Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplementary Information

Ultrasound-Promoted Chiral Fluorescent Organogel

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1. Gelation test toward typical organic fluids at room temperature.

Table S1. Gel-forming Abilities of (*S*)-**1-7** in Various Solvents.[a]

Solvents	(*S*)-**1**	(*S*)-**2**	(*S*)-**3**	(*S*)-**4**	(*S*)-**5**	(*S*)-**6**	(*S*)-**7**
n-Hexane	I	I	I	I	I	I	I
Dichloromethane	S	S	S	S	S	S	S
Chloroform	S	S	S	S	S	S	S
Ethyl acetate	PG+G*[b]	C	C	C	S	C	C
Acetone	PG[c]+G*[b]	S	S	S	S	S	S
Tetrahydrofuran	S	S	S	S	S	S	S
Acetonitrile	P	I	I	I	I	I	I
Benzene	P	S	S	S	S	S	S
Toluene	PG[c]+G*	S	S	S	S	S	S
ethylbenzene	PG[c]+G*	S	S	S	S	S	S
Xylene	PG[c]+G*	S	S	S	S	S	S
1,3,5-Trimethylbenzene	PG[c]+G*	S	S	S	S	S	S
Tetrahydronaphthene	S	S	S	S	S	S	S
o-Dichlorobenzene	S	S	S	S	S	S	S
Chlorobenzene	S	S	S	S	S	S	S
DMF	S	S	S	S	S	S	S
Methanol	I	I	I	I	I	I	I
Ethanol	I	I	I	I	I	I	I
i-Propanol	I	I	I	I	I	I	I

[a] The concentration of solution is 5 wt% in general.
[b] The concentration of sonciated solution is 2.5 wt%.
[c] The partial gel is formed when standing at –10 ºC for at least 6 hr.
I = almost insoluble; S = isotropic solution; P = precipitation; C = crystallization; PG = partial gel; G* = gel formed via ultrasound.

2. SEM images of (*S*)-**1**

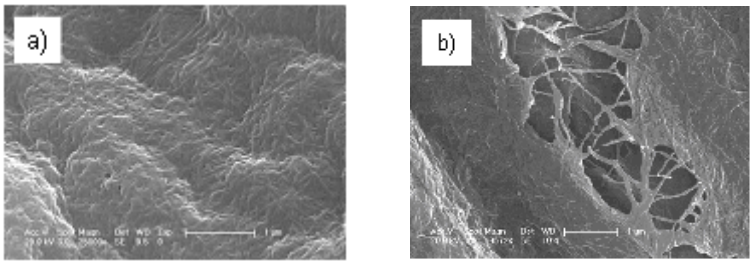

Fig. S1 SEM image of xerogel from ethyl acetate (a) and toluene (b).

3. UV-vis absorption and fluorescence emission spectra of (*S*)-**1** in various organic solvents

Table S2. Absorption Maxima and Extinction Coefficients of (*S*)-**1** in Different Solvents.[a]

Solvents	λ_{max} (nm)	ε ($M^{-1}cm^{-1}$)
n-Hexane	309.0	94400
Methylene chloride	313.0	104000
THF	314.0	115600
Ethyl acetate	311.0	116800
Toluene	314.0	104400
Acetonitrile	309.5	107200

[a] $c = 2.5 \times 10^{-6}$ M, room temperature.

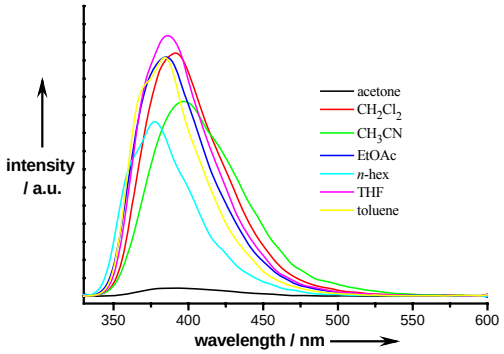

Fig. S2 Fluorescence spectra of (*S*)-**1** in different solvents (2.5×10^{-6} M), λ_{ex}=320 nm. Both UV-Vis absorption and fluorescence spectra of (*S*)-**1** show only a subtle solvent effect.

4. Comparison of UV-vis absorption and fluorescence emission spectra of (*S*)-**1** and its model compound **8**

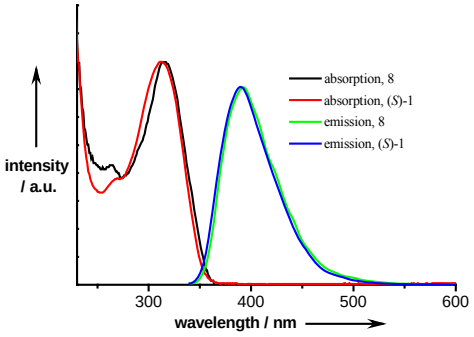

Fig. S3 Comparison of UV-vis absorption and emission of (*S*)-**1** and its model compound **8** in dichloromethane (2.5×10^{-6} M). Note: The spectra are normalized for comparison.

5. Fluorescence spectra of (*S*)-**1** in toluene at different concentration

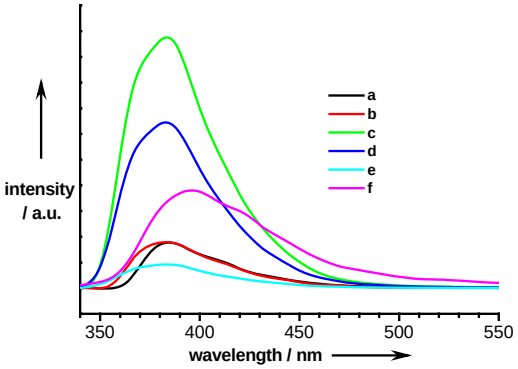

Fig. S4 Fluorescence spectra of (*S*)-**1** in toluene at different concentration (a) 2.5×10^{-3} M, (b) 2.5×10^{-4} M, (c) 2.5×10^{-5} M, (d) 2.5×10^{-6} M, (e) 2.5×10^{-7} M and (f) in thin film. excitation wavelength, λ_{ex}=320 nm.

