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Supplementary Information

A novel magnetic fluid for ultra-fast and highly efficient extraction of N^1-Methylnicotinamide in urine samples

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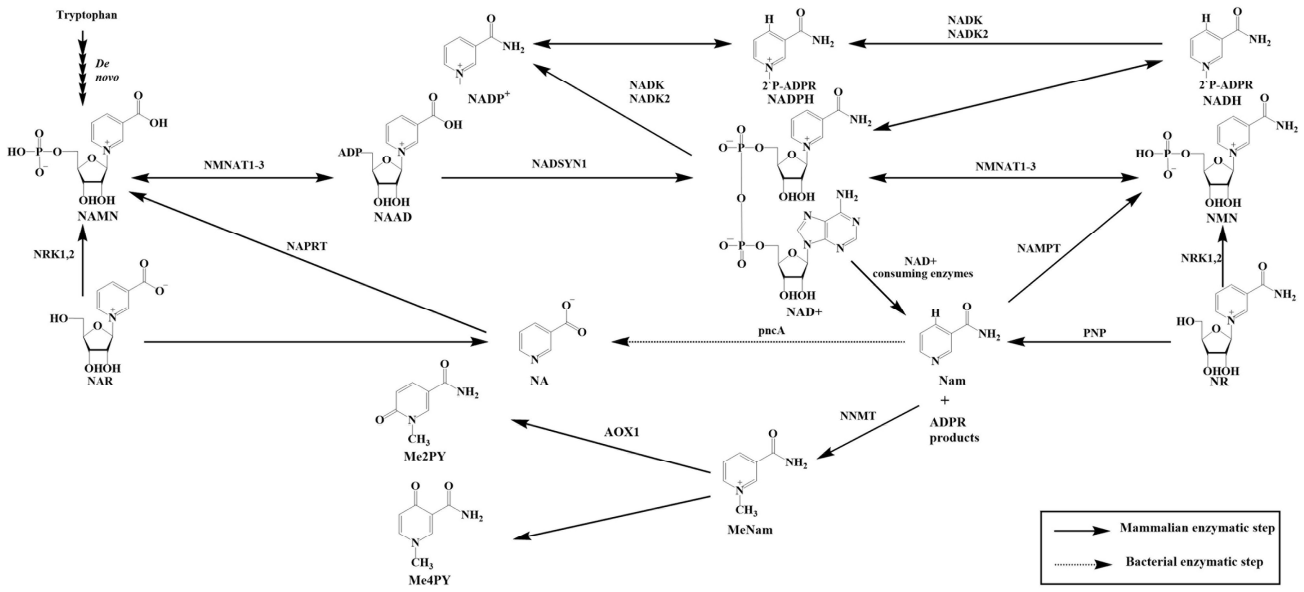

Fig. S1 NAD+ metabolome. NAD+ is synthesized by salvaging vitamin precursors or obtained from tryptophan in a novel pathway. NAD+ can be consumed to generate Nam. Nam can also be methylated and oxidized to metabolites.

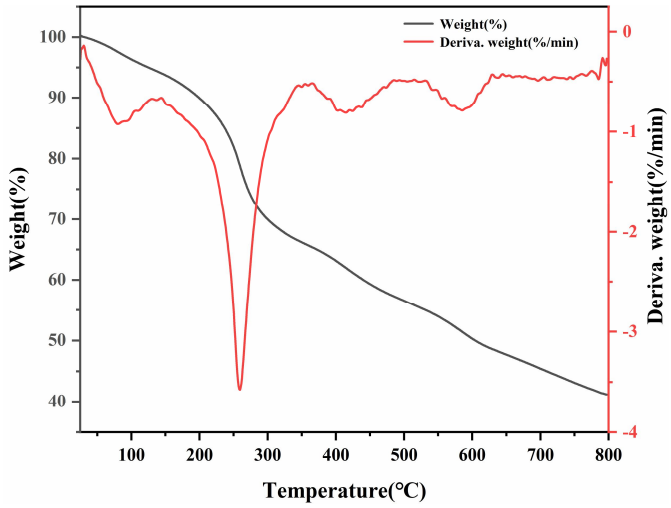

Fig. S2 TGA curve of the Fe_3O_4@HPMC@DMSA NPs.

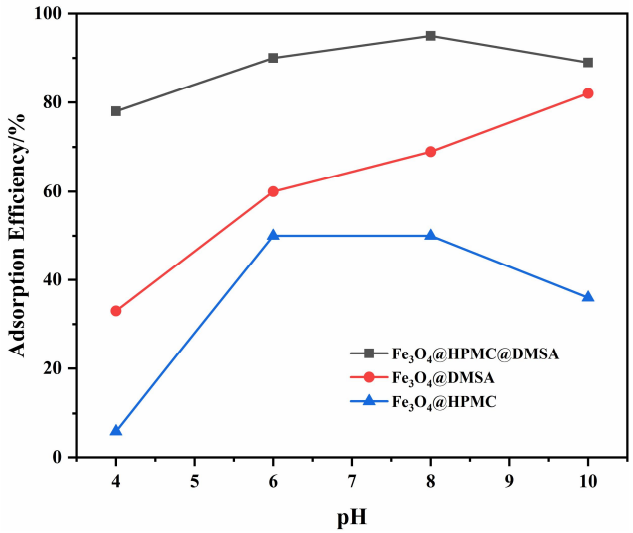

Fig. S3 Graph of the effect of pH on the adsorption efficiency of the three materials.

