Figure S1. TG profiles of MET–RHE, MET–RHE–H₂O, MET–RHE–ethanol–H₂O, MET–RHE–acetonitrile.
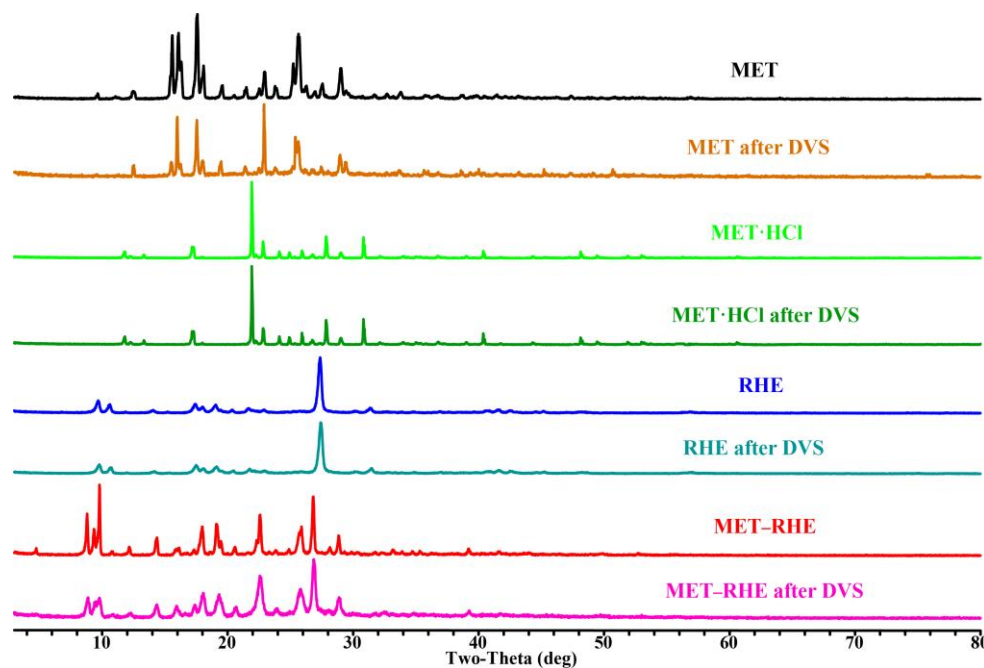

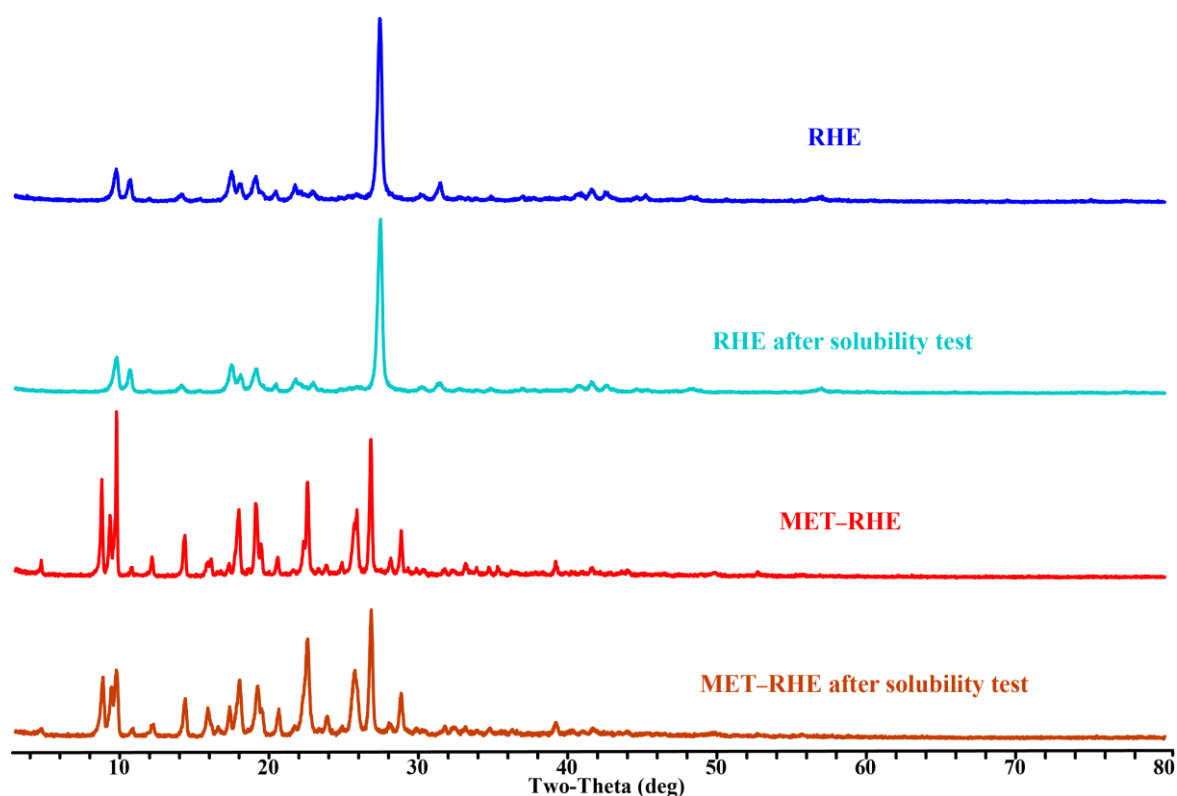**Figure S2.** The PXRD patterns of samples after DVS experiments