6. ESI-MS spectra of (*S*)-**1**

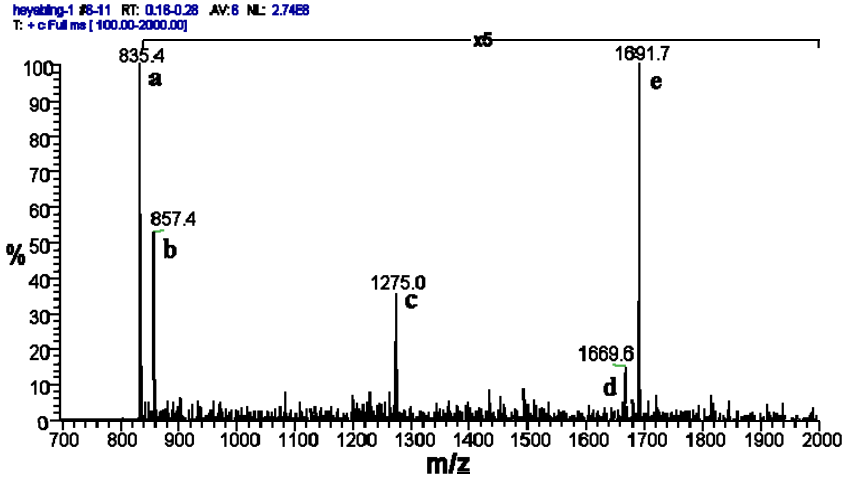

Fig. S5 ESI-MS spectra of (*S*)-**1** exhibit singly and doubly charged species. a: $[(\mathbf{1})+H]^+$, b: $[(\mathbf{1})+Na]^+$, c: $[(\mathbf{1})_3+Na_2]^{2+}$, d: $[(\mathbf{1})_2+H]^+$, e: $[(\mathbf{1})_2+Na]^+$.

7. Concentration-dependent ^{1}H NMR spectra of (*S*)-**1** in $CDCl_3$ at 298 K.

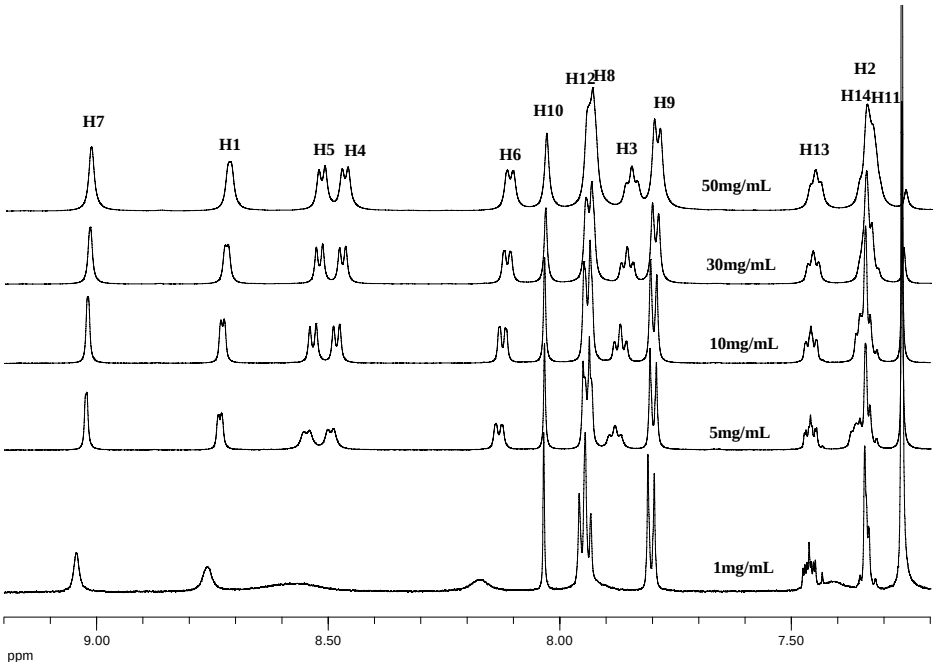

Fig. S6 Concentration-dependent ^{1}H NMR spectra of (*S*)-**1** in $CDCl_3$ at 298K.

8. Concentration- independent ^{1}H NMR spectra of (*S*)-**1** in [D_8]toluene at 298 K.

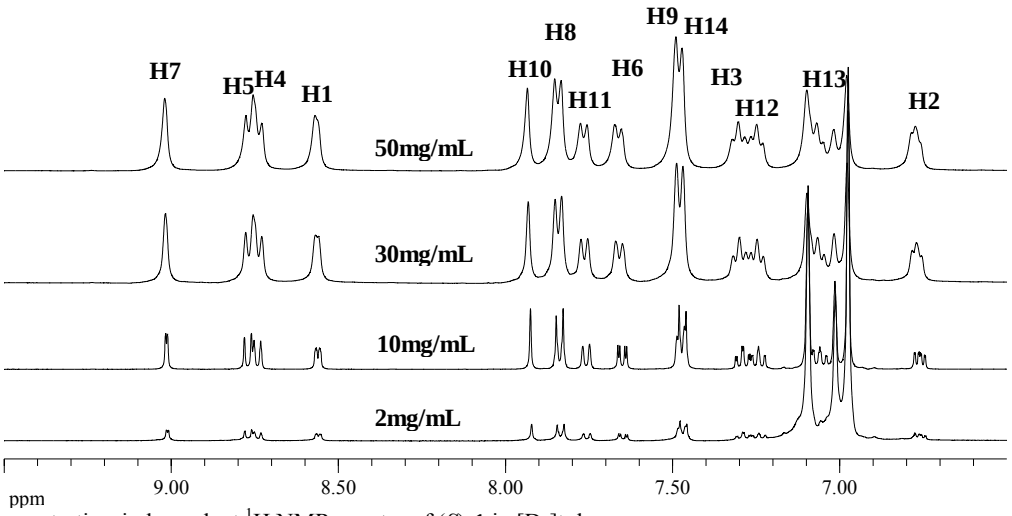

Fig. S7 Concentration-independent ^{1}H NMR spectra of (*S*)-**1** in [D_8]toluene.

