

Squaramide-Catalyzed Asymmetric Mannich Reactions Between 3-Fluorooxindoles and Pyrazolinone Ketimines

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Supporting Information

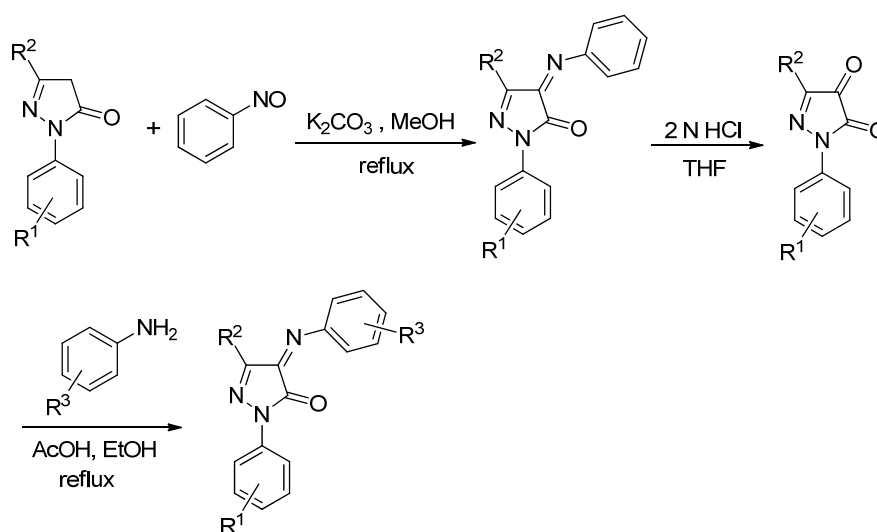
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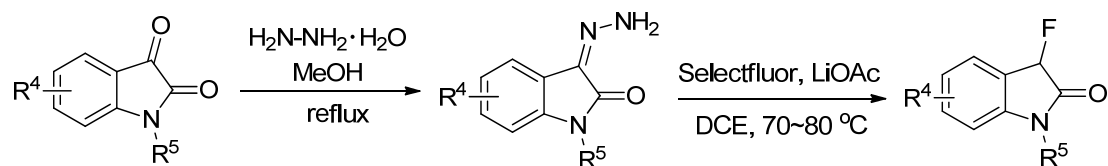
1. General information and starting materials

General information. All solvents commercially and available chemicals were used without further purification. The column chromatography was performed with silica gel (200–300 mesh) using mixtures of petroleum ether and ethyl acetate. Melting points were determined with a XT-4 melting-point apparatus without corrected. ^1H NMR spectra were measured with Bruker Ascend 400 MHz spectrometer, and chemical shifts were reported in δ (ppm) units relative to tetramethylsilane (TMS) as the internal standard. ^{13}C NMR spectra were measured at 101 MHz with Bruker Ascend 400 MHz spectrometer or 176 MHz with Bruker Avance III HD 700 MHz spectrometer, and chemical shifts are reported in δ (ppm) units relative to tetramethylsilane and referenced to the solvent peak (CDCl_3 , $\delta(\text{C}) = 77.00$ ppm). ^{19}F NMR spectra were measured at 376 MHz with Bruker Ascend 400 MHz spectrometer. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br). High-resolution mass spectra were obtained with an Agilent 6520 Accurate-Mass-Q-TOF MS system equipped with an electrospray ionization (ESI) source. The enantiomeric excesses were determined by chiral HPLC analysis using an Agilent 1200 LC instrument with Daicel Chiralpak IA, IB, IC or AD-H columns. Optical rotations were measured with Krüss P8000 polarimeter at the indicated concentration with the units of grams per 100 mL at 20 °C using sodium D light.

Starting materials. **1a–1p** were prepared according to the literature.^[1]



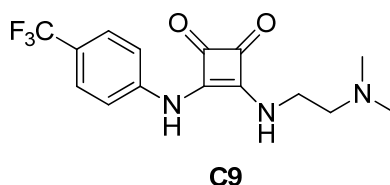
2a–2h were prepared according to the literature.^[2]



The squaramide organocatalysts **C1–C8** were prepared by the reported procedures.^[3]

2. General procedure for the synthesis of compound **3**

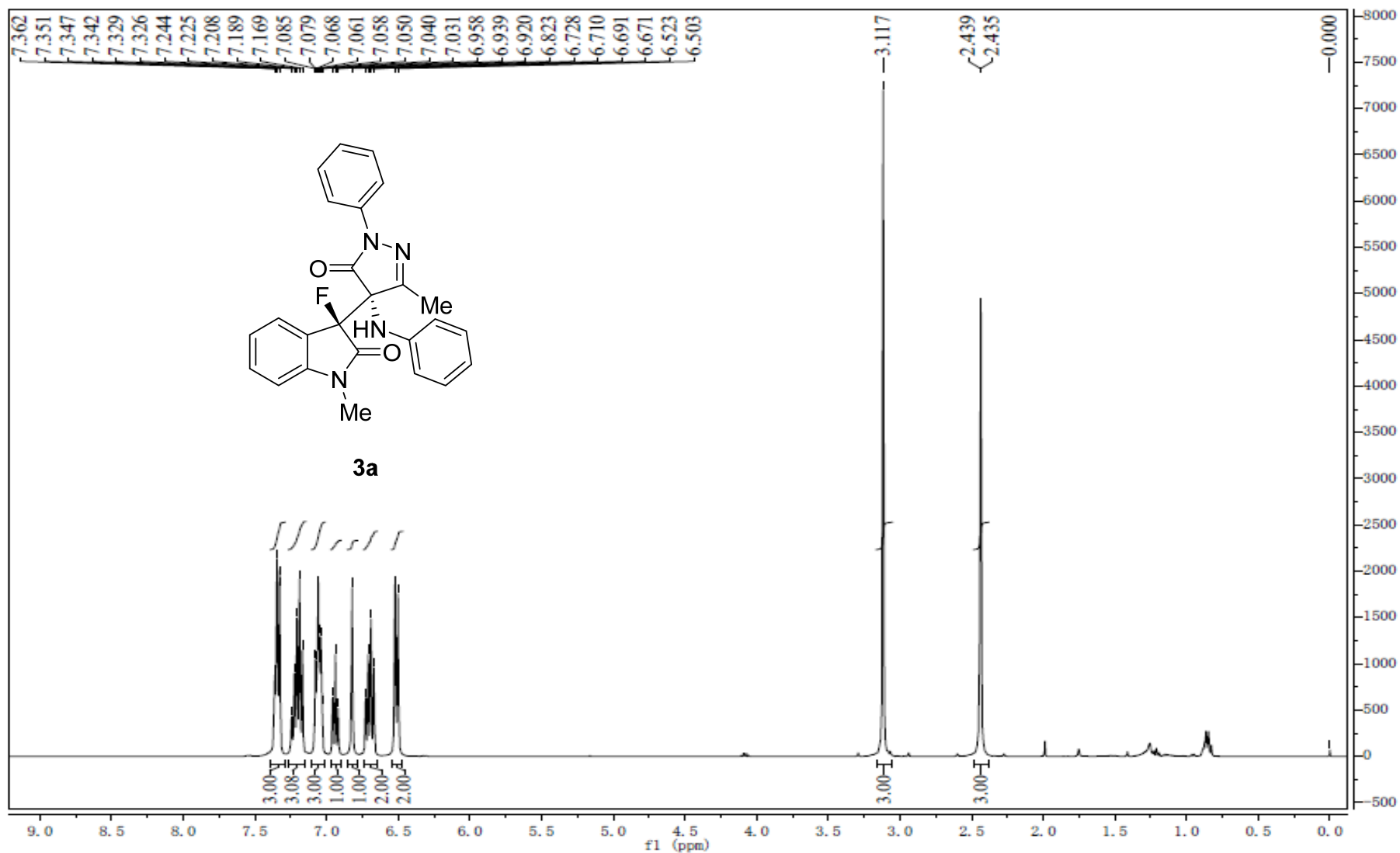
To a dried small bottle were added pyrazolone imine **1** (0.22mmol), 3-fluorooxindole **2** (0.2 mmol), and squaramide catalyst **C5** (5 mol%) in MeCN (2.0 mL) at room temperature. The reaction mixture was stirred for 36 h and the progress of the reaction was monitored by TLC analysis (Petroleum ether/ ethyl acetate = 2:1). After the completion of the reaction, the crude product mixture was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 5:1) to afford the pure product **3**. The racemic standard of **3** was prepared using achiral catalyst **C9**.^[4]

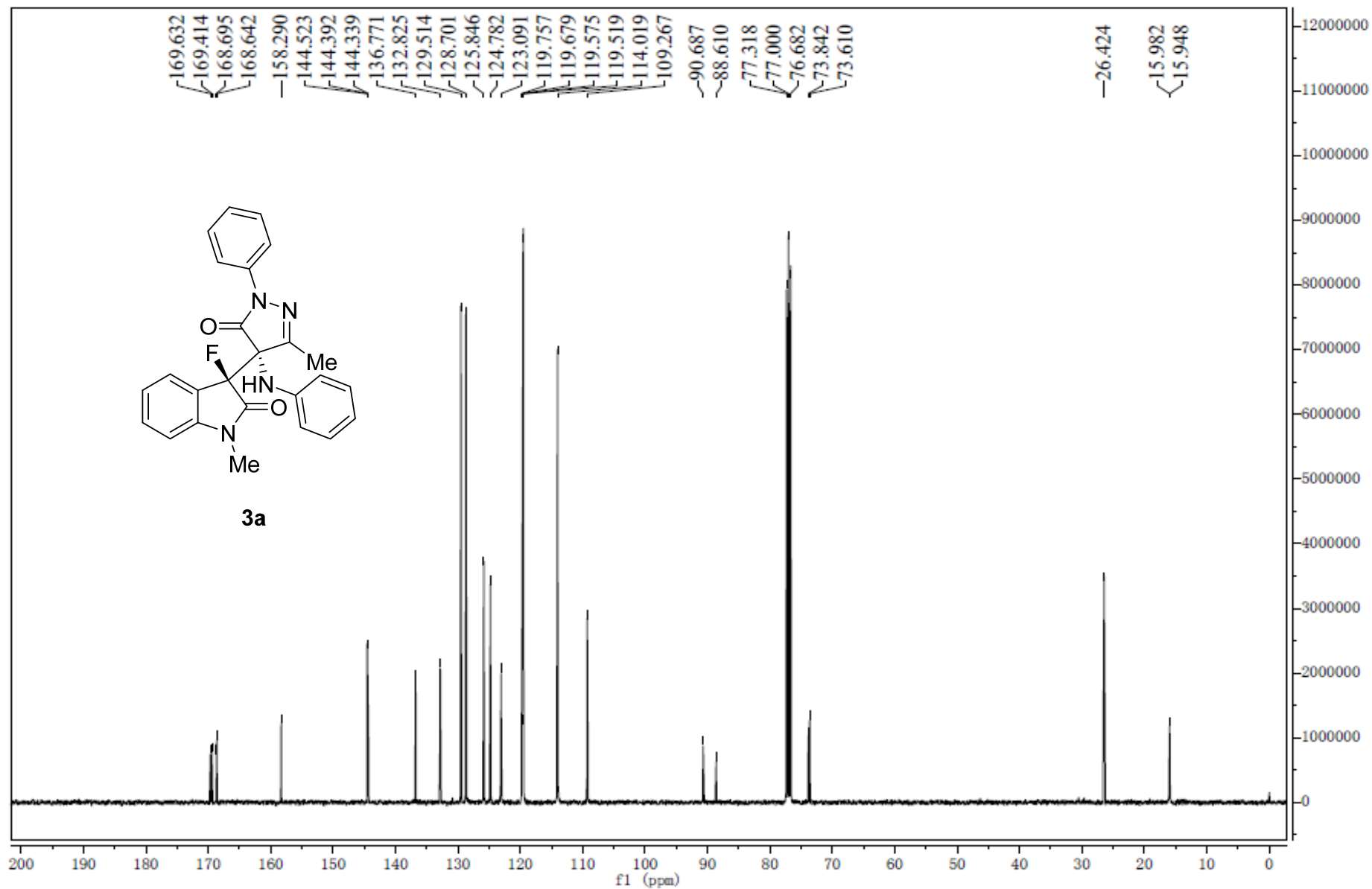


References

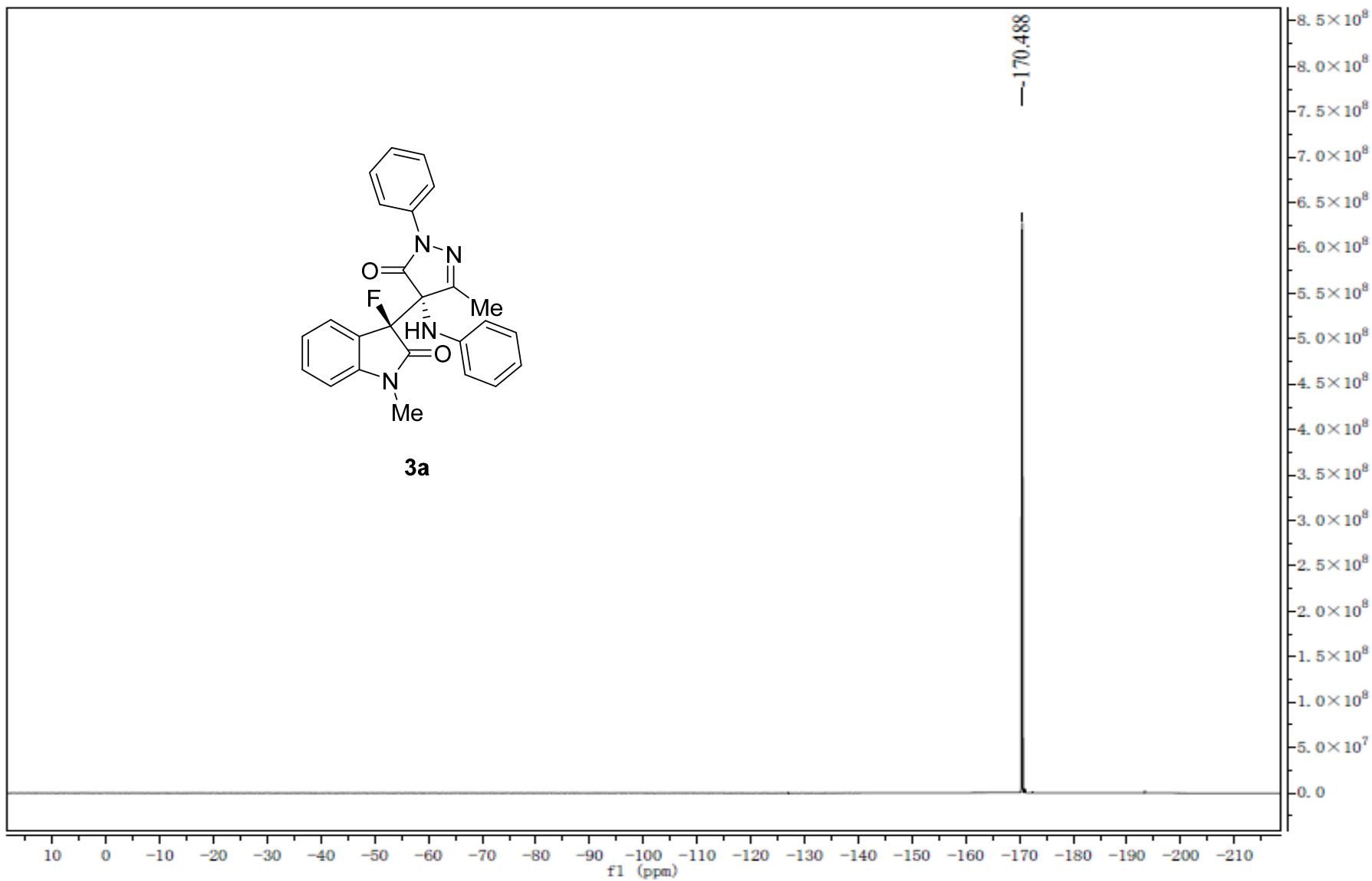
- [1] P. Chauhan, S. Mahajan, U. Kaya, A. Peuronen and K. Rissanen, *J. Org. Chem.* 2017, **82**, 7050.
- [2] Q. Yang, G. -L. Dai, Y.-M. Yang, Z.-Z. Luo and Z.-Y. Tang, *J. Org. Chem.* 2018, **83**, 6762.
- [3] (a) Y. Zhu, J. P. Malerich and V. -H. Rawal, *Angew. Chem., Int. Ed.* 2010, **49**, 153; (b) W. Yang and D.-M. Du, *Org. Lett.* 2010, **12**, 5450; (c) C. Cassani, R.-M. Rapún, E. Arceol, F. Bravo and P. Melchiorre, *Nat. Protoc.* 2013, **8**, 325; (d) E. Massolo, M. Benaglia, A. Genoni, R. Annunziata, G. Celentanob and N. Gaggero, *Org. Biomol. Chem.* 2015, **13**, 5591.
- [4] S. Sopena, E. Martin, E. -C. Escuder and A. -W. Kleij, *ACS Catal.* 2017, **7**, 3532.

3. Copies of ^1H , ^{13}C and ^{19}F NMR spectra of new products

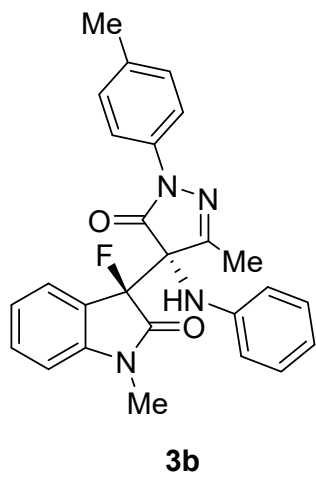
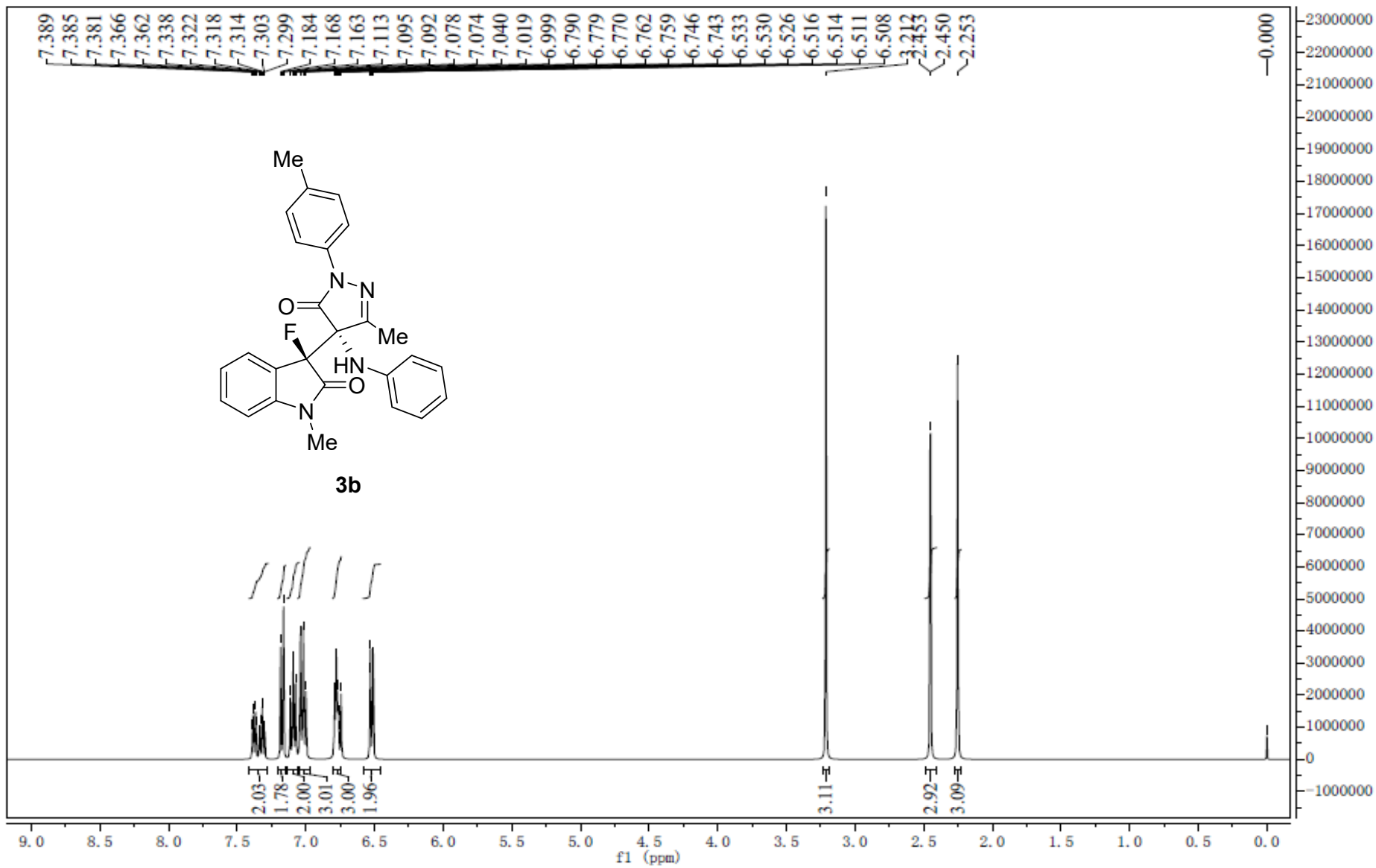




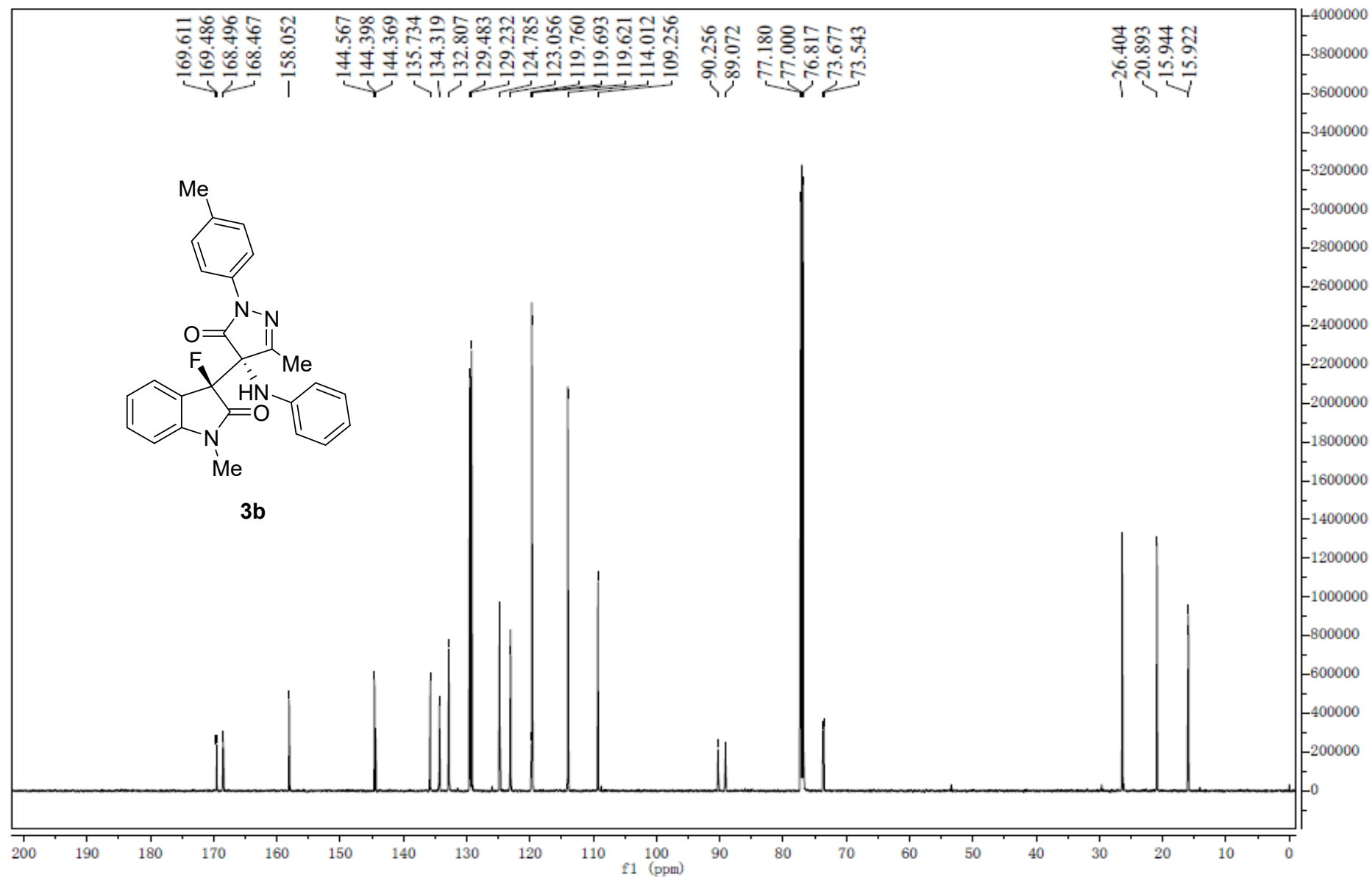
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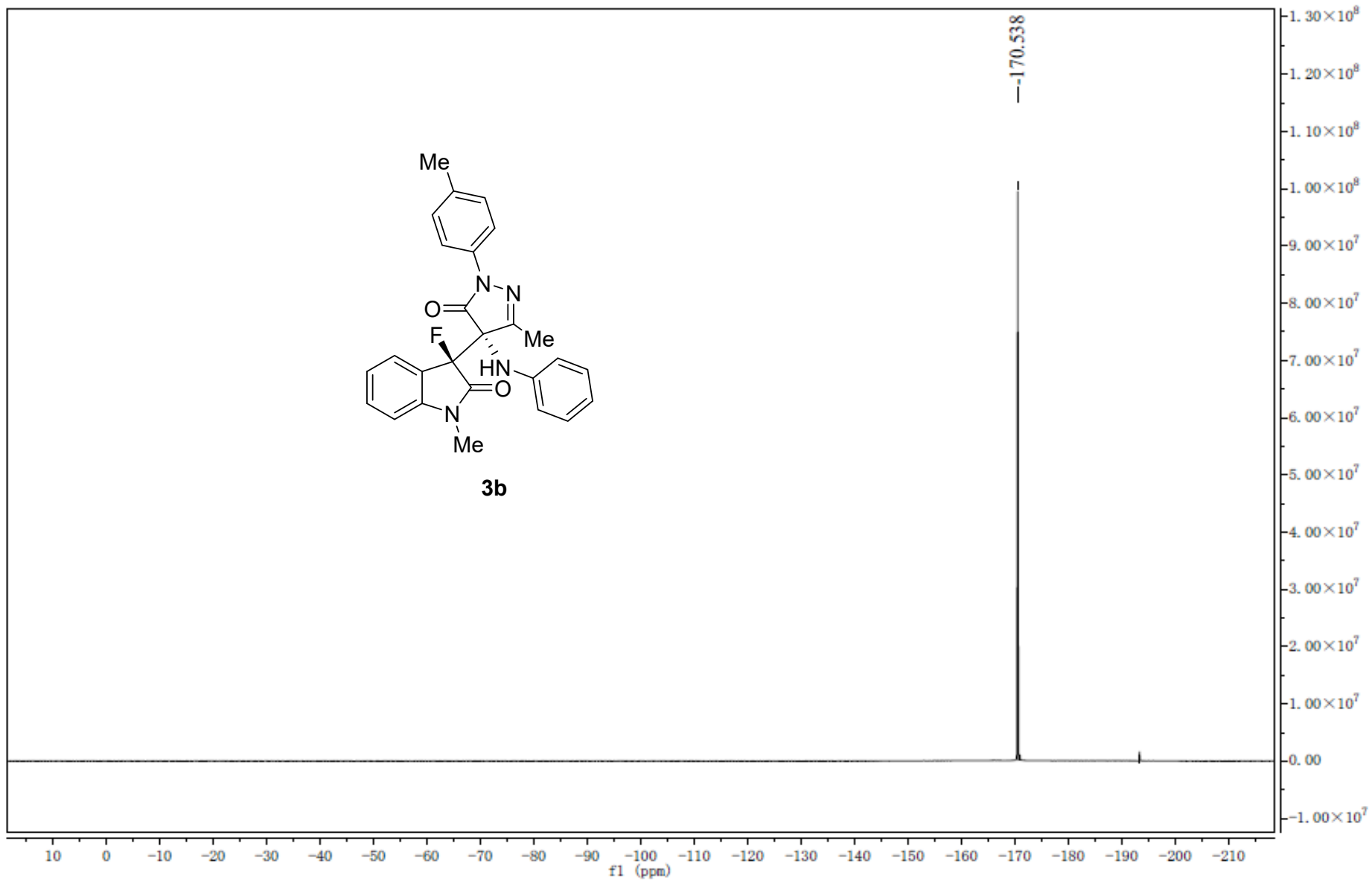
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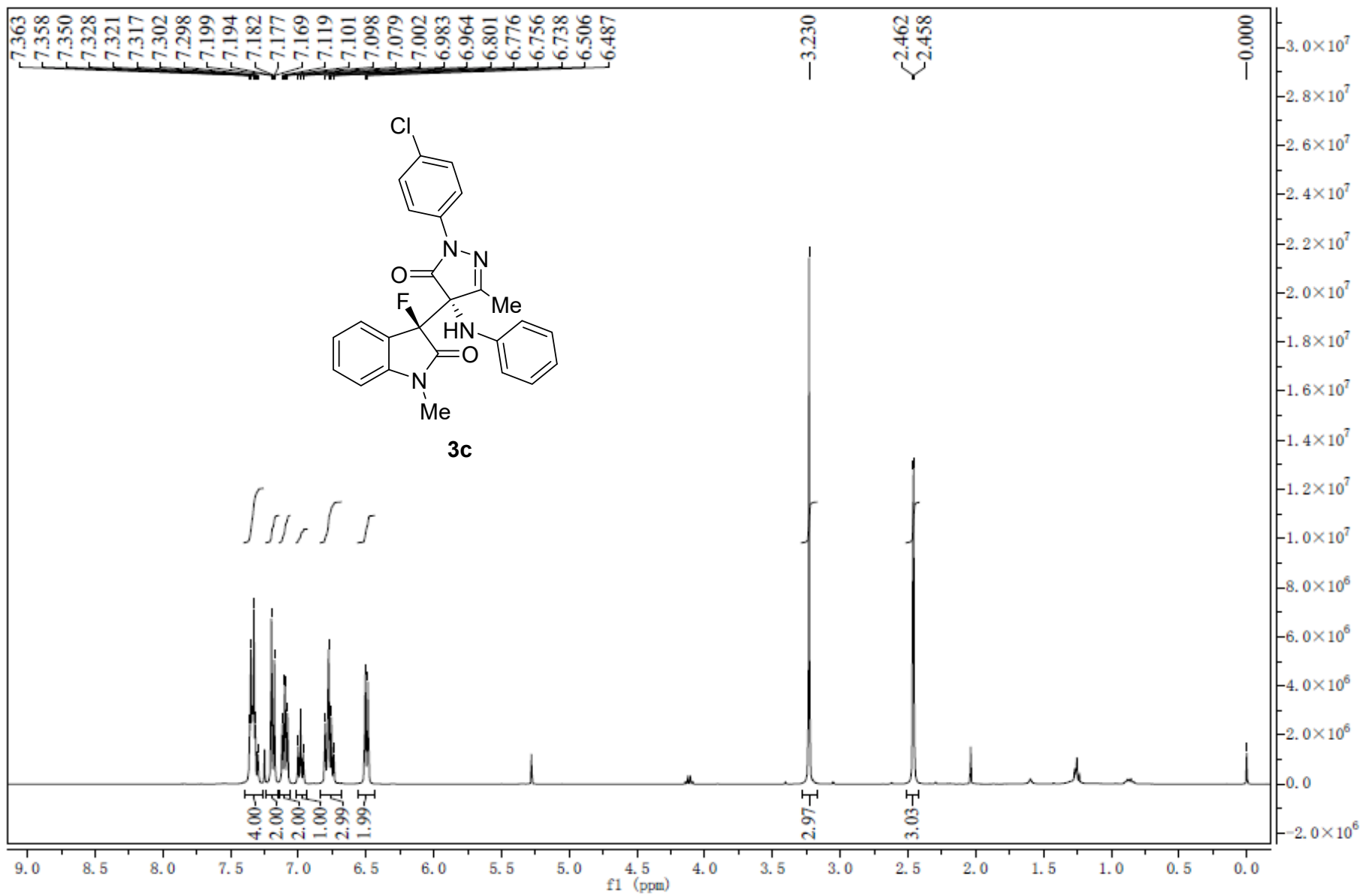
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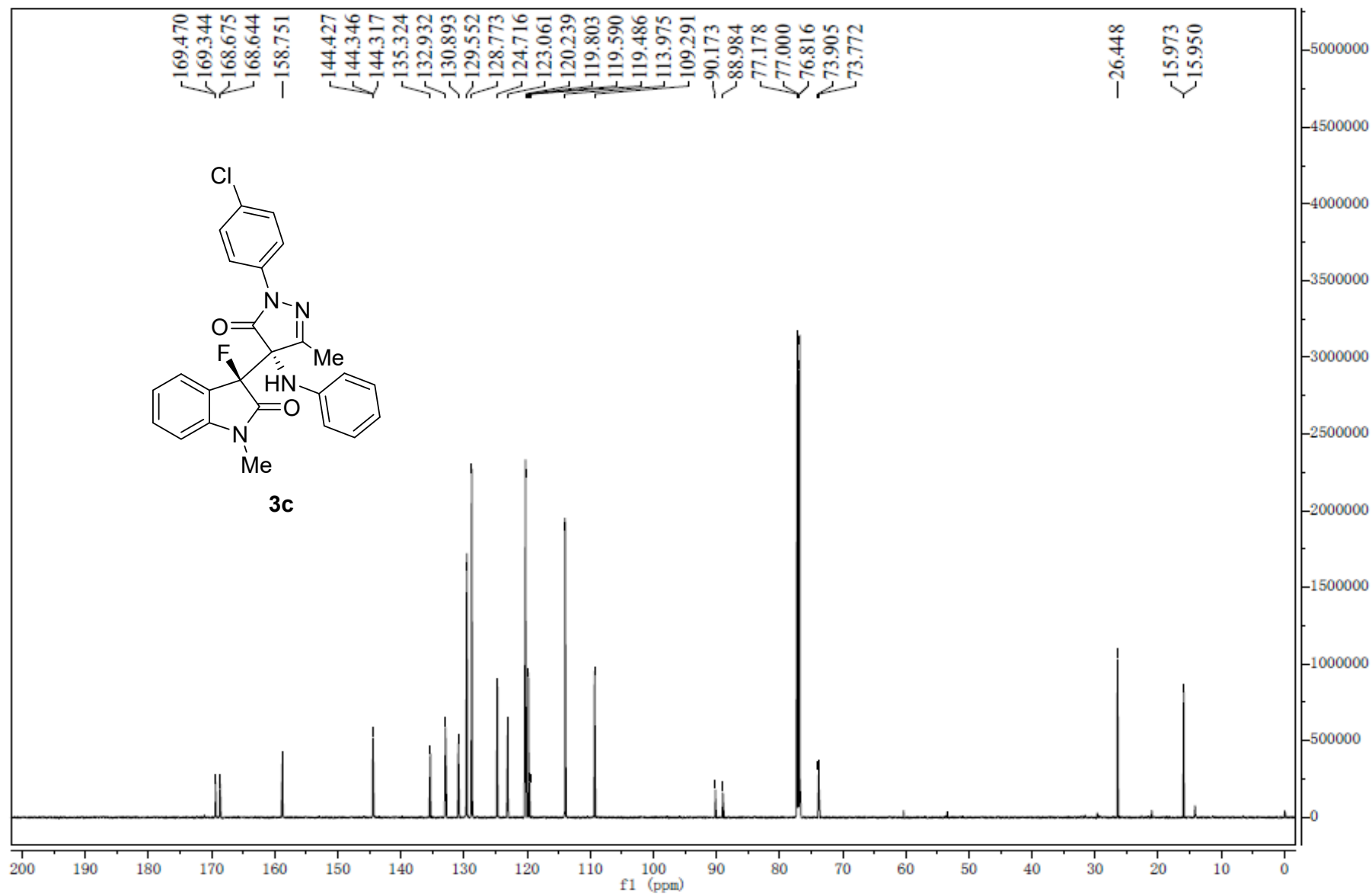
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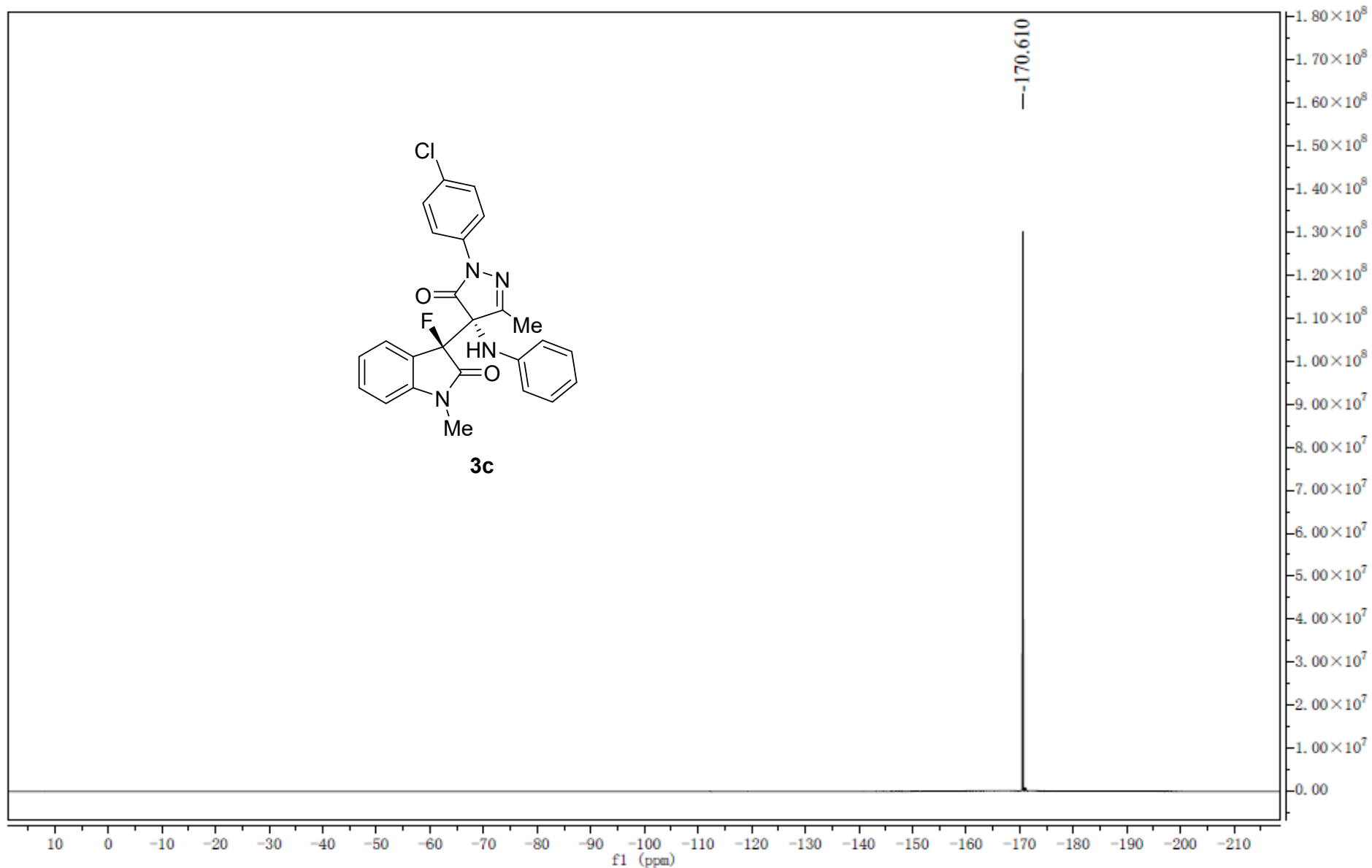
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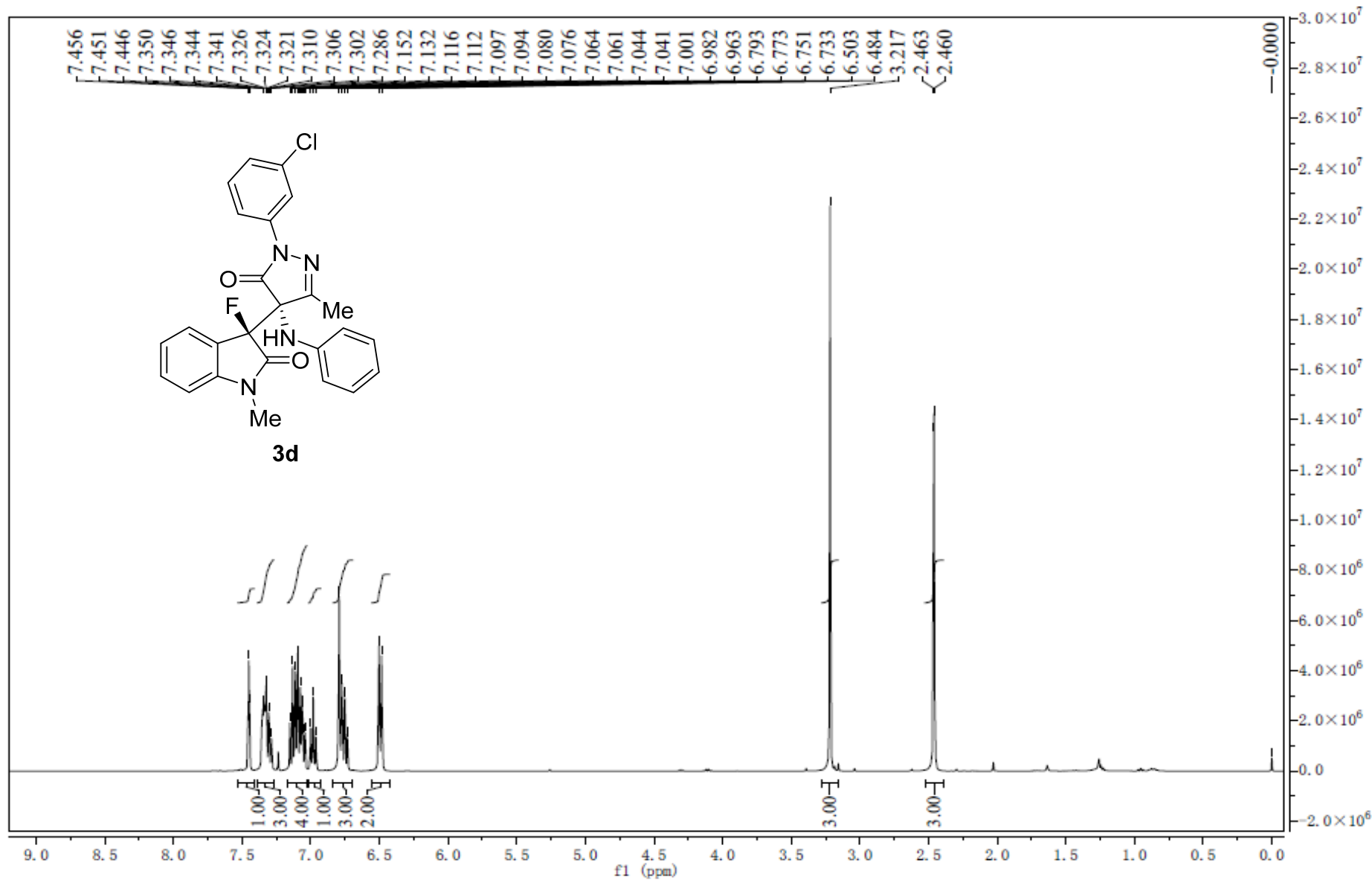
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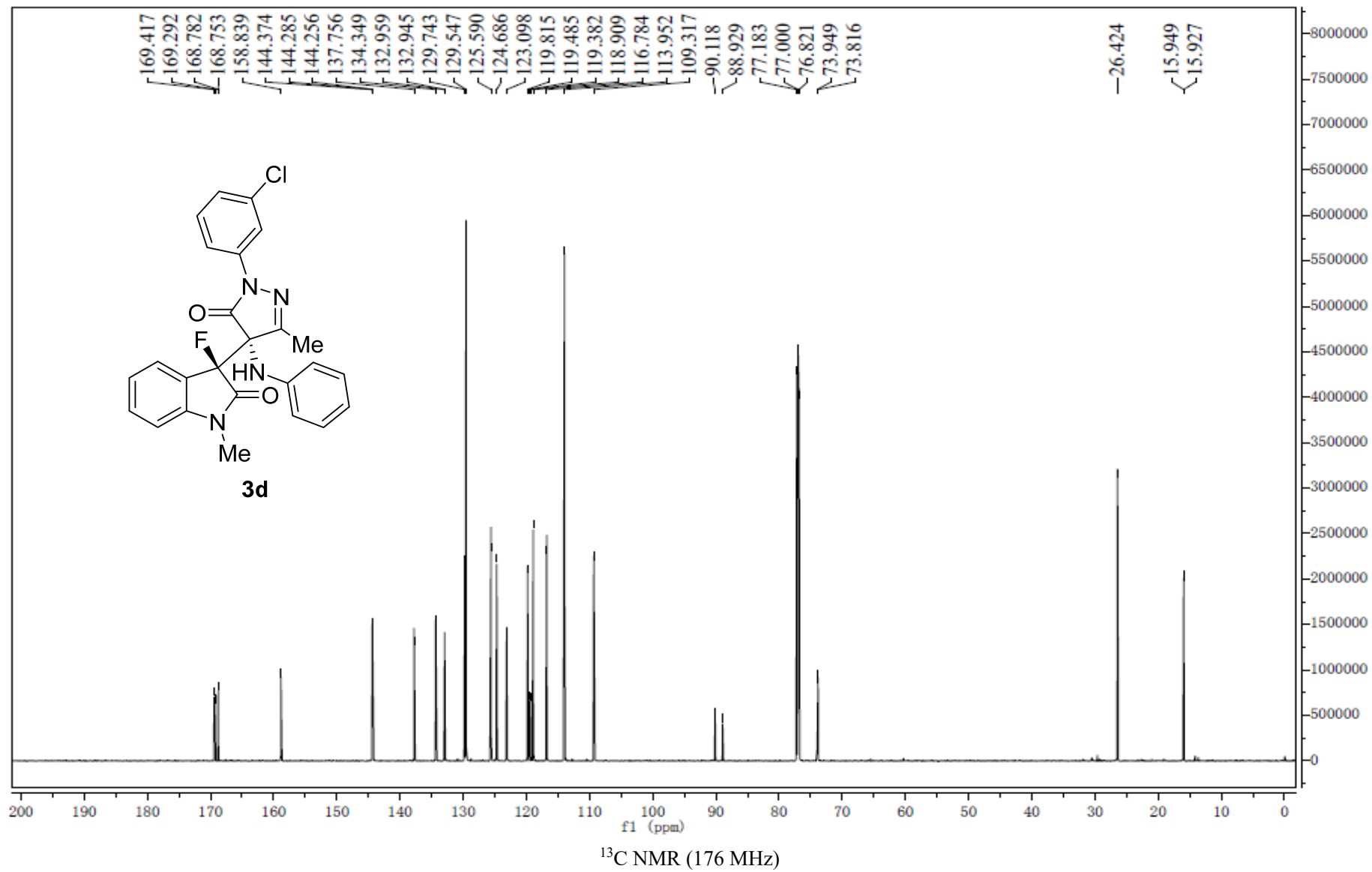
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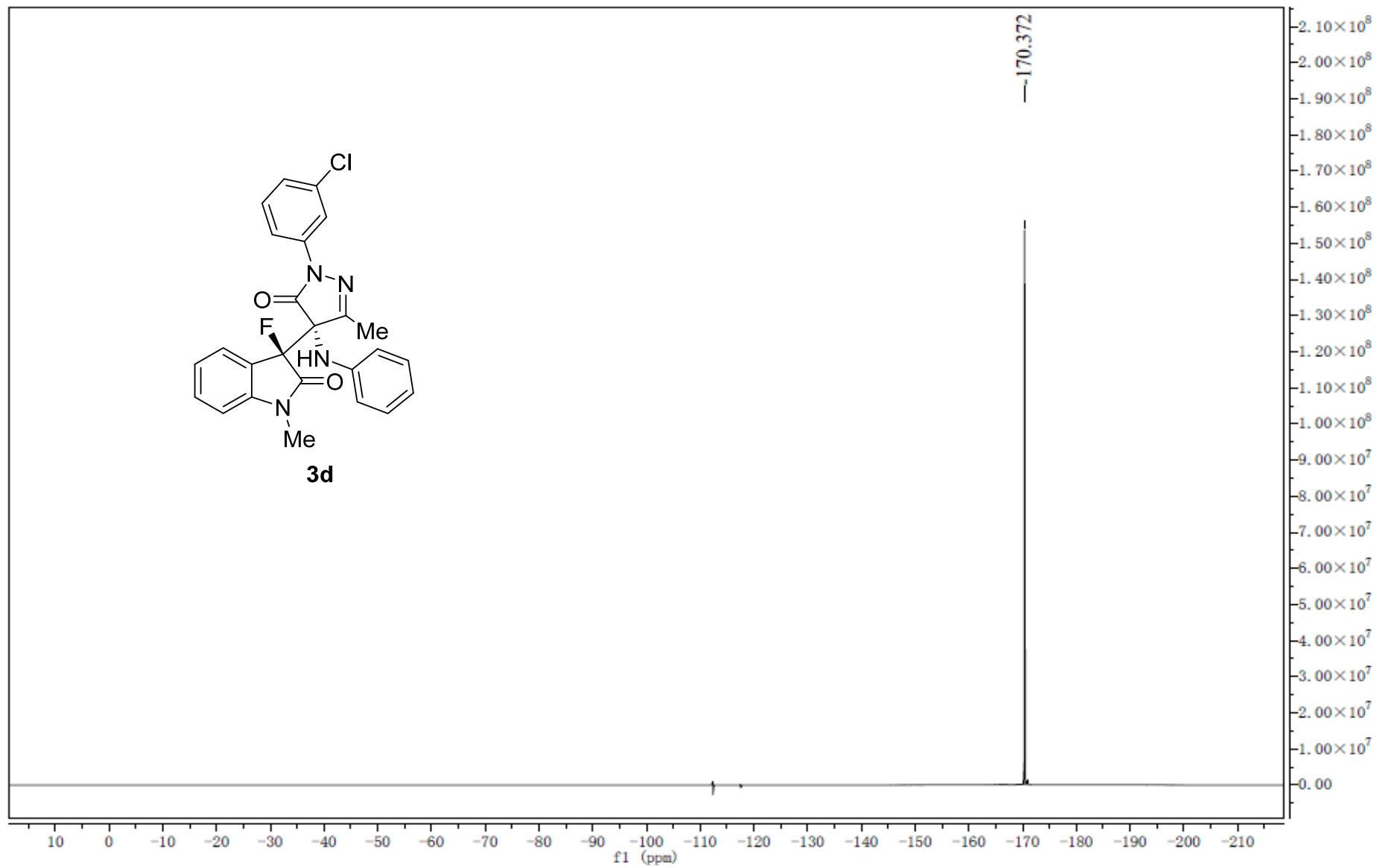


