Supporting Information for

A Vibrational Circular Dichroism Approach to the Determination of the Absolute Configurations of Flavorous 5-Substituted-2(5*H*)-furanones

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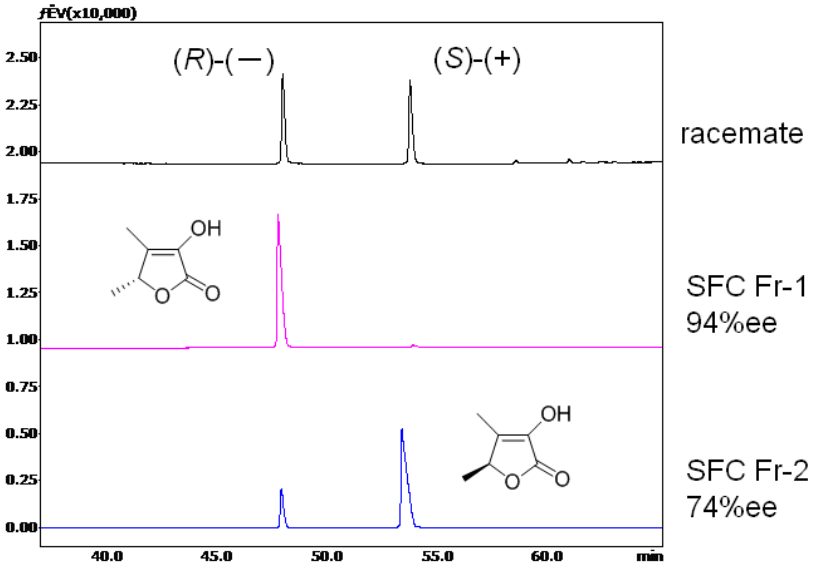
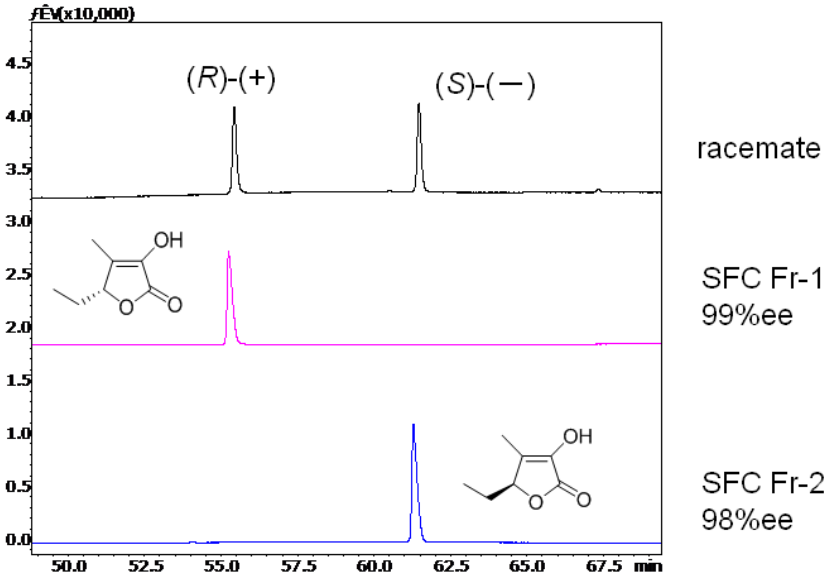
Contents

SI1. Chiral GC analysis of sotolon (1).



