

Supporting Information

Drug Repurposing of the Antiviral Drug Acyclovir: New Pharmaceutical Salts

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Table of Contents

I. Figure S1: Fingerprint images (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H and (f) Total of Acv hydrogen-sulfate salt.....	S1
II. Figure S2: Fingerprint images (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H and (f) Total of Acv nitrate salt.....	S2
III. Figure S3: Fingerprint images (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H (f) H-Cl and (g) Total of Acv hydrochloride salt	S3
IV. Figure S4: Detail Hirshfeld surfaces mapped in shape index (a) Acv nitrate and (b) Acv hydrochloride salts.....	S4
V. Figure S5: Full interaction Maps of (a) Acyclovir free solvent and (b) Acv hydrogen-sulfate salt. ...	S5
VI. Figure S6: Full interaction Maps of (a) Acv hydrochloride (b) Acv nitrate salts	S6
VII. Table S1: Hydrogen Bonds for the Acv salts	S7
VIII. Table S2: Bond Length Table S2: Bond Lengths for the Acv salts	S8
IX. Figure S7: % of contacts contribution in Acv salts	S8
X. Figure S8: ¹ H NMR (400 MHz) spectrum of commercial Acv in DMSO-d ₆	S8
XI. Figure S9: ¹ H NMR (400 MHz) spectrum of commercial HAcv·HSO ₄ in DMSO-d ₆	S8
XII. Figure S10: ¹ H NMR (400 MHz) spectrum of commercial HAcv·NO ₃ in DMSO-d ₆	S8
XIII. Figure S11: ¹ H NMR (400 MHz) spectrum of commercial HAcv·Cl in DMSO-d ₆	S8
XIV. Figure S12: Aqueous solubility of Acv salts	S8

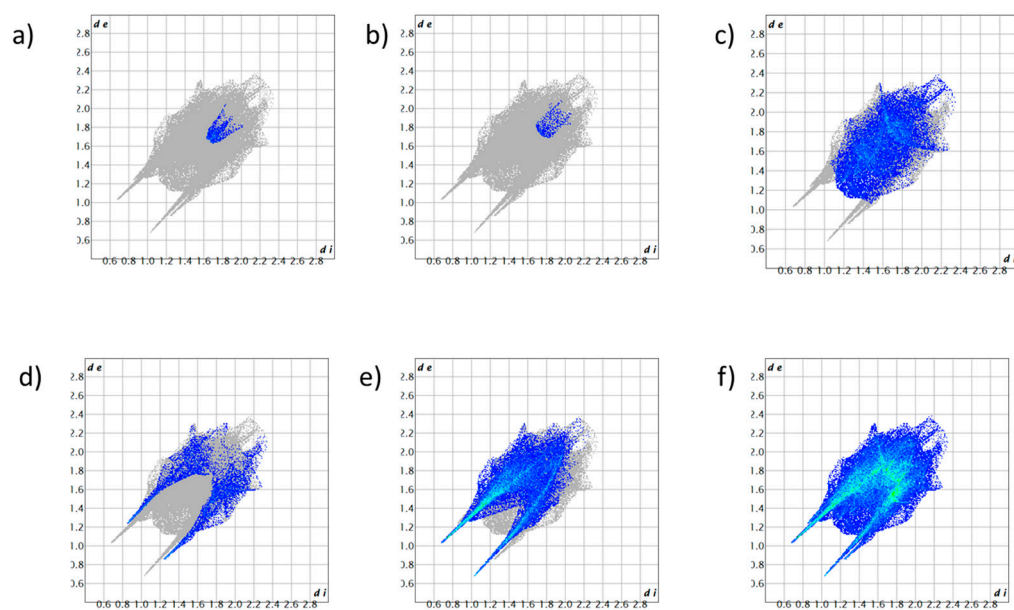


Figure S1. Fingerprint images of (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H and (f) Total Acv hydrogen-sulfate salt.

