

Supplementary Material

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

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^b *Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad de Alicante, Apdo. 99, Ctra. Alicante-San Vicente s/n, 03690-Alicante, Spain*

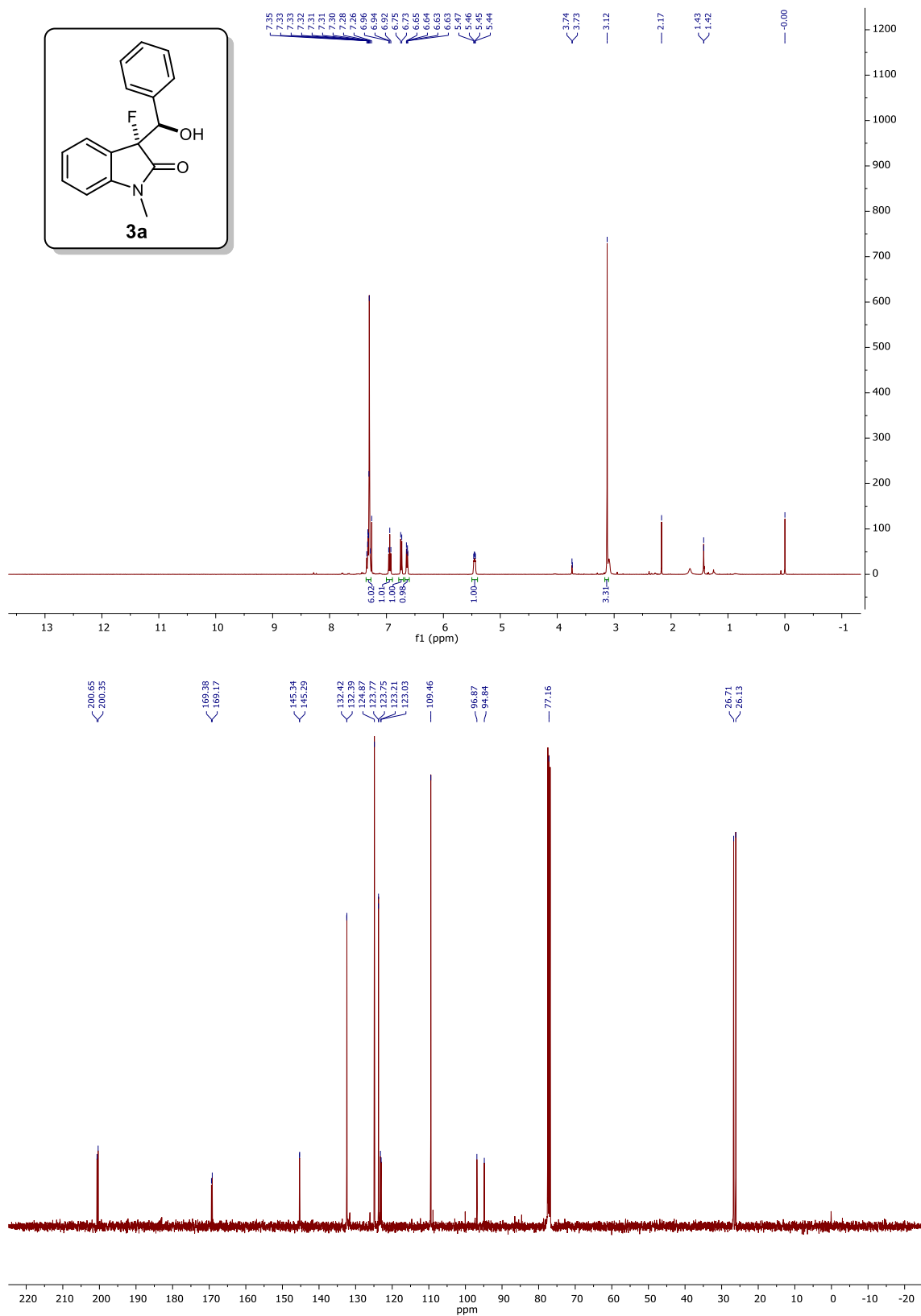
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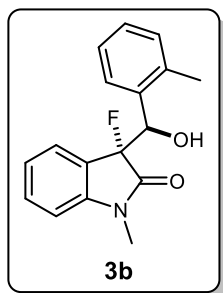
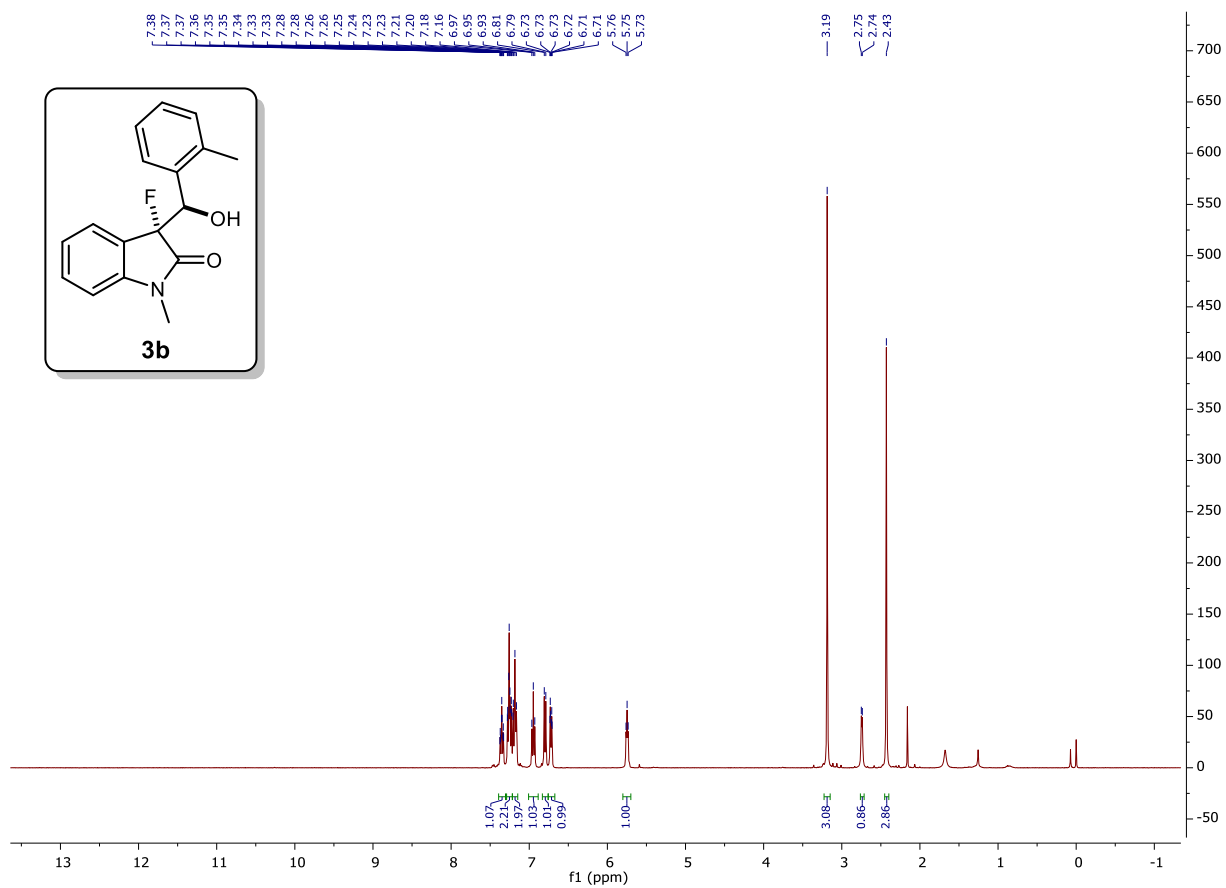
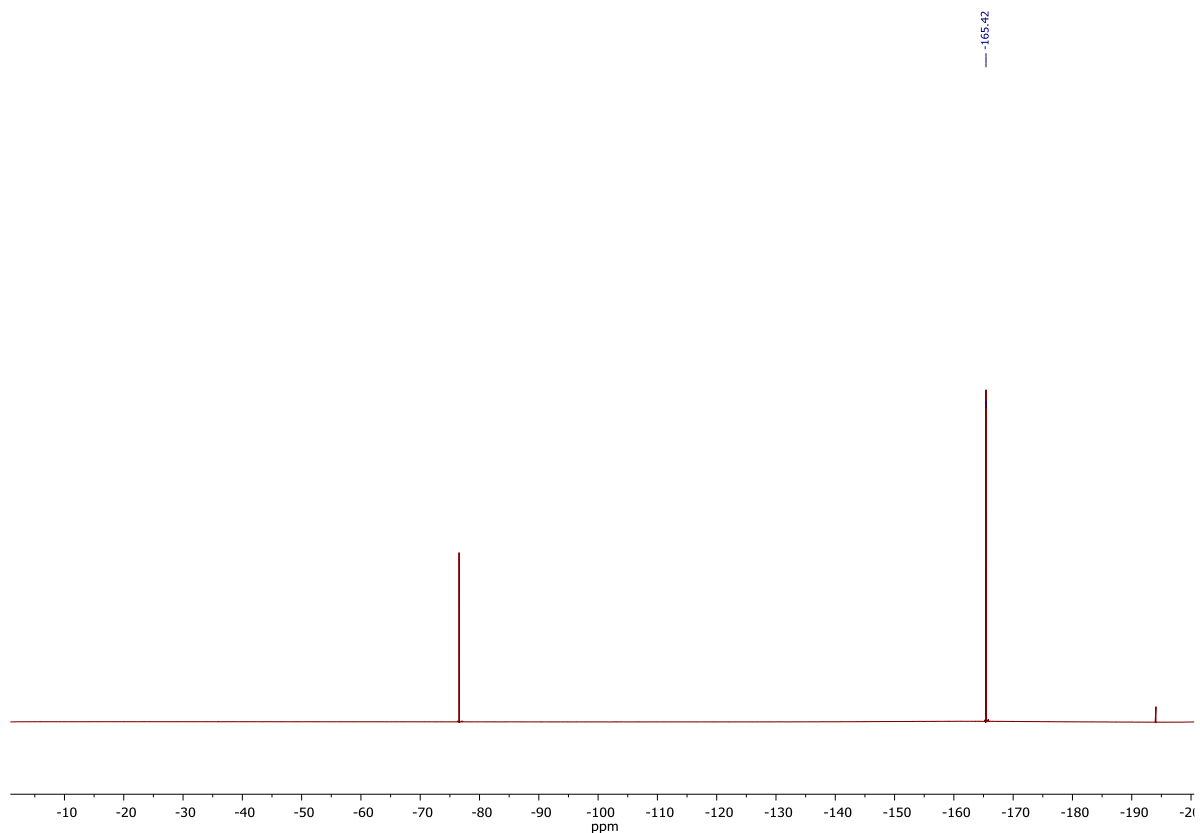
Email: cnajera@ua.es; jmsansano@ua.es

