STRUCTURAL
CHEMISTRY

Volume 78 (2022)

Supporting information for article:

Zwitterionic *versus* neutral molecules of fluoroquinolones: crystal structure of danofloxacin dihydrate

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Table S1 The results of the database survey.

CSD refcodes of the analysed fluoroquinolones, two C–O bond lengths (Å), the molecular form, the associated solvents and substituents at positions 5 and 8.

d_1 and d_2 are the C–O bond lengths in the carboxylic/carboxylate group, where $d_1 \leq d_2$.

No.	Refcode	d_1(C–O)	d_2(C–O)	molecular form	solvate/hydrate	substituent* at positions 5 and 8
1	ASUSIS	1.207	1.325	neutral	dichloromethane solvate	8-Cl
2	COQWOU	1.250	1.258	zwitterion	hydrate	5-NH_2, 8-F
2a	COQWOU01	1.246	1.266	zwitterion	hydrate	
2b	COQWOU02	1.255	1.260	zwitterion	hydrate	
3	COVPIN	1.251	1.254	zwitterion	hydrate	
3a	COVPIN01	1.258	1.26	zwitterion	hydrate	
3b	COVPIN03	1.261	1.261	zwitterion	hydrate	
3c	COVPIN04	1.259	1.260	zwitterion	hydrate	
3d	COVPIN05	1.256	1.259	zwitterion	hydrate	
4	EJOBOW	1.213	1.337	neutral	methanol solvate hydrate	
5	ENODOB	1.252	1.262	zwitterion	difluoroethanol solvate	
	ENODOB	1.249	1.278	zwitterion		
6	ENODUH	1.258	1.262	zwitterion	hydrate	
	ENODUH	1.253	1.265	zwitterion		
	ENODUH	1.249	1.270	zwitterion		
6a	ENODUH01	1.253	1.269	zwitterion	hydrate	
	ENODUH01	1.253	1.260	zwitterion		
	ENODUH01	1.250	1.272	zwitterion		
7	EVERUV	1.211	1.326	neutral		8-Cl
8	GEHLIR	1.210	1.324	neutral		
9	GEHLOX	1.207	1.326	neutral	acetonitrile solvate	
10	JEKMOB	1.208	1.324	neutral		5-NH_2, 8-F

11	LONTUE01	1.199	1.325	neutral		
12	MAPKEU	1.205	1.328	neutral		
13	MOCYAF	1.215	1.334	neutral		
14	MUBKIE	1.210	1.330	neutral		
15	NUQWIF	1.205	1.335	neutral		
16	PAZSAN	1.249	1.251	zwitterion	hydrate	5-F, 8-F
17	PIKVIO	1.251	1.253	zwitterion	hydrate	8-OMe
18	PIKVOU	1.226	1.255	zwitterion	hydrate	8-OMe
19	RIFHEV	1.212	1.336	neutral		
20	SESZEW	1.241	1.272	zwitterion	methanol solvate	
21	TUNJAP	1.208	1.325	neutral		5-NH_2, 8-F
22	UHITOV01	1.195	1.341	neutral		
23	UHITOV02	1.247	1.266	zwitterion		
24	ULOSEW	1.194	1.302	neutral	acetic acid solvate	
25	XEBWOS	1.206	1.335	neutral		
26	XICPAC	1.206	1.34	neutral		
26a	XICPAC01	1.206	1.332	neutral		
27	XICPEG	1.247	1.265	zwitterion	hydrate	
28	XITMAQ	1.215	1.324	neutral	acetone solvate	
29	XITMEU	1.218	1.327	neutral	methanol solvate hydrate	
	XITMEU	1.220	1.329	neutral		
30	XITMIY	1.216	1.320	neutral	dichloromethane solvate	
31	YAPMEJ	1.261	1.261	zwitterion	hydrate	
	YAPMEJ	1.252	1.265	zwitterion		
	YAPMEJ	1.244	1.274	zwitterion		
32	YIHHAY	1.198	1.318	neutral		
33	YIHHEC	1.211	1.318	neutral		8-F
34	YIHHIG	1.237	1.274	zwitterion		
35	YOPWUV	1.180	1.337	neutral		8-Cl

* Substituent other than H-atom

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