

## Supplementary Material

### Diastereoselective deacylative aldol reaction of 3-acetyl-3-fluorooxindoles with aldehydes

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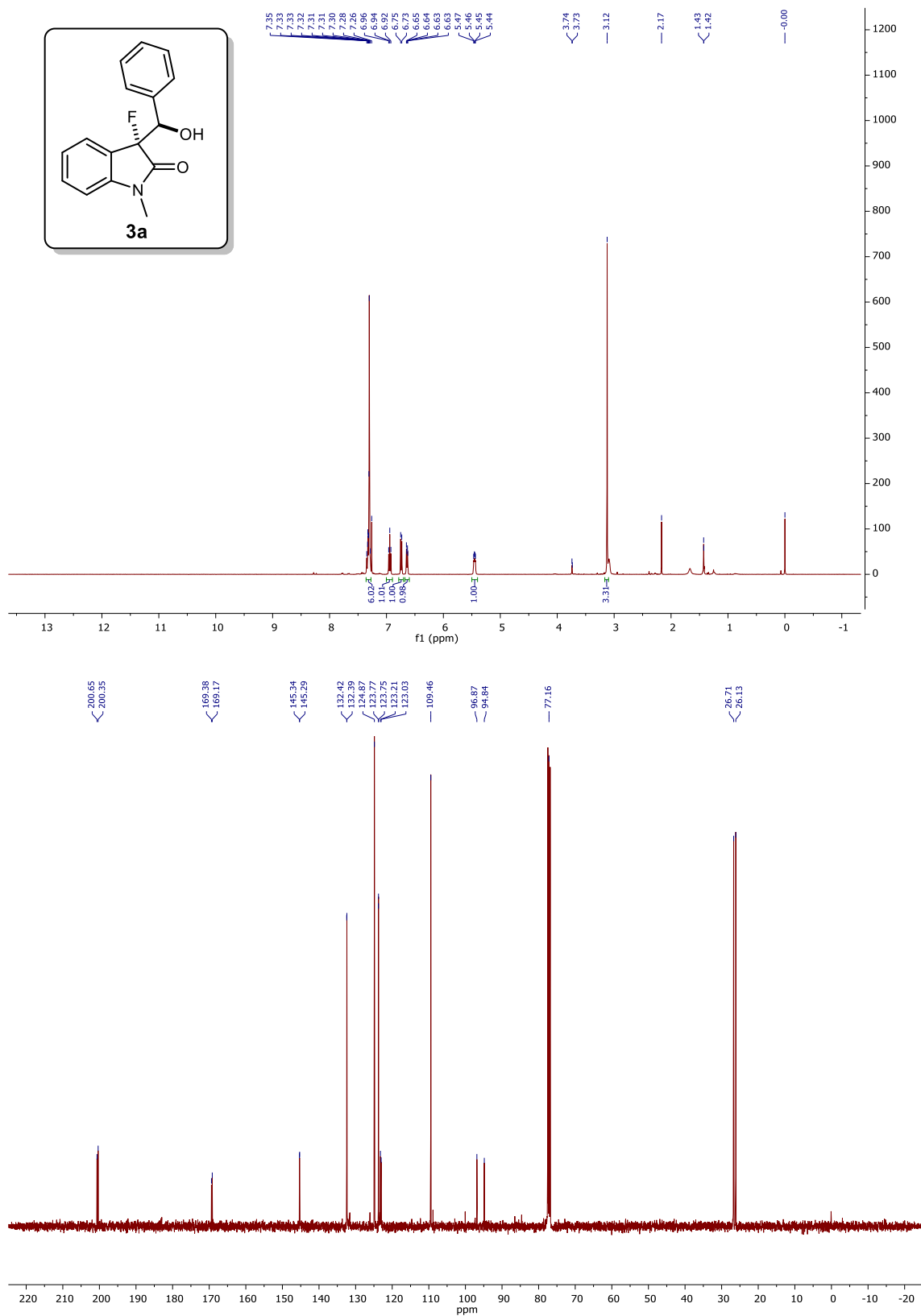
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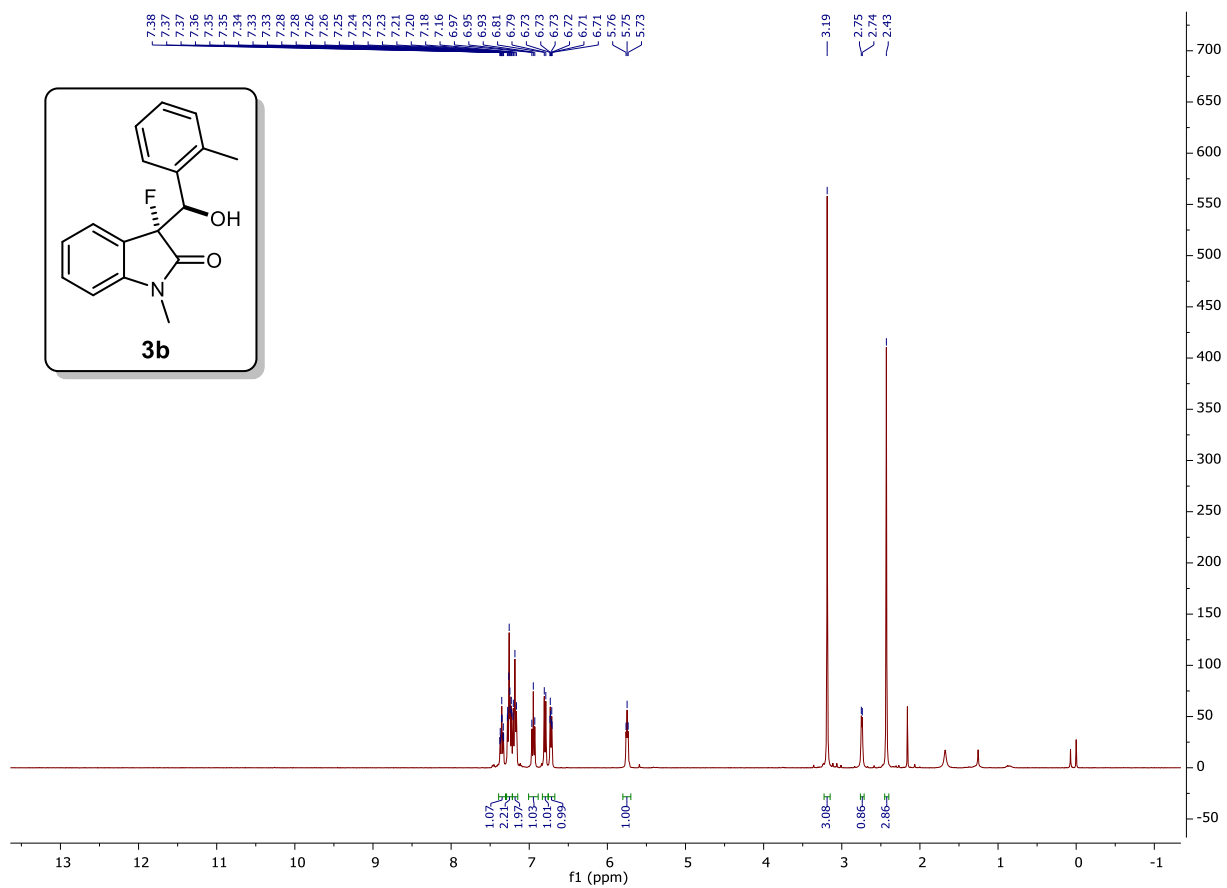
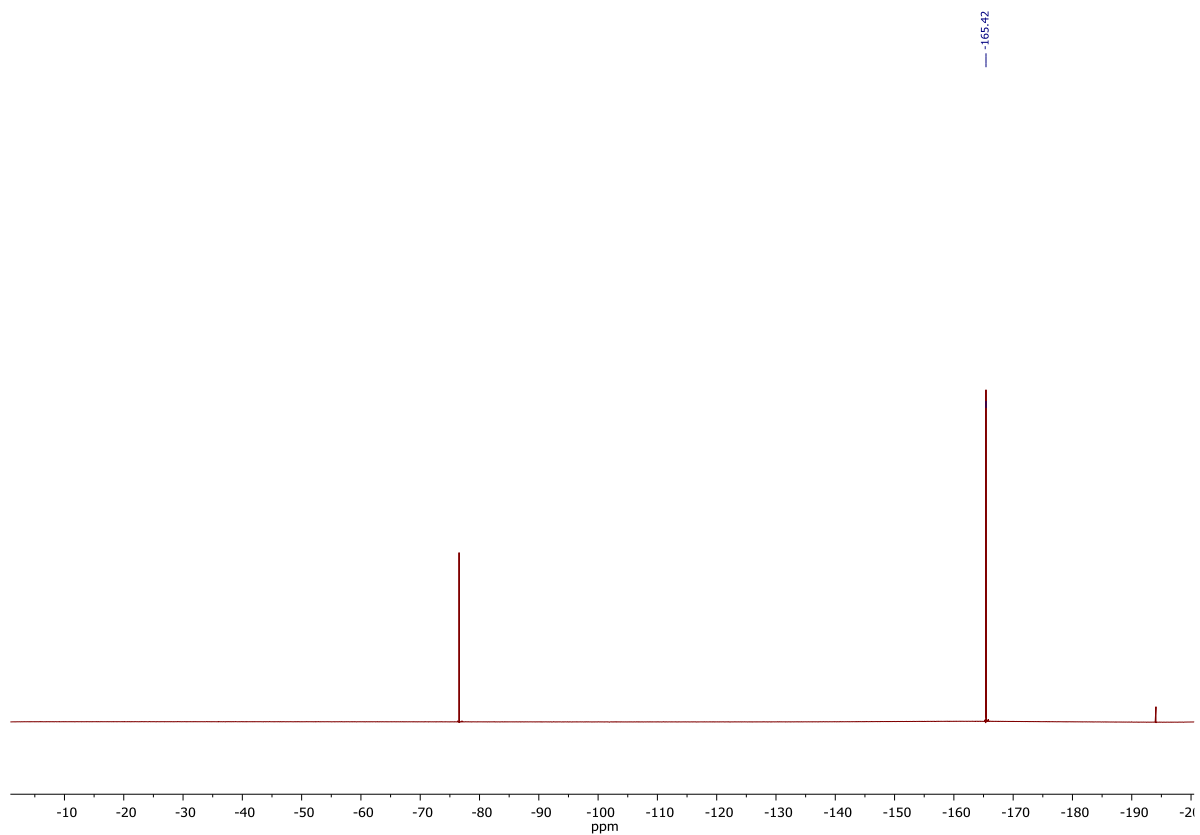
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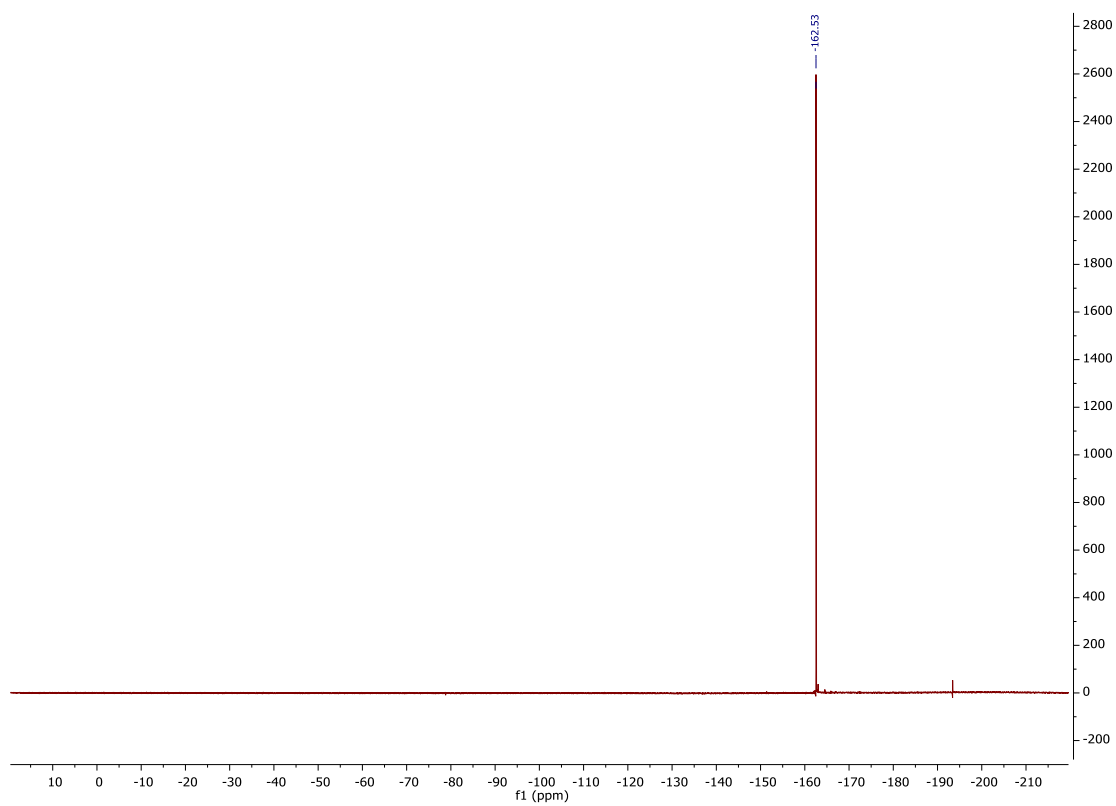
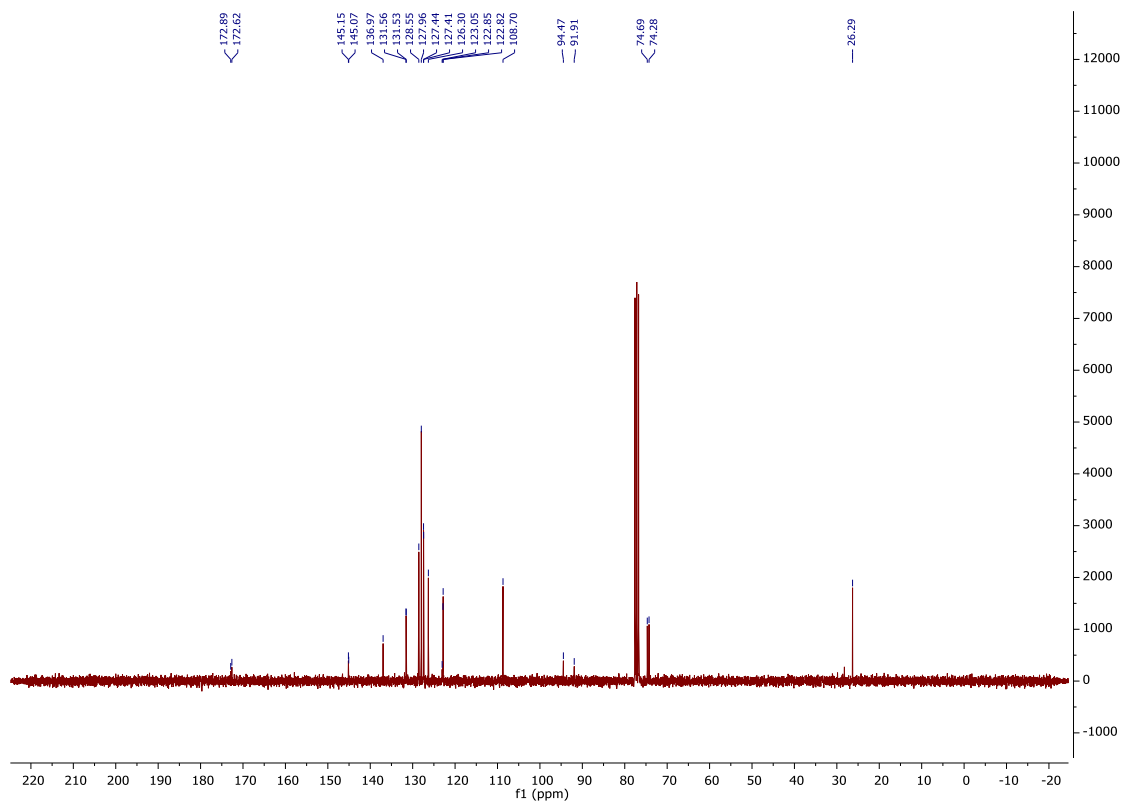
