

Electronic Supporting Information for

Polydiacetylene Paper-Based Colorimetric Sensor Array for Vapor Phase Detection and Identification of VOCs

*Thichamporn Eaidkong,^a Radeemada Mungkarndee,^b Chaiwat Phollookin,^c Gamonwarn Tumcharern^d
Mongkol Sukwattanasinitt^c and Sumrit Wacharasindhu^{*c}*

^a Graduate Program for Petrochemical and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

^b Program in Biotechnology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

^c Center for Petroleum Petrochemicals, and Advanced Materials, Department of Chemistry, Chulalongkorn University, Bangkok 10330, Thailand Fax: +66-2-2187634 ; Tel: +662-218-7598

^d National Nanotechnology Center, National Science and Technology Development Agency, Pathumthani 12120, Thailand

sumrit.w@chula.ac.th

Fig. S1-S12	¹ H- ¹³ C NMR Spectrum of monomer 3-8	S3-S8	page
Fig. S13-S18	MS characterization of monomer 3-8 in MeOH	S9-S11	page
Fig. S19	PCA loading plots in the PC1–PC2 plane of the eight element sensors (1-8) in the developed arrays	S12	page
Fig. S20	PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from 2 and 8 after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)	S12	page
Fig. S21	PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from 3 and 8 after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)	S13	page
Fig. S22	PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from 2 and 3 after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)	S13	page
Fig. S23	Appearance of tested automotive fuels in this investigation	S14	page

Fig. S24

RGB color change profile of paper-based PDA sensor array
prepared from **2,3** and **8** after exposure to saturated vapors of
automotive fuels

