Supplementary Data

Cyclic tetraureas with variable flexibility – synthesis, crystal structures and properties

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Supplementary data for the Molecular dynamics simulation chapter.

Table S1 Average energies (kcal/mol) for the complexes of **12** and **17** with chloride and dihydrogenphosphate in chloroform and acetonitrile.

	chloroform				acetonitrile			
	12 (XXXX)		**17** (DDDD)		**12** (XXXX)		**17** (DDDD)	
	Cl^-	$H_2PO_4^-$	Cl^-	$H_2PO_4^-$	Cl^-	$H_2PO_4^-$	Cl^-	$H_2PO_4^-$
Macrocycle MC								
$E_{MC,complex}$	241.5	245.5	-72.7	-89.3	243.4	243.3	-71.8	-88.0
$E_{MC,\ free}$	191.3	191.3	-142.8	-142.8	247.2	247.2	-100.0	-100.0
Ions								
$E_{X^-,complex}$		-82.4		-81.1		-82.2		-80.8
$E_{X^-,free}$		-82.5		-82.5		-82.8		-82.8
$E_{TBA,complex}$	95.7	95.2	94.7	95.3	95.9	95.7	95.2	95.2
$E_{TBA,free}$	95.5	95.3	95.5	95.3	95.2	96.7	95.2	96.7
Interaction energies								
$\Delta E_{interact,MC\_X^-,complex}$	-121.2	-101.4	-145.2	-110.1	-126.8	-102.1	-146.7	-113.3
$\Delta E_{interact,MC\_TBA,complex}$	-26.9	-29.4	-21.4	-19.9	-7.7	0.0	-1.8	-2.5
$\Delta E_{interact,X^-\_tba,complex}$	-44.7	-43.5	-52.8	-52.8	-14.9	-0.4	-5.1	-7.4
$\Delta E_{interact,X^-\_tba,free}$	-70.4	-71.2	-70.4	-71.2	-23.7	-15.2	-23.7	-15.2
$\Sigma E_{total,complex}$	144.3	84.0	-197.5	-257.9	189.8	154.3	-130.3	-196.7
$\Sigma E_{total,free}$	216.4	132.9	-117.7	-201.2	318.7	245.8	-28.5	-101.3
$\Delta E_{total,complex-free}$	-72.1	-48.9	-79.8	-56.7	-128.8	-91.5	-101.8	-95.4

