Supplementary Material (ESI) for Chemical Communications

Probing the Na^+ binding site in a calix[4]arene-guanosine conjugate dimer by solid-state ^{23}Na NMR and quantum chemical calculation

By

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Electronic Supplementary Information (ESI)

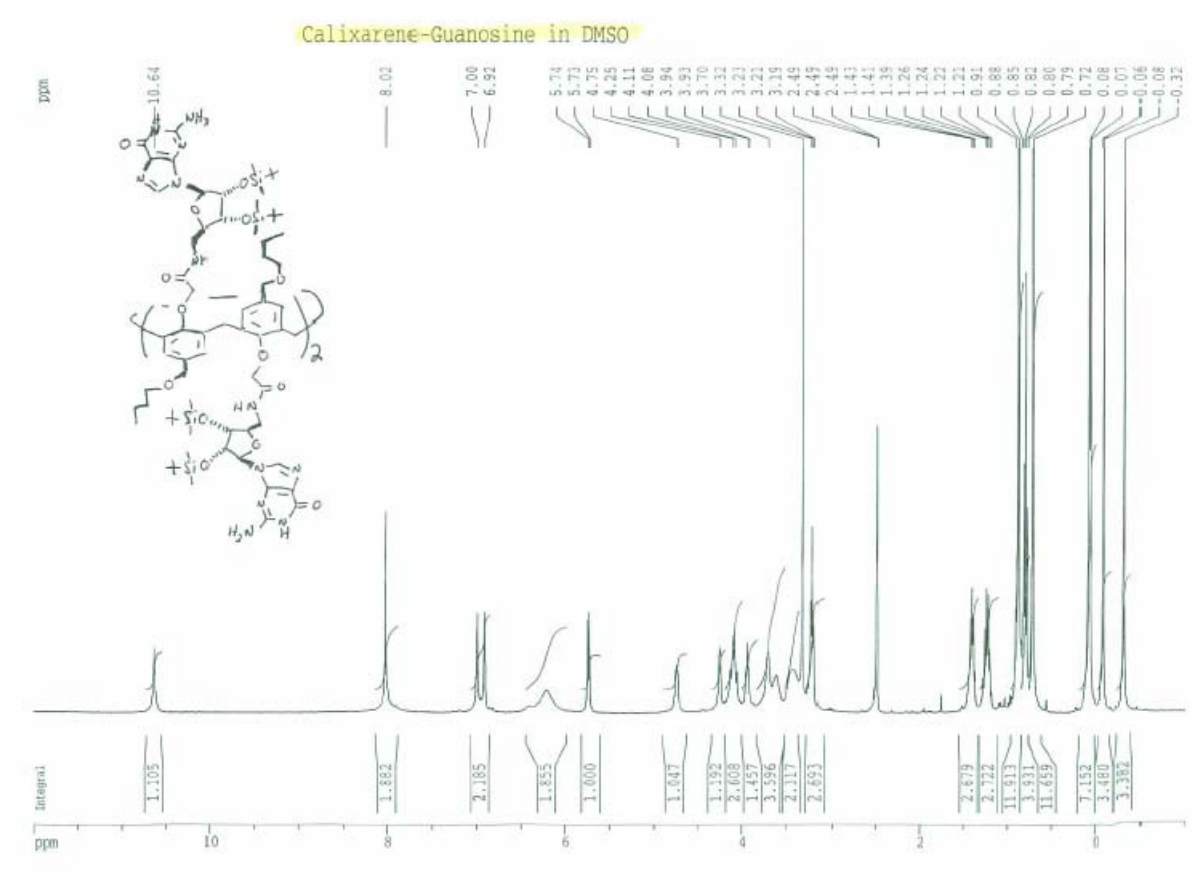

Figure S1. Experimental ^{1}H NMR spectrum of CG in DMSO.

