Electronic Supplementary Information

Reducing Properties of 1,2-Dipyridyl-1,2-disodioethanes: Chemical Validation of Theoretical and Electrochemical Predictions

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ASSOCIATED CONTENT

Table S1: Sum of the Electronic and Zero Point Energy for minimum energy of compounds **1a-d**, **2a-d, 3a-d** calculated *in vacuo* at the PBE0/6-311+G(d,p) level

	Conf Name	Ce=Ce-Ci=N		E(Hartree)	
		Ar	Ar'	In vacuo	PCM
3a	aZ	0°	-	-571.9840	-572.2642
2a		0°	-	-572.0907	-572.1846
1a		0°	-	-572.0509	-572.0819
3a	aE	180°	-	-571.9851	-572.2629
2a		180°	-	-572.0904	-572.1839
1a		180°	-	-572.0492	-572.0811
3b	bZZ	0°	0°	-571.9724	-572.2589
2b		0°	0°	-572.0858	-572.1827
1b		0°	0°	-572.0546	-572.0834
3b	bZE	0°	180°	-571.9724	-572.2573
2b		0°	180°	-572.0844	-572.1816
1b		0°	180°	-572.0518	-572.0826
3b	bEE	180°	180°	-571.9744	-572.2561
2b		180°	180°	-572.0854	-572.1809
1b		180°	180°	-572.0516	-572.0822
3c	cZ	0°	0°	-555.9193	-556.1930
2c		0°	0°	-556.0369	-556.1260
1c		0°	0°	-556.0102	-556.0342
3c	cE	0°	180°	-555.9204	-556.1912
2c		0°	180°	-556.0365	-556.1249
1c		0°	180°	-556.0085	-556.0335
3d	d	-	-	-539.8663	-540.1257
2d		-	-	-539.9874	-540.0677
1d		-	-	-539.9655	-539.9843

Table S2. LUMO energies (eV) for compounds 1, and SOMO energies (eV) for compounds 2

	Vacuo	DMF
1d	-1,641	-1,628
1c	-1,777	-1,828
1b	-1,905	-2,005
1a	-2,161	-2,115
2d	0,676	-2,648
2c	0,543	-2,899
2b	0,411	-3,107
2a	0,176	-3,212