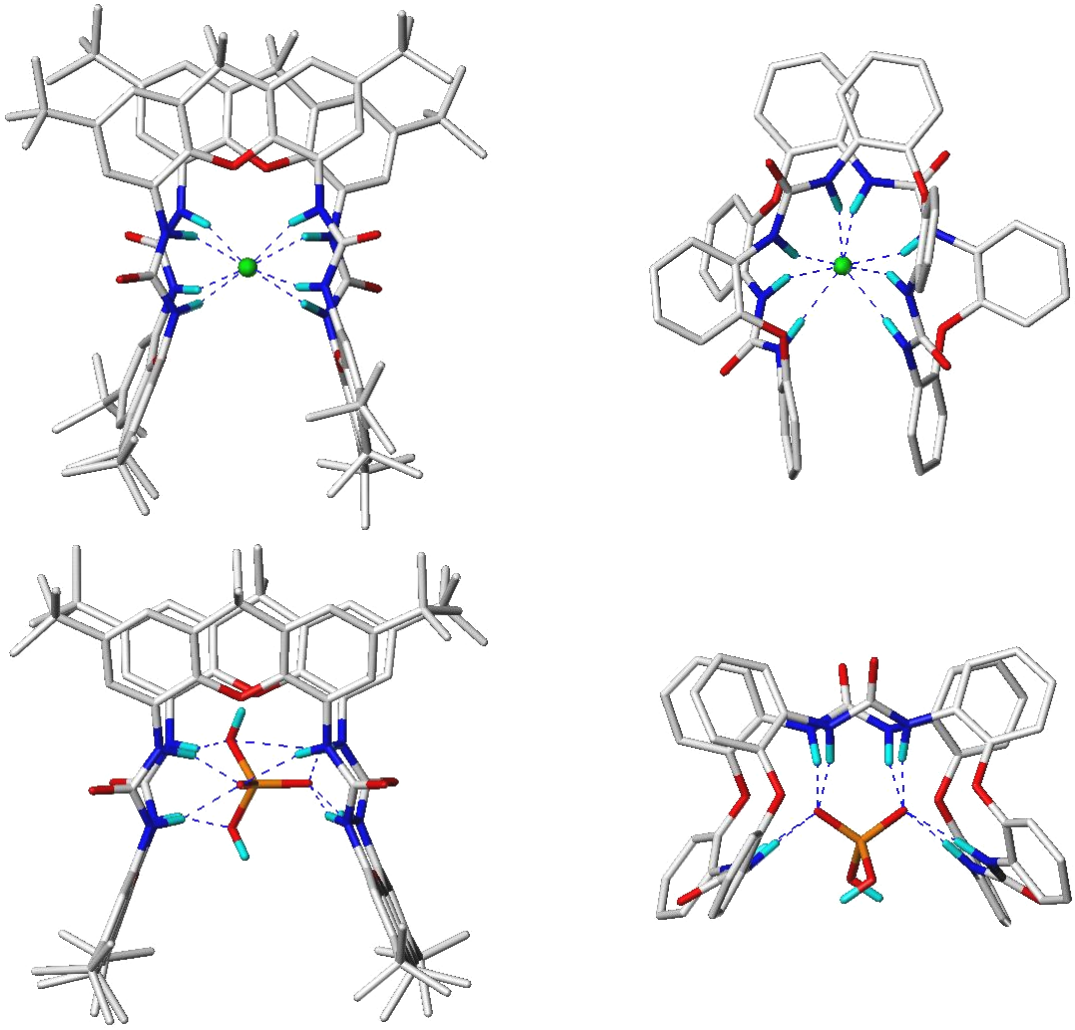


Figure S1 Minimized average structures of the complexes of **12** and **17** with chloride (top) and dihydrogenphosphate (bottom) in chloroform. Nonpolar hydrogen atoms have been omitted.

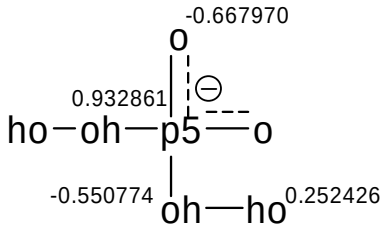
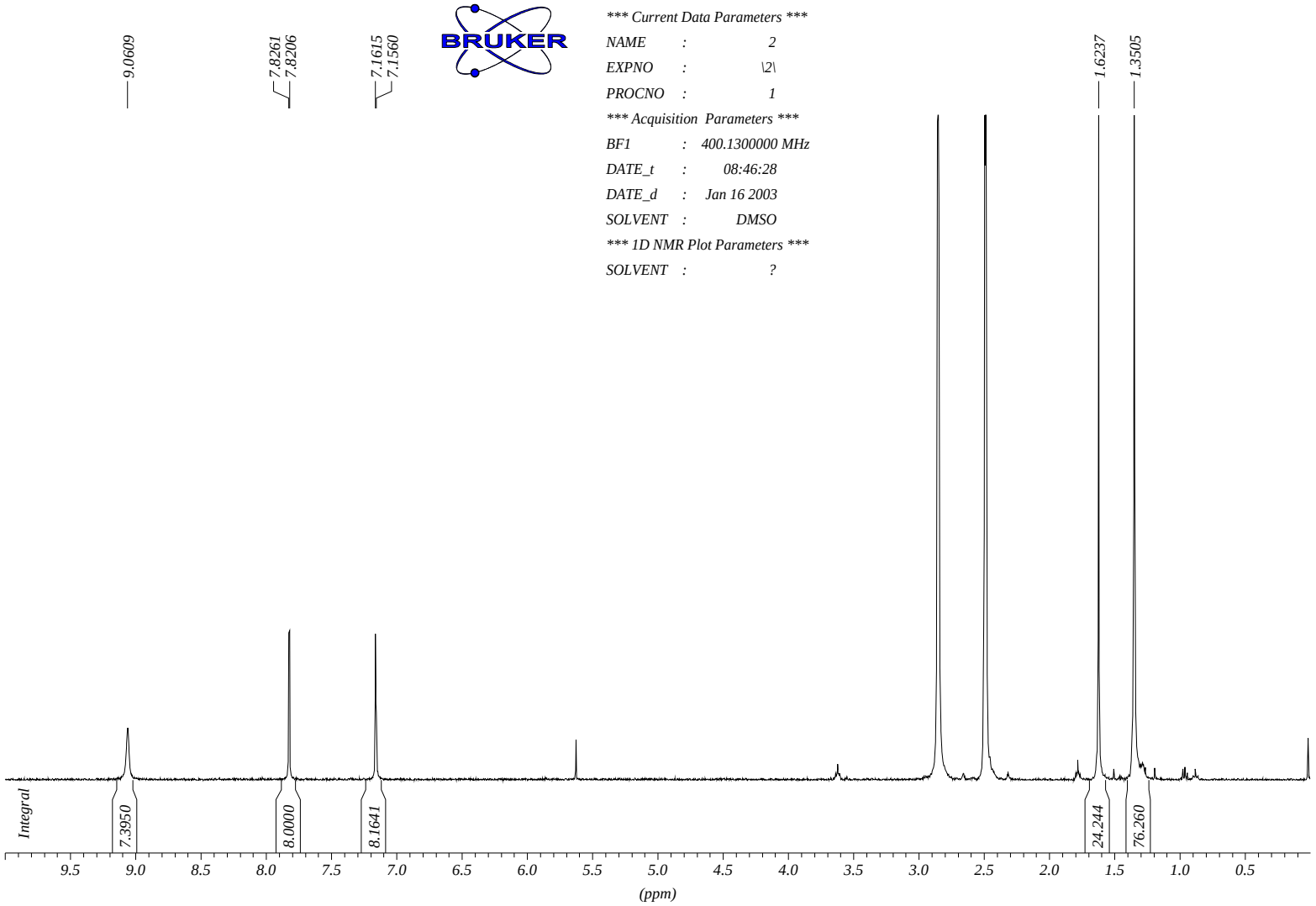


