

Electronic Supplementary Information
For

**Febuxostat-minoxidil salt solvates: crystal structures, characterization,
interconversion and solubility performance**

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Table S1 The detailed PXRD values of FEB-MIN·ACE.

Number	Simulated values		Experimental values	
	2-Theta	d(Å)	2-Theta	d(Å)
1	7.557	11.6883	7.549	11.7005
2	7.981	11.0682	7.956	11.103
3	10.218	8.6501	10.19	8.6737
4	11.478	7.7031	11.418	7.7431
5	12.042	7.3435	11.994	7.3729
6	12.994	6.8075	12.947	6.8319
7	13.403	6.6009	13.337	6.6333
8	14.257	6.2072	14.174	6.2434
9	15.178	5.8324	15.092	5.8656
10	16.024	5.5265	15.96	5.5484
11	17.416	5.0878	17.3	5.1215
12	18.107	4.8952	17.985	4.928
13	18.578	4.7721	18.328	4.8365
14	19.9	4.4579	19.754	4.4928
15	21.159	4.1955	21.06	4.2149
16	22.119	4.0154	22.001	4.0367
17	22.841	3.8902	22.709	3.9125
18	24.398	3.6452	24.263	3.6652
19	24.779	3.5901	24.63	3.6115
20	26.177	3.4014	26.052	3.4175

Table S2. The detailed PXRD values of FEB-MIN·THF

Number	Simulated values		Experimental values	
	2-Theta	d(Å)	2-Theta	d(Å)
1	7.461	11.8394	7.424	11.898
2	7.963	11.0942	7.922	11.1503
3	10.163	8.6965	10.15	8.7073
4	11.341	7.7958	11.289	7.8317
5	11.859	7.4564	11.813	7.4851
6	12.939	6.8363	12.898	6.8582
7	13.343	6.6303	13.313	6.6453
8	14.099	6.2764	14.062	6.2928
9	14.958	5.9176	14.887	5.9458
10	15.978	5.5424	15.888	5.5734
11	16.838	5.2612	16.755	5.2869
12	17.401	5.0921	17.332	5.1123
13	18.182	4.875	18.117	4.8924
14	19.137	4.6339	19.09	4.6452
15	19.46	4.5578	19.48	4.5764
16	19.836	4.4722	19.744	4.4928
17	22.503	3.9477	22.473	3.9529
18	24.099	3.6898	24.051	3.6971
19	24.682	3.604	24.631	3.6114
20	26.001	3.4241	25.966	3.4286

Table S3. The detailed PXRD values of FEB-MIN·IPA

Number	Simulated values		Experimental values	
	2-Theta	d(Å)	2-Theta	d(Å)
1	7.299	12.1019	7.339	12.0362
2	7.799	11.3267	7.82	11.2955
3	10.217	8.6509	10.162	8.6977
4	11.52	7.6753	11.473	7.7061
5	13.518	6.5447	13.492	6.5575
6	14.621	6.0536	14.648	6.0424
7	15.636	5.6625	15.625	5.6668
8	16.841	5.2602	16.728	5.2955
9	17.2	5.1512	17.171	5.1597
10	17.922	4.9453	17.854	4.964
11	18.199	4.8706	18.166	4.8792
12	19.003	4.6664	19.033	4.6589
13	19.738	4.4941	19.767	4.4877
14	20.501	4.3285	20.532	4.3221
15	21.86	4.0625	21.77	4.079
16	22.44	3.9587	22.346	3.9753
17	23.562	3.7727	23.554	3.774
18	24.08	3.6928	24.002	3.7045
19	24.881	3.5756	24.816	3.5849
20	25.703	3.4631	25.683	3.4658

Table S4. The mole percentage of the three salt solvates in ACE, THF, and IPA solution.

Entry	Salt solvates	ACE			THF			IPA		
		FEB- MIN·ACE	FEB- MIN·TH	FEB- MIN·IP	FEB- MIN·ACE	FEB- MIN·TH	FEB- MIN·IP	FEB- MIN·ACE	FEB- MIN·THF	FEB- MIN·IPA
		(%)	F (%)	A (%)	(%)	F (%)	A (%)	(%)	(%)	(%)
1	FEB- MIN·AC E	100	0	0	23.7	76.3	0	6.0	0	94.0
2	FEB- MIN·TH F	78.8	21.2	0	0	100	0	0	5.0	95.0
3	FEB- MIN·IPA	95.8	0	4.2	0	100	0	0	0	100