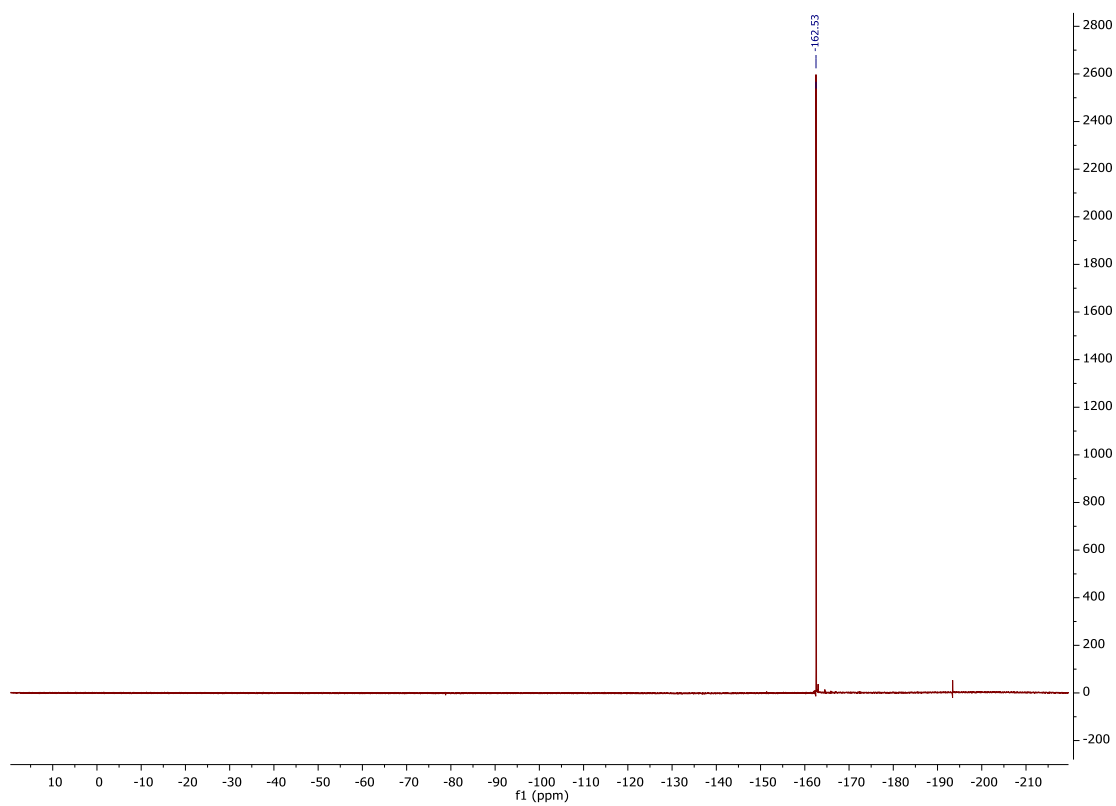
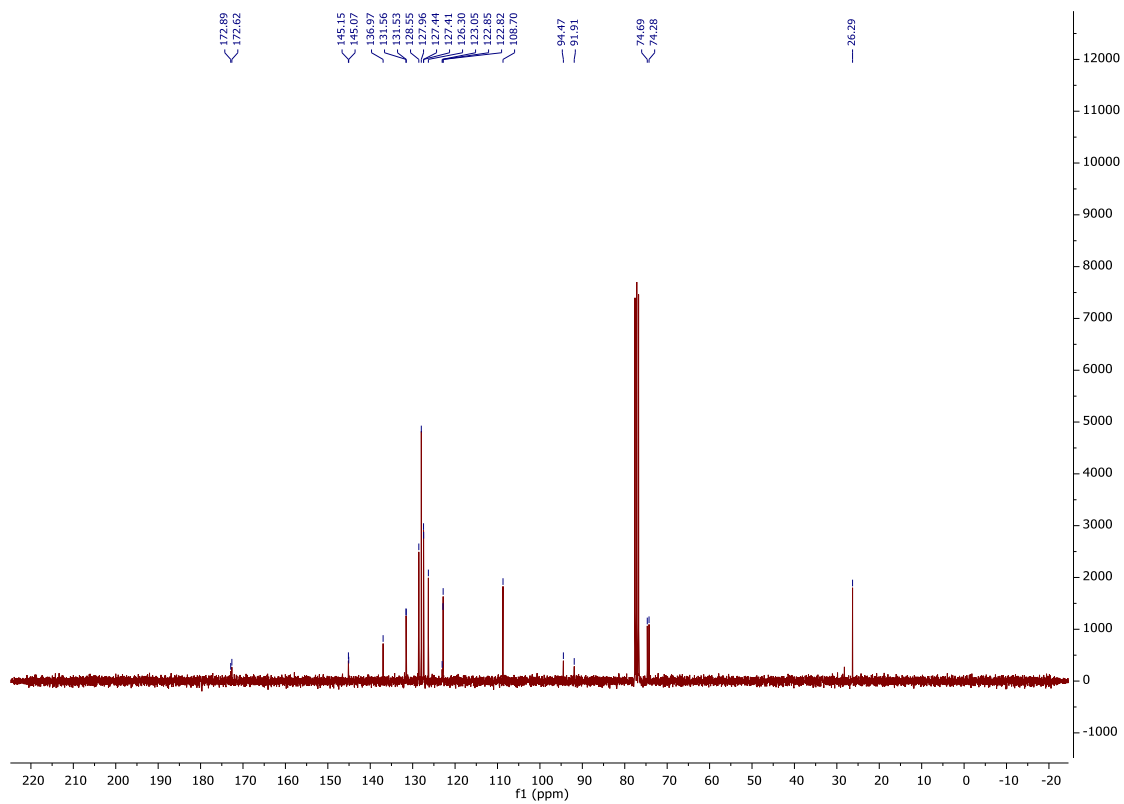
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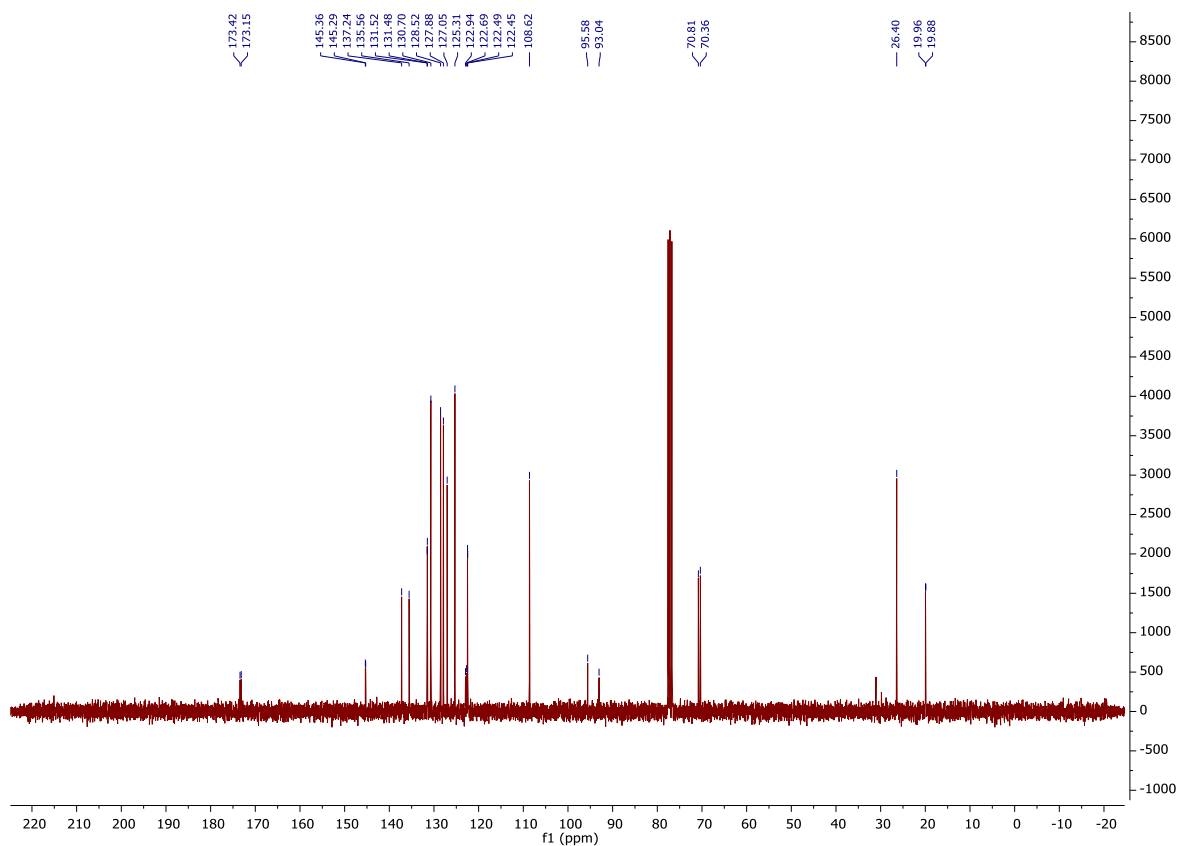
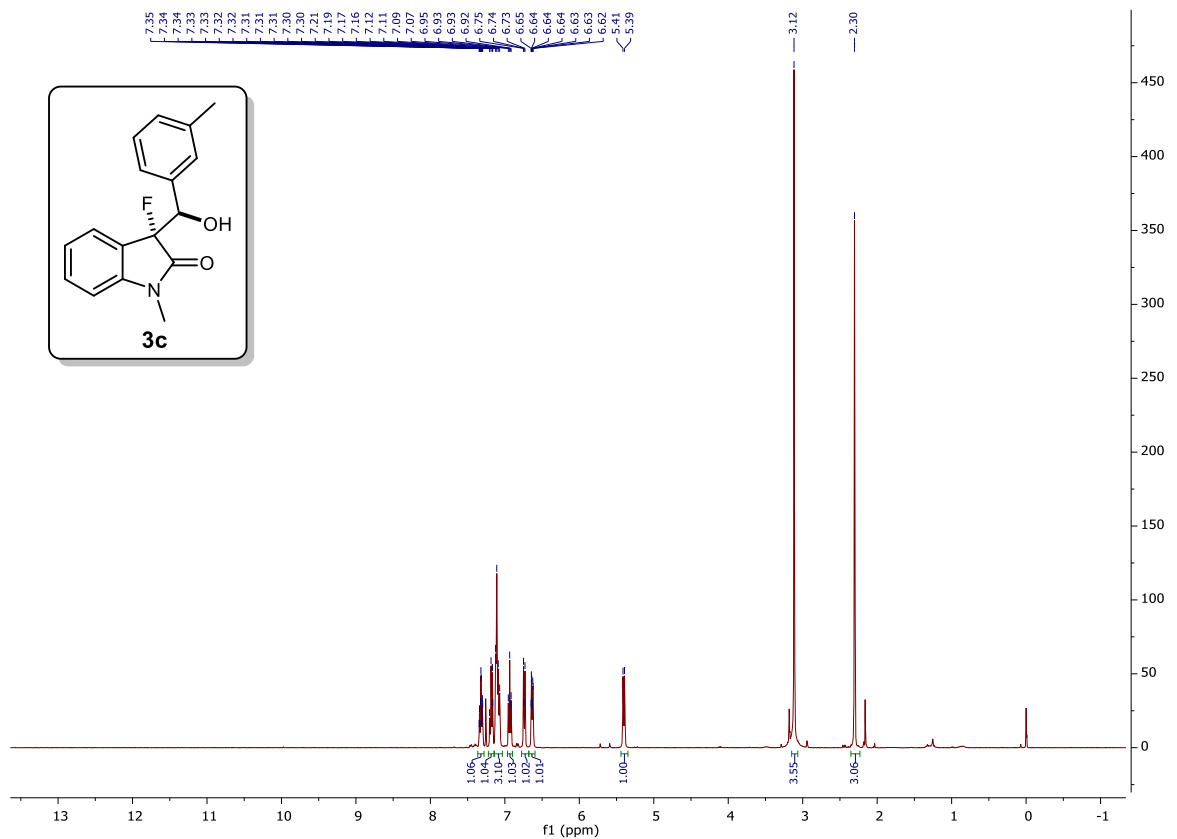
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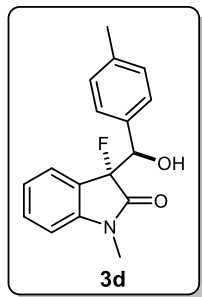
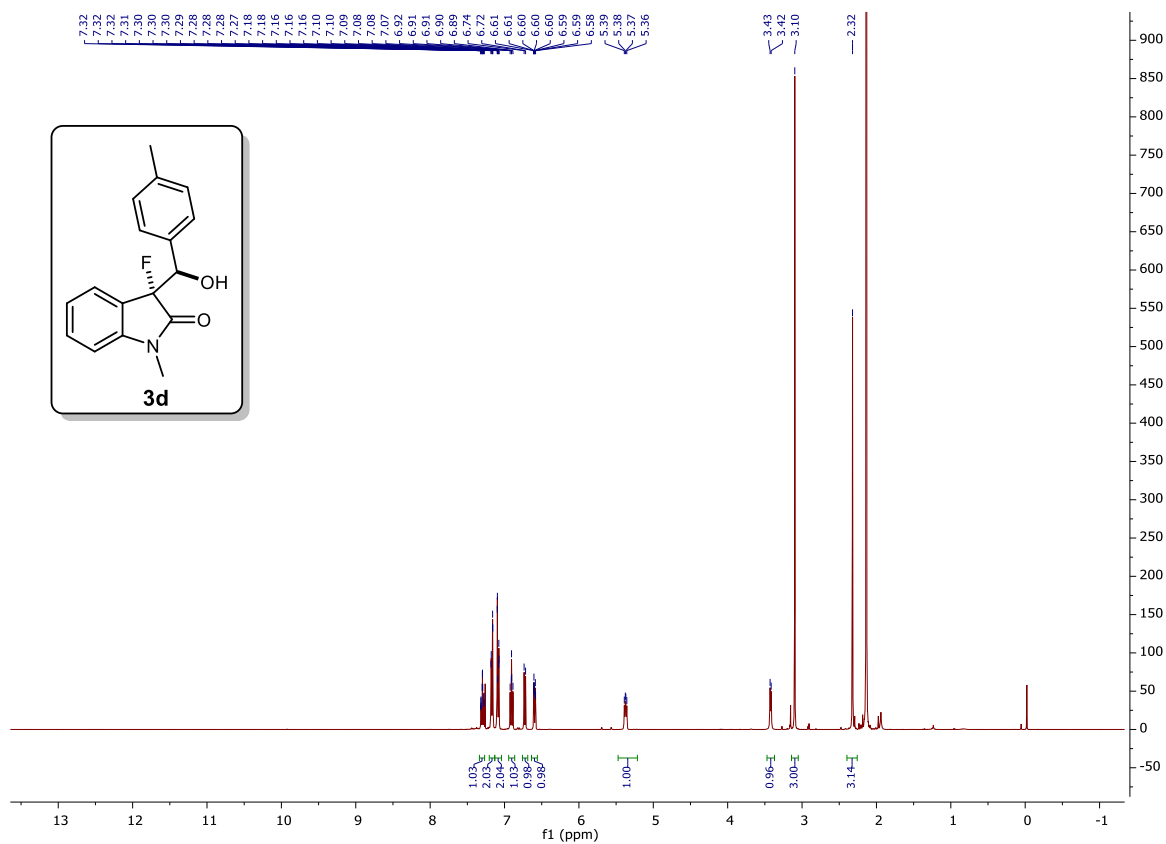
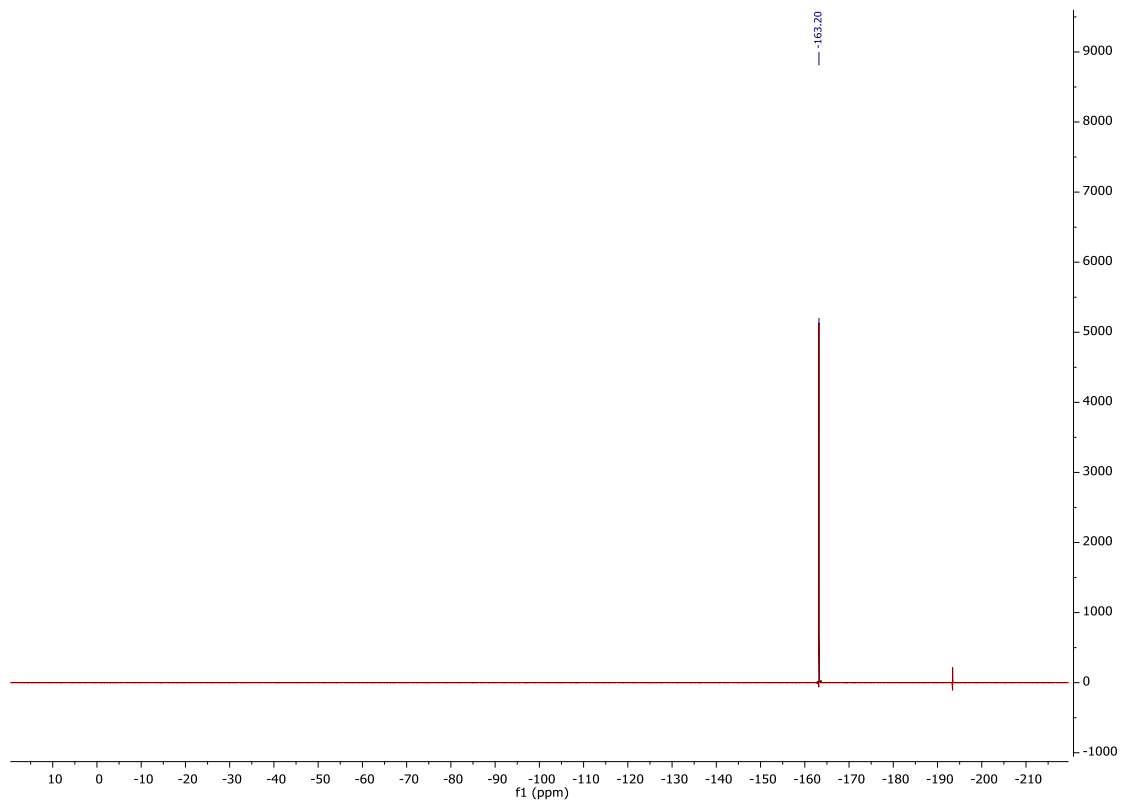
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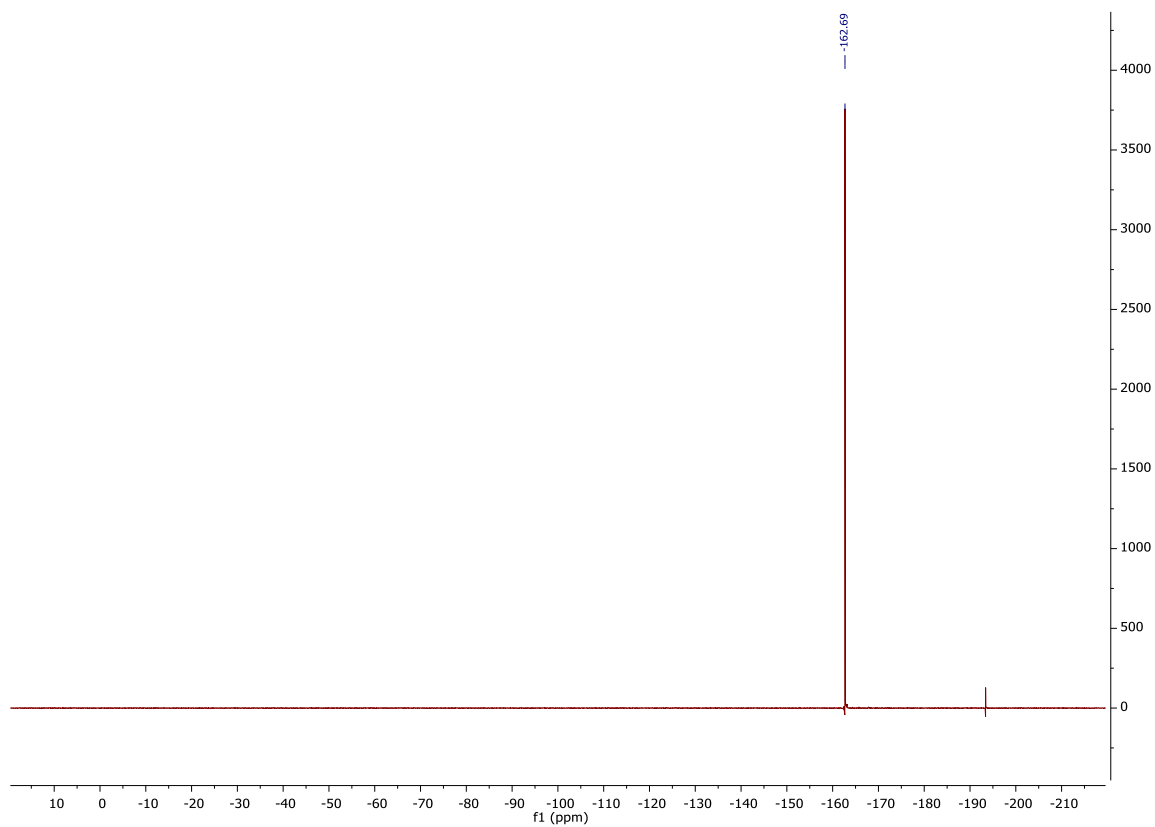
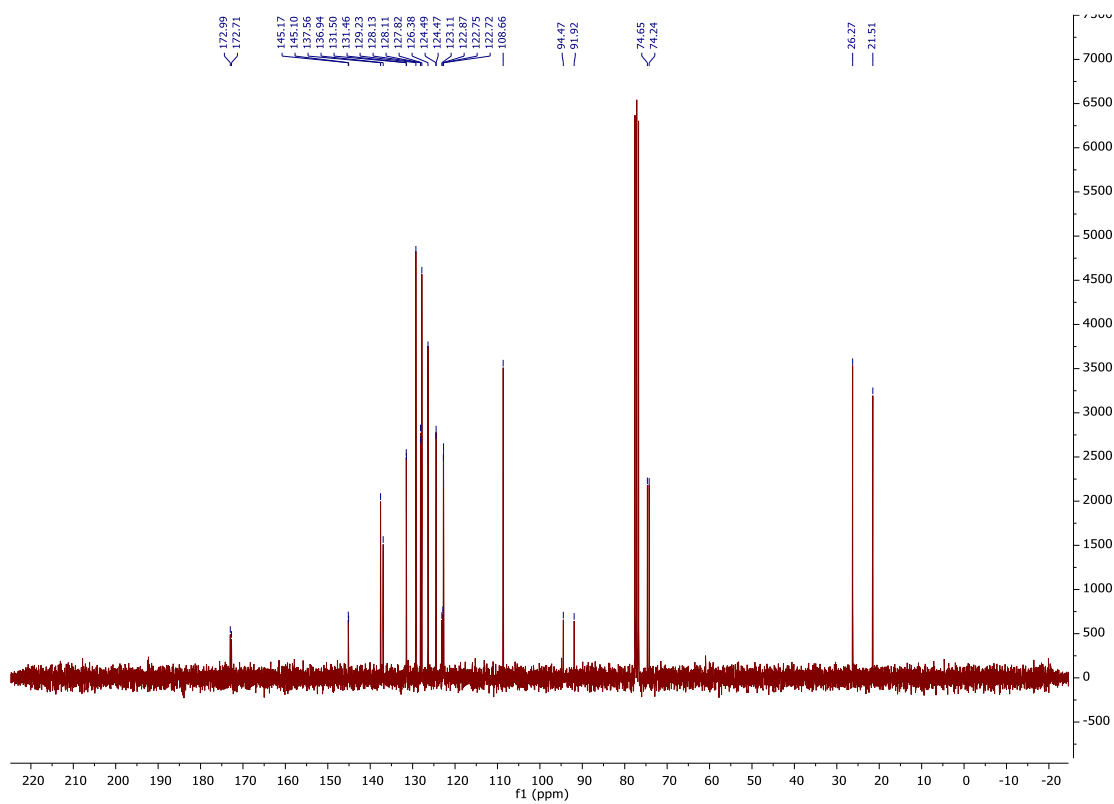


