

Supplementary Information

Virtual Screening of Organic Quinones as Cathode Materials for Sodium-Ion Batteries

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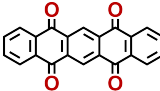
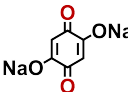
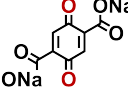
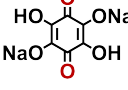
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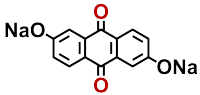
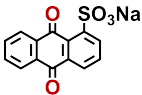
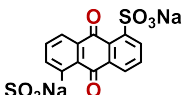
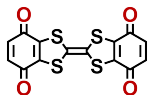
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Table S1: A summary of key experimental data on molecules that have been used to develop an equation of calibration between the measured reduction potentials and the calculated LUMO energies.

No.	2D structures	Organic electrolyte	Average reduction potential (V vs Na/Na ⁺)	Discharge condition
1		1 M NaClO ₄ /EC+PC+DMC (v/v/v=4.5:4.5:1)	2.73	10 mA/g
2		1 M NaClO ₄ /EC+PC+DMC (v/v/v=4.5:4.5:1)	2.70	10 mA/g
3		0.3 M NaTFSI/DME	2.06	34 mA/g
4		0.3 M NaTFSI/DME	1.96	26 mA/g
5		0.3 M NaTFSI/DME	1.64	26 mA/g
6		0.3 M NaTFSI/DME	1.97	20 mA/g
7		1 M NaClO ₄ /EC+DMC (v/v=1:1)	1.15	50 mA/g
8		1 M NaClO ₄ /EC+DMC (v/v=1:1)	2.32	19 mA/g
9		1 M NaClO ₄ /EC+DMC (v/v=1:1)	1.81	24.8 mA/g

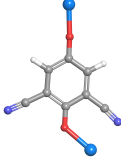
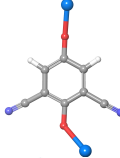
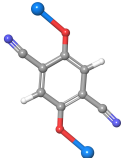
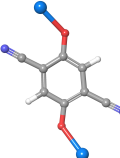
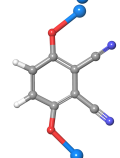
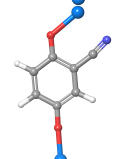
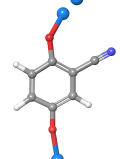
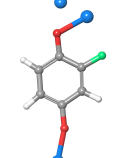
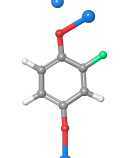
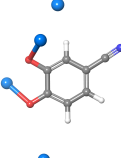
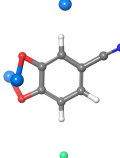
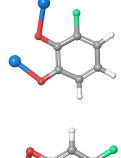
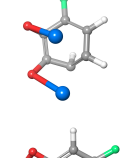
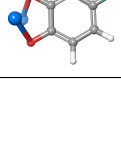
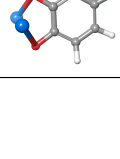
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Table S1 – continued from previous page

No.	2D structures	Organic electrolyte	Average reduction potential (V vs Na/Na ⁺)	Discharge condition
10		1 M NaPF ₆ /DME	1.14	50 mA/g
11		1 M NaClO ₄ /EC+DEC (v/v=1:1)	2.05	30 mA/g
12		1 M NaClO ₄ /EC+DEC (v/v=1:1)	2.11	30 mA/g
13		1 M NaClO ₄ /EC+DMC (v/v=1:1)	2.01	0.1 C
14		2.5 M NaTFSI/PC	2.59	40 mA/g

The abbreviations of organic solvents in the above table are denoted as: EC = ethylene carbonate, PC = propylene carbonate, DMC = dimethyl carbonate, DME= dimethyl ether, DEC = diethyl carbonate. The v/v indicates the volume fraction of organic solvents in a mixture.

Table S2: The initial and final geometries of the 21 sodiated product molecules and the bond distances between O and Na atoms ($d_{\text{O-Na}}$) as measured prior to and post MD simulations.

