# Supporting Information

**Starch-Polyvinyl alcoholpolymer film based on-site sensor for ammonia: A cost effective day to day monitoring technique of fish and meat spoilage**

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**Determination of limit of detection (LOD):**

The detection limit of response towards$NH_3$ was calculated by using the following equation:

Detection limit = 3σ/K, where σ is standard deviation. The standard deviation was determined by 10 blank replicate measurements of compounds BP. Here, K is the slop of the linear curve obtained from absorbance of BP versus $NH_3$ concentration.

**Determination of Limit of Quantification (LOQ):**

Mathematically, the Limit of quantification is defined as equal to 10 times the standard deviation of the results for a series of replicates used to determine a justifiable limit of detection**[1]**.LOQ can be calculated according the formula:

$$LOQ = 10\ \sigma/S$$

where, σ = Standard deviation of the response based on either the standard deviation of the blank, the residual standard deviation of the regression line or the standard deviation of y= Intercepts of regression lines and S = Slope of the calibration curve.

**Synthesis of paper strips sensor:**

The strips of the BP are prepared by dipping the filter paper strips in a methanolic solution of Triphenyl methane based sensor (BP) (5 mM) and dried for 5 minutes in an oven (60 ºC).

**Synthesis of HBP:**

0.75 gm of hydroxyl ethyl cellulose (HEC) was added into 50 mL of distilled water. Then, the mixture was allowed to stir for around 10 min at room temperature until a clear solution was obtained. After getting a clear solution, 0.25 gm of carboxy methyl cellulose (CMC) was added to the solution as a result a highly viscous solution was obtained, followed by addition of 0.05 gm of Triphenyl methane based derivative (BP) to the solution. Again, 0.03 gm of citric acid was used as a cross linkers. After stirring for 2 hours final homogeneous composite with red in color was obtained. The homogeneous mixture was poured in a Petridis to make a thick film by being pre-dried for 24 hours at 40°C.

**Preparation of Solutions for spectral measurements:**For spectral investigation the solutions of BP were prepared in THF/ DMSO with different concentrations $10^{-4}$ M in THF and $10^{-3}$ M in DMSO. Ammonia solutions were prepared in THF/Hexane/Water of 2% (V/V), 3% (V/V) and 5% (V/V). The 2% (V/V) $NH_3$ solution was prepared by adding 200µL in 9800µL of THF/Hexane/ Water by making total volume of 10000µL. By using the similar procedure 3% (V/V) and 5% (V/V) $NH_3$ solutions were prepared by adding 300 µL of NH3in 9700µL of THF/Hexane/ Water and 500µL of NH3 in 9500µL of THF/Hexane/ Water by making the volume 10000µL respectively. For investigating the optical properties of BP@SPC film, the solutions were prepared with similar concentrations as prepared in spectral study. In case of aerial reversibility hexane was preferred as solvent and optical properties were studied by considering the solutions in hexane.

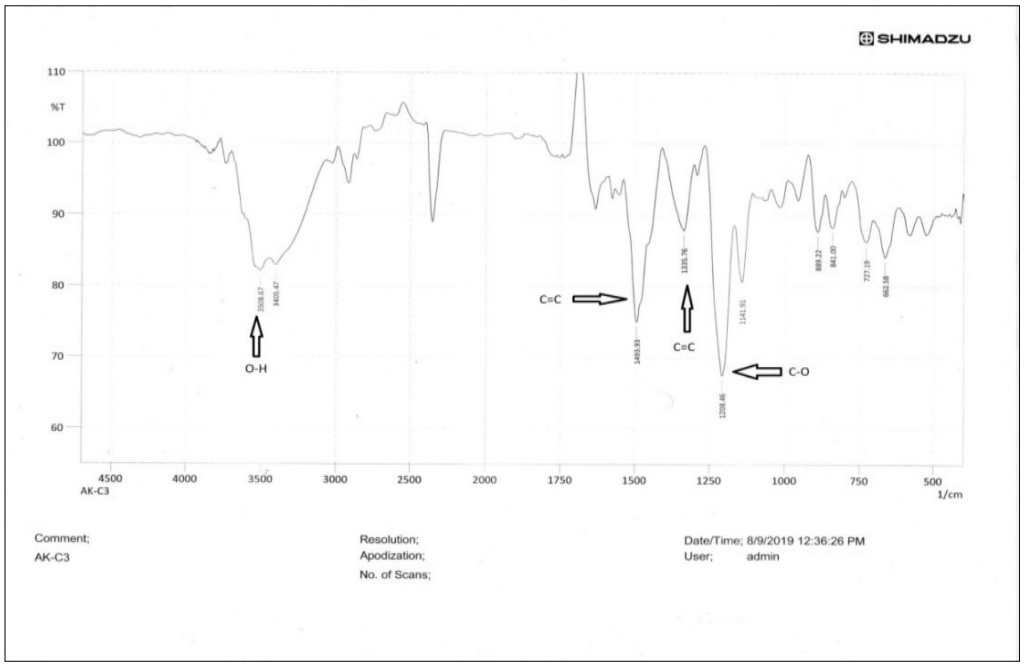


**Fig. S1** FTIR spectra of compound **BP**

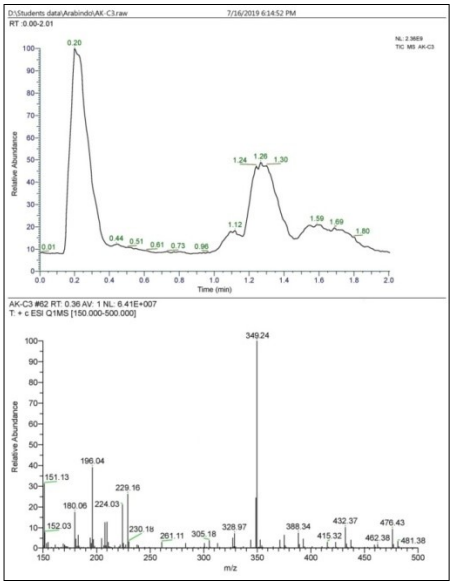


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**Fig. S2** LC-MS spectra of compound **BP**.