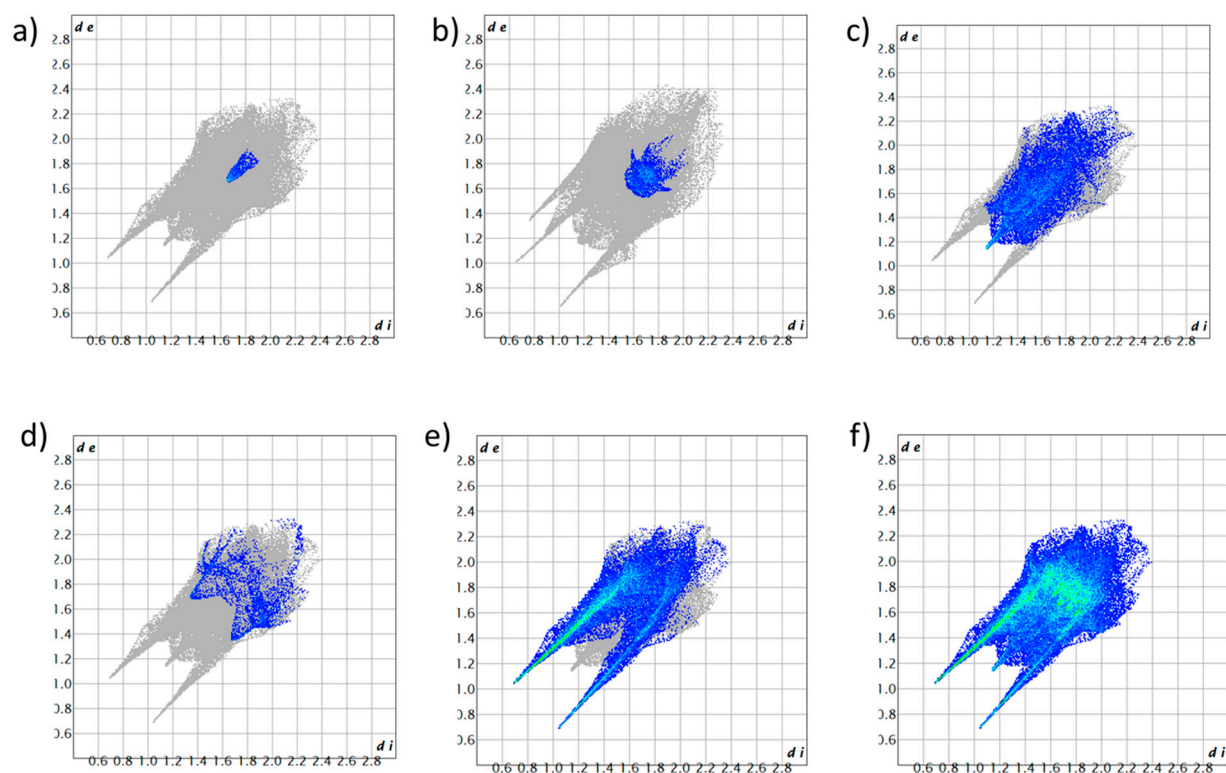


Figure S2. Fingerprint images of (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H and (f) Total Acv nitrate salt.

