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Supporting Information

Polydiacetylene (PDA) Impregnated Poly(vinylidene fluoride) (PVDF) Membrane for Sensitive Detection of Fluoride Ions

Ankit Thakuri,[a] Raghunath Acharya,[b,c] Mainak Banerjee,*[a] and Amrita Chatterjee*[a]

[a]*Department of Chemistry, BITS-Pilani, K.K. Birla Goa Campus, NH 17B, Bypass Road, Zuarinagar, Sancoale, Goa-403726, INDIA.*

[b]*Radiochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, INDIA.*

[c]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400085, INDIA.*

**Email id: amrita@goa.bits-pilani.ac.in, mainak@goa.bits-pilani.ac.in*

Table of contents

Sr. No.	Title	Page No.
1	Images of the experimental setup of **PDABA@PVDF** membrane based fluoride detection	S2
2	Synthesis of the probe **PDABA**	S2
3	NMR Spectra of **PDABA**	S3
4	IR spectra	S4
5	HRMS spectra of **PDABA**	S5
6	Images of strips with varying PCDA:**PDABA** ratio	S5
7	Images of **PDABA@PVDF** strips under long UV (365 nm)	S6
8	Liposome Preparation	S5
9	Variation in response time with concentration	S6
10	Linear trend in response of **PDABA@PVDF** strips towards fluoride.	S7
11	Comparison of **PDABA@PVDF** membranes with IC for fluoride detection	S7
12	Comparative table of solid-phase detection of fluoride ions	S9
13	References	S11

1. Experimental setup

Figure S1: Images of the experimental setup of **PDABA@PVDF** membrane based fluoride detection.

2. Synthesis of the probe PDABA[1]

10,12-Pentacosadiynoic acid (0.374 g, 1 mmol) was dissolved in dichloromethane (5 mL) and to the solution, oxalyl chloride (0.3 mL, 3.5 mmol) was added dropwise under nitrogen atmosphere. After 1 h of stirring, one drop of DMF was added to the solution, and the resulting mixture was stirred for another 4 h. After the solvent was evaporated, the crude acid chloride was dissolved in 5 mL anhydrous THF, placed in an ice bath under nitrogen atmosphere and to it, a solution of 4-hydroxyphenyl boronic acid (0.41 g, 3 mmol) and triethylamine (1.4 mL, 10 mmol) in 5 mL of THF was slowly added and the mixture was stirred overnight at room temperature. The crude residue obtained after solvent removal was dissolved in a small amount of methanol and was added dropwise to cold water. The precipitates formed were collected and subjected to column chromatography on a silica gel and eluted with dichloromethane-methanol (10:1) to give the desired product (yield 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.24 (d, *J* = 8 Hz, 2H), 2.61–2.54 (m, 2H), 2.28–2.22 (m, 4H), 1.82–1.73 (m, 2H), 1.53–1.47 (m, 4H), 1.41–1.25 (m, 26H), 0.87 (t, *J* = 8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 172.3, 153.0, 135.2, 129.8, 121.1, 65.3, 46.0, 34.4, 31.9, 29.6, 29.5, 29.4, 29.1, 28.9, 28.8, 28.4, 28.3, 24.9, 22.7, 19.2, 14.1; IR (ν, ATR): 3318, 2916, 2851, 1751, 1600, 1469, 1348, 1220, 1117, 1016, 807, 719 cm^{-1}; HRMS (ESI, *m/z*) calcd for $C_{31}H_{47}BO_4$ $[M+H]^+$ 495.3646, found: 495.3649.