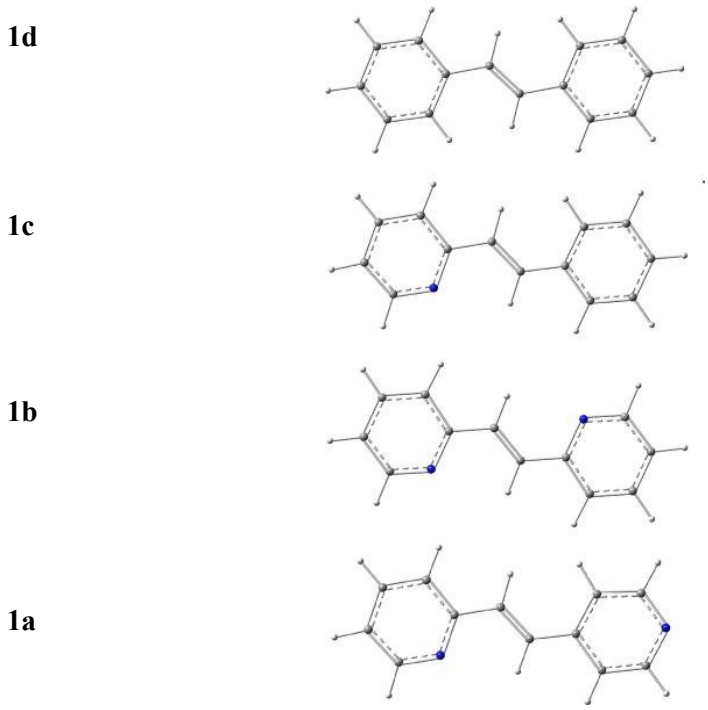


Figure S1. PBE0/6-311+G(d,p)/IEFPCM(DMF) global minima for compounds **1a-d**

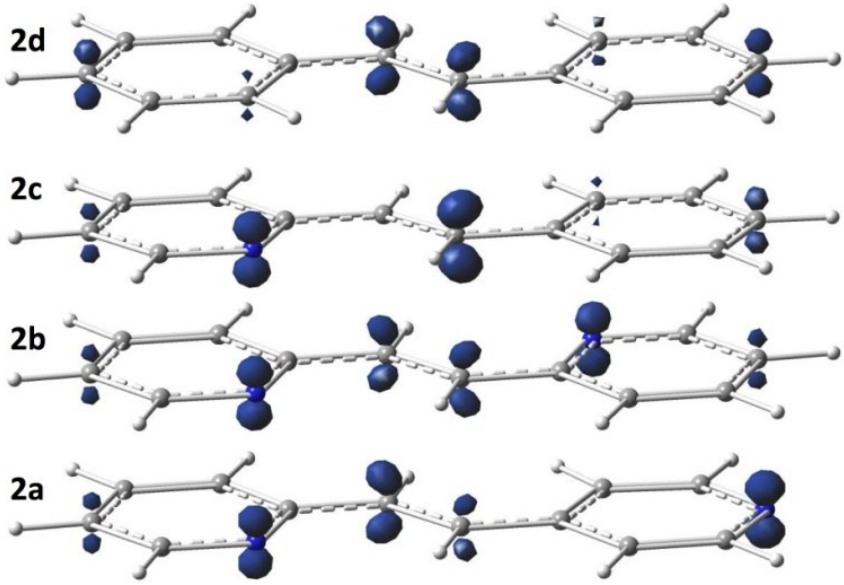
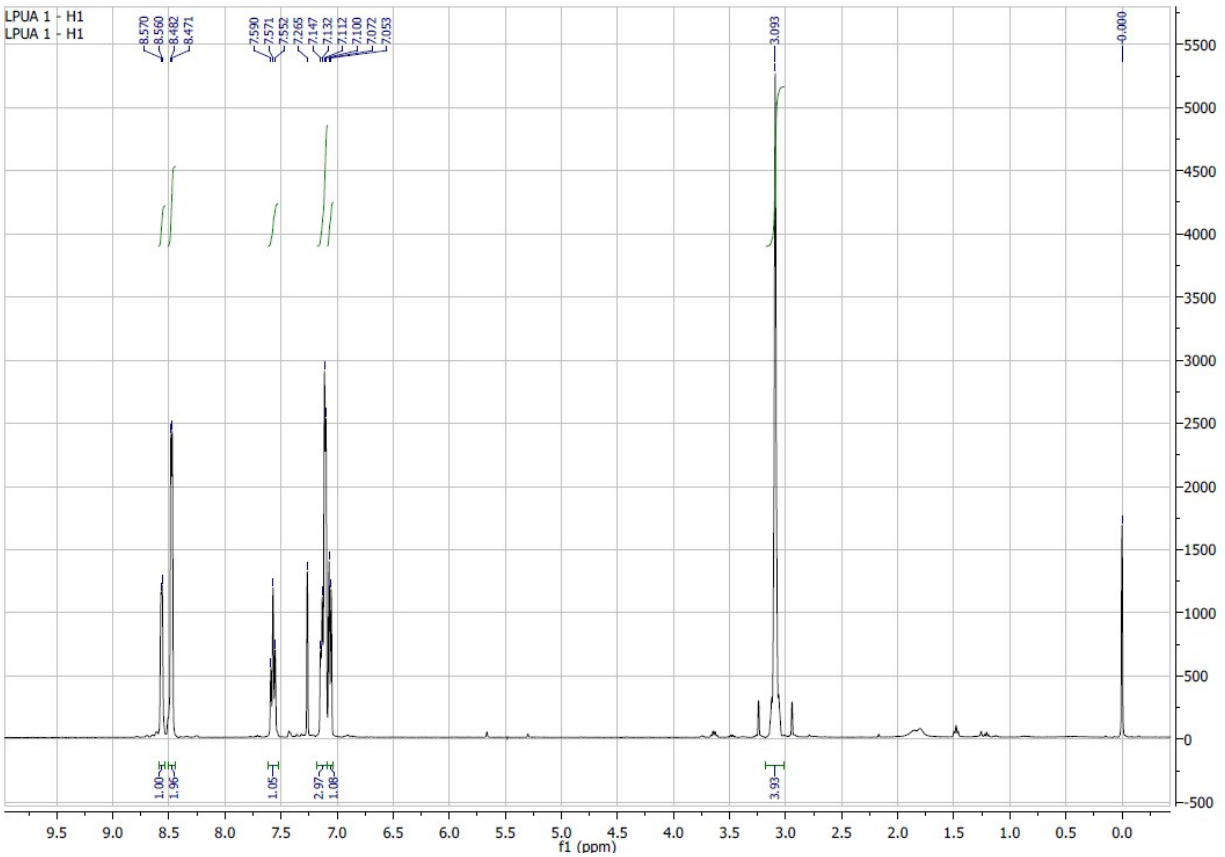
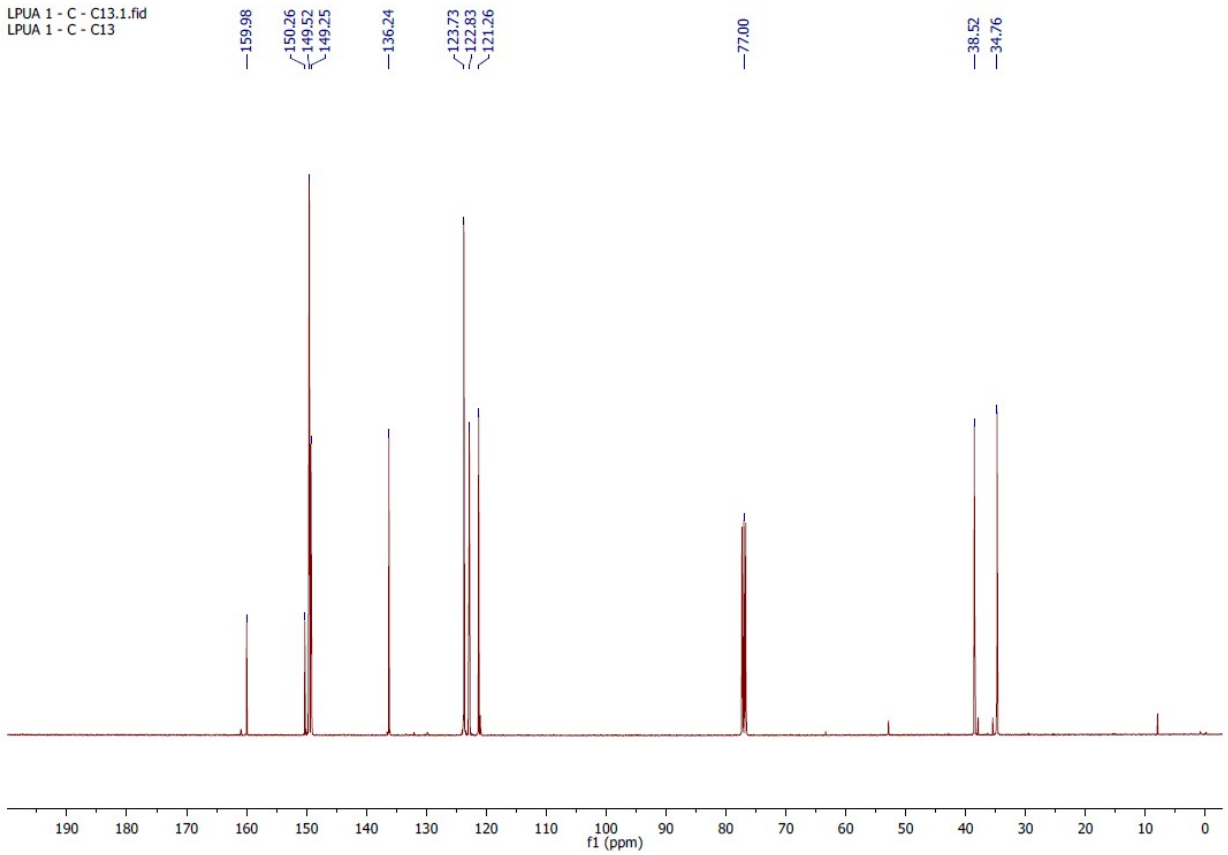


