

Triethylamine-Promoted Oxidative Cyclodimerization of 2H-Azirine-2-carboxylates to Pyrimidine-4,6-dicarboxylates: Experimental and DFT Study

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and Nikolai V. Rostovskii ***

Institute of Chemistry, St. Petersburg State University, 7/9 Universitetskaya Nab.,
199034 St. Petersburg, Russia

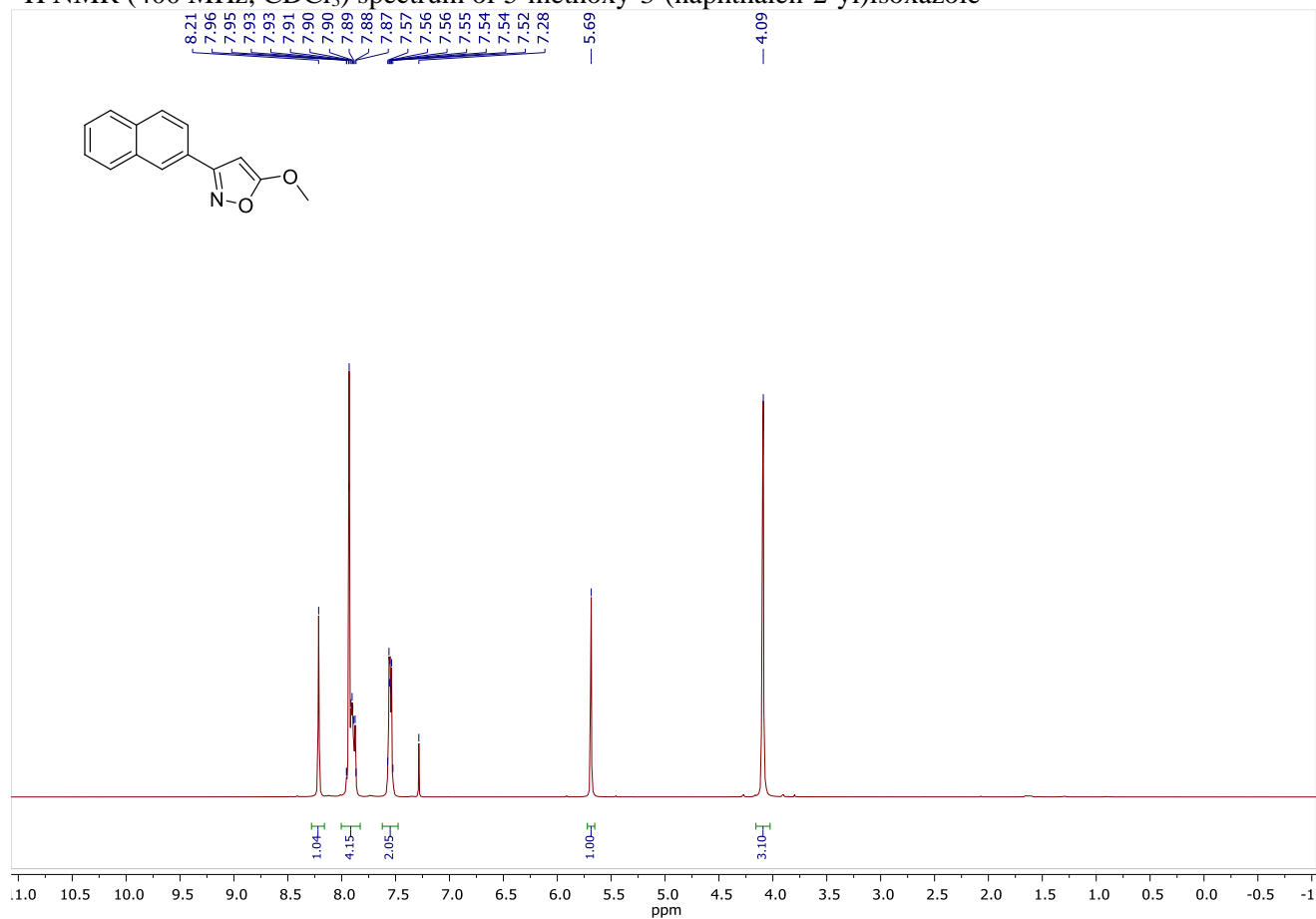
* Correspondence: n.rostovskiy@spbu.ru

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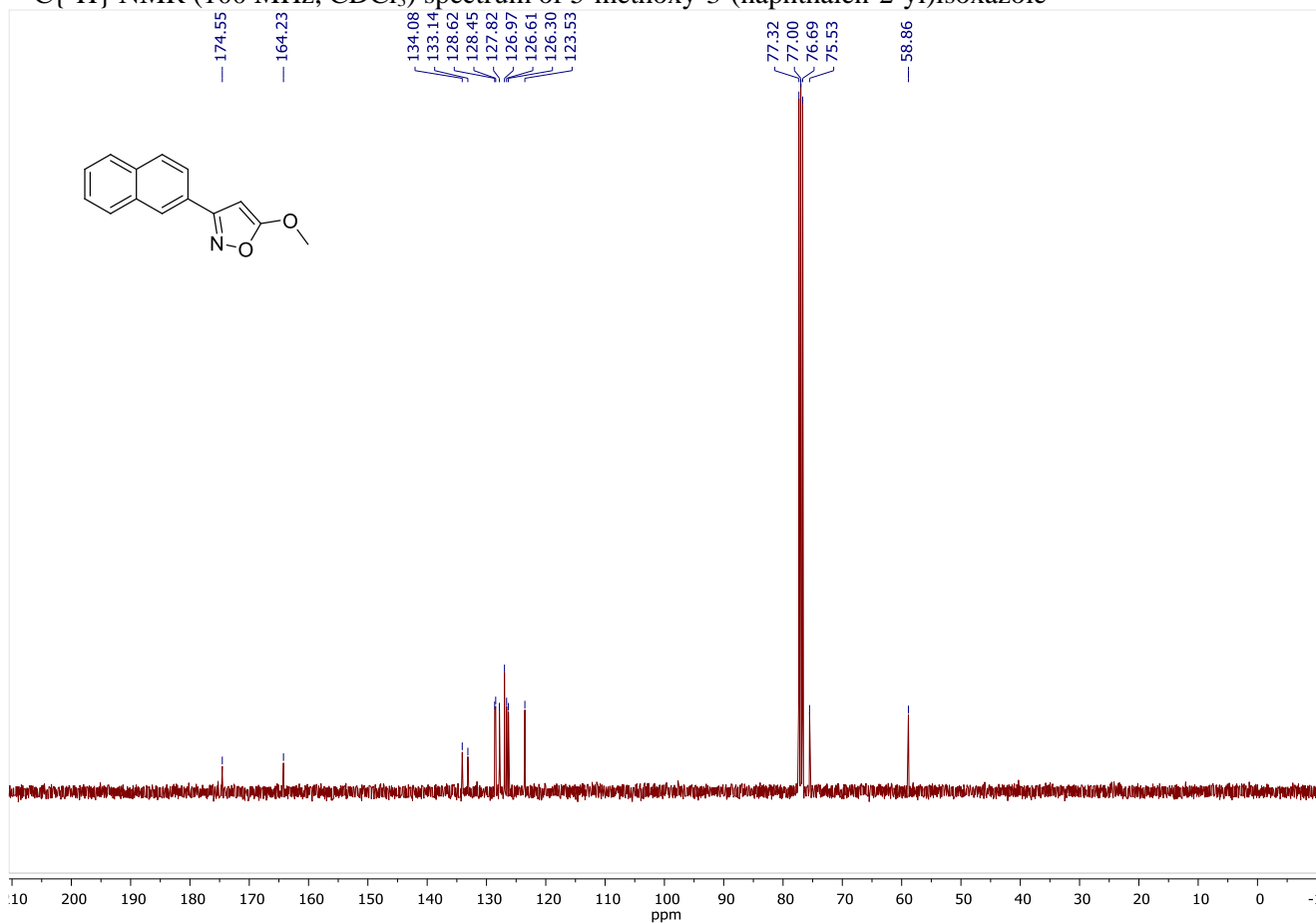
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I. NMR spectroscopy

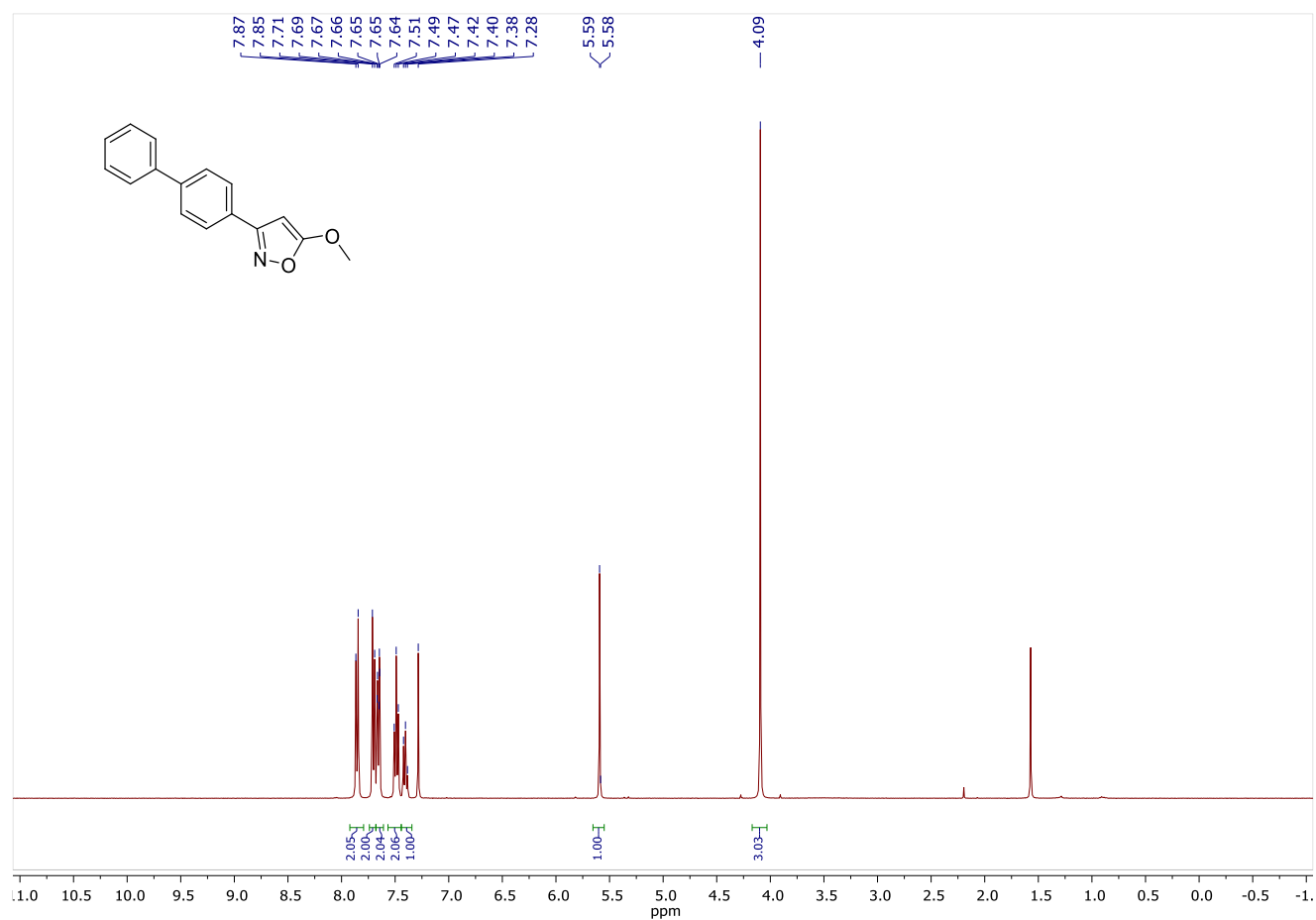
^1H NMR (400 MHz, CDCl_3) spectrum of 5-methoxy-3-(naphthalen-2-yl)isoxazole



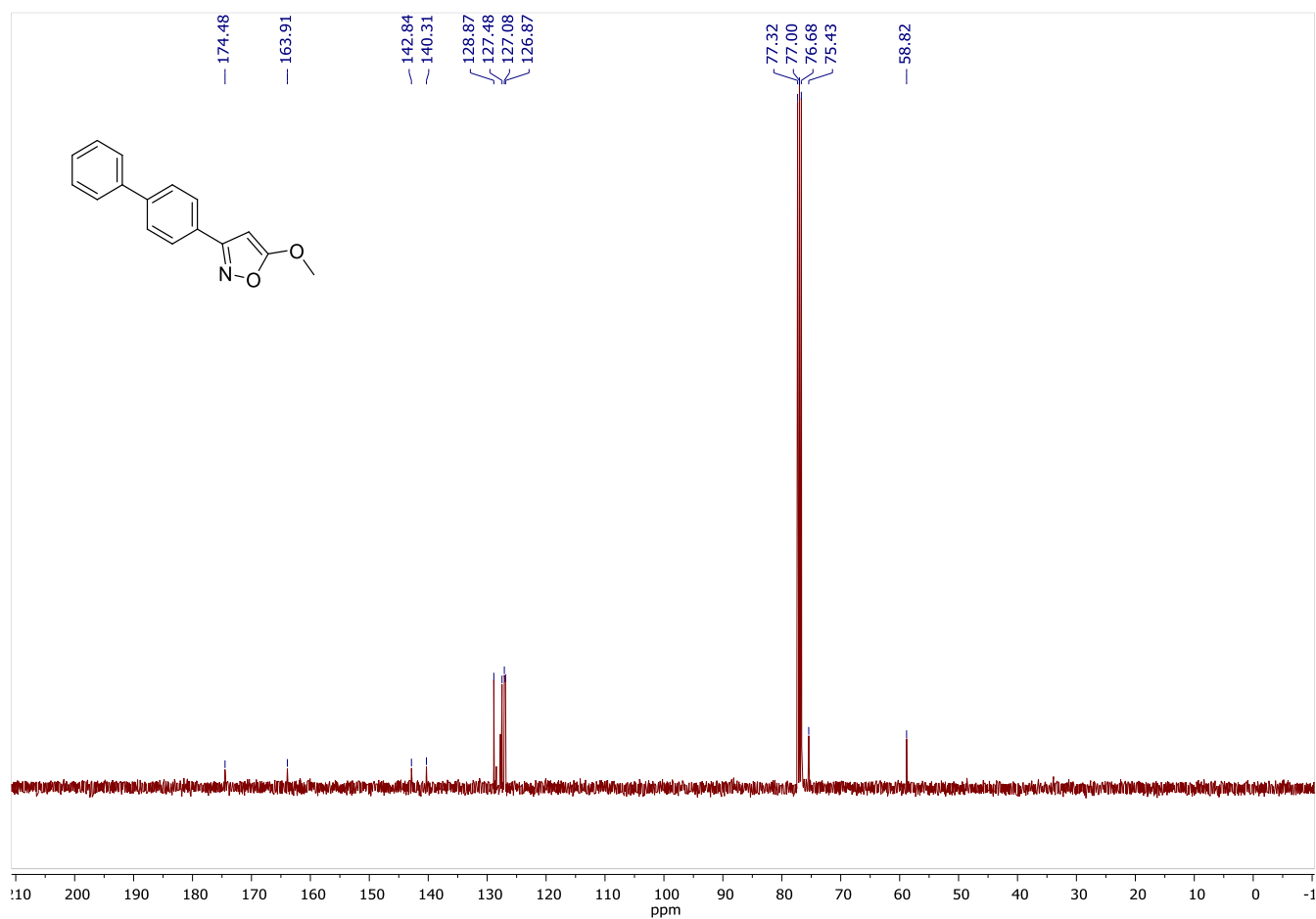
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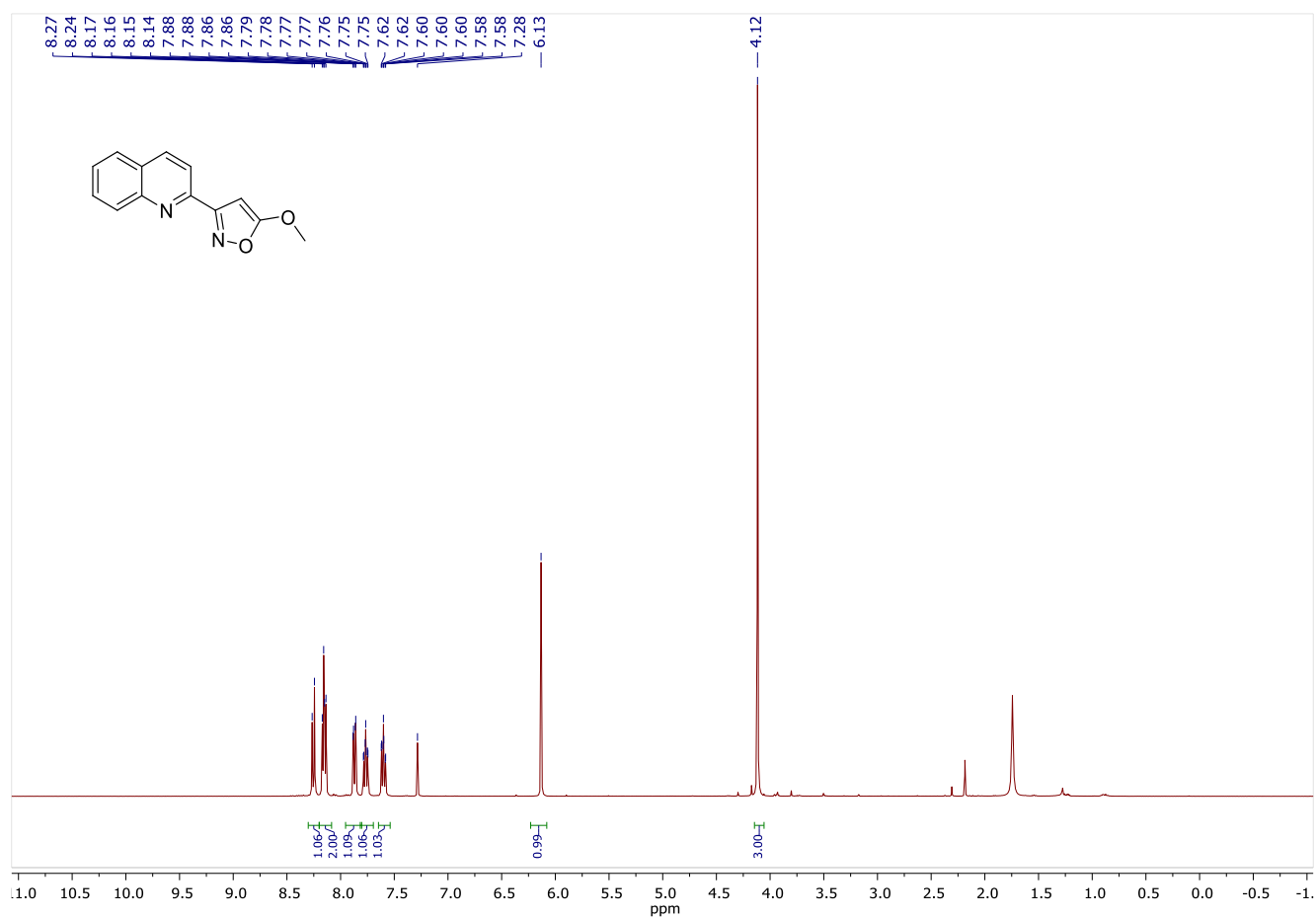
^1H NMR (400 MHz, CDCl_3) spectrum of 3-(biphenyl-4-yl)-5-methoxyisoxazole



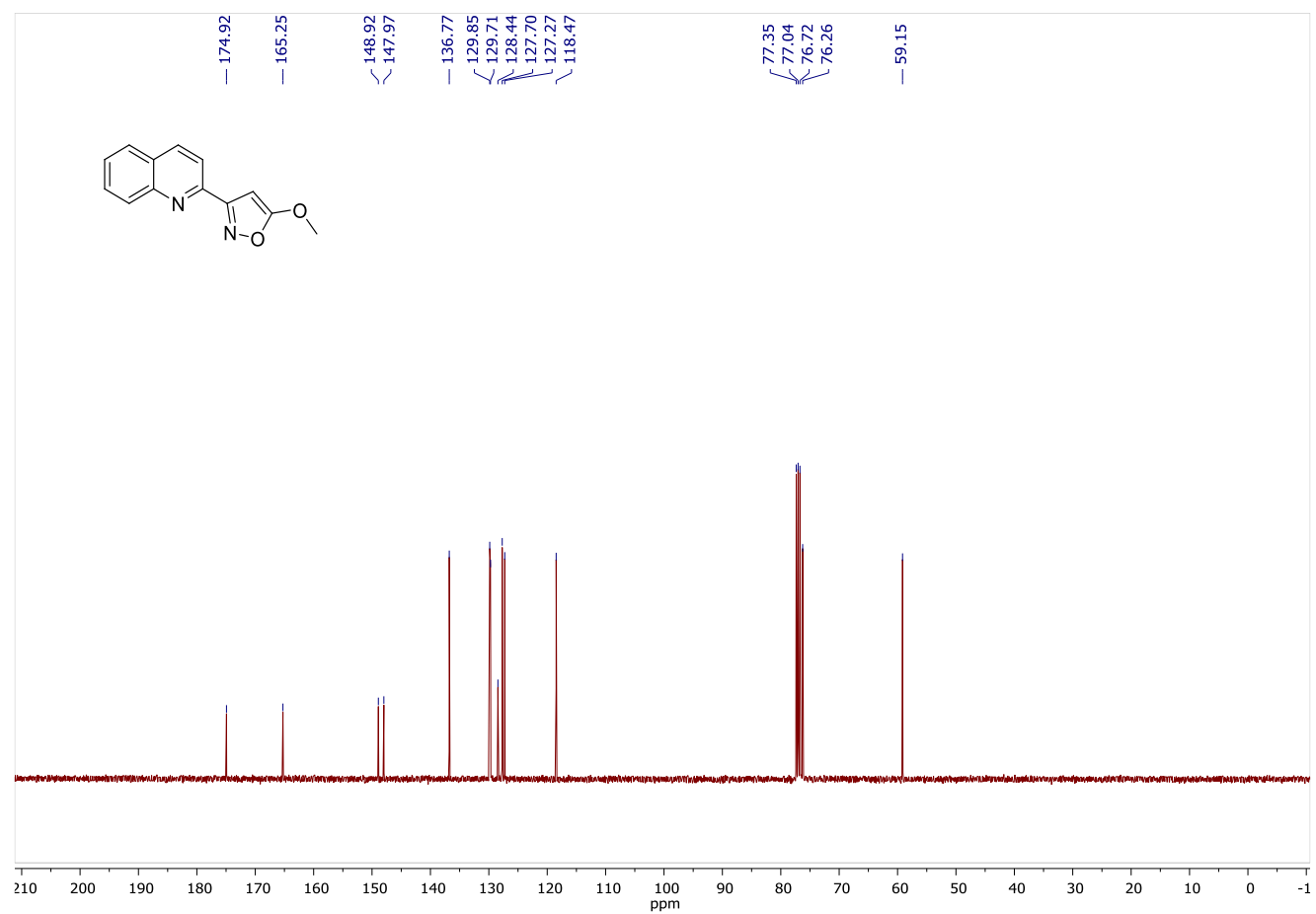
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of 3-(biphenyl-4-yl)-5-methoxyisoxazole



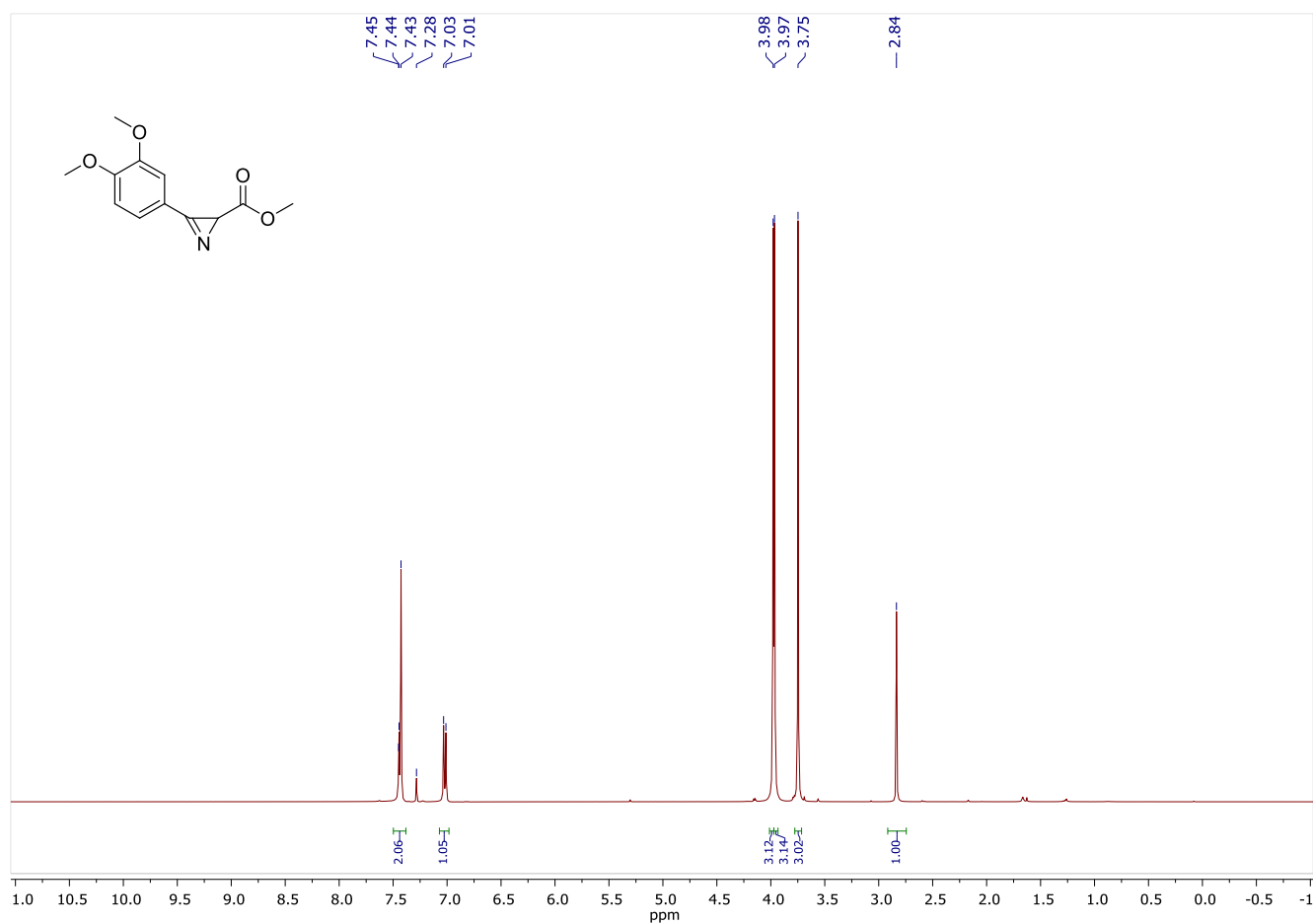
^1H NMR (400 MHz, CDCl_3) spectrum of 5-methoxy-3-(quinolin-2-yl)isoxazole



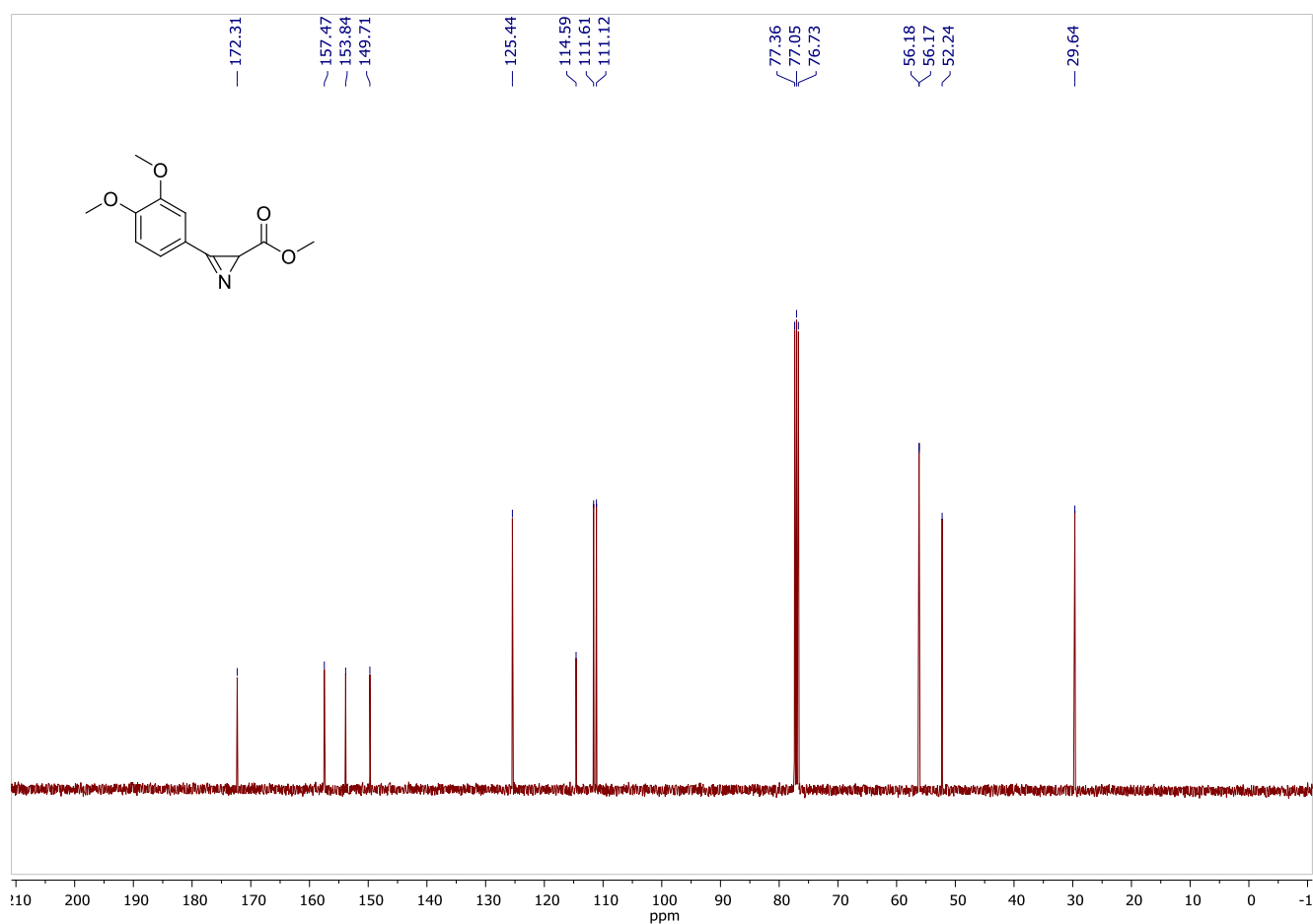
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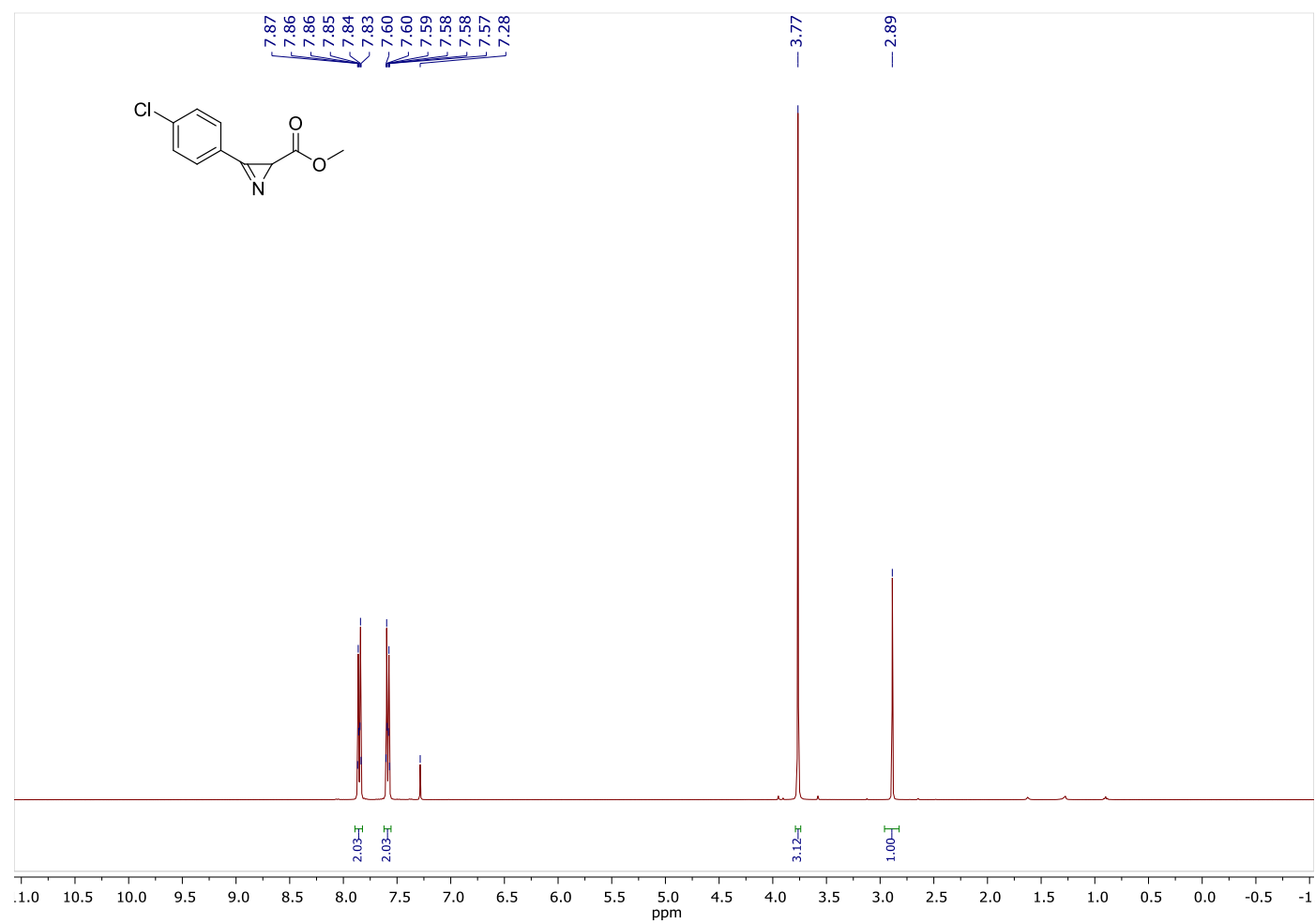
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(3,4-dimethoxyphenyl)-2*H*-azirine-2-carboxylate (**1c**)



