Supplementary Information (SI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2025

Pharmaceutical Salts of Venetoclax with Dicarboxylic and Sulfonic Acids: Solid-state Characterization and Dissolution Performance

Supporting information

Tereza Havlůjová[1], Erika Hriňová[1], Eliška Zmeškalová[1,3], Monika Kučeráková[3], Luděk Ridvan[2], Miroslav Šoóš[1]

[1]Department of Chemical Engineering, University of Chemistry and Technology in Prague, Technická 3, 16628, Prague 6, Czech Republic

[2]Zentiva k.s., U Kabelovny 130, 10237, Prague 10, Czech Republic

[3]Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 00, Prague 8, Czech Republic

Table I: Crystallographic data

	venetoclax acetonitrile solvate (1:1)	venetoclax oxalate acetonitrile solvate (1:1:1)	venetoclax fumurate acetonitrile solvate (1:1:3)	venetoclax napsylate acetonitrile solvate (1:2:0.5)	venetoclax tosylate (1:2)
Crystal data					
Chemical formula	$C_{47}H_{53}ClN_8O_7S$	$C_{49}H_{55}ClN_8O_{11}S$	$C_{55}H_{63}ClN_{10}O_{11}S$	$C_{66}H_{67.50}ClN_{7.50}O_{13}S_3$	$C_{59}H_{66}ClN_7O_{13}S_3$
M_r	909.50	999.54	1107.68	1305.45	1212.86
Crystal system, space group	Triclinic, *P*-1	Triclinic, *P*-1	Monoclinic, $P2_1/c$	Triclinic, *P*1	Triclinic, *P*-1
Temperature (K)	95	120	95	95	95
a, *b*, *c* (Å)	12.2261 (5), 14.0822 (6), 15.1150 (5)	11.1533 (4), 12.6185 (5), 19.2633 (7)	12.6958 (5), 43.0206 (12), 10.8969 (5)	10.8016 (1), 10.8223 (1), 14.0795 (1)	12.1935 (1), 15.7385 (1), 17.4811 (2)
α, β, γ (°)	67.388 (4), 72.278 (3), 74.731 (3)	71.723 (3), 85.508 (3), 73.590 (3)	90, 110.267 (5), 90	84.7041 (9), 83.8240 (9), 76.704 (1)	109.4801 (9), 95.9264 (8), 109.2612 (9)
V (Å^3)	2256.41 (17)	2469.28 (17)	5583.2 (4)	1588.57 (2)	2898.70 (5)
Z	2	2	4	1	2
Radiation type	Cu *K*α	Mo *K*α	Cu *K*α	Cu *K*α	Cu *K*α
μ (mm^{-1})	1.68	0.19	1.52	2.04	2.18
Crystal size (mm)	0.08 × 0.06 × 0.02	0.49 × 0.23 × 0.14	0.13 × 0.08 × 0.04	0.21 × 0.11 × 0.09	0.16 × 0.14 × 0.10

Data collection					
Diffractometer	Oxford Diffraction SuperNova	Oxford Diffraction SuperNova	Oxford Diffraction SuperNova	Oxford Diffraction SuperNova	Oxford Diffraction SuperNova
Absorption correction	Multi-scan *CrysAlis PRO* (Rigaku Oxford Diffraction, 2017)	Multi-scan *CrysAlis PRO* (Rigaku Oxford Diffraction, 2017)	Multi-scan *CrysAlis PRO* (Rigaku Oxford Diffraction, 2017)	Multi-scan *CrysAlis PRO* (Rigaku Oxford Diffraction, 2017)	Multi-scan *CrysAlis PRO* (Rigaku Oxford Diffraction, 2017)
T_{min}, T_{max}	0.37, 0.96	0.85, 0.97	0.57, 0.95	0.40, 0.83	0.56, 0.81
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	16343, 8774, 7093	18873, 11173, 7533	34290, 11044, 8249	54398, 11525, 11444	100705, 11510, 10350
R_{int}	0.035	0.029	0.065	0.036	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.621	0.677	0.622	0.621	0.622
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.098, 0.99	0.053, 0.165, 0.99	0.053, 0.138, 0.98	0.055, 0.150, 1.05	0.047, 0.137, 0.91
No. of reflections	8773	11173	11040	11525	11458
No. of parameters	589	651	703	835	768
No. of restraints	12	19	0	1146	21
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.54	1.56, −0.73	0.62, −0.69	0.70, −0.33	0.71, −0.75
CCDC	2377711	2377712	2377714	2393684	2393682

Table II: Selected bond distances (Å) and angles (°) of venetoclax acetonitrile solvate.