Figure S3. The PXRD patterns of samples after solubility tests

Table S1. Weight loss steps of solvents in the TG curves of A, B and C compared with theoretical weight loss percentage.

Sample	Actual Weight Loss (%)	Theoretical Weight Loss (%)
MET–RHE–H_2O	4.8	4.2
MET–RHE–ethanol–H_2O	12.6	13.4
MET–RHE–acetonitrile	4.7	4.7

Table S2. Detailed hydrogen bonding information of MET–RHE.

D–H⋯A (Å)	d(D–H) (Å)	d(H⋯A) (Å)	d(D⋯A) (Å)	∠D–H⋯A (deg)
O_3–H_3⋯O_4	0.82	1.90	2.60	143.92
O_3–H_3⋯O_5[a]	0.82	2.60	3.23	133.77
O_5–H_5⋯O_4	0.82	1.89	2.61	145.33
O_5–H_5⋯O_4[b]	0.82	2.50	2.99	119.37
N_2–H_{2A}⋯O_2[c]	0.86	2.16	2.92	147.49
N_2–H_{2B}⋯O_2[d]	0.86	2.24	2.98	144.19
N_2–H_{2B}⋯N_4	0.86	2.38	2.86	115.64
N_3–H_{3B}⋯N_5[e]	0.86	2.34	3.01	135.48
N_4–H_{4A}⋯O_2[f]	0.86	2.20	2.89	137.08
N_4–H_{4A}⋯N_2	0.86	2.41	2.86	112.35
N_4–H_{4B}⋯O_1	0.86	2.17	2.93	145.94
N_5–H_{5A}⋯O_1	0.99	1.83	2.77	156.83

Symmetry codes: (a) -x+3, -y+1, -z (b) -x+3, -y+1, -z (c) -x, -y+1, -z+1 (d) x-1, y, z (e) -x, -y+2, -z+1 (f) -x+1, -y+1, -z+1.

Table S3. Detailed hydrogen bonding information of MET–RHE–ethanol–H_2O.

D–H⋯A (Å)	d(D–H) (Å)	d(H⋯A) (Å)	d(D⋯A) (Å)	∠D–H⋯A (deg)
$O_3–H_3⋯O_4$	0.84	1.86	2.58	144.02
$O_3–H_3⋯O_4$[a]	0.84	2.47	2.88	110.80
$O_5–H_5⋯O_4$	0.84	1.85	2.59	145.13
$O_5–H_5⋯O_3$[b]	0.84	2.65	3.29	134.44
$N_5–H_{5A}⋯O_1$	0.88	2.11	2.91	151.32
$N_5–H_{5B}⋯N_3$[c]	0.88	2.20	3.08	174.13
$N_4–H_{4A}⋯O_7$	0.88	2.12	2.96	159.47
$N_4–H_{4B}⋯O_7$[d]	0.88	2.10	2.88	147.47
$N_2–H_{2A}⋯O_8$[e]	0.88	2.22	2.92	136.78
$N_2–H_{2B}⋯O_1$[f]	0.88	2.19	2.89	137.07
$O_7–H_{7A}⋯O_2$	0.84	1.80	2.64	173.09
$O_8–H_{8A}⋯O_6$	0.86	2.07	2.92	176.41
$O_8–H_{8B}⋯O_2$[g]	0.85	0.98	2.82	169.88

Symmetry codes: (a) -x+1, -y, -z (b) -x+1, -y, -z (c) -x+1, -y+1, -z-1 (d) -x, -y, -z-1 (e) -x,-y+1,-z-1 (f) -x,-y+1,-z-1 (g) x, y+1, z.

Table S4. Detailed hydrogen bonding information of MET–RHE–acetonitrile.