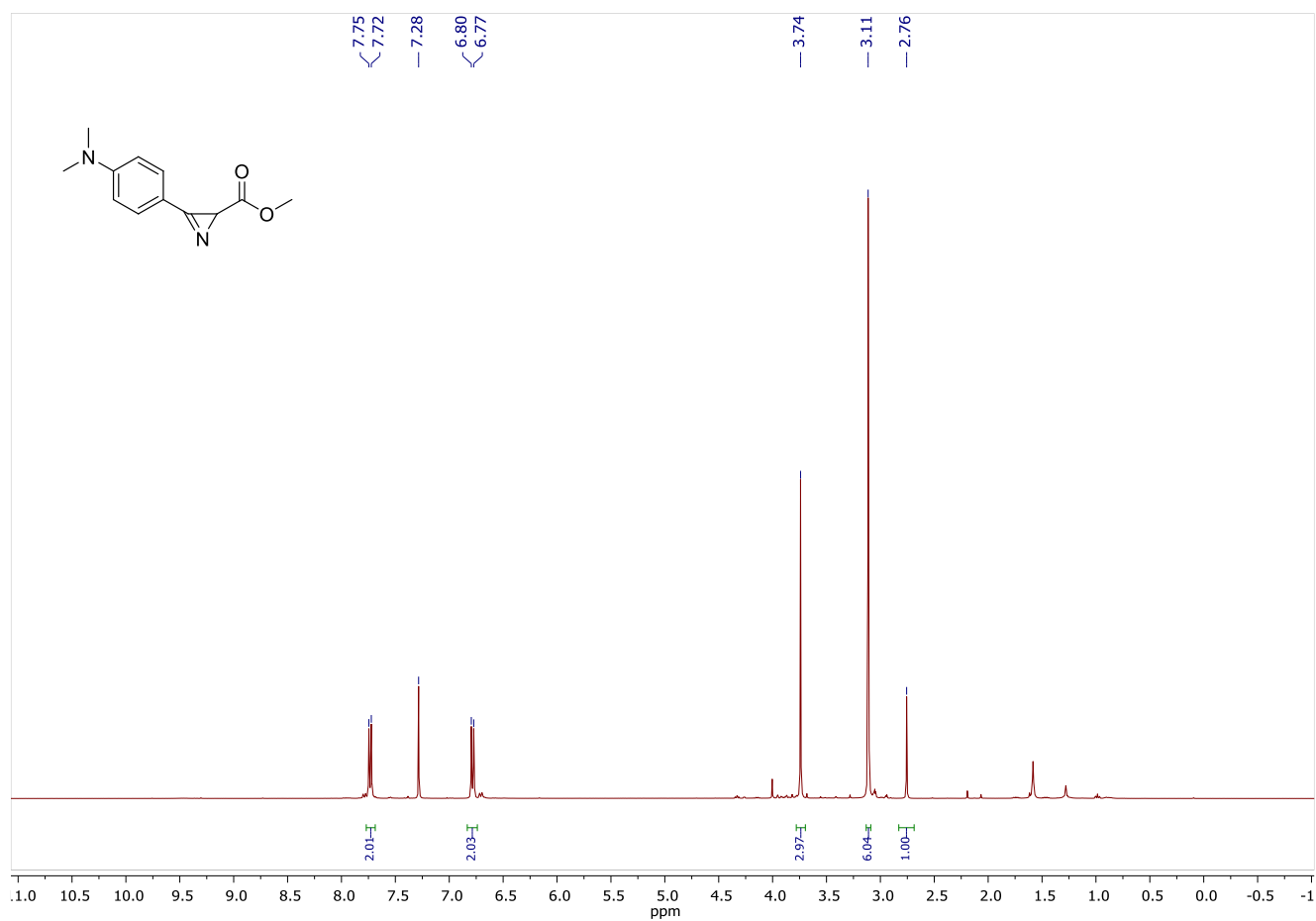
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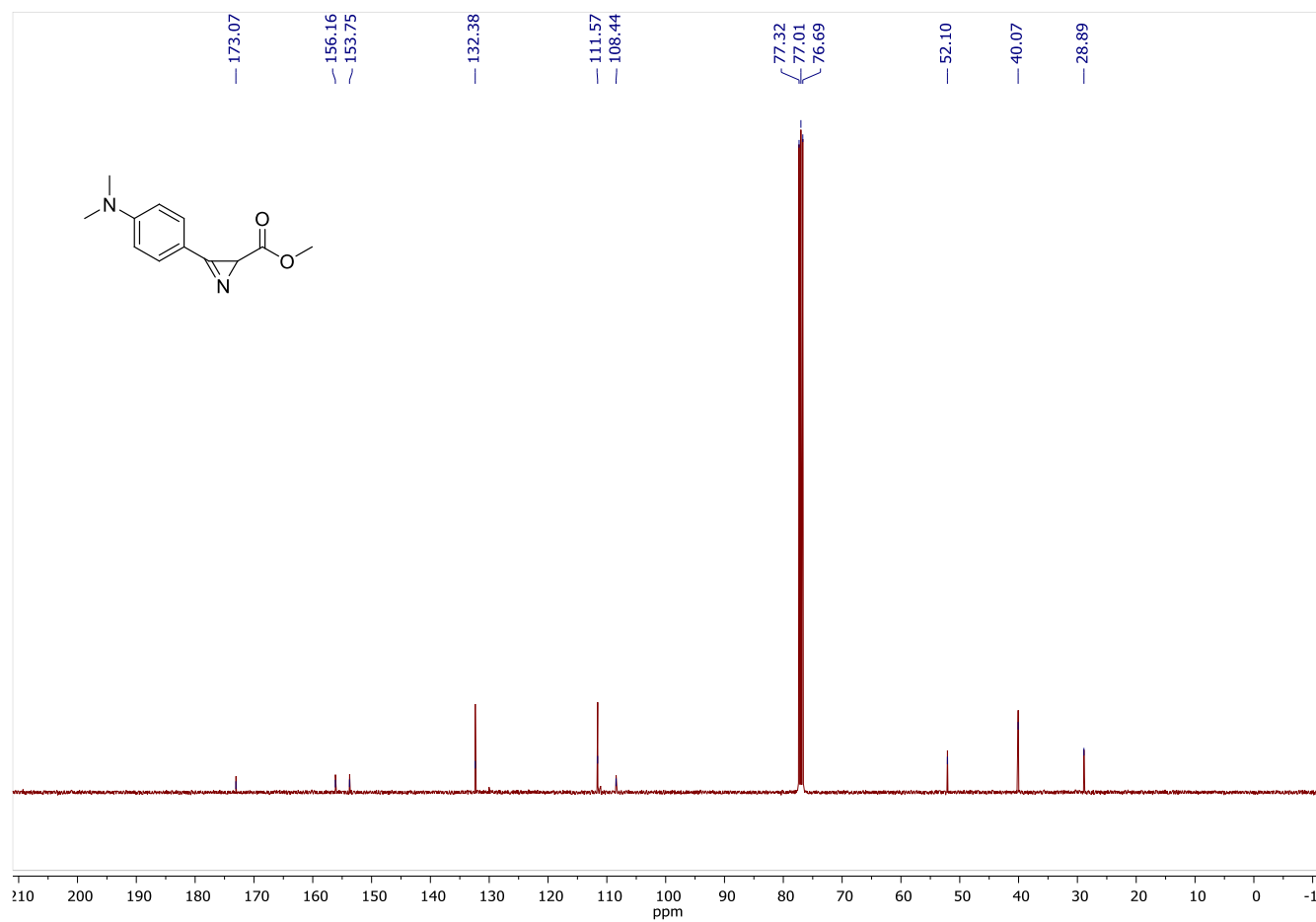
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(4-chlorophenyl)-2*H*-azirine-2-carboxylate (**1e**)



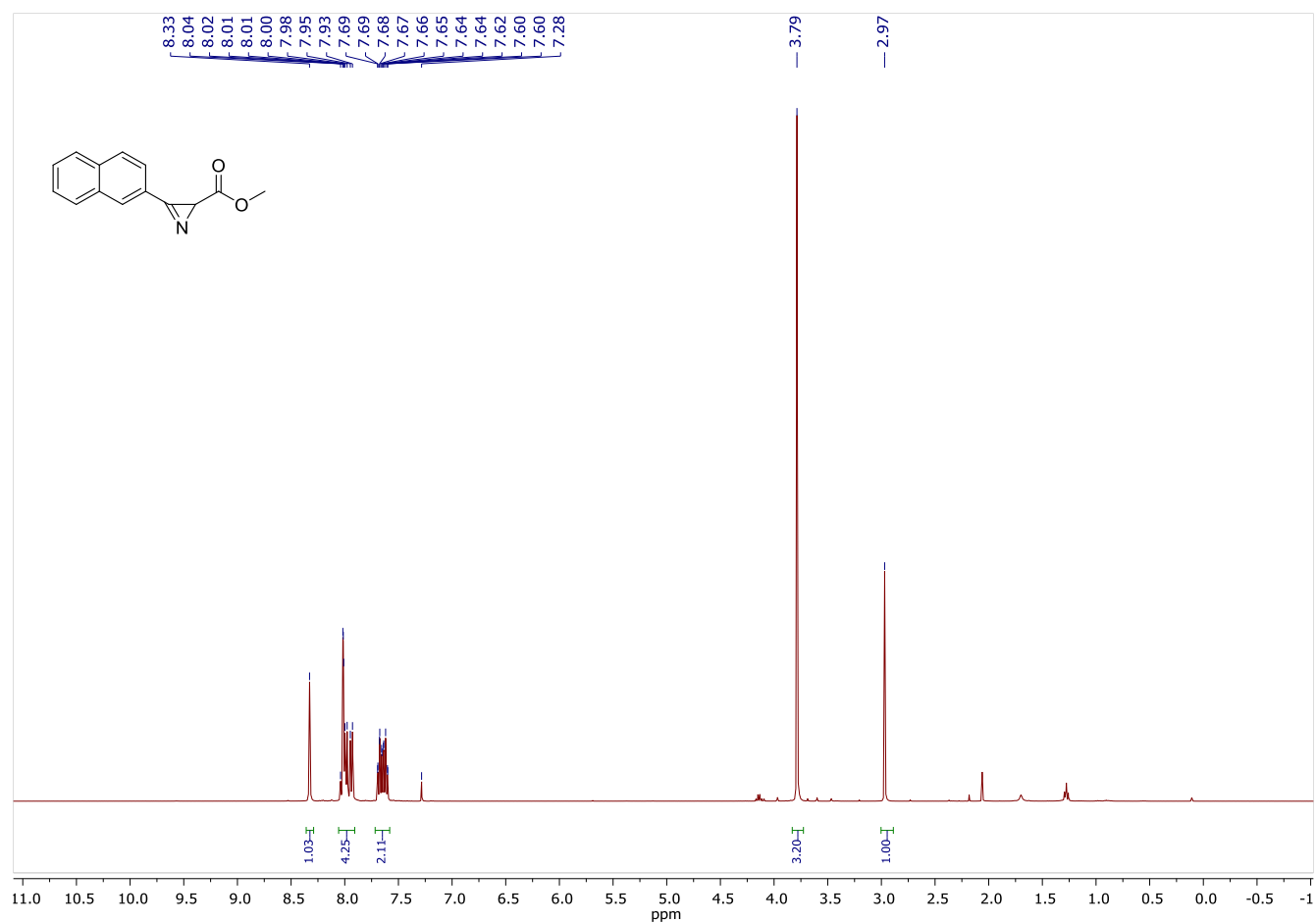
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(4-(dimethylamino)phenyl)-2*H*-azirine-2-carboxylate (**1f**)



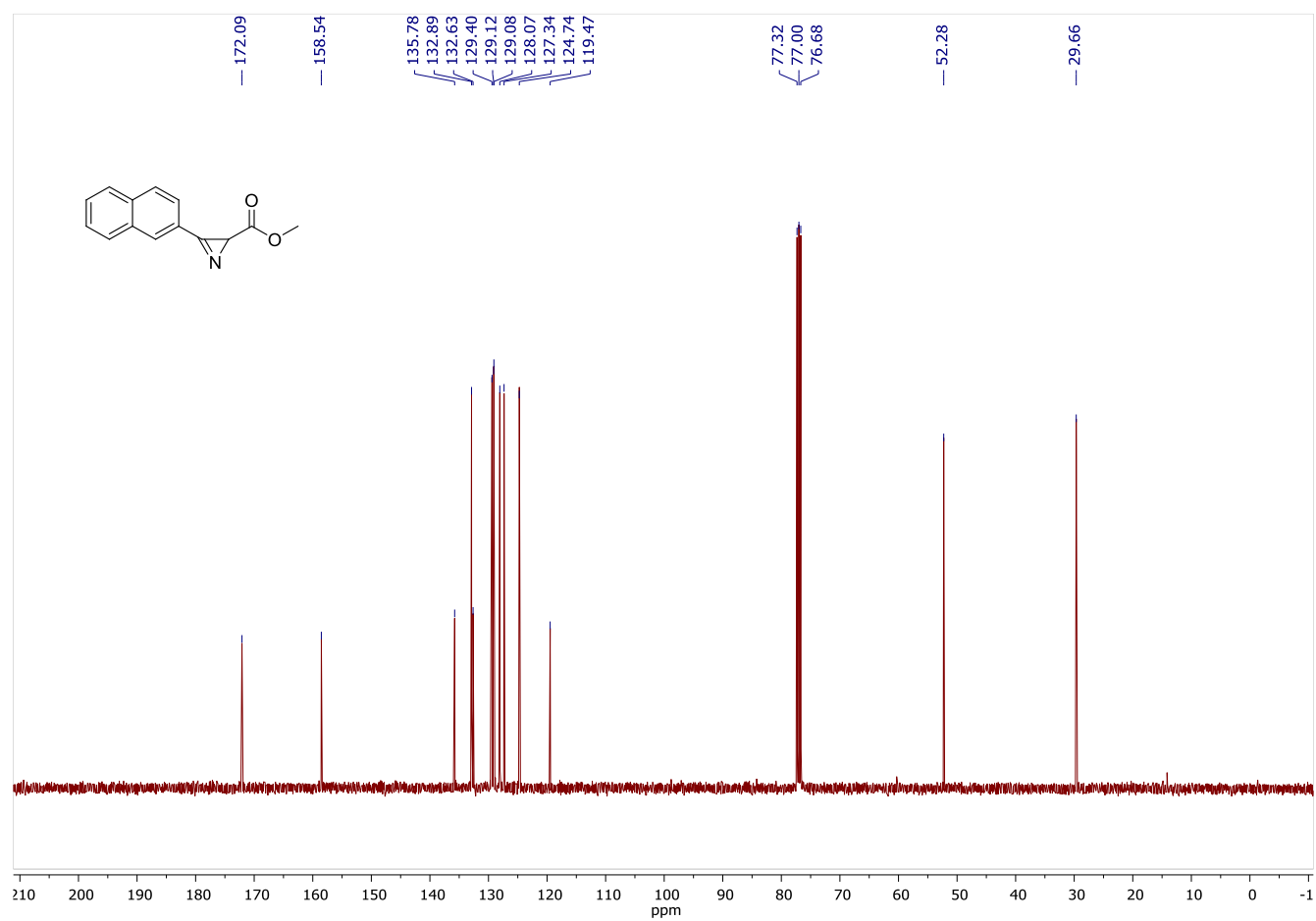
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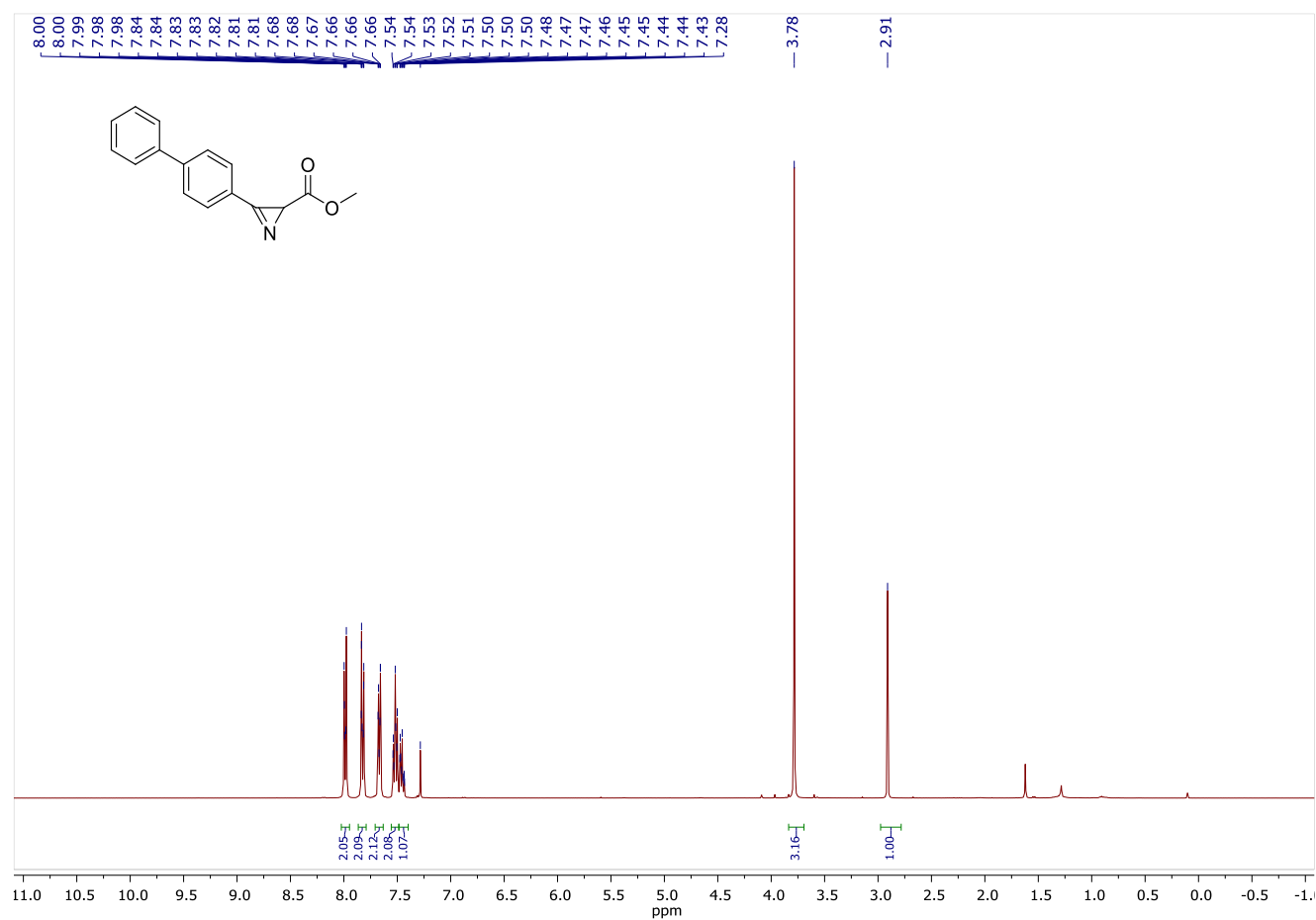
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(naphthalen-2-yl)-2*H*-azirine-2-carboxylate (**1g**)



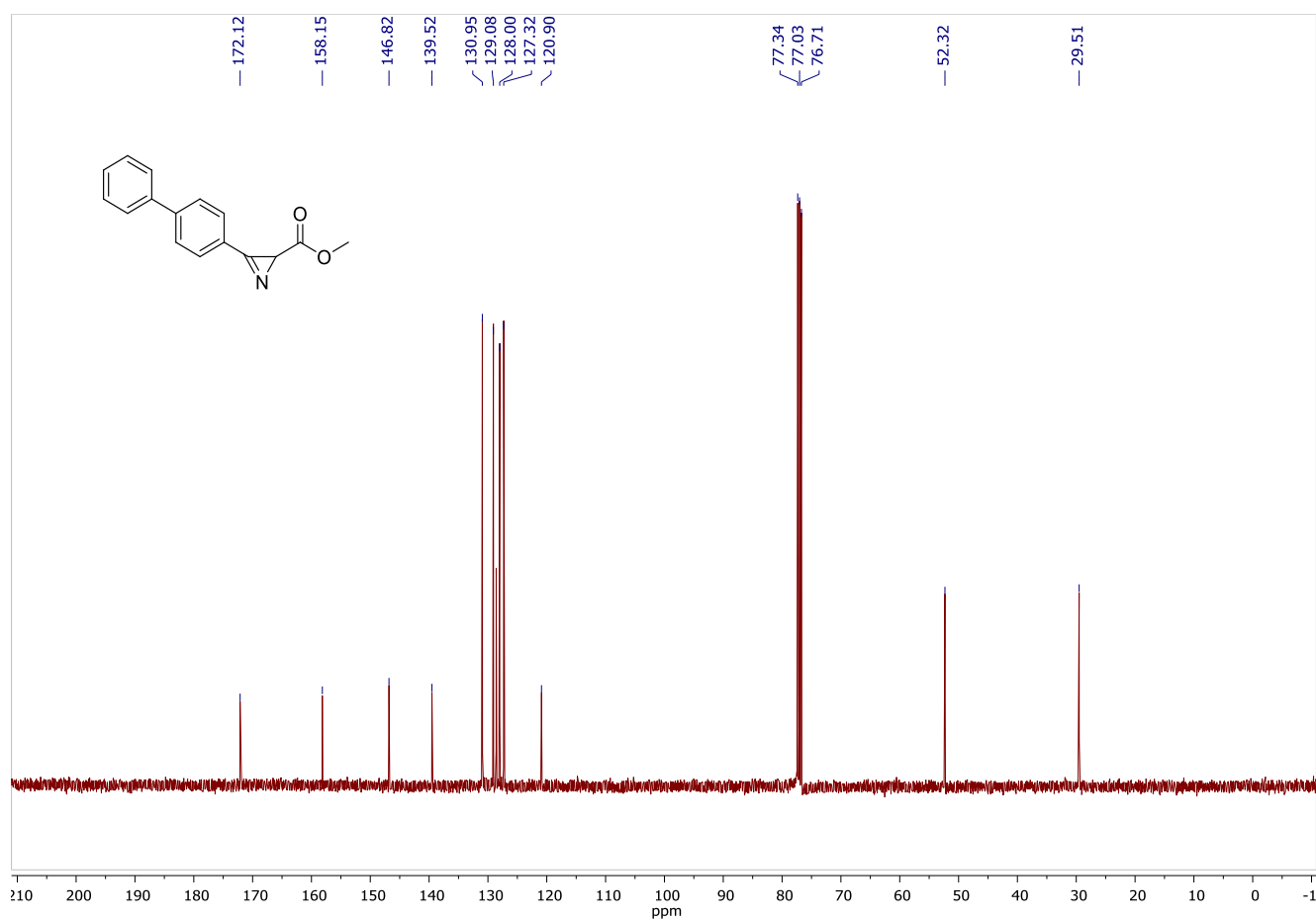
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of methyl 3-(naphthalen-2-yl)-2*H*-azirine-2-carboxylate (**1g**)



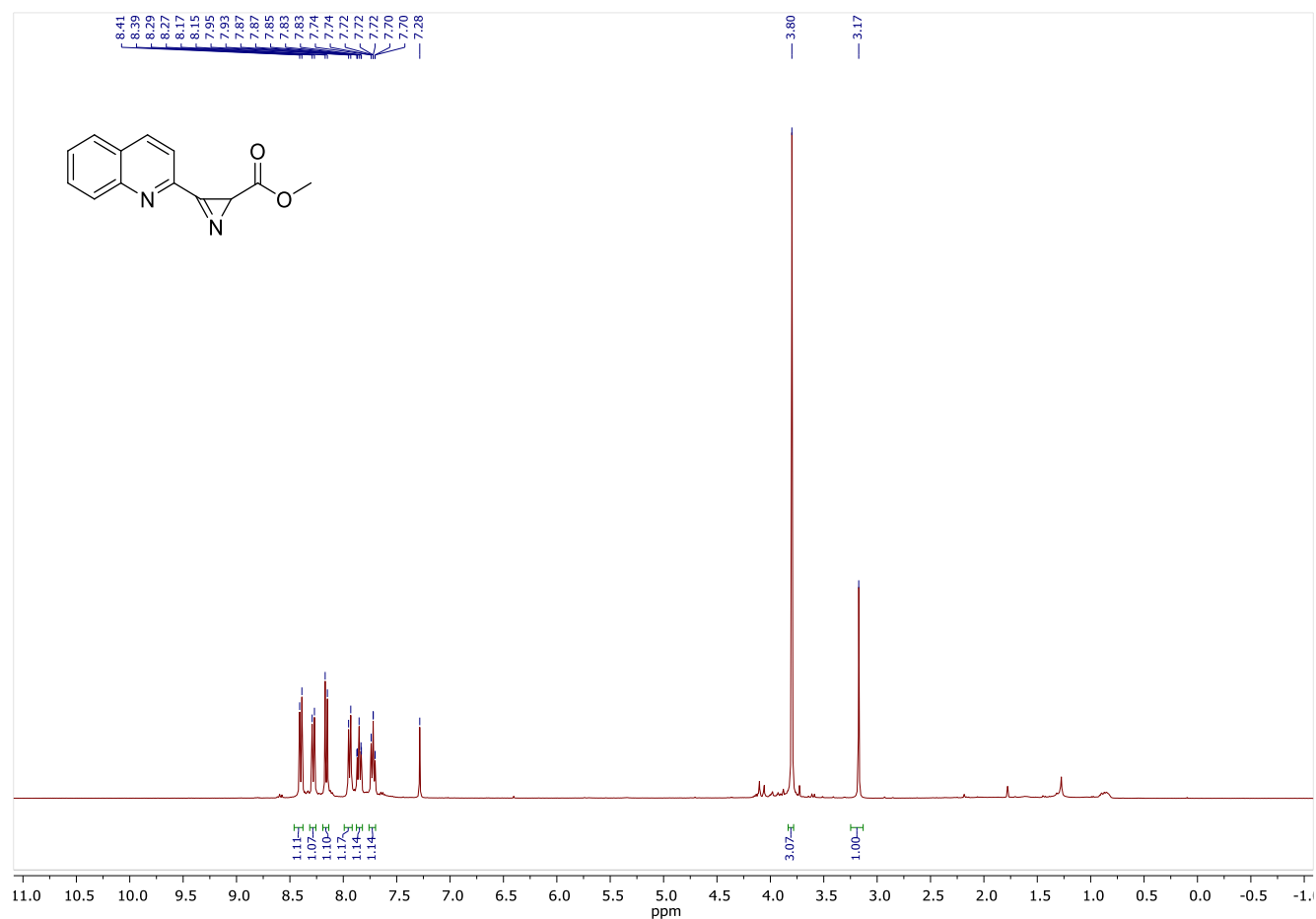
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(biphenyl-4-yl)-2*H*-azirine-2-carboxylate (**1h**)



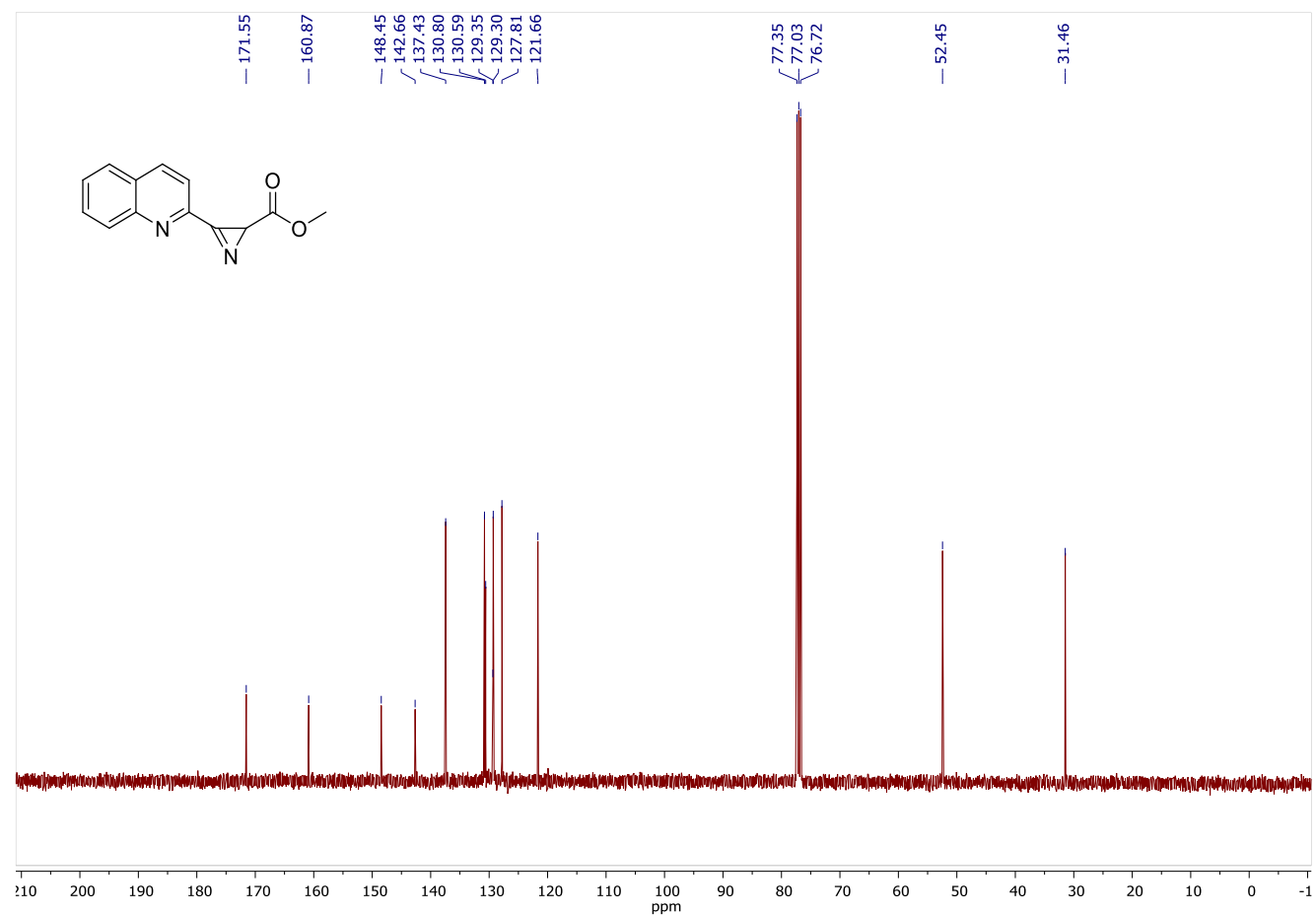
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of methyl 3-(biphenyl-4-yl)-2*H*-azirine-2-carboxylate (**1h**)



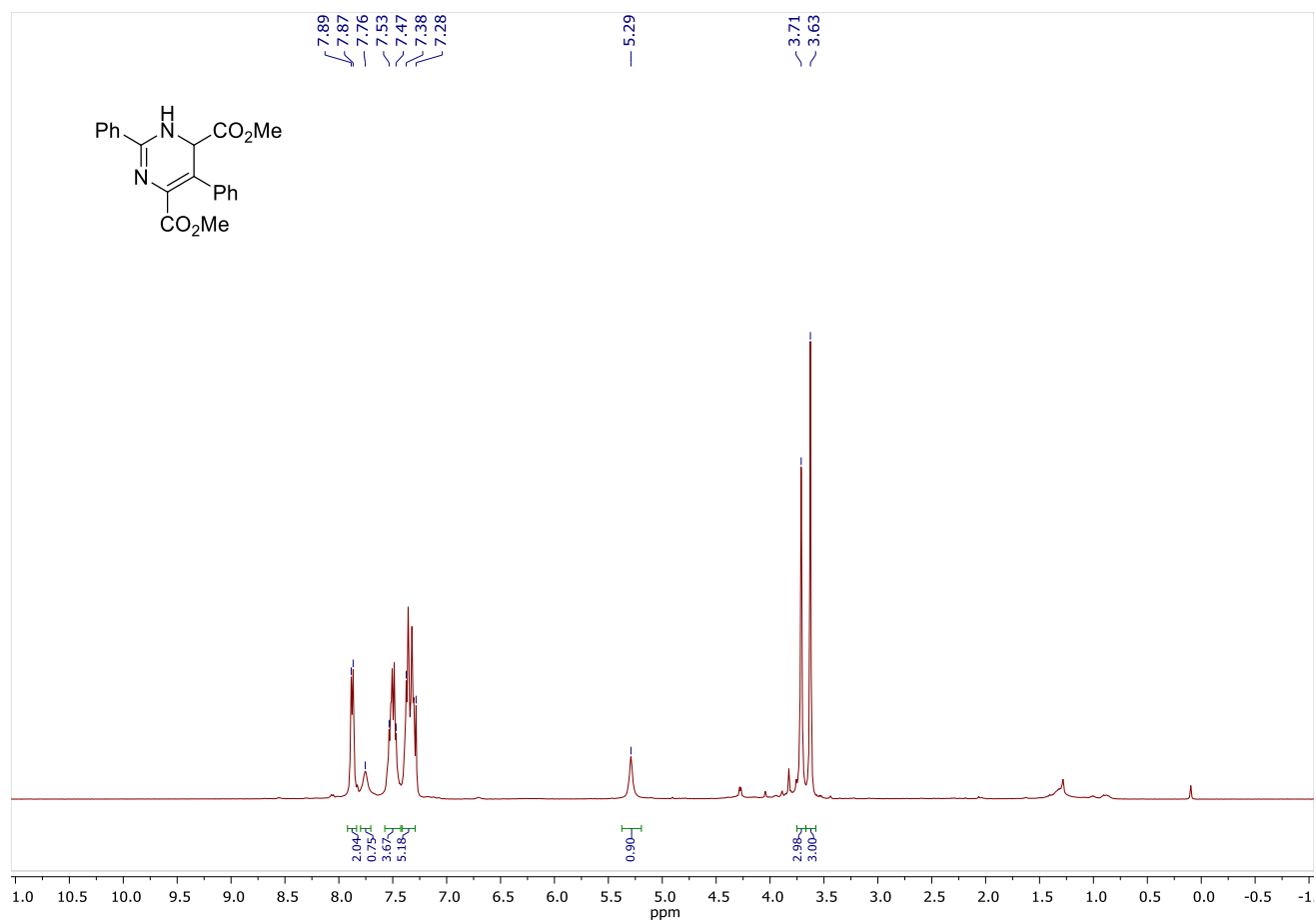
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 3-(quinolin-2-yl)-2*H*-azirine-2-carboxylate (**1k**)



