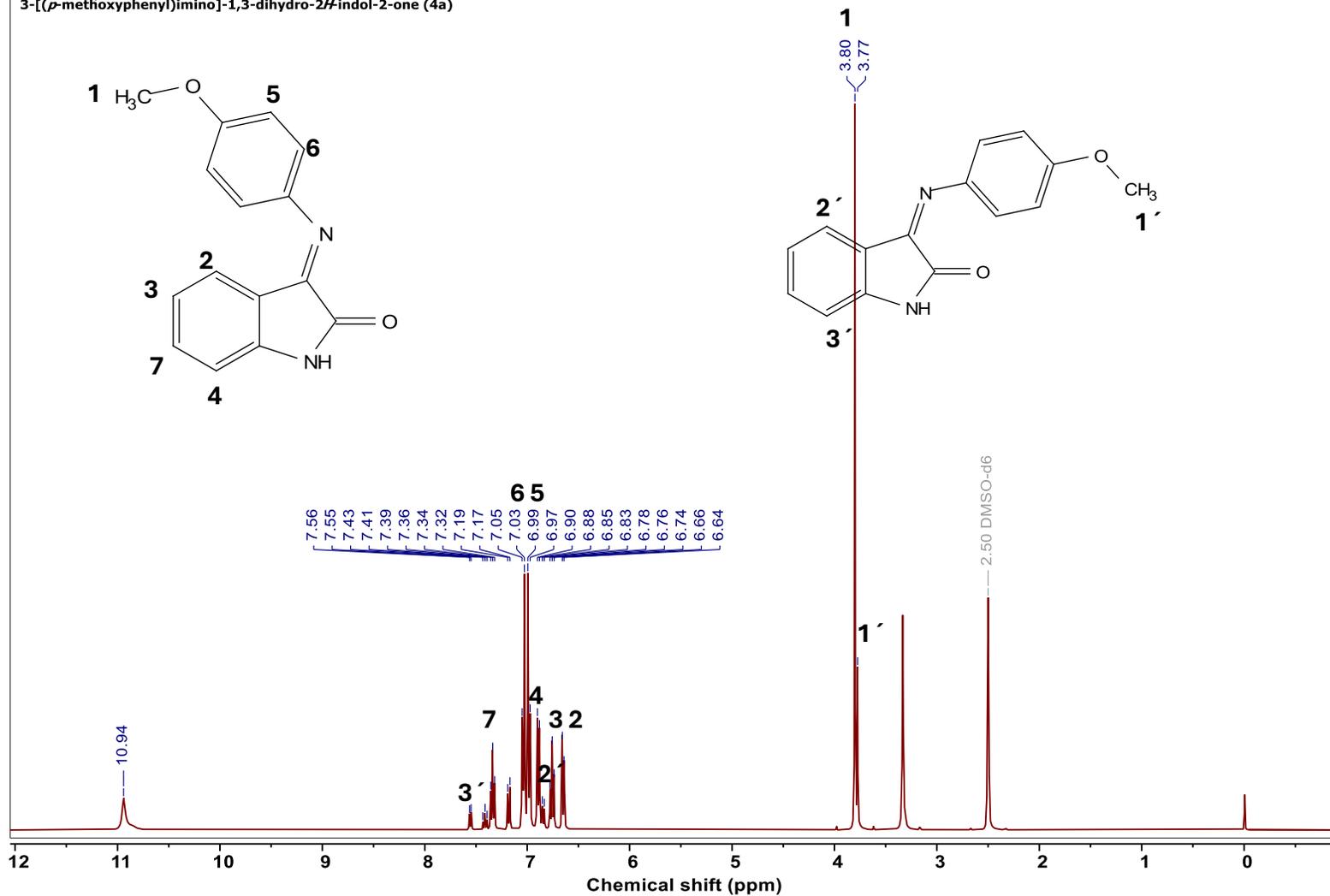


Figure S14: ¹H-NMR of 4a in d₆-DMSO

¹³C-NMR (d₆-DMSO)
3-[[p-methoxyphenyl]imino]-1,3-dihydro-2H-indol-2-one (4a)