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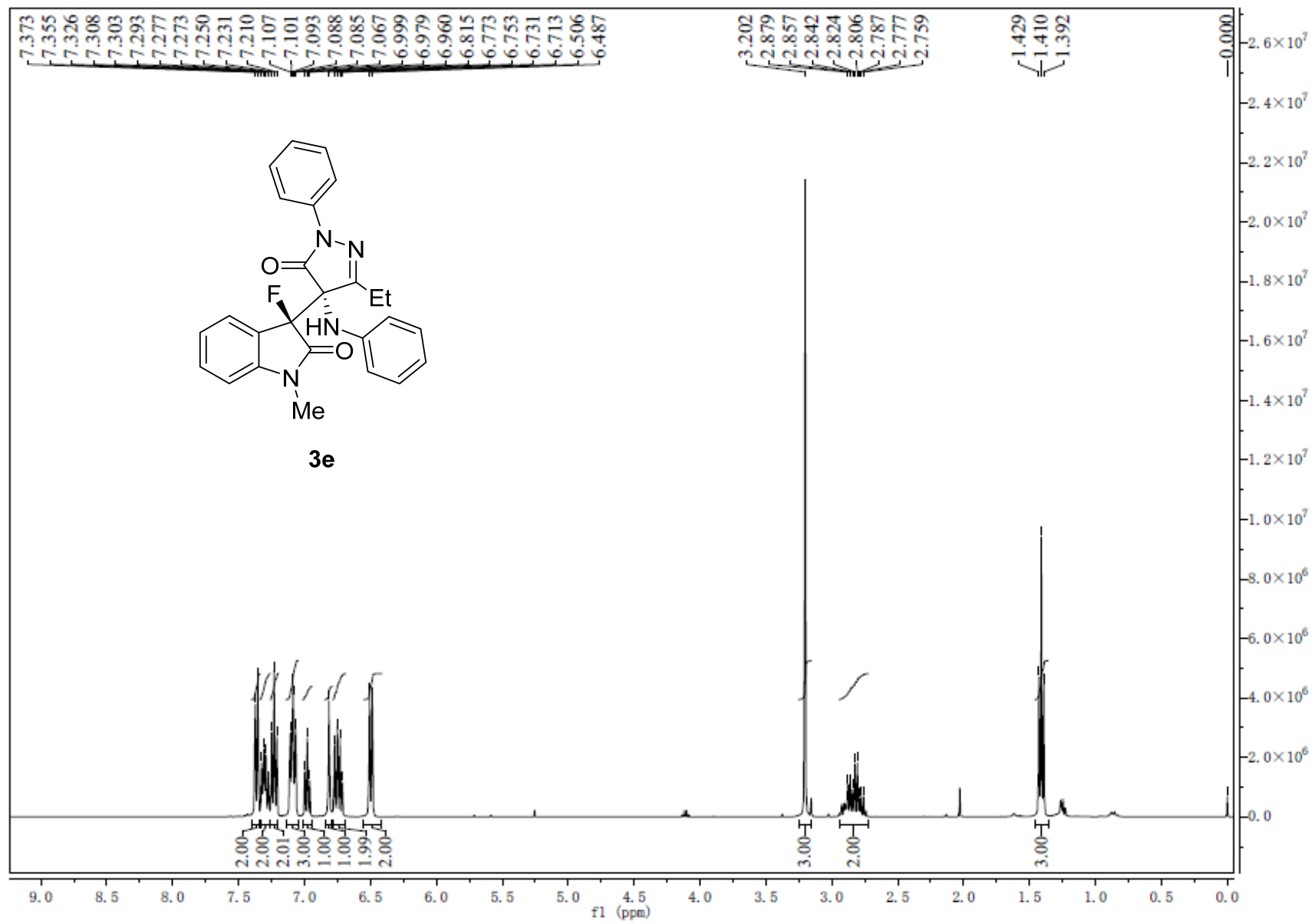
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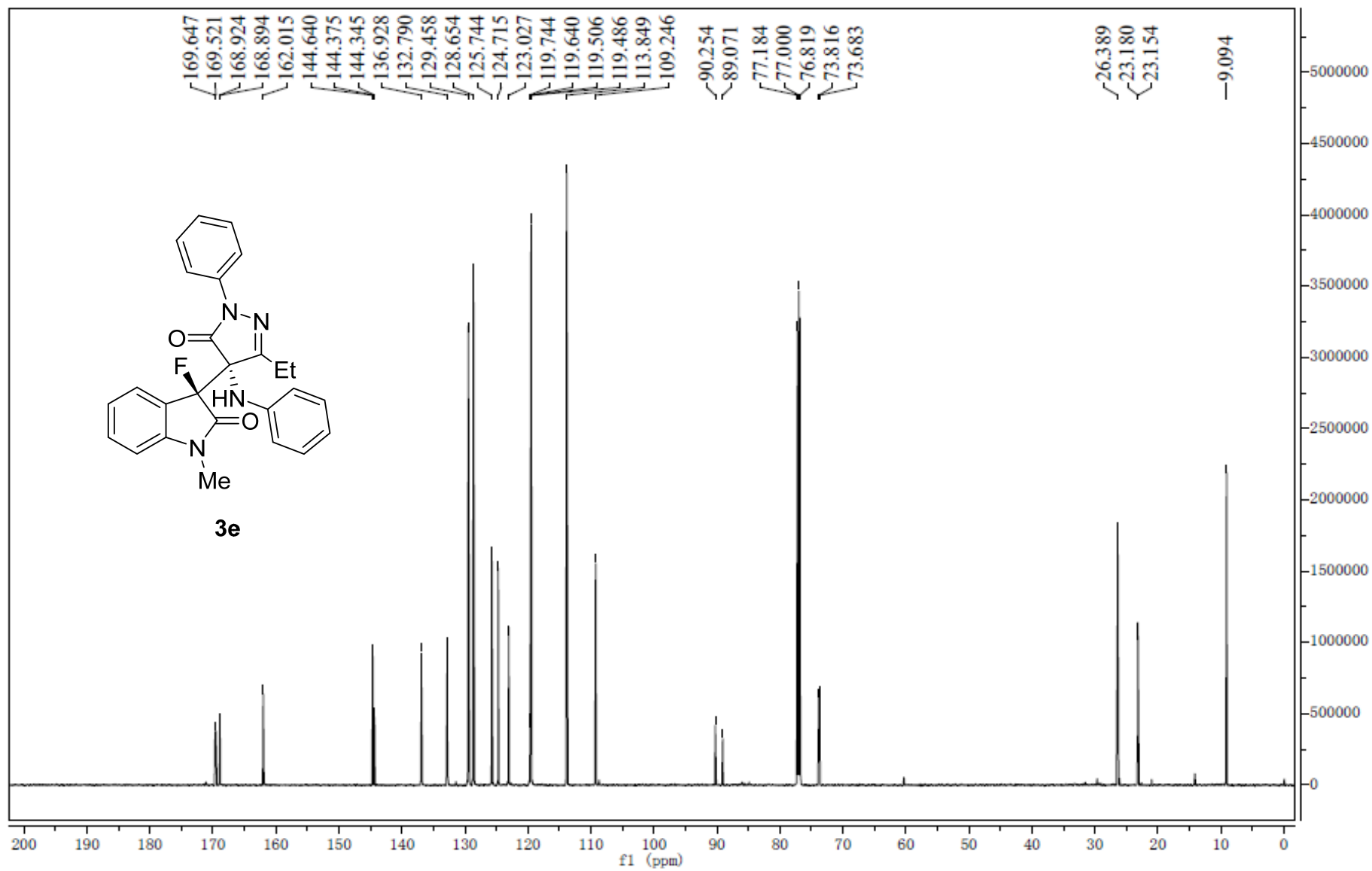


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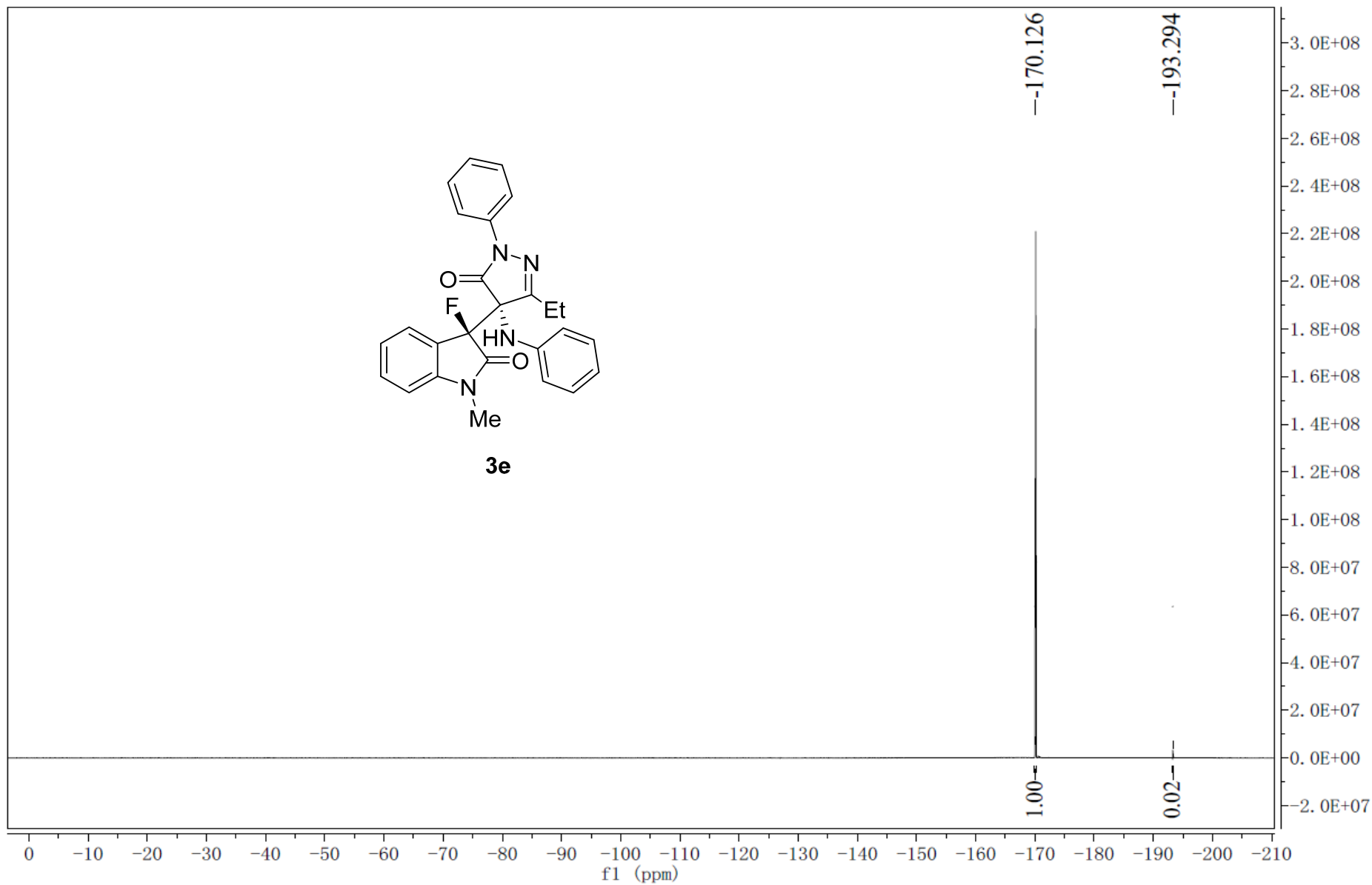
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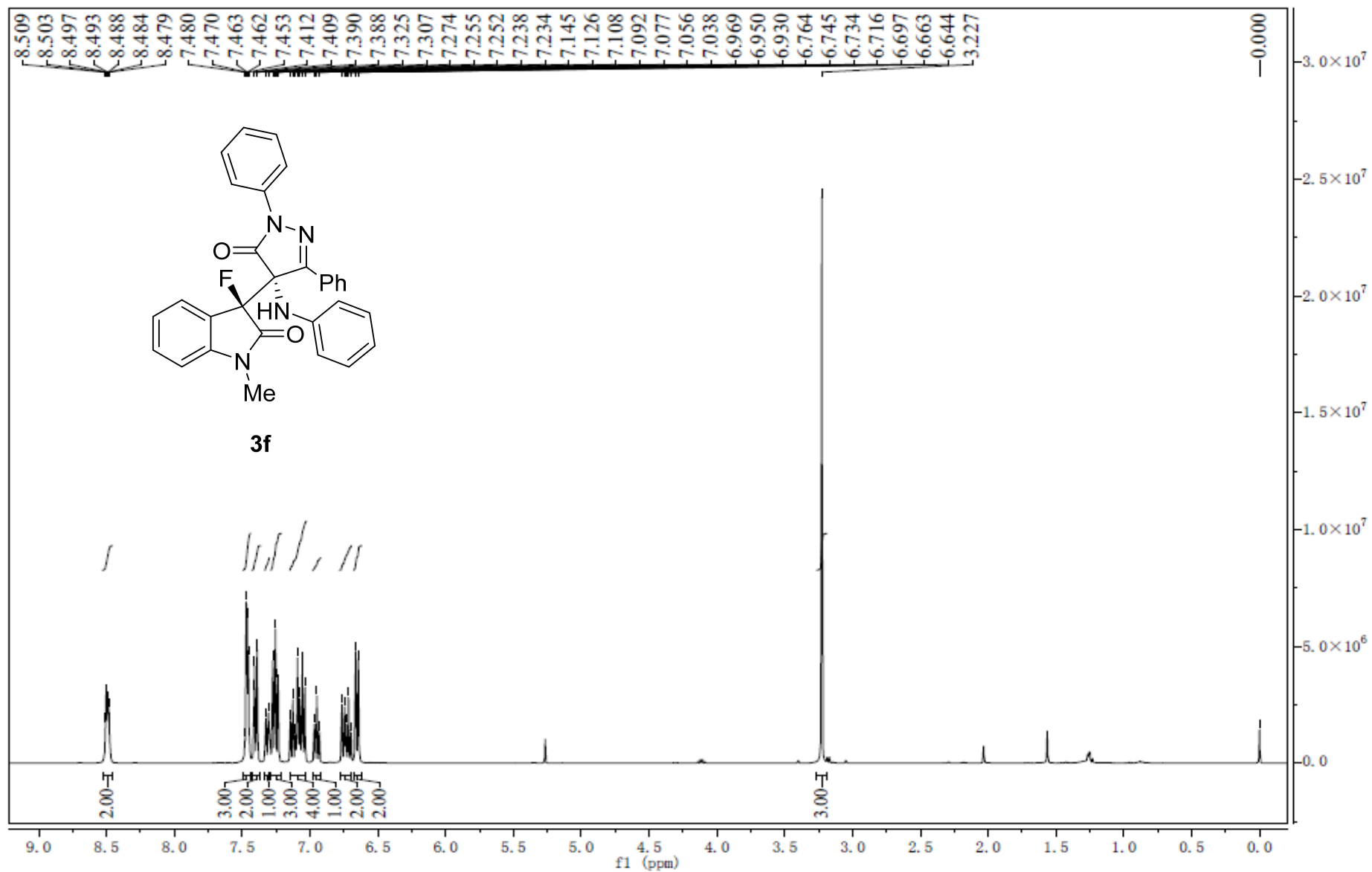
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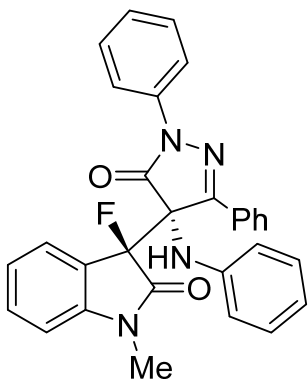
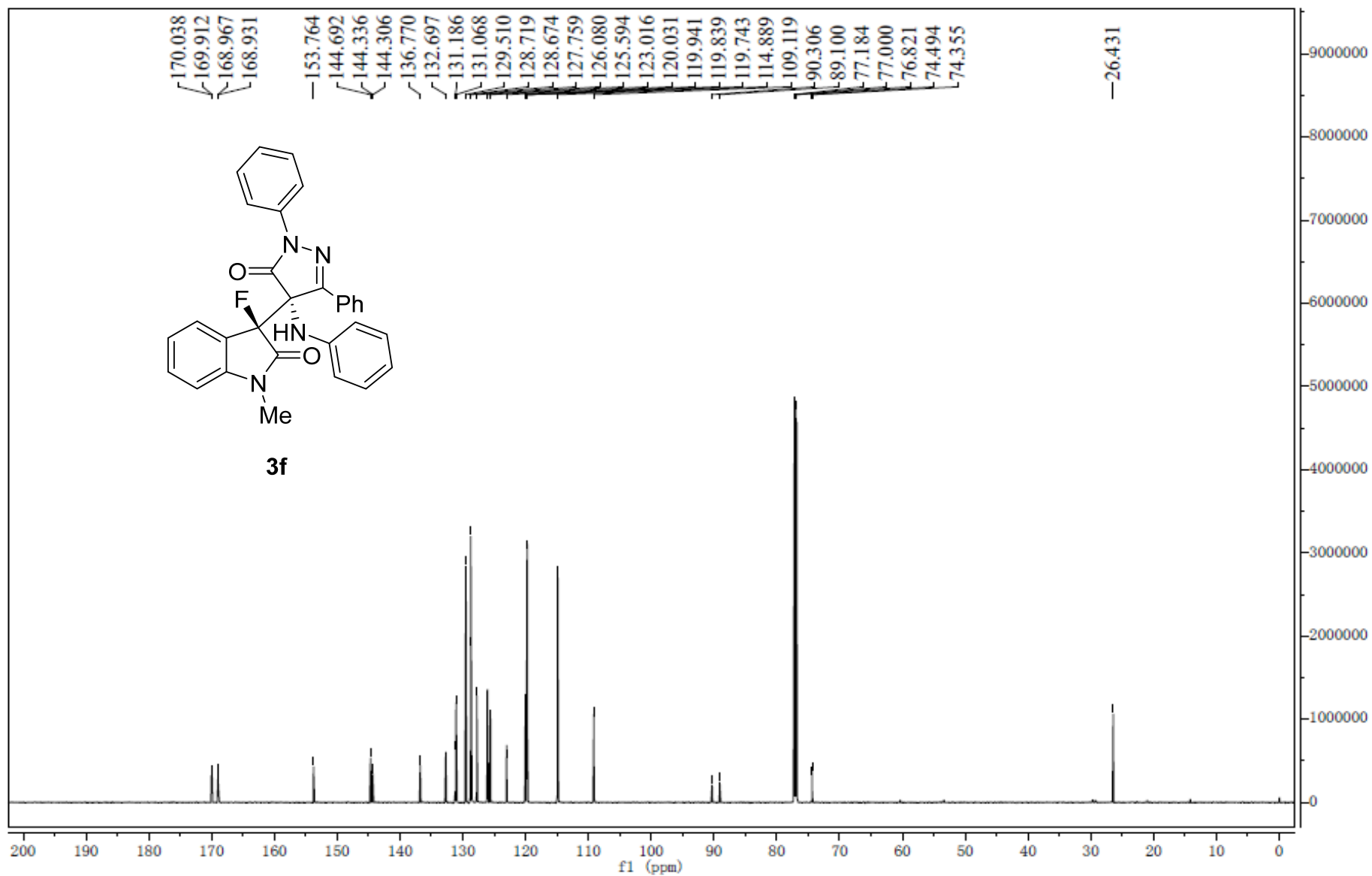
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¹⁹F NMR (376 MHz)

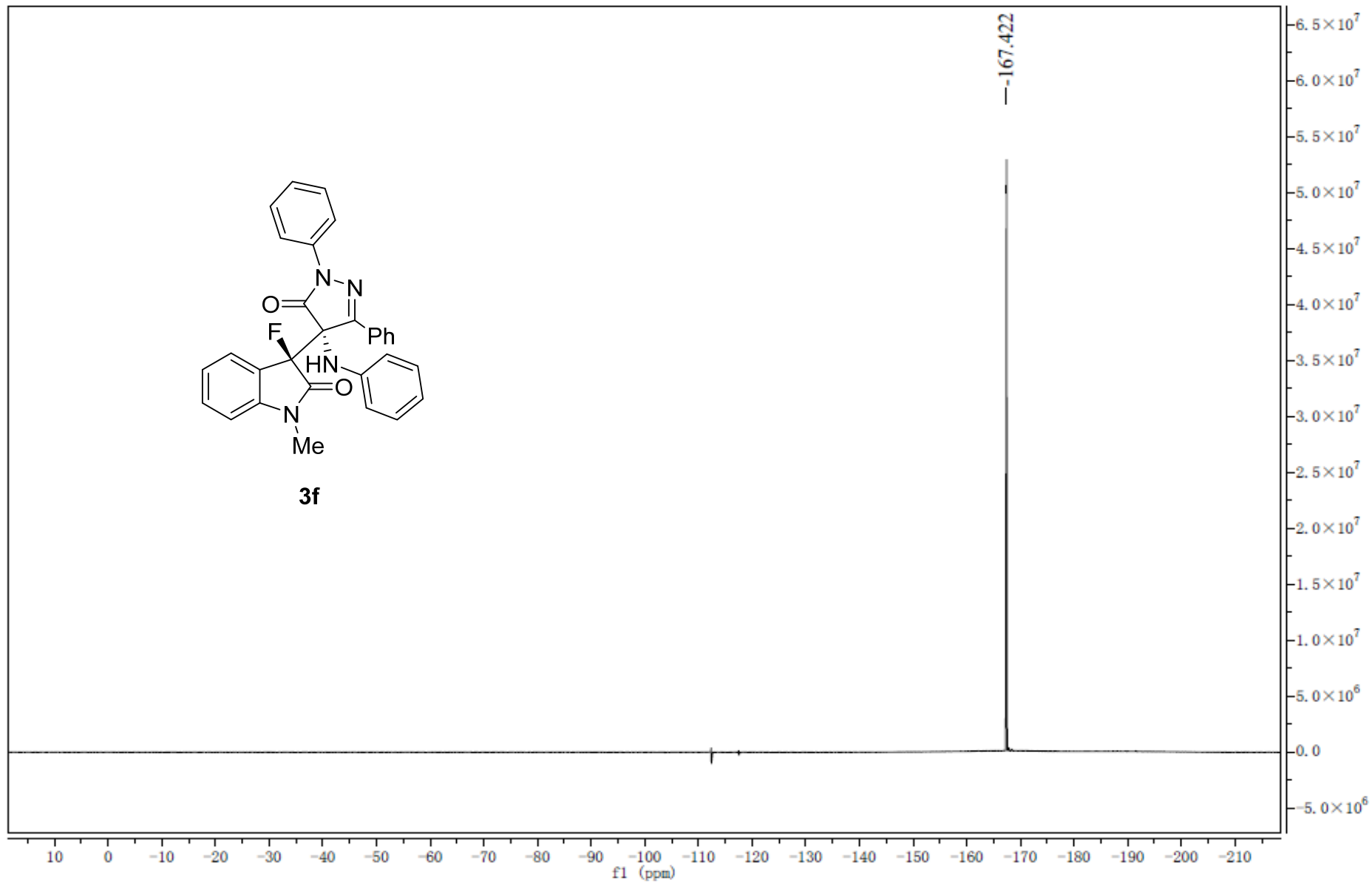


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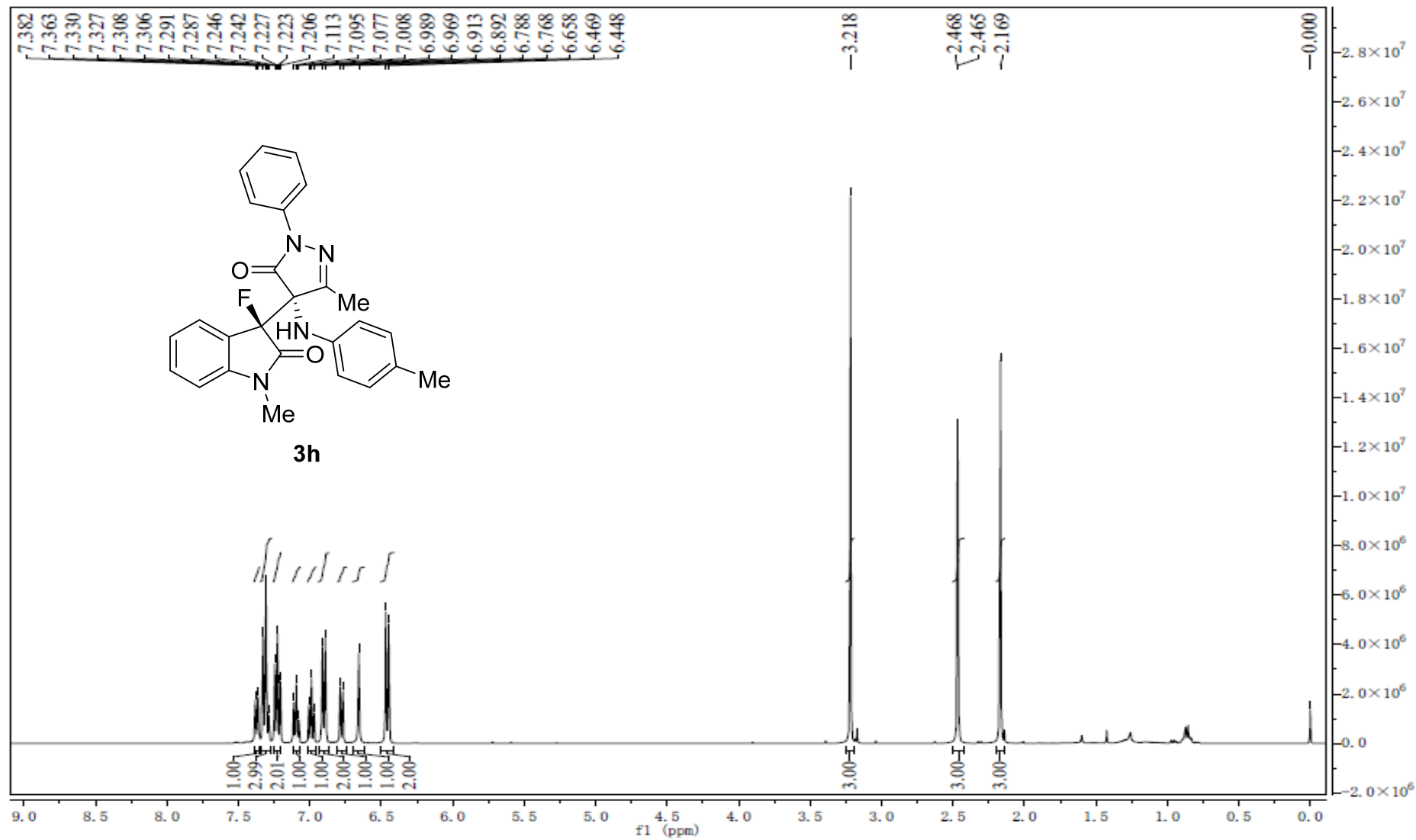


3f

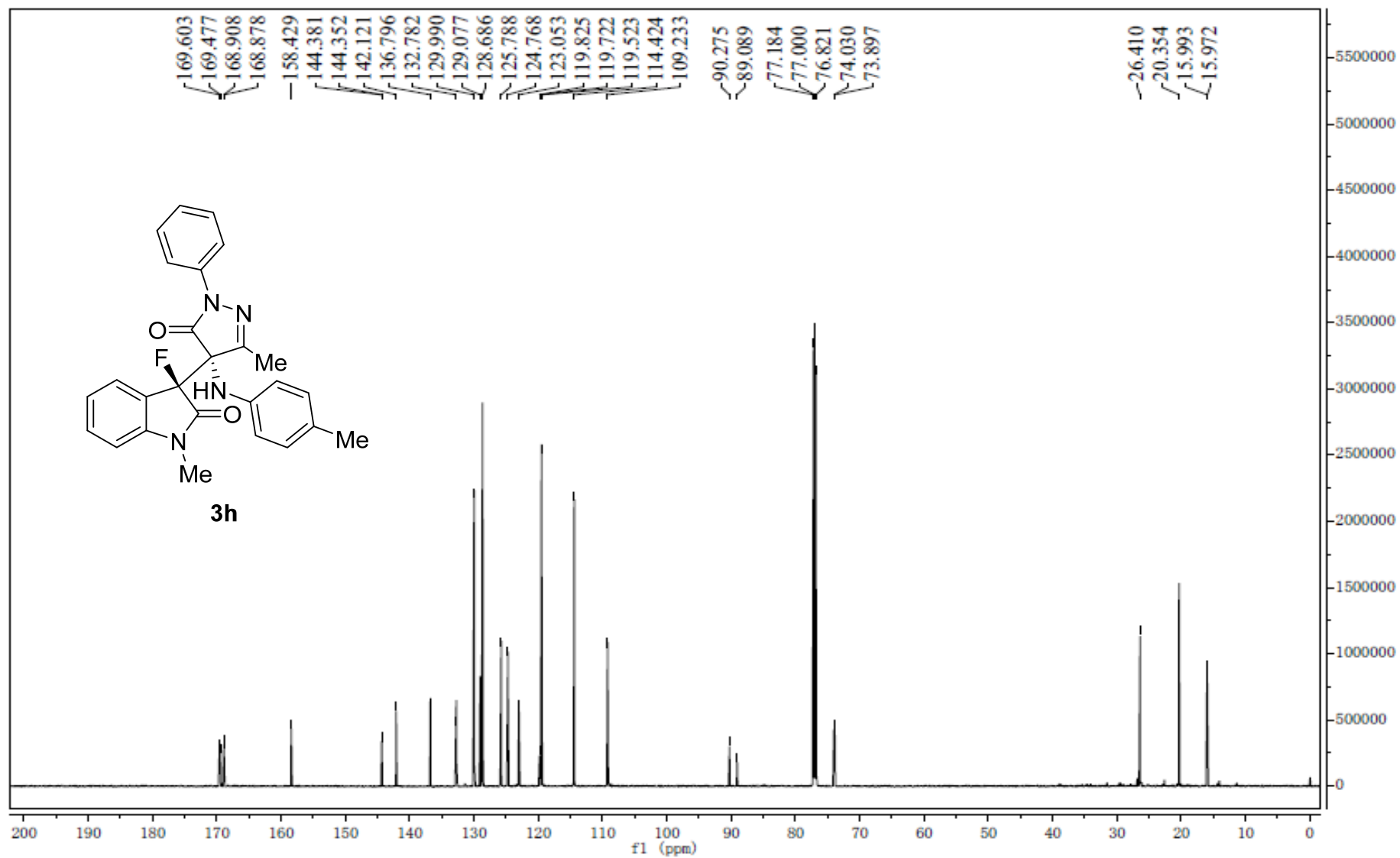
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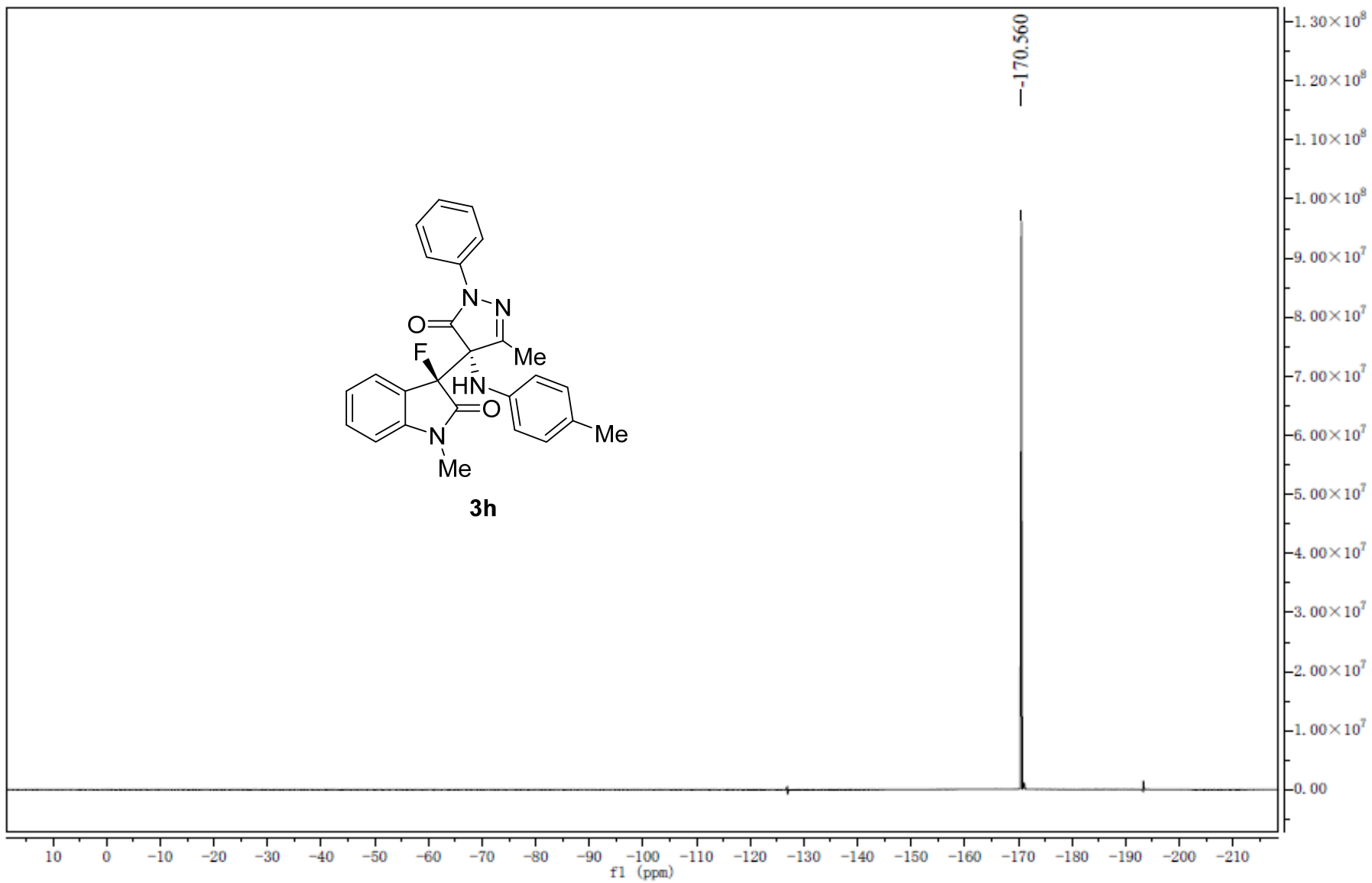
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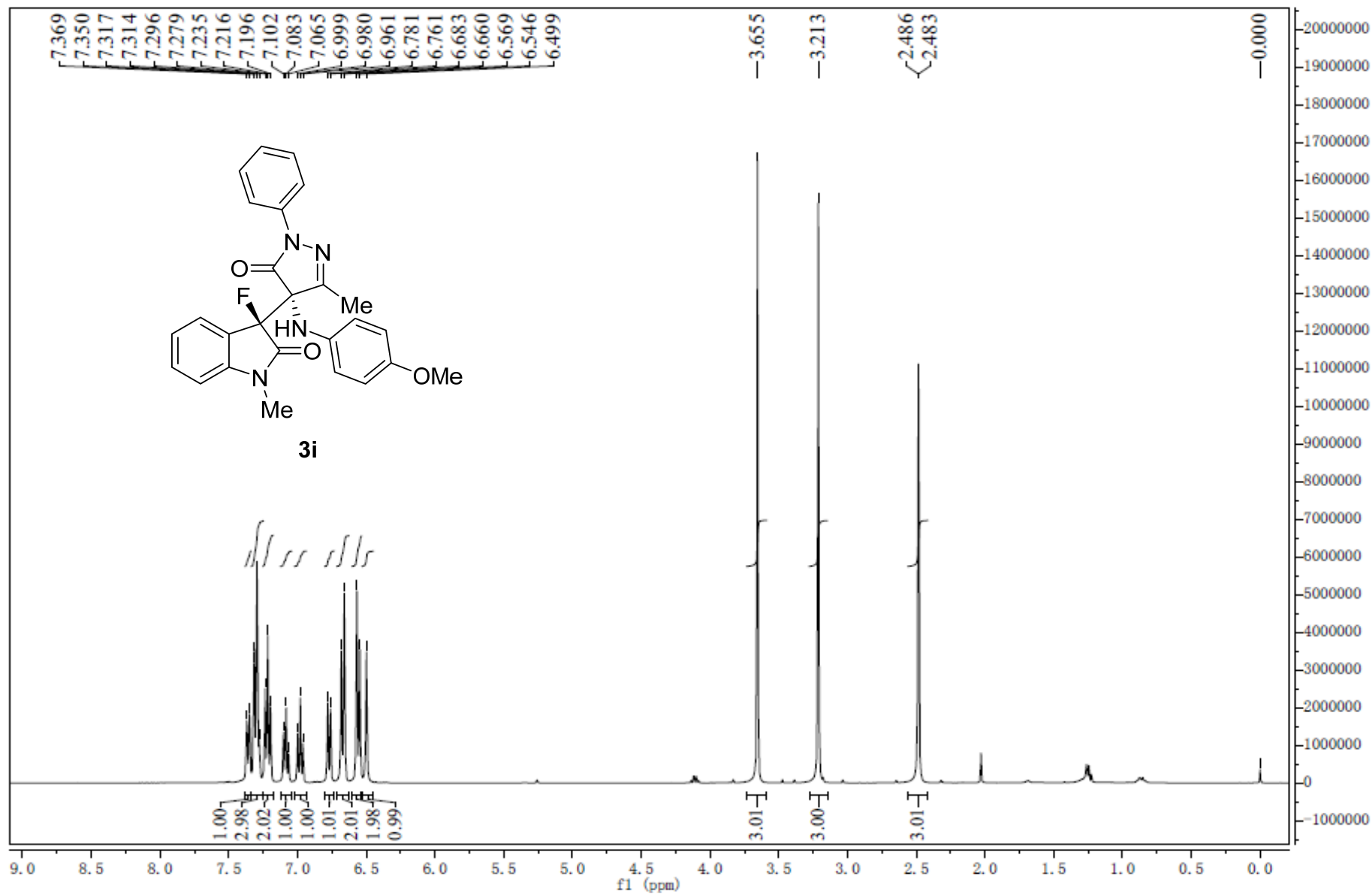
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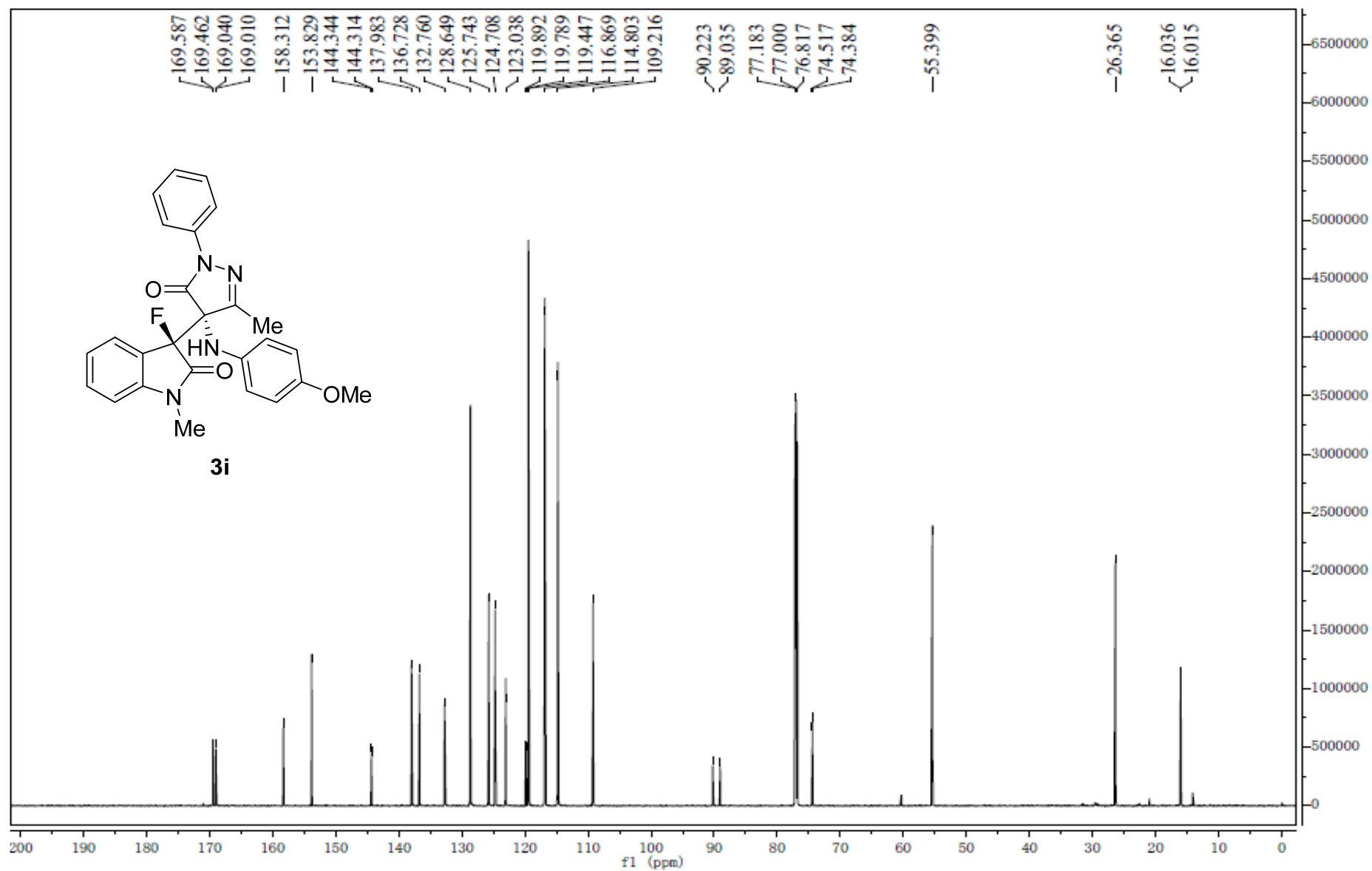
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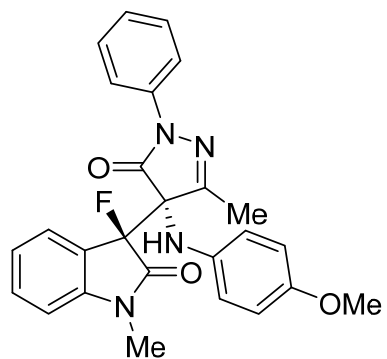
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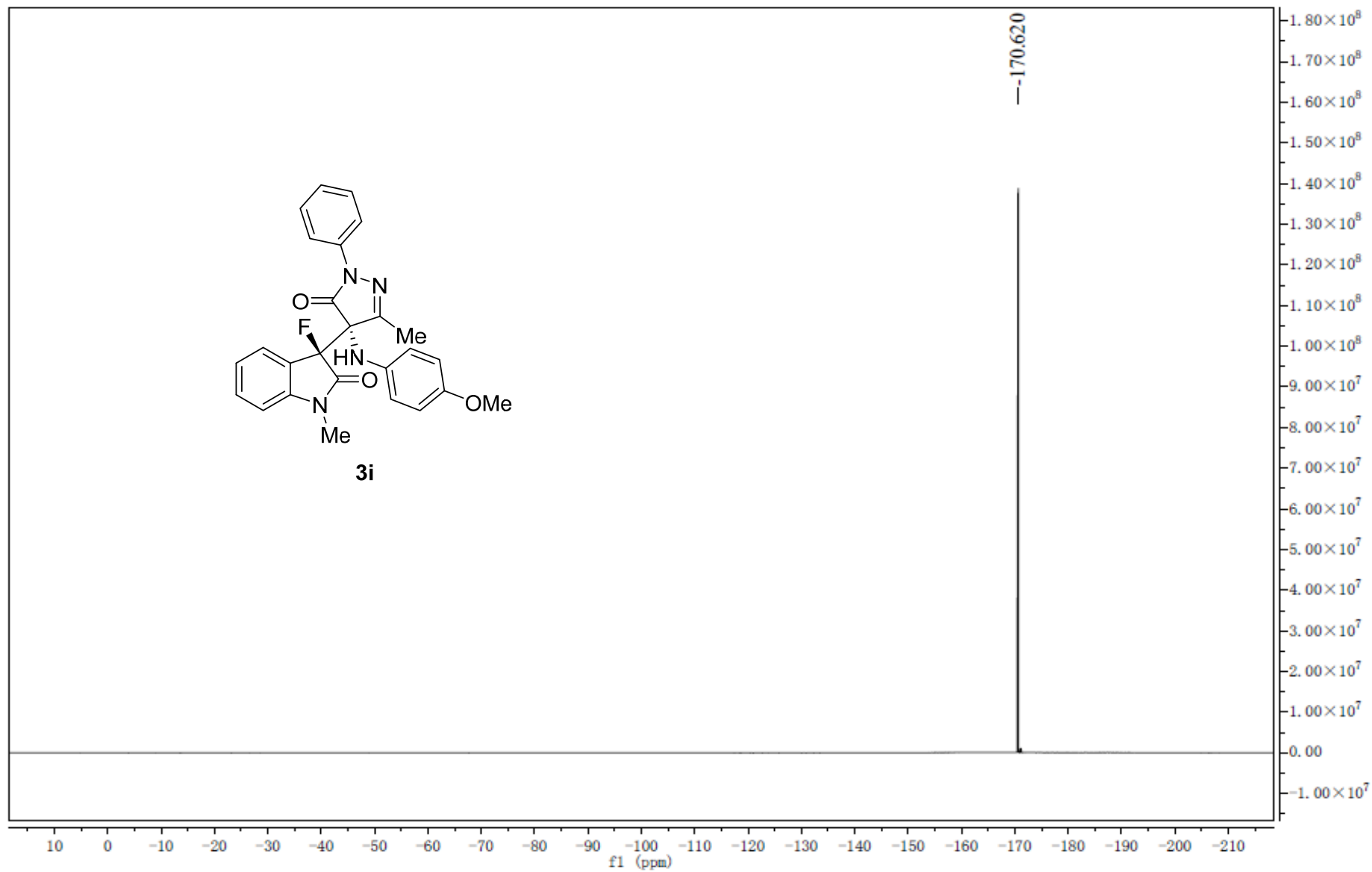
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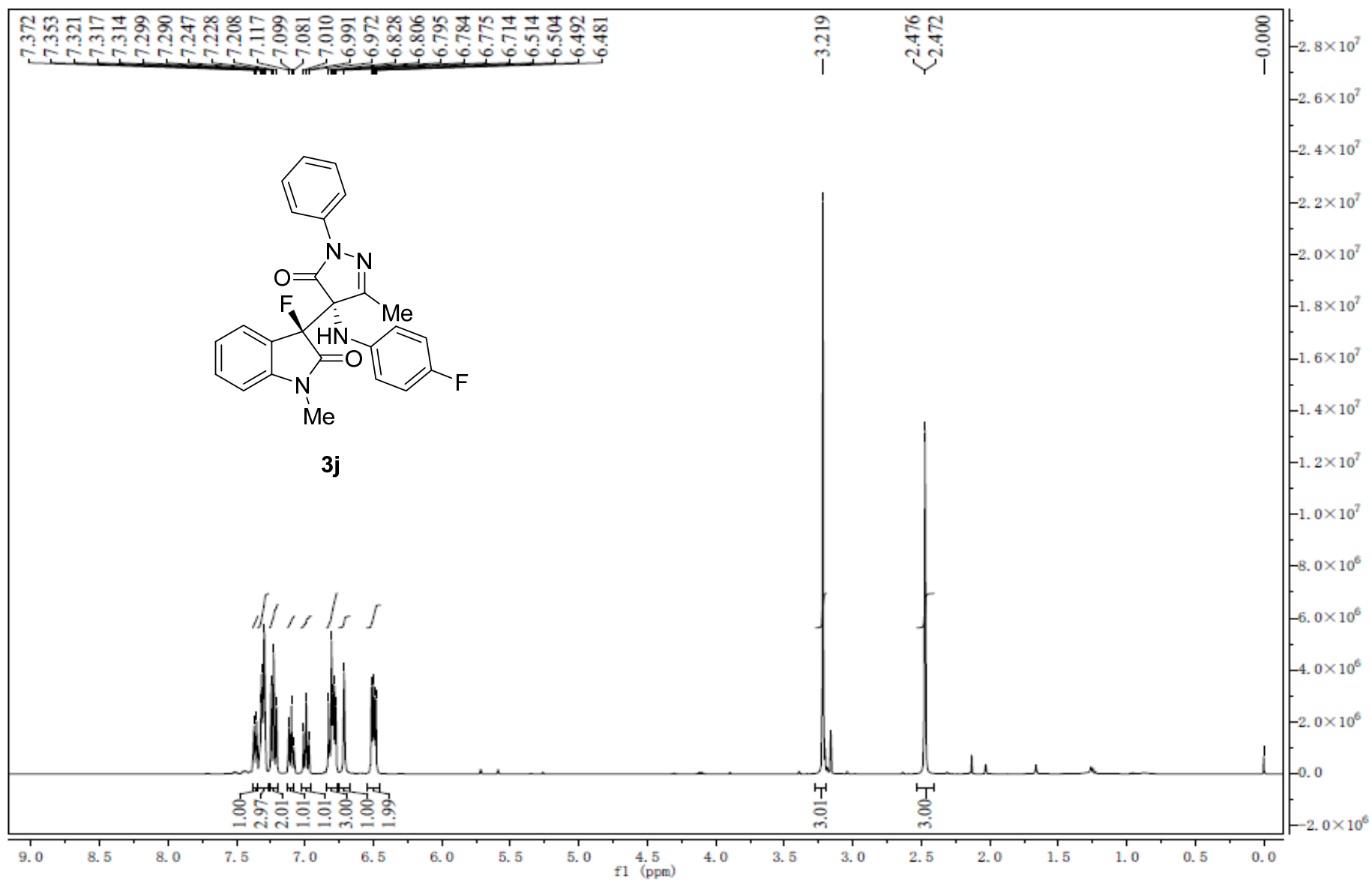
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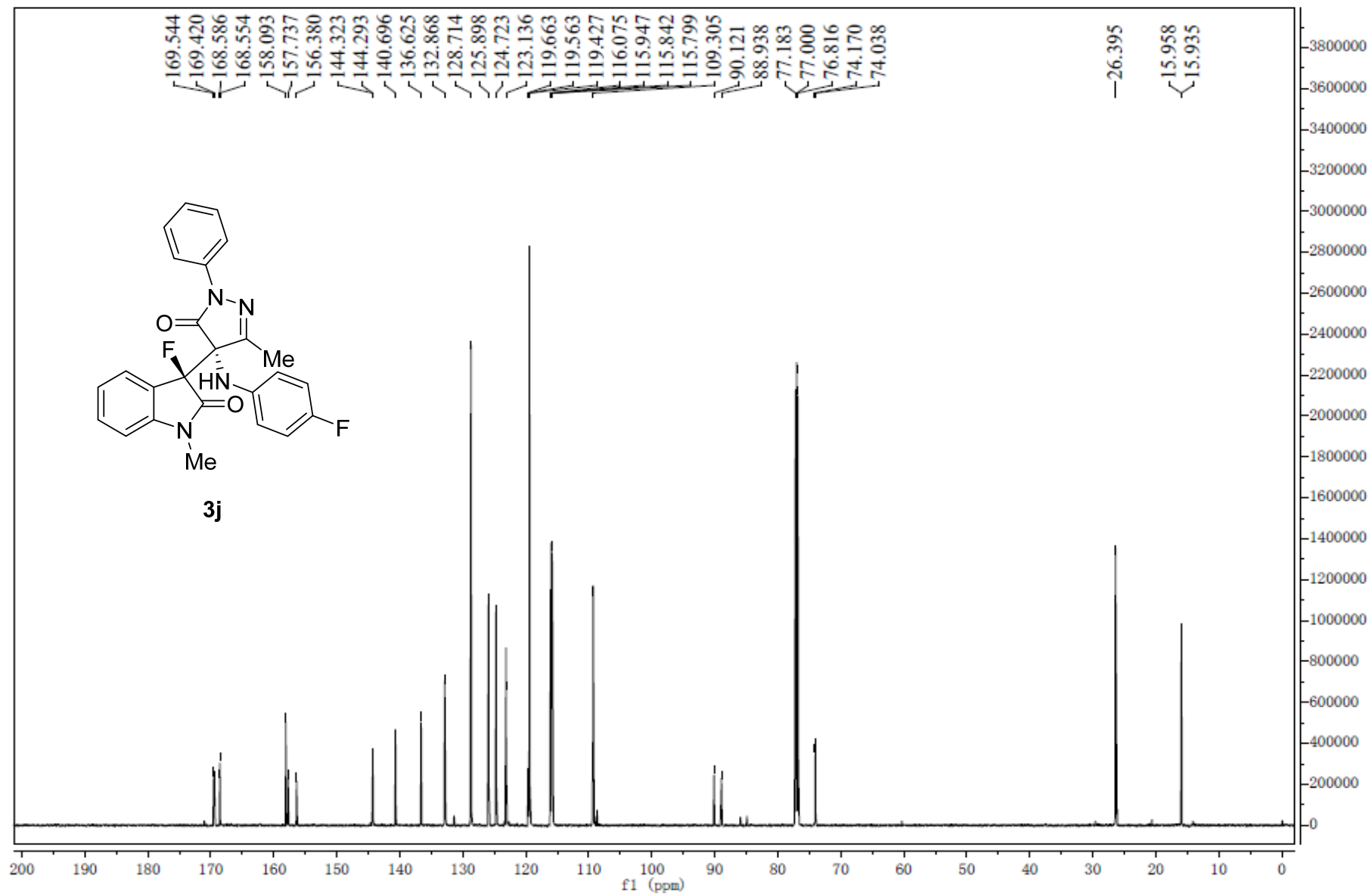
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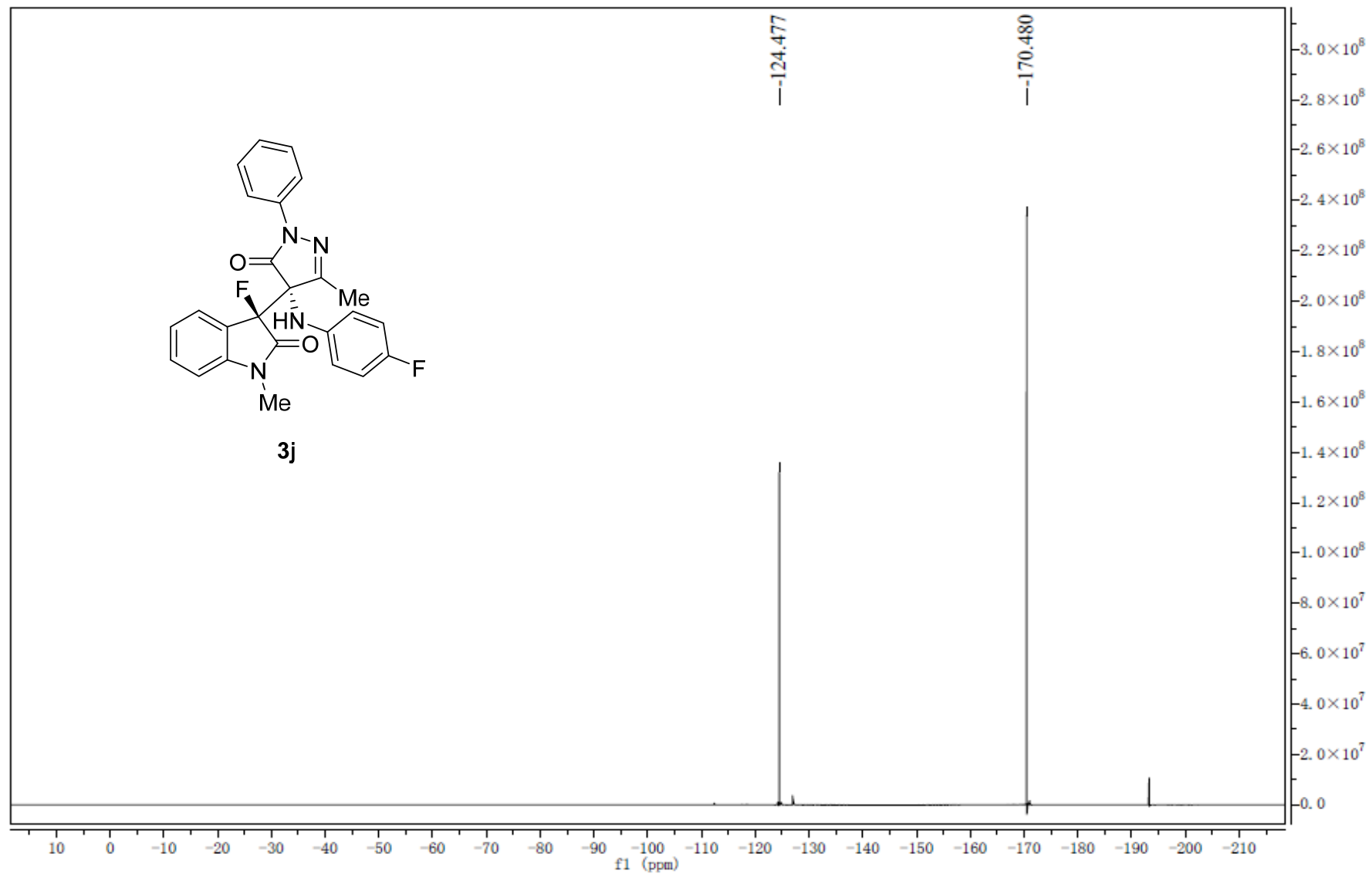
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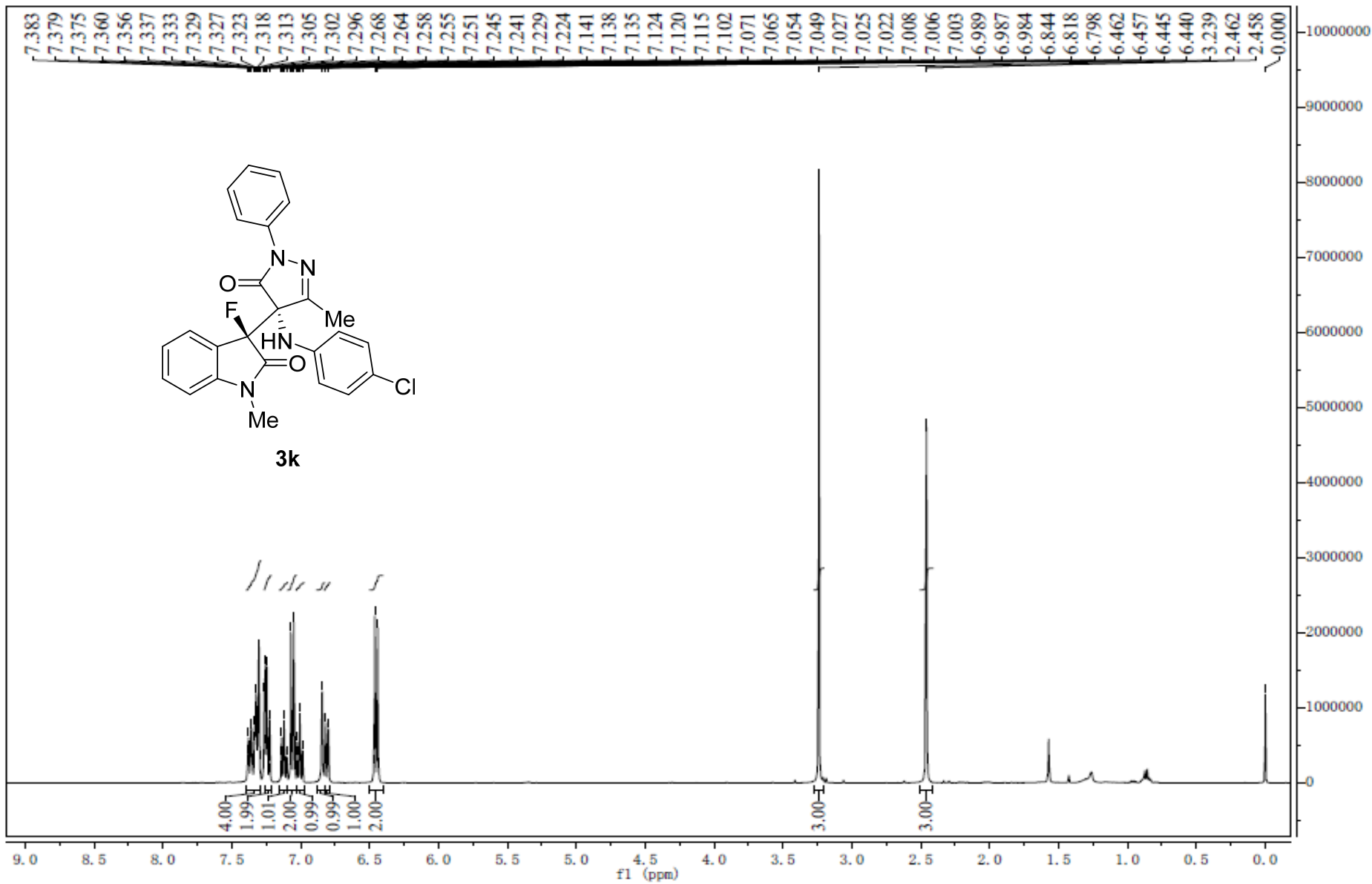
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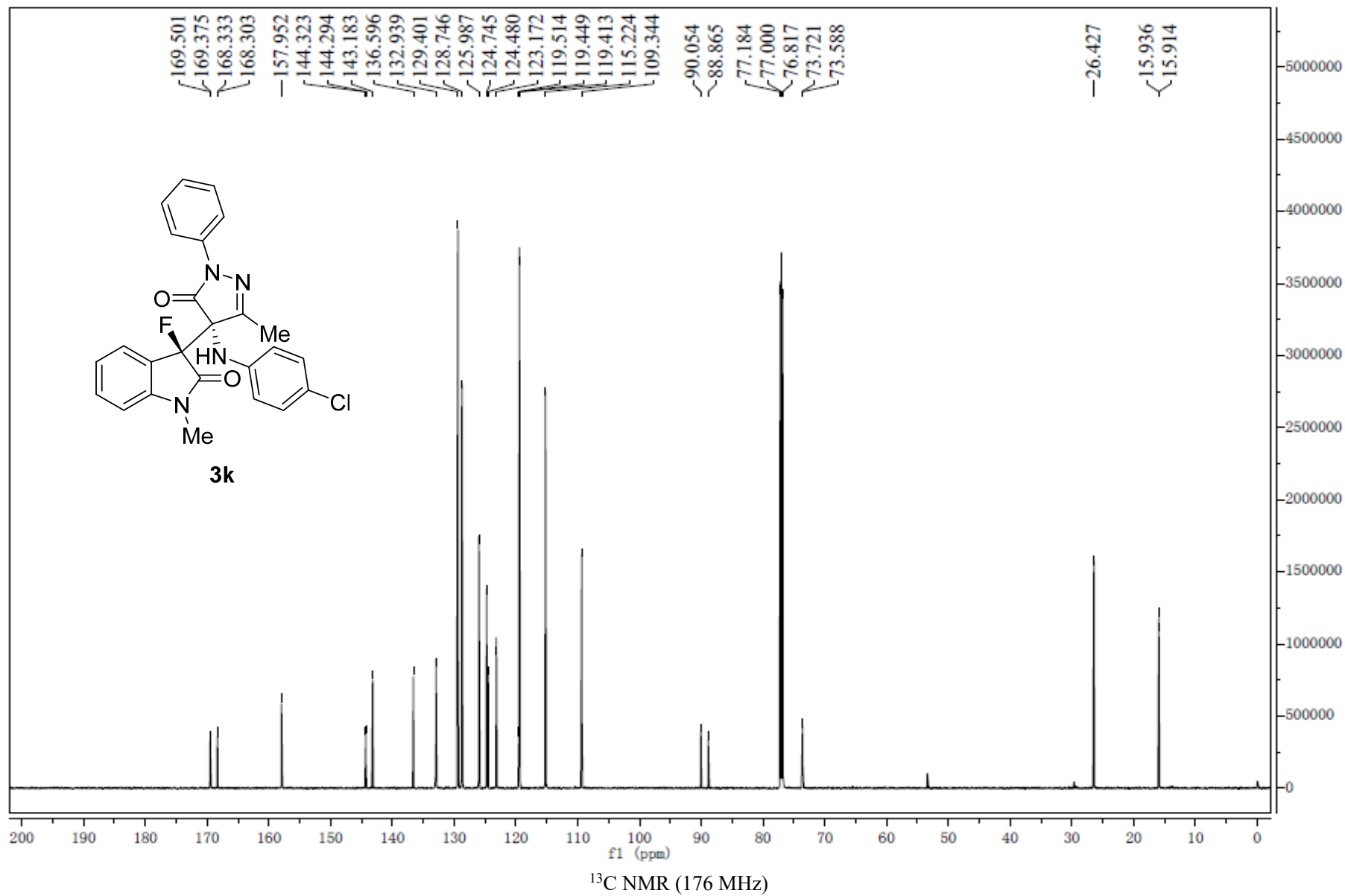
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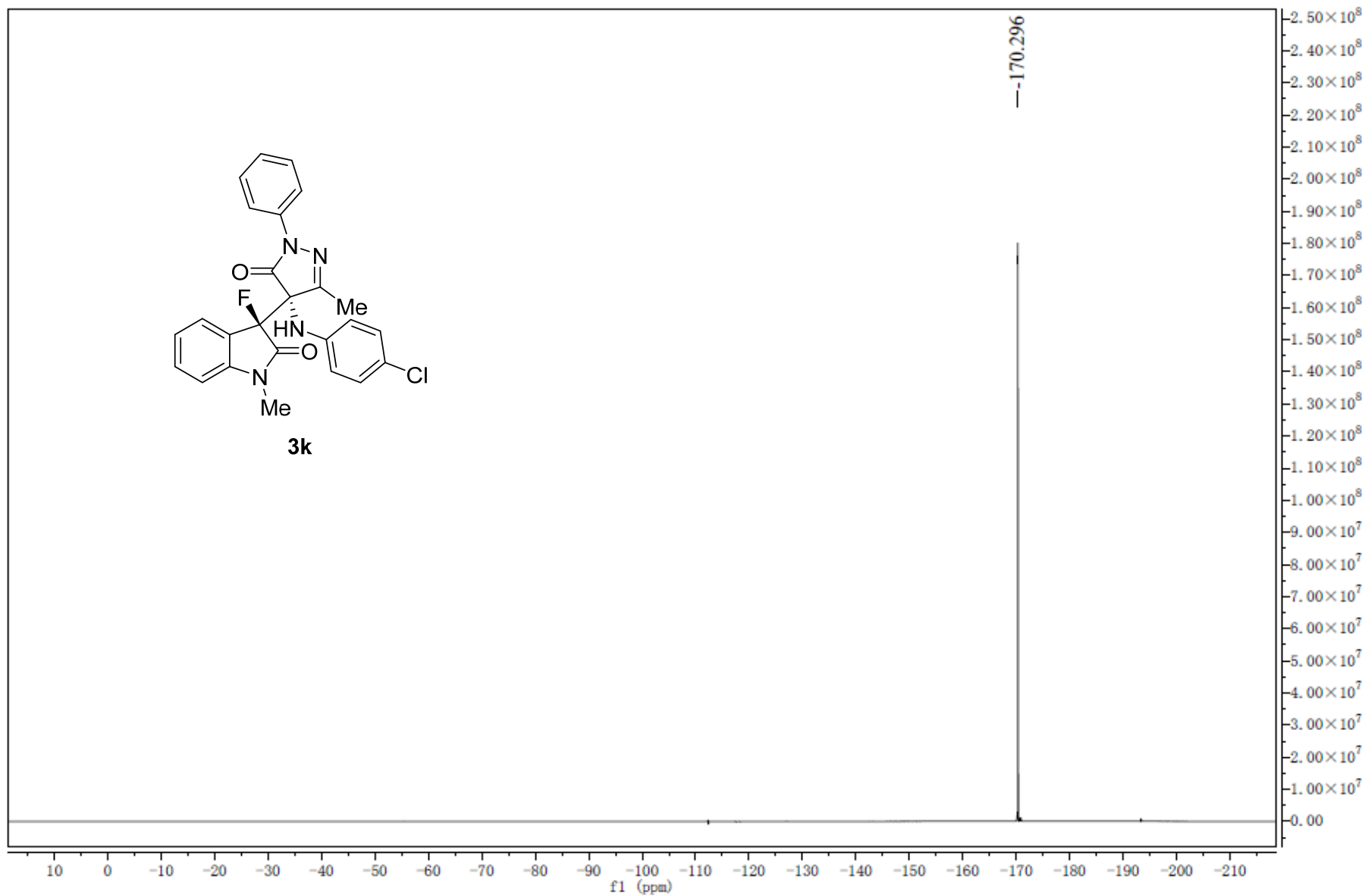