S14 page

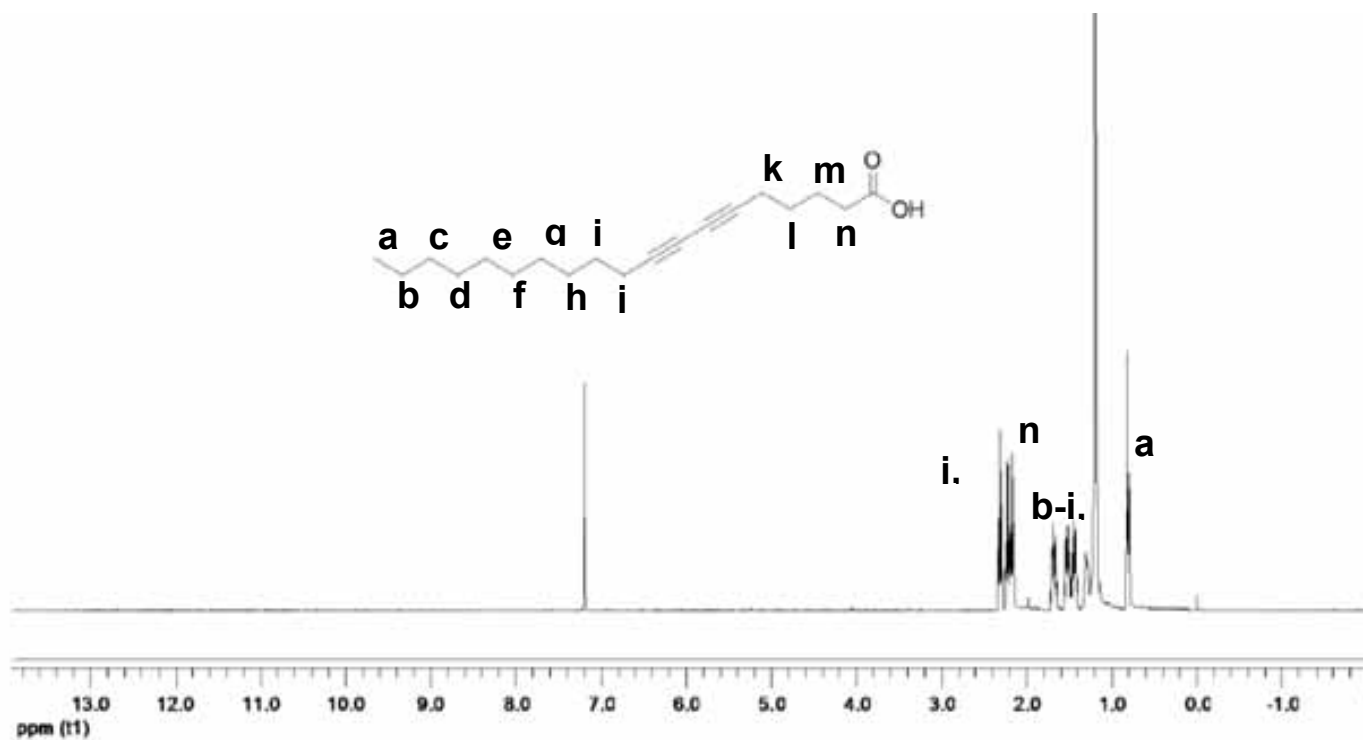


Fig. S1: ^1H NMR of 3 in CDCl_3

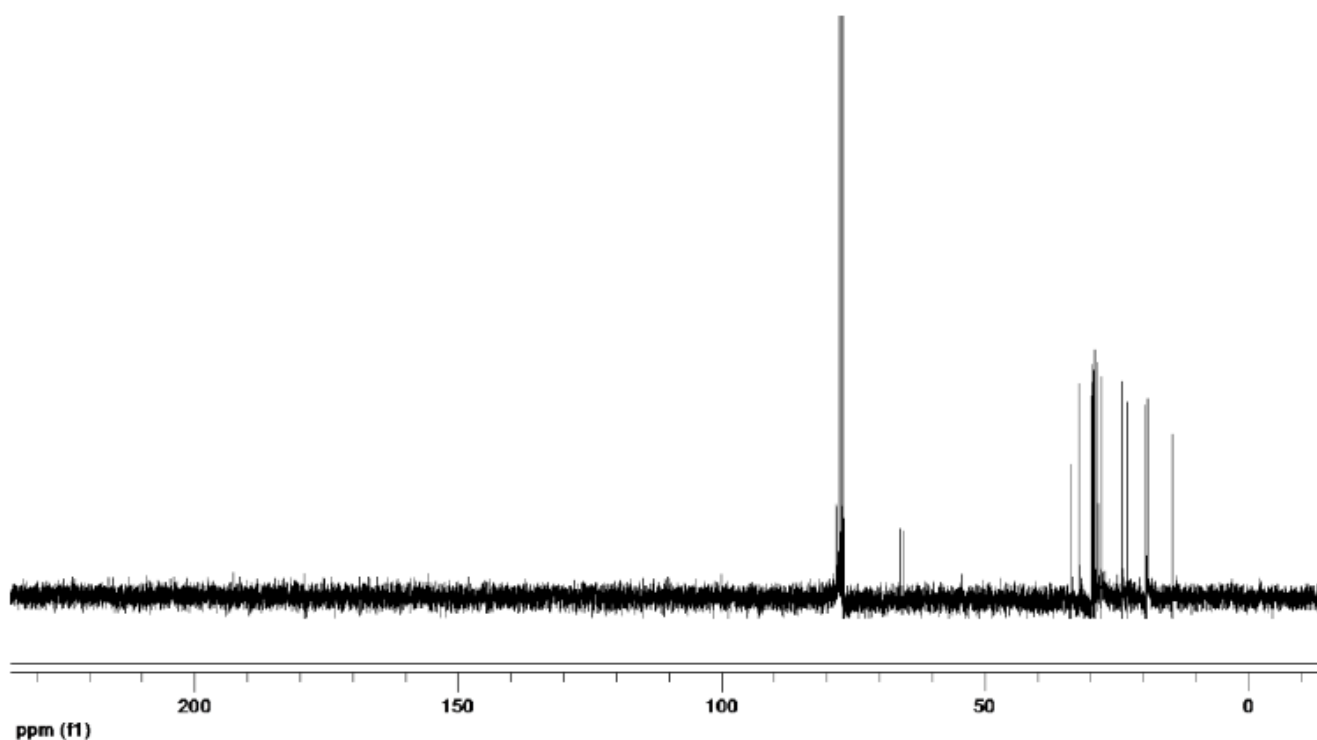


Fig. S2: ^{13}C NMR of 3 in CDCl_3

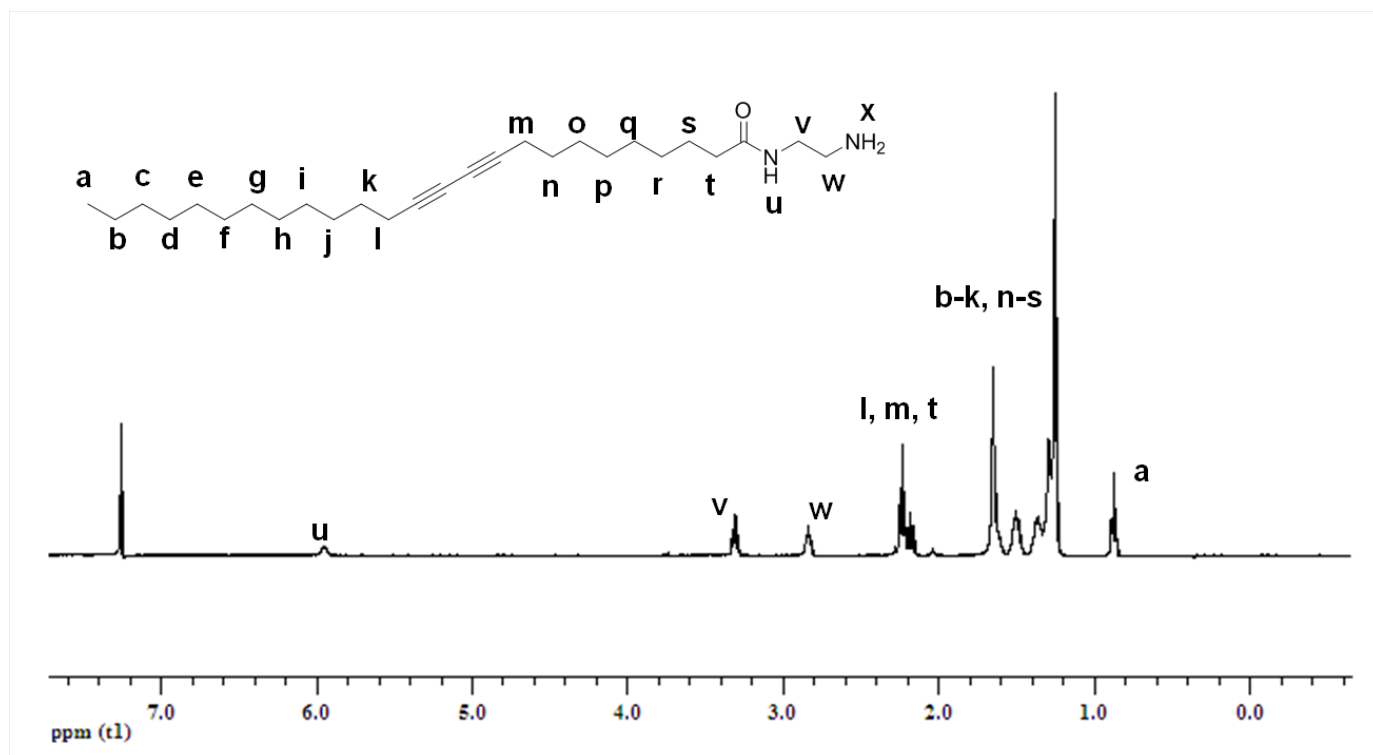


Fig. S3: ^1H NMR of 4 in CDCl_3

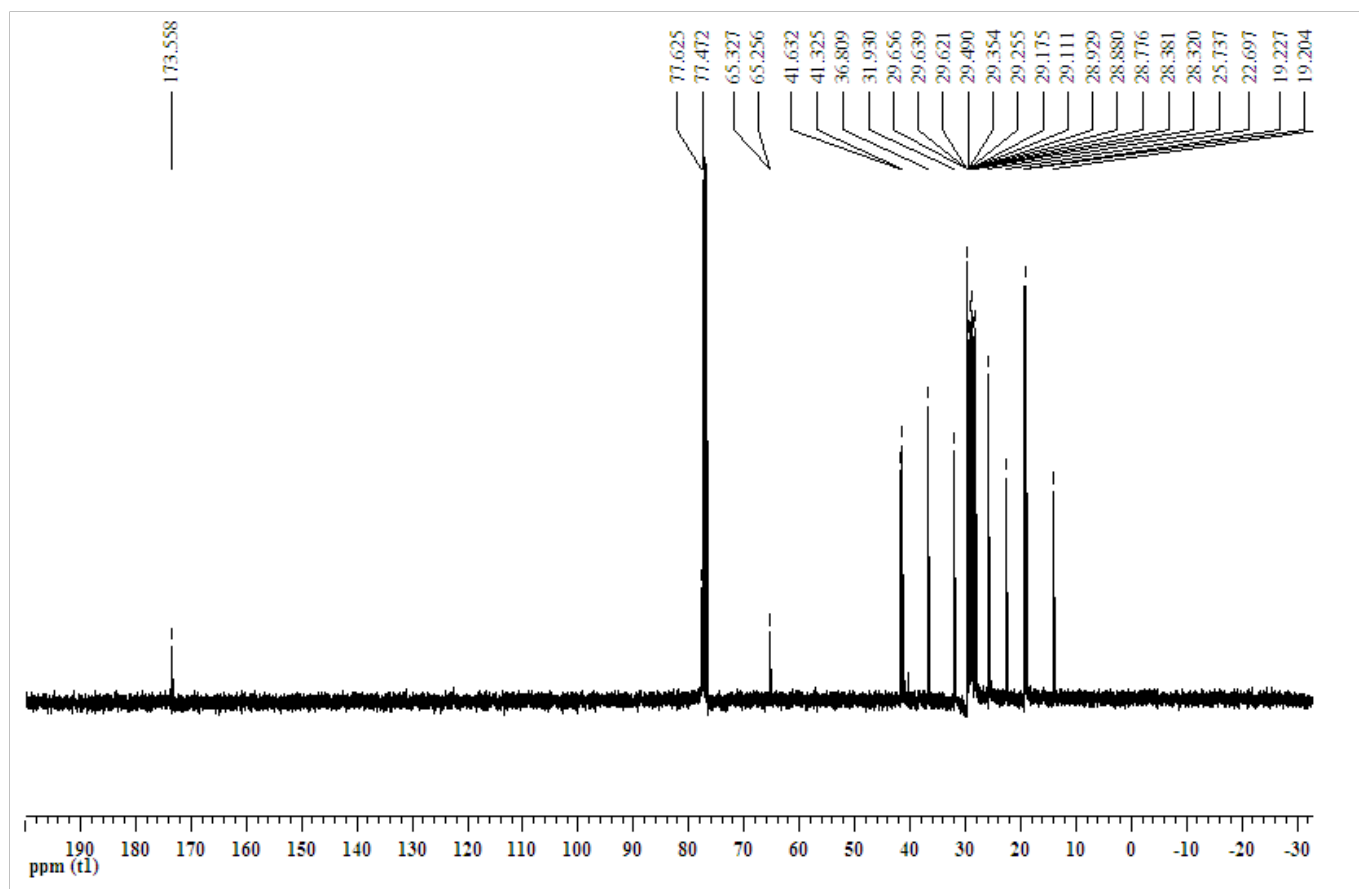


