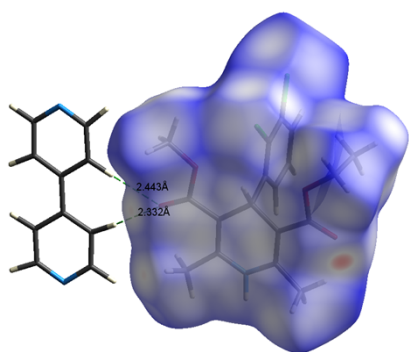


Polymorphism of felodipine co-crystals with 4,4'- bipyridine

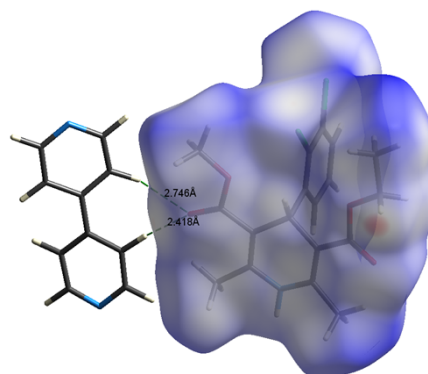
Artem O. Surov, Katarzyna A. Solanko, Andrew D. Bond,
Annette Bauer-Brandl and German L. Perlovich

Supporting Information

S1. Hirshfeld surface analysis



[FeI+BP] (1:1) form I



[FeI+BP] (1:1) form II

Fig. S1. Illustrations of the O...H contacts in the co-crystals.

S2. Experimental PXRD patterns

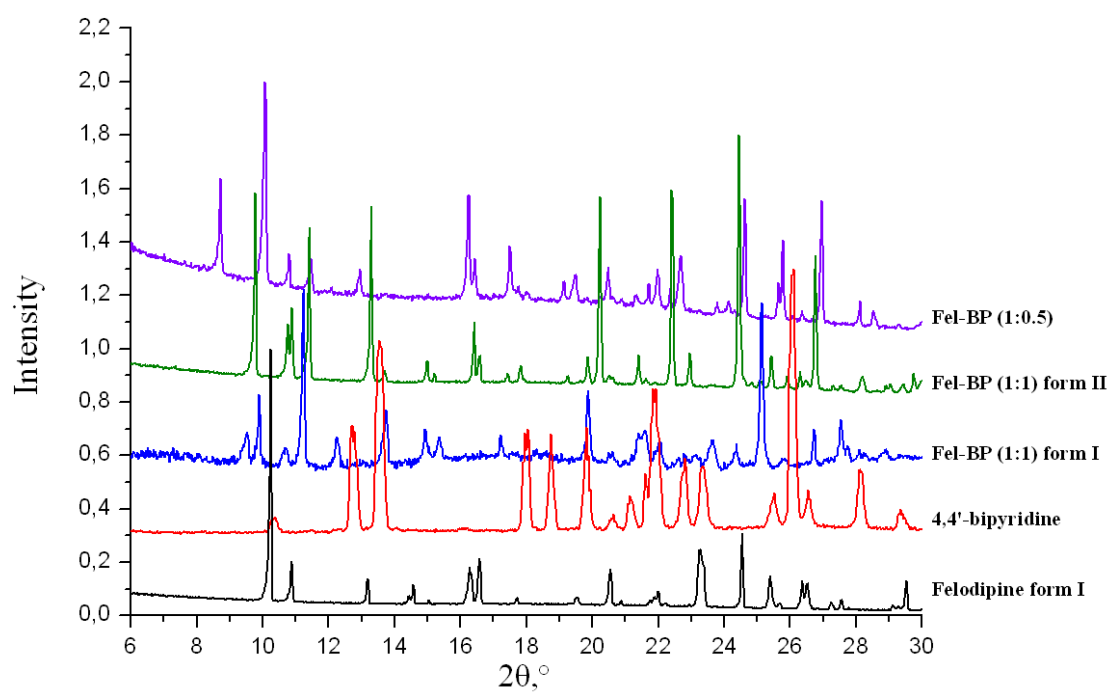


Fig. S2. Measured PXRD patterns of felodipine, 4,4'-bipyridine and the felodipine co-crystals

