Supporting Information

Absolute Configuration Assignment to Chiral Natural Products by Biphenyl Chiroptical Probes: the Case of the Phytotoxins Colletochlorin A and Agropyrenol

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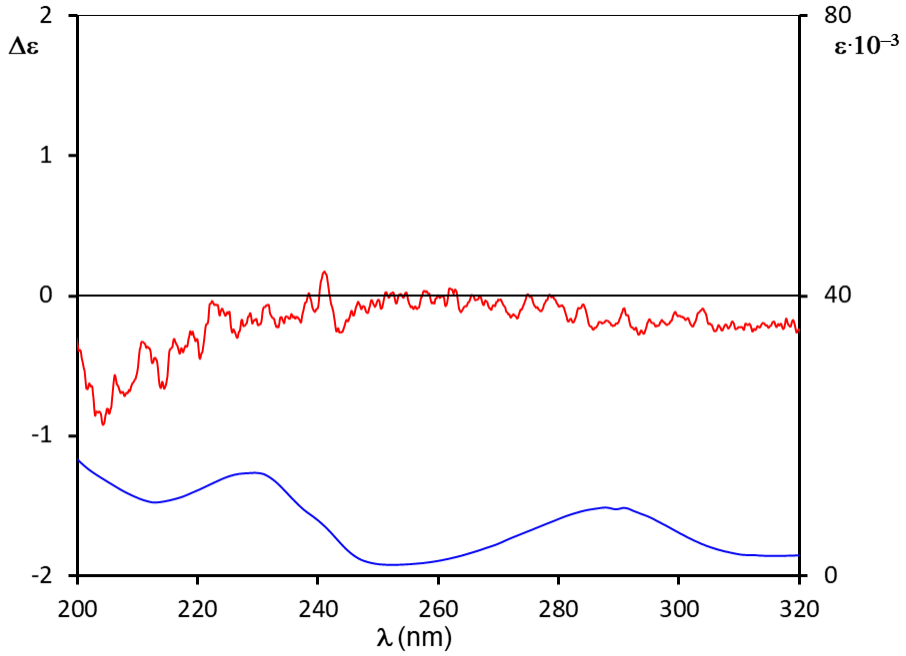

Figure S1. Experimental ECD spectrum of colletochlorin A (-)-**1** in CH_3CN.

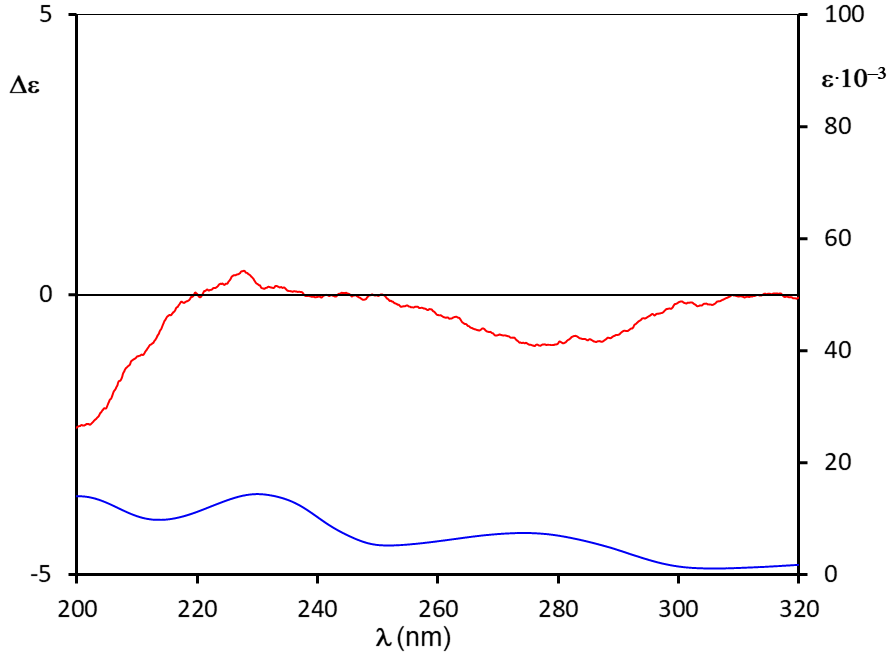

Figure S2. Experimental ECD spectrum for agropyrenol (-)-**2** in CH_3CN.