3. [1]HMNR spectra

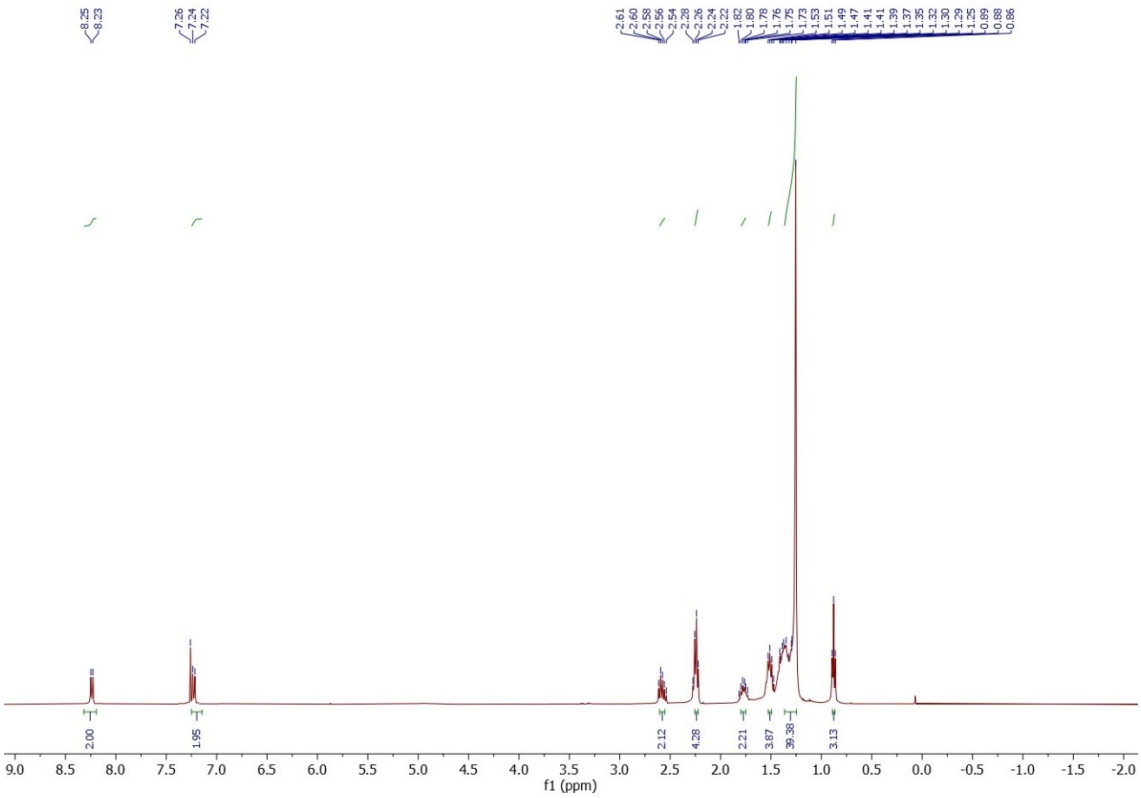


Figure S2. [1]H NMR (400 MHz, $CDCl_3$) spectra of **PDABA**.