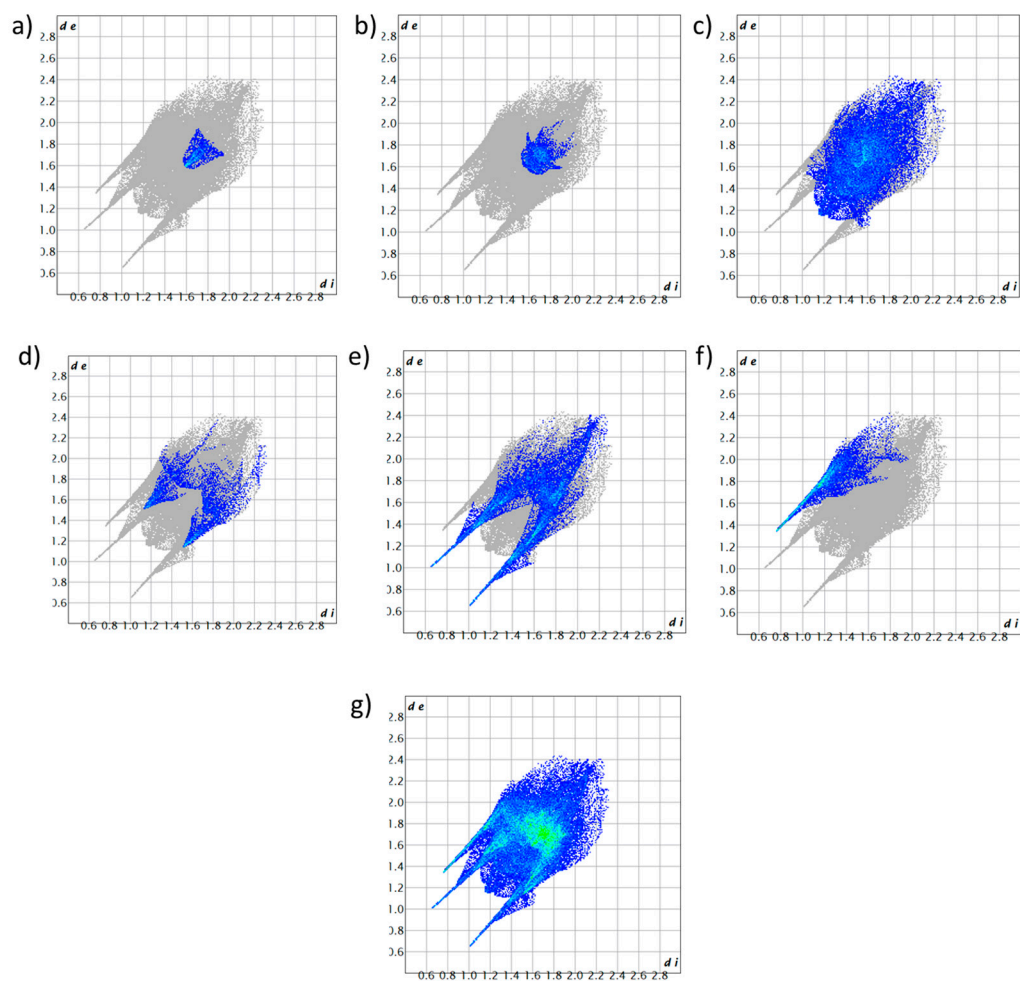


Figure S3. Fingerprint images of (a) C-C (b) C-N (c) H-H (d) N-H (e) O-H (f) H-Cl and (g) Total Acv hydrochloride salt.

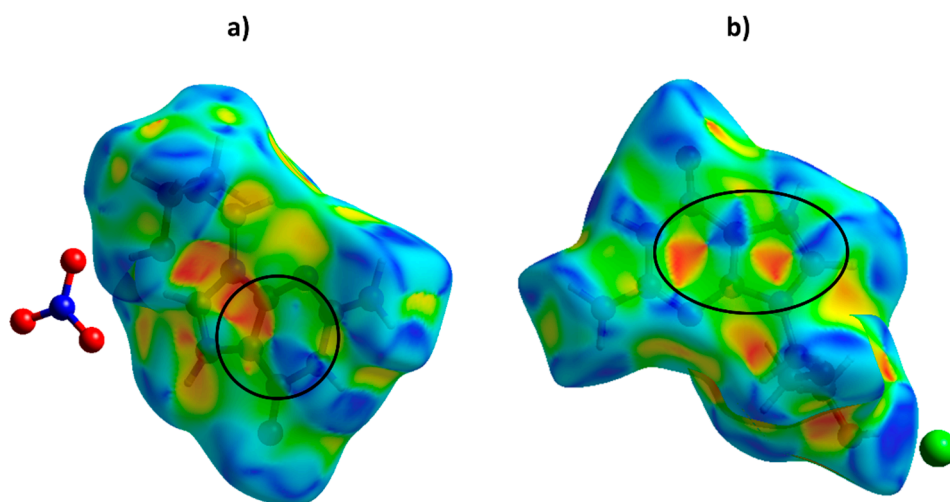
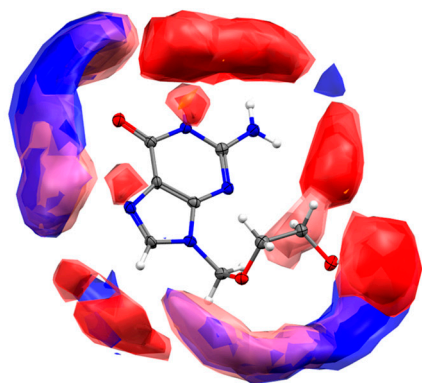