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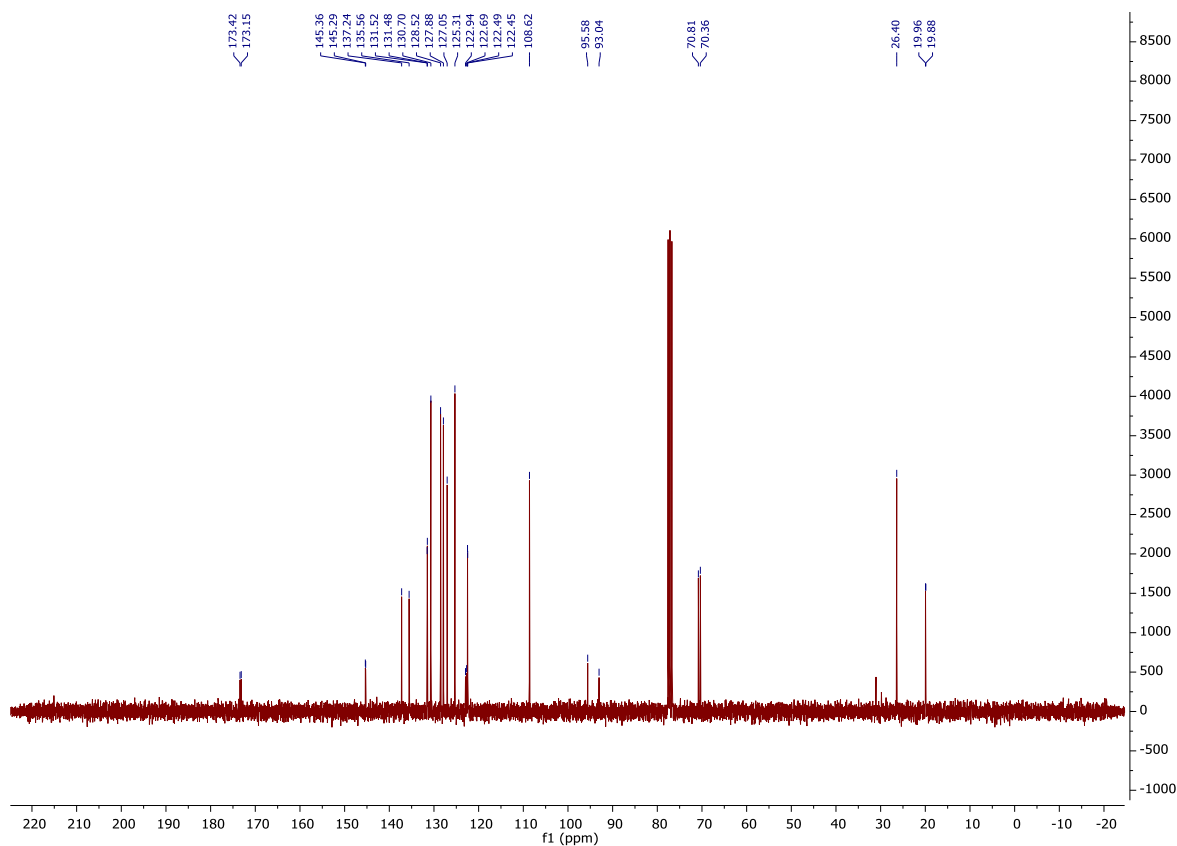
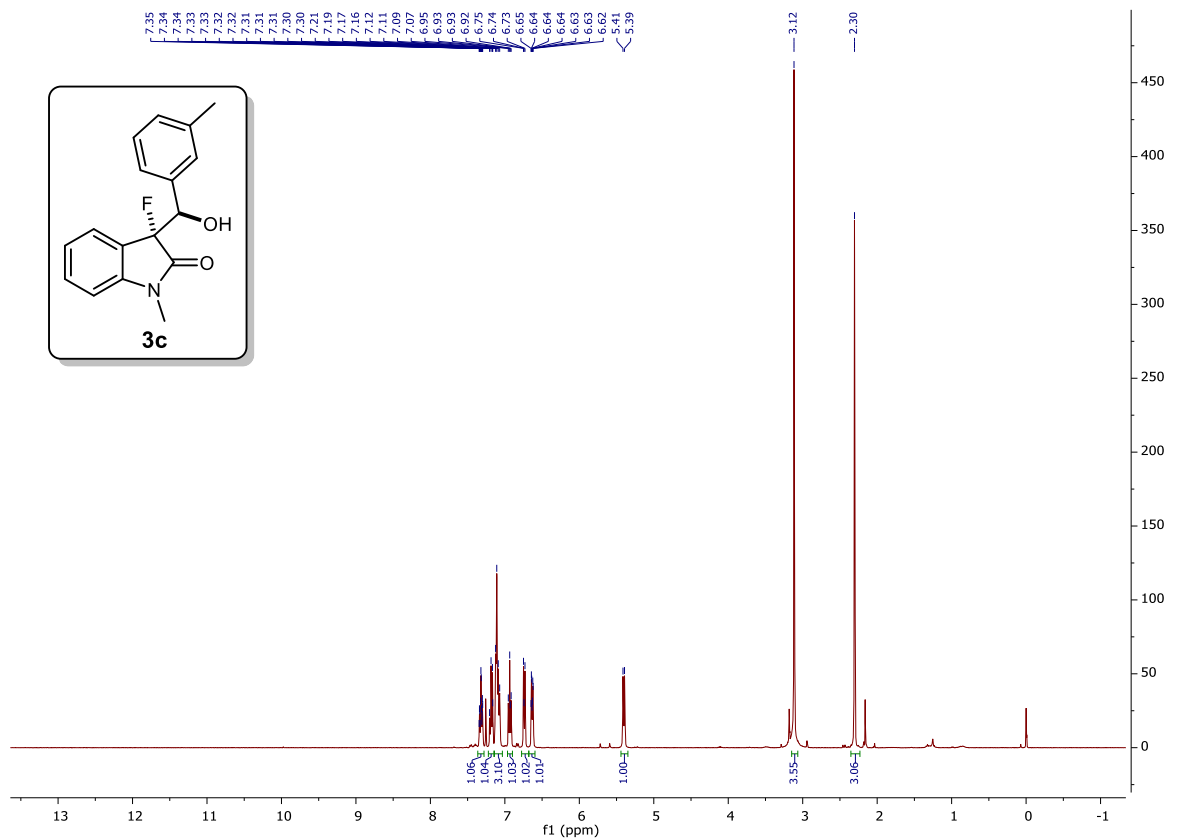
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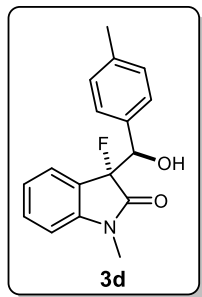
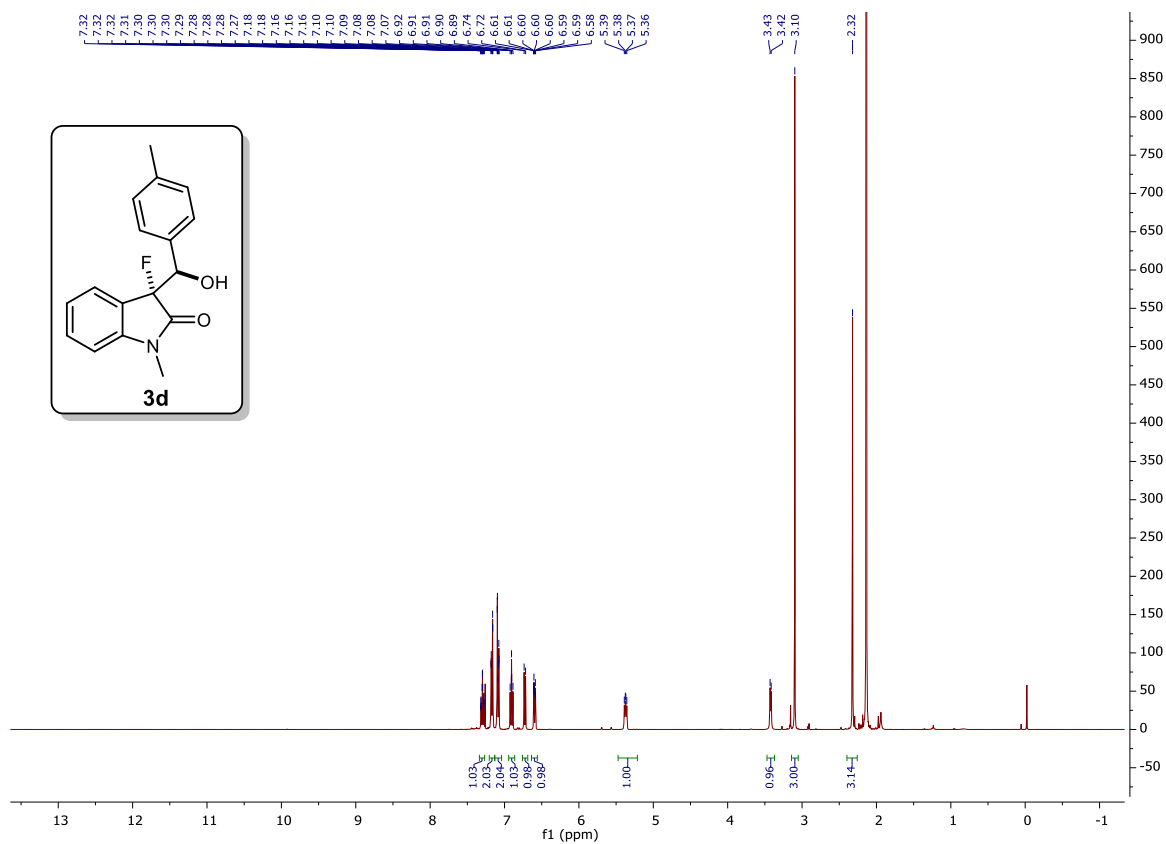
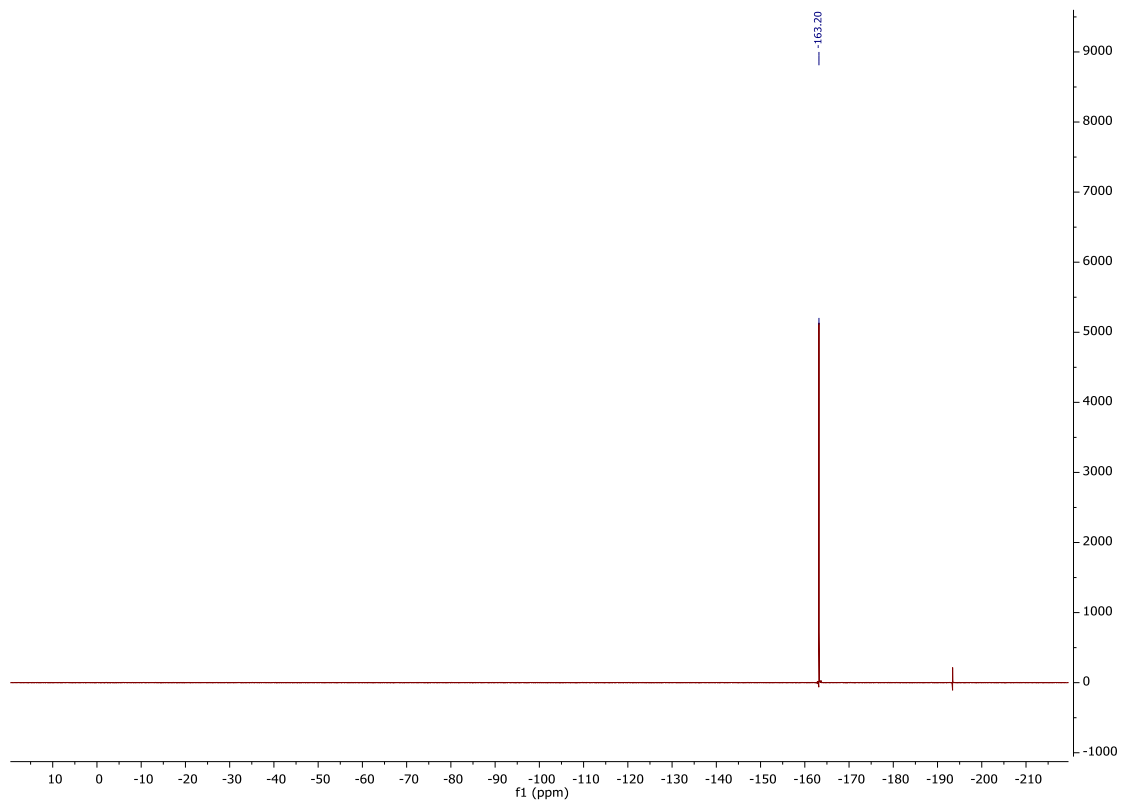
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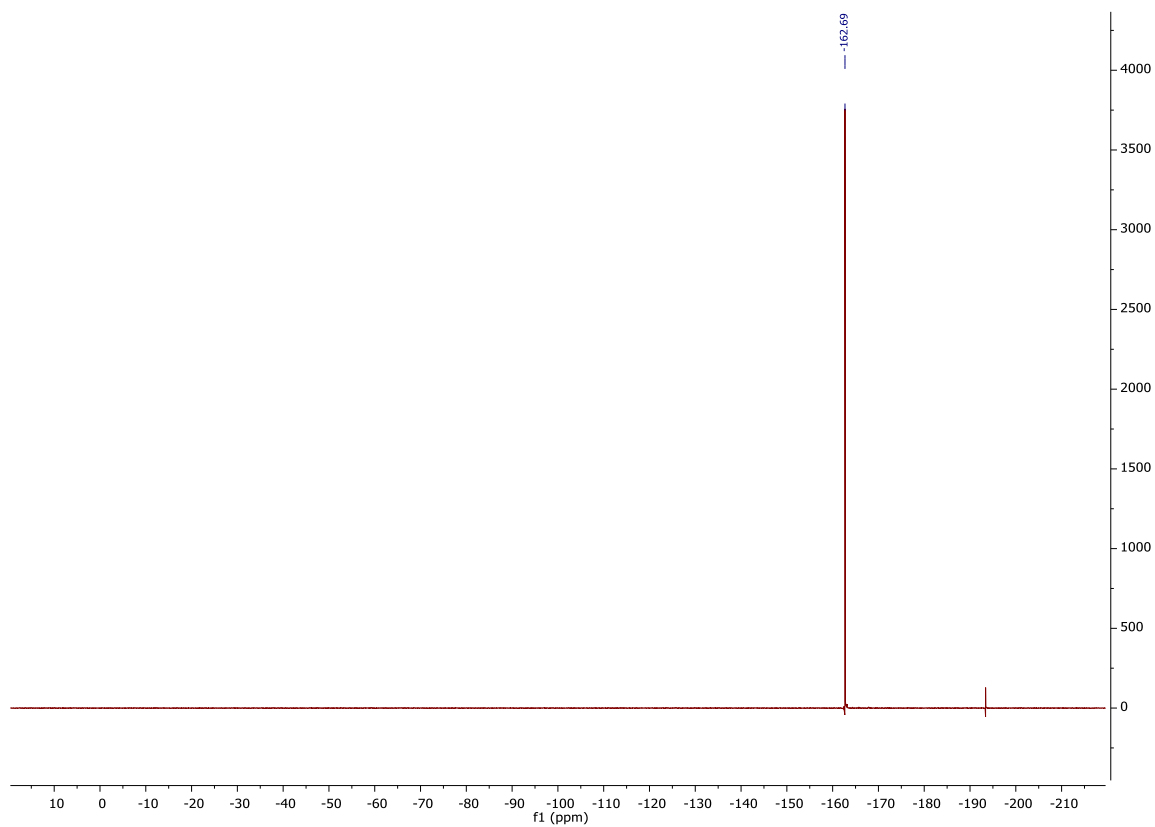
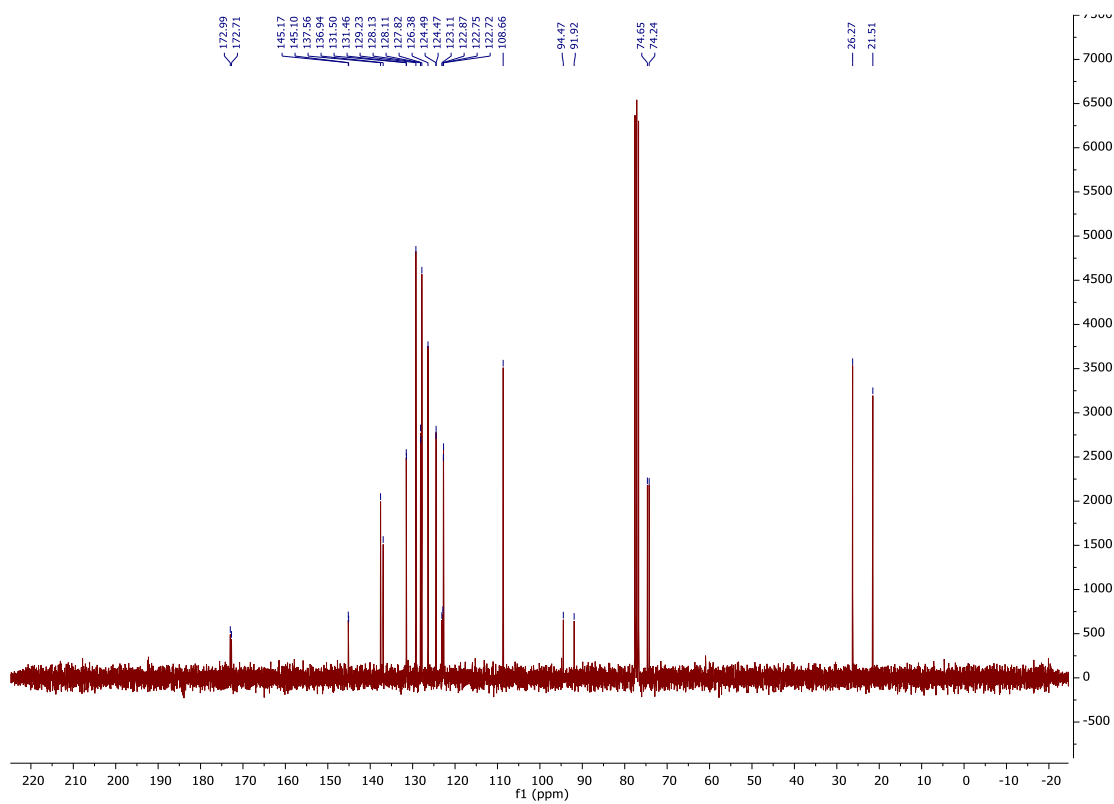