S3. Single-crystal X-ray diffraction data

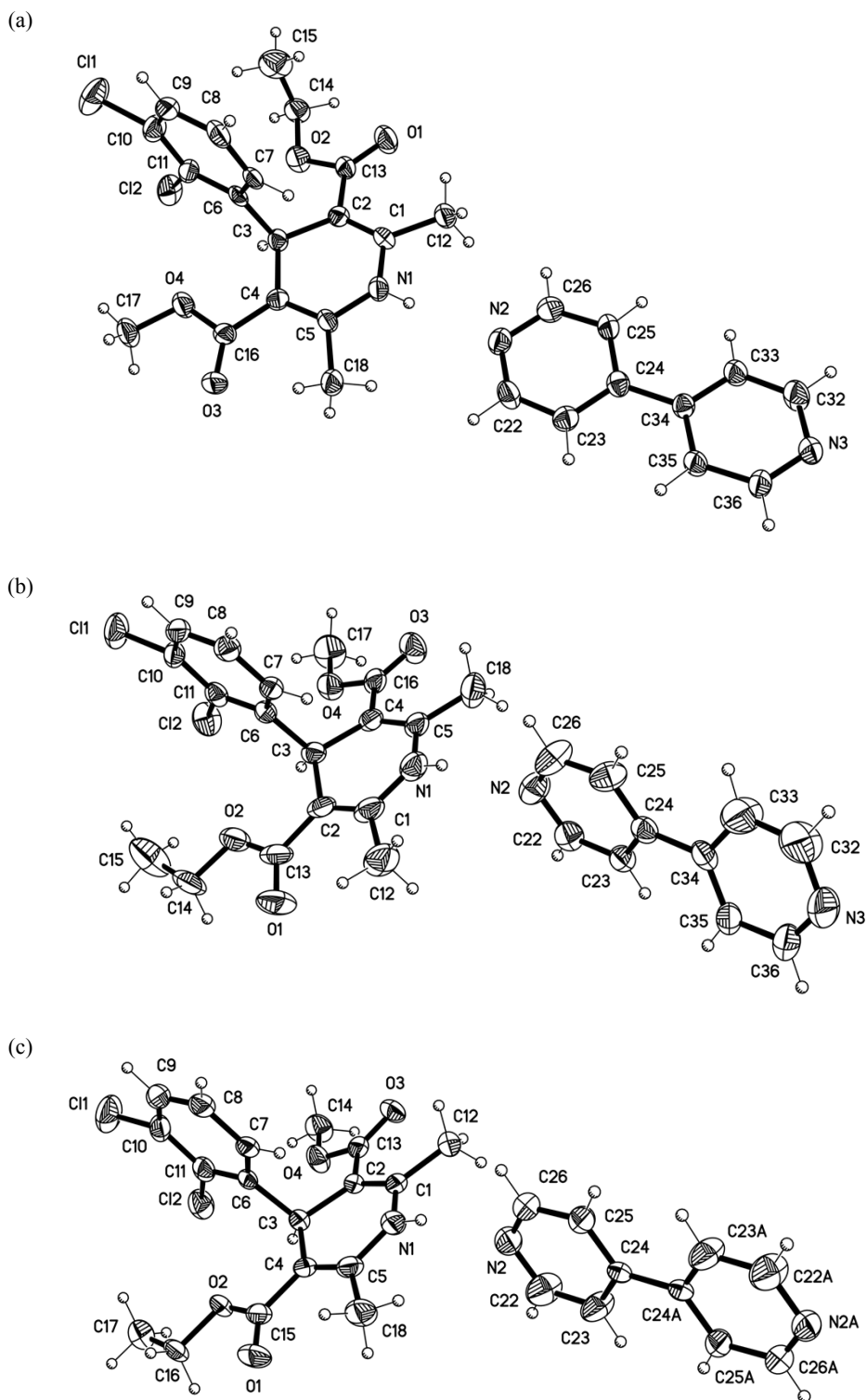


Fig. S3. Molecular units with atomic numbering in (a) [Fe+BP] (1:1) form I; (b) [Fe+BP] (1:1) form II; (c) [Fe+BP] (2:1). Displacement ellipsoids are shown at 50% probability.