Table S1 Conformers Boltzmann distribution of **2.**

	DFT/B3LYP/TZVP (Gas Phase)	
Conformers	ΔG (kcal/mol)	% Pop
a	0.00	40.3
b	0.42	19.8
c	0.91	8.7
d	1.10	6.3
e	1.15	5.8
f	1.20	5.3
g	1.30	4.5
h	1.42	3.7
i	1.99	1.4
j	2.11	1.1
k	2.23	0.9
l	2.42	0.7
m	2.60	0.5
n	2.62	0.5
o	2.65	0.5

Table S2. Conformers Boltzmann distribution of (*S*,*S*)-**2a** (*M* and P).

	DFT/B3LYP/TZVP (Gas Phase)	
Conformers	ΔG (kcal/mol)	% Pop
1-*p*	0.00	14.3
2-*p*	-0.15	18.5
3-*p*	0.56	5.5
4-*p*	-0.61	40.3
1-*m*	0.60	5.1
2-*m*	0.74	4.1
3-*m*	1.33	1.5
4-*m*	0.17	10.7

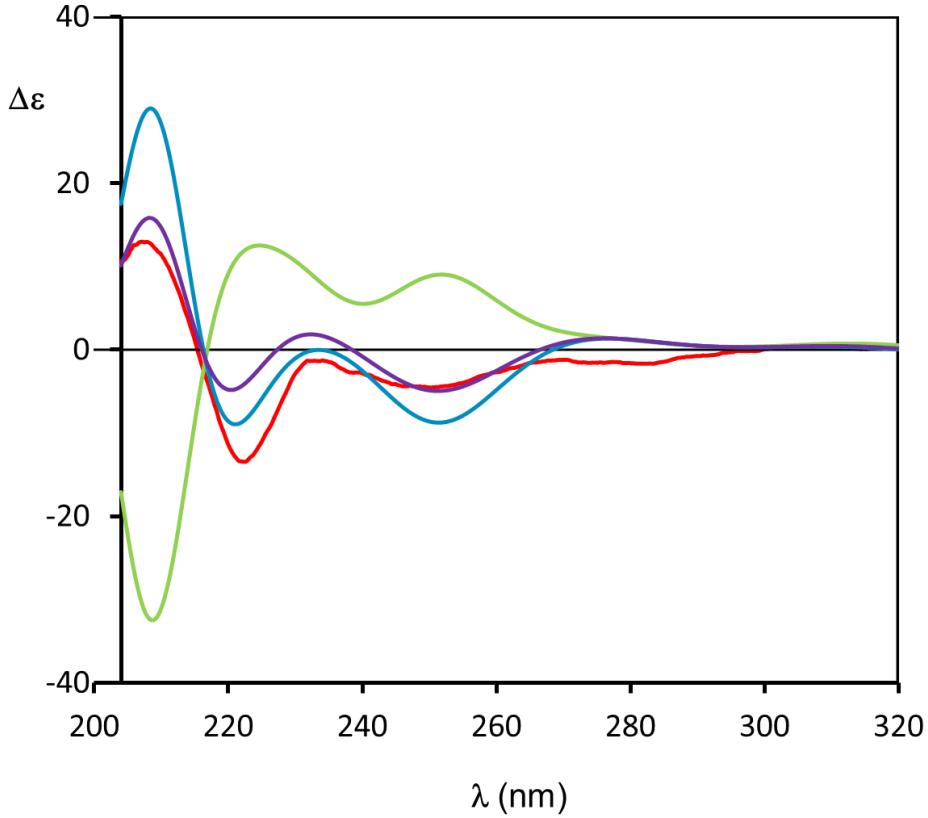

Figure S3. Experimental ECD spectrum of **2a** (red line, THF) and theoretical ECD spectra of (*S*,*S*,*P*)-**2a** (blue line) and (*S*,*S*,*M*)-**2a** (green line) computed at TDDFT/CAM-B3LYP/aug-cc-pVDZ//DFT/B3LYP/TZVP/gas phase and computed spectrum weighed on Boltzmann population of (*S*,*S*,*P*)-**2a** and (*S*,*S*,*M*)-**2a** (violet line). (computed spectra are divided by 5).