9. Temperature-dependent ^{1}H NMR spectra of (*S*)-**1** in [D_8]toluene.

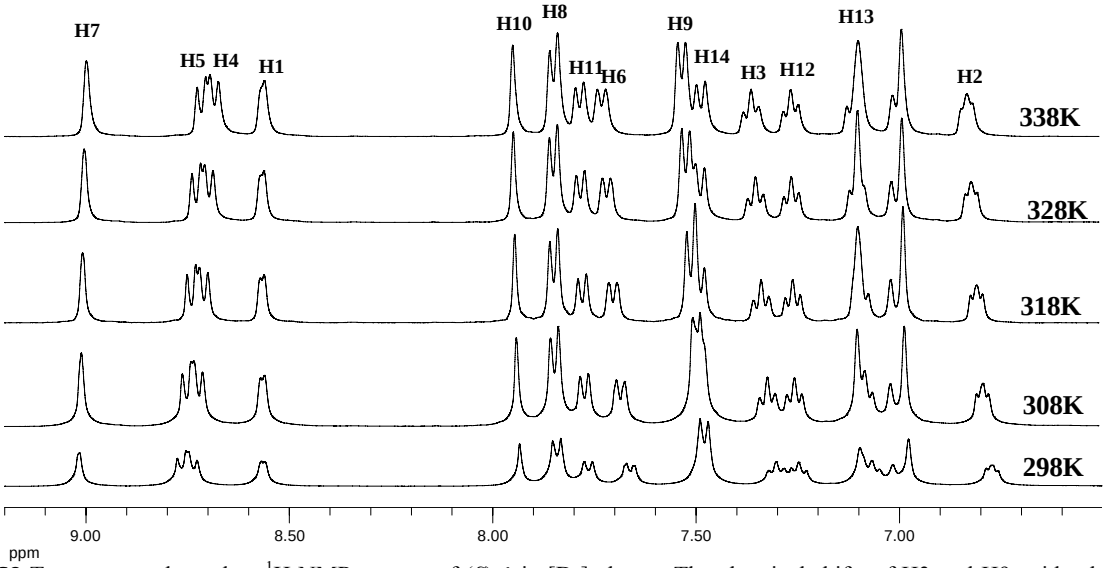

Fig. S8 Temperature-dependent ^{1}H NMR spectra of (*S*)-**1** in [D_8]toluene. The chemical shifts of H3 and H9 evidently shift downfield upon increasing the temperature, indicative of the reduction of intermolecular π-π interactions.

10. ^{1}H NMR and ^{13}C NMR spectra of the compounds investigated.

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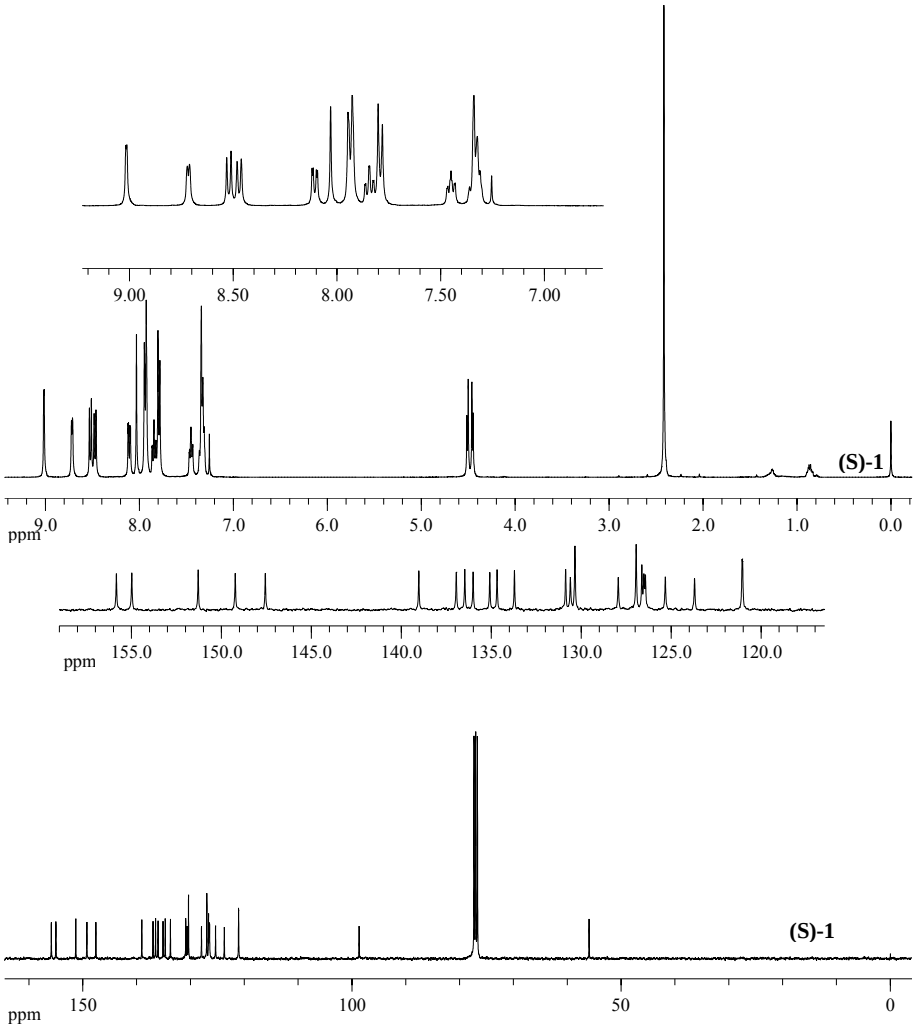

