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Selective removal of isoquinoline and quinoline from simulated fuel using 1,1'binaphthyl-2,2'-diol (BINOL): Crystal structure and evaluation of the adduct electronic properties

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Supplementary data



Fig. S1. 1H-NMR spectra of 1,1'-binaphthyl-2,2'-diol.



Fig. S2 GC-MS fragmentation pattern of 6-bromo-1,1'-binaphthyl-2,2'-diol.



Fig. S3 GC-MS chromatogrm of (A) 1,1'-binaphthyl-2,2'-diol (8.3%) and (B) 6-bromo-1,1'-binaphthyl-2,2'-diol. The observed retention time @ 20.228 min indicate 1-bromo-2-Naphthalenol (13.2%).







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Fig. S4. 1H-NMR spectra of 6-bromo-1,1'-binaphthyl-2,2'-diol (**II**); 6-bromo-1,1'-binaphthyl-2,2'-diyl dibenzoate (**III**); 6-vinyl-1,1'-binaphthyl-2,2'-diyl dibenzoate (**IV**) and 6-vinyl-1,1'-binaphthyl-2,2'-diol (**V**).



Fig. S5 FT-IR spectra of **(I)** 1,1'-binaphthyl-2,2'-diol; **(II)** 6-bromo-1,1'-binaphthyl-2,2'-diol; **(III)** 6-bromo-1,1'-binaphthyl-2,2'-diyl dibenzoate; **(IV)** 6-vinyl-1,1'-binaphthyl-2,2'-diyl dibenzoate and **(V)** 6-vinyl-1,1'-binaphthyl-2,2'-diol.

TG profile

The TG profile of 1,1'-binaphthyl-2,2'-diol (BINOL) shows a one-step degradation pattern (Fig. S6), a rapid decomposition of the BINOL (100 wt% loss) occurred at a temperature range of 200-245°C. The DSC displayed a complementary endotherms at T=220°C.



Fig. S6 TG and DSC curves for 1,1'-binaphthyl-2,2'-diol (BINOL).

Energy Dispersive Spectroscopy (EDS)

Chemical characterization of [DBN-*co*-STY] nanofibers after electrospinning was explored. Energy Dispersive Spectroscopy (EDS) spectra of [DBN-*co*-STY] polymer nanofibers are presented in Fig. S7. The presence of oxygen, nitrogen and carbon was also confirmed. The elemental % distribution of carbon and oxygen as shown by the EDS analysis are 96.53% and 3.47% respectively. The EDS analysis confirmed the presence of 1,1'-binaphthyl-2,2'-diol *via* the identification of oxygen atom.



Fig. S7 EDS spectra of [DBN-co-STY] polymer nanofibers.



Fig. S8 UV spectra of polymer material [DBN-co-STY] and the resulting polymer nanofibers.

TG profile

The TG profile of [DBN-co-STY] polymer shows a one-step degradation pattern (Fig. S9), a rapid decomposition of the [DBN-co-STY] polymer (100 wt% loss) occurred at a temperature range of 400-440°C. The DSC displayed a complementary endotherms at T=430°C.



Fig. S9 TG and DSC curves for [DBN-co-STY] polymer.



Fig. S10 ¹H-NMR spectra of [DBN-co-STY] (a: confirmed the presence of –OH).



Fig. S11 Molecular weight distribution of DBN-co-STY as a function of time.



Fig. S12 The distribution plot, $dw/d(log M_w)$ vs log M_w



Fig. S13 ITC titration involving 1,1'-binaphthyl-2,2'-diol (BINOL) (0.998 mM) and carbazole (9.98 mM).



Fig S14. ¹³C-NMR spectra of [DBN-co-STY].