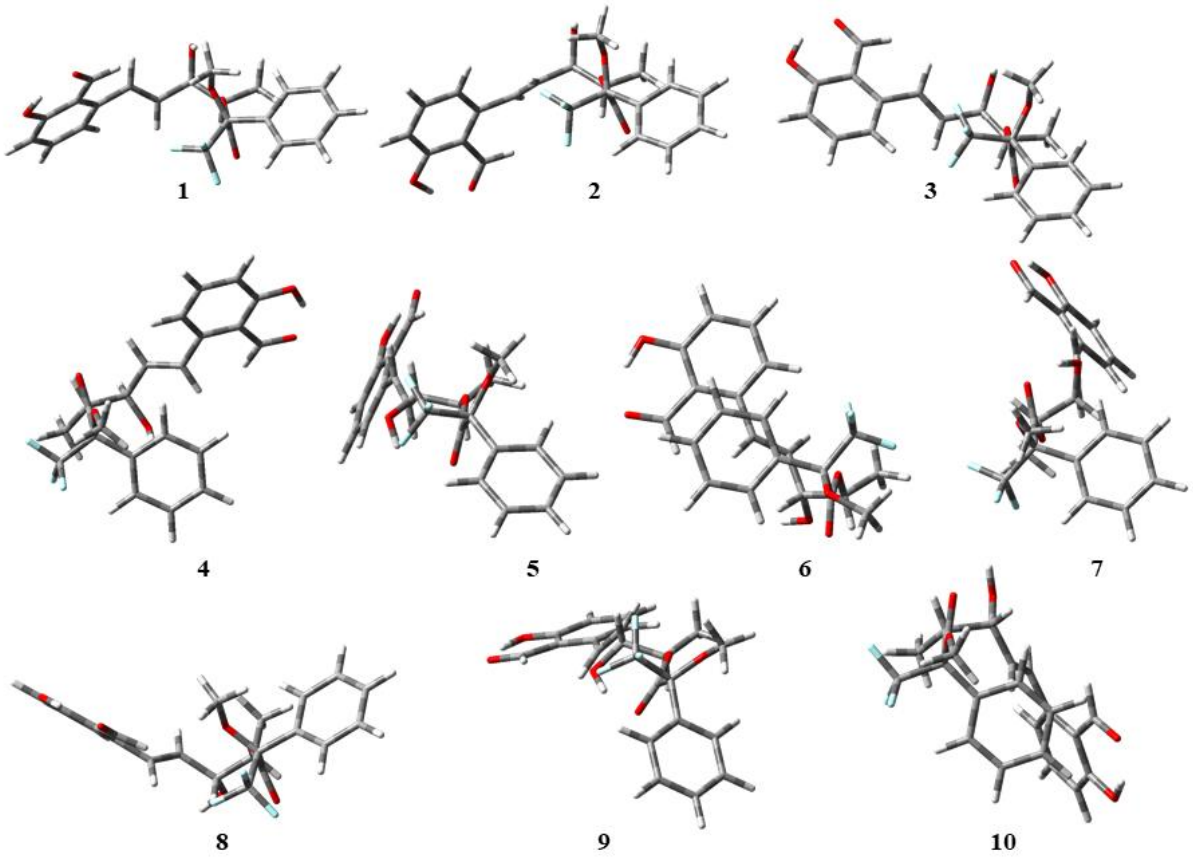

Figure S4. Structures of conformers of 4'-(*R*)-MTPA-**2** computed at DFT/B2LYP/TZVP/ IEFPCM($CHCl_3$) level.

Table S3. Conformers Boltzmann distribution of 4'-(*R*)-MTPA ester of (3'*R*,4'*R*)-**2** computed at DFT/B3LYP/TZVP/IEFPCM($CHCl_3$) level of theory.