Fig. S4: ^{13}C NMR of 4 in CDCl_3

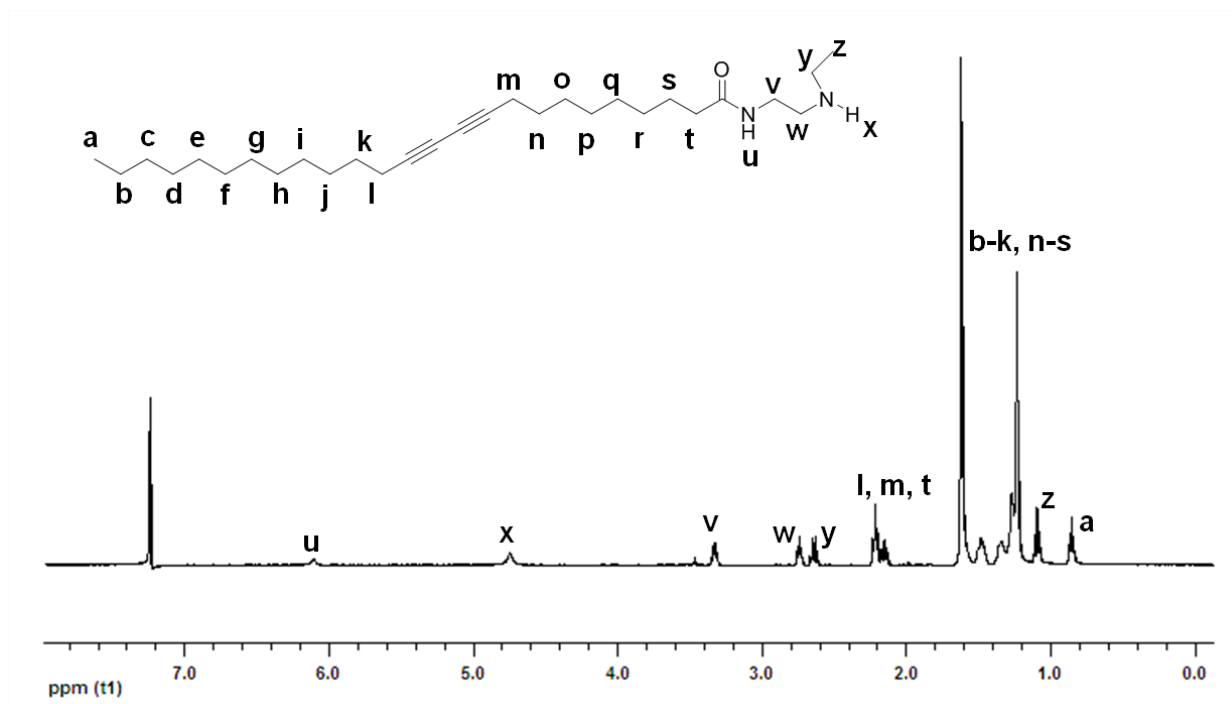


Fig. S5: ^1H NMR of 5 in CDCl_3

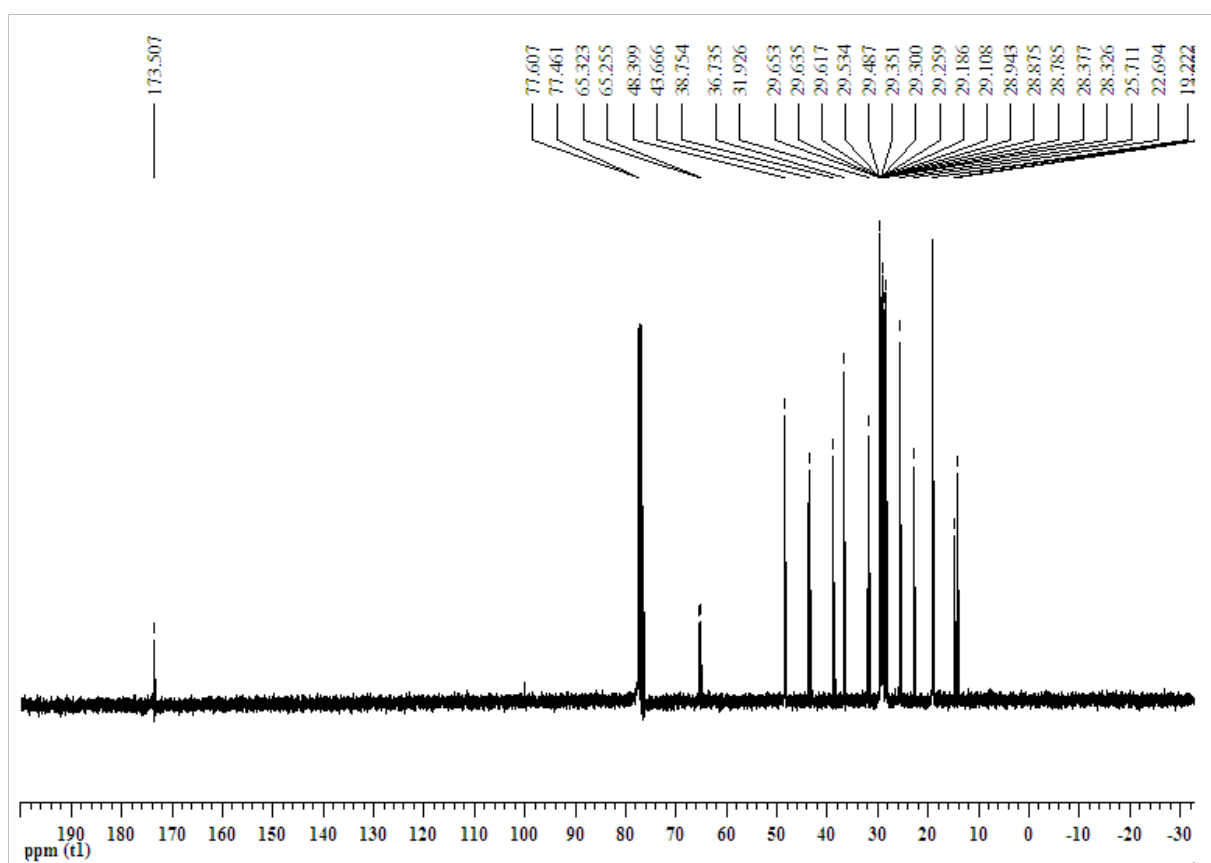


Fig. S6: ^{13}C NMR of 5 in CDCl_3

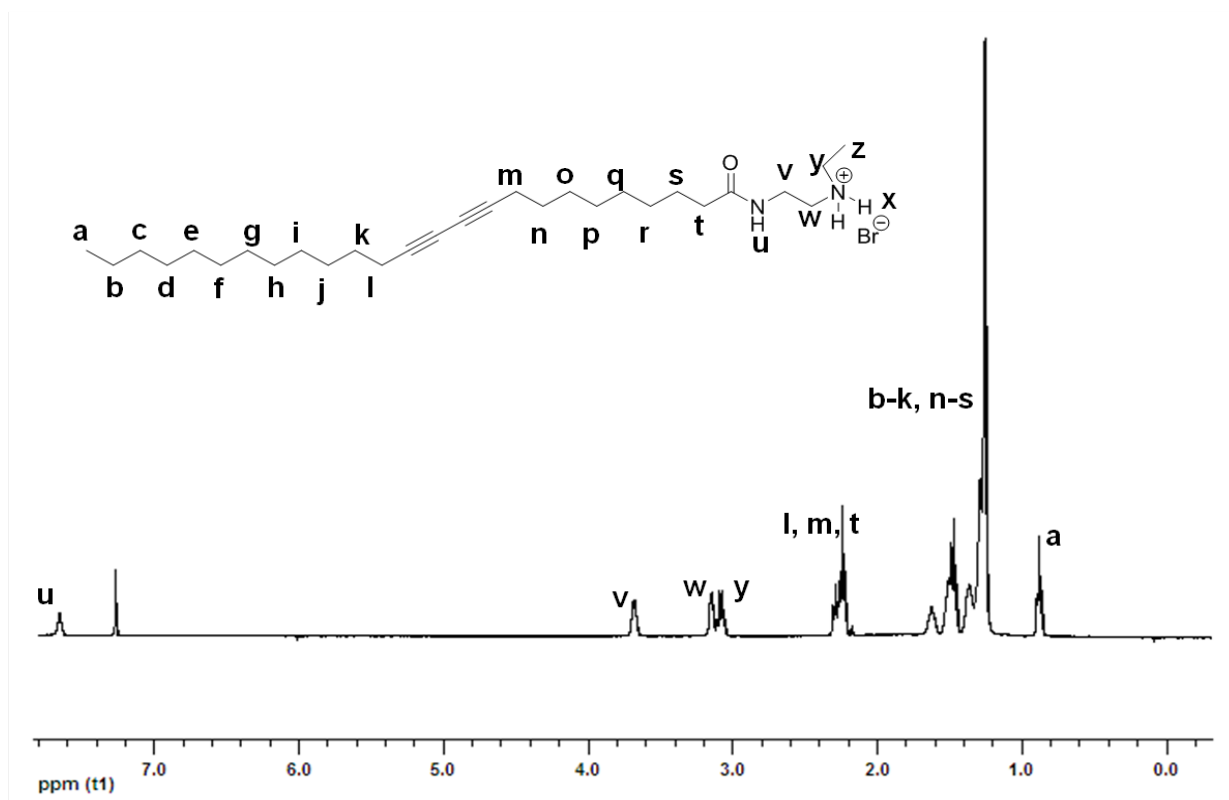


Fig. S7: ^1H NMR of 6 in CDCl_3

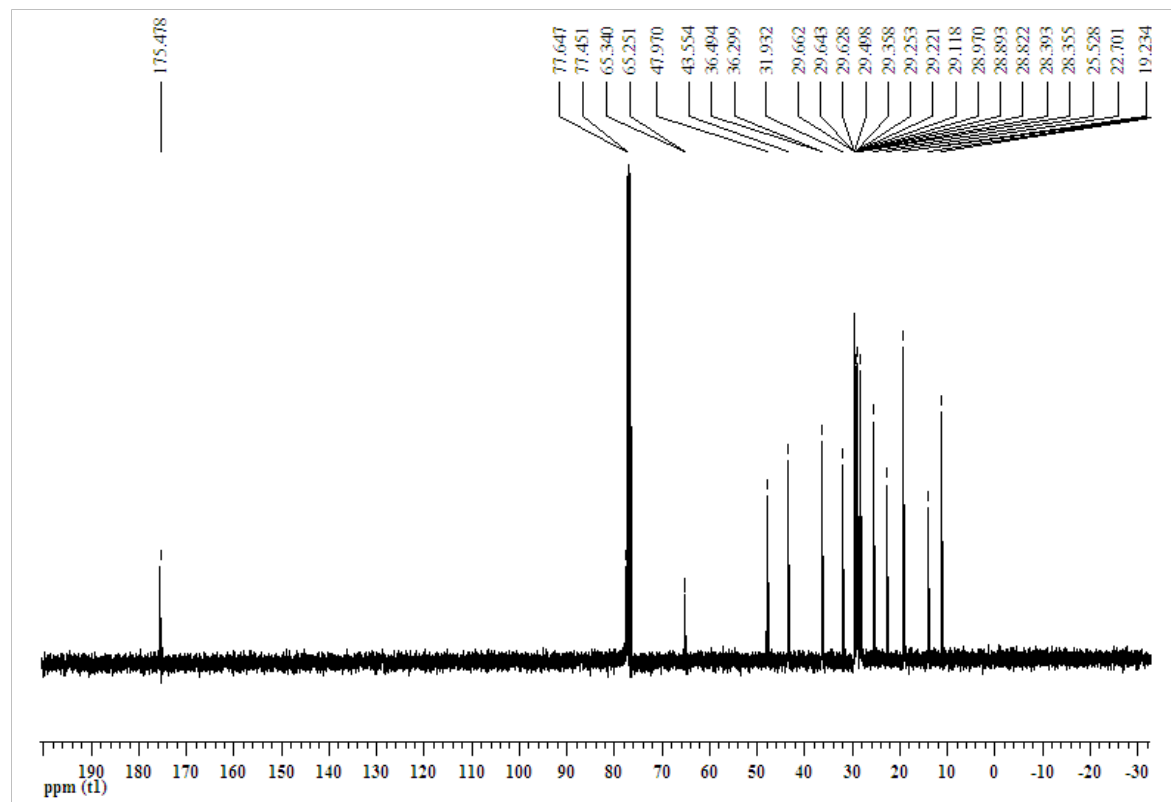