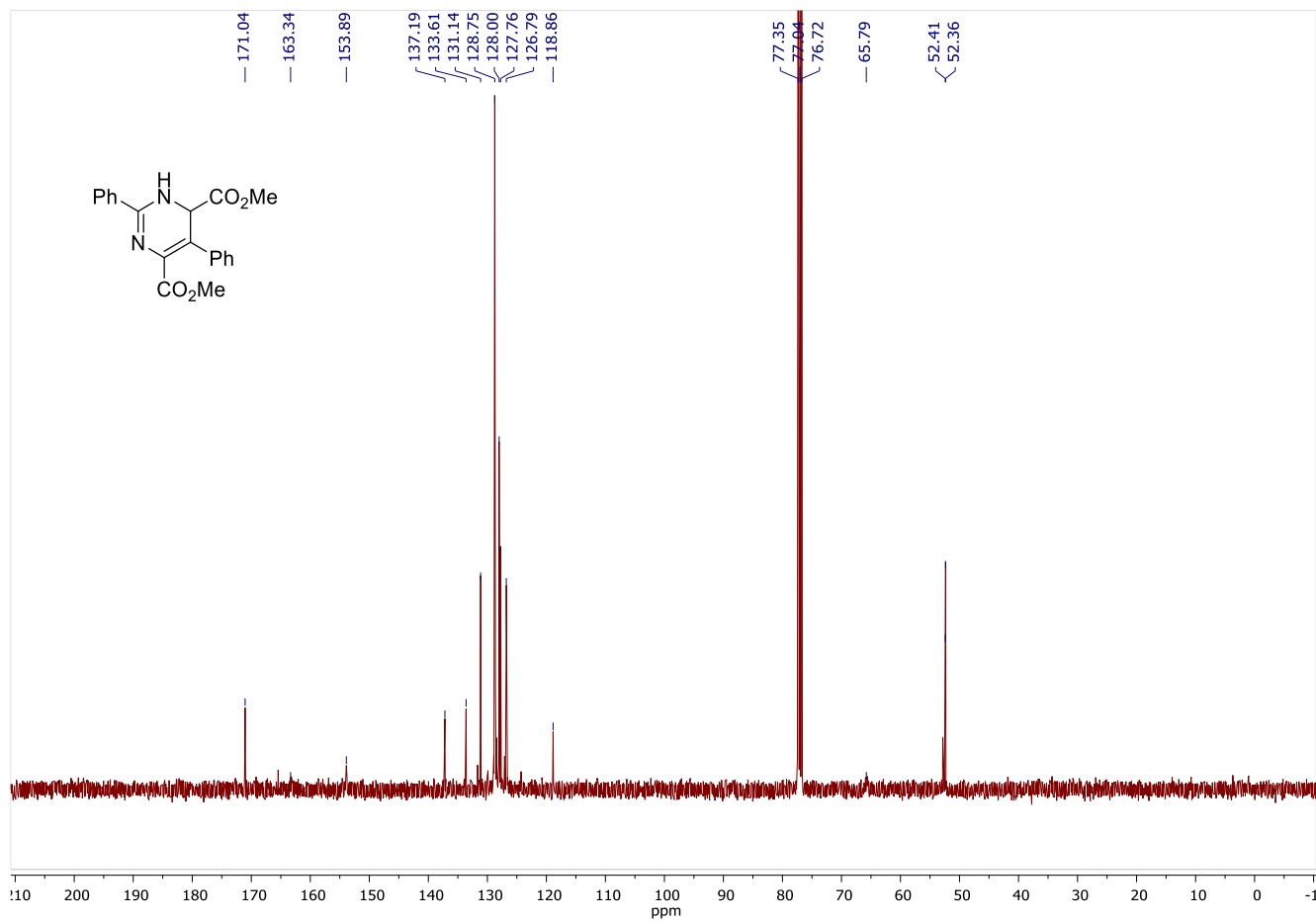
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of methyl 3-(quinolin-2-yl)-2*H*-azirine-2-carboxylate (**1k**)



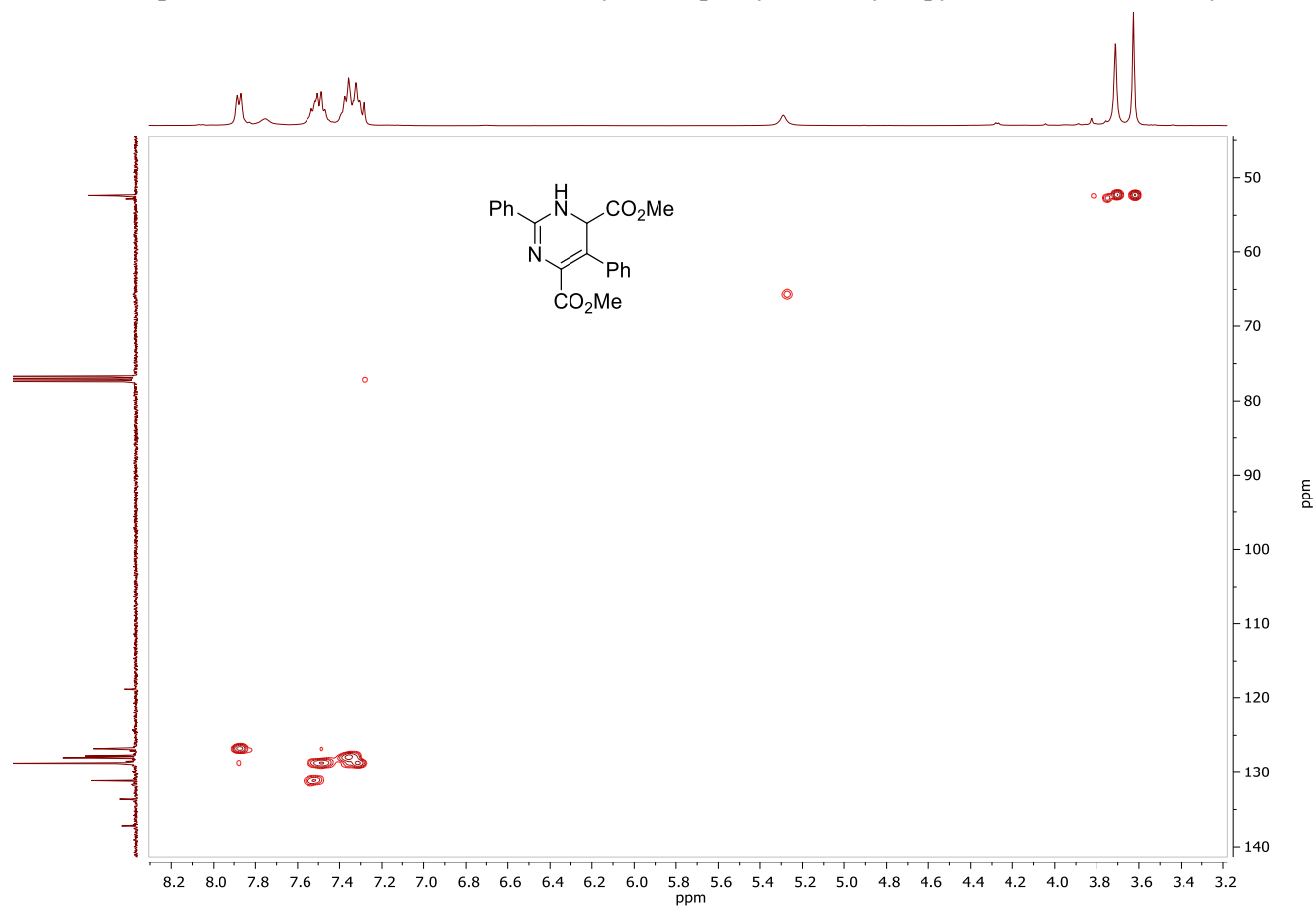
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-diphenyl-1,6-dihydropyrimidine-4,6-dicarboxylate (**2a**)



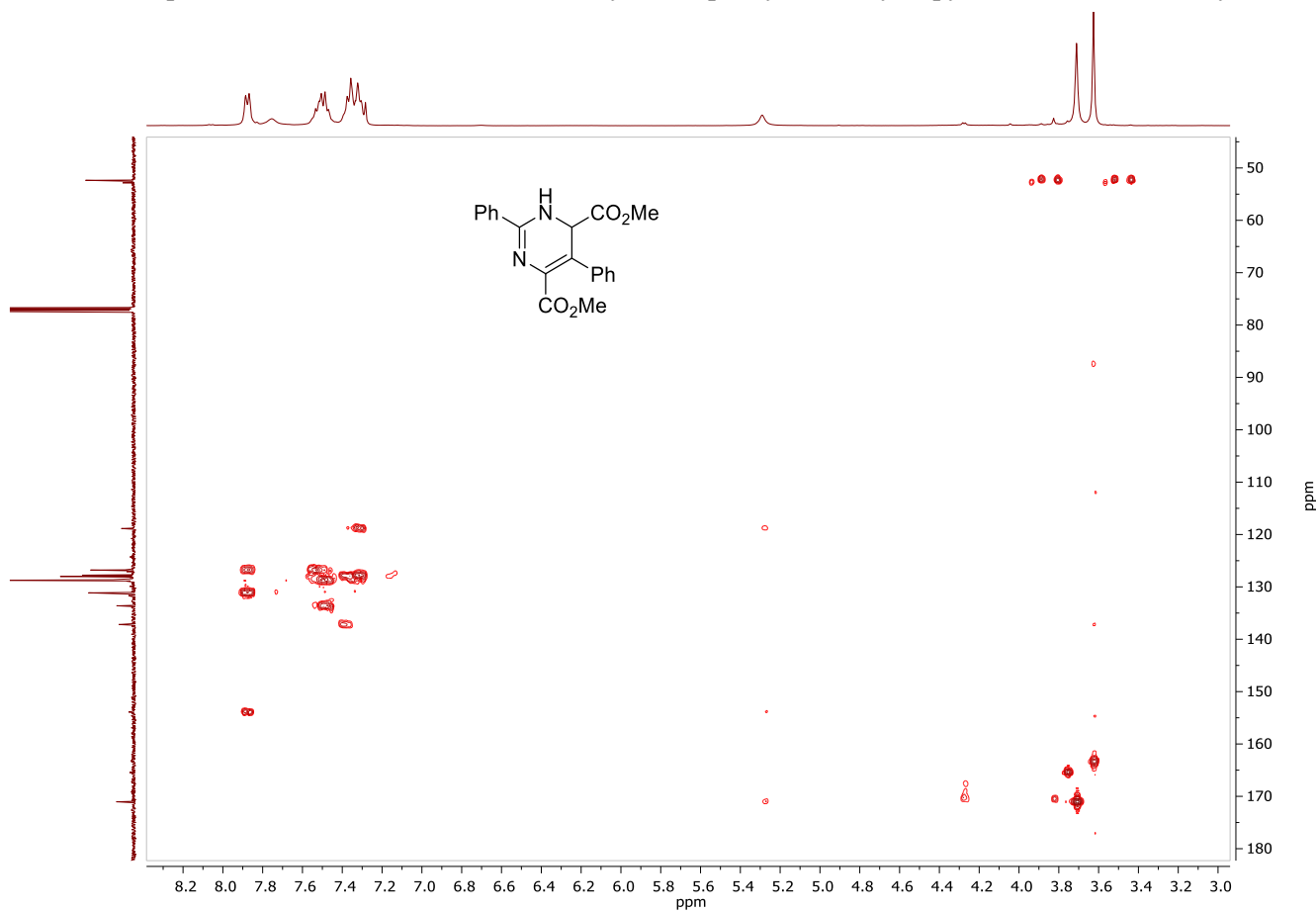
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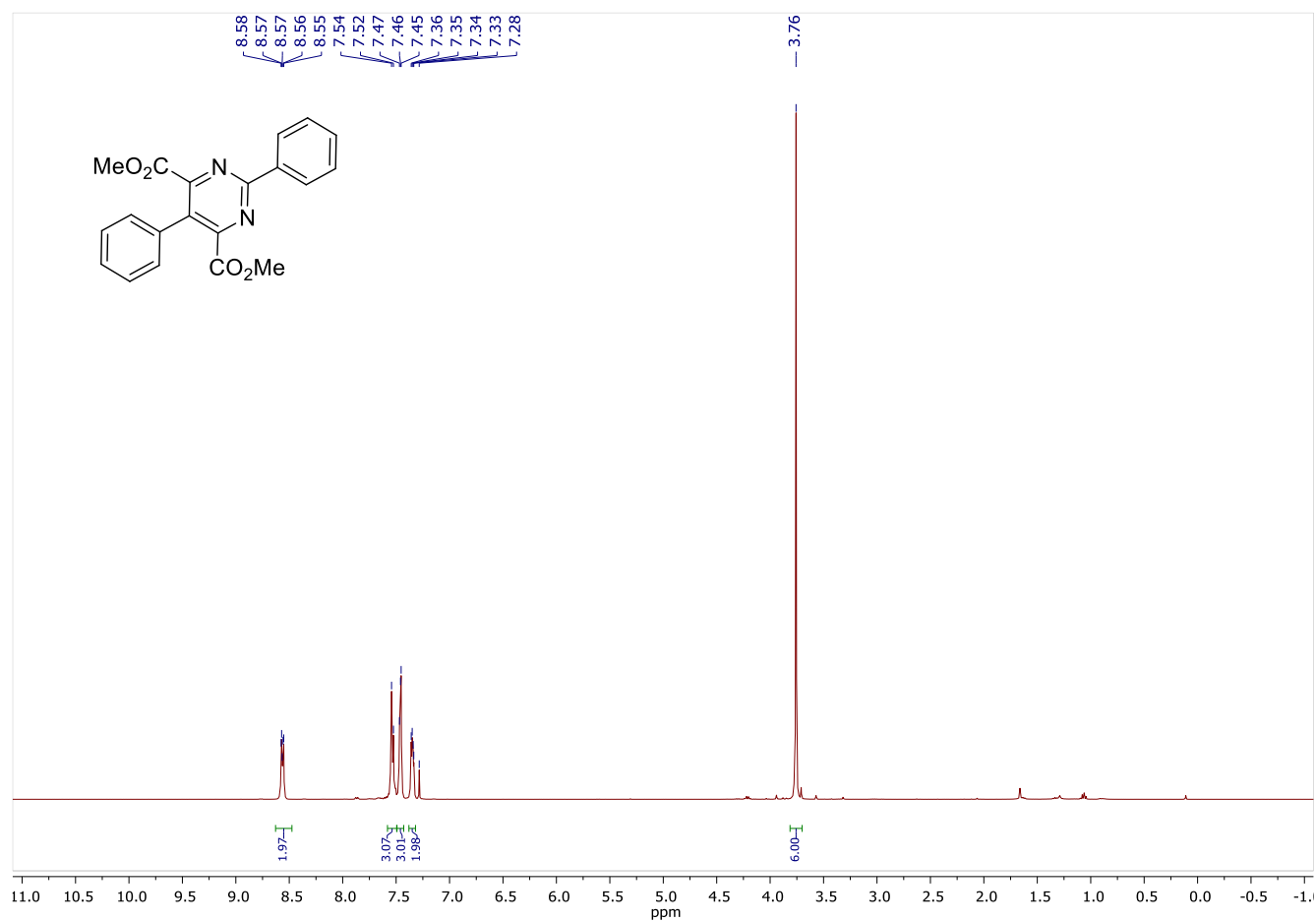
^1H - ^{13}C HSQC spectrum (400 MHz, CDCl_3) of dimethyl 2,5-diphenyl-1,6-dihydropyrimidine-4,6-dicarboxylate (**2a**)



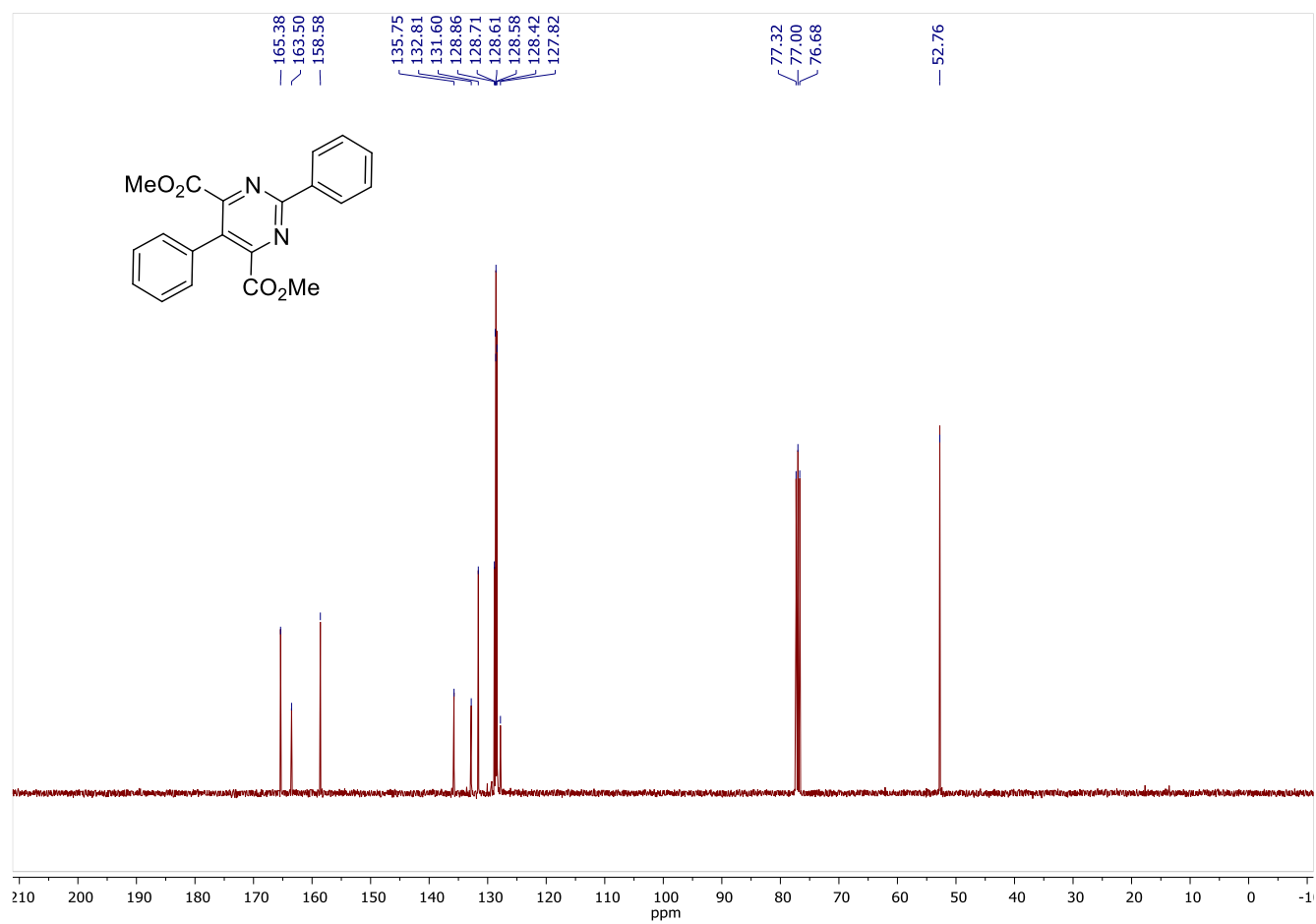
^1H - ^{13}C HMBC spectrum (400 MHz, CDCl_3) of dimethyl 2,5-diphenyl-1,6-dihydropyrimidine-4,6-dicarboxylate (**2a**)



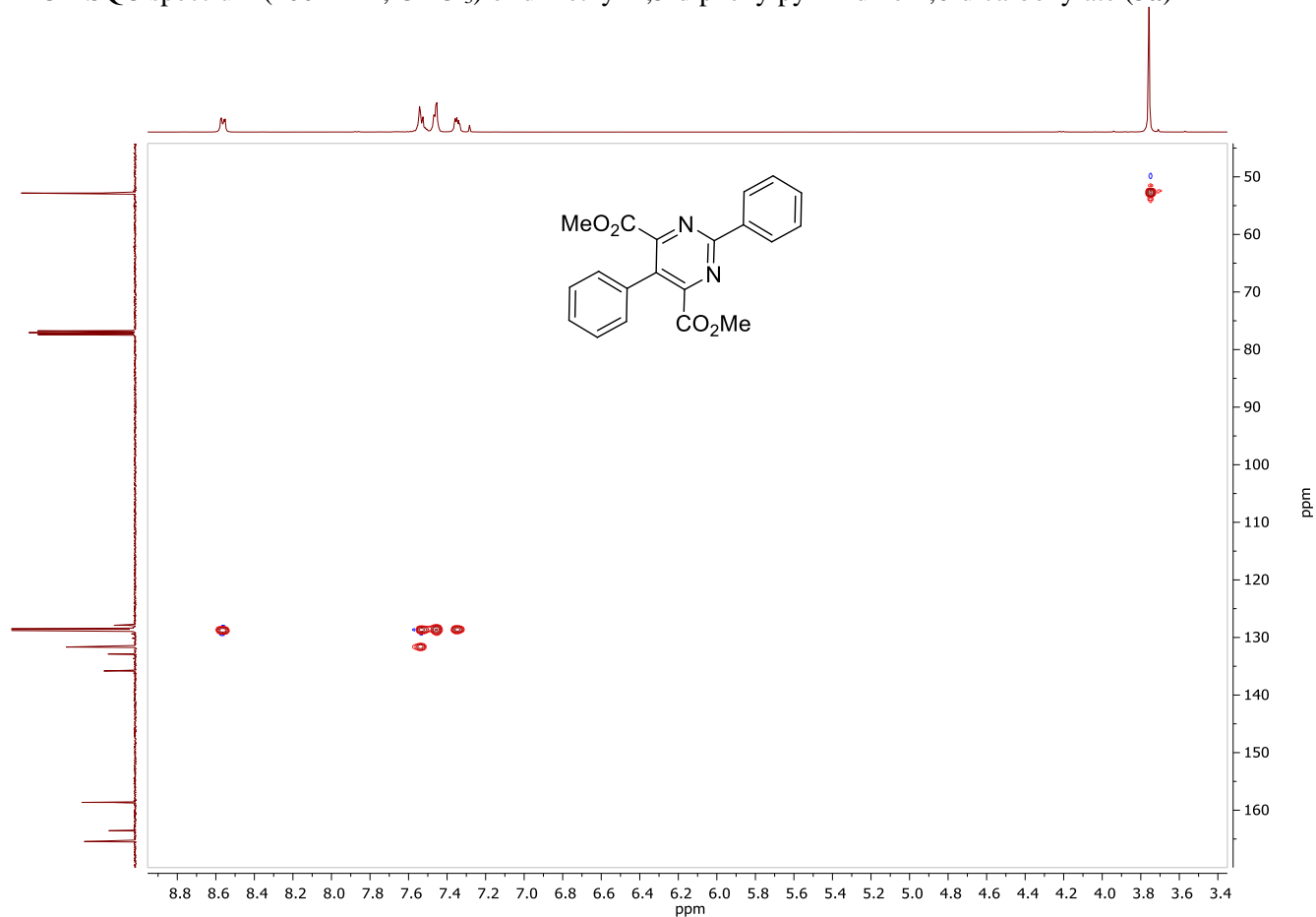
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3a**)



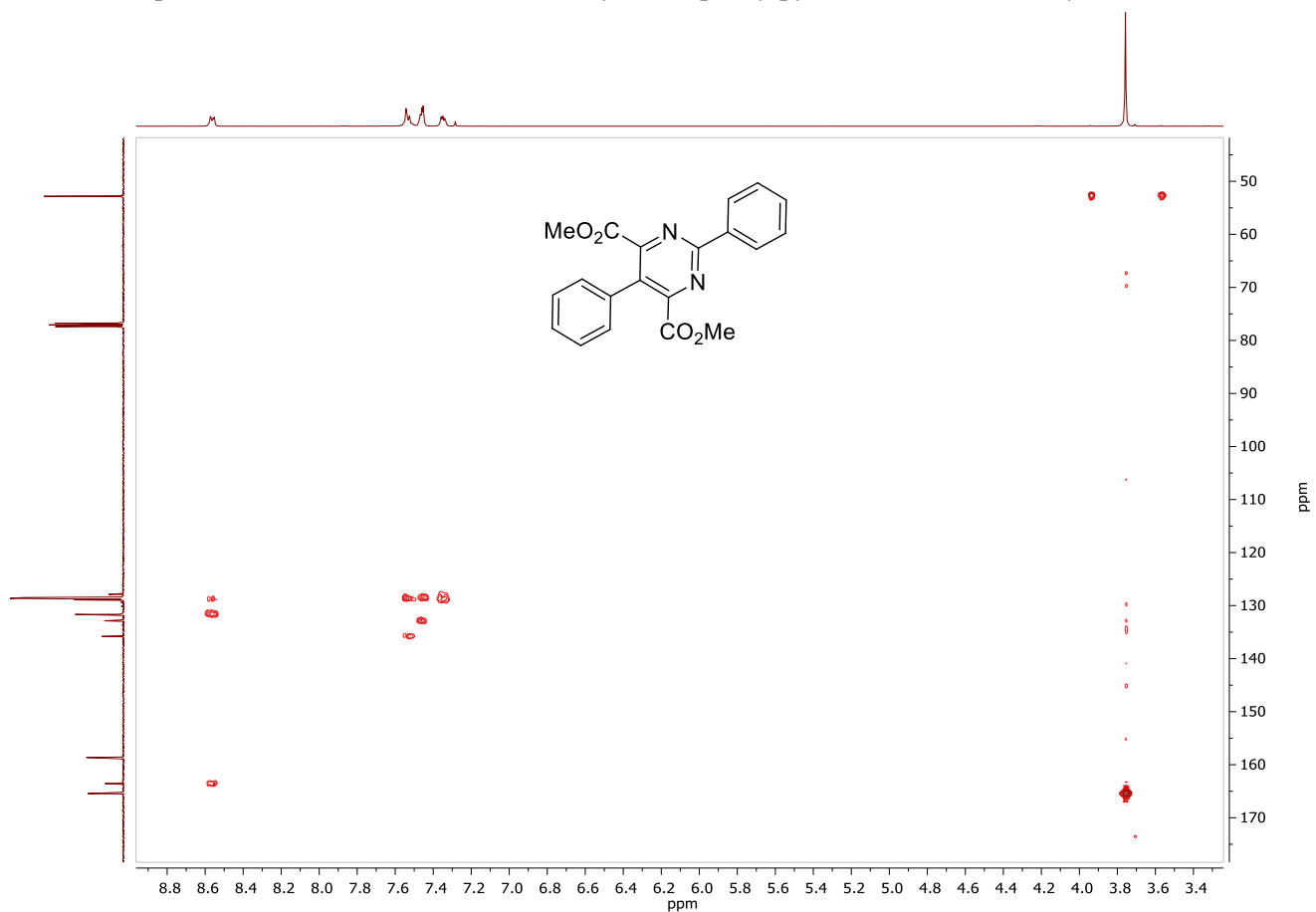
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of dimethyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3a**)



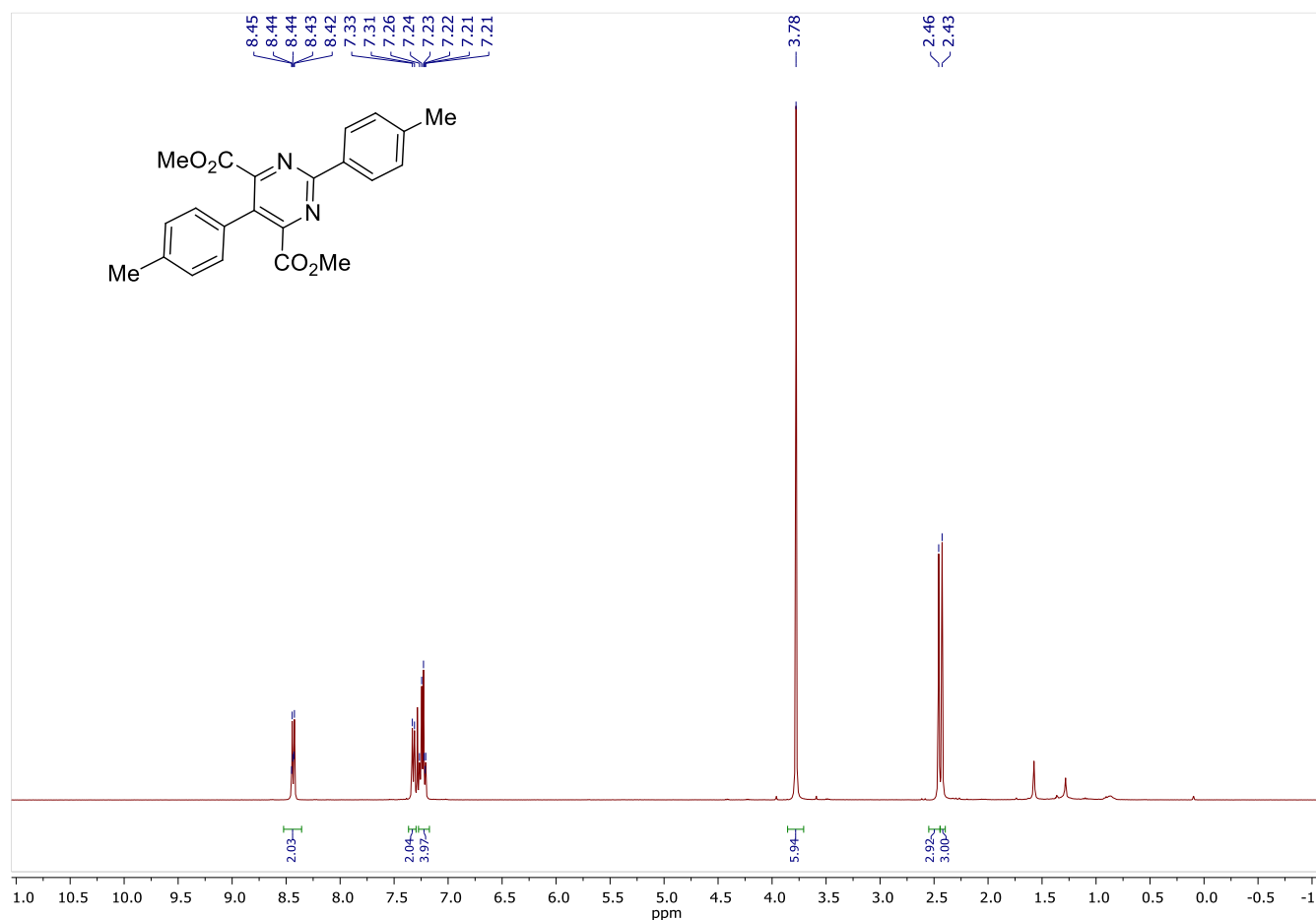
^1H - ^{13}C HSQC spectrum (400 MHz, CDCl_3) of dimethyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3a**)



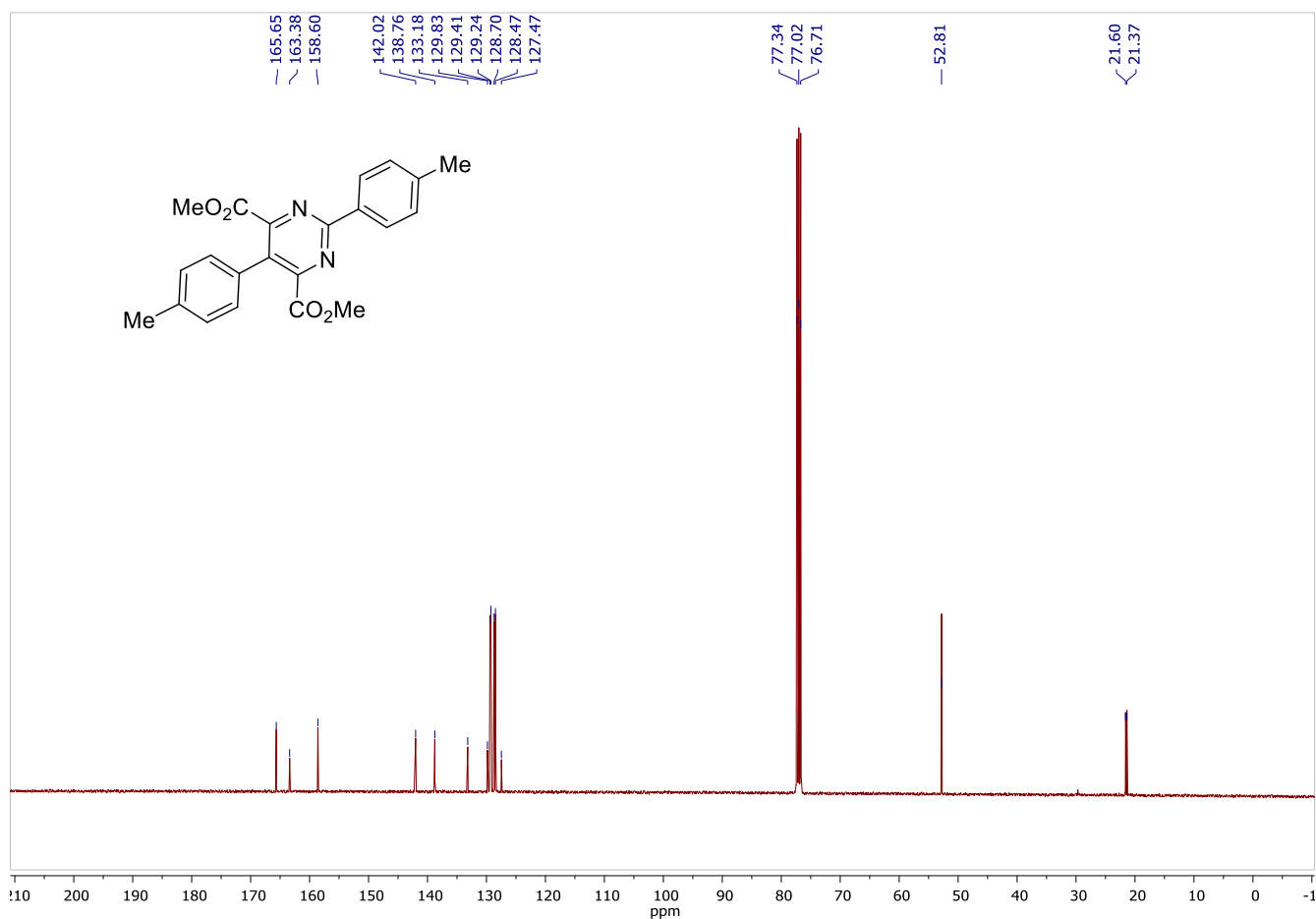
^1H - ^{13}C HMBC spectrum (400 MHz, CDCl_3) of dimethyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3a**)



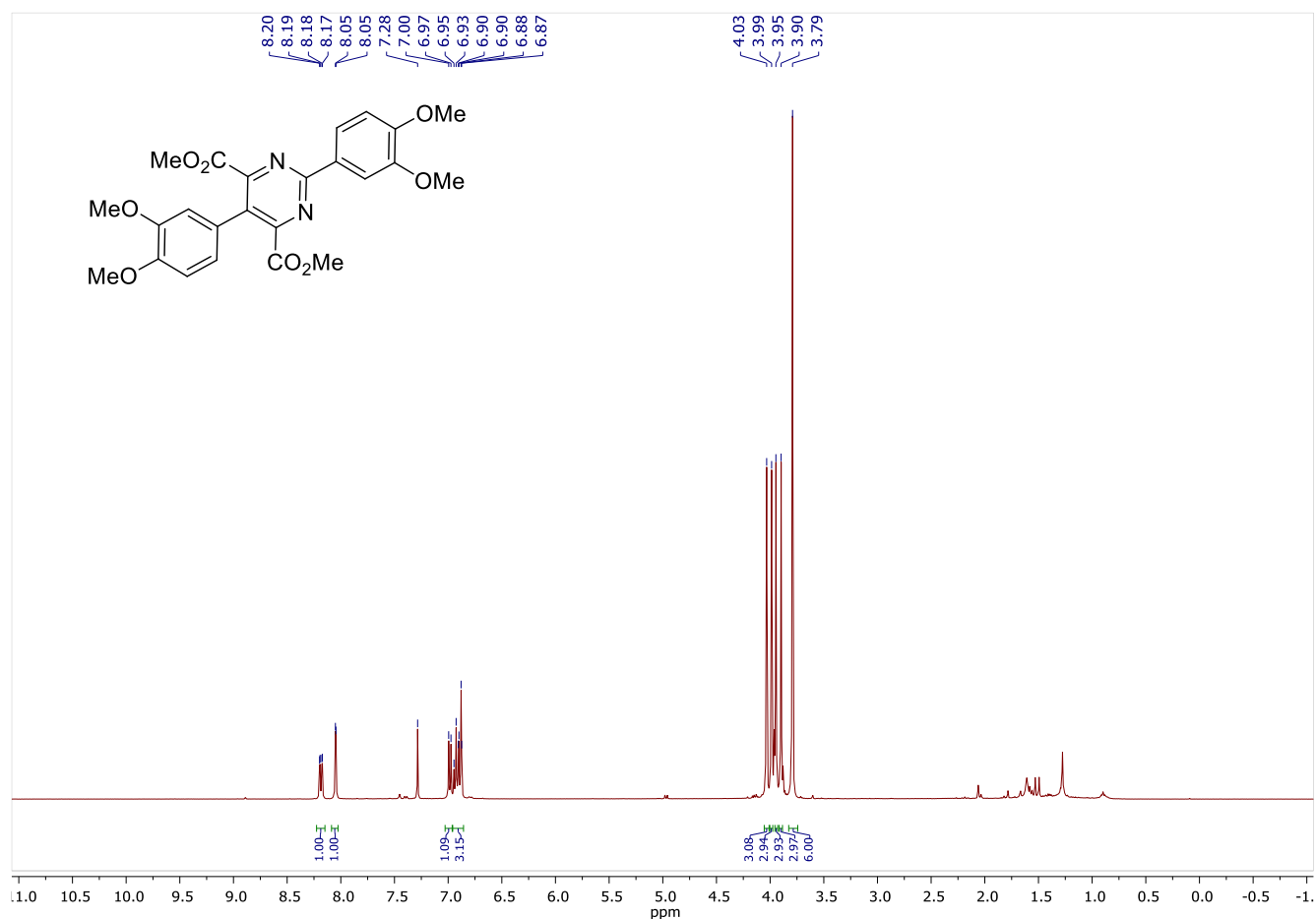
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(*p*-tolyl)pyrimidine-4,6-dicarboxylate (**3b**)