		DFT/B3LYP/TZVP (IEFPCM = $CHCl_3$)	
Conformer[a]	rotamer[a]	ΔG (kcal/mol)	% Pop
1	d	0.00	40.6
2	a	0.52	17.0
3	b	0.74	11.6
4	d	0.86	9.5
5	d	0.89	9.0
6	d	1.42	3.7
7	d	1.50	3.2
8	c	1.53	3.1
9	b	1.98	1.4
10	d	2.34	0.8

[a]See Figure S4 for conformers structures. [b]See Figure 6 in text for rotamers structures.

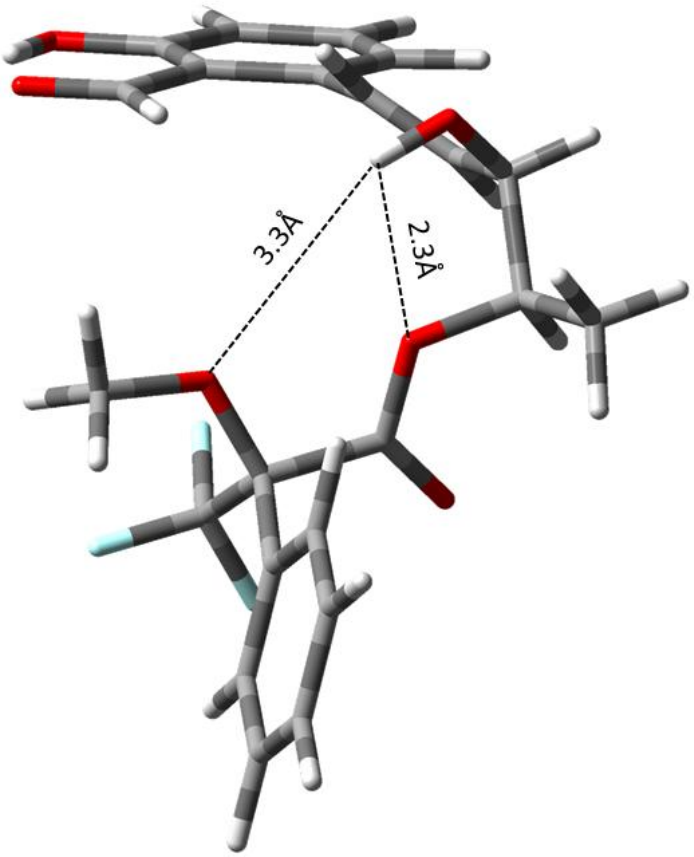

Figure S5. Structure of conformer 1 (rotamer (d)) of (*R*)-MTPA-**2.**

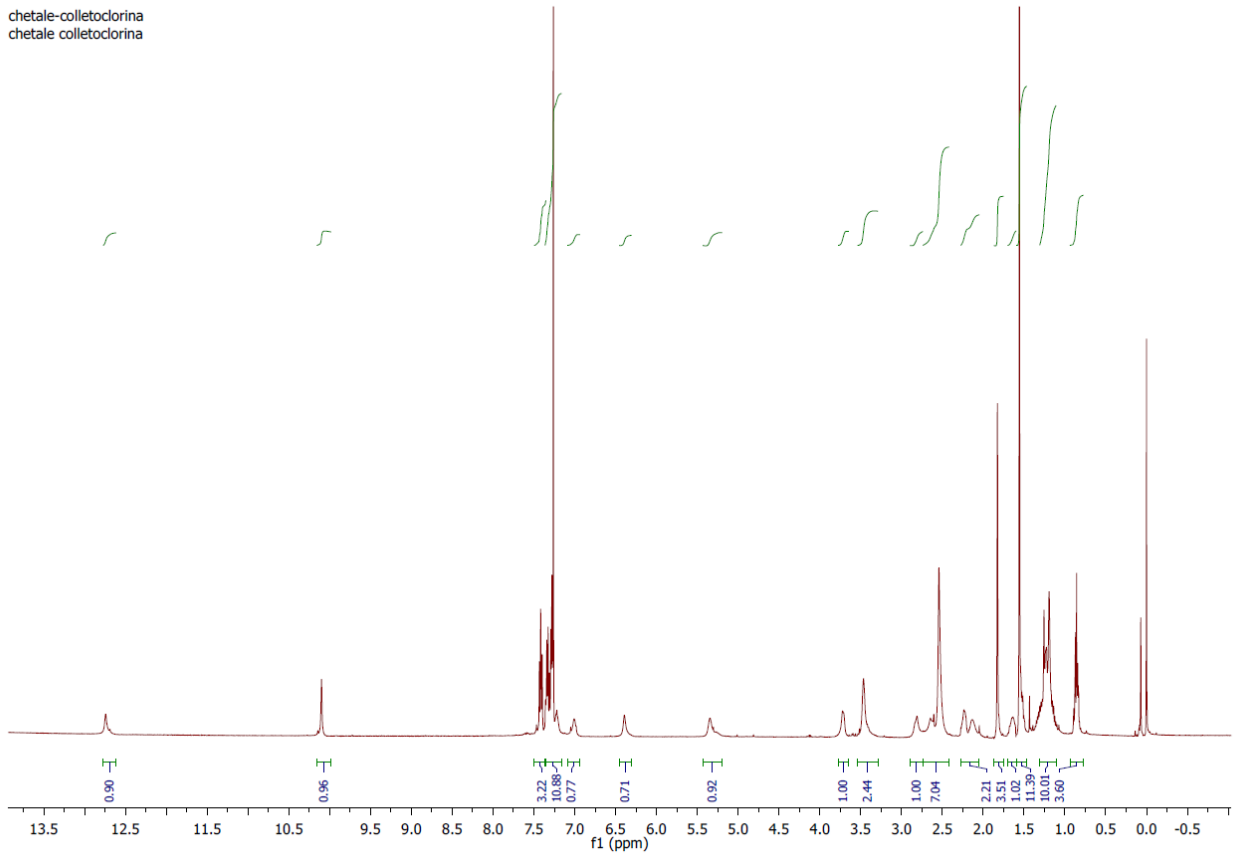

Figure S6. [1]HNMR spectrum of **1a**.