Fig. S8: ^{13}C NMR of 6 in CDCl_3

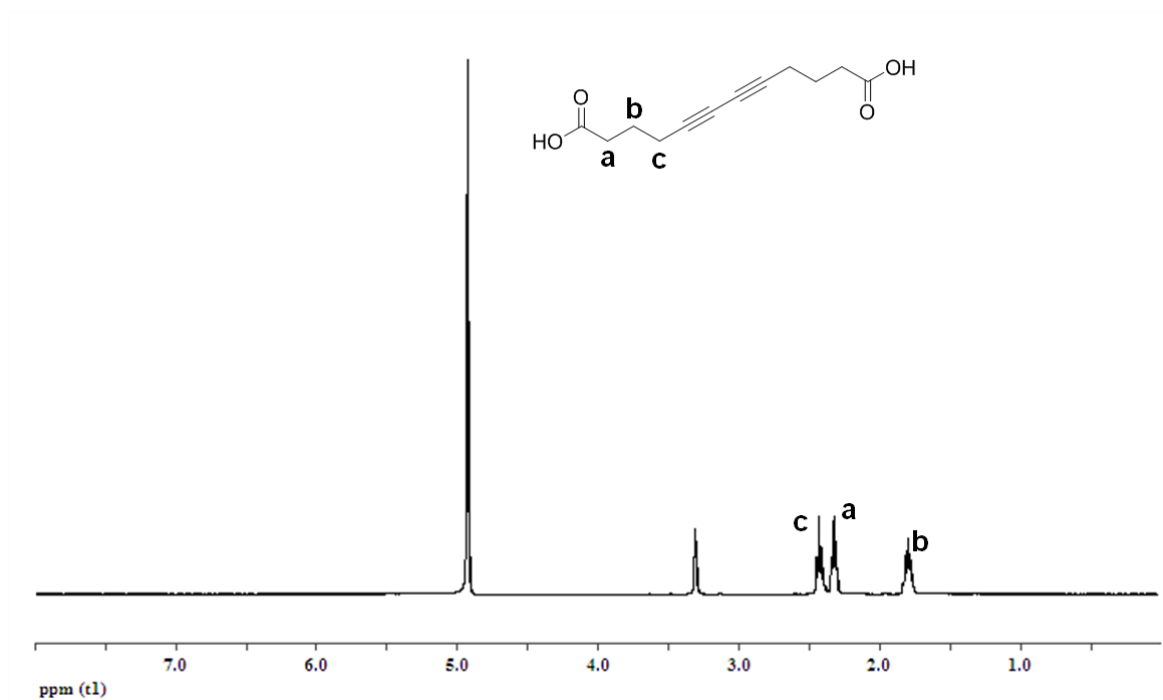


Fig. S9: ¹H NMR of 7 in CDCl₃

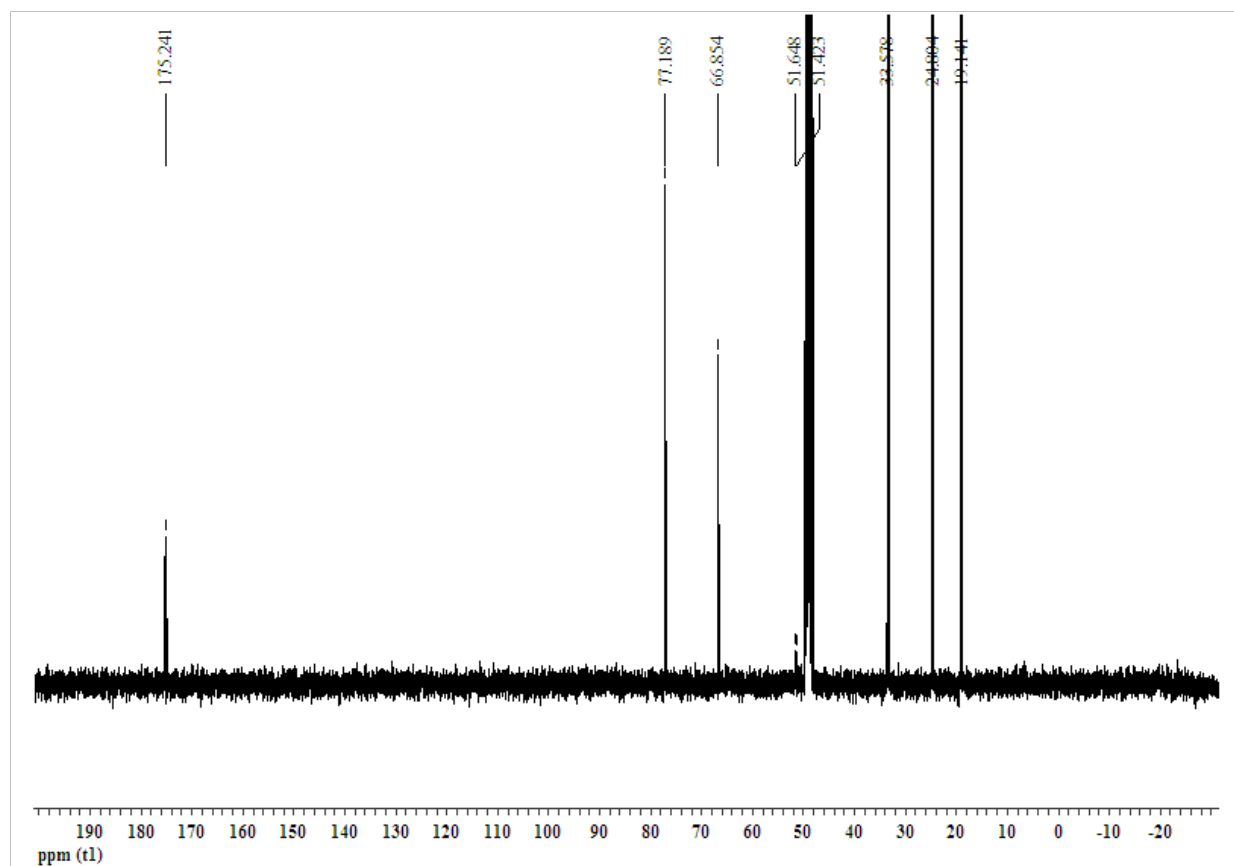


Fig. S10: ¹³C NMR of 7 in CDCl₃

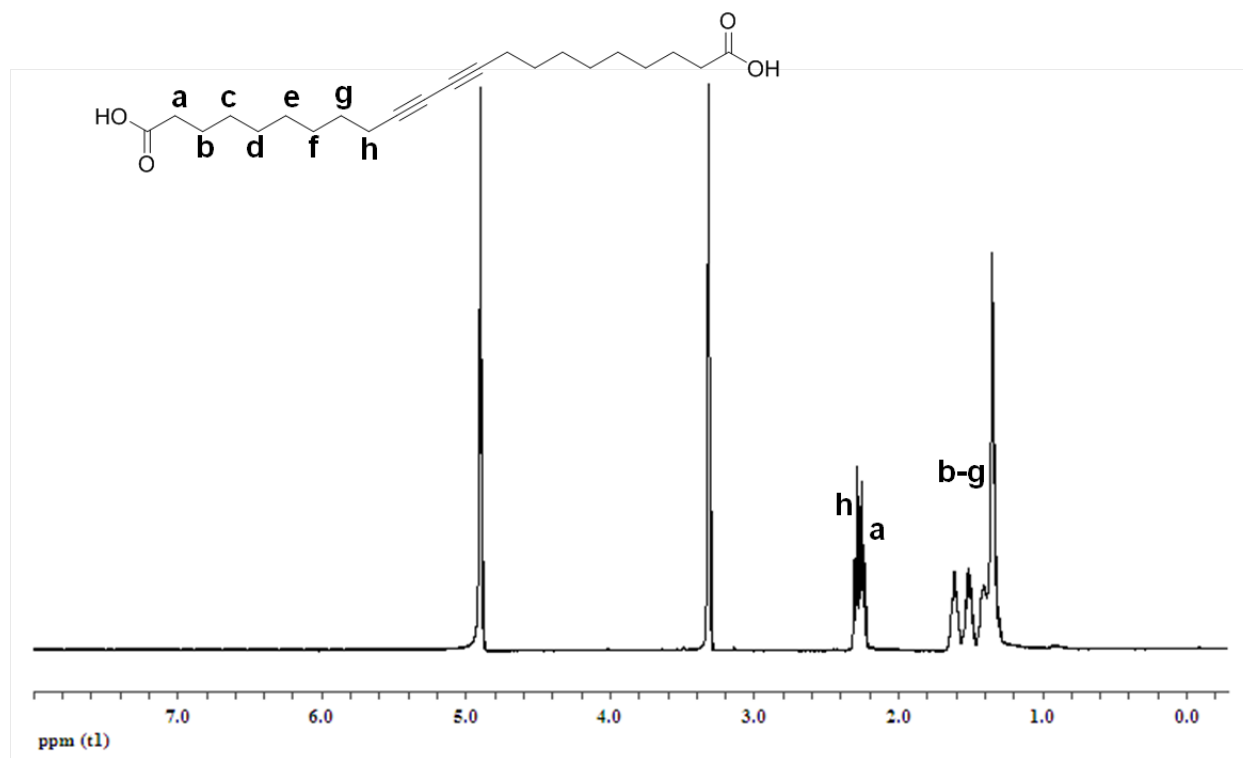


Fig. S11: ¹H NMR of 8 in CDCl₃

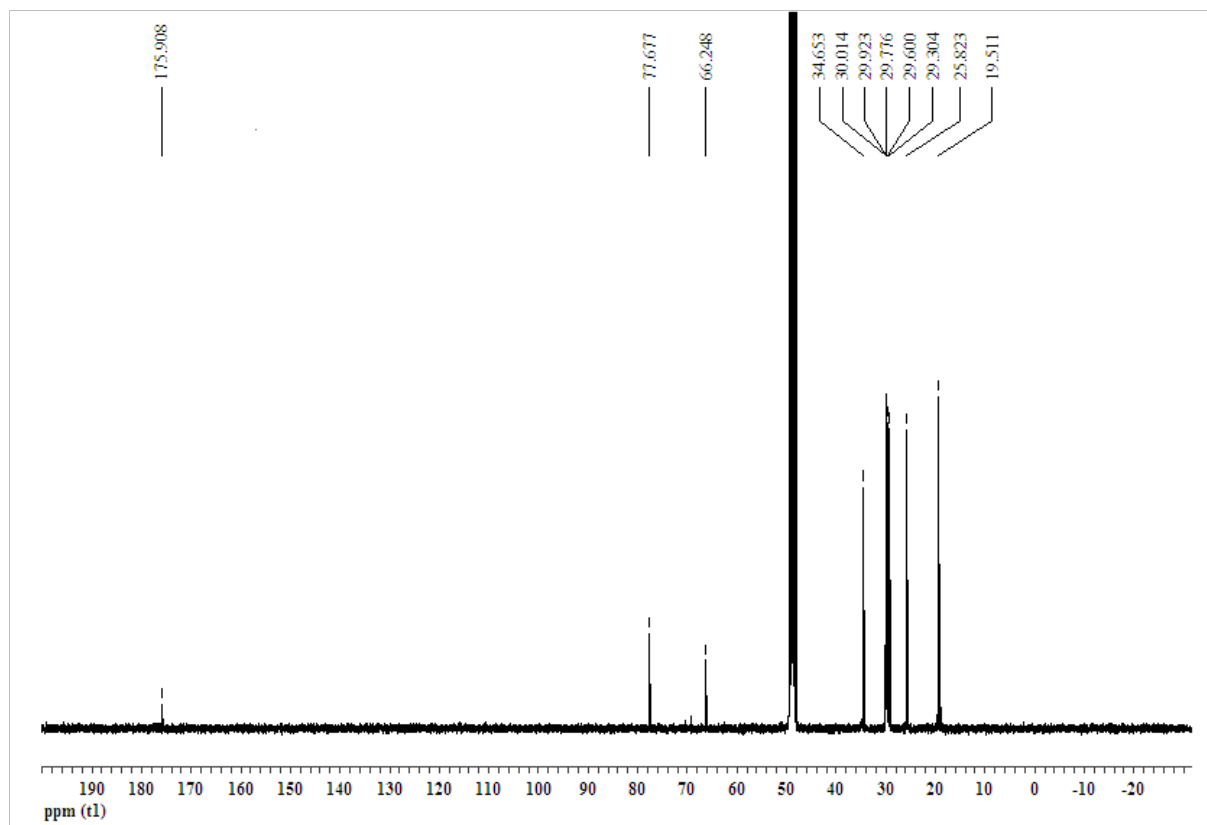