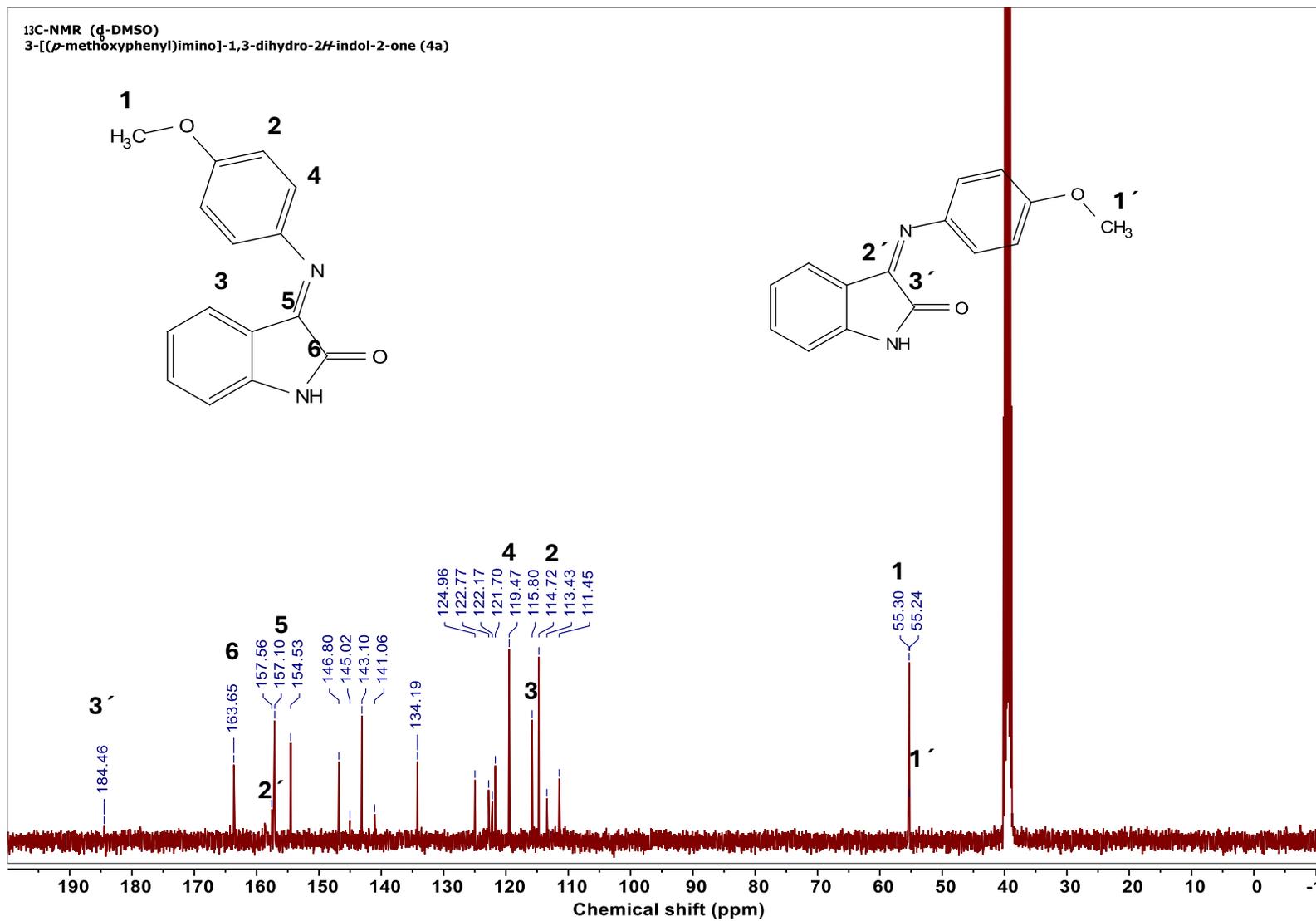


Figure S15: ¹³C-NMR of 4a in d₆-DMSO

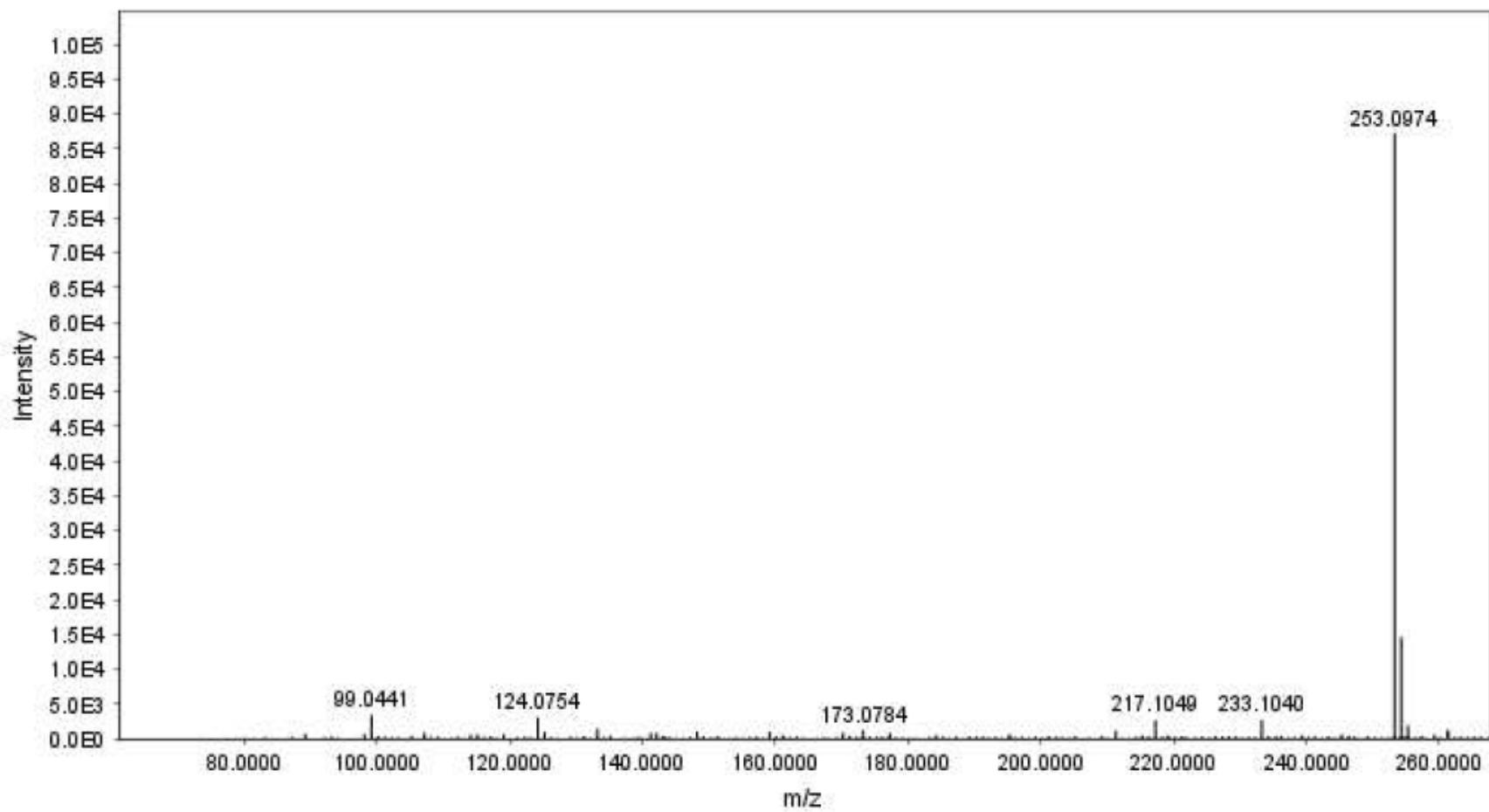


Figure S16: Mass spectra (ESI-MS) of 4a

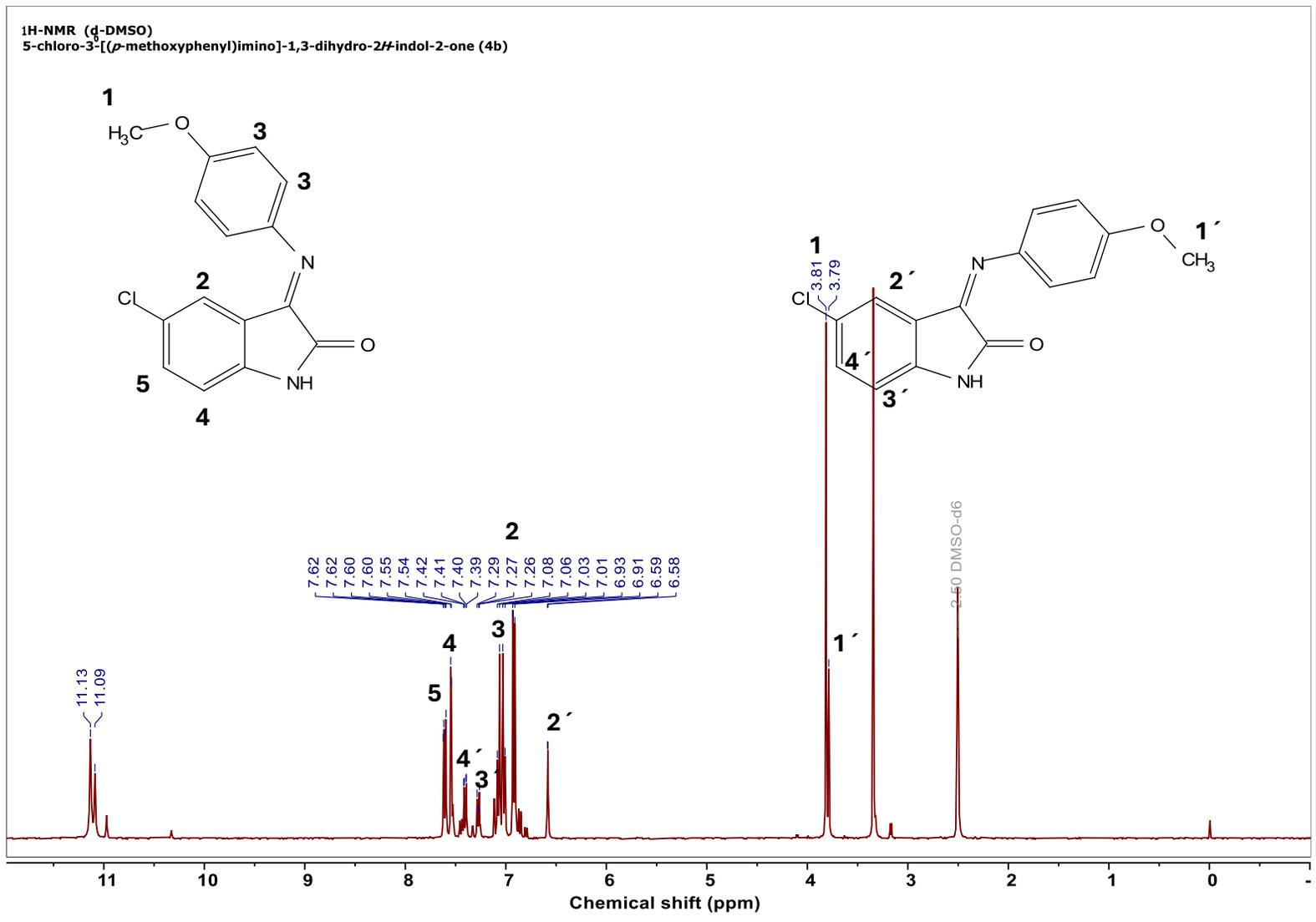


Figure S17: ¹H-NMR of **4b** in d₆-DMSO

¹³C-NMR (d₆-DMSO)
5-chloro-3-[(*p*-methoxyphenyl)imino]-1,3-dihydro-2*H*-indol-2-one (4b)

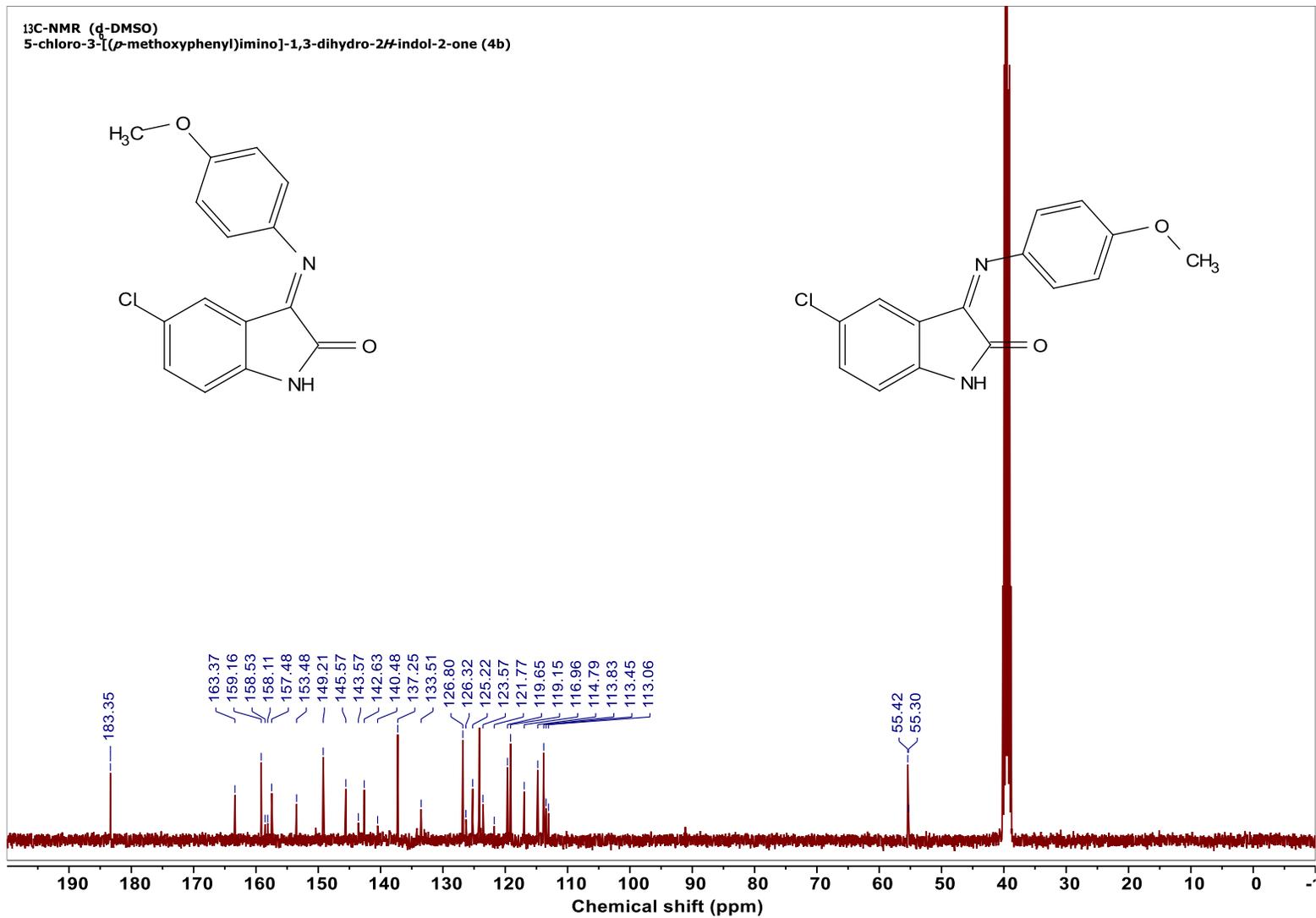


Figure S18: ¹³C-NMR of 4b in d₆-DMSO

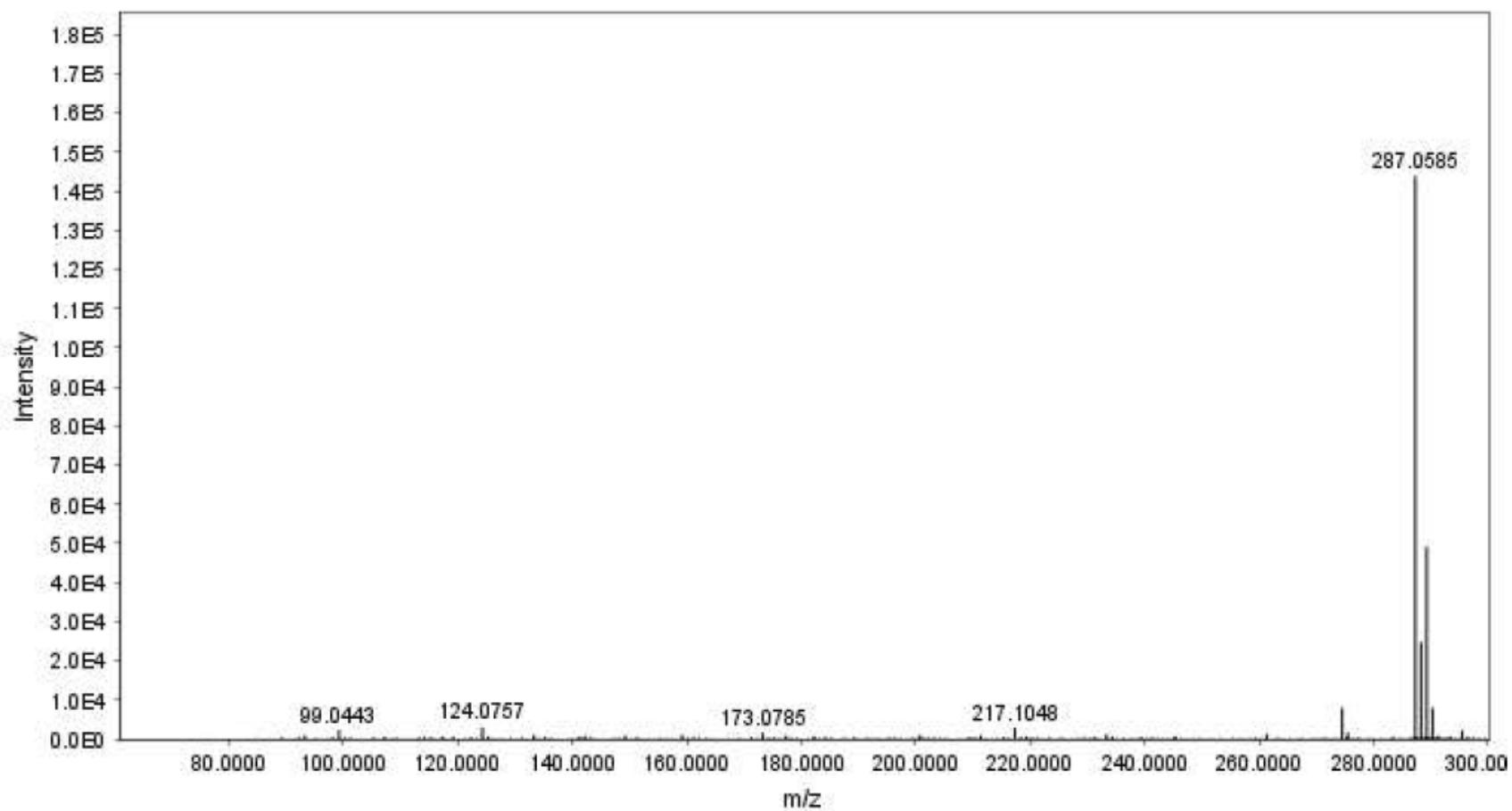


Figure S19: Mass spectra (ESI-MS) of **4b**

¹H-NMR (d₆-DMSO)
5-nitro-3-[(*p*-methoxyphenyl)imino]-1,3-dihydro-2*H*-indol-2-one (**4c**)

