

Supporting information

Amorphous Poly-N-vinylcarbazole polymer as a novel matrix for determination of low molecular weight compounds by MALDI-TOF MS

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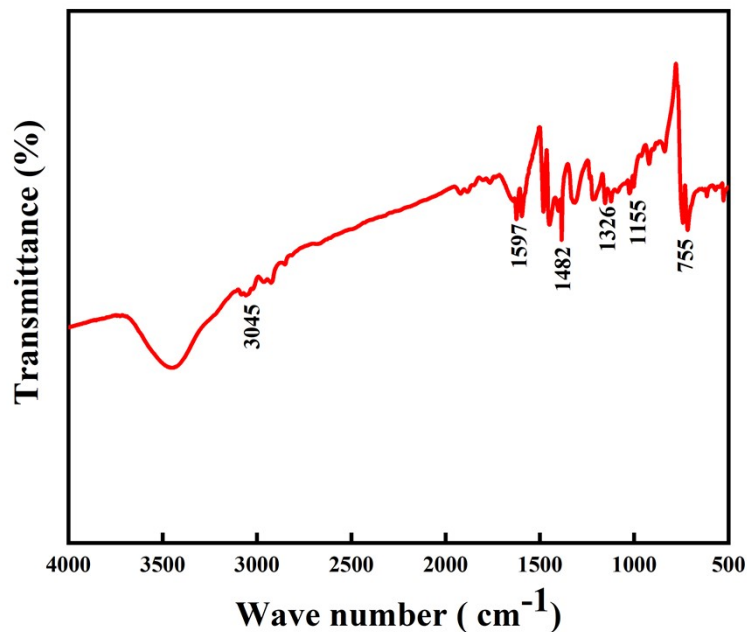


Fig. S1 Fourier-transform infrared spectroscopy of PVK

C–H stretching vibration peaks in aromatic rings (3045 cm^{-1}), and those in aliphatic groups ($2800 - 2970\text{ cm}^{-1}$). C = C vibration peak in benzene ring skeleton (1597 and 1482 cm^{-1}). The C–N Tensile vibration peak in carbazole ring (1326 cm^{-1}) and the C–H out of plane bending vibration peak of benzene ring (745 cm^{-1}). C–C tensile vibration peak (1155 cm^{-1}) in benzene ring skeleton, and the position of each peak is consistent with the literature²⁹.

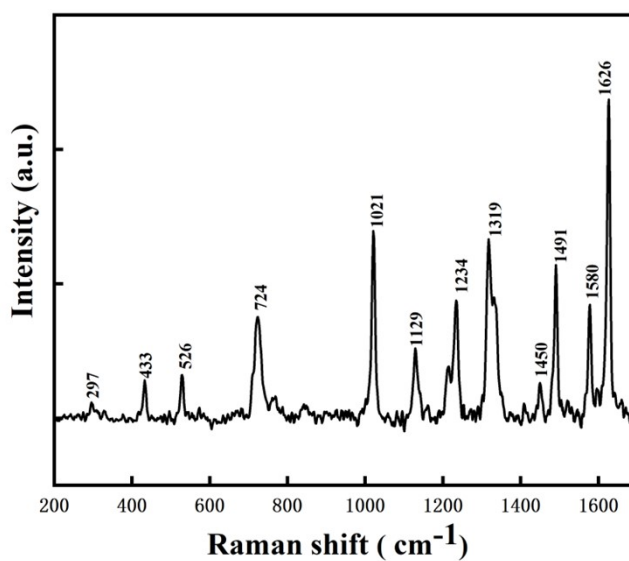


Fig. S2 The Raman spectra of PVK

Table S1 Raman vibrational frequencies (cm⁻¹) of PVK and the vibrational assignments