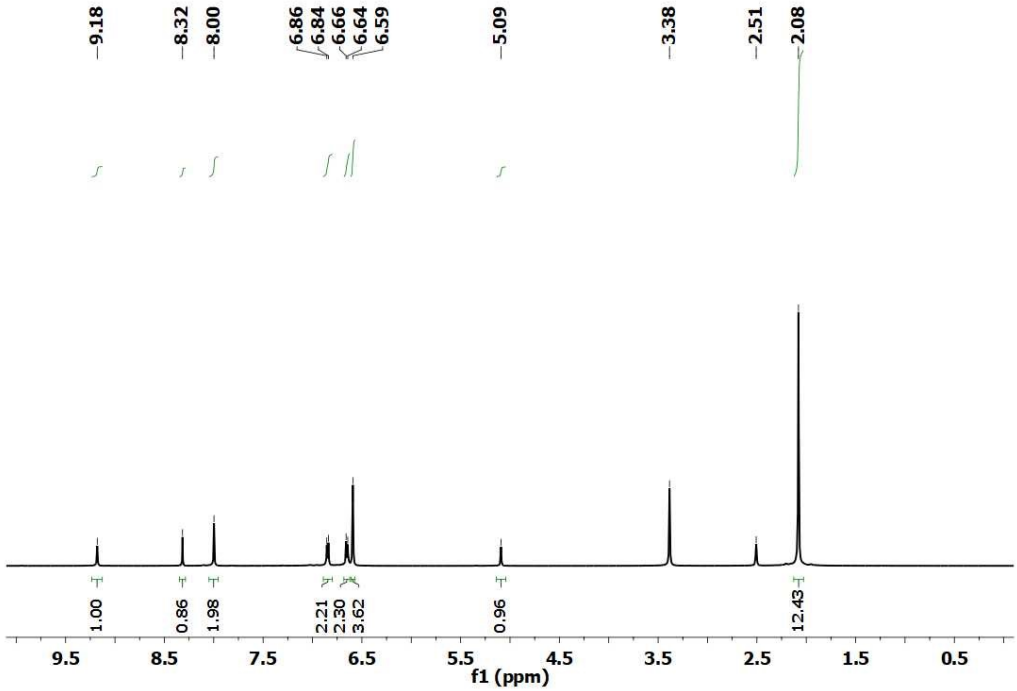



**Fig. S3**[1]H NMR (500MHz, DMSO-$d_6$) spectra of compound **BP**.

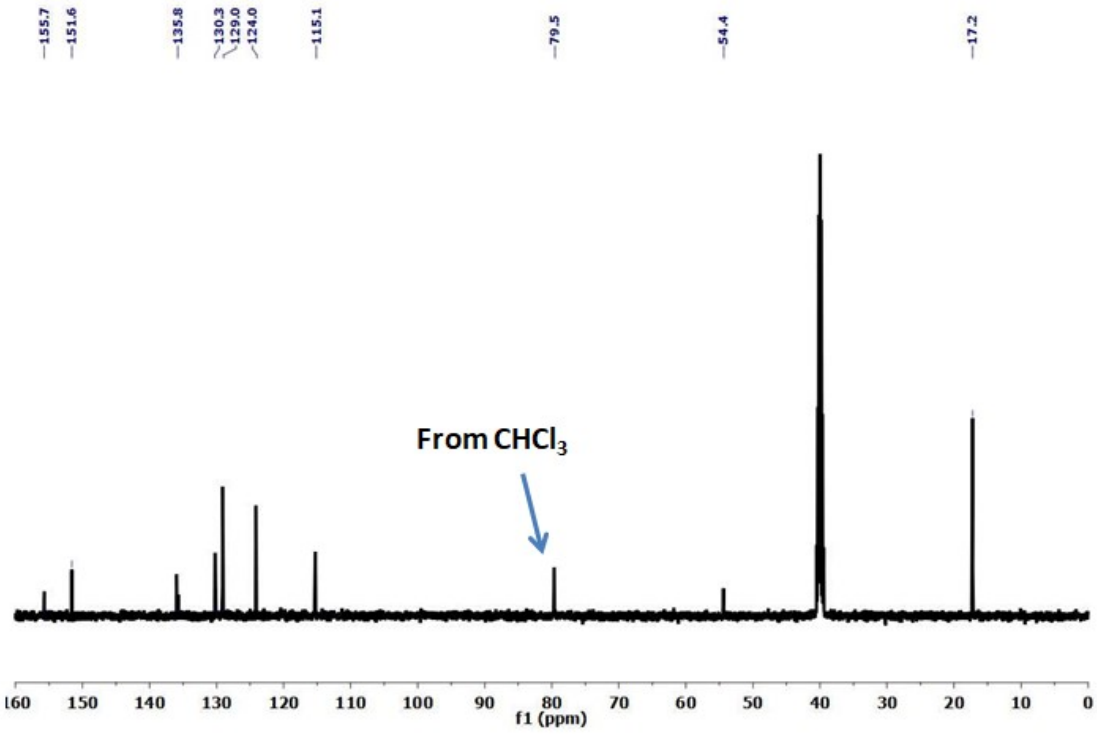



**Fig. S4**[13]C NMR (126 MHz, DMSO-$d_6$) spectra of compound **BP**.

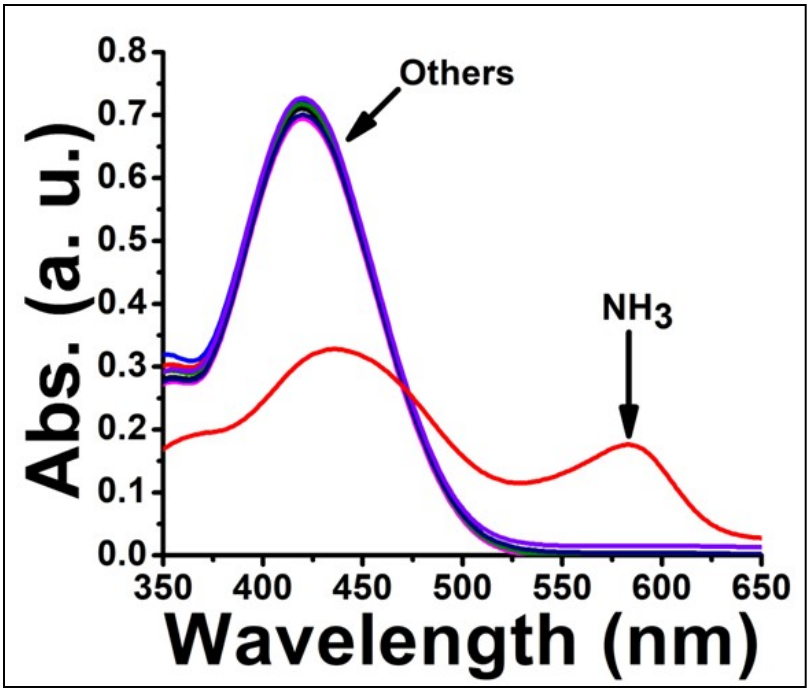



Figure S5: The changes in the absorption in the presence of ammonia and ammonia derivatives

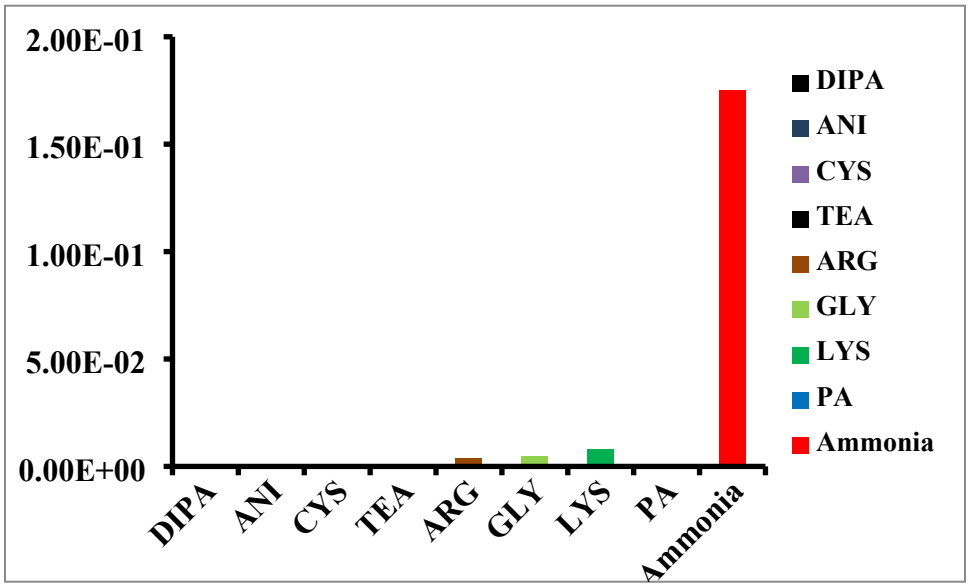



Figure S6: Bar diagram for selectivity of ammonia sensing at absorption wavelength 580 nm

