Supporting Information

Chiral Spherical Molecule Constructed from Aromatic Amides: Facile Synthesis and Highly Ordered Network Structure in the Crystal

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Details of chiral separation

The chiral separation of **1** was carried out by chiral HPLC. HPLC was performed on a Waters delta-600 systems with column, SUMICHIRAL OA-4800. Other details are described on Figure S1.

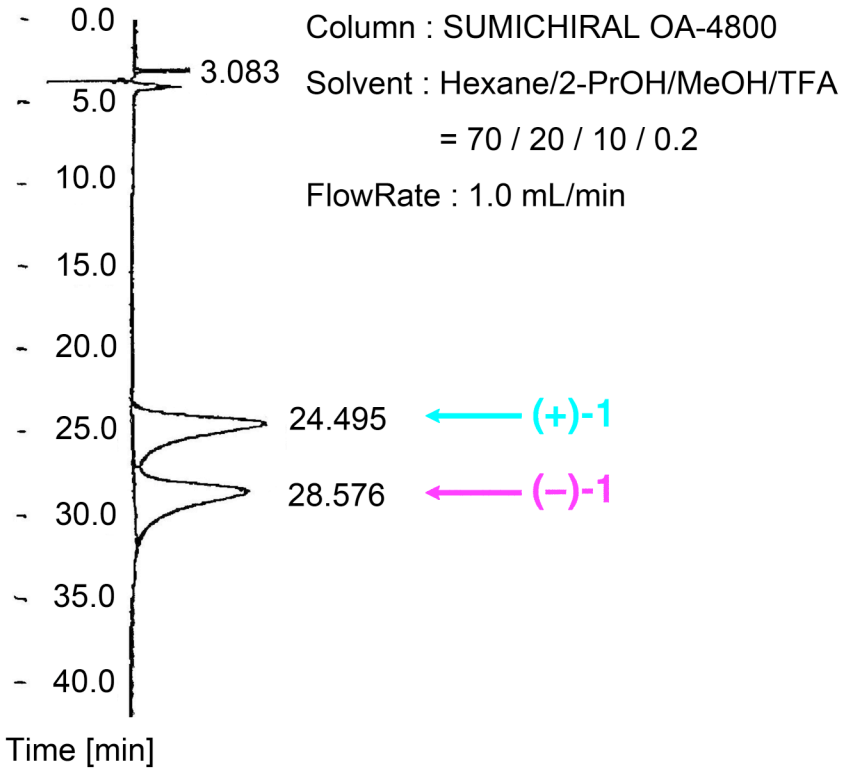


Figure S1. Chart of chiral HPLC for chiral separation of compound **1**.

X-ray crystallographic analysis and ORTEP diagrams

General. The X-ray crystallographic analyses were under taken using CCD diffractometer with graphite monocromated MoKα (λ = 0.71073 Å). The crystal structures were solved by using SHELXS 97 (Sheldrick, 1997). Refinements were carried out by full-matrix least squares (on F^2) with anisotropic temperature factors for non-H atoms. In all of the structures H atoms were included as their calculated positions. For refinement of the structure and structure analysis, the program package SHELXTL was used.

Crystal of racemic 1. Three oxygen atoms of water molecules (O7, O8 and O9) have 0.5 of occupancy respectively (Figure S2). The positions of hydrogen atoms included in the water molecules were not calculated. The Friedel pairs were averaged in refinement.

Crystal of enantio-pure (+)-1: Two spherical molecules and three water molecules (O13, O14 and O15) exist independently in an asymmetric unit (Figure S3). The positions of hydrogen atoms included in the water molecules were not calculated. The Flack parameter for estimation of the absolute structure is indeterminate. The Friedel pairs were averaged in refinement.

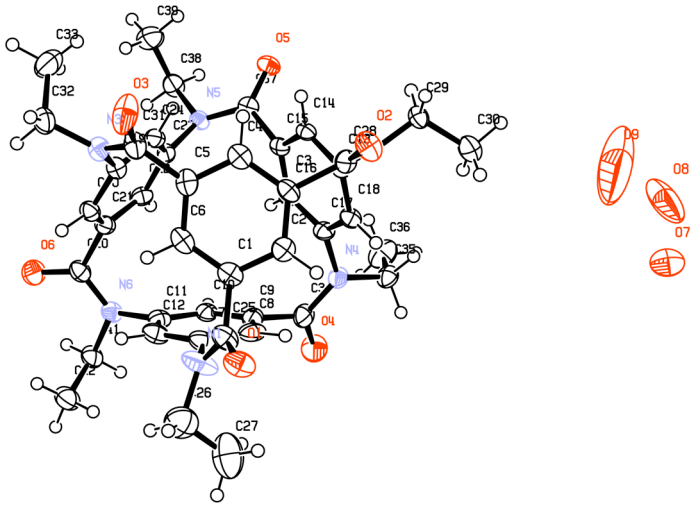


Figure S2. ORTEP diagram of asymmetric unit in a crystal of racemic **1**. The ellipsoids of non–hydrogen atoms are drawn at the 50% probability level.

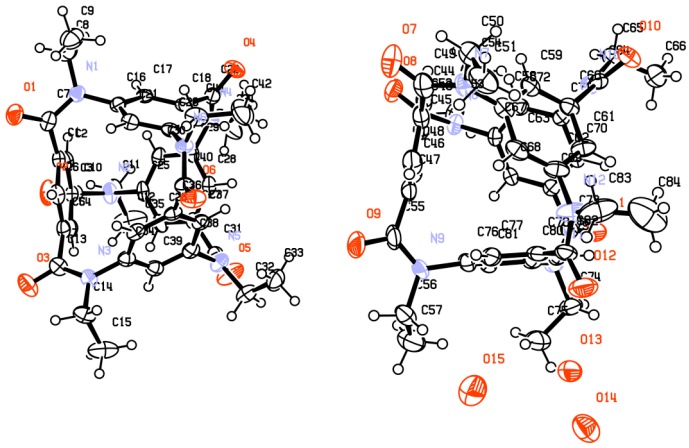


Figure S3. ORTEP diagram of asymmetric unit in a crystal of enantio-pure (+)-**1**. The ellipsoids of non–hydrogen atoms are drawn at the 50% probability level.