Figure S4. Detail Hirshfeld surfaces mapped in shape index (a) Acv nitrate and (b) Acv hydrochloride salts.

a)



b)

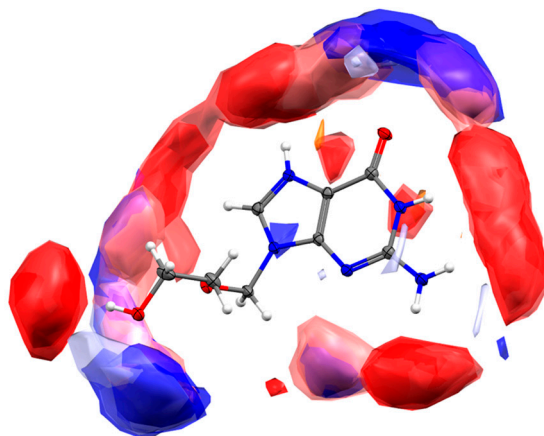
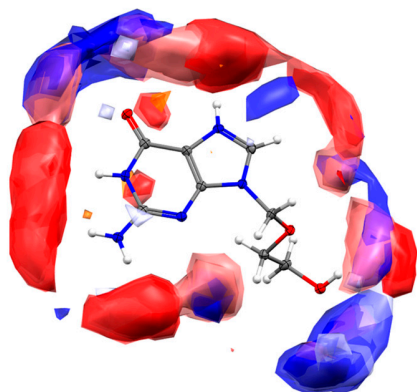


Figure S5. Full interaction Maps of (a) Acyclovir free solvent and (b) Acv hydrogen-sulfate salt.

c)



d)

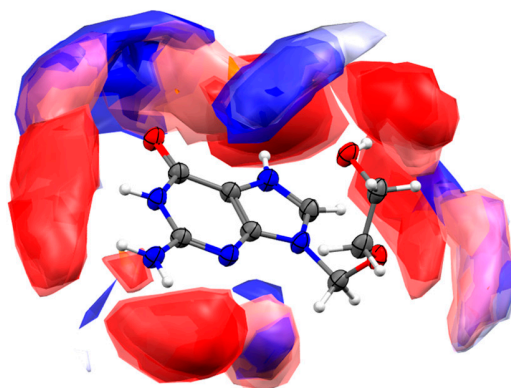


Figure S6. Full interaction Maps of (a) Acv hydrochloride (b) Acv nitrate salts.