Fig. S12: ¹³C NMR of 8 in CDCl₃

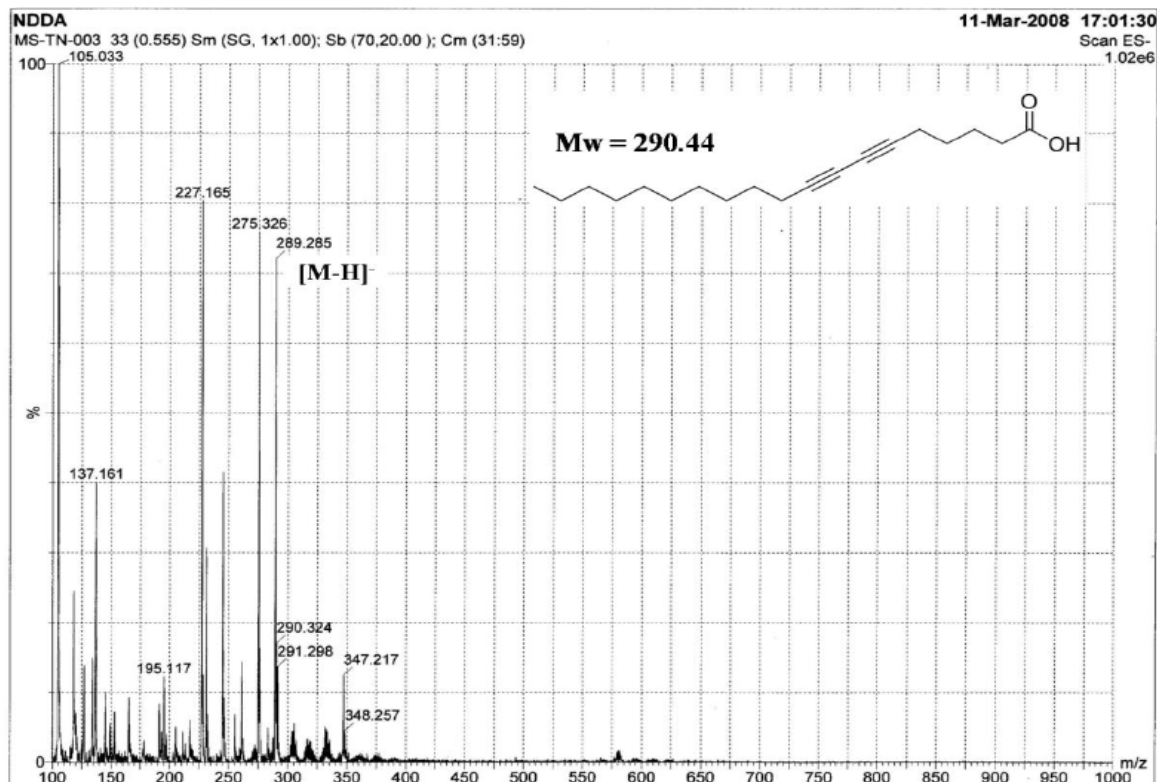


Fig. S13: Mass Spectra (ESI-) of monomer 3

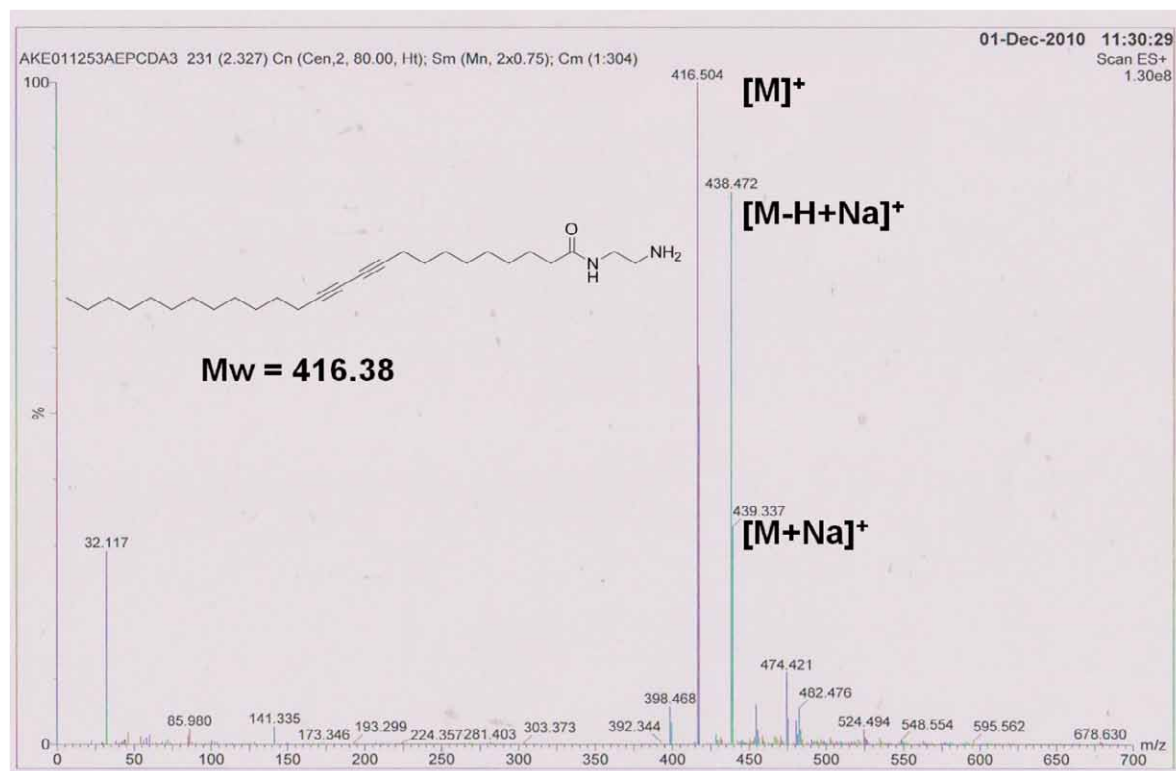


Fig. S14: Mass Spectra (ESI+) of monomer 4

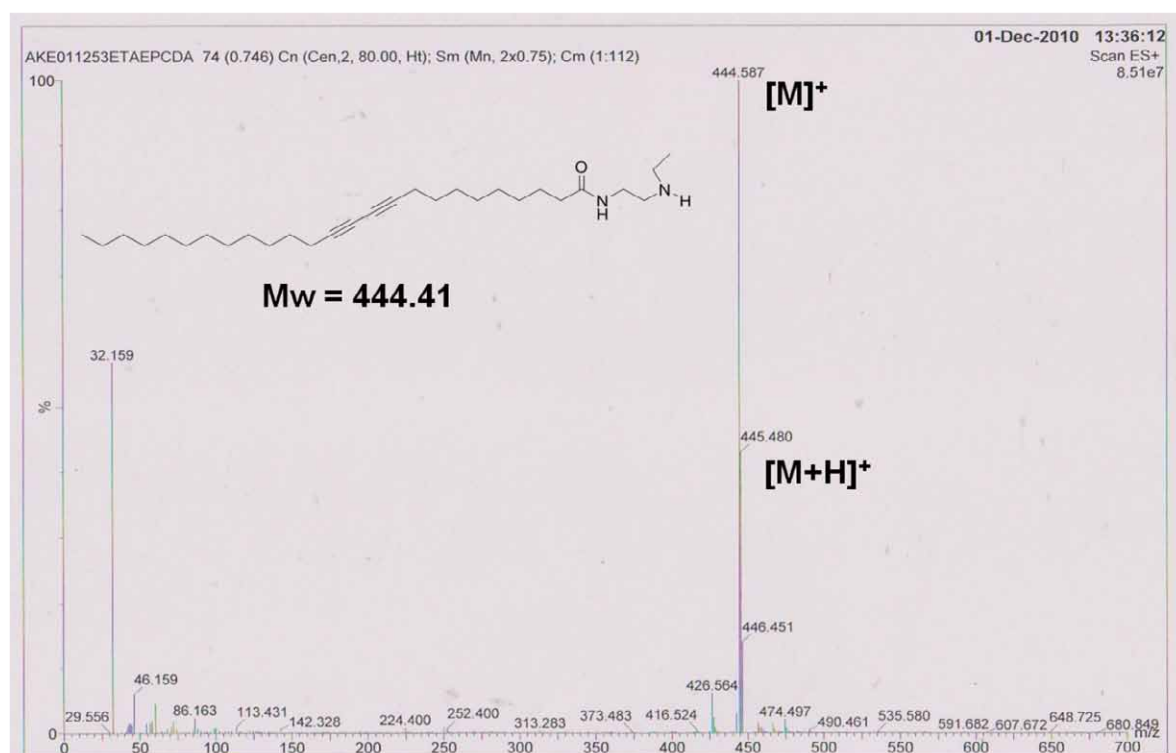


Fig. S15: Mass Spectra (ESI⁺) of monomer 5