Details of intermolecular CH/O and CH/π interactions

In the crystal of racemic **1**, eight molecules are joined to one molecule by multiple CH/O interactions (Figure S4). In contrast, six molecules are joined to one molecule by multiple CH/O and CH/π interactions in the crystal of enatio-pure (+)-**1** (Figure S5).

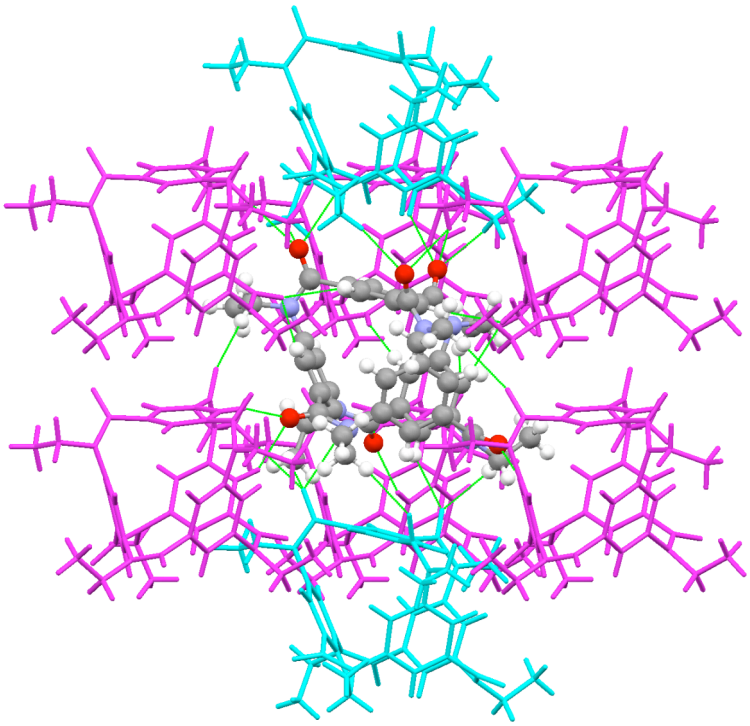


Figure S4. Intermolecular interactions around one molecule in the crystal of racemic **1**. Green lines show CH/O interactions. Magenta- and cyan-colored molecules are enantiomers of each other.

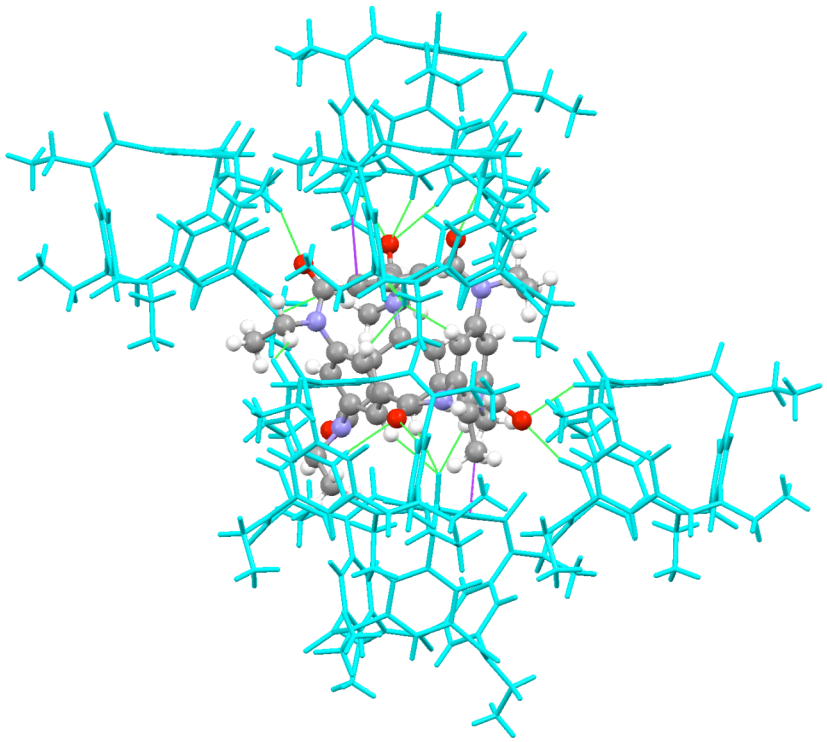
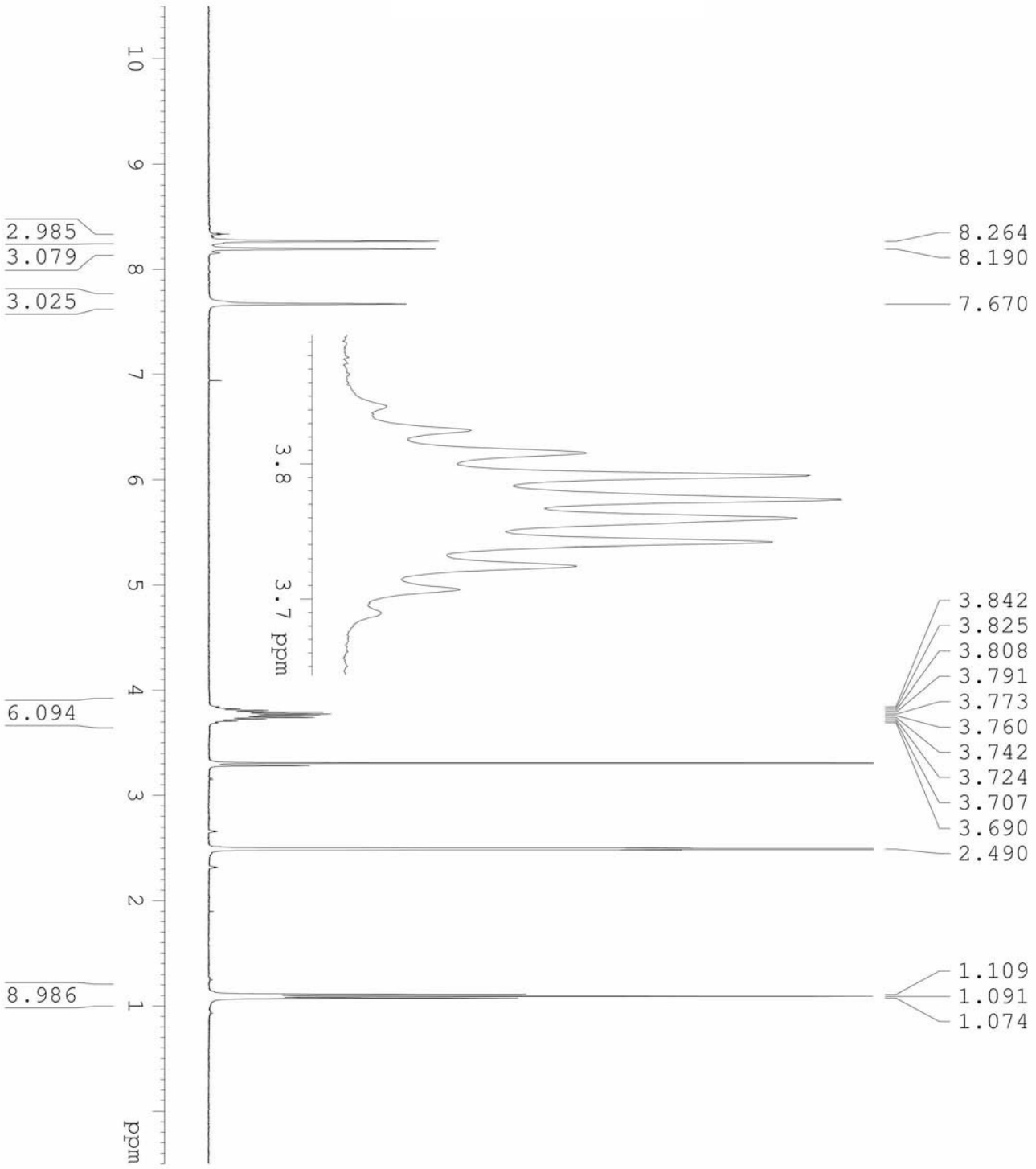
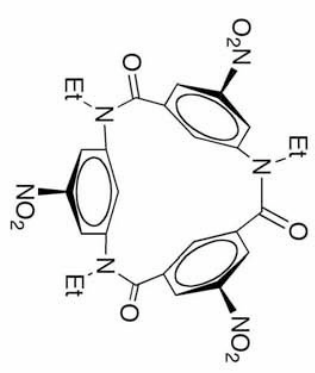