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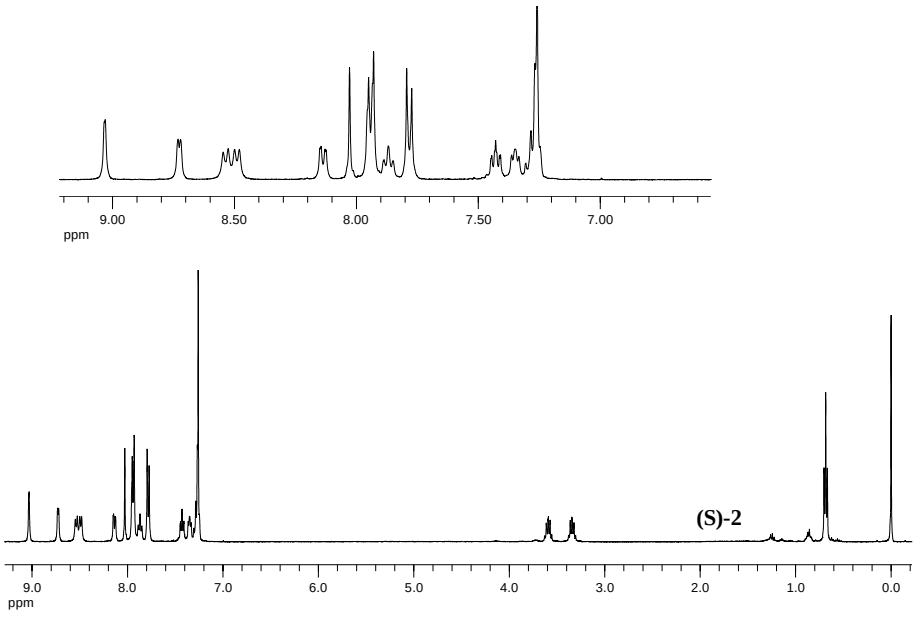

