

Supporting Information

Synthesis, Alkali Cation Binding and Computational Analysis of Adamantane-substituted Hexaaza Crown Ethers

Tatjana Šumanovac, Mihaela Jakić, Kata Mlinarić-Majerski* and Marina Šekutor*

Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička
cesta 54, 10 000 Zagreb, Croatia

Email: majerski@irb.hr, msekutor@irb.hr

* Corresponding authors

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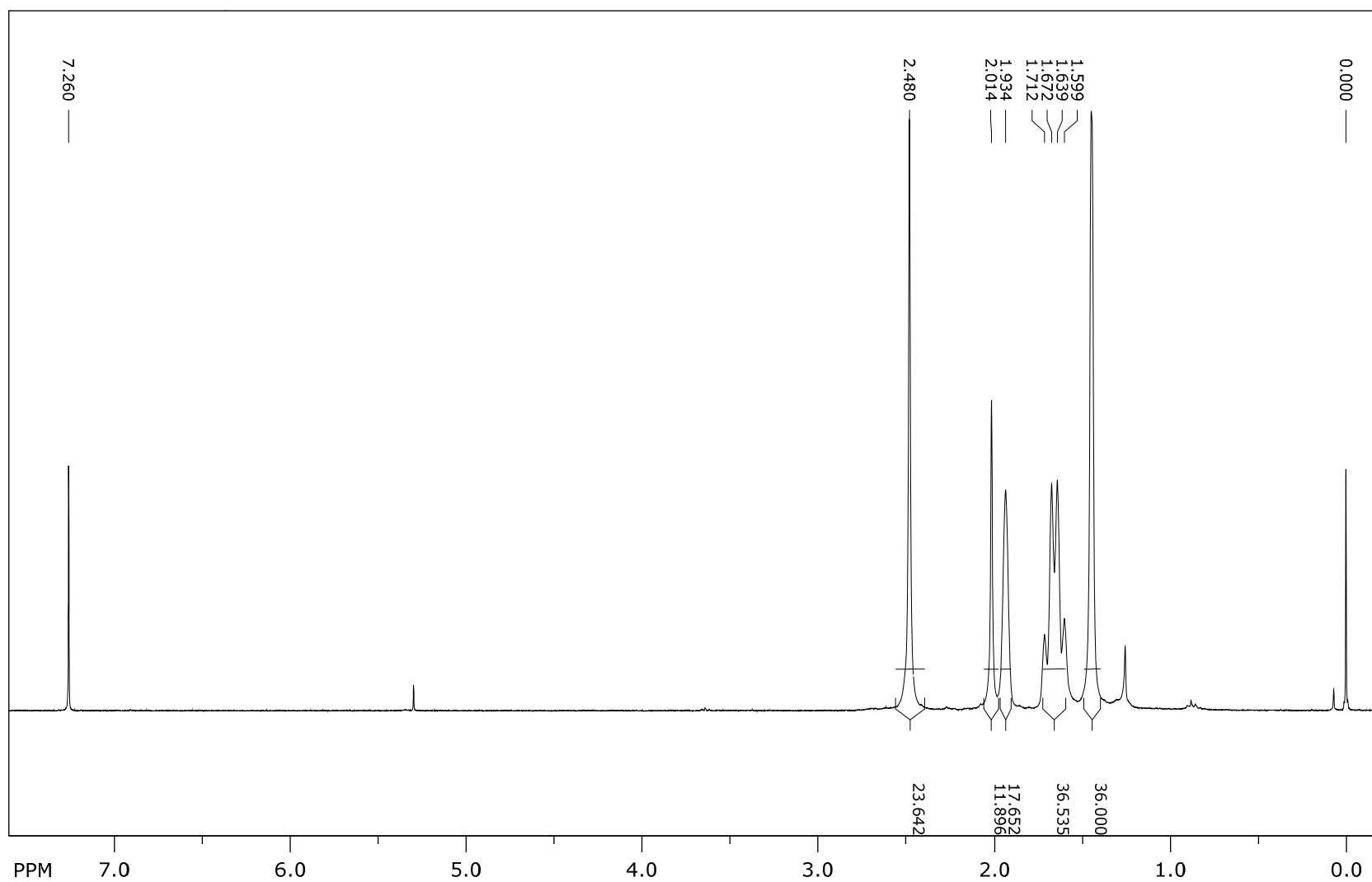


Figure S1. ¹H NMR (300 MHz, CDCl₃) spectrum of compound **1**.

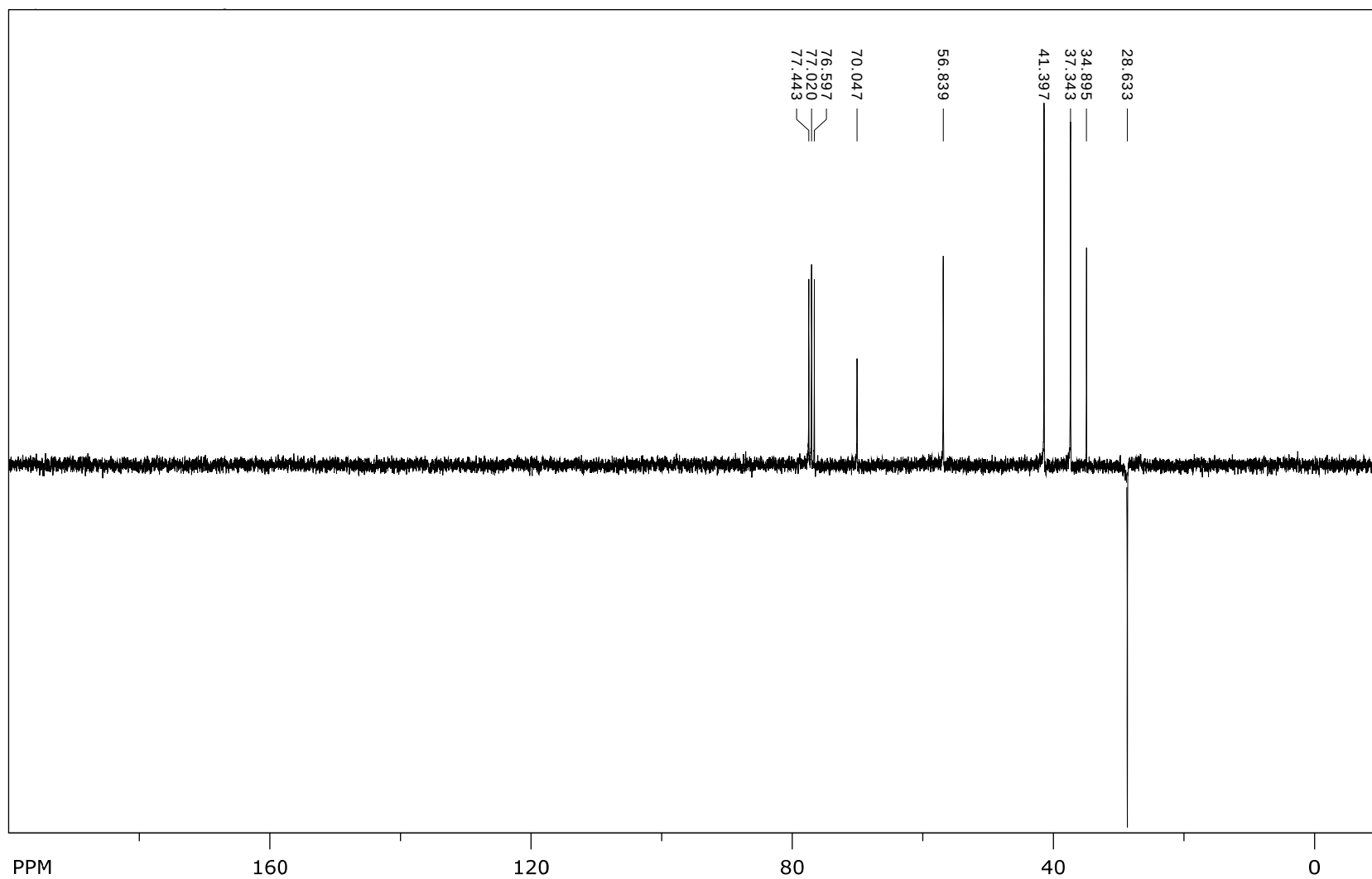


Figure S2. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound **1**.