Figure S2 RESP charges and AMBER atom types for dihydrogenphosphate.

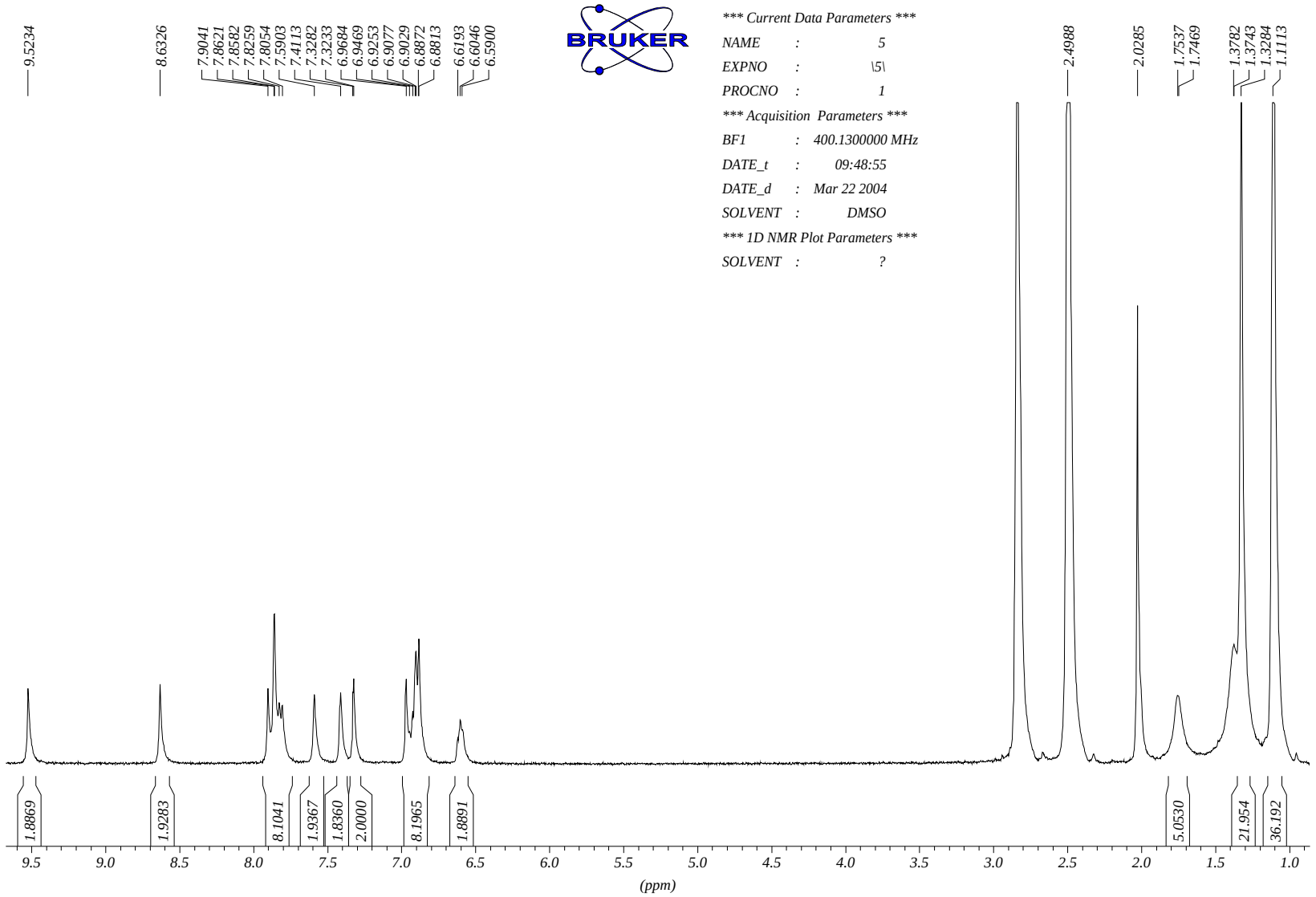
Supporting information for the synthetic chapter.