Ring count	Initial geometries	Final geometries	$d_{\text{O-Na}}^{\text{Initial}}$ (Å) (Top → Bottom)	$d_{\text{O-Na}}^{\text{Final}}$ (Å) (Top → Bottom)
1			1.98	2.00
			2.11	2.17
			2.11	2.15
			2.11	2.14
			2.13	2.16
			2.13	2.12
			2.11	2.12
			1.97	2.00
			2.08	2.07
			2.04	1.99
			2.14	2.16
			2.13	2.14
			2.11	2.10
			2.09	2.12
			2.22	2.29
			2.21	2.28

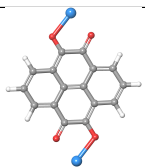
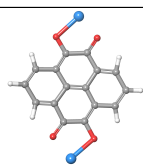
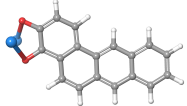
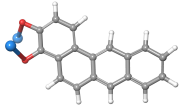
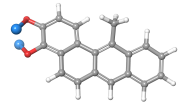
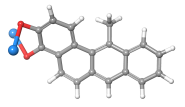
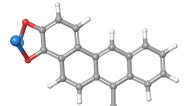
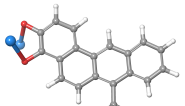
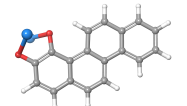
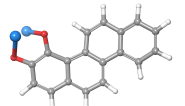
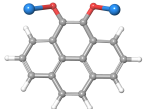
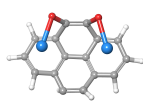
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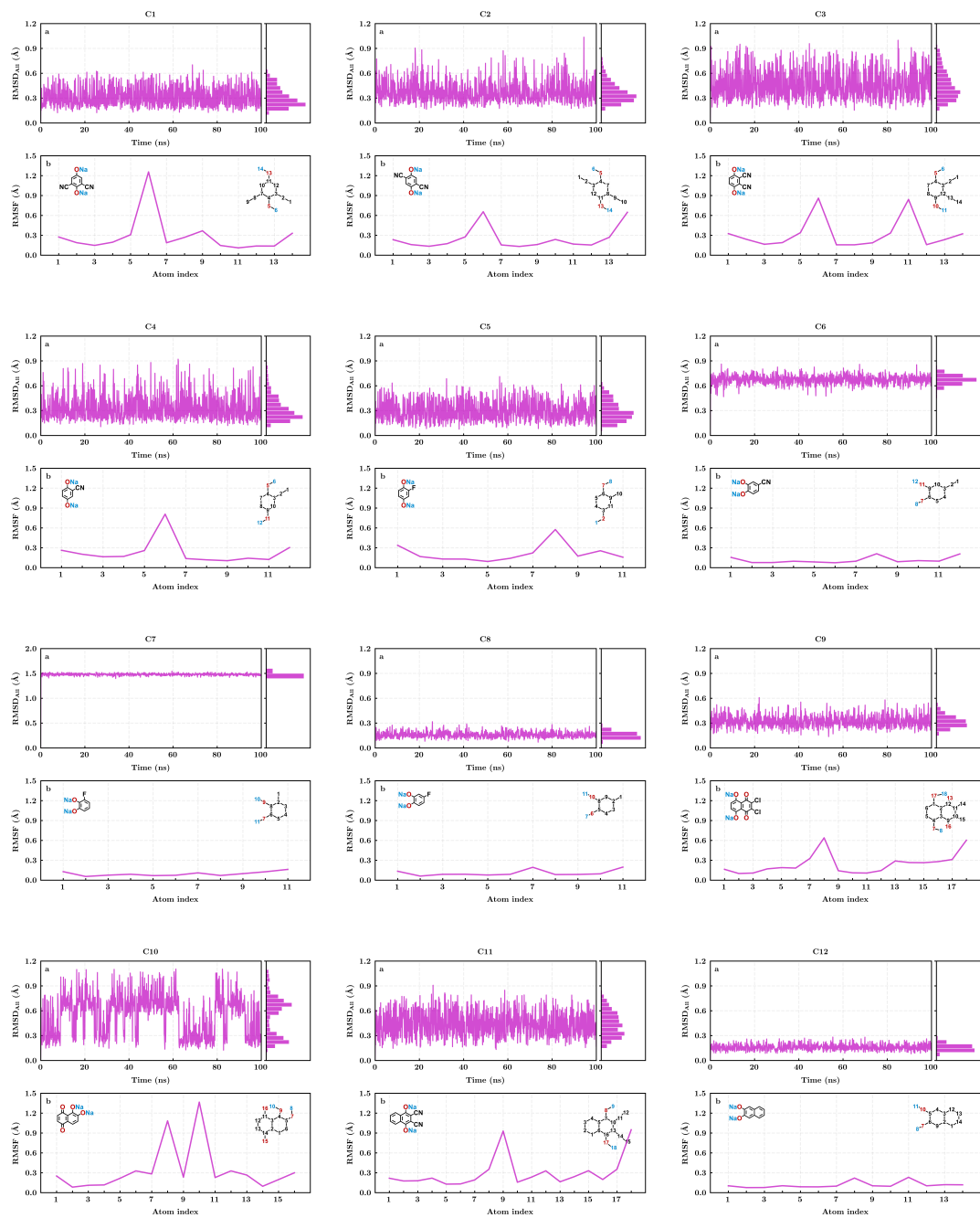
Table S2 – continued from previous page