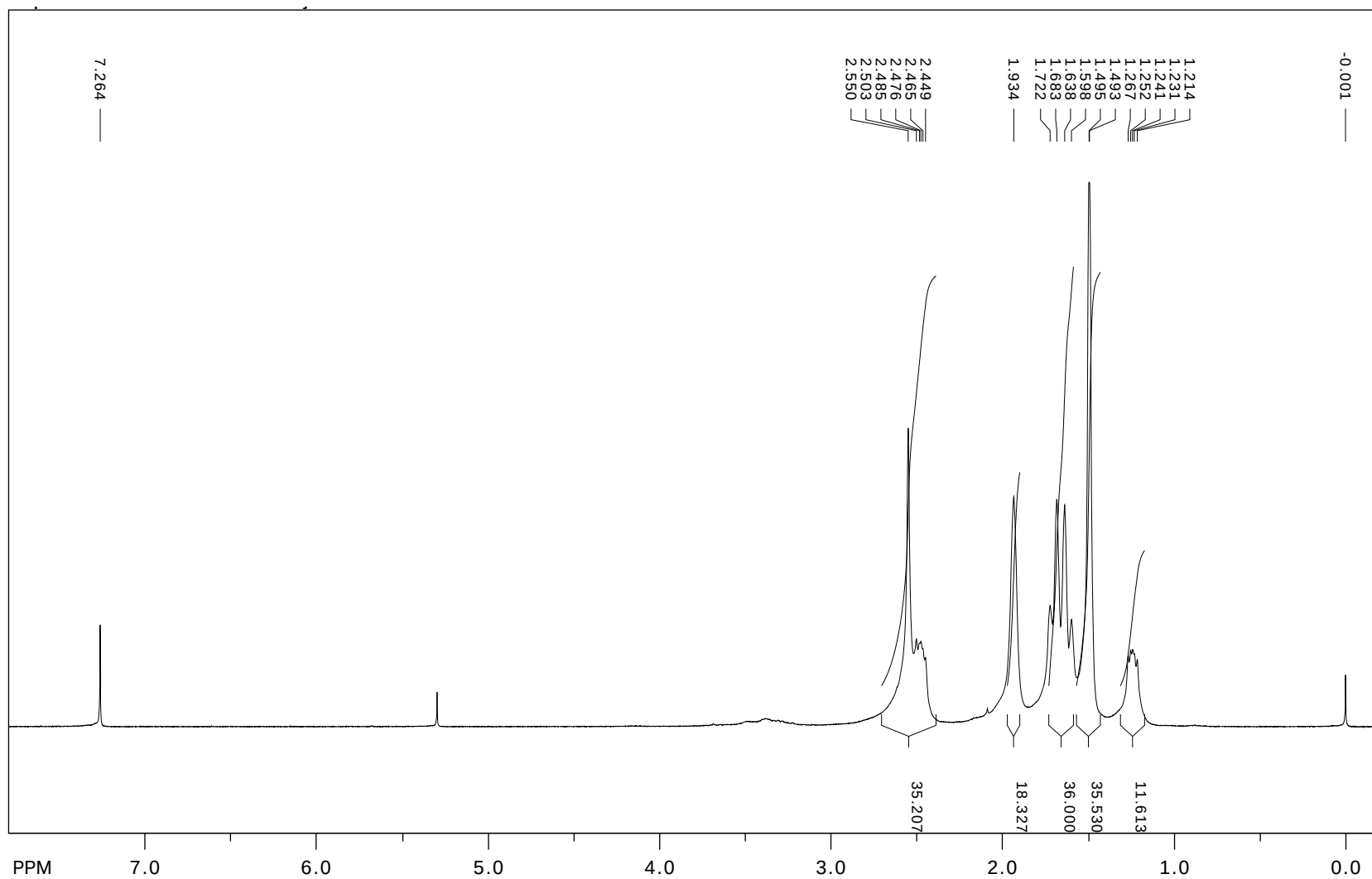


Figure S3. ¹H NMR (300 MHz, CDCl₃) spectrum of compound **2**.