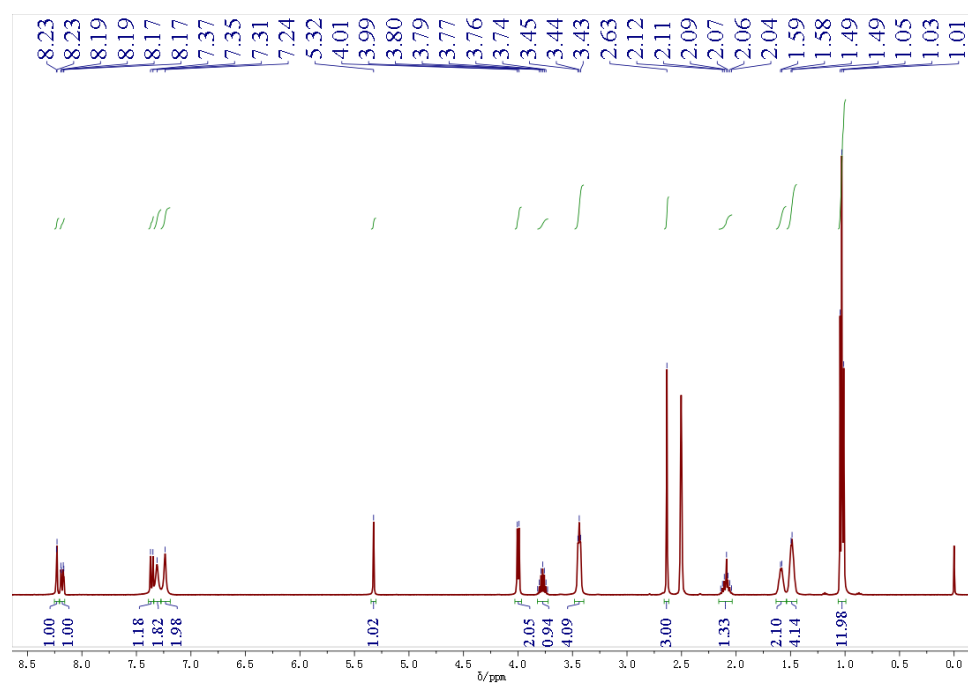


Figure S1. ^1H -NMR spectra of FEB-MIN-ACE in IPA solution after 24h.

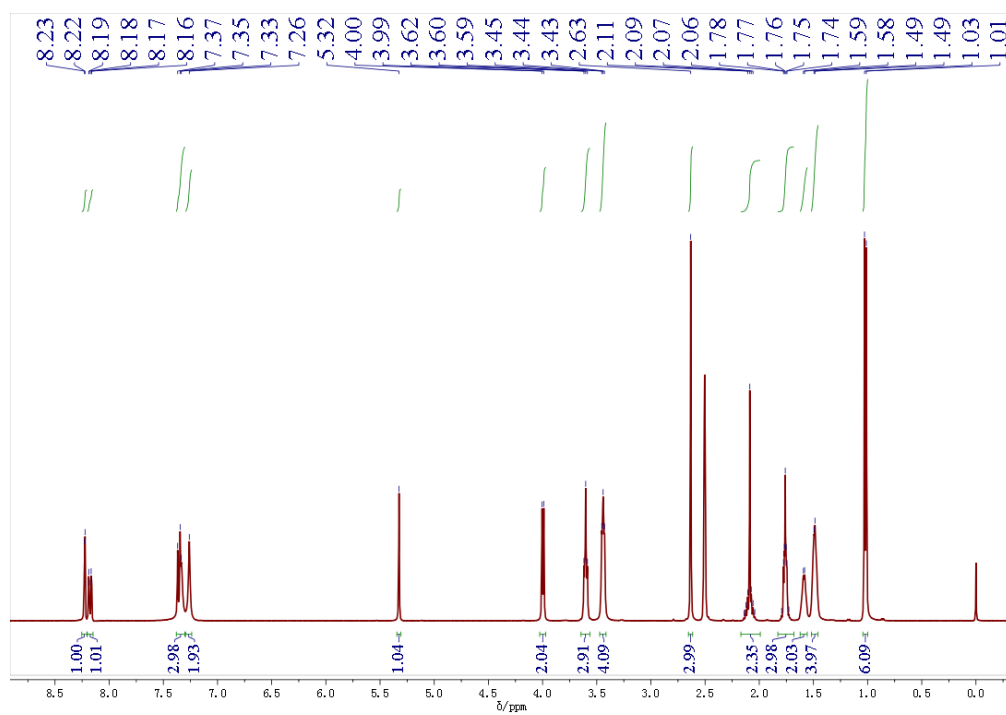


Figure S2. ^1H -NMR spectra of FEB-MIN-ACE in THF solution after 24h.

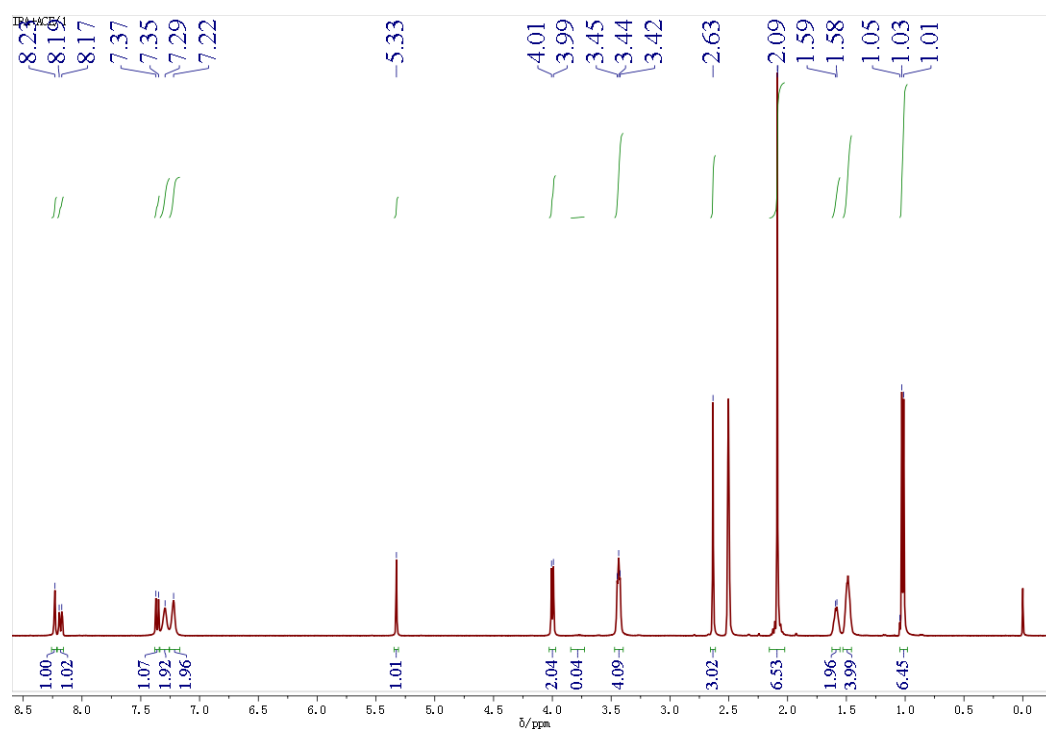


Figure S3. ^1H -NMR spectra of FEB-MIN-IPA in ACE solution after 24h.