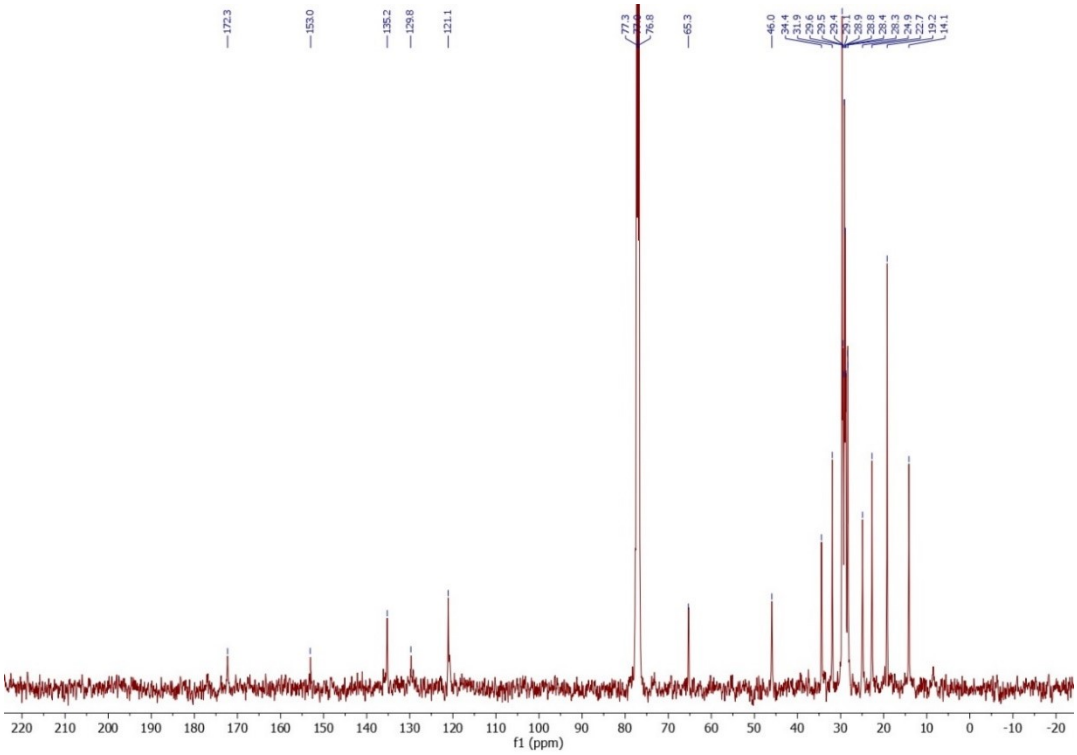


Figure S3. [13]CNMR (100 MHz, $CDCl_3$) spectra of **PDABA**.

4. IR spectra of PCDA and PDABA

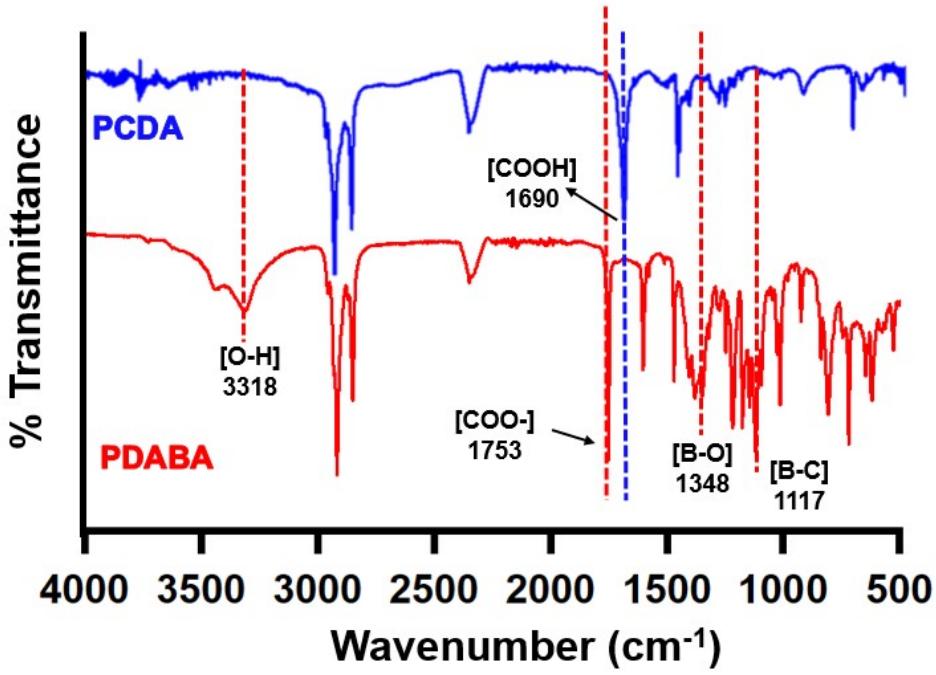
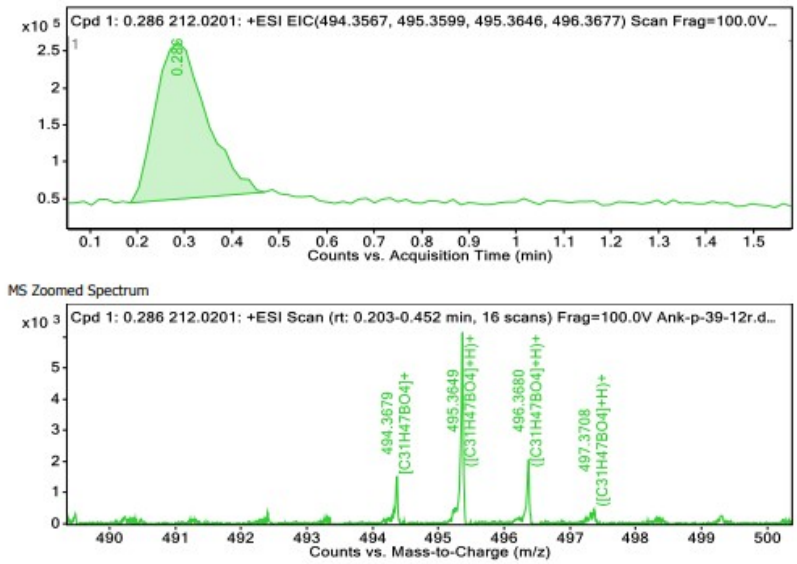