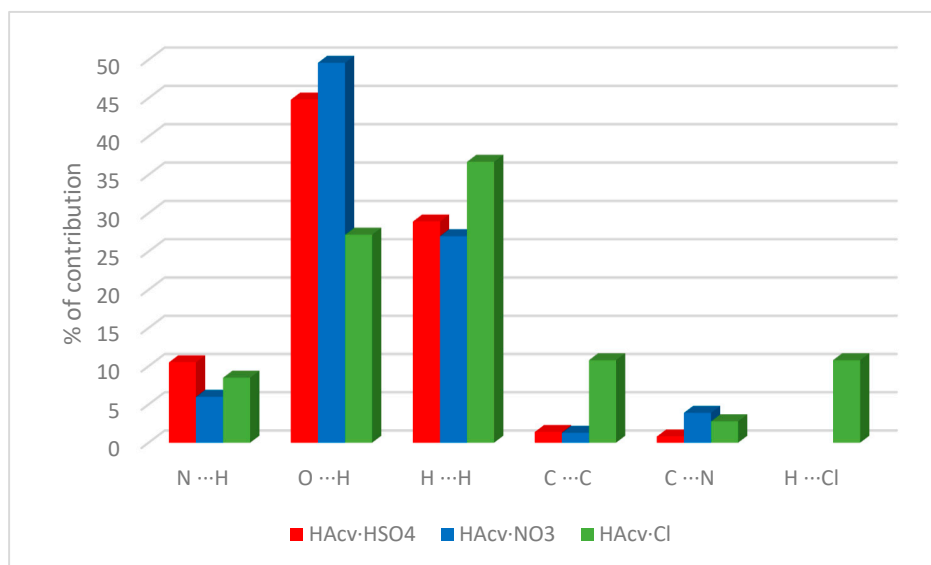
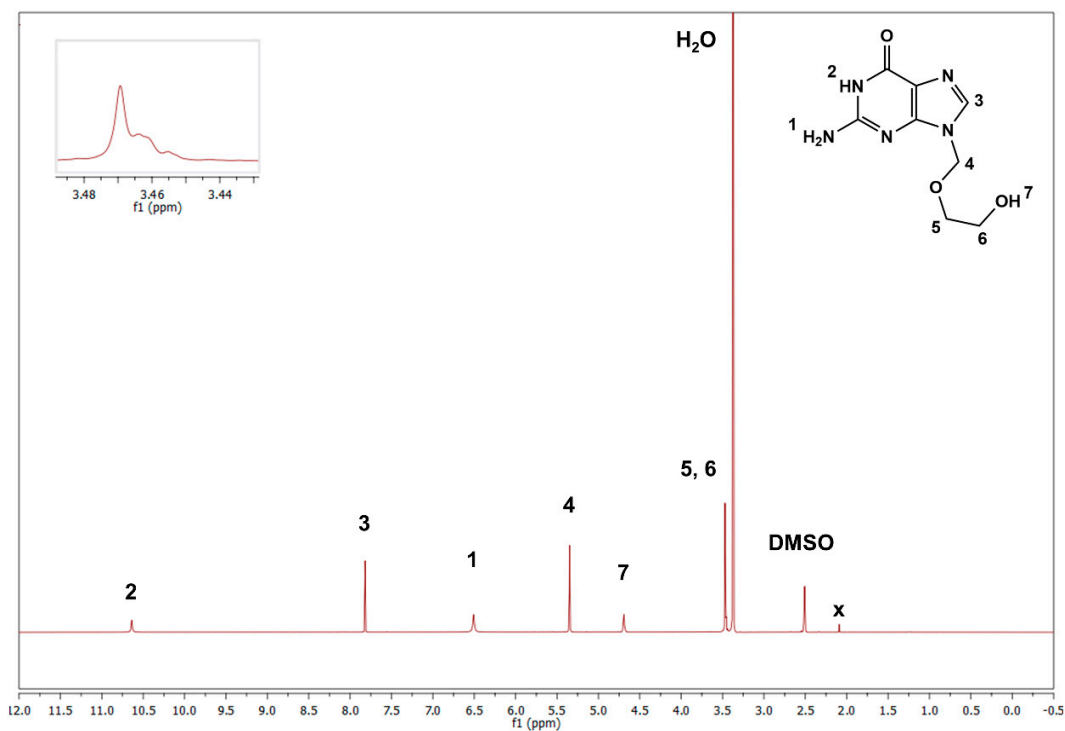


Figure S7. Contributions (%) of the contacts for the structure of the Acv salts.