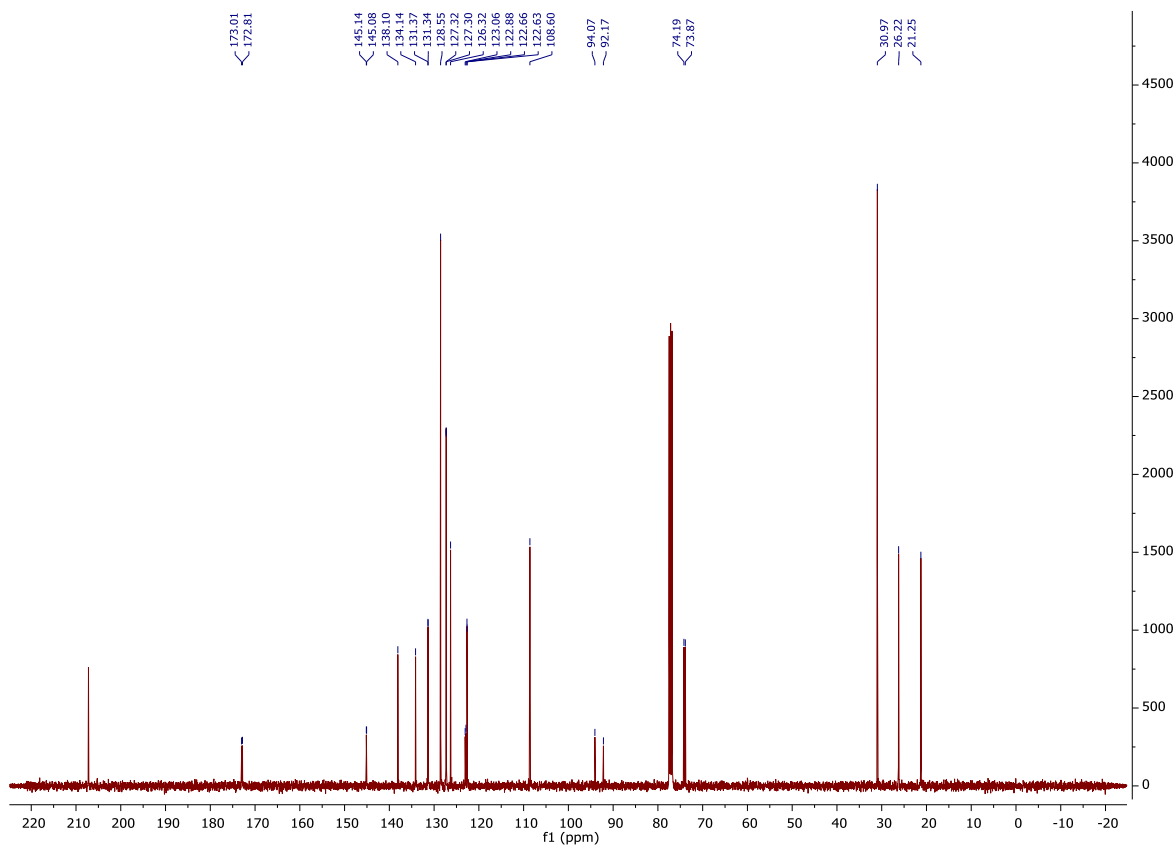
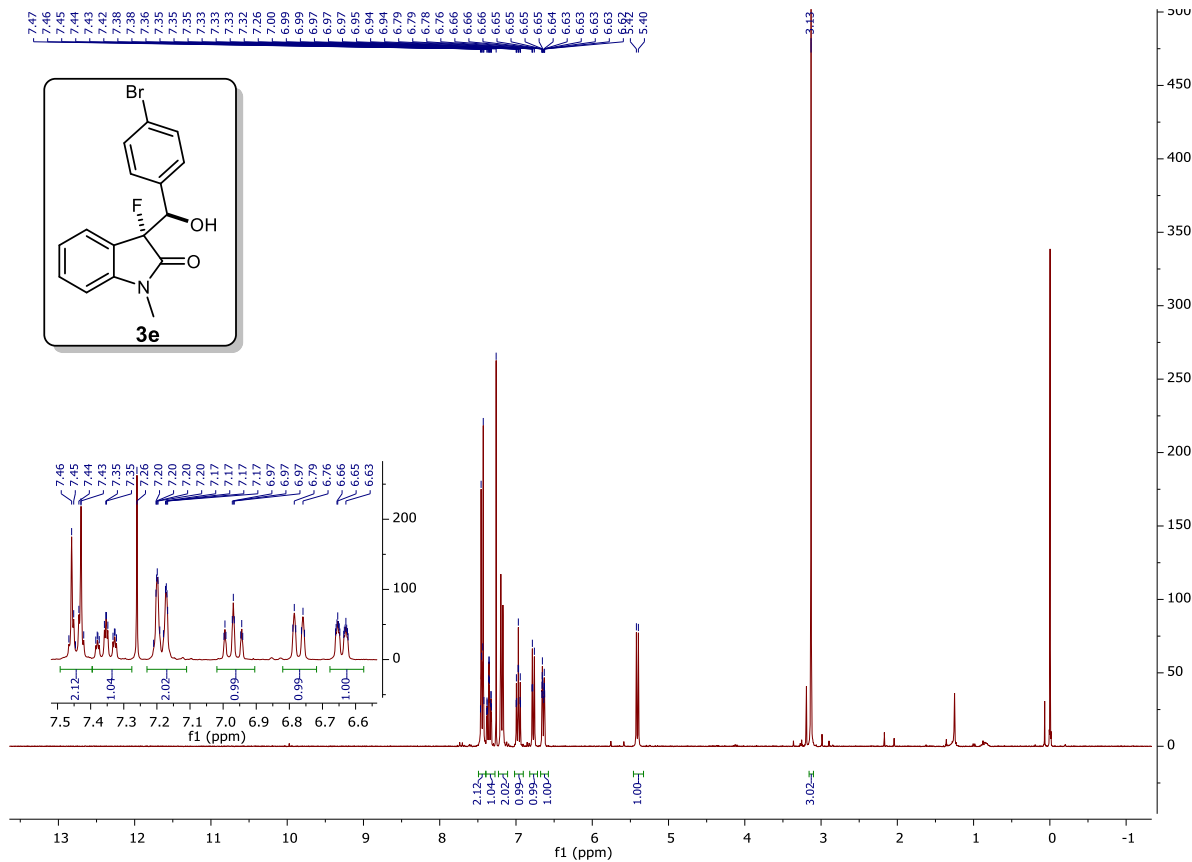