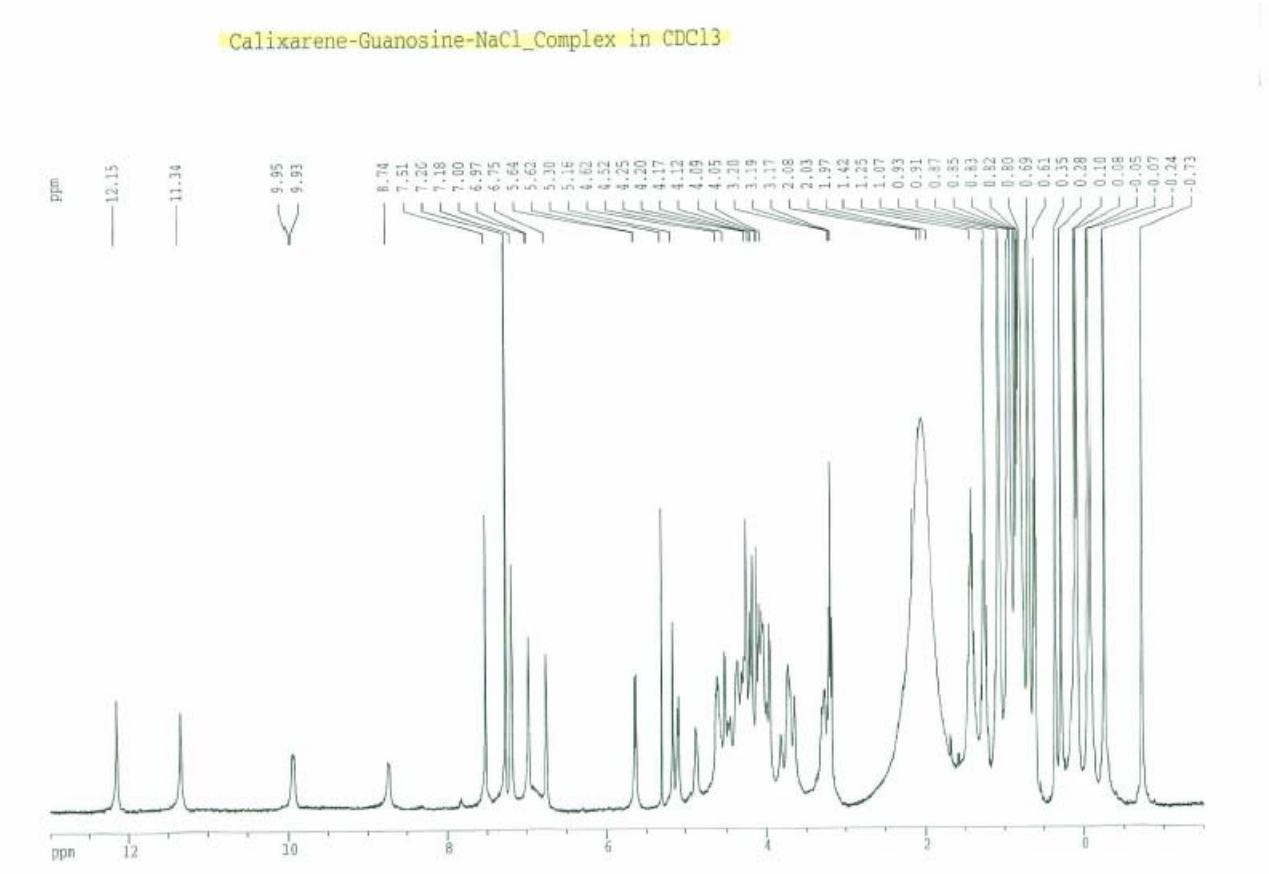

Figure S2. Experimental ^{1}H NMR spectrum of $(CG)_2 \cdot NaCl \cdot (H_2O)_n$ in $CDCl_3$.