The NMR spectra of the tetramers.

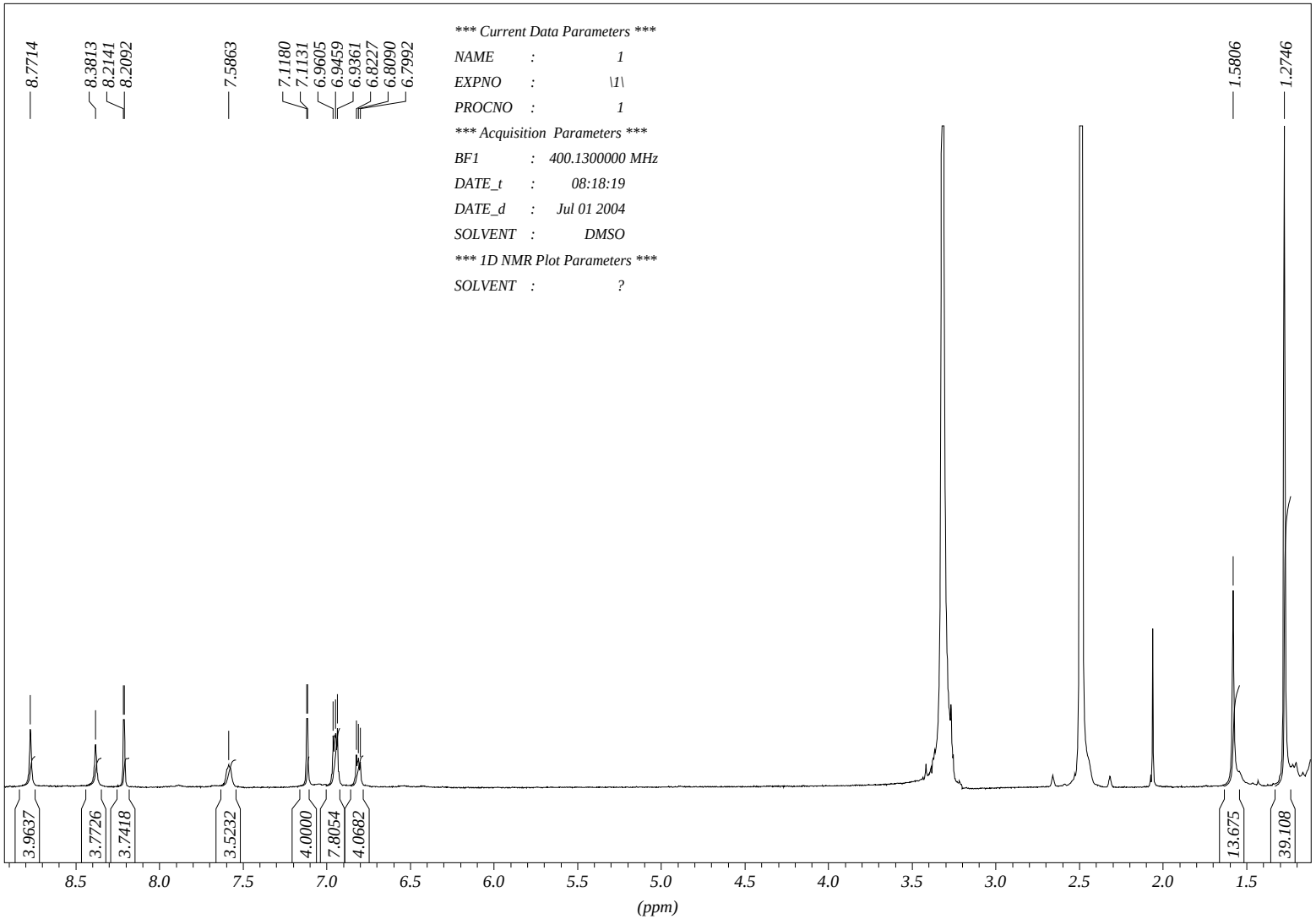
Tetramer 12 (XXXX) DMSO-d6, 120°C



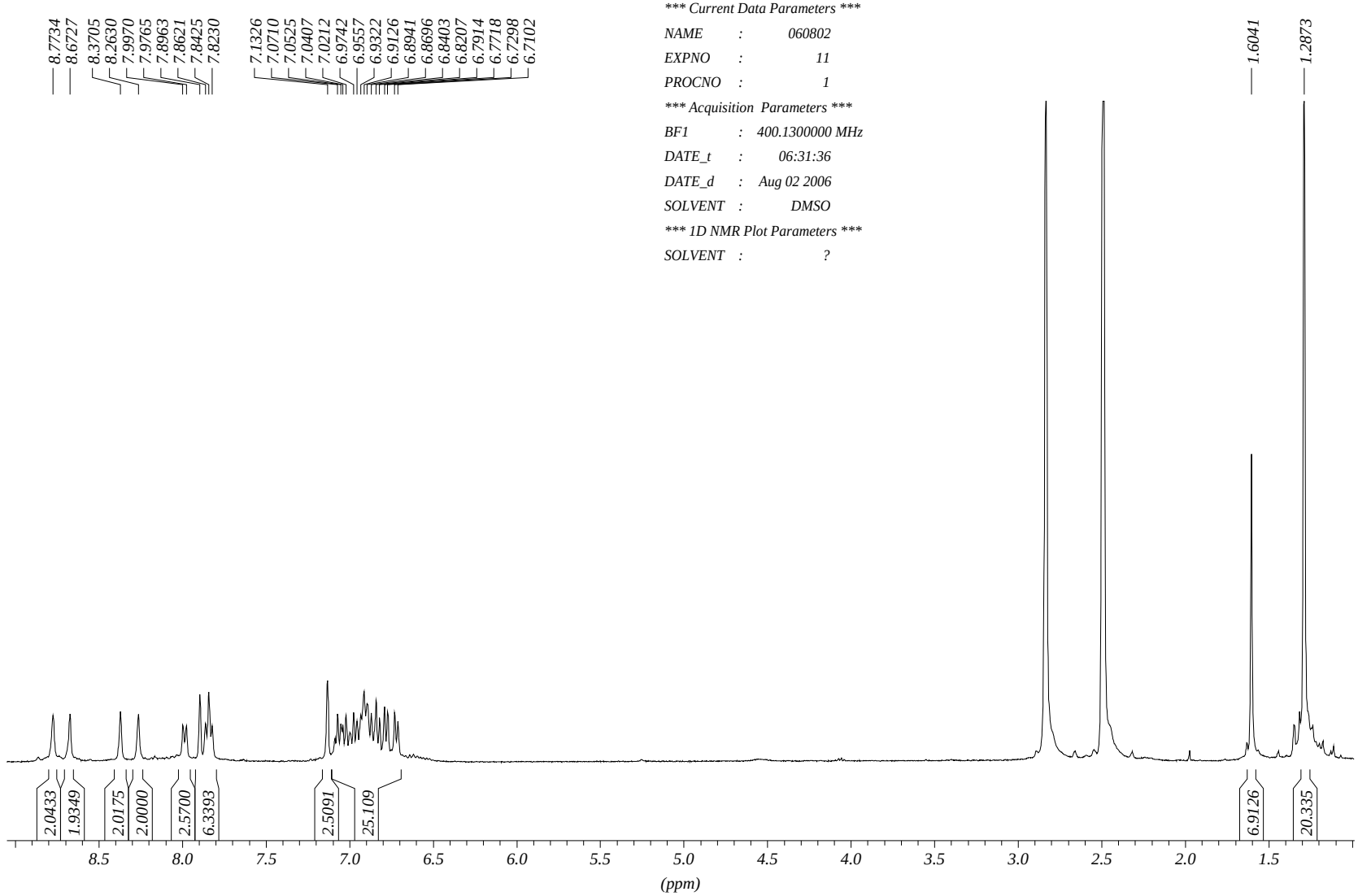
Tetramer 13 (XXXD),) DMSO-d6, 120°C