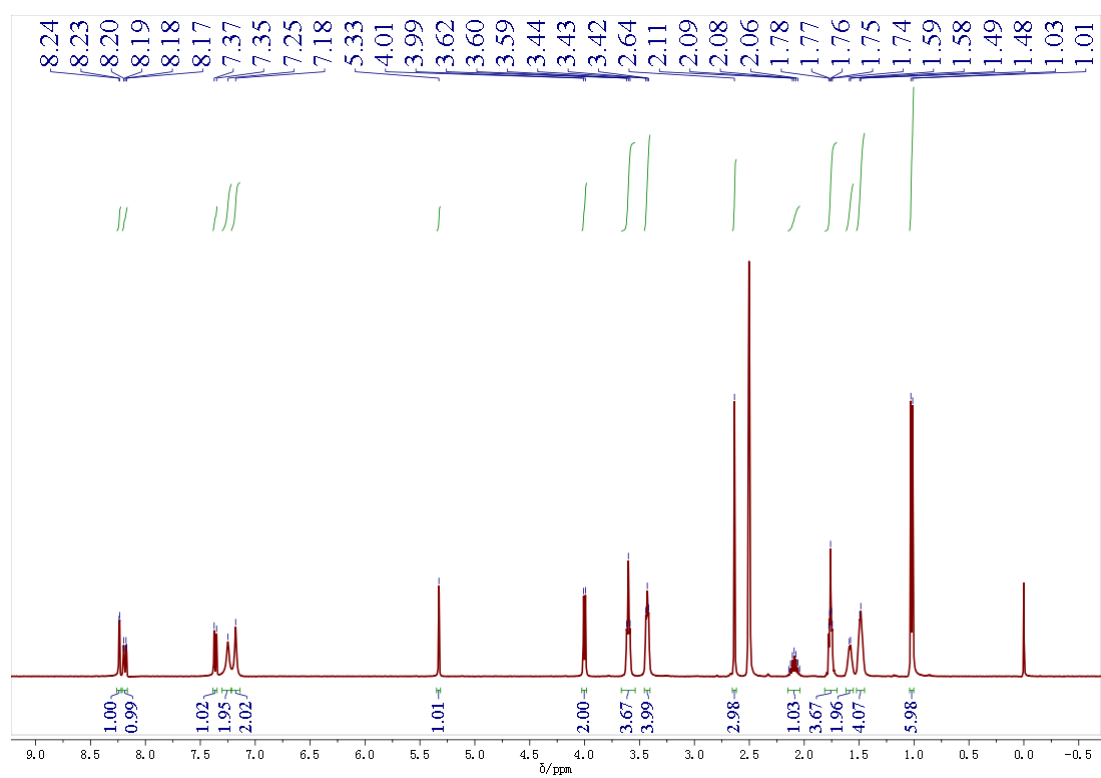


Figure S4. ^1H -NMR spectra of FEB-MIN-IPA in THF solution after 24h.

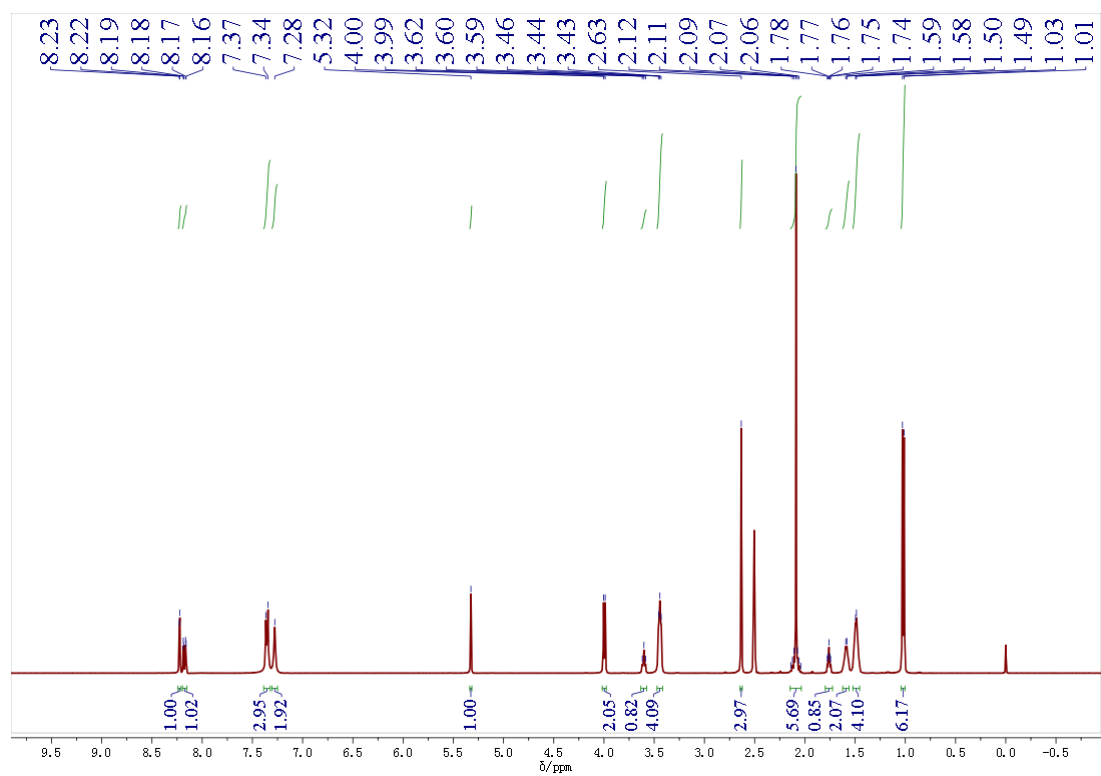


Figure S5. ^1H -NMR spectra of FEB-MIN·THF in ACE solution after 24h.