Cl1—C2	1.747 (2)	N27—C28	1.459 (2)
C8—N9	1.476 (2)	C31—O32	1.437 (2)
N9—C10	1.461 (2)	O32—C33	1.431 (2)
N9—C53	1.463 (2)	C33—C34	1.524 (3)
C11—N12	1.465 (2)	C35—N37	1.443 (2)
N12—C13	1.401 (2)	N37—O38	1.236 (2)
N12—C52	1.468 (2)	N37—O39	1.242 (2)
C17—O18	1.218 (2)	C40—O42	1.390 (2)
C17—N19	1.385 (2)	O42—C43	1.404 (2)
N19—S20	1.6518 (15)	C46—N47	1.374 (2)
S20—O21	1.4271 (13)	C46—N50	1.332 (3)
S20—O22	1.4412 (14)	N47—C48	1.368 (3)
S20—C23	1.7453 (18)	N50—C51	1.339 (3)
C26—N27	1.336 (2)	N62—C63	1.143 (4)
C8—N9—C10	109.46 (15)	C35—N37—O38	118.79 (15)
C8—N9—C53	110.89 (15)	C35—N37—O39	119.29 (14)
C10—N9—C53	110.15 (15)	O38—N37—O39	121.93 (15)
C11—N12—C13	115.25 (15)	C40—O42—C43	117.68 (14)
C11—N12—C52	110.78 (15)	C46—N47—C48	108.73 (16)
C13—N12—C52	117.18 (15)	N19—S20—C23	104.48 (8)
C17—N19—S20	124.37 (13)	O21—S20—C23	109.03 (8)
N19—S20—O21	110.47 (8)	O22—S20—C23	108.98 (8)
N19—S20—O22	102.56 (8)	C46—N50—C51	114.50 (16)
O21—S20—O22	120.12 (8)	C26—N27—C28	124.73 (15)

Table III: Hydrogen-bond geometry (Å, °) for venetoclax acetonitrile solvate.

D-H … A	D-H	H … A	D … A	D-H … A
N19—H191···O42	0.85	2.292(19)	2.724 (2)	111.9 (16)
N27—H271···O18^{i}	0.86	2.24	2.945 (3)	140 (1)

N47—H471⋯O22^{ii}	0.87	2.28	3.108 (3)	161 (2)

Symmetry codes: (i) −x+1, −y+2, −z+1; (ii) −x+1, −y+1, −z+1

Table IV Hydrogen-bond geometry (Å, °) for venetoclax oxalate acetonitrile solvate

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C4—H41⋯O67^{i}	0.93	2.57	3.274 (4)	132
C8—H82⋯C60	1.01	2.58	3.296 (4)	128
C8—H81⋯O66^{ii}	0.99	2.59	3.262 (4)	125
C10—H102⋯O66^{ii}	0.98	2.50	3.184 (4)	127
C11—H111⋯O51^{iii}	0.99	2.40	3.345 (4)	159
C53—H532⋯O44^{iv}	0.95	2.47	3.322 (4)	149
C60—H601⋯O30^{v}	0.93	2.43	3.108 (4)	129
N31—H311⋯O16	0.888 (16)	1.923 (18)	2.643 (4)	137.0 (16)
N9—H91⋯O62^{ii}	0.901 (16)	1.905 (17)	2.782 (4)	163.8 (17)
N21—H211⋯N19^{vi}	0.871 (16)	2.015 (17)	2.871 (4)	167 (2)
O67—H671⋯O64^{i}	0.853 (18)	1.93 (3)	2.658 (4)	143 (3)
N39—H391⋯O51	0.865 (16)	1.992 (17)	2.636 (4)	130.3 (15)

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*+1; (iv) −*x*+2, −*y*+2, −*z*+1; (v) *x*, *y*−1, *z*; (vi) −*x*, −*y*+2, −*z*+1.

Table V: Selected bond distances (Å) and angles (°) of venetoclax fumarate acetonitrile solvate

Cl1—C2	1.746 (3)	S30—C33	1.744 (3)
C7—C8	1.512 (3)	C36—N37	1.339 (3)
C8—N9	1.516 (3)	N37—C38	1.456 (3)
N9—C10	1.497 (3)	C41—O42	1.414 (4)
N9—C53	1.502 (3)	O42—C43	1.420 (4)
C11—N12	1.466 (3)	C45—N47	1.447 (3)
N12—C13	1.371 (3)	N47—O48	1.240 (3)
N12—C52	1.465 (3)	N47—O49	1.231 (3)
C15—O16	1.391 (3)	C21—N22	1.375 (3)
O16—C17	1.402 (3)	N22—C23	1.368 (3)