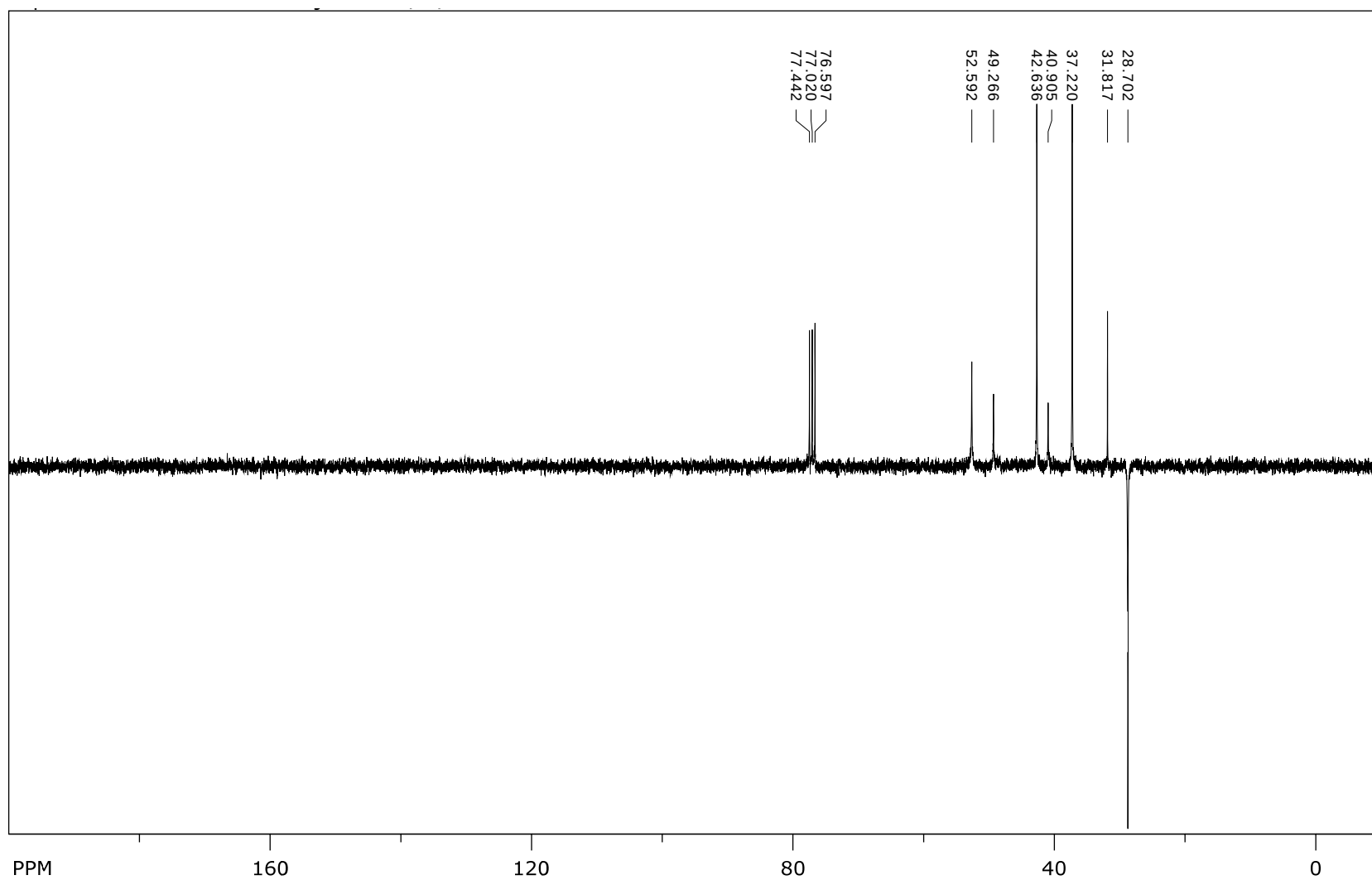


Figure S4. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound **2**.

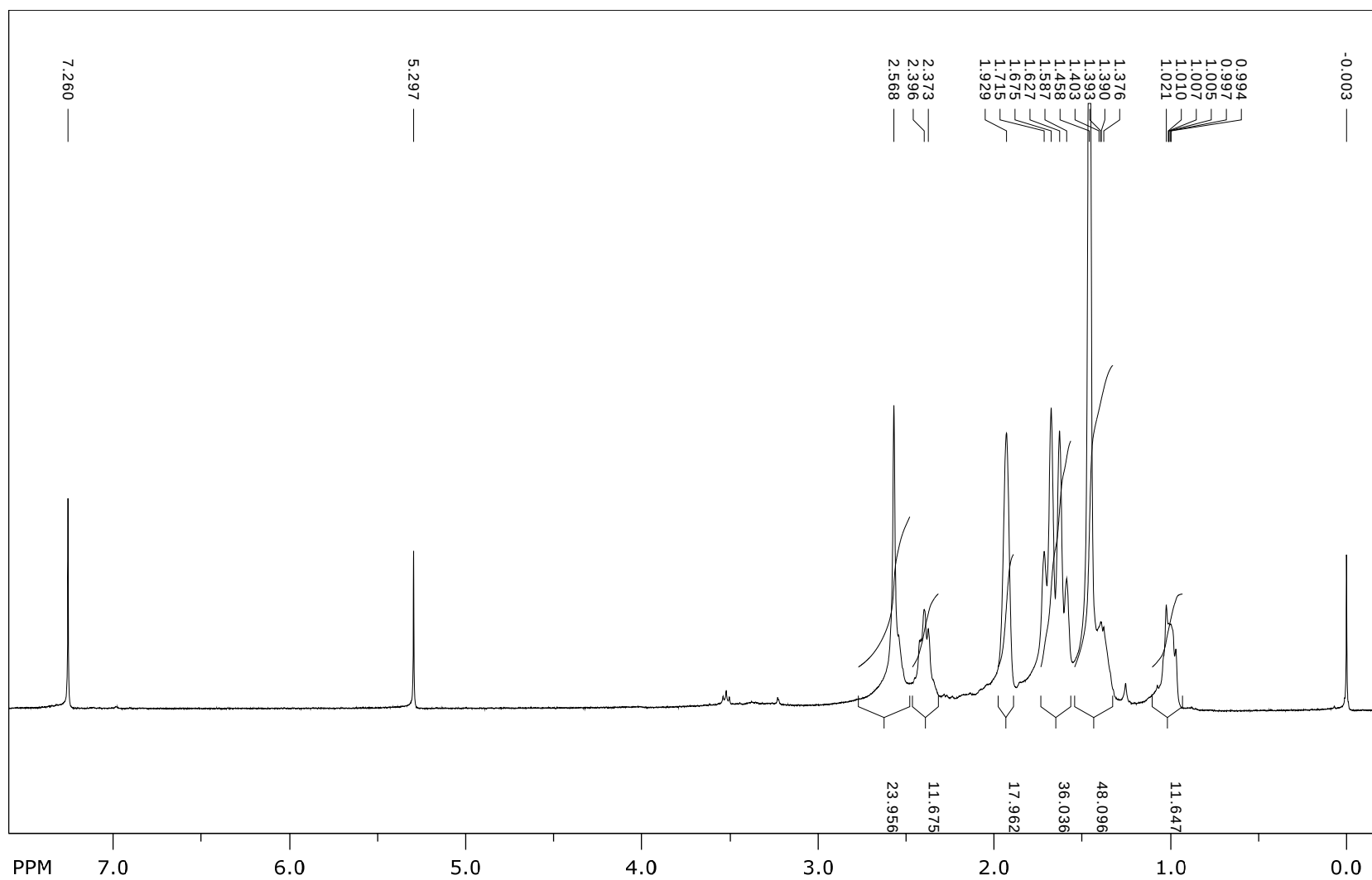


Figure S5. ^1H NMR (300 MHz, CDCl_3) spectrum of compound **3**.