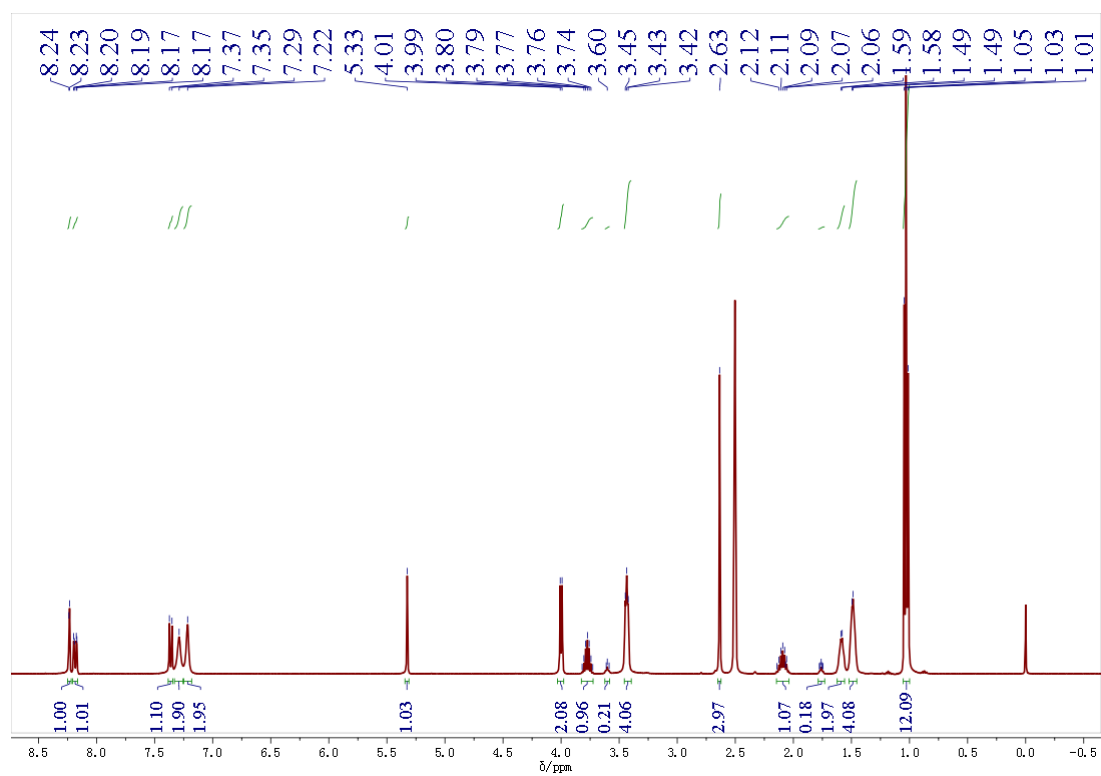


Figure S6. ^1H -NMR spectra of FEB-MIN·THF in IPA solution after 24h.

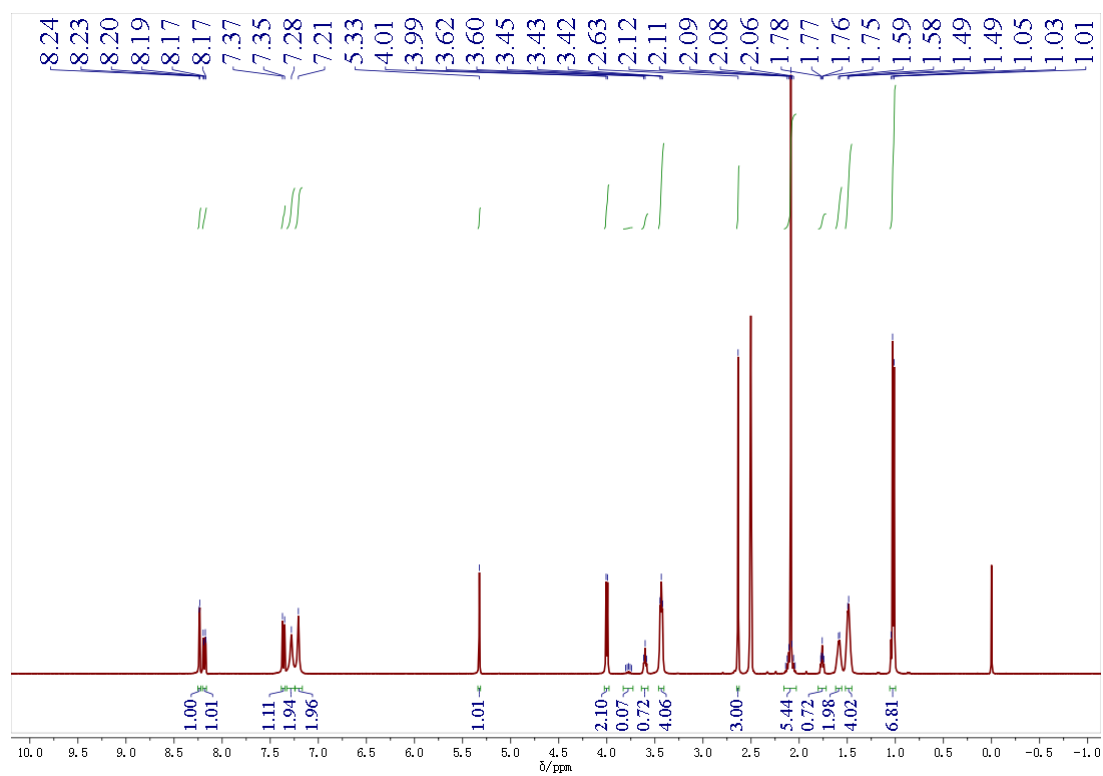


Figure S7. ^1H -NMR spectra of FEB-MIN-ACE in mixed solution after 24h.

