Supplementary Material for *N*-Methyl-(*R*)-3-(*tert*-Butyl)-Sulfinyl-1,4-Dihydropyridine: A Novel NADH Model Compound, by Kun Xie, You-Cheng Liu \*, Yi Cui, Jian-Ge Wang, Yao Fu and Thomas C.W. Mak, *Molecules*, 2007, *12*, 415-422

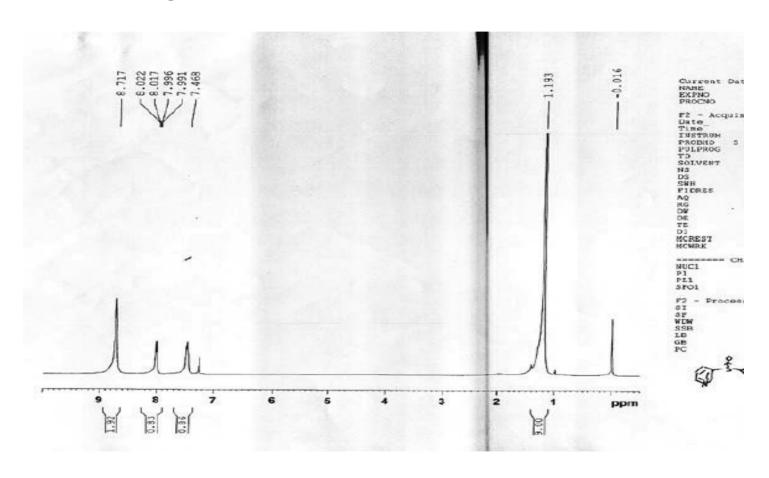
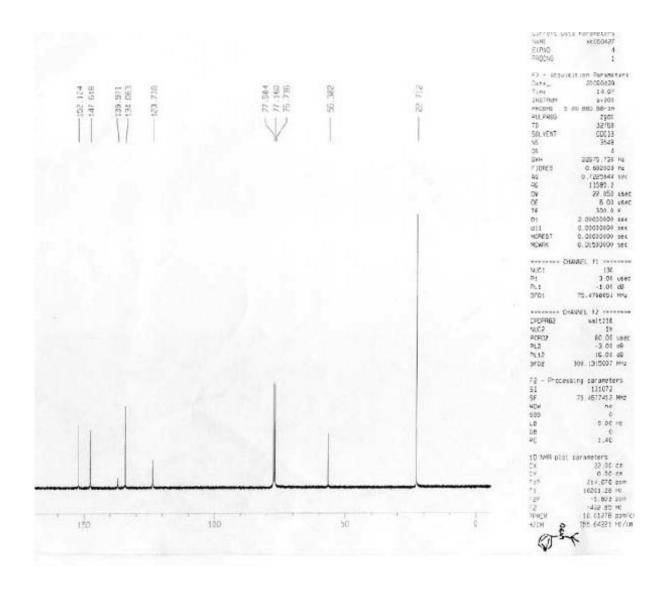