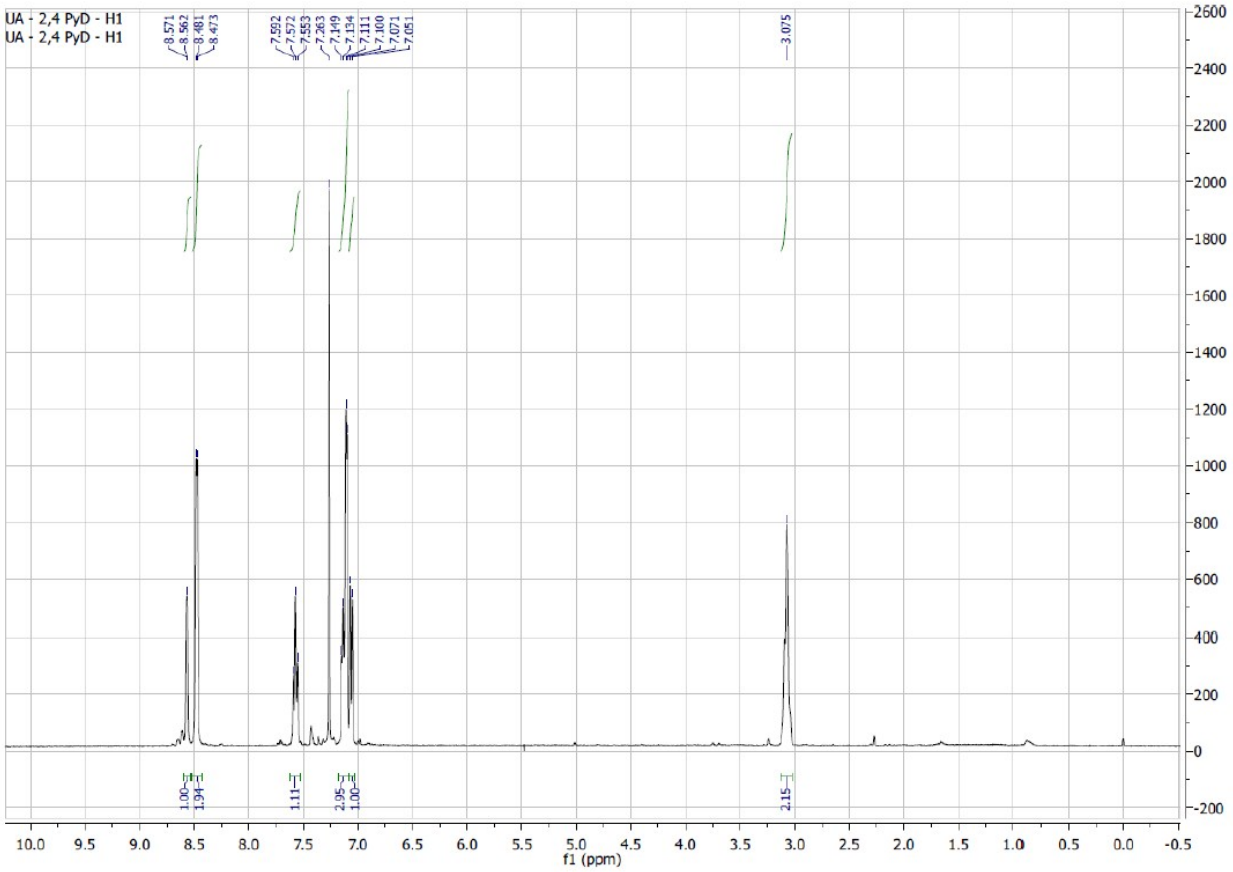
Figure S2 Spin density, calculated at the PBE0/6-311+G(d,p)/IEFPCM(DMF) level. The blue surfaces connect the points where the spin density is 0.02 au/A^3