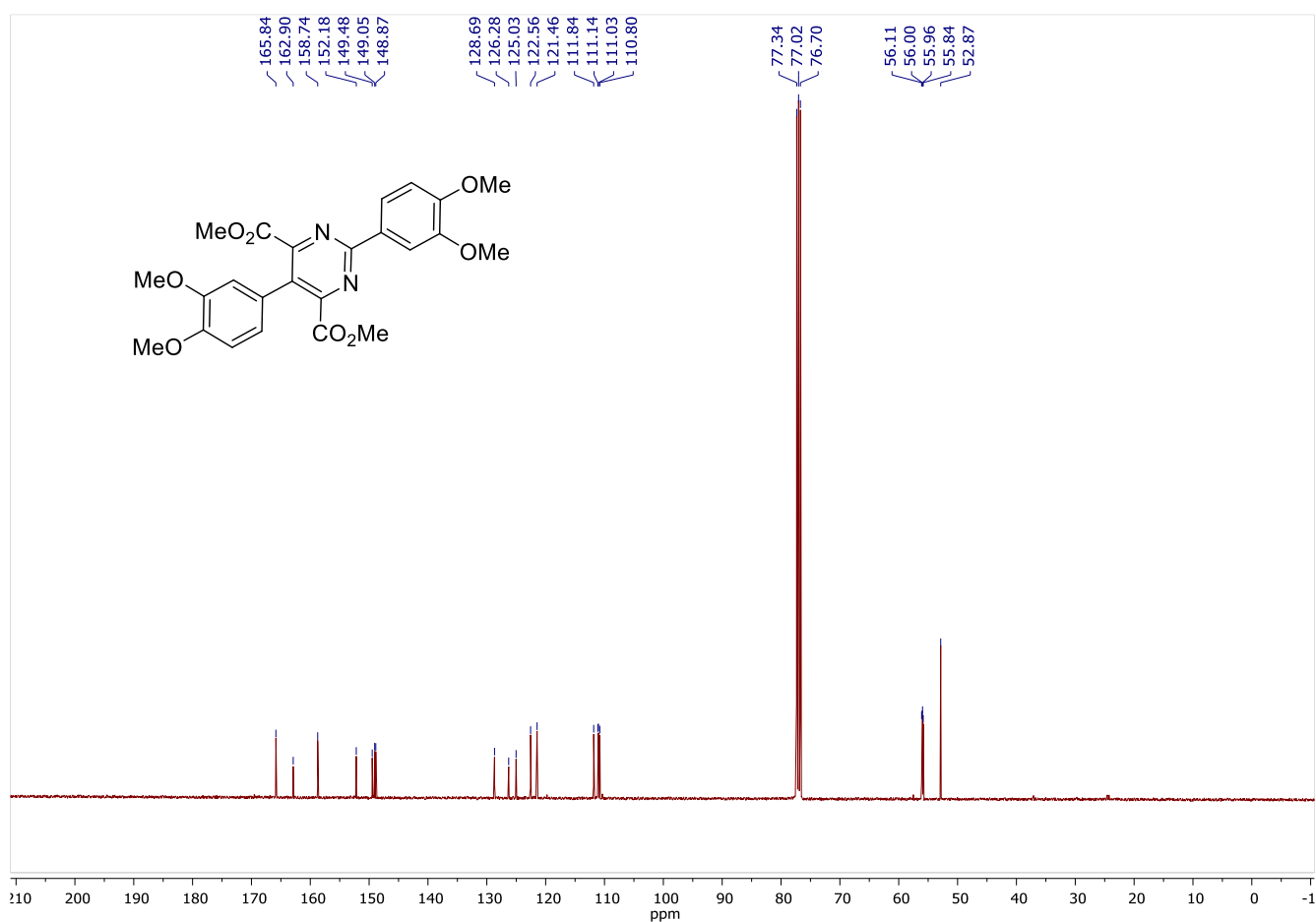
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of dimethyl 2,5-di(*p*-tolyl)pyrimidine-4,6-dicarboxylate (**3b**)



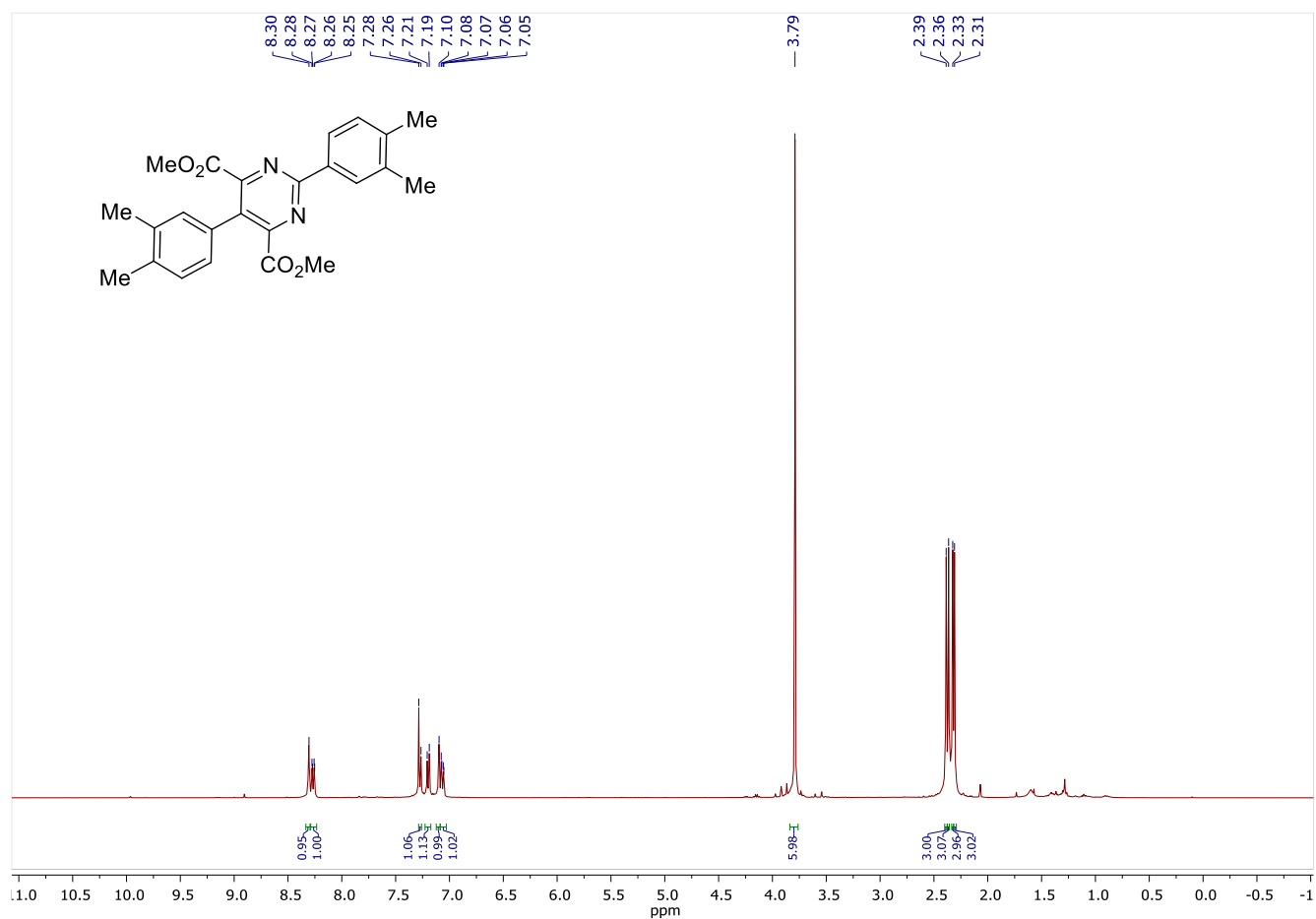
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(3,4-dimethoxyphenyl)pyrimidine-4,6-dicarboxylate (**3c**)



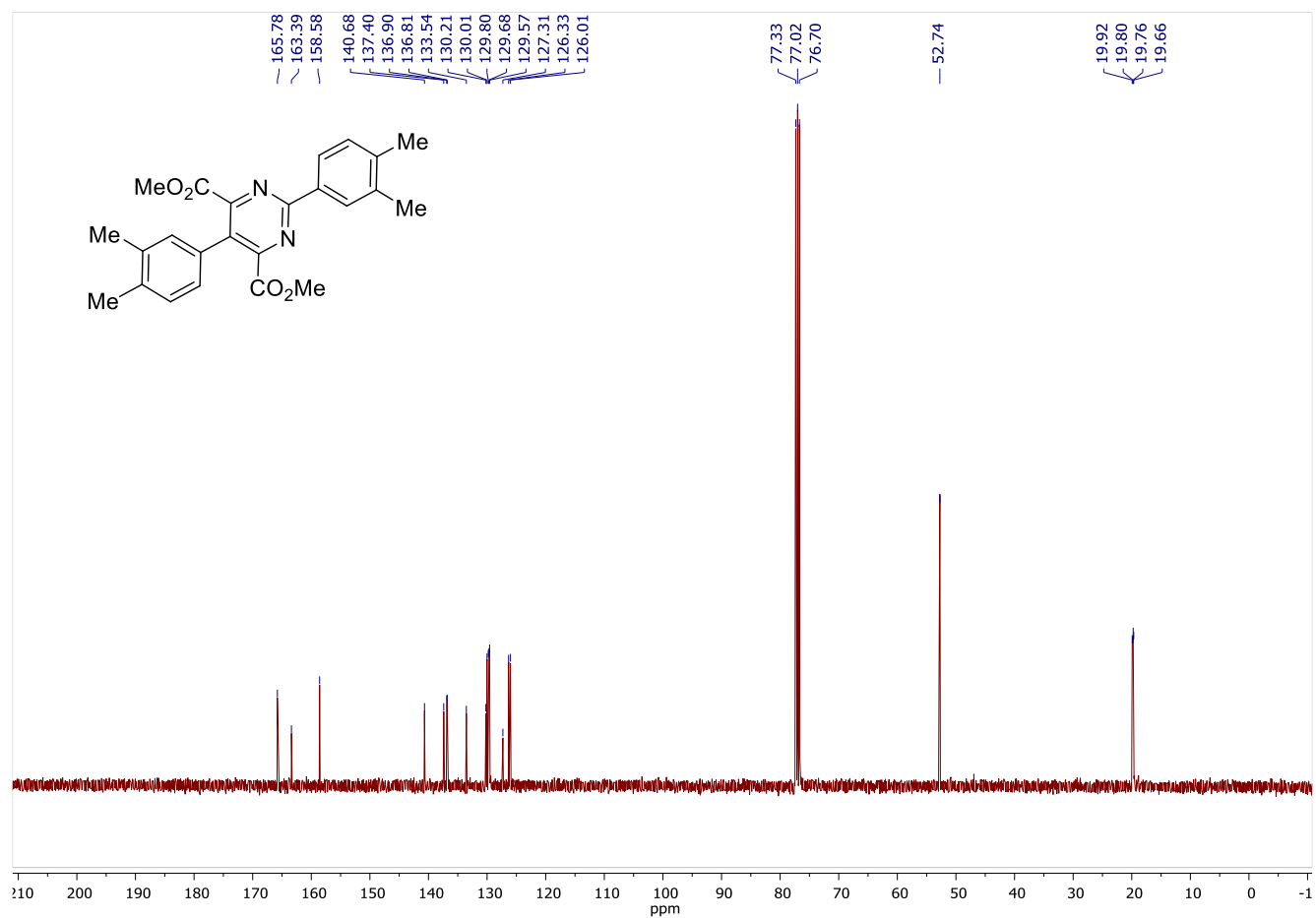
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of dimethyl 2,5-di(3,4-dimethoxyphenyl)pyrimidine-4,6-dicarboxylate (**3c**)



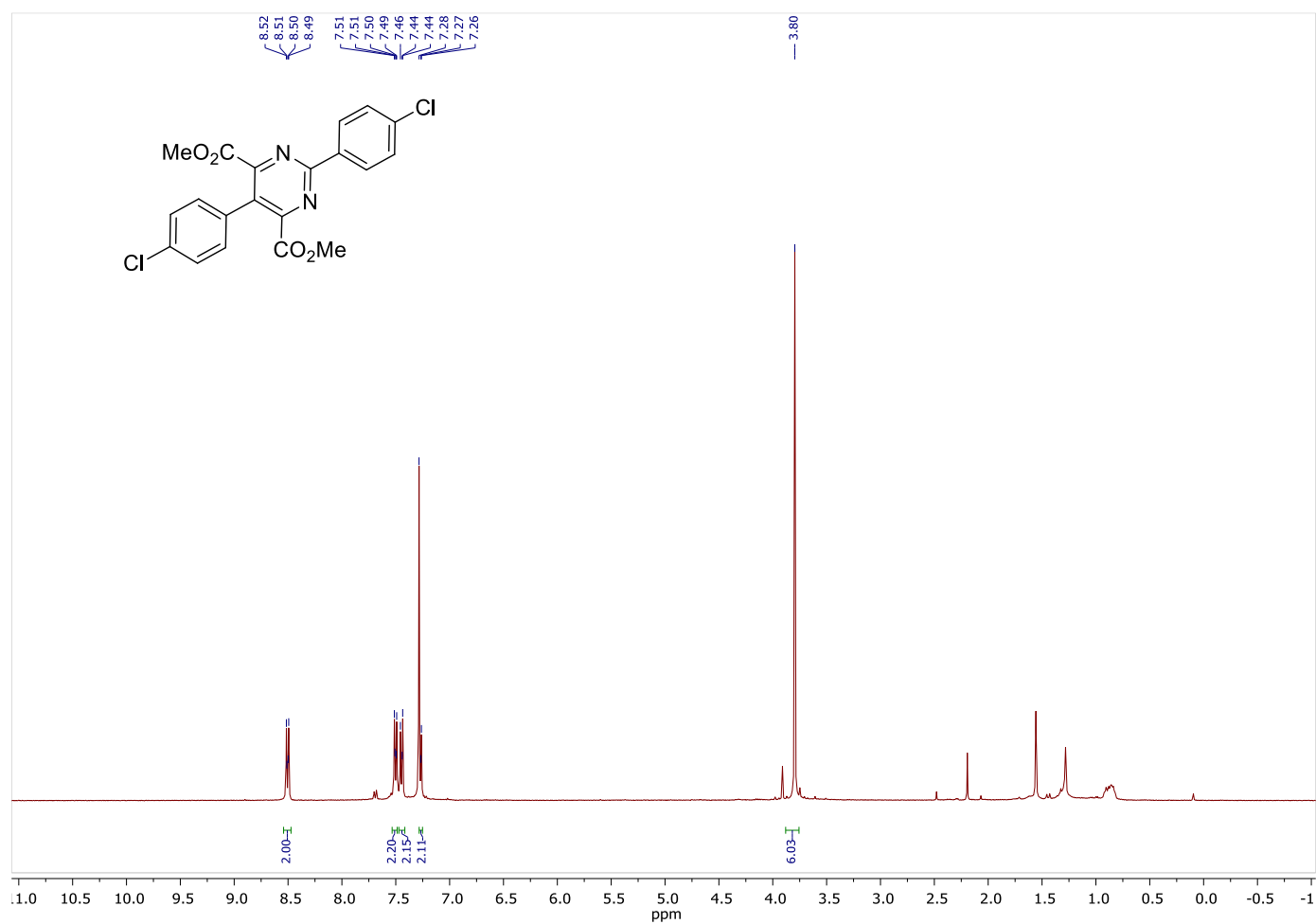
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(3,4-dimethylphenyl)pyrimidine-4,6-dicarboxylate (**3d**)



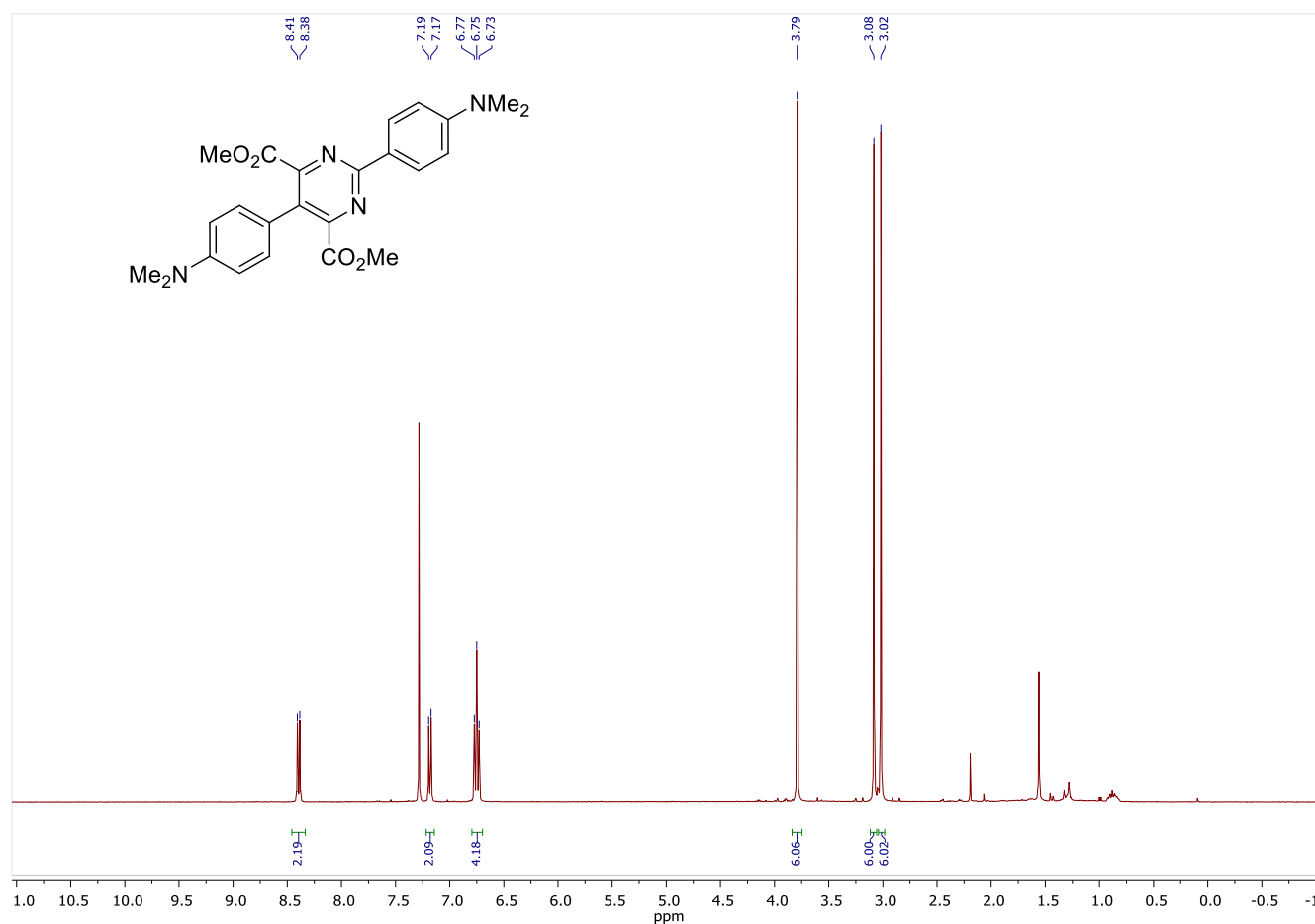
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) spectrum of dimethyl 2,5-di(3,4-dimethylphenyl)pyrimidine-4,6-dicarboxylate (**3d**)



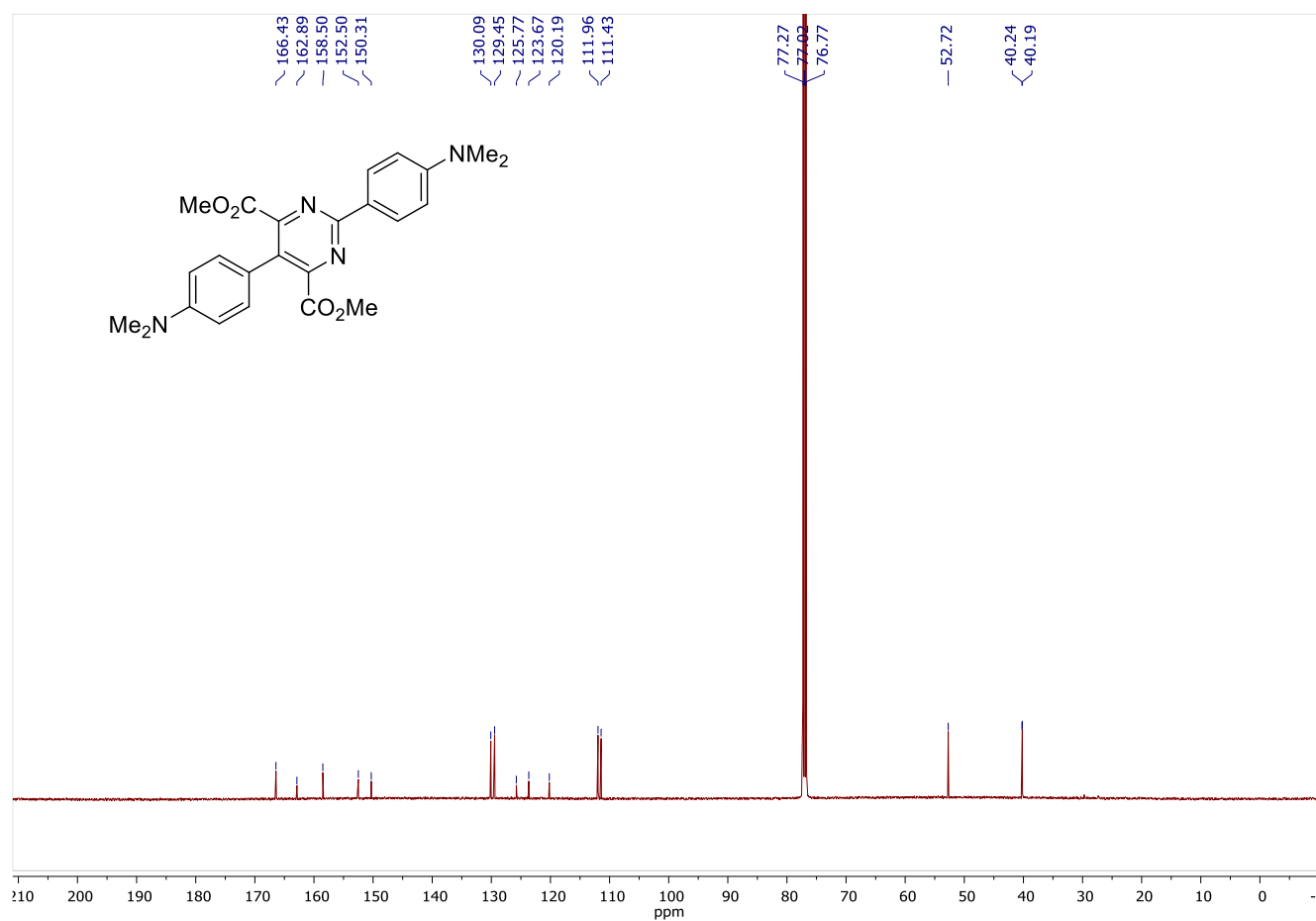
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(4-chlorophenyl)pyrimidine-4,6-dicarboxylate (**3e**)



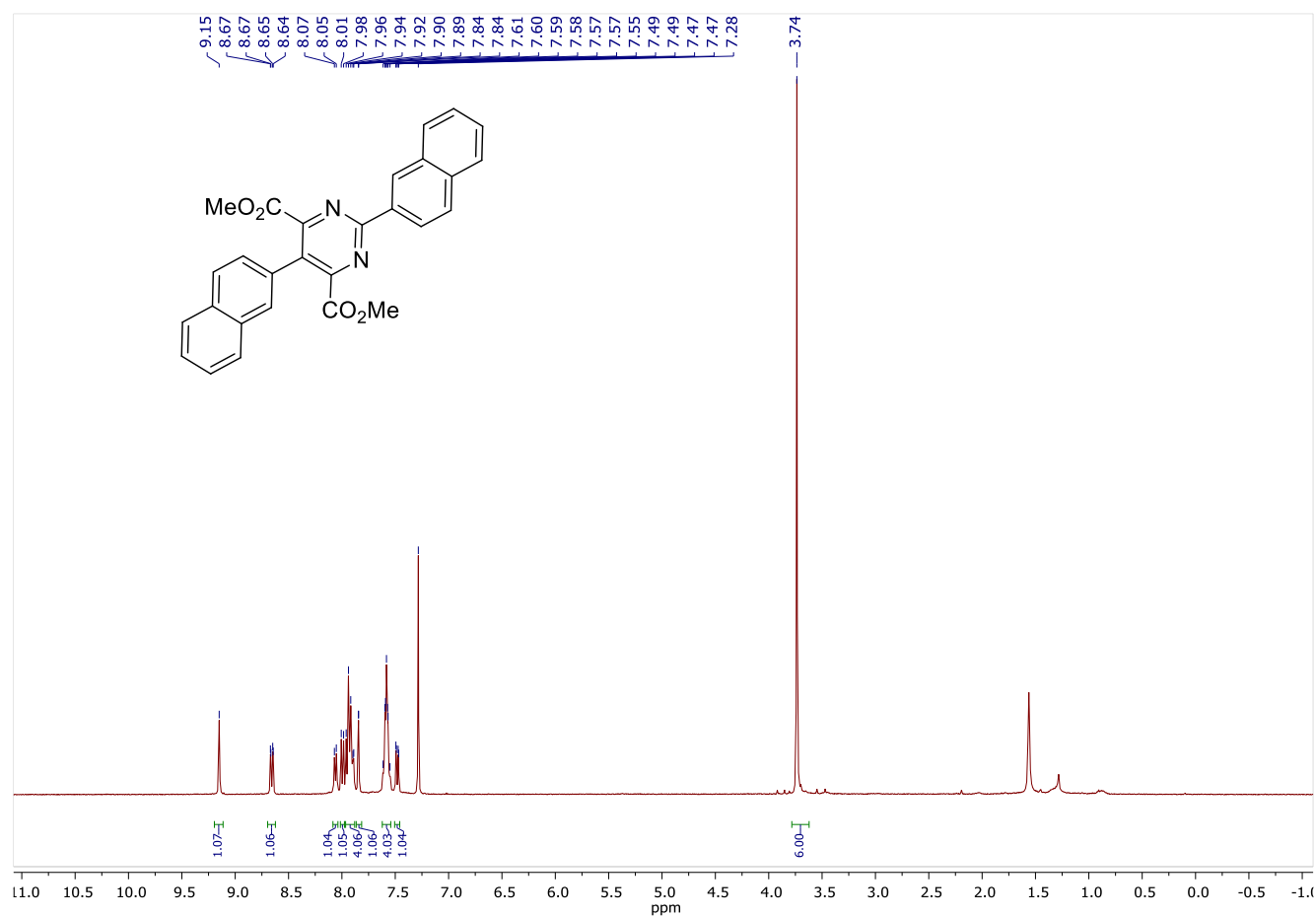
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(4-dimethylaminophenyl)pyrimidine-4,6-dicarboxylate (**3f**)



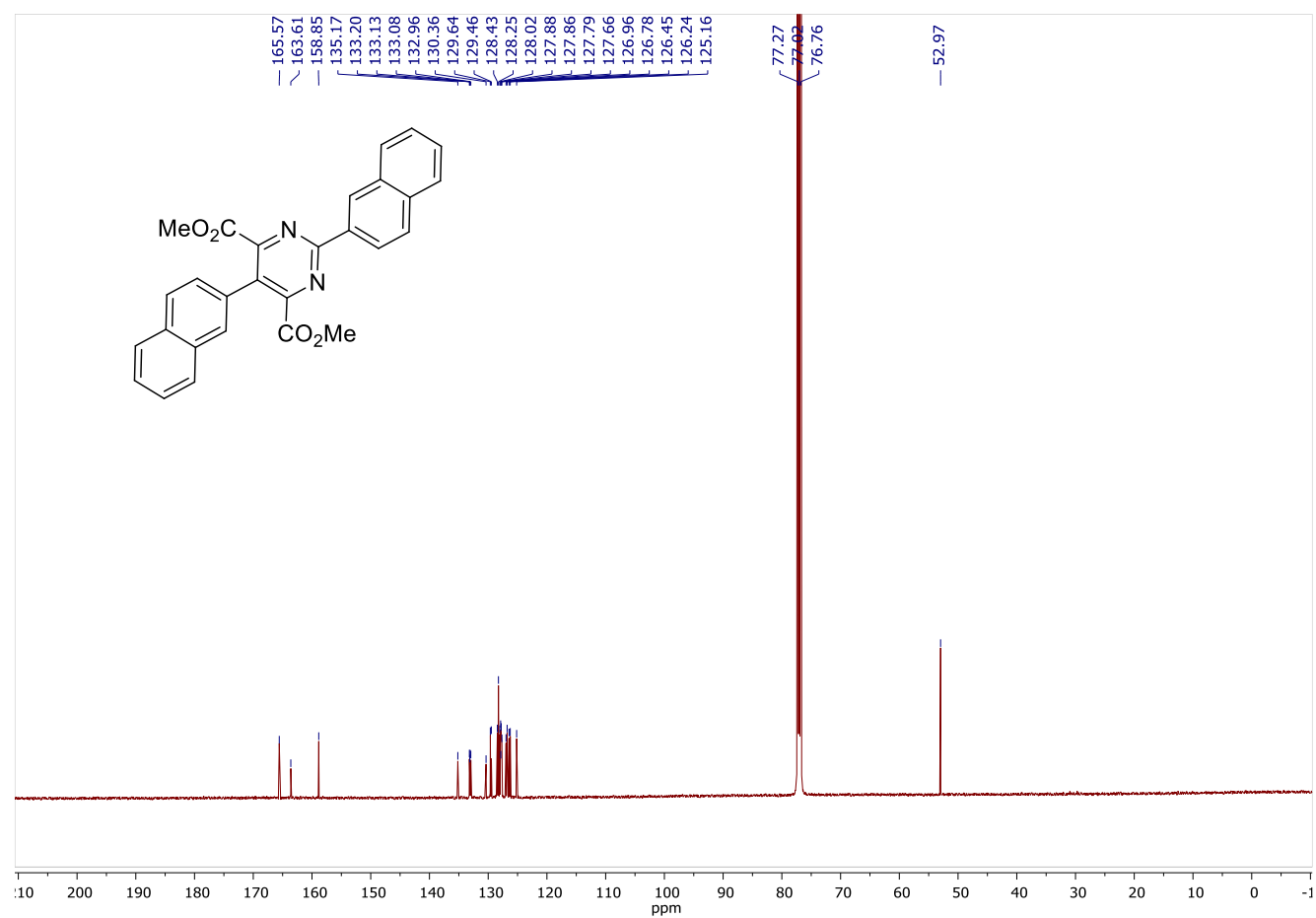
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) spectrum of dimethyl 2,5-di(4-dimethylaminophenyl)pyrimidine-4,6-dicarboxylate (**3f**)



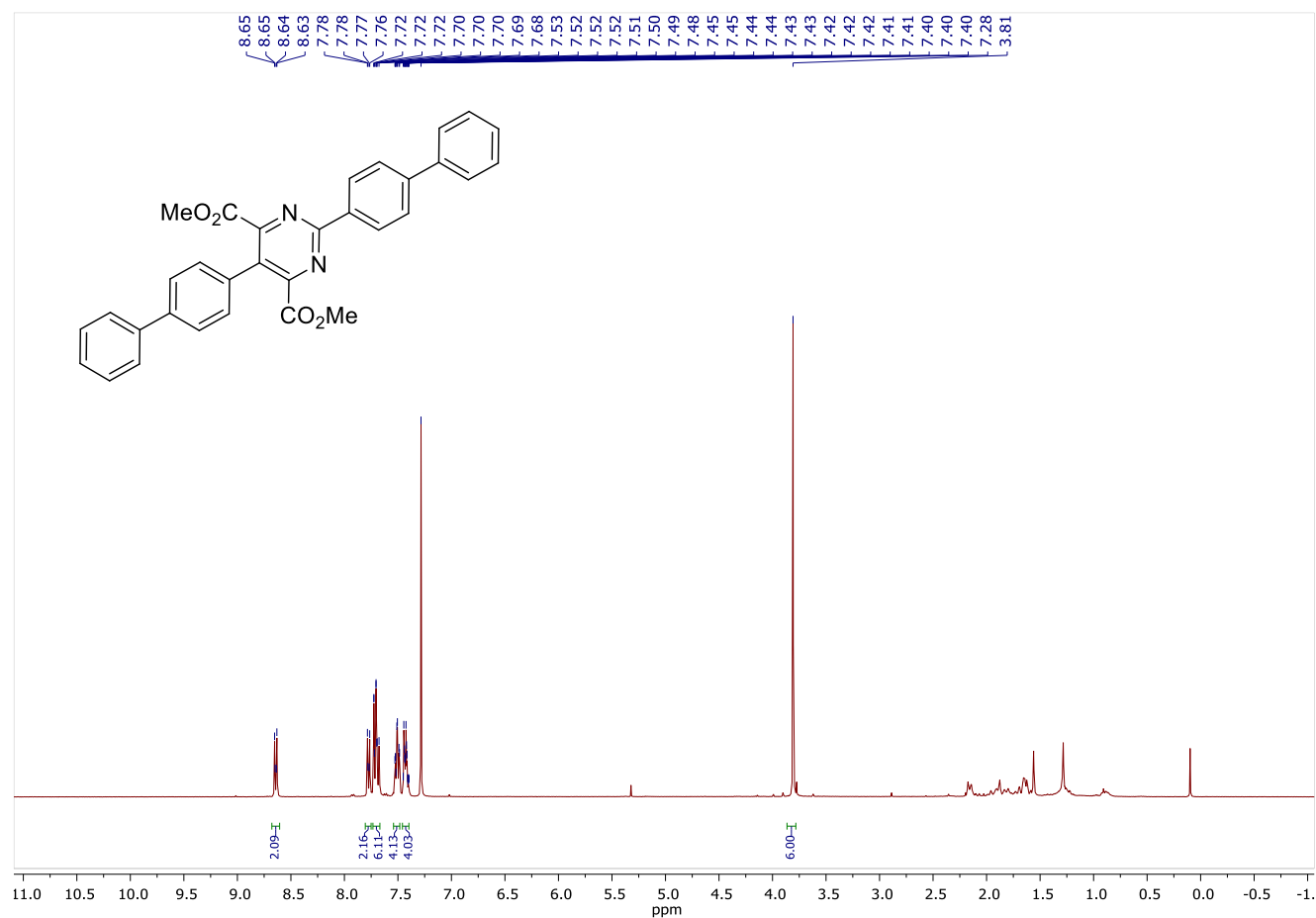
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(naphthalen-2-yl)pyrimidine-4,6-dicarboxylate (**3g**)