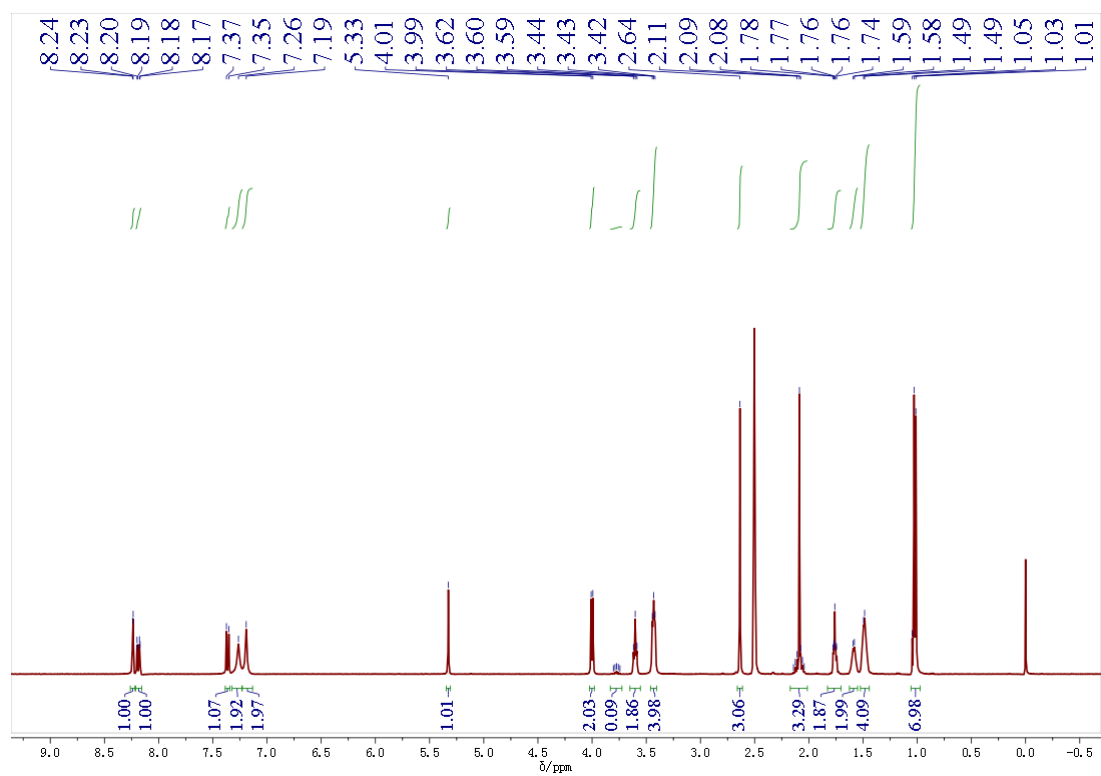


Figure S8. ^1H -NMR spectra of FEB-MIN·THF in mixed solution after 24h.

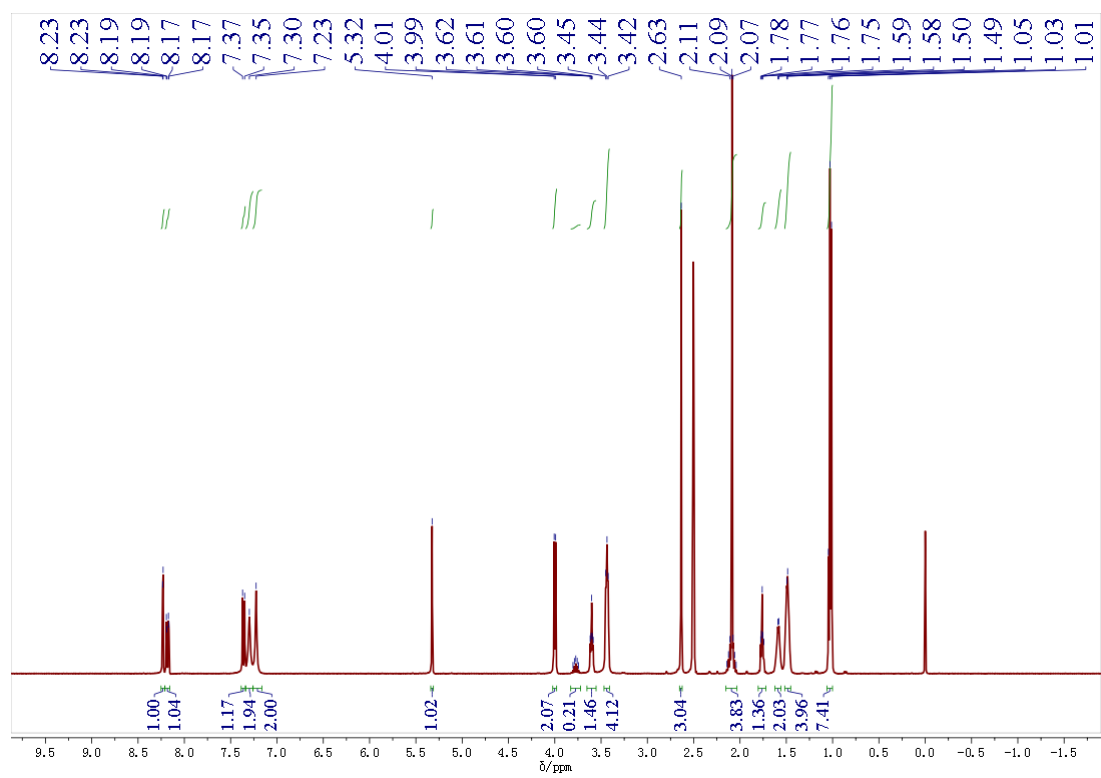


Figure S9. ^1H -NMR spectra of FEB-MIN-IPA in mixed solution after 24h.