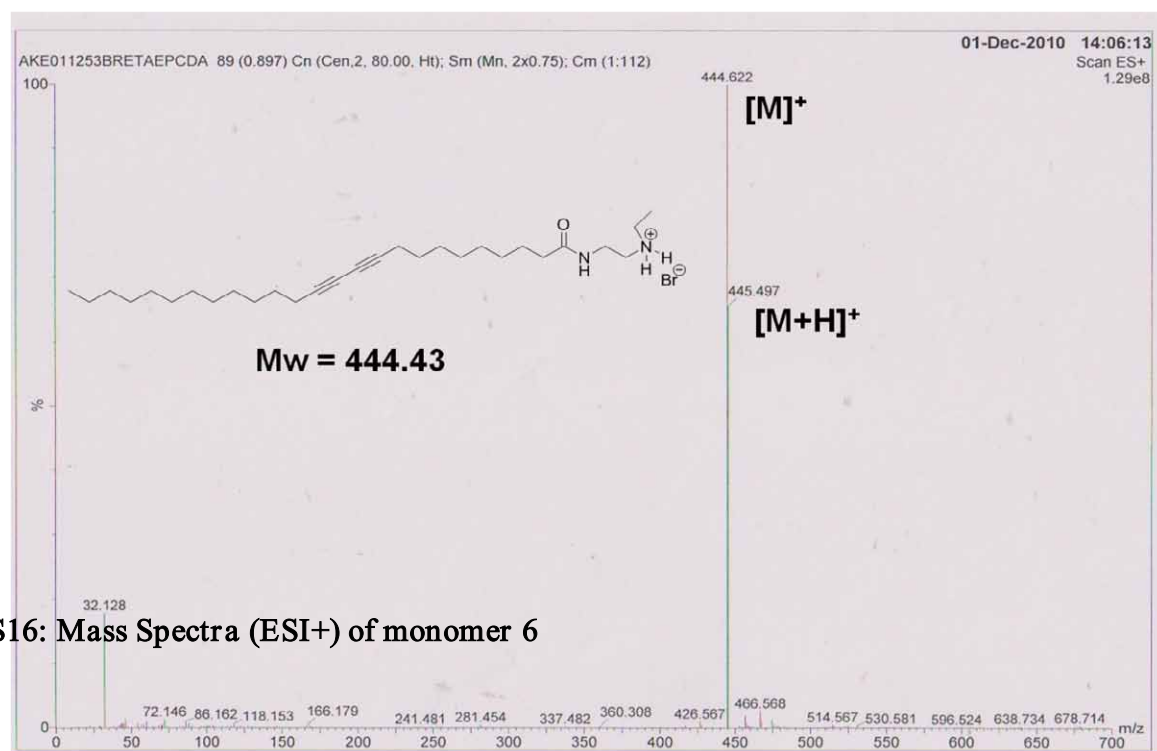


Fig. S16: Mass Spectra (ESI⁺) of monomer 6

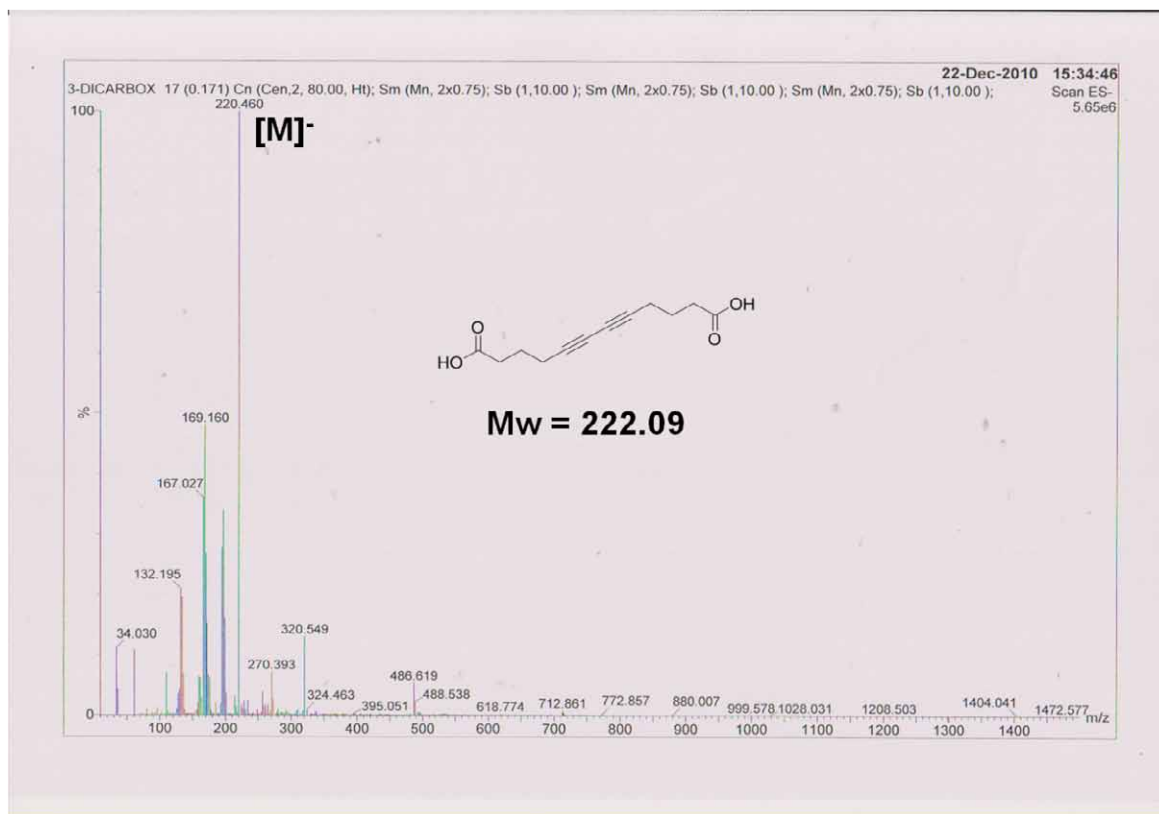


Fig. S17: Mass Spectra (ESI+) of monomer 7

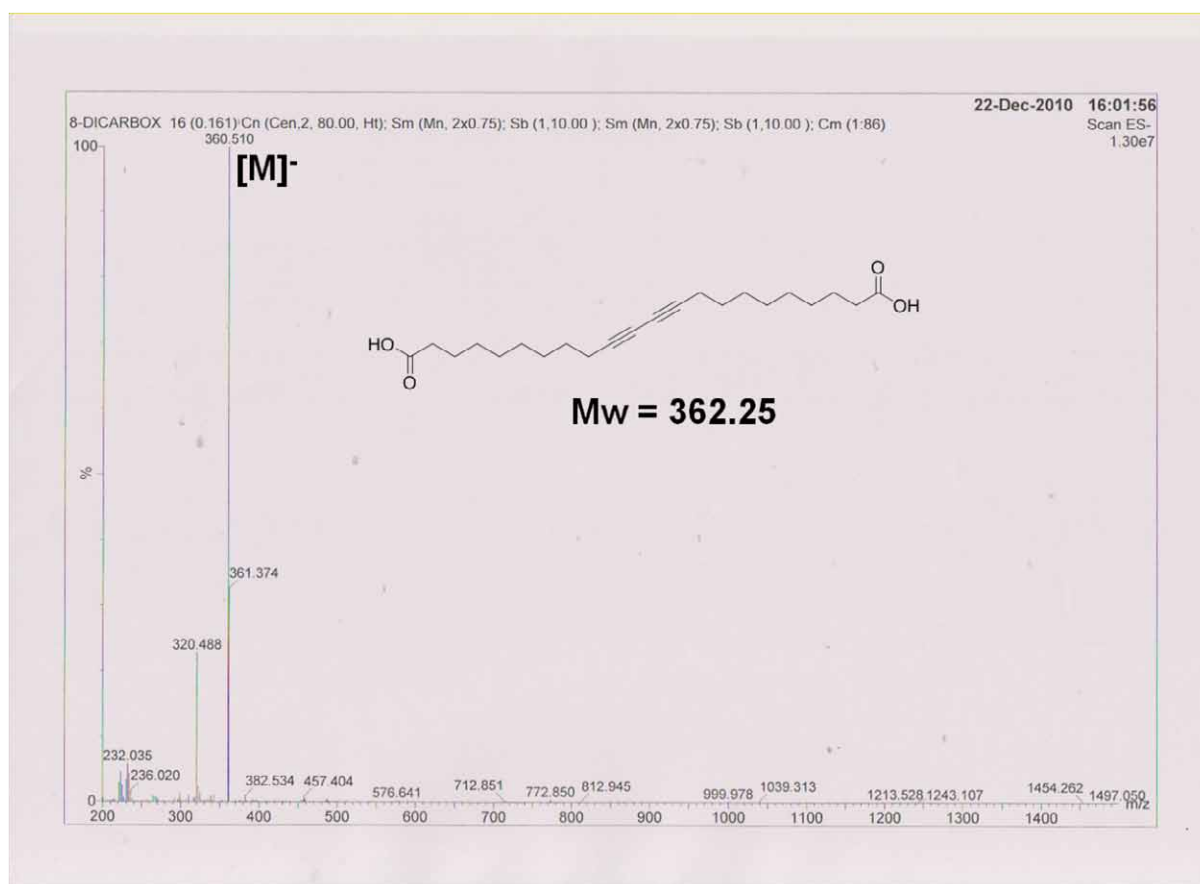


Fig. S18: Mass Spectra (ESI+) of monomer 8

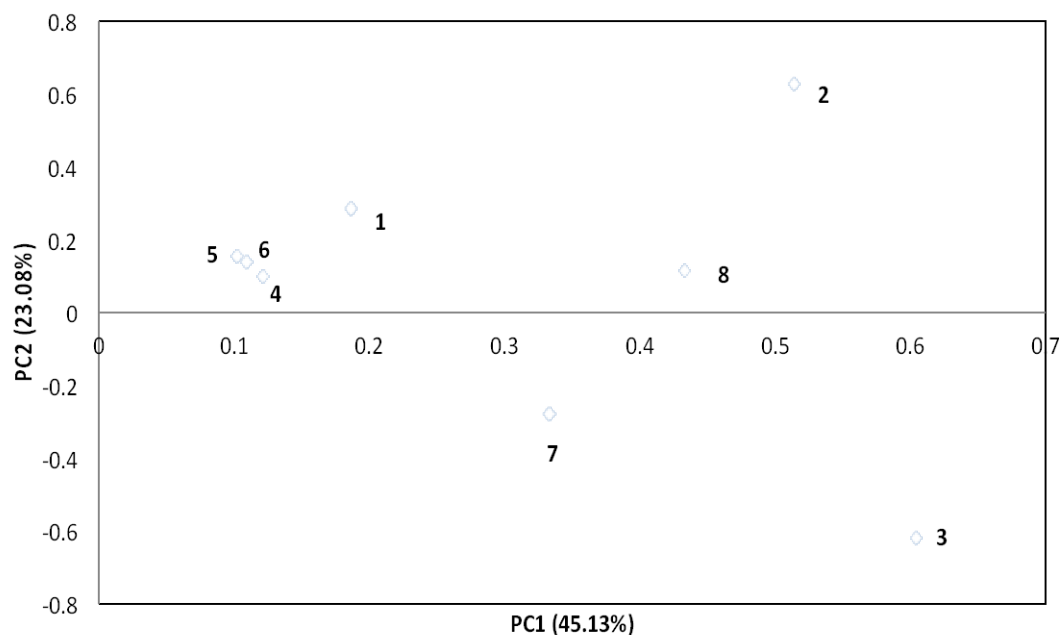