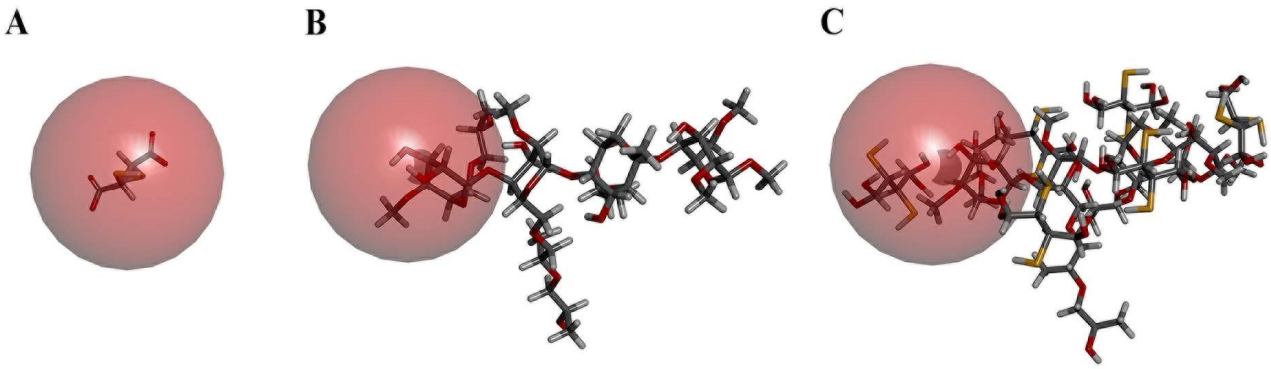

Fig. S4 The active docking site of HPMC, DMSA and HPMC @ DMSA.

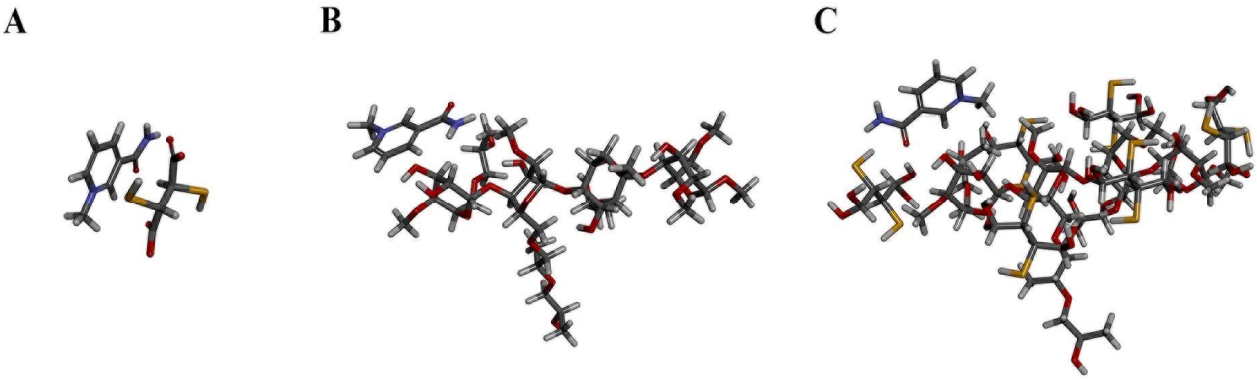

Fig. S5 The docking conformation of MeNam with HPMC, DMSA and HPMC @ DMSA.

Table S1. Docking energy of MeNam with HPMC, DMSA and HPMC@DMSA.

Docking Conformation	-CDOCKER-ENERGY (kcal/mol)	-CDOCKER-INTERACTION-ENERGY (kcal/mol)	Electrostatic Energy (kcal/mol)	Hydrogen Bond Energy (kcal/mol)	Van der Waals Energy (kcal/mol)	RMS Gradient
MeNam-HPMC	4.0136	7.1170	-1.7666	-4.3756	1.7537	0.0097
MeNam-DMSA	12.0203	17.0409	-9.9746	-0.1534	1.9453	0.0066
MeNam-HPMC@DMSA	7.8374	11.0266	-7.6778	-3.5324	1.5395	0.0089

Table S2. Comparison of analytical performance of the proposed method with other methods.

Preconcentration	Detection technique	Column	Analytes	Linearity	LOD	Intra-assay CVs	Inter-assay CVs	Recovery	Sample	Reference
Without extraction	LC/MS	C18-BDS Column (150 × 2.0 mm,3μm)	NA, N-methylnicotinamide (NMA), 2PY, 4PY, M2PY, NOX，M4PY, and 4PYR	/	/	＜10%	＞20%	/	human and rat plasma and urine	[1]
	HPLC-ESI-MS/MS	Synergi 4u polar-RP column (250 × 4.6 mm)	N^1-Methylnicotinamide (NMNAM), nicotinic acid (NA), nicotinamide (NAM), N^1-methyl-2-pyridone-5-carboxamide(2-Py), nicotinuric acid (NUA)	10-1000 ng mL^{-1} (N^1-methylnicotinamide)	/	≤3.1%	≤5.6%	113 ± 13%	Urine	[2]
	LC–MS/MS	a Waters Spherisorb S5 CN microbore column (2.0 × 100 mm, 5 μm)	Nicotinamide, N^1-methylnicotinamide	2.500–80.00 ng/mL (N^1-methylnicotinamide)	/	6.90%	6.90%	>88%	human serum	[3]
liquid/liquid extraction	HPLC-UV	Biphenyl Column (100 × 2.1 mm,2.6μm)	N-methyl-2-pyridone-5-carboxamide (2PYr) and N-1-methylnicotinamide (NMN)	0.8630-25.89 μg/mL (N-1-methylnicotinamide)	/	＜8%	＜8%	91 ±5.4%	Urine	[4]
MSPE	HPLC-UV	BaseLine C18 Column (4.6 × 150 mm, 5 μm)	N^1-methylnicotinamide (MeNam)	0.1–80 μg/mL	0.0375 μg/mL	＜10%	＜10%	＞95%	Urine	This work

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