| Raman spectra in the molecular powder state of PVK | Ascription |
|--|--|
| 297(w) | CCC deformation vibration in long polyethylene chains |
| 433(w) | Out of plane deformation and vibration of o-bis-p-benzene ring |
| 526(m) | Out of plane deformation and vibration of o-bis-p-benzene ring |
| 724(m) | Methylene in-plane rocking twisting vibration in long polyethylene chains |
| 1021(s) | Methylene in-plane rocking twisting vibration in long polyethylene chains |
| 1129(w) | In plane deformation and vibration of C-H in o-di-p-benzene ring |
| 1234(m) | Out-of-plane rocking vibration of methylene groups in long polyethylene chains |
| 1319(s) | Methylene in-plane rocking twisting vibration in long polyethylene chains |
| 1450(w) | HCH deformation vibration in long polyethylene chains |
| 1491(m) | Heteropentacyclic ring stretching vibration |
| 1580(m) | O-bis-substituted para-phenyl ring stretching vibration |
| 1626(s) | O-bis-substituted para-phenyl ring stretching vibration |

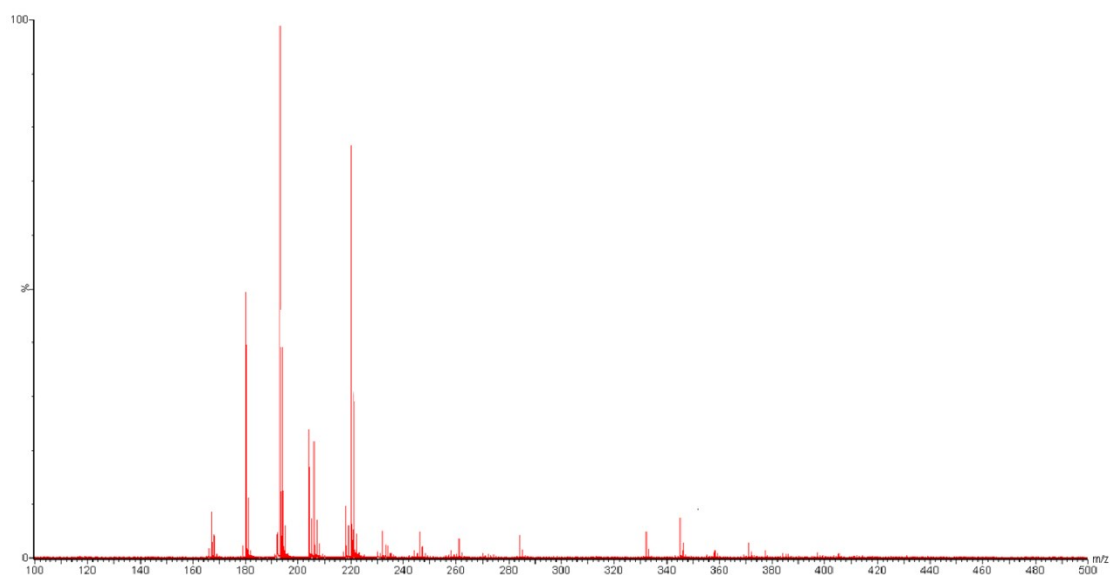


Fig.S3 LDI MS spectrum of purification PVK in positive ion mode

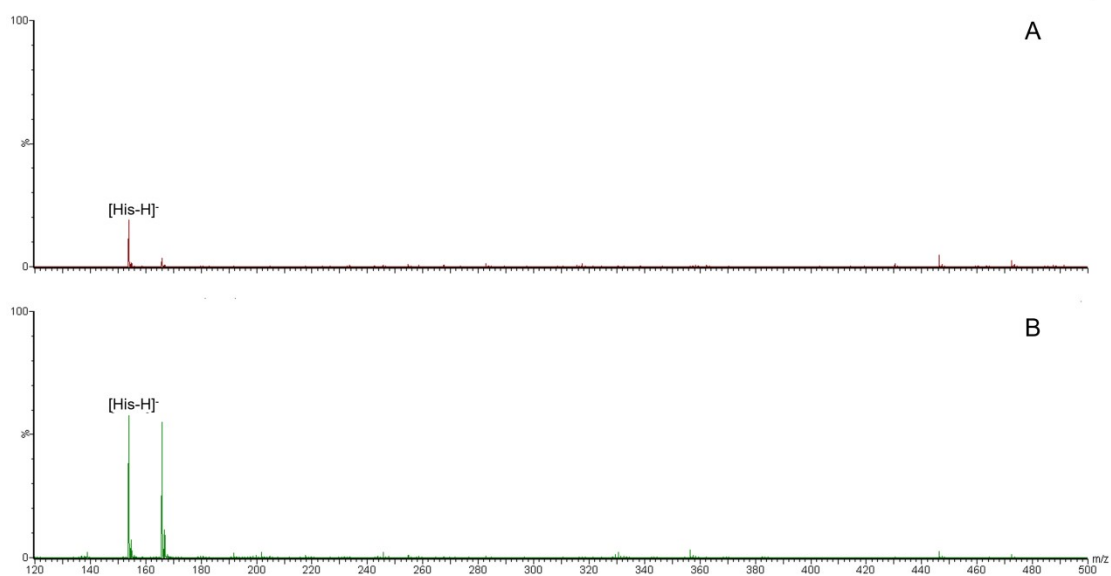


Fig. S4 Comparison of mass spectra of different solvents (A) THF, and (B) DCM dissolved matrix PVK for histidine detection by MALDI-TOF MS in negative ion mode

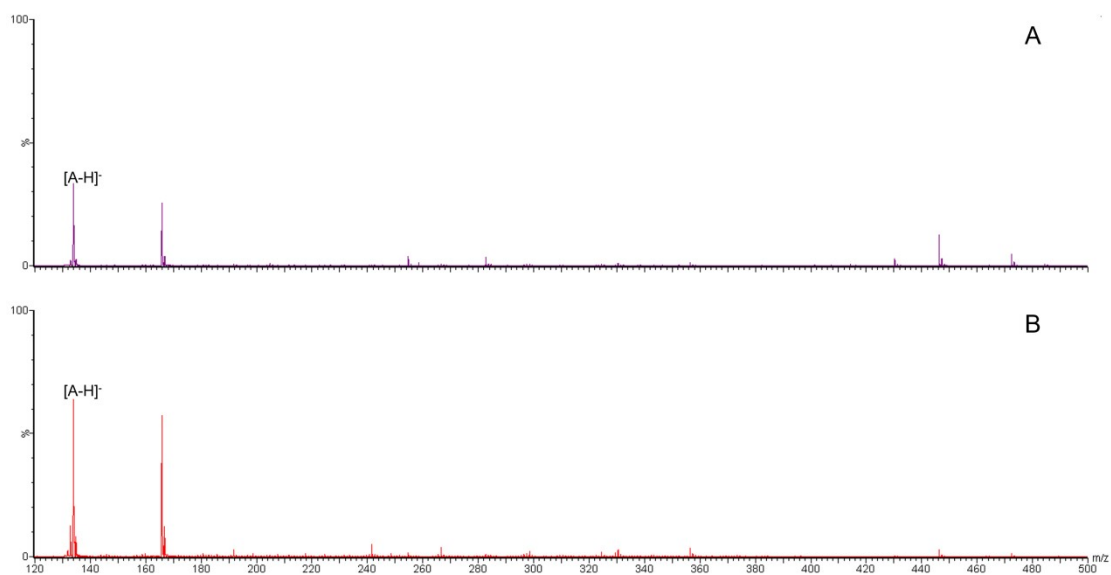


Fig. S5 Comparison of mass spectra of different solvents (A) THF, and (B) DCM dissolved matrix PVK for adenine detection by MALDI-TOF MS in negative ion mode