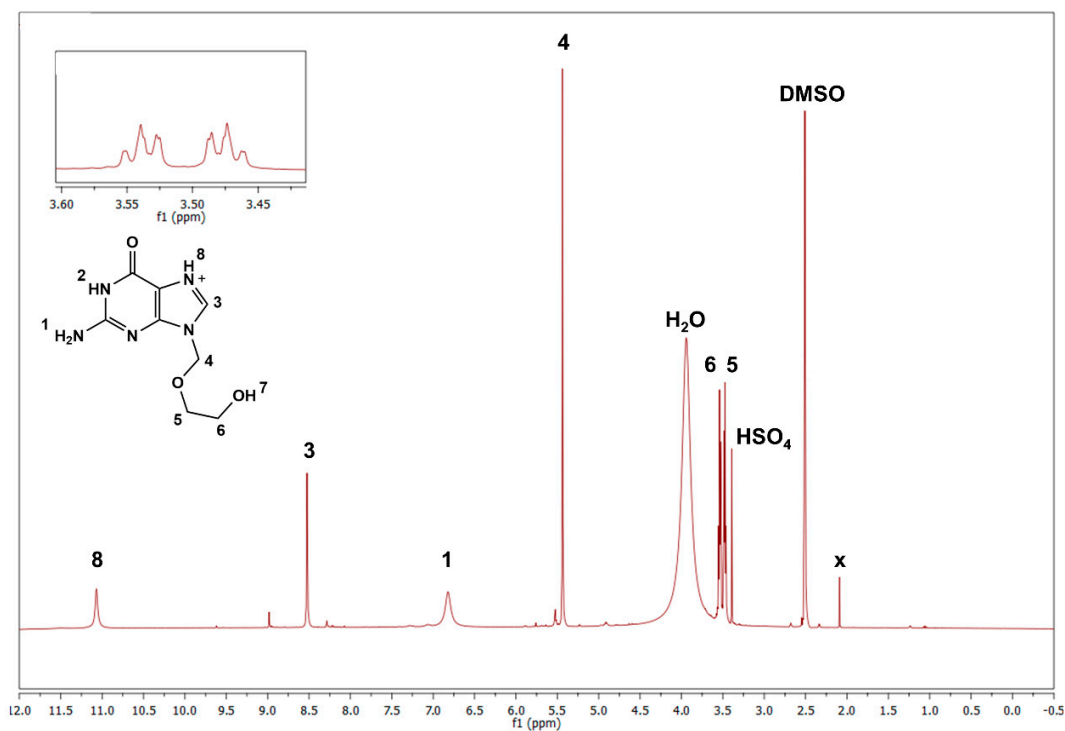


Figure S9. ^1H NMR (400 MHz) spectrum of $\text{HAcv} \cdot \text{HSO}_4$ in DMSO-d_6 .

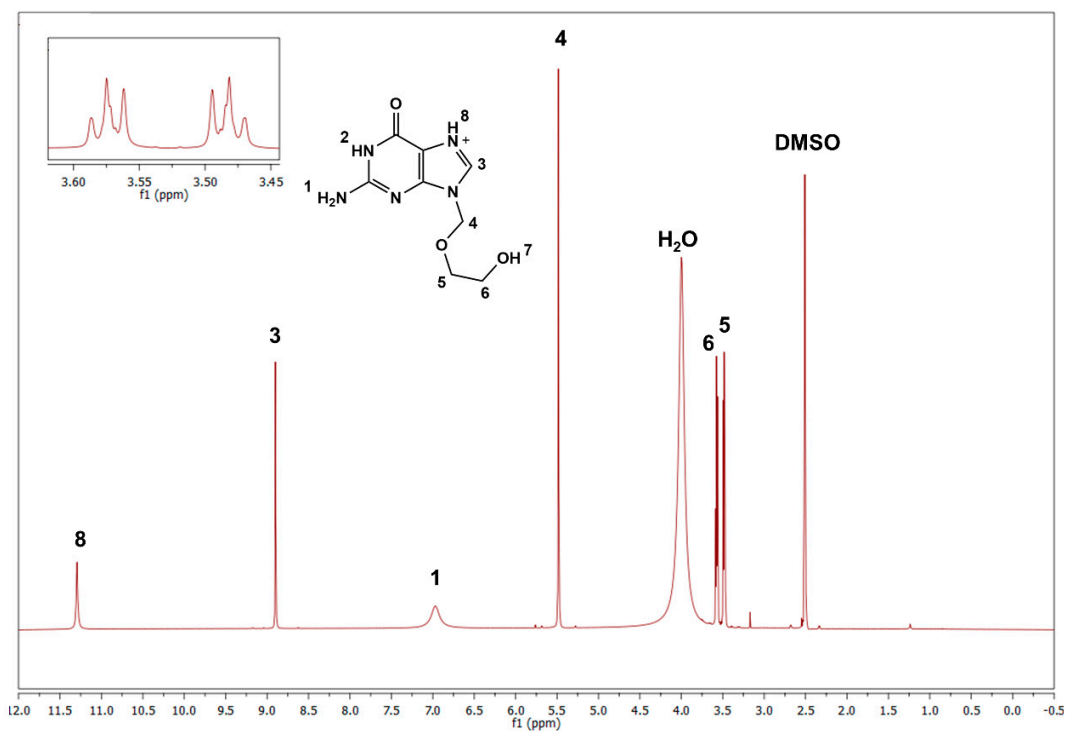


Figure S10. ^1H NMR (400 MHz) spectrum of $\text{HAcv}\cdot\text{NO}_3$ in DMSO-d_6 .