D–H⋯A (Å)	d(D–H) (Å)	d(H⋯A) (Å)	d(D⋯A) (Å)	∠D–H⋯A (deg)
$O_{1B}–H_{1B}⋯O_{4B}$	0.82	1.87	2.59	144.87
$O_{1B}–H_{1B}⋯O_{4A}$[a]	0.82	2.37	2.86	118.83
$O_{1A}–H_{1A}⋯O_{4B}$[b]	0.82	2.36	2.84	118.38
$O_{1A}–H_{1A}⋯O_{4A}$	0.82	1.87	2.58	145.30
$O_{3B}–H_{3B}⋯O_{4B}$	0.82	1.89	2.60	144.37
$O_{3B}–H_{3B}⋯O_{1A}$[c]	0.82	2.48	3.11	134.85
$N_{4B}–H_{4BA}⋯O_{5A}$[d]	0.86	2.18	2.99	155.89
$N_{4B}–H_{4BB}⋯N_{2B}$	0.86	2.47	2.89	111.31
$N_{4B}–H_{4BB}⋯N_{1Y}$[e]	0.86	2.37	3.06	137.90
$N_{2B}–H_{2BA}⋯O_{6B}$[f]	0.86	2.18	3.03	171.95
$N_{2B}–H_{2BB}⋯O_{6B}$	0.86	2.21	2.90	137.70
$N_{2B}–H_{2BB}⋯N_{4B}$	0.86	2.47	2.89	110.96
$N_{1A}–H_{1AA}⋯O_{5B}$	0.86	2.29	3.04	146.16
$N_{1A}–H_{1AB}⋯O_{6A}$[g]	0.86	2.02	2.82	152.75
$O_{3A}–H_{3A}⋯O_{1B}$[h]	0.82	2.49	3.12	135.20
$O_{3A}–H_{3A}⋯O_{4A}$	0.82	1.88	2.59	143.38
$N_{1B}–H_{1BA}⋯O_{6A}$[i]	0.86	2.06	2.83	148.75
$N_{1B}–H_{1BB}⋯O_{5B}$[j]	0.86	2.12	2.90	151.21
$N_{2A}–H_{2AA}⋯O_{5B}$[k]	0.86	2.54	3.18	132.31
$N_{2A}–H_{2AA}⋯N_{4A}$	0.86	2.47	2.89	110.79
$N_{2A}–H_{2AB}⋯O_{5A}$[l]	0.86	2.11	2.95	167.25
$N_{4A}–H_{4AA}⋯O_{6B}$[m]	0.86	2.22	3.02	153.76
$N_{4A}–H_{4AB}⋯O_{2A}$	0.86	2.43	2.89	113.64
$N_{4A}–H_{4AB}⋯N_{1Y}$	0.86	2.62	3.19	125.55

Symmetry codes: (a) x, -y+3/2, z+1/2 (b) x, -y+3/2, z-1/2 (c) x, -y+3/2, z+1/2 (d) -x+1, y-1/2, -z+1/2 (e) -x, y-1/2, -z+1/2 (f) -x, -y+1, -z (g) x-1, y, z (h) x, -y+3/2, z-1/2 (i) -x+1, -y+1, -z (j) -x, -y+1, -z (k) -x, y+1/2, -z+1/2 (l) x-1, y, z (m) x, -y+3/2, z+1/2.

Table S5. The DVS data of MET, MET·HCl, MET–RHE

Target RH (%)	Change in Mass (%)		
	MET	**MET–RHE**	**MET·HCl**
20	0.00	0.00	0.00
25	0.02	0.04	0.00
30	0.04	0.09	0.00
35	0.05	0.14	0.01
40	0.07	0.20	0.01
45	0.09	0.26	0.01
50	0.13	0.34	0.02
55	0.23	0.44	0.02
60	0.45	0.57	0.02
65	0.97	0.71	0.03
70	1.67	0.86	0.04
75	4.06	1.04	0.05
80	9.59	1.28	0.06
85	18.49	1.61	0.08
90	31.79	2.03	0.11
95	49.41	2.66	0.17
90	60.50	2.41	0.11
85	64.68	1.72	0.08
80	64.48	1.37	0.06
75	59.09	1.15	0.05
70	51.50	0.99	0.04
65	43.17	0.87	0.04
60	35.20	0.77	0.03
55	27.05	0.58	0.02
50	18.04	0.60	0.02
45	11.92	0.52	0.01
40	10.71	0.44	0.01
35	10.34	0.36	0.01
30	10.05	0.28	0.01
25	9.84	0.22	0.00
20	9.66	0.15	0.00