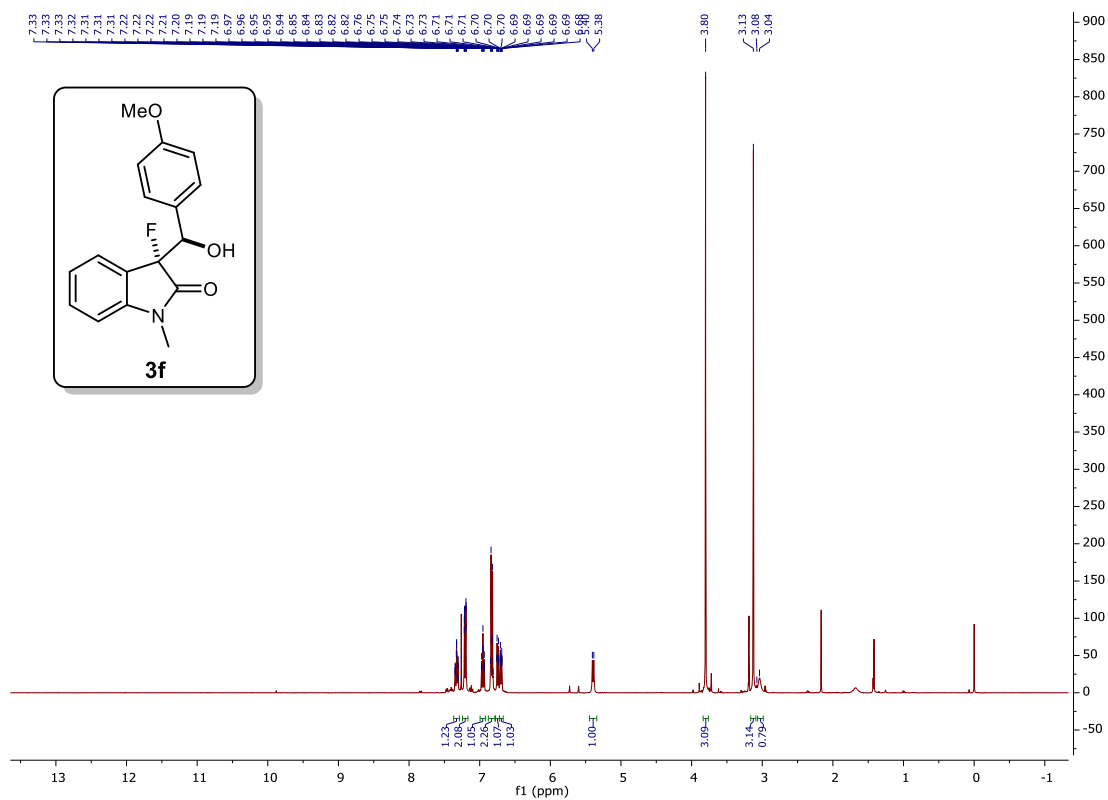
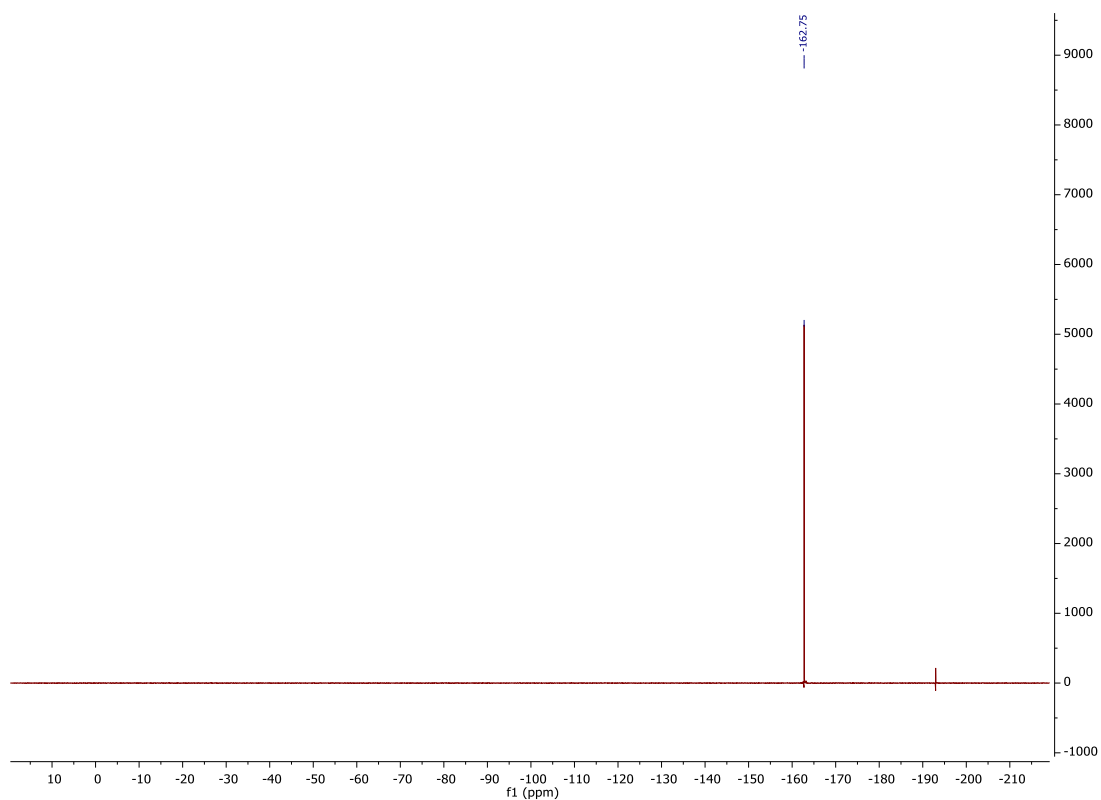