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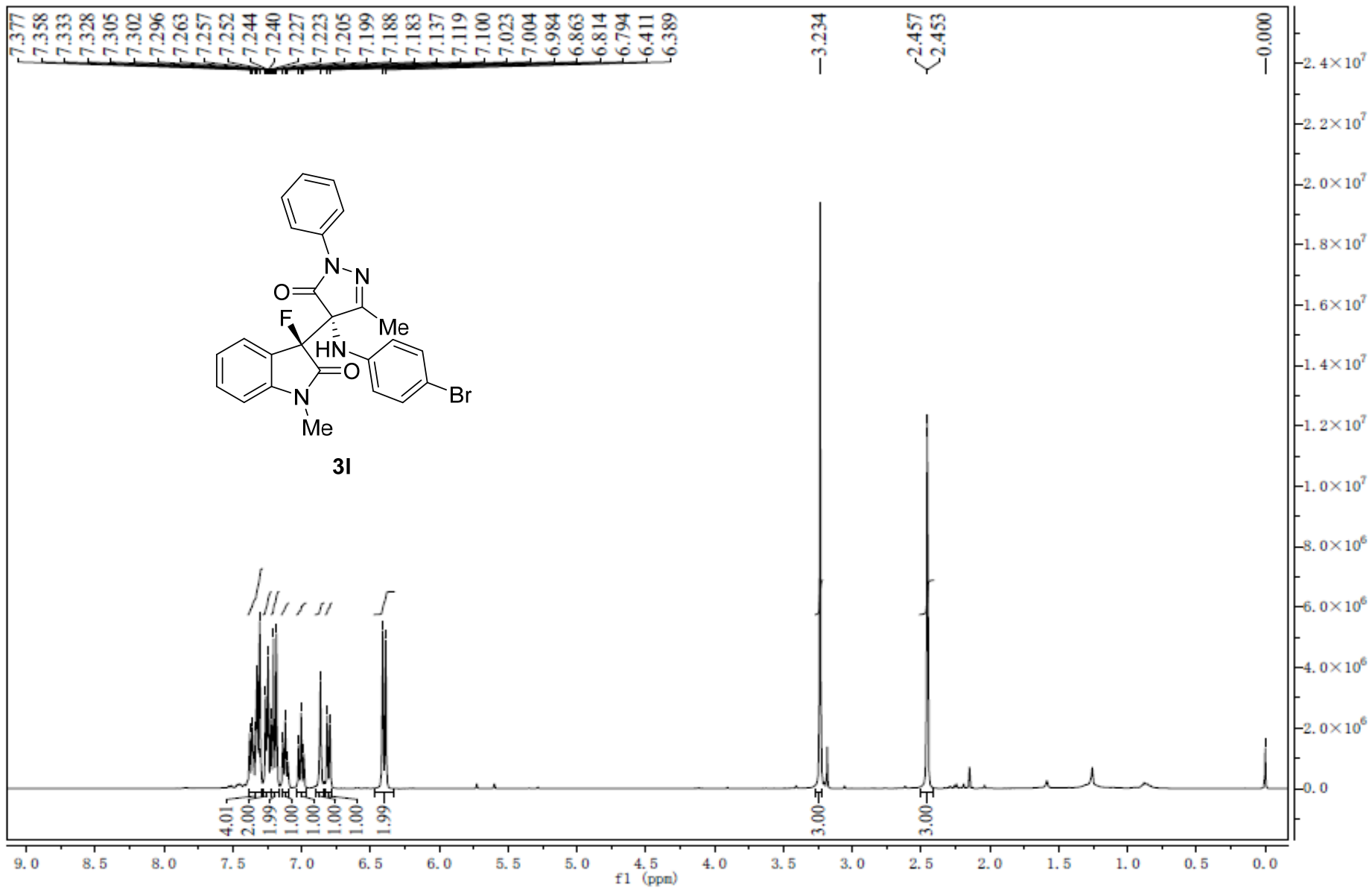


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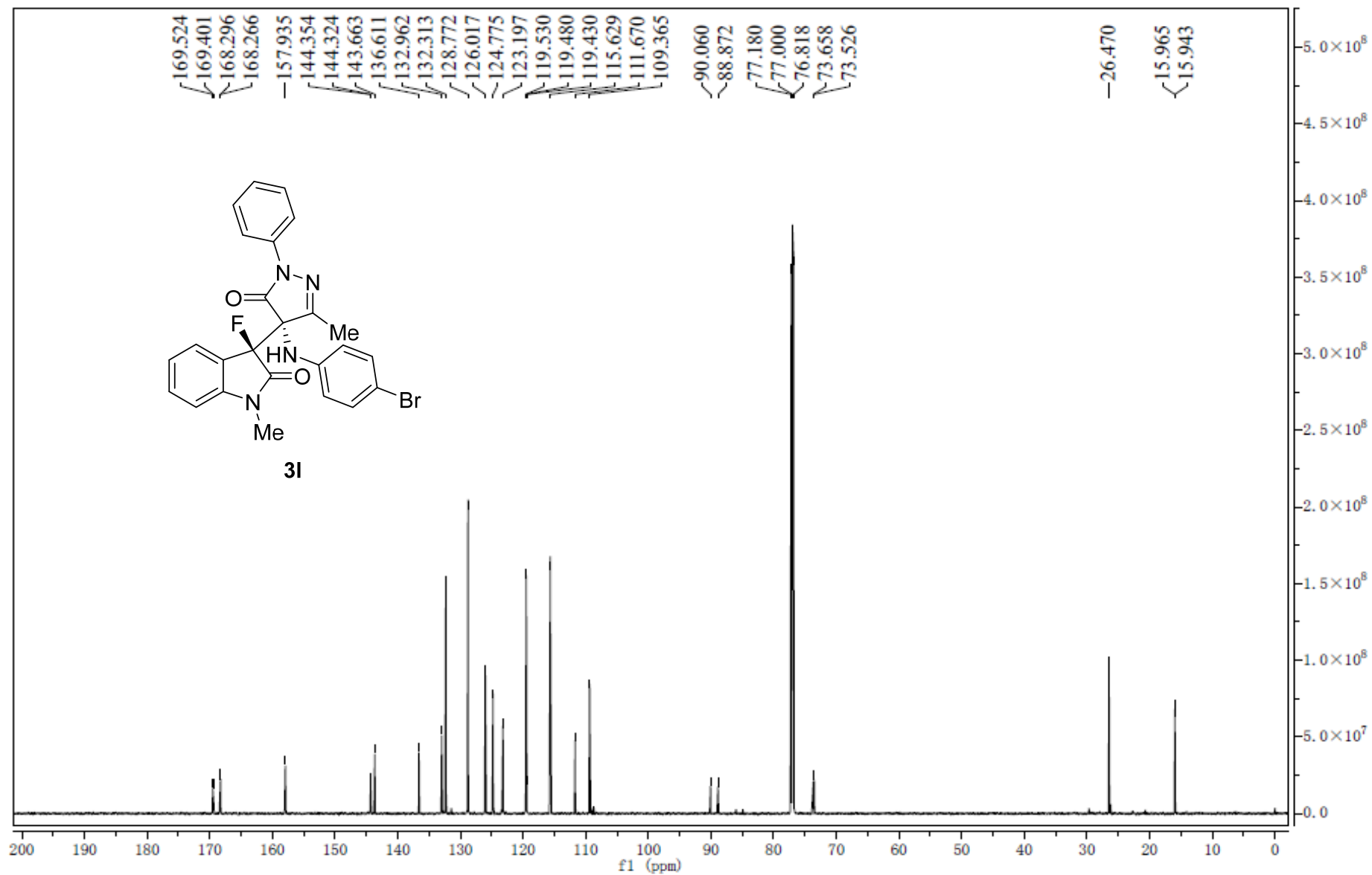




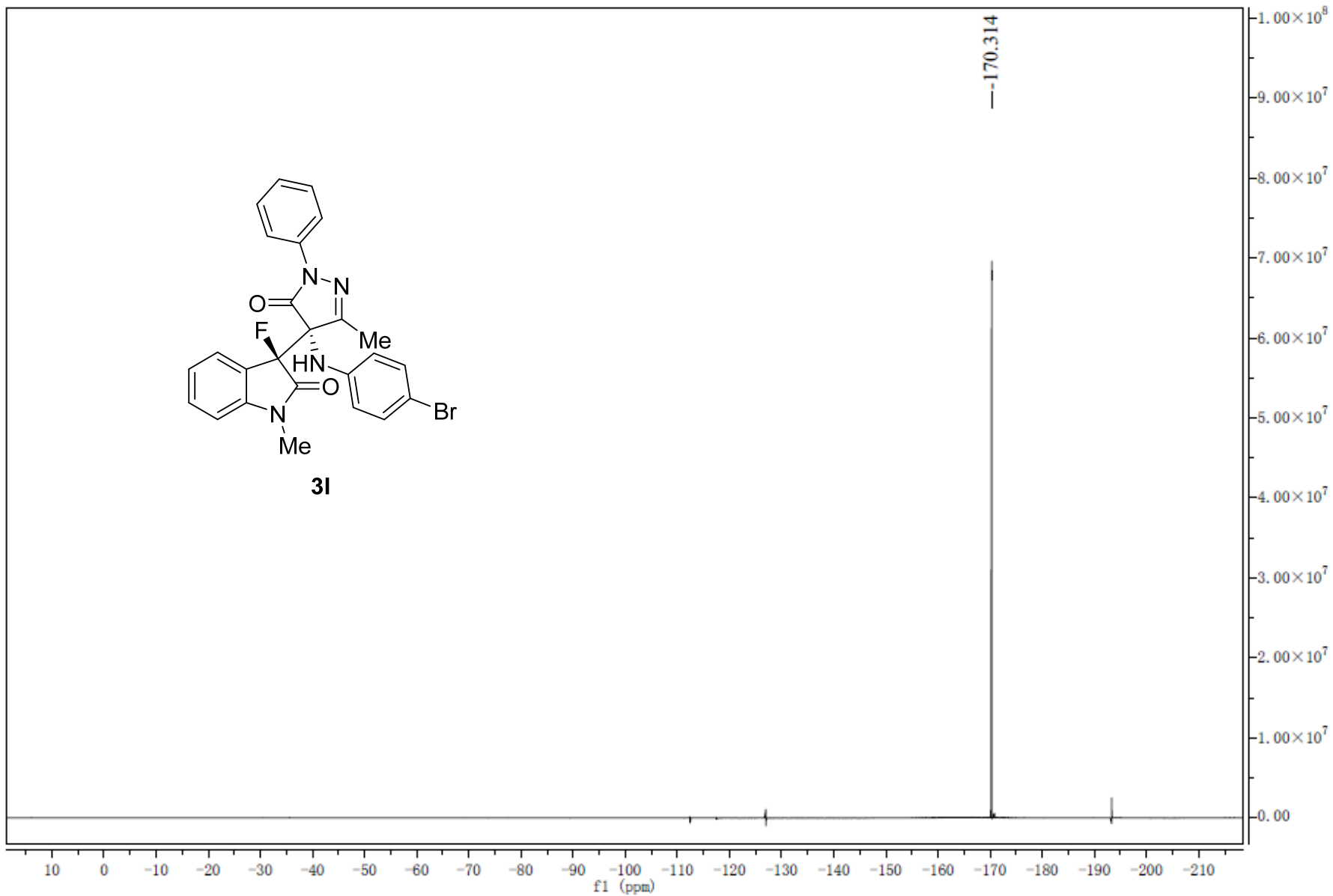
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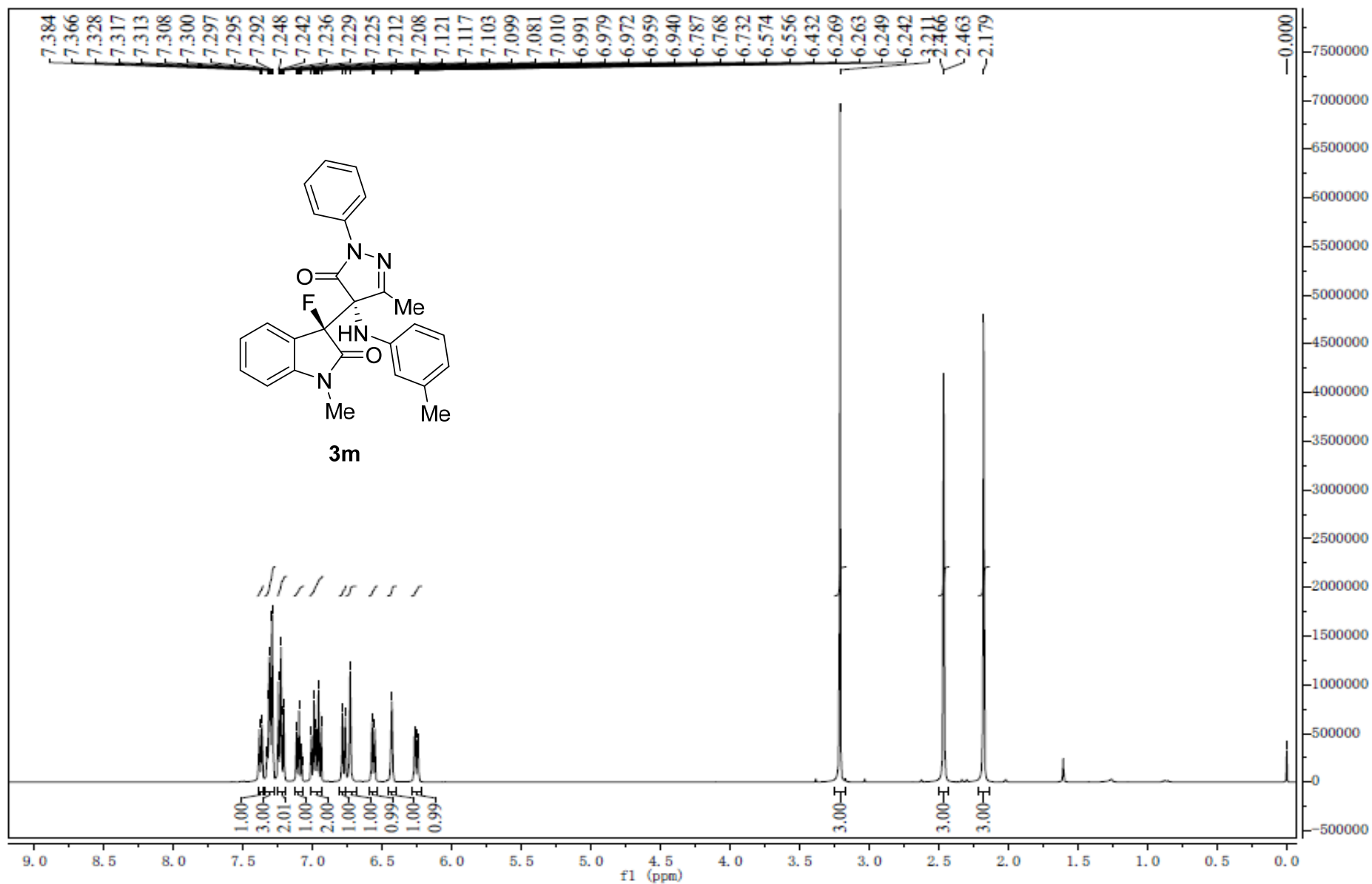
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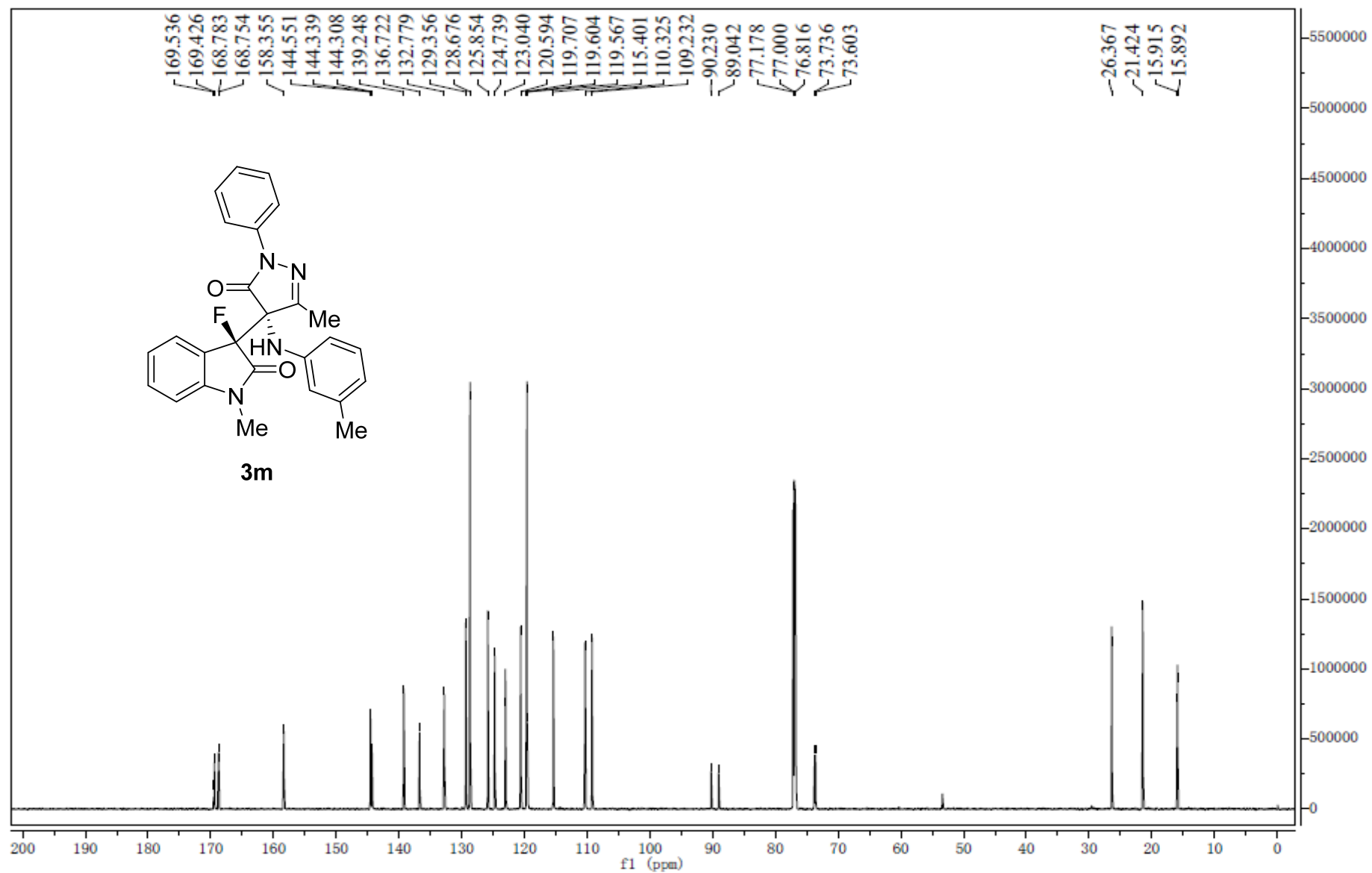
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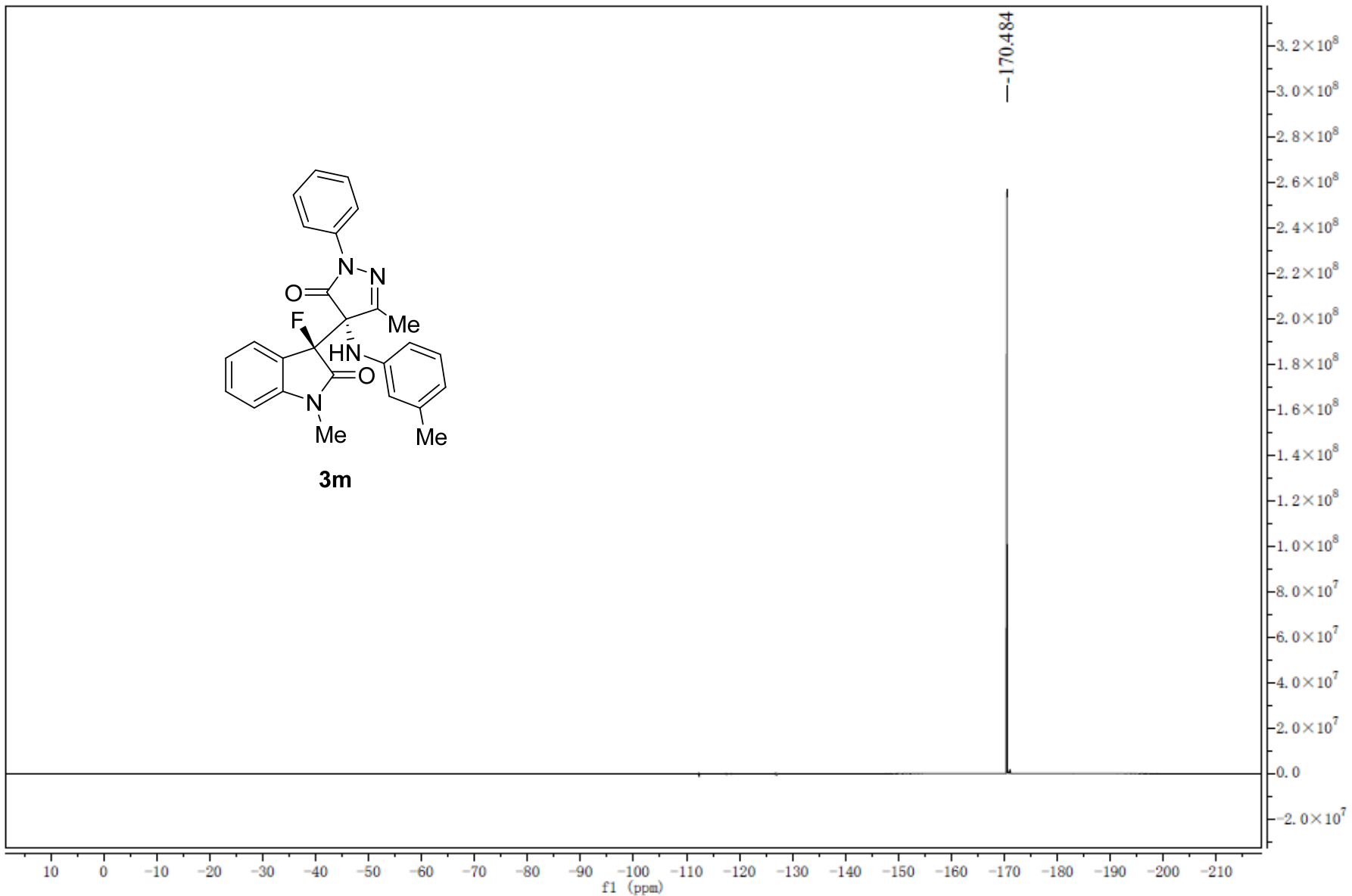
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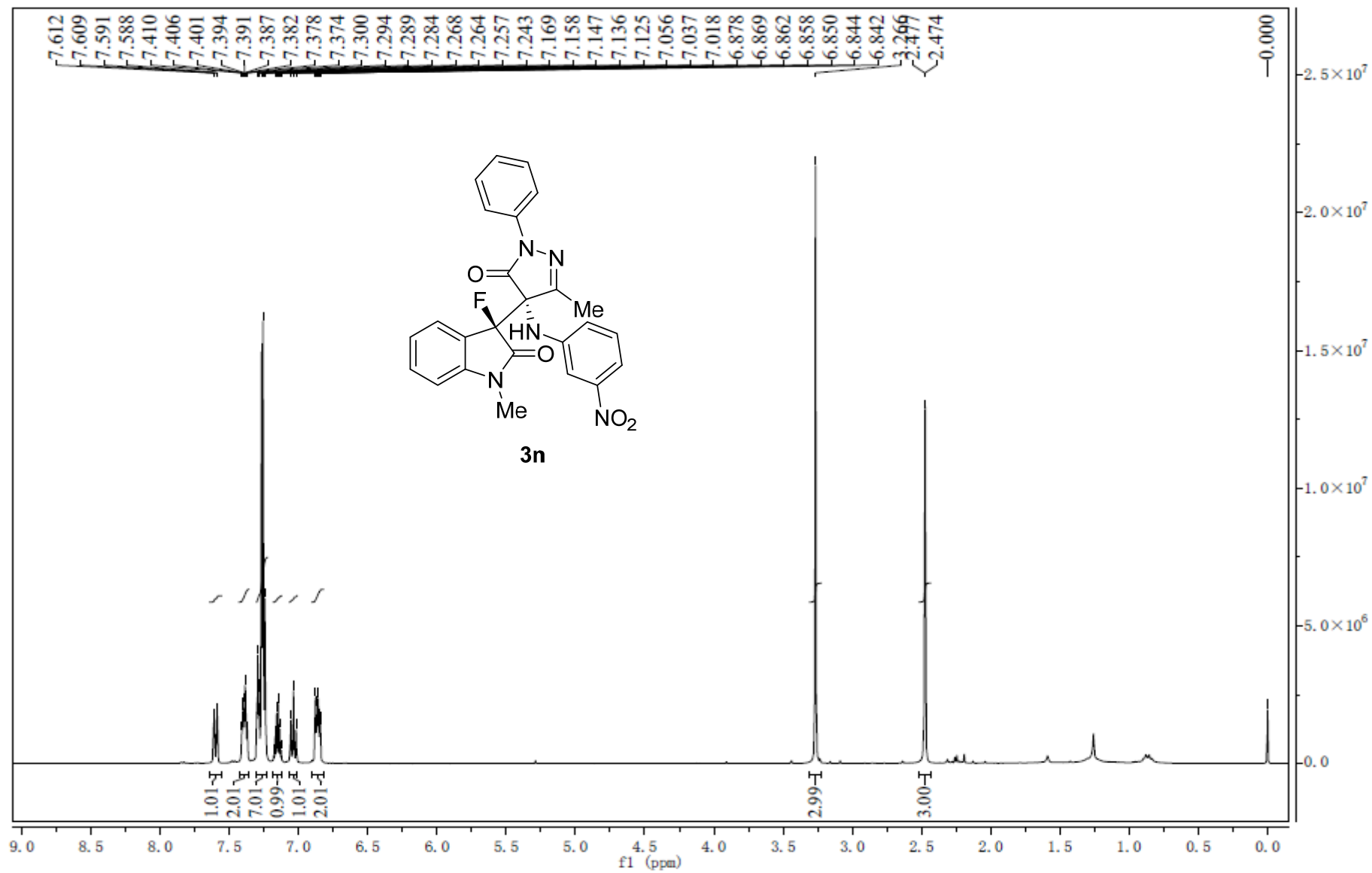
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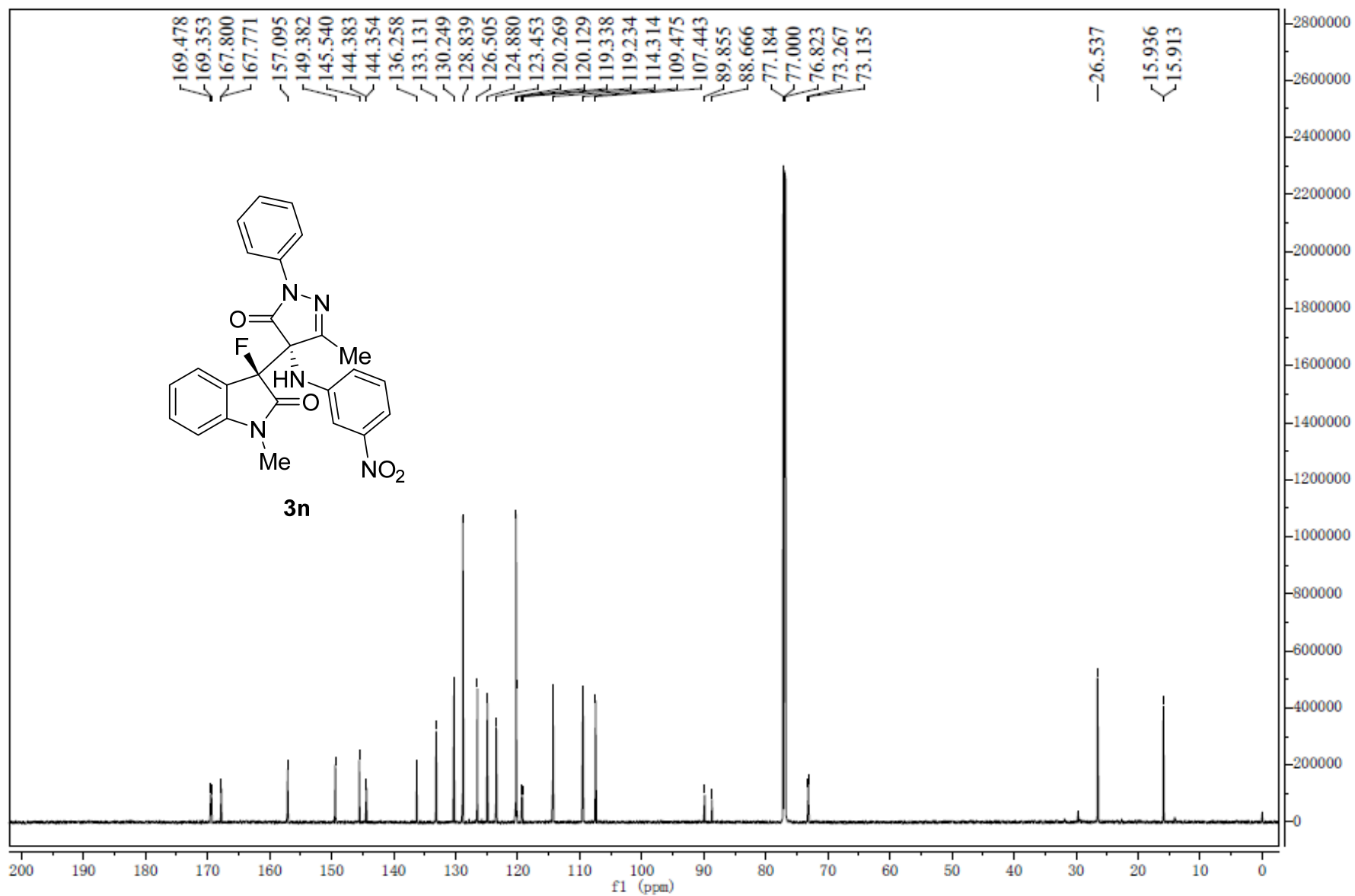
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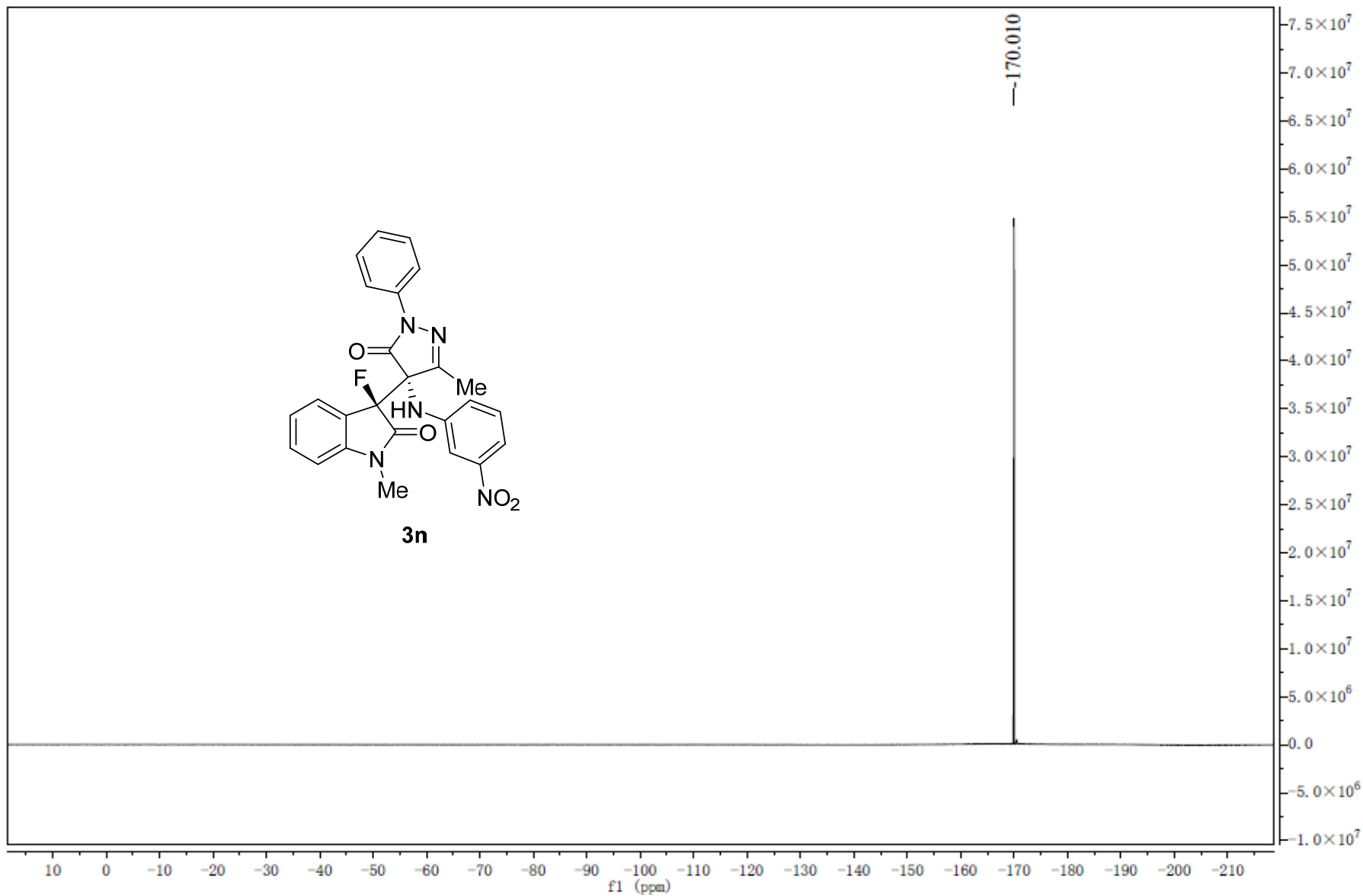
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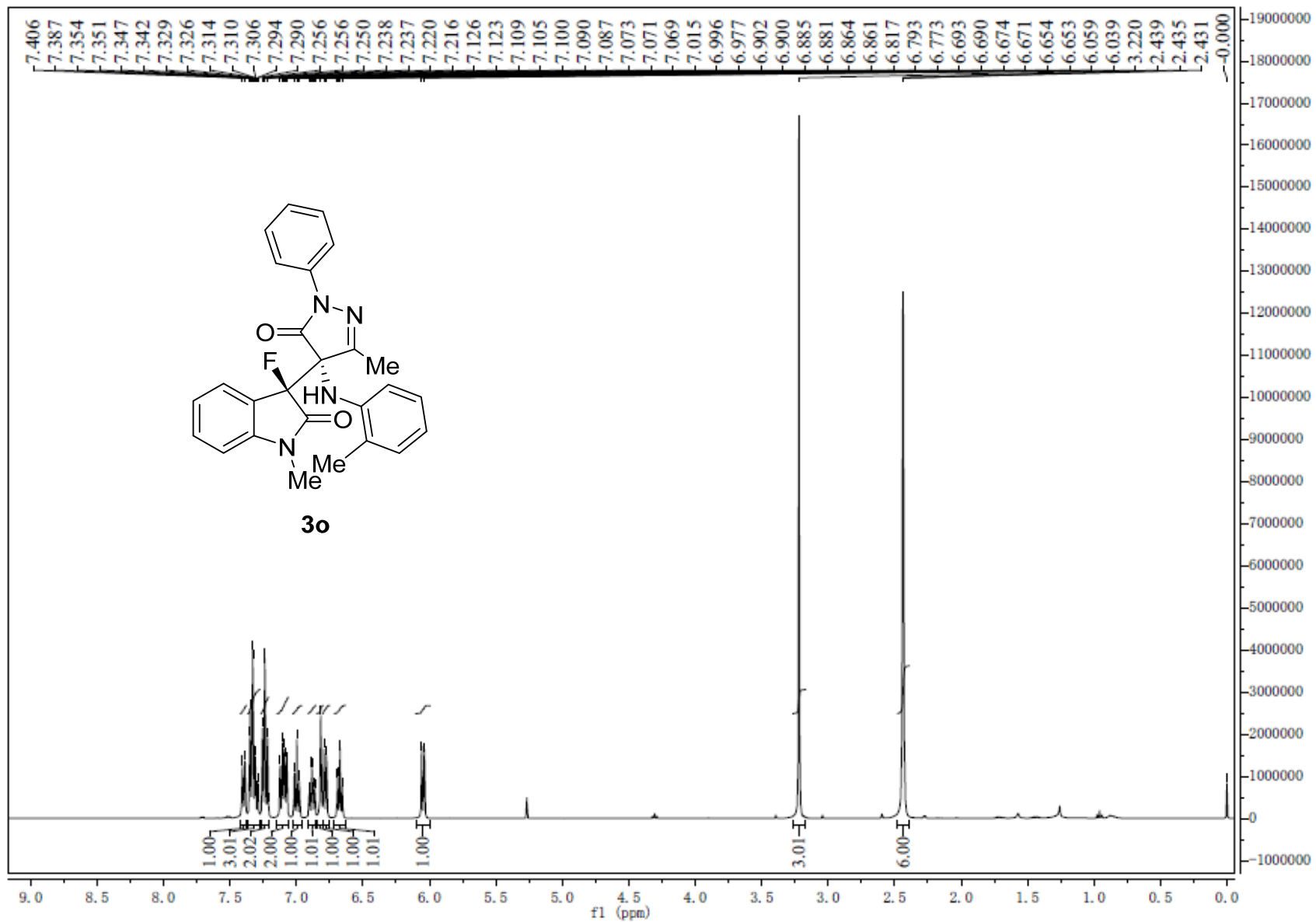
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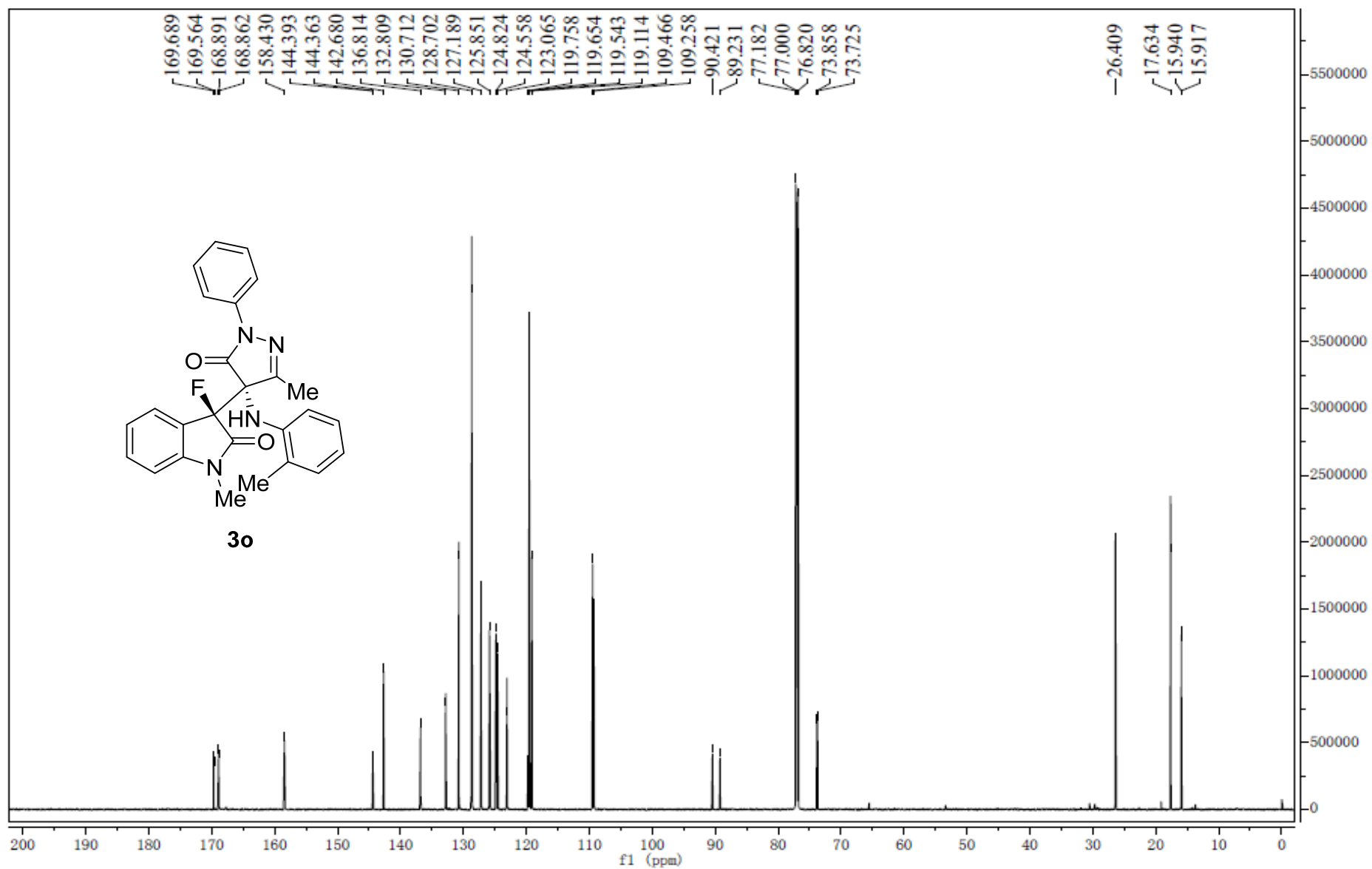
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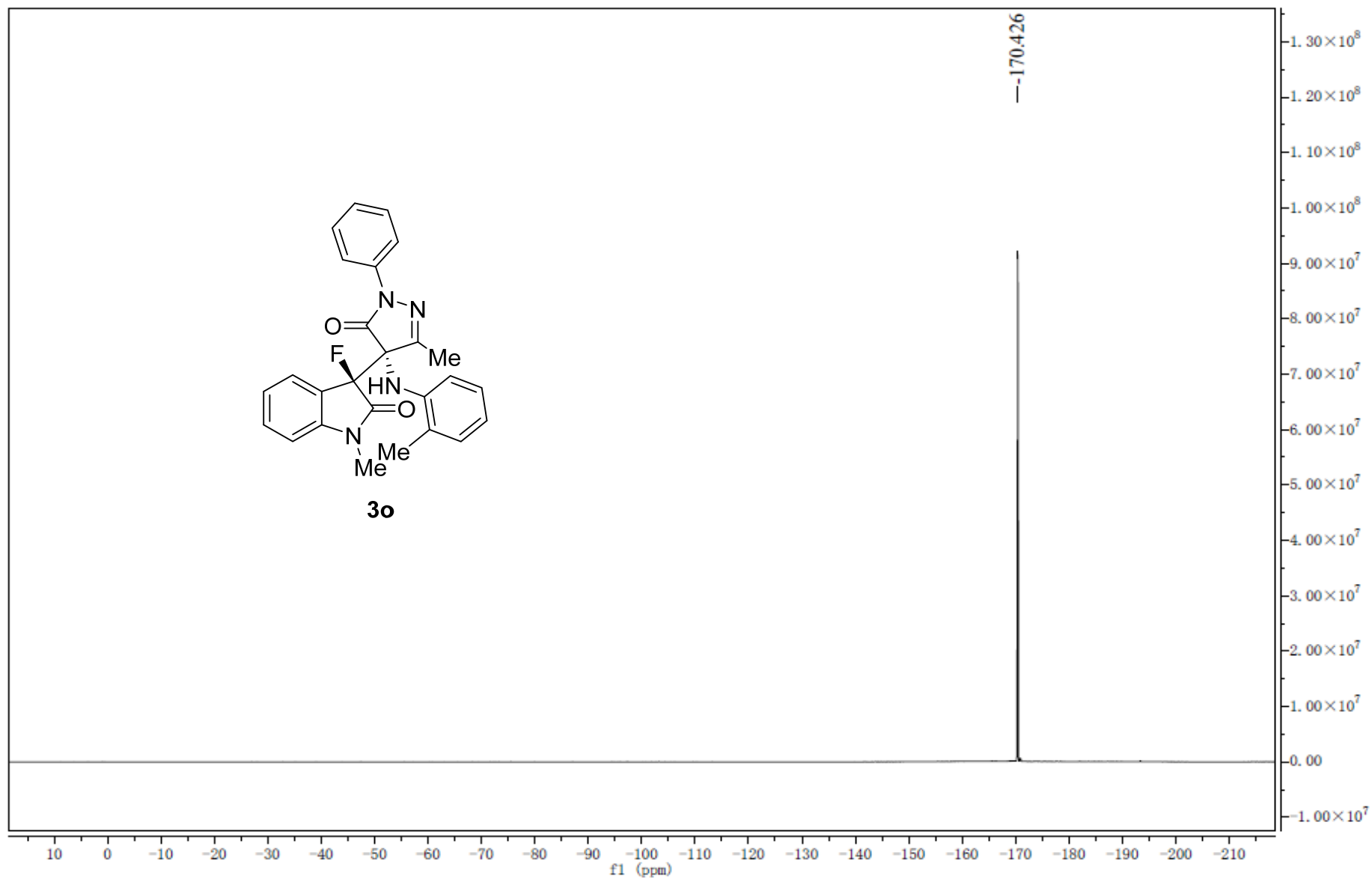
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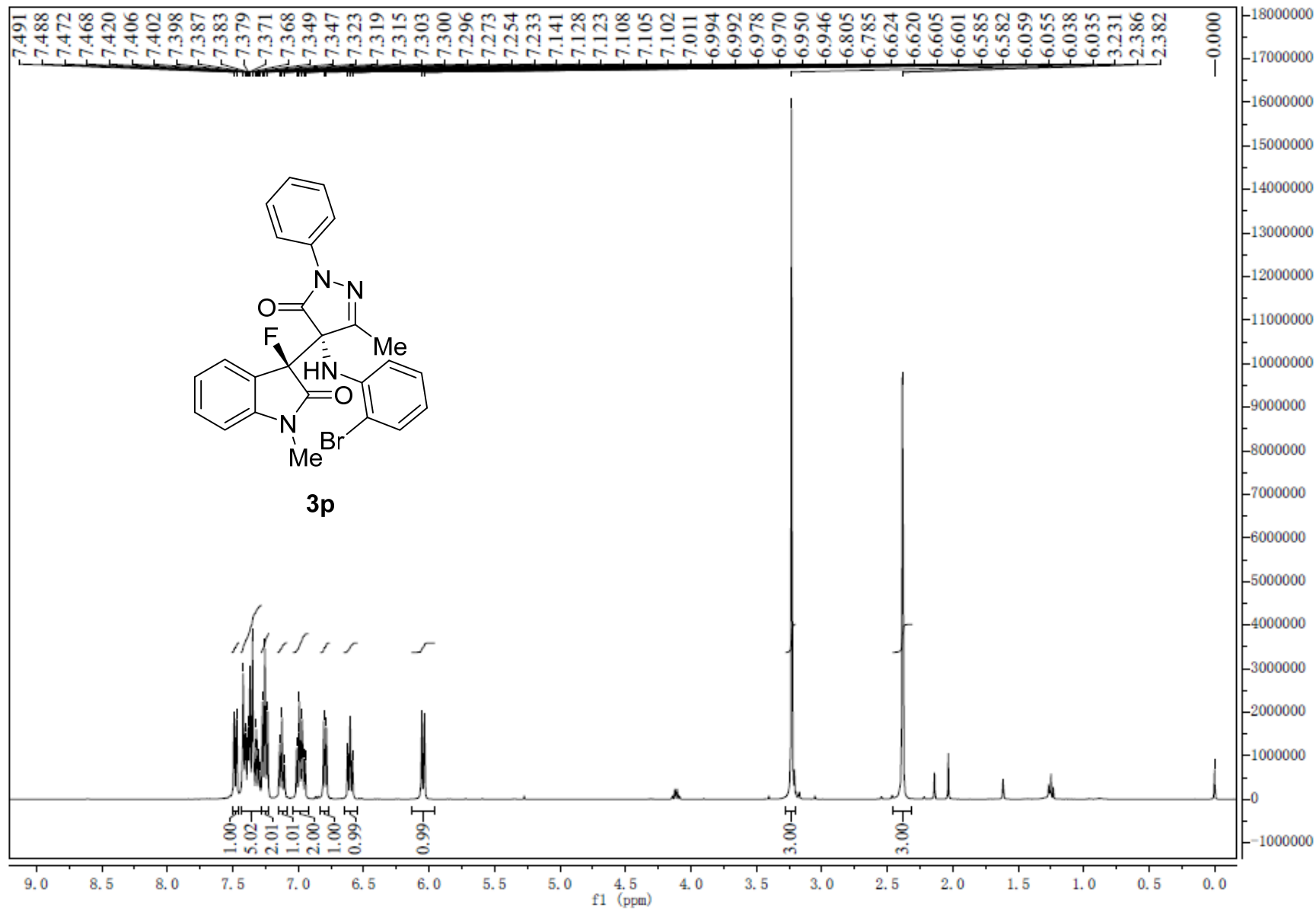
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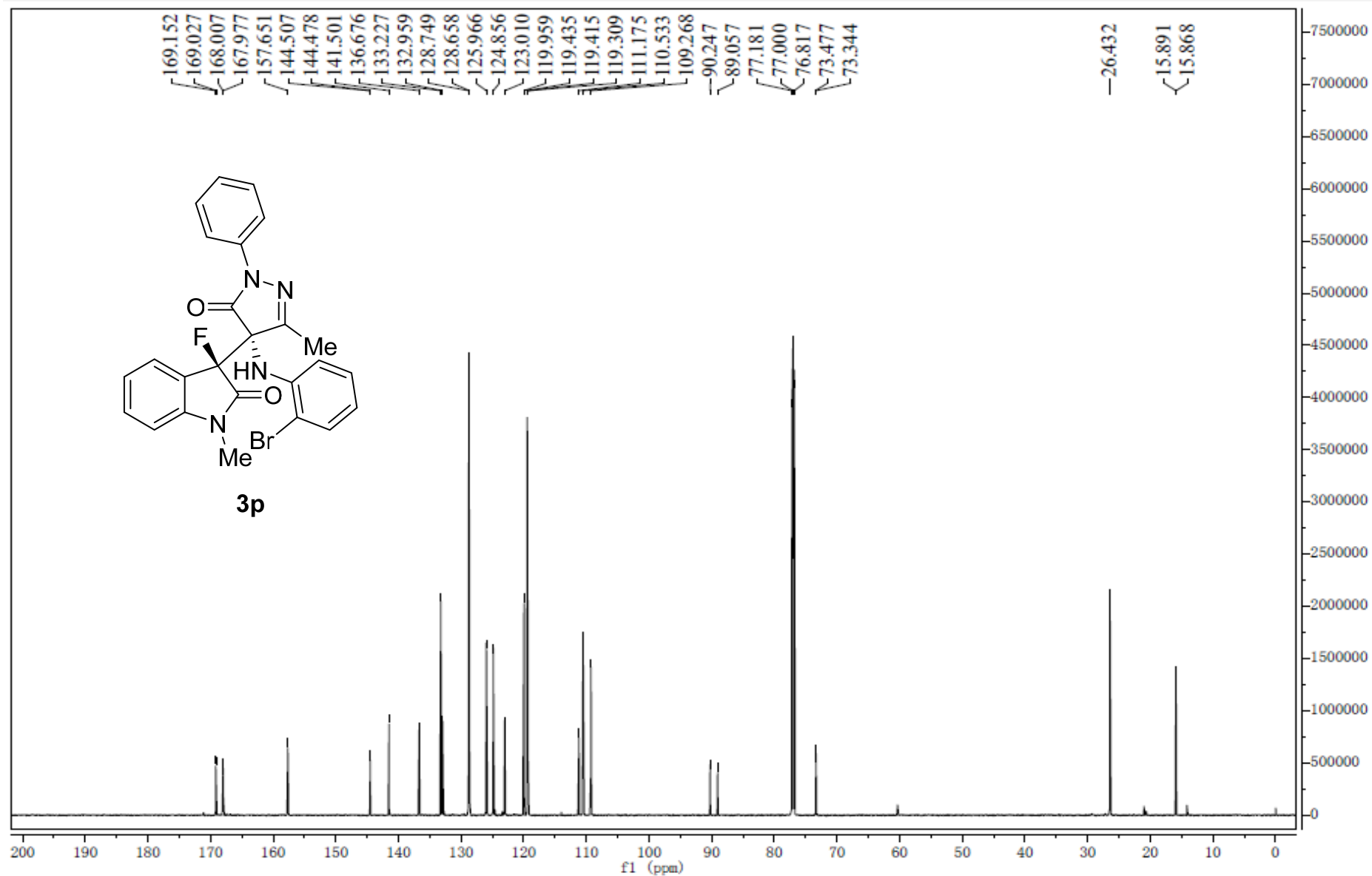
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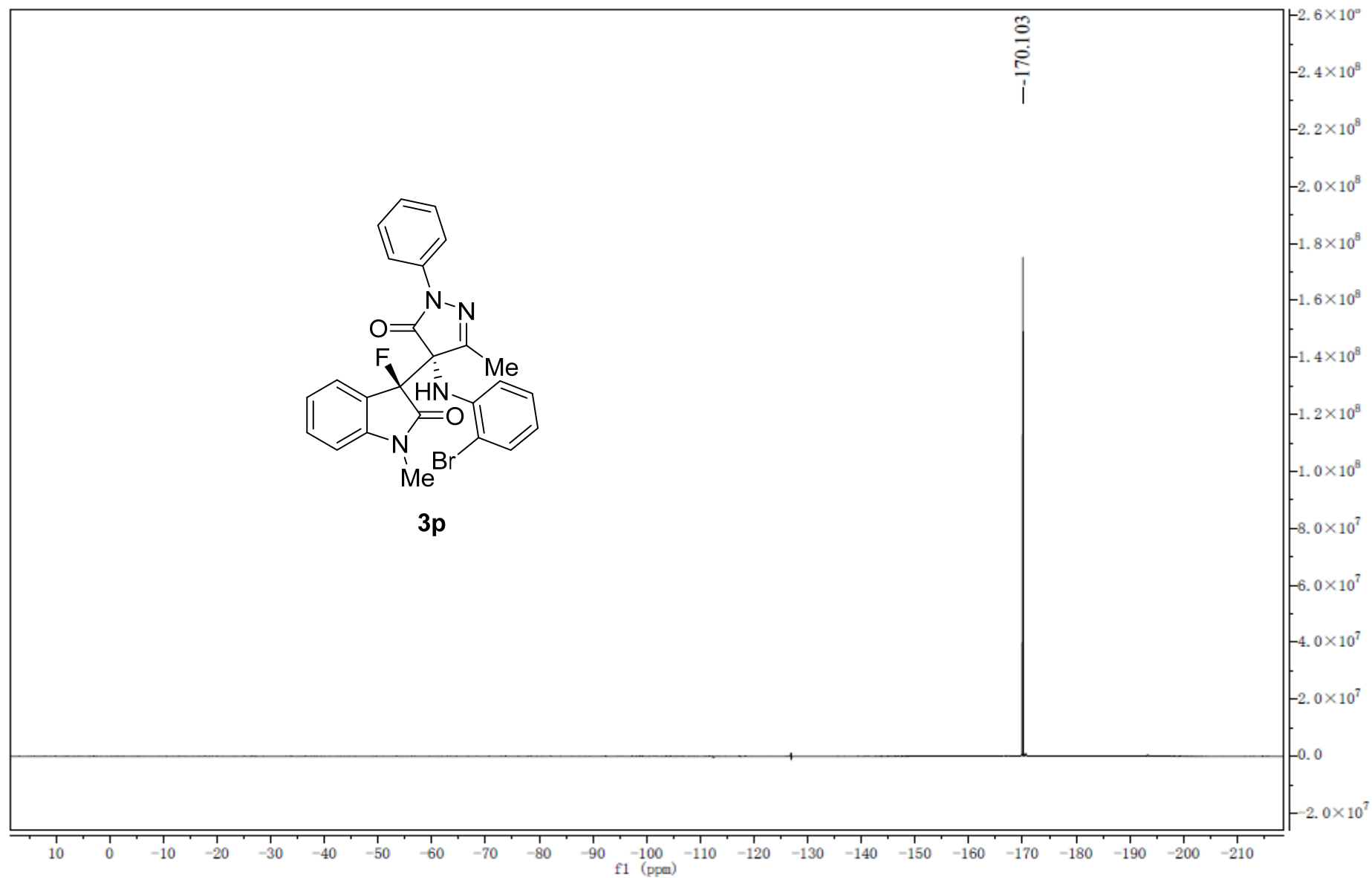
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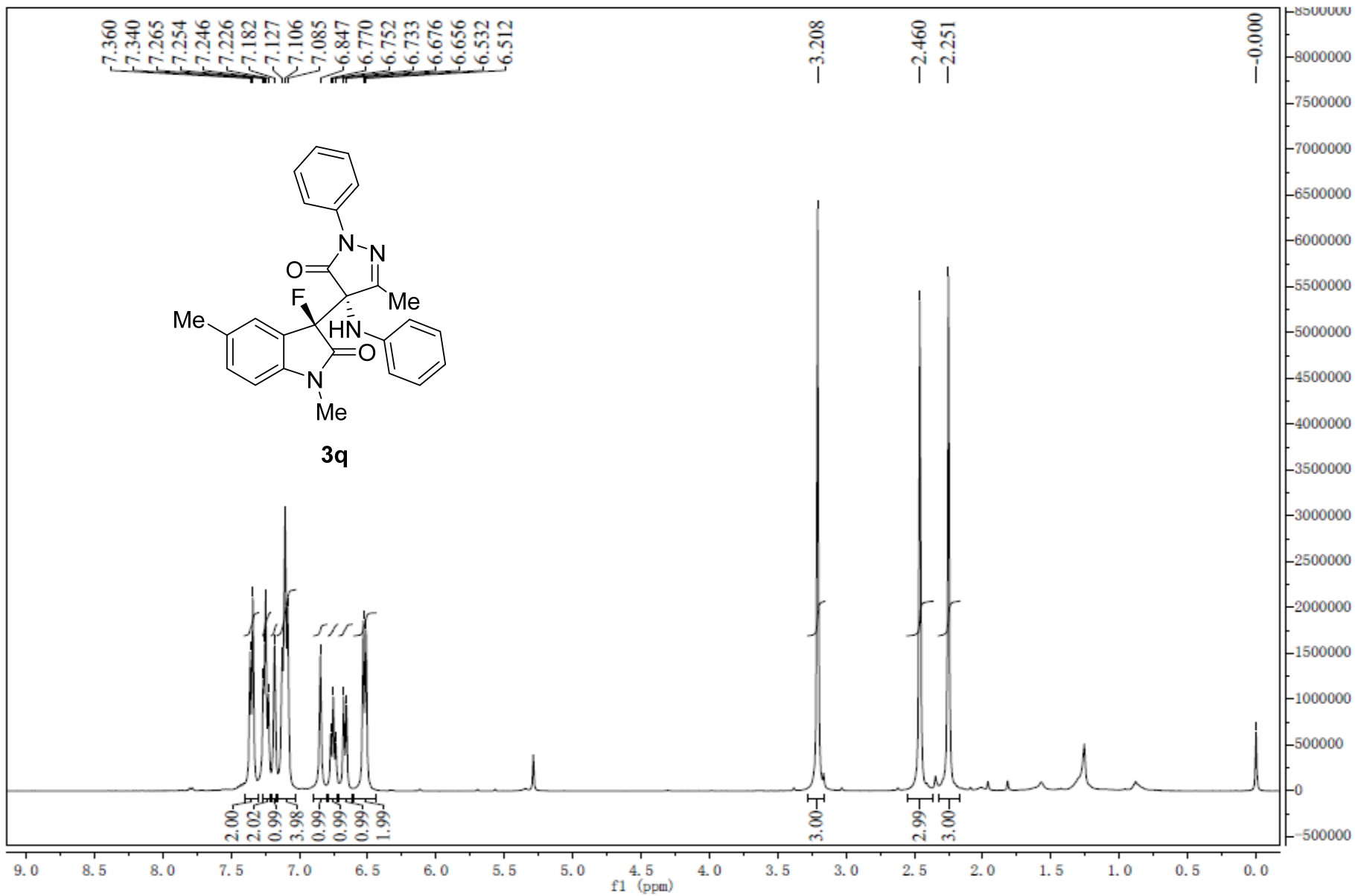
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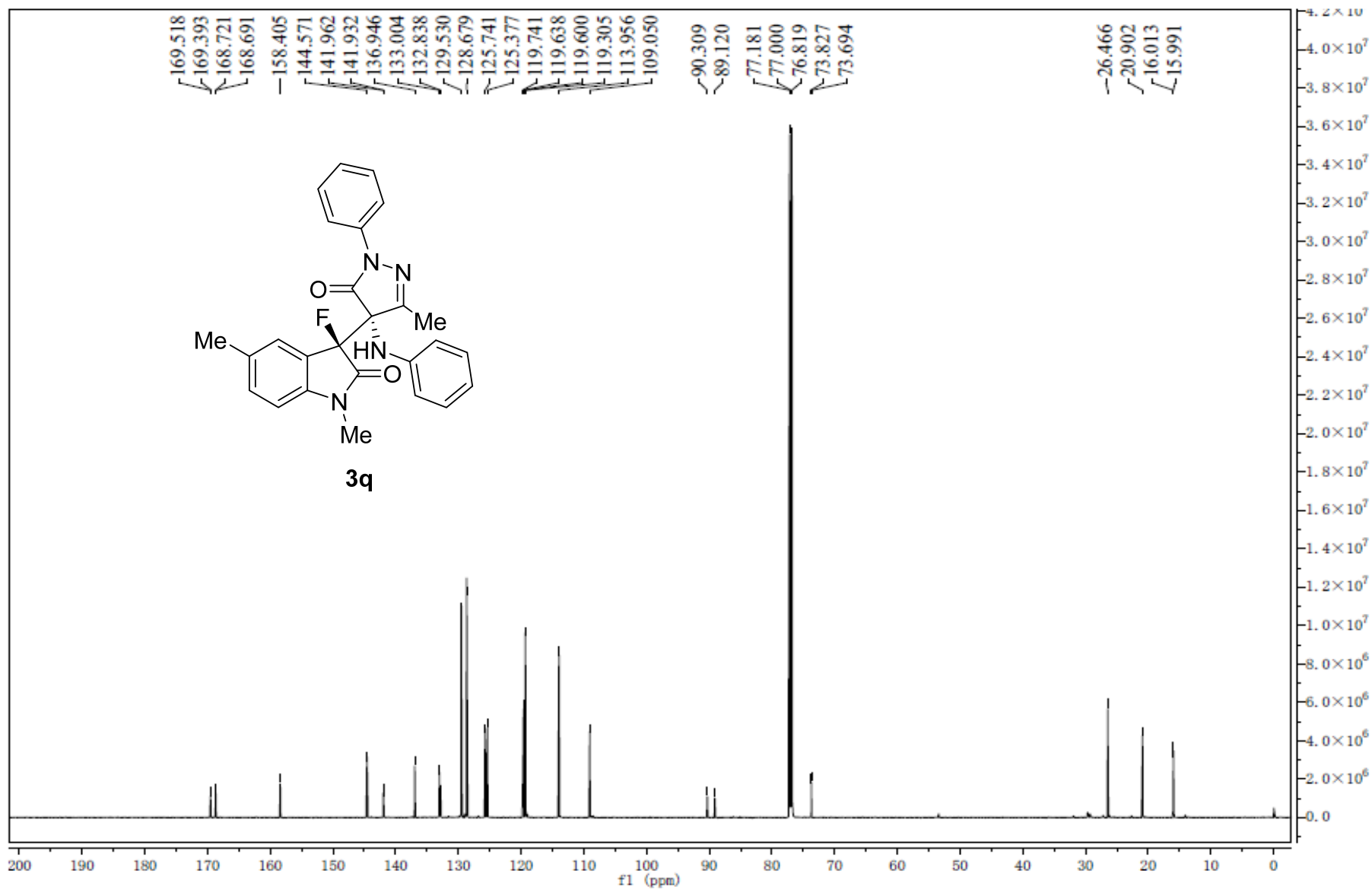
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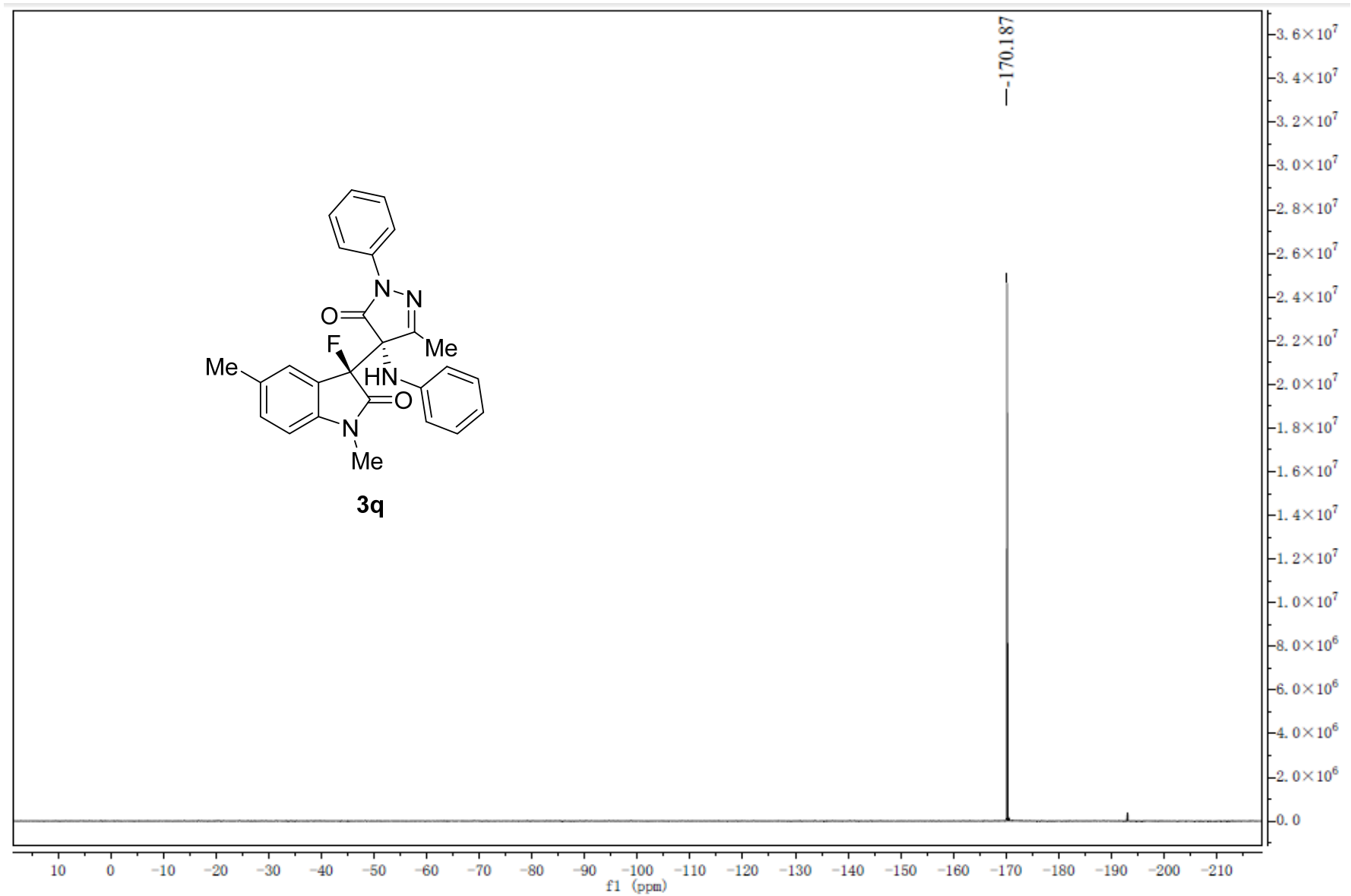
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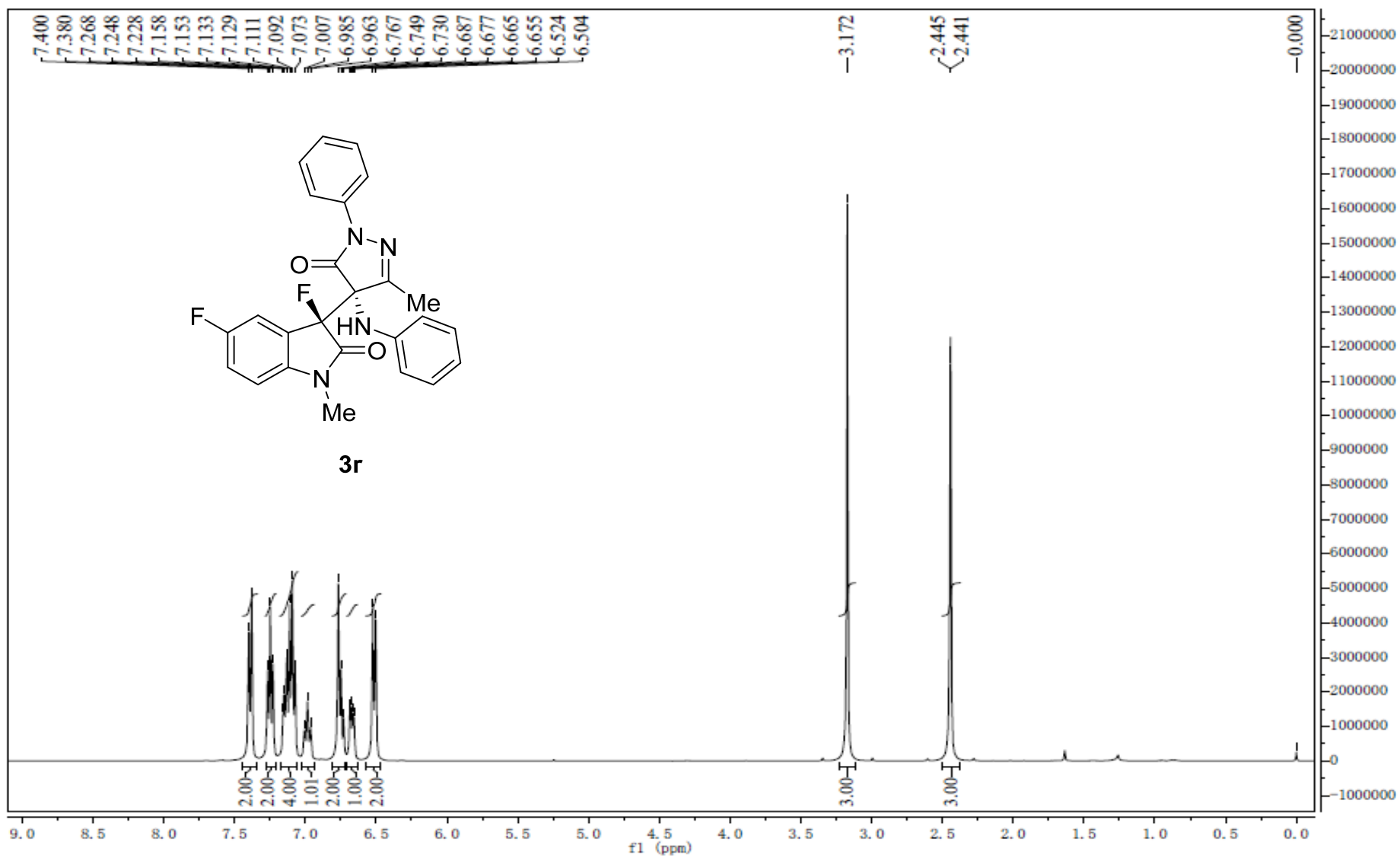