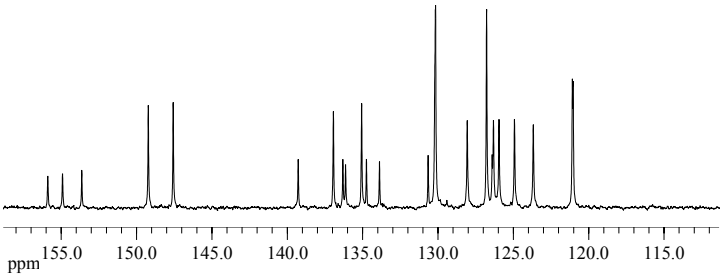
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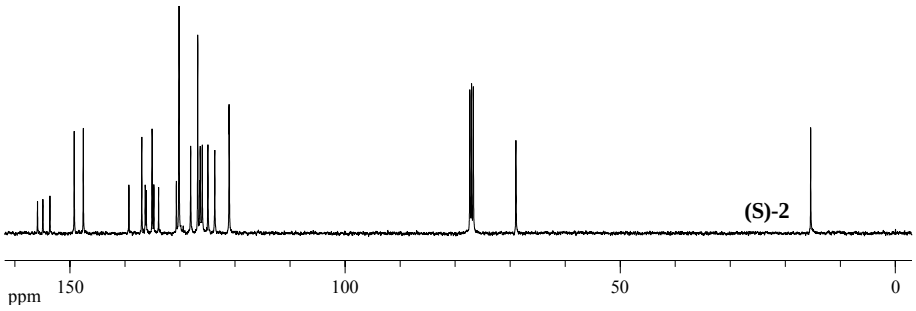
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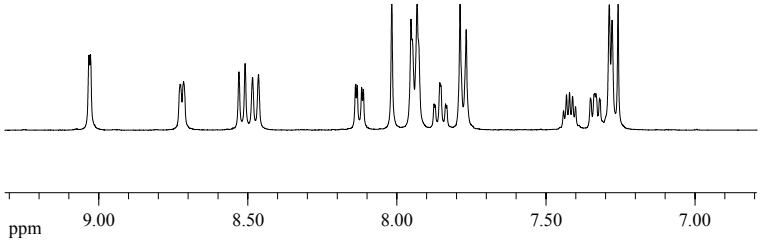
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7.50
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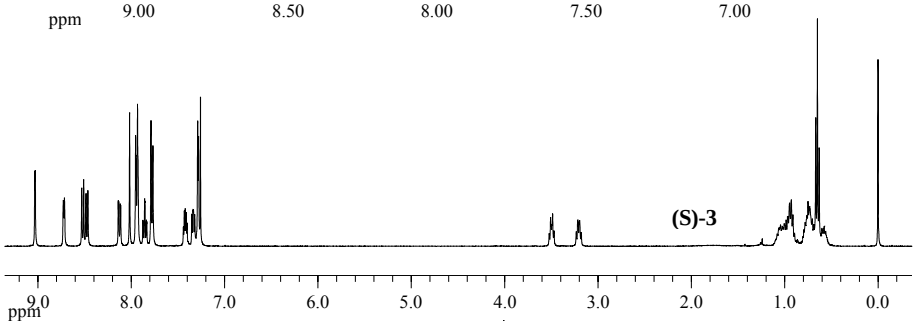
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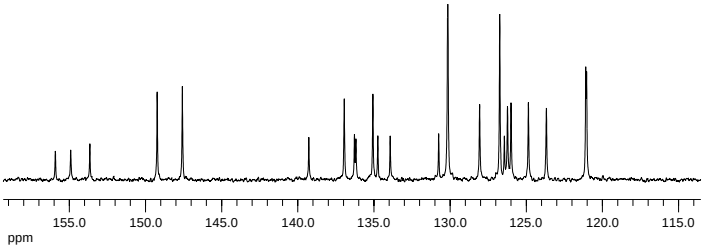
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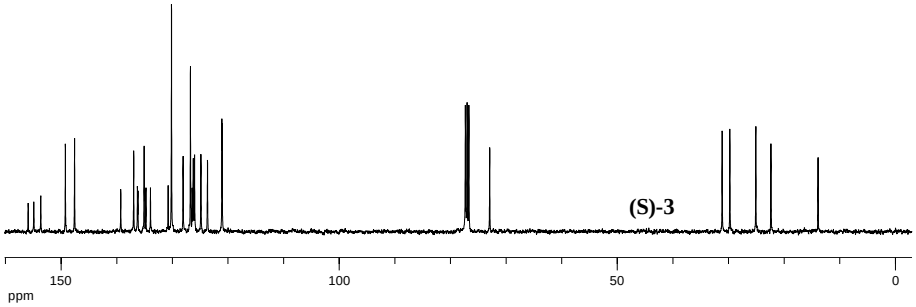
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100
50
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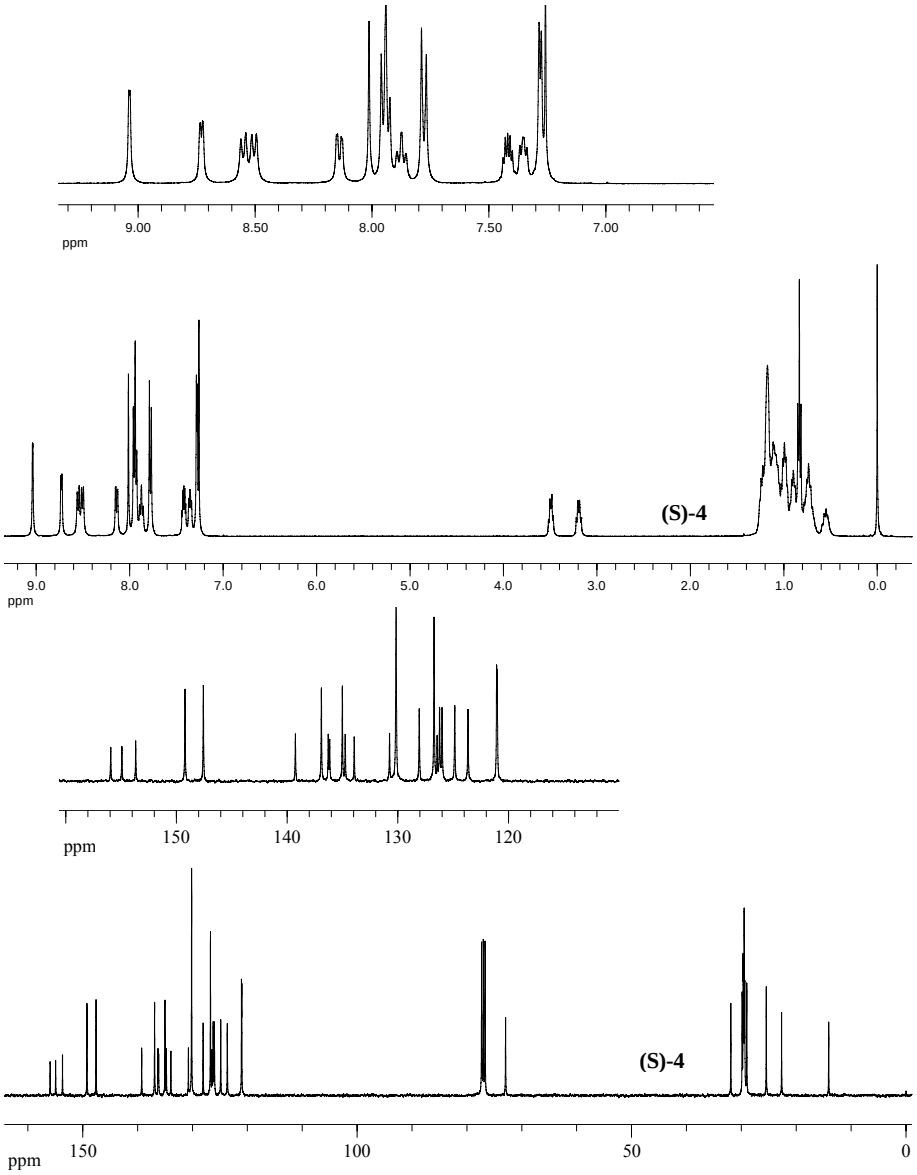
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7.00
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7.0
6.0
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4.0
3.0
2.0
1.0
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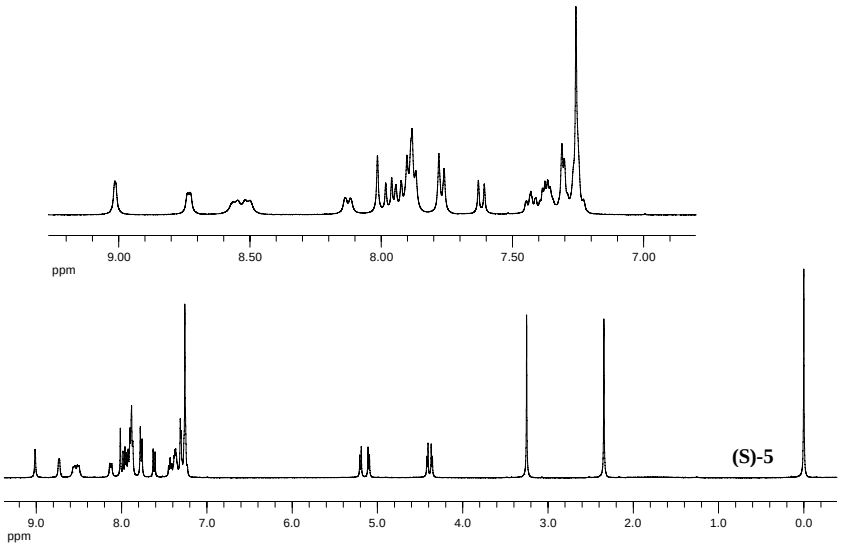
ppm
150
140
130
120
ppm
(S)-4
150
100
50
0
ppm