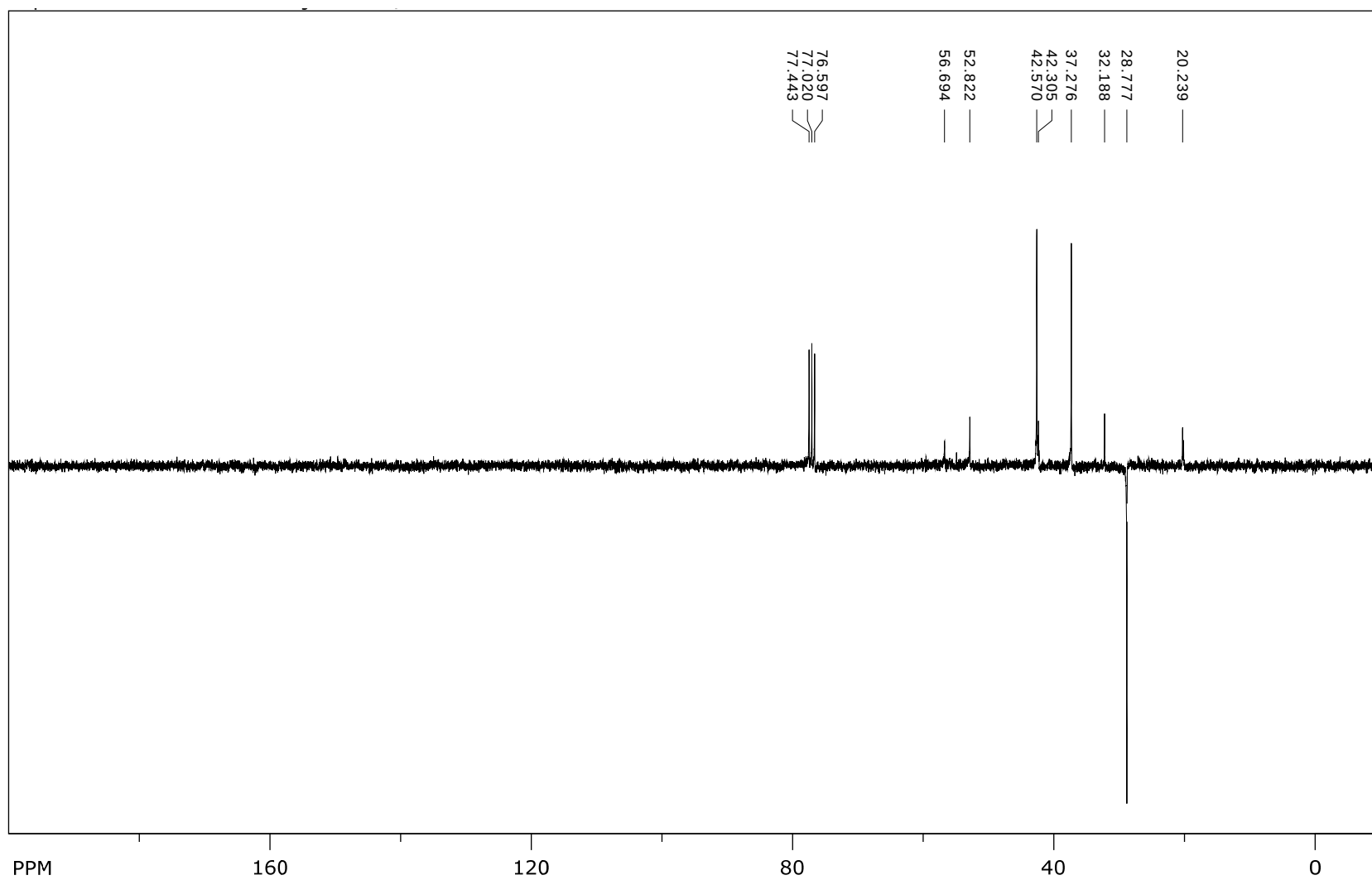


Figure S6. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound **3**.

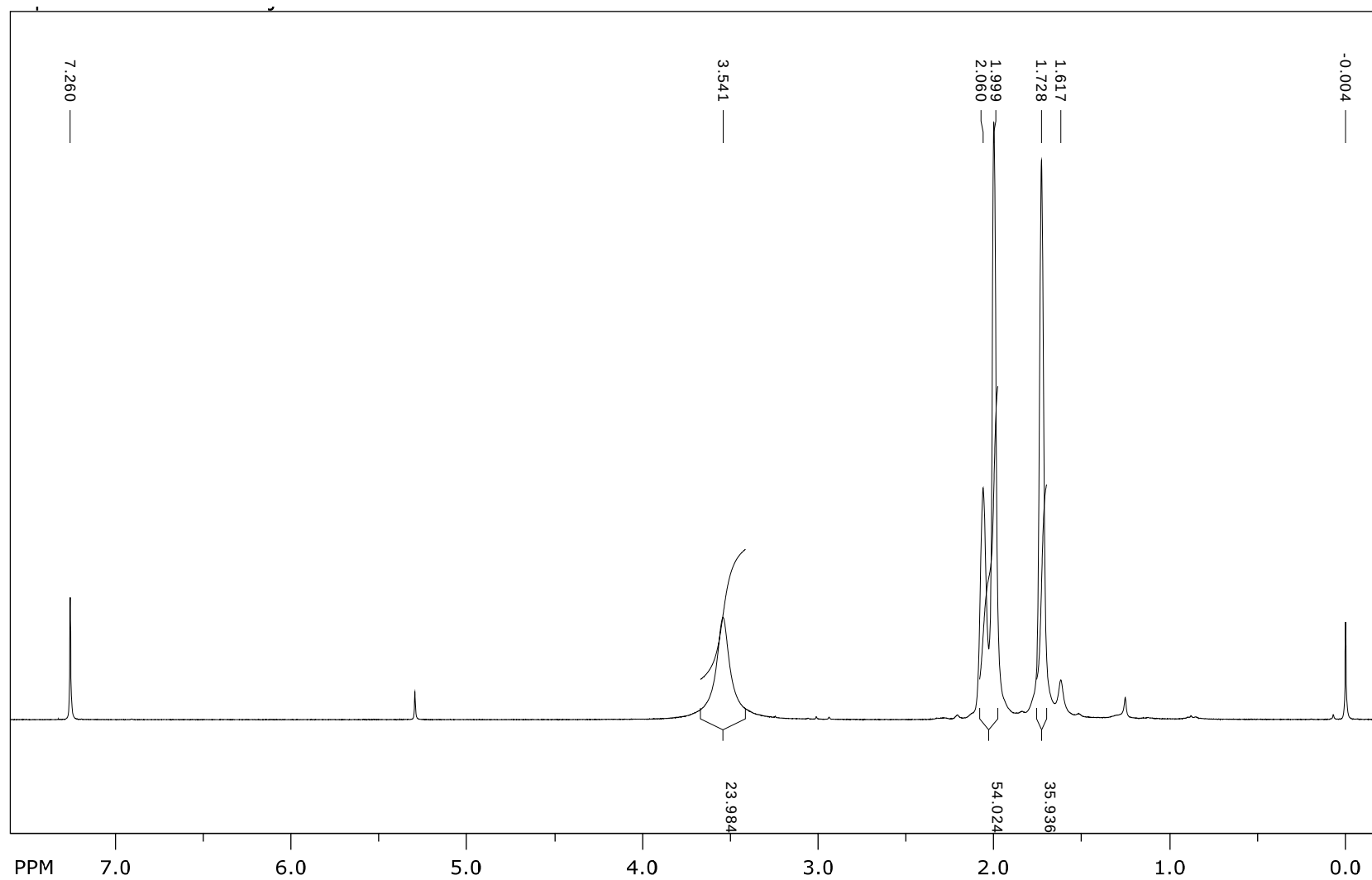


Figure S7. ¹H NMR (300 MHz, CDCl₃) spectrum of compound 4.