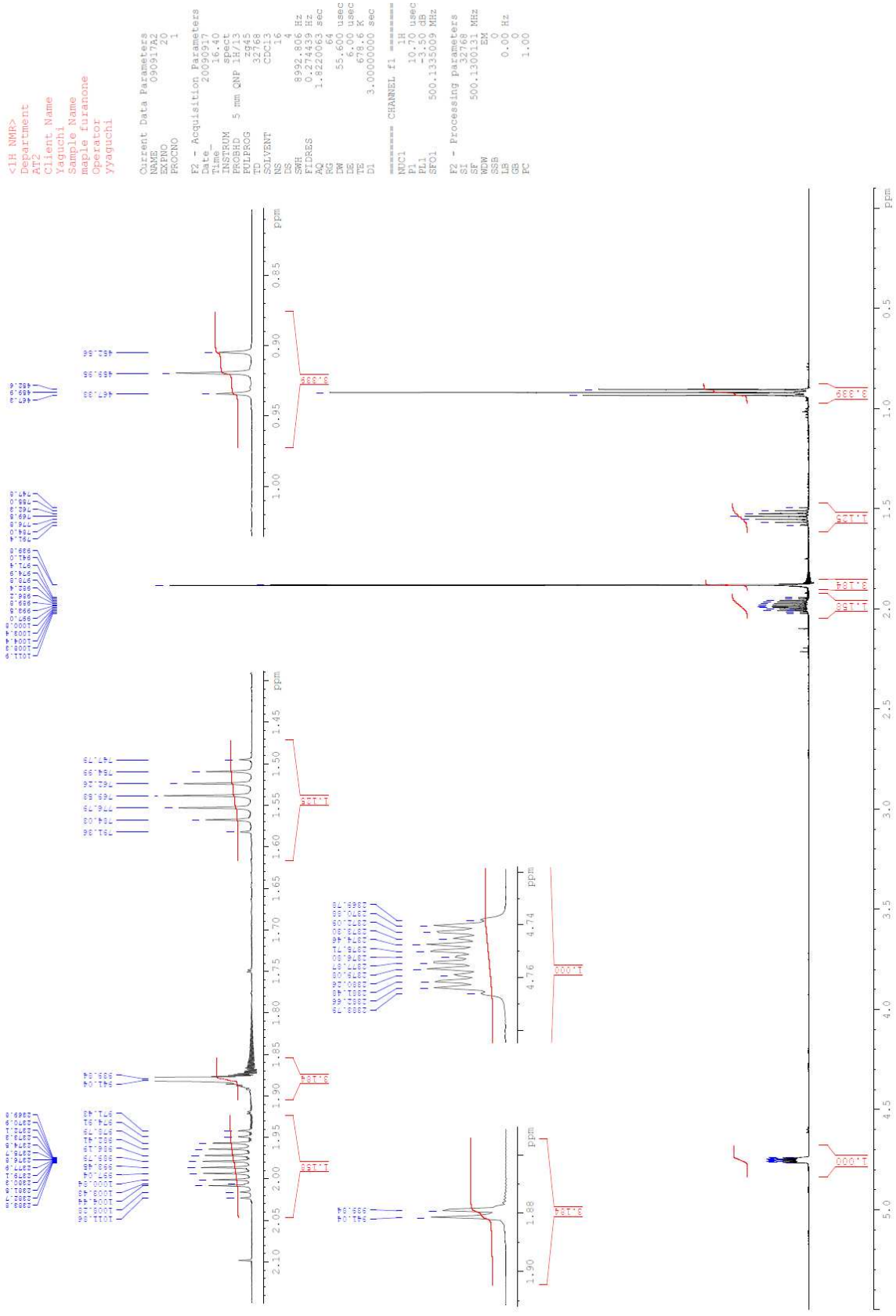
Sotolon (**1**) : β-DEX325 (Supelco)

SI2. Chiral GC analysis of maple furanone (2).