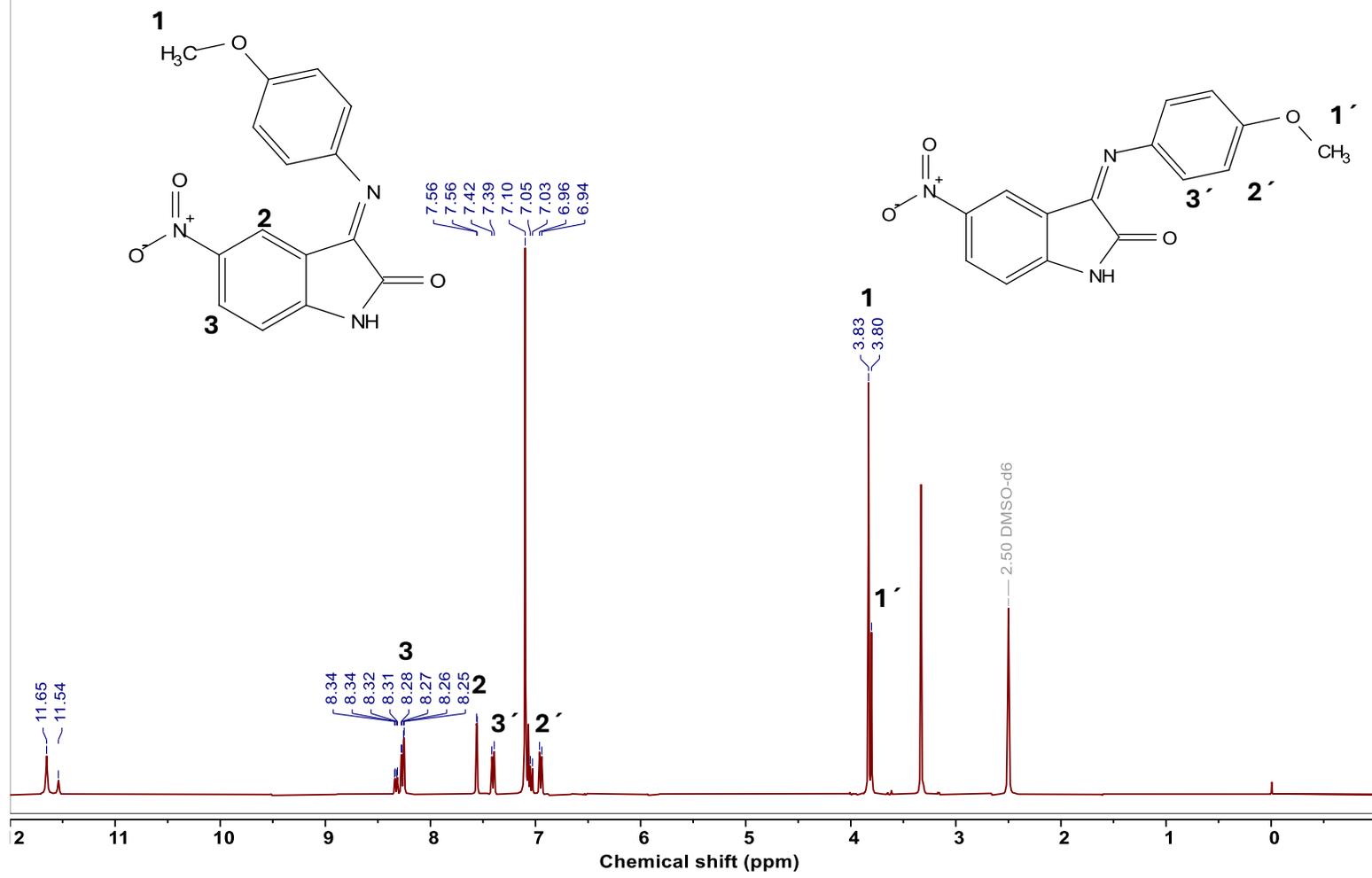


Figure S20: ¹H-NMR of **4c** in d₆-DMSO

¹³C-NMR (d₆-DMSO)
5-nitro-3-[(*p*-methoxyphenyl)imino]-1,3-dihydro-2*H*-indol-2-one (4c)