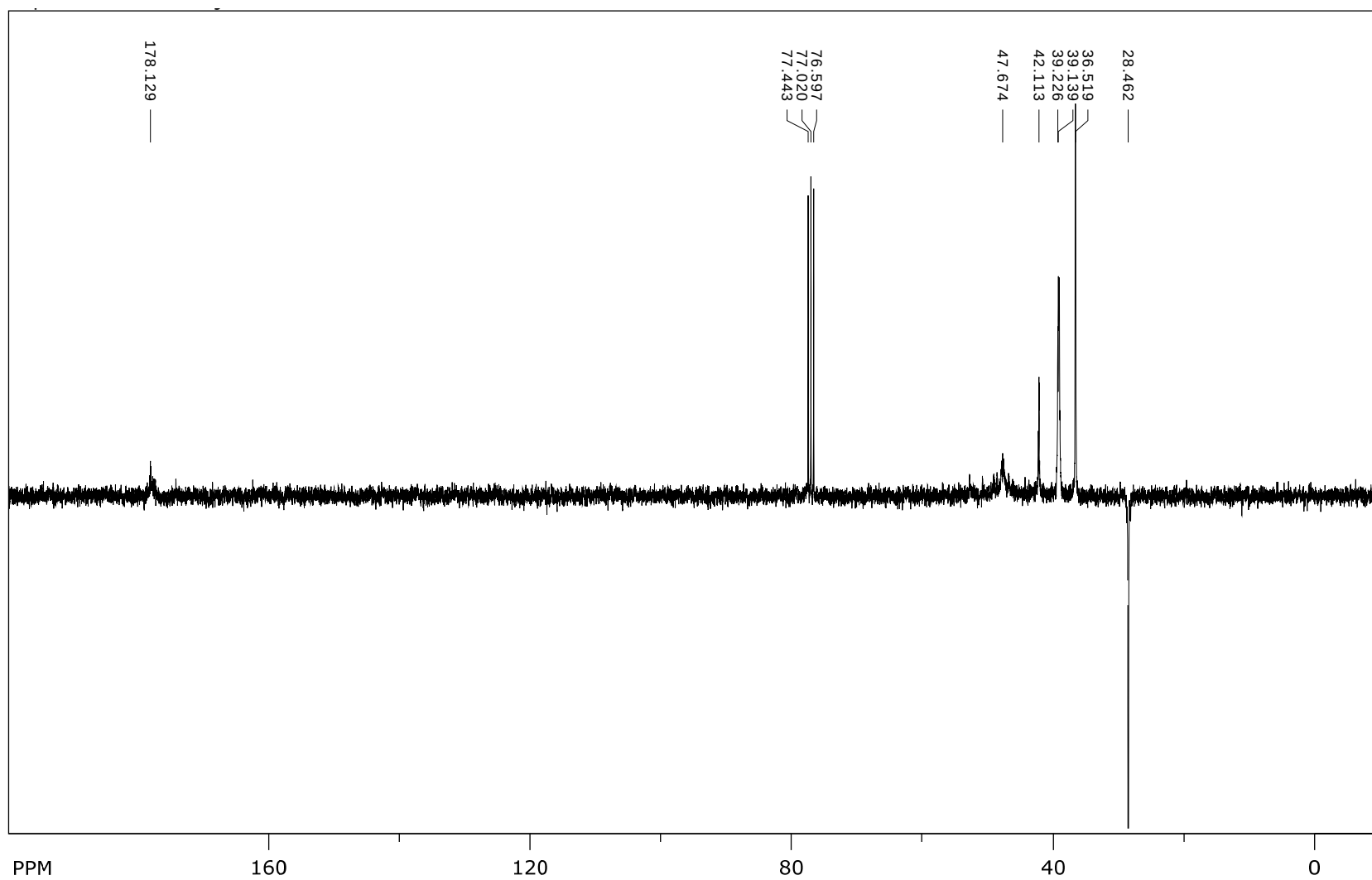


Figure S8. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound 4.

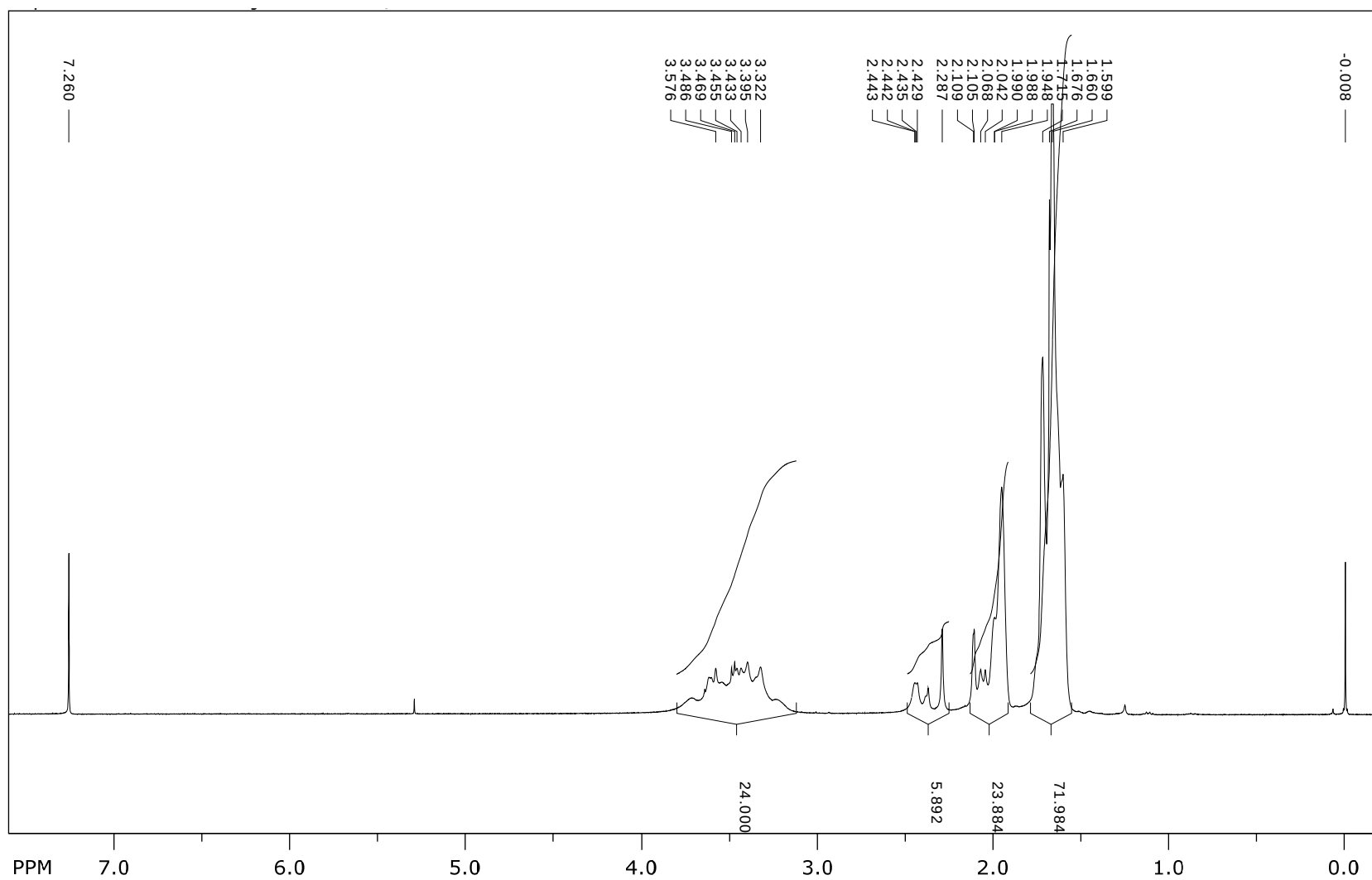


Figure S9. ¹H NMR (300 MHz, CDCl₃) spectrum of compound **5**.