Figure S4. IR spectra of PCDA (blue) and **PDABA** (red).

5. HRMS spectra



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
494.3679	494.3567	-22.59	1	1503.4	C31H47BO4	M+
495.3649	495.3646	-0.75	1	6166.98	C31H47BO4	(M+H)+
496.368	496.3677	-0.65	1	2058.43	C31H47BO4	(M+H)+
497.3708	497.3707	-0.08	1	472.48	C31H47BO4	(M+H)+

Figure S5. HRMS spectra of **PDABA**.

6. Strips bearing different compositions of PCDA: PDABA

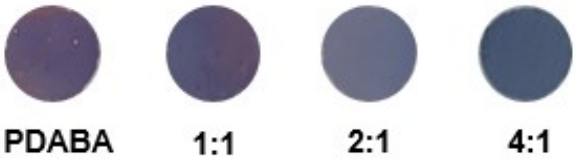


Figure S6: Images of strips prepared using varying concentrations of PCDA:**PDABA**. The strips were dipped irradiated for 1 min under UV light (254 nm) and the images were taken after 5 min.

7. Images of strips under UV

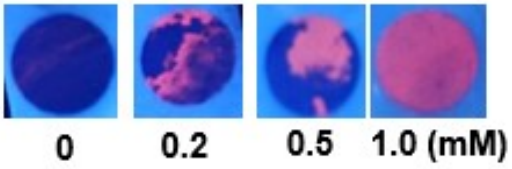


Figure S7: Fluorescent images of **PDABA@PVDF** strips dipped in fluoride solution for 1 h and images were taken under long UV light (365 nm)**.**

8. Liposome preparation

For the preparation of liposomes the mixture of PCDA:**PDABA** was dissolved in chloroform and then, the organic solvent was evaporated under nitrogen flow, and HEPES buffer (10 mM, pH 7.4) was added to attain a total concentration of 1 mM. The solution was then probe-sonicated at 80 ^{o}C for 20 min to afford a turbid solution. The suspension was then filtered through a syringe filter (0.45 μm) and stored overnight at 4 ^{o}C. This liposome suspension was then utilized for fluoride detection.

Figure S8. Schematic representation of liposome formation between PCDA and **PDABA**.