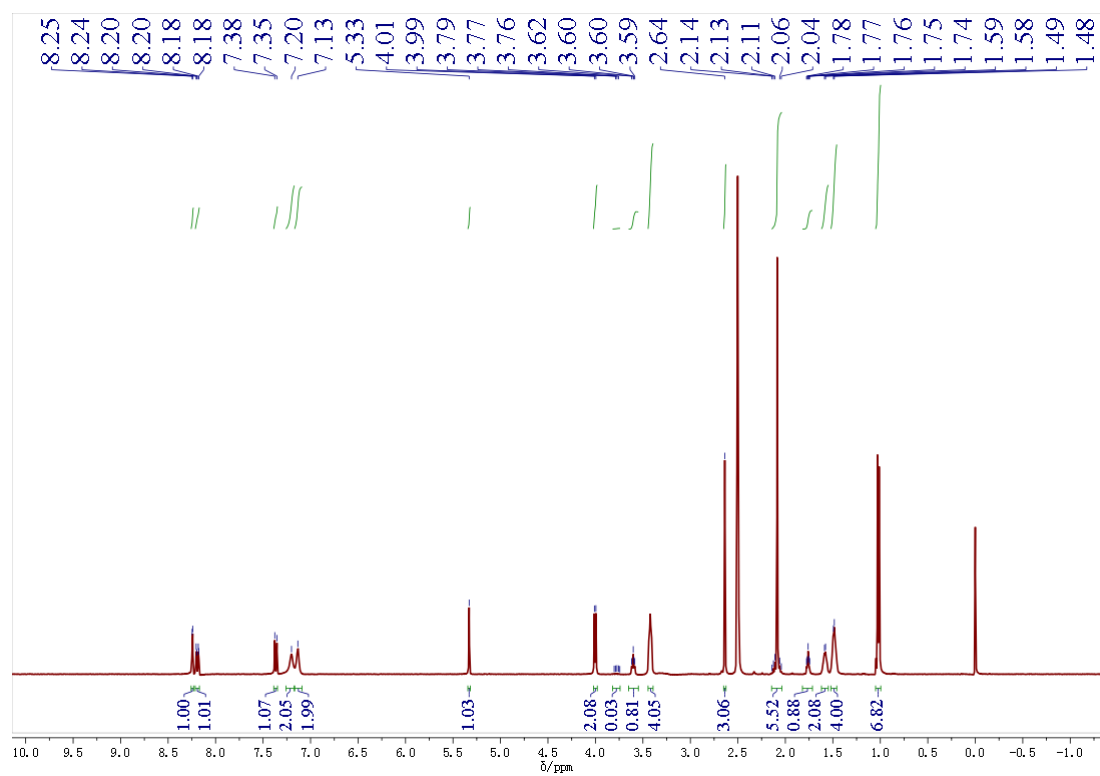


Figure S10. ^1H -NMR spectra of FEB-MIN·ACE in mixed solution after 48h.

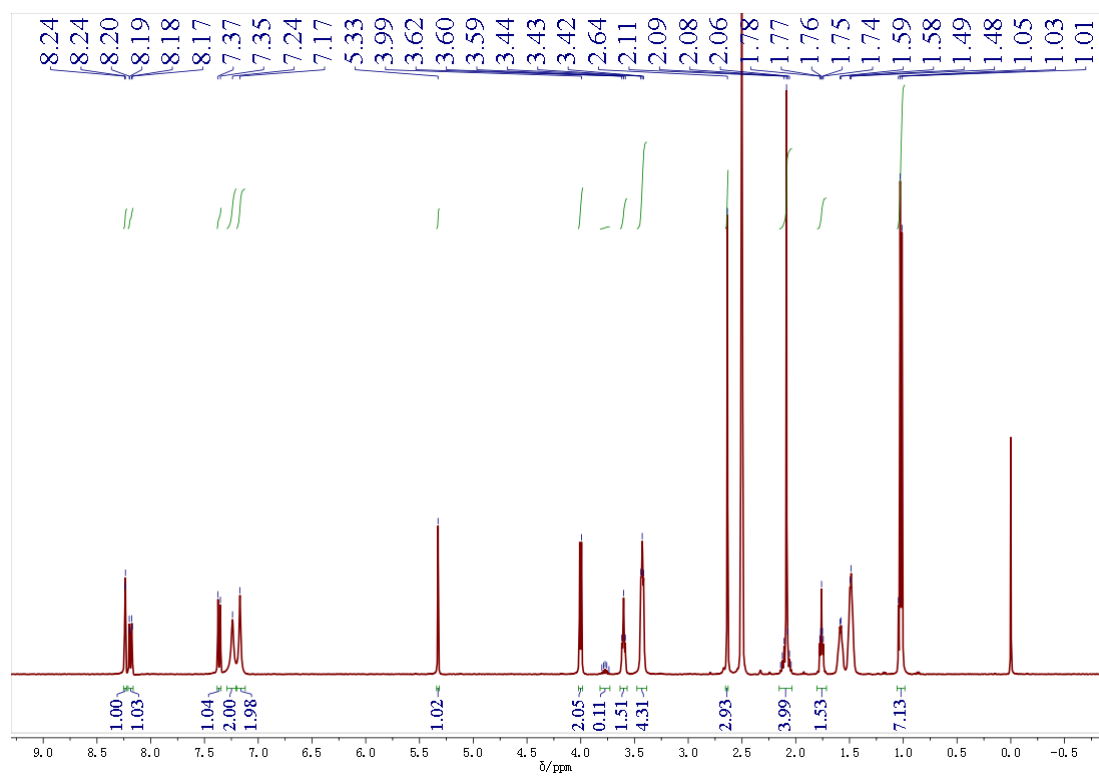


Figure S11. ^1H -NMR spectra of FEB-MIN-IPA in mixed solution after 48h.