Figure S5. Intermolecular interactions around one molecule in the crystal of enantio-pure (+)-**1**. Green lines and purple lines show CH/O and CH/π interactions respectively.

^{1}H NMR Spectra of Compounds





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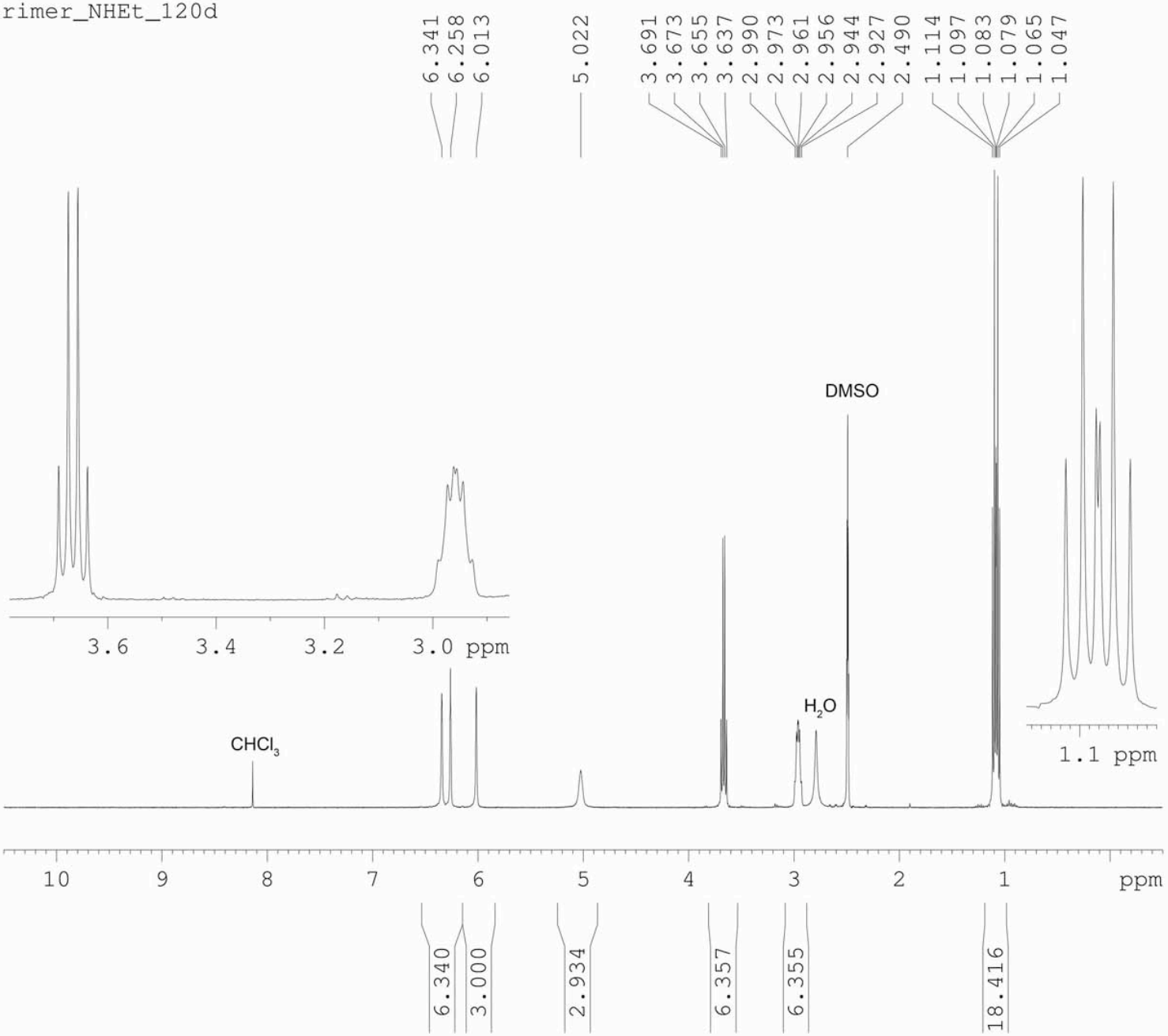