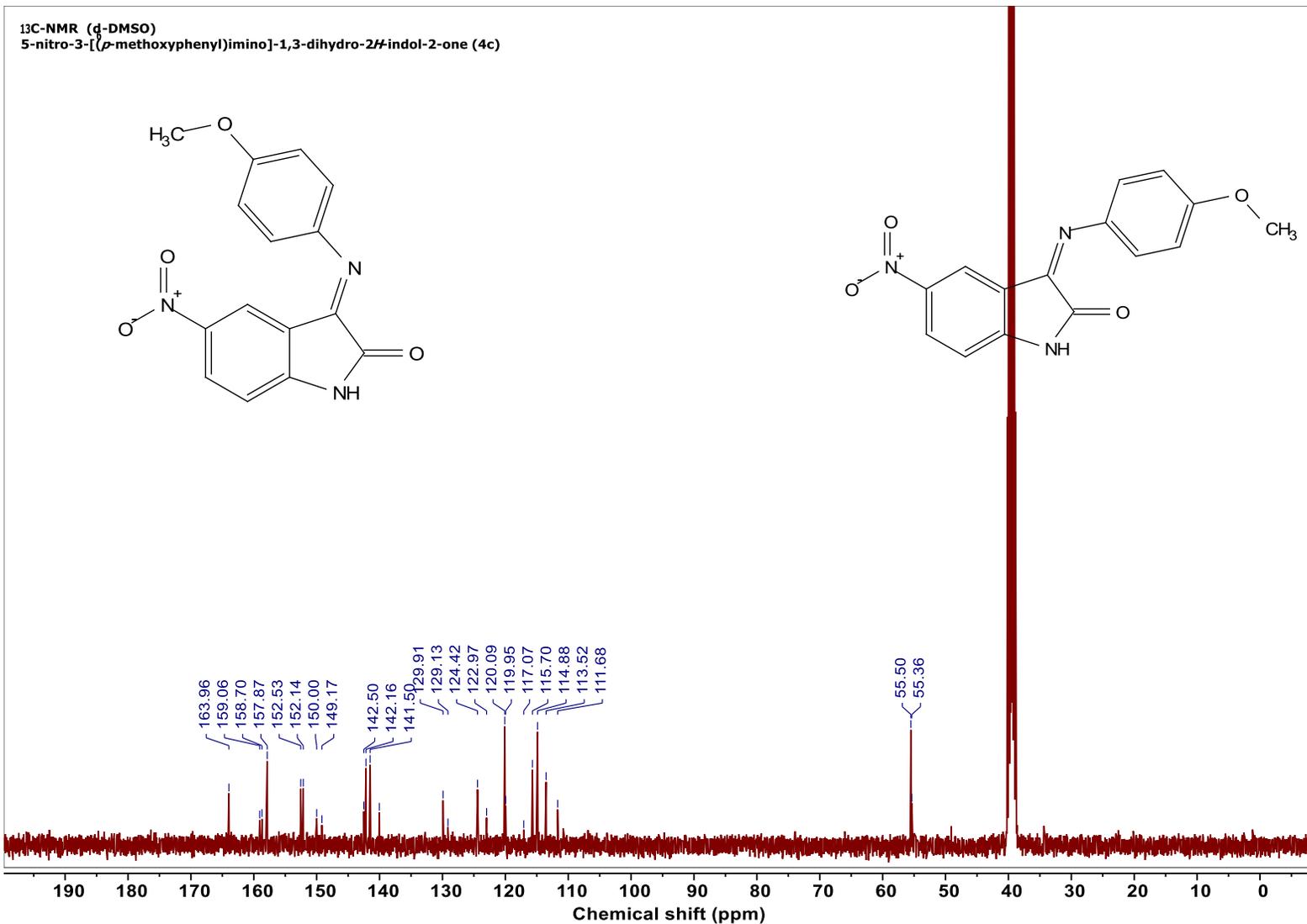


Figure S21: ¹³C-NMR of 4c in d₆-DMSO

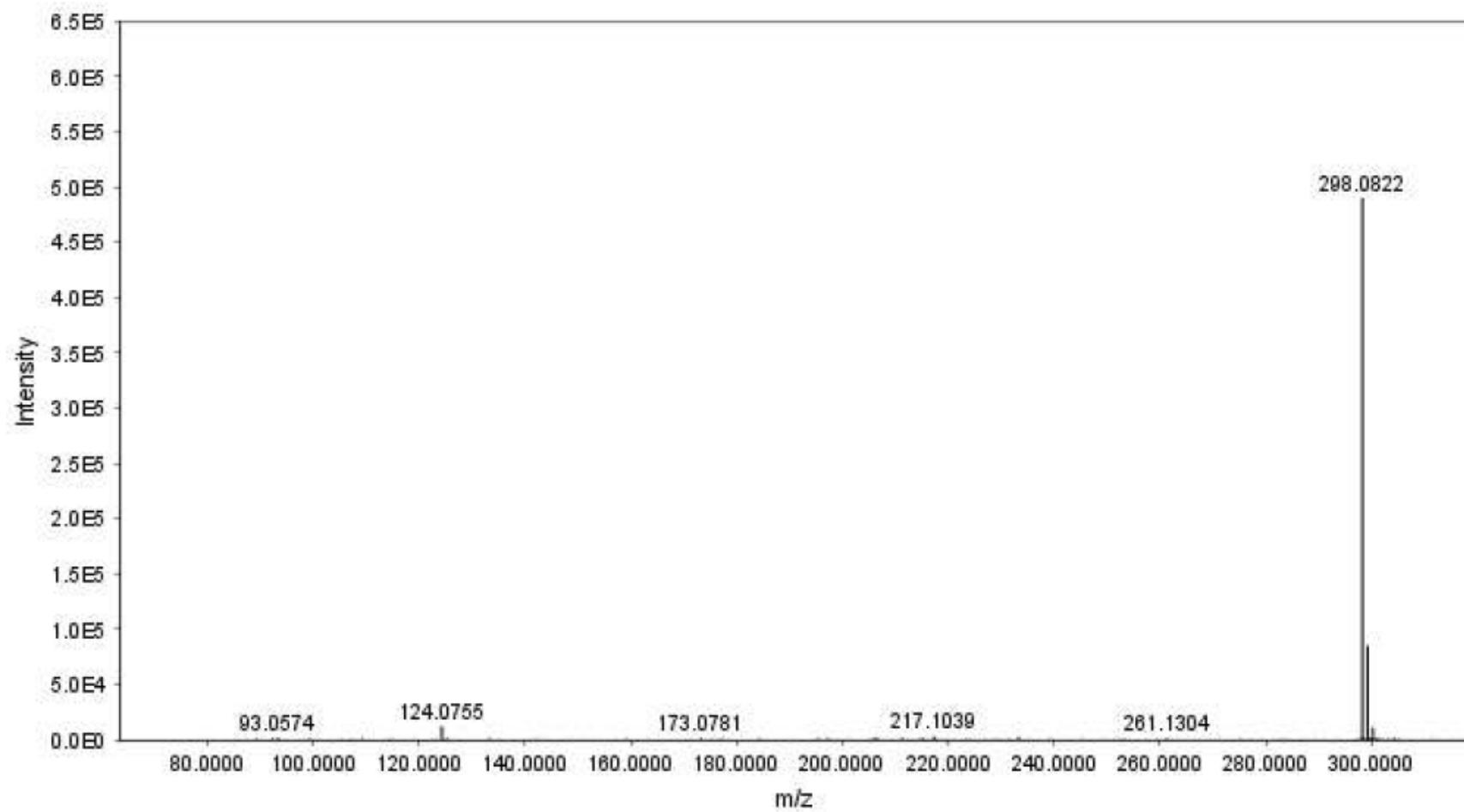


Figure S22: Mass spectra (ESI-MS) of 4c

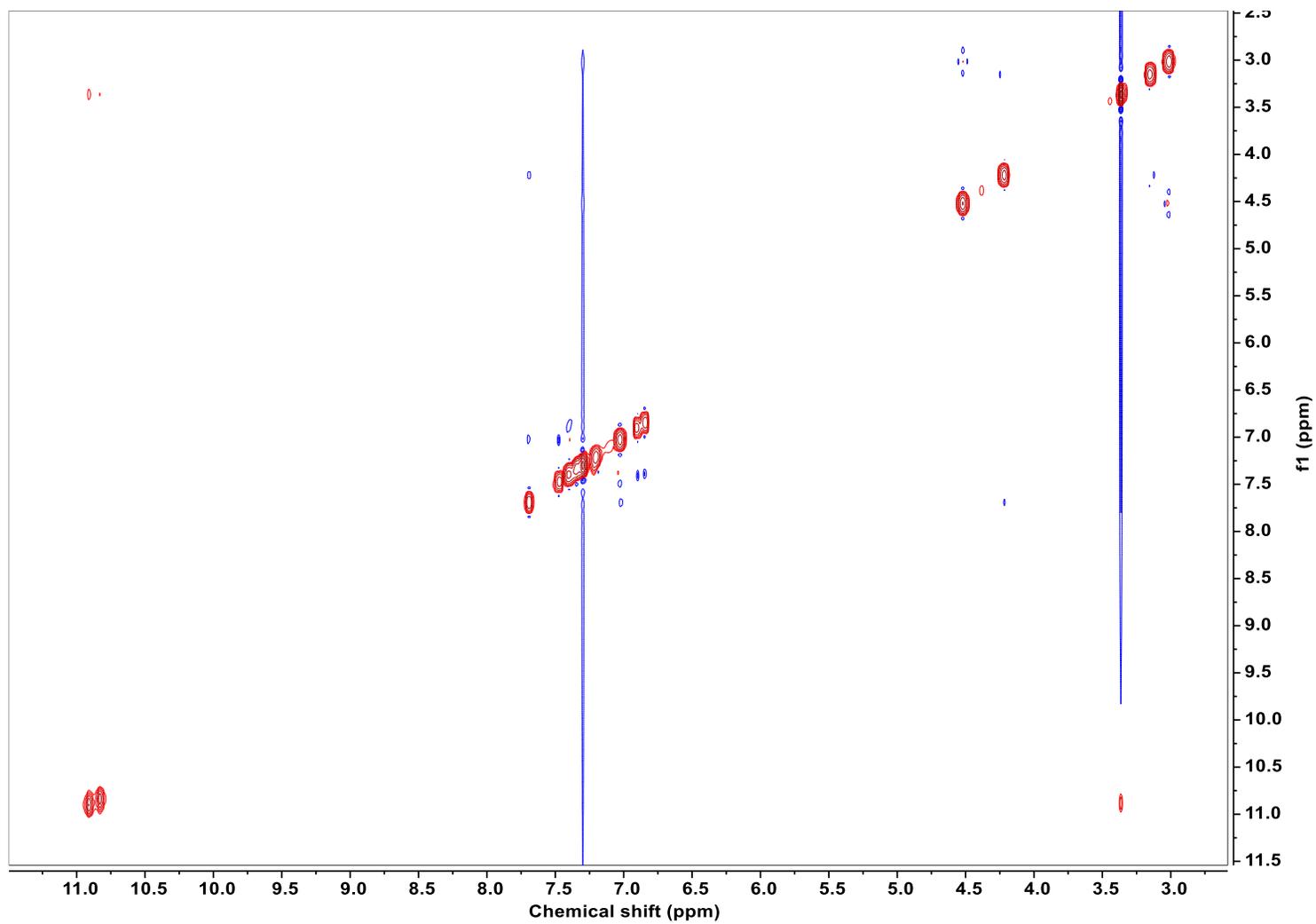


Figure S23: EXSY spectra of **3a** (Mixing time 150 ms)

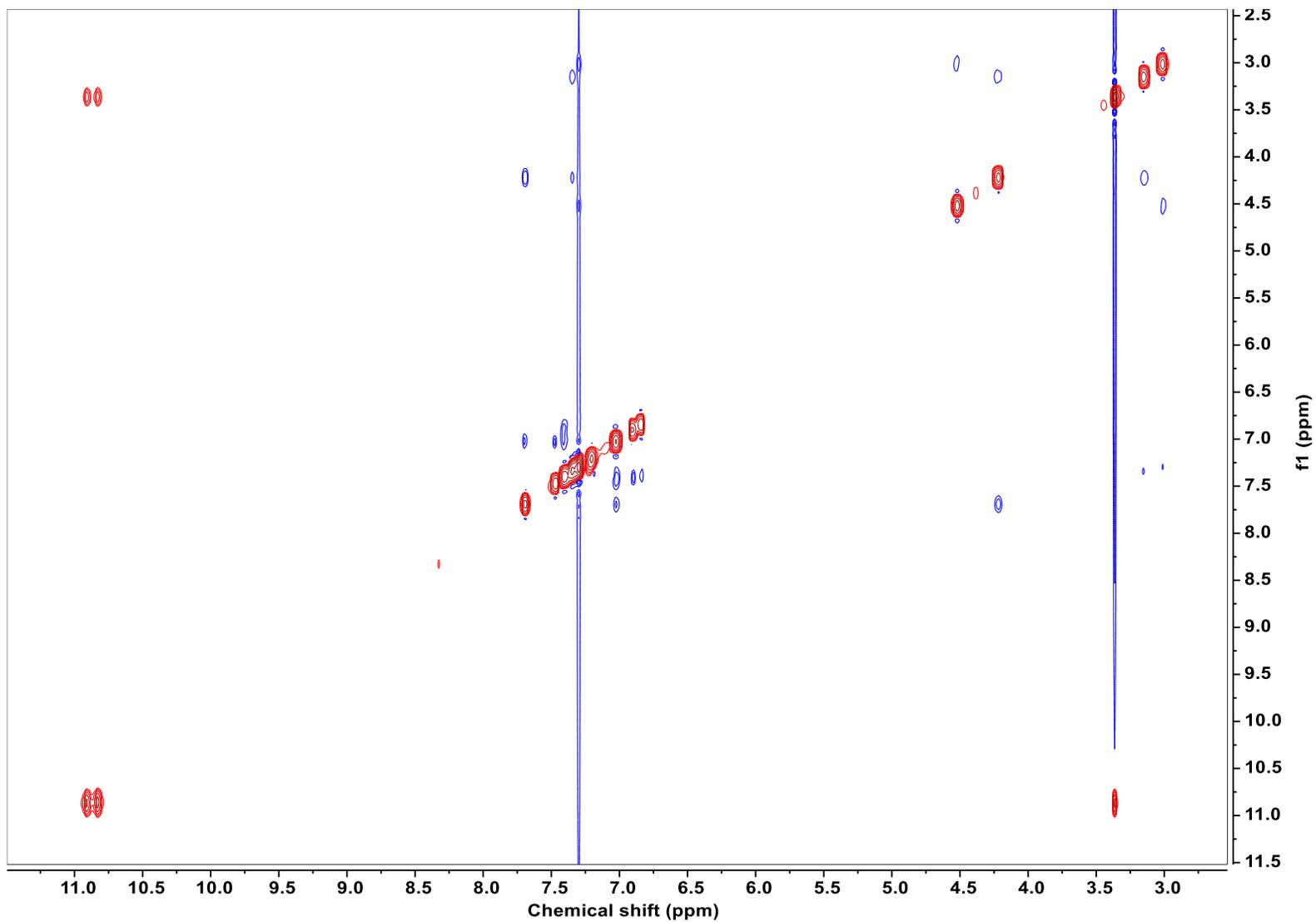


Figure S24: EXSY spectra of **3a** (Mixing time 500 ms)

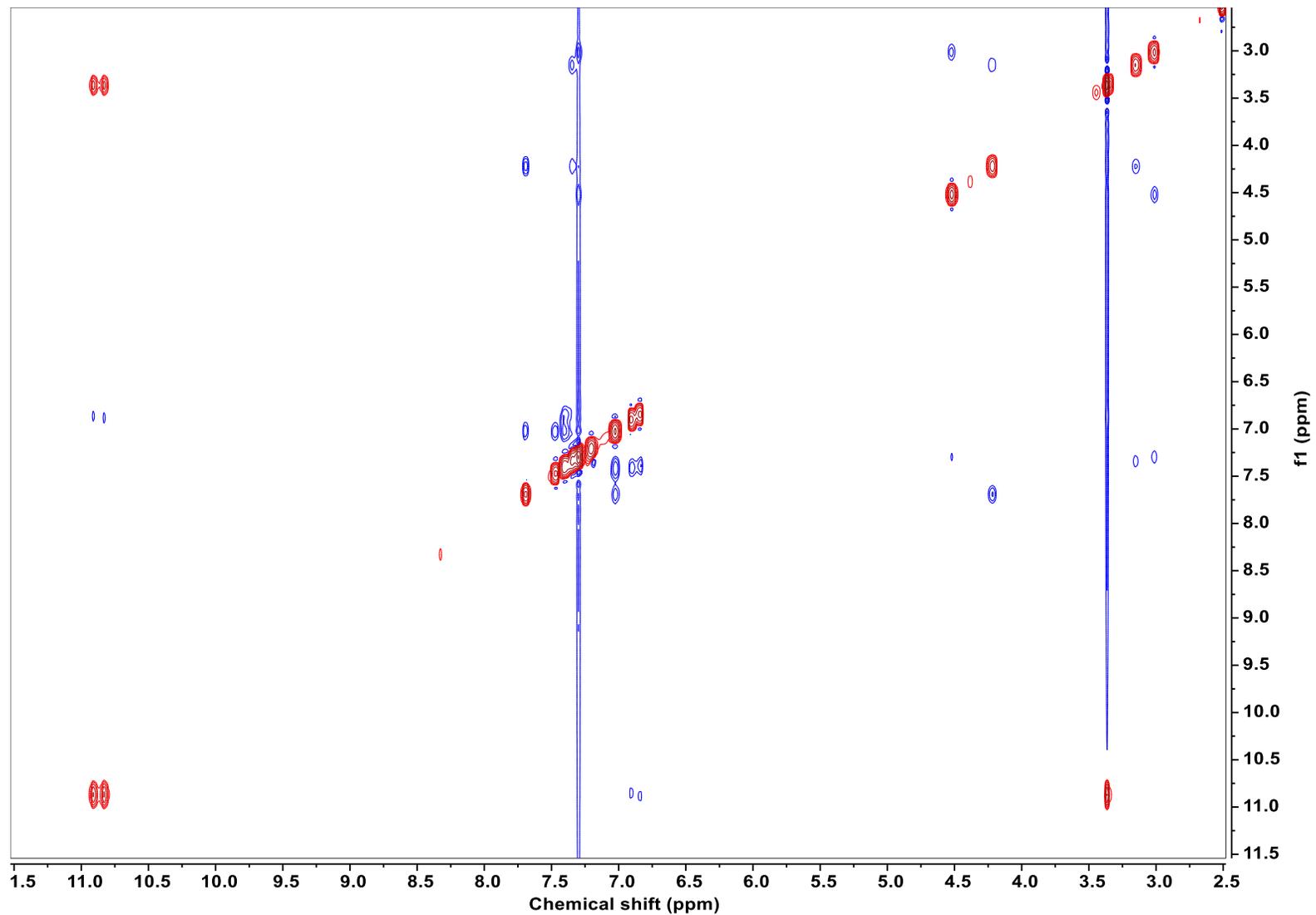


Figure S25: EXSY spectra of **3a** (Mixing time 1000 ms)