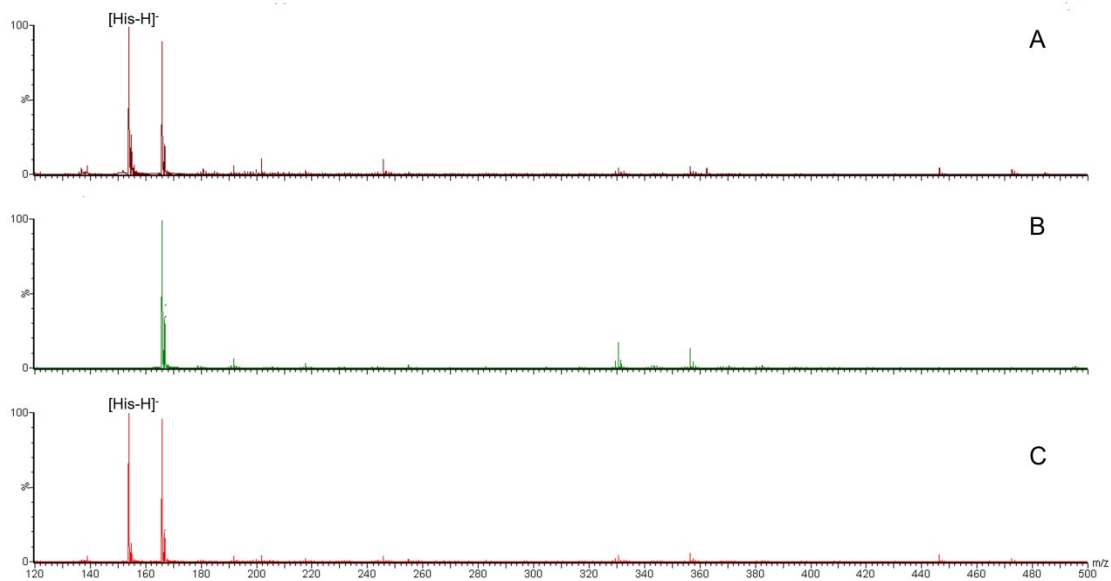


Fig. S6 MALDI-TOF MS spectrum of histidine with different spotting method included the sample first technique (A) the matrix first technique (B), and the dried-droplet technique (C) in negative ion mode

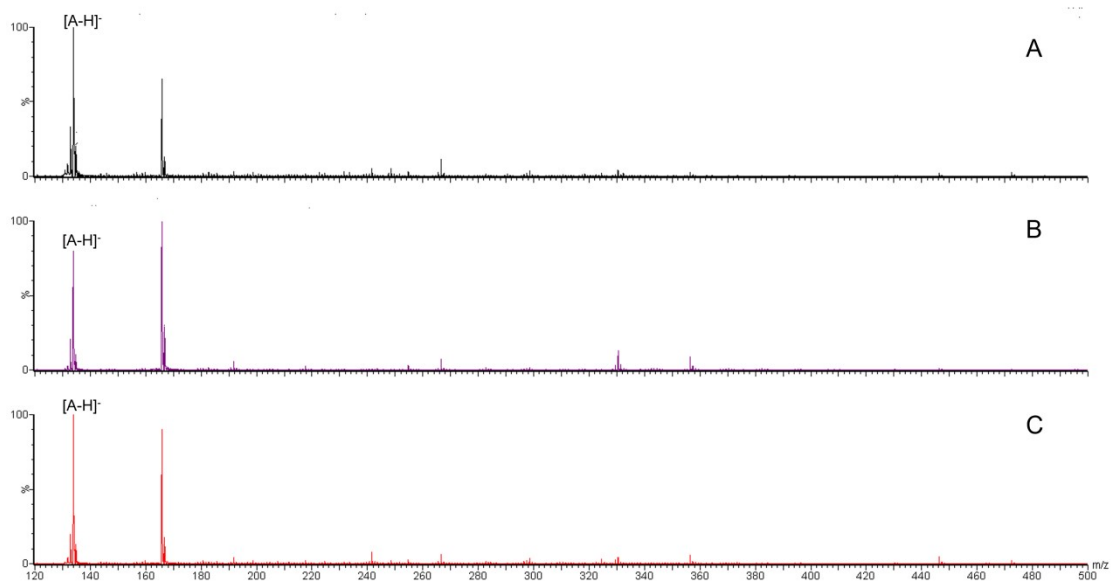


Fig. S7 MALDI-TOF MS spectrum of adenine with different spotting method included the sample first technique (A) the matrix first technique (B), and the dried-droplet technique (C) in negative ion mode