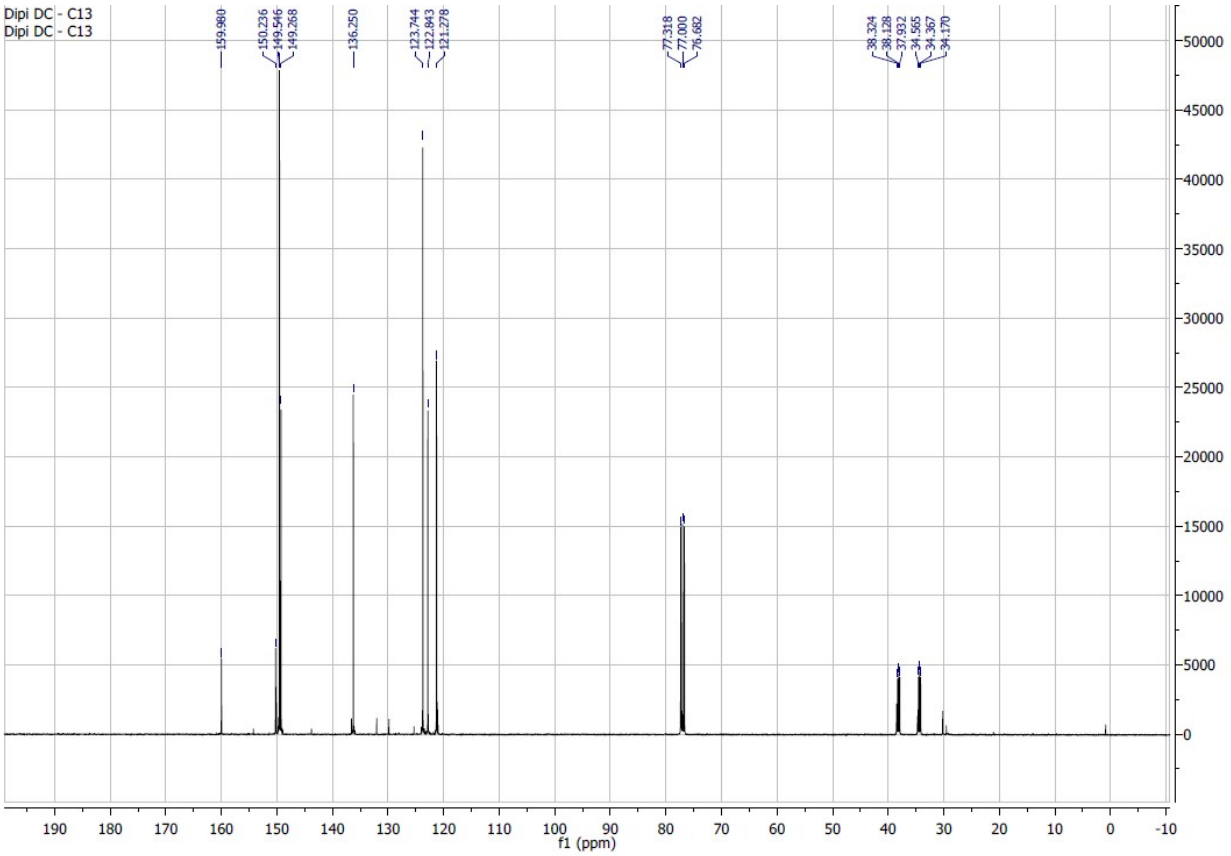
^{1}H NMR (400 MHz) in $CDCl_3$ of 1-(2-Pyridyl)-2-(4-pirydyl)ethane (**4a**)