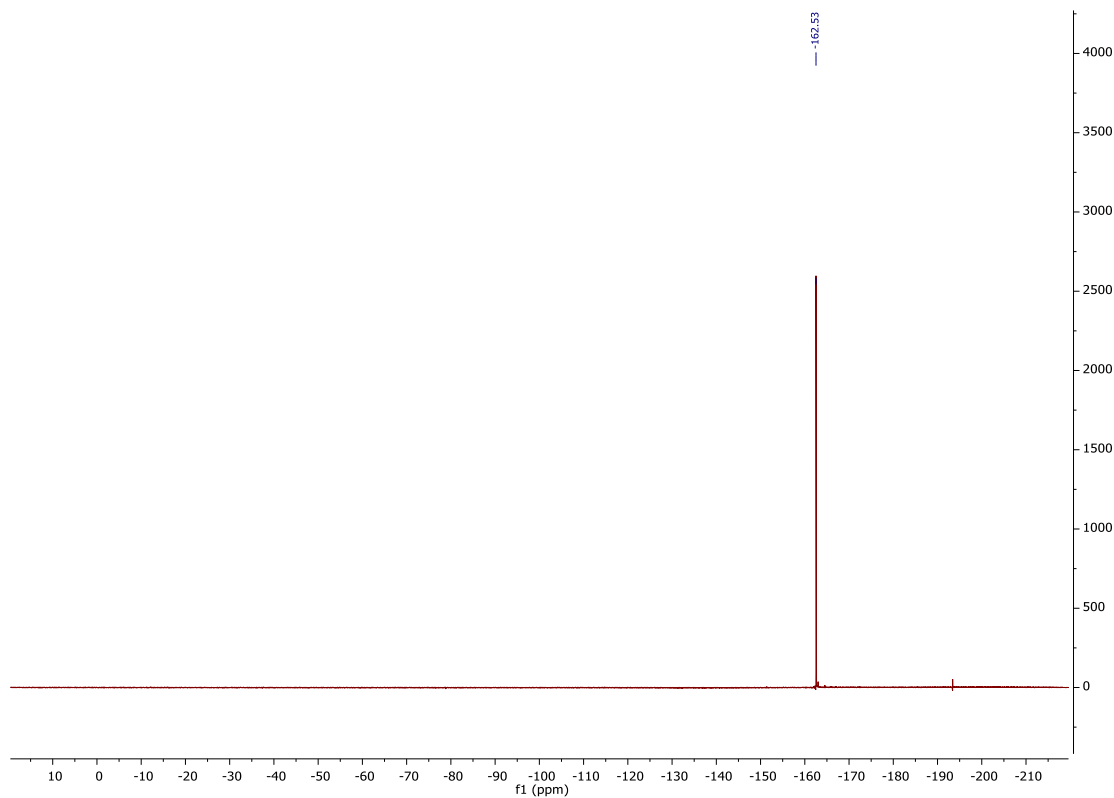
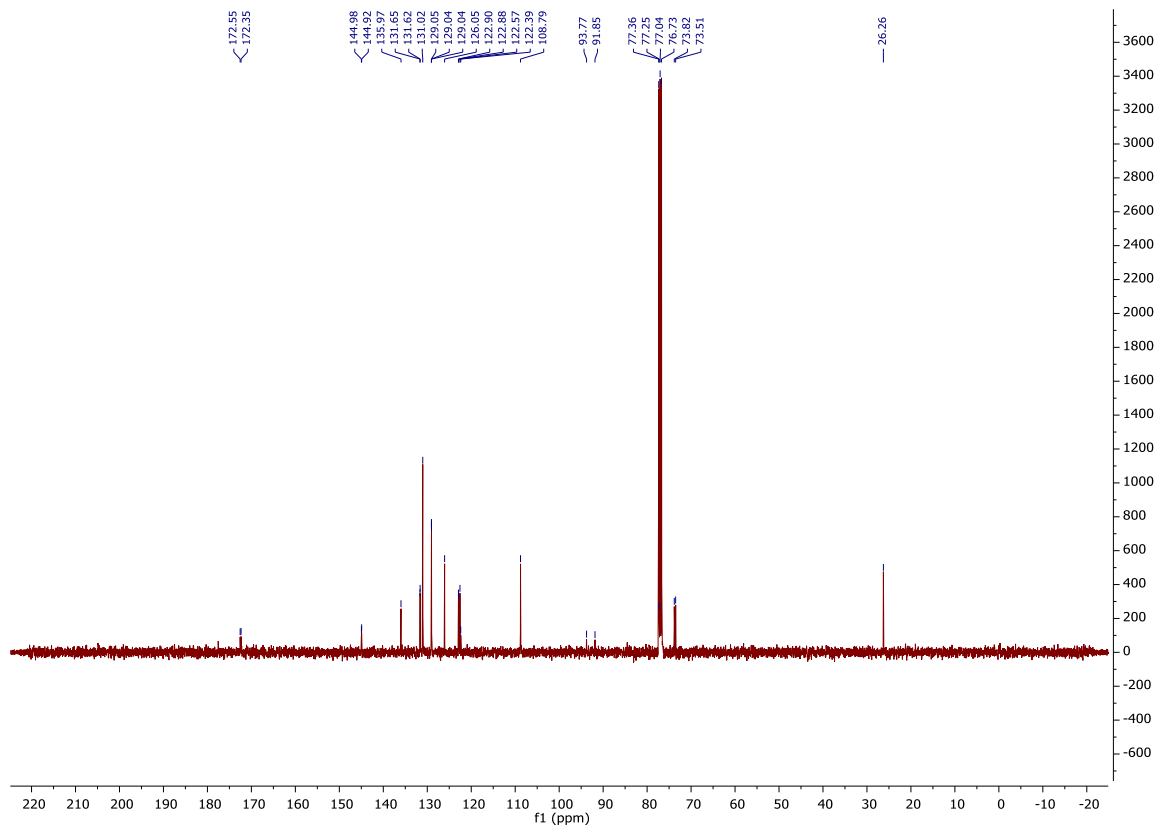


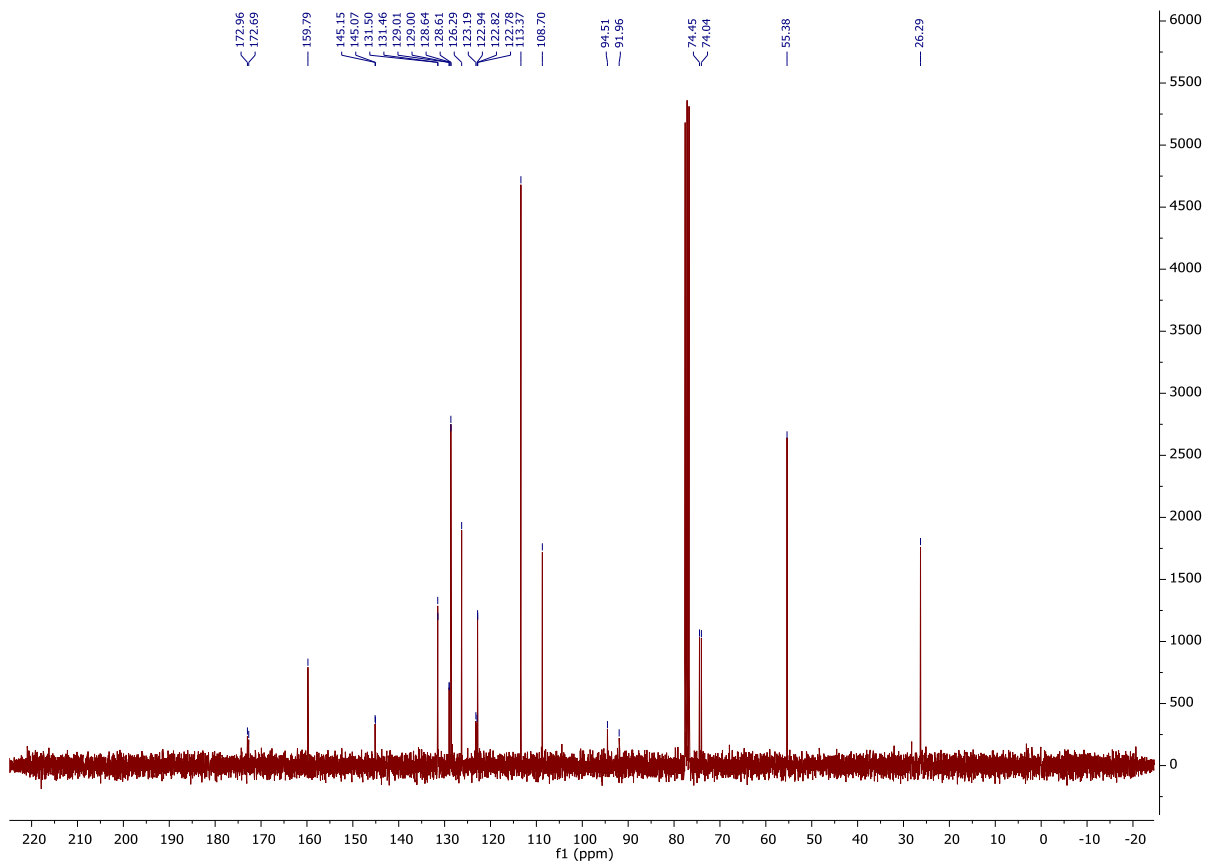
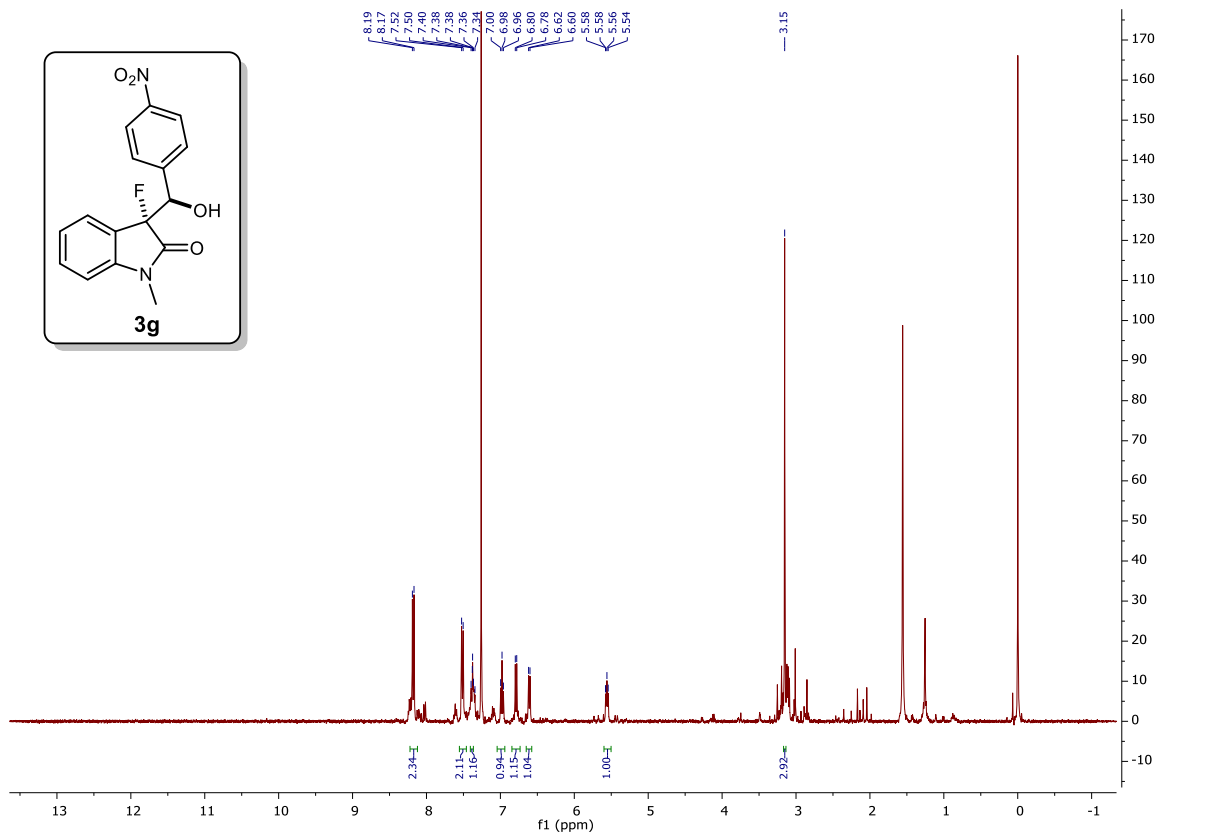