Figure 1: <sup>1</sup>H-NMR of (Rs)-2



**Figure 2:** <sup>13</sup>C-NMR of (Rs)-2

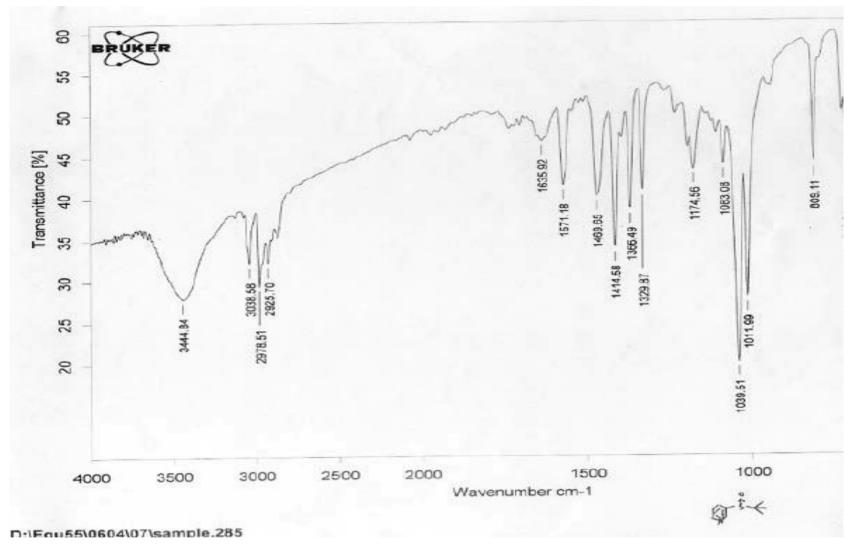
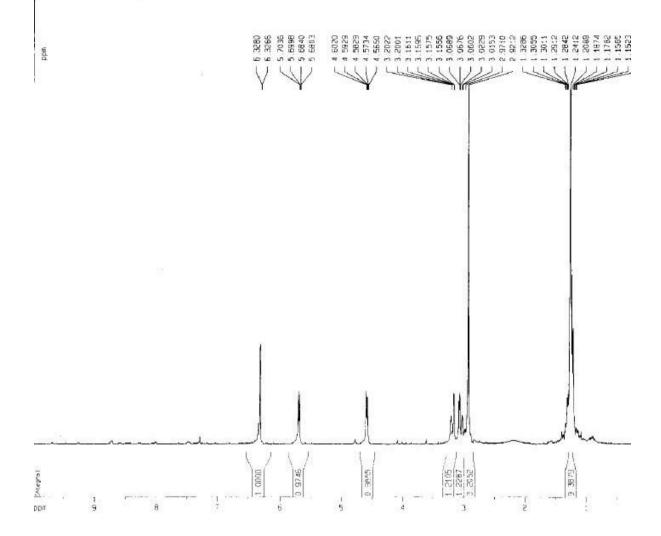
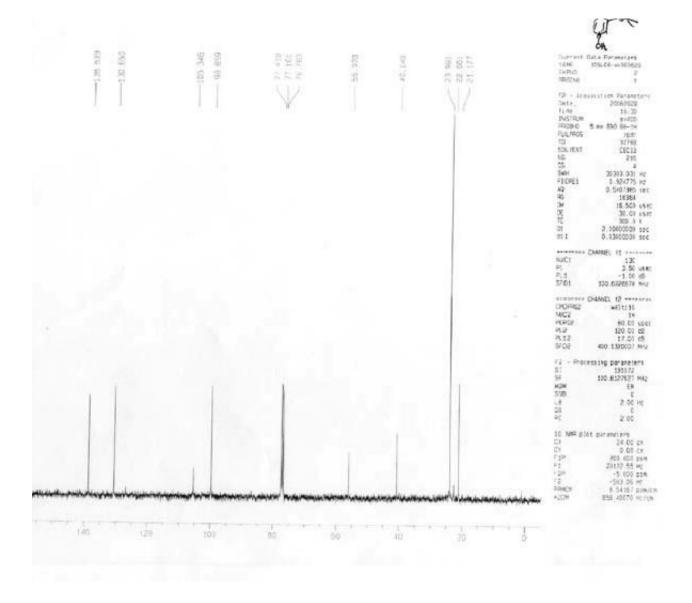