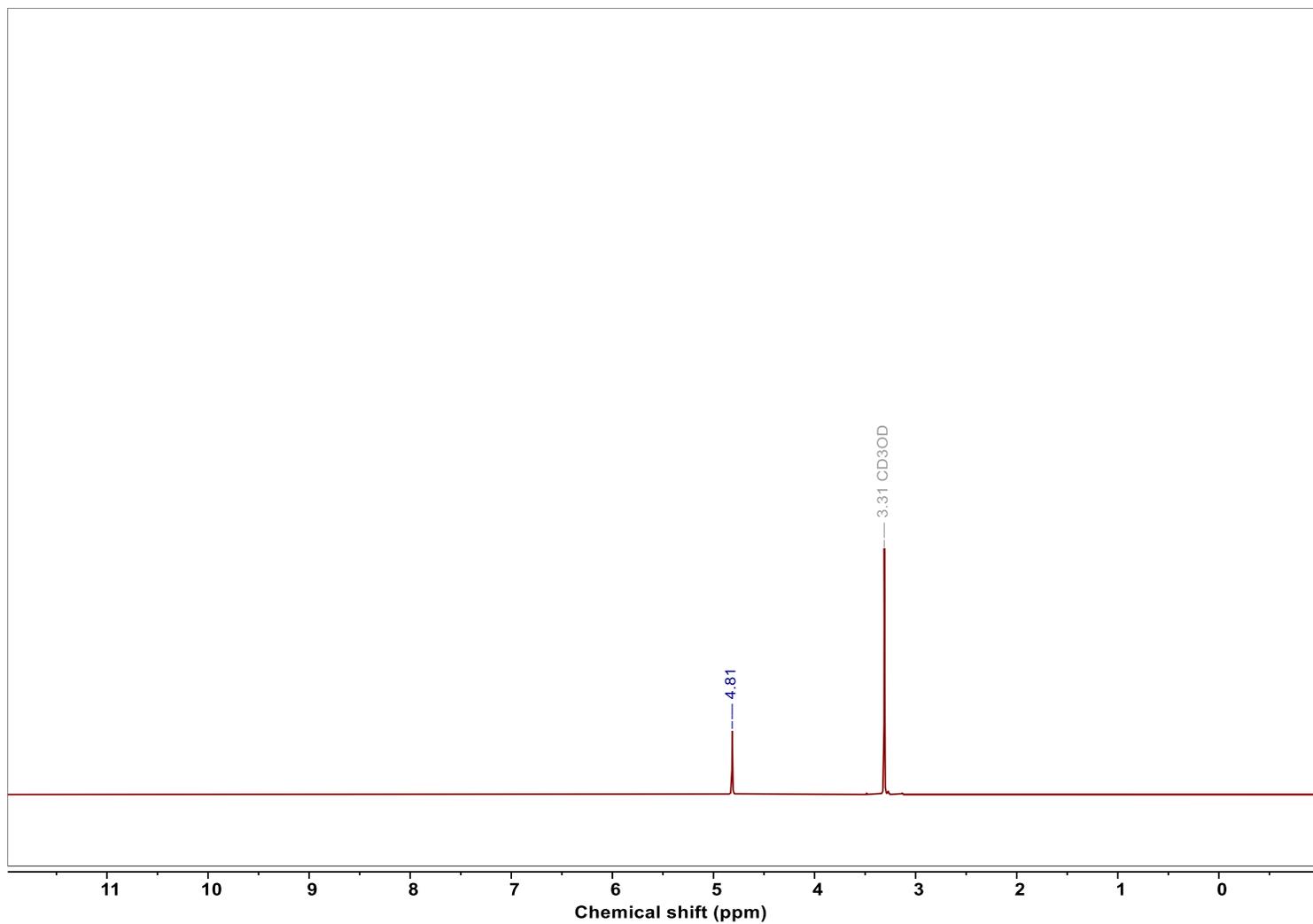


Figure S26: Temperature calibration spectra (4% Methanol in d_4 -Methanol). Calibration equation (VTU calibration) for 4% Methanol in d_4 -Methanol in a temperature range from 270K to 300K. $T = (4.109 - \Delta\delta) / 0,008708$

Computational data (Cartesian coordinates)

Geometrical optimizations and frequency calculations in the gas phase were carried out using *Gaussian 16* with the B3LYP DFT functional, Grimme's D3BJ dispersion correction, and the 6-311++G(d,p) basis set. To include solvent effects, the SMD solution model was employed through single-point energy calculations on the optimized gas-phase geometries. To confirm that the gas-phase optimized geometry is consistent with that obtained upon optimization in each solvent, the RMSDs of the two isomers of 3a were compared.

Table S1: Comparison of the optimized structures in different solvents based on their RMSD.

Comparison of the optimized structures	RMSD (Å)
Z-3a (gas phase) vs Z-3a (Chloroform)	0.088
Z-3a (gas phase) vs Z-3a (DMSO)	0.135
Z-3a (Chloroform) vs Z-3a (DMSO)	0.072
E-3a (gas phase) vs E-3a (Chloroform)	0.055
E-3a (gas phase) vs E-3a (DMSO)	0.053
E-3a (Chloroform) vs E-3a (DMSO)	0.068

Only structures exhibiting RMSD values greater than 2 are regarded as distinct.

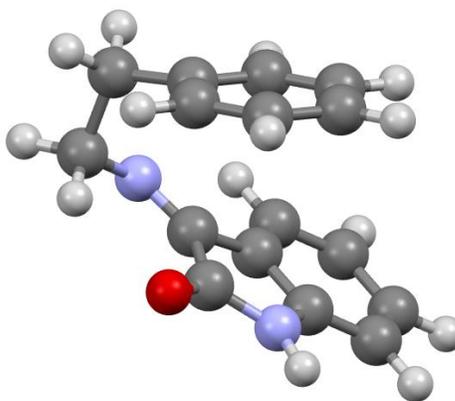
Table S2: Comparison of calculated free energy of isomerization and free energy of activation with different basis set.

Process		6-311G++(d,p)	def2-TZVP	Energy difference
ΔG_{Isom}^{gp} (kcal/mol)	E-3a ---> Z-3a	-2.5	-2.5	0.0
	E-3b ---> Z-3b	-2.0	-2.2	0.2

	<i>E-3c</i> ---> <i>Z-3c</i>	-1.3	-1.4	0.1
	<i>E-4a</i> ---> <i>Z-4a</i>	-1.4	-1.7	0.3
	<i>E-4b</i> ---> <i>Z-4b</i>	-1.8	-2.0	0.2
	<i>E-4c</i> ---> <i>Z-4c</i>	-2.0	-2.1	0.1
ΔG^\ddagger (kcal/mol)	<i>E-3a</i> ---> TS- 3a	19.8	19.1	0.7
	<i>E-3b</i> ---> TS- 3b	19.4	19.3	0.1
	<i>E-3c</i> ---> TS- 3c	22.7	23.1	0.4
	<i>E-4a</i> ---> TS- 4a	15.0	14.6	0.4
	<i>E-4b</i> ---> TS- 4b	14.7	14.3	0.4
	<i>E-4c</i> ---> TS- 4c	14.1	13.8	0.7

- Cartesian coordinates of molecules optimized in chloroform:

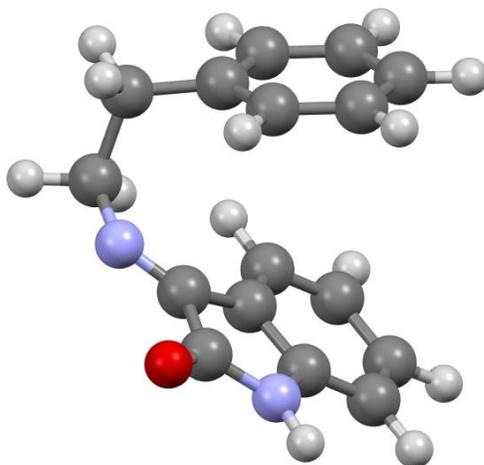
- **Z-3a**



H	1.6843070000	2.1210290000	1.2393880000
H	1.5025250000	3.5244930000	0.1568140000
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N	0.0728660000	2.0720950000	-0.1604450000

C	-0.5479330000	1.1099200000	0.3901290000
O	0.8125320000	0.3274960000	2.3371100000
C	-0.1490700000	0.2290590000	1.5986380000
C	-2.6862560000	0.9501730000	-1.0952140000
C	-1.8438670000	0.5780450000	-0.0568190000
H	-2.4369990000	1.7993920000	-1.7204080000
C	1.4967890000	-1.8259630000	-1.4198880000
C	2.3531610000	-2.4917670000	-0.5449480000
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C	-3.8521920000	0.2105250000	-1.3105490000
N	-1.1506630000	-0.7044860000	1.7078330000
C	-2.1584930000	-0.5279100000	0.7490870000
H	2.3211650000	-3.5727220000	-0.4659430000
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C	3.2551550000	-1.7580050000	0.2260540000
C	-4.1525140000	-0.8860350000	-0.4984000000
C	-3.3065840000	-1.2760060000	0.5465740000
H	-4.5265980000	0.4859110000	-2.1123810000
C	2.4342410000	0.3120020000	-0.7427710000
H	0.8684700000	0.0760340000	-2.1976060000
C	3.2915720000	-0.3696140000	0.1271790000
H	-1.1547680000	-1.4154010000	2.4266620000
H	3.9267820000	-2.2674800000	0.9082660000
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H	-5.0595460000	-1.4514440000	-0.6793000000
H	-3.5417140000	-2.1302510000	1.1699960000
H	3.9844060000	0.1955790000	0.7420190000
H	2.1557000000	2.1667520000	-1.7881250000
H	3.4118980000	2.2133160000	-0.5475160000

- E-3a

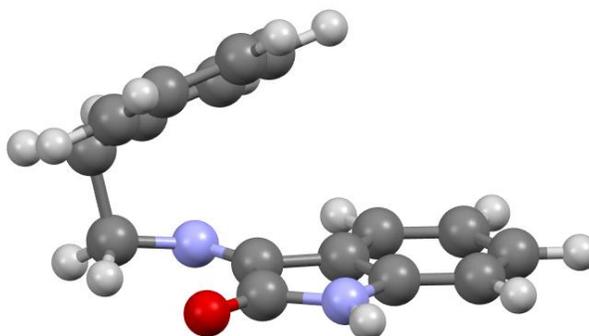


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C	1.8700380000	2.8892370000	-0.5992130000
C	2.5980240000	1.9779660000	0.1712390000
C	2.1994860000	0.6520580000	0.1463990000
C	1.1020540000	0.2063500000	-0.6214770000
C	0.9786810000	-1.2492710000	-0.3832090000
C	2.1084180000	-1.5991210000	0.6025780000
N	2.7678930000	-0.4204830000	0.8435990000
H	0.2199000000	3.2004730000	-1.9424930000
H	-0.4769170000	0.8418920000	-1.9491090000
H	3.4425100000	2.2967250000	0.7704140000
H	2.1591040000	3.9339250000	-0.5964240000
O	2.3727870000	-2.6837570000	1.0804780000
N	0.2166520000	-2.1877370000	-0.7713720000
H	3.5581140000	-0.3456510000	1.4695260000
C	-0.9130450000	-1.9678330000	-1.6507010000
C	-2.2209200000	-1.9063540000	-0.8228300000