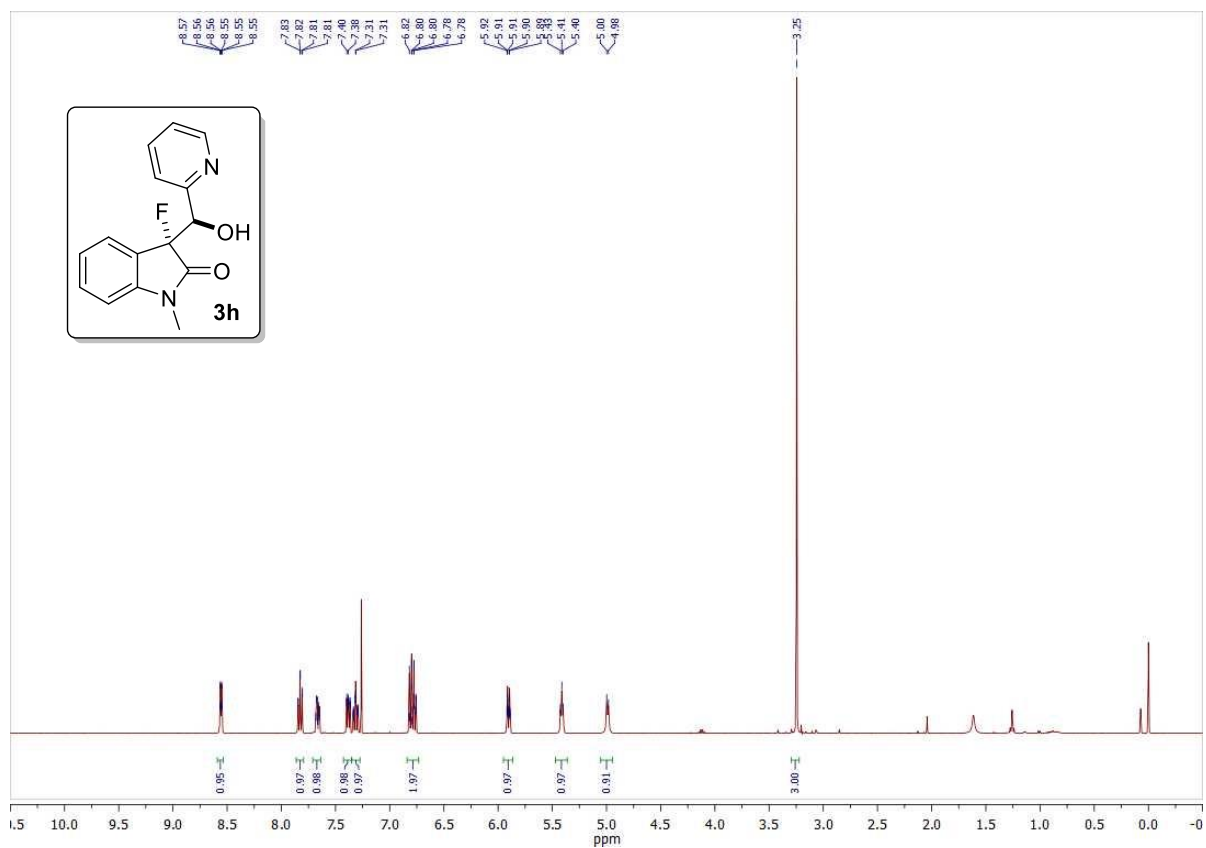
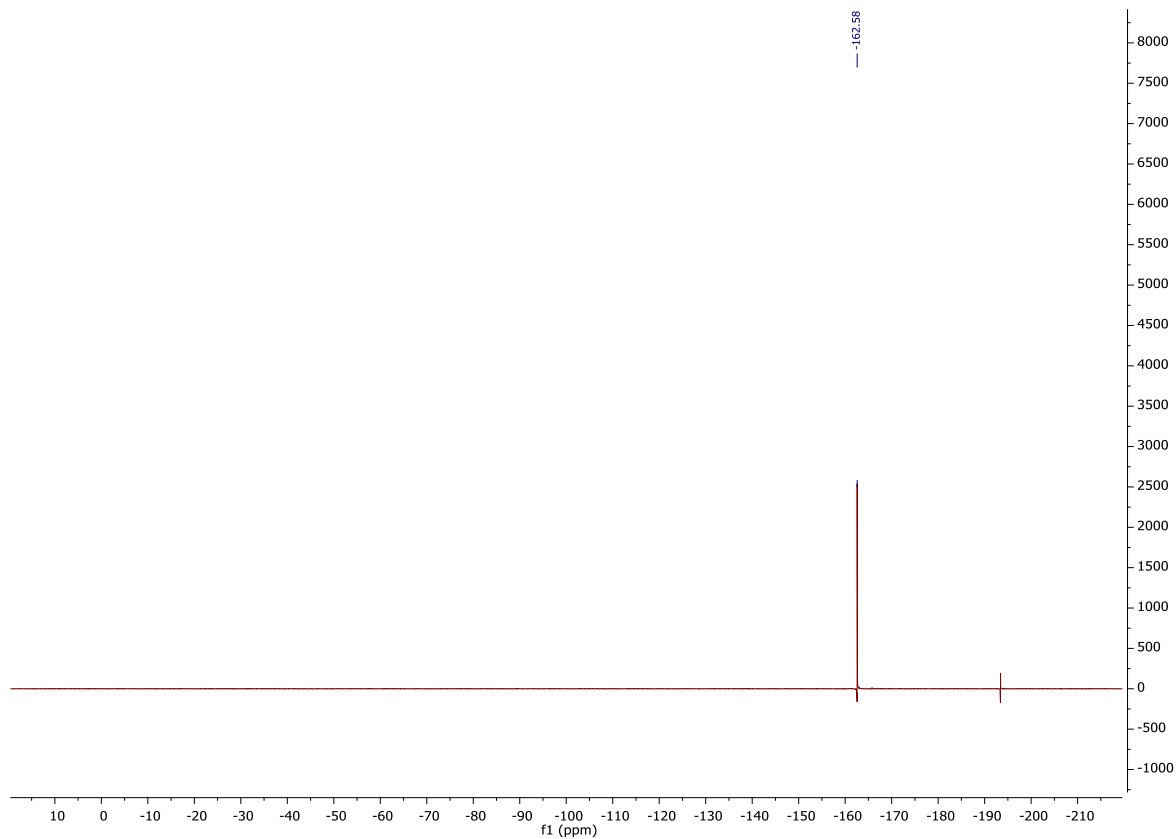


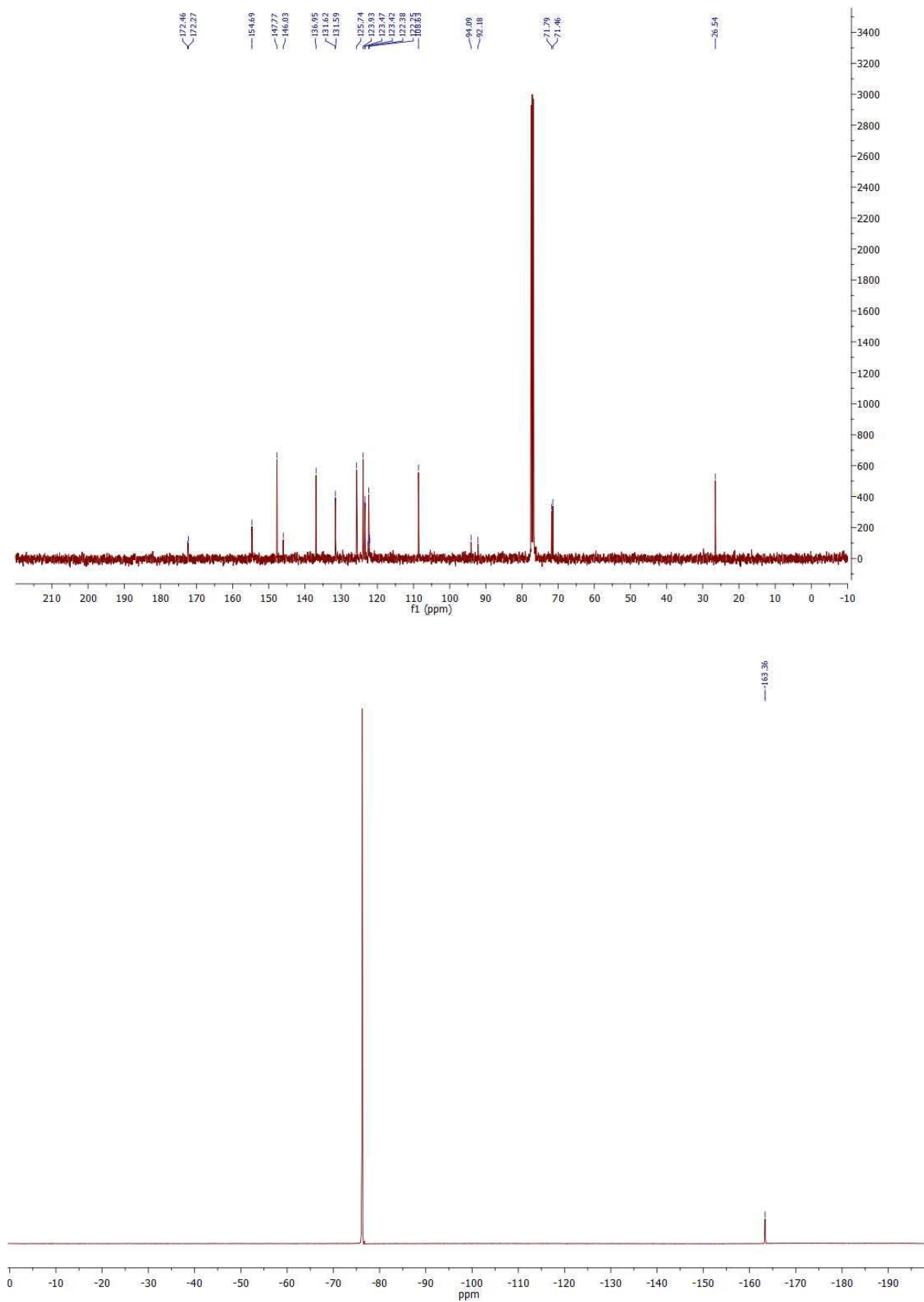


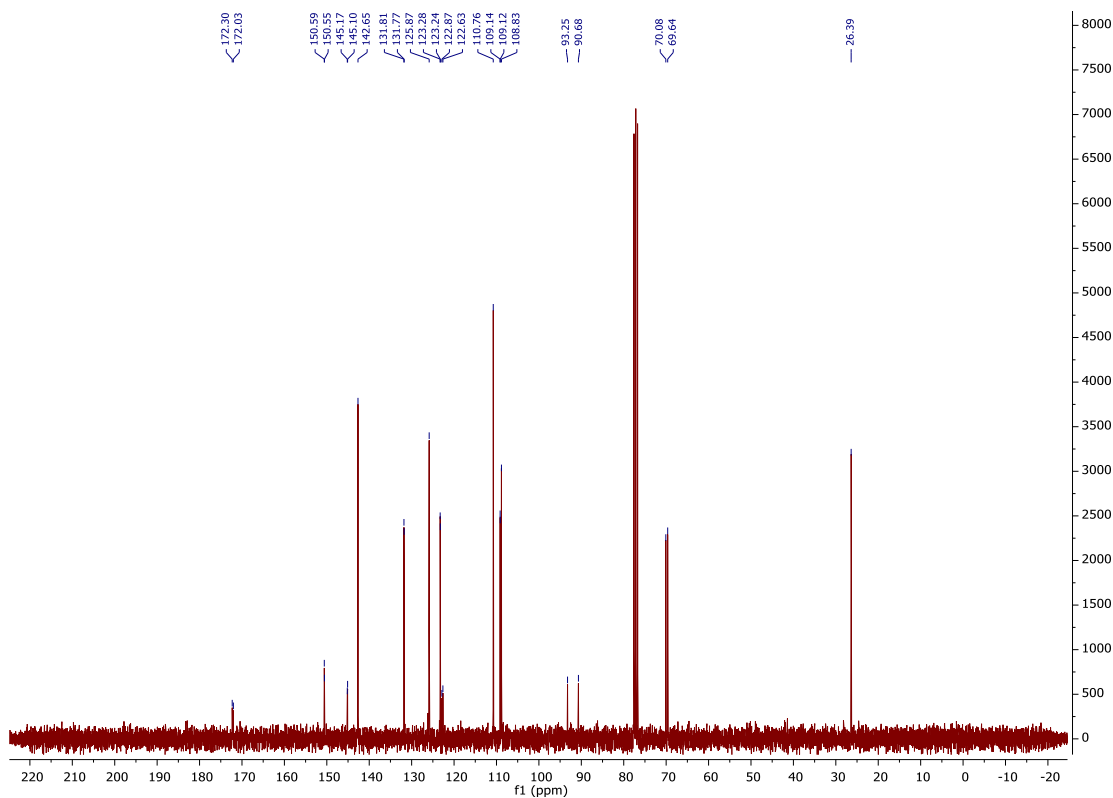
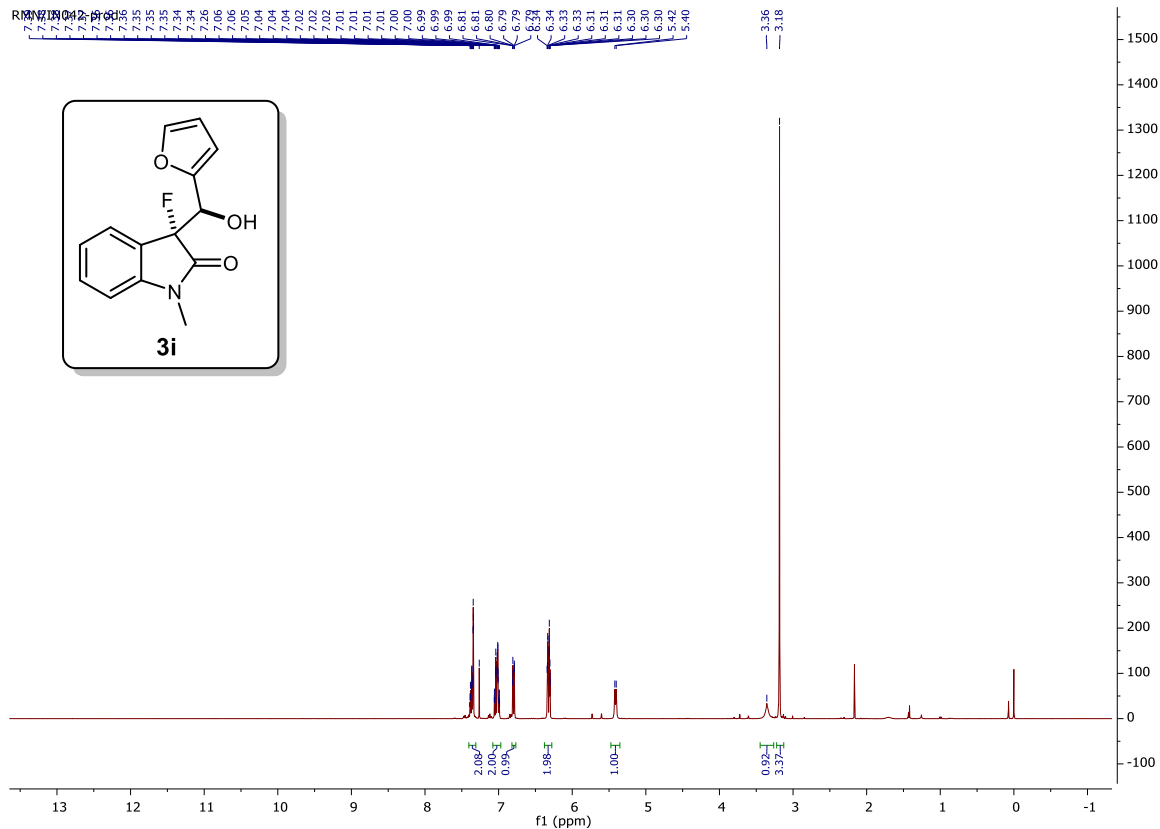