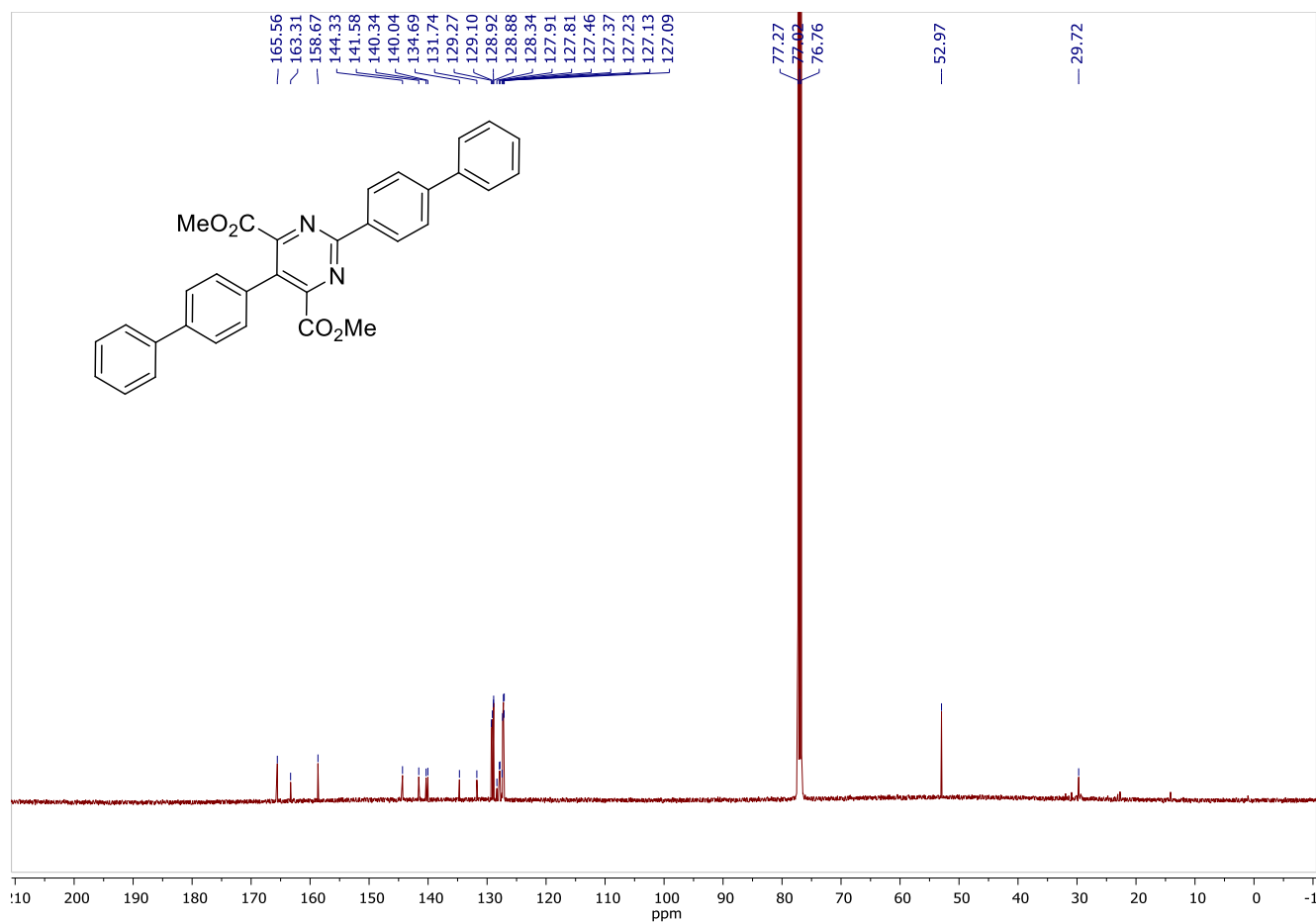
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) spectrum of dimethyl 2,5-di(naphthalen-2-yl)pyrimidine-4,6-dicarboxylate (**3g**)



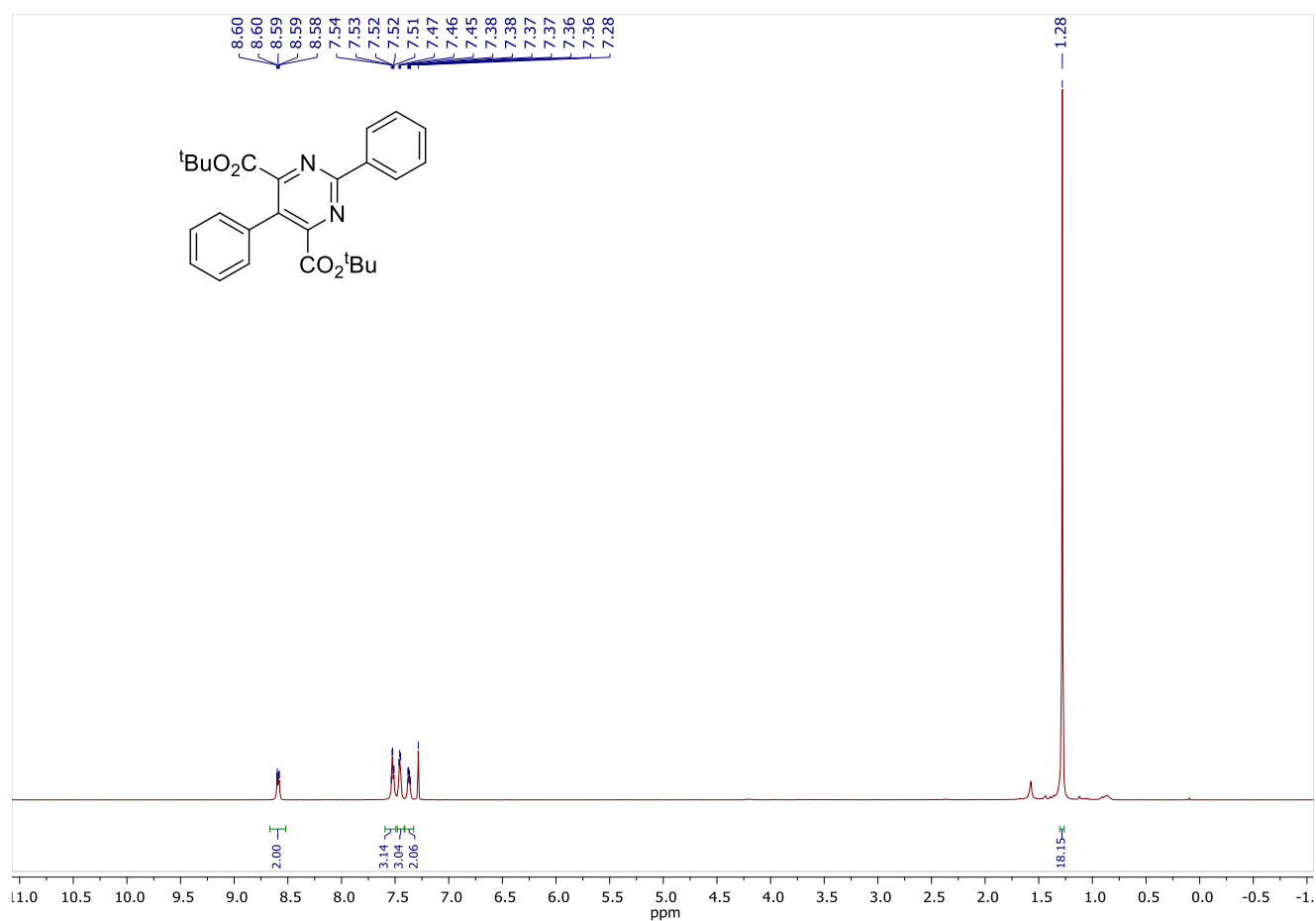
^1H NMR (400 MHz, CDCl_3) spectrum of dimethyl 2,5-di(4-biphenyl)pyrimidine-4,6-dicarboxylate (**3h**)



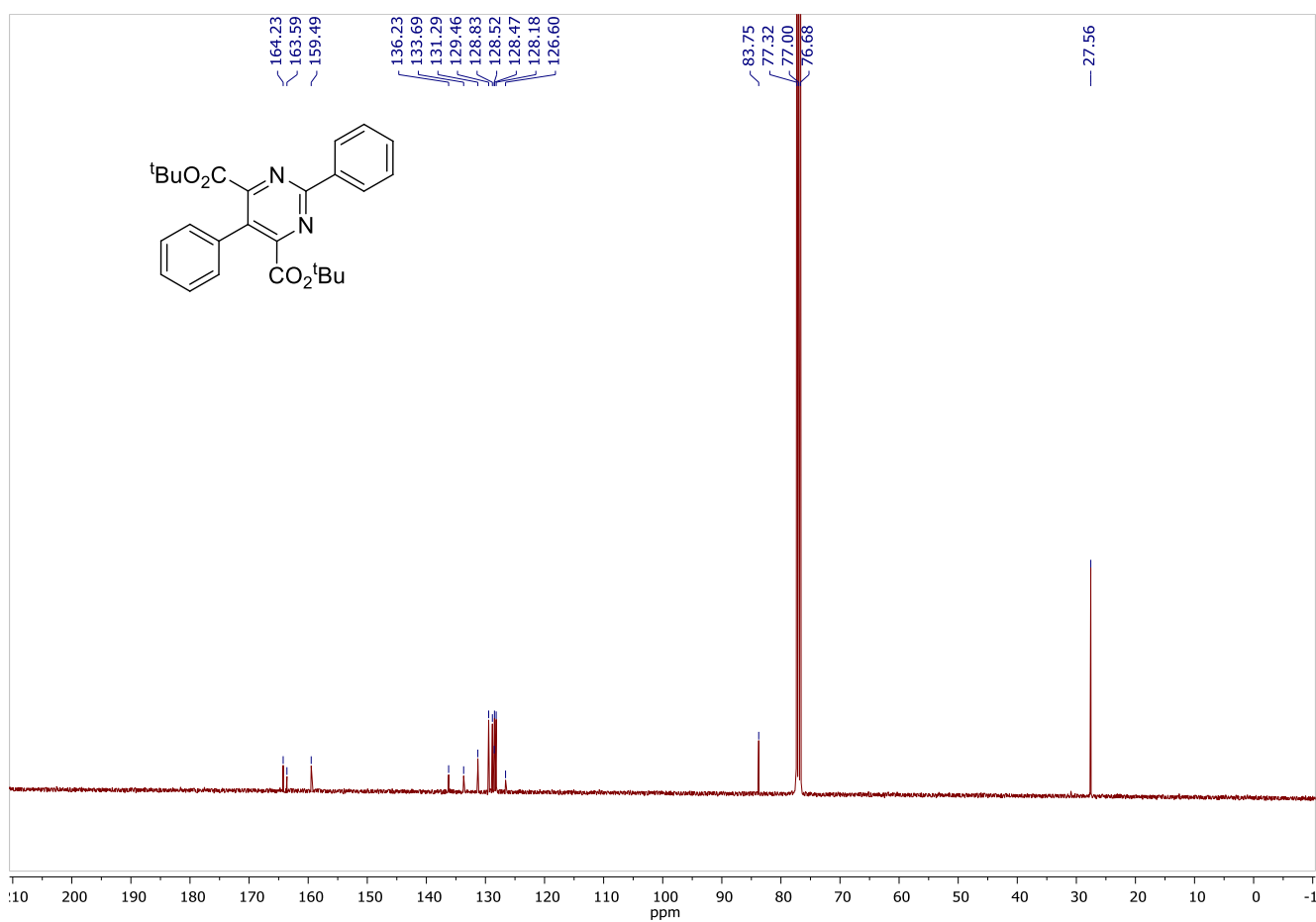
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) spectrum of dimethyl 2,5-di(4-biphenyl)pyrimidine-4,6-dicarboxylate (**3h**)



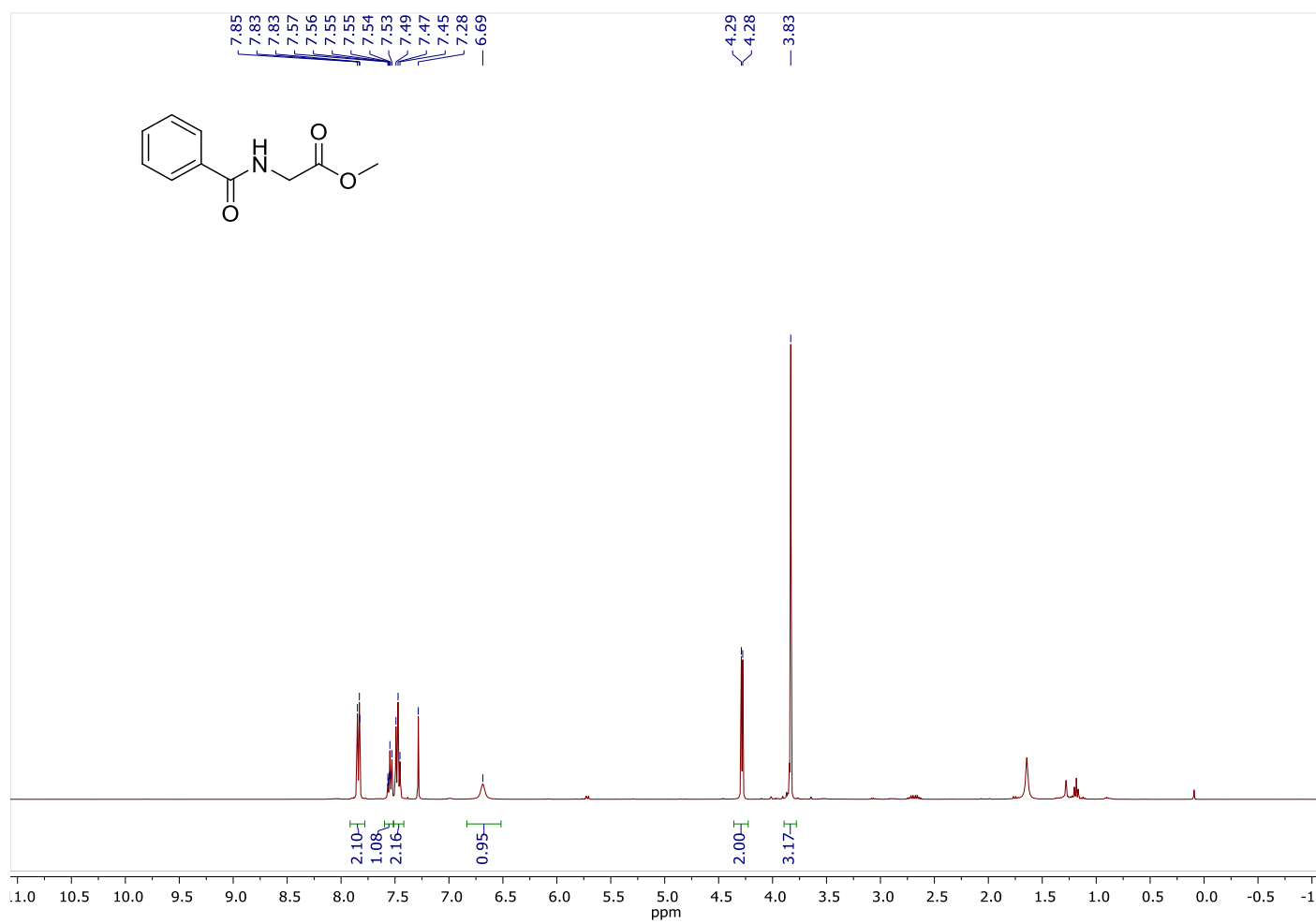
^1H NMR (400 MHz, CDCl_3) spectrum of di-*tert*-butyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3i**)



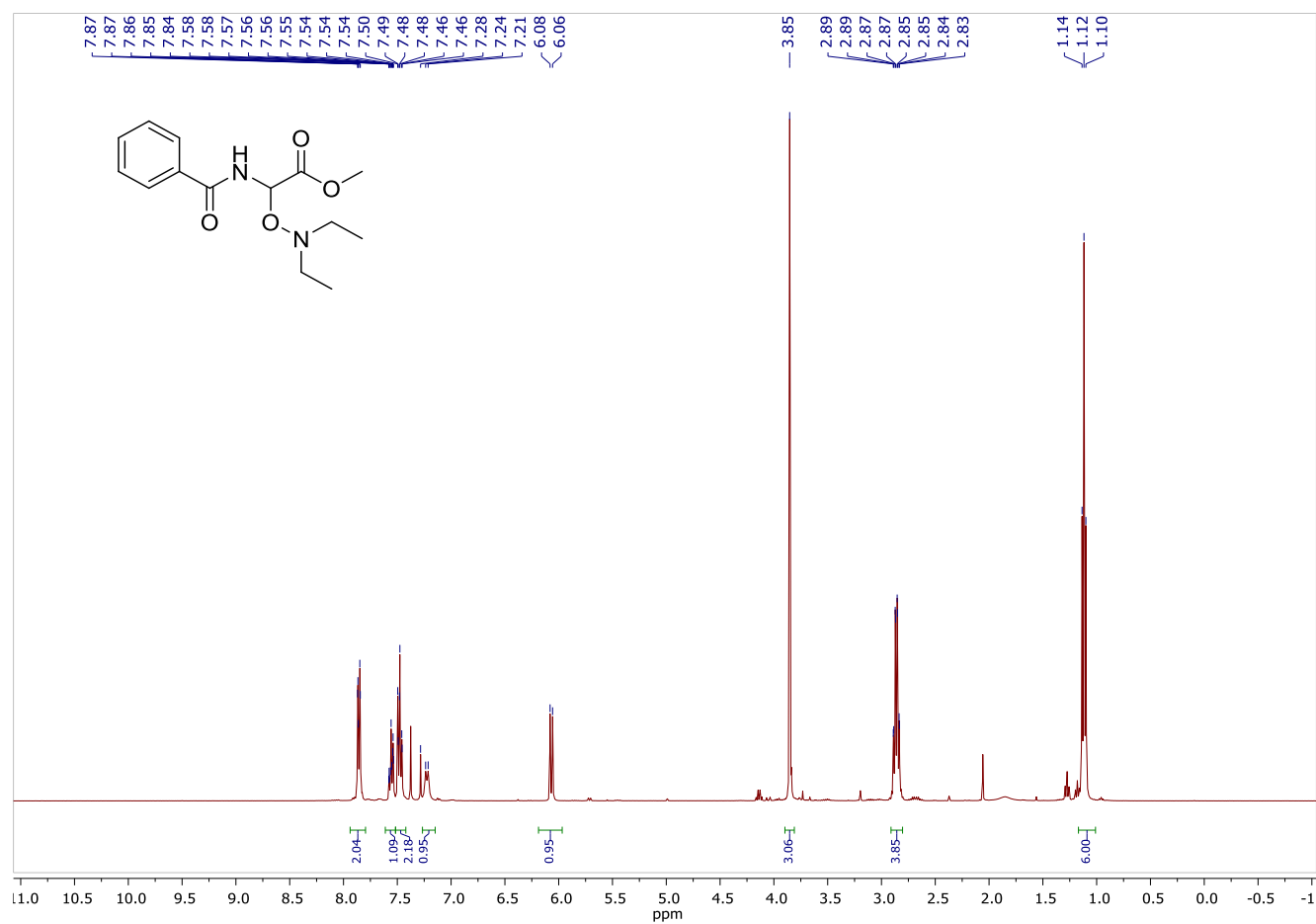
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of di-*tert*-butyl 2,5-diphenylpyrimidine-4,6-dicarboxylate (**3i**)



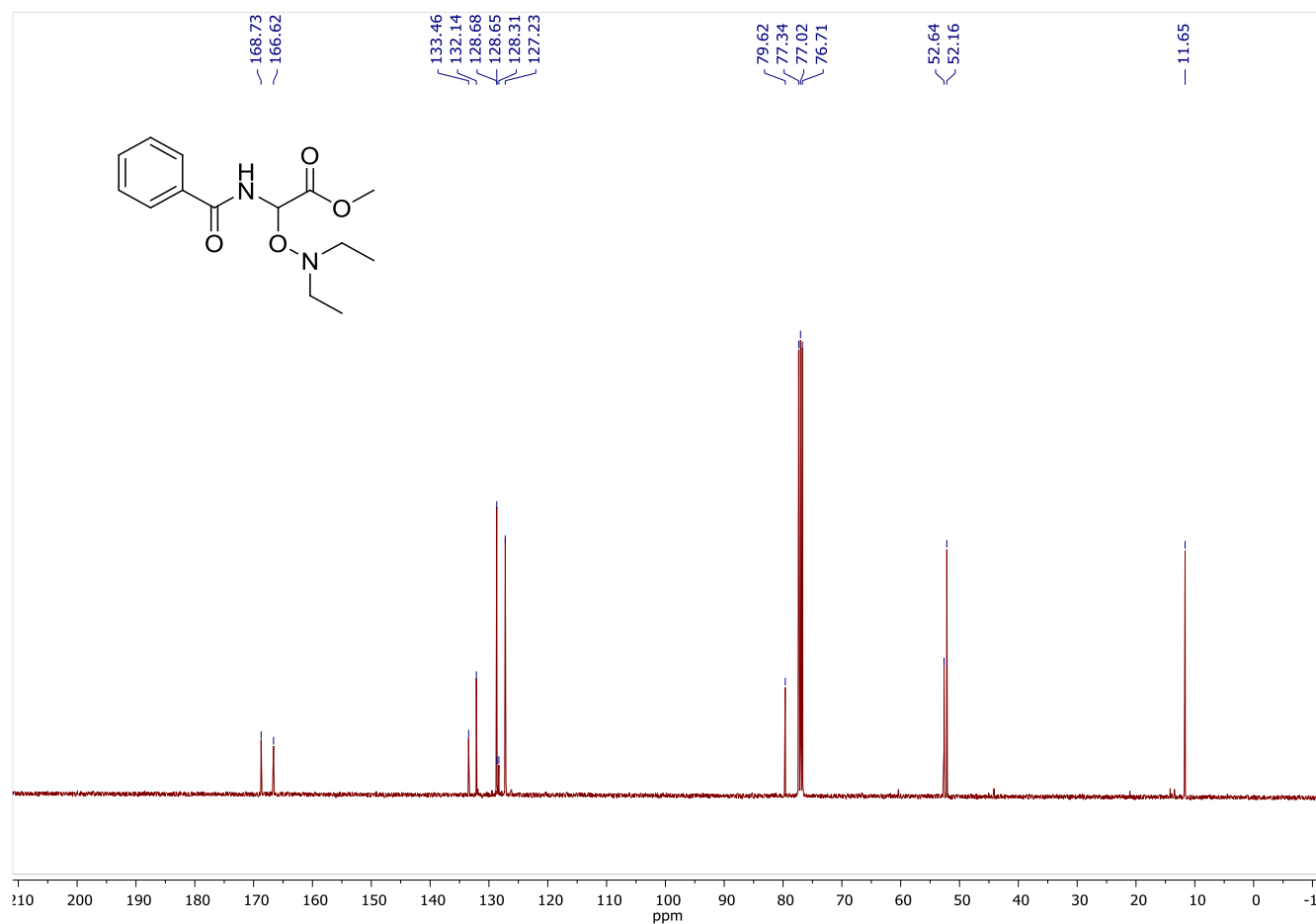
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 2-benzamidoacetate (**4a**)



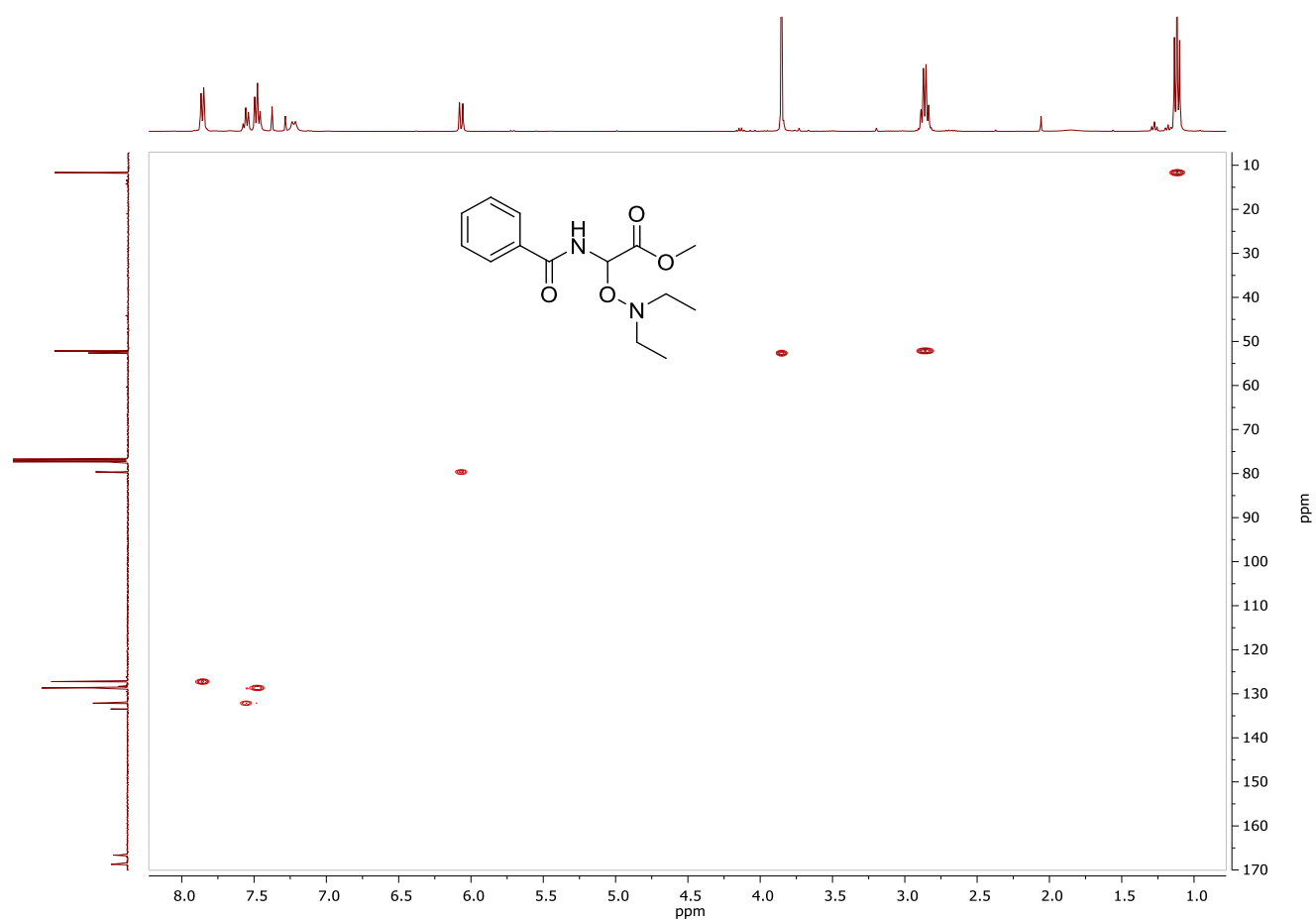
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 2-benzamido-2-((diethylamino)oxy)acetate (**4b**)



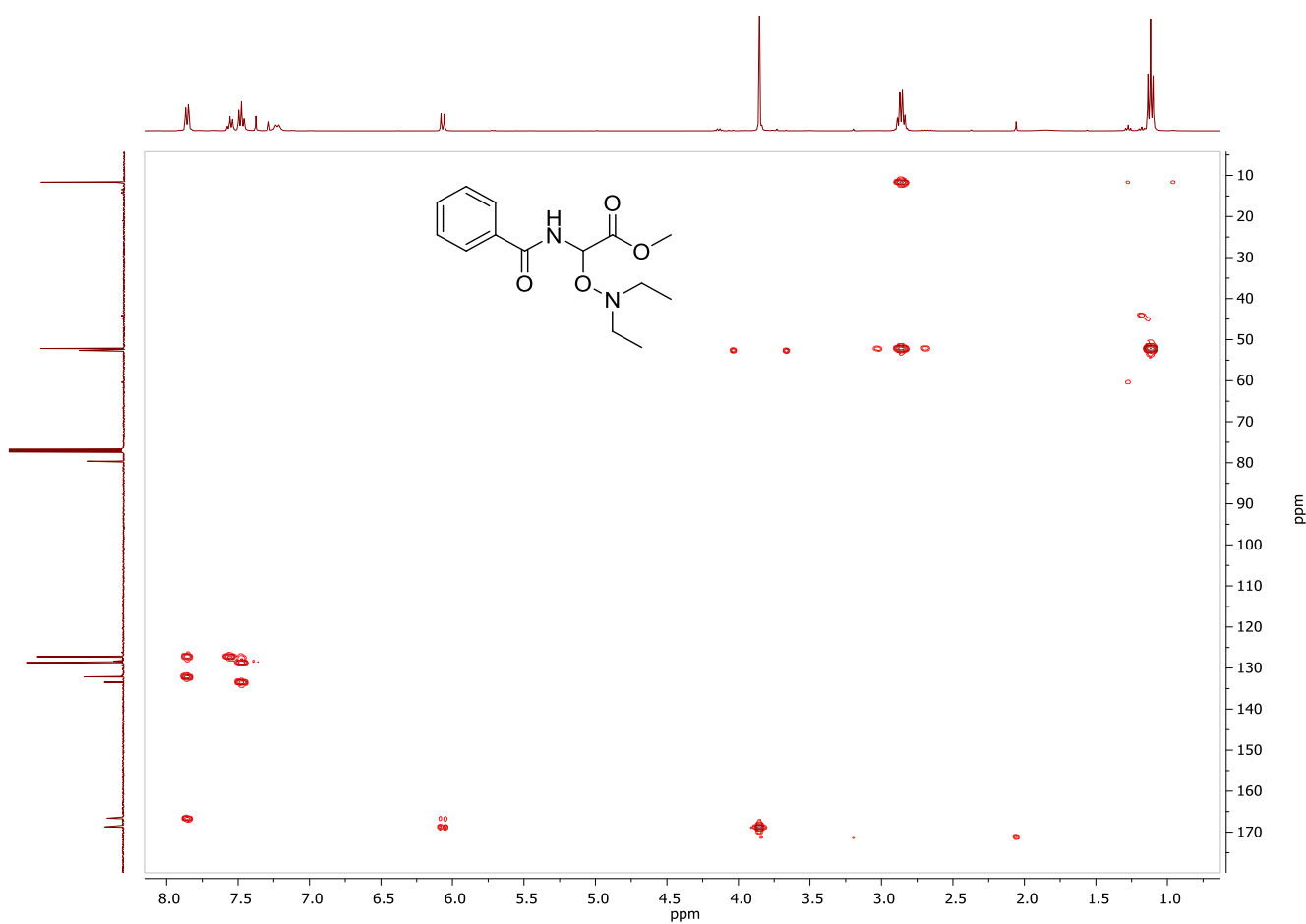
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectrum of methyl 2-benzamido-2-((diethylamino)oxy)acetate (**4b**)



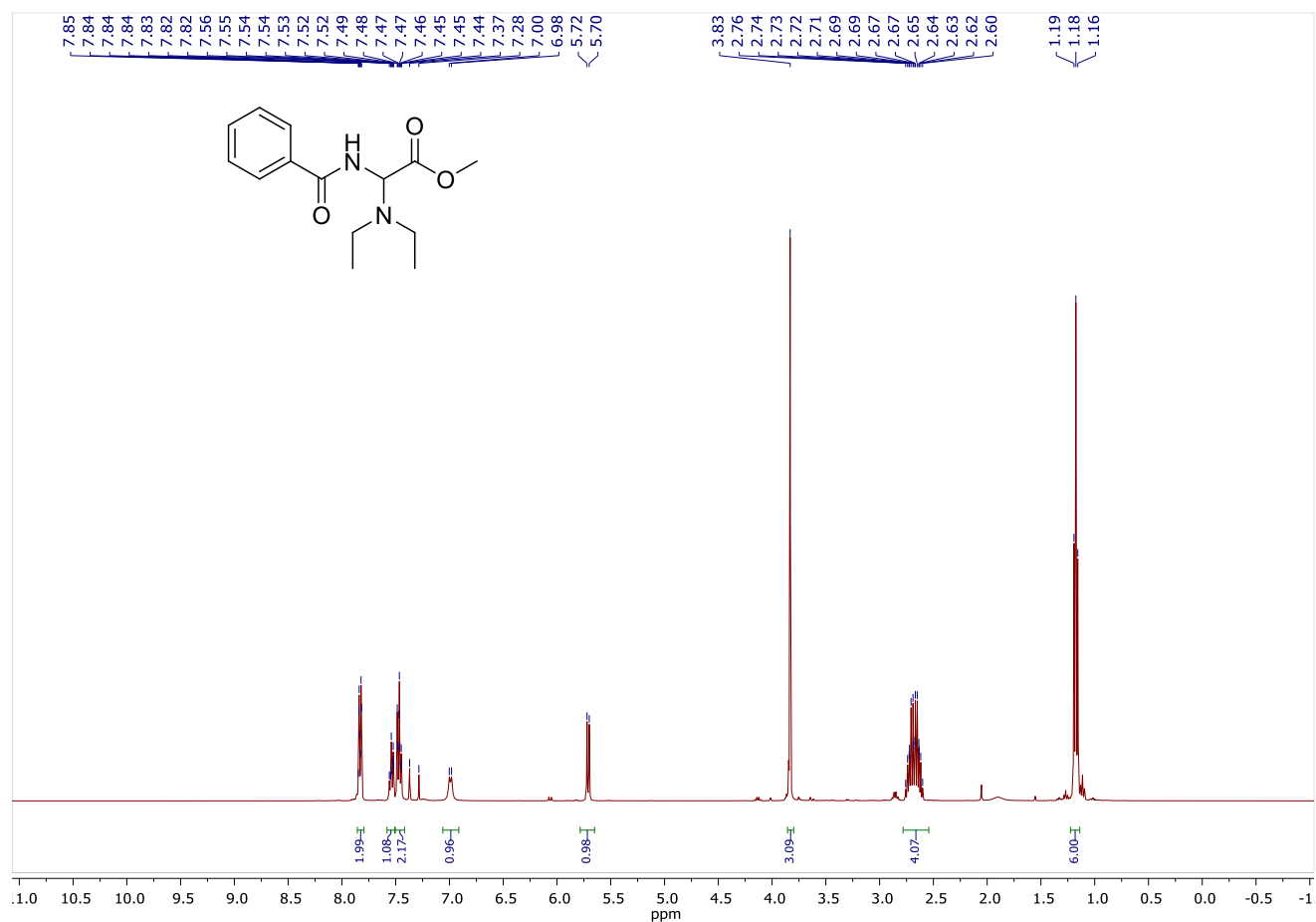
^1H - ^{13}C HSQC spectrum (400 MHz, CDCl_3) of methyl 2-benzamido-2-((diethylamino)oxy)acetate (**4b**)