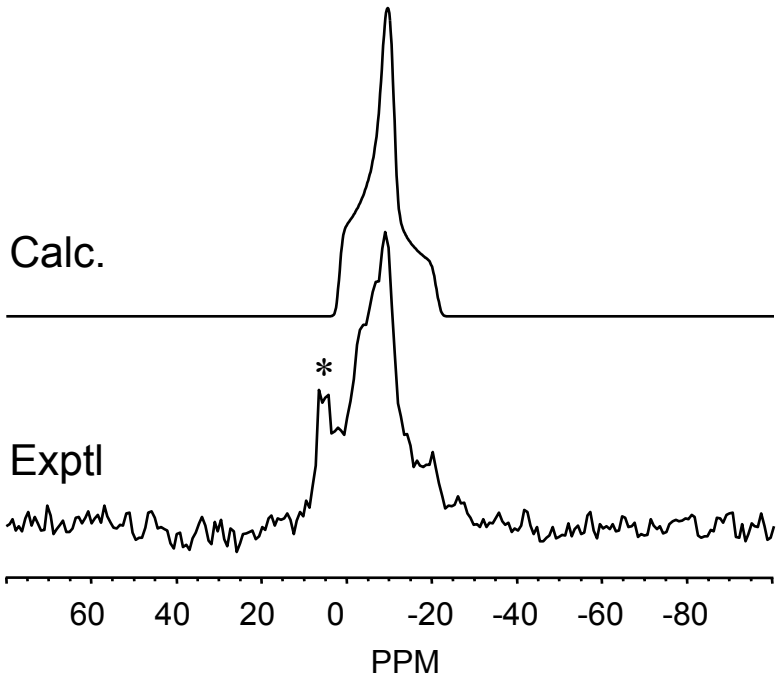

Figure S3. Experimental and calculated ^{23}Na MAS spectra of $(CG)_2$·NaBr·(H_2O)n at 11.75 T. The ^{23}Na NMR parameters used in the calculation are: C_Q = 2.4 MHz, η_Q = 0.9, δ_{iso} = 2 ppm. The asterisk (*) indicates the presence of a small amount of free NaBr.