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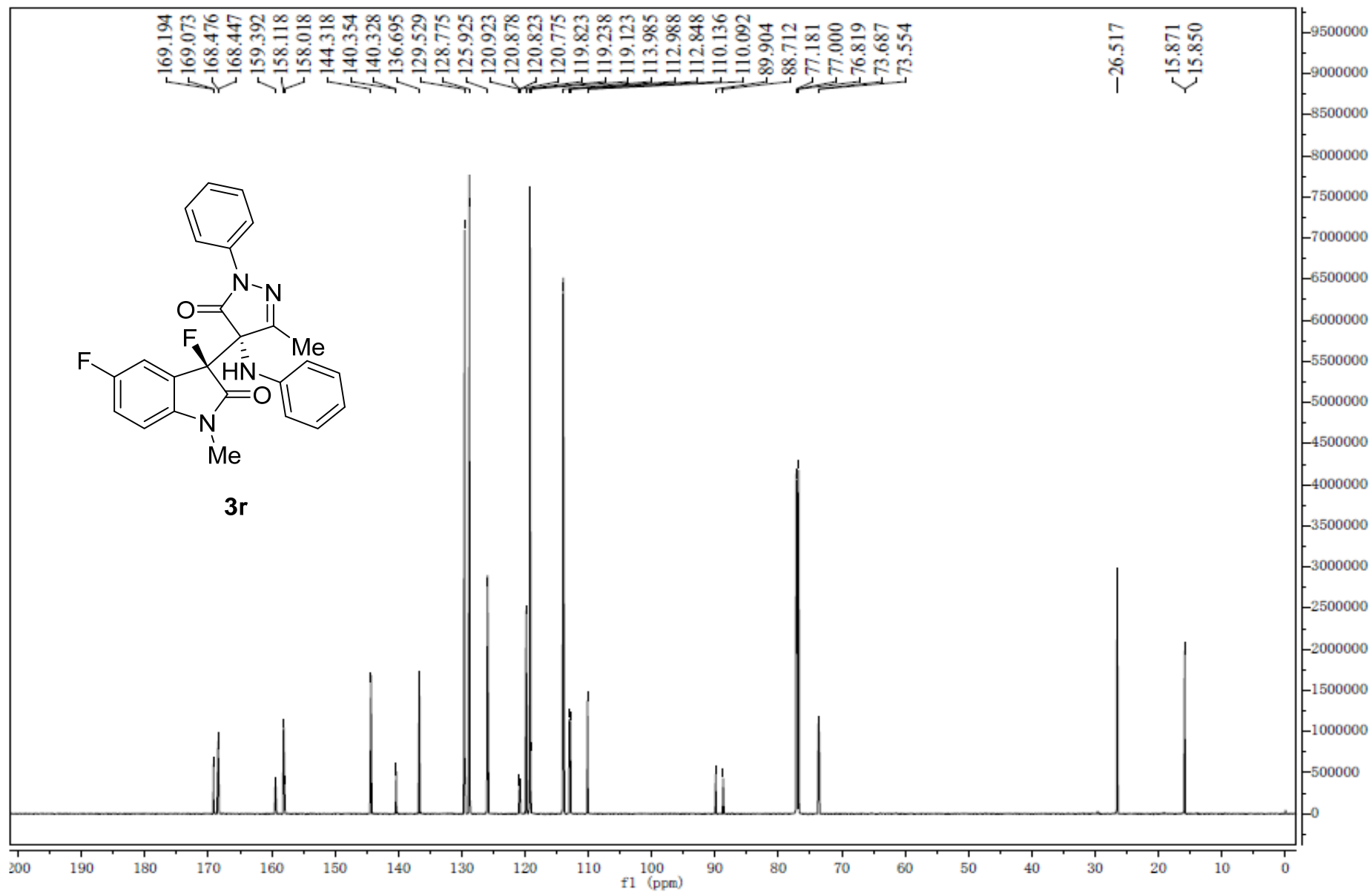