9. Variation in response time with concentration

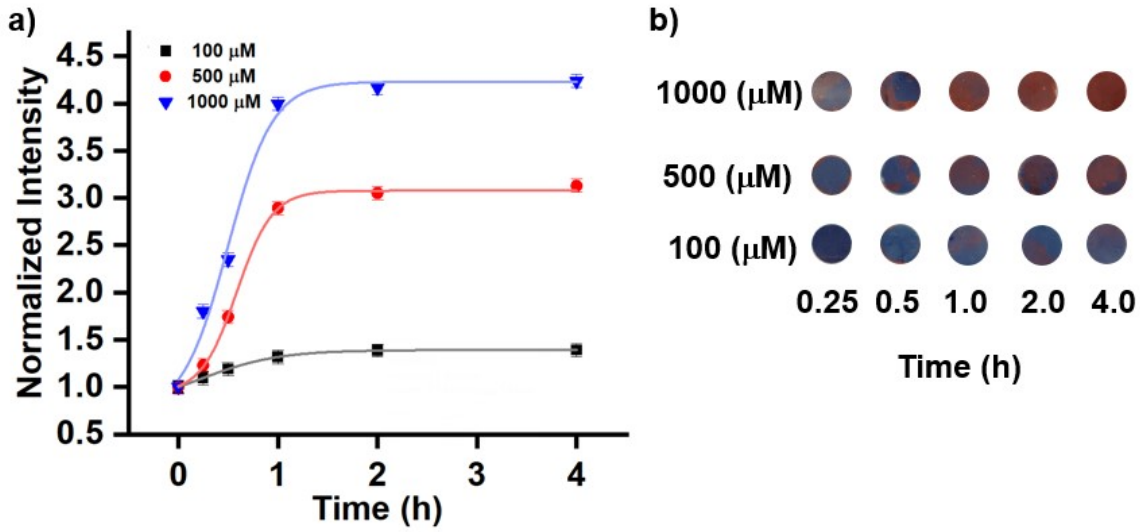


Figure S9. (a) Response-time variation of the **PDABA@PVDF** strips against different concentrations of fluoride. The RGB data were collected using the images captured through three different cameras viz. Mi 10i (108 MP), Redmi Note 8 pro (64 MP), Redmi Note 9 pro max (64 MP) and the average value of the data were presented. (b) Images of the strips exposed to different concentrations for varying times.

10. Linear trend in response of PDABA@PVDF strips towards fluoride.

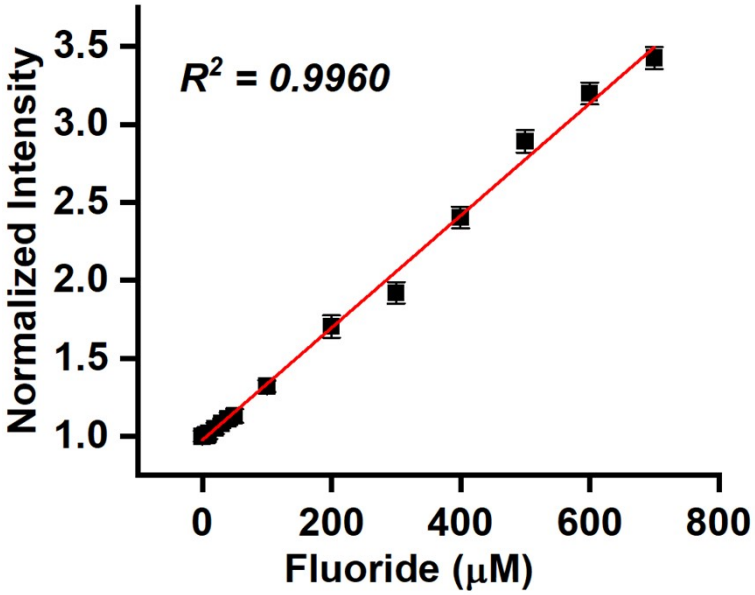


Figure S10. Response of **PDABA@PVDF** strips against higher concentration of fluoride.