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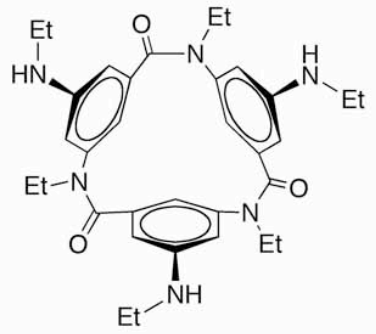

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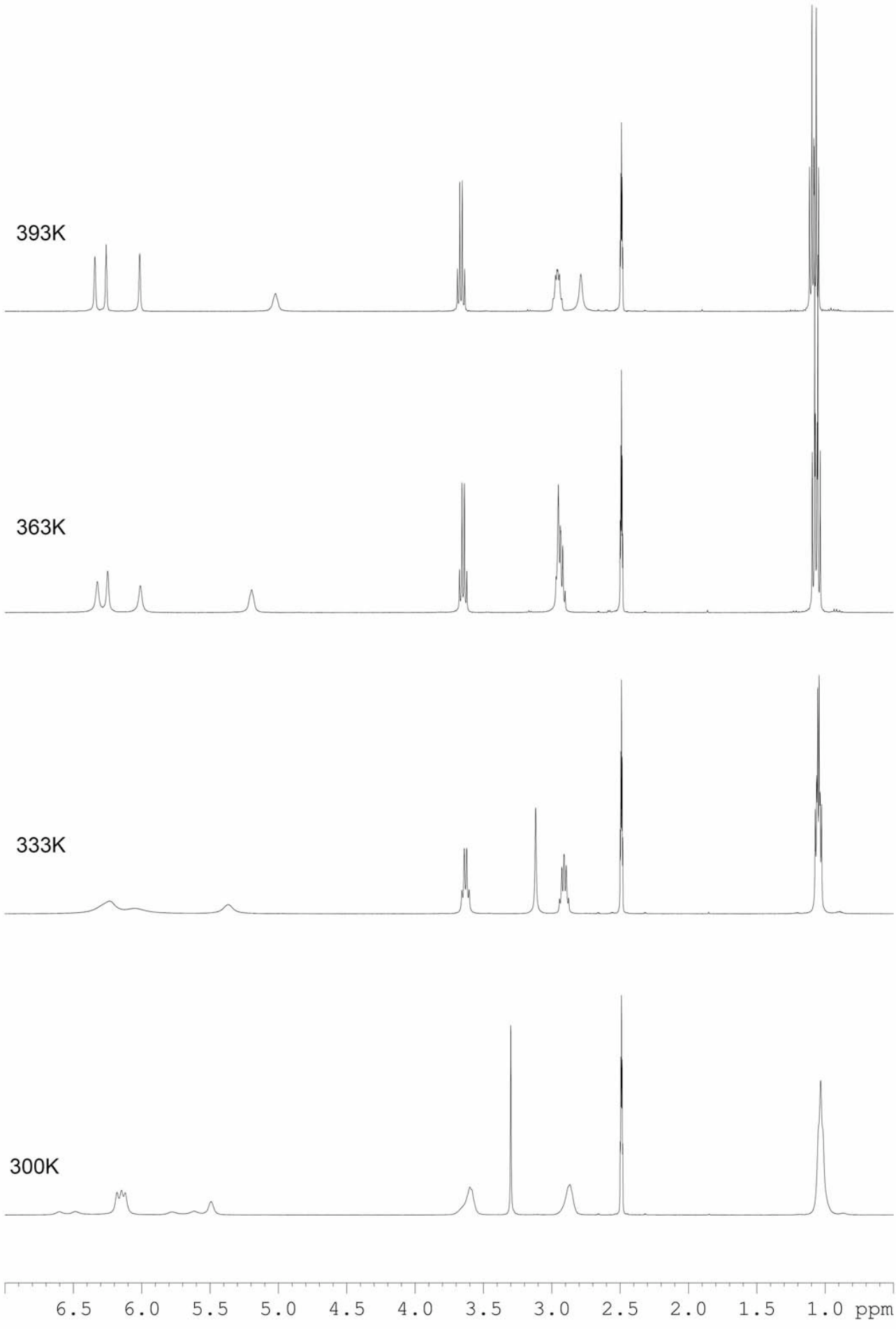
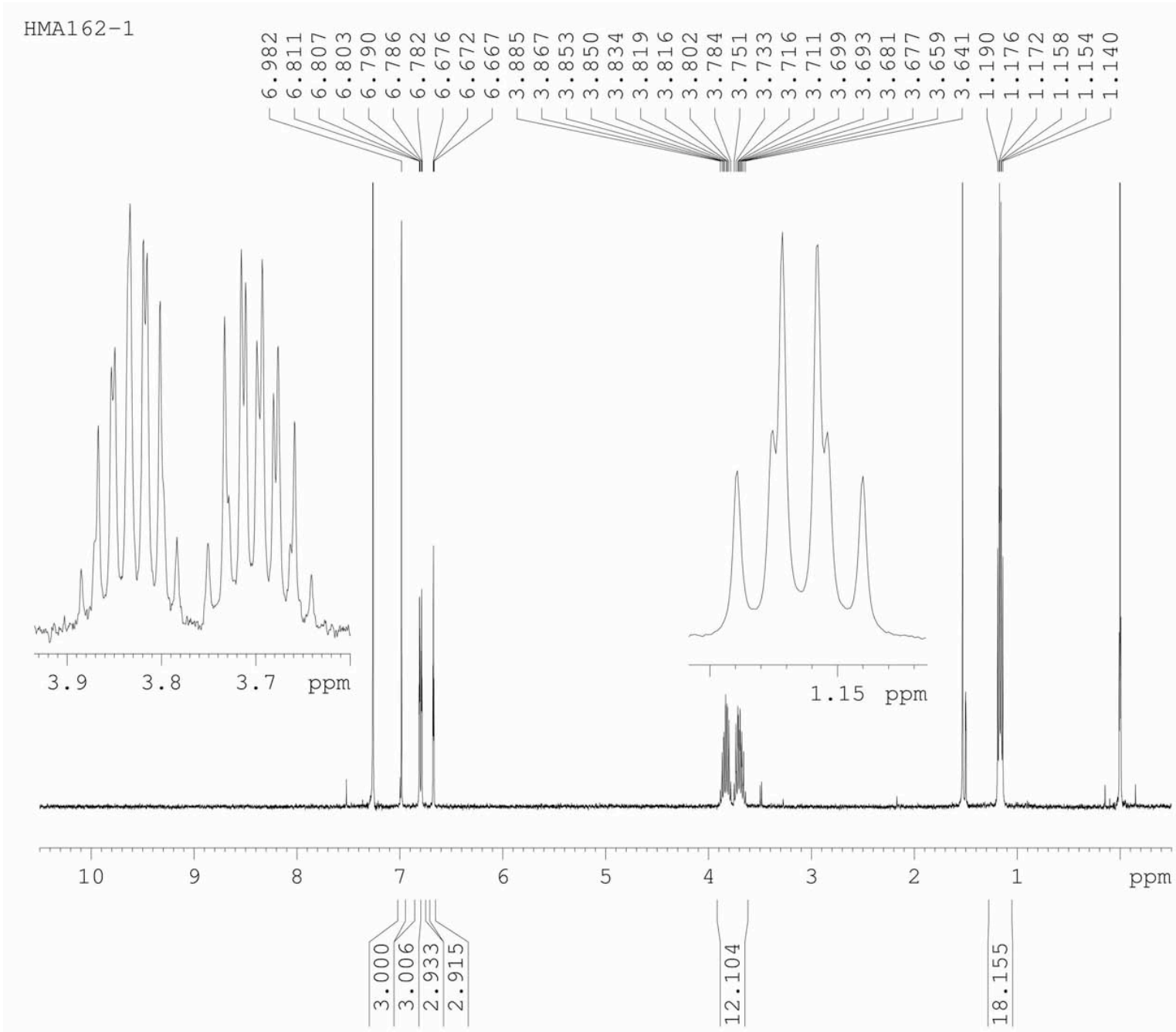
VT-NMR for compound **4** in DMSO.