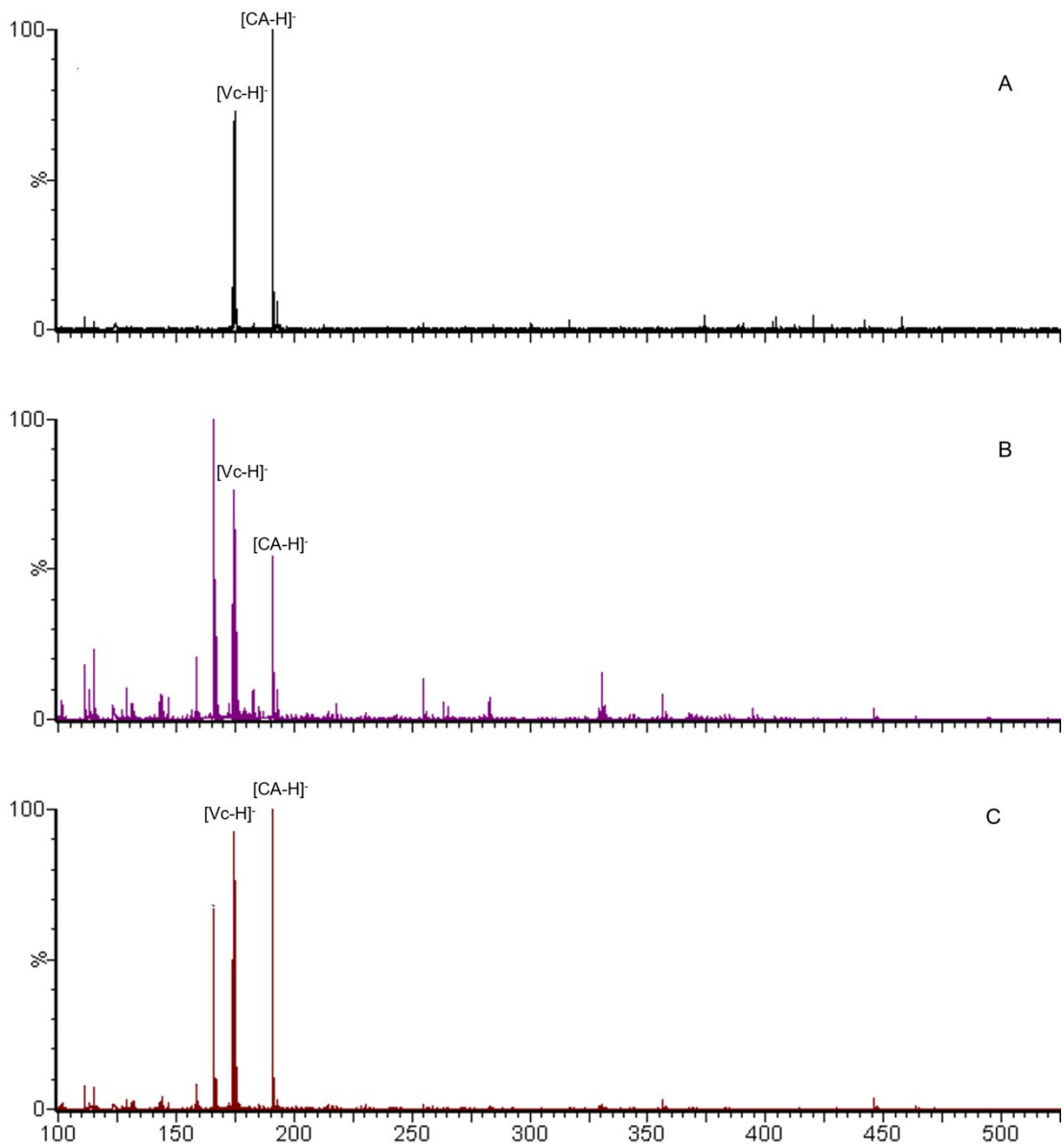