H	-0.9787220000	-2.8362380000	-2.3113320000
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C	-1.7347300000	0.5162440000	2.0800410000
C	-2.3132480000	1.6799860000	1.5763420000
H	-2.3089060000	2.5906970000	2.1645360000
H	-3.3657290000	2.5612730000	-0.0826060000
H	-1.2825150000	-1.5537200000	1.7172970000
H	-1.2801020000	0.5175570000	3.0645500000
H	-3.3532160000	0.4900520000	-1.4298540000

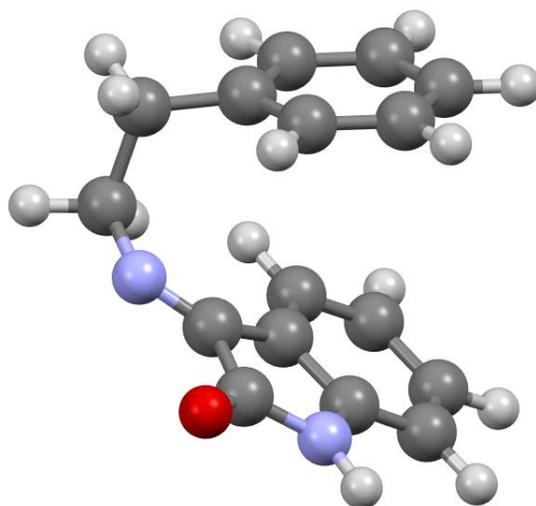
- Cartesian coordinates of molecules optimized in DMSO:

- Z-3a



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C	1.3917700000	2.4318540000	0.2679230000
N	0.0417090000	2.0659000000	-0.1253840000
C	-0.5771750000	1.0917770000	0.4066660000

O	0.7758750000	0.2802010000	2.3481780000
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C	-1.8697450000	0.5650580000	-0.0547880000
H	-2.4666570000	1.8170670000	-1.6974420000
C	1.5326070000	-1.8155390000	-1.3695710000
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N	-1.1755000000	-0.7529820000	1.6838620000
C	-2.1820780000	-0.5577770000	0.7282980000
H	2.4654250000	-3.5414190000	-0.4786640000
C	1.5297860000	-0.4240190000	-1.4634910000
C	3.3886360000	-1.7023950000	0.1638310000
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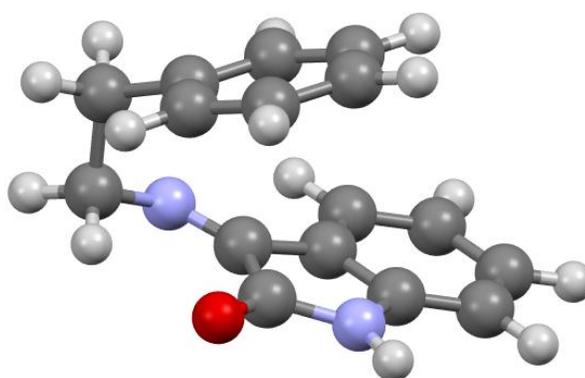


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C	1.0538820000	0.2077960000	-0.6443470000
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H	1.9658610000	3.9743430000	-0.6345920000
O	2.4649710000	-2.6259820000	1.0451970000
N	0.2457860000	-2.2153960000	-0.7593030000
H	3.5414850000	-0.2293830000	1.4360610000
C	-0.9139070000	-2.0314000000	-1.6107520000
C	-2.1981930000	-1.9623310000	-0.7464790000
H	-0.9907200000	-2.9161110000	-2.2478280000

H	-0.8504470000	-1.1533220000	-2.2565150000
C	-2.2648710000	-0.7150690000	0.0960080000
H	-2.2360560000	-2.8536250000	-0.1148010000
H	-3.0493060000	-2.0004700000	-1.4307820000
C	-2.8657420000	0.4456870000	-0.4034430000
C	-1.6584430000	-0.6634990000	1.3561180000
C	-2.8428640000	1.6331390000	0.3239220000
C	-1.6276690000	0.5244430000	2.0855440000
C	-2.2136310000	1.6789470000	1.5682880000
H	-2.1855200000	2.6048140000	2.1318380000
H	-3.3077640000	2.5244460000	-0.0829750000
H	-1.1966360000	-1.5563030000	1.7625180000
H	-1.1429400000	0.5484750000	3.0553660000
H	-3.3409920000	0.4199600000	-1.3788190000

- Cartesian coordinates of gas-phase optimized molecules:

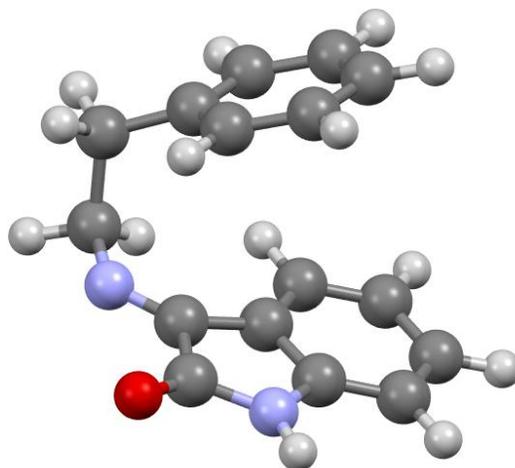
- Z-3a



H	1.75416	2.10276	1.26509
H	1.58209	3.52643	0.20344
C	1.47540	2.44068	0.26637
N	0.10711	2.11494	-0.09395
C	-0.49187	1.12357	0.42684
O	0.92461	0.24787	2.29060
C	-0.05083	0.18583	1.57544
C	-2.66750	1.03403	-1.00097
C	-1.79771	0.60858	-0.00849
H	-2.43083	1.91923	-1.57873
C	1.32137	-1.78514	-1.44248
C	2.16754	-2.50065	-0.59864
H	0.57560	-2.30334	-2.03457
C	-3.83607	0.30301	-1.22857
N	-1.05296	-0.76219	1.66399
C	-2.08602	-0.54216	0.74298
H	2.08589	-3.57945	-0.53050
C	1.42946	-0.39833	-1.52640
C	3.12335	-1.82077	0.15525
C	-4.11087	-0.83866	-0.47316
C	-3.23686	-1.28224	0.52588
H	-4.53264	0.62008	-1.99487
C	2.37764	0.29569	-0.76704
H	0.76223	0.15463	-2.17757
C	3.22363	-0.43580	0.07082
H	-1.01769	-1.51206	2.33708
H	3.78486	-2.36935	0.81586
C	2.42533	1.80221	-0.78481
H	-5.02012	-1.39744	-0.66183

H	-3.45631	-2.17183	1.10410
H	3.95323	0.08806	0.67889
H	2.14975	2.17891	-1.77307
H	3.43793	2.15204	-0.56643

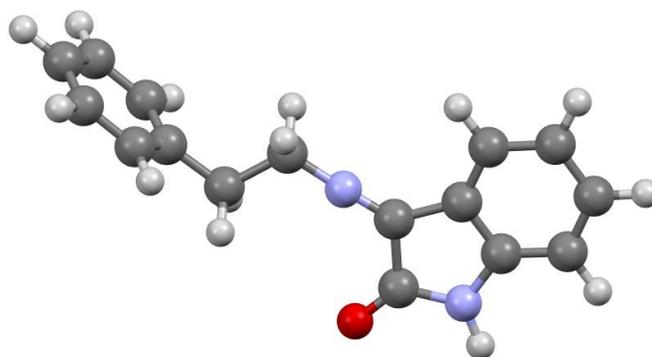
- ***E*-3a**



C	0.29903	1.12266	-1.35421
C	0.65070	2.47329	-1.35796
C	1.75513	2.91816	-0.63393
C	2.53145	2.02898	0.11312
C	2.17148	0.69115	0.10572
C	1.06284	0.21318	-0.62757
C	0.98295	-1.24629	-0.38407
C	2.14208	-1.56836	0.57883
N	2.78666	-0.36058	0.78860
H	0.05242	3.17998	-1.91926
H	-0.57803	0.80626	-1.89571
H	3.38483	2.37579	0.68368
H	2.01503	3.97027	-0.64181
O	2.44411	-2.62940	1.06585

N	0.24040	-2.20494	-0.75748
H	3.58619	-0.27181	1.39598
C	-0.90918	-2.01614	-1.61309
C	-2.19867	-1.96317	-0.75318
H	-0.97436	-2.89423	-2.26126
H	-0.84940	-1.13004	-2.25242
C	-2.27872	-0.71660	0.08937
H	-2.22042	-2.85592	-0.12378
H	-3.05379	-2.01478	-1.43257
C	-2.92269	0.42662	-0.39354
C	-1.64214	-0.64906	1.33287
C	-2.90800	1.61584	0.32989
C	-1.62010	0.54035	2.05707
C	-2.24554	1.67887	1.55411
H	-2.22372	2.60597	2.11484
H	-3.40985	2.49317	-0.06219
H	-1.14930	-1.53066	1.72601
H	-1.11221	0.57765	3.01402
H	-3.43341	0.38541	-1.35080

- TS-3a

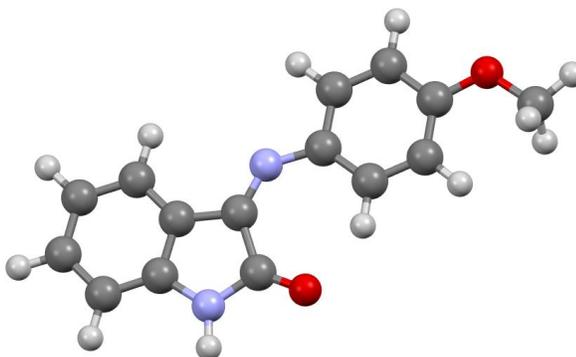


C	2.87943	-1.85132	0.00021
C	4.17717	-2.36911	0.00025

C	5.27445	-1.50605	0.00014
C	5.11238	-0.11602	-0.00001
C	3.81829	0.38053	-0.00005
C	2.70516	-0.47641	0.00006
C	1.47925	0.36115	-0.00002
C	2.01241	1.82942	-0.00019
N	3.39204	1.71772	-0.00020
H	4.33549	-3.44052	0.00037
H	2.01412	-2.50479	0.00029
H	5.97162	0.54437	-0.00009
H	6.27699	-1.91784	0.00018
O	1.37089	2.85252	-0.00029
N	0.28155	0.05716	0.00002
H	4.00448	2.51921	-0.00028
C	-1.05901	-0.34376	0.00007
C	-2.08546	0.81582	-0.00018
H	-1.23862	-0.98946	0.87156
H	-1.23861	-0.98983	-0.87115
C	-3.49715	0.29171	-0.00008
H	-1.89872	1.43789	-0.87854
H	-1.89872	1.43827	0.87791
C	-4.15632	0.00970	1.20113
C	-4.15630	0.00916	-1.20116
C	-5.43823	-0.53535	1.20416
C	-5.43821	-0.53589	-1.20398
C	-6.08335	-0.81125	0.00015
H	-7.08227	-1.23169	0.00023
H	-5.93510	-0.74114	-2.14545
H	-3.66240	0.22824	-2.14247