Ring count	Initial geometries	Final geometries	$d_{\text{O-Na}}^{\text{Initial}}$ (Å) (Top → Bottom)	$d_{\text{O-Na}}^{\text{Final}}$ (Å) (Top → Bottom)
2			2.11	2.14
			2.11	2.10
			2.13	2.19
			2.09	2.09
			2.13	2.16
			2.13	2.11
			2.22	2.27
			2.22	2.22
3			2.10	2.08
			2.10	2.12
			2.11	2.10
			2.11	2.07
			2.15	2.11
			2.15	2.13

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Table S2 – continued from previous page

Ring count	Initial geometries	Final geometries	$d_{\text{O-Na}}^{\text{Initial}}$ (Å)	$d_{\text{O-Na}}^{\text{Final}}$ (Å)
			(Top → Bottom)	(Top → Bottom)
4			2.15	2.23
			2.15	2.20
			2.22	2.20
			2.22	2.26
			2.22	2.26
			2.22	2.20
			2.22	2.26
			2.22	2.29
			2.21	2.27
			2.21	2.29
			2.09	2.15
			2.09	2.14



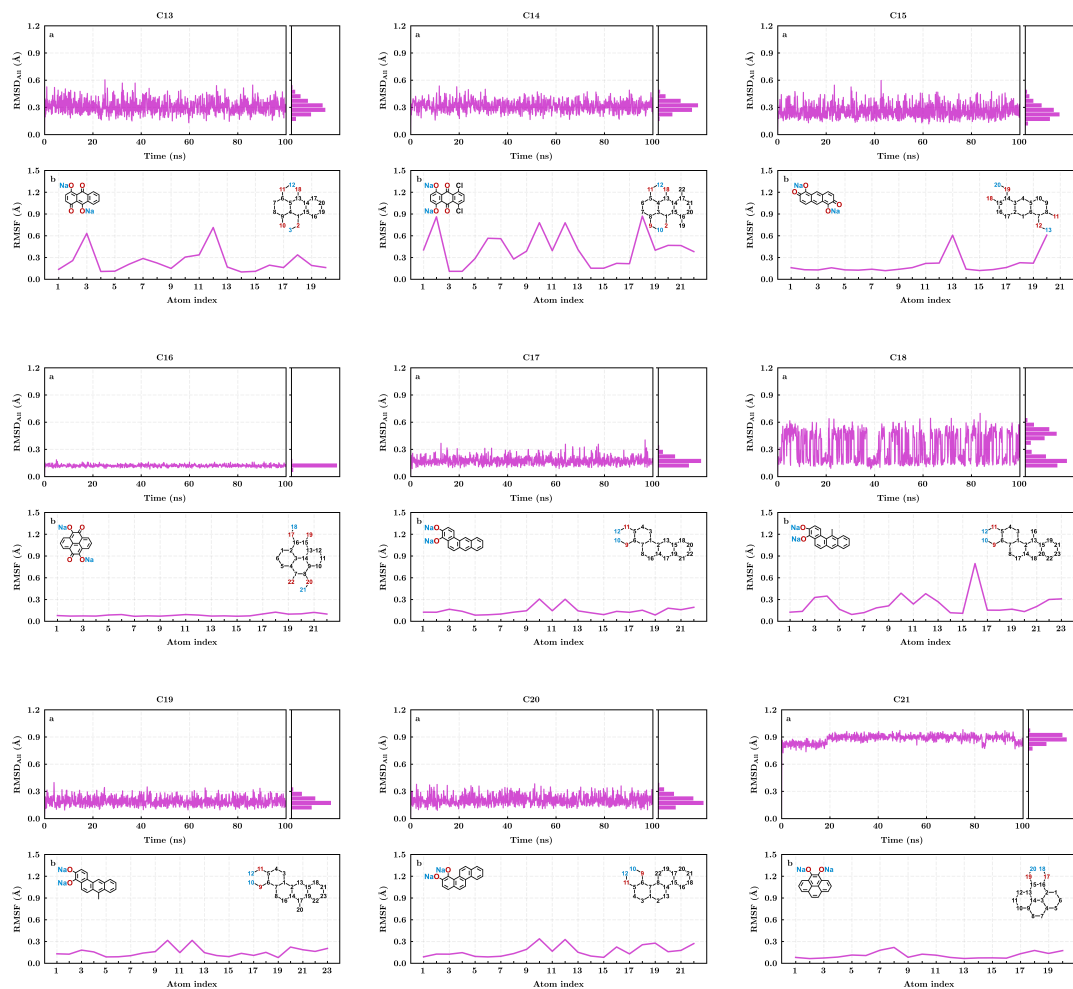


Figure S1: The MD simulation data of a total of 21 candidate (C) sodiated quinone molecules. For each molecule, (a) is the MD trajectory that shows the RMSD of all atoms in the sodiated product molecule, while the distribution of RMSD values is shown in the histogram on the right, and (b) is the root mean square fluctuation (RMSF) of the heavy atoms in the sodiated product molecule, where the top-left and top-right images represent the molecule's 2D structure and the atomic index of the heavy atoms, respectively. The C1-21 represent the 21 candidate molecules.

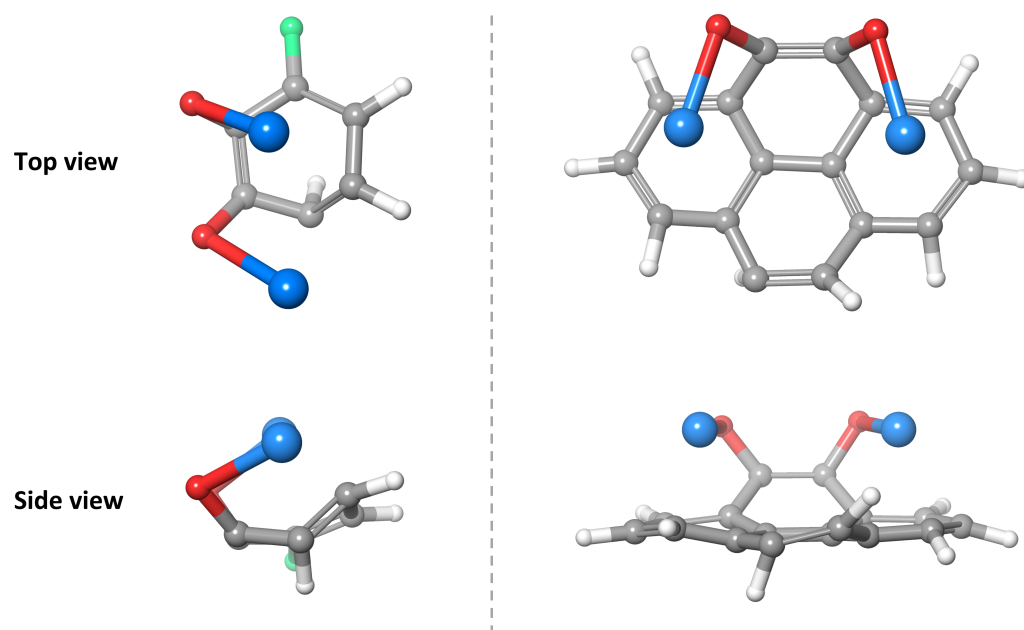


Figure S2: Top and side views of sodiated quinone geometries with high average RMSD_{All} and low RMSF_{Max} values.