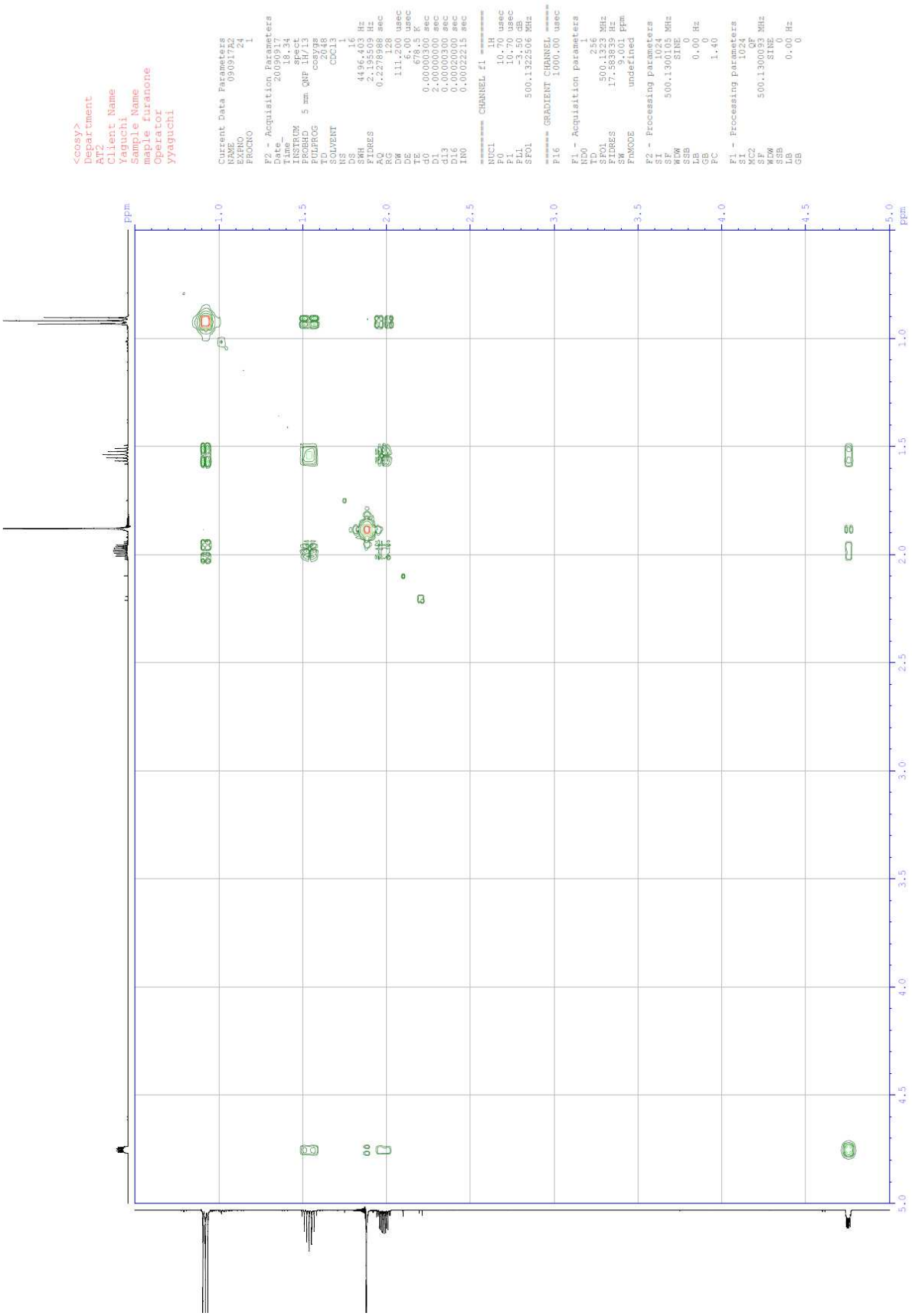


Maple furanone (**2**) : β-DEX325 (Supelco)