(*S*)-**5**: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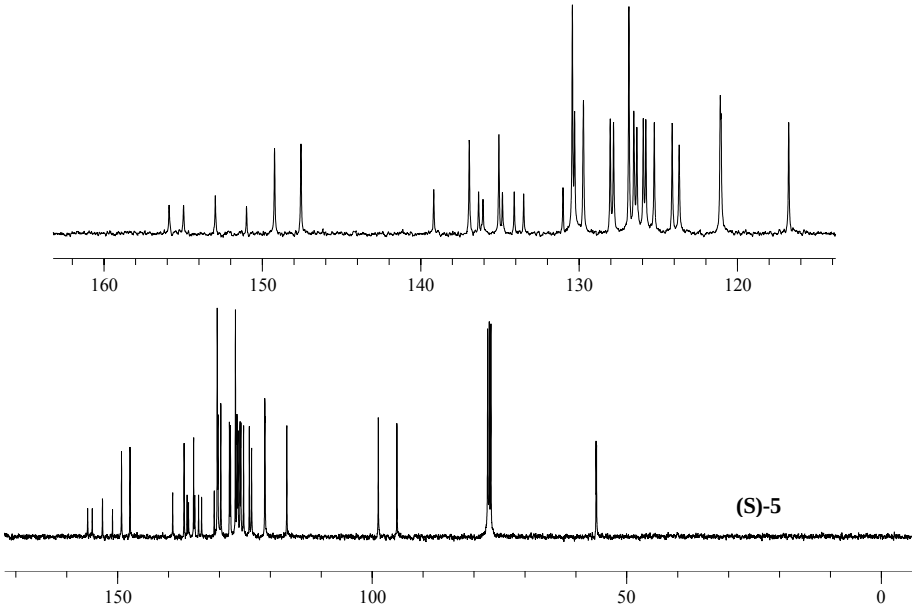
ppm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150
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50
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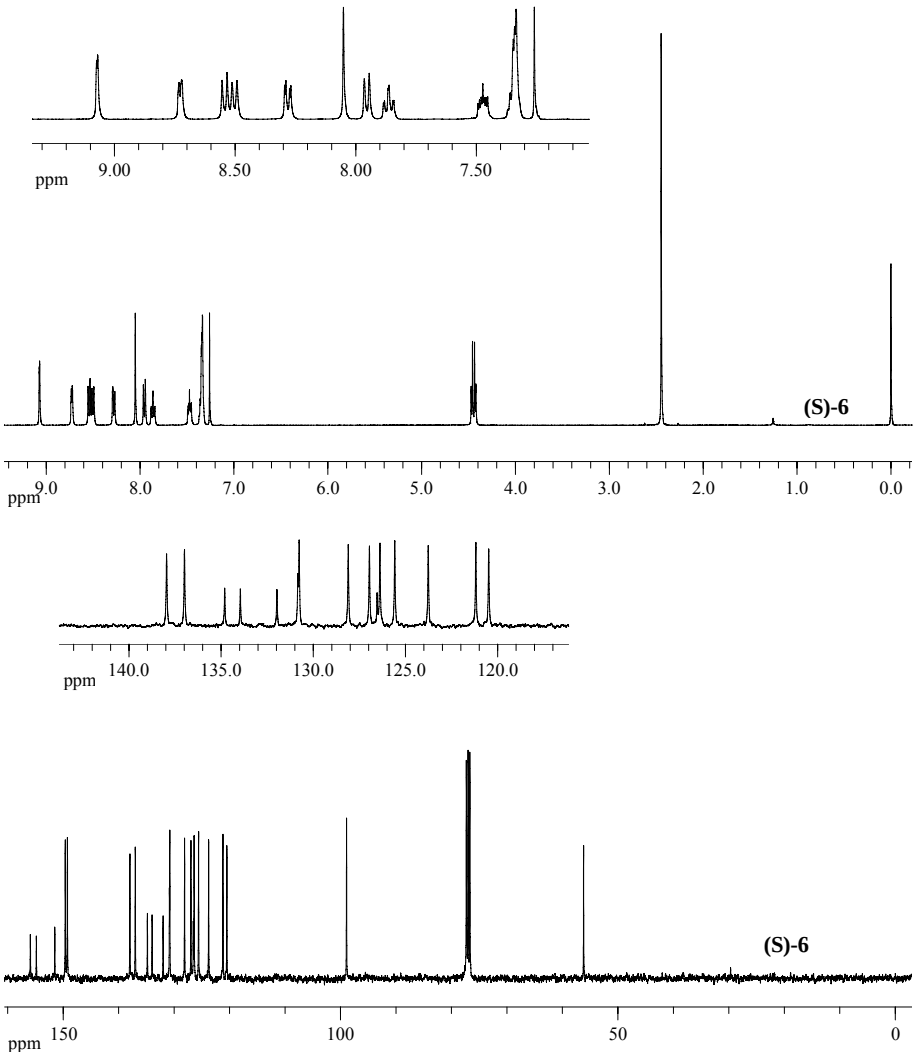
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3.0
2.0
1.0
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ppm
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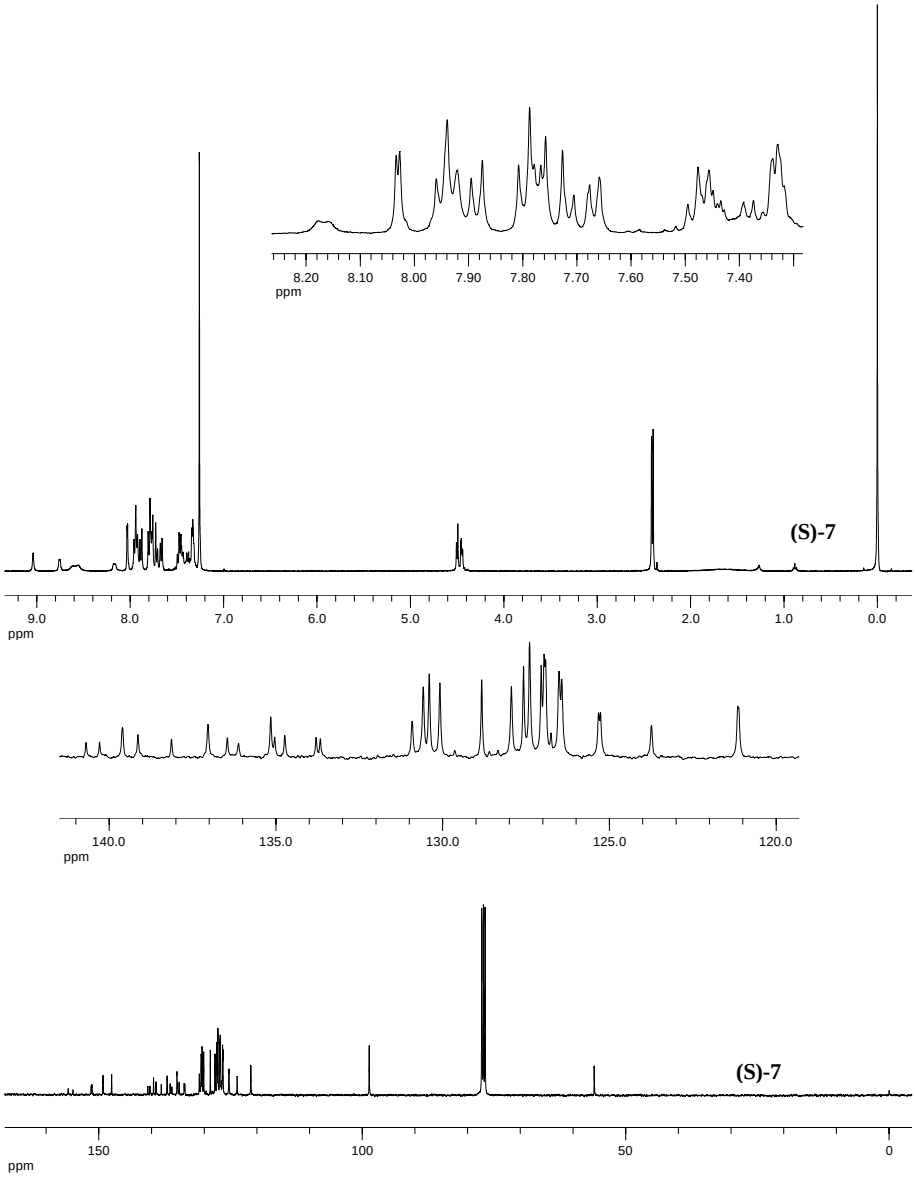
100
50
0

