Identification of unusual C–Cl…π contacts in 2-(alkylamino)-3-chloro-1,4-naphthoquinones: Effect of N-substituents on crystal packings, fluorescence, redox and anti-microbial properties

Vinay K Singh, *a Sanjay K Verma, a Rahul Kadu a and Shaikh M. Mobin b

a Department of Chemistry, Faculty of Science, The M. S. University of Baroda, Vadodara-390 002, India;
b National Single Crystal X-ray Diffraction Facility, IIT Bombay, Powai, Mumbai 400 076, India

Email: vks.msu@gmail.com

Supplementary Information

1. IR spectra: The IR spectra of secondary amines summarized below as Fig. S1 to S7.

Fig. S1: IR Spectrum of compound 1
Fig. S2: IR Spectrum of compound 2

Fig. S3: IR Spectrum of compound 3
Fig. S4: IR Spectrum of compound 4

Fig. S5: IR Spectrum of compound 5
Fig. S6: IR Spectrum of compound 6

Fig. S7: IR Spectrum of compound 7
2. **NMR spectra:** The NMR spectra of secondary amines summarized below as Fig. S8 to S21.

Fig. S8: $^1$H NMR spectrum of compound 1
Fig. S9: $^{13}$C NMR spectrum of compound 1

Fig. S10: $^1$H NMR spectrum of compound 2
Fig. S11: $^{13}$C NMR spectrum of compound 2

Fig. S12: $^1$H NMR spectrum of compound 3

Fig. S13: $^{13}$C NMR spectrum of compound 3
Fig. S14: $^1$H NMR spectrum of compound 4

Fig. S15: $^{13}$C NMR spectrum of compound 4
Fig. S16: $^1$H NMR spectrum of compound 5

Fig. S17: $^{13}$C NMR spectrum of compound 5
Fig. S18: $^1$H NMR spectrum of compound 6

Fig. S19: $^{13}$C NMR spectrum of compound 6
Fig. S20: $^1$H NMR spectrum of compound 7

Fig. S21: $^{13}$C NMR spectrum of compound 7
3. **GC MS spectra:** The GC MS spectra of compounds are summarized below as Fig. S22 to S28

Fig. S22: GC MS spectra of compound 1

Fig. S23: GC MS spectra of compound 2
Fig. S24: GC MS spectra of compound 3

Fig. S25: GC MS spectra of compound 4
Fig. S26: GC MS spectra of compound 5

Fig. S27: GC MS spectra of compound 6
Fig. S28: GC MS spectra of compound 7

4. Figures: TG/DTA of the compounds is summarized below as Fig. S29
Fig. S29: TG/DTA of the compounds 1-7.