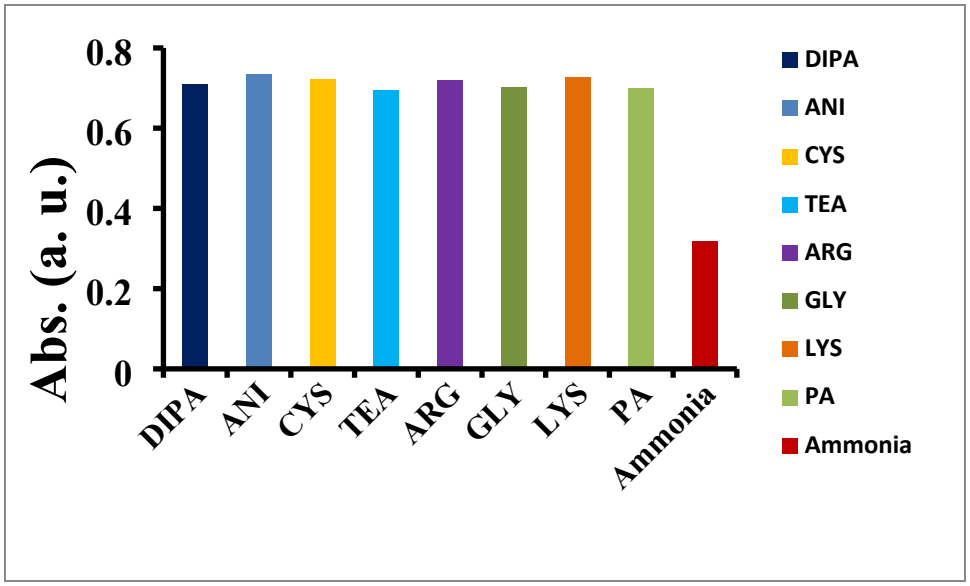



Figure S7: Bar diagram for selectivity of ammonia sensing at absorption wavelength 420 nm

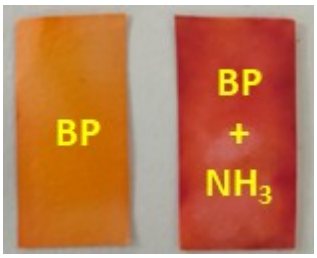



Figure S8: The change in colour of the paper strips after dipping in solution of ammonia in water

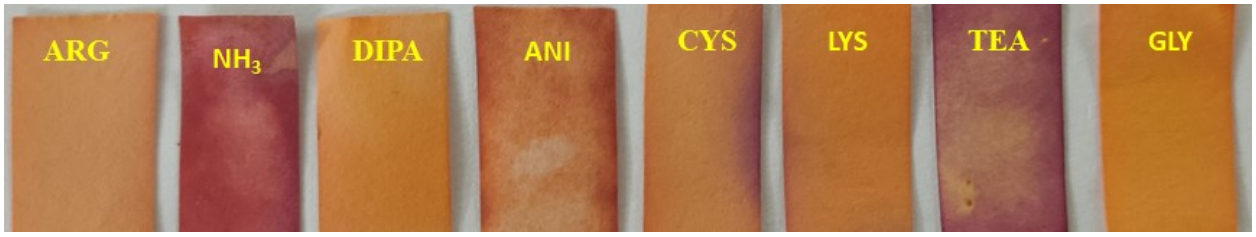



Figure S9: The change in colour of the paper strips after dipping in solution of ammonia and ammonia derivatives in THF

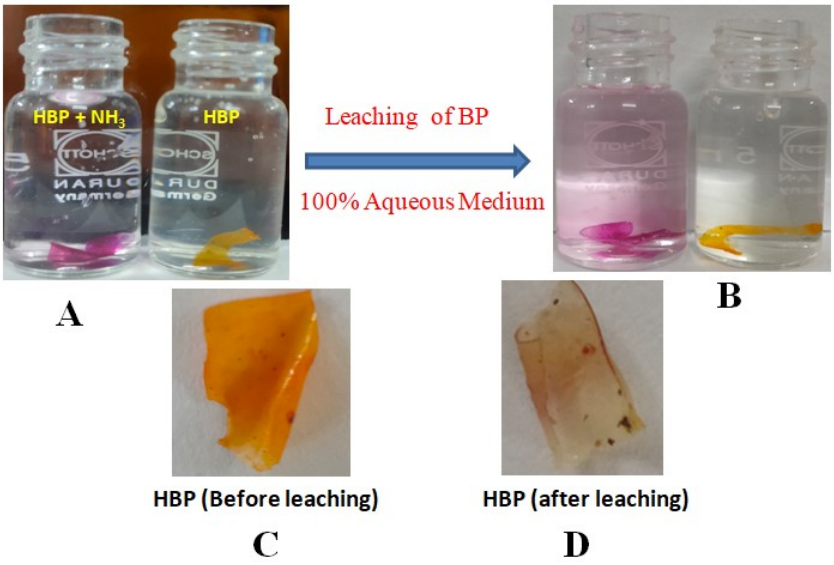



Figure S10: The changes in colour of the hydrogel (HBP) composite strips, A.on dipping into ammonia solution in water, B. change in colour of the solution due to leaching of BP, C. the original colour of the HBP film, D. change in colour of the HBP film after leaching

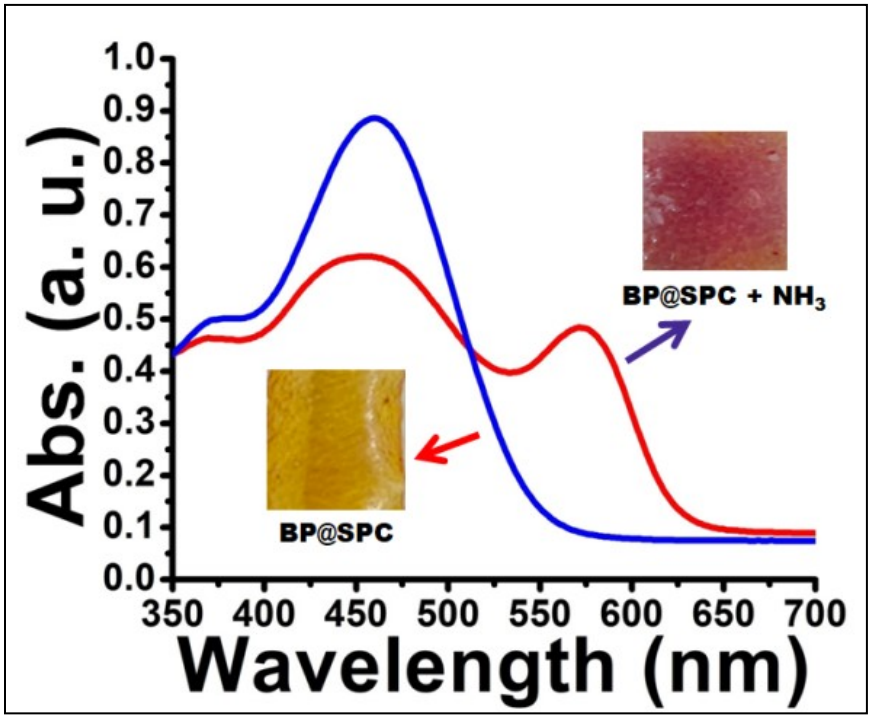



Figure S11: Solid UV-visible absorption spectra of **BP@SPC** before and after addition of $NH_3$ solution (3%, V/V). (Inset: colour of the composite films)