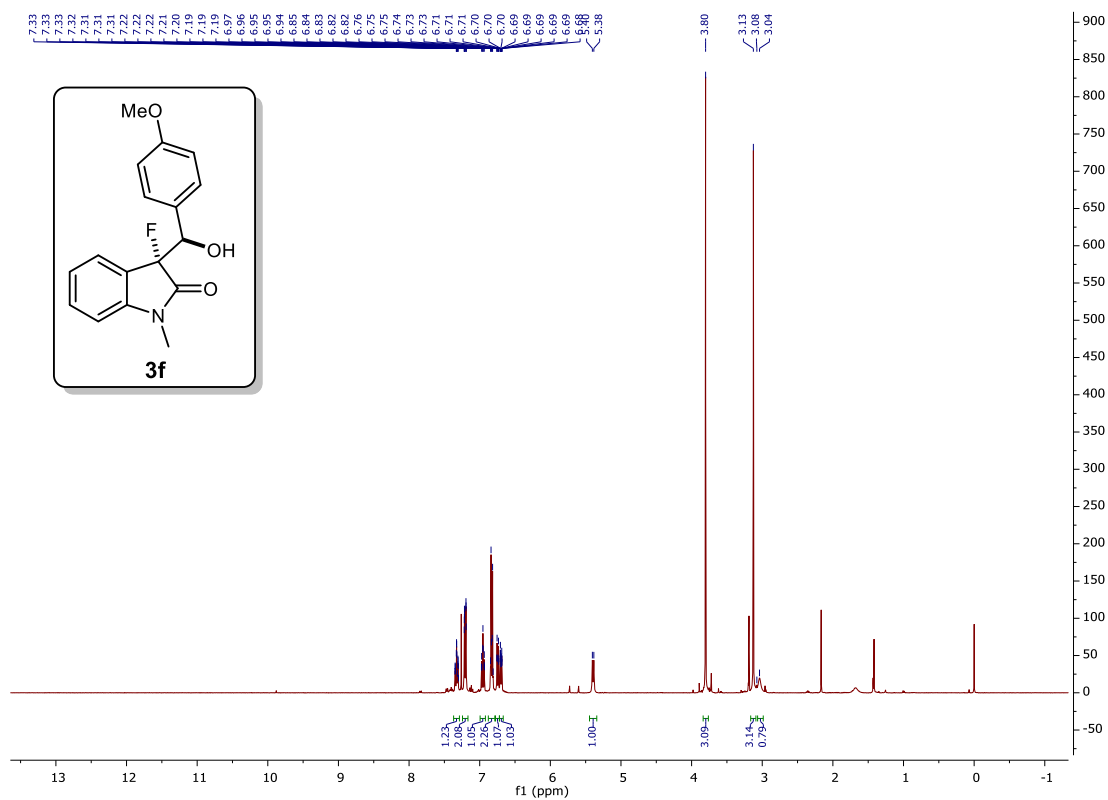
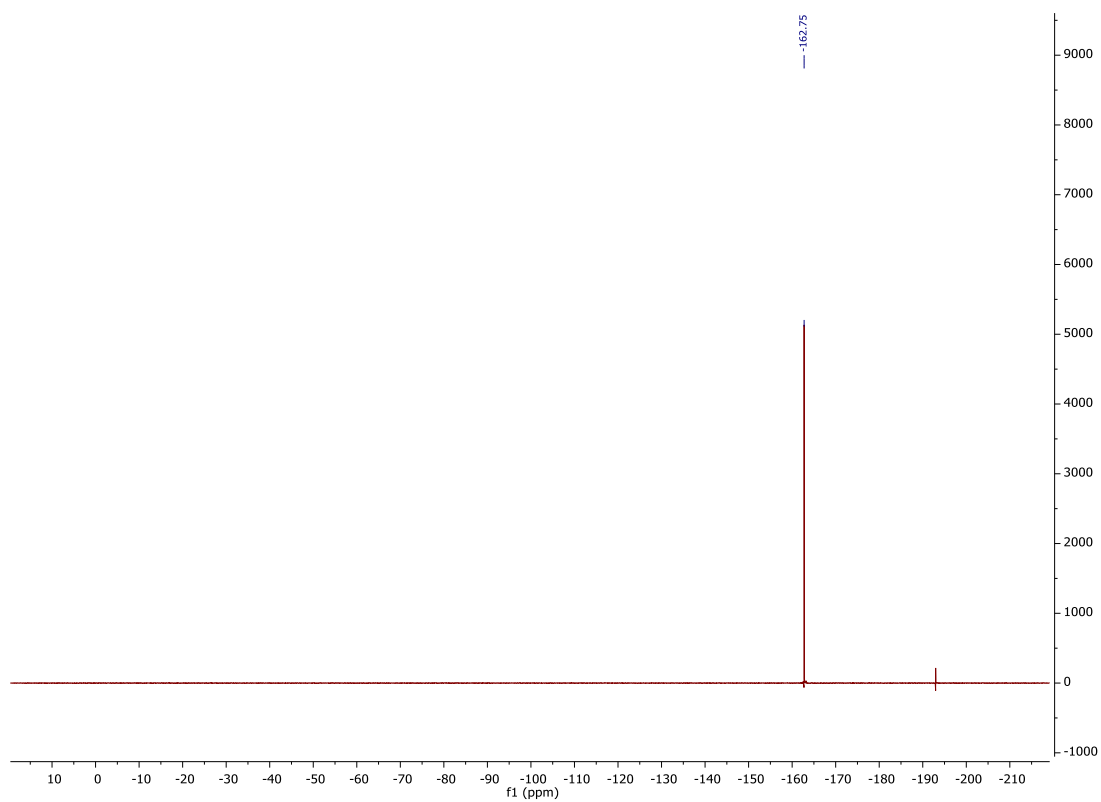


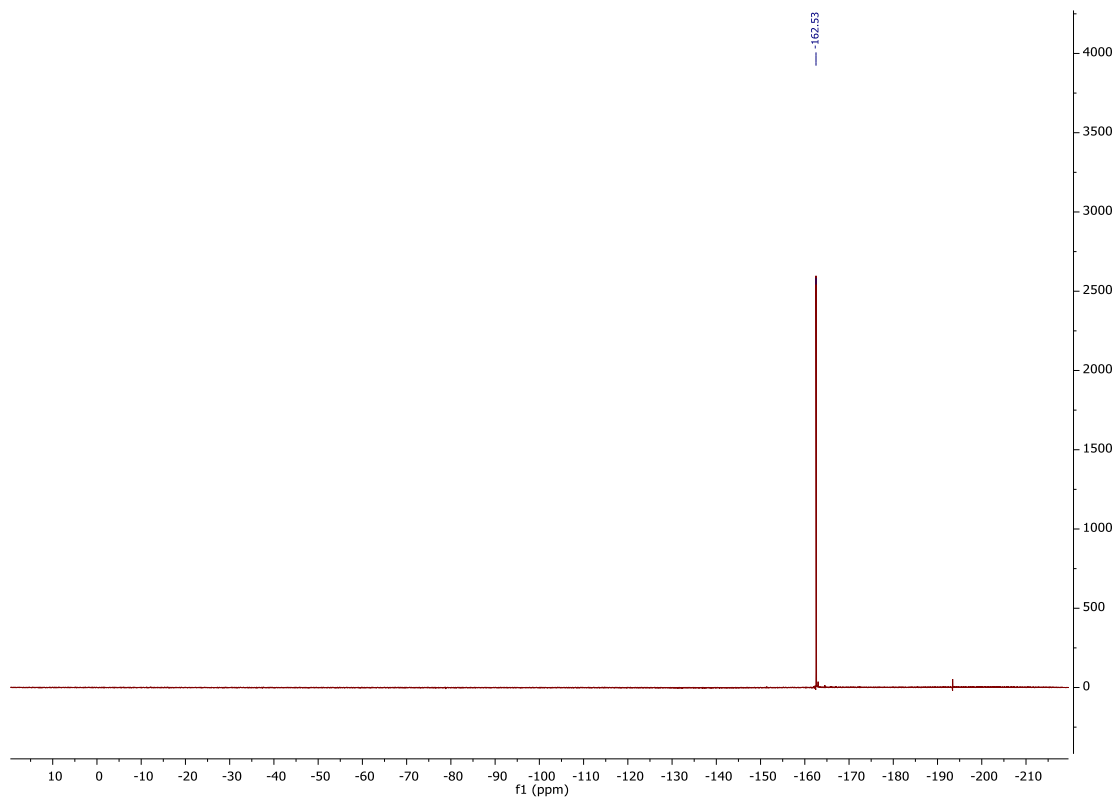
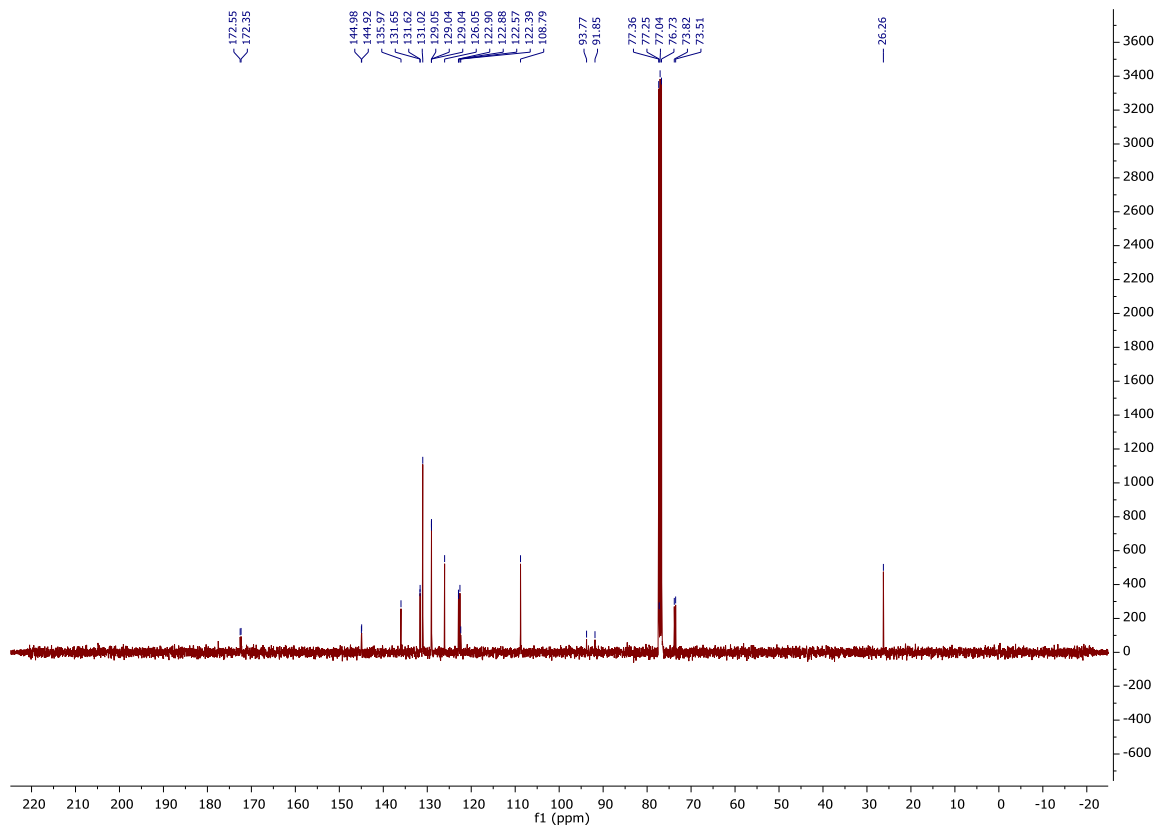


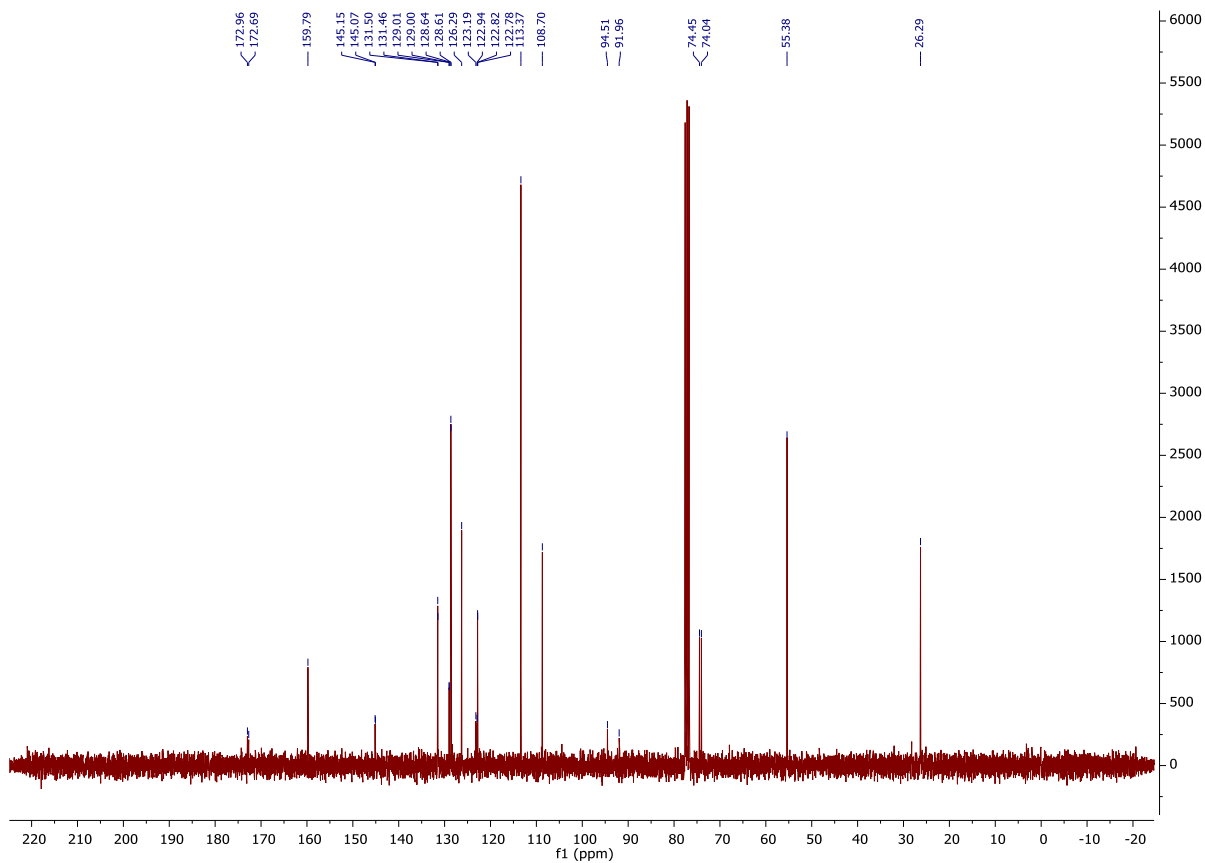
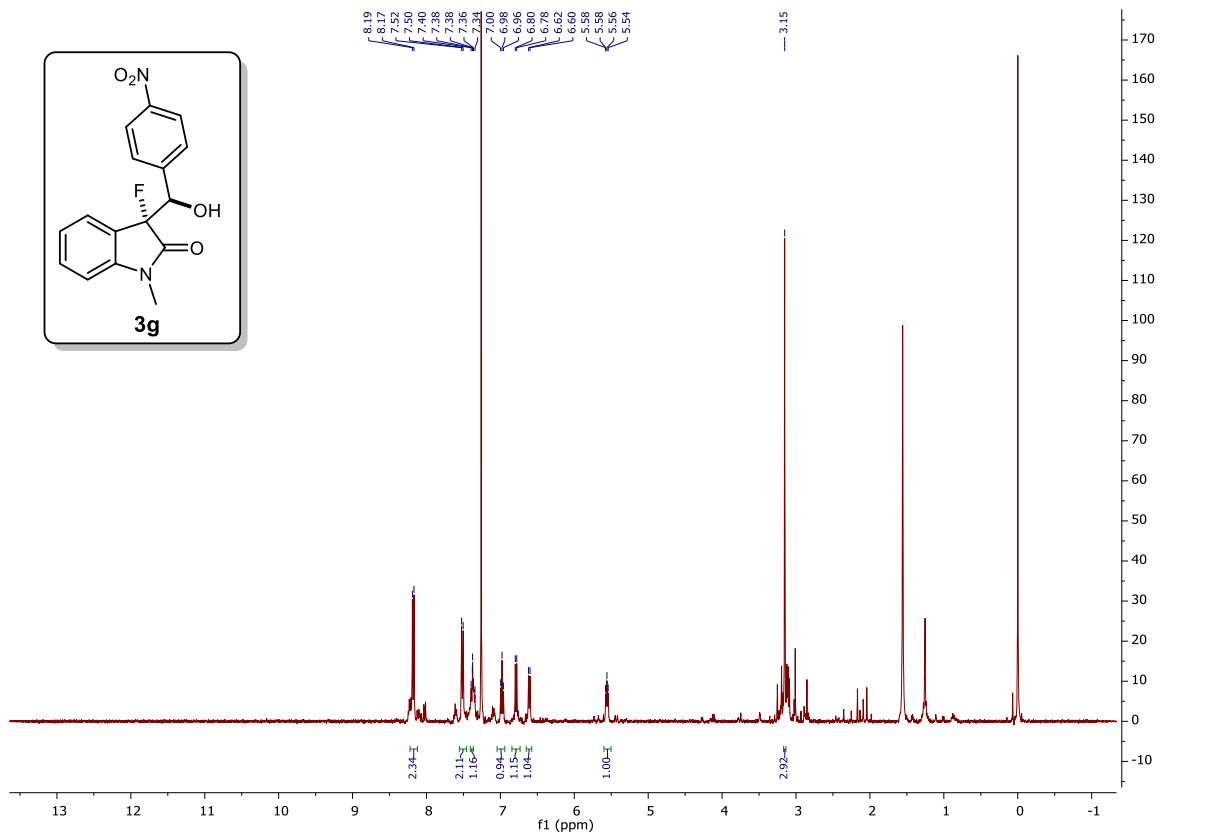