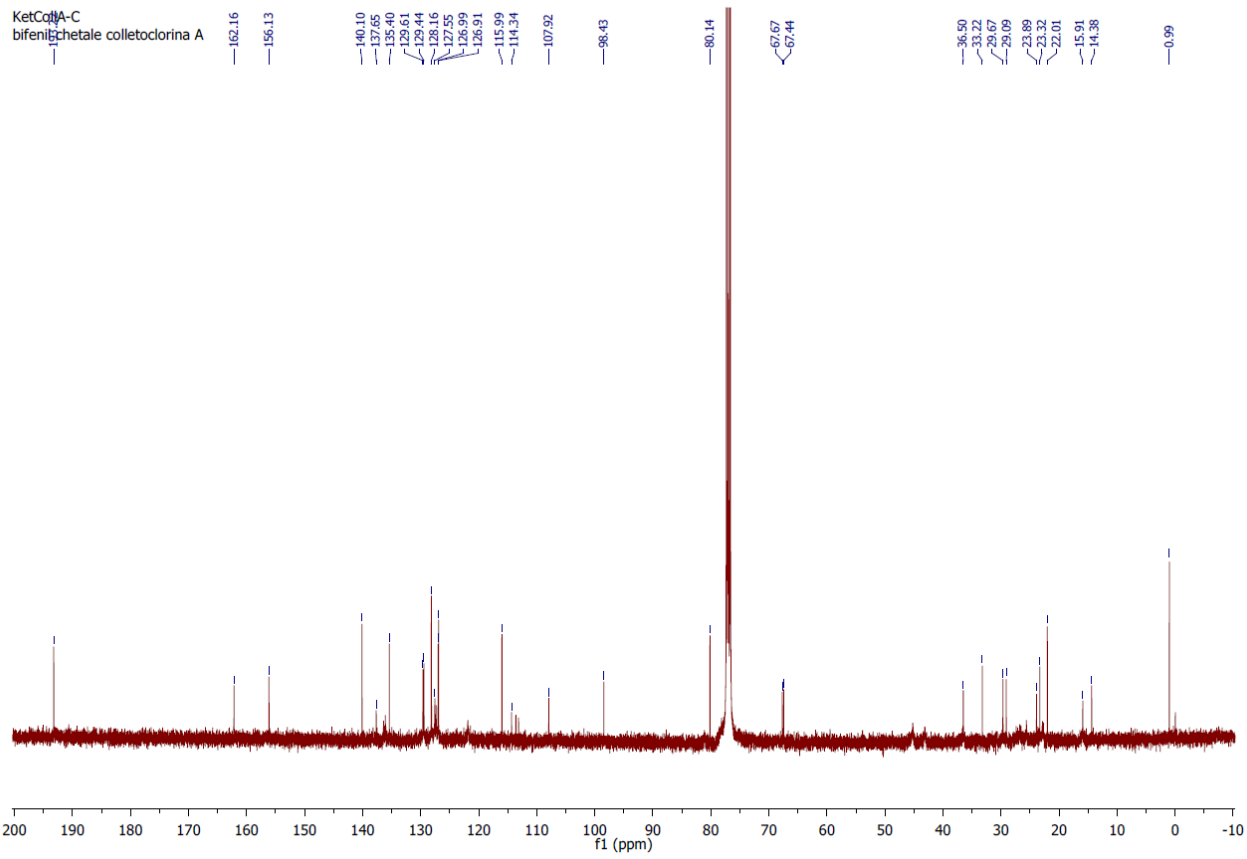

Figure S7. [13]CNMR spectrum of **1a**.