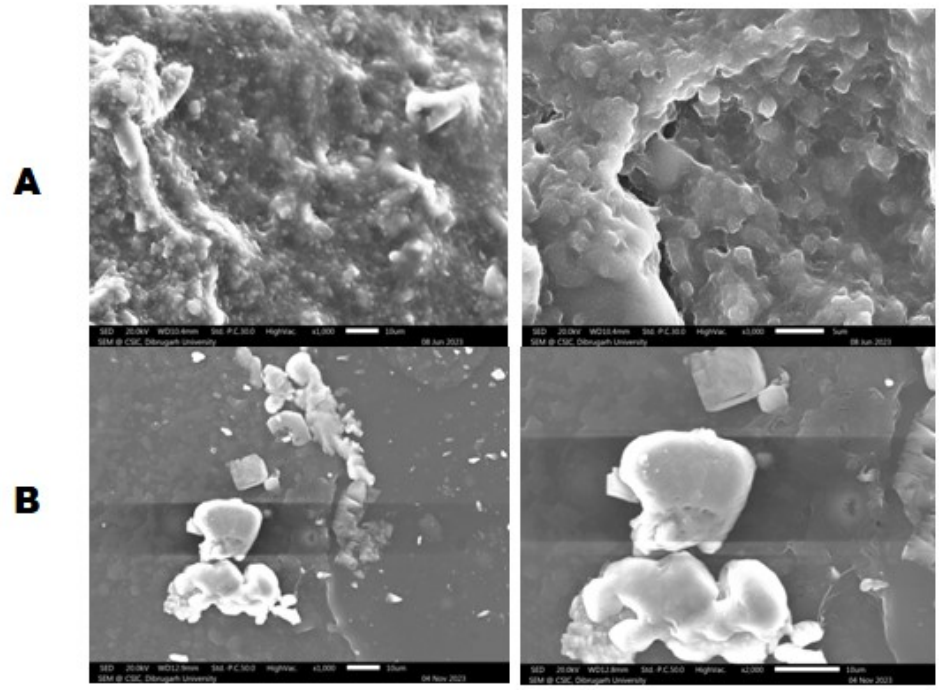
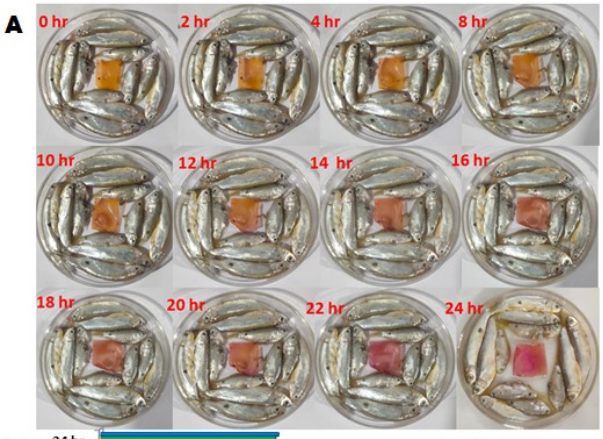
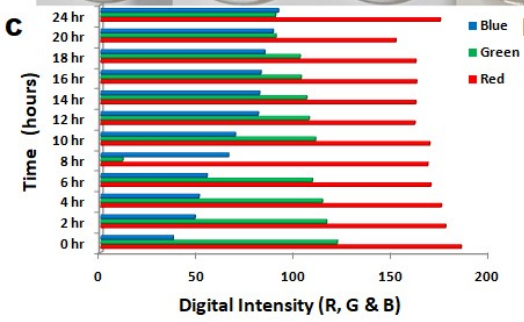



Figure S12: SEM images of (a) **BP@SPC** film only and (b) **BP@SPC** with ammonia.




B

| Time | Red | Green | Blue |
|---|---|---|---|
| 0 hr | 185.526 | 121.675 | 37.217 |
| 2 hr | 177.542 | 116.22 | 48.445 |
| 4 hr | 175.362 | 114.009 | 50.545 |
| 6 hr | 169.85 | 108.892 | 54.684 |
| 8 hr | 168.278 | 11.26 | 65.721 |
| 10 hr | 169.273 | 110.467 | 69.176 |
| 12 hr | 161.652 | 107.218 | 80.985 |
| 14 hr | 162.159 | 105.983 | 81.719 |
| 16 hr | 162.553 | 103.092 | 82.384 |
| 18 hr | 162.159 | 102.54 | 84.384 |
| 20 hr | 151.872 | 90.164 | 88.729 |
| 24 hr | 174.782 | 89.89 | 91.457 |



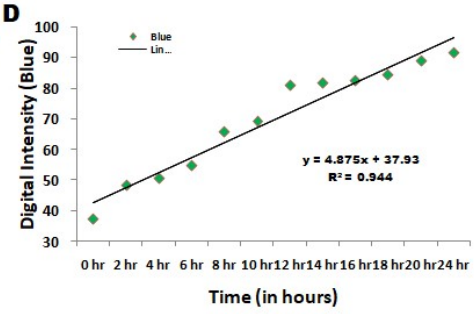



Figure13. A. Changes in the colours of **BP@SPC** film in hourly monitoring the fish spoilage environment, B. Table containing digital intensities of colour of the films (R, G & B), C. the bar diagram of digital intensities with respect to time in hours, D. The linear calibration curve digital blue contents of the respective colour of the **BP@SPC** films vs time (in hours).

| BP@SPC | Blank | 1 Min | 2 Min | 3 Min | 4 Min | 5 Min | 6 Min | 8 Min |
|---|---|---|---|---|---|---|---|---|
| Film + $NH_3$ (Gas) |  |  |  |  |  |  |  |  |
| RED | 193.711 | 171.007 | 160.377 | 164.336 | 163.768 | 164.382 | 163.546 | 173.785 |
| GREEN | 113.579 | 83.116 | 68.801 | 68.343 | 63.859 | 60.705 | 61.192 | 107.479 |
| BLUE | 1.353 | 22.140 | 42.956 | 59.162 | 65.768 | 86.879 | 87.440 | 107.551 |

Table S1: The R, G and B contents of the composite films due to exposure of ammonia vapour