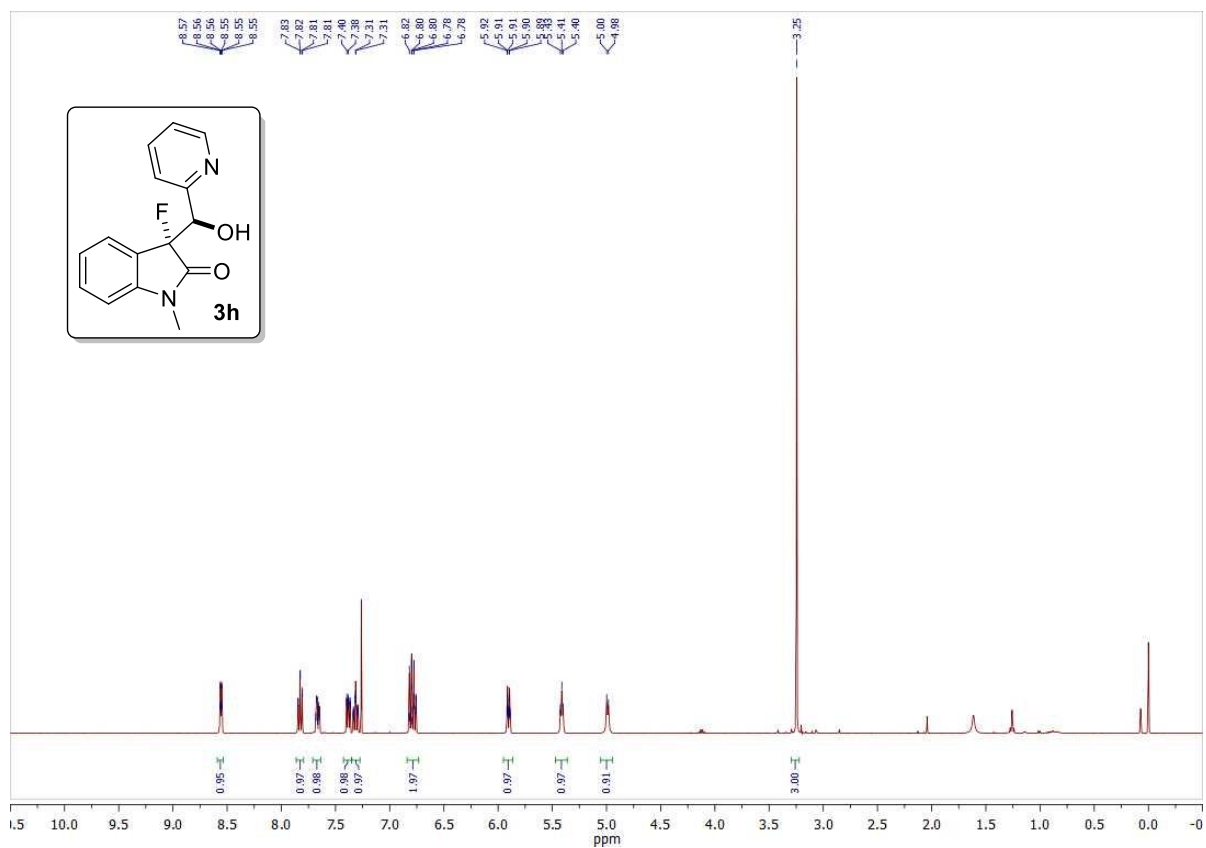
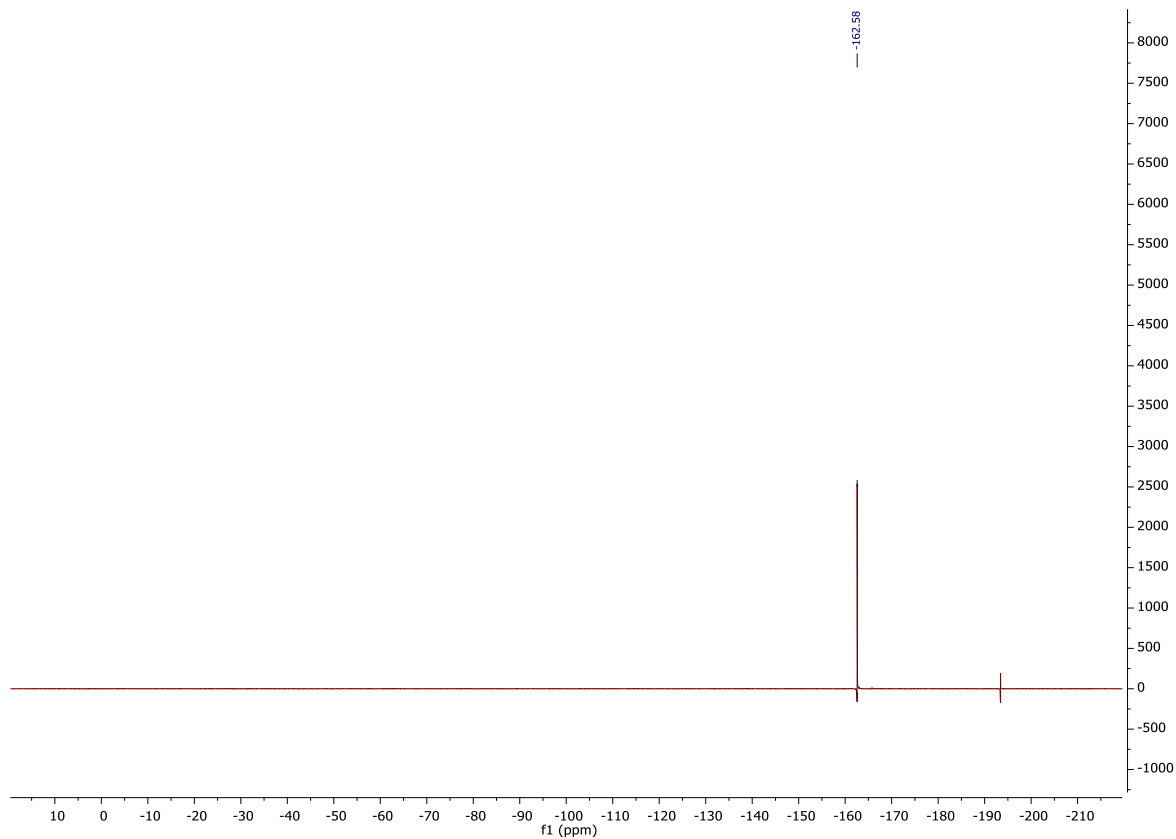


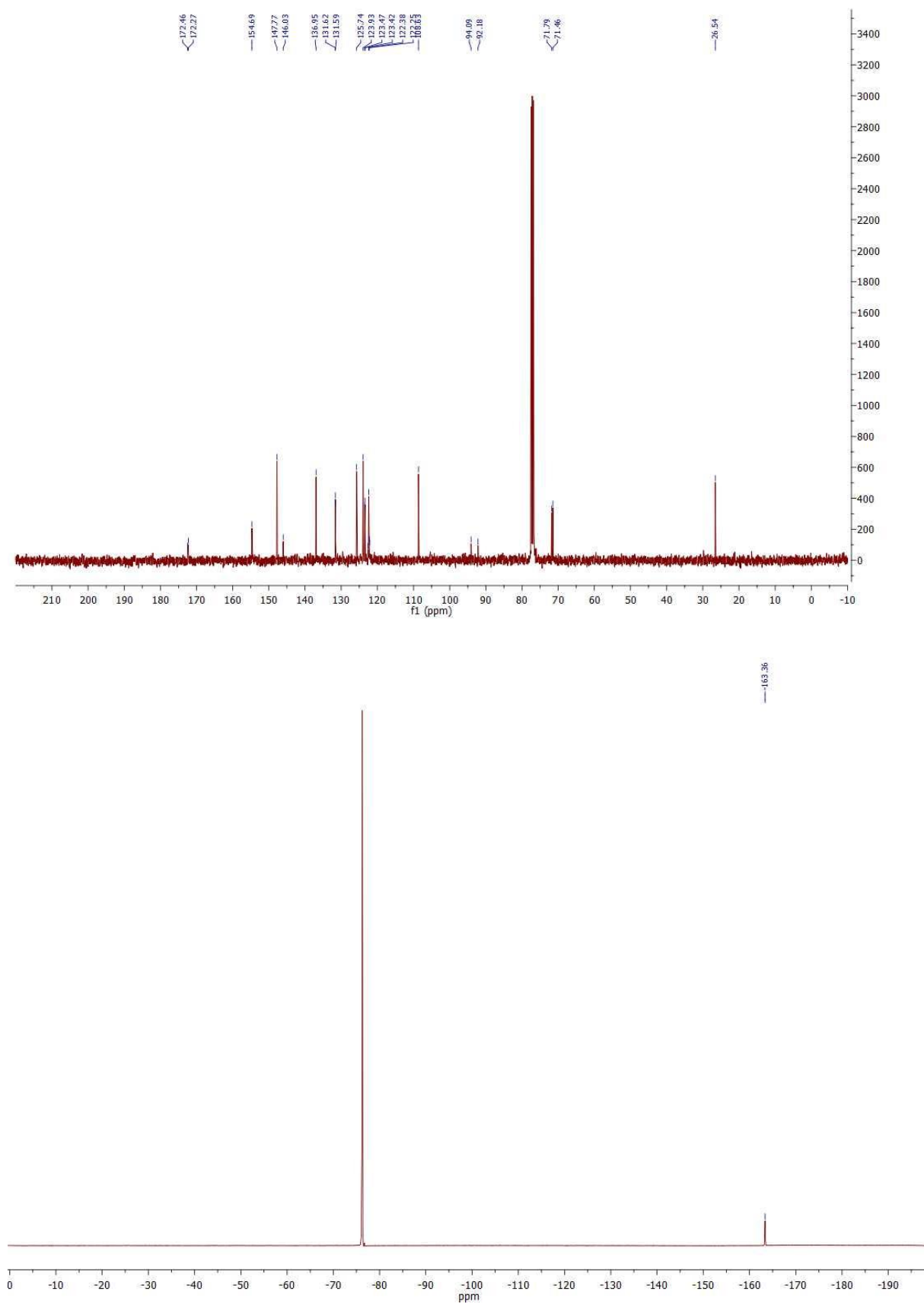


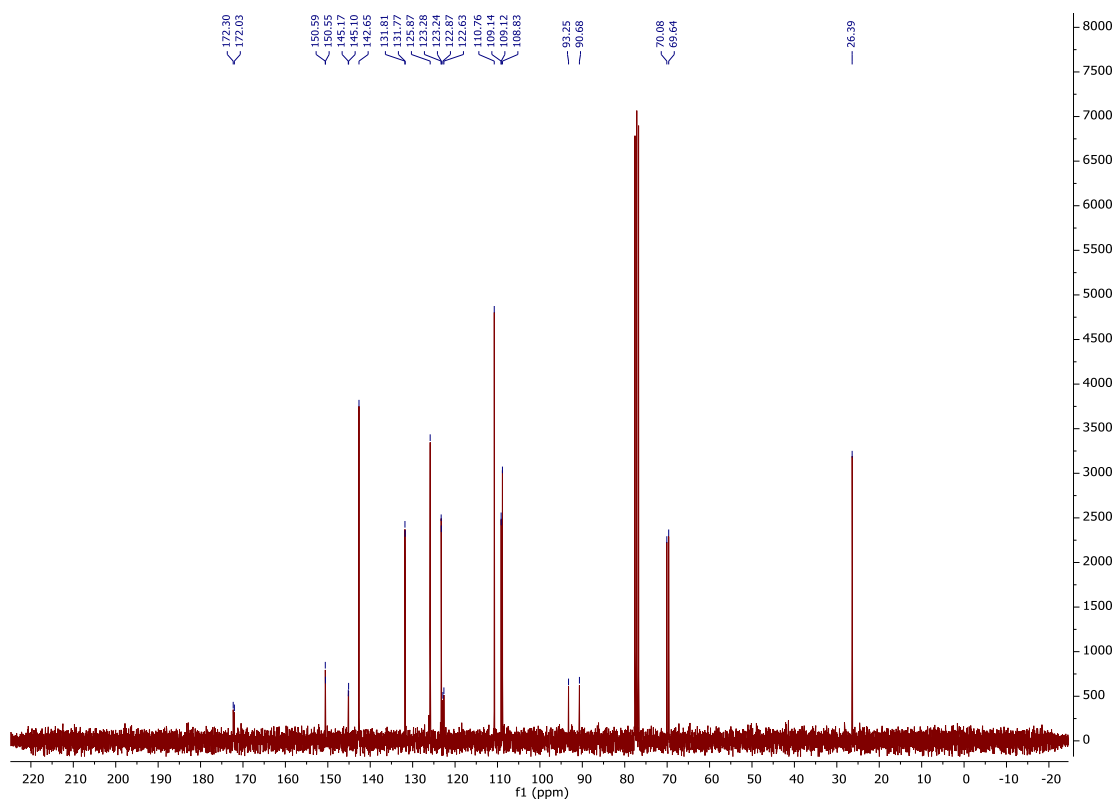
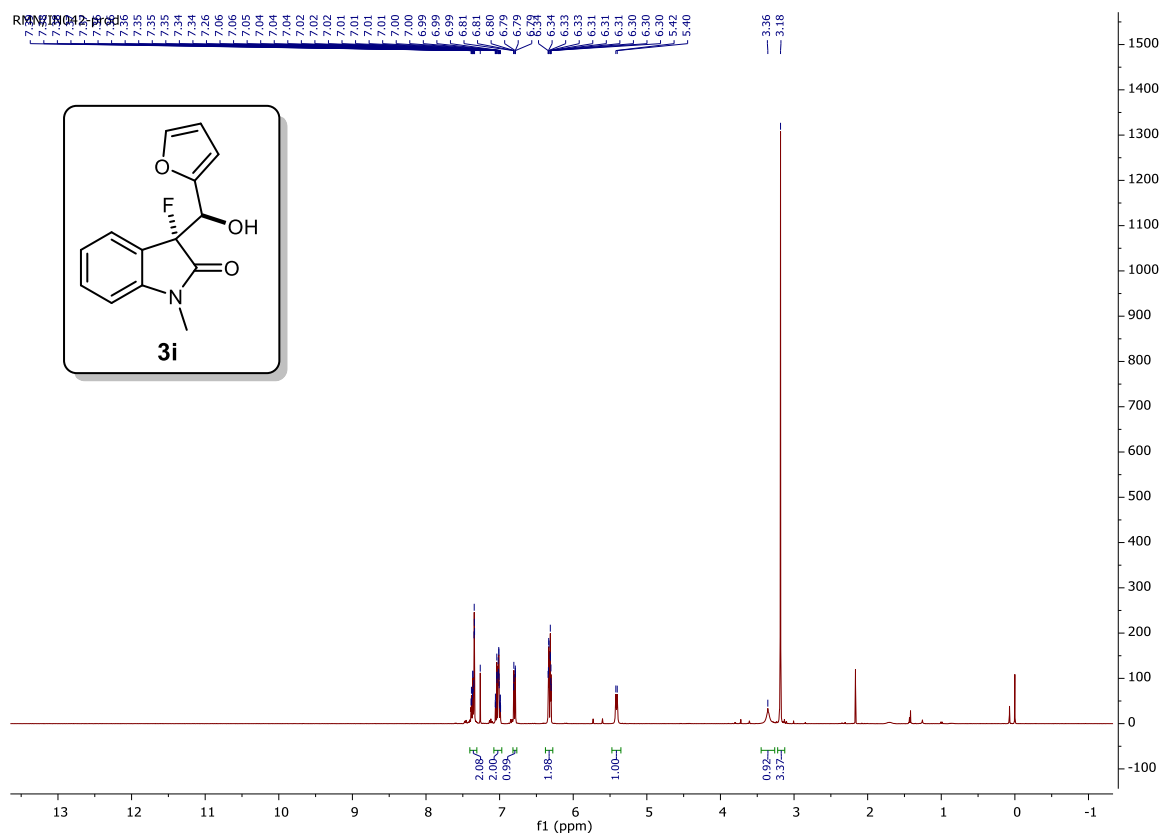