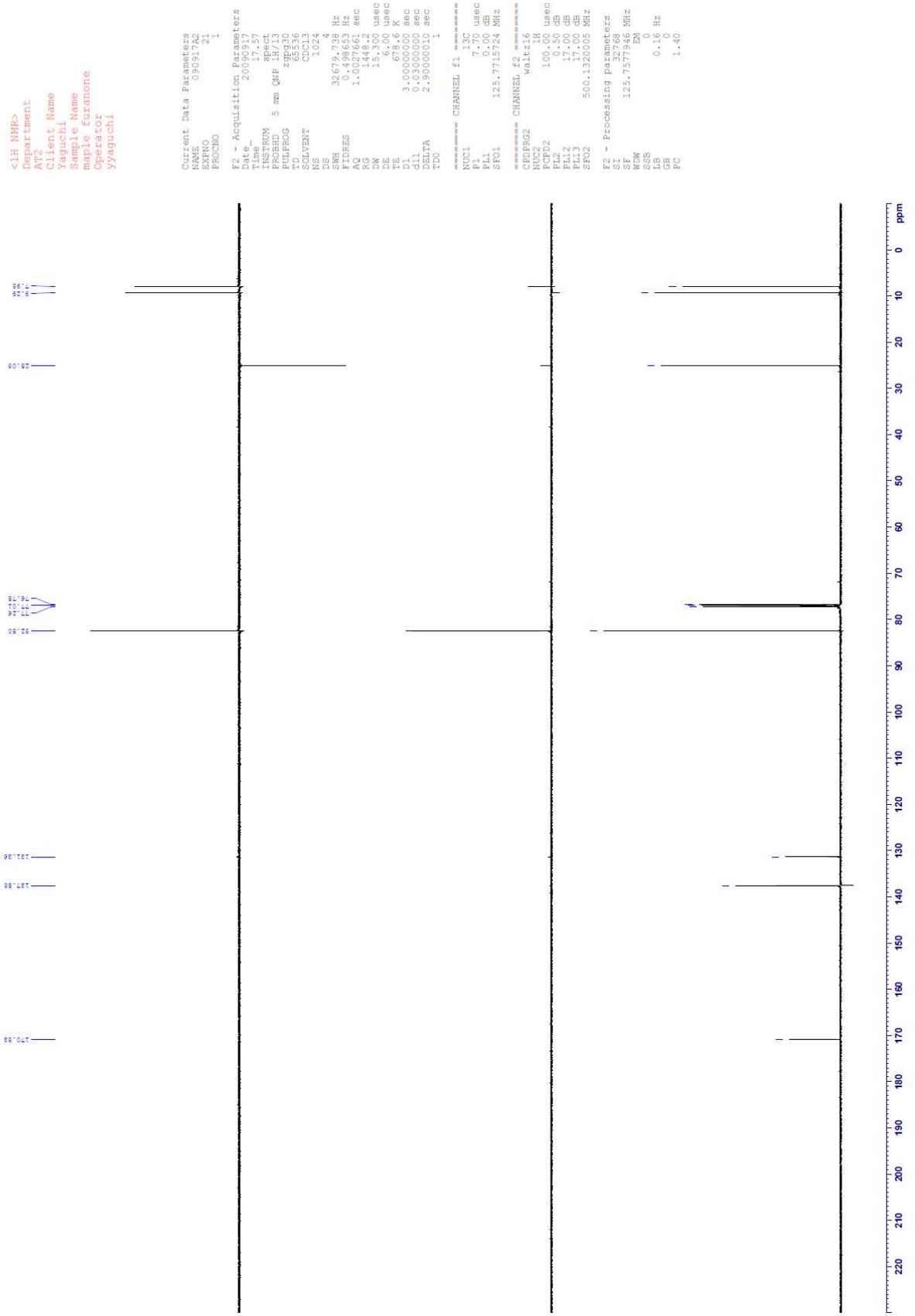
SI3. ^{1}H NMR spectrum of maple furanone (2)