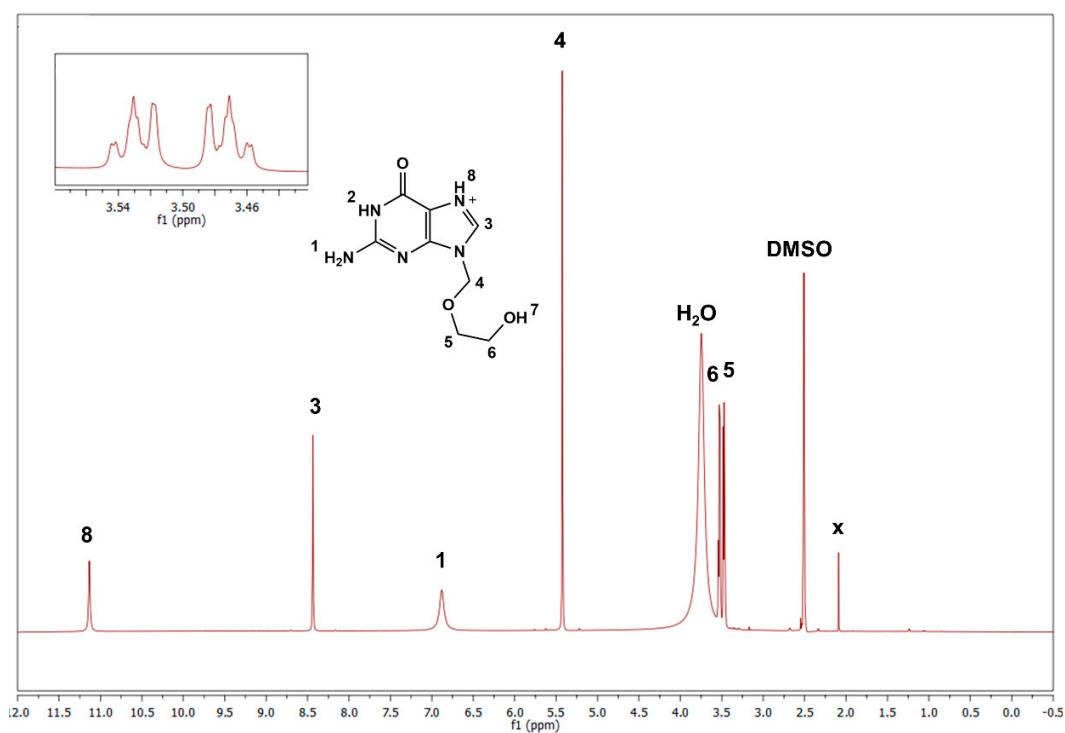


Figure S11. ^1H NMR (400 MHz) spectrum of HAcv-Cl in DMSO- d_6 .

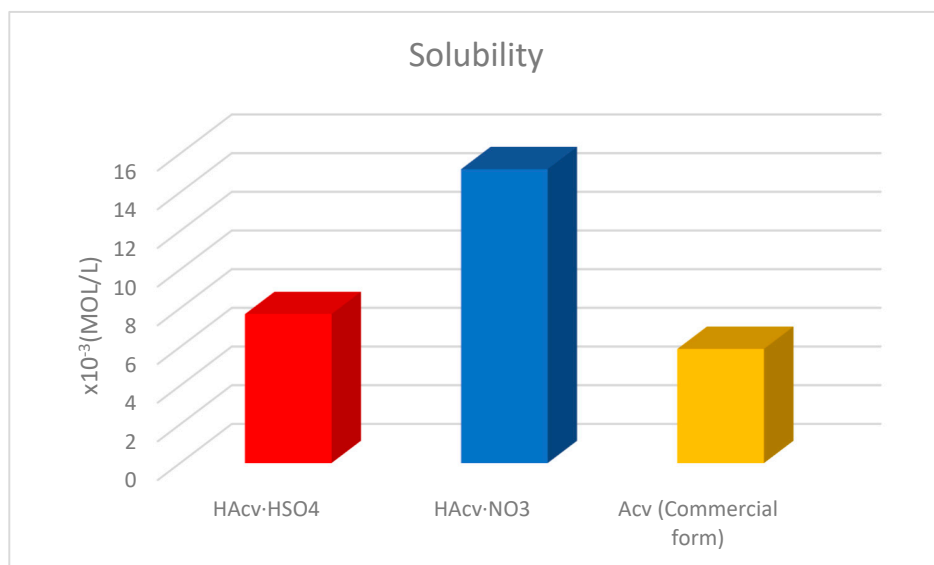


Figure S12. Aqueous solubility of Acv salts.