Figure 19. PCA loading plots in the PC1–PC2 plane of the eight element sensors in the developed arrays

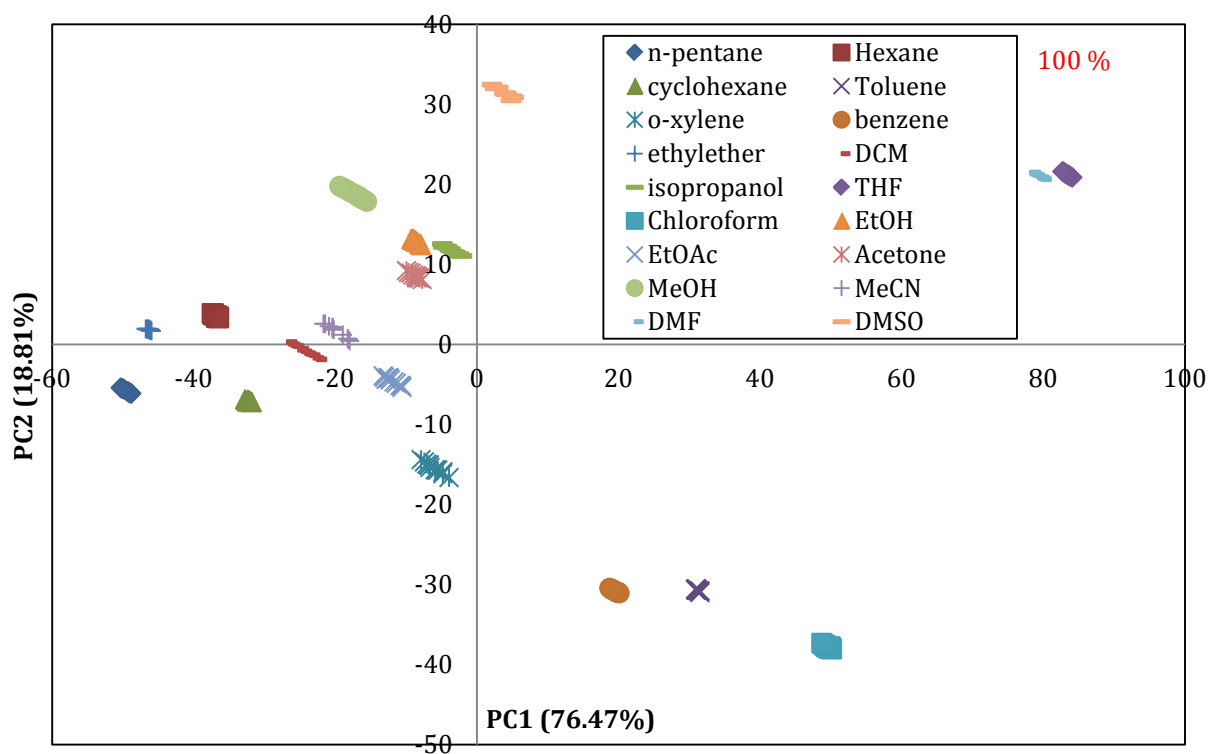


Figure S20. PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from **2** and **8** after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)