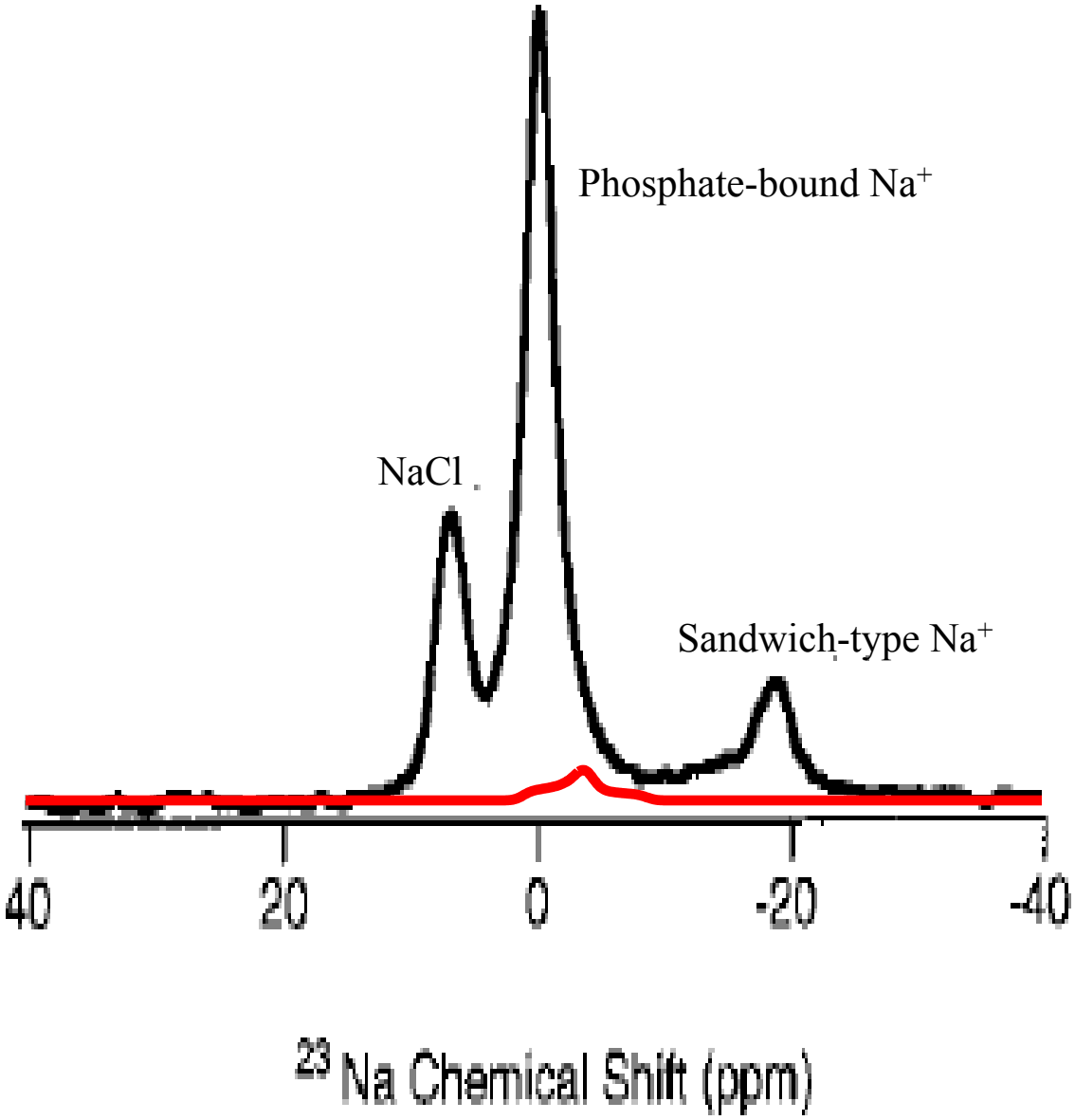

Figure S4: (Black trace) Solid-state ^{23}Na NMR spectrum of $[d(TG_4T)]_4$ at 17.6 T (from Rovnyak et al. J. Am. Chem. Soc. **2000**, *112*, 11423). (Red trace) Calculated ^{23}Na NMR spectrum of $(CG)_2 \cdot NaCl \cdot (H_2O)_n$ at 17.6 T. In the dimeric quadruplex structure of $[d(TG_4T)]_4$, there are five sandwich-type Na^+ ions but only two in-plane Na^+ ions. In addition, because the in-plane Na^+ ions have a much larger C_Q than the sandwich-type Na^+, their signal intensities are considerably lower.

Table S1: Atomic coordinates (in Å) of Model (a)

N	-1.257	6.709	0.0843
C	0.117	6.595	0.0843
N	0.517	5.348	0.0843
C	-0.65	4.599	0.0843
C	-0.863	3.194	0.0843
O	0.	2.284	0.0843
N	-2.221	2.866	0.0843
C	-3.259	3.782	0.0843
N	-4.509	3.3	0.0843
N	-3.065	5.098	0.0843
C	-1.771	5.436	0.0843
H	-1.8	7.561	0.0843
H	0.761	7.463	0.0843
H	-2.43	1.855	0.0843
H	-5.243	3.99	0.0843
H	-4.748	2.299	0.0843
N	-6.709	-1.257	0.0843
C	-6.595	0.117	0.0843
N	-5.348	0.517	0.0843
C	-4.599	-0.65	0.0843
C	-3.194	-0.863	0.0843
O	-2.284	0.	0.0843
N	-2.866	-2.221	0.0843
C	-3.782	-3.259	0.0843
N	-3.3	-4.509	0.0843
N	-5.098	-3.065	0.0843
C	-5.436	-1.771	0.0843
H	-7.561	-1.8	0.0843
H	-7.463	0.761	0.0843
H	-1.855	-2.43	0.0843
H	-3.99	-5.243	0.0843
H	-2.299	-4.748	0.0843
N	1.257	-6.709	0.0843
C	-0.117	-6.595	0.0843
N	-0.517	-5.348	0.0843
C	0.65	-4.599	0.0843
C	0.863	-3.194	0.0843
O	0.	-2.284	0.0843
N	2.221	-2.866	0.0843
C	3.259	-3.782	0.0843
N	4.509	-3.3	0.0843
N	3.065	-5.098	0.0843
C	1.771	-5.436	0.0843
H	1.8	-7.561	0.0843
H	-0.761	-7.463	0.0843
H	2.43	-1.855	0.0843
H	5.243	-3.99	0.0843
H	4.748	-2.299	0.0843
N	6.709	1.257	0.0843
C	6.595	-0.117	0.0843
N	5.348	-0.517	0.0843
C	4.599	0.65	0.0843
C	3.194	0.863	0.0843
O	2.284	0.	0.0843
N	2.866	2.221	0.0843