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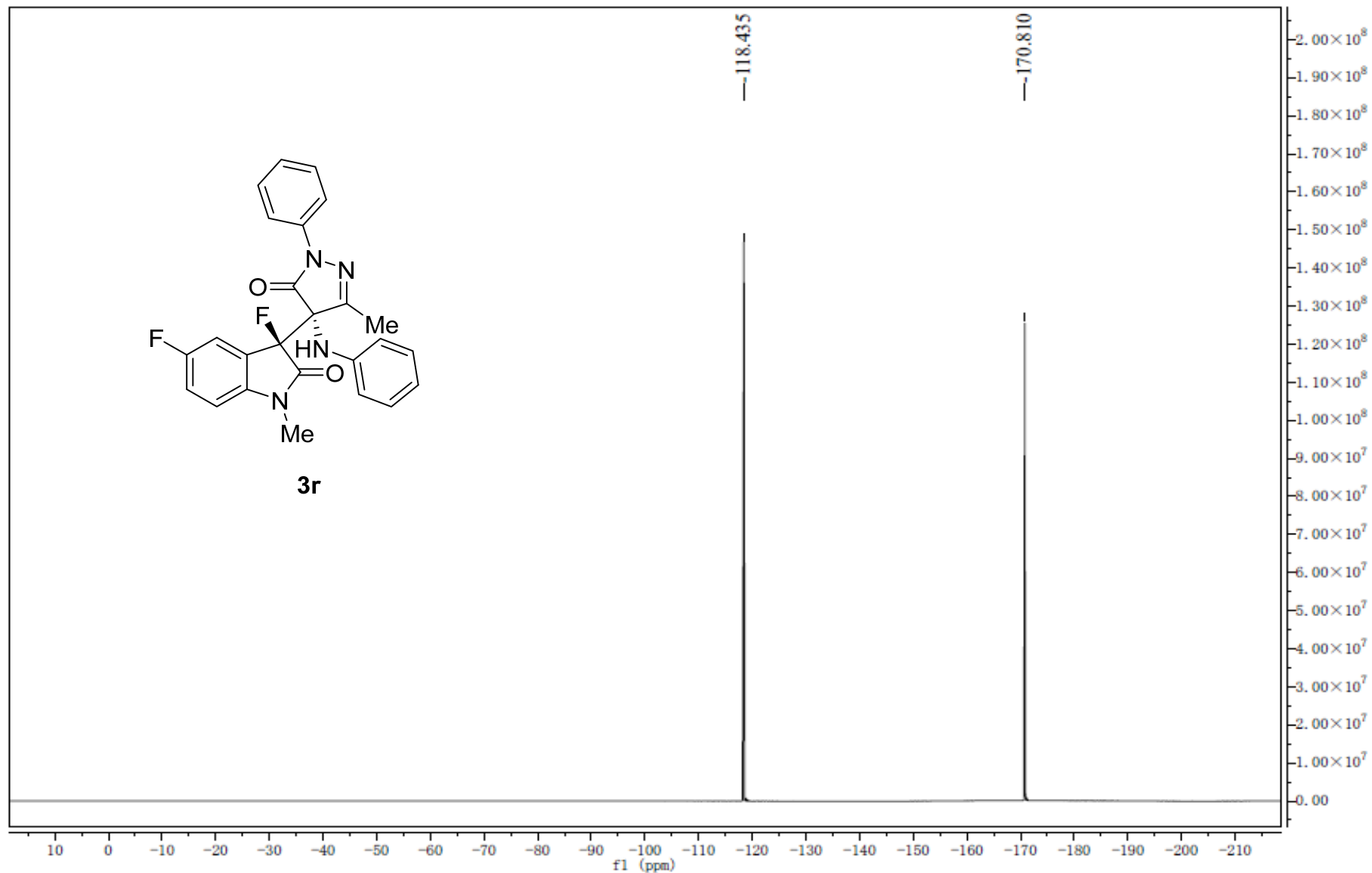
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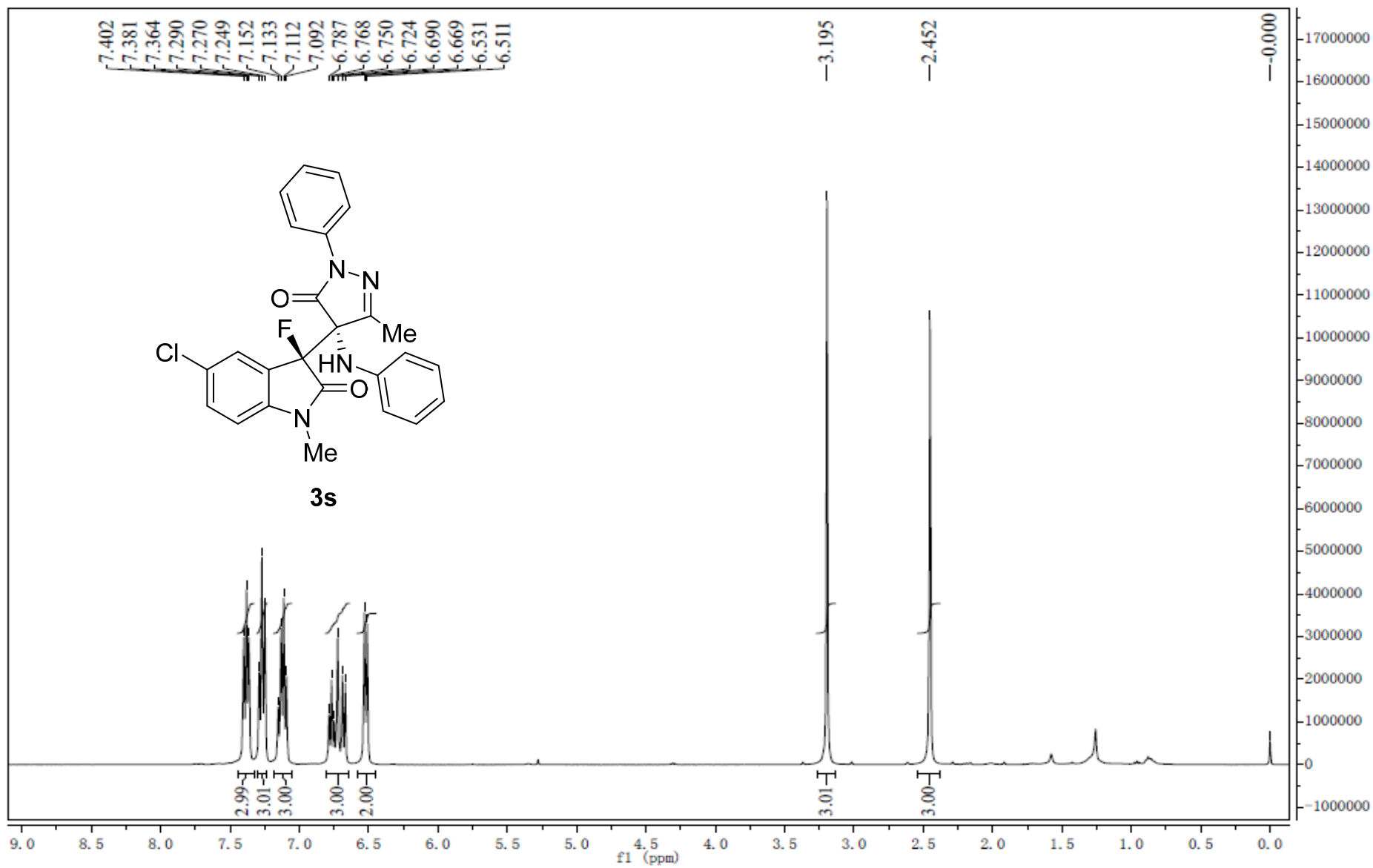
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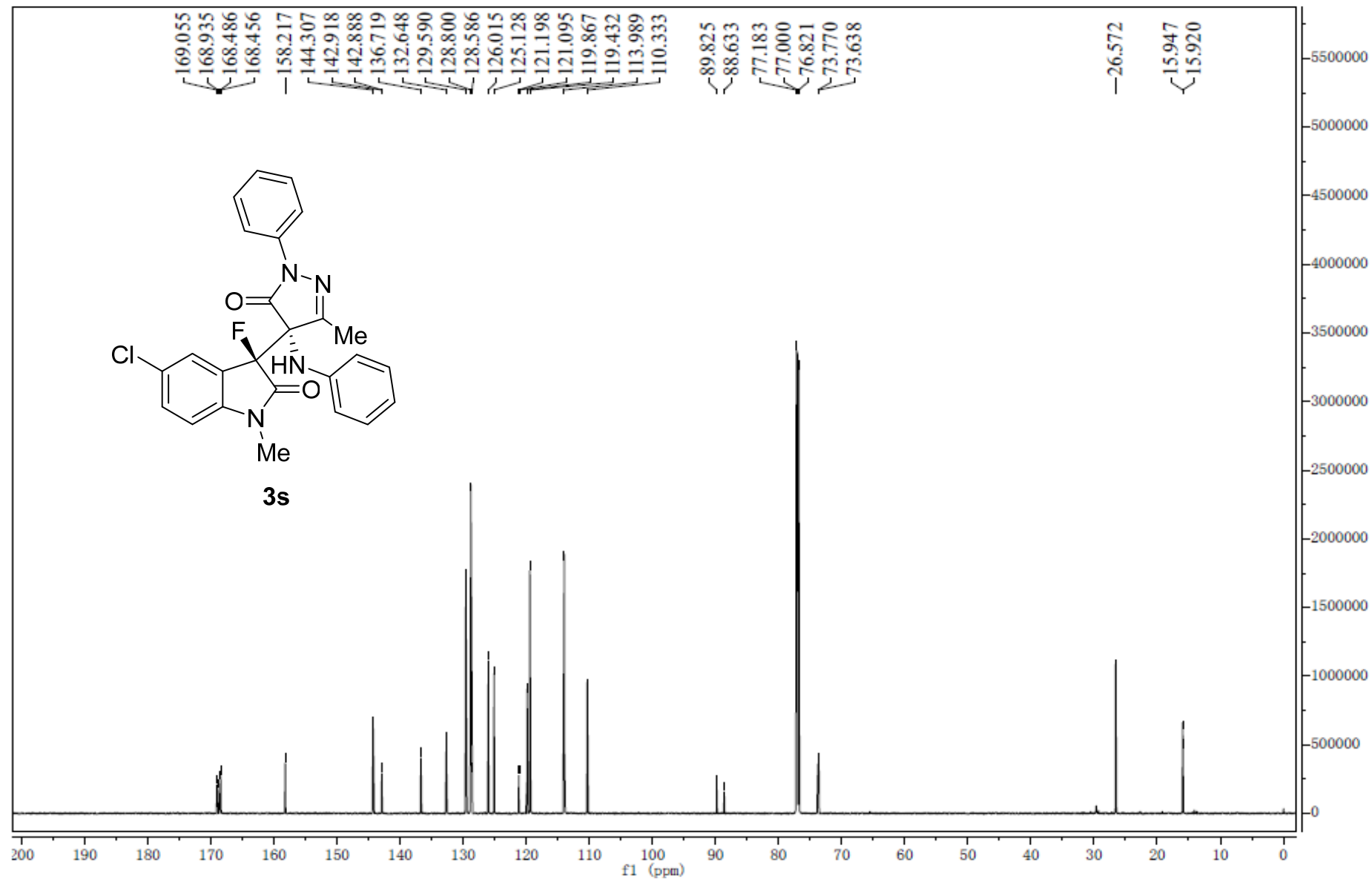
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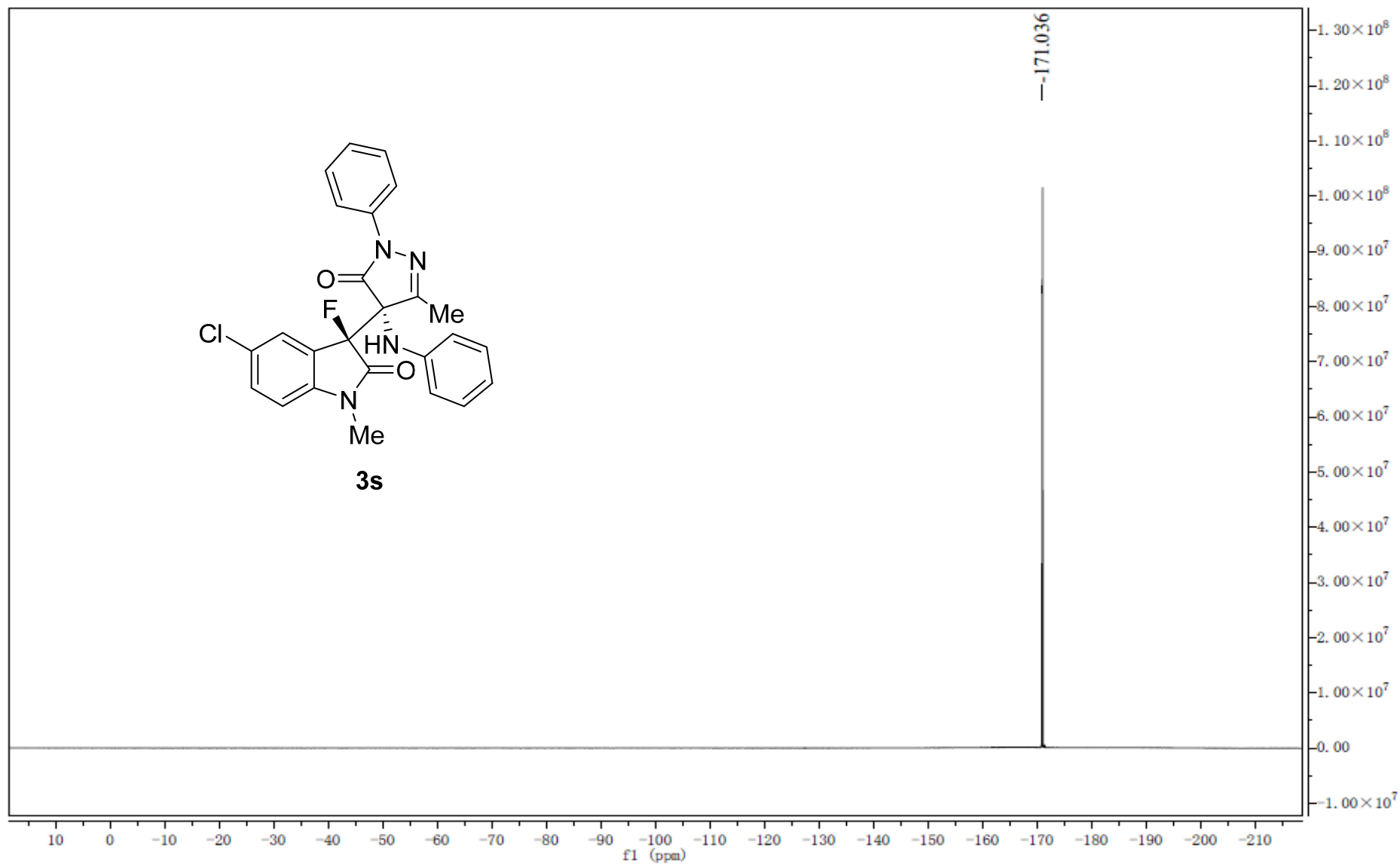
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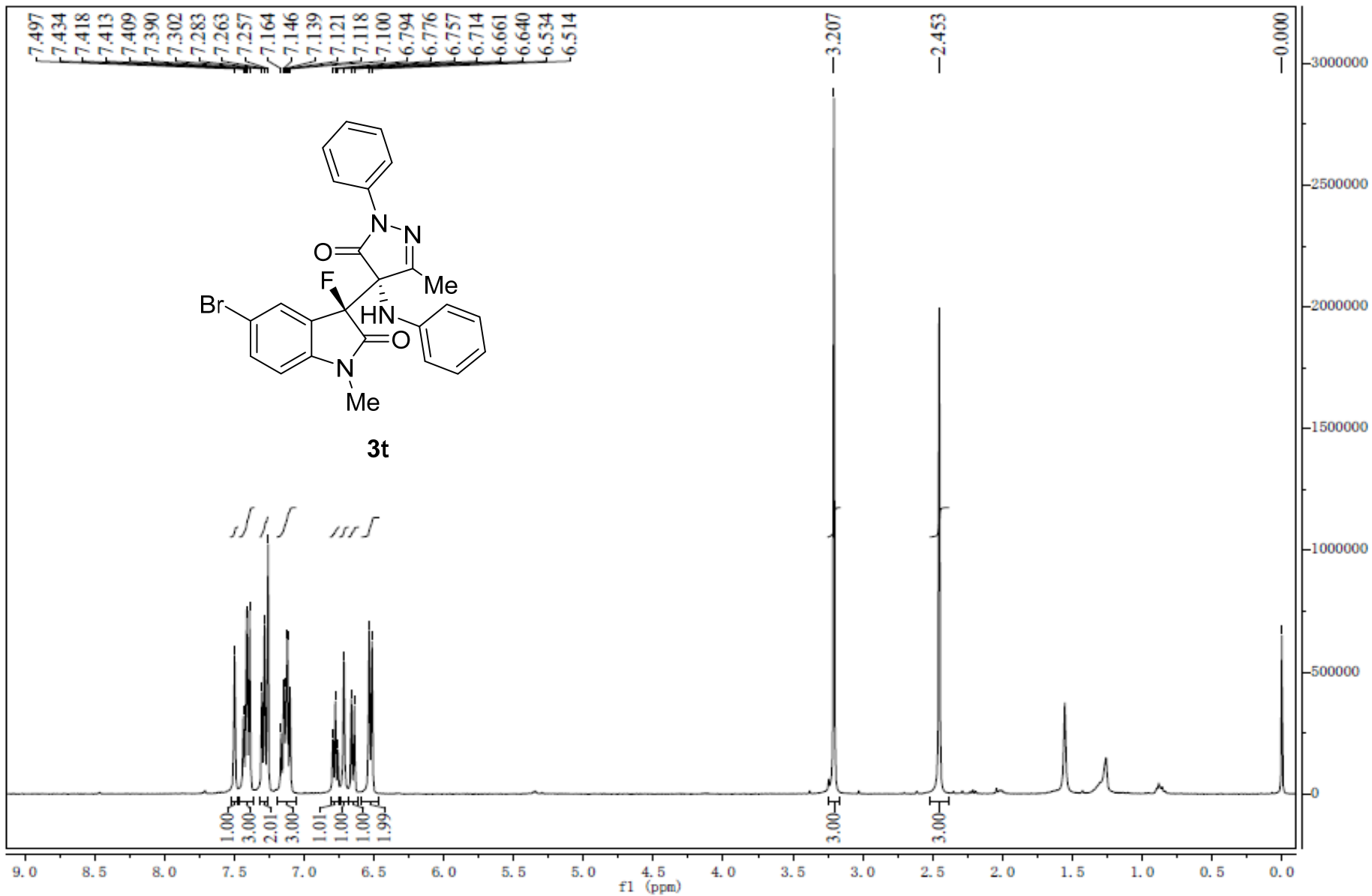
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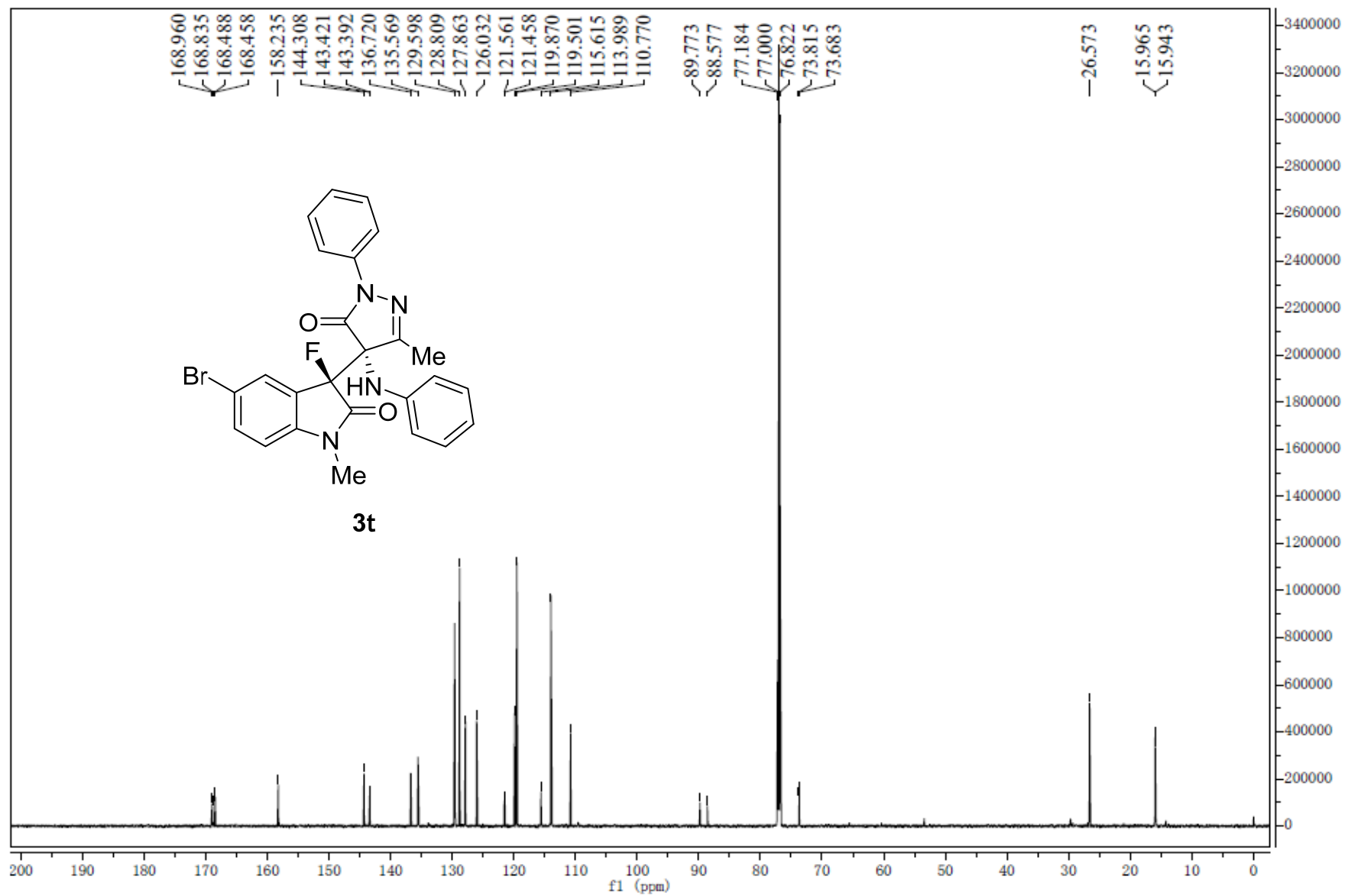
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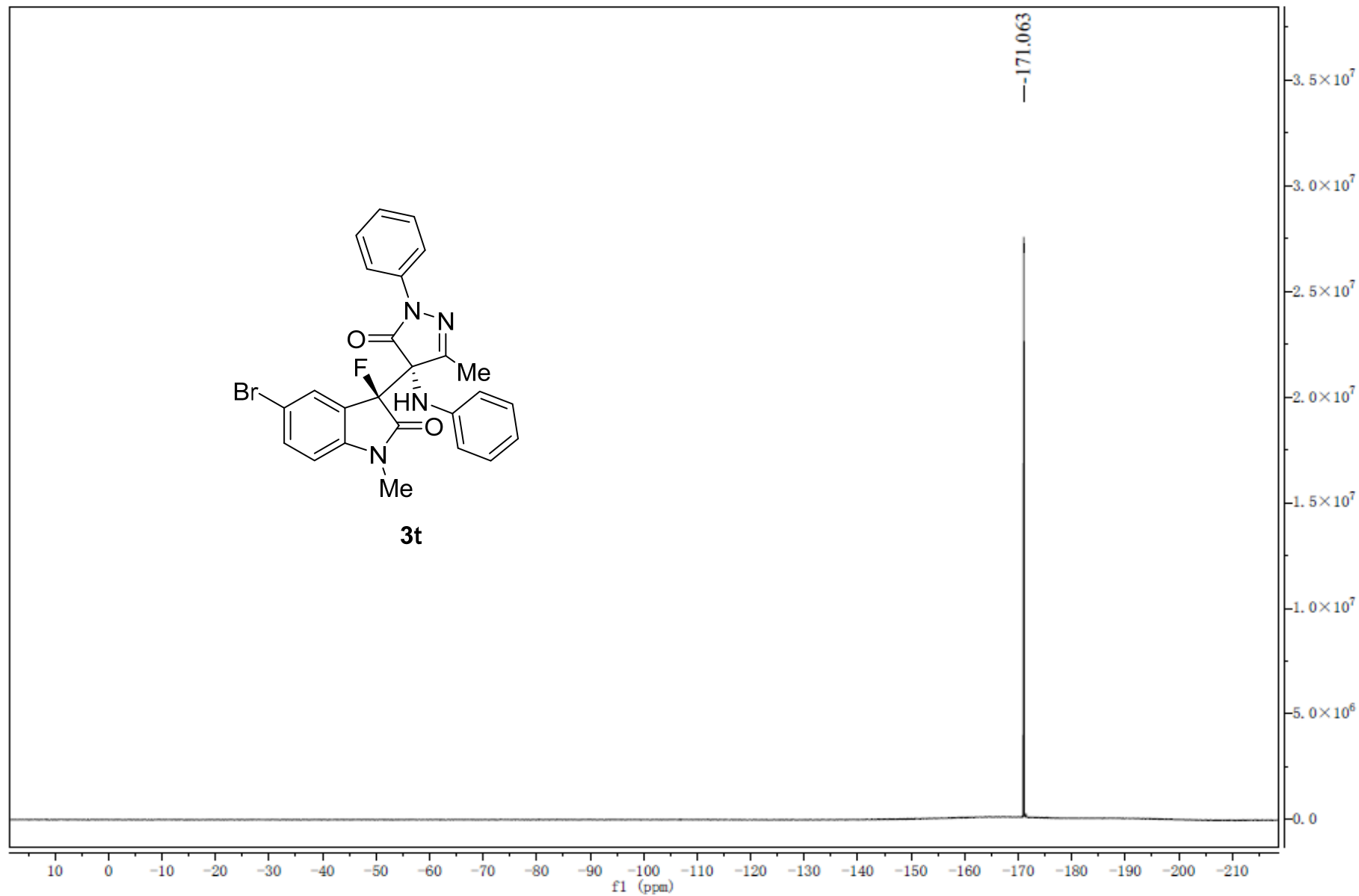
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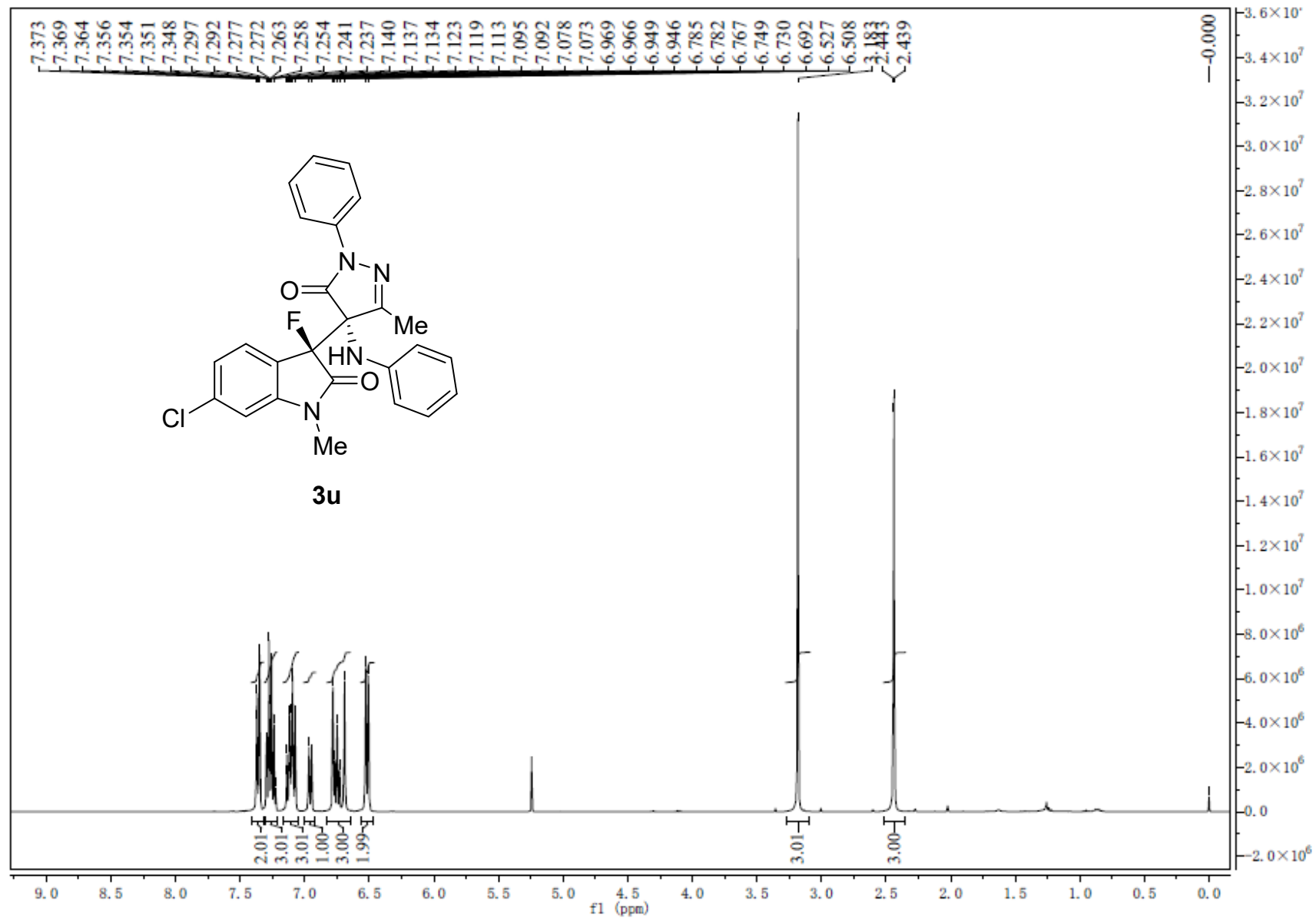
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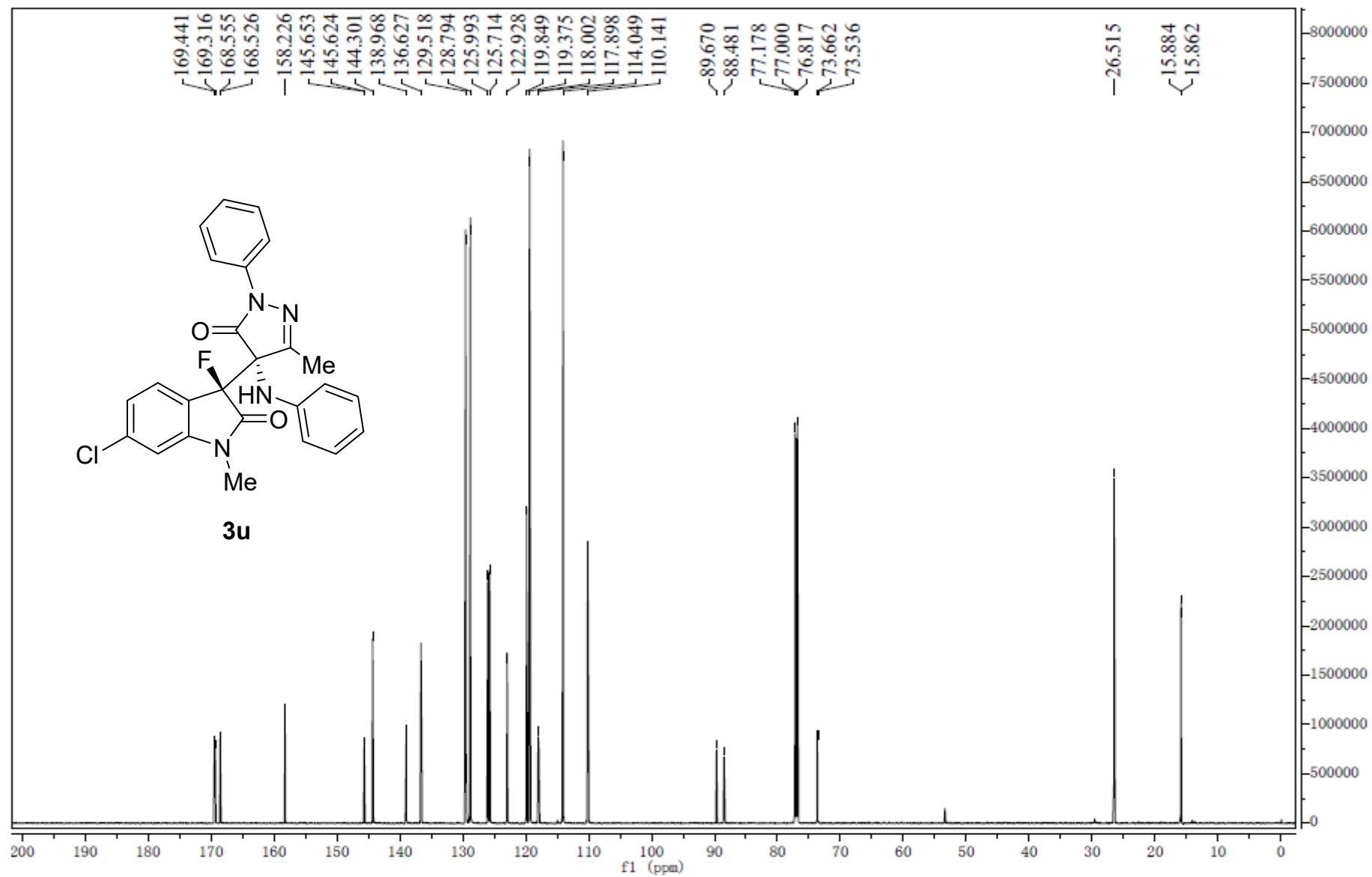
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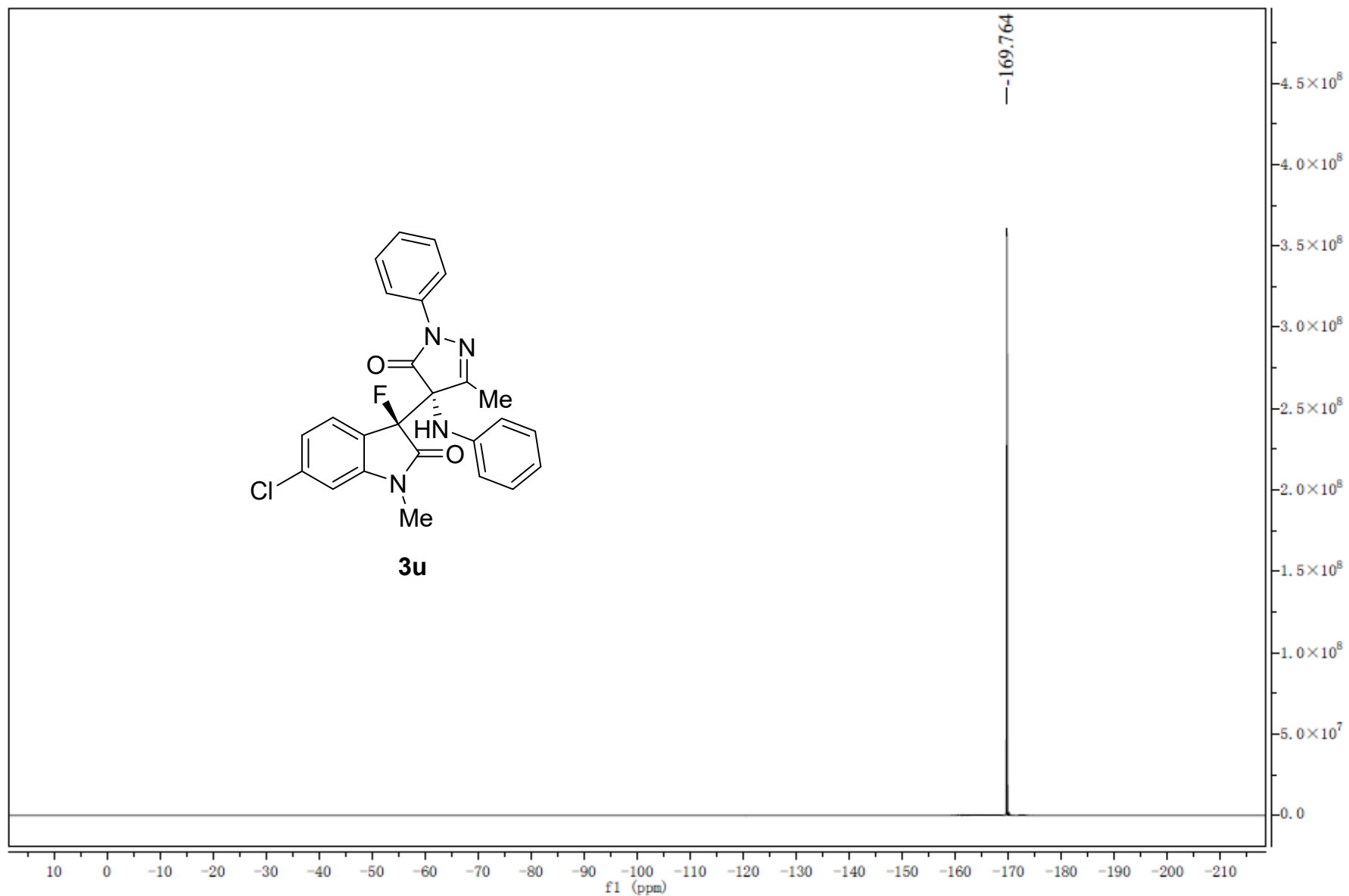
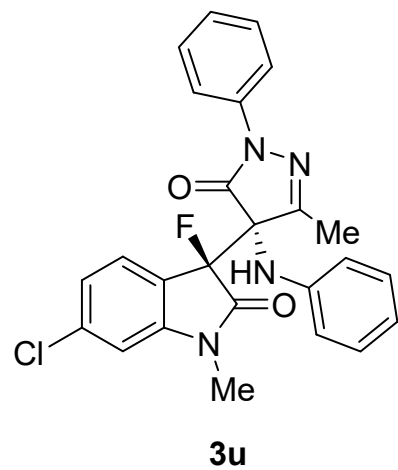
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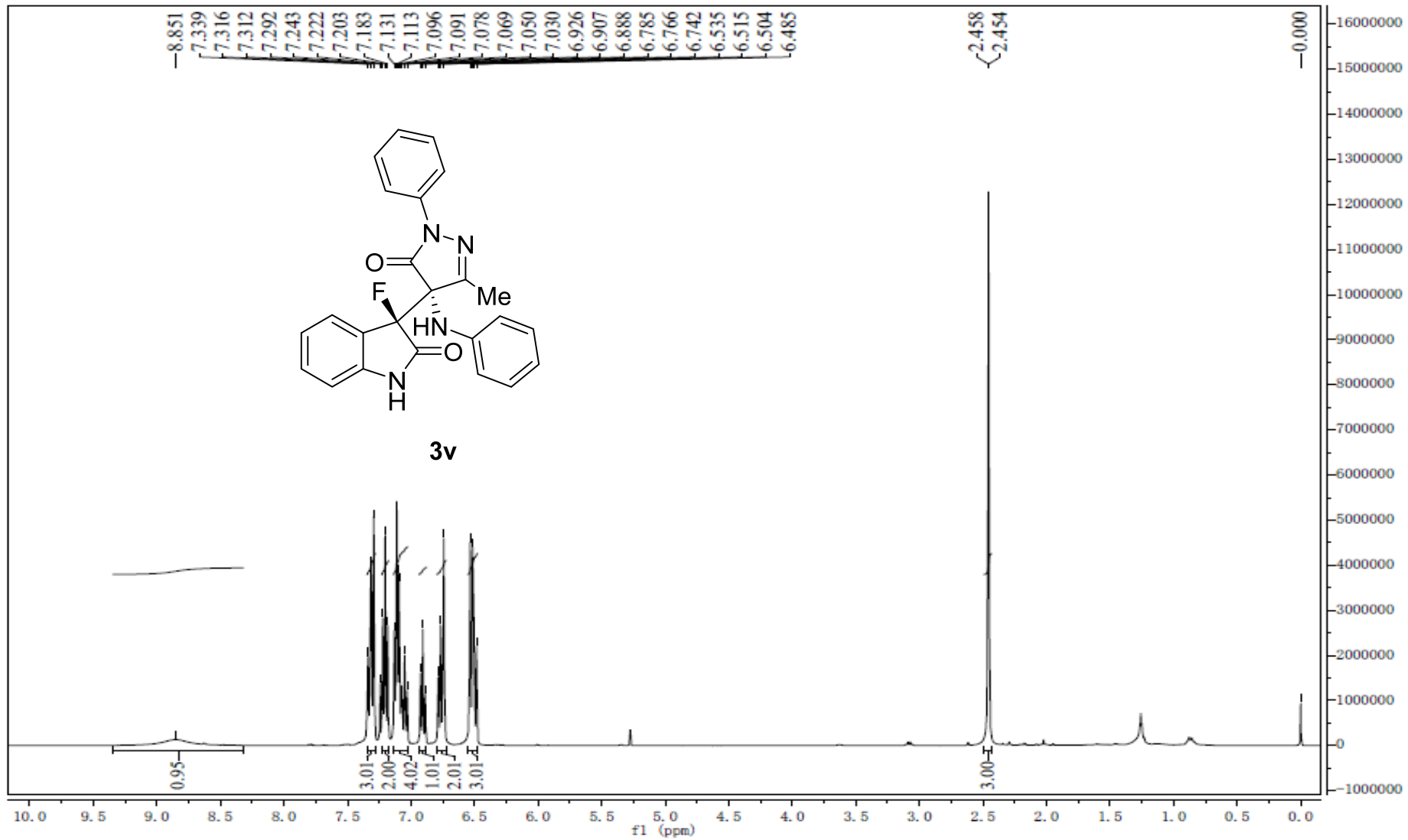
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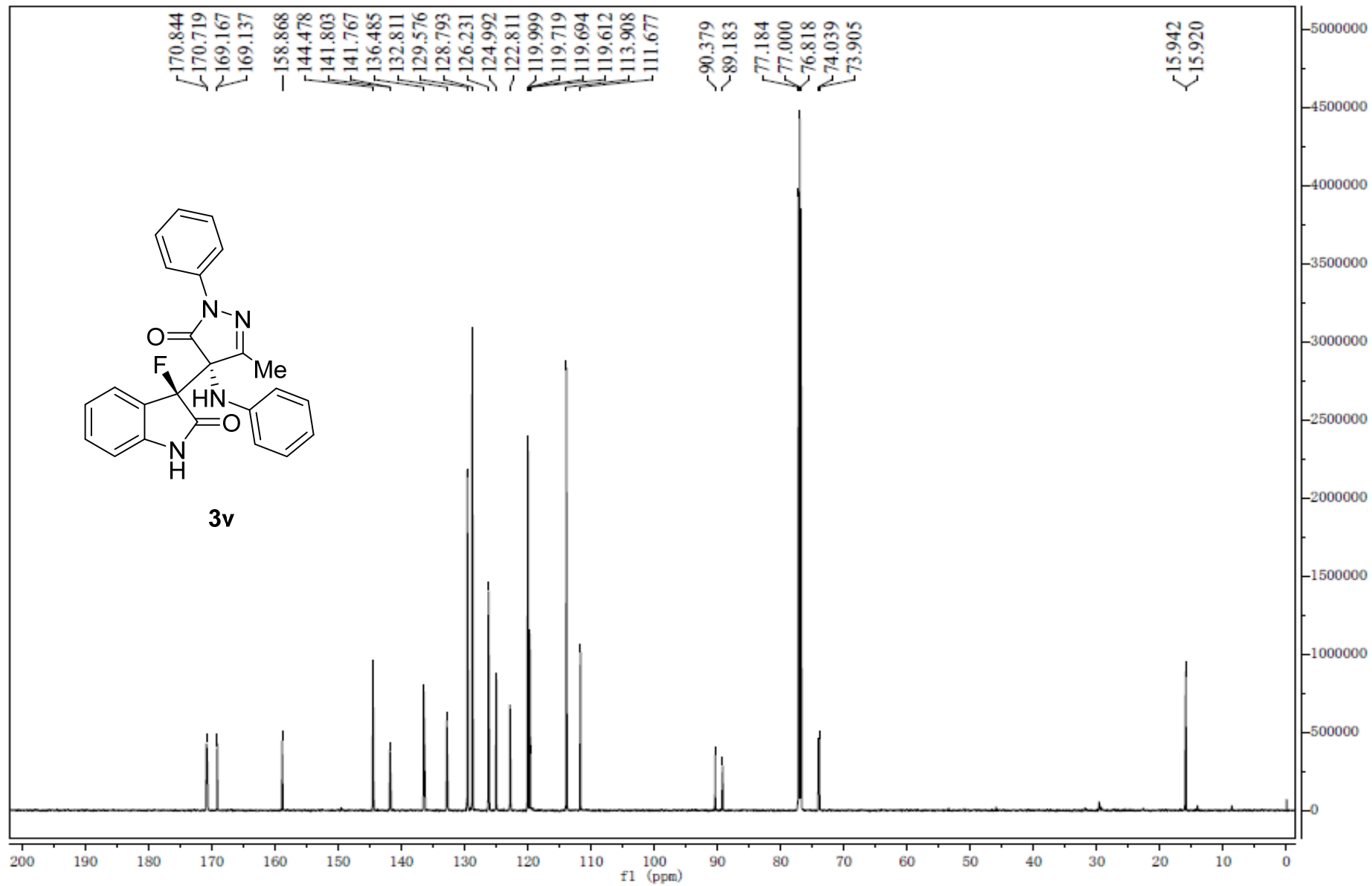
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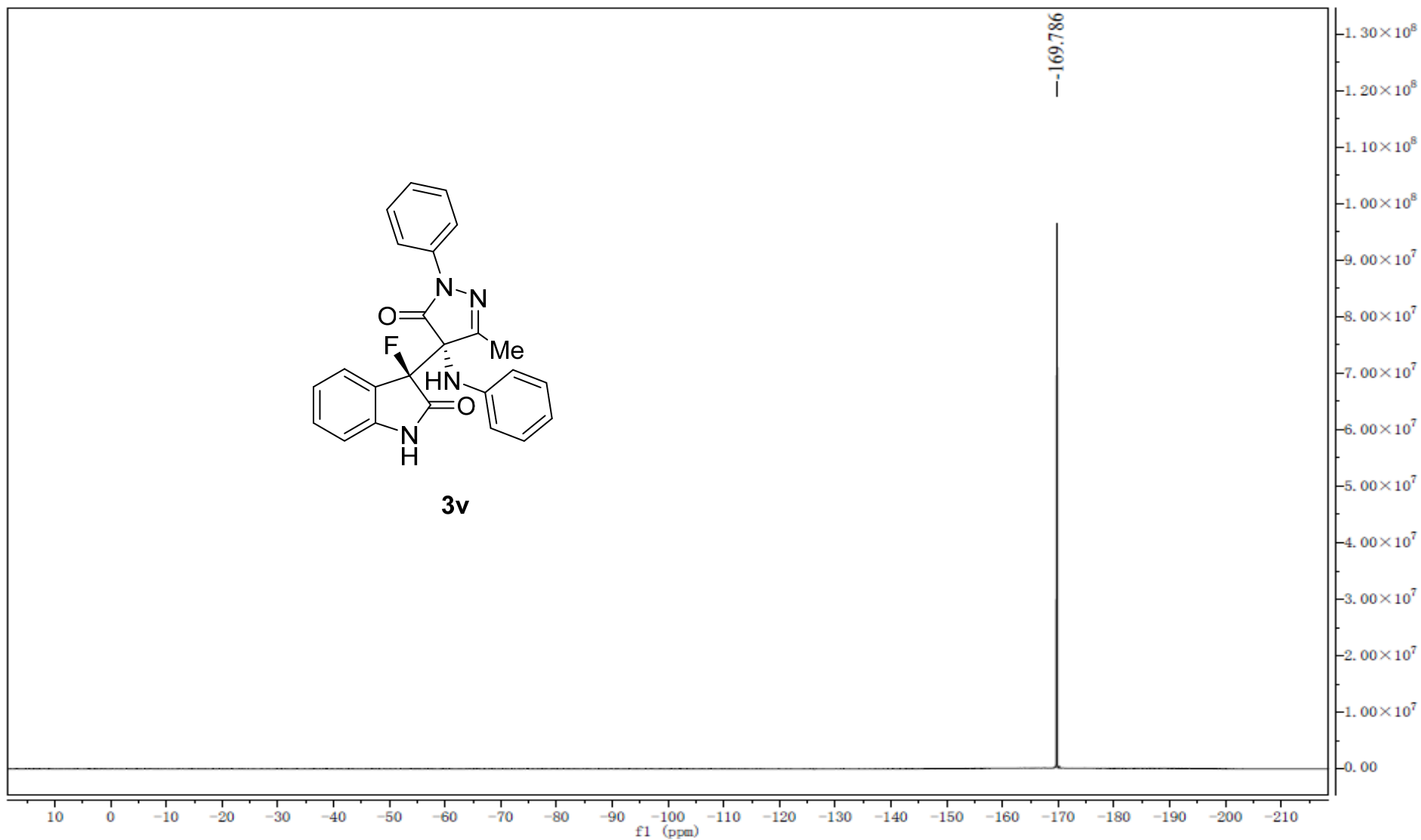
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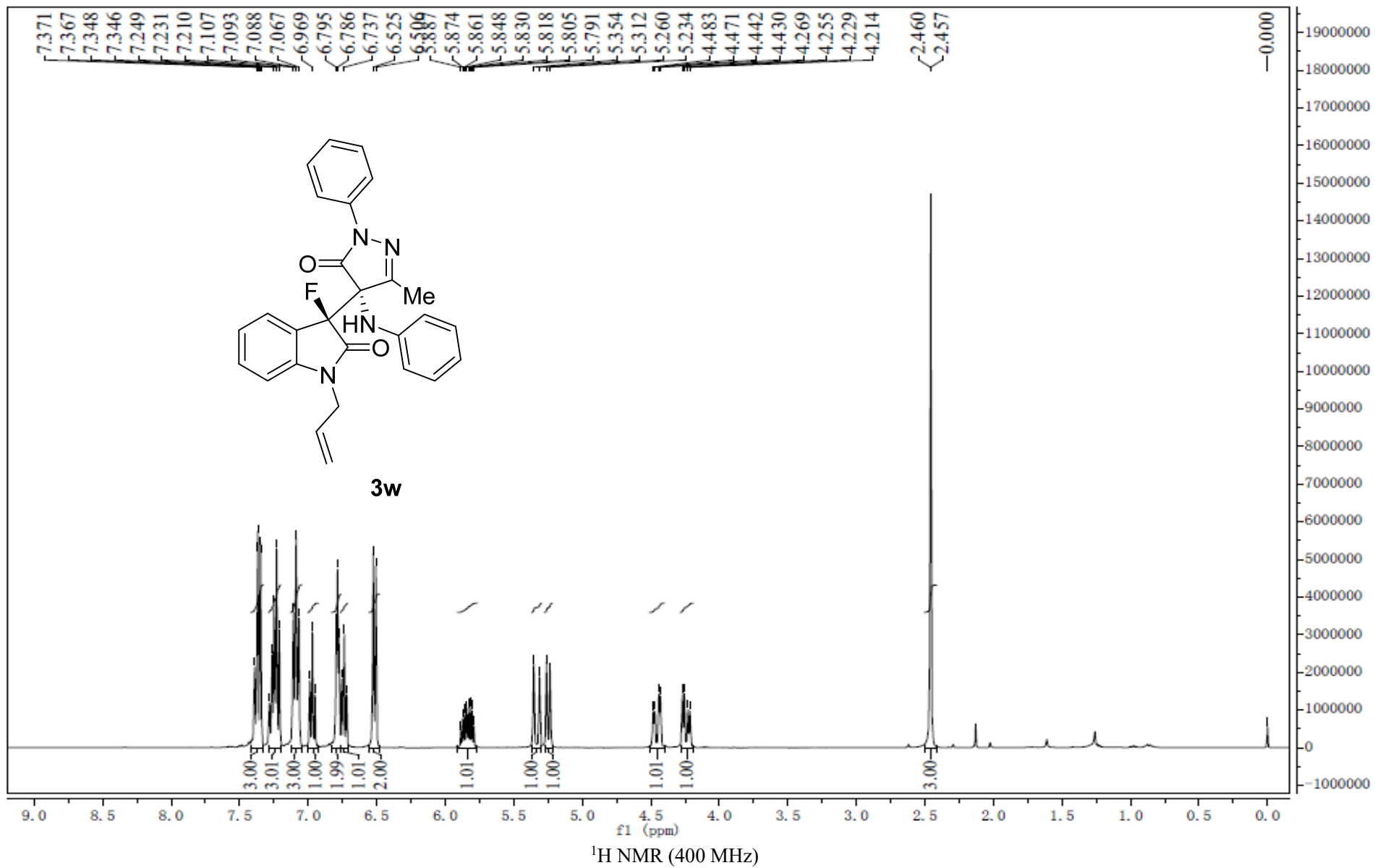
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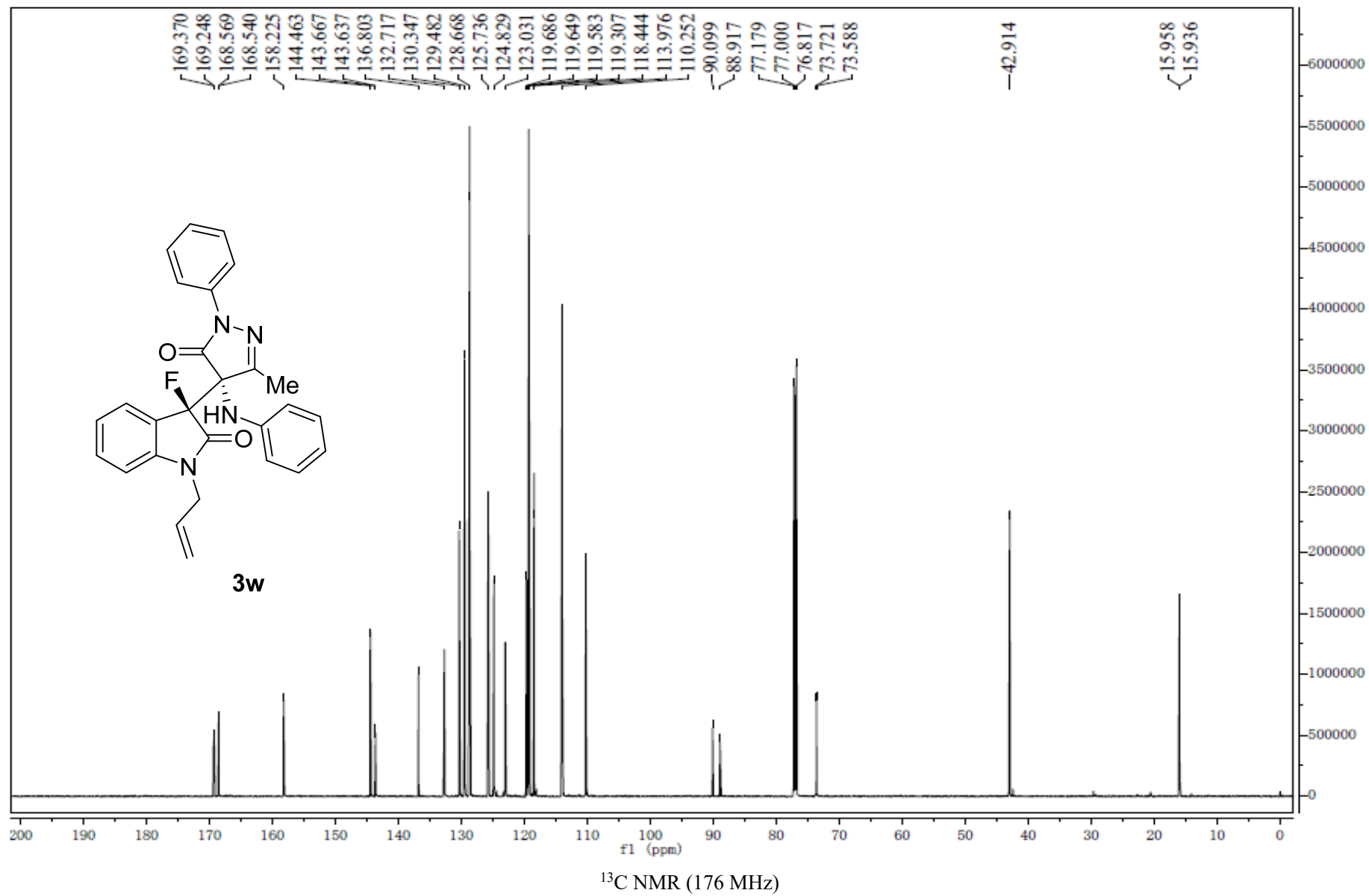


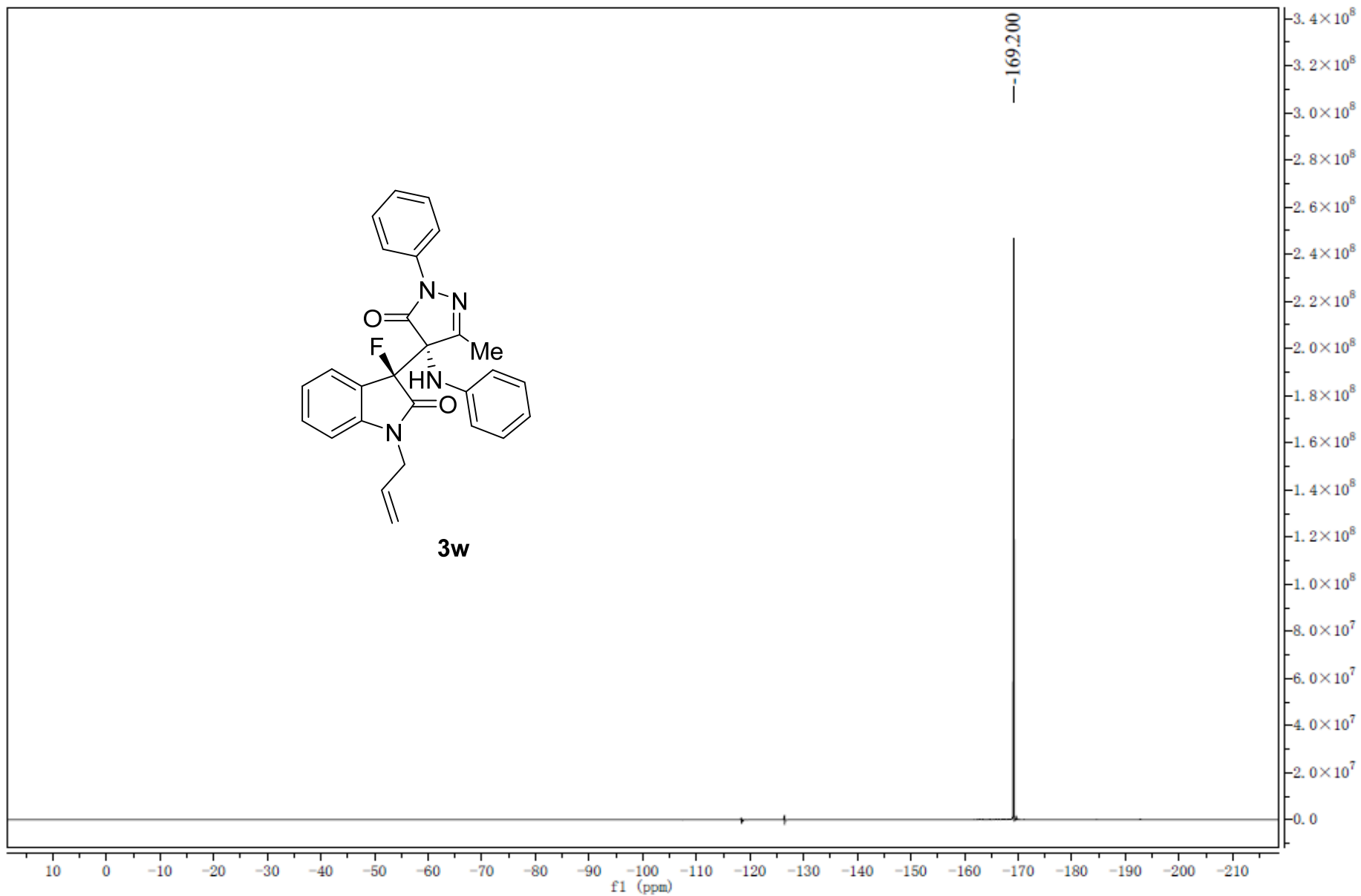
¹³C NMR (176 MHz)



^{19}F NMR (376 MHz)

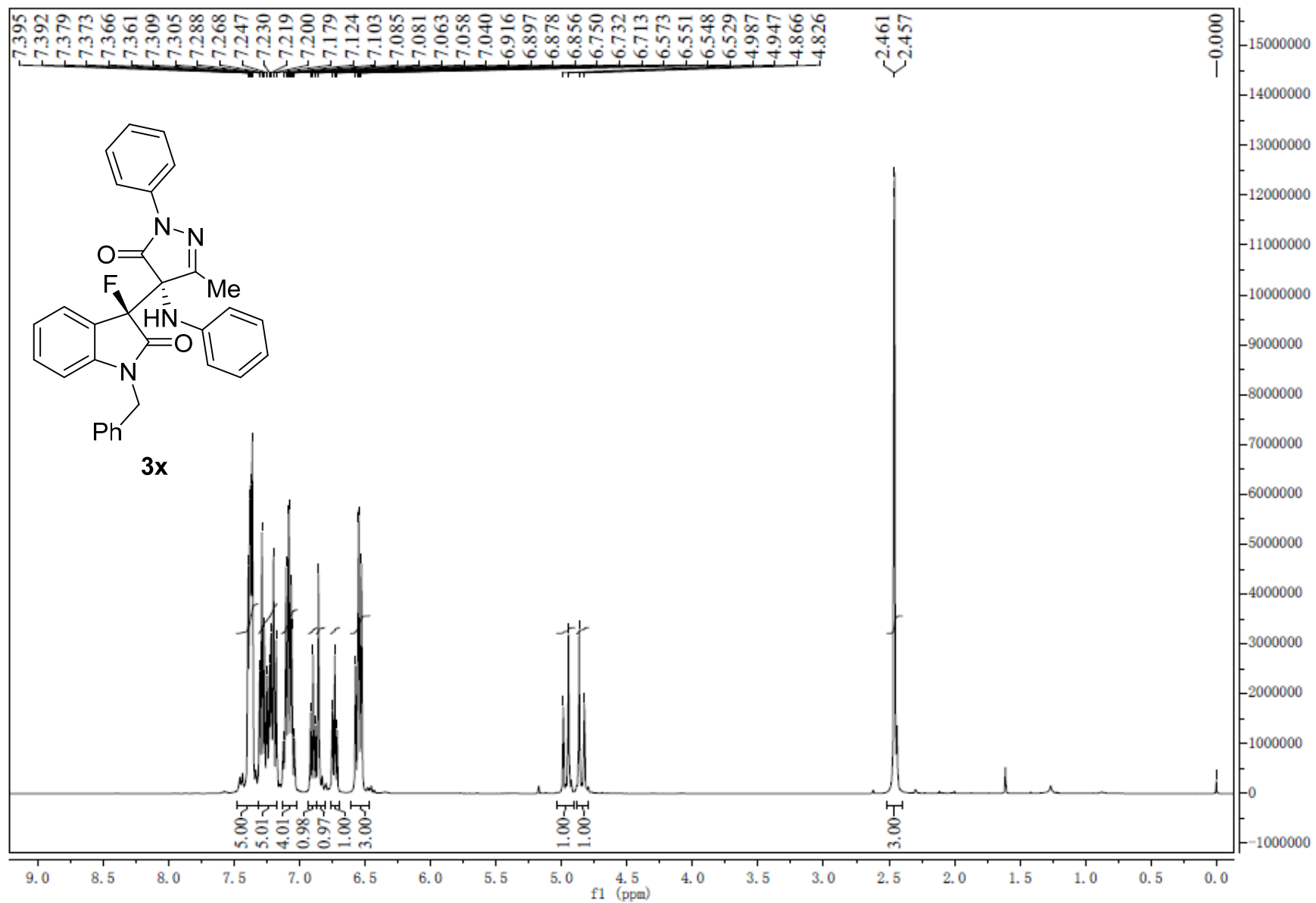




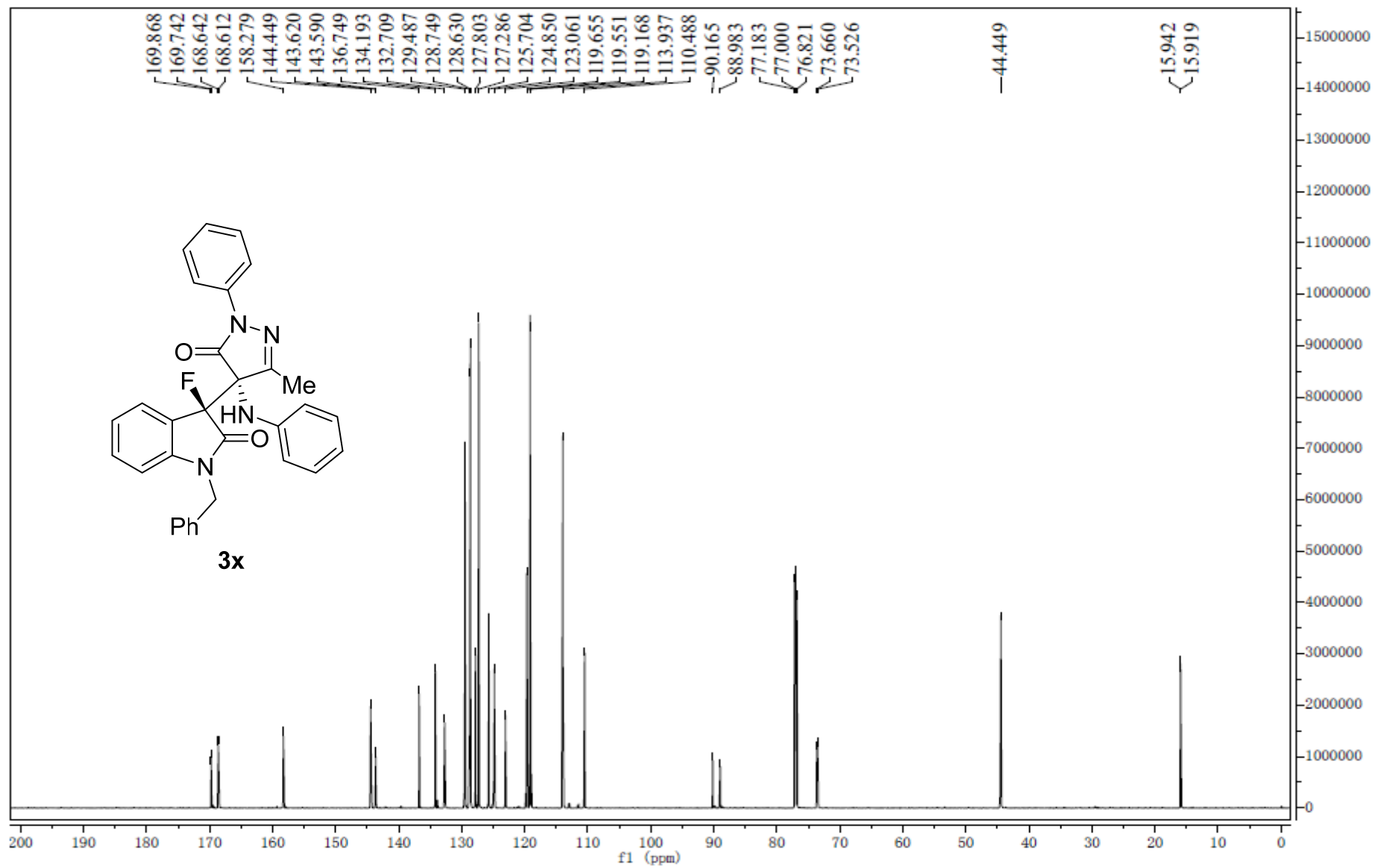


^{19}F NMR (376 MHz)

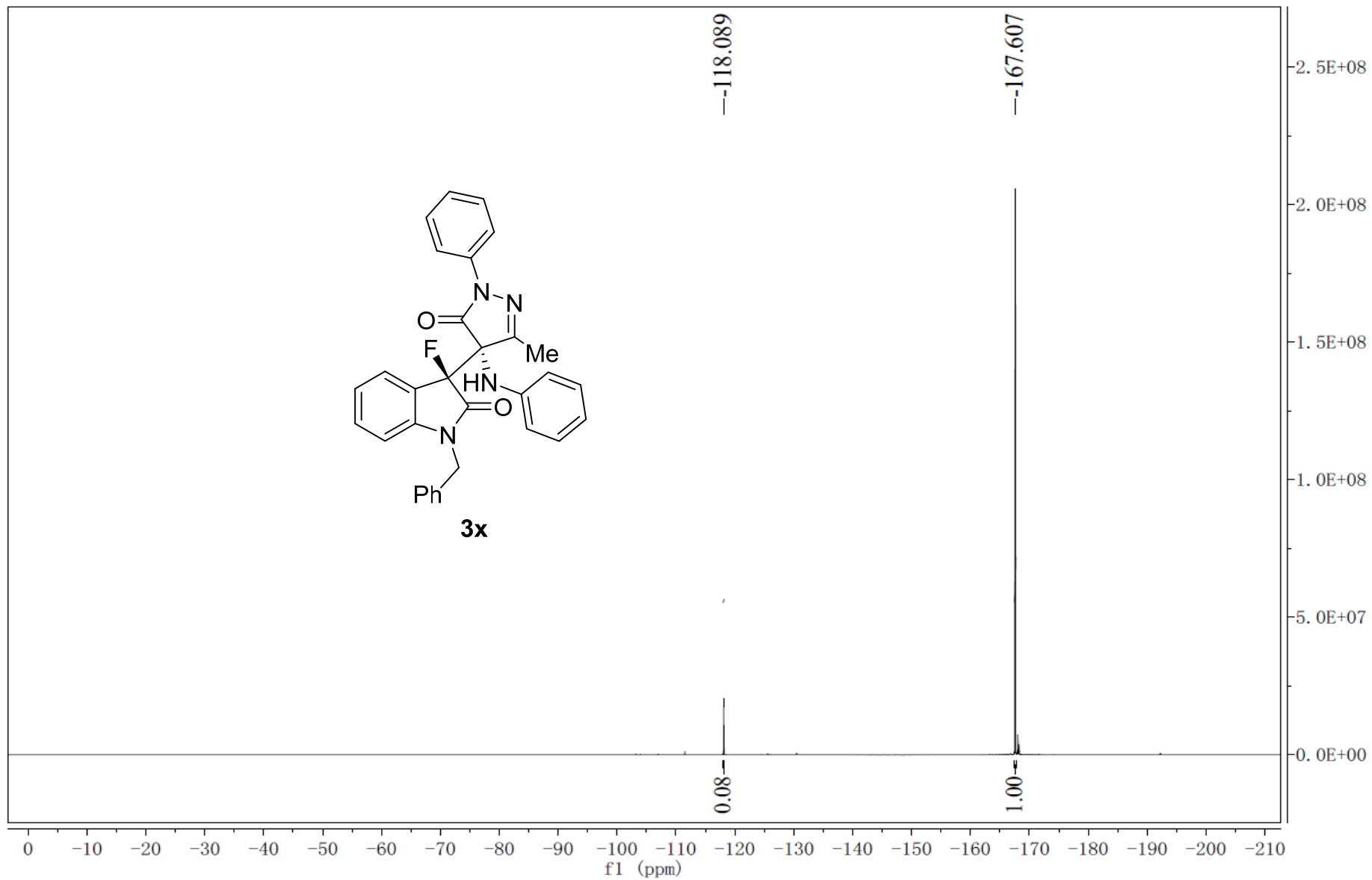
S68



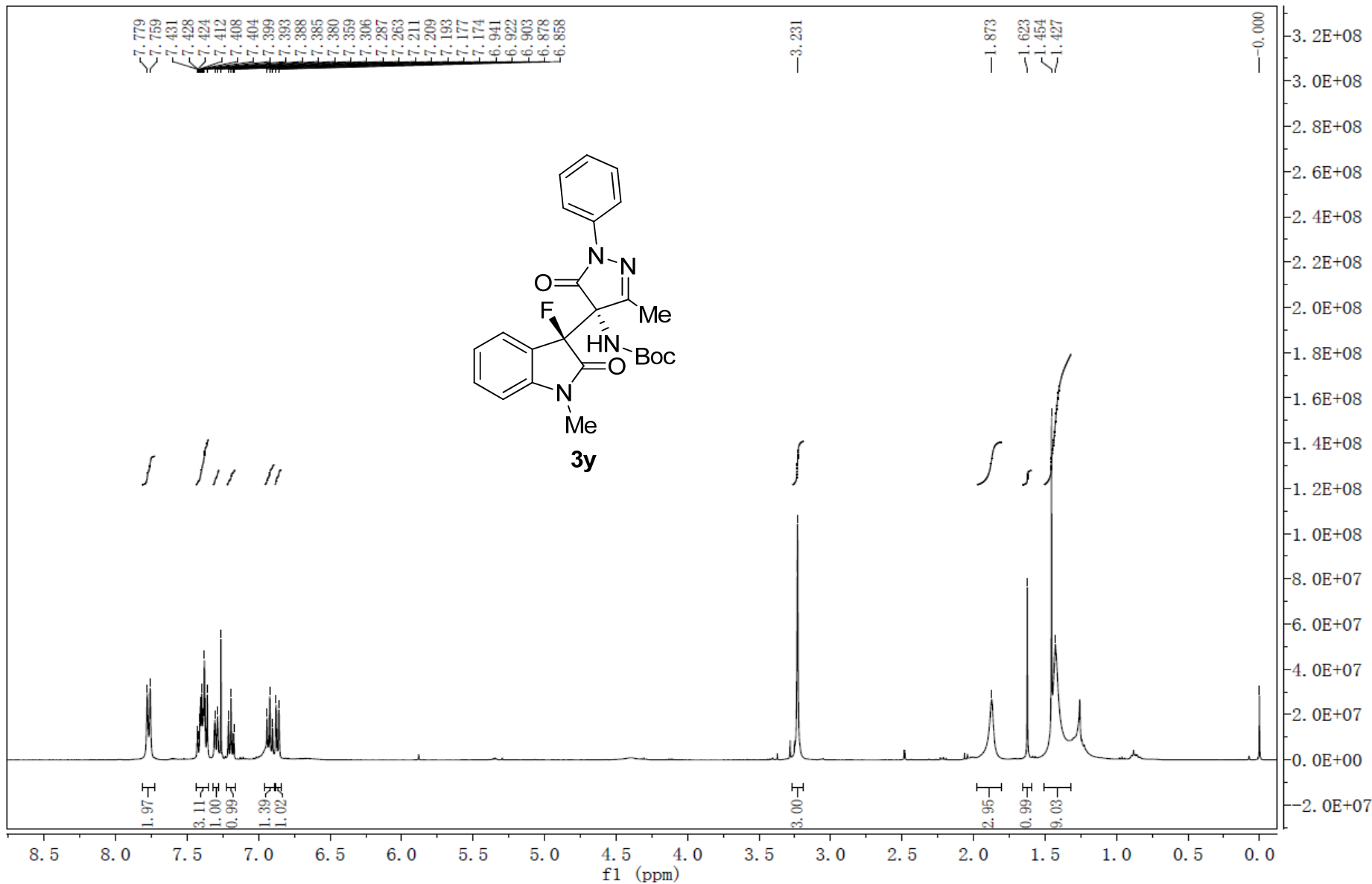
¹H NMR (400 MHz)



