

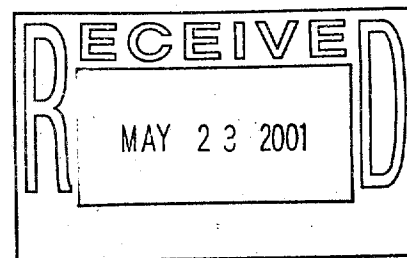
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Supporting Information

Toward the Creation of NMR Databases in Chiral Solvents for Assignments of Relative and Absolute Stereochemistry: NMR Desymmetrization of meso-Compounds

Yoshihisa Kobayashi, Nobuyuki Hayashi, and Yoshito Kishi*

*Department of Chemistry and Chemical Biology, Harvard University
12 Oxford Street, Cambridge, Massachusetts 02138*



¹³C NMR Chemical shifts of 2a,b and 3a,b in DMBA

DMBA	2a		2b (R) (S)	
1	14.113		14.114	14.123
2	18.658	18.650	19.182	19.181
3	40.881	40.858	40.520	40.495
4	71.250		67.331	67.418
5	43.613		44.592	44.451
6	71.250		67.331	67.418
7	40.858	40.881	40.520	40.495
8	18.650	18.658	19.182	19.181
9	14.113		14.114	14.123

DMBA	3a	3b (R) (S)	
1	24.351	24.103	24.121
2	67.108	63.746	63.756
3	47.330	47.706	47.657
4	67.108	63.746	63.756
5	24.351	24.103	24.121

(Also see Figure 1 in text)

¹³C NMR Chemical shifts of 4 and 5 in DMBA

DMBA	4	
1	14.213	
2	19.436	
3	34.674	
4	74.173	74.158
5	74.158	74.173
6	34.674	
7	19.436	
8	14.213	

DMBA	5	
1	14.171	
2	19.138	
3	40.292	40.282
4	70.229	70.203
5	solvent	solvent
6	solvent	solvent
7	70.203	70.229
8	40.282	40.292
9	19.138	
10	14.171	

(Also see Figure 2 in text)

¹³C NMR Chemical shifts of 6a~c in DMBA

DMBA	6a		6b		6c	
1	14.111		14.137		14.090	
2	18.699		19.158		18.695	
3	40.771	40.745	40.564		40.776	40.796
4	70.373		67.387	67.484	70.724	
5	44.551	44.530	44.993	44.886	44.387	
6	71.568		65.209		68.389	68.443
7	44.530	44.551	44.886	44.993	45.298	45.173
8	70.373		67.484	67.387	66.707	66.782
9	40.745	40.771	40.564		40.717	
10	18.699		19.158		19.102	
11	14.111		14.137		14.128	

(Also see Figure 3)

¹³C NMR Chemical shifts of 7a~e in DMBA

	7a		7b		7c		7e		7e	
1	13.980		14.013		14.040		14.040		14.049	
2	22.894		22.841		22.897		22.889		22.902	
3	28.107	28.118	28.092		28.261		28.221		28.226	
4	33.605	33.625	38.001	38.011	37.859	37.849	37.804		38.168	
5	71.675	71.695	69.201	69.305	70.316	70.306	70.162		70.106	70.129
6	66.652	66.665	40.031	40.062	35.059	35.046	37.892	37.877	37.829	
7	*	*	59.612	59.67	29.800		22.512	22.495	25.946	
8	*	*	*	*	61.676		33.352		26.382	
9	*	*	*	*	*	*	61.278		33.401	
10	*	*	*	*	*	*	*	*	61.264	

(Also see Figure 4 in text)