(*S*)-**7**: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7.40
ppm
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7.0
6.0
5.0
4.0
3.0
2.0
1.0
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ppm
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135.0
130.0
125.0
120.0
ppm
(S)-7
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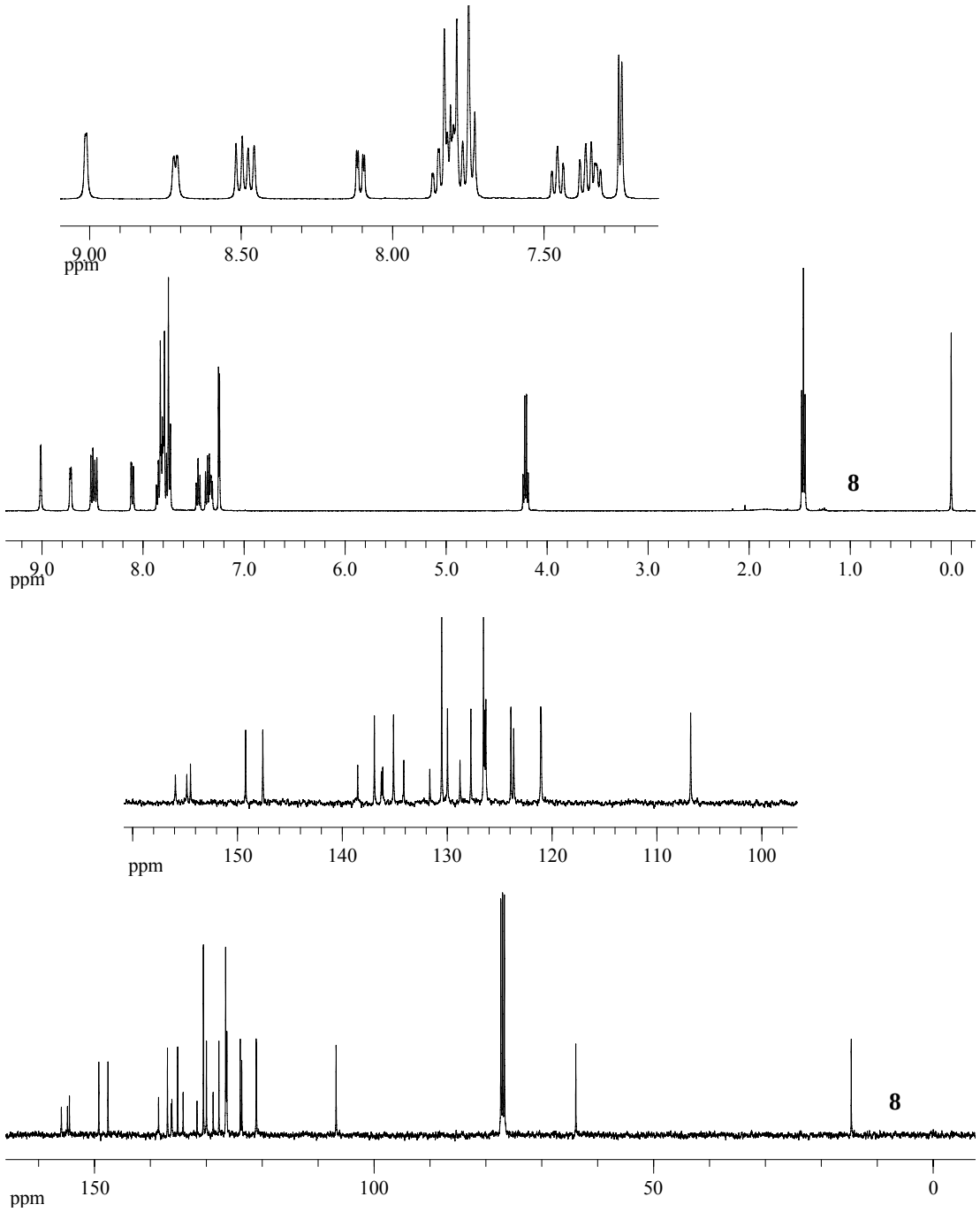
100
50
0
ppm