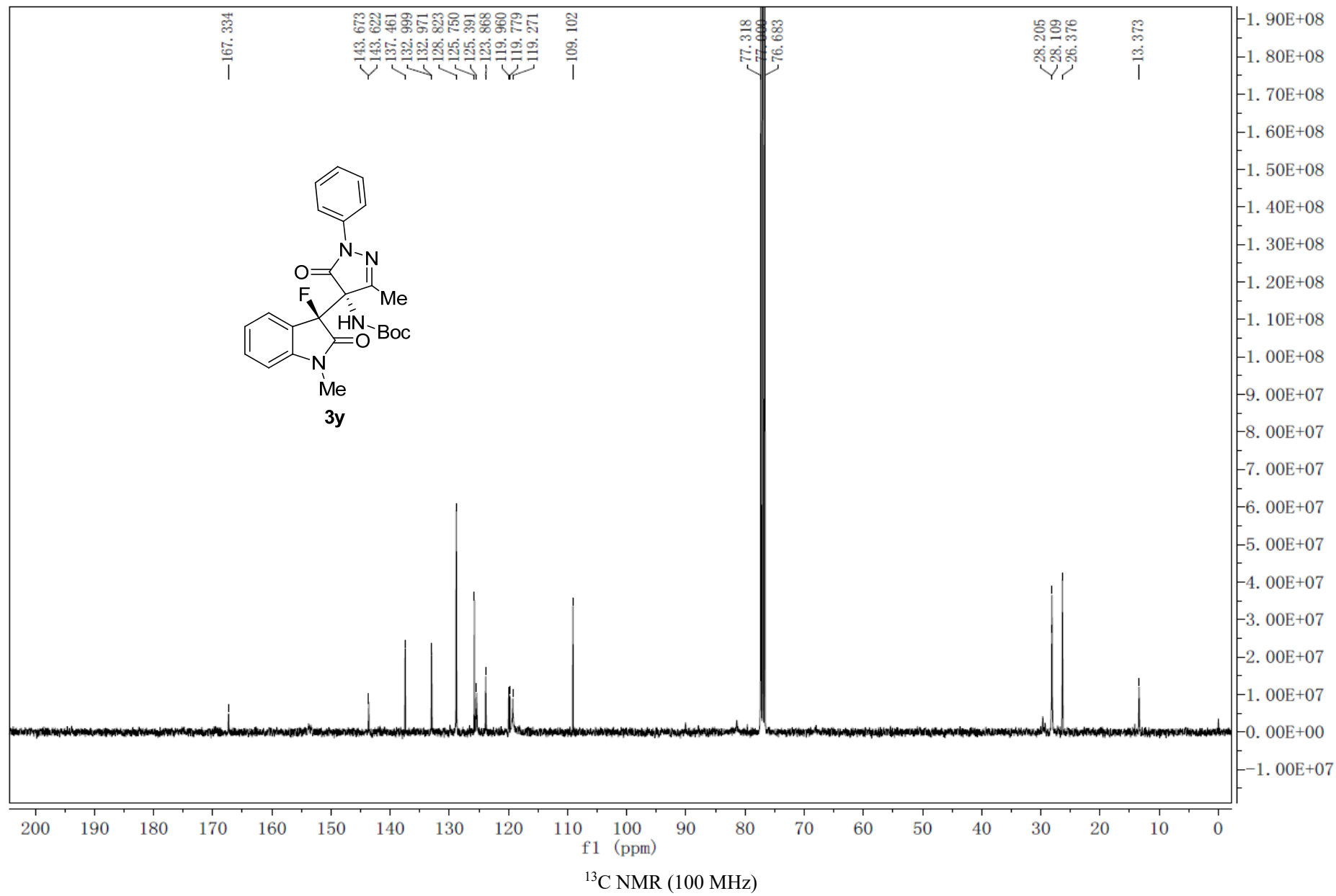
^{13}C NMR (176 MHz)

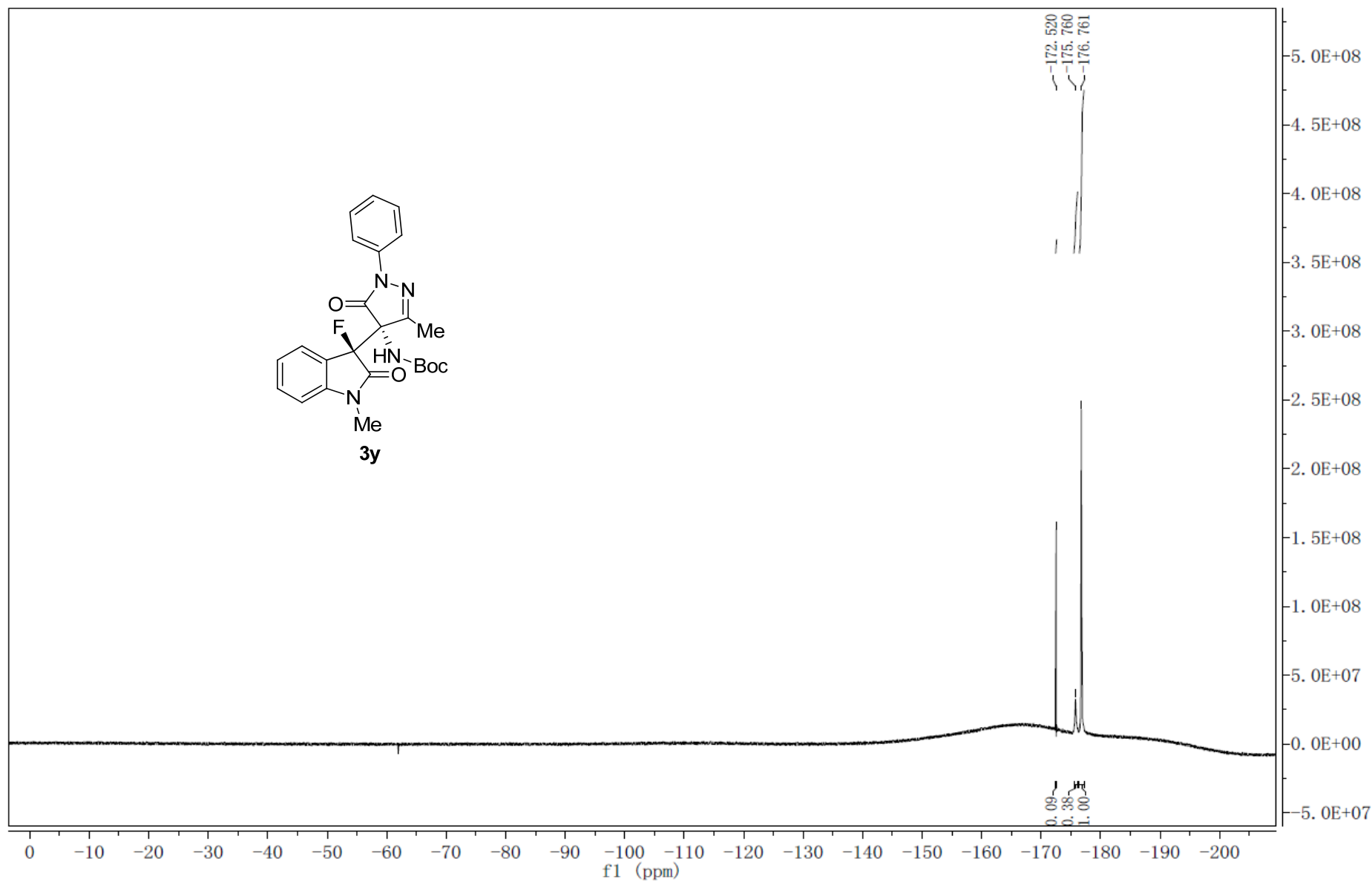


¹⁹F NMR (376 MHz)

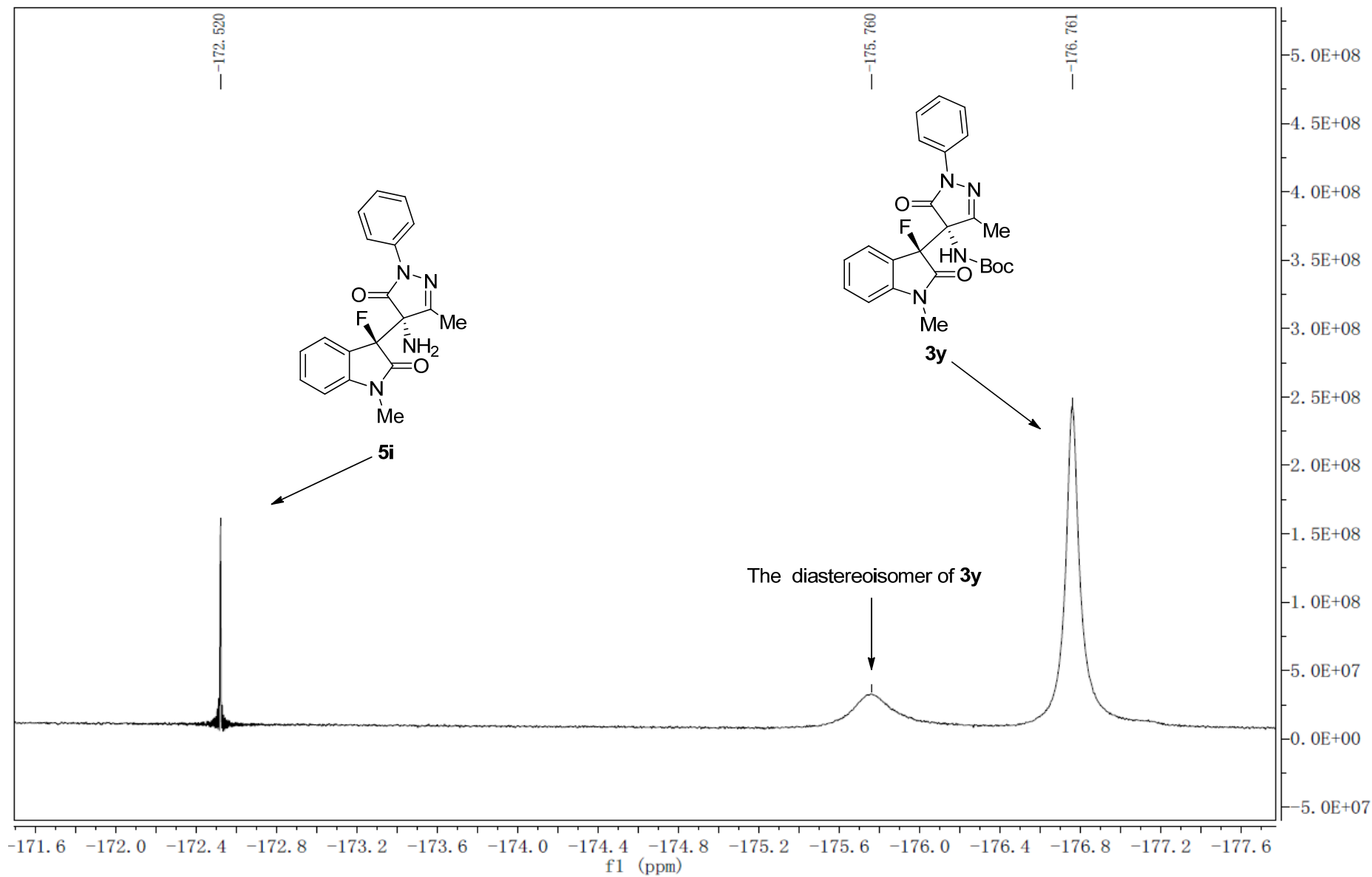


¹H NMR (400 MHz)

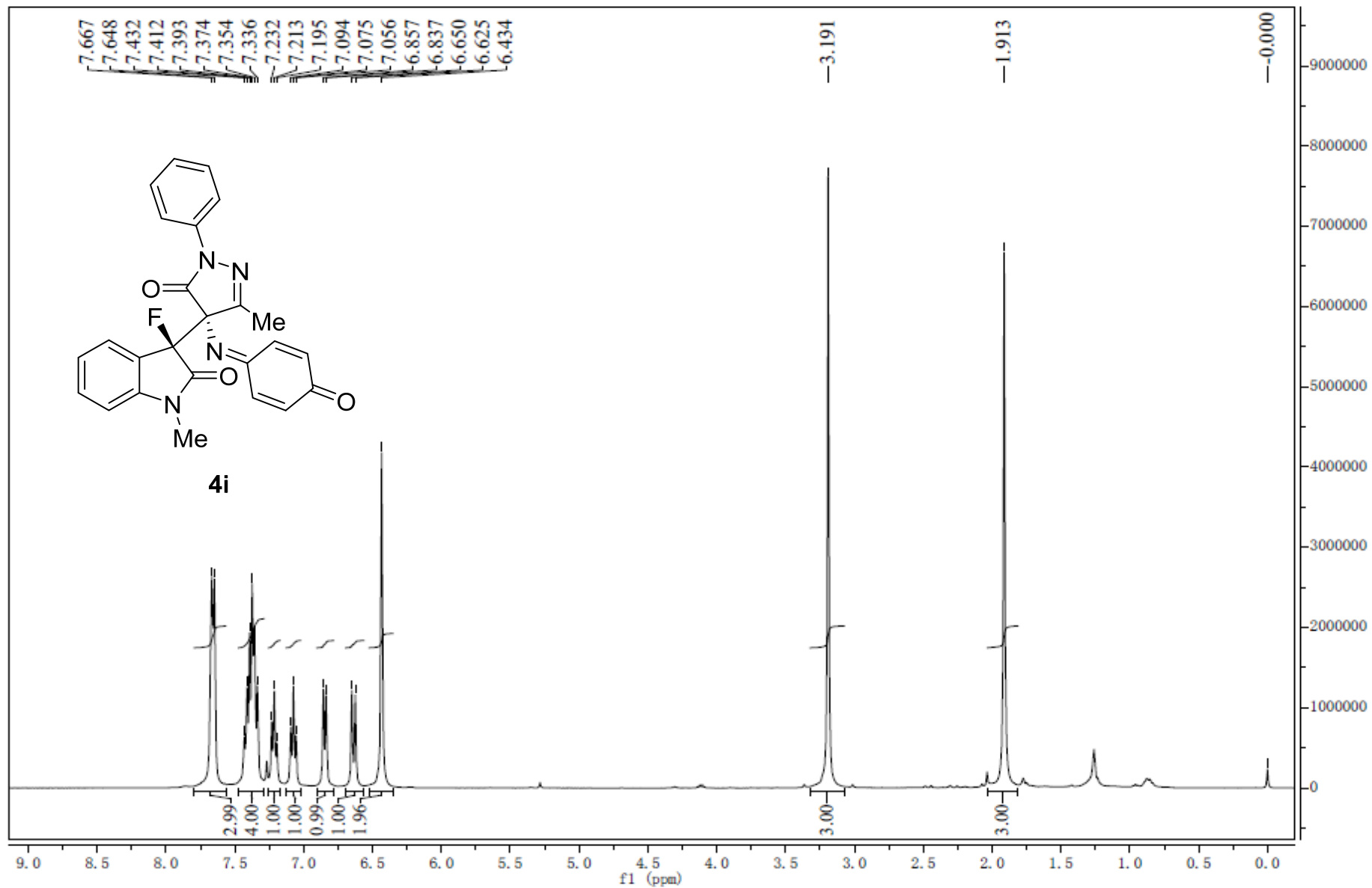




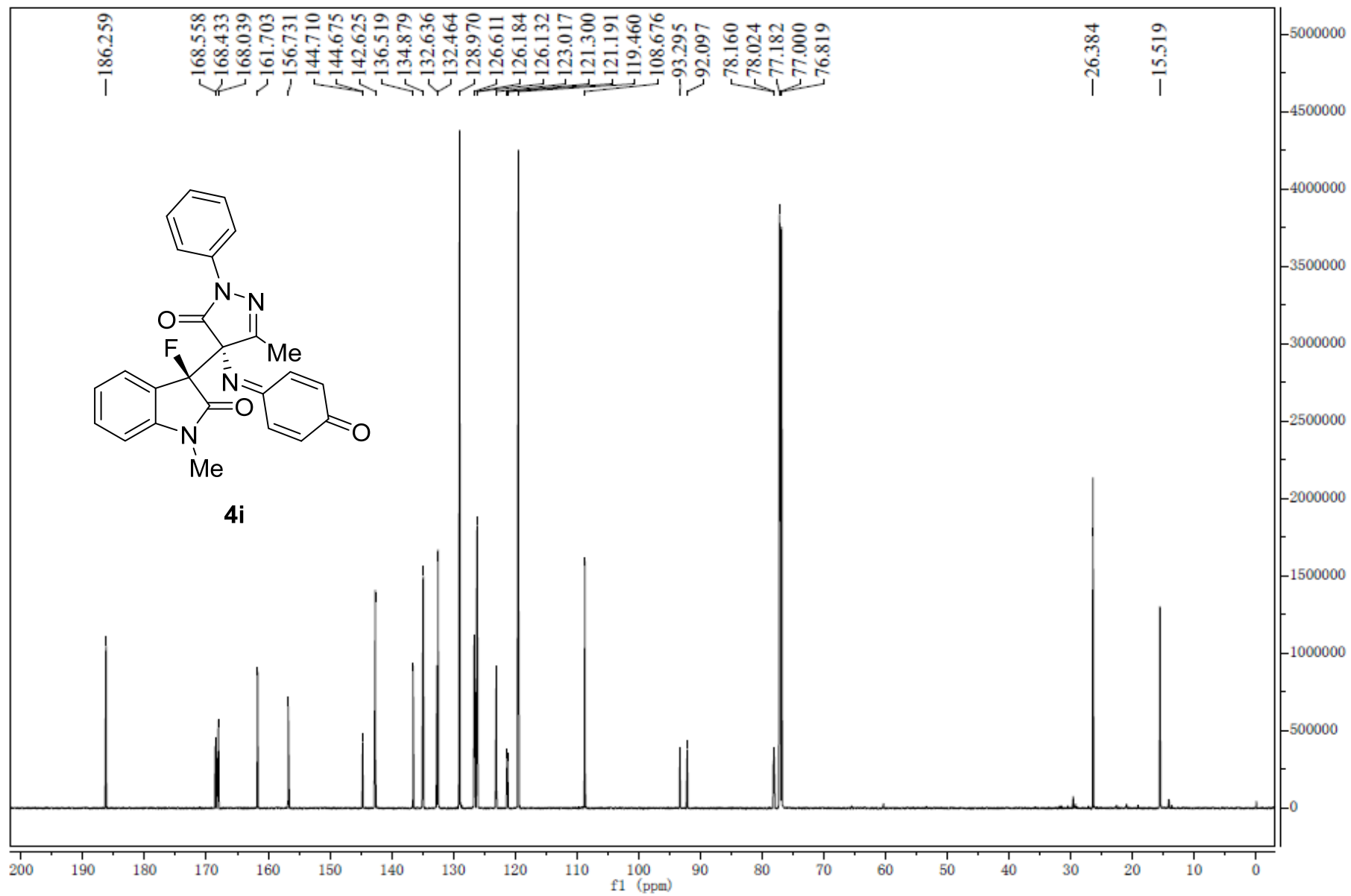
^{19}F NMR (376 MHz)



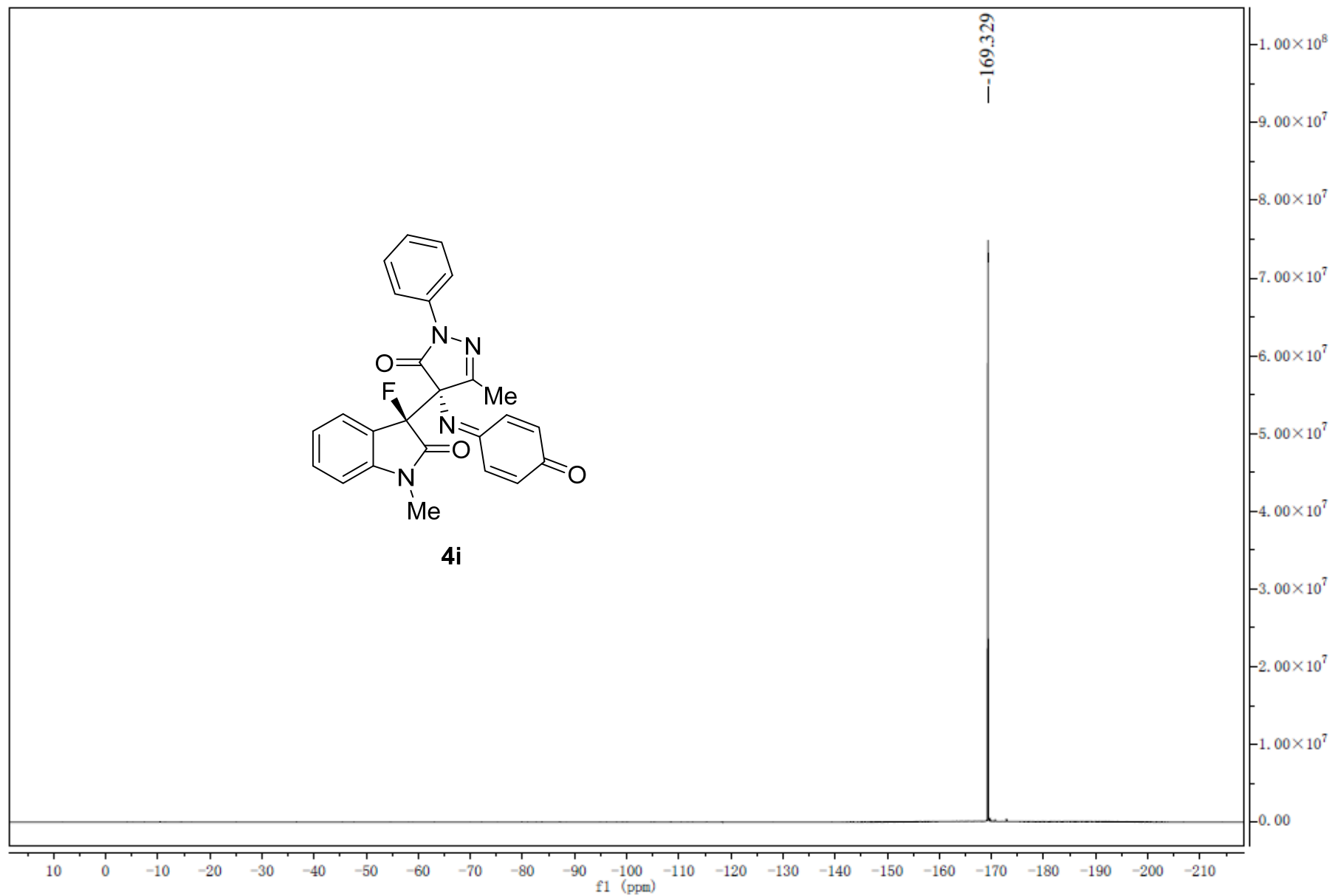
^{19}F NMR (376 MHz)



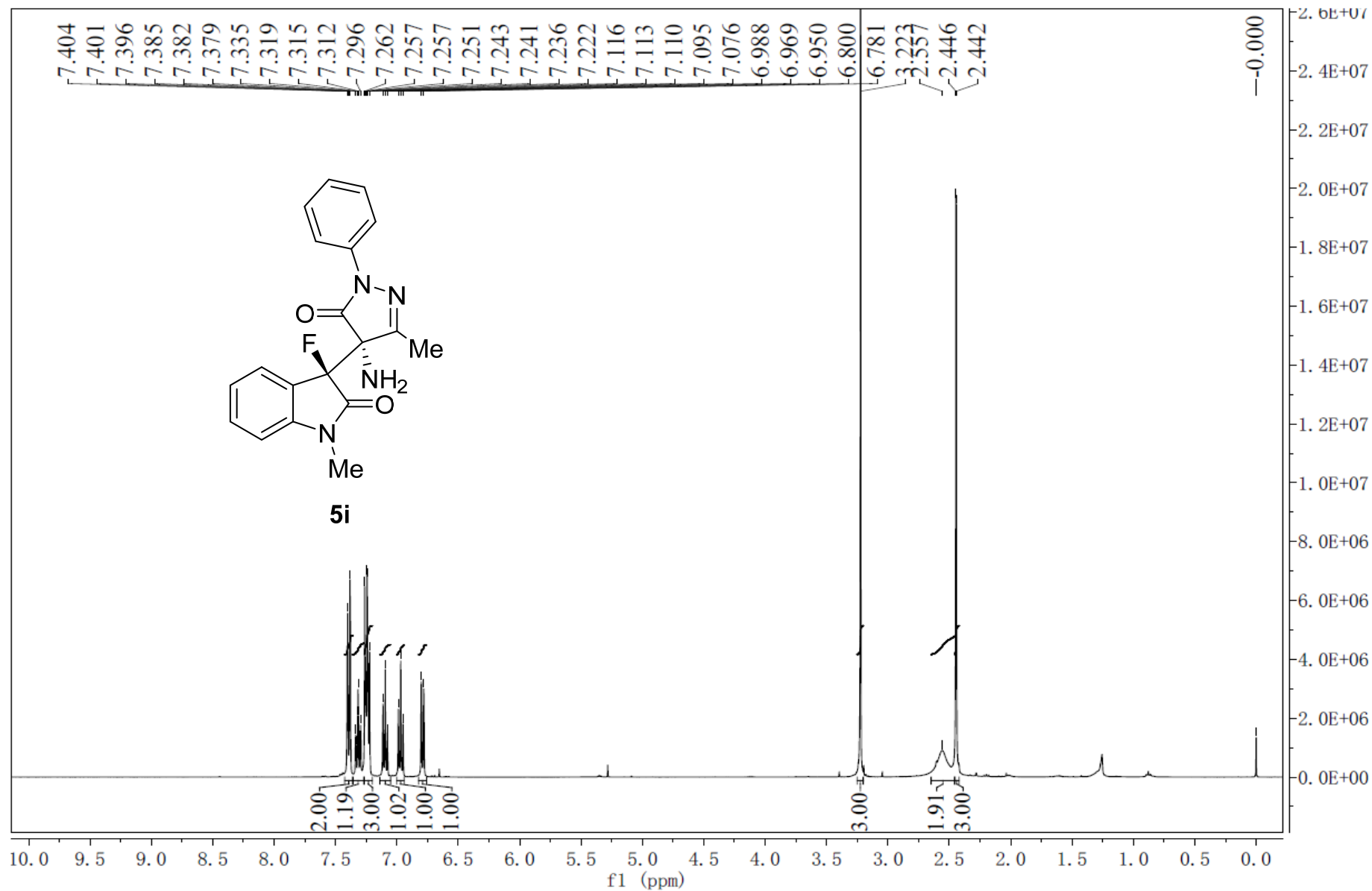
¹H NMR (400 MHz)



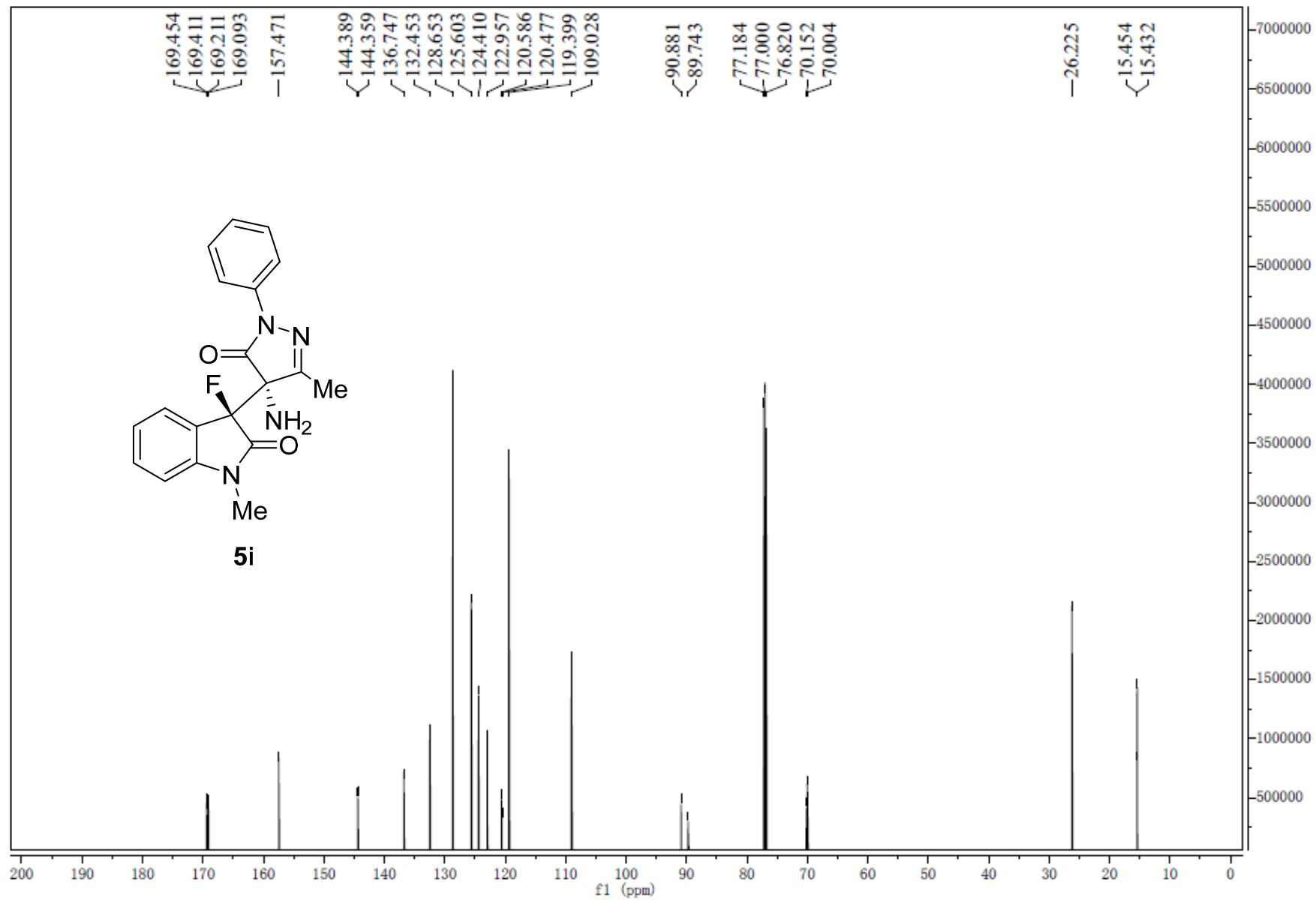
^{13}C NMR (176 MHz)



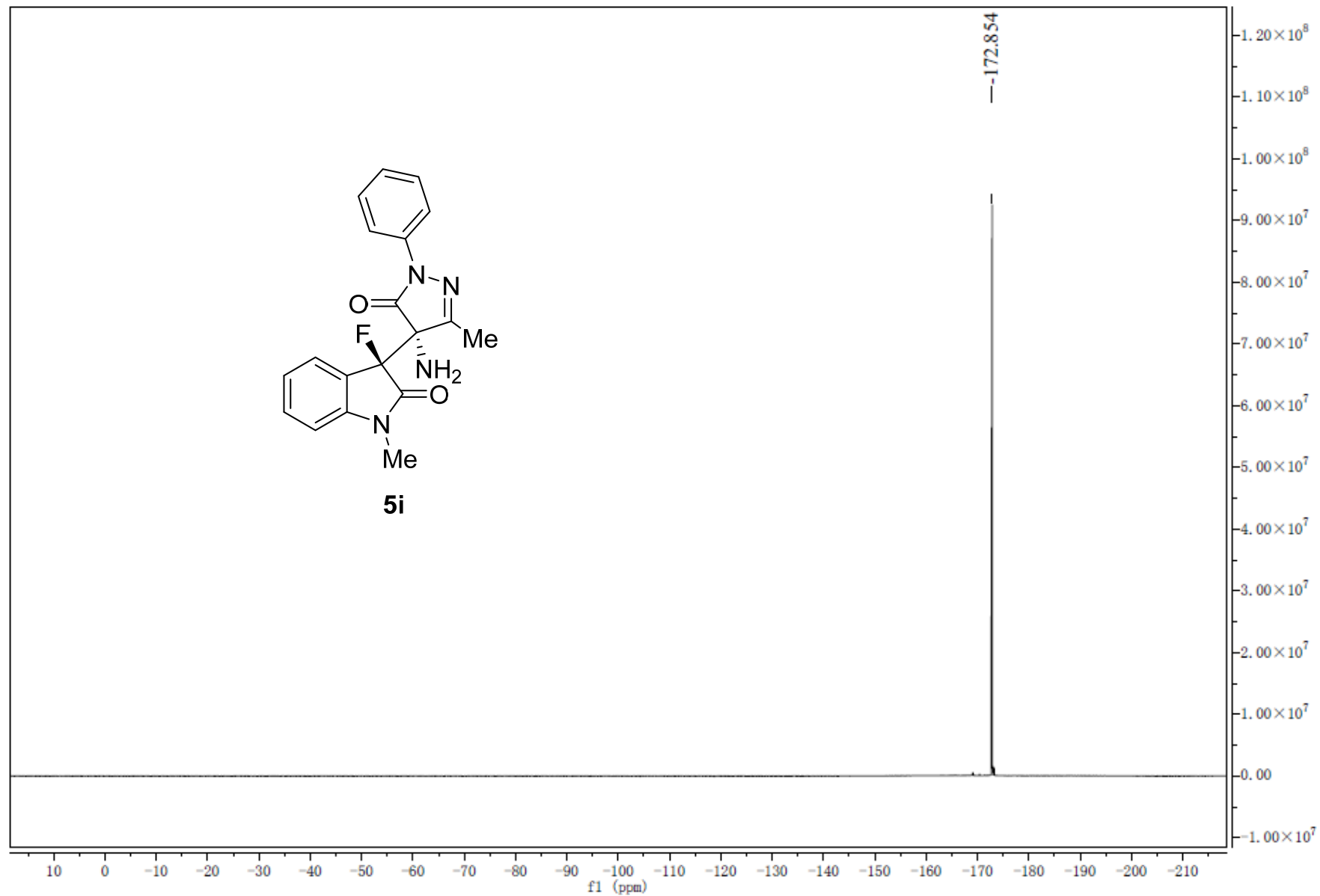
^{19}F NMR (376 MHz)



¹H NMR (400 MHz)

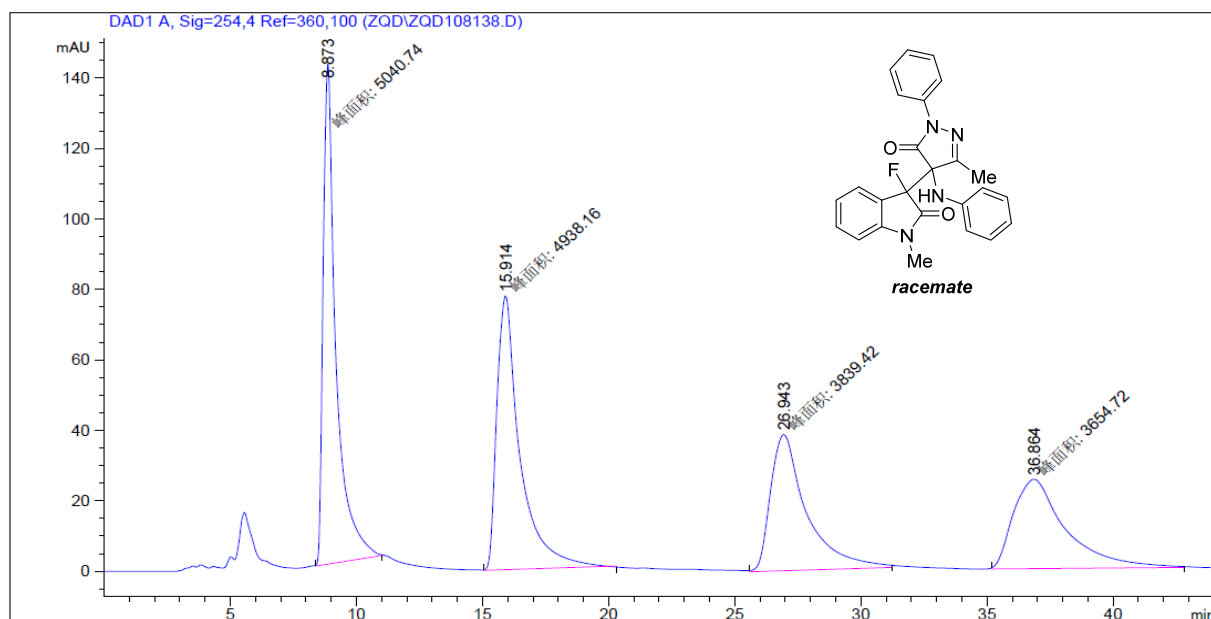


^{13}C NMR (176 MHz)

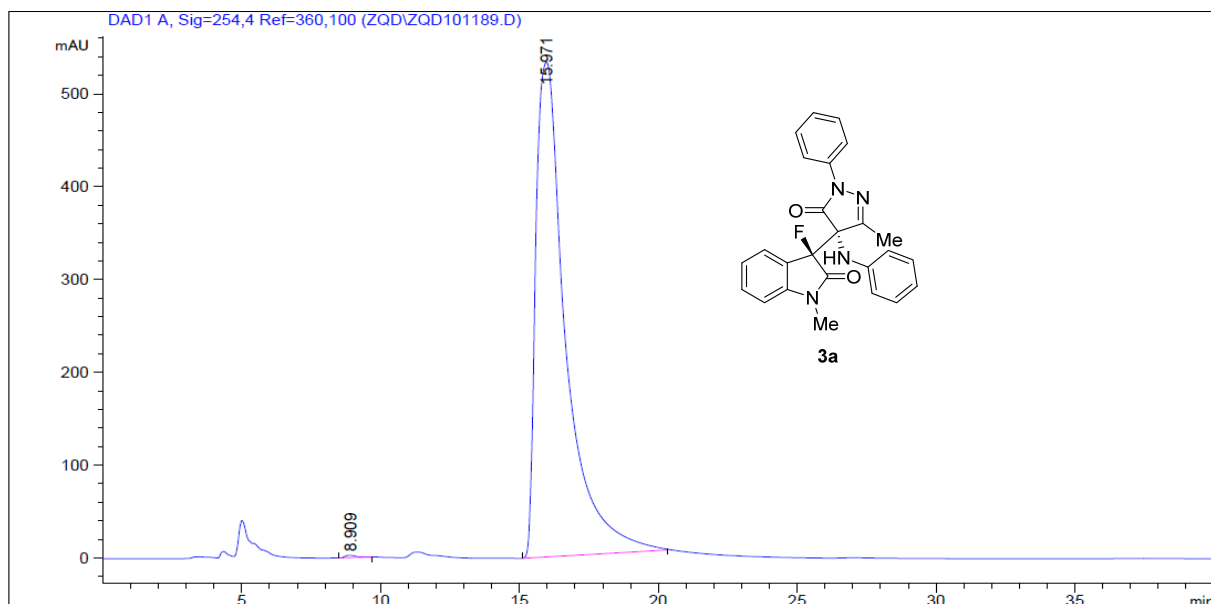


^{19}F NMR (376 MHz)

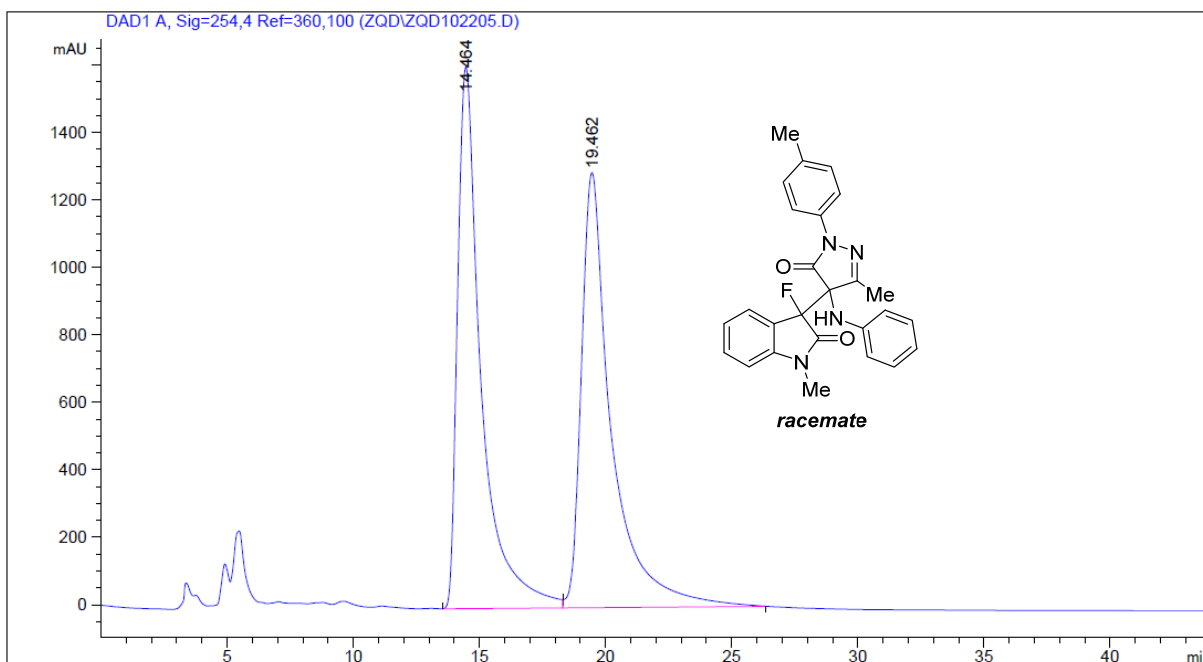
4. Copies of HPLC chromatograms of products



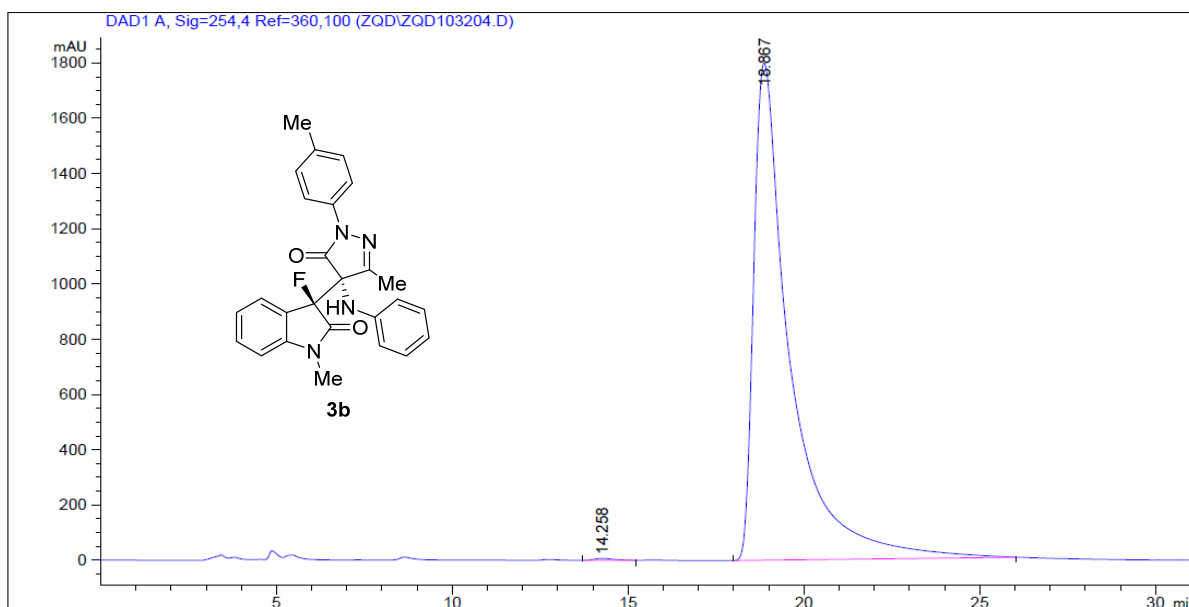
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.873	MM	0.5921	5040.73828	141.89995	28.8487
2	15.914	MM	1.0596	4938.16113	77.67131	28.2616
3	26.943	MM	1.6551	3839.41943	38.66217	21.9734
4	36.864	MM	2.4032	3654.71680	25.34659	20.9163



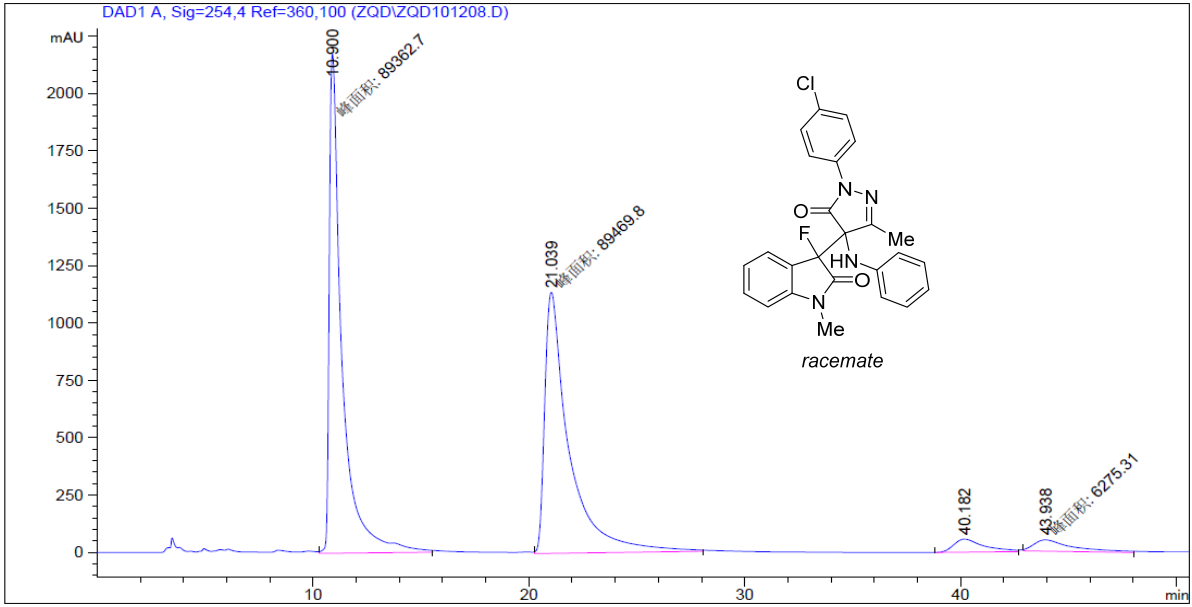
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.909	BB	0.3543	70.18701	2.35088	0.1754
2	15.971	BB	1.1176	3.99395e4	533.37372	99.8246



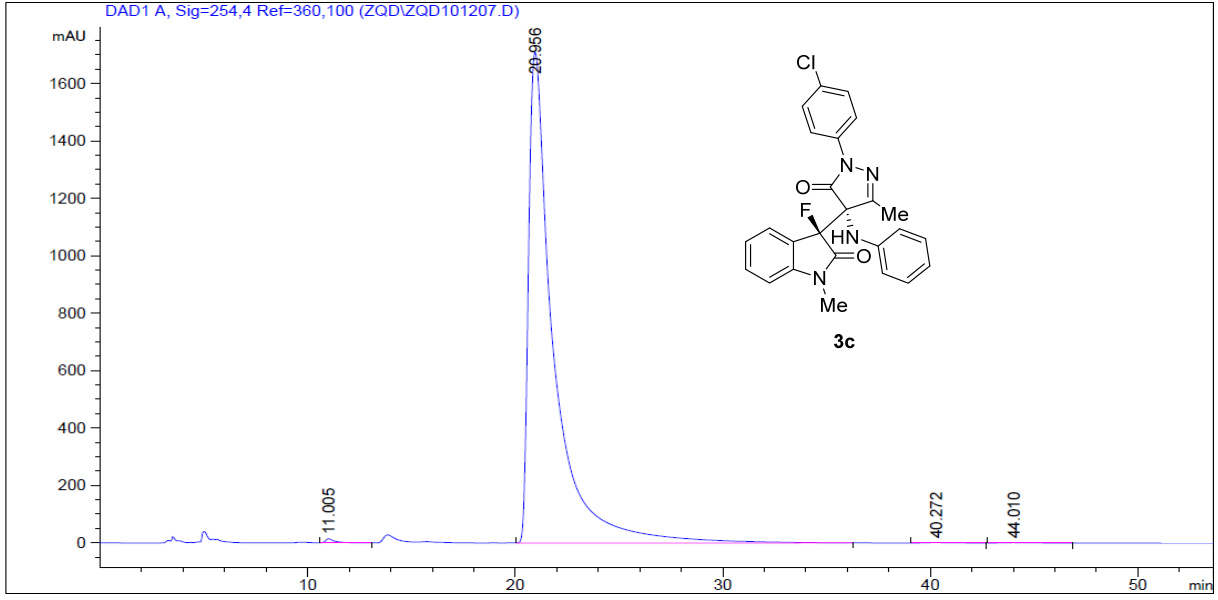
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.464	BB	0.9638	1.04534e5	1605.20154	49.4334
2	19.462	BB	1.1893	1.06930e5	1289.69202	50.5666



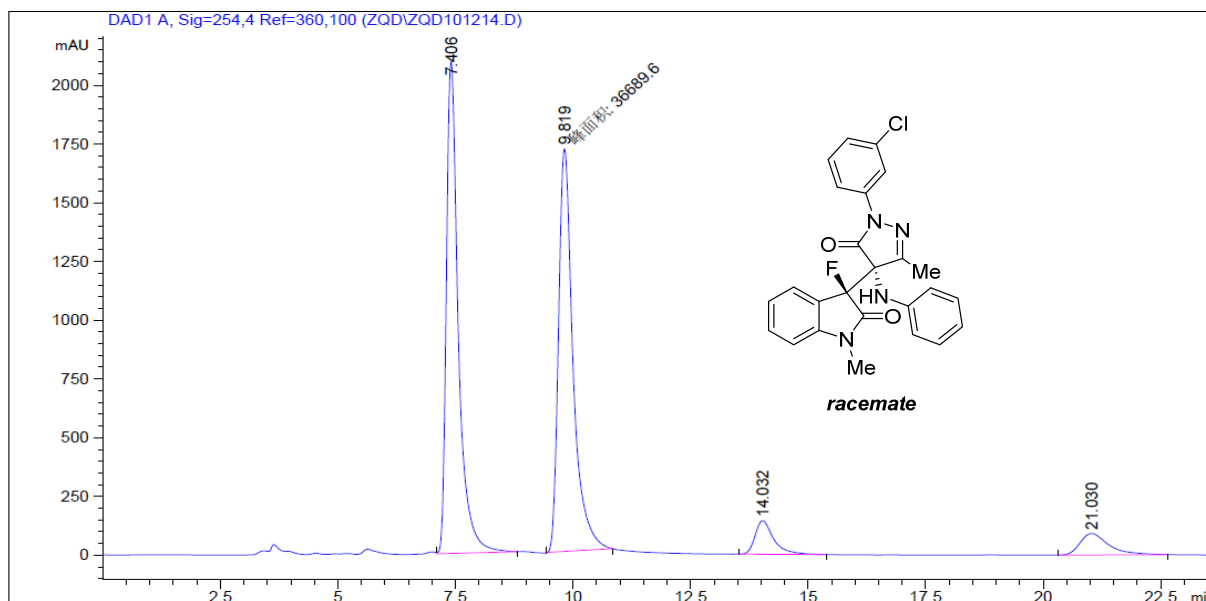
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.258	BB	0.5678	278.42581	7.19024	0.2131
2	18.867	BB	1.0273	1.30399e5	1799.71021	99.7869



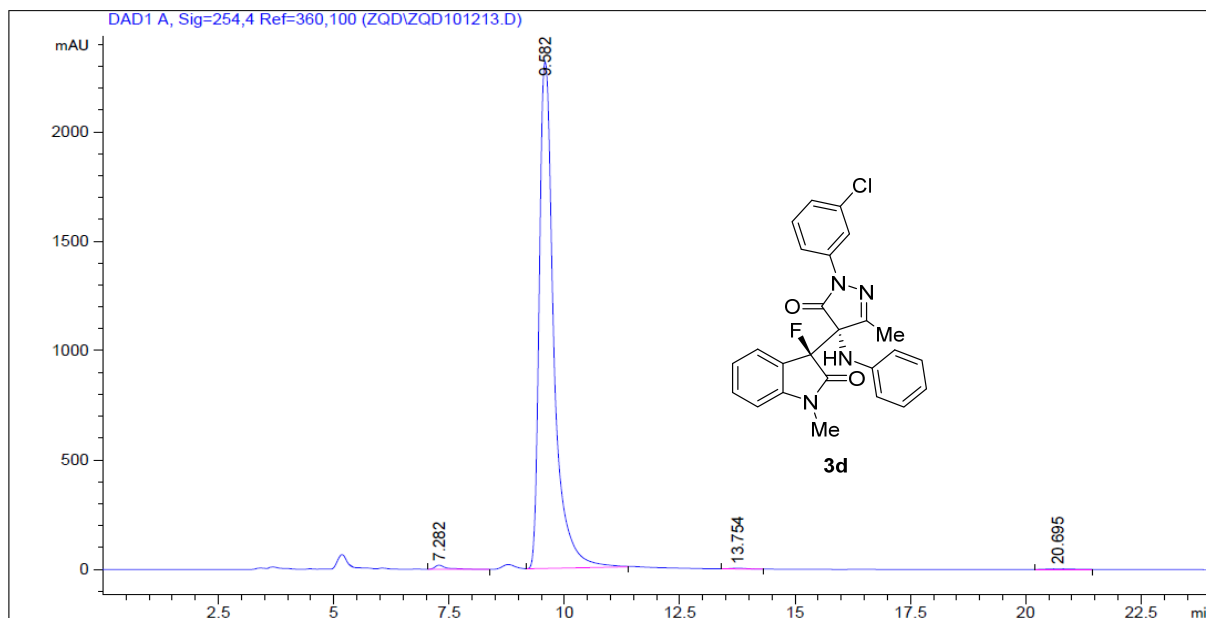
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.900	MM	0.6848	8.93627e4	2175.01904	46.8642
2	21.039	MM	1.3104	8.94697e4	1137.94421	46.9204
3	40.182	BB	1.3971	5576.49316	56.91363	2.9245
4	43.938	MM	2.1108	6275.31152	49.55000	3.2909



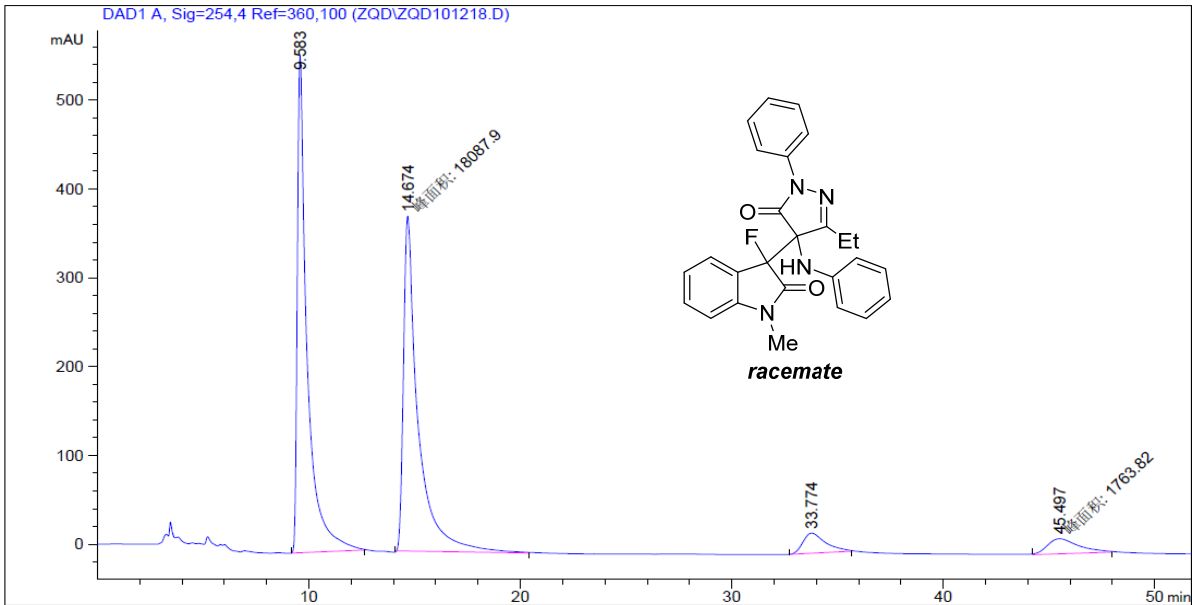
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.005	VB	0.4748	506.68384	14.82362	0.3495
2	20.956	VB	1.1955	1.44136e5	1709.79968	99.4348
3	40.272	BB	1.1332	150.14992	1.63840	0.1036
4	44.010	BB	1.3212	162.51303	1.54753	0.1121