H	-5.93514	-0.74019	2.14572
H	-3.66243	0.22919	2.14234

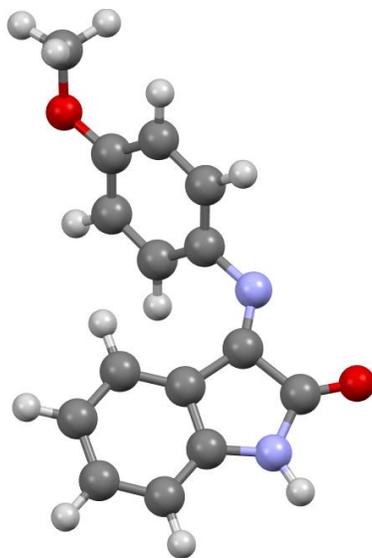
- Z-4a



C	-3.07361	-1.67727	-0.00012
C	-4.45872	-1.85253	-0.00017
C	-5.31206	-0.74638	-0.00014
C	-4.81063	0.56025	-0.00004
C	-3.43427	0.71493	0.00001
C	-2.56319	-0.38594	-0.00003
C	-1.18063	0.10827	-0.00001
C	-1.31041	1.64144	0.00017
N	-2.67020	1.88808	0.00015
H	-4.87709	-2.85163	-0.00025
H	-2.39411	-2.52068	-0.00017
H	-5.47752	1.41425	-0.00001
H	-6.38501	-0.89870	-0.00018
O	-0.45926	2.51096	-0.00004
N	-0.18184	-0.69635	-0.00007
H	-3.03419	2.82833	-0.00018
C	1.18728	-0.50000	-0.00004
C	1.94178	-1.69671	-0.00008

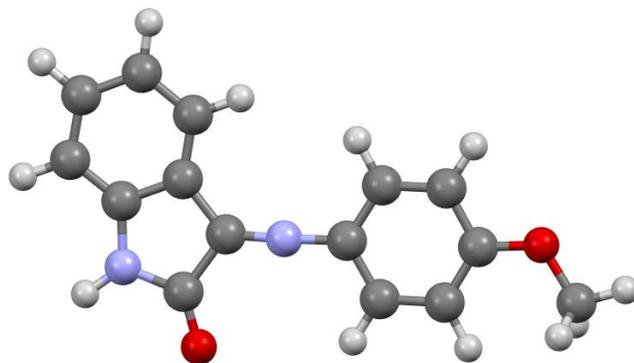
C	1.89111	0.71973	0.00002
C	3.32018	-1.68432	-0.00005
C	4.00417	-0.46011	0.00001
C	3.28022	0.73814	0.00005
H	3.89504	-2.60184	-0.00008
H	1.39769	-2.63286	-0.00013
H	1.34435	1.65044	0.00003
H	3.78790	1.69278	0.00008
O	5.35858	-0.53829	0.00003
C	6.11077	0.67006	0.00031
H	5.90252	1.26580	-0.89390
H	7.15603	0.36771	0.00044
H	5.90222	1.26557	0.89461

- ***E-4a***



C	1.12096	1.57339	-0.20091
C	1.84631	2.76057	-0.30903
C	3.24078	2.74527	-0.25668
C	3.94656	1.54794	-0.11540
C	3.21590	0.37397	-0.01892

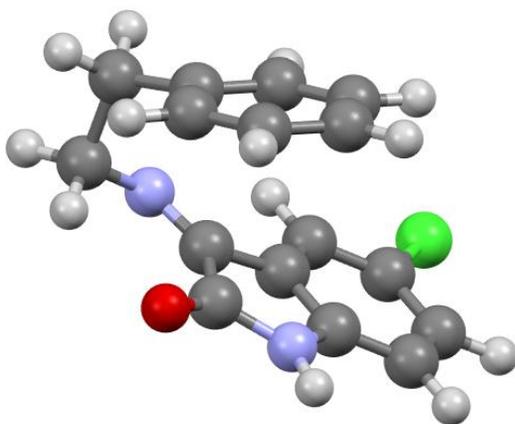
C	1.80364	0.36884	-0.04047
C	1.37841	-1.04302	0.01984
C	2.67231	-1.86932	0.06692
N	3.69690	-0.93316	0.07997
H	1.32194	3.70035	-0.42927
H	0.04132	1.59168	-0.23839
H	5.02975	1.53798	-0.09268
H	3.79032	3.67626	-0.33278
O	2.80269	-3.06739	0.10304
N	0.26055	-1.65254	-0.01067
H	4.66954	-1.19771	0.08173
C	-0.97140	-0.99173	0.07269
C	-1.28021	-0.10519	1.11849
C	-1.97050	-1.31272	-0.84883
C	-3.22514	-0.71064	-0.78565
C	-3.51449	0.18383	0.24792
C	-2.53613	0.46780	1.20946
H	-0.53097	0.11248	1.86981
H	-2.78700	1.13822	2.02218
H	-1.74872	-2.03070	-1.62870
H	-3.96701	-0.96181	-1.53075
O	-4.71286	0.81151	0.41528
C	-5.75156	0.53545	-0.51392
H	-5.46426	0.82592	-1.53018
H	-6.60352	1.13258	-0.19447
H	-6.02481	-0.52497	-0.50124



H	6.25278	0.77295	-0.89429
C	3.09595	-1.55354	-0.00019
C	1.74390	-1.28115	-0.00018
C	1.26514	0.05264	-0.00002
C	-1.90040	1.96462	0.00002
C	4.02503	-0.50067	-0.00002
C	2.21779	1.09275	0.00014
C	3.57973	0.82777	0.00015
C	-1.27964	0.55132	-0.00000
C	-2.42977	-0.37179	-0.00001
C	-3.60568	0.40283	0.00000
C	-2.50899	-1.75714	-0.00003
C	-3.76622	-2.36553	-0.00003
C	-4.86027	-0.18570	-0.00000
C	-4.92333	-1.58391	-0.00002
C	6.32685	0.14664	0.00012
N	-0.04866	0.33886	-0.00001
N	-3.27272	1.76408	0.00002
O	-1.32941	3.03197	0.00004
O	5.32977	-0.86965	-0.00004
H	-3.93596	2.52357	0.00002
H	3.46921	-2.57010	-0.00033

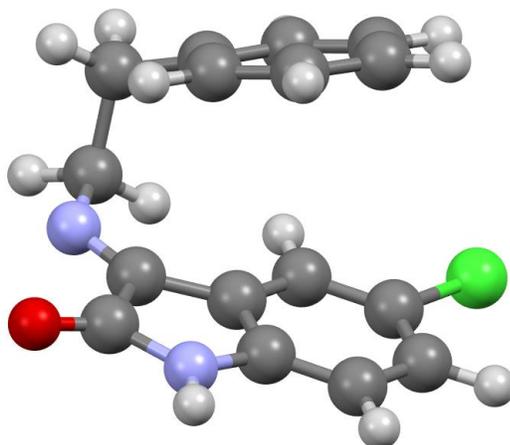
H	1.02174	-2.08831	-0.00030
H	1.84980	2.11140	0.00026
H	4.28154	1.65008	0.00028
H	-1.60133	-2.34996	-0.00004
H	-3.84729	-3.44565	-0.00005
H	-5.76448	0.41176	0.00001
H	-5.89372	-2.06660	-0.00002
H	7.28115	-0.37589	0.00008
H	6.25274	0.77270	0.89471

- **Z-3b**



H	2.41236	1.83091	1.59825
H	1.92148	3.44374	1.01215
C	1.90843	2.37265	0.79716
N	0.52278	1.97980	0.61625
C	0.12019	0.82166	0.94382
O	1.94284	-0.31427	2.21874
C	0.85175	-0.31502	1.69501
C	-2.27813	0.83427	-0.05516
C	-1.20499	0.27359	0.61822
H	-2.23712	1.85815	-0.40221

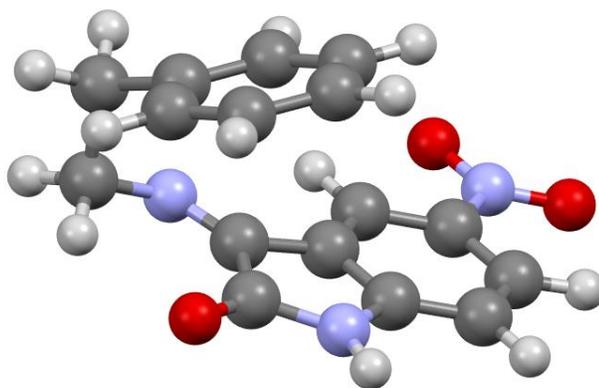
C	1.68124	-1.26194	-1.95307
C	2.72325	-2.06661	-1.49834
H	0.86822	-1.69372	-2.52560
C	-3.40046	0.03499	-0.26542
N	-0.03896	-1.37356	1.69226
C	-1.24846	-1.05752	1.06126
H	2.72723	-3.12870	-1.71515
C	1.68067	0.10304	-1.67223
C	3.76453	-1.49642	-0.76695
C	-3.45029	-1.28629	0.17421
C	-2.36248	-1.85232	0.84668
C	2.71464	0.68451	-0.93033
H	0.86341	0.72354	-2.02185
C	3.75644	-0.13394	-0.48587
H	0.18723	-2.26029	2.11560
H	4.57897	-2.11534	-0.40849
C	2.65982	2.14045	-0.54400
H	-4.33879	-1.87590	-0.00938
H	-2.40215	-2.88121	1.18271
H	4.55776	0.29758	0.10413
H	2.16220	2.72184	-1.32410
H	3.67030	2.54038	-0.42492
Cl	-4.78809	0.70817	-1.11062



C	0.85136	-0.51854	-0.92622
C	1.99869	-1.19883	-0.52678
C	1.93859	-2.32661	0.28398
C	0.70237	-2.80409	0.72332
C	-0.44065	-2.12486	0.33398
C	-0.38537	-0.97988	-0.48951
C	-1.77905	-0.50150	-0.65948
C	-2.65295	-1.49700	0.12774
N	-1.76410	-2.41076	0.67238
H	0.95018	0.36205	-1.53725
H	0.64768	-3.67977	1.35854
H	2.85178	-2.82748	0.57719
O	-3.84978	-1.49944	0.26876
N	-2.35425	0.47514	-1.22792
H	-2.06459	-3.17886	1.25187
C	-1.63020	1.52240	-1.91315
C	-1.42546	2.72769	-0.95638
H	-2.25590	1.85505	-2.74520
H	-0.66727	1.20439	-2.32410
C	-0.46773	2.41301	0.16349
H	-2.40260	3.01457	-0.56111

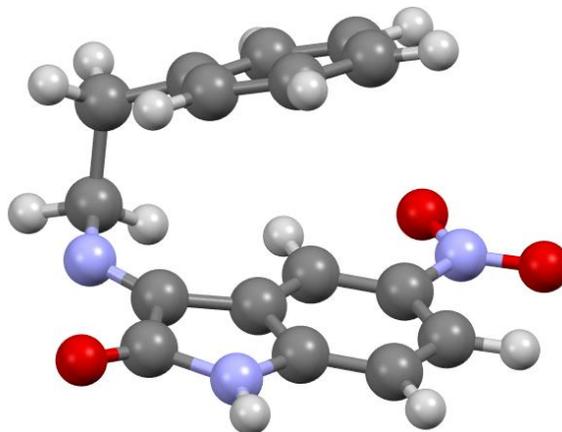
H	-1.04979	3.56286	-1.55356
C	0.90395	2.63531	0.00688
C	-0.91489	1.80082	1.33856
C	1.81170	2.22312	0.97798
C	-0.00971	1.38426	2.31207
C	1.35671	1.58355	2.12938
H	2.06222	1.24949	2.88102
H	2.87249	2.38697	0.83005
H	-1.97645	1.63330	1.48026
H	-0.37261	0.89958	3.21125
H	1.26590	3.11935	-0.89502
Cl	3.56596	-0.59352	-1.04650