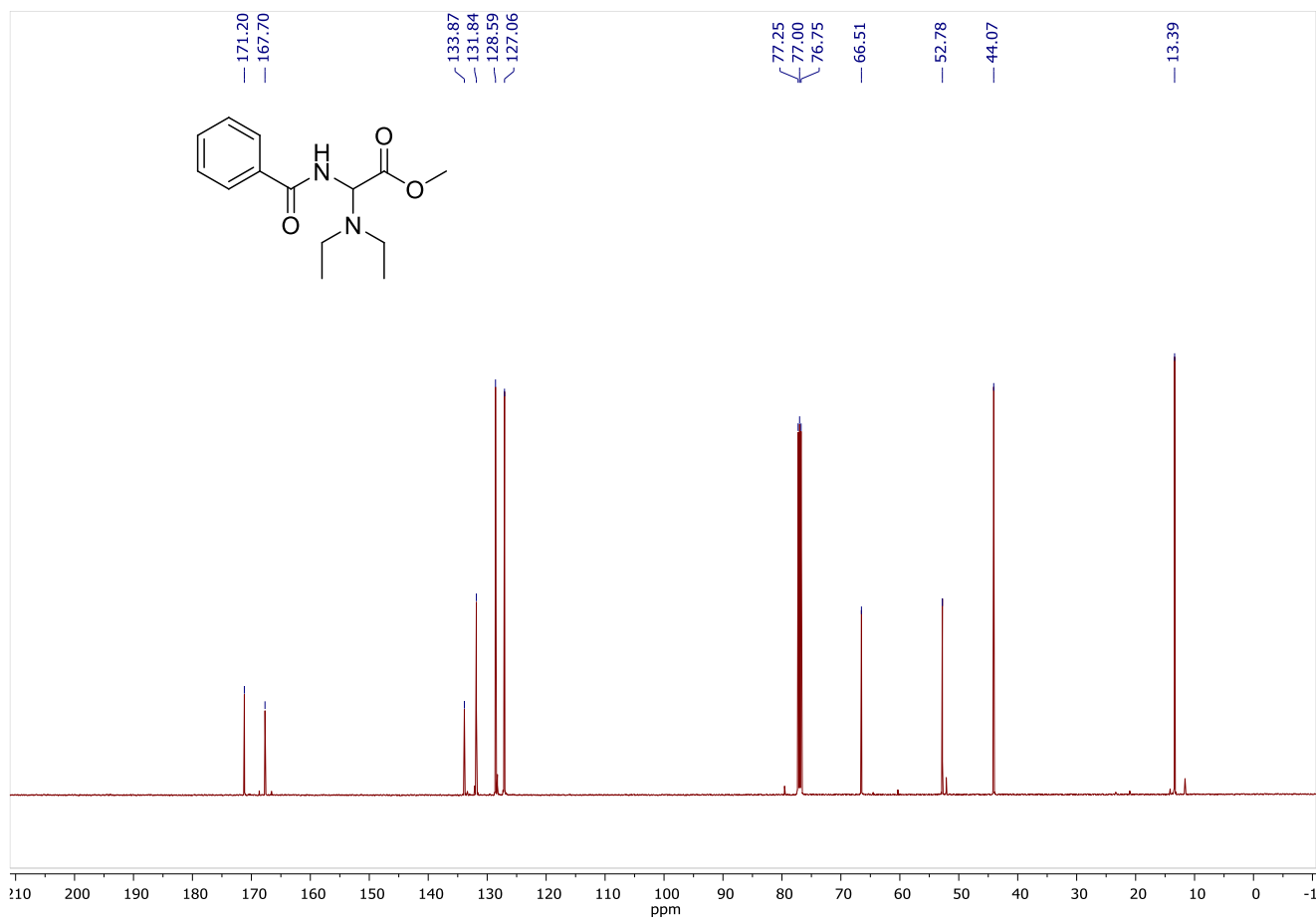
^1H - ^{13}C HMBC spectrum (400 MHz, CDCl_3) of methyl 2-benzamido-2-((diethylamino)oxy)acetate (**4b**)



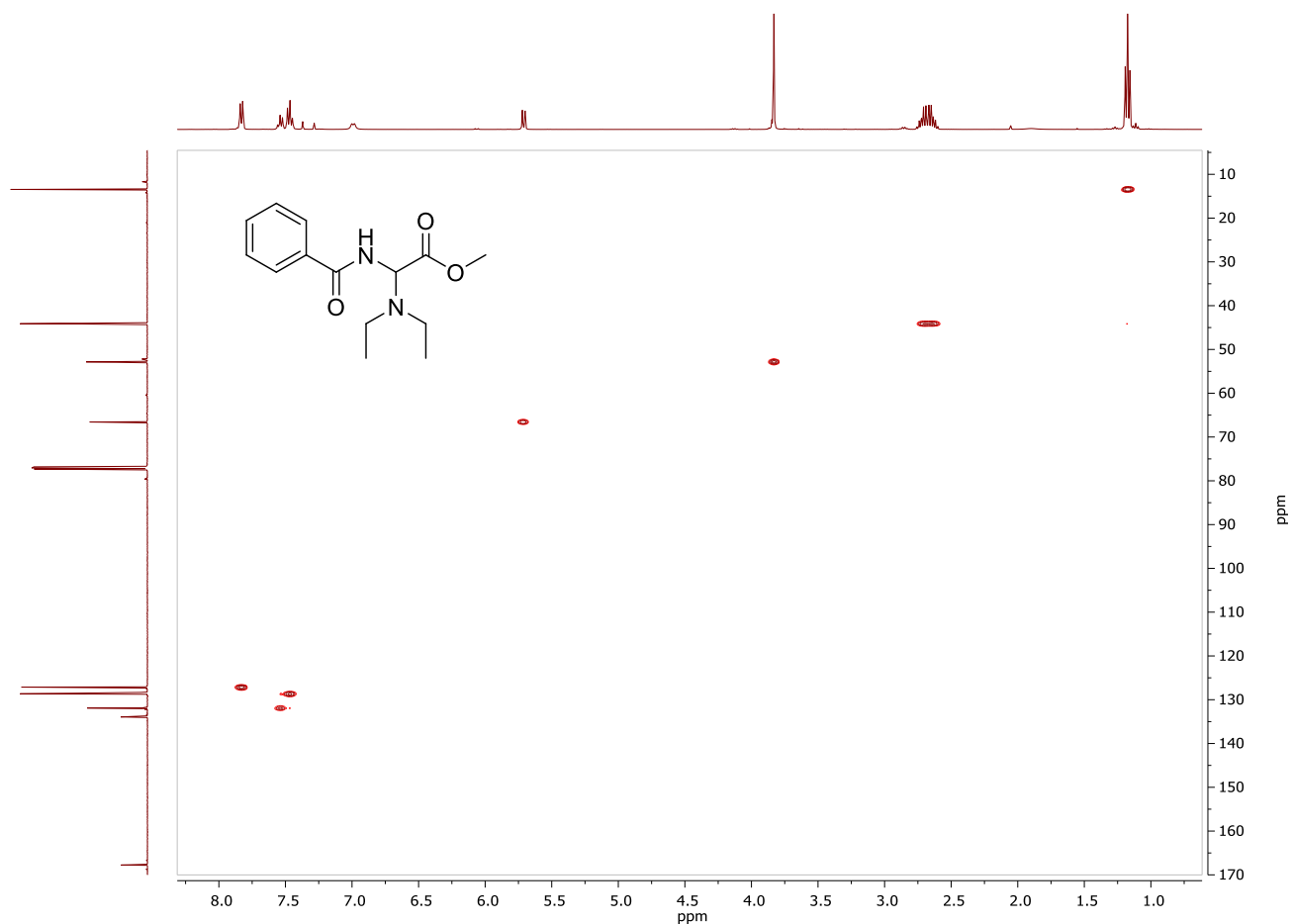
^1H NMR (400 MHz, CDCl_3) spectrum of methyl 2-benzamido-2-(diethylamino)acetate (**4c**)



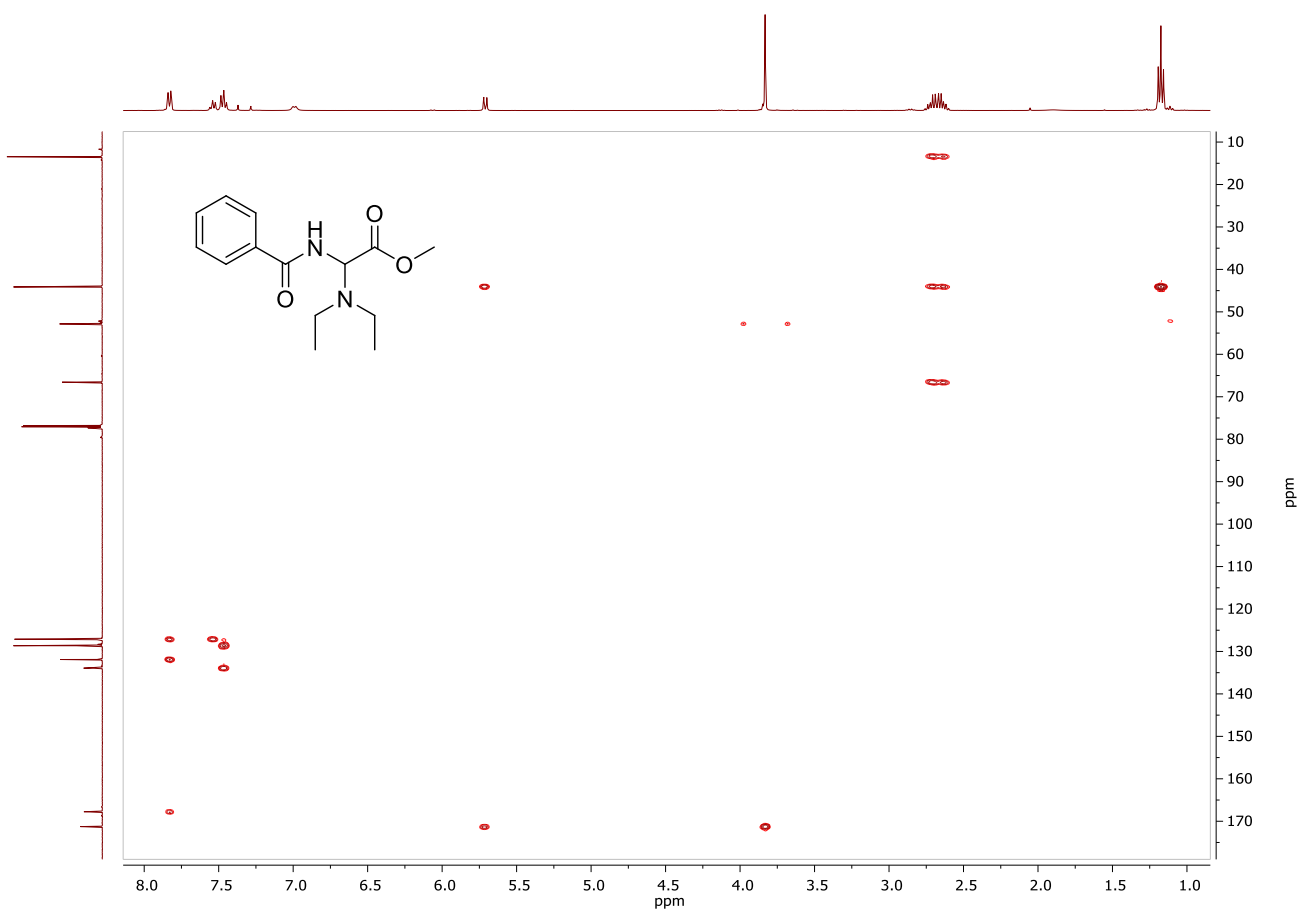
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) spectrum of methyl 2-benzamido-2-(diethylamino)acetate (**4c**)



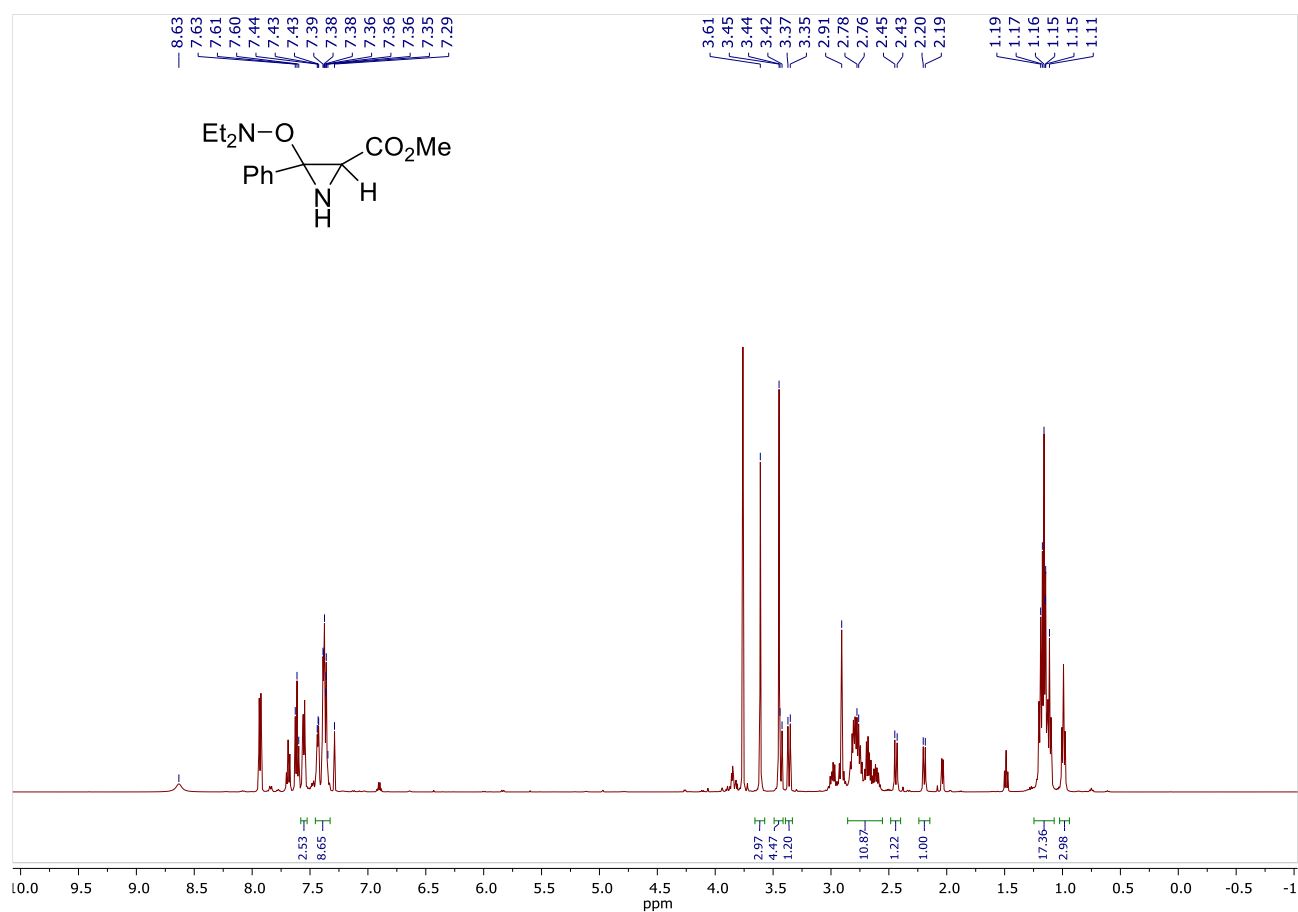
^1H - ^{13}C HSQC spectrum (500 MHz, CDCl_3) of methyl 2-benzamido-2-(diethylamino)acetate (**4c**)



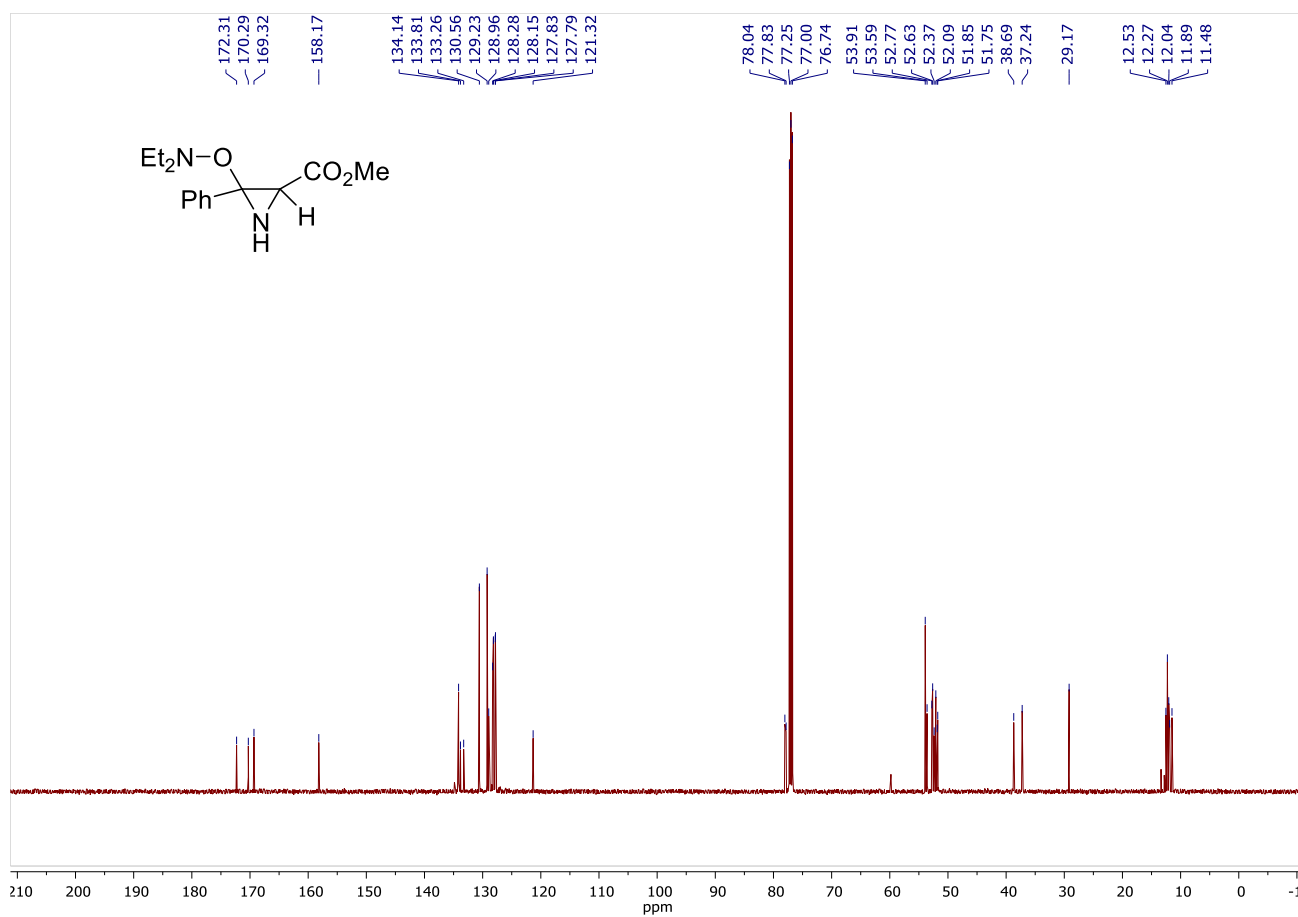
^1H - ^{13}C HMBC spectrum (500 MHz, CDCl_3) of methyl 2-benzamido-2-(diethylamino)acetate (**4c**)



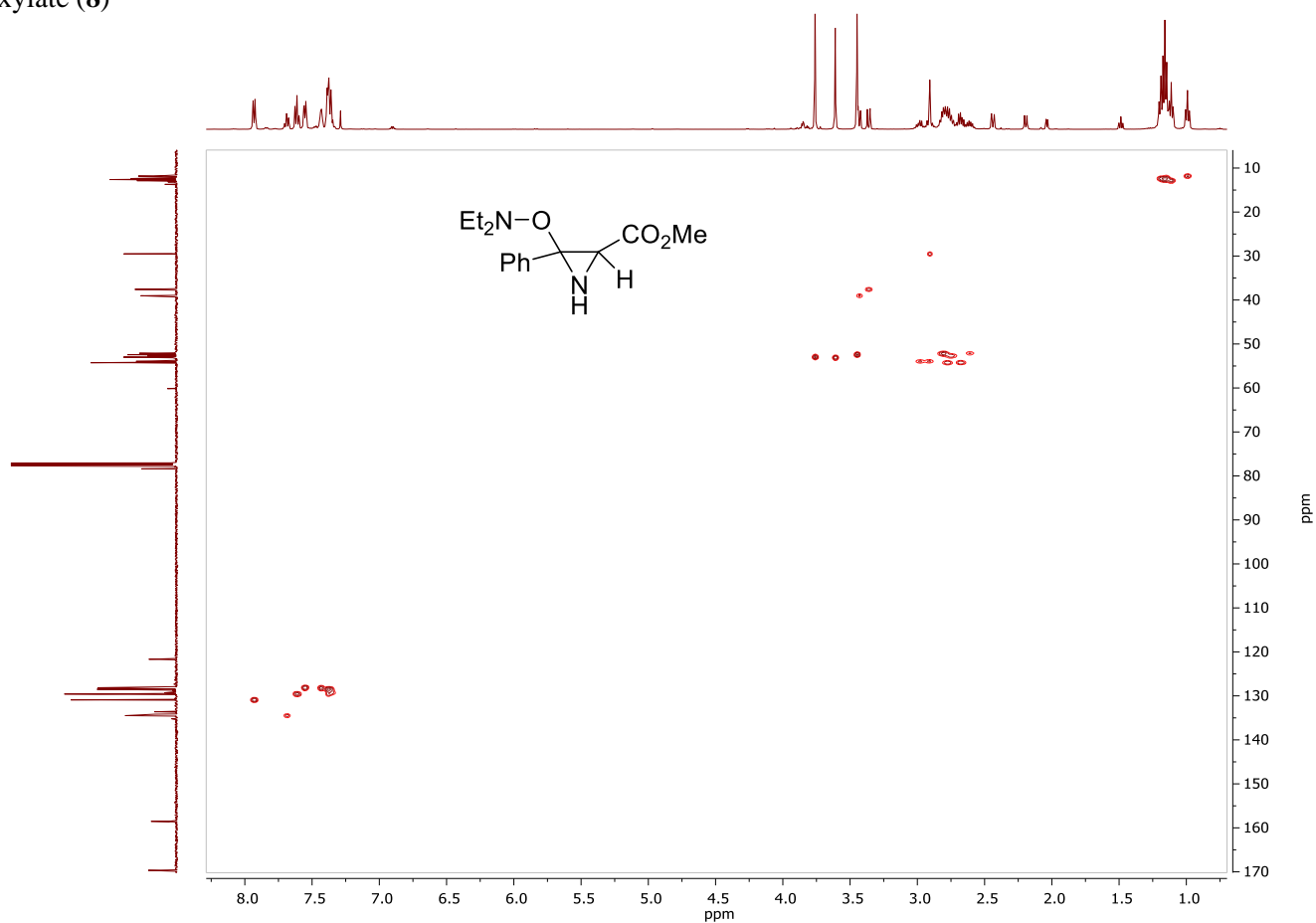
^1H NMR (500 MHz, CDCl_3 , $-40\text{ }^\circ\text{C}$) spectrum of crude methyl 3-(diethylaminoxy)-3-phenylaziridine-2-carboxylate (**8**)



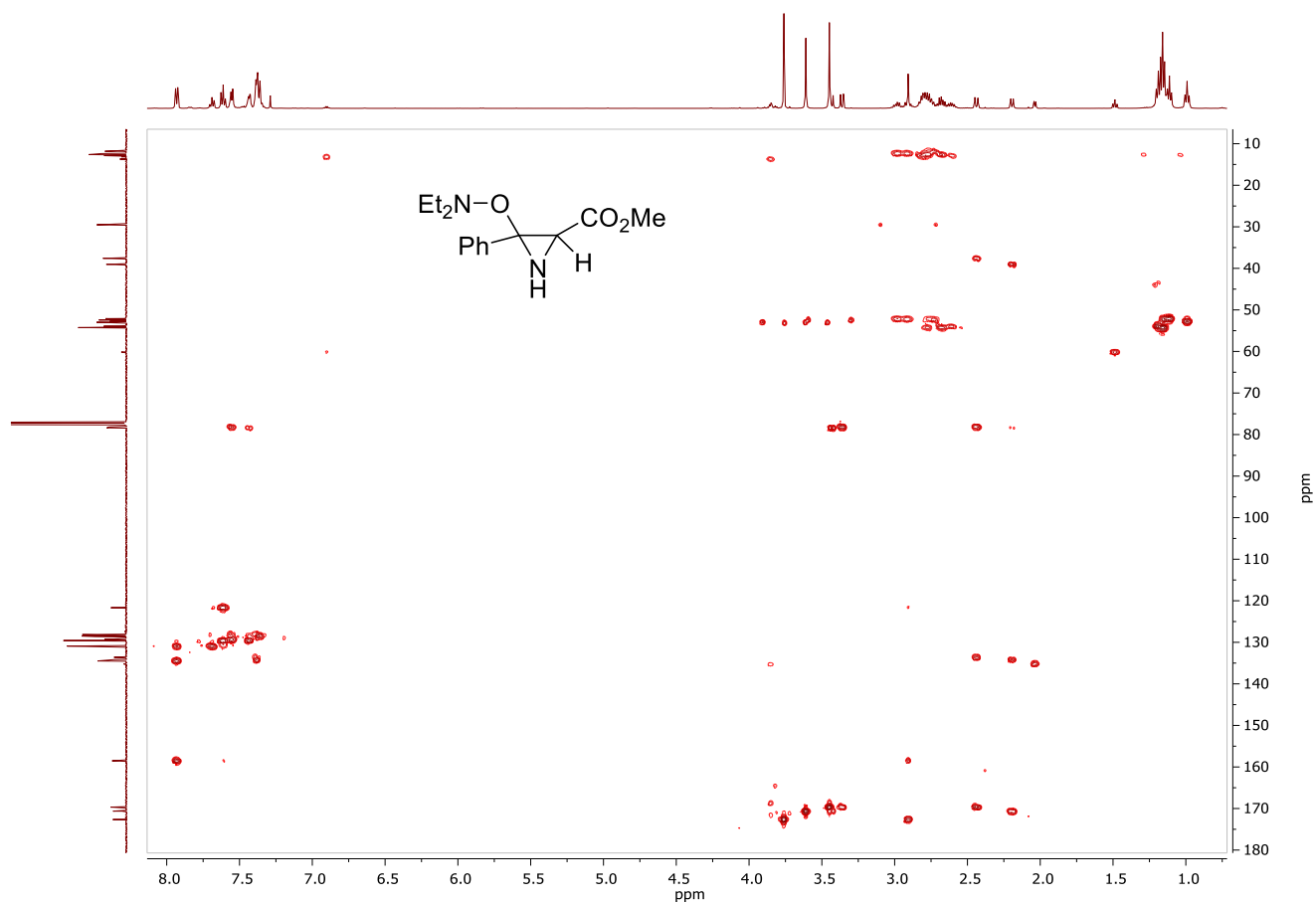
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3 , $-40\text{ }^\circ\text{C}$) spectrum of crude methyl 3-(diethylaminoxy)-3-phenylaziridine-2-carboxylate (**8**)



^1H - ^{13}C HSQC spectrum (500 MHz, CDCl_3 , -40°C) of crude methyl 3-(diethylaminooxy)-3-phenylaziridine-2-carboxylate (**8**)

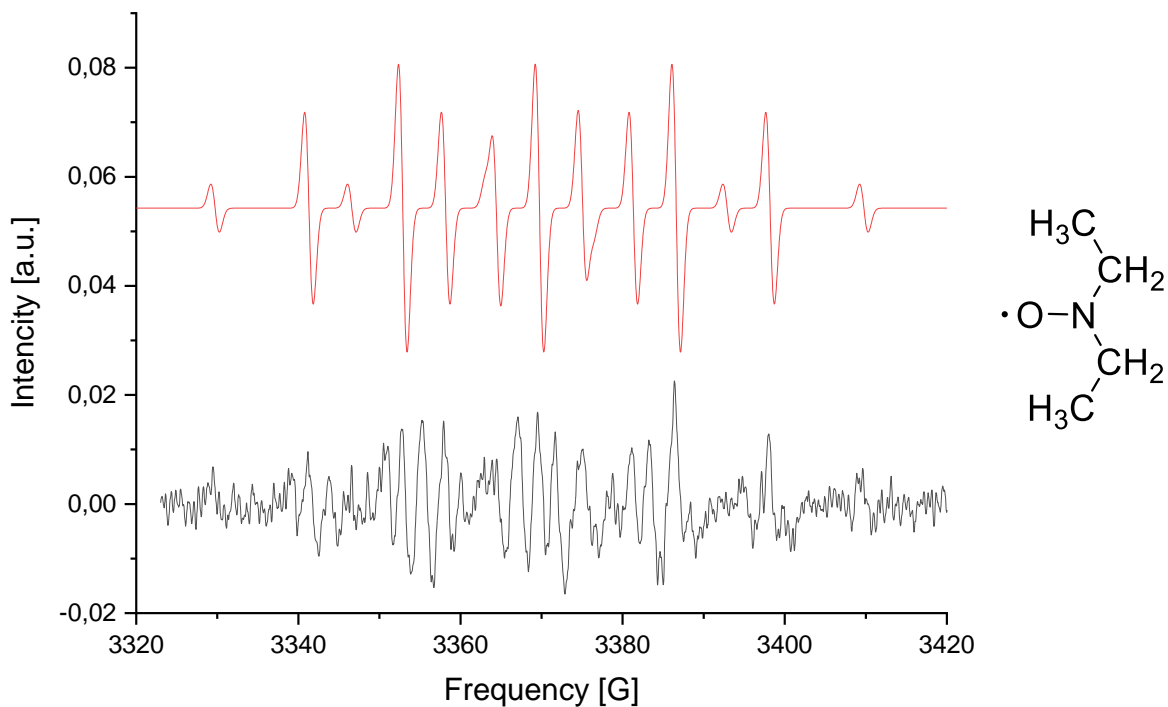


^1H - ^{13}C HMBC spectrum (500 MHz, CDCl_3 , -40°C) of crude methyl 3-(diethylaminooxy)-3-phenylaziridine-2-carboxylate (**8**)



II. EPR spectroscopy

The reaction mixture of azirine **1a** (60 mg, 0.34 mmol) and triethylamine (90 mg, 0.88 mmol) in acetonitrile (1.5 mL) was stirred at 70 °C for 12 h. After cooling, a few drops of water were added to this reaction mixture to increase the signal resolution. The mixture was transferred into an EPR vial. The EPR experiment was carried out on a Bruker Elexsys E580 with a modulation amplitude of 1 G and at 323 K.

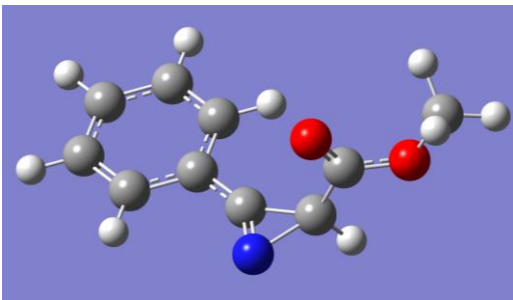
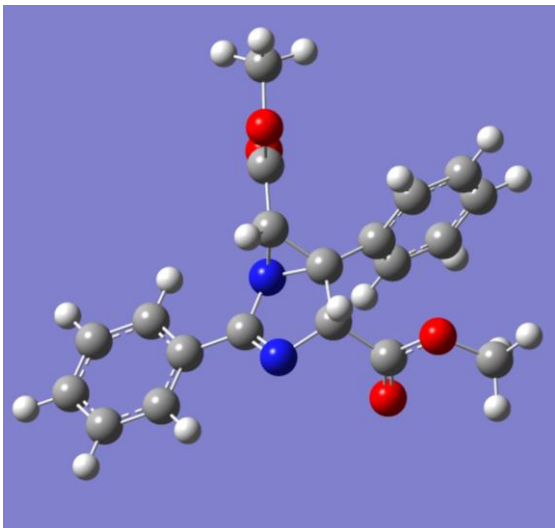


g-factor	2.00558
a_N	11.58 G
a_H	16.87 G

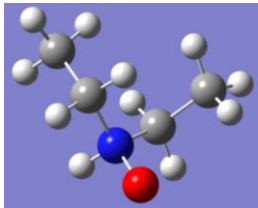
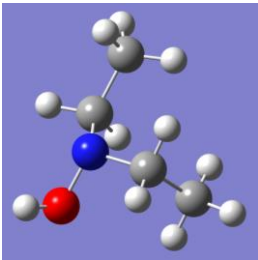
III. Calculations details

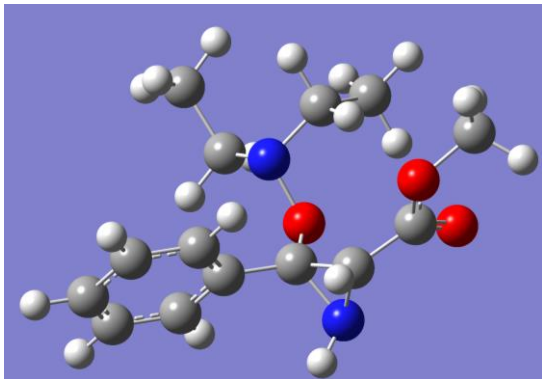
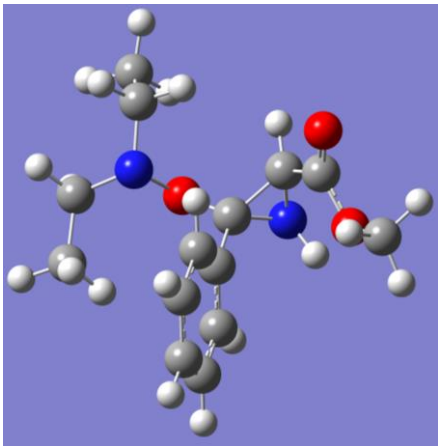
All calculations were performed by using the Gaussian 09 D.01 suit of quantum chemical programs.¹ The calculations were performed at the DFT rwb97xd/6-311+g(d,p) (Table S1) or ub3lyp/6-31g(d) (Table S2) level using PCM model for acetonitrile (343 K). The optimized structures were characterized by frequency analysis. Structures of the transition states were found by qst3 optimization model and optimized using Berny saddle point optimization algorithm.