	HAcv·HSO₄		HAcv·NO₃		HAcv·Cl
D H A	D(D-A)(Å)	D H A	D(D-A)(Å)	D H A	D(D-A)(Å)
O3 H3 O6	2.7907(14)	O3 H3 O4	2.734(4)	O3 H3 O6	2.7907(14)
O5 H5B O7	2.5892(13)	N1 H1 O3	2.752(4)	O5 H5B O7	2.5892(13)
N5 H5 O3	2.7191(15)	N2 H2A O1	2.943(4)	N5 H5 O3	2.7191(15)
N1 H1 O4	2.8068(14)	N2 H2B O5	2.895(4)	N1 H1 O4	2.8068(14)
N2 H2A N3	3.1112(16)	N5 H5 O5	2.724(4)	N2 H2A N3	3.1112(16)
N2 H2B O5	3.0860(15)			N2 H2B O5	3.0860(15)

Table S1. Hydrogen Bonds for the Acv salts.

	HAcv·HSO₄		HAcv·NO₃		HAcv·Cl
Atom-Atom	Length (Å)	Atom-Atom	Length (Å)	Atom-Atom	Length (Å)
S1 O6	1.4461(10)	O1 C4	1.234(5)	O2 C7	1.447(2)
S1 O7	1.4641(10)	O2 C7	1.445(5)	O2 C6	1.401(2)
S1 O4	1.4436(10)	O2 C6	1.389(5)	O3 C8	1.441(2)
S1 O5	1.5766(9)	O5 N6	1.269(4)	O1 C2	1.222(2)
O2 C6	1.3956(16)	O3 C8	1.427(5)	N5 C1	1.385(2)
O2 C7	1.4405(16)	O6 N6	1.232(4)	N5 C5	1.315(2)
O1 C4	1.2188(16)	N3 C1	1.319(5)	N3 C4	1.345(2)
O3 C4	1.4357(17)	N3 C2	1.341(5)	N3 C3	1.326(2)
N5 C3	1.3832(17)	N1 C4	1.395(5)	N4 C4	1.389(2)
N5 C5	1.3154(17)	N1 C1	1.382(5)	N4 C5	549.43(7)
N3 C2	1.3511(17)	N2 C1	1.325(5)	N4 C6	1.470(2)
N3 C1	1.3271(17)	N5 C3	1.386(5)	N2 C3	1.343(2)
N4 C2	1.3830(17)	N5 C5	1.316(5)	N1 C3	1.380(2)
N4 C5	1.3444(17)	N4 C2	1.387(4)	N1 C2	1.398(2)
N4 C6	1.4705(16)	N4 C6	1.468(4)	C4 C1	1.378(2)
N1 C4	1.4010(17)	N4 C5	1.351(5)	C2 C1	1.428(2)
N1 C1	1.3728(17)	C4 C3	1.423(5)	C7 C8	1.508(2)
N2 C1	1.3363(18)	C3 C2	1.378(5)		
C4 C3	1.4268(18)	C7 C8	1.486(6)		
C3 C2	1.3740(18)				
C7 C8	1.500(2)				

Table S2. Bond Lengths for the Acv salts.

Hydrogen atom	Chemical Shifts δ (ppm)			
	Acv	HAcv-HSO ₄	HAcv-NO ₃	HAcv-Cl
1	6.51	6.82	6.97	6.88
2	10.64	—	—	—
3	7.82	8.52	8.90	8.44
4	5.35	5.44	5.48	5.43
5	3.47	3.47	3.48	3.47
6	3.47	3.54	3.58	3.53
7	4.69	—	—	—
8	—	11.07	11.29	11.13

Table S3. ¹H NMR data for commercial acyclovir and its salts.