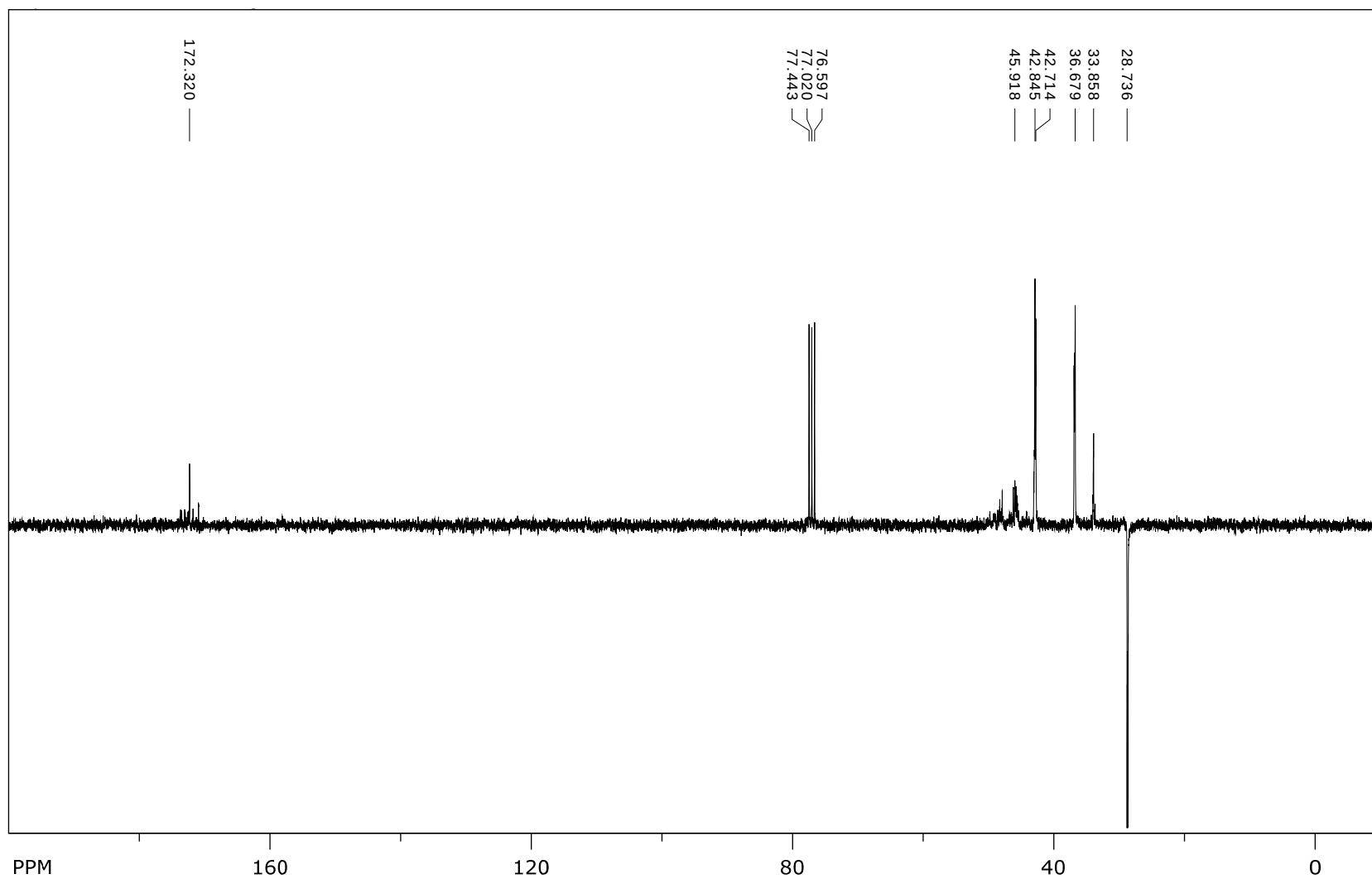


Figure S10. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound 5.

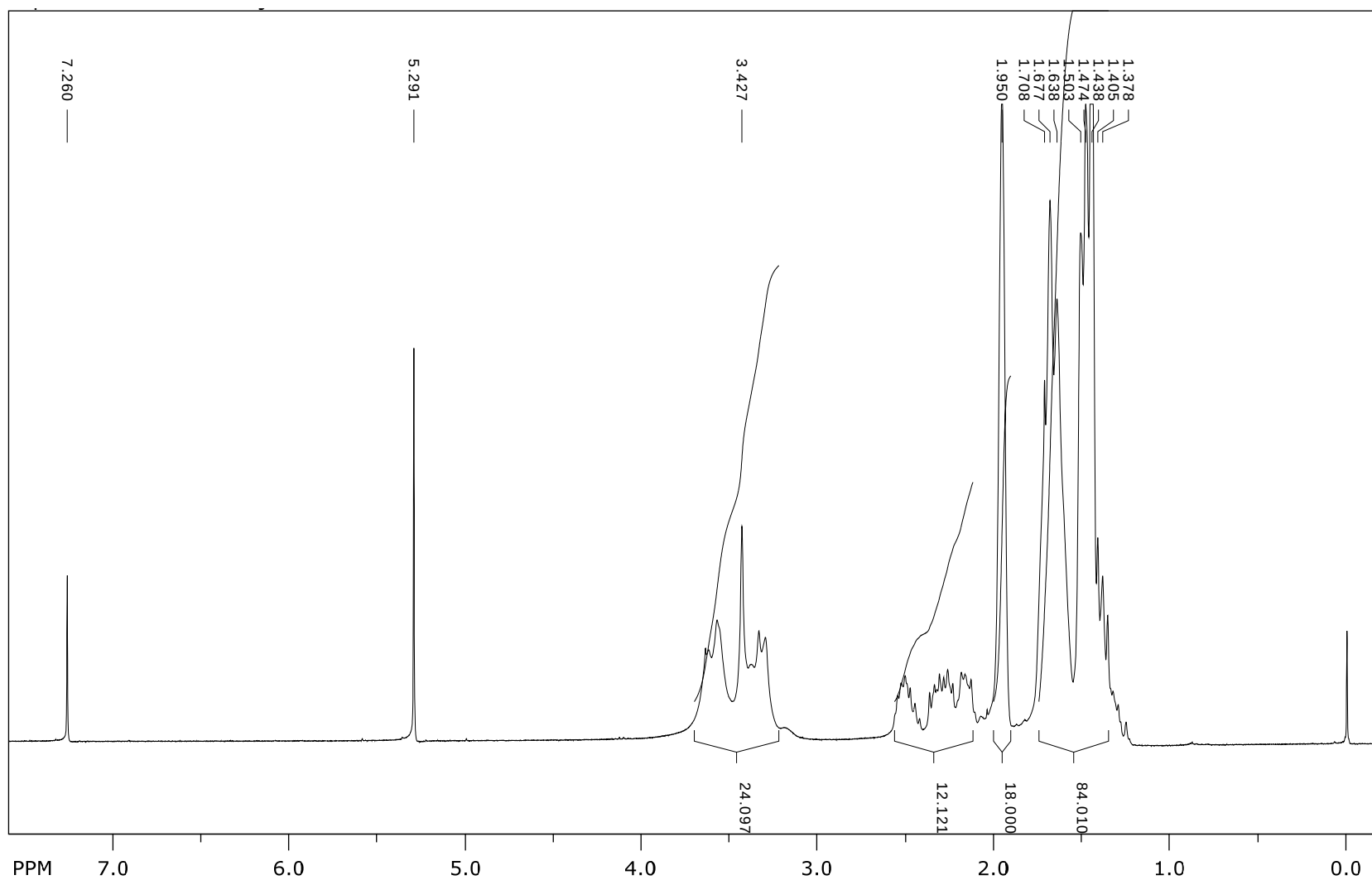


Figure S11. ¹H NMR (300 MHz, CDCl₃) spectrum of compound **6**.