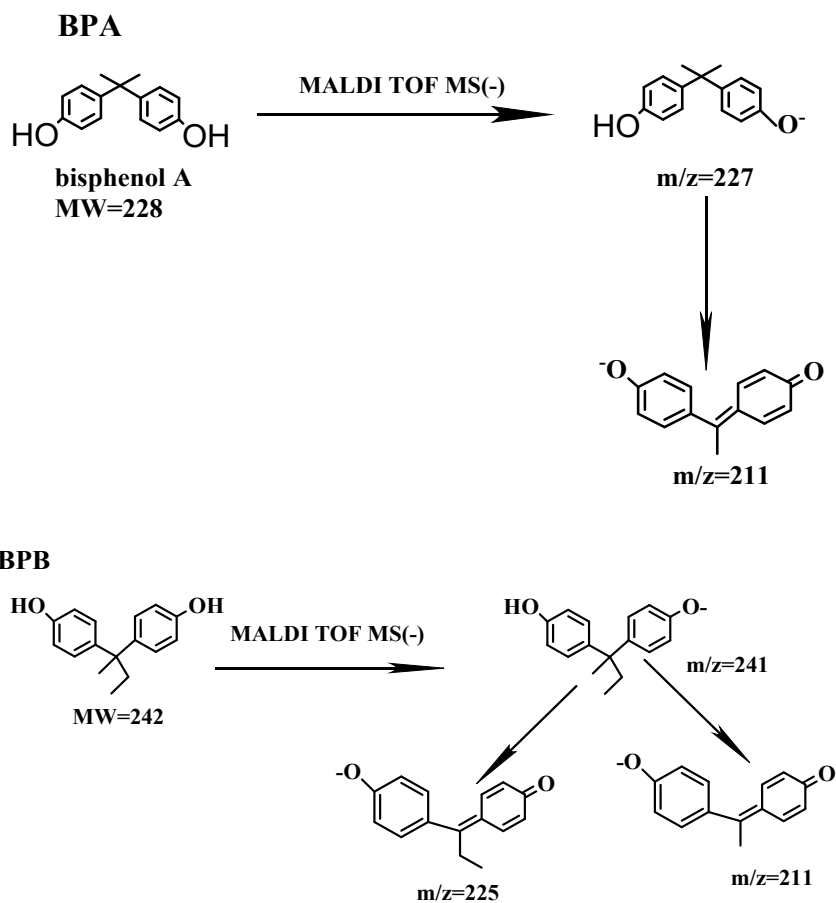