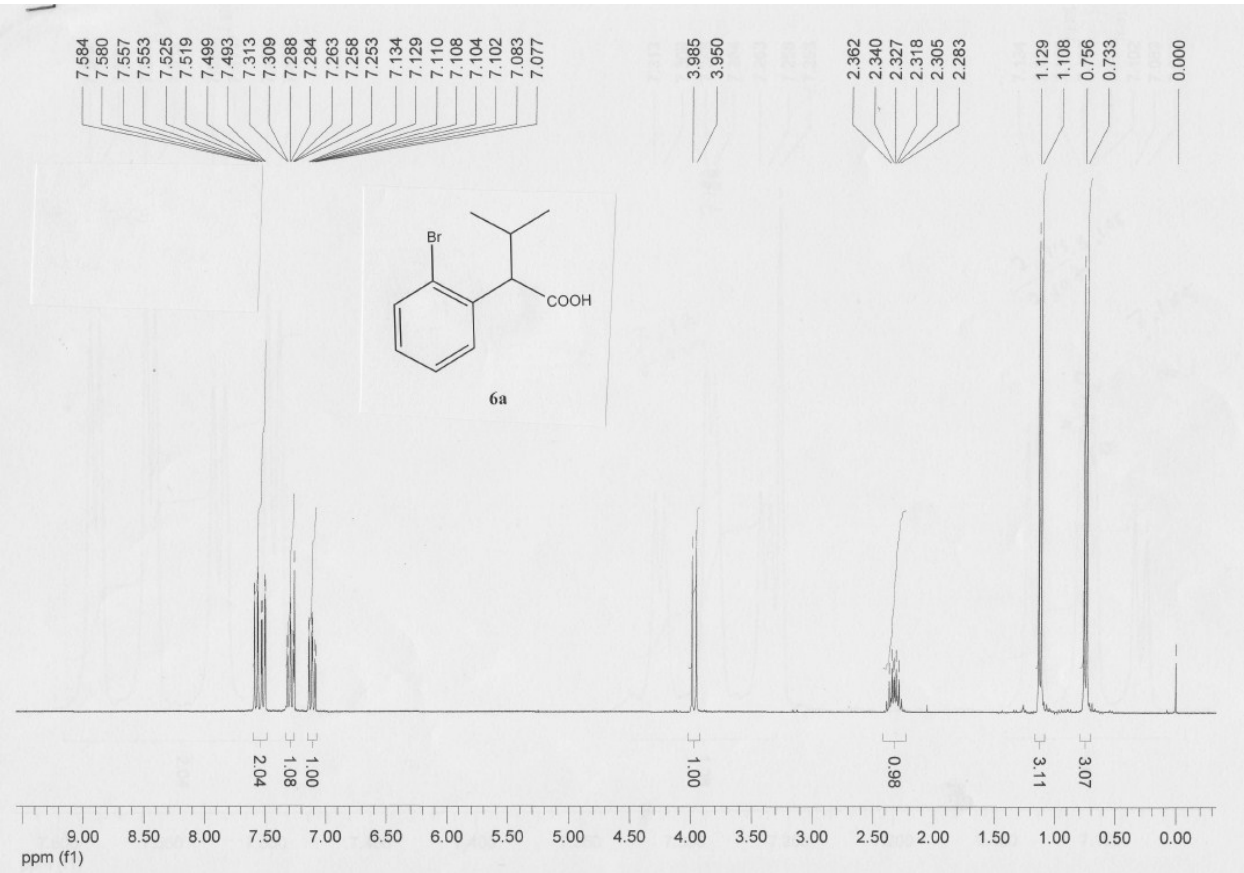
^{13}C NMR (100 MHz) in $CDCl_3$ of 1-(2-Pyridyl)-2-(4-pirydyl)ethane (**4a**)