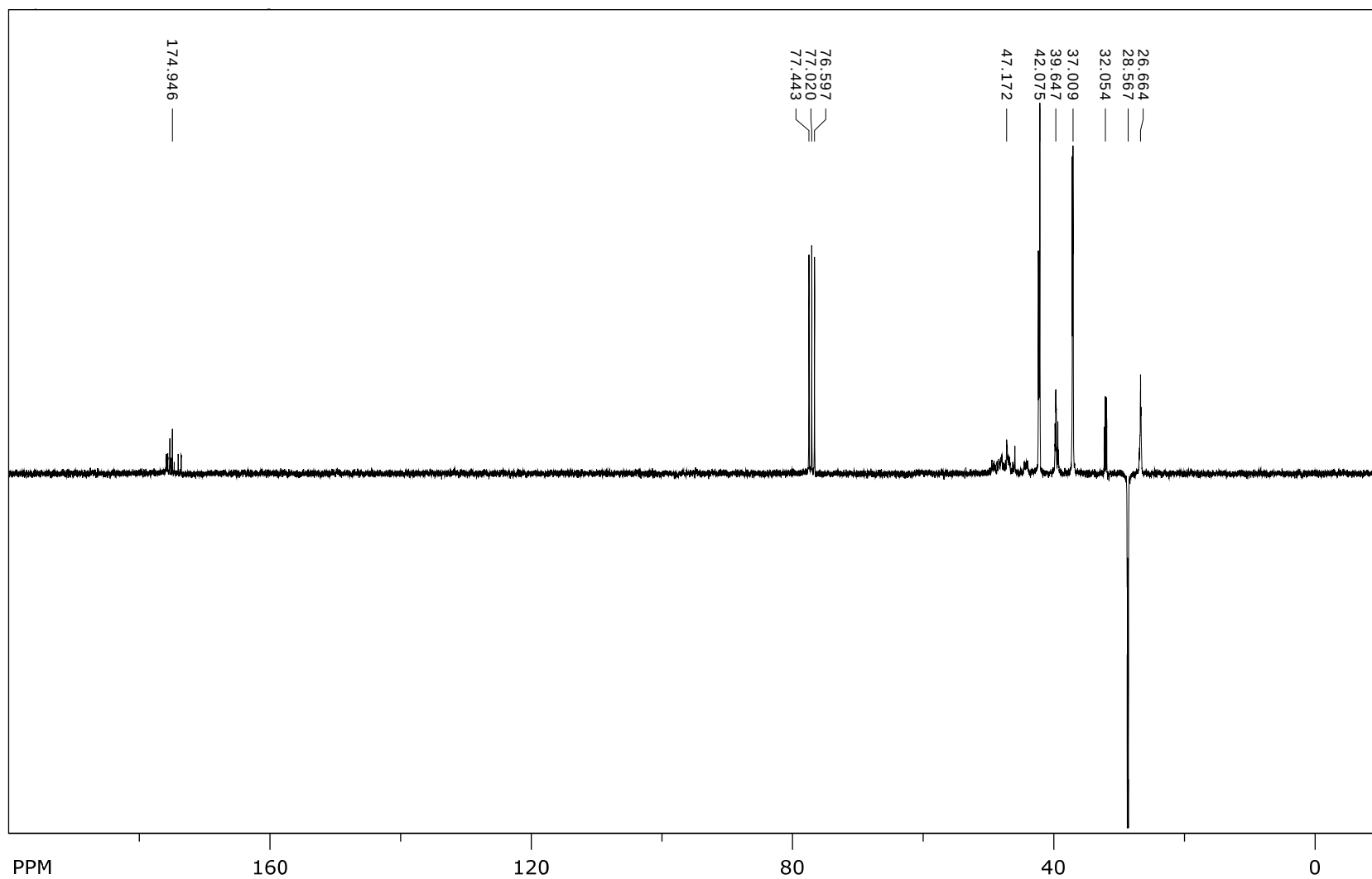


Figure S12. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound **6**.

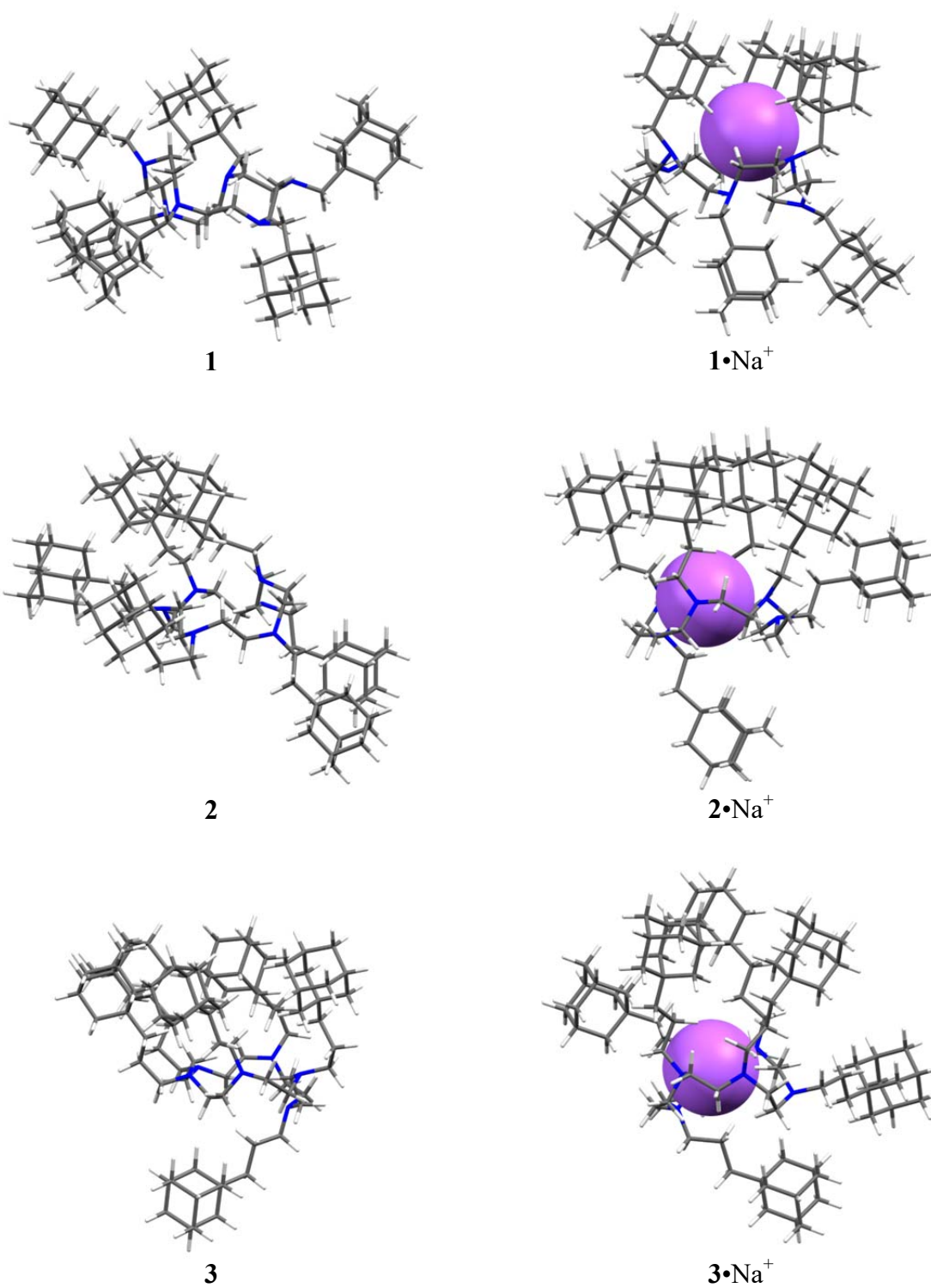
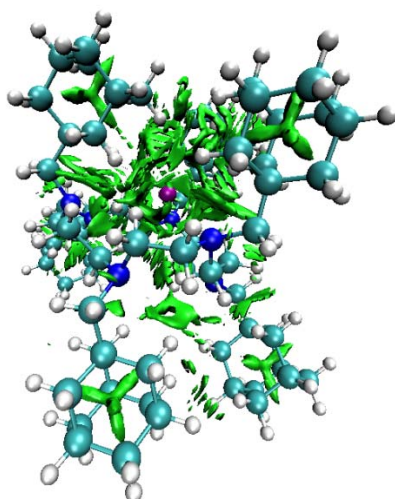
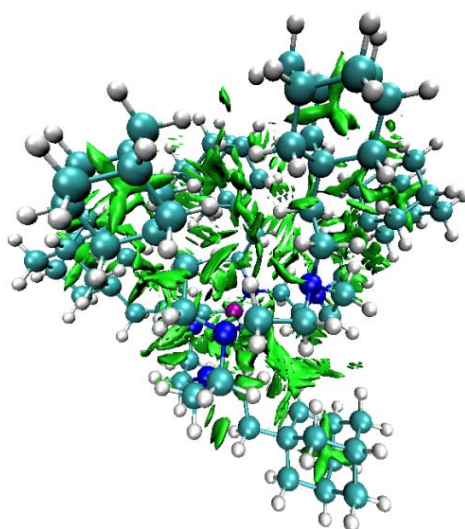