Figure 3: IR of (Rs)-2



**Figure 4:** <sup>1</sup>H-NMR of (Rs)-3



**Figure 5:** <sup>13</sup>C-NMR of (Rs)-**3** 

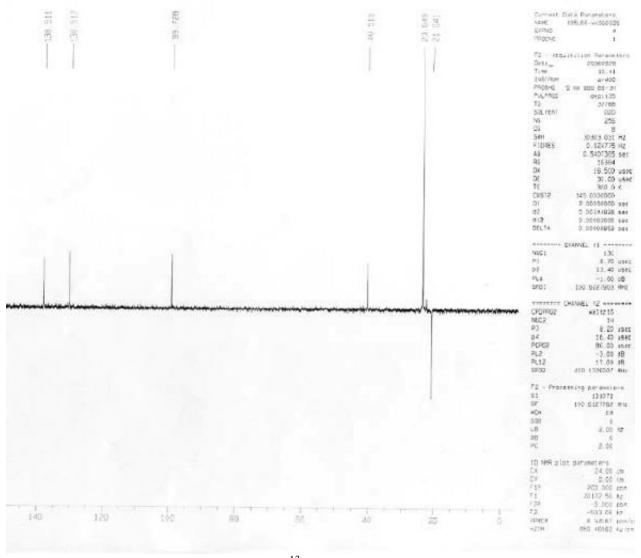


Figure 6: <sup>13</sup>C-NMR-DEPT of (Rs)-3

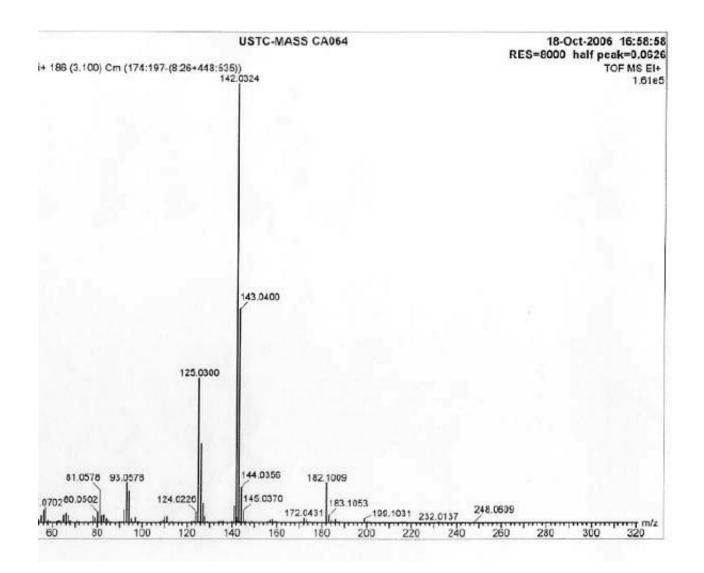


Figure7: HRMS of (Rs)-3

Multiple Mass Analysis: 51 mass(es) processed - displaying only valid results Tolerance = 5.0 mDa / DBE: min = -10.0, max = 50.0

Monoisotopic Mass, Odd and Even Electron Ions 1996 formula(e) evaluated with 158 results within limits (up to 50 closest results for each mass)

Minimum: Maximum:	100.00		5.0	5.0	-10.0 50.0	
Mass	RA	Calc. Mass	mpa	PPM	DBE	Formula
		128.0318	1.4	10.6	-6.0	H15 N 328 338
		128.0296	3.6	28.2	2 0	345
		128.0369	-3.7	-29.0	3.0	C6 H6 O 32S
		128.0285	4.7	36.9	-1.5	C3 H12 N 328 348
141.0251	3.64	141.0248	0.3	1.9	-1.0 4.0	C3 H11 N 335 34:
		141.0215	3.6	25.8		C6 H7 N D 325
		141.0290	-3.9	-27.5	9.0 4.0	C9 H3 N O
		141.0209	4.2			C7 H8 O 335
142.0324	100.00	142.0327	-0.3	29.6	-0.5	C4 H11 0 325 34
112.0321	100.00	142.0293	3.1	-1.8	3.5	C6 H8 N O 328
		142.0288		21.9	8.5	C9 H4 N O
		142.0368	3.6	25.7	-1.0	C4 H12 0 328 345
			-4.4	-31.0	3.5	C7 H9 C 338
		142.0276	4.8	33.8	-1.0	C3 H11 N O 325
143.0400	48.29	143.0405	-0.5	-3.4	3.0	
		143.0371	2.9	20.2		
		143.0366	3.4	23.9	8.0	C9 H5 N O
		143.0354	4.6	32.0	-1.5	C4 H13 C 32s 34s
		113.0331	9.0	32.0	-1.5	C3 H12 N O 32S
		143.0446	-4.5	-32.3	3.0	C7 H10 0 335
144.0356	7.98	144.0360	-0.4	-2.5	-1.5	C4 H13 O 335 345
		144.0393	-3.7	-26.0	-6.5	C H17 O 328 338
				20.0	0.3	345
		144.0318	3.8	26.2	-1.5	C3 H12 N C 328
		144.0399	-4.3	-29.7	3.0	34s C6 H9 N O 33s
145.0370	2.52	145.0363	0.7	5.0	3.0	
		145.0346	2.4	16.6	-6.5	C6 H9 N O 345 H16 N O 325 335
			4.7	+0.0	-6.3	H16 N O 325 338
		145.0397	-2.7	-18.3	-2.0	C3 H13 N O 32S
182.1009 183.1053	9.01	182.1003			200	345
	3-01		0.6	3.0	3.5	C10 H16 N 32s
		182.1045	-3.6	-19.7	3.5	C11 H17 33S
	1.46	182.0964	4.5	24.5	-1.0	C8 H20 325 34S
	1.46	183.1031	2.2	12.0	-1.5	C7 H20 N 325 339
		183.1082	-2.9	-15.7	3.0	C10 H17 N 32S
		183,1009	4.4	24.1	3.5	C11 H17 34S
184.0991	0.51	184.0995	-0.4	-2.3	-1.5	C7 H20 N 325 345
186,0262	2.32	184.0961	3.0	16.1	3.5	C10 H16 N 34S
	0.64	186.0254	0.8	4.3	4.5	C9 H11 335 348
		186.0288	-2.6	-13.8	-0.5	C6 H15 328 338
		186.0293	-3.1	-16.7	9.0	345 C11 H7 N 335
		186.0305	-4.3	-22.9	9.0	C12 H8 345
		186.0213	4.9	26.5	4.5	C8 H10 N 32S 34S
199.1031	0.85	199.1031	0.0	0.1	3.0	C10_H17_N 0 325
		199.1072	-4.1	-20.7	3.0	
		102.0317	5,2	51.0	2.0	
103.0487	5.18	103.0429	5.8	56.4	-3.5	
		103.0548	-6.1	-59.0		C H11 03 S
		103.0395			5.5	CB H7
		103.0333	9.2	89.1	1.5	C4 H7 Q3

Figure 8: HRMS of (Rs)-3 - Elemental Composition Report