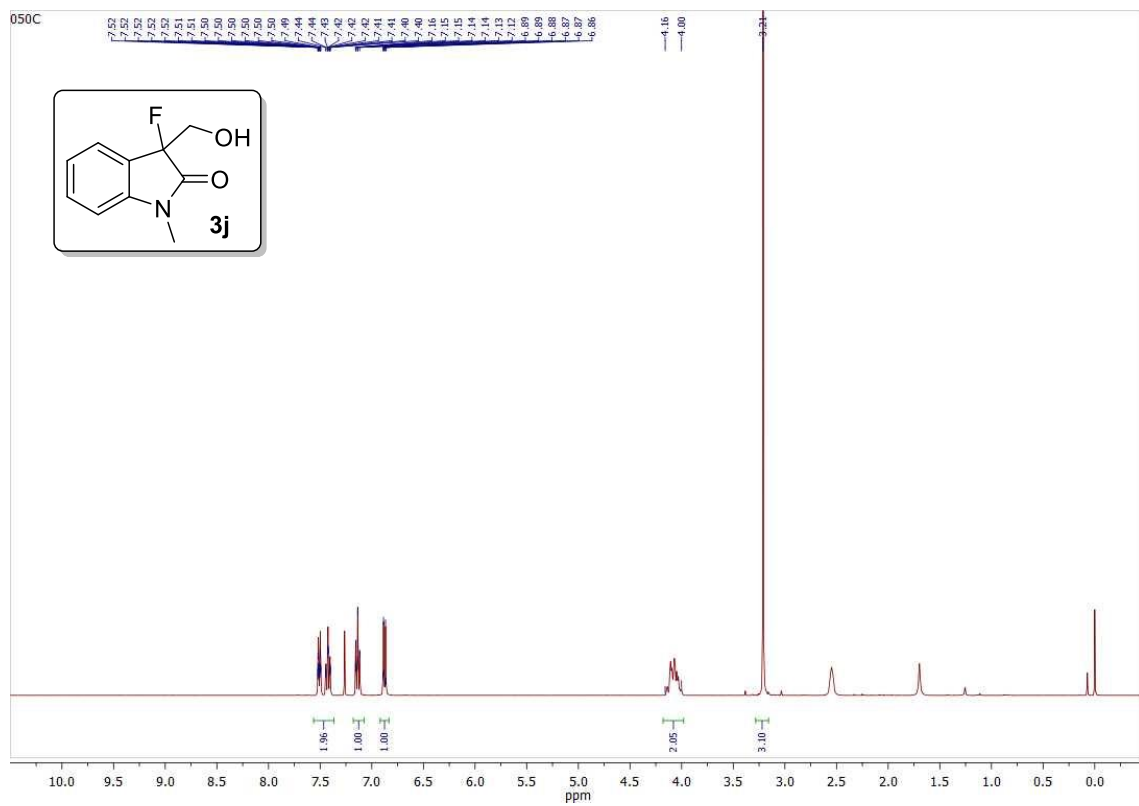


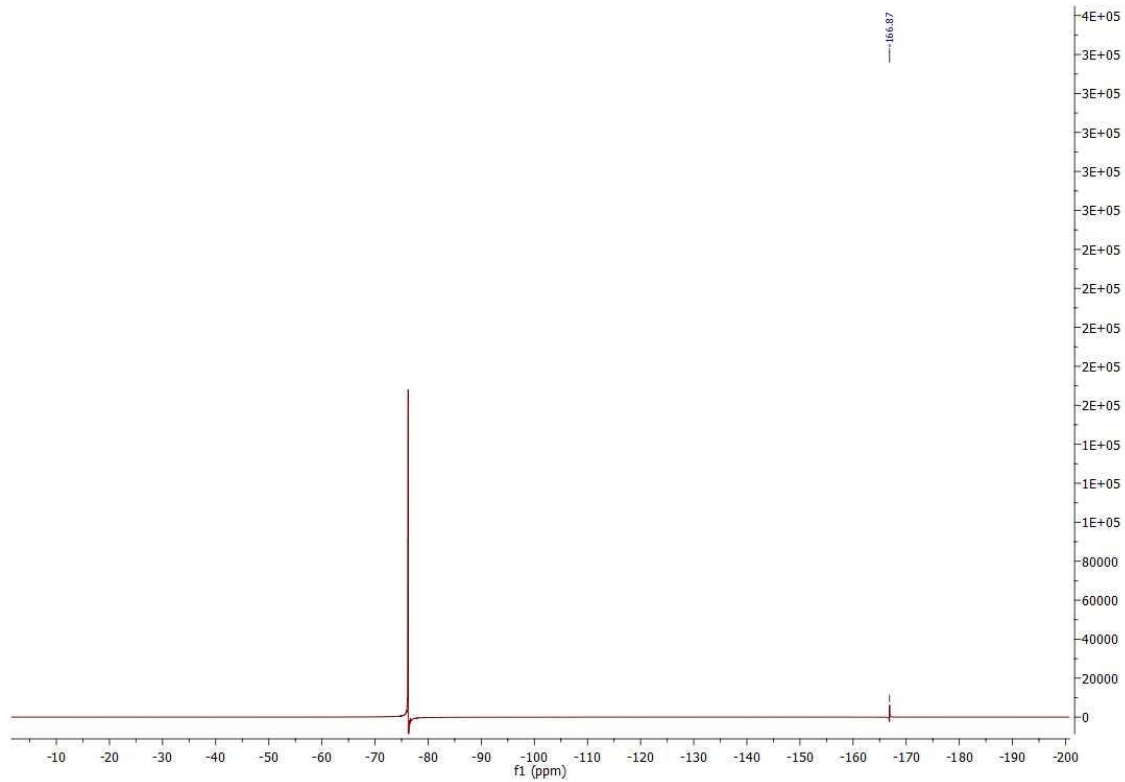
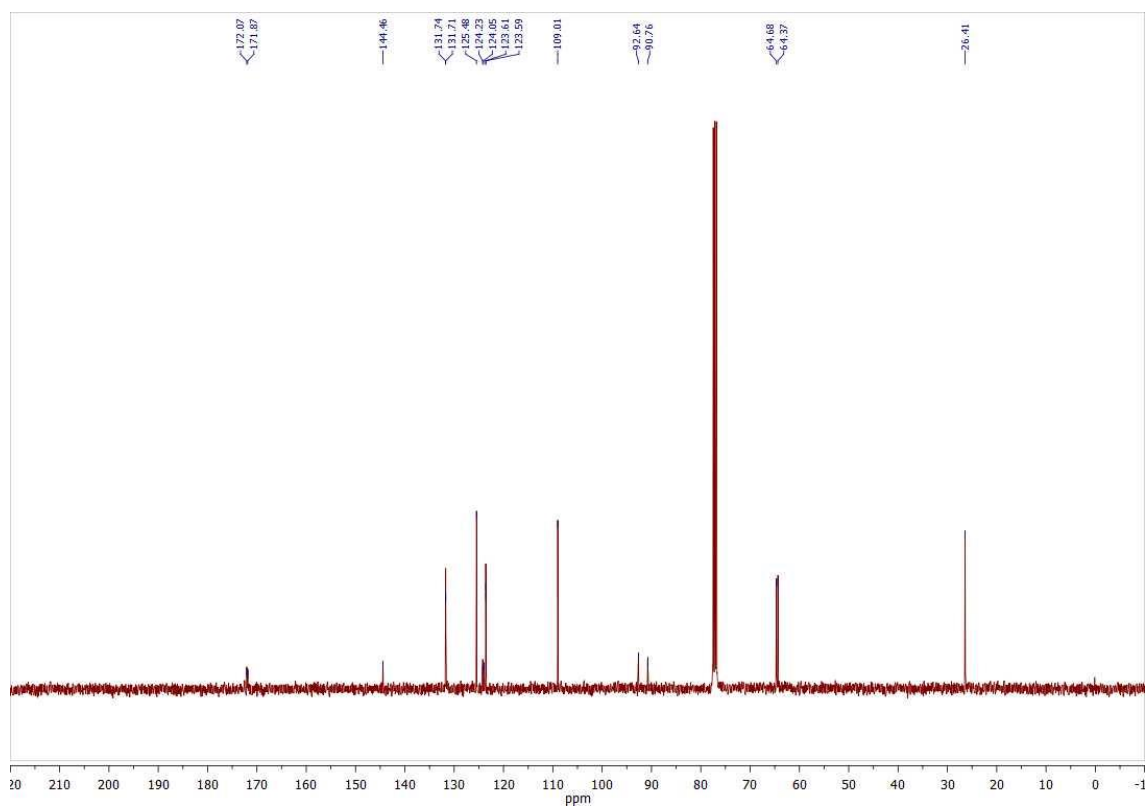




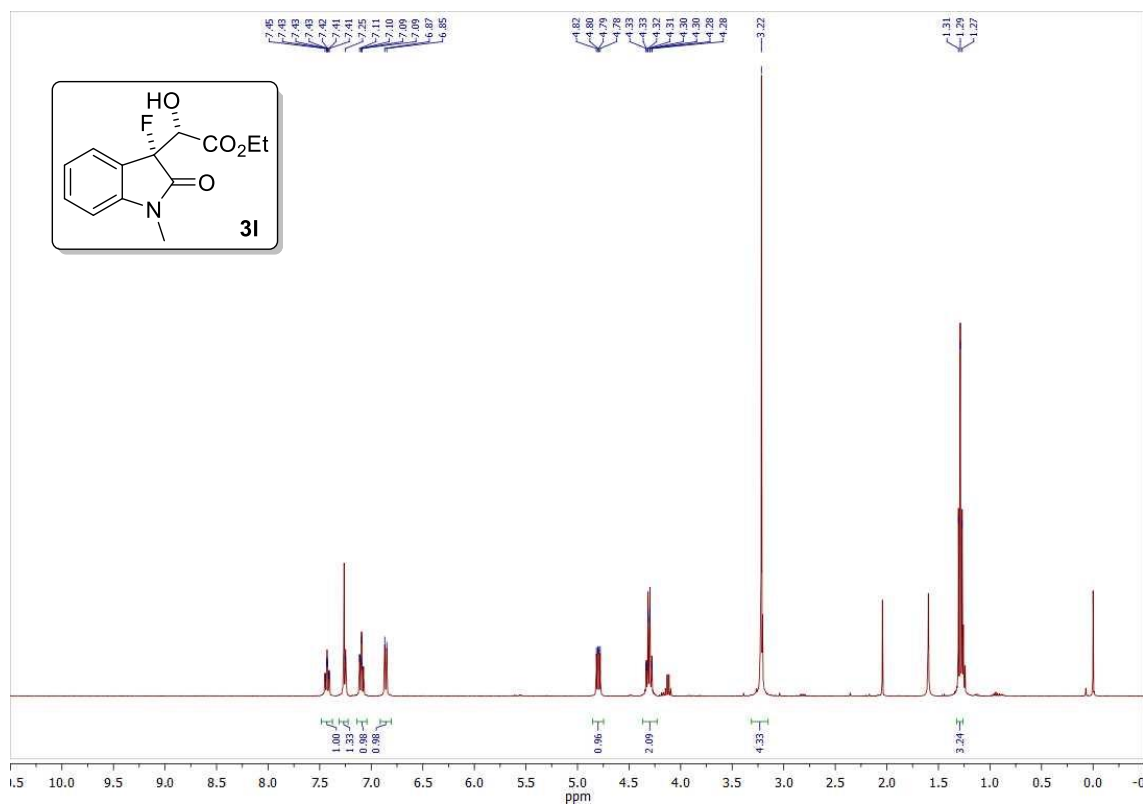
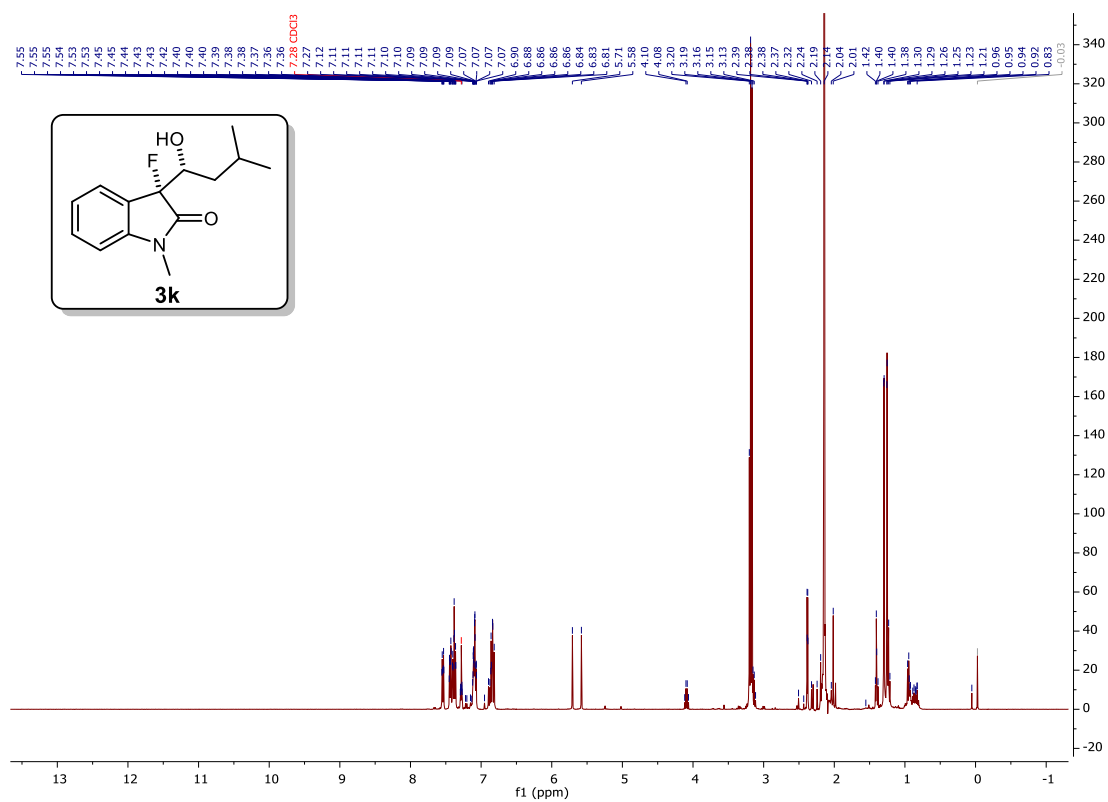