C	3.782	3.259	0.0843
N	3.3	4.509	0.0843
N	5.098	3.065	0.0843
C	5.436	1.771	0.0843
H	7.561	1.8	0.0843
H	7.463	-0.761	0.0843
H	1.855	2.43	0.0843
H	3.99	5.243	0.0843
H	2.299	4.748	0.0843
Na	0.	0.	0.0843

Table S2: Atomic coordinates (in Å) of Model (b)

G-quartet			
Na	0.	0.	0.
O	0.	0.	2.432
H	0.779	0.	2.882
H	-0.779	0.	2.882
O	0.	0.	-2.432
H	-0.779	0.	-2.882
H	0.779	0.	-2.882

Table S3: Atomic coordinates (in Å) of Model (c)

G-quartet			
Na	0.	0.	0.0843
O	0.8752	0.9543	-2.4545
H	0.8752	1.6733	-2.9965
H	0.8752	0.2353	-2.9965
H	-1.0329	-1.3056	-3.3348
O	-0.8147	-0.8884	-2.4982
H	-1.1352	0.0166	-2.4982

Table S4: Atomic coordinates (in Å) of Model (d)

G-quartet			
Na	0.	0.	0.
O	0.	0.	2.432
H	0.779	0.	2.882
H	-0.779	0.	2.882

Table S5: Atomic coordinates (in Å) of Model (e)

G-quartet			
Na	0.	0.	0.500
O	0.	0.	2.932
H	0.779	0.	3.382
H	-0.779	0.	3.382

Table S6: Atomic coordinates (in Å) of Model (f)

G-quartet			
Na	0.0028	0.001	-0.0569
Cl	-0.1795	-0.005	2.6369

Table S7: Atomic coordinates (in Å) of Model (g)

G-quartet			
Na	0.	0.	0.0843
O	-0.003	-0.1609	-2.4105
H	-0.2044	0.2885	-3.1643
H	-0.1395	-1.0312	-2.5968
Cl	0.0033	0.1737	2.7787

Table S8: Atomic coordinates (in Å) of Model (h)

G-quartet			
Na	0.	0.	0.5
O	0.	0.	2.932
H	0.779	0.	3.382
H	-0.779	0.	3.382
Cl	0.	0.	5.878

Table S9: Atomic coordinates (in Å) of Model (i)

N	-1.257	6.709	0.
C	0.117	6.595	0.
N	0.517	5.348	0.
C	-0.65	4.599	0.
C	-0.863	3.194	0.
O	0.	2.284	0.
N	-2.221	2.866	0.
C	-3.259	3.782	0.
N	-4.509	3.3	0.
N	-3.065	5.098	0.
C	-1.771	5.436	0.
H	-1.8	7.561	0.
H	0.761	7.463	0.
H	-2.43	1.855	0.
H	-5.243	3.99	0.
H	-4.748	2.299	0.
N	-6.709	-1.257	0.
C	-6.595	0.117	0.
N	-5.348	0.517	0.
C	-4.599	-0.65	0.
C	-3.194	-0.863	0.
O	-2.284	0.	0.
N	-2.866	-2.221	0.
C	-3.782	-3.259	0.
N	-3.3	-4.509	0.
N	-5.098	-3.065	0.
C	-5.436	-1.771	0.
H	-7.561	-1.8	0.