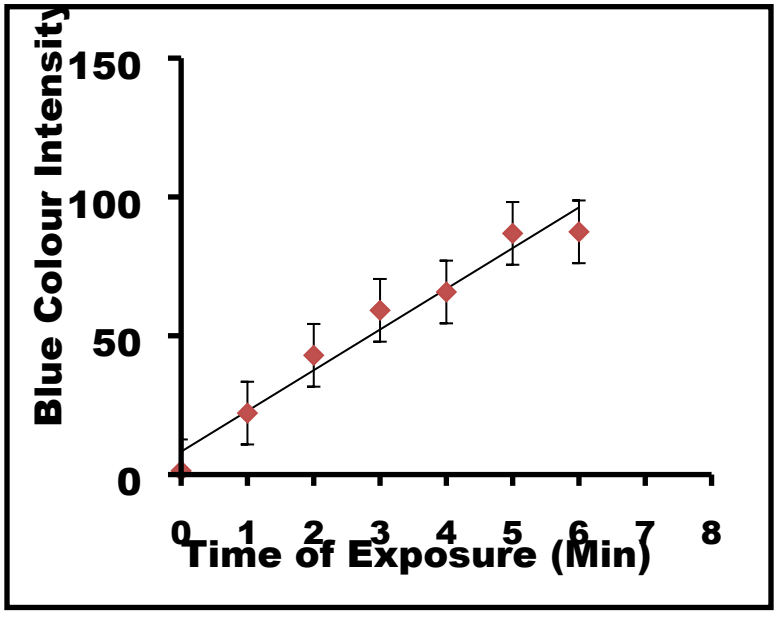



Figure S14: The linear curve between the blue colour intensity with time of exposure

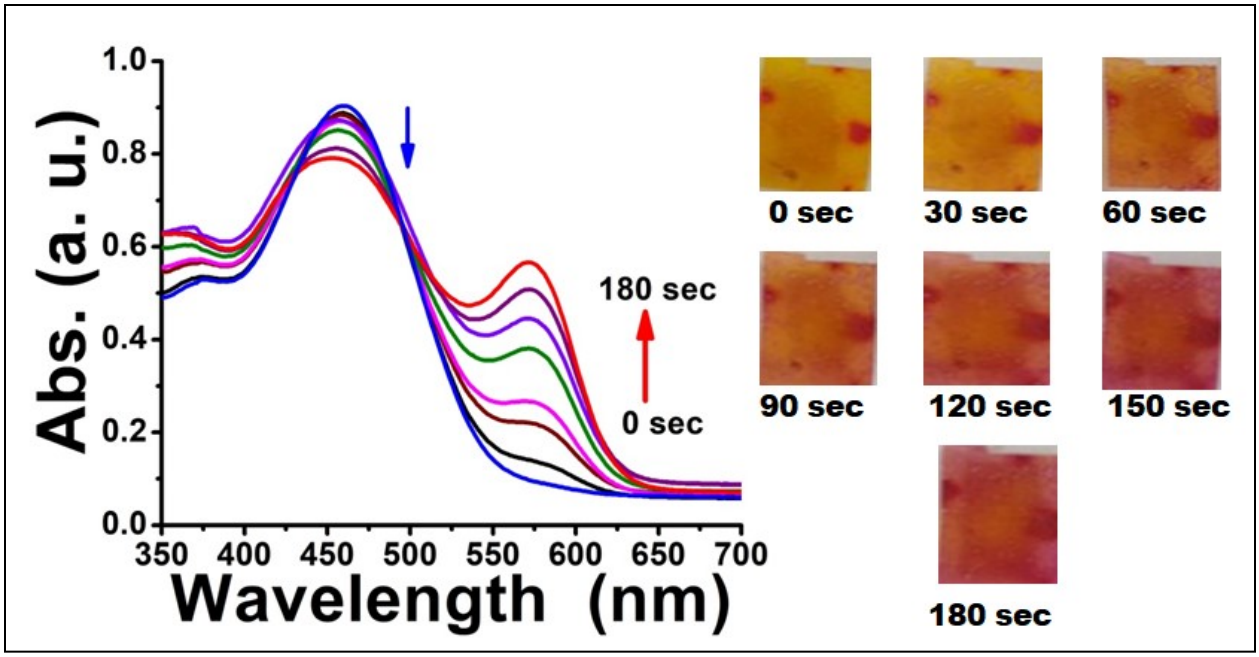



Figure S15: The change in the absorbance of the composite film (on day 3) on exposing them in the fish spoilage environment (inset: the colour changes of the films in the respective time intervals)

| Test time | 0 sec | 30 sec | 60 sec | 90 sec | 120 sec | 150 sec | 180 sec |
|---|---|---|---|---|---|---|---|
| Film + Fish sample |  | | | | | | |
| RED | 193.711 | 171.007 | 160.377 | 164.336 | 163.768 | 164.382 | 163.546 |
| GREEN | 113.579 | 83.116 | 68.801 | 68.343 | 63.859 | 60.705 | 61.192 |
| BLUE | 1.353 | 22.140 | 42.956 | 59.162 | 65.768 | 86.879 | 87.440 |

Table S2: The values of R, G and B contents of the films on day 3 in the presence of fish spoilage environment.

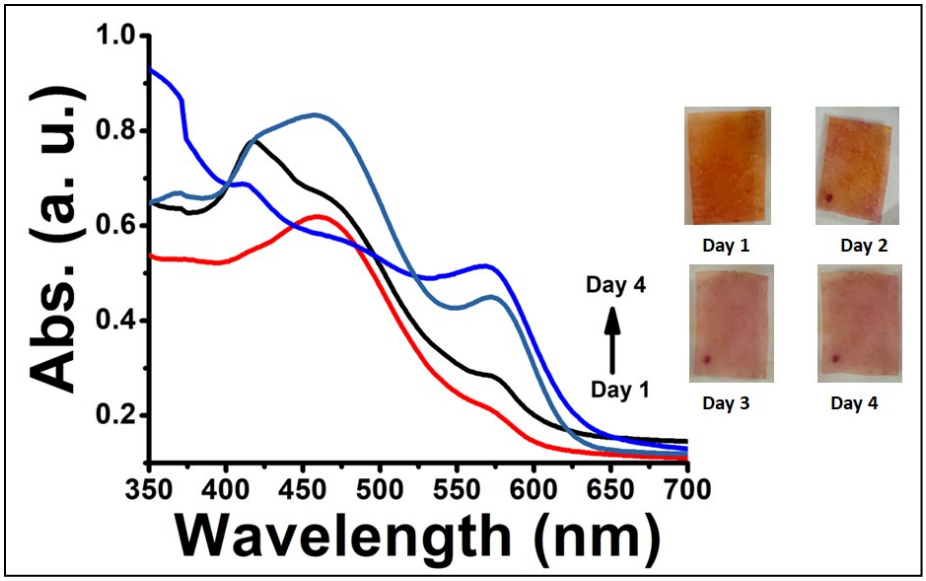



Figure S16: The changes in the absorption of composite film from day 1 to day 4 in the presence of meat spoilage environment.