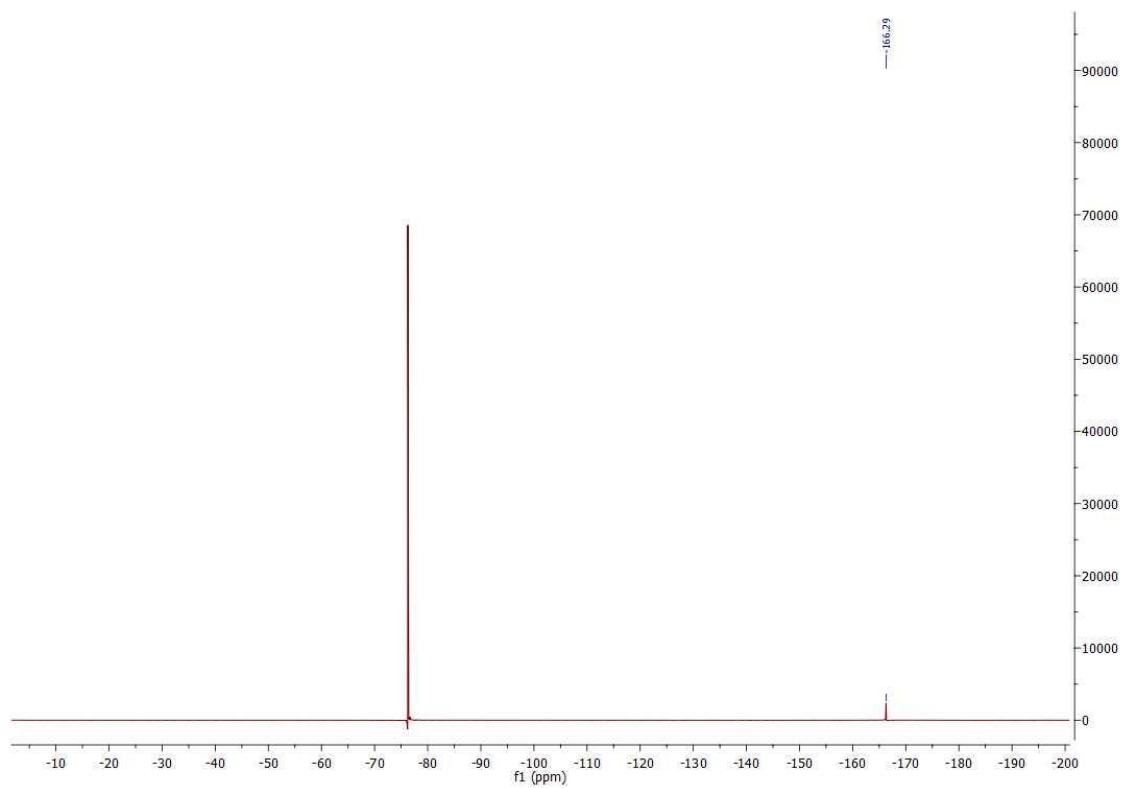
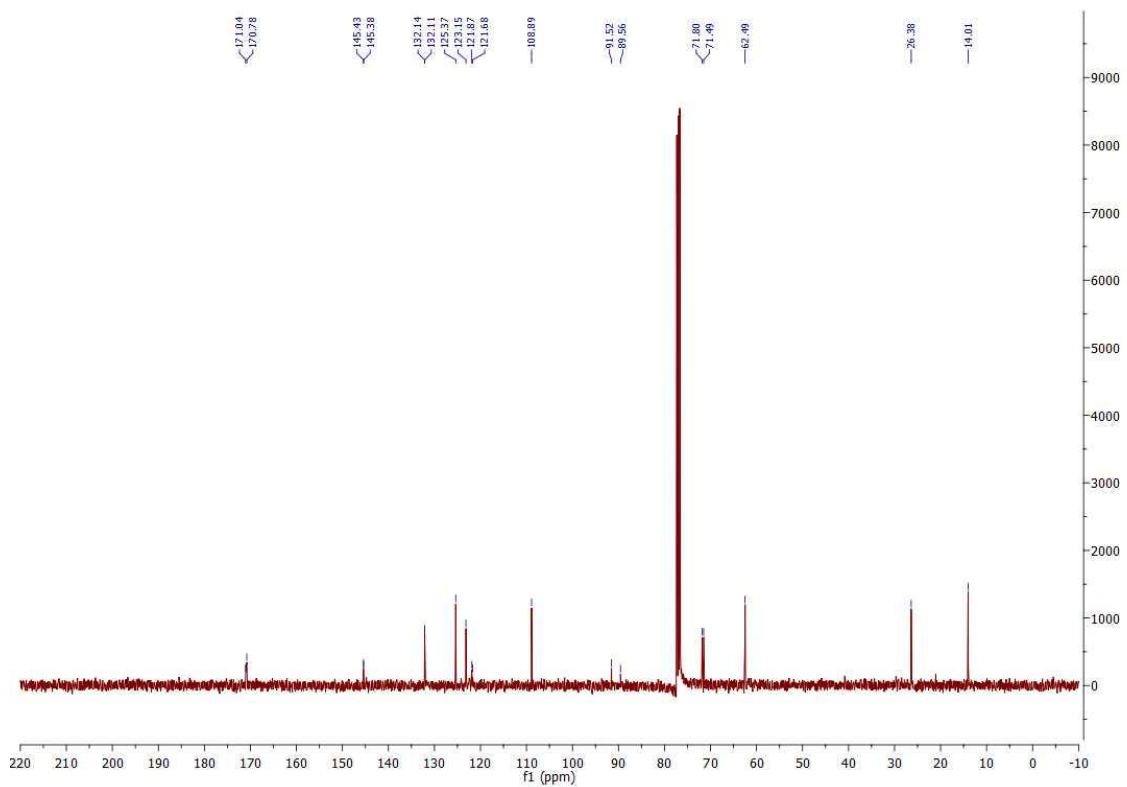


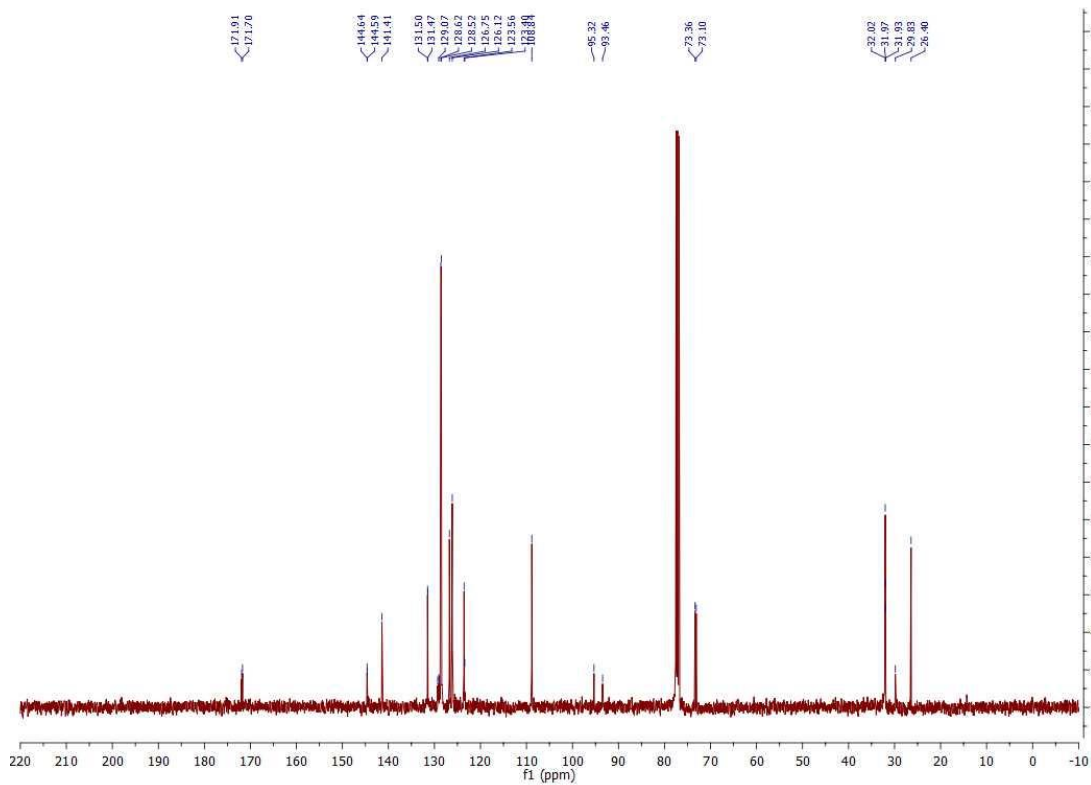
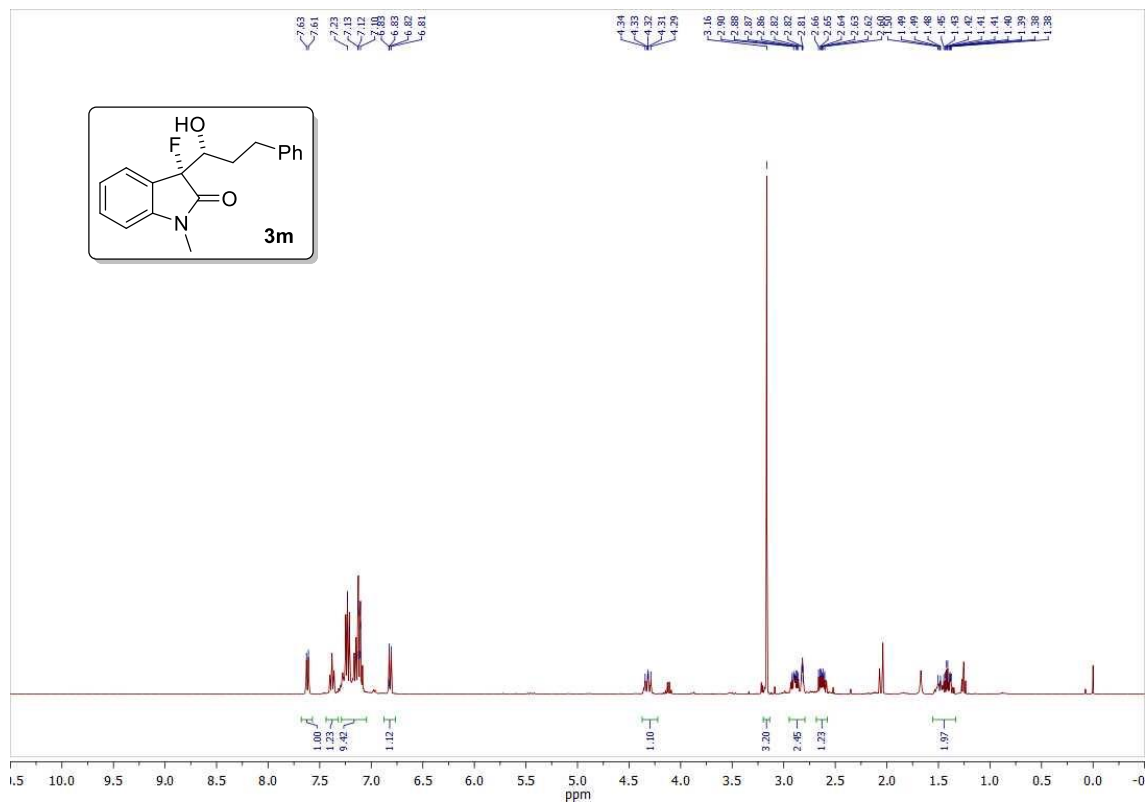