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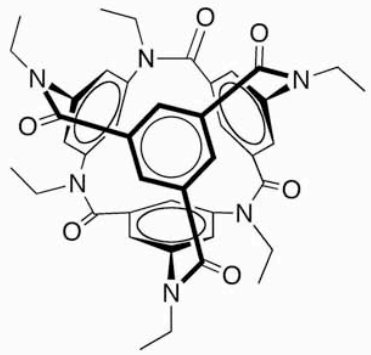
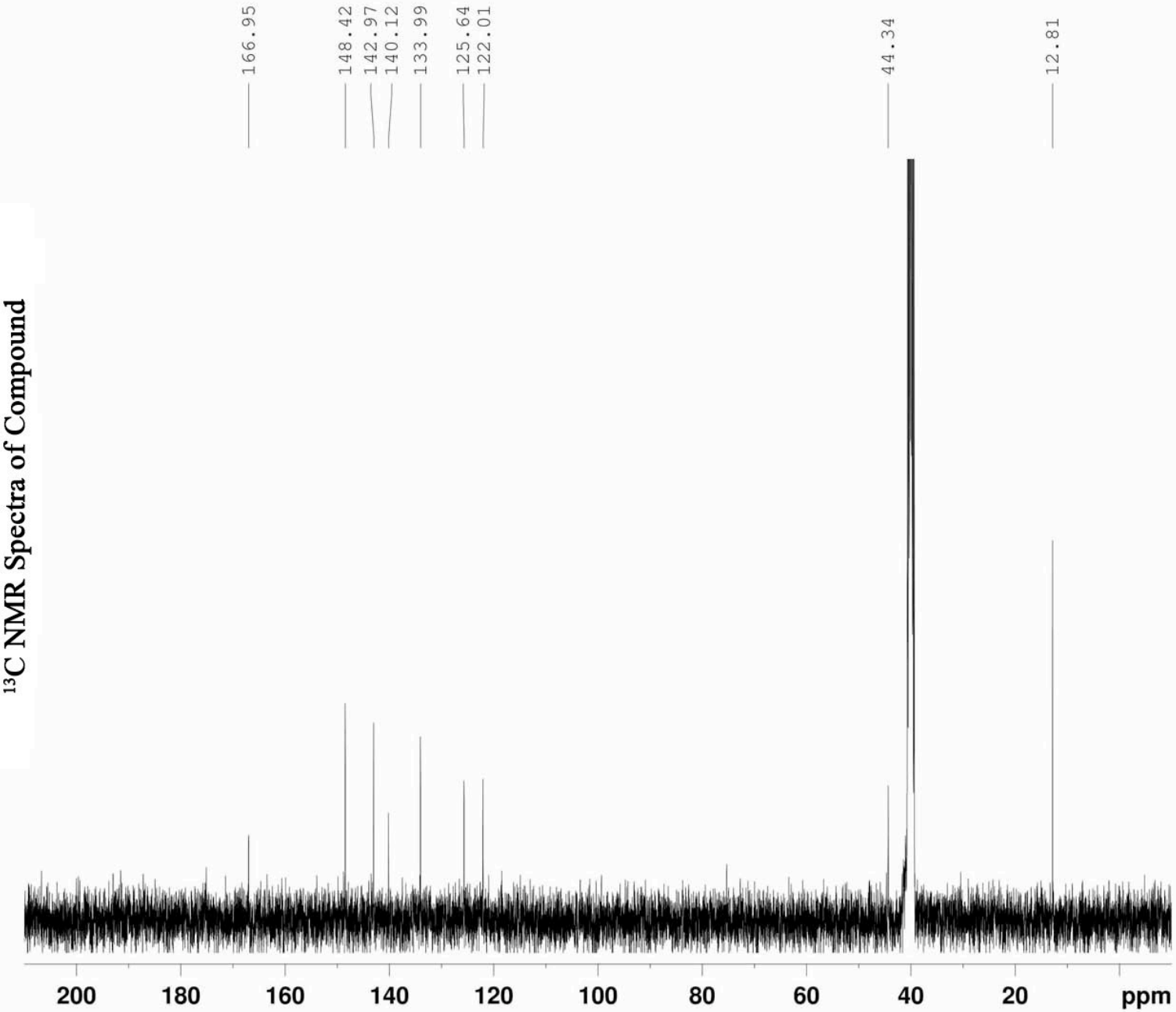