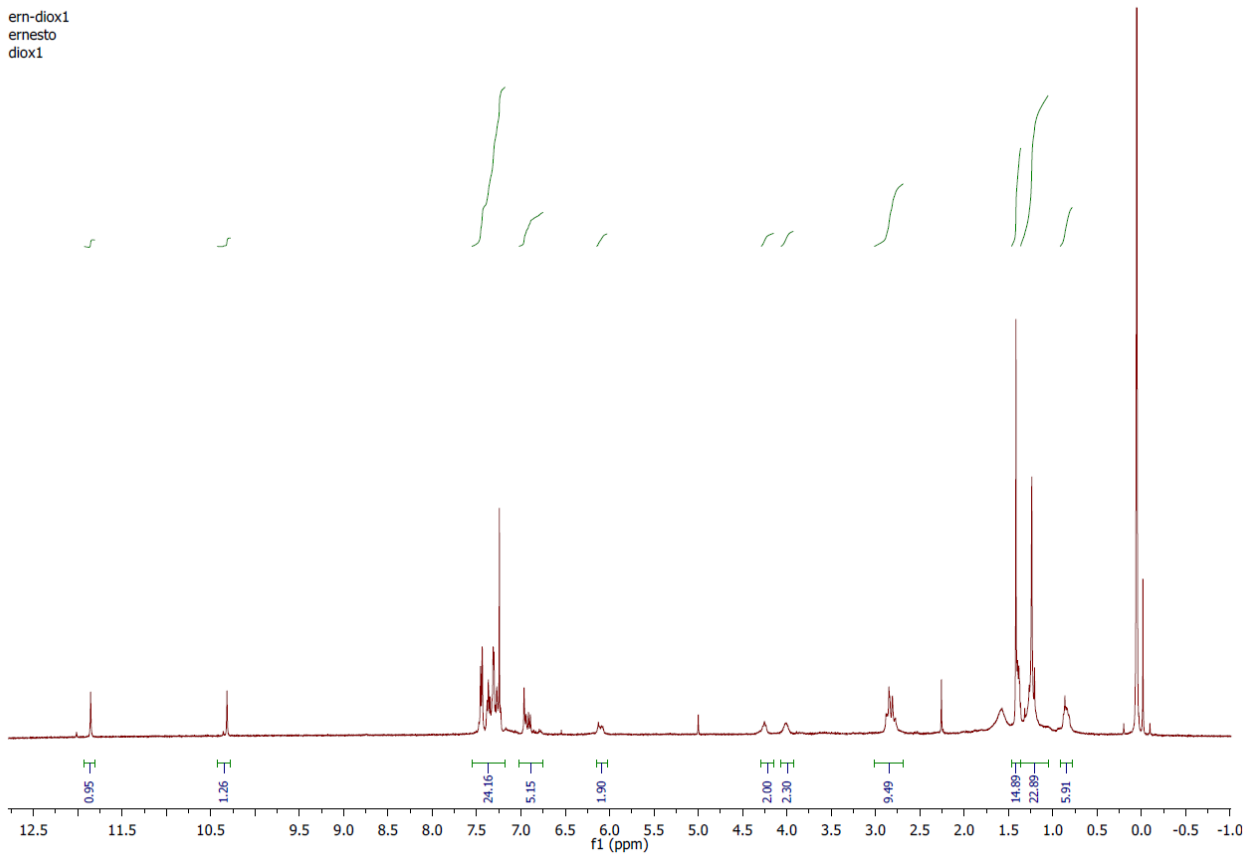

Figure S8. [1]HNMR spectrum of **2a**.