H	-7.463	0.761	0.
H	-1.855	-2.43	0.
H	-3.99	-5.243	0.
H	-2.299	-4.748	0.
N	1.257	-6.709	0.
C	-0.117	-6.595	0.
N	-0.517	-5.348	0.
C	0.65	-4.599	0.
C	0.863	-3.194	0.
O	0.	-2.284	0.
N	2.221	-2.866	0.
C	3.259	-3.782	0.
N	4.509	-3.3	0.
N	3.065	-5.098	0.
C	1.771	-5.436	0.
H	1.8	-7.561	0.
H	-0.761	-7.463	0.
H	2.43	-1.855	0.
H	5.243	-3.99	0.
H	4.748	-2.299	0.
N	6.709	1.257	0.
C	6.595	-0.117	0.
N	5.348	-0.517	0.
C	4.599	0.65	0.
C	3.194	0.863	0.
O	2.284	0.	0.
N	2.866	2.221	0.
C	3.782	3.259	0.
N	3.3	4.509	0.
N	5.098	3.065	0.
C	5.436	1.771	0.
H	7.561	1.8	0.
H	7.463	-0.761	0.
H	1.855	2.43	0.
H	3.99	5.243	0.
H	2.299	4.748	0.
N	-1.257	6.709	3.45
C	0.117	6.595	3.45
N	0.517	5.348	3.45
C	-0.65	4.599	3.45
C	-0.863	3.194	3.45
O	0.	2.284	3.45
N	-2.221	2.866	3.45
C	-3.259	3.782	3.45
N	-4.509	3.3	3.45
N	-3.065	5.098	3.45
C	-1.771	5.436	3.45
H	-1.8	7.561	3.45
H	0.761	7.463	3.45
H	-2.43	1.855	3.45
H	-5.243	3.99	3.45
H	-4.748	2.299	3.45
N	-6.709	-1.257	3.45
C	-6.595	0.117	3.45
N	-5.348	0.517	3.45
C	-4.599	-0.65	3.45
C	-3.194	-0.863	3.45

O	-2.284	0.	3.45
N	-2.866	-2.221	3.45
C	-3.782	-3.259	3.45
N	-3.3	-4.509	3.45
N	-5.098	-3.065	3.45
C	-5.436	-1.771	3.45
H	-7.561	-1.8	3.45
H	-7.463	0.761	3.45
H	-1.855	-2.43	3.45
H	-3.99	-5.243	3.45
H	-2.299	-4.748	3.45
N	1.257	-6.709	3.45
C	-0.117	-6.595	3.45
N	-0.517	-5.348	3.45
C	0.65	-4.599	3.45
C	0.863	-3.194	3.45
O	0.	-2.284	3.45
N	2.221	-2.866	3.45
C	3.259	-3.782	3.45
N	4.509	-3.3	3.45
N	3.065	-5.098	3.45
C	1.771	-5.436	3.45
H	1.8	-7.561	3.45
H	-0.761	-7.463	3.45
H	2.43	-1.855	3.45
H	5.243	-3.99	3.45
H	4.748	-2.299	3.45
N	6.709	1.257	3.45
C	6.595	-0.117	3.45
N	5.348	-0.517	3.45
C	4.599	0.65	3.45
C	3.194	0.863	3.45
O	2.284	0.	3.45
N	2.866	2.221	3.45
C	3.782	3.259	3.45
N	3.3	4.509	3.45
N	5.098	3.065	3.45
C	5.436	1.771	3.45
H	7.561	1.8	3.45
H	7.463	-0.761	3.45
H	1.855	2.43	3.45
H	3.99	5.243	3.45
H	2.299	4.748	3.45
Na	0.	0.	1.725