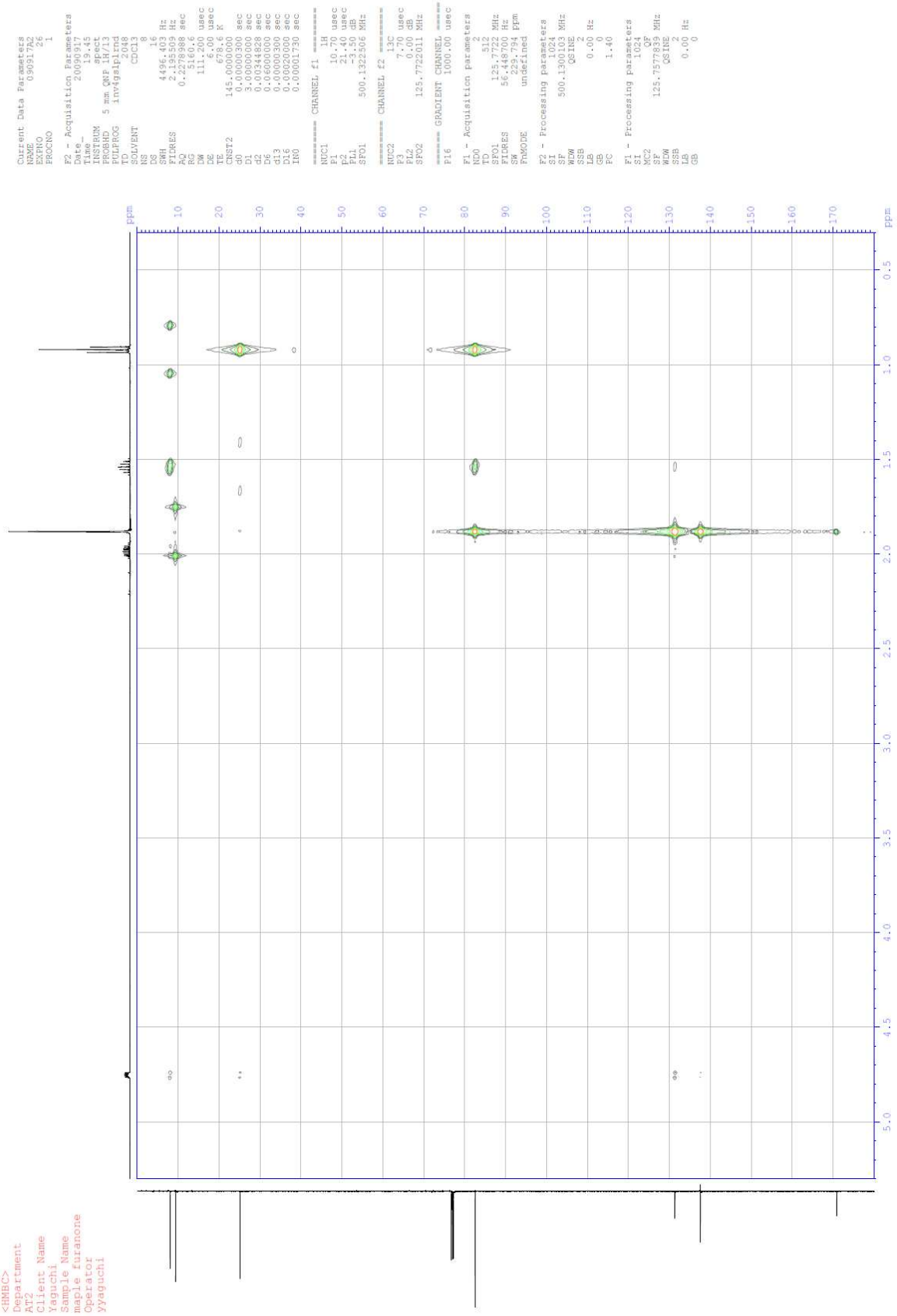
SI4. COSY spectrum of maple furanone (2)



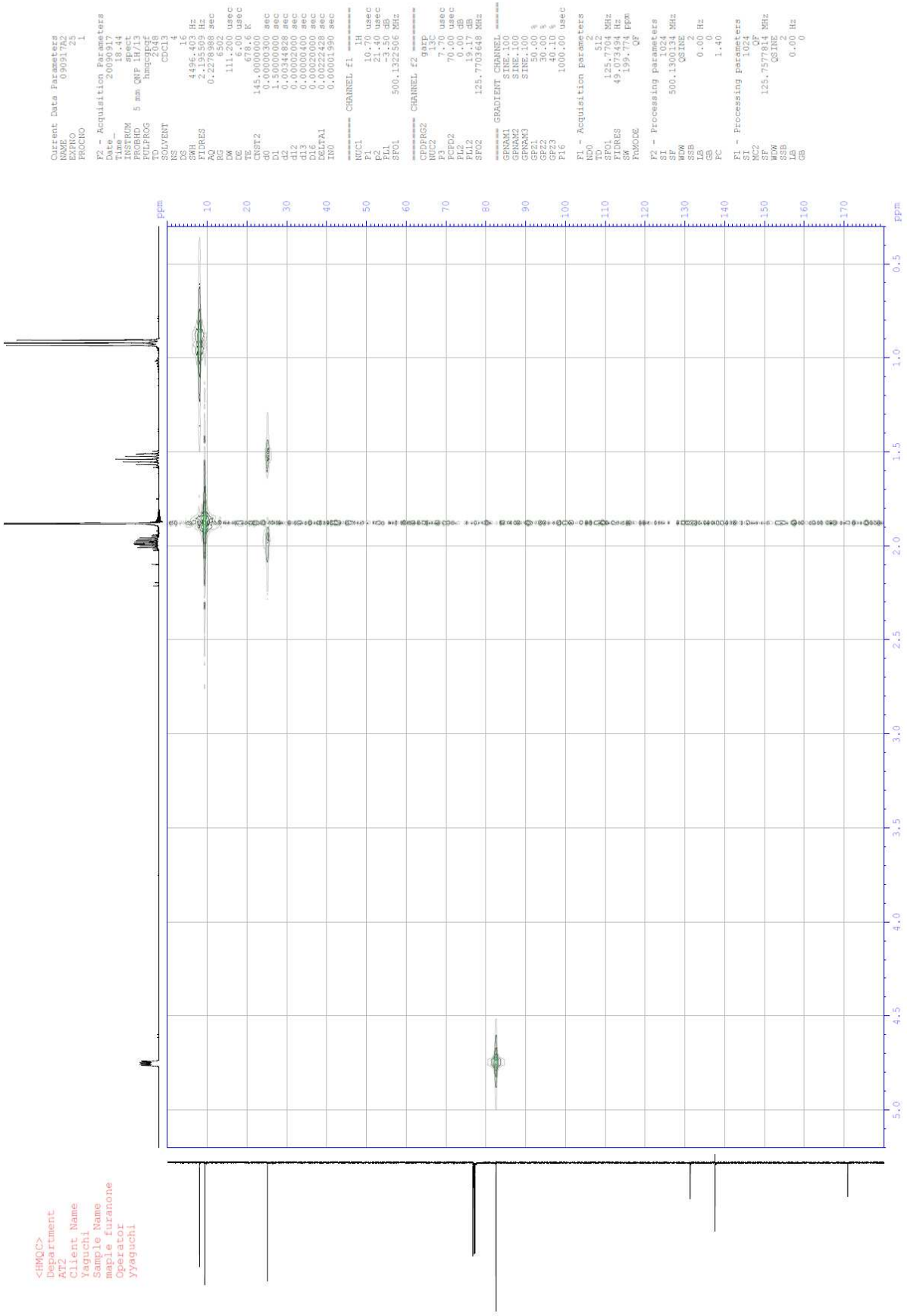
SI5. ^{13}C NMR spectrum of maple furanone (2)