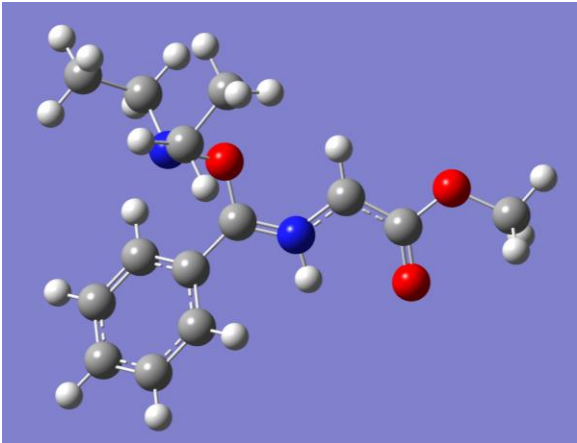
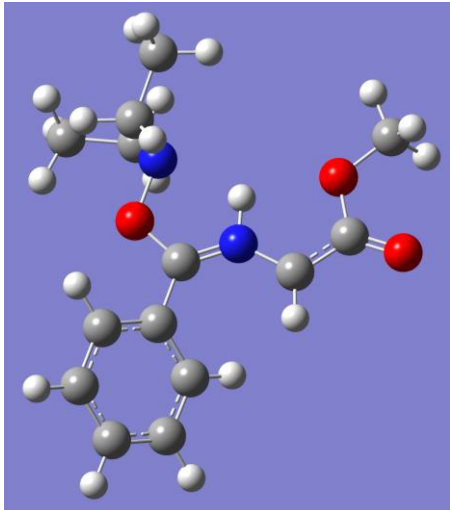
Table S1. Energies (au) and cartesian coordinates of stationary points for compounds **1a**, **7**, **7'**, *anti*-**8**, *syn*-**8**, *E*-**9**, *Z*-**9**, *anti*-**10**, *syn*-**10**, **11** and transition states TS1, TS1a, TS1b, TS2a, TS2b, TS3a, TS3b, TS4a, TS4b (calculations in rwb97xd/6-311+g(d,p)).

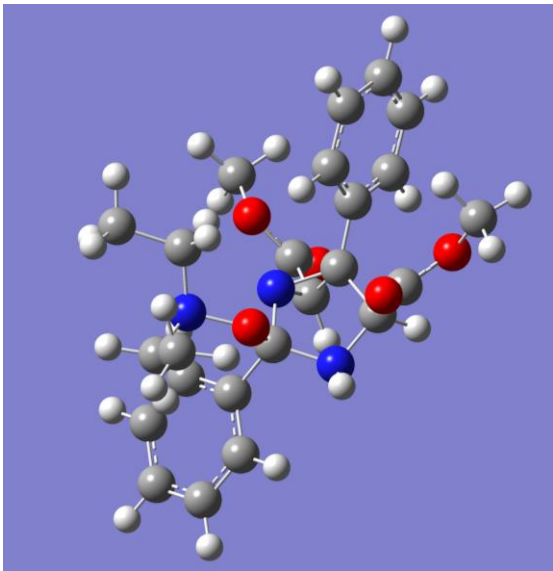
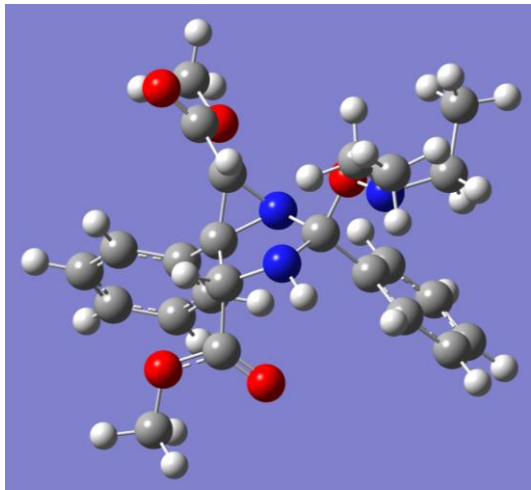
azirine 1a				azirinopyrroline 11			
							
Zero-point correction = 0.171506 (Hartree/Particle)				Zero-point correction = 0.349063 (Hartree/Particle)			
Thermal correction to Energy = 0.186245				Thermal correction to Energy = 0.378390			
Thermal correction to Enthalpy = 0.187331				Thermal correction to Enthalpy = 0.379476			
Thermal correction to Gibbs Free Energy = 0.124140				Thermal correction to Gibbs Free Energy = 0.281616			
Sum of electronic and zero-point Energies = -591.422847				Sum of electronic and zero-point Energies = -1182.930276			
Sum of electronic and thermal Energies = -591.408107				Sum of electronic and thermal Energies = -1182.900950			
Sum of electronic and thermal Enthalpies = -591.407021				Sum of electronic and thermal Enthalpies = -1182.899863			
Sum of electronic and thermal Free Energies = -591.470212				Sum of electronic and thermal Free Energies = -1182.997724			
Imaginary frequencies = 0				Imaginary frequencies = 0			
C	-3.835753000	0.908175000	0.211051000	N	1.204429000	-1.448845000	-1.076269000
C	-3.682270000	-0.452503000	0.472147000	C	1.663859000	-0.565347000	-0.280230000
C	-2.453138000	-1.061626000	0.274946000	N	0.723261000	0.365023000	0.273018000
C	-1.374205000	-0.300975000	-0.186864000	C	-0.536477000	0.019363000	-0.379212000
C	-1.527313000	1.061186000	-0.448183000	C	-0.226775000	-1.243652000	-1.221571000
C	-2.761655000	1.664330000	-0.247669000	C	0.214157000	1.241234000	-0.796062000
C	-0.087146000	-0.921268000	-0.397132000				
N	0.546686000	-1.995658000	-0.314714000				
C	1.299771000	-0.762125000	-0.814846000				
C	2.275140000	-0.159528000	0.134987000				
O	3.265817000	0.444255000	-0.518332000				
O	2.183086000	-0.203411000	1.339511000				
C	4.261781000	1.094546000	0.282768000				
H	-4.799023000	1.380199000	0.366695000				

¹ Gaussian 09, Revision D.01, 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. 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, N. J.; 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 09, Revision C.01; Gaussian: Wallingford CT, 2013.

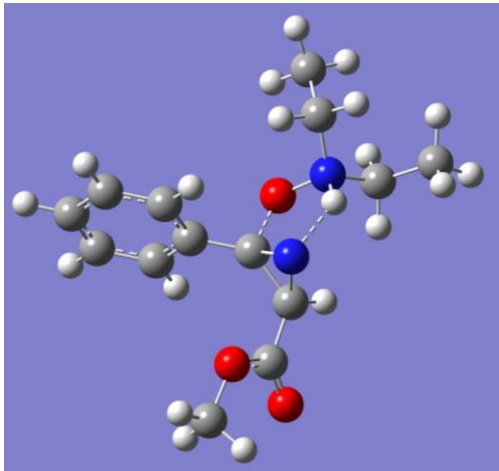
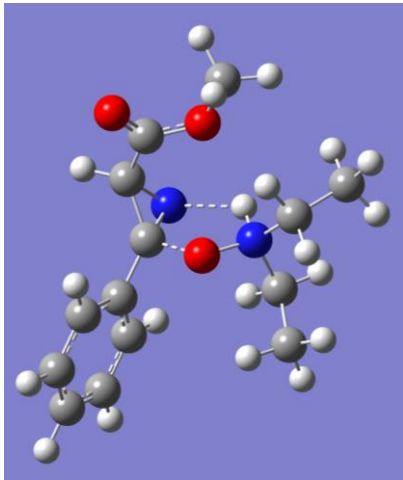
H	-4.523124000	-1.034805000	0.829543000	C	3.079281000	-0.425743000	0.091982000
H	-2.320382000	-2.118785000	0.474153000	C	-1.008554000	-2.435279000	-0.681471000
H	-0.680708000	1.636681000	-0.805473000	O	-2.207960000	-2.499009000	-1.246161000
H	-2.886902000	2.721595000	-0.447798000	O	-0.613330000	-3.186012000	0.173173000
H	1.566212000	-0.735285000	-1.865857000	C	-3.125230000	-3.453238000	-0.691951000
H	3.810853000	1.898008000	0.866255000	C	-0.267548000	2.594649000	-0.372111000
H	4.738891000	0.376872000	0.950523000	O	-0.614995000	3.298322000	-1.445780000
H	4.984882000	1.497109000	-0.421704000	O	-0.353766000	2.987346000	0.762492000
				C	-1.161937000	4.603706000	-1.206736000
				C	-1.816537000	0.110592000	0.383115000
				C	3.483359000	0.597577000	0.950750000
				C	4.826282000	0.738293000	1.280749000
				C	5.767143000	-0.142996000	0.760527000
				C	5.366089000	-1.168118000	-0.094176000
				C	4.028579000	-1.309924000	-0.429402000
				C	-2.946666000	0.639578000	-0.236321000
				C	-4.161152000	0.669499000	0.437153000
				C	-4.251209000	0.167964000	1.732112000
				C	-3.122969000	-0.358458000	2.352706000
				C	-1.906666000	-0.387039000	1.680076000
				H	0.720153000	1.215514000	-1.756174000
				H	-4.048783000	-3.330018000	-1.250966000
				H	-2.737387000	-4.465026000	-0.810642000
				H	-3.287842000	-3.238015000	0.365269000
				H	-1.347428000	5.026689000	-2.190291000
				H	-2.092887000	4.521053000	-0.644907000
				H	-0.449568000	5.217631000	-0.655588000
				H	2.744549000	1.278183000	1.356083000
				H	5.136608000	1.534908000	1.946788000
				H	6.814357000	-0.031894000	1.018143000
				H	6.099467000	-1.856162000	-0.498460000
				H	3.706953000	-2.099967000	-1.097232000
				H	-2.874684000	1.024889000	-1.248310000
				H	-5.037303000	1.084421000	-0.047766000
				H	-5.199162000	0.190604000	2.257611000
				H	-3.189371000	-0.746982000	3.362545000
				H	-1.022842000	-0.792027000	2.159965000
				H	-0.490426000	-1.108181000	-2.272677000
diethylamine oxide 7'				<i>N,N</i> -diethylhydroxylamine 7			
							
Zero-point correction = 0.156980 (Hartree/Particle)				Zero-point correction = 0.154088 (Hartree/Particle)			
Thermal correction to Energy = 0.166107				Thermal correction to Energy = 0.163974			
Thermal correction to Enthalpy = 0.167193				Thermal correction to Enthalpy = 0.165060			
Thermal correction to Gibbs Free Energy = 0.120367				Thermal correction to Gibbs Free Energy = 0.116705			
Sum of electronic and zero-point Energies = -288.801494				Sum of electronic and zero-point Energies = -288.814055			
Sum of electronic and thermal Energies = -288.792367				Sum of electronic and thermal Energies = -288.804170			
Sum of electronic and thermal Enthalpies = -288.791281				Sum of electronic and thermal Enthalpies = -288.803083			
Sum of electronic and thermal Free Energies = -288.838107				Sum of electronic and thermal Free Energies = -288.851438			
Imaginary frequencies = 0				Imaginary frequencies = 0			
N	0.084890000	0.691608000	0.358546000				

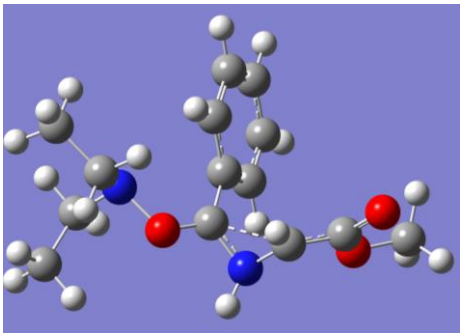
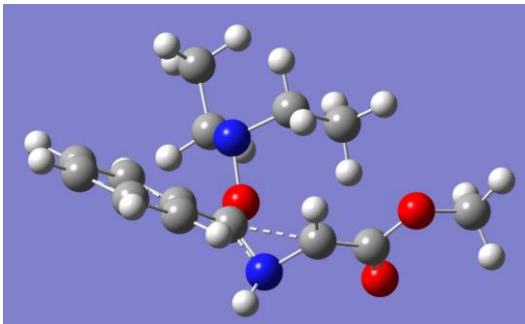
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H	1.726004000	-0.106364000	1.321410000	H	0.748324000	0.102561000	-1.451822000
H	0.305137000	-1.159166000	1.346907000	H	1.563329000	1.399417000	-0.577141000
C	-1.106025000	0.370921000	-0.490082000	C	2.082408000	-0.570927000	0.114972000
H	-1.615409000	1.325869000	-0.615879000	H	1.685494000	-1.588925000	0.126552000
H	-0.712105000	0.070789000	-1.460344000	H	2.984886000	-0.574236000	-0.499877000
C	-2.030500000	-0.675383000	0.107286000	H	2.364273000	-0.299561000	1.135779000
H	-2.936291000	-0.729566000	-0.499072000	C	-0.848152000	-0.565635000	0.715778000
H	-1.577441000	-1.668558000	0.119984000	H	-0.226783000	-1.212428000	1.341278000
H	-2.328998000	-0.414454000	1.126450000	H	-1.684788000	-0.241174000	1.338650000
C	1.448122000	-1.241939000	-0.497048000	C	-1.364220000	-1.336475000	-0.497527000
H	2.163837000	-1.995534000	-0.163883000	H	-0.551080000	-1.790499000	-1.069447000
H	0.657563000	-1.755630000	-1.048347000	H	-2.024410000	-2.140831000	-0.164064000
H	1.961120000	-0.551942000	-1.167979000	H	-1.934092000	-0.684159000	-1.162791000
O	0.836798000	1.679612000	-0.216694000	N	-0.053521000	0.635159000	0.441676000
H	-0.287958000	1.034015000	1.249688000	O	-0.912906000	1.570777000	-0.221540000
aziridine <i>syn</i> -8				H	-0.969343000	2.301977000	0.397643000
				aziridine <i>anti</i> -8			
Zero-point correction = 0.330375 (Hartree/Particle)							
Thermal correction to Energy = 0.355002				Zero-point correction = 0.330177 (Hartree/Particle)			
Thermal correction to Enthalpy = 0.356088				Thermal correction to Energy = 0.354845			
Thermal correction to Gibbs Free Energy = 0.270431				Thermal correction to Enthalpy = 0.355931			
Sum of electronic and zero-point Energies = -880.262914				Thermal correction to Gibbs Free Energy = 0.270731			
Sum of electronic and thermal Energies = -880.238287				Sum of electronic and zero-point Energies = -880.265085			
Sum of electronic and thermal Enthalpies = -880.237201				Sum of electronic and thermal Energies = -880.240417			
Sum of electronic and thermal Free Energies = -880.322858				Sum of electronic and thermal Enthalpies = -880.239330			
Imaginary frequencies = 0				Sum of electronic and thermal Free Energies = -880.324531			
C	0.837995000	-1.733995000	-0.394290000	Imaginary frequencies = 0			
C	-0.189783000	-0.690555000	-0.736986000	C	-0.394883000	-1.796793000	-0.563255000
H	0.511486000	-2.552193000	0.238283000	C	0.193253000	-0.427437000	-0.771874000
C	-1.583076000	-0.807016000	-0.195078000	H	0.289053000	-2.622351000	-0.410879000
C	-2.653802000	-0.495146000	-1.032885000	C	-0.494169000	0.811566000	-0.285042000
C	-1.828675000	-1.200078000	1.116150000	C	-0.835718000	1.806709000	-1.196682000
C	-3.958332000	-0.583103000	-0.563361000	C	-0.751551000	0.999978000	1.069552000
H	-2.462805000	-0.182306000	-2.054189000	C	-1.432294000	2.982664000	-0.757914000
C	-3.134608000	-1.288899000	1.586761000	H	-0.631372000	1.664962000	-2.253066000
H	-0.998249000	-1.426061000	1.775847000	C	-1.350058000	2.174507000	1.509817000
C	-4.200504000	-0.980442000	0.748514000	H	-0.475210000	0.228715000	1.779077000
H	-4.785510000	-0.341565000	-1.221198000	C	-1.688607000	3.168397000	0.596880000
H	-3.318507000	-1.592369000	2.611106000	H	-1.697356000	3.752920000	-1.473157000
H	-5.217993000	-1.049661000	1.116528000	H	-1.548356000	2.316091000	2.566169000
C	-0.742050000	2.595157000	-0.395586000	H	-2.154339000	4.085121000	0.940815000
H	-0.244862000	3.075420000	-1.250205000	C	3.170921000	0.949495000	0.227116000
H	-1.683231000	2.178208000	-0.760495000				

C	-1.021214000	3.614983000	0.697701000	H	3.745532000	0.990606000	1.156845000
H	-1.742085000	4.348721000	0.331245000	H	3.865980000	0.665354000	-0.575673000
H	-1.444534000	3.131950000	1.582194000	C	2.560166000	2.309772000	-0.067164000
H	-0.120615000	4.156718000	0.995912000	H	3.348132000	3.064619000	-0.127952000
C	1.361444000	1.799159000	0.633042000	H	2.023218000	2.299761000	-1.017214000
H	1.181635000	2.387065000	1.536735000	H	1.856211000	2.597615000	0.717397000
H	1.808287000	0.863522000	0.974353000	C	2.693351000	-1.338726000	0.965340000
C	2.312775000	2.532706000	-0.306573000	H	3.100094000	-1.091246000	1.949991000
H	1.939834000	3.526101000	-0.569039000	H	1.841545000	-1.999078000	1.143589000
H	3.281313000	2.659993000	0.183289000	C	3.741790000	-2.052392000	0.115935000
H	2.467642000	1.962096000	-1.223999000	H	4.661309000	-1.469563000	0.025395000
C	2.278536000	-1.374411000	-0.238730000	H	3.996696000	-3.007752000	0.580772000
C	4.009869000	-1.226357000	1.349464000	H	3.357004000	-2.252354000	-0.886182000
H	4.126932000	-1.449847000	2.406574000	C	-1.684000000	-1.949726000	0.167337000
H	4.703515000	-1.820878000	0.754339000	C	-3.944187000	-1.294522000	0.261003000
H	4.182996000	-0.165017000	1.164279000	H	-4.612577000	-0.714879000	-0.369797000
N	0.272352000	-1.607734000	-1.737538000	H	-4.325973000	-2.306747000	0.394801000
H	-0.410287000	-2.336492000	-1.915005000	H	-3.820989000	-0.811960000	1.231222000
N	0.038562000	1.462350000	0.102253000	N	-0.323955000	-1.165147000	-1.886728000
O	3.008250000	-0.952208000	-1.098778000	H	-1.238309000	-0.812448000	-2.155413000
O	0.225192000	0.607589000	-1.034179000	N	2.157807000	-0.081231000	0.434932000
O	2.656208000	-1.571349000	1.028155000	O	-1.786662000	-2.569053000	1.200398000
				O	1.586355000	-0.348270000	-0.852513000
				O	-2.689861000	-1.321889000	-0.432943000
azomethine-ylide Z-9				azomethine-ylide E-9			
							
Zero-point correction = 0.329622 (Hartree/Particle) Thermal correction to Energy = 0.354836 Thermal correction to Enthalpy = 0.355923 Thermal correction to Gibbs Free Energy = 0.269126 Sum of electronic and zero-point Energies = -880.257721 Sum of electronic and thermal Energies = -880.232506 Sum of electronic and thermal Enthalpies = -880.231420 Sum of electronic and thermal Free Energies = -880.318217 Imaginary frequencies = 0				Zero-point correction = 0.329472 (Hartree/Particle) Thermal correction to Energy = 0.354824 Thermal correction to Enthalpy = 0.355910 Thermal correction to Gibbs Free Energy = 0.267916 Sum of electronic and zero-point Energies = -880.257783 Sum of electronic and thermal Energies = -880.232430 Sum of electronic and thermal Enthalpies = -880.231344 Sum of electronic and thermal Free Energies = -880.319338 Imaginary frequencies = 0			
C	2.226036000	0.320690000	-0.280002000	C	2.226036000	0.320690000	-0.280002000
C	-0.126341000	-0.279022000	-0.262532000	C	-0.126341000	-0.279022000	-0.262532000
H	2.060240000	1.367340000	-0.460781000	H	2.060240000	1.367340000	-0.460781000
C	-1.137467000	-1.325829000	-0.087217000	C	-1.137467000	-1.325829000	-0.087217000
C	-2.271867000	-1.350677000	-0.904945000	C	-2.271867000	-1.350677000	-0.904945000
C	-0.964389000	-2.317069000	0.881416000	C	-0.964389000	-2.317069000	0.881416000
C	-3.206943000	-2.363220000	-0.762974000	C	-3.206943000	-2.363220000	-0.762974000
H	-2.412367000	-0.583131000	-1.655779000	C	-0.964389000	-2.317069000	0.881416000

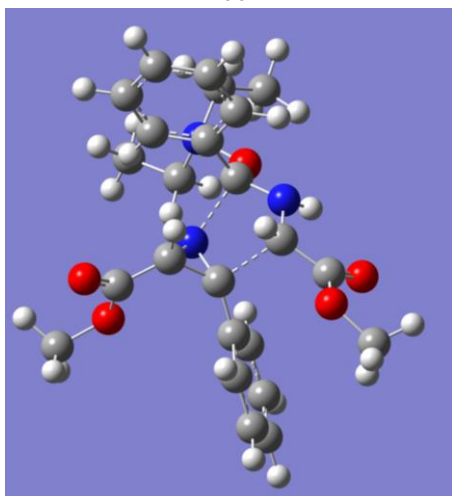
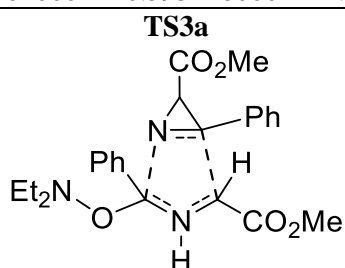
C	-1.904163000	-3.332158000	1.016468000	C	-3.206943000	-2.363220000	-0.762974000
H	-0.111667000	-2.284417000	1.551199000	H	-2.412367000	-0.583131000	-1.655779000
C	-3.025725000	-3.357381000	0.196607000	C	-1.904163000	-3.332158000	1.016468000
H	-4.080295000	-2.380124000	-1.404569000	H	-0.111667000	-2.284417000	1.551199000
H	-1.764381000	-4.094633000	1.773710000	C	-3.025725000	-3.357381000	0.196607000
H	-3.762134000	-4.145014000	0.306776000	H	-4.080295000	-2.380124000	-1.404569000
C	-2.207389000	2.397171000	-0.925942000	H	-1.764381000	-4.094633000	1.773710000
H	-1.493217000	3.184884000	-1.199242000	H	-3.762134000	-4.145014000	0.306776000
H	-2.415044000	1.817512000	-1.827885000	C	-2.207389000	2.397171000	-0.925942000
C	-3.496992000	3.002560000	-0.393469000	H	-1.493217000	3.184884000	-1.199242000
H	-3.985553000	3.562756000	-1.192758000	H	-2.415044000	1.817512000	-1.827885000
H	-4.182148000	2.222859000	-0.052213000	C	-3.496992000	3.002560000	-0.393469000
H	-3.315371000	3.693485000	0.432775000	H	-3.985553000	3.562756000	-1.192758000
C	-1.215383000	2.055959000	1.321337000	H	-4.182148000	2.222859000	-0.052213000
H	-2.144645000	2.292552000	1.845238000	H	-3.315371000	3.693485000	0.432775000
H	-0.742972000	1.250096000	1.890386000	C	-1.215383000	2.055959000	1.321337000
C	-0.300329000	3.273826000	1.260968000	H	-2.144645000	2.292552000	1.845238000
H	-0.792345000	4.133559000	0.800164000	H	-0.742972000	1.250096000	1.890386000
H	-0.015739000	3.558127000	2.276353000	C	-0.300329000	3.273826000	1.260968000
H	0.612480000	3.054337000	0.703403000	H	-0.792345000	4.133559000	0.800164000
C	3.476592000	-0.304390000	-0.164219000	H	-0.015739000	3.558127000	2.276353000
C	5.822989000	-0.005456000	-0.162255000	H	0.612480000	3.054337000	0.703403000
H	6.517579000	0.825395000	-0.273100000	C	3.476592000	-0.304390000	-0.164219000
H	5.964177000	-0.478765000	0.811687000	C	5.822989000	-0.005456000	-0.162255000
H	6.000100000	-0.743318000	-0.947509000	H	6.517579000	0.825395000	-0.273100000
N	1.146347000	-0.530494000	-0.166472000	H	5.964177000	-0.478765000	0.811687000
H	1.423475000	-1.503231000	-0.037787000	H	6.000100000	-0.743318000	-0.947509000
N	-1.629808000	1.466508000	0.042761000	N	1.146347000	-0.530494000	-0.166472000
O	3.655951000	-1.517039000	0.019773000	H	1.423475000	-1.503231000	-0.037787000
O	-0.426053000	0.982096000	-0.605130000	N	-1.629808000	1.466508000	0.042761000
O	4.521638000	0.560893000	-0.273835000	O	3.655951000	-1.517039000	0.019773000
				O	-0.426053000	0.982096000	-0.605130000
				O	4.521638000	0.560893000	-0.273835000
azirinopyrrolidine <i>anti</i> -10				azirinopyrrolidine <i>syn</i> -10			
							
Zero-point correction = 0.506513 (Hartree/Particle)				Zero-point correction = 0.506089 (Hartree/Particle)			
Thermal correction to Energy = 0.546387				Thermal correction to Energy = 0.546031			
Thermal correction to Enthalpy = 0.547473				Thermal correction to Enthalpy = 0.547117			
Thermal correction to Gibbs Free Energy = 0.427259				Thermal correction to Gibbs Free Energy = 0.425761			
Sum of electronic and zero-point Energies = -1471.758865				Sum of electronic and zero-point Energies = -1471.755864			
				Sum of electronic and thermal Energies = -1471.715922			
				Sum of electronic and thermal Enthalpies = -1471.714836			

Sum of electronic and thermal Energies = -1471.718991				Sum of electronic and thermal Free Energies = -			
Sum of electronic and thermal Enthalpies = -				1471.836192			
1471.717905				Imaginary frequencies = 0			
Sum of electronic and thermal Free Energies = -							
1471.838119							
Imaginary frequencies = 0							
C	0.833320000	-0.606941000	-1.873546000	C	0.575152000	-0.470327000	-1.686415000
C	1.091988000	0.376573000	-0.716891000	C	1.138861000	0.417212000	-0.562023000
C	0.327904000	1.656905000	-0.878047000	C	0.491103000	1.763998000	-0.517695000
C	-1.178433000	-0.256190000	-0.642044000	C	-1.137882000	0.006800000	-0.096690000
H	-0.152252000	1.817597000	-1.837968000	H	-0.149531000	2.027325000	-1.351333000
H	1.222601000	-0.187114000	-2.806135000	H	0.858002000	-0.066231000	-2.662715000
C	-2.503056000	0.472101000	-0.817433000	C	-1.494920000	-1.136565000	0.852667000
C	-3.407803000	0.032371000	-1.780668000	C	-1.082872000	-1.090489000	2.182420000
C	-2.848524000	1.543900000	0.001065000	C	-2.297126000	-2.196247000	0.432425000
C	-4.643267000	0.652685000	-1.923288000	C	-1.458148000	-2.089795000	3.074987000
H	-3.152342000	-0.797891000	-2.429207000	H	-0.462170000	-0.268318000	2.515618000
C	-4.080274000	2.172217000	-0.146466000	C	-2.679557000	-3.190238000	1.323526000
H	-2.153861000	1.881822000	0.760114000	H	-2.650136000	-2.246639000	-0.590283000
C	-4.982426000	1.726518000	-1.106541000	C	-2.259141000	-3.142403000	2.649418000
H	-5.339723000	0.299588000	-2.675484000	H	-1.123615000	-2.041381000	4.105441000
H	-4.337441000	3.007917000	0.494894000	H	-3.308328000	-4.004521000	0.981009000
H	-5.944146000	2.214327000	-1.219610000	H	-2.555124000	-3.920057000	3.344641000
C	2.367682000	0.288594000	0.053660000	C	2.513413000	0.161093000	-0.040128000
C	3.450508000	1.096267000	-0.280185000	C	3.614107000	0.763422000	-0.642632000
C	2.497076000	-0.652618000	1.072303000	C	2.700582000	-0.723384000	1.018846000
C	4.655051000	0.967277000	0.402240000	C	4.897371000	0.483000000	-0.188376000
H	3.353879000	1.825771000	-1.077766000	H	3.466479000	1.452489000	-1.467967000
C	3.701347000	-0.784699000	1.751932000	C	3.984191000	-1.007375000	1.469832000
H	1.653992000	-1.285835000	1.325751000	H	1.837533000	-1.181537000	1.490267000
C	4.782865000	0.025298000	1.417618000	C	5.083965000	-0.405625000	0.865918000
H	5.494008000	1.601298000	0.138844000	H	5.751888000	0.957014000	-0.657696000
H	3.795923000	-1.520788000	2.542197000	H	4.125775000	-1.697637000	2.293750000
H	5.723257000	-0.077963000	1.947049000	H	6.085067000	-0.624635000	1.219864000
C	-3.215962000	-1.983633000	1.389624000	C	-4.390085000	0.543922000	0.395976000
H	-3.801884000	-1.673666000	0.521235000	H	-4.039418000	-0.113981000	1.193656000
H	-3.790316000	-1.691508000	2.272790000	H	-5.270767000	0.063843000	-0.039258000
C	-1.052224000	-1.429110000	2.454846000	C	-3.608335000	1.387994000	-1.792662000
H	-0.241105000	-0.711978000	2.322090000	H	-2.733674000	1.292474000	-2.437579000
H	-0.625451000	-2.438157000	2.357799000	H	-3.679131000	2.441744000	-1.488027000
C	-1.671484000	-1.245155000	3.832343000	C	-4.860766000	0.968113000	-2.547216000
H	-0.888006000	-1.299390000	4.591165000	H	-4.925877000	1.526950000	-3.483209000
H	-2.158345000	-0.269721000	3.913388000	H	-4.830308000	-0.098262000	-2.786419000
H	-2.408302000	-2.018835000	4.060950000	H	-5.772226000	1.167735000	-1.978499000
C	-2.999022000	-3.494802000	1.368767000	C	-4.754418000	1.913265000	0.963592000
H	-2.507955000	-3.848815000	2.279062000	H	-5.209007000	2.562518000	0.210882000
H	-3.963837000	-4.002133000	1.292281000	H	-5.476829000	1.790205000	1.774199000
H	-2.389677000	-3.788879000	0.511460000	H	-3.872551000	2.415729000	1.366546000
C	1.545330000	-1.943878000	-1.675377000	C	1.154951000	-1.880986000	-1.594145000
C	3.661069000	-2.969249000	-1.736540000	C	3.074573000	-3.155056000	-2.060463000
H	3.290107000	-3.842616000	-2.272929000	H	2.525956000	-3.991916000	-2.493117000
H	4.651077000	-2.695244000	-2.091285000	H	4.007866000	-2.994678000	-2.593588000
H	3.684811000	-3.172128000	-0.664522000	H	3.268095000	-3.343414000	-1.003356000
N	-0.613664000	-0.691897000	-1.908208000	N	-0.851978000	-0.382073000	-1.471759000
H	-0.948924000	-1.608354000	-2.176053000	H	-1.363411000	-1.191525000	-1.789084000
N	-0.163597000	0.586955000	-0.017803000	N	0.062409000	0.689367000	0.375748000
O	-1.330999000	-1.423585000	0.157824000	O	-2.151371000	1.004613000	-0.046345000
O	2.829577000	-1.830361000	-1.994580000	O	2.331530000	-1.937672000	-2.207919000
				N	-3.354244000	0.519505000	-0.641388000
				C	1.208132000	2.940749000	0.059775000
				C	2.315907000	3.852962000	1.913472000

N	-2.011006000	-1.152407000	1.385479000	H	2.476289000	3.561882000	2.948148000
C	0.797063000	2.929627000	-0.249582000	H	3.269155000	3.943546000	1.391211000
C	1.379243000	4.042315000	1.730321000	H	1.776054000	4.798795000	1.863002000
H	1.305270000	3.831631000	2.793850000	O	1.480718000	3.910430000	-0.610899000
H	2.421023000	4.190873000	1.443195000	O	1.535081000	2.799154000	1.334496000
H	0.795609000	4.927087000	1.475138000	O	0.629827000	-2.812695000	-1.039431000
O	1.116346000	3.889104000	-0.913882000				
O	0.848080000	2.884539000	1.072180000				
O	1.022254000	-2.965160000	-1.308699000				
TS1a				TS1b			
							
Zero-point correction = 0.328547 (Hartree/Particle)				Zero-point correction = 0.330106 (Hartree/Particle)			
Thermal correction to Energy = 0.353297				Thermal correction to Energy = 0.354351			
Thermal correction to Enthalpy = 0.354384				Thermal correction to Enthalpy = 0.355437			
Thermal correction to Gibbs Free Energy = 0.267724				Thermal correction to Gibbs Free Energy = 0.271823			
Sum of electronic and zero-point Energies = -880.227722				Sum of electronic and zero-point Energies = -880.223548			
Sum of electronic and thermal Energies = -880.202972				Sum of electronic and thermal Energies = -880.199303			
Sum of electronic and thermal Enthalpies = -880.201885				Sum of electronic and thermal Enthalpies = -880.198216			
Sum of electronic and thermal Free Energies = -880.288545				Sum of electronic and thermal Free Energies = -880.281830			
Imaginary frequencies = 1				Imaginary frequencies = 1			
C	2.348443000	3.436725000	0.296413000	C	-4.597455000	-0.226519000	-0.451774000
C	2.290808000	2.530750000	1.350672000	C	-3.753777000	-0.948883000	-1.291447000
C	1.582650000	1.342745000	1.208644000	C	-2.414726000	-1.114022000	-0.959171000
C	0.933628000	1.058714000	0.010191000	C	-1.915163000	-0.558321000	0.216707000
C	0.999114000	1.961835000	-1.049060000	C	-2.763800000	0.150750000	1.064106000
C	1.702878000	3.150335000	-0.904109000	C	-4.101352000	0.320808000	0.727679000
C	0.179427000	-0.193455000	-0.140492000	C	-0.496569000	-0.722412000	0.580025000
N	-0.116709000	-0.986129000	-1.131028000	N	0.169423000	-0.663876000	1.696159000
C	0.384997000	-1.618946000	0.137415000	C	0.395092000	-1.859342000	0.829414000
C	1.739090000	-2.230199000	0.174353000	C	1.673123000	-2.090153000	0.100261000
O	2.588692000	-1.692640000	-0.699404000	O	2.597753000	-1.149578000	0.314251000
O	2.043599000	-3.120086000	0.940822000	O	1.878889000	-3.073403000	-0.576866000
C	3.924727000	-2.205373000	-0.691654000	C	3.865404000	-1.346290000	-0.324257000
O	-1.385834000	0.318999000	0.739258000	O	0.211299000	0.428919000	-0.725038000
N	-2.370154000	-0.218917000	-0.040282000	N	0.995338000	1.287699000	-0.000366000
C	-3.252800000	-1.111277000	0.765204000	C	2.183380000	1.696457000	-0.801901000
C	-4.295928000	-1.824272000	-0.075334000	C	3.256861000	2.359594000	0.040783000
C	-3.069341000	0.839406000	-0.831412000	C	0.192824000	2.426614000	0.555293000
C	-3.881057000	1.785739000	0.028591000	C	-0.524576000	3.229153000	-0.509028000
H	2.898005000	4.364620000	0.407967000	H	-5.641835000	-0.096370000	-0.712138000
H	2.797538000	2.748789000	2.283896000	H	-4.141111000	-1.384160000	-2.205712000
				H	-1.751342000	-1.672894000	-1.610284000