1 (racemic)

^{13}C NMR Spectra of Compound

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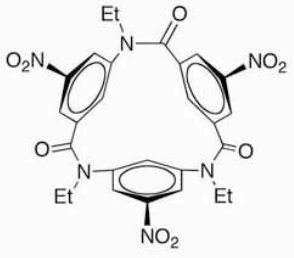

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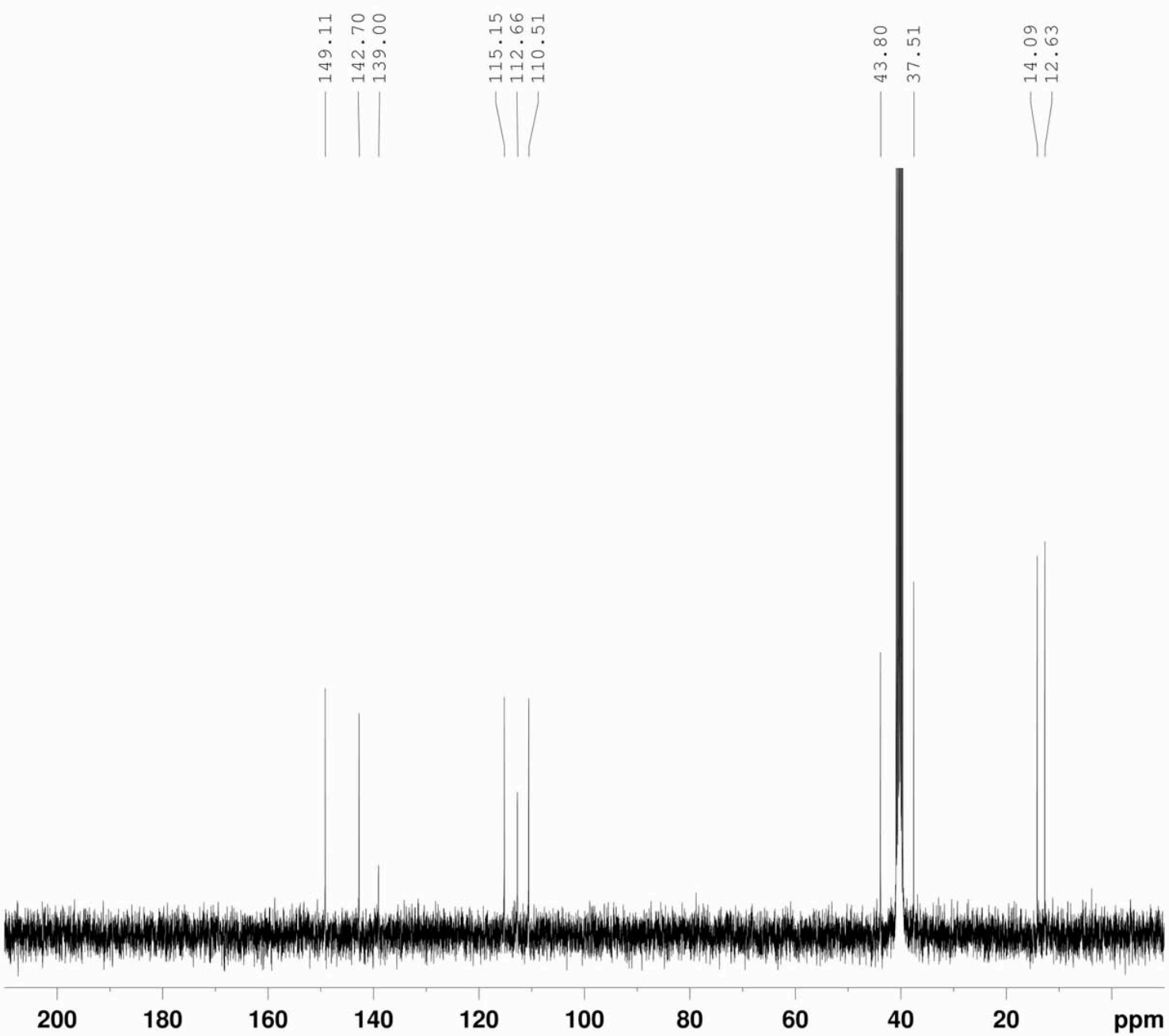


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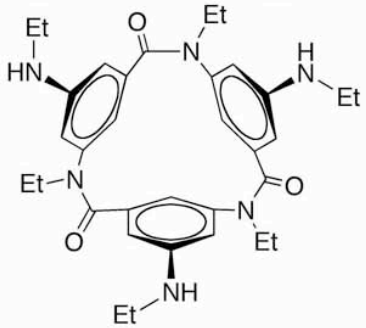