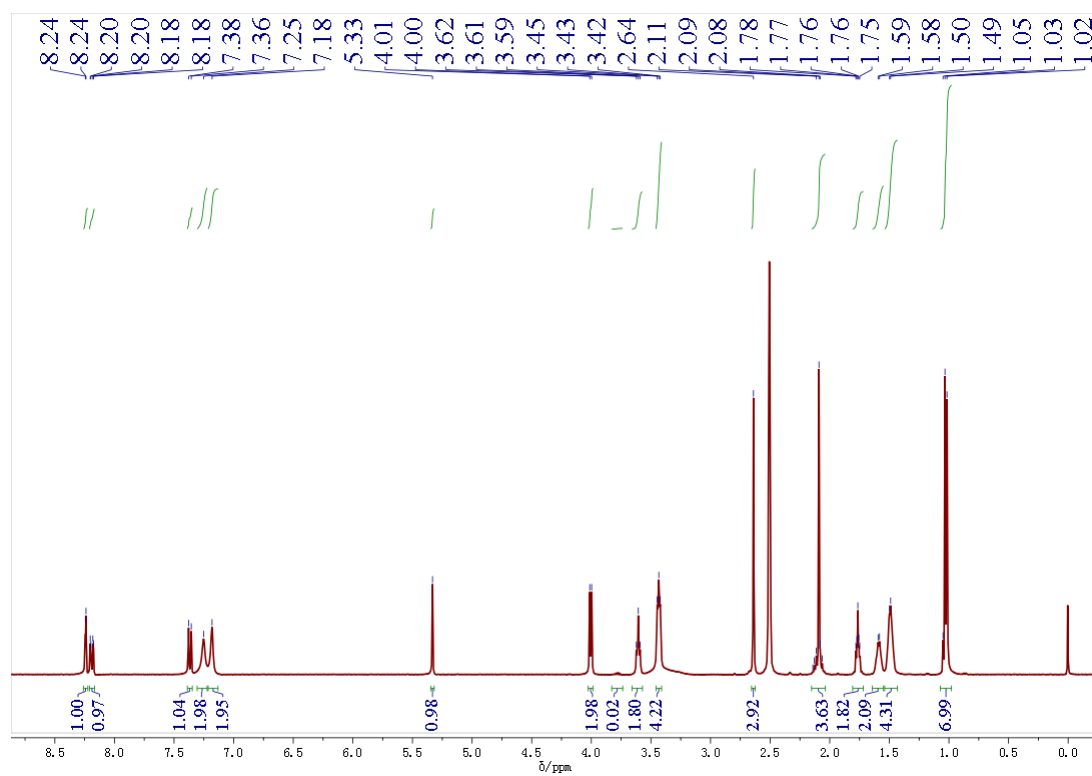


Figure S12. ^1H -NMR spectra of FEB-MIN·THF in mixed solution after 48h.

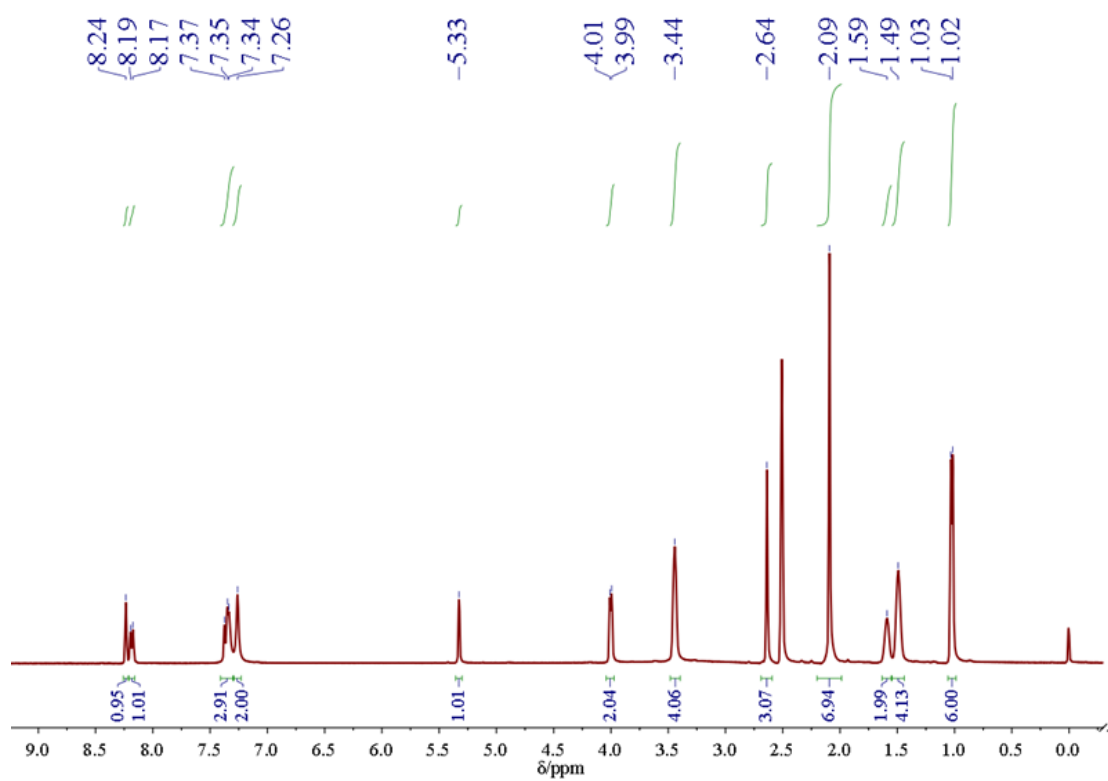


Figure S13. ¹H-NMR spectra of FEB-MIN-ACE.