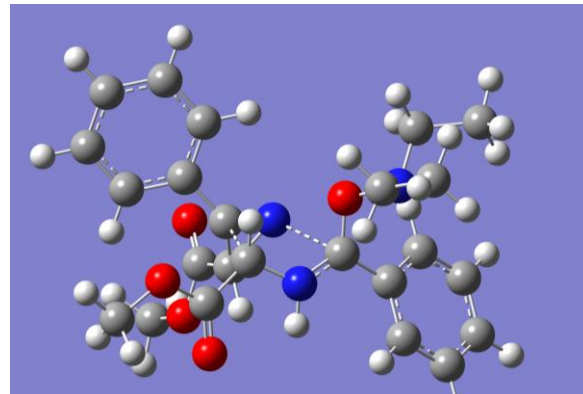
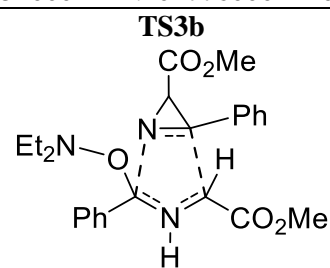
H	1.532626000	0.630369000	2.025234000	H	-2.374413000	0.559889000	1.990214000
H	0.502646000	1.727292000	-1.984491000	H	-4.757647000	0.876784000	1.387593000
H	1.751644000	3.853945000	-1.727457000	H	-0.047073000	-2.806069000	1.141115000
H	-0.314695000	-2.135525000	0.790124000	H	4.467306000	-0.480862000	-0.056320000
H	4.453787000	-1.655409000	-1.465969000	H	4.334353000	-2.259774000	0.042021000
H	4.391637000	-2.036507000	0.279639000	H	3.743465000	-1.406901000	-1.406570000
H	3.925626000	-3.272626000	-0.916704000	H	2.542953000	0.777155000	-1.255475000
H	-2.577971000	-1.819309000	1.244096000	H	1.825205000	2.346645000	-1.598985000
H	-3.702555000	-0.496105000	1.544105000	H	4.144334000	2.505066000	-0.577170000
H	-4.800531000	-2.562598000	0.549540000	H	2.950041000	3.337319000	0.415723000
H	-5.054081000	-1.139131000	-0.458950000	H	3.538237000	1.731139000	0.890209000
H	-3.839181000	-2.351636000	-0.916575000	H	-0.516924000	1.963885000	1.239675000
H	-2.269507000	1.364233000	-1.354035000	H	0.874163000	3.039898000	1.147075000
H	-3.685569000	0.330582000	-1.574908000	H	-1.143382000	2.577906000	-1.126831000
H	-4.258464000	2.593652000	-0.600304000	H	-1.172653000	3.954840000	-0.014500000
H	-4.740455000	1.291142000	0.485855000	H	0.164811000	3.783373000	-1.148734000
H	-3.260790000	2.220661000	0.813373000	H	1.309051000	0.734255000	0.829626000
H	-1.833149000	-0.807669000	-0.747213000				
TS2a				TS2b			
							
Zero-point correction = 0.327842 (Hartree/Particle)				Zero-point correction = 0.327914 (Hartree/Particle)			
Thermal correction to Energy = 0.352446				Thermal correction to Energy = 0.352455			
Thermal correction to Enthalpy = 0.353532				Thermal correction to Enthalpy = 0.353541			
Thermal correction to Gibbs Free Energy = 0.268483				Thermal correction to Gibbs Free Energy = 0.269252			
Sum of electronic and zero-point Energies = -880.219514				Sum of electronic and zero-point Energies = -880.216309			
Sum of electronic and thermal Energies = -880.194910				Sum of electronic and thermal Energies = -880.191768			
Sum of electronic and thermal Enthalpies = -880.193824				Sum of electronic and thermal Enthalpies = -880.190682			
Sum of electronic and thermal Free Energies = -880.278873				Sum of electronic and thermal Free Energies = -880.274972			
Imaginary frequencies = 1				Imaginary frequencies = 1			
C	1.092989000	1.178366000	-1.164384000	C	-1.221948000	-1.671975000	0.088930000
C	0.216324000	0.705942000	-0.184874000	C	0.486143000	-0.560767000	0.730743000
C	-0.229393000	1.569511000	0.821416000	H	-0.851425000	-1.911296000	-0.899414000
C	0.202491000	2.885241000	0.842837000	C	1.844211000	-0.765184000	0.233161000
C	1.071021000	3.357506000	-0.140243000	C	2.846230000	0.204507000	0.380538000
C	1.513490000	2.502647000	-1.141797000	C	2.161008000	-2.001098000	-0.344794000
H	1.447526000	0.500270000	-1.929373000	C	4.136709000	-0.066541000	-0.039088000
H	-0.893080000	1.208747000	1.595113000	H	2.621631000	1.154864000	0.842871000
H	-0.136103000	3.547443000	1.631174000	C	3.452909000	-2.257942000	-0.782417000
H	1.402620000	4.389464000	-0.119889000	H	1.393001000	-2.754717000	-0.475864000
H	2.191288000	2.862452000	-1.907166000	C	4.440537000	-1.292764000	-0.628810000
C	-0.178643000	-0.712820000	-0.254801000	H	4.910938000	0.679937000	0.091480000
C	1.425664000	-1.702484000	0.613233000	H	3.685419000	-3.210837000	-1.241987000
H	0.907379000	-2.021280000	1.507954000	H	5.451128000	-1.493978000	-0.965120000
C	2.789048000	-1.339972000	0.695443000	C	0.401723000	2.882368000	0.684170000
C	4.683350000	-0.531514000	-0.468061000	H	-0.526872000	3.101503000	1.225912000
H	4.793480000	0.353715000	0.162221000	H	1.183954000	2.731134000	1.431396000
H	4.934111000	-0.284232000	-1.498421000	C	0.779429000	4.037496000	-0.229896000

H	5.349496000	-1.315588000	-0.101974000	H	0.992903000	4.919354000	0.376729000
O	3.331571000	-0.971853000	-0.496889000	H	1.671975000	3.795995000	-0.812142000
O	3.460078000	-1.326335000	1.730761000	H	-0.026914000	4.295830000	-0.919584000
N	0.696492000	-1.661302000	-0.624110000	C	-0.796138000	1.598597000	-1.059192000
H	0.313359000	-2.515971000	-1.012892000	H	-0.461958000	2.248154000	-1.871783000
O	-1.419232000	-1.145192000	-0.105321000	H	-0.815169000	0.583538000	-1.459606000
N	-2.448265000	-0.136515000	0.044519000	C	-2.184773000	1.999045000	-0.573120000
C	-3.930508000	-1.379400000	-1.616756000	H	-2.242419000	3.059850000	-0.317628000
H	-4.740295000	-1.604875000	-0.919104000	H	-2.907843000	1.810611000	-1.369986000
H	-3.258550000	-2.239159000	-1.659322000	H	-2.482609000	1.410364000	0.297039000
H	-4.372588000	-1.244168000	-2.606098000	C	-2.574208000	-1.328255000	0.298870000
C	-4.326007000	0.429936000	1.517417000	C	-4.663000000	-1.034482000	-0.780902000
H	-5.108900000	0.408455000	0.756510000	H	-5.065359000	-1.151912000	-1.785969000
H	-3.930774000	1.446378000	1.584032000	H	-5.207592000	-1.680057000	-0.088344000
H	-4.785198000	0.175757000	2.474230000	H	-4.770821000	0.004107000	-0.458872000
C	-3.180365000	-0.110409000	-1.226369000	N	-0.282542000	-1.582958000	1.164283000
C	-3.213737000	-0.563137000	1.218051000	H	0.191838000	-2.415270000	1.491326000
H	-2.451277000	0.160437000	-1.993755000	N	0.293939000	1.635001000	-0.074563000
H	-3.866705000	0.735664000	-1.143880000	O	-3.112335000	-0.986853000	1.351326000
H	-3.618155000	-1.575069000	1.090562000	O	-0.029187000	0.639691000	0.939962000
H	-2.508902000	-0.593148000	2.052143000	O	-3.293051000	-1.402776000	-0.864744000



Zero-point correction = 0.496989 (Hartree/Particle)
Thermal correction to Energy = 0.536593
Thermal correction to Enthalpy = 0.537680
Thermal correction to Gibbs Free Energy = 0.422861
Sum of electronic and zero-point Energies = -1471.680757
Sum of electronic and thermal Energies = -1471.641153
Sum of electronic and thermal Enthalpies = -1471.640067
Sum of electronic and thermal Free Energies = -1471.754885
Imaginary frequencies = 1

C	0.804745000	-1.737929000	-0.707951000
C	1.177313000	0.233358000	-0.285842000

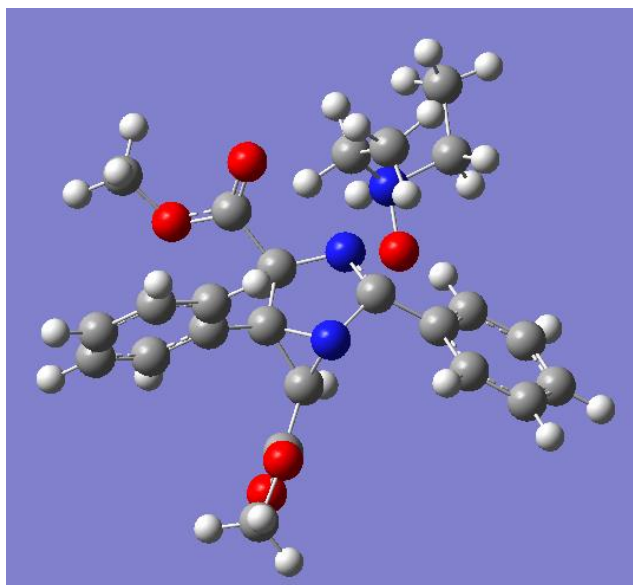


Zero-point correction = 0.500088 (Hartree/Particle)
Thermal correction to Energy = 0.540923
Thermal correction to Enthalpy = 0.542009
Thermal correction to Gibbs Free Energy = 0.420230
Sum of electronic and zero-point Energies = -1471.679379
Sum of electronic and thermal Energies = -1471.638544
Sum of electronic and thermal Enthalpies = -1471.637458
Sum of electronic and thermal Free Energies = -1471.759237
Imaginary frequencies = 1

C	-2.894009000	1.933867000	1.428598000
C	-2.490562000	1.220280000	0.290522000
C	-3.035397000	1.557141000	-0.957570000
C	-3.953815000	2.594549000	-1.064019000
C	-4.346959000	3.306333000	0.071474000

C	0.451014000	1.029452000	-1.319175000	C	-3.816173000	2.971490000	1.316231000
C	-1.283507000	-0.868830000	0.119096000	H	-2.519649000	1.665765000	2.410109000
H	0.025498000	0.502849000	-2.167898000	H	-2.717241000	1.018284000	-1.840210000
H	0.638604000	-1.688800000	-1.778884000	H	-4.360834000	2.852492000	-2.034797000
C	-2.169280000	-0.704998000	-1.075739000	H	-5.065203000	4.113464000	-0.013978000
C	-2.434958000	-1.826977000	-1.882008000	H	-4.126551000	3.509561000	2.204193000
C	-2.772541000	0.525047000	-1.391246000	C	-1.481174000	0.154443000	0.365157000
C	-3.288621000	-1.720539000	-2.985293000	C	0.553446000	-0.653726000	1.346225000
H	-1.978027000	-2.778057000	-1.631546000	H	0.431079000	-1.677892000	1.027291000
C	-3.626057000	0.626246000	-2.491858000	C	1.440271000	-0.375068000	2.472982000
H	-2.558914000	1.389374000	-0.778880000	C	3.349205000	-1.116143000	3.671573000
C	-3.887585000	-0.494334000	-3.291442000	H	2.868514000	-1.035950000	4.646819000
H	-3.484916000	-2.593418000	-3.599687000	H	3.999578000	-1.986582000	3.639697000
H	-4.080073000	1.582089000	-2.731707000	H	3.917258000	-0.208690000	3.465312000
H	-4.548430000	-0.409218000	-4.148318000	C	-3.224543000	-2.096796000	-1.637437000
C	2.452803000	0.416598000	0.421301000	H	-2.895687000	-3.140060000	-1.736787000
C	3.664644000	0.486740000	-0.289710000	H	-2.624708000	-1.505187000	-2.328152000
C	2.476680000	0.484618000	1.825465000	C	-4.702395000	-1.949466000	-1.999282000
C	4.876522000	0.624264000	0.393051000	H	-5.351649000	-2.524656000	-1.338206000
H	3.650558000	0.431259000	-1.373464000	H	-5.007324000	-0.902008000	-1.952240000
C	3.690155000	0.615765000	2.505673000	H	-4.860299000	-2.308316000	-3.020123000
H	1.539242000	0.446645000	2.369993000	C	-2.769034000	-2.646649000	0.735967000
C	4.893541000	0.686378000	1.792890000	H	-2.403064000	-2.163859000	1.644139000
H	5.805611000	0.688004000	-0.165335000	H	-2.012670000	-3.373164000	0.407484000
H	3.697211000	0.666530000	3.590033000	C	-4.086365000	-3.355855000	1.044888000
H	5.835409000	0.792826000	2.322077000	H	-4.443484000	-3.951245000	0.203045000
C	-4.122151000	-0.621004000	2.053463000	H	-3.928289000	-4.035633000	1.885473000
H	-4.368596000	-1.301006000	1.233046000	H	-4.864236000	-2.641692000	1.324700000
H	-4.937759000	0.108462000	2.118749000	N	-2.935225000	-1.586214000	-0.277168000
C	-2.367474000	1.144398000	2.548858000	N	-0.590640000	0.130383000	1.355689000
H	-1.450419000	1.499737000	2.073813000	H	-0.505502000	0.971470000	1.921939000
H	-2.097278000	0.677104000	3.507402000	O	-1.578097000	-0.962232000	-0.386900000
C	-3.343142000	2.305467000	2.765337000	O	1.383380000	0.636485000	3.161062000
H	-2.851919000	3.089476000	3.351636000	O	2.362441000	-1.338626000	2.641823000
H	-3.649988000	2.736345000	1.806675000	C	2.300685000	-0.998462000	-0.879826000
H	-4.243393000	1.999660000	3.310246000	C	1.844431000	-2.031684000	-1.709405000
C	-3.977086000	-1.398289000	3.369167000	C	2.715845000	-3.035256000	-2.124480000
H	-3.819969000	-0.734022000	4.226056000	C	4.052510000	-3.016244000	-1.720449000
H	-4.889135000	-1.975378000	3.560105000	C	4.511593000	-1.987817000	-0.897373000
H	-3.136035000	-2.095534000	3.315534000	C	3.639397000	-0.986216000	-0.473693000
C	1.934885000	-2.560126000	-0.260588000	H	0.809046000	-2.038719000	-2.030223000
C	4.167309000	-3.308431000	-0.811966000	H	2.354435000	-3.829830000	-2.767811000
H	3.947926000	-4.305773000	-0.426469000	H	4.731060000	-3.795960000	-2.047399000
H	4.757759000	-3.357805000	-1.724683000	H	5.549302000	-1.964880000	-0.583938000
H	4.677301000	-2.721207000	-0.045599000	H	3.998651000	-0.189885000	0.168139000
N	-0.334347000	-1.882586000	0.110981000	C	1.369344000	0.063587000	-0.456631000
H	-0.120234000	-2.265706000	1.031680000	C	1.392115000	1.533239000	-0.324424000
N	-0.092252000	0.701442000	0.085133000	H	1.089464000	1.977068000	0.621915000
O	-1.849348000	-0.861978000	1.409506000	C	2.310965000	2.384171000	-1.126259000
O	2.922557000	-2.632330000	-1.208508000	C	3.627023000	4.363305000	-1.061101000
N	-2.939038000	0.152606000	1.599059000	H	3.169780000	4.786264000	-1.956029000
C	0.730174000	2.447967000	-1.645471000	H	3.828251000	5.144576000	-0.332280000
C	1.522026000	4.581448000	-0.834581000	H	4.548951000	3.846511000	-1.329471000
H	1.892942000	4.958180000	0.116441000	N	0.400961000	0.695318000	-1.084806000
H	2.280579000	4.667564000	-1.615911000	O	2.713112000	3.455805000	-0.410374000
H	0.622559000	5.116581000	-1.147748000	O	2.672532000	2.172843000	-2.266188000
O	0.565346000	2.942905000	-2.770514000				
O	1.210708000	3.169719000	-0.581116000				
O	2.024100000	-3.083908000	0.864113000				

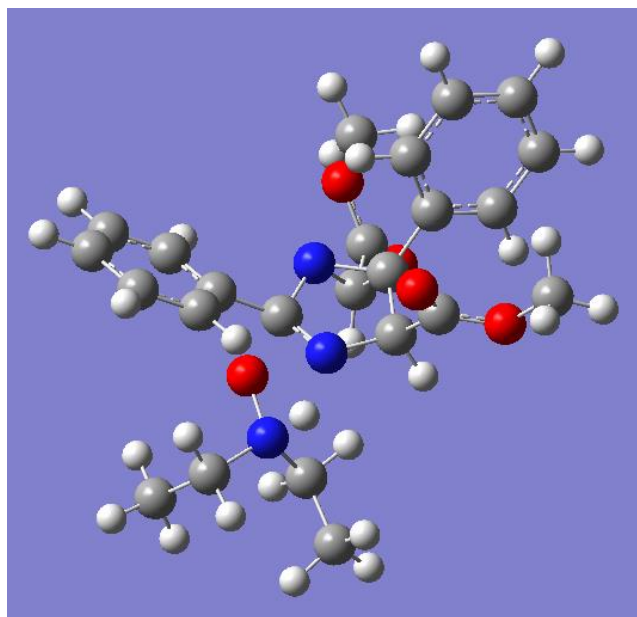
TS4a



Zero-point correction = 0.503884 (Hartree/Particle)
 Thermal correction to Energy = 0.542955
 Thermal correction to Enthalpy = 0.544041
 Thermal correction to Gibbs Free Energy = 0.425685
 Sum of electronic and zero-point Energies = -1471.729582
 Sum of electronic and thermal Energies = -1471.690511
 Sum of electronic and thermal Enthalpies = -1471.689425
 Sum of electronic and thermal Free Energies = -1471.807782
 Imaginary frequencies = 1

C	0.386840000	-0.583815000	-1.544726000
C	0.994465000	0.418052000	-0.524441000
C	0.435731000	1.798569000	-0.700754000
C	-1.293461000	0.193692000	-0.177270000
H	-0.141381000	1.973166000	-1.604112000
H	0.558484000	-0.203679000	-2.560001000
C	-2.484285000	1.122289000	-0.276060000
C	-3.330971000	1.069483000	-1.377525000
C	-2.734201000	2.048932000	0.737283000
C	-4.427127000	1.923867000	-1.462096000
H	-3.114218000	0.356790000	-2.164428000
C	-3.821764000	2.907847000	0.649234000
H	-2.069846000	2.097921000	1.592750000
C	-4.674446000	2.844956000	-0.450703000
H	-5.083892000	1.874522000	-2.323769000
H	-4.005289000	3.629375000	1.437740000
H	-5.523554000	3.515969000	-0.519234000
C	2.325818000	0.170145000	0.102064000
C	3.494874000	0.547806000	-0.554614000
C	2.406035000	-0.475335000	1.332596000
C	4.733827000	0.279895000	0.014231000
H	3.432488000	1.049951000	-1.514362000
C	3.645178000	-0.748047000	1.900739000
H	1.491642000	-0.743075000	1.850671000
C	4.811139000	-0.371712000	1.241757000
H	5.639906000	0.579764000	-0.500060000

TS4b

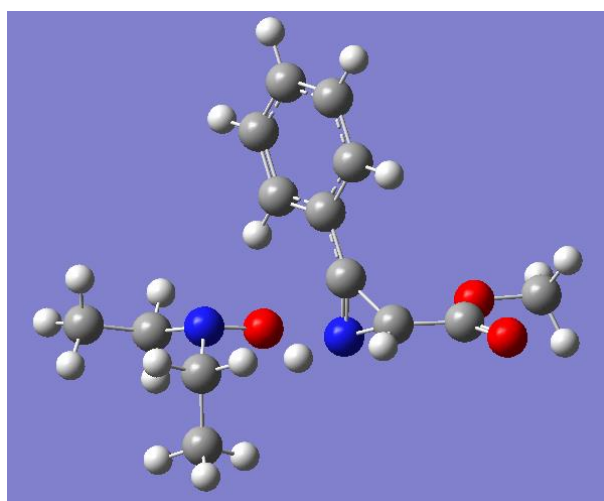


Zero-point correction = 0.502817 (Hartree/Particle)
 Thermal correction to Energy = 0.542170
 Thermal correction to Enthalpy = 0.543256
 Thermal correction to Gibbs Free Energy = 0.424047
 Sum of electronic and zero-point Energies = -1471.723603
 Sum of electronic and thermal Energies = -1471.684249
 Sum of electronic and thermal Enthalpies = -1471.683163
 Sum of electronic and thermal Free Energies = -1471.802373
 Imaginary frequencies = 1

C	0.393791000	1.448066000	-0.430208000
C	1.087910000	0.237716000	0.254157000
C	0.503790000	-0.138924000	1.570458000
C	-1.120663000	-0.253948000	-0.268675000
H	-0.182570000	0.555820000	2.032490000
H	0.370739000	2.307227000	0.249550000
C	-1.915804000	-1.273349000	-1.029416000
C	-2.102299000	-2.551856000	-0.503243000
C	-2.482939000	-0.948965000	-2.257747000
C	-2.860191000	-3.488569000	-1.192084000
H	-1.649258000	-2.808021000	0.447551000
C	-3.245687000	-1.887219000	-2.947368000
H	-2.315621000	0.039976000	-2.667741000
C	-3.437898000	-3.157271000	-2.415930000
H	-3.000977000	-4.479667000	-0.775249000
H	-3.684759000	-1.626404000	-3.903949000
H	-4.029257000	-3.889205000	-2.954814000
C	2.486580000	-0.135645000	-0.118089000
C	3.561952000	0.479636000	0.518875000
C	2.721905000	-1.066057000	-1.126508000
C	4.864904000	0.166636000	0.149842000
H	3.377203000	1.207237000	1.302365000
C	4.024601000	-1.379716000	-1.495506000
H	1.879858000	-1.546535000	-1.612066000
C	5.097430000	-0.763241000	-0.858774000

H	3.700575000	-1.248228000	2.861051000	H	5.698308000	0.646901000	0.649868000
H	5.777791000	-0.579149000	1.686734000	H	4.202728000	-2.107841000	-2.278797000
C	-1.006611000	-2.913895000	1.512665000	H	6.113841000	-1.008715000	-1.145591000
H	0.001017000	-2.504820000	1.498824000	C	-4.100427000	1.264125000	0.284951000
H	-0.970530000	-3.874951000	0.999980000	H	-4.058127000	0.589240000	-0.569822000
C	-3.245262000	-2.351765000	0.500894000	H	-4.319441000	2.264406000	-0.093088000
H	-3.645699000	-1.594657000	-0.174234000	C	-2.503081000	2.166269000	2.002603000
H	-3.735265000	-2.234129000	1.468298000	H	-1.439246000	2.105495000	2.230484000
C	-3.436549000	-3.743285000	-0.075075000	H	-3.048689000	1.744937000	2.848904000
H	-4.493671000	-3.886084000	-0.304609000	C	-2.894652000	3.609791000	1.737860000
H	-2.869048000	-3.868948000	-1.000499000	H	-2.578583000	4.219373000	2.585976000
H	-3.140024000	-4.524065000	0.627825000	H	-2.401026000	3.995533000	0.842295000
C	-1.537905000	-3.044828000	2.927867000	H	-3.973255000	3.732762000	1.623973000
H	-2.511020000	-3.539979000	2.957120000	C	-5.137831000	0.802419000	1.291533000
H	-0.841637000	-3.650068000	3.511339000	H	-5.264163000	1.518290000	2.107012000
H	-1.625843000	-2.067452000	3.405434000	H	-6.101245000	0.697958000	0.789254000
C	1.098876000	-1.929182000	-1.496442000	H	-4.862623000	-0.166481000	1.711650000
C	3.087765000	-3.036054000	-2.091558000	C	1.202369000	1.872751000	-1.652021000
H	2.592917000	-3.910092000	-2.515941000	C	3.102021000	3.100691000	-2.299262000
H	3.978046000	-2.788304000	-2.663910000	H	2.619595000	3.545724000	-3.169791000
H	3.347627000	-3.227654000	-1.049363000	H	3.770545000	3.816553000	-1.827941000
N	-1.022468000	-0.650384000	-1.229583000	H	3.652174000	2.206349000	-2.597173000
H	-1.359574000	-1.840991000	-0.376064000	N	-0.925206000	0.975431000	-0.797629000
N	-0.099457000	0.883170000	0.304355000	H	-1.958697000	1.553003000	-0.049279000
O	-1.688347000	-0.705365000	1.110060000	N	0.076944000	-0.813489000	0.344655000
O	2.238803000	-1.885801000	-2.180331000	O	-2.256053000	0.023528000	1.064343000
N	-1.810351000	-2.005253000	0.662631000	O	2.130262000	2.763043000	-1.302318000
C	1.195890000	3.006724000	-0.264992000	N	-2.717654000	1.293645000	0.825565000
C	2.294162000	4.108958000	1.489282000	C	1.303759000	-0.898634000	2.579618000
H	2.427559000	3.940330000	2.554592000	C	2.507147000	-2.849876000	3.073140000
H	3.257402000	4.093479000	0.978053000	H	2.678057000	-3.804602000	2.582929000
H	1.798073000	5.063939000	1.313817000	H	3.450515000	-2.322184000	3.218437000
O	1.544640000	3.859815000	-1.050089000	H	2.014030000	-2.997613000	4.034190000
O	1.474119000	3.026965000	1.029543000	O	1.607408000	-0.410086000	3.644477000
O	0.698883000	-2.913289000	-0.922885000	O	1.659685000	-2.109925000	2.184370000
				O	1.066353000	1.444986000	-2.769495000

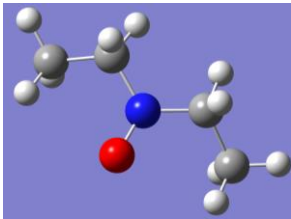
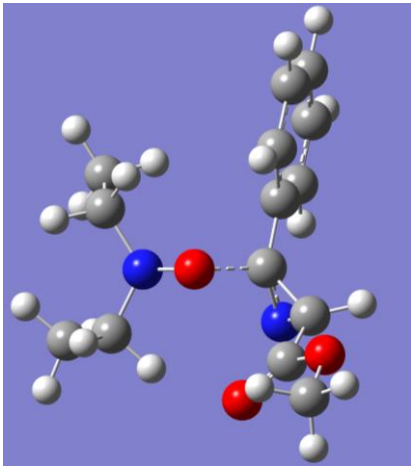
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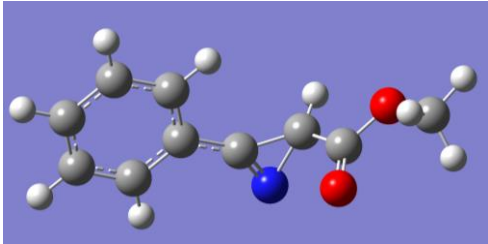


Zero-point correction = 0.322641 (Hartree/Particle)
 Thermal correction to Energy = 0.348182
 Thermal correction to Enthalpy = 0.349268
 Thermal correction to Gibbs Free Energy = 0.259824
 Sum of electronic and zero-point Energies = -880.178147
 Sum of electronic and thermal Energies = -880.152606

Sum of electronic and thermal Enthalpies = -880.151520			
Sum of electronic and thermal Free Energies = -880.240964			
Imaginary frequencies = 1			
C	0.854573000	4.049693000	0.402547000
C	1.346775000	3.198968000	1.388500000
C	1.309060000	1.825582000	1.199586000
C	0.776056000	1.303841000	0.015792000
C	0.281646000	2.161303000	-0.976335000
C	0.324044000	3.530814000	-0.778471000
C	0.729875000	-0.109832000	-0.172244000
N	0.550957000	-1.036466000	-1.088453000
C	1.189135000	-1.431568000	0.220126000
C	2.637739000	-1.806124000	0.211972000
O	3.324613000	-1.176792000	-0.731527000
O	3.113636000	-2.582532000	1.005347000
C	4.730053000	-1.457081000	-0.801177000
O	-1.397385000	-0.692774000	0.057607000
N	-2.677600000	-0.378631000	0.375754000
C	-3.368799000	0.138249000	-0.805025000
C	-4.779005000	0.625628000	-0.509937000
C	-3.333846000	-1.486544000	1.073251000
C	-3.587252000	-2.733225000	0.226257000
H	0.885936000	5.122738000	0.552585000
H	1.759971000	3.608082000	2.302621000
H	1.687227000	1.150581000	1.959042000
H	-0.130146000	1.744013000	-1.887871000
H	-0.055076000	4.199891000	-1.541745000
H	0.581076000	-1.997001000	0.917248000
H	5.104348000	-0.859678000	-1.628005000
H	5.217547000	-1.168328000	0.130317000
H	4.894413000	-2.517872000	-0.991320000
H	-2.757566000	0.965624000	-1.171512000
H	-3.387541000	-0.624707000	-1.600579000
H	-5.190347000	1.113706000	-1.396435000
H	-5.450753000	-0.194364000	-0.244014000
H	-4.777929000	1.349457000	0.309383000
H	-2.687761000	-1.733929000	1.918775000
H	-4.273129000	-1.111541000	1.489189000
H	-3.971125000	-3.539137000	0.856766000
H	-4.322727000	-2.546977000	-0.561087000
H	-2.661351000	-3.077936000	-0.241156000
H	-0.565815000	-1.218385000	-1.003773000

Table S2. Energies (au) and cartesian coordinates of stationary points for compounds **1a** and Et₂N-O· and transition state TS1^{rad} (calculations in ub3lyp/6-31g(d)).

nitroxyl radical Et ₂ N-O·				TS1 ^{rad}			
							
Zero-point correction = 0.141765 (Hartree/Particle)				Zero-point correction = 0.312280 (Hartree/Particle)			
Thermal correction to Energy = 0.151635				Thermal correction to Energy = 0.337673			
Thermal correction to Enthalpy = 0.152721				Thermal correction to Enthalpy = 0.338759			
Thermal correction to Gibbs Free Energy = 0.101605				Thermal correction to Gibbs Free Energy = 0.249729			
Sum of electronic and zero-point Energies = -288.216750				Sum of electronic and zero-point Energies = -879.639735			
Sum of electronic and thermal Energies = -288.206879				Sum of electronic and thermal Energies = -879.614341			
Sum of electronic and thermal Enthalpies = -288.205793				Sum of electronic and thermal Enthalpies = -879.613255			
Sum of electronic and thermal Free Energies = -288.256909				Sum of electronic and thermal Free Energies = -879.702285			
Imaginary frequencies = 0				Imaginary frequencies = 1			
C	0.273864000	0.662649000	1.269491000	C	-3.728395000	-2.228520000	-0.187310000
N	-0.106237000	0.018409000	0.000000000	C	-3.408642000	-1.715282000	1.071373000
C	0.273864000	0.662649000	-1.269491000	C	-2.147307000	-1.161531000	1.302125000
O	-1.144763000	-0.740507000	0.000000000	C	-1.201681000	-1.109543000	0.270034000
C	0.273864000	-0.326314000	2.429648000	C	-1.525173000	-1.628432000	-0.991891000
C	0.273864000	-0.326314000	-2.429648000	C	-2.782738000	-2.186389000	-1.217332000
H	1.265613000	1.101956000	1.127064000	C	0.141970000	-0.527530000	0.536013000
H	-0.428483000	1.487113000	1.466252000	N	0.691735000	-0.262888000	1.739420000
H	-0.428483000	1.487113000	-1.466252000	C	1.412345000	-1.217075000	0.857816000
H	1.265613000	1.101956000	-1.127064000	C	2.733035000	-0.797509000	0.282637000
H	0.536470000	0.194398000	3.355895000	O	3.243106000	0.302608000	0.361356000
H	-0.713158000	-0.778644000	2.549982000	O	3.320207000	-1.851054000	-0.326048000
H	1.004066000	-1.125230000	2.262643000	C	4.616890000	-1.601169000	-0.900214000
H	0.536470000	0.194398000	-3.355895000	N	-0.151340000	1.811134000	-0.391650000
H	1.004066000	-1.125230000	-2.262643000	C	0.808955000	2.825807000	0.048989000
H	-0.713158000	-0.778644000	-2.549982000	C	-1.280623000	2.143309000	-1.273299000
				C	0.150826000	4.039641000	0.699957000
				C	-2.613554000	2.315369000	-0.539482000
				H	-4.707812000	-2.663658000	-0.365731000
				H	-4.137879000	-1.749057000	1.876125000
				H	-1.884166000	-0.773928000	2.281597000
				H	-0.791659000	-1.589022000	-1.791813000
				H	-3.026069000	-2.589006000	-2.196709000
				H	1.367176000	-2.276245000	1.117851000
				H	4.932809000	-2.549999000	-1.333236000
				H	4.551428000	-0.831617000	-1.673462000
				H	5.321319000	-1.279931000	-0.128796000
				H	1.470565000	2.311406000	0.750870000

	H	1.426446000	3.138732000	-0.808769000
	H	-1.348296000	1.334712000	-2.004316000
	H	-1.024631000	3.061261000	-1.818805000
	H	0.932711000	4.729547000	1.033614000
	H	-0.494373000	4.585509000	0.004140000
	H	-0.443767000	3.748135000	1.571633000
	H	-3.401112000	2.544924000	-1.266073000
	H	-2.571360000	3.133551000	0.185386000
	H	-2.887011000	1.398124000	-0.010324000
	O	0.421371000	0.619941000	-0.612067000
<p>azirine 1a</p>  <p>Zero-point correction = 0.170668 (Hartree/Particle) Thermal correction to Energy = 0.185582 Thermal correction to Enthalpy = 0.186668 Thermal correction to Gibbs Free Energy = 0.123117 Sum of electronic and zero-point Energies = -591.469160 Sum of electronic and thermal Energies = -591.454246 Sum of electronic and thermal Enthalpies = -591.453160 Sum of electronic and thermal Free Energies = -591.516711 Imaginary frequencies = 0</p>				
C	3.872165000	0.891656000	-0.220373000	
C	3.702029000	-0.475254000	-0.470888000	
C	2.461196000	-1.070937000	-0.268590000	
C	1.382240000	-0.292542000	0.188249000	
C	1.555249000	1.077617000	0.439368000	
C	2.801156000	1.666522000	0.233790000	
C	0.089095000	-0.901502000	0.401807000	
N	-0.546310000	-1.989042000	0.335579000	
C	-1.298893000	-0.725135000	0.820753000	
C	-2.291077000	-0.151825000	-0.134052000	
O	-3.294039000	0.453459000	0.528515000	
O	-2.211279000	-0.215200000	-1.347002000	
C	-4.310554000	1.065103000	-0.289985000	
H	4.842785000	1.352382000	-0.380035000	
H	4.537808000	-1.072043000	-0.823505000	
H	2.315877000	-2.129966000	-0.459686000	
H	0.714453000	1.667306000	0.792324000	
H	2.937736000	2.726165000	0.426855000	
H	-1.561891000	-0.684082000	1.875068000	
H	-3.874264000	1.842562000	-0.921834000	
H	-4.795291000	0.314867000	-0.919216000	
H	-5.026128000	1.497811000	0.408391000	