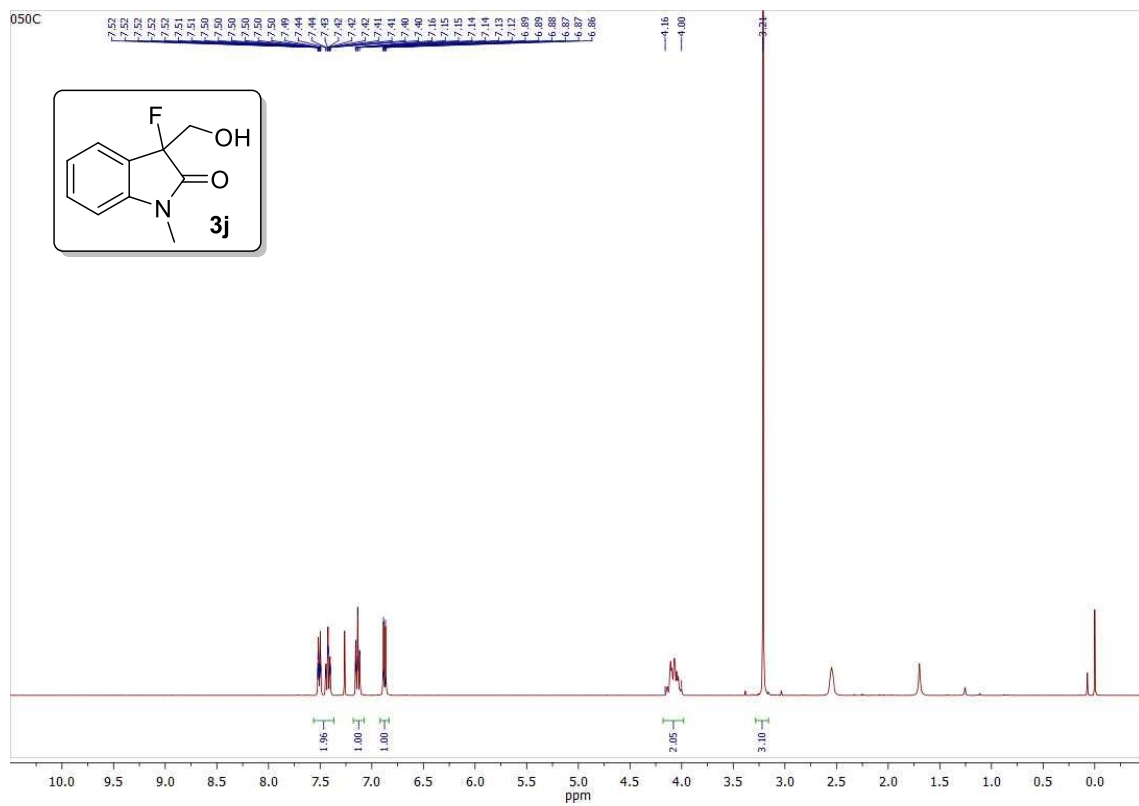
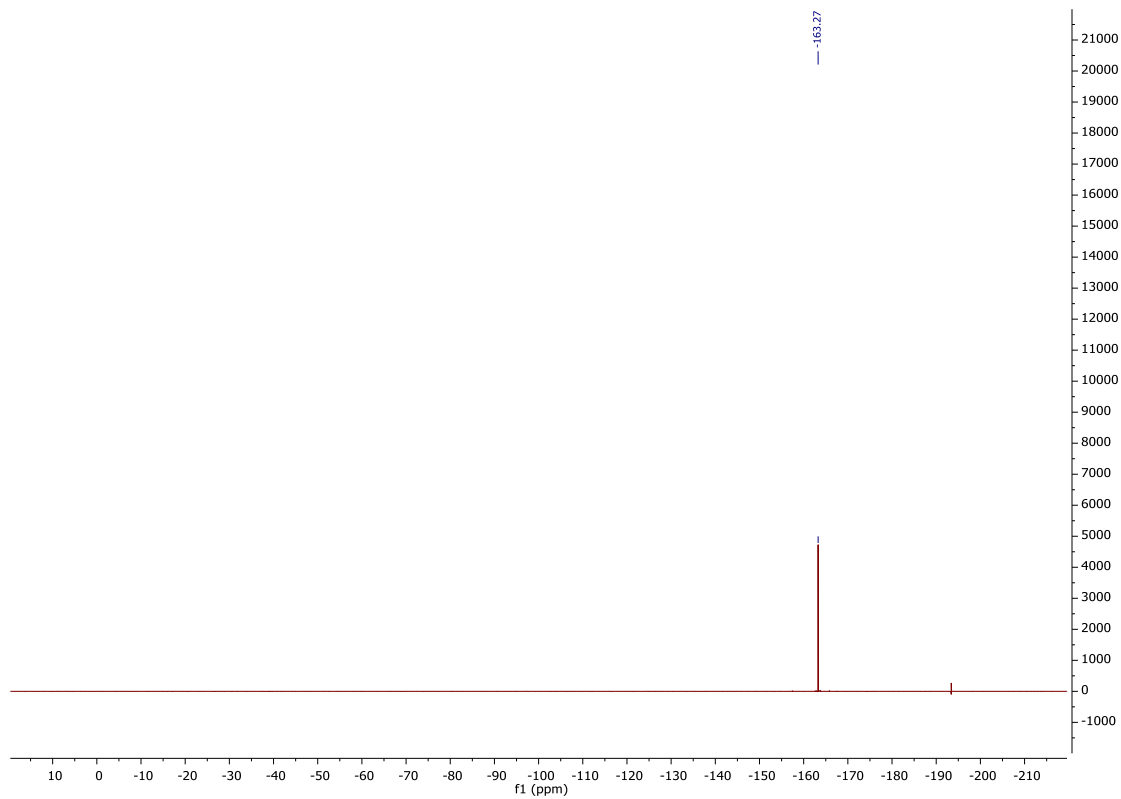


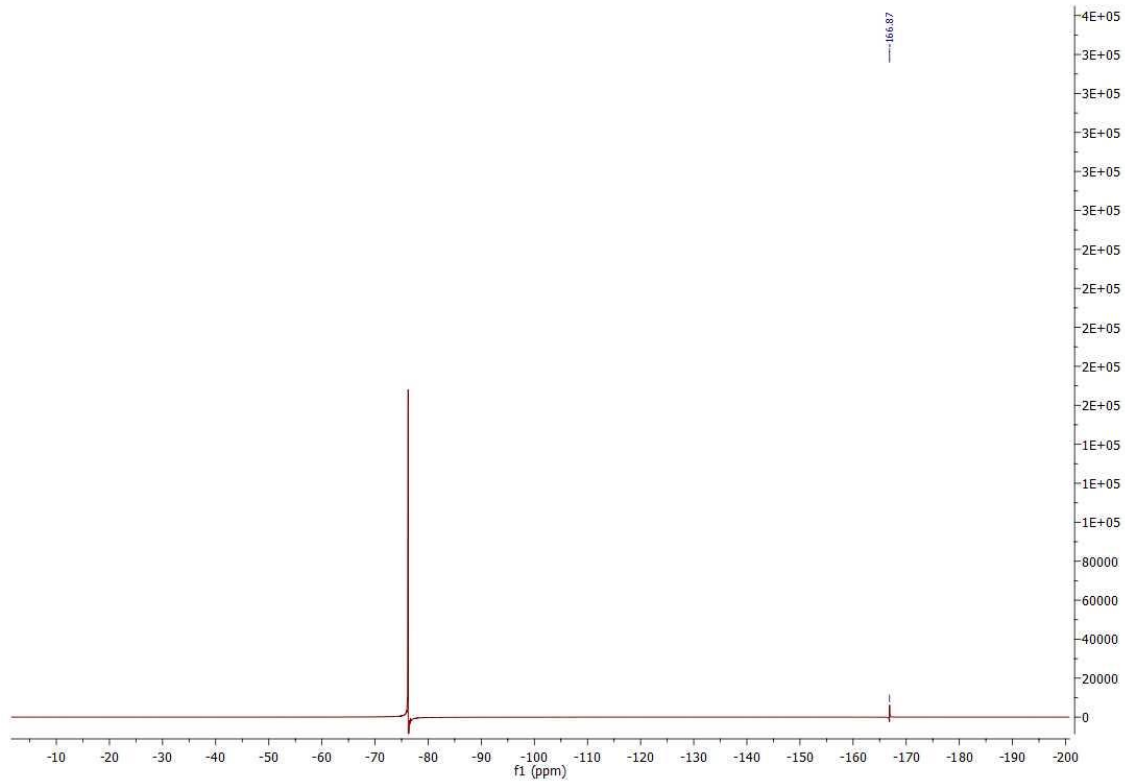
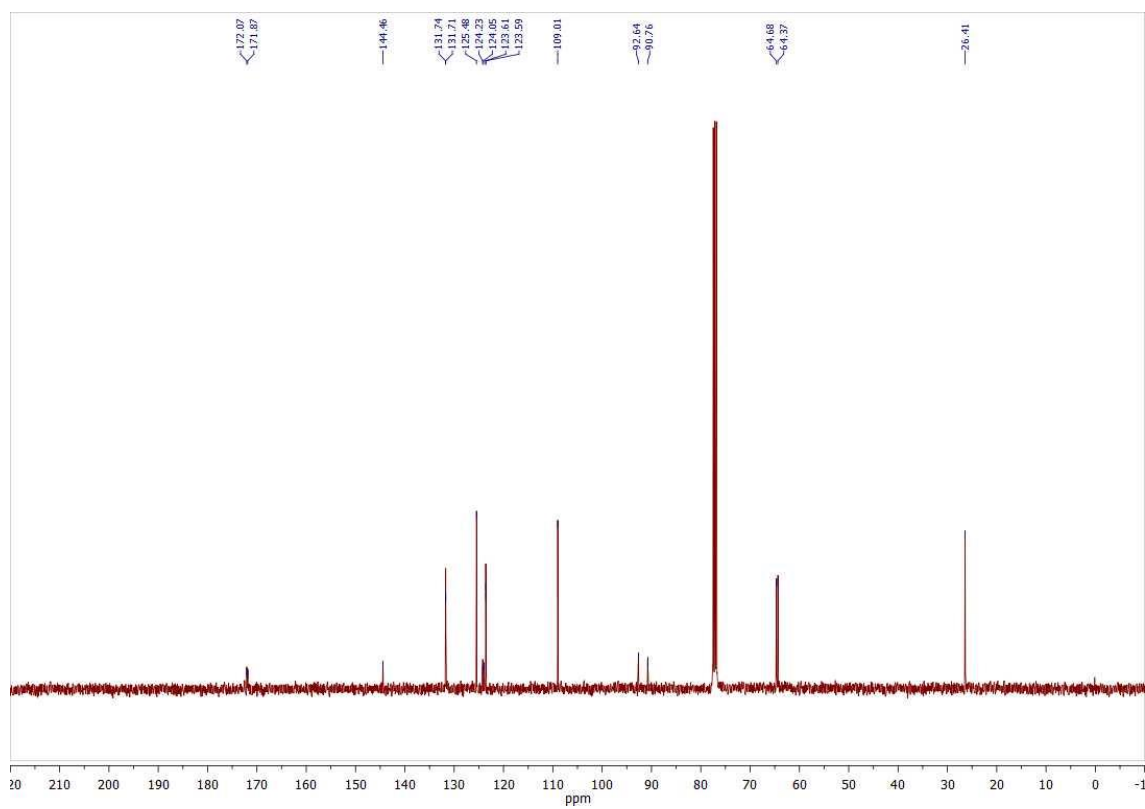