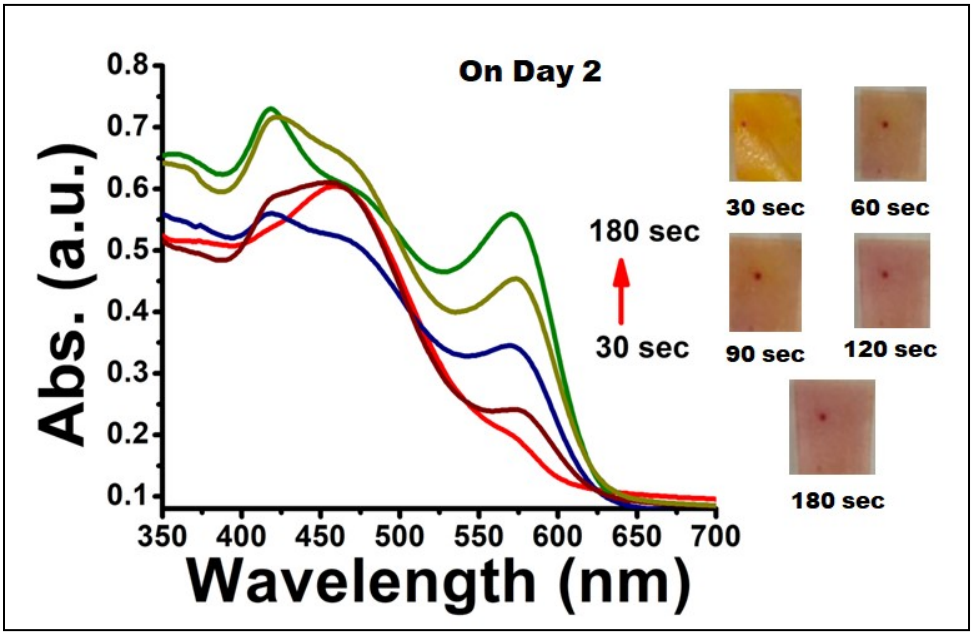



Figure S17: Changes in the absorption spectra of the composite film on day 2 with meat spoilage environment in different time intervals. (inset: the changes in the colour of the films)

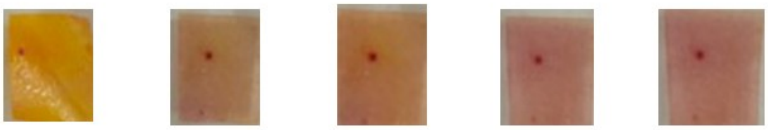
| BP@SPC | 30 sec | 60 sec | 90 sec | 120 sec | 180 sec |
|---|---|---|---|---|---|
| Film + Meat sample |  | | | | |
| RED | 186.433 | 156.432 | 163.987 | 162.699 | 161.960 |
| GREEN | 133.267 | 117.395 | 111.684 | 117.154 | 114.104 |
| BLUE | 33.836 | 73.026 | 85.341 | 98.745 | 101.342 |

Table S3: The values of R, G and B contents of the films in the presence of meat spoilage environment in the respective time intervals

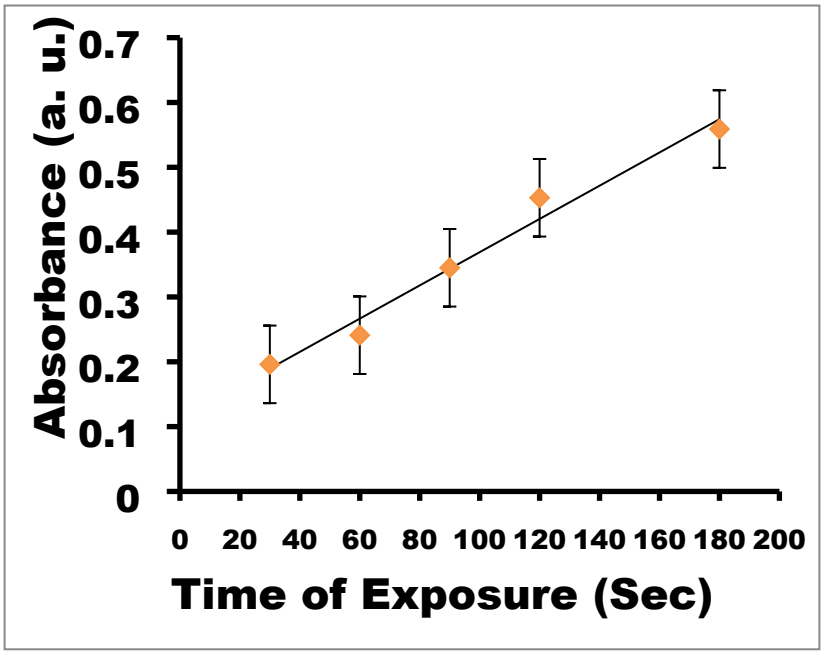



Figure S18: The linear curve between the change in the absorbance of the composite films in the presence of meat spoilage environment and time of exposure

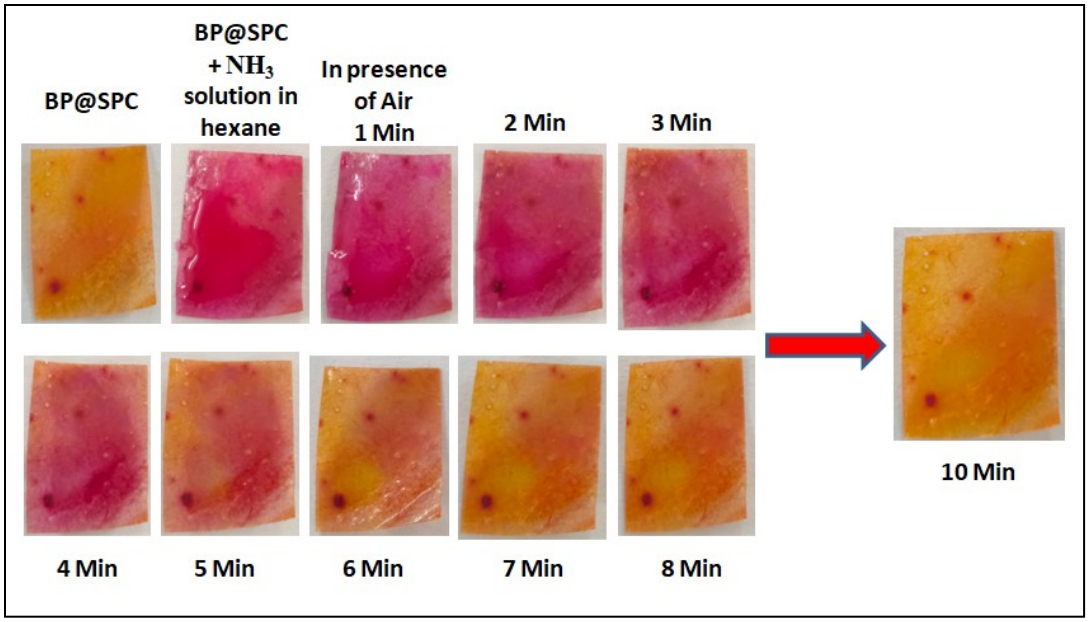



Figure S19: Optical responses of **BP@SPC** film towards $NH_3$ vapor in hexane (2%, V/V)

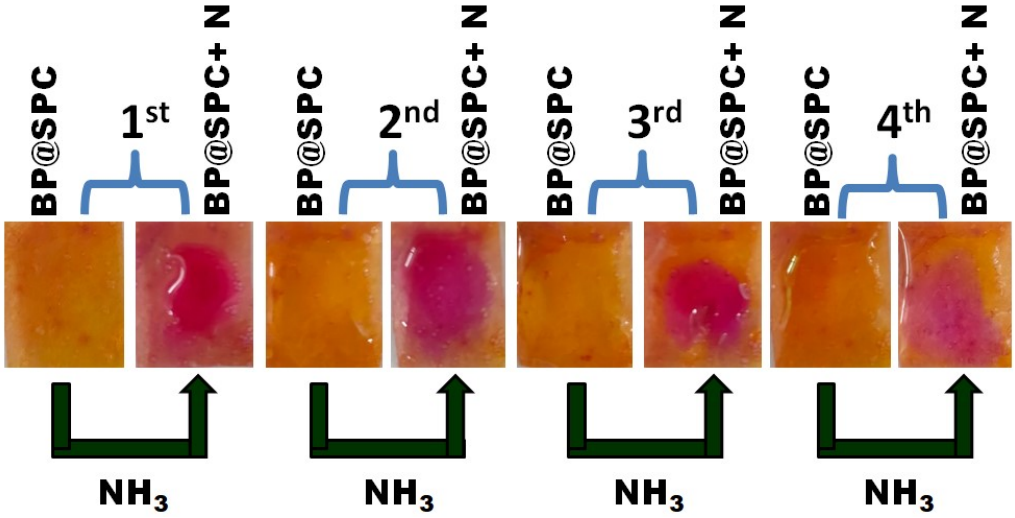



Figure S20: Photographs of reversibility of the composite films up to 4$^{th}$ cycle