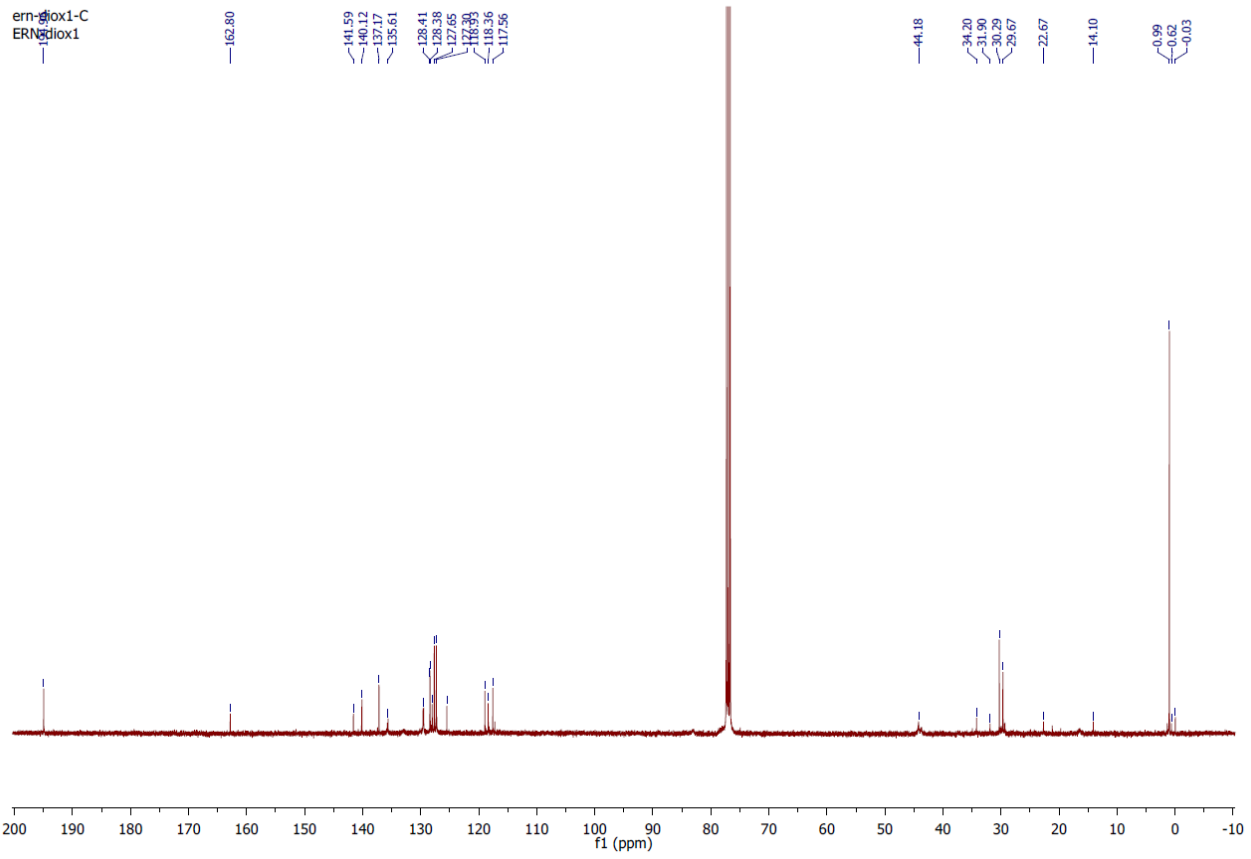

Figure S9. [13]HNMR spectrum of **2a**.