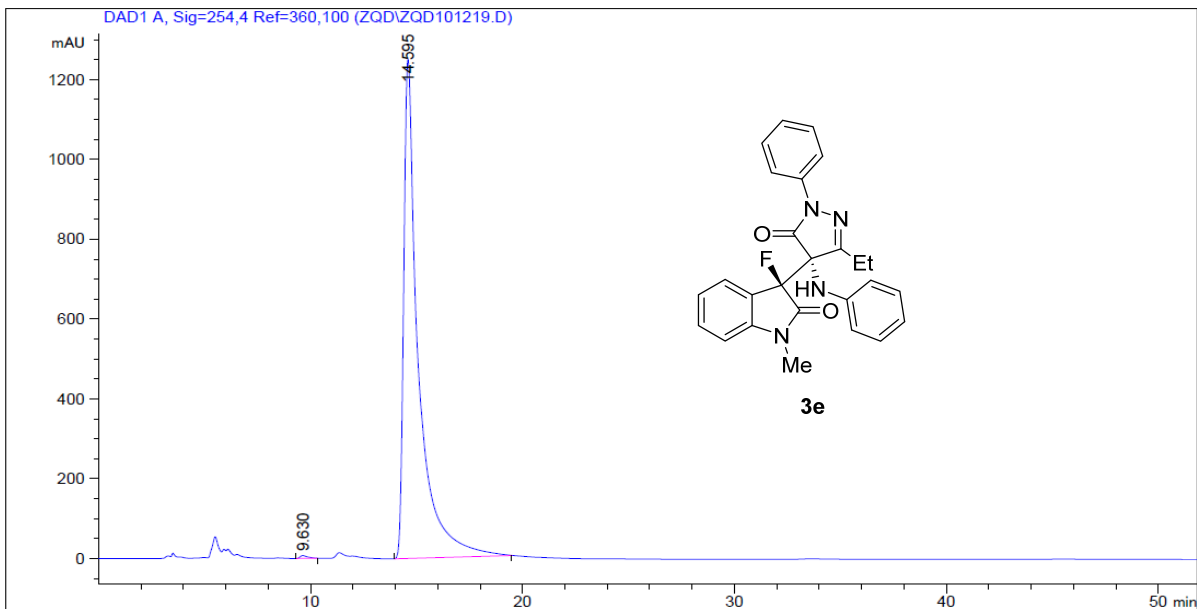
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.406	VB	0.2640	3.69661e4	2093.37915	45.3552
2	9.819	MM	0.3568	3.66896e4	1713.91394	45.0160
3	14.032	BB	0.4120	3946.61157	143.01100	4.8423
4	21.030	BB	0.6426	3901.19507	91.27499	4.7865



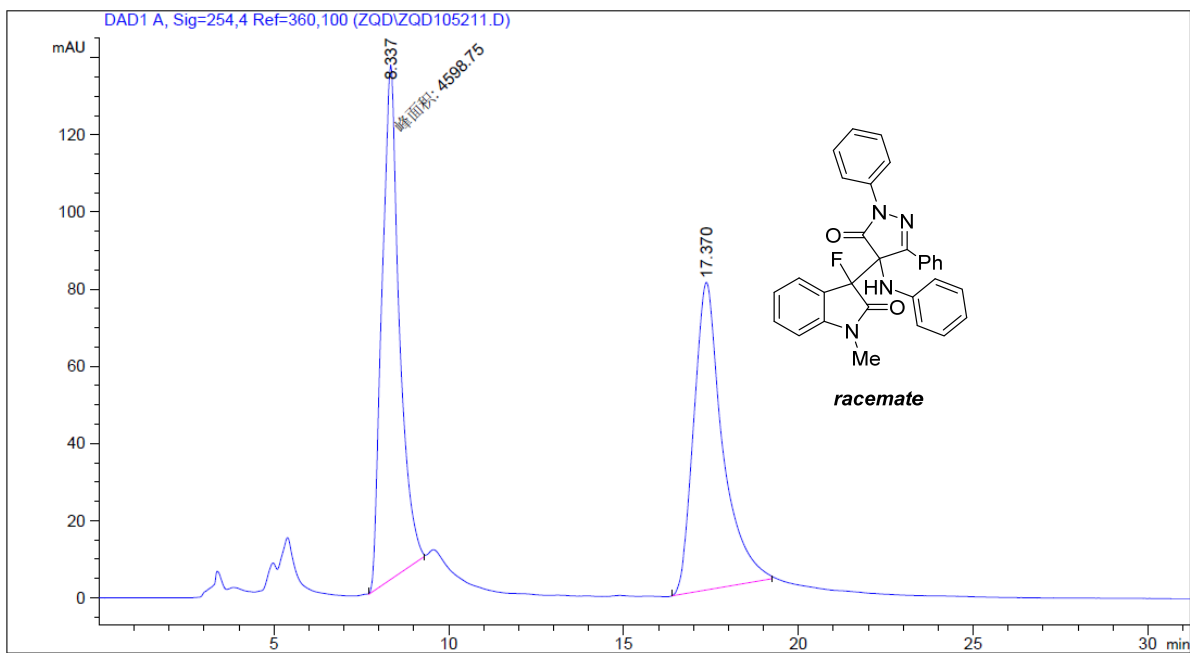
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.282	BV	0.2532	336.53128	19.13636	0.6546
2	9.582	VB	0.3306	5.09015e4	2313.86938	99.0066
3	13.754	BB	0.3337	71.97612	3.20918	0.1400
4	20.695	BB	0.4916	102.20467	2.77572	0.1988



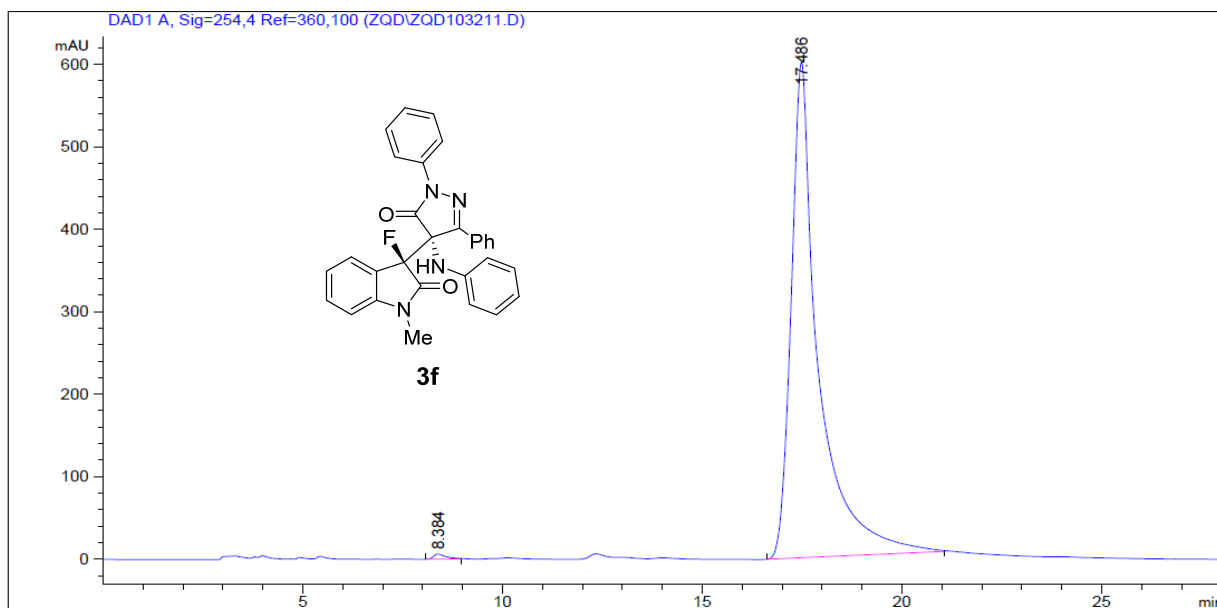
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.583	BB	0.4529	1.81558e4	559.10504	45.7360
2	14.674	MM	0.7995	1.80879e4	377.09079	45.5652
3	33.774	BB	1.0907	1689.34192	22.58285	4.2556
4	45.497	MM	1.7254	1763.82019	17.03795	4.4432



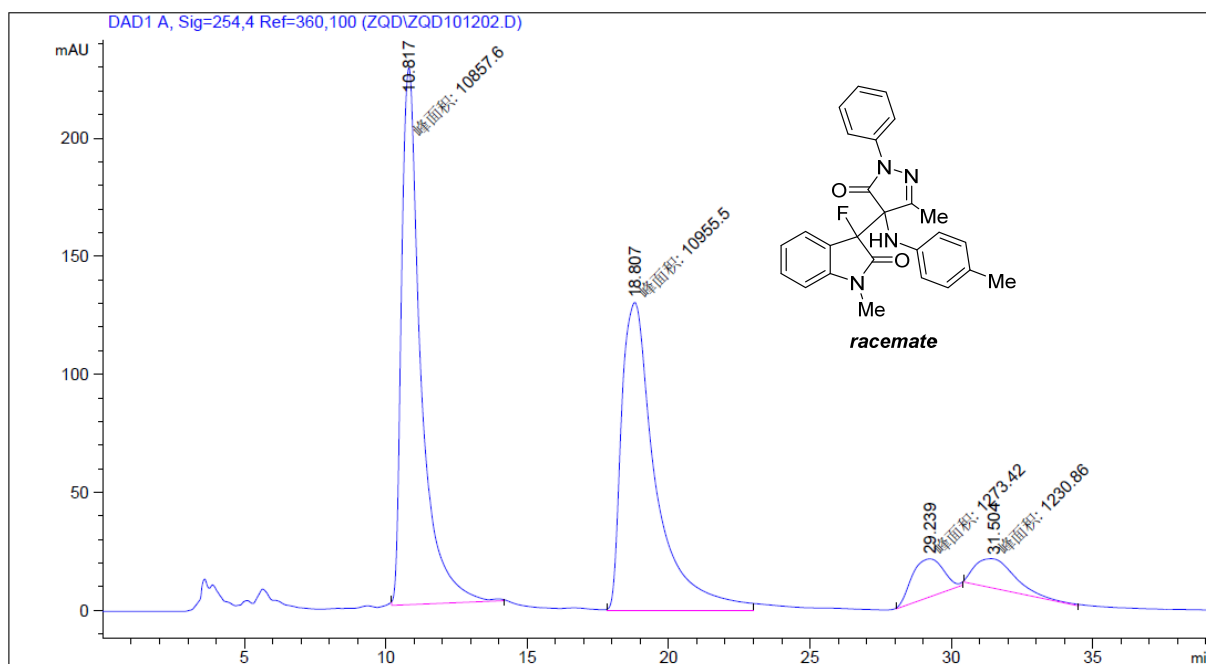
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.630	BB	0.3560	180.88950	7.27824	0.2993
2	14.595	BB	0.6742	6.02471e4	1250.31116	99.7007



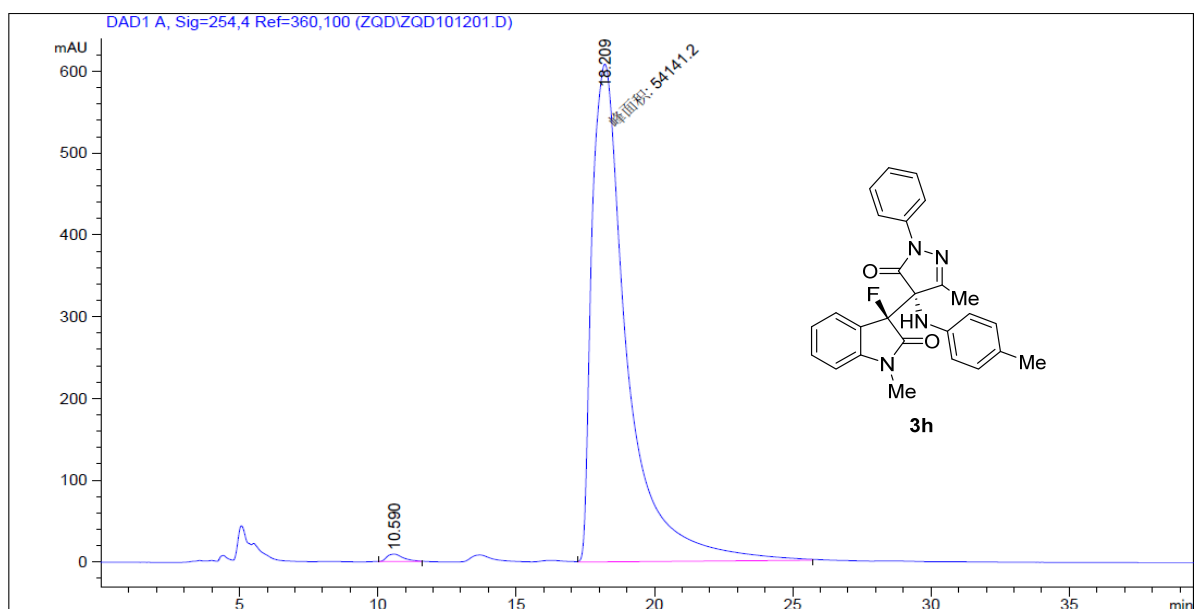
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.337	MM	0.5746	4598.74902	133.38606	50.1886
2	17.370	BB	0.8360	4564.19531	79.71053	49.8114



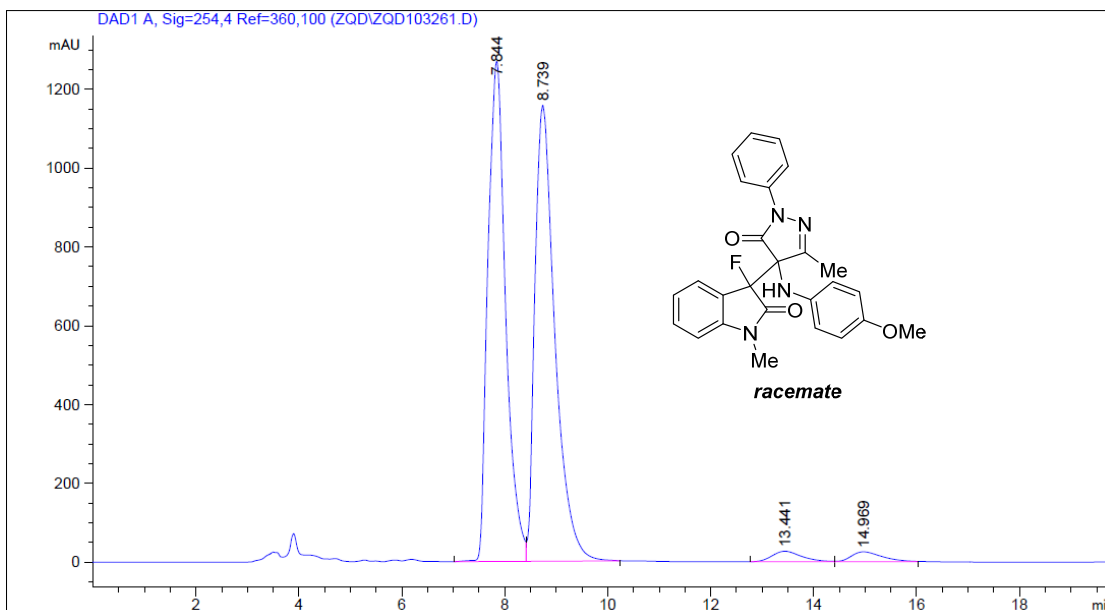
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.384	BB	0.3070	135.01965	6.22742	0.4706
2	17.486	BB	0.6540	2.85536e4	601.28241	99.5294



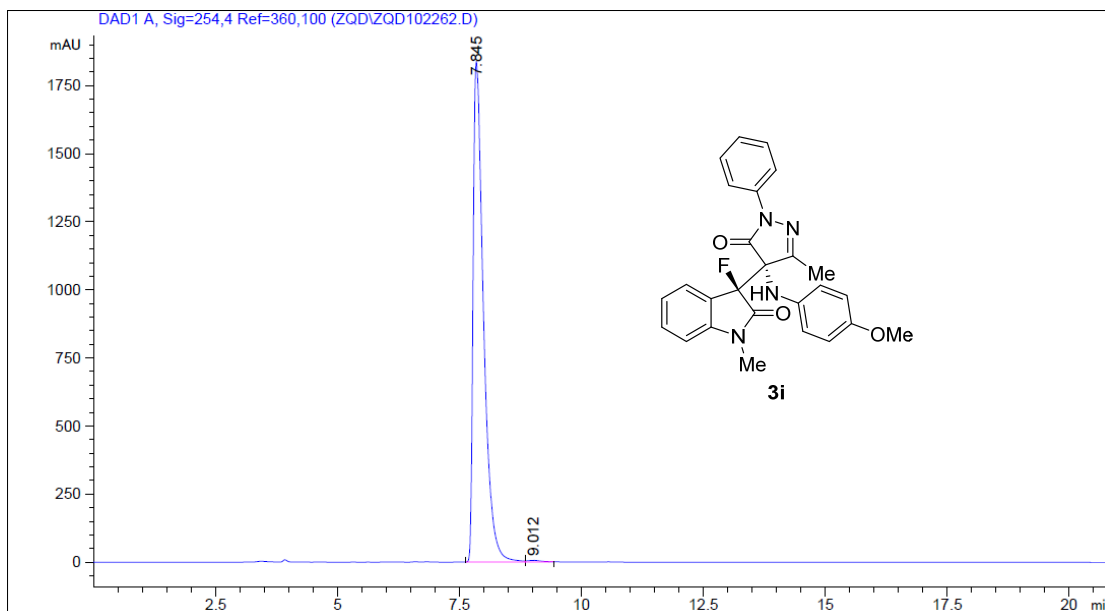
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.817	MM	0.7960	1.08576e4	227.33813	44.6497
2	18.807	MM	1.4015	1.09555e4	130.27798	45.0520
3	29.239	MM	1.3184	1273.42004	16.09828	5.2367
4	31.504	MM	1.6482	1230.86389	12.44635	5.0617



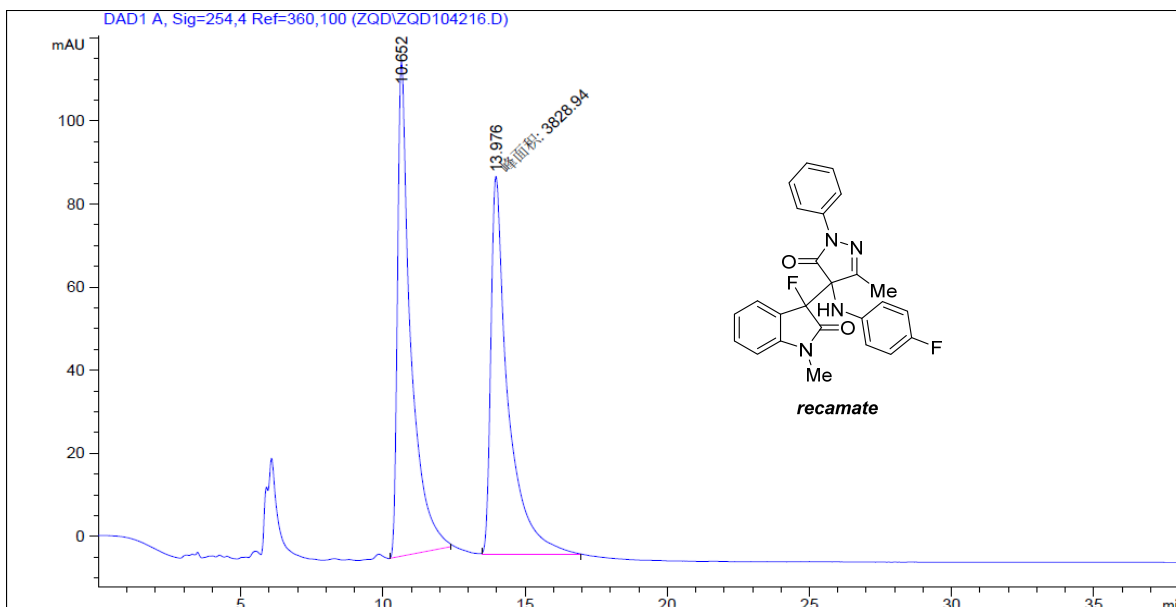
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.590	BB	0.6218	367.08743	8.96258	0.6735
2	18.209	MM	1.4825	5.41412e4	608.66223	99.3265



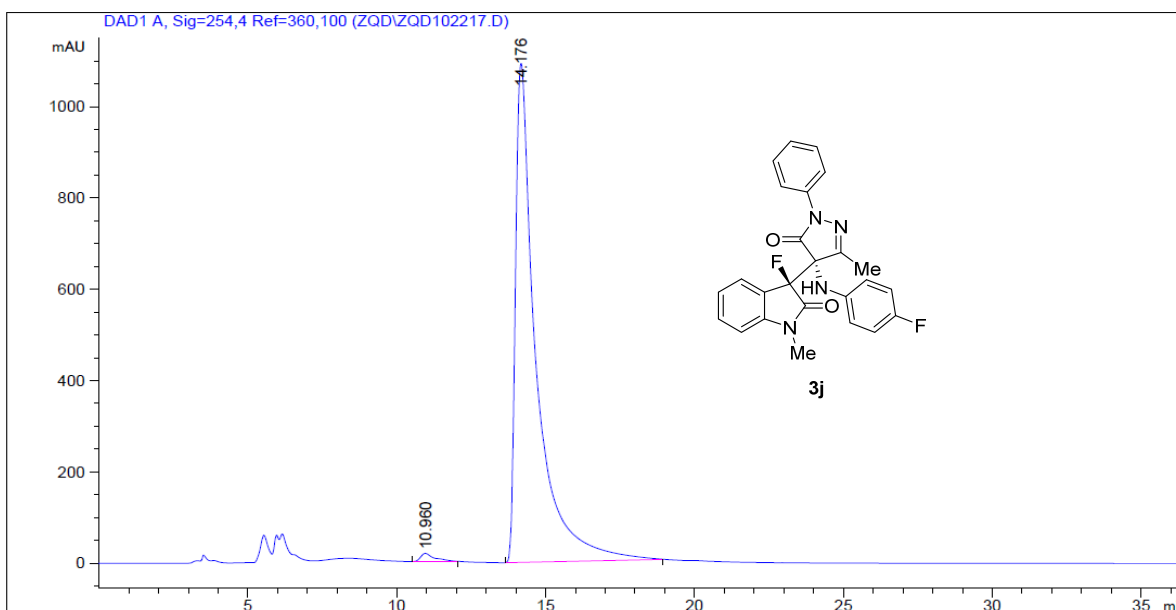
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.844	BV	0.3833	3.03734e4	1268.94324	47.6205
2	8.739	VB	0.4198	3.13241e4	1157.21655	49.1110
3	13.441	BV	0.5981	1060.04395	26.64782	1.6620
4	14.969	VB	0.6251	1024.67969	24.95120	1.6065



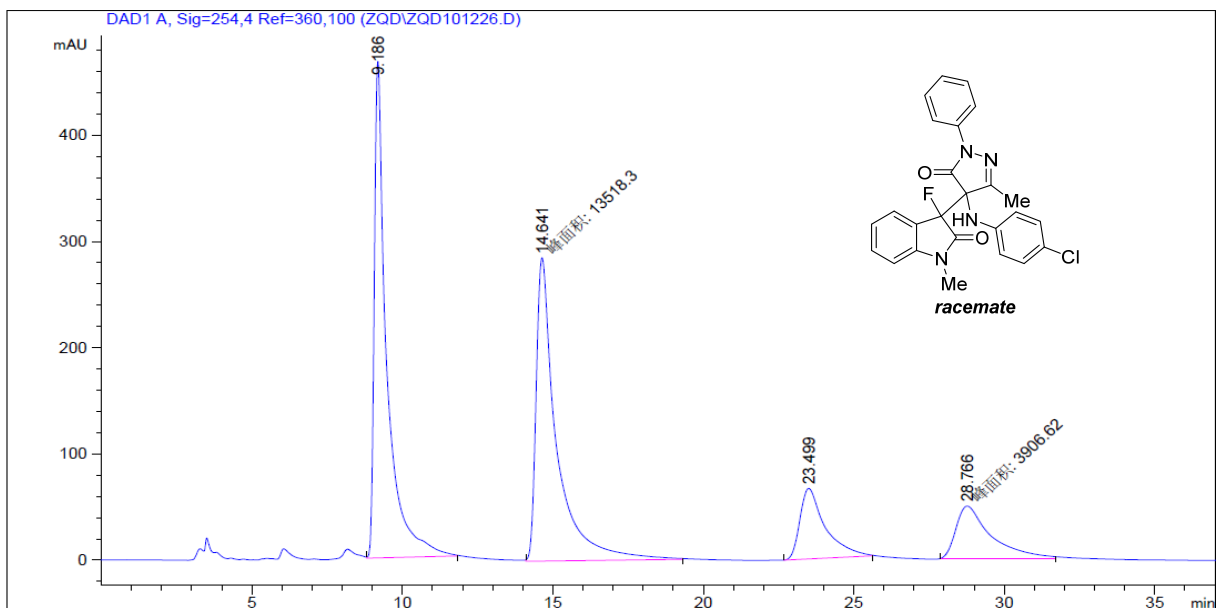
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.845	BV	0.2223	2.71564e4	1839.10437	99.5643
2	9.012	VB	0.2779	118.84081	6.08492	0.4357



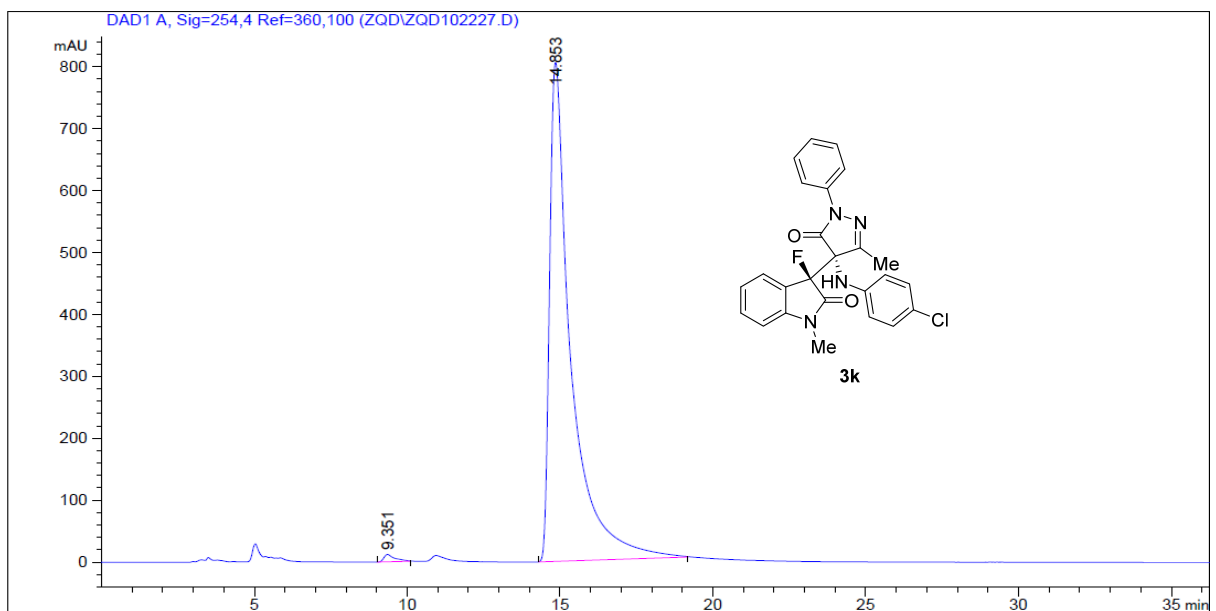
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.652	BB	0.4568	3887.01978	119.08190	50.3764
2	13.976	MM	0.7013	3828.93872	90.99483	49.6236



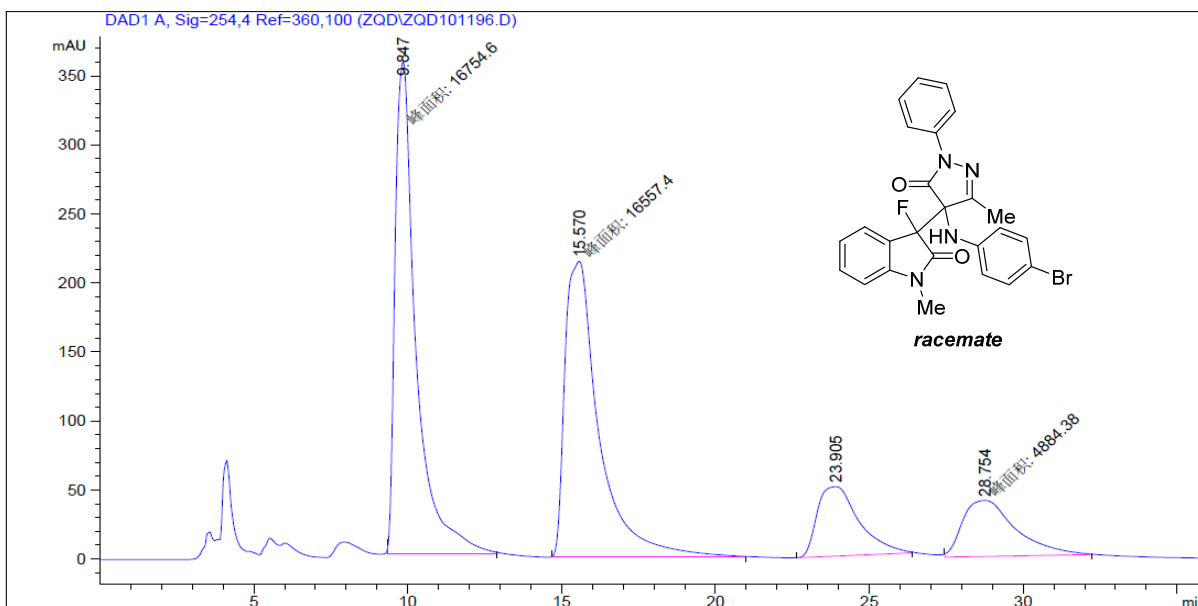
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.960	BB	0.4705	606.92633	18.22639	1.1405
2	14.176	BB	0.6777	5.26074e4	1092.74207	98.8595



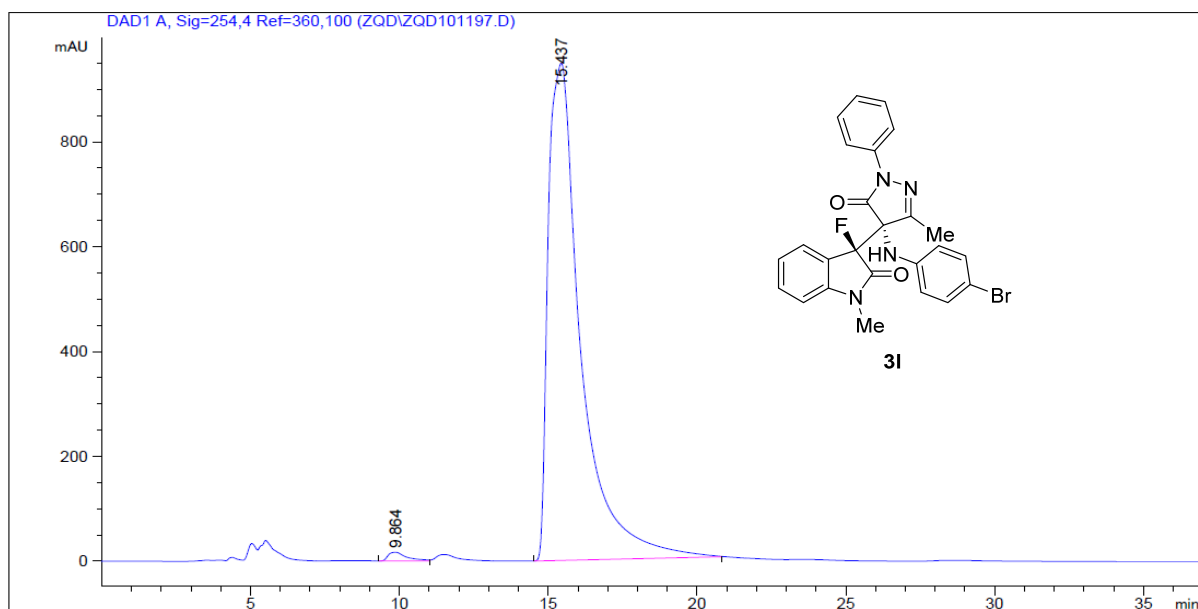
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.186	VB	0.4014	1.35247e4	467.61603	38.8308
2	14.641	MM	0.7888	1.35183e4	285.63370	38.8124
3	23.499	BB	0.8432	3880.23950	66.45439	11.1406
4	28.766	MM	1.3282	3906.62183	49.02090	11.2163



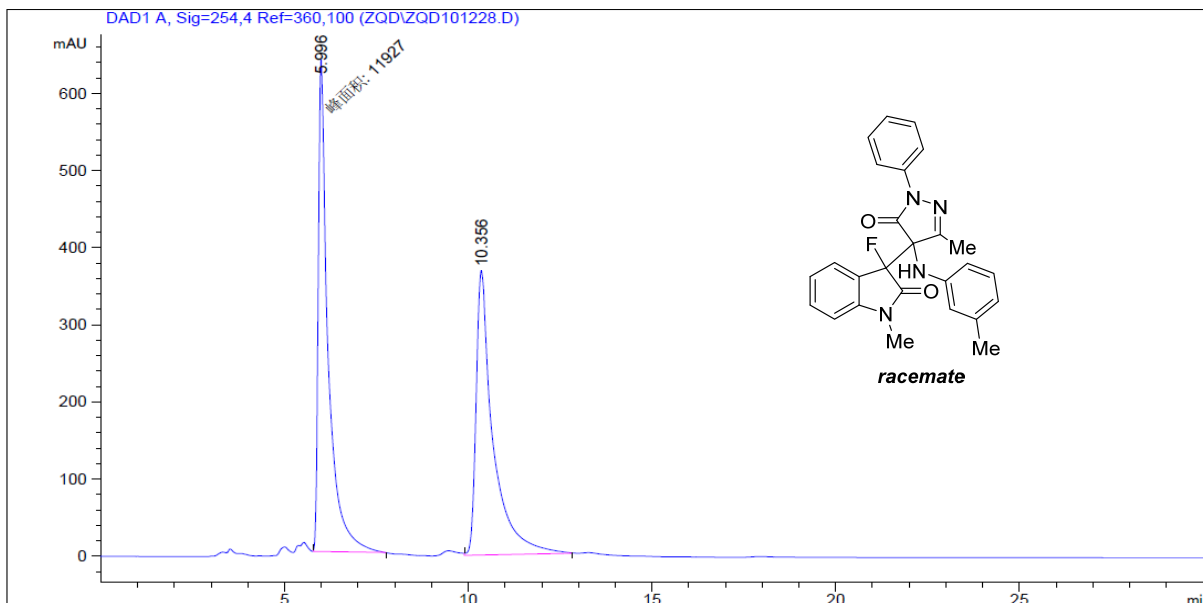
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.351	BB	0.3541	302.01068	11.97911	0.7624
2	14.853	BB	0.6911	3.93110e4	805.87976	99.2376



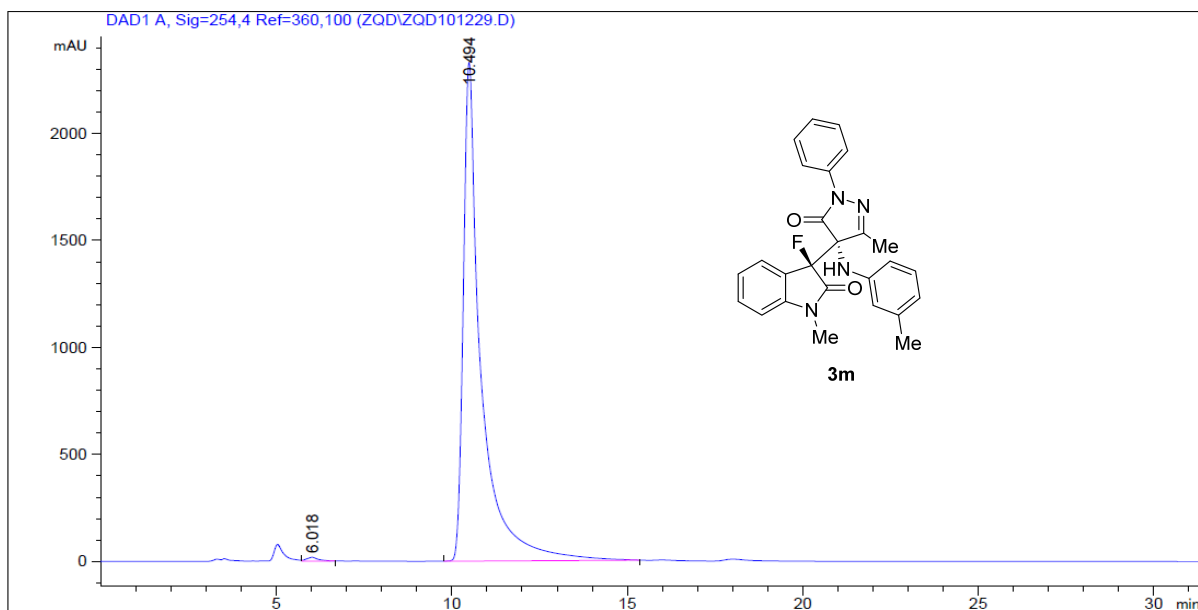
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.847	MM	0.7844	1.67546e4	355.98157	39.0125
2	15.570	MM	1.2875	1.65574e4	214.32971	38.5533
3	23.905	BB	1.2264	4750.44971	50.36625	11.0612
4	28.754	MM	2.0052	4884.37939	40.59732	11.3731



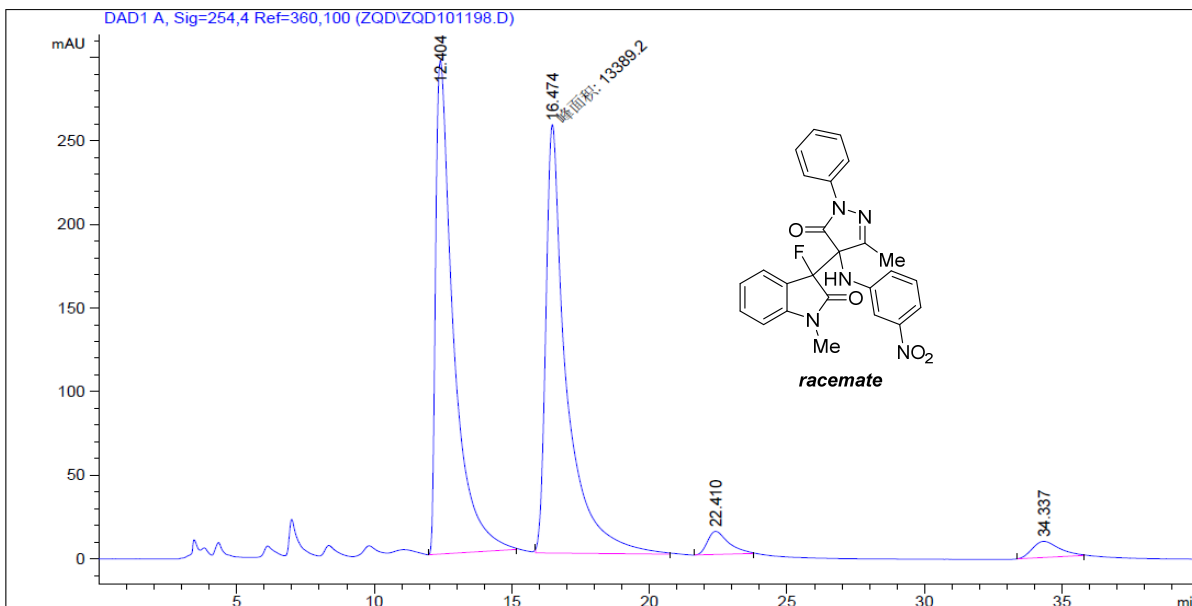
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.864	BB	0.6421	716.93677	16.52725	0.9795
2	15.437	BB	1.1414	7.24741e4	948.50500	99.0205



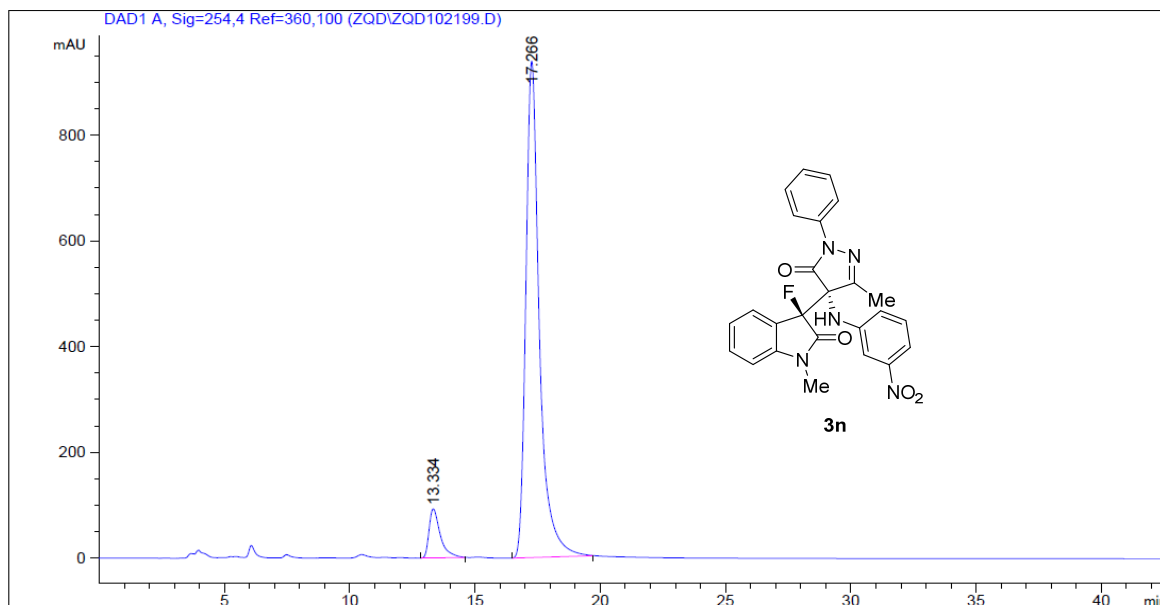
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.996	MM	0.3116	1.19270e4	637.84229	50.2761
2	10.356	VB	0.4449	1.17960e4	369.07785	49.7239



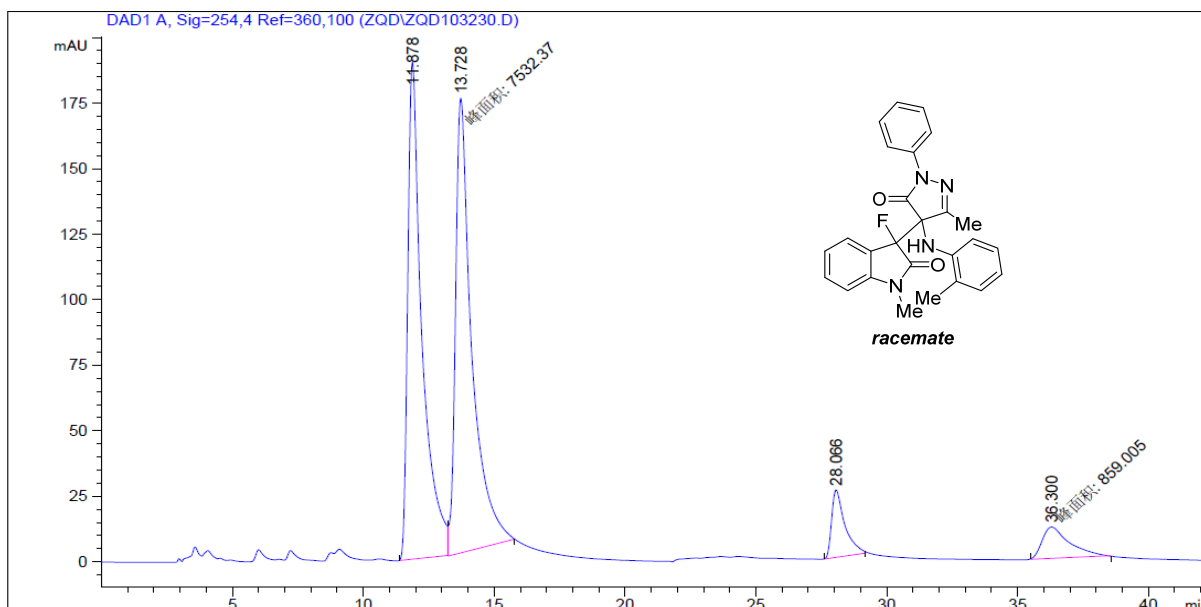
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.018	VB	0.3113	419.89084	18.46594	0.5052
2	10.494	BB	0.4899	8.26909e4	2330.98950	99.4948



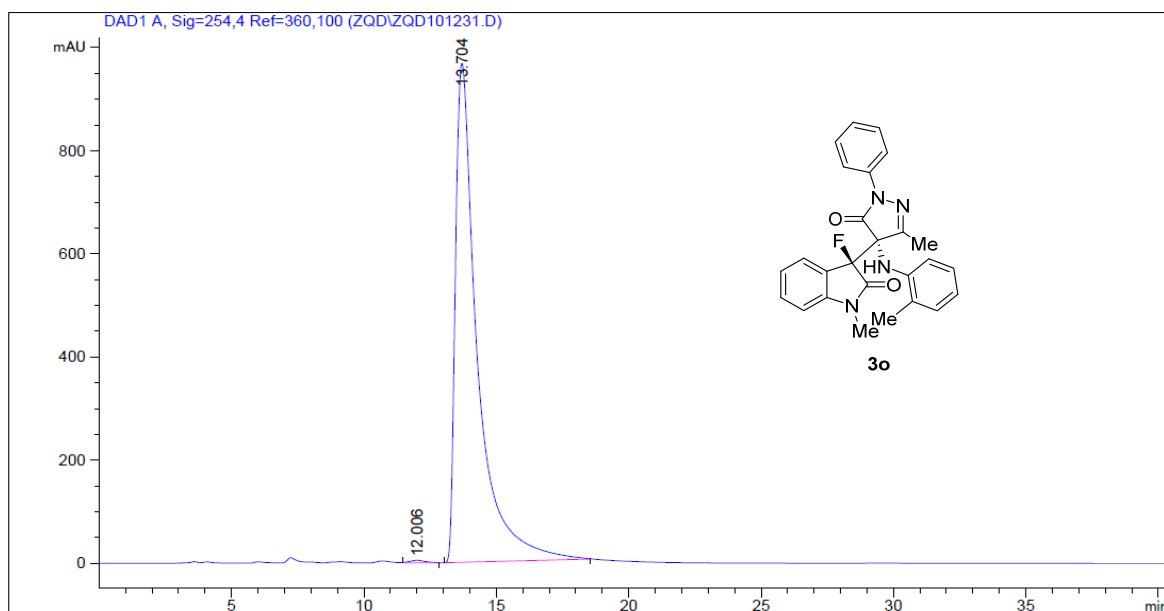
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.404	BB	0.6521	1.33200e4	295.37213	47.3851
2	16.474	MM	0.8707	1.33892e4	256.29105	47.6314
3	22.410	BB	0.7689	741.49408	13.84439	2.6378
4	34.337	BB	0.8455	659.37006	9.67033	2.3457



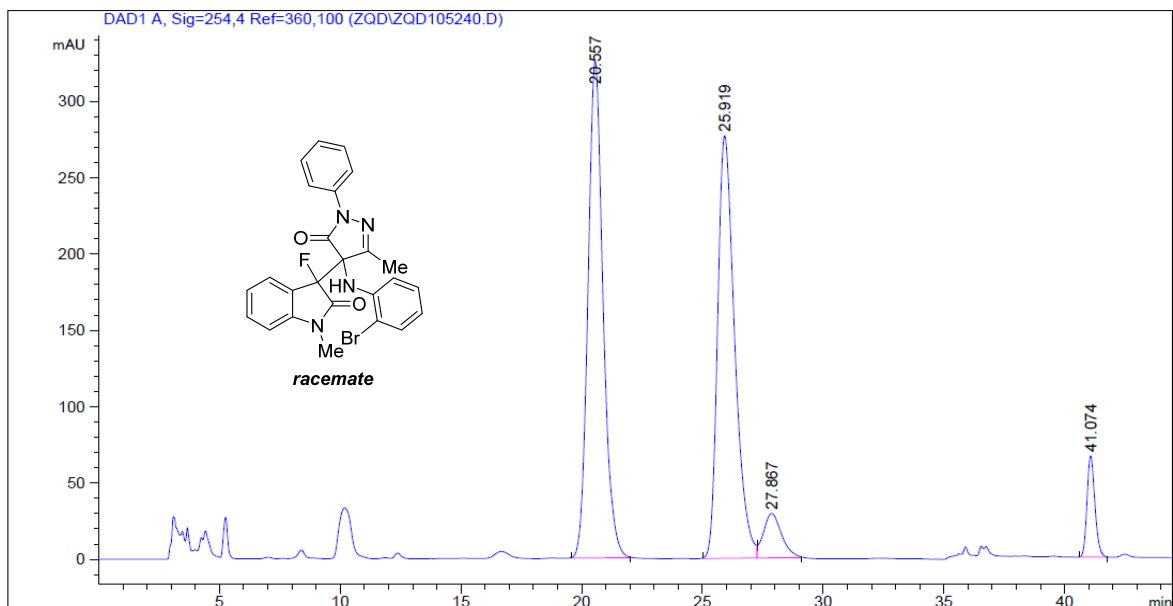
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.334	BB	0.4674	2896.23560	92.98054	7.5842
2	17.266	BB	0.5624	3.52918e4	939.15857	92.4158



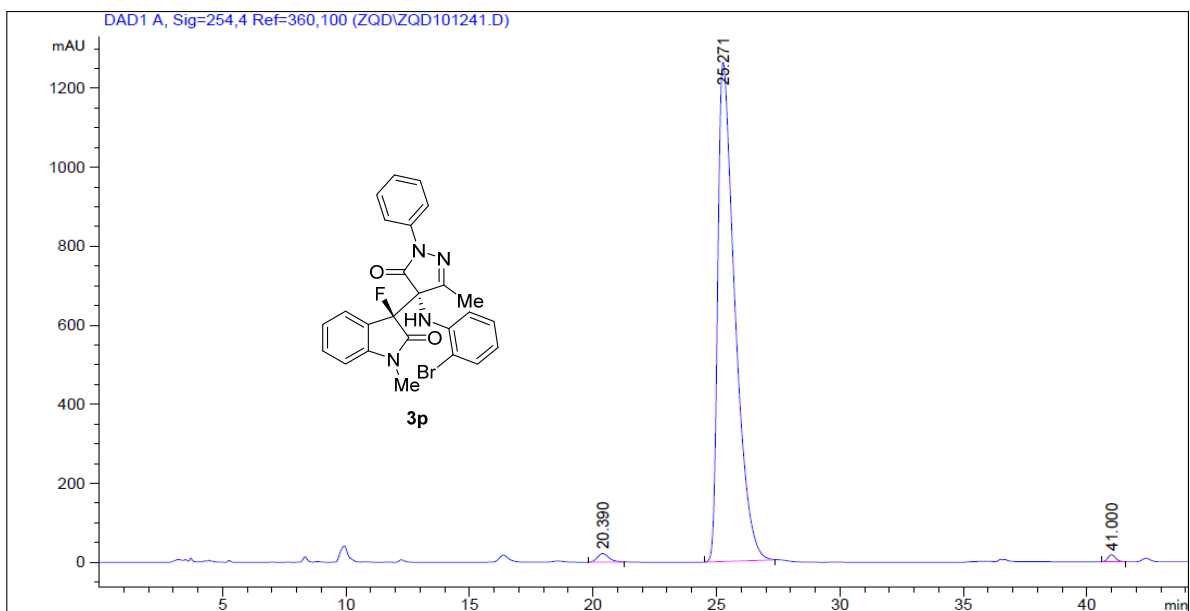
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.878	BV	0.5458	7211.27637	189.57137	43.6915
2	13.728	MM	0.7236	7532.36816	173.49495	45.6370
3	28.066	BB	0.5129	902.32495	25.74213	5.4670
4	36.300	MM	1.1983	859.00519	11.94770	5.2045



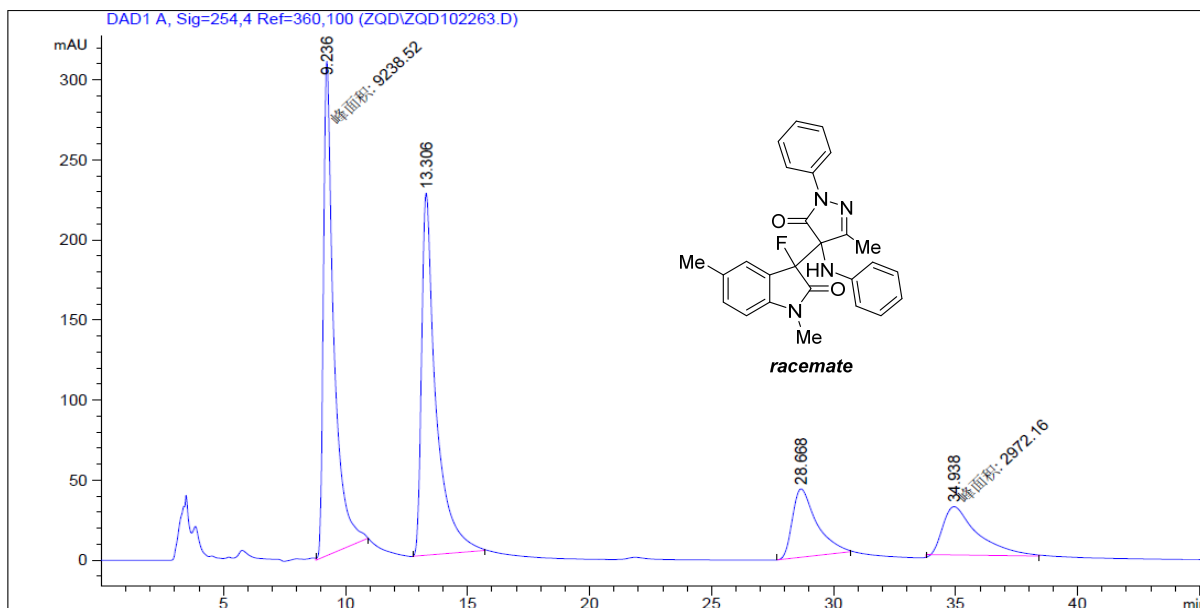
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.006	BB	0.5380	194.39804	4.88788	0.3486
2	13.704	BB	0.8361	5.55787e4	967.71069	99.6514