Fig. S8. MALDI-TOF MS spectrum of 1 mg/mL ascorbic acid and citric acid solution with 9-AA (A), VK(B), and PVK (C) matrix



Fig. S9 MALDI-TOF MS spectrum of (A) phenylalanine and (B) adenine Using amorphous PVK as the matrix



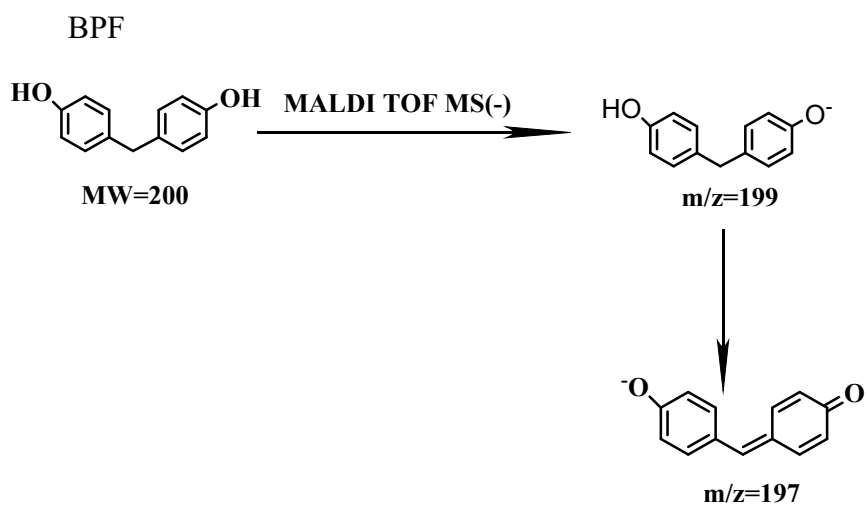


Fig.S10 Fragmentation pathways of BPs

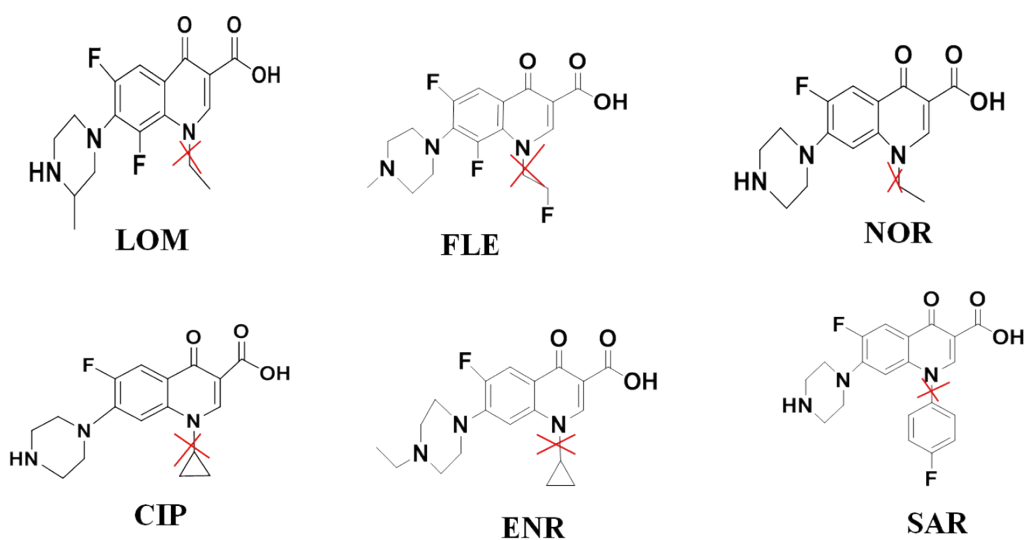


Fig. S11 Fragmentation pathways of quinolones

Table S2 The LOD of analytes measurement with the matrices of PVK.

| Analyte | Detection limit (mg/mL) |
|---------------|-------------------------|
| ascorbic acid | 0.01 |
| citric acid | 0.001 |
| phenylalanine | 0.001 |

| | |
|----------------------------|--------|
| methionine | 0.001 |
| threonine | 0.001 |
| adenine | 0.001 |
| uracil | 0.001 |
| thymine | 0.001 |
| stearic acid | 0.001 |
| palmitic acid | 0.001 |
| bisphenol A | 0.0001 |
| bisphenol B | 0.0001 |
| bisphenol F | 0.001 |
| bisphenol S | 0.0001 |
| lomefloxacin | 0.001 |
| fleroxacin | 0.0001 |
| norfloxacin | 0.001 |
| ciprofloxacin | 0.001 |
| sarafloxacin hydrochloride | 0.001 |
| enrofloxacin | 0.001 |