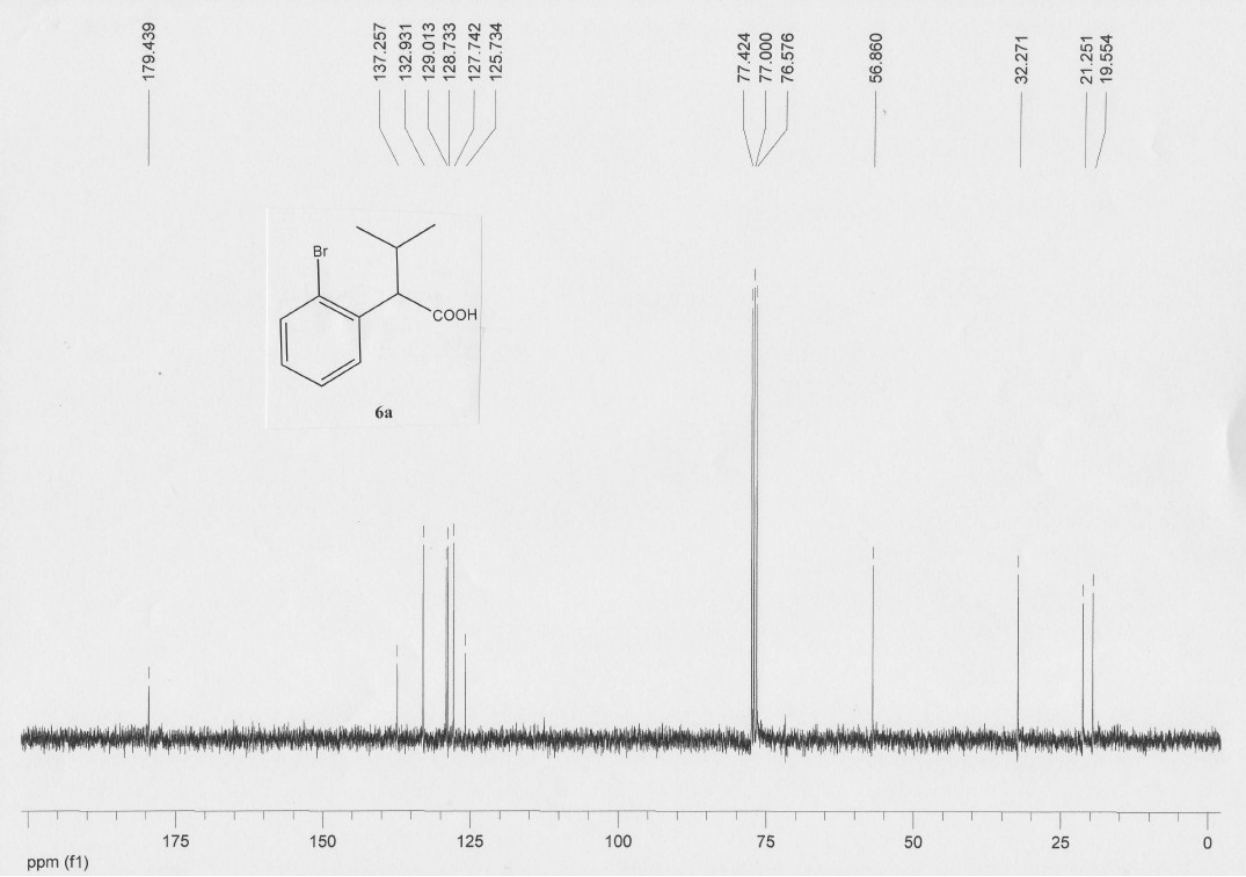
^{1}H NMR (400 MHz) in $CDCl_3$ of 1,2-Dideutero-1-(2-Pyridyl)-2-(4-pirydyl)ethane (**4a**$_{d2}$)