11. Comparison of PDABA@PVDF membranes with IC for fluoride detection in real samples

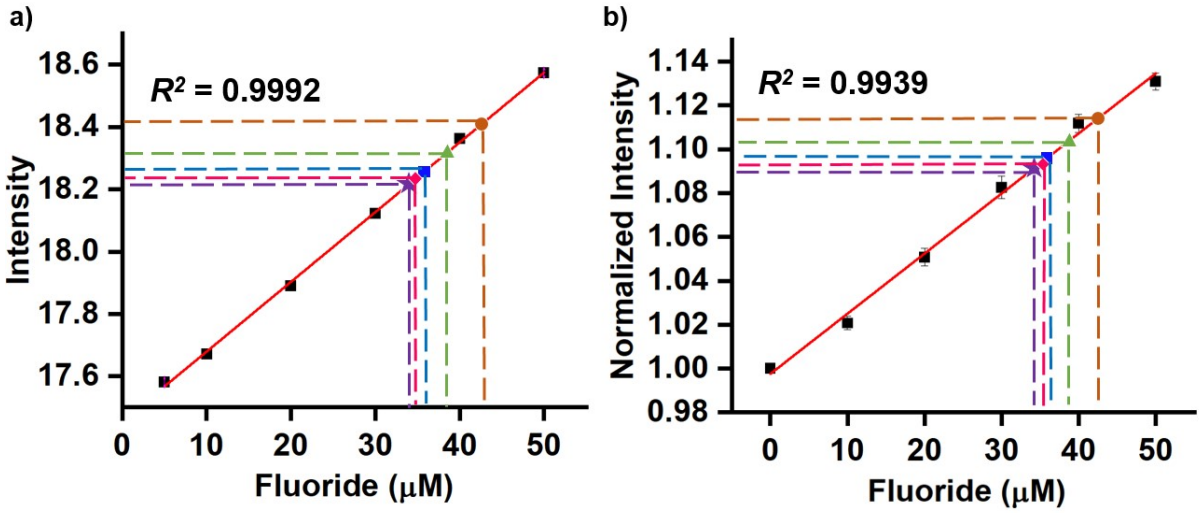
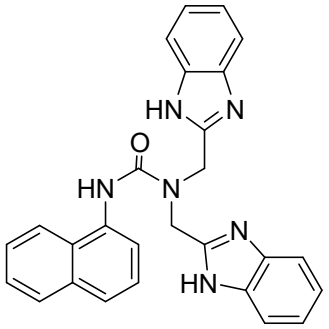
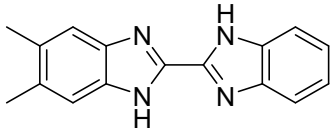
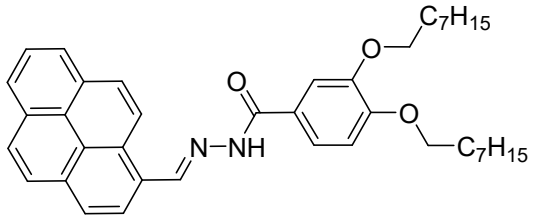
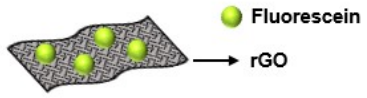
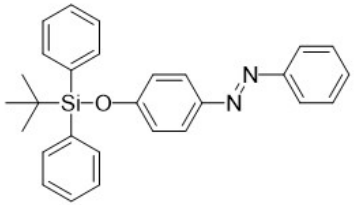
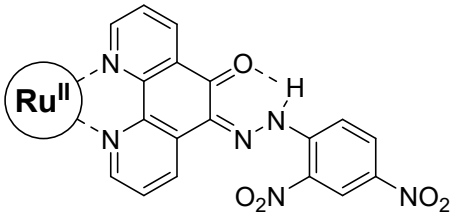
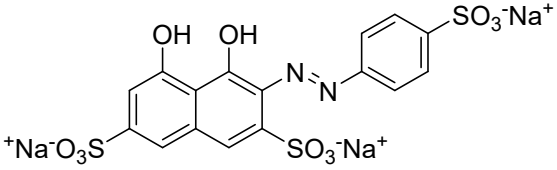


Figure S11. Fluoride ion content analysis of different toothpaste via (a) IC and (b) **PDABA@PVDF** strips (five different toothpaste were used).

12. Comparative table of molecular sensor based solid-phase detection of fluoride ions

Sr. No.	Probe structure	Solid platform	Mode of detection	LOD (μM)	Time	Working range (μM)	Ref.
1		Filter paper	Fluorimetric	100	< 2 min	NA	S2
2		NA	Fluorimetric	NA	< 2 min	NA	S3
3		Organogel	Colorimetric	NA	< 30 sec	NA	S4
4		Filter paper	Fluorimetric	157	< 2 min	NA	S5

5		Filter paper	Colorimetric	60	< 30 sec	60-250	S6
6			Colorimetric	520	< 2 min	NA	S7
7	 SPADNS reagent	Micropad (μPAD)	Colorimetric	6.85	2 min	12-118	S8
8	PCDA**:PDABA**	PVDF membrane	Colorimetric and Image Analysis	6	60 min	0-700	This work

13. References

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