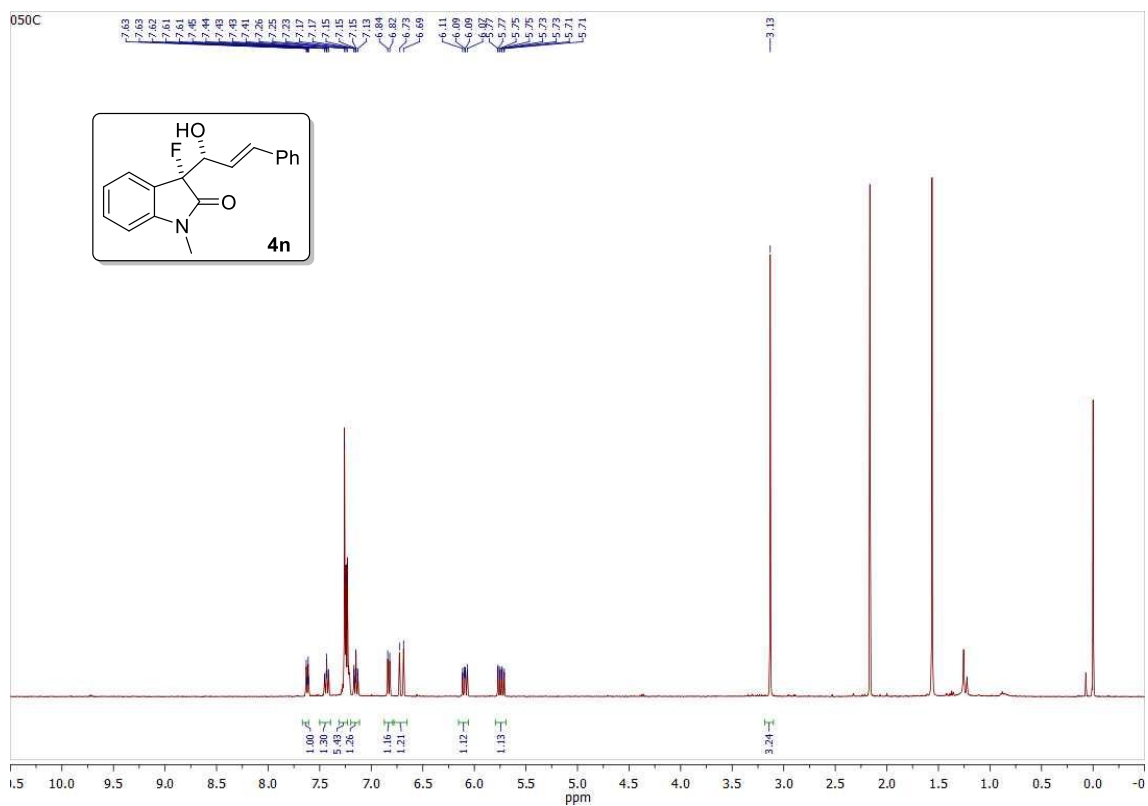
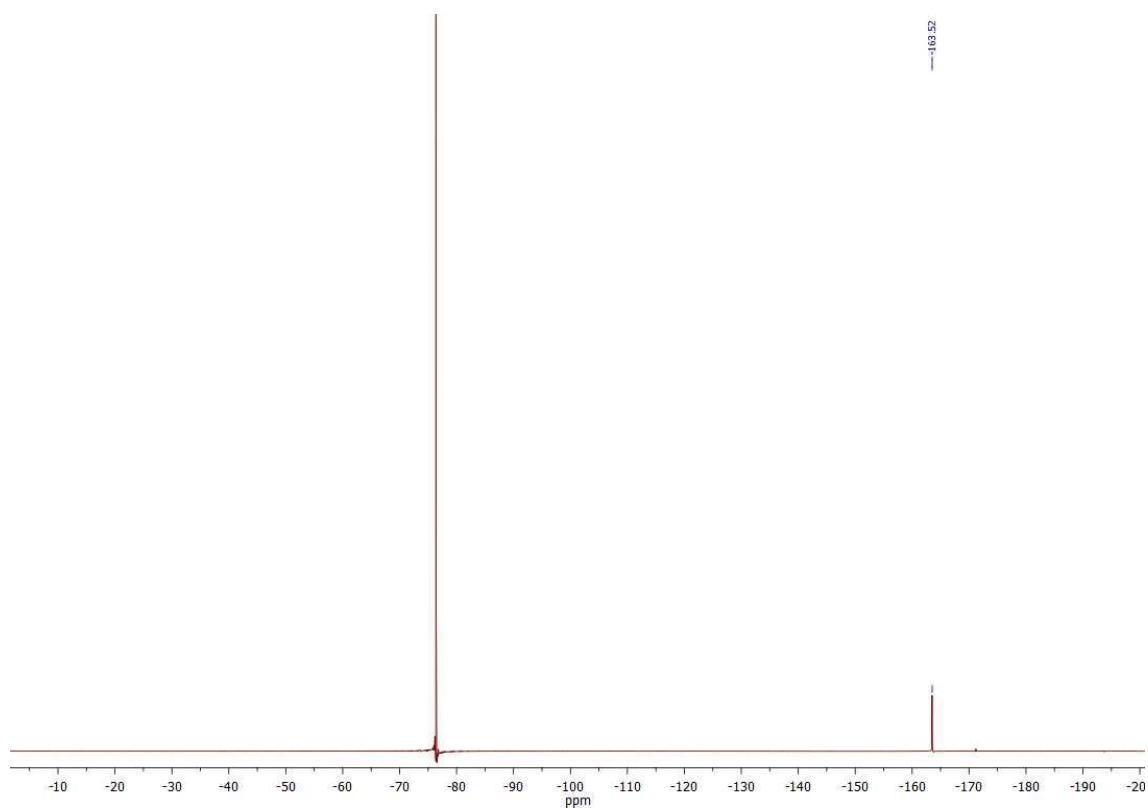


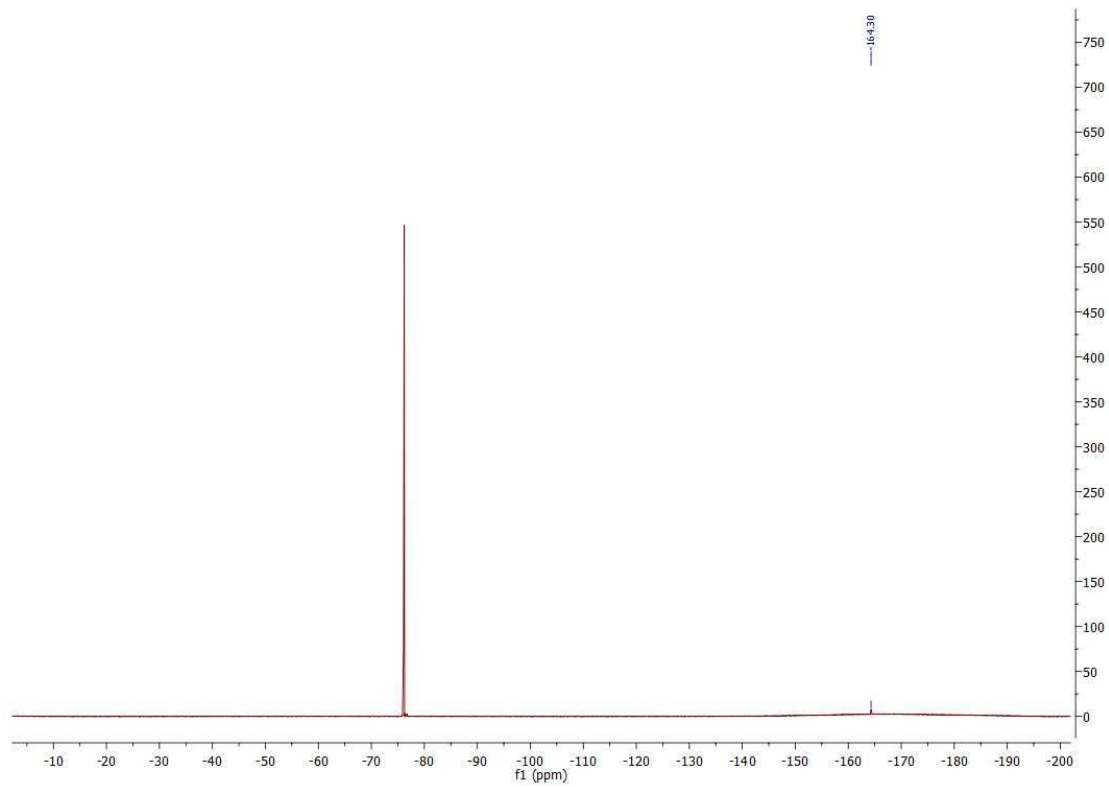
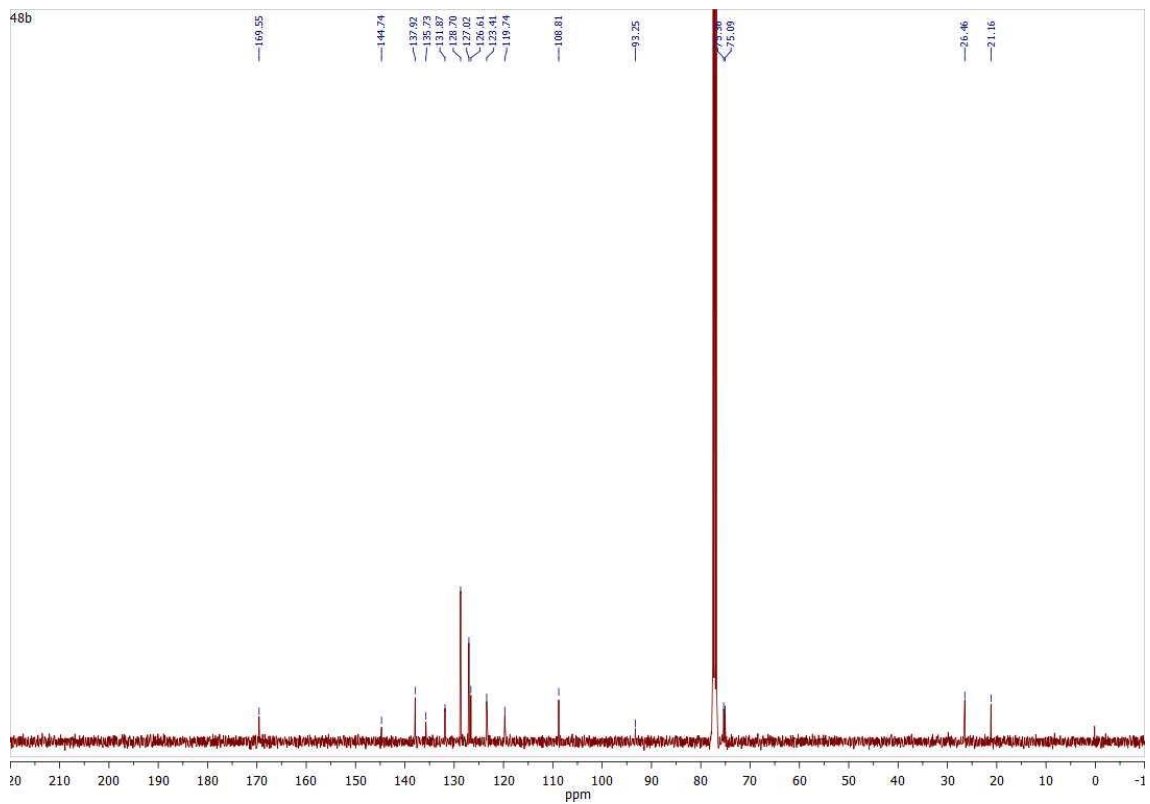












## 2. COMPUTATIONAL DETAILS

All of the calculations were performed using the Gaussian09 program.<sup>1</sup> Computations were done using B3LYP functional<sup>2</sup> in conjunction with Grimme's dispersion correction.<sup>3</sup> Standard basis sets def2SVP was employed.<sup>4</sup> The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). The optimizations were carried out using the Berny analytical gradient optimization method.<sup>5</sup> Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis),<sup>6</sup> using the Hratchian-Schlegel algorithm.<sup>7</sup> Analytical second derivatives of the energy were calculated to classify the nature of every stationary point, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies. Correction to free energy was made by subtracting  $S_{\text{trans}}$  contribution and considering a 1M concentration.<sup>8</sup> Structural representations were generated using CYLView.<sup>9</sup>

### Energies

**Table S1.** Calculated (B3lyp-3dbj/def2tzvp/PCM=THF//b3lyp-3dbj/def2svp/PCM=THF) absolute (hartree) and relative (kcal/mol) energies

	$E_0$	$\Delta E_0$	G	$\Delta G$	im. freq
<b>EN</b>	-1282.122492		-1282.187897		
<b>BA</b>	-345.627457		-345.657969		
REAGENTS <sup>a</sup>	-1395.305108	0.0	-1395.374081	0.0	
<b>SC</b>	-1395.301210	2.4	-1395.366492	4.8	
( <i>R,R</i> )- <b>TS</b>	-1395.302850	1.4	-1395.367677	4.0	-354.0
( <i>R,S</i> )- <b>TS</b>	-1395.298237	4.3	-1395.363829	6.4	-354.4
( <i>R,R</i> )- <b>PR</b>	-1395.308442	-2.1	-1395.373290	0.5	
( <i>R,S</i> )- <b>PR</b>	-1395.305077	0.0	-1395.368071	3.8	

### Cartesian Coordinates

<sup>1</sup> Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT.: 2009.

<sup>2</sup> (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.

<sup>3</sup> (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104-154119. (b) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456-1465.

<sup>4</sup> (a) Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, *8*, 227-236. (b) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

<sup>5</sup> (a) Schlegel, H. B. *J. Comput. Chem.* **1982**, *3*, 214-218. (b) Schlegel, H. B. In *Modern Electronic Structure Theory*; Yarkony, D. R., Ed.; World Scientific Publishing: Singapore, 1994.

<sup>6</sup> (a) Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363-368. (b) Fukui, K. *J. Phys. Chem.* **1970**, *74*, 4161-4163.

<sup>7</sup> Hratchian, H. P.; Schlegel, H. B. *J. Phys. Chem. A* **2002**, *106*, 165-169.

<sup>8</sup> Tanaka, R.; Yamashita, M.; Chung, L. W.; Morokuma, K.; Nozaki, K. *Organometallics* **2011**, *30*, 6742-6750

<sup>9</sup> C. Y. Legault, *Université de Sherbrooke*, 2009, <http://www.cylview.org>.

**Cartesian Coordinates**

PR-RR

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## PR-RS

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SC

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TS-RR

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TS-RS

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