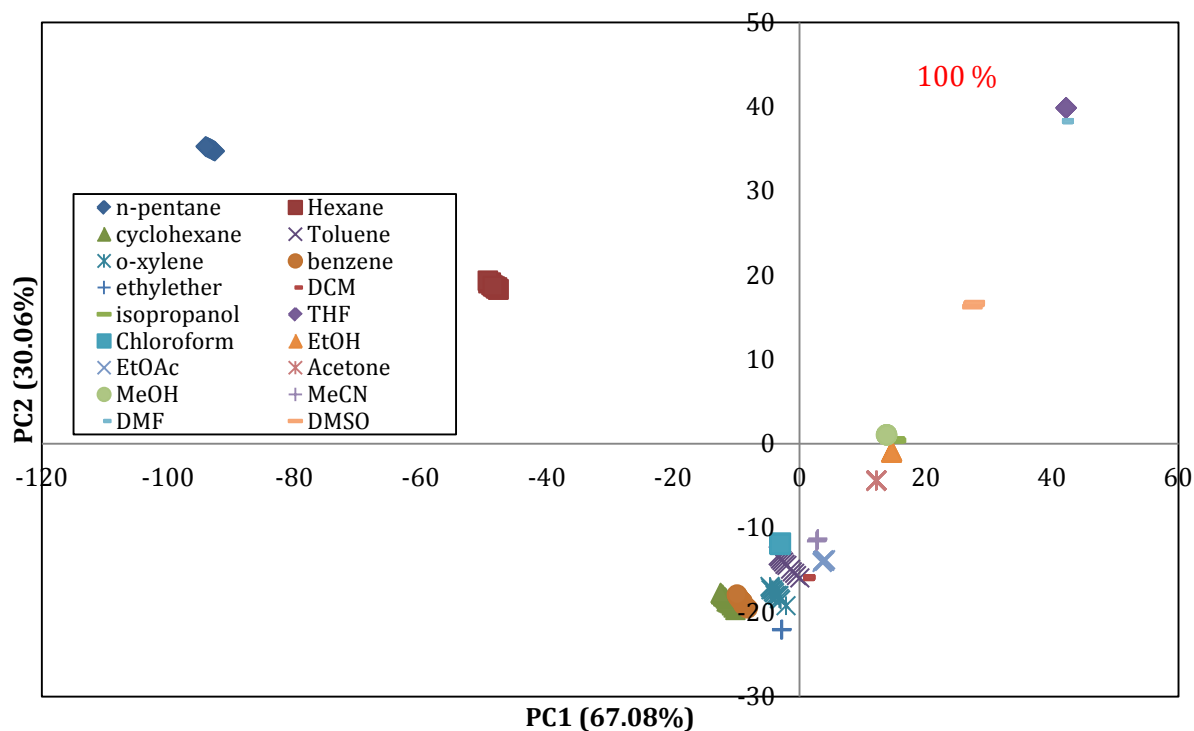


Figure S21. PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from **3** and **8** after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)

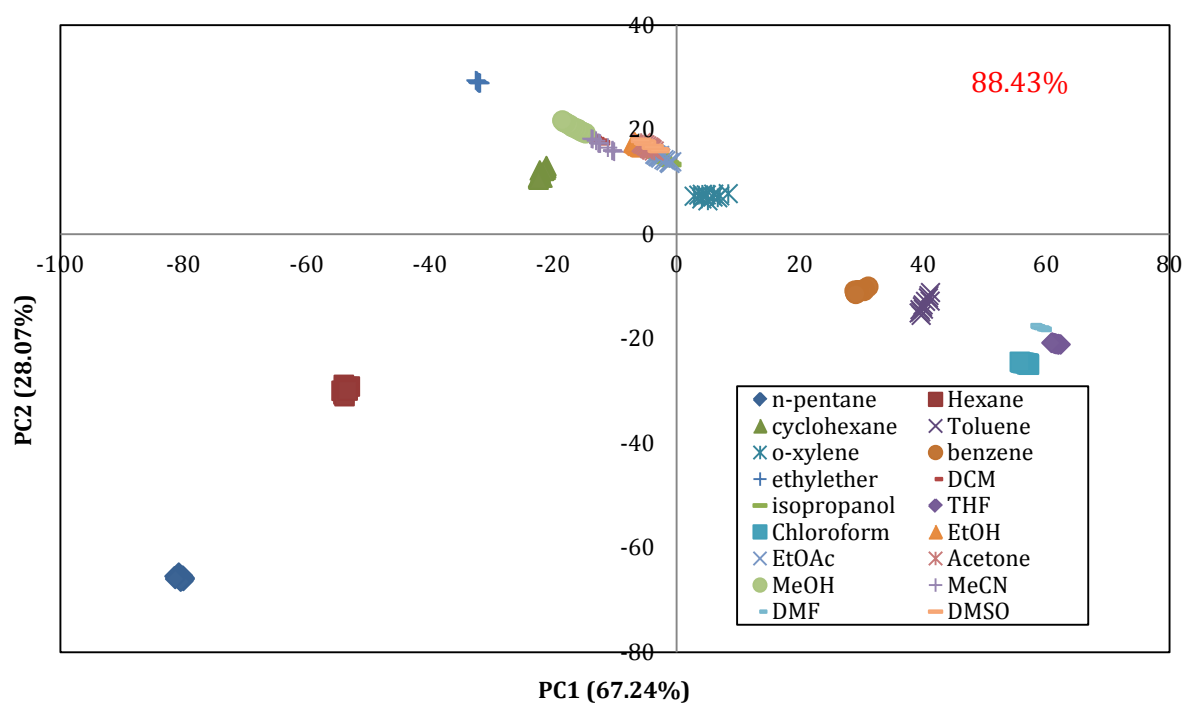


Figure S22. PCA score plot of RGB color changes obtained from the paper-based PDA sensor array prepared from **2** and **3** after exposure to 18 VOC vapors (2 PDAs x 4 replicates x 18 VOCs x 3 measurements)

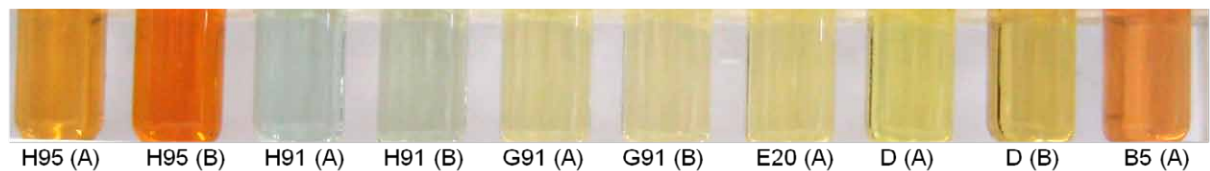


Figure S23. Color of tested automotive fuels in this investigation

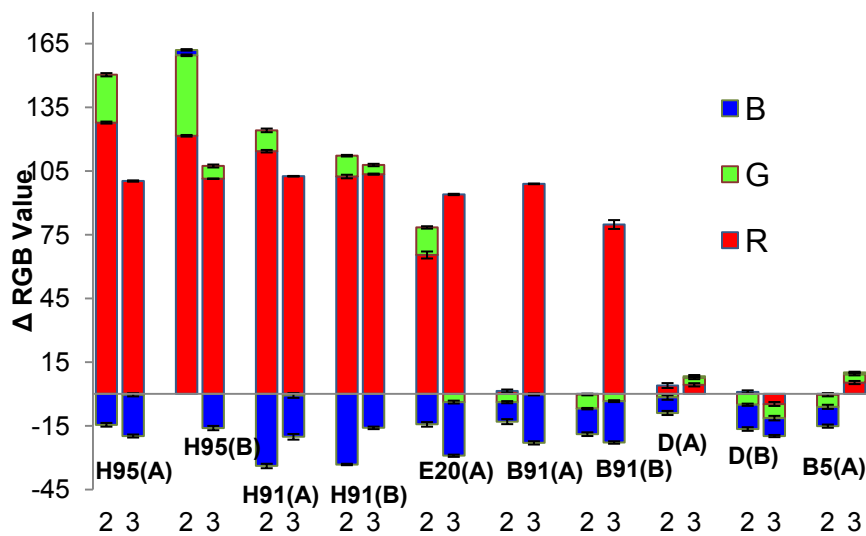


Figure S24. RGB color change profile of paper-based PDA sensor array prepared from **2** and **3** after exposure to saturated vapors of automotive fuels