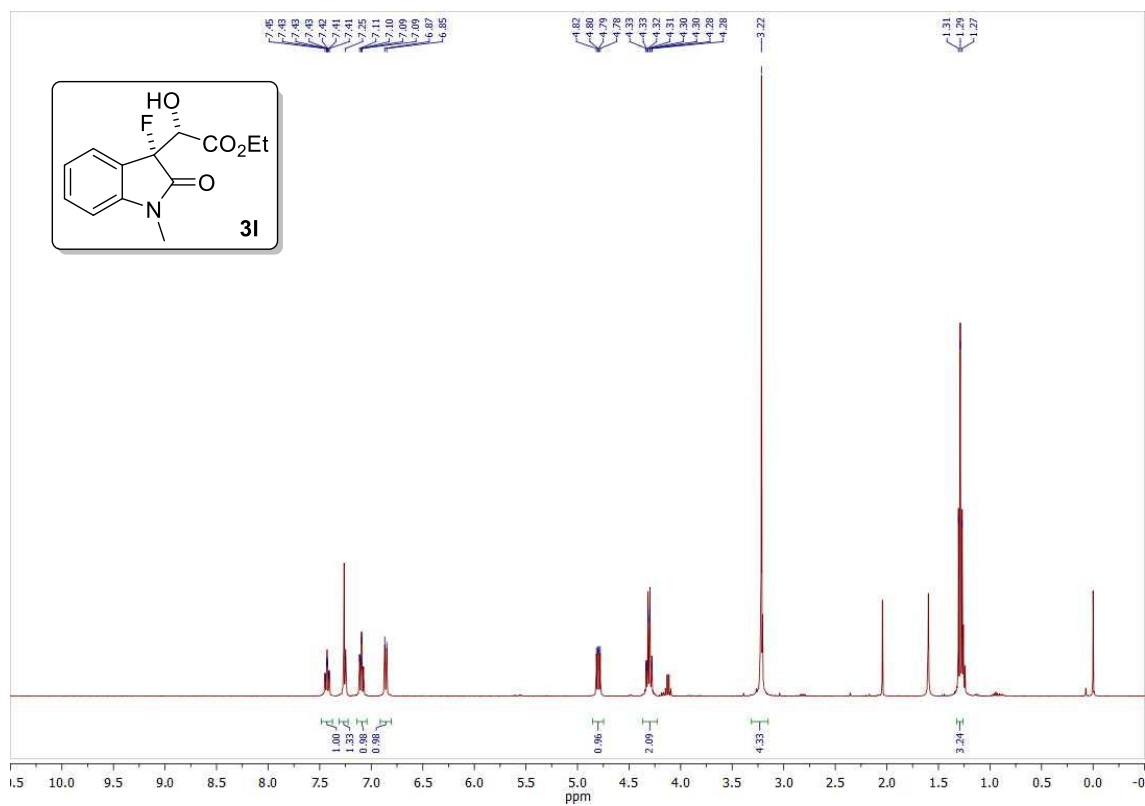
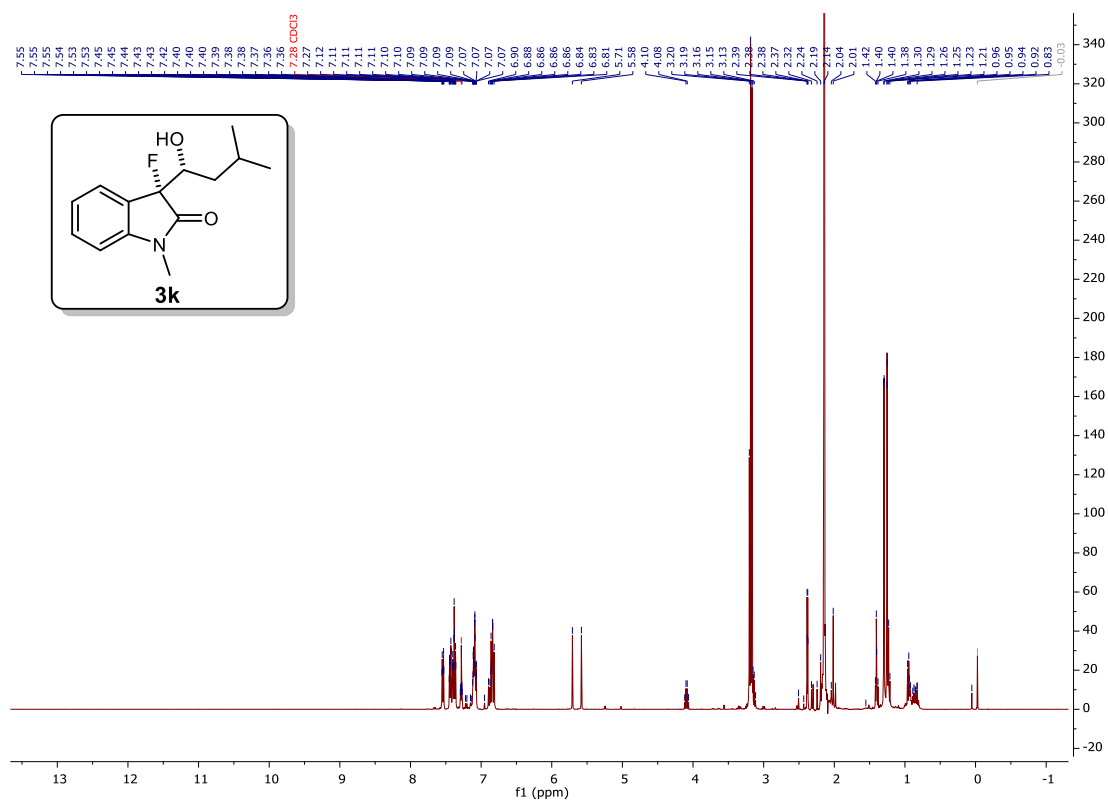


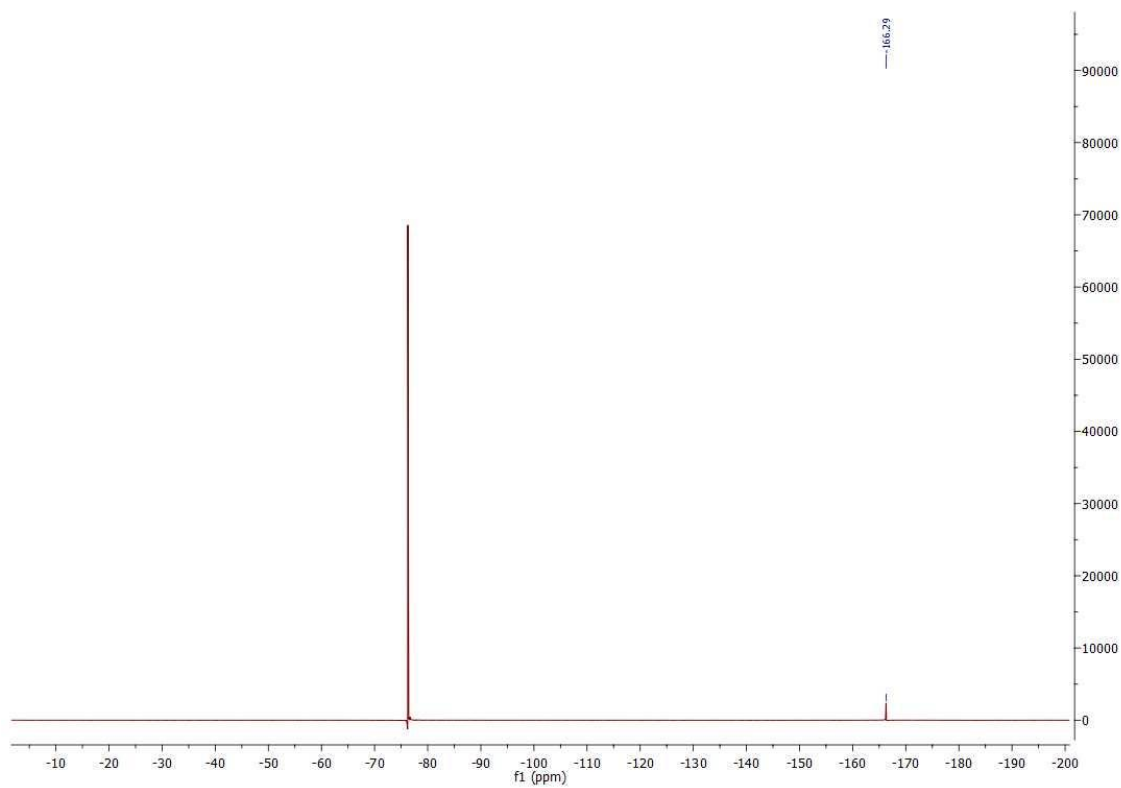
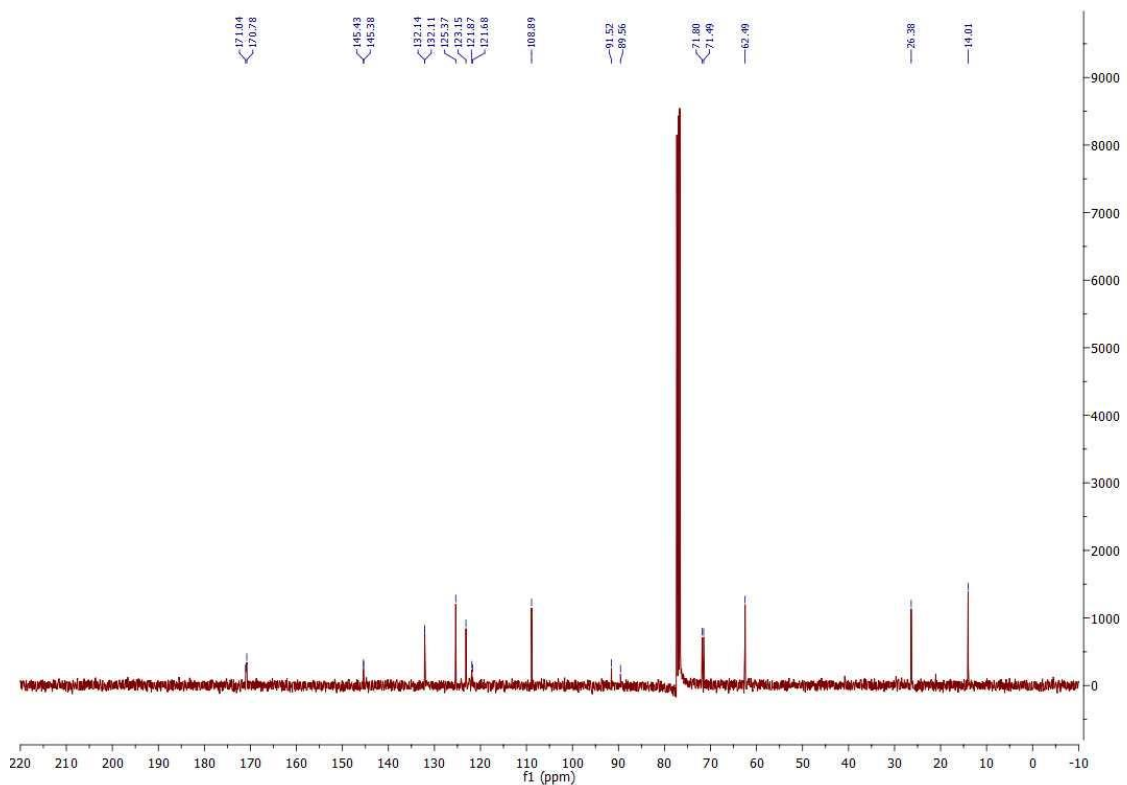


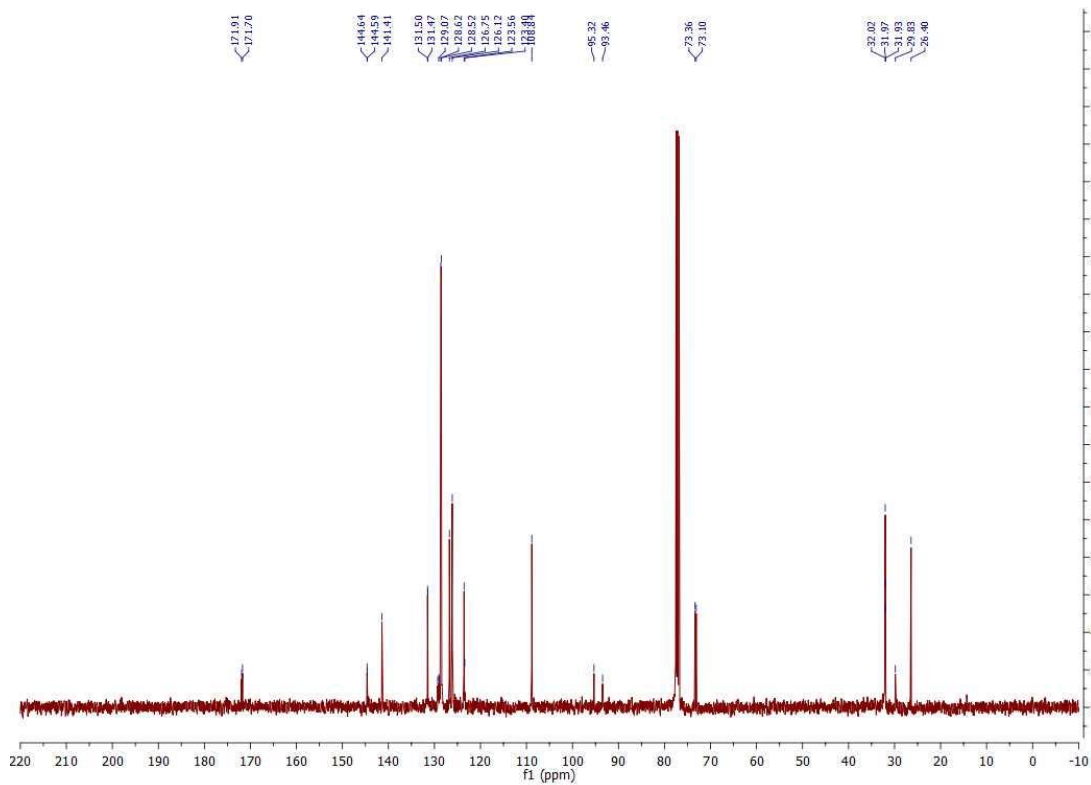
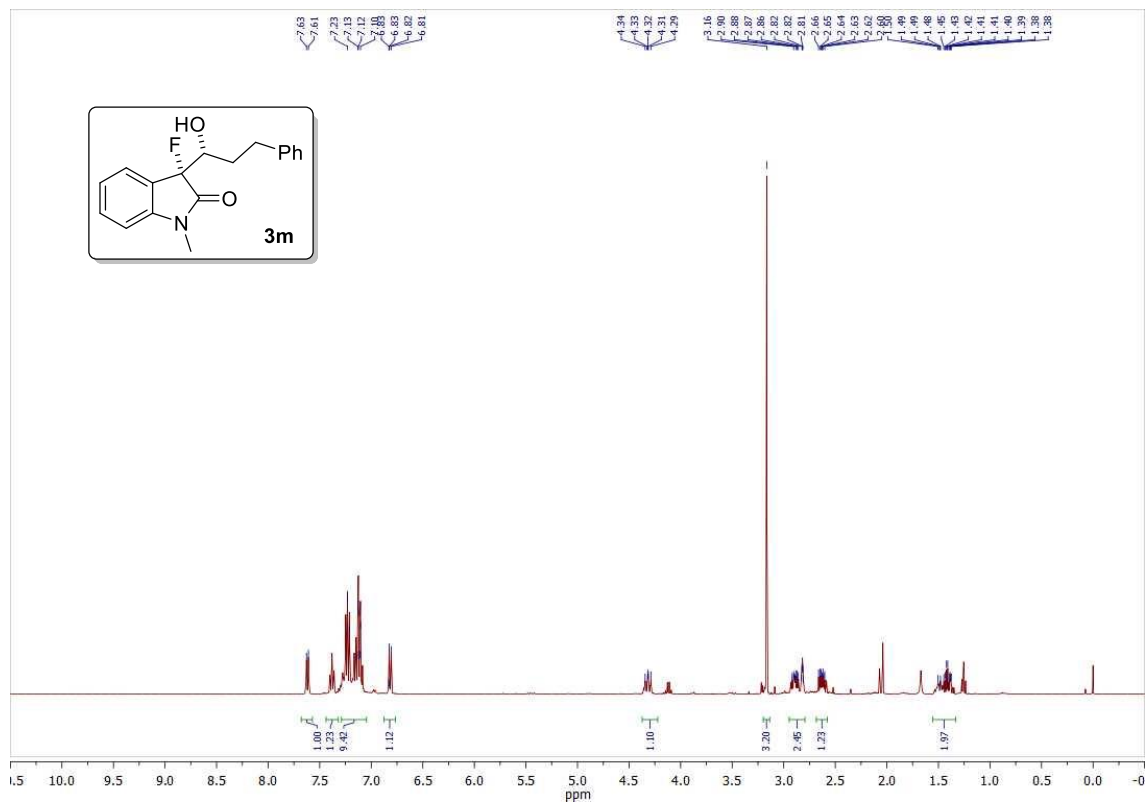