8: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3.0
2.0
1.0
0.0
ppm
150
140
130
120
110
100
ppm
8
150
100
50
0
ppm

11. The single crystal structures of model compound **8**, (*S*)-**2** and (*S*)-**4**

Table S3. Crystal data and structure refinement for model compound **8**, (*S*)-**2** and (*S*)-**4**

.Compound	**8**	(*S*)-**2**	(*S*)-**4**
Empirical formula	$C_{28}H_{22}N_2O$	$C_{56}H_{42}N_4O_2$	$C_{76}H_{82}N_4O_2$
Formula weight	402.48	802.94	1083.46
Temperature	187(2) K	187(2) K	187(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic	Triclinic
space group	P2(1)/n	$P2_12_12_1$	P1
Unit cell dimensions	a = 7.6624(6) Å b = 24.225 (2) Å c = 11.3419(10) Å α = 90° β = 102.6110(10)° γ = 90°	a = 13.0290(18) Å b = 19.014(3) Å c = 34.024(5) Å α = 90° β = 90° γ = 90°	a = 7.8840(5) Å b = 24.1800(15) Å c = 26.8060(16) Å α = 114.619(9)° β = 92.681(9)° γ = 96.014(10)°
Volume, Z	2054.5(3) $Å^3$, 4	8429(2) $Å^3$, 8	4596.9(5) $Å^3$, 3
Calculated density	1.426 Mg/m^3	1.265 Mg/m^3	1.174 Mg/m^3
Absorption coefficient	0.128 mm^{-1}	0.077 mm^{-1}	0.0701 mm^{-1}
F(000)	902	6752	5238
Crystal size	0.30 × 0.20 × 0.15 mm	0.30 × 0.21 × 0.12 mm	0.4 × 0.35 × 0.28 mm
θ range for data collection	1.68 to 26.03°	1.61 to 25.04°	1.50 to 26.03°
Limiting indices	-9≤h≤8 -29≤k≤28 -10≤l≤14	-15≤h≤14 -21≤k≤22 -40≤l≤29	-8≤h≤9 -29≤k≤28 -33≤l≤30
Reflections collected / unique	11505 / 4031 [R_{int} = 0.0358]	43434 / 8100 [R_{int} = 0.0888]	26057/ 17732 [R_{int} = 0.0336]
Completeness to theta	26.03, 99.4 %	25.00, 99.1 %	25.00, 98.6 %
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Data / restraints / parameters	4031 / 0 / 281	8100 / 6 / 1104	17732 / 4 /2195
Goodness-of-fit on F^2	1.029	1.024	0.955
Final R indices, I>2sigma(I)	R_1 = 0.0487; wR_2 = 0.0995	R_1 = 0.0866; wR_2 = 0.2166	R_1 = 0.0577, wR_2 = 0.1290
R indices (all data)	R_1 = 0.0749; wR_2 = 0.1111	R_1 = 0.1441; wR_2 = 0.2625	R_1 = 0.0914, wR_2 = 0.1474
Largest diff. peak and hole	0.190 and -0.157 $e.Å^{-3}$	1.063 and -0.522 $e.Å^{-3}$	0.431/-0.306 $e.Å^{-3}$
CCDC	664579	709732	709733

It should be pointed out that the X-ray analyses for (*S*)-**2** and (*S*)-**4** only show the relative, not absolute stereochemistry. CCDC-664579, 709732-709733 contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.