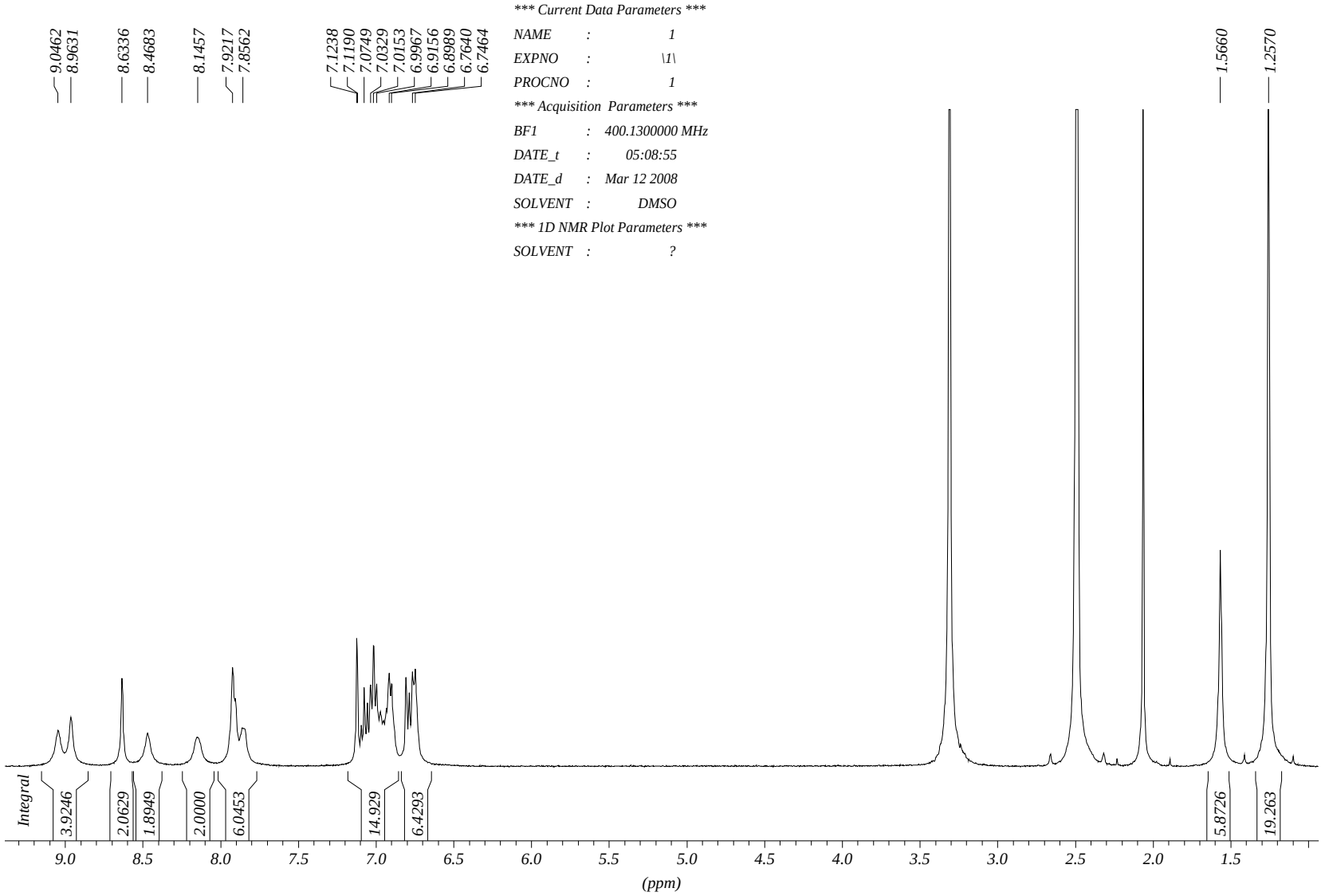
Tetramer 14 (XDXD)



Tetramer 15 (XXDD) DMSO-d6



Tetramer 16 (XDDD)) DMSO-d6, 120°C



Tetramer 17 (DDDD) DMSO-d6