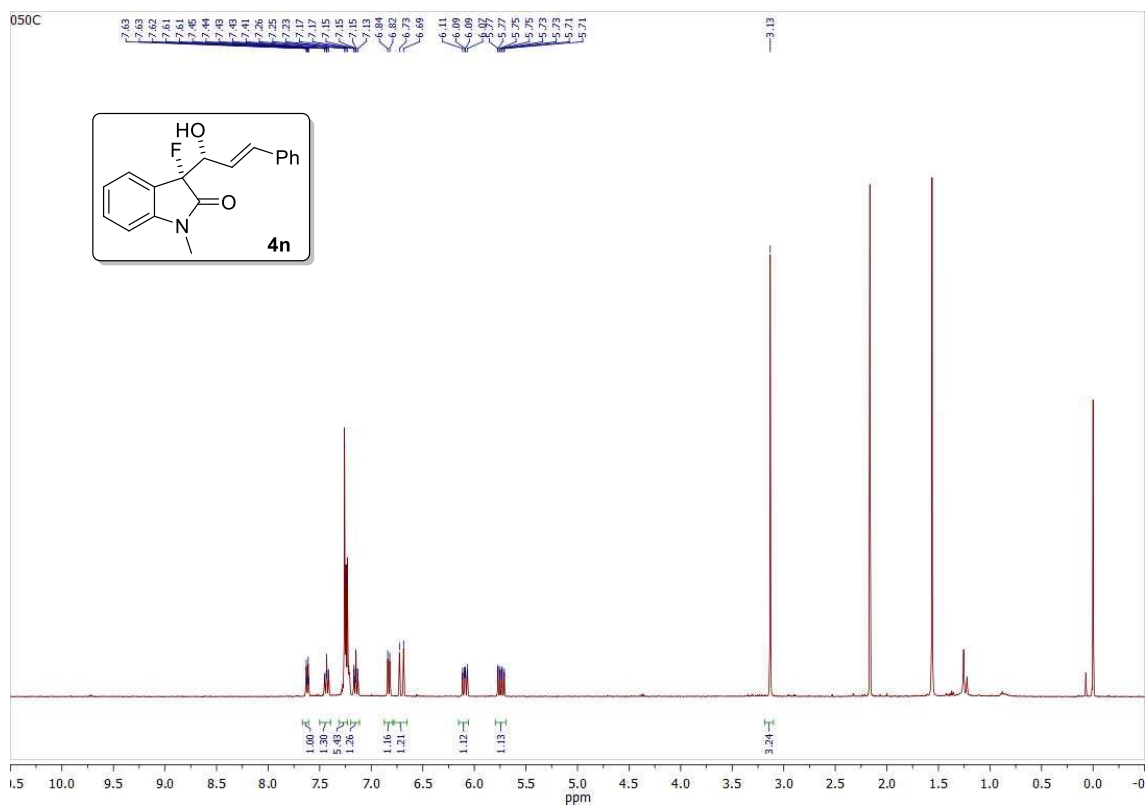
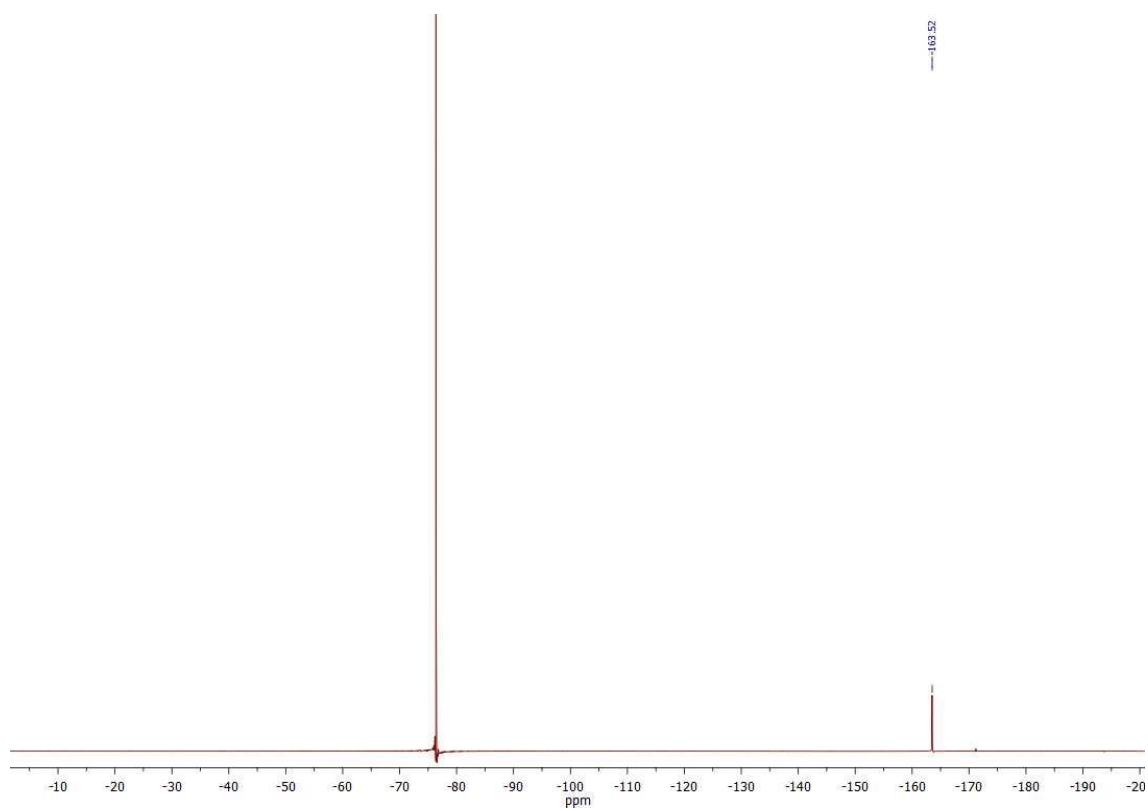


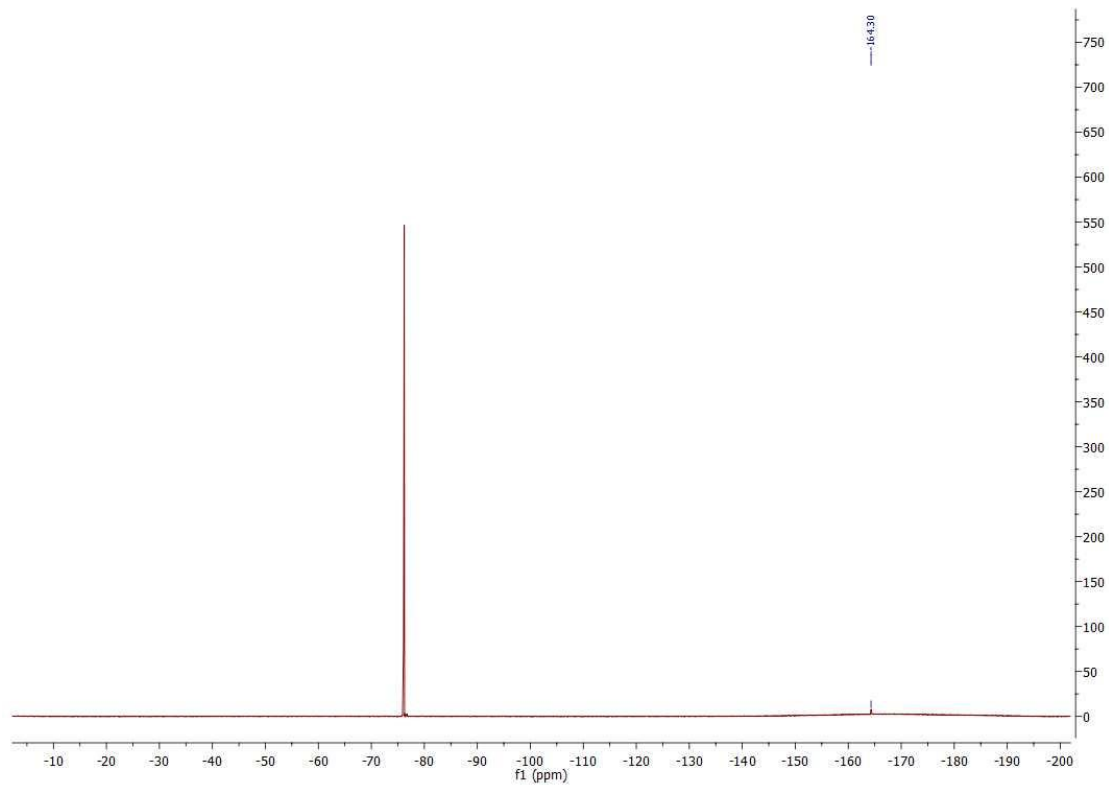
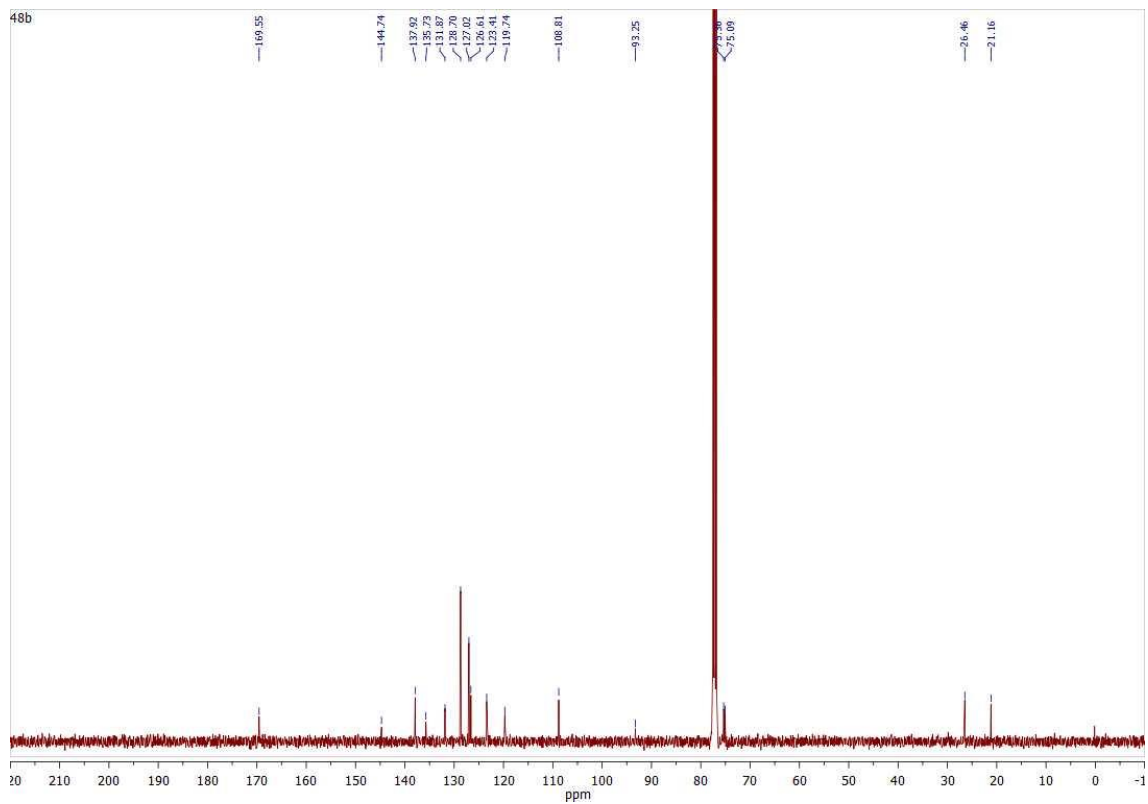












2. COMPUTATIONAL DETAILS

All of the calculations were performed using the Gaussian09 program.¹ Computations were done using B3LYP functional² in conjunction with Grimme's dispersion correction.³ Standard basis sets def2SVP was employed.⁴ 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.⁵ 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),⁶ using the Hratchian-Schlegel algorithm.⁷ 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_{trans} contribution and considering a 1M concentration.⁸ Structural representations were generated using CYLView.⁹

Energies

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

	E_0	ΔE_0	G	ΔG	im. freq
EN	-1282.122492		-1282.187897		
BA	-345.627457		-345.657969		
REAGENTS ^a	-1395.305108	0.0	-1395.374081	0.0	
SC	-1395.301210	2.4	-1395.366492	4.8	
(<i>R,R</i>)- TS	-1395.302850	1.4	-1395.367677	4.0	-354.0
(<i>R,S</i>)- TS	-1395.298237	4.3	-1395.363829	6.4	-354.4
(<i>R,R</i>)- PR	-1395.308442	-2.1	-1395.373290	0.5	
(<i>R,S</i>)- PR	-1395.305077	0.0	-1395.368071	3.8	

Cartesian Coordinates

¹ 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.

² (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.

³ (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.

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

⁵ (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.

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

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

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

⁹ 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

O 1

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