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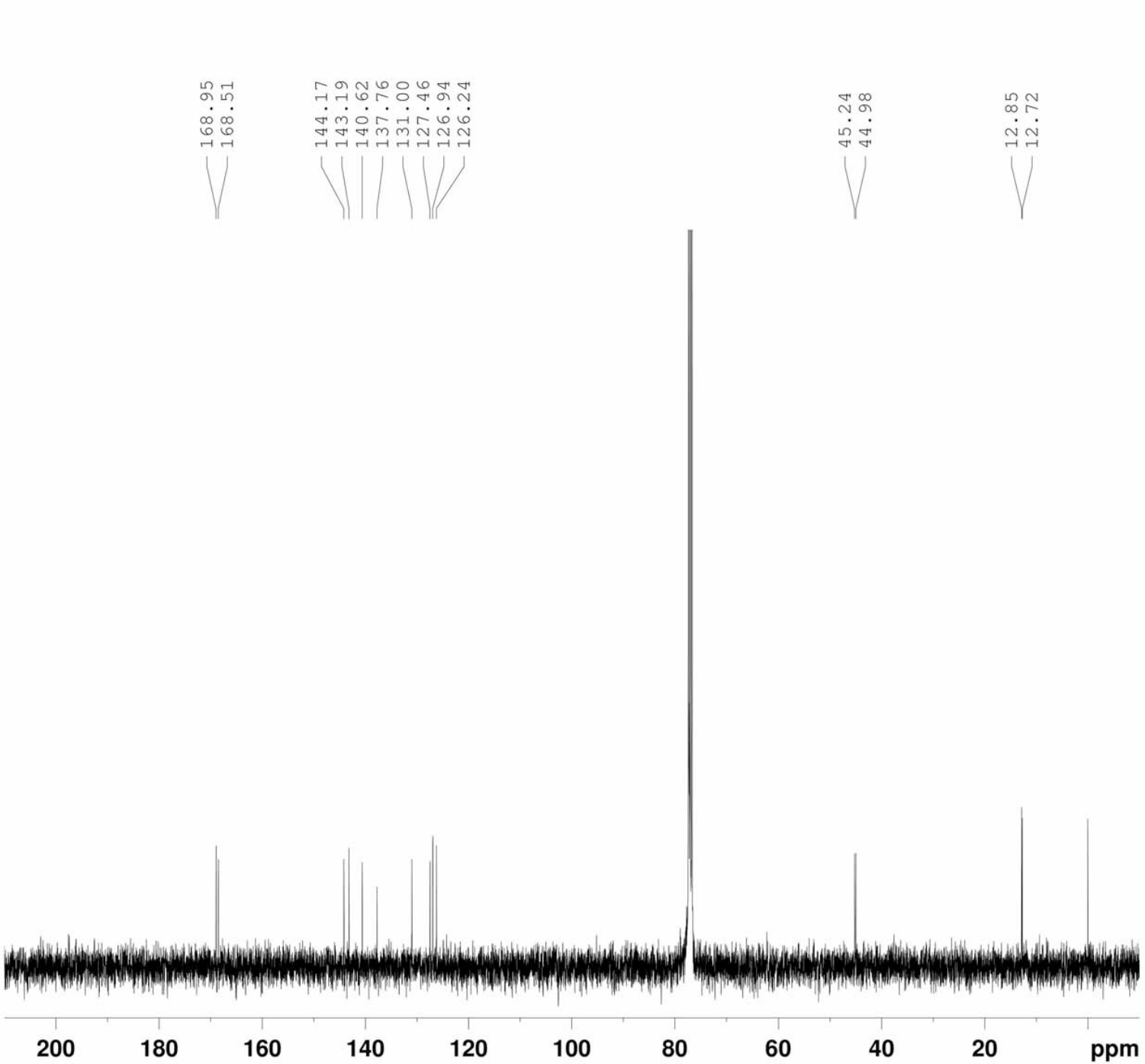


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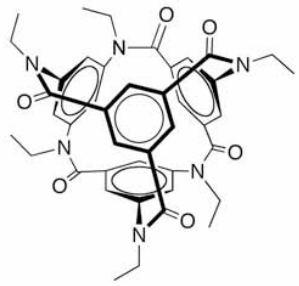
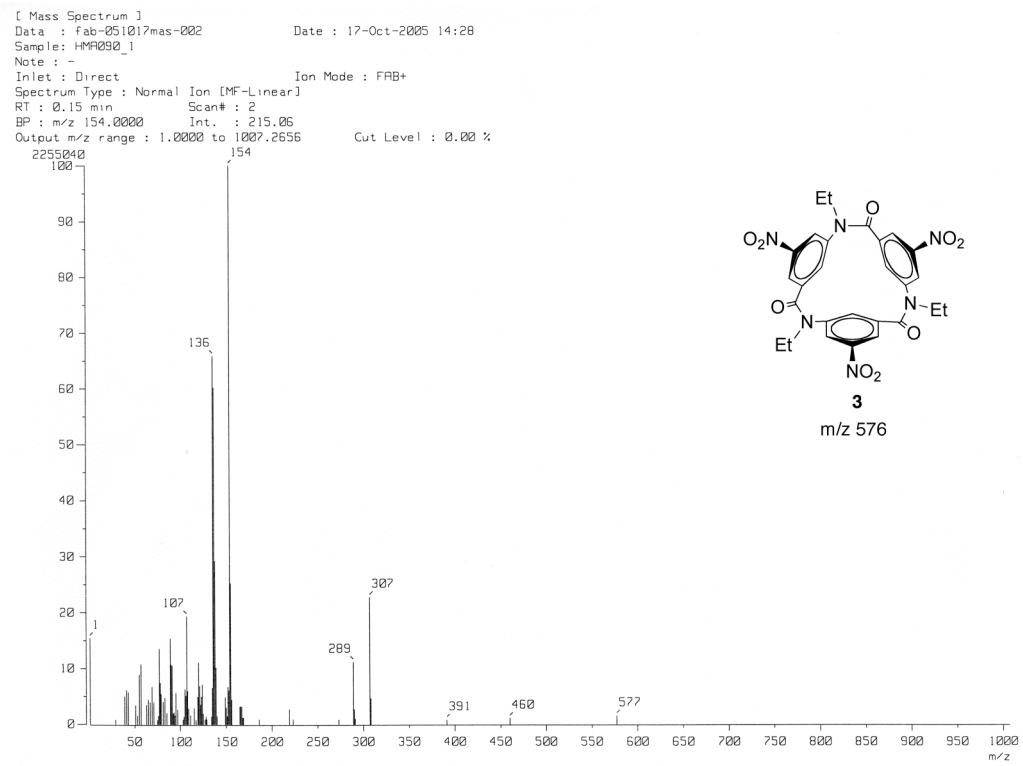