Figure S13. Optimized structures of compounds **1–3** (left) and their Na⁺ complexes (right) computed at the r²SCAN-3c level of theory.

1•Na⁺



2•Na⁺



3•Na⁺

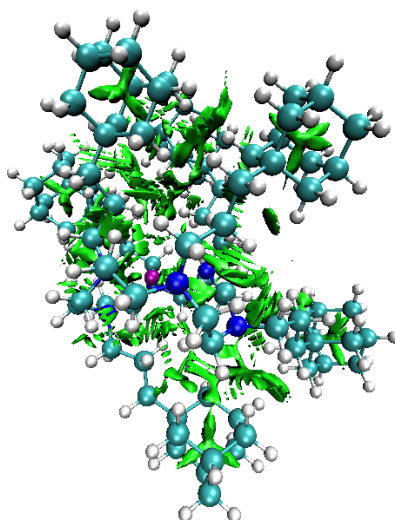


Figure S14. NCI plots for Na⁺ complexes of compounds **1–3**. Attractive non-covalent interactions are depicted in green.

Table S1. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of compounds **1–3** and their Na⁺ complexes in hartree and complex binding energies in kcal mol⁻¹ optimized at the r²SCAN-3c level of theory.

Structure	<i>E</i>	<i>ZPVE</i>	<i>H</i>	<i>G</i>	ΔG^a
1	-3375.889831	1.944322	-3373.873559	-3374.036064	–
2	-3611.697641	2.114991	-3609.504894	-3609.676466	–
3	-3847.517959	2.284316	-3845.146554	-3845.336462	–
1•Na⁺	-3538.035689	1.948192	-3536.014830	-3536.176380	-44.1
2•Na⁺	-3773.893022	2.119465	-3771.693845	-3771.869009	-76.9
3•Na⁺	-4009.696107	2.289828	-4007.318904	-4007.508587	-64.1

^a Binding energies are defined as a difference between the Gibbs energy of the complex and the energies of the optimized corresponding hexaaza crown ether and the sodium cation (*G* (Na⁺) = -162.070051 hartree).

Table S2. Geometries of compounds **1–3** and their Na⁺ complexes in Cartesian coordinates in Å computed at the r²SCAN-3c level of theory.

1			
6	1.453079000	2.499967000	2.025341000
1	1.324859000	3.560401000	1.721021000
1	1.815140000	2.525128000	3.060803000
6	3.849833000	2.152201000	1.544430000
1	3.886529000	3.025382000	2.217565000
1	4.388602000	2.452584000	0.630519000
6	2.189129000	1.764385000	-0.210356000
1	1.259983000	1.202289000	-0.376698000
1	2.985374000	1.183951000	-0.694762000
6	2.103536000	3.130134000	-0.905992000
1	1.184971000	3.663138000	-0.589961000
1	2.945258000	3.744742000	-0.561555000
6	2.365056000	4.301531000	-3.035969000
1	2.117454000	5.132061000	-2.351310000
1	1.653718000	4.377967000	-3.874697000
6	1.188394000	2.147251000	-2.968064000
1	1.337037000	1.118821000	-2.612556000
1	1.378956000	2.118848000	-4.049153000
6	-0.266941000	2.583705000	-2.711024000
1	-0.492630000	2.502423000	-1.639109000
1	-0.374625000	3.648479000	-2.956544000
6	-1.353644000	2.201934000	-4.881443000
1	-1.218384000	1.305688000	-5.510384000
1	-0.529242000	2.885451000	-5.145835000
6	-1.307231000	0.407625000	-3.209341000
1	-0.386370000	-0.099886000	-3.556900000

1	-2.131741000	-0.017714000	-3.795561000
7	2.461030000	1.804683000	1.222911000
7	2.209285000	3.007181000	-2.361016000
7	-1.287952000	1.848901000	-3.459304000
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1	-3.378020000	0.733375000	7.070217000
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1	-0.083586000	-1.934408000	7.870343000
6	-4.869033000	-2.415222000	2.088806000
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1	-2.744853000	-3.001949000	0.424544000
1	-3.610432000	-4.093106000	-0.668678000

2			
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6	0.302210000	-2.237406000	0.604777000
7	3.864502000	0.503888000	0.933150000
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6	1.810321000	-0.640556000	1.734984000
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6	2.684789000	2.633123000	0.090379000
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1	-2.291434000	-3.803221000	-4.411309000
1	-0.697398000	-3.093073000	-4.339682000
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1	4.647773000	-0.125140000	-4.883452000
1	2.987169000	-2.030955000	-5.024506000
1	2.598553000	-1.789360000	-3.325636000
1	2.529419000	3.361394000	-0.491822000
1	1.838897000	3.300921000	1.131996000
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1	2.619835000	1.447178000	2.769607000
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