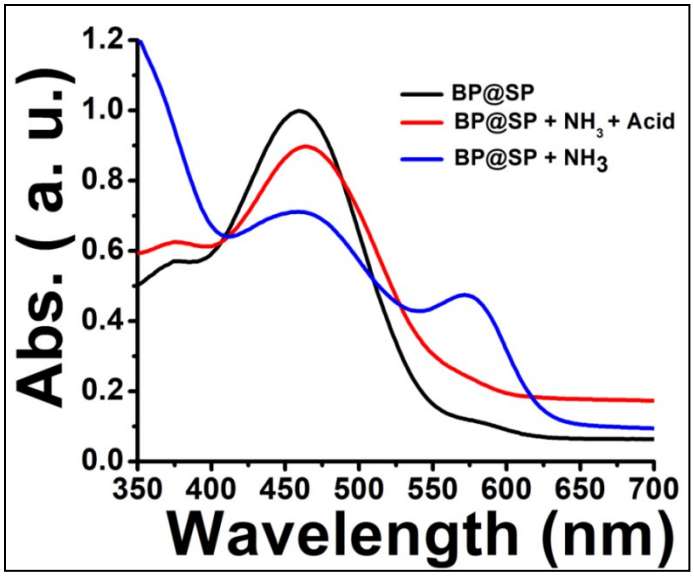
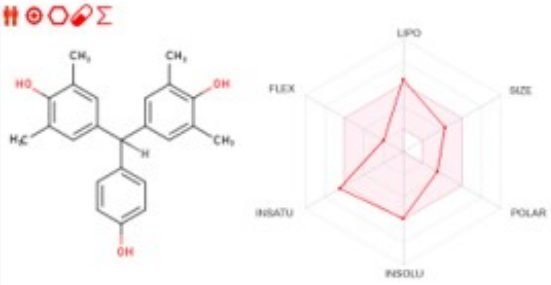



Figure S21: The change in absorption of the composite film in reversibility test




SMILES Oc1ccc(cc1)C(c1cc(C)c(o)c(c1)C)O)c1cc(C)c(o)c(c1)C)O

Physicochemical Properties

| | |
|---|---|
| Formula | C23H24O3 |
| Molecular weight | 348.43 g/mol |
| Num. heavy atoms | 26 |
| Num. arom. heavy atoms | 18 |
| Fraction Csp3 | 0.22 |
| Num. rotatable bonds | 3 |
| Num. H-bond acceptors | 3 |
| Num. H-bond donors | 3 |
| Molar Refractivity | 106.31 |
| TPSA | |
| **Topological Polar Surface Area:** Calculated from Ertl P. et al. 2000 J. Med. Chem. | 60.69 Å² |

Lipophilicity

| | |
|---|---|
| Log $P_{o/w}$ (iLOGP) | |
| **iLOGP:** in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model. | 3.25 |
| Log $P_{o/w}$ (XLOGP3) | |
| **XLOGP3:** Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry | 5.69 |
| Log $P_{o/w}$ (WLOGP) | |
| **WLOGP:** Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model. | 5.22 |
| Log $P_{o/w}$ (MLOGP) | |
| **MLOGP:** Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev. | 4.21 |
| Log $P_{o/w}$ (SILICOS-IT) | |
| **SILICOS-IT:** Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com | 5.76 |
| Consensus Log $P_{o/w}$ | |
| **Consensus Log $P_{o/w}$:** Average of all five predictions | 4.82 |

Water Solubility

| | |
|---|---|
| Log *S* (ESOL) | |
| **ESOL:** Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model. | -5.90 |
| Solubility | 4.39e-04 mg/ml ; 1.26e-06 mol/l |
| Class | |
| **Solubility class:** Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly | Moderately soluble |
| Log *S* (Ali) | |
| **Ali:** Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model. | -6.73 |
| Solubility | 6.49e-05 mg/ml ; 1.86e-07 mol/l |
| Class | |
| **Solubility class:** Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly | Poorly soluble |
| Log *S* (SILICOS-IT) | |
| **SILICOS-IT:** Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com | -7.26 |
| Solubility | 1.89e-05 mg/ml ; 5.43e-08 mol/l |
| Class | |
| **Solubility class:** Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly | Poorly soluble |

Pharmacokinetics

| | |
|---|---|
| GI absorption | |
| **Gatrointestinal absorption:** according to the white of the BOILED-Egg | High |
| BBB permeant | |
| **BBB permeation:** according to the yolk of the BOILED-Egg | Yes |
| P-gp substrate | |
| **P-glycoprotein substrate:** SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94 | Yes |
| CYP1A2 inhibitor | |
| **Cytochrome P450 1A2 inhibitor:** SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91 | No |
| CYP2C19 inhibitor | Yes |
| **Cytochrome P450 2C19 inhibitor:** SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) | |

| | |
|---|---|
| 10-fold CV: ACC=0.80 / AUC=0.86<br>External: ACC=0.80 / AUC=0.87 | |
| CYP2C9 inhibitor | |
| **Cytochrome P450 2C9 inhibitor:** SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set)<br>10-fold CV: ACC=0.78 / AUC=0.85<br>External: ACC=0.71 / AUC=0.81 | No |
| CYP2D6 inhibitor | |
| **Cytochrome P450 2D6 inhibitor:** SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set)<br>10-fold CV: ACC=0.79 / AUC=0.85<br>External: ACC=0.81 / AUC=0.87 | Yes |
| CYP3A4 inhibitor | |
| **Cytochrome P450 3A4 inhibitor:** SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set)<br>10-fold CV: ACC=0.77 / AUC=0.85<br>External: ACC=0.78 / AUC=0.86 | Yes |
| Log $K_p$ (skin permeation) | |
| **Skin permeation:** QSPR model implemented from Potts RO and Guy RH. 1992 Pharm. Res. | -4.39 cm/s |
| | Druglikeness |
| Lipinski | |
| **Lipinski (Pfizer) filter:** implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev.<br>MW ≤ 500<br>MLOGP ≤ 4.15<br>N or O ≤ 10<br>NH or OH ≤ 5 | Yes; 1 violation: MLOGP>4.15 |
| Ghose | |
| **Ghose filter:** implemented from Ghose AK. et al. 1999 J. Comb. Chem.<br>160 ≤ MW ≤ 480<br>-0.4 ≤ WLOGP ≤ 5.6<br>40 ≤ MR ≤ 130<br>20 ≤ atoms ≤ 70 | Yes |
| Veber | |
| **Veber (GSK) filter:** implemented from Veber DF. et al. 2002 J. Med. Chem.<br>Rotatable bonds ≤ 10<br>TPSA ≤ 140 | Yes |
| Egan | |
| **Egan (Pharmacia) filter:** implemented from Egan WJ. et al. 2000 J. Med. Chem.<br>WLOGP ≤ 5.88<br>TPSA ≤ 131.6 | Yes |
| Muegge | No; 1 violation: XLOGP3>5 |
| **Muegge (Bayer) filter:** implemented from Muegge I. et al. 2001 J. Med. Chem. | |