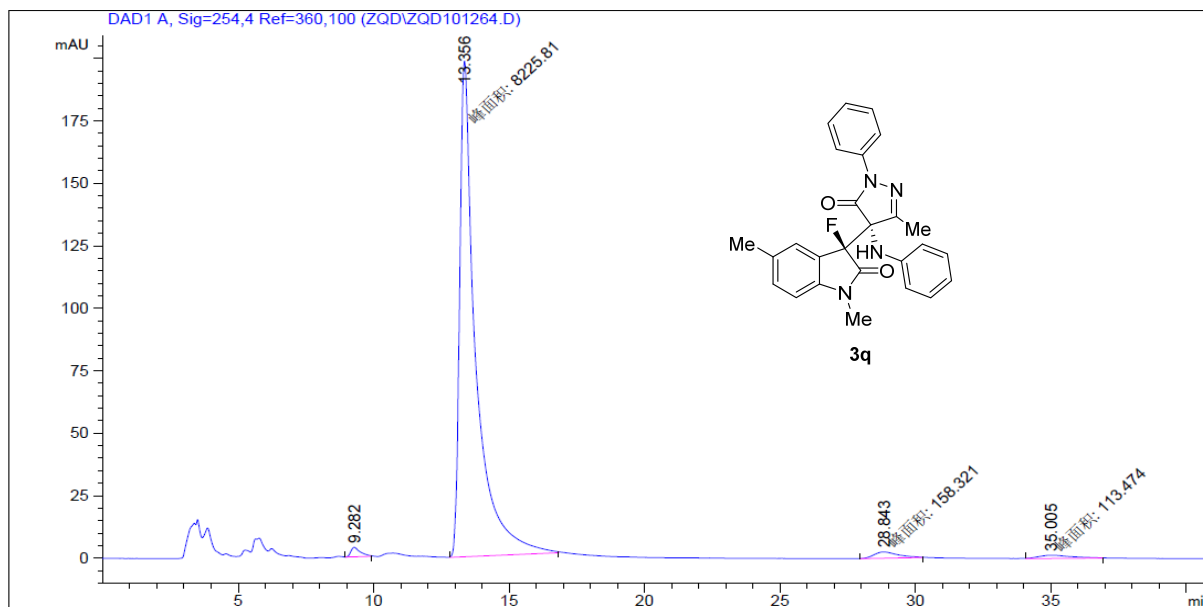
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.557	BB	0.6621	1.41142e4	325.36551	45.9671
2	25.919	BB	0.7459	1.35676e4	276.79010	44.1869
3	27.867	BB	0.7837	1520.21301	29.08757	4.9510
4	41.074	BB	0.3480	1503.03674	66.42085	4.8951



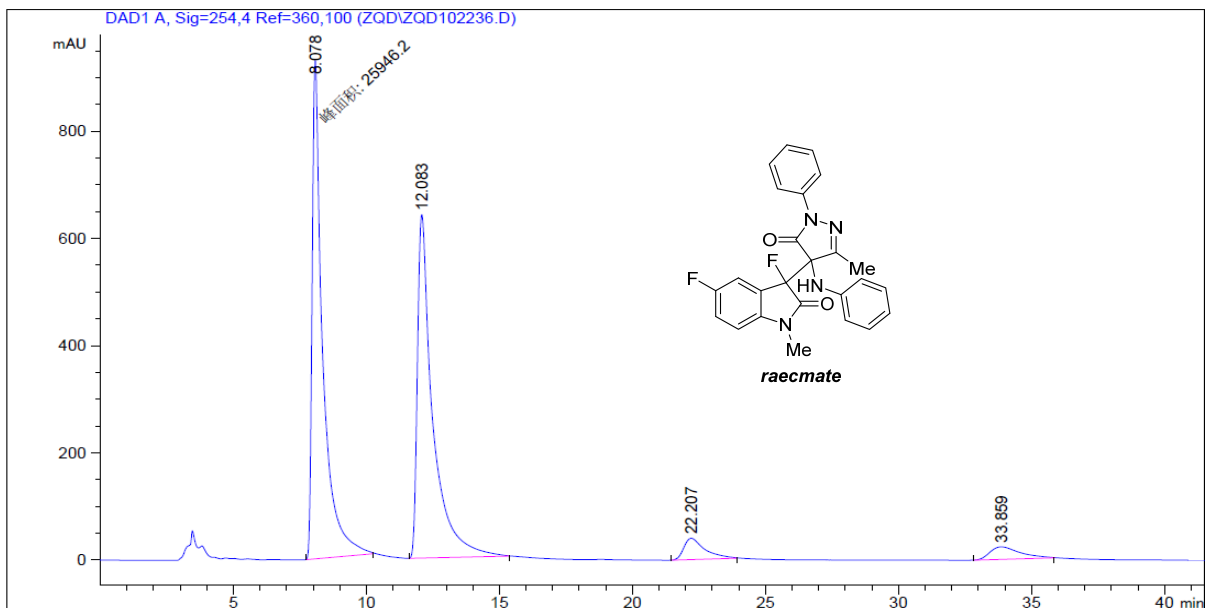
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.390	BB	0.4981	720.13251	21.87251	1.1621
2	25.271	BB	0.7181	6.08550e4	1263.13513	98.2070
3	41.000	BB	0.3360	390.90961	17.95379	0.6308



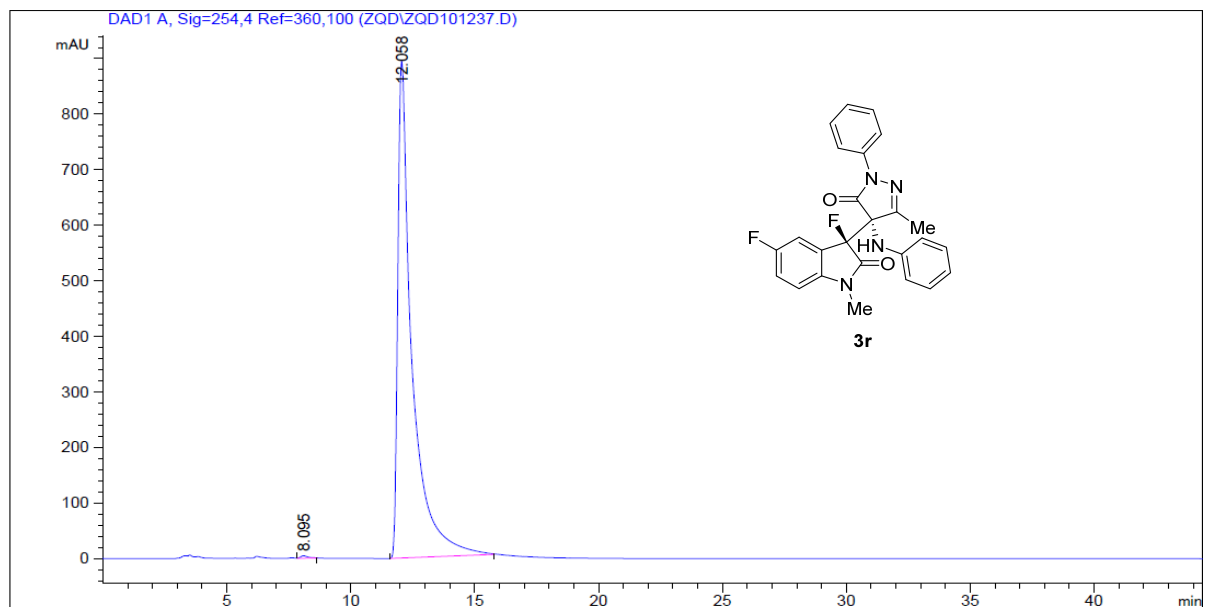
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.236	MM	0.4989	9238.51660	308.62634	37.8803
2	13.306	BB	0.5806	9237.08398	226.13391	37.8745
3	28.688	BB	0.9952	2940.92456	42.71903	12.0586
4	34.938	MM	1.6443	2972.15747	30.12531	12.1866



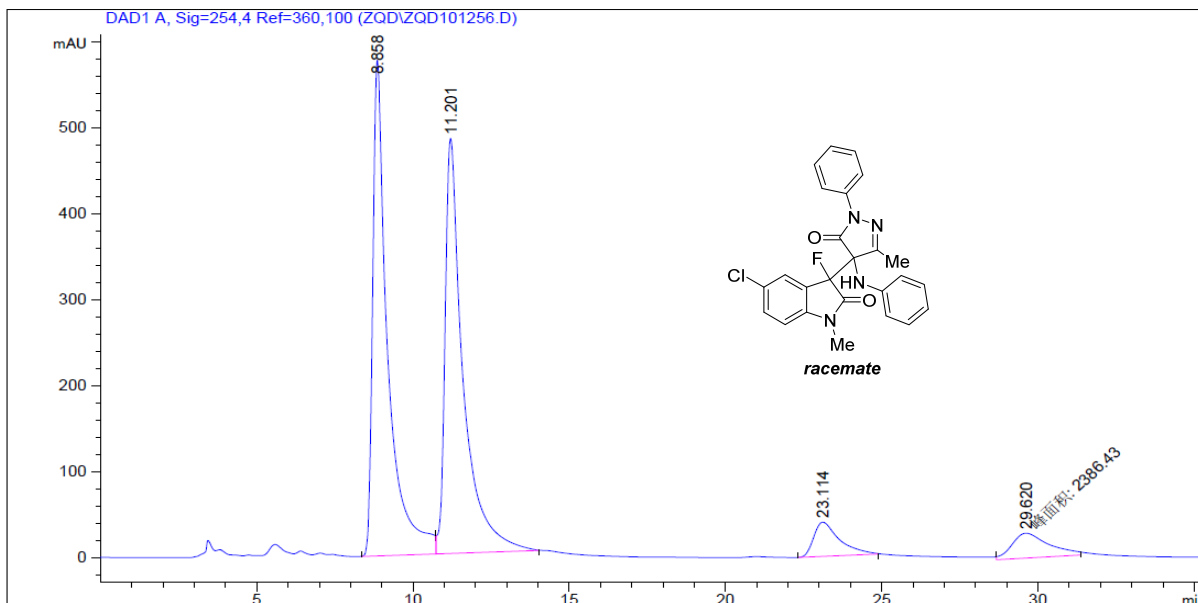
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.282	BB	0.3463	92.07326	3.77869	1.0719
2	13.356	MM	0.6912	8225.80957	198.35567	95.7639
3	28.843	MM	1.0388	158.32072	2.54024	1.8432
4	35.005	MM	1.4511	113.47414	1.30327	1.3211



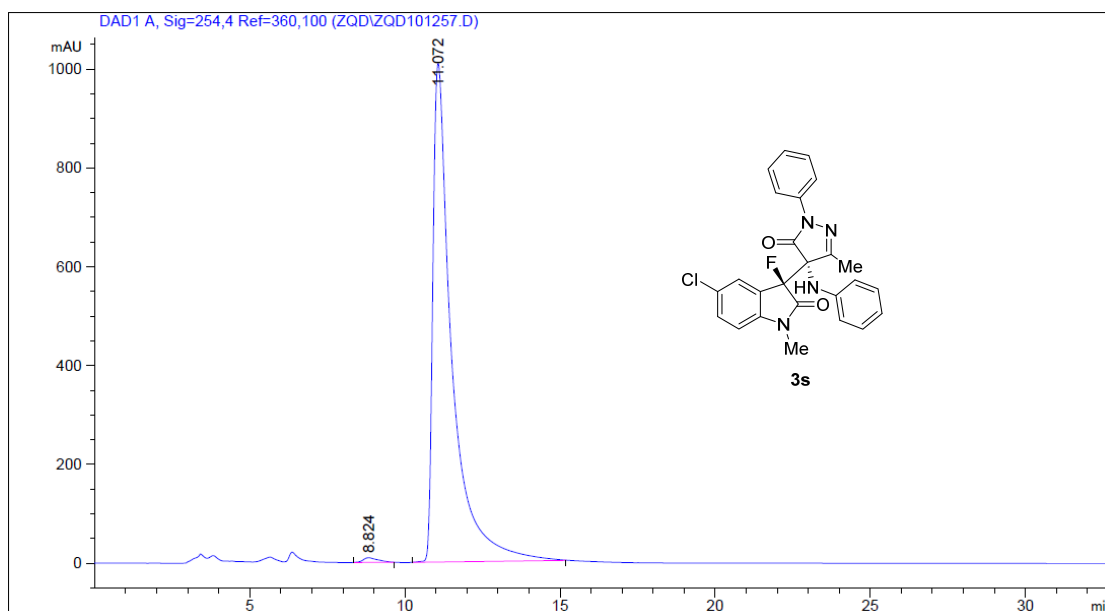
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.078	MM	0.4646	2.59462e4	930.67548	46.6451
2	12.083	BB	0.5627	2.56467e4	641.13300	46.1065
3	22.207	BB	0.7947	2184.98560	39.91110	3.9281
4	33.859	BB	1.1127	1846.95117	23.35297	3.3204



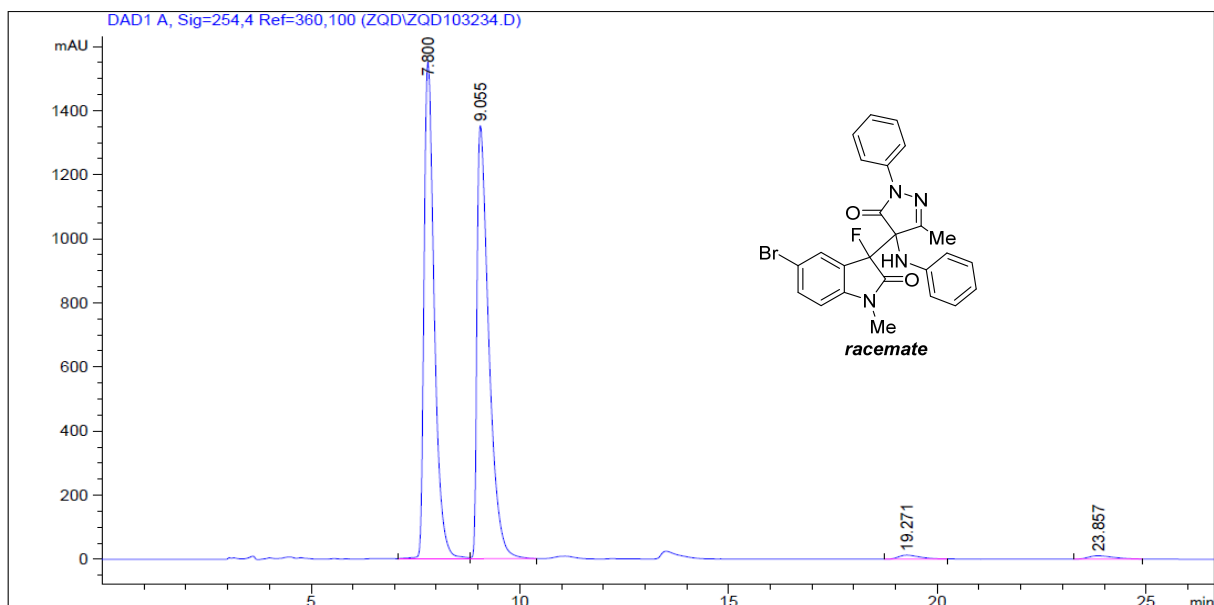
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.095	BB	0.3105	97.19876	4.49139	0.2714
2	12.058	BB	0.5599	3.57206e4	894.49554	99.7286



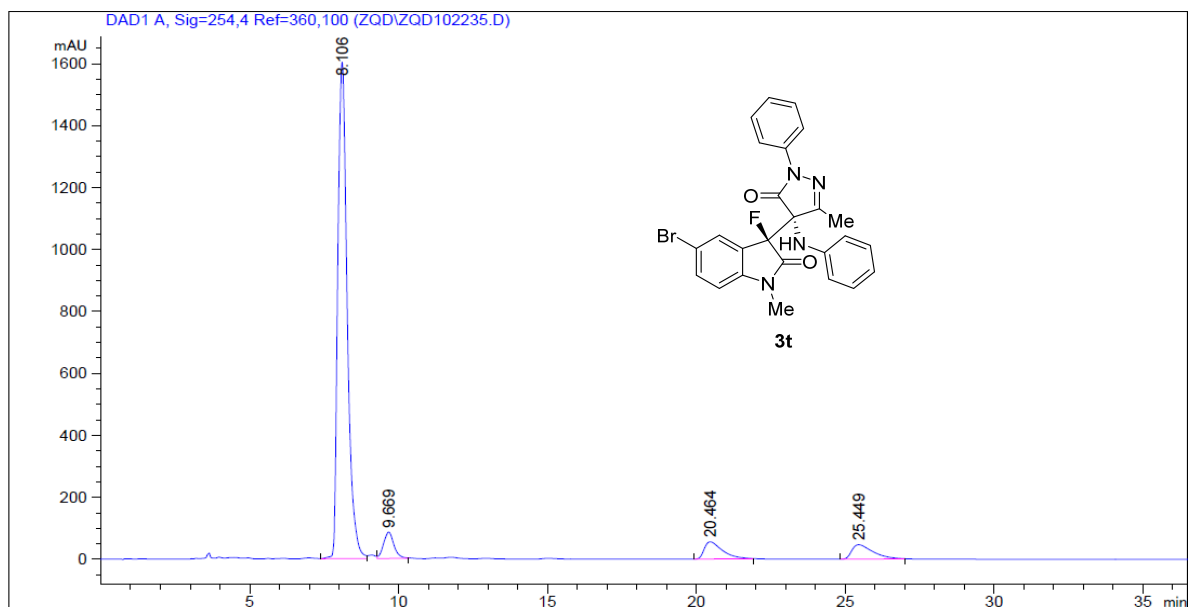
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.858	BV	0.4699	1.93798e4	576.99146	44.5575
2	11.201	VB	0.5694	1.94331e4	482.95026	44.6800
3	23.114	BB	0.8403	2294.59033	39.93878	5.2757
4	29.620	MM	1.3743	2386.43188	28.94032	5.4868



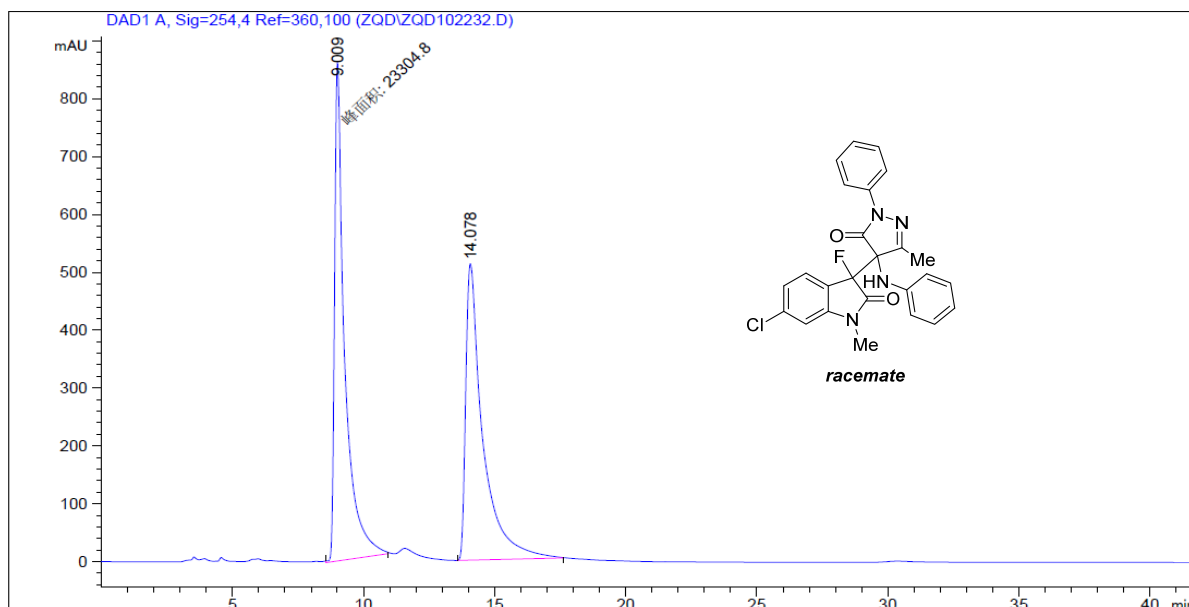
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.824	BB	0.4721	322.96133	9.65921	0.7474
2	11.072	BB	0.6056	4.28855e4	1009.59741	99.2526



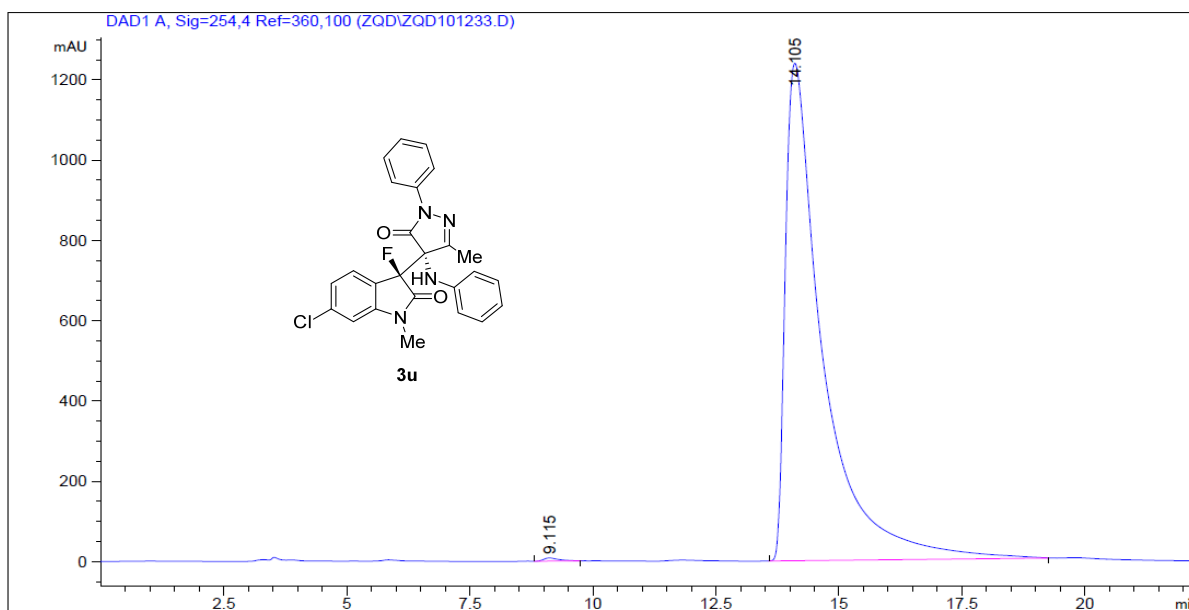
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.800	BV	0.2637	2.65402e4	1550.65125	49.1481
2	9.055	VB	0.2974	2.65760e4	1351.54614	49.2145
3	19.271	BB	0.5463	437.56903	12.32246	0.8103
4	23.857	BB	0.6314	446.65436	10.56210	0.8271



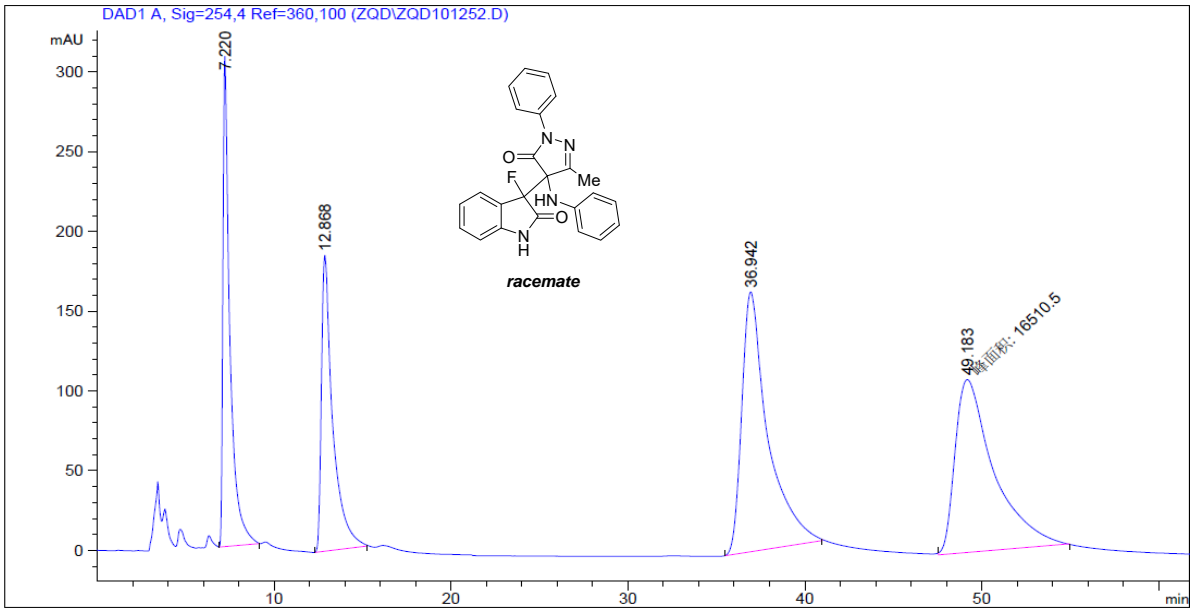
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.106	VV	0.3485	3.52454e4	1603.17969	83.9849
2	9.669	VB	0.3793	2069.67163	85.22997	4.9317
3	20.464	BB	0.6416	2363.24316	55.63307	5.6313
4	25.449	BB	0.7343	2288.02808	46.47846	5.4520



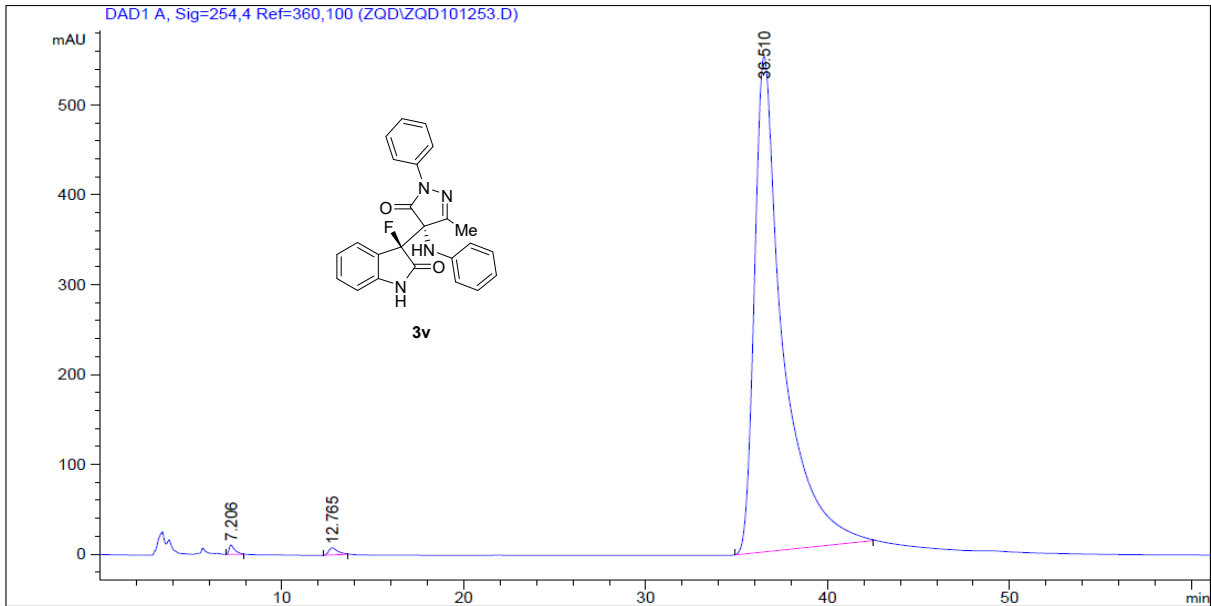
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.009	MM	0.4506	2.33048e4	862.04279	50.0705
2	14.078	BB	0.6409	2.32392e4	512.65649	49.9295



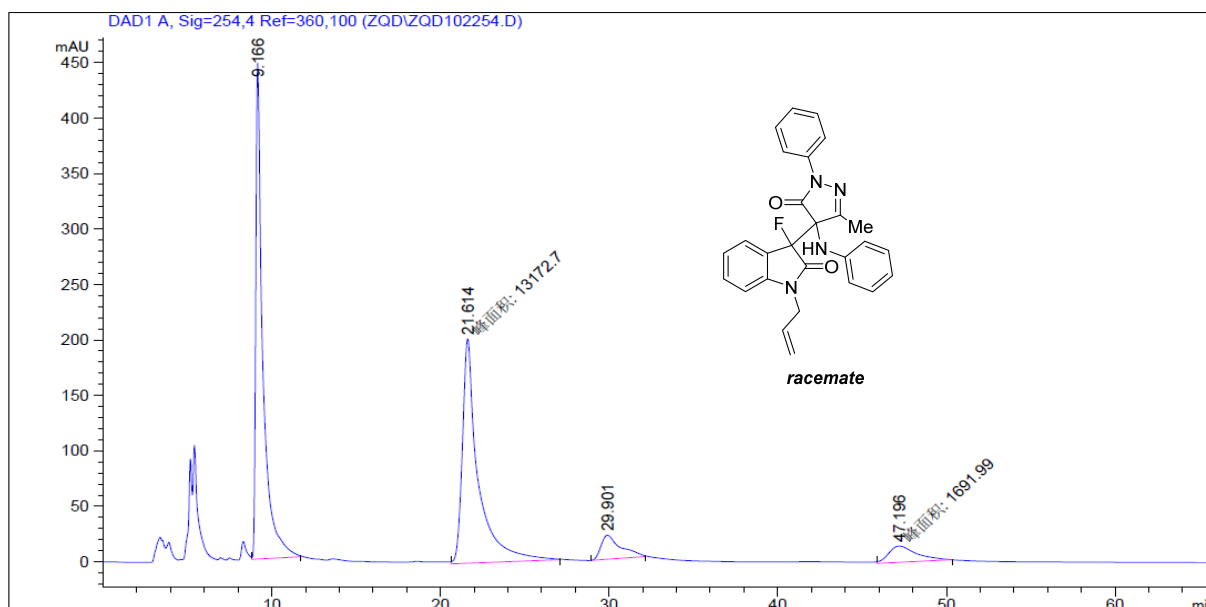
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.115	BB	0.3180	174.03249	7.93242	0.2627
2	14.105	BB	0.7620	6.60634e4	1239.10413	99.7373



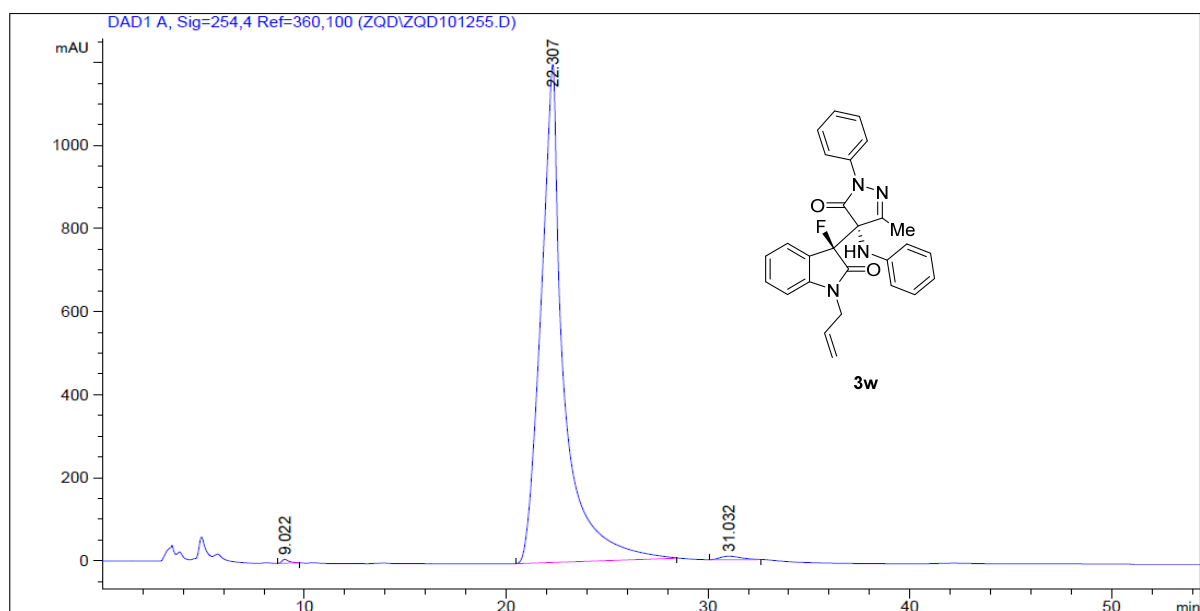
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.220	VB	0.3846	8448.24902	307.43680	16.9451
2	12.868	BB	0.6299	8236.50293	185.54865	16.5204
3	36.942	BB	1.4535	1.66613e4	162.86472	33.4185
4	49.183	MM	2.5391	1.65105e4	108.37518	33.1160



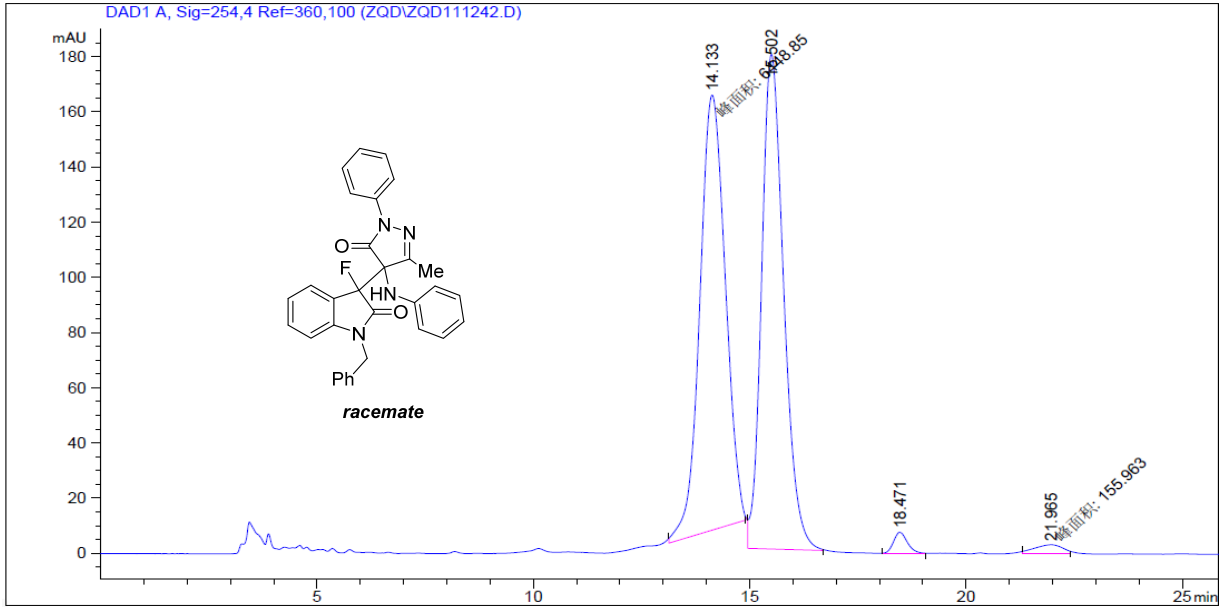
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.206	BB	0.3127	230.23994	10.54505	0.3795
2	12.765	BB	0.5052	276.29623	7.95599	0.4554
3	36.510	BB	1.5383	6.01635e4	551.69360	99.1651



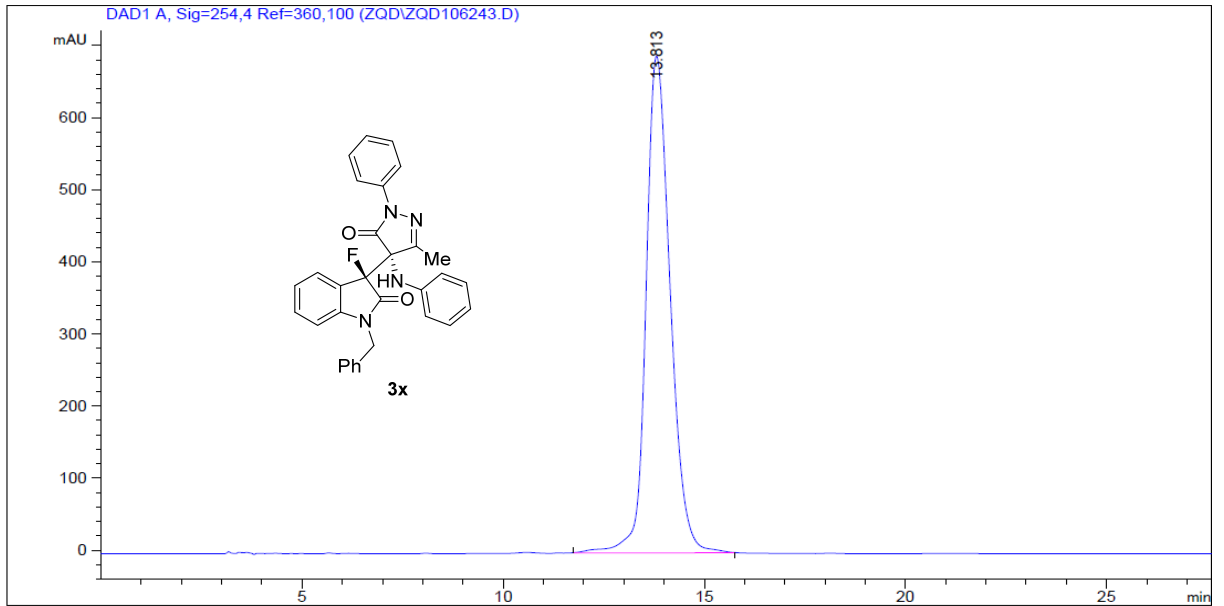
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.166	VB	0.4080	1.30991e4	446.84305	44.0523
2	21.614	MM	1.0853	1.31727e4	202.29279	44.2998
3	29.901	BB	1.1414	1771.57434	21.67915	5.9578
4	47.196	MM	1.9238	1691.98840	14.65837	5.6901



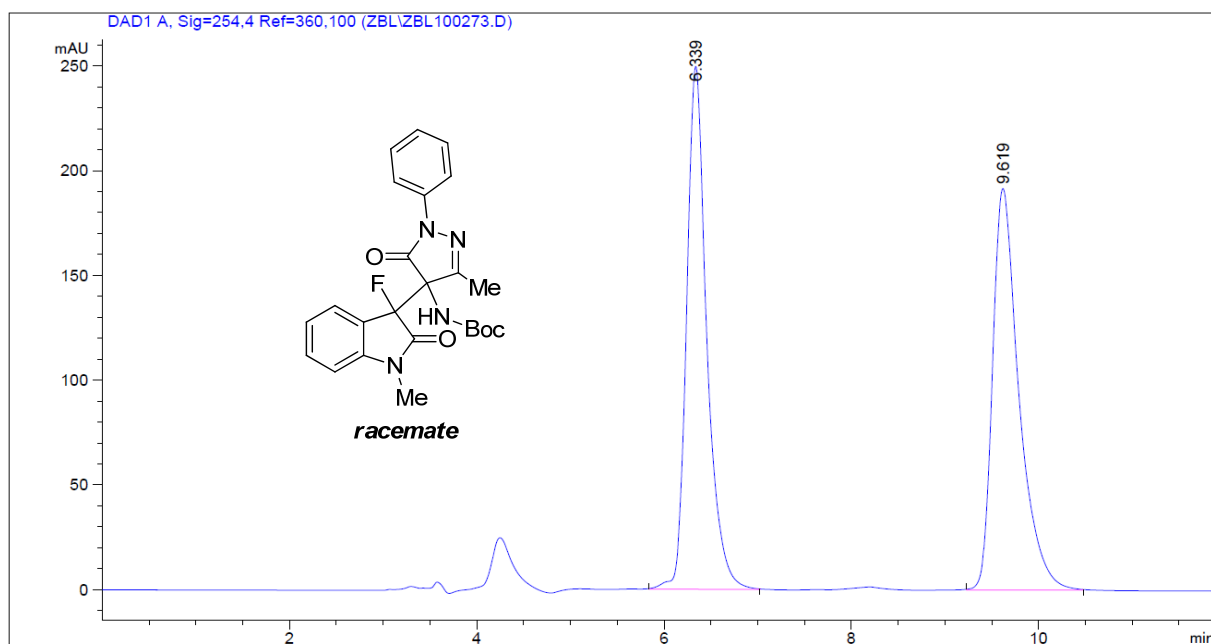
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.022	BB	0.3625	233.52469	9.51062	0.2444
2	22.307	BB	1.0430	9.46863e4	1199.36938	99.1045
3	31.032	BB	0.8682	622.03369	8.49580	0.6511



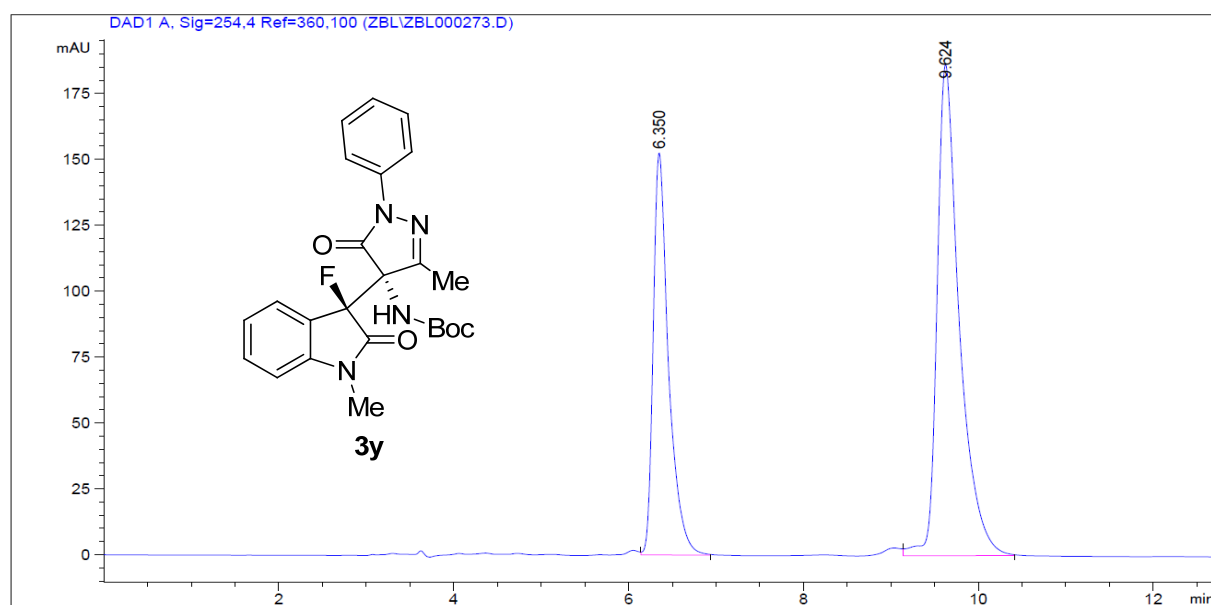
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.133	MM	0.6817	6448.85400	157.66197	49.1050
2	15.502	VB	0.5440	6360.57764	179.25342	48.4328
3	18.471	BB	0.3356	167.38147	7.64107	1.2745
4	21.965	MM	0.7643	155.96283	3.40093	1.1876



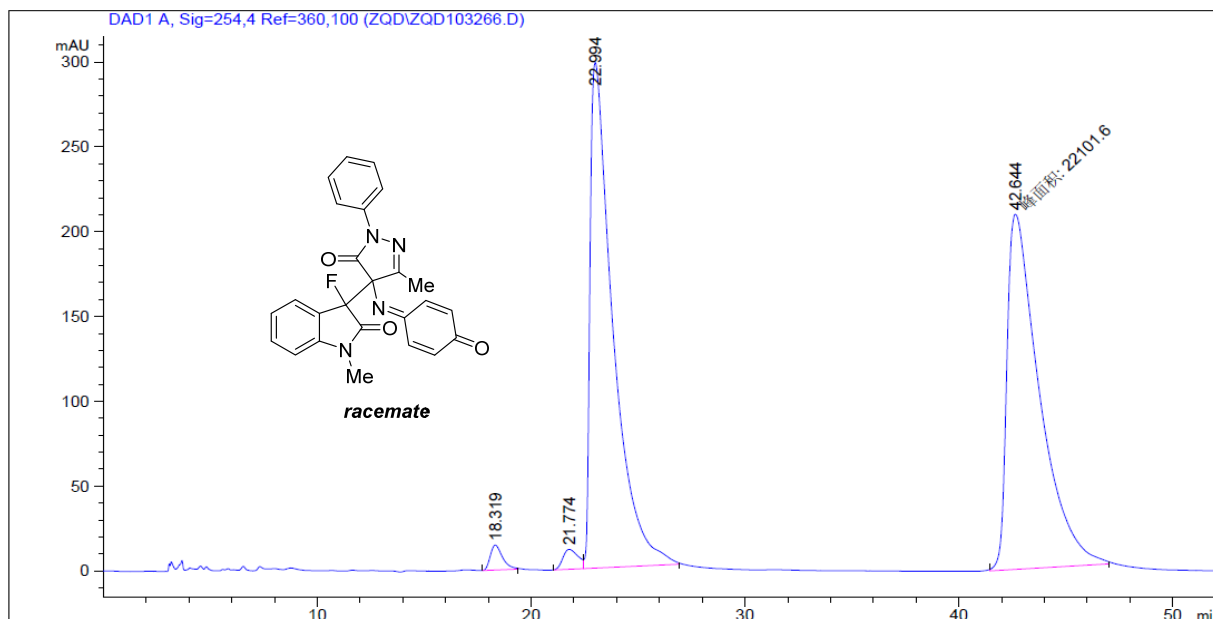
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.813	BB	0.6434	2.88967e4	688.80420	100.0000



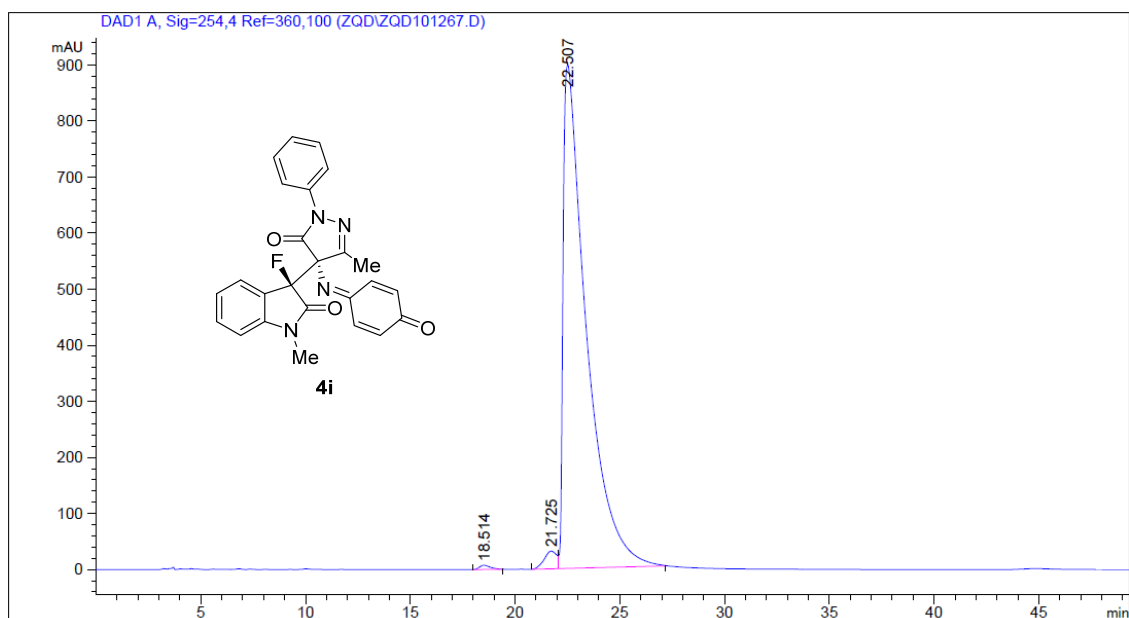
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.339	BB	0.2247	3738.05493	249.65070	49.8961
2	9.619	BB	0.2925	3753.62915	191.63785	50.1039



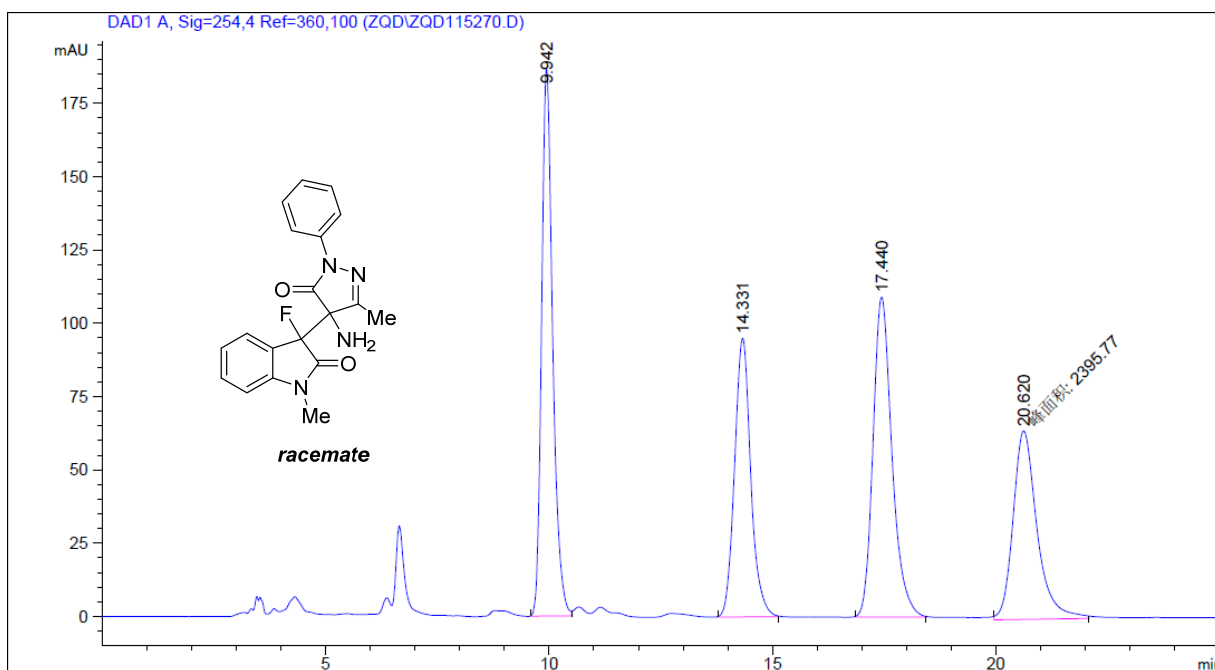
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.350	VB	0.1802	1859.23254	152.59227	36.0015
2	9.624	VB	0.2590	3305.08252	186.27971	63.9985



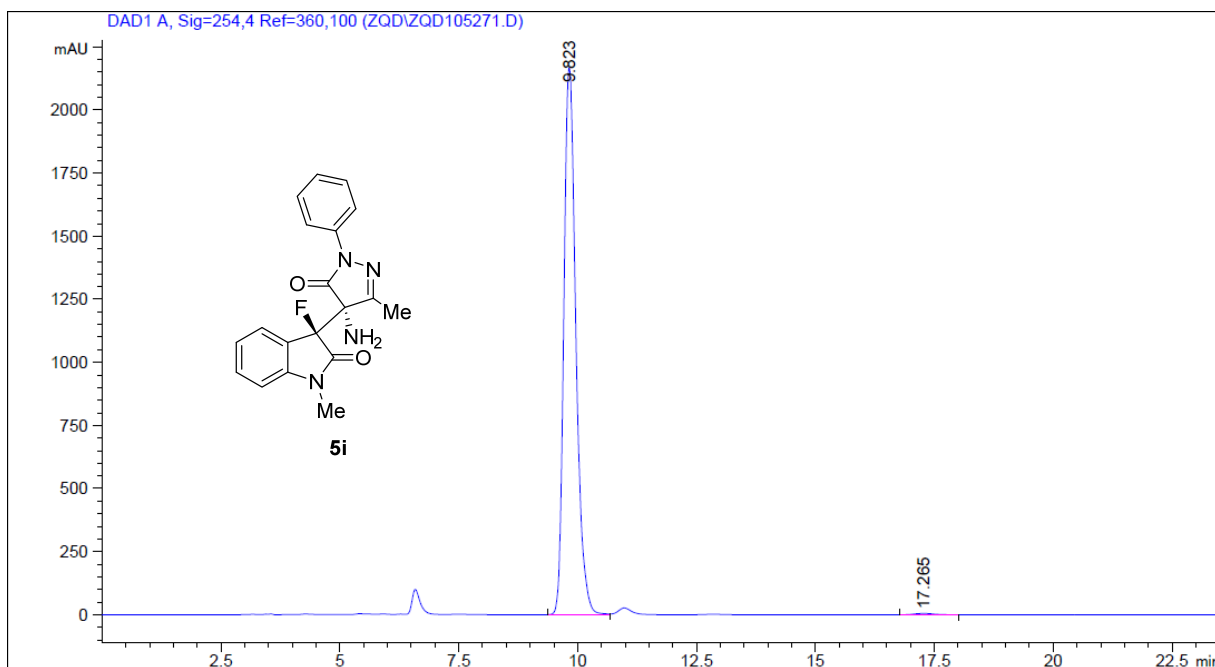
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.319	BB	0.5936	581.98480	14.70881	1.2838
2	21.774	BV	0.7228	576.01465	11.73281	1.2707
3	22.994	VB	1.0497	2.20716e4	298.13214	48.6896
4	42.644	MM	1.7590	2.21016e4	209.41531	48.7559



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.514	BB	0.5286	271.26550	7.56021	0.3844
2	21.725	BV	0.6244	1294.98901	31.44894	1.8353
3	22.507	VB	1.0887	6.89941e4	899.71576	97.7803



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.942	BV	0.2614	3224.00806	186.72260	28.7145
2	14.331	BB	0.3855	2391.47046	95.05723	21.2995
3	17.440	BB	0.4499	3216.56323	109.13490	28.6482
4	20.620	MM	0.6210	2395.76831	64.29482	21.3378



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.823	BV	0.2695	3.82099e4	2169.16821	99.6090
2	17.265	BB	0.4247	150.00024	5.32477	0.3910