1 (racemic)

Mass Spectra of Compounds



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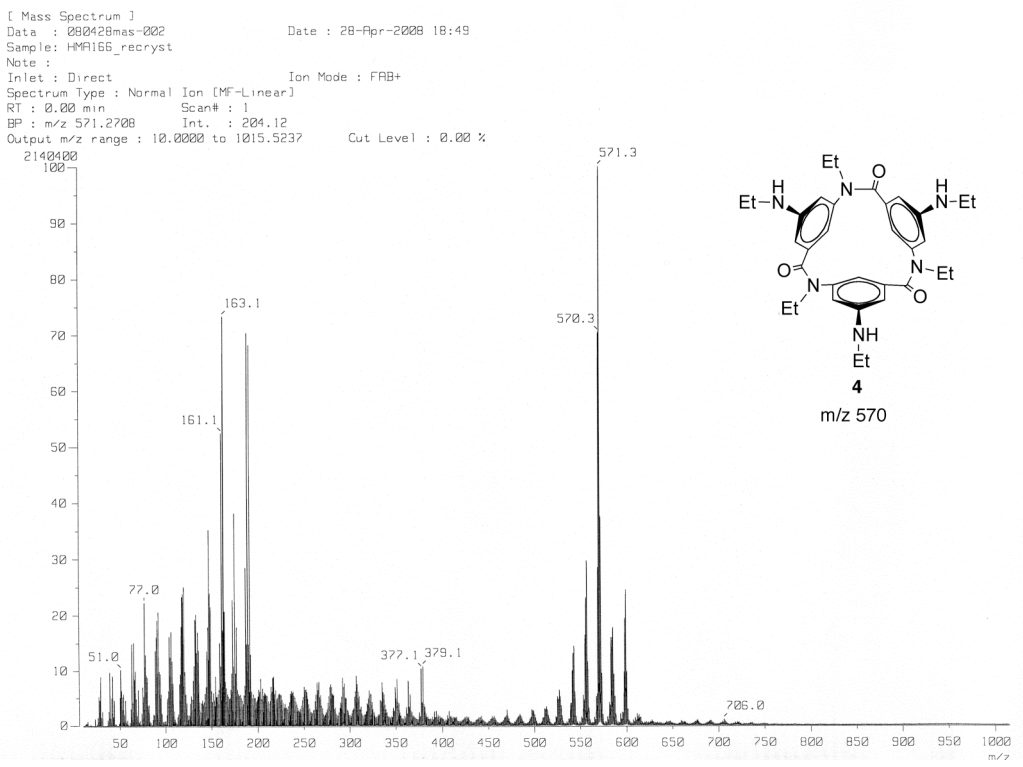

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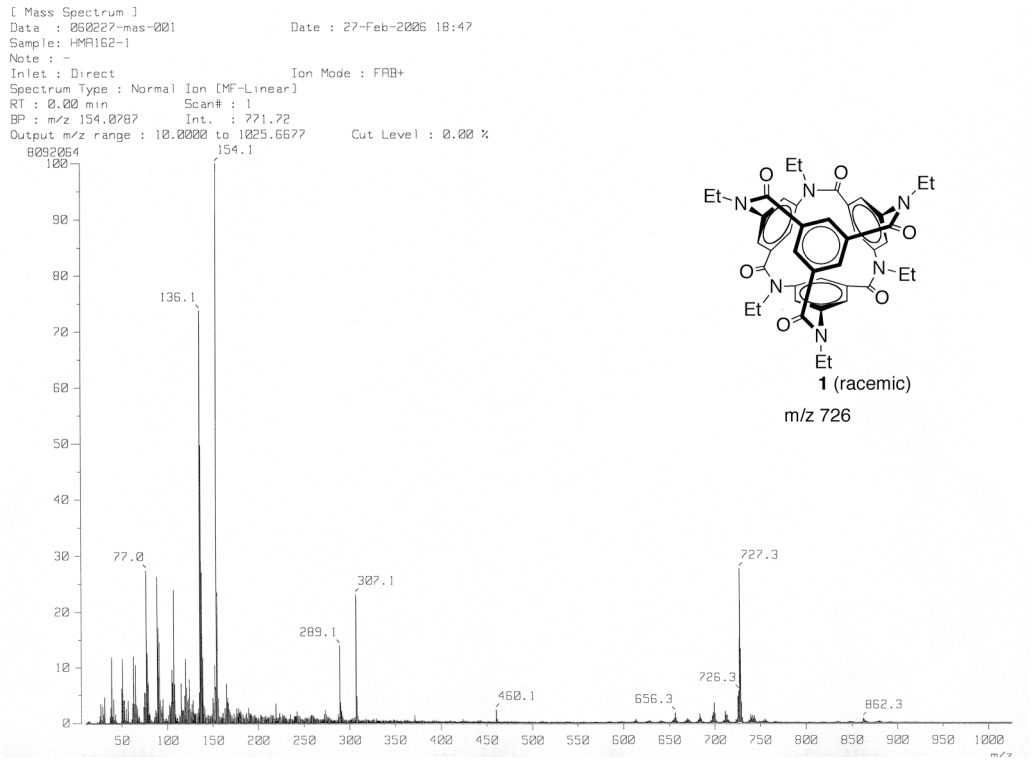
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m/z
1 (racemic)
m/z 726