200 ≤ MW ≤ 600
-2 ≤ XLOGP ≤ 5
TPSA ≤ 150
Num. rings ≤ 7
Num. carbon > 4
Num. heteroatoms > 1
Num. rotatable bonds ≤ 15
H-bond acc. ≤ 10
H-bond don. ≤ 5

Bioavailability Score

| | |
|---|---|
| **Abbott Bioavailability Score:** Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem. | 0.55 |

Medicinal Chemistry

PAINS

| | |
|---|---|
| **Pan Assay Interference Structures:** implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem. | 0 alert |

Brenk

| | |
|---|---|
| **Structural Alert:** implemented from Brenk R. et al. 2008 ChemMedChem | 0 alert |

Leadlikeness

| | |
|---|---|
| **Leadlikeness:** implemented from Teague SJ. 1999 Angew. Chem. Int. Ed.<br>250 ≤ MW ≤ 350<br>XLOGP ≤ 3.5<br>Num. rotatable bonds ≤ 7 | No; 1 violation: XLOGP3>3.5 |

Synthetic accessibility

| | |
|---|---|
| **Synthetic accessibility score:** from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2$ = 0.94) | 2.23 |



Figure S22: In-Silico toxicity data for BP

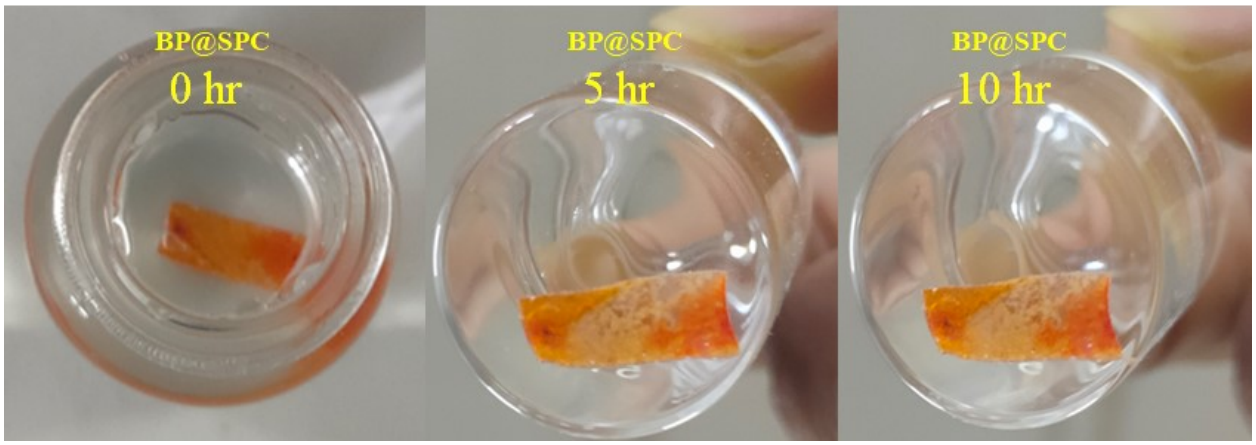



Figure S23: The stability of **BP@SPC** film under water before treating with $NH_3$

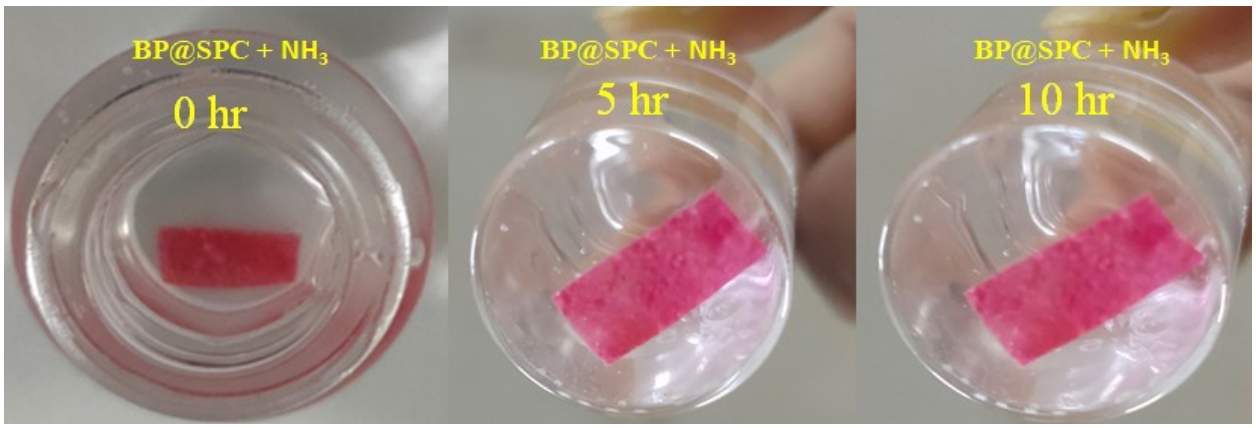



Figure S24: The stability of **BP@SPC** film under water after treating with $NH_3$

**Deep Freezing condition (at -5°C )** **Under water condition** **Thermal condition in Oven (at 70°C )**

Figure S25: Stability of **BP@SPC** film under different environmental conditions

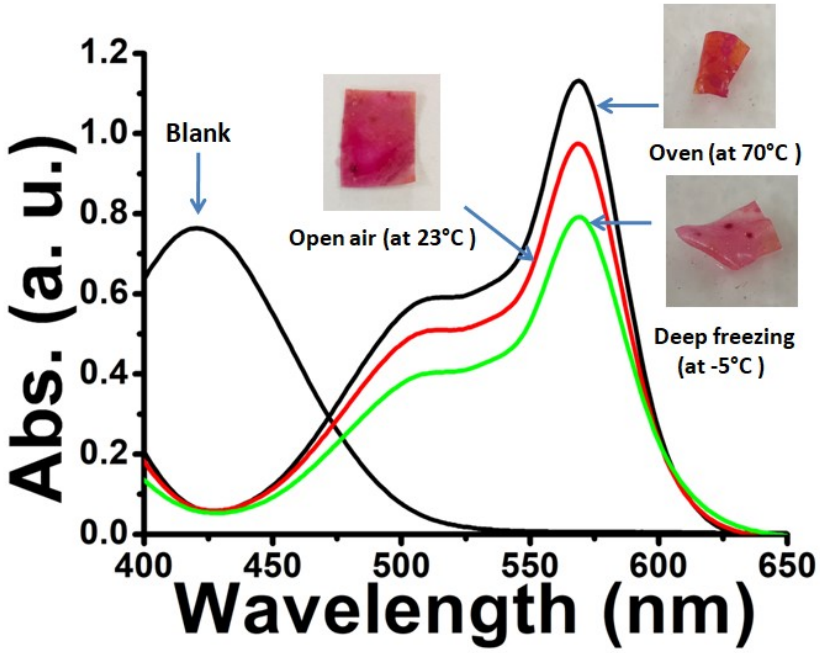



Figure S26: The spectral changes of **BP@SPC** film after treating with $NH_3$ under different thermal conditions