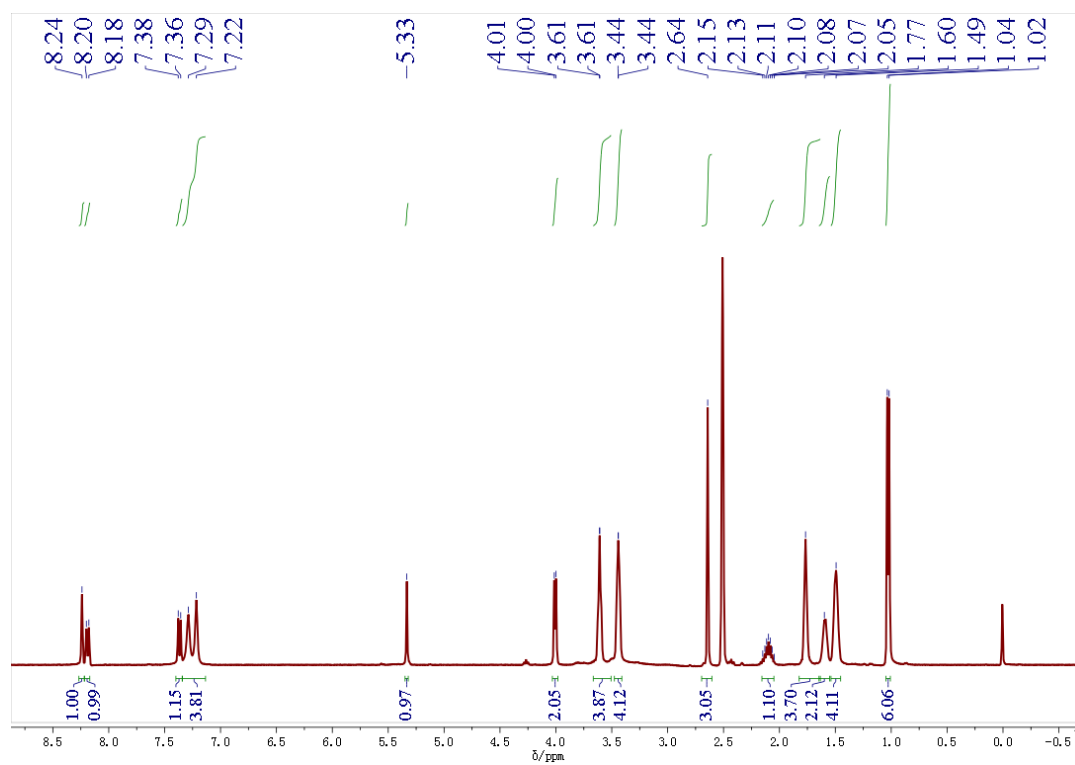


Figure S14. ¹H-NMR spectra of FEB-MIN·THF.

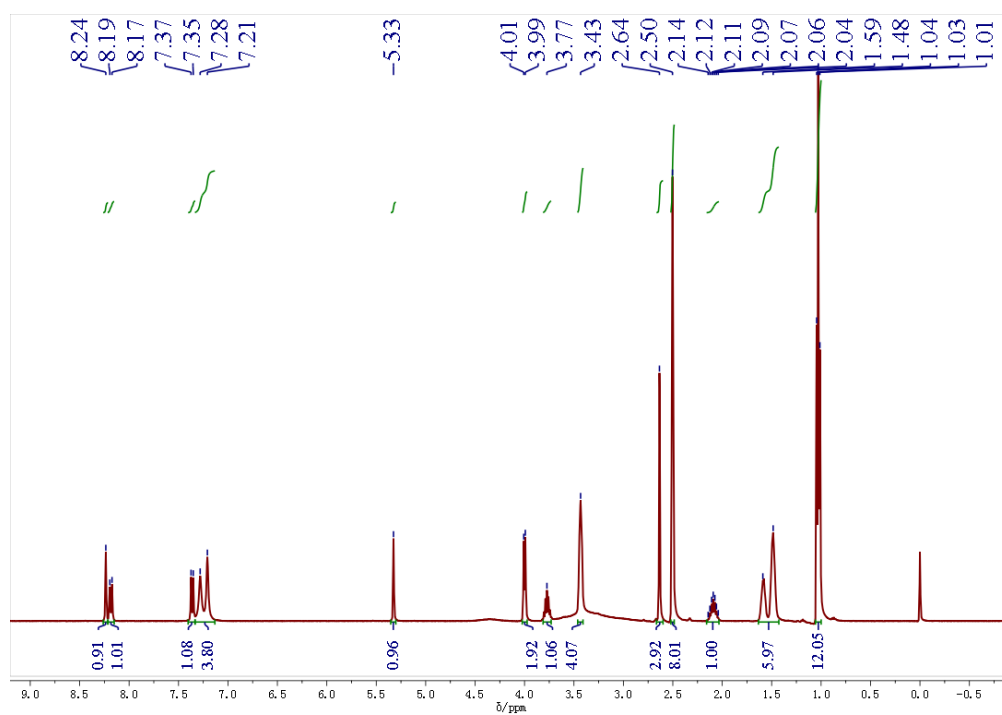


Figure S15. ^1H -NMR spectra of FEB-MIN-IPA.