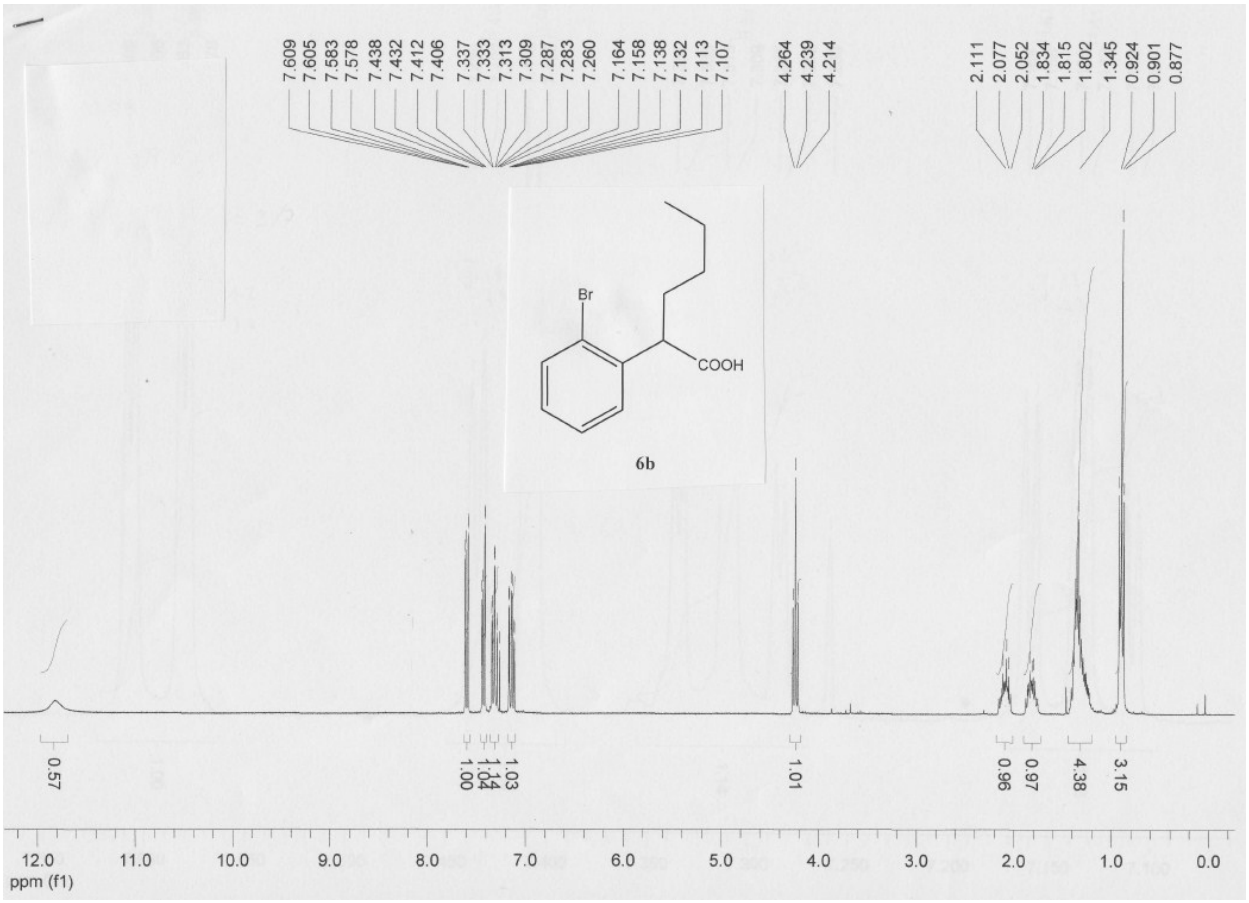
^{13}C NMR (100 MHz) in $CDCl_3$ of 1,2-Dideutero-1-(2-Pyridyl)-2-(4-pirydyl)ethane (**4a**$_{d2}$)