- **Z-3c**



H	-2.64400	1.70292	-1.71749
H	-2.10306	3.35065	-1.29527
C	-2.09961	2.30277	-0.98728
N	-0.71560	1.89971	-0.82370
C	-0.34644	0.70730	-1.04961
O	-2.22810	-0.51721	-2.14141
C	-1.12265	-0.47985	-1.65698
C	2.08604	0.76095	-0.14416

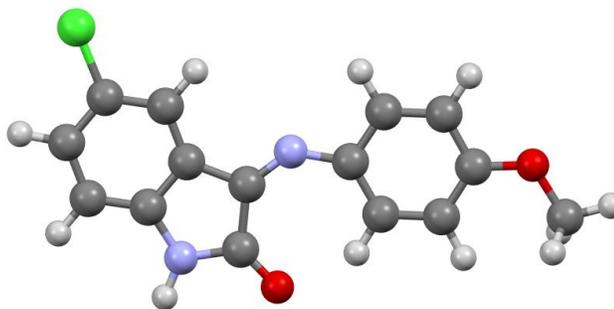
C	0.98077	0.16620	-0.71893
H	2.09595	1.81146	0.10990
C	-1.82259	-1.07719	2.07165
C	-2.89099	-1.90067	1.72441
H	-0.99875	-1.47002	2.65669
C	3.19694	-0.04924	0.09724
N	-0.24433	-1.55613	-1.58014
C	0.98381	-1.20739	-1.03047
H	-2.90384	-2.93867	2.03644
C	-1.81166	0.25741	1.67008
C	-3.94877	-1.37914	0.98027
C	3.21086	-1.40958	-0.21121
C	2.09133	-2.00928	-0.78242
C	-2.86223	0.78887	0.91380
H	-0.97571	0.89317	1.93907
C	-3.93091	-0.04714	0.57925
H	-0.50311	-2.47703	-1.90086
H	-4.78468	-2.01259	0.70690
C	-2.80009	2.20379	0.39829
H	4.10141	-1.98375	0.00199
H	2.09217	-3.06553	-1.02013
H	-4.74688	0.34487	-0.01818
H	-2.26281	2.84257	1.10328
H	-3.80769	2.61122	0.28161
O	4.35683	1.74348	0.97681
O	5.36096	-0.17958	0.90161
N	4.39433	0.54930	0.70333



C	0.74807	-0.42608	-0.87970
C	1.91827	-1.04511	-0.44138
C	1.90780	-2.19066	0.35087
C	0.69461	-2.75455	0.72761
C	-0.47635	-2.13708	0.30201
C	-0.46655	-0.97098	-0.50177
C	-1.88067	-0.57718	-0.71216
C	-2.71340	-1.64318	0.01810
N	-1.77993	-2.51248	0.58196
H	0.83240	0.46642	-1.47354
H	0.66682	-3.64401	1.34442
H	2.84758	-2.62067	0.66722
O	-3.90822	-1.73582	0.11784
N	-2.49332	0.37867	-1.27557
H	-2.05091	-3.31098	1.13552
C	-1.80783	1.48754	-1.90174
C	-1.69769	2.66601	-0.89625
H	-2.42626	1.81597	-2.74041
H	-0.81747	1.23601	-2.29225
C	-0.76319	2.36191	0.24625
H	-2.70084	2.89024	-0.52662

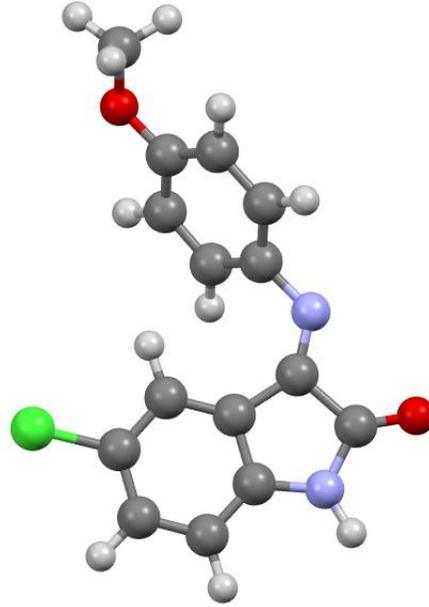
H	-1.34543	3.53839	-1.45270
C	0.60119	2.64910	0.14142
C	-1.22121	1.70090	1.39072
C	1.49349	2.25726	1.13539
C	-0.33135	1.30288	2.38595
C	1.02992	1.57079	2.25617
H	1.72371	1.25629	3.02703
H	2.54891	2.47774	1.02778
H	-2.27863	1.48463	1.49296
H	-0.70170	0.78360	3.26256
H	0.97378	3.16598	-0.73707
O	4.22452	-0.95462	-0.35683
O	3.18484	0.56015	-1.51282
N	3.20301	-0.43857	-0.79917

- Z-4b



C	-2.67334	-0.90228	-0.00006
C	-4.06518	-0.85368	-0.00015
C	-4.75918	0.35534	-0.00017
C	-4.06400	1.56898	-0.00010
C	-2.68009	1.52148	0.00002
C	-1.98484	0.30240	0.00003
C	-0.54310	0.58236	0.00006

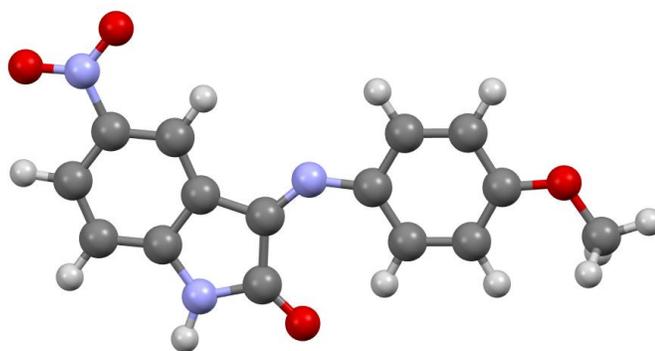
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H	-5.84105	0.35023	-0.00025
O	0.53184	2.84594	0.00004
N	0.32016	-0.36619	-0.00002
H	-1.96672	3.54992	-0.00016
C	1.70156	-0.38342	0.00001
C	2.26295	-1.68245	-0.00005
C	2.58382	0.71490	0.00008
C	3.62643	-1.88124	-0.00003
C	4.48992	-0.77571	0.00006
C	3.95857	0.52015	0.00011
H	4.05426	-2.87576	-0.00006
H	1.58159	-2.52391	-0.00011
H	2.18585	1.71833	0.00012
H	4.60723	1.38515	0.00016
O	5.81483	-1.06003	0.00007
C	6.74473	0.01843	0.00026
H	6.63039	0.63855	-0.89413
H	7.73053	-0.44191	0.00032
H	6.63020	0.63840	0.89472
Cl	-4.97591	-2.35970	-0.00026



C	1.10520	1.01812	-0.07858
C	1.94246	2.12998	-0.11846
C	3.32875	2.00788	-0.06470
C	3.91959	0.74533	0.01103
C	3.09189	-0.36604	0.04174
C	1.68554	-0.24438	0.01764
C	1.13555	-1.61512	-0.00519
C	2.35082	-2.55286	-0.00364
N	3.45496	-1.71284	0.06745
H	0.03403	1.14444	-0.11792
H	4.99791	0.64609	0.03514
H	3.94601	2.89627	-0.08794
O	2.37494	-3.75723	-0.03728
N	-0.03192	-2.11842	-0.07833
H	4.40037	-2.06224	0.05477
C	-1.20241	-1.36111	0.04247
C	-1.43170	-0.49148	1.12294
C	-2.22855	-1.56310	-0.88378

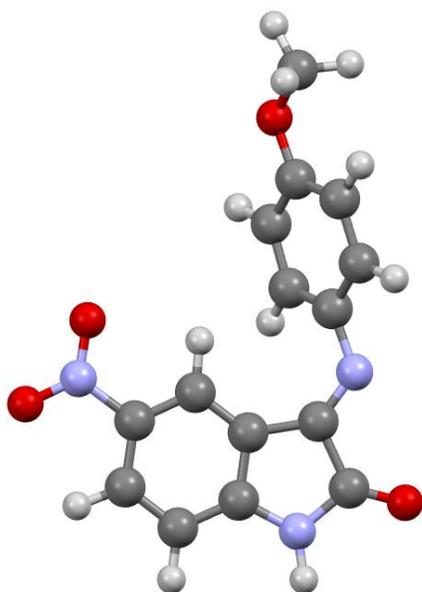
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C	-2.63318	0.18282	1.24193
H	-0.66672	-0.36883	1.87988
H	-2.82375	0.84194	2.07972
H	-2.07063	-2.26865	-1.69003
H	-4.18804	-1.01587	-1.54220
O	-4.77176	0.74163	0.47093
C	-5.82837	0.60317	-0.46978
H	-5.51028	0.90871	-1.47213
H	-6.62178	1.26327	-0.12491
H	-6.19923	-0.42664	-0.50171
Cl	1.22707	3.73231	-0.23063

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H	6.85926	0.47531	0.89473
C	6.94855	-0.14810	0.00003
C	-3.79908	1.82458	-0.00002
C	-4.53893	0.64472	-0.00012
C	-2.41395	1.71829	0.00007
C	-3.88587	-0.58896	-0.00016
C	-1.76172	0.47026	0.00004
C	3.75802	-1.92533	0.00004

C	2.40400	-1.67437	0.00006
C	-2.49520	-0.70172	-0.00007
C	-0.31086	0.69818	0.00017
C	4.66379	-0.85325	0.00003
C	1.89382	-0.35346	0.00006
C	2.81818	0.71104	0.00005
C	4.18334	0.46339	0.00004
C	-0.15300	2.22083	0.00021
N	-1.45198	2.72010	0.00014
N	0.51690	-0.28227	0.00011
O	5.97445	-1.18814	0.00001
O	0.83850	2.92123	0.00016
H	7.91409	-0.64918	0.00003
H	-4.29495	2.78714	-0.00002
H	-5.61938	0.66448	-0.00018
H	4.14754	-2.93538	0.00003
H	1.69015	-2.48838	0.00007
H	-2.01298	-1.66871	-0.00008
H	-1.63360	3.71243	0.00007
H	2.46024	1.72930	0.00005
H	4.86573	1.30194	0.00004
H	6.85928	0.47534	-0.89466
O	-4.10562	-2.88880	-0.00029
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N	-4.69641	-1.81470	-0.00023



H	-2.80005	0.97991	2.00743
H	-0.72666	-0.36501	1.81592
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C	-1.51546	-0.47662	1.08235
O	-4.79529	0.91087	0.45989
C	-3.70989	0.11751	0.26961
C	-1.36841	-1.41145	0.04102
O	2.01910	-4.06191	-0.05026
C	2.08202	-2.86116	-0.00827
C	0.95139	-1.83123	0.00089
N	-0.25277	-2.24054	-0.08581
N	3.25833	-2.10977	0.06558
C	1.61249	-0.51031	0.03492
C	3.01006	-0.74829	0.05118
H	4.17192	-2.53688	0.05026
C	3.93578	0.28930	0.02522
C	1.14681	0.79321	-0.05452
H	-6.62002	1.53048	-0.12024
C	-5.88169	0.80359	-0.45222

C	3.45819	1.59301	-0.04284
C	2.08417	1.82491	-0.09154
H	-6.32074	-0.19907	-0.42938
H	5.00017	0.09190	0.04666
H	0.09553	1.03121	-0.09261
C	-3.58563	-0.82510	-0.75601
C	-2.43575	-1.60318	-0.84203
H	4.13425	2.43598	-0.06439
H	-4.37930	-0.97591	-1.47405
H	-5.56647	1.04379	-1.47272
H	-2.34247	-2.35891	-1.61200
O	0.38973	3.39146	-0.19754
O	2.43996	4.10496	-0.21697
N	1.60214	3.20999	-0.17488