Table S1. The retrieved CSD set of 4,4'-bipyridine cocrystals*

1	AMIDEF	31	HUPPAJ	61	NUCJEB	91	SOVDIQ	121	XOLHUC
2	AMIDIJ	32	HUPPEN	62	OFOKEA	92	SOVFIS	122	XOLHUC01
3	BEQWAV	33	IDUBUF	63	OFOKIE	93	SOVFOY	123	XOLHUC02
4	BIHZAU	34	IFABUN	64	OFOKOK	94	SOVHEQ	124	XOTYUB
5	BOQDOA	35	IFUQAC	65	OGEPOG	95	SUXVOW	125	XOZJAY
6	COBLAG	36	IKUJIH	66	OJENIA	96	TEKKID	126	XUNGIW
7	COZXUL	37	IKUJON	67	PANKAR	97	TEKKOJ	127	XUNGUI
8	DAQZIF	38	IKUJUT	68	PEGDAH	98	TIJKOM	128	XUNHAP
9	DATQEV	39	JAWVAF	69	POVJAL	99	TUQBIR	129	YAKVAI
10	DEBJAW	40	JAWVIN	70	PUFFUS	100	UCEXIJ	130	YUCQUJ
11	DEZHIA	41	JAZBAO	71	PUHFAA	101	UDUZEY	131	ZINZUR
12	DIWGOG	42	JEHXAW	72	PUJHUY	102	UDUZIC	121	XOLHUC
13	DOKGEQ	43	KASYEJ	73	PULWUO	103	UDUZOI	122	XOLHUC01
14	DOYJUX	44	KIHYAC	74	QAMRUS	104	UHELLO	123	XOLHUC02
15	EGUXAG	45	KIHZOR	75	QANRUS	105	UHOSIU	124	XOTYUB
16	EJEVUK	46	LAPLIY	76	QETMOS	106	UJORAM	125	XOZJAY
17	FAWXUX	47	LAPLOE	77	QIHBAK	107	UJOREQ	126	XUNGIW
18	FIDKOT	48	LEDJIO	78	QIHBEO	108	VEFWAF	127	XUNGUI
19	FIHYEA	49	LIDVAW	79	QIHBIS	109	VEXQOE	128	XUNHAP
20	FIJCIK	50	LIPWUC	80	QIJCUH	110	VEXQUK	129	YAKVAI
21	FOWSAM	51	LOMHUR	81	QOQDIJ	111	VEXWUQ	130	YUCQUJ
22	FUHRAC	52	LUJCOJ	82	RADDOQ	112	VUJTAW	131	ZINZUR
23	GAWJEU	53	MAQYAF	83	RADFOS	113	VUXRAI		
24	GEHROB	54	MIYKOU	84	RAPHAR	114	WEJHID		
25	GIPQAX	55	MIYKOU01	85	RAPXAI	115	WEXWEC		
26	GIPQEB	56	MOXRUN	86	RASBOD	116	WOVYEL		
27	GIYHUS	57	MUFNIK	87	RIRGUV	117	XAPWIU		
28	GODTUO	58	MUFNIK01	88	SIMHAY	118	XAPWUG		
29	HONVAI	59	MUPQAP	89	SITDIJ	119	XAQQUC		
30	HOXHAE	60	MURFEK	90	SOVBOU	120	XEZDIQ		

* CSD Version 5.34 (2013 Release with Nov 2012 update). Search constraints: 3-D coordinates determined, two-component, only organics.

Table S2. The weight, g (mg), solution concentrations, m (mol kg⁻¹), and solution enthalpies, ΔH_{sol}^0 (kJ·mol⁻¹), of felodipine cocrystals in methanol at 298 K.

Fel-BP (1:1) form I			Fel-BP (1:1) form II			Fel-BP (1:0.5)		
g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}	g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}	g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}
20.49	0.81	43.2	12.59	0.49	41.2	9.41	0.42	36.6
15.13	0.59	43.4	14.95	0.60	41.6	10.09	0.46	35.4
12.28	0.47	44.0	12.84	0.49	41.2	10.97	0.47	35.9
11.32	0.43	44.6	12.83	0.48	42.1	10.83	0.47	36.0
$\Delta H_{sol}^0 = 43.8 \pm 0.3$			$\Delta H_{sol}^0 = 41.5 \pm 0.2$			$\Delta H_{sol}^0 = 36.0 \pm 0.2$		

Table S3. The weight, g (mg), solution concentrations, m (mol kg⁻¹), and solution enthalpies, ΔH_{sol}^0 (kJ·mol⁻¹), of felodipine form I in 4,4'-bipyridine methanol solution and 4,4'-bipyridine in felodipine methanol solution at 298 K.

Felodipine form I in 1.38 <i>m</i> 4,4'-bipyridine methanol solution			4,4'-bipyridine in 1.37 <i>m</i> felodipine methanol solution		
g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}	g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}
25.23	1.38	21.2	10.05	1.35	17.2
25.52	1.29	21.1	11.47	1.42	17.6
24.88	1.37	21.1	10.54	1.41	17.6
25.09	1.38	21.6	11.11	1.51	17.1
$\Delta H_{sol}^0 = 21.3 \pm 0.1$			$\Delta H_{sol}^0 = 17.4 \pm 0.1$		
Felodipine form I in 0.79 <i>m</i> 4,4'-bipyridine methanol solution			4,4'-bipyridine in 2.71 <i>m</i> felodipine methanol solution		
g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}	g	$m \cdot 10^{-3}$	ΔH_{sol}^{298}
28.93	1.54	20.3	10.08	1.36	21.6
28.84	1.49	21.7	10.04	1.36	21.4
29.48	1.59	21.5	10.44	1.38	21.8
28.78	1.57	21.5	10.53	1.36	21.6
$\Delta H_{sol}^0 = 21.3 \pm 0.3$			$\Delta H_{sol}^0 = 21.6 \pm 0.1$		