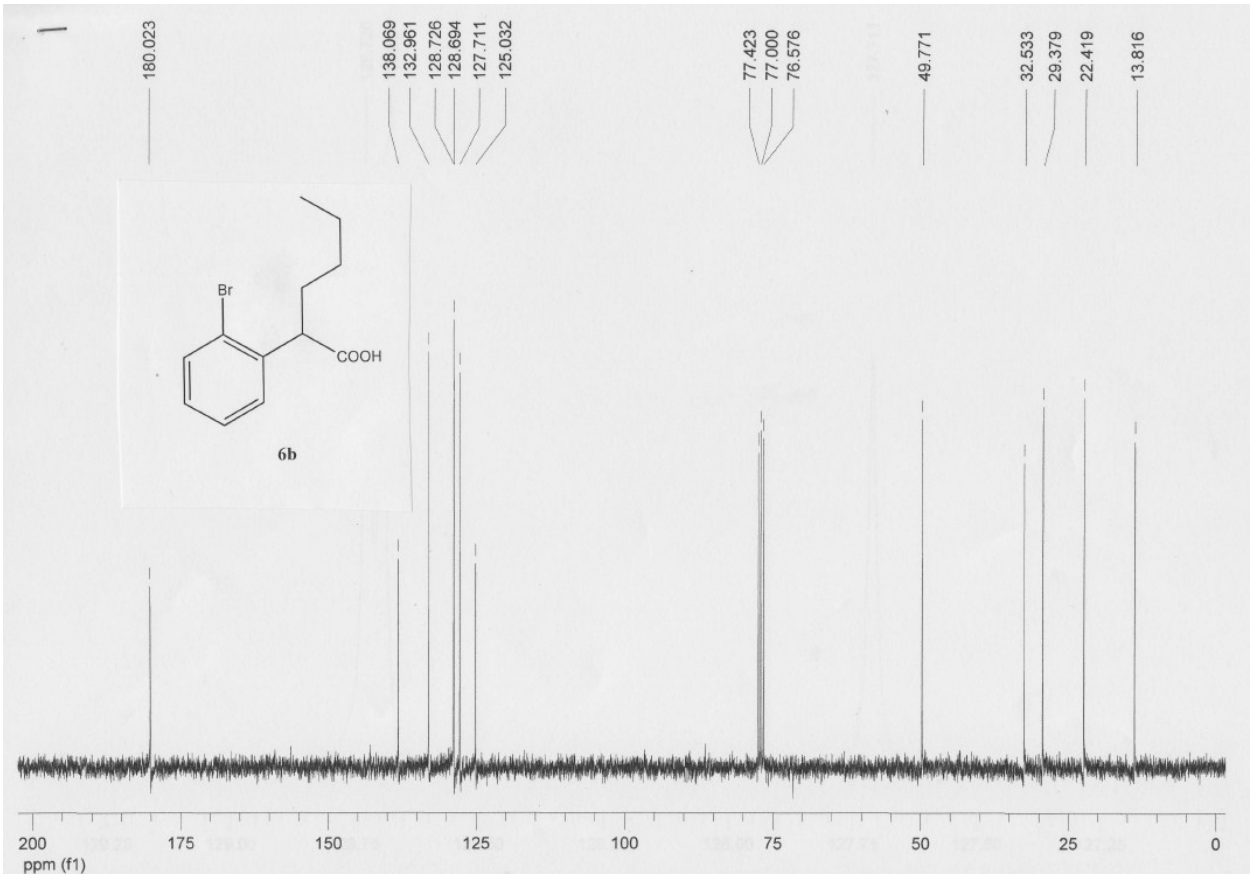
^{1}H-NMR (300 MHz) in $CDCl_3$ of 2-(2-Bromophenyl)-3-methylbutanoic acid (**6a**)



^{13}C-NMR (75 MHz) in $CDCl_3$ of 2-(2-Bromophenyl)-3-methylbutanoic acid (**6a**)



^{1}H-NMR (300 MHz) in $CDCl_3$ of 2-(2-Bromophenyl)hexanoic acid (**6b**)



^{13}C-NMR (75 MHz) in $CDCl_3$ of 2-(2-Bromophenyl)hexanoic acid (**6b**)