SI6. HMBC spectrum of maple furanone (2)



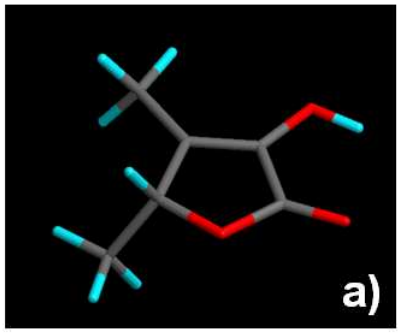
SI7. HMQC spectrum of maple furanone (2)



SI8. VCD calculation of sotolon (1).

The IR and VCD spectra of **1** were theoretically calculated based on the density functional theory (DFT) at the B3PW91/6-31G(d,P) level of theory. Conformational analysis offered a sole stable conformer (a) as shown below.

The conformations of (*R*)-**1**



SI9. VCD calculation of maple furanone (2).

1. CONFLEX search with MMFF94S force fields.

6 non-redundant conformers were found in conformational search with CONFLEX program code. Table 1 shows the energy and Boltzmann weight of the selected low-lying conformers. The DFT calculations were performed for low-lying three conformers whose sum of the weights was over 99.9994%.

Table 1 Results of the conformational search for (*R*)-**2**

conformation ID	Energy (kcal/mol)	Relative energy (kcal/mol)	Boltzmann Weight	Cumulative sum of Boltzmann Weight
0000	8.8952	0.0000	53.0877	53.0877
0001	9.0325	0.1372	42.1106	95.1983
0002	10.3190	1.4238	4.8011	99.9994
0003	15.9797	7.0845	0.0003	99.9997
0004	16.0977	7.2025	0.0003	100.0000
0005	17.4906	8.5953	0.0000	100.0000

2. Results of DFT calculations

Table 2 shows the energy and Boltzmann weight of the DFT calculations. The IR and VCD spectra were calculated for 3 low-lying conformers.

Table 2 Results of the DFT calculations for (*R*)-**2**

Conformation ID	Total Energy (au)	Relative energy (kcal/mol)	Boltzmann weight	Cumulative sum of Boltzmann weight
b(0000)	-498.145647	0.000	0.65874	0.65874
c(0001)	-498.144934	0.447	0.30945	0.96819
d(0002)	-498.142787	1.795	0.03181	1.00000

The conformations of (*R*)-**2**