N29—S30	1.6506 (19)	C23—N24	1.337 (3)
S30—O31	1.4287 (17)	N24—C25	1.340 (3)
S30—O32	1.4299 (18)	C2—C3	1.382 (4)
O31—S30—O32	119.91 (11)	C27—N29—S30	125.54 (17)
N29—S30—C33	106.04 (11)	N29—S30—O31	110.09 (10)
O31—S30—C33	108.19 (11)	N29—S30—O32	102.61 (10)
O32—S30—C33	109.14 (11)	C11—N12—C13	123.3 (2)
C7—C8—N9	112.81 (19)	C11—N12—C52	110.11 (18)
C8—N9—C10	109.35 (17)	C13—N12—C52	123.83 (19)
C8—N9—C53	110.94 (19)	C36—N37—C38	123.9 (2)
C10—N9—C53	110.51 (17)	C41—O42—C43	110.2 (2)
C15—O16—C17	120.74 (18)	C45—N47—O48	119.8 (2)
C21—N22—C23	108.2 (2)	C45—N47—O49	118.5 (2)
C23—N24—C25	115.1 (2)	O48—N47—O49	121.7 (2)

Table VI: Hydrogen-bond geometry (Å, °) for venetoclax fumarate acetonitrile solvate.

D-H … A	D-H	H … A	D … A	D-H … A
N29—H291···O16	0.85	1.89	2.604 (4)	140
N22—H221···N24^{i}	0.86	2.01	2.845 (4)	162
N37—H371···O48	0.86	1.95	2.622 (4)	134
O62—H621···O68^{ii}	0.84	1.73	2.551 (4)	164
N9—H91···O68^{ii}	0.93	1.77	2.691 (4)	171

Symmetry codes: (i) *x*+1, *y*, *z*; (v) *x*, −*y*+1/2, *z*+1/2; (ii) x, −y+1/2, z−1/2.

Table VII: Selected geometric parameters (Å, °) of venetoclax napsylate acetonitrile hemisolvate

Cl1—C2	1.753 (3)	C43—C56	1.375 (4)
C2—C3	1.379 (5)	C44—C45	1.375 (4)
C2—C7	1.382 (4)	C45—C46	1.422 (4)
C3—C4	1.386 (4)	C46—N47	1.344 (3)
C4—C5	1.401 (4)	C46—C55	1.422 (4)
C5—C6	1.390 (4)	N47—C48	1.458 (4)

C5—C8	1.494 (4)	C48—C49	1.529 (4)
C6—C7	1.401 (4)	C49—C50	1.524 (4)
C8—C9	1.336 (4)	C49—C54	1.529 (4)
C8—C13	1.507 (4)	C50—C51	1.516 (4)
C9—C10	1.523 (4)	C51—O52	1.442 (4)
C9—C16	1.503 (4)	O52—C53	1.426 (4)
C10—C11	1.518 (4)	C53—C54	1.522 (4)
C11—C12	1.532 (4)	C55—C56	1.398 (4)
C12—C13	1.542 (4)	C55—N57	1.451 (3)
C12—C14	1.525 (4)	N57—O58	1.222 (3)
C12—C15	1.528 (4)	N57—O59	1.241 (3)
C16—N17	1.518 (3)	C60—C61	1.385 (4)
N17—C18	1.499 (3)	S62—O63	1.433 (2)
N17—C22	1.484 (4)	S62—O64	1.475 (2)
C18—C19	1.523 (4)	S62—O65	1.465 (2)
C19—N20	1.464 (4)	S62—C66	1.773 (3)
N20—C21	1.467 (3)	C66—C67	1.422 (4)
N20—C23	1.398 (3)	C66—C71	1.361 (4)
C21—C22	1.525 (3)	C67—C68	1.371 (5)
C23—C24	1.406 (4)	C68—C69	1.416 (4)
C23—C61	1.404 (4)	C69—C70	1.424 (4)
C24—C25	1.383 (4)	C69—C75	1.416 (4)
C25—O26	1.387 (3)	C70—C71	1.425 (4)
C25—C36	1.406 (3)	C70—C72	1.413 (5)
O26—C27	1.389 (3)	C72—C73	1.380 (5)
C27—C28	1.387 (4)	C73—C74	1.406 (6)
C27—C35	1.379 (4)	C74—C75	1.359 (5)
C28—C29	1.396 (4)	S76—O77	1.466 (2)
C29—C30	1.415 (4)	S76—O78	1.446 (2)
C29—C33	1.432 (3)	S76—O79	1.457 (2)
C30—N31	1.349 (3)	S76—C80	1.778 (3)

C30—N34	1.345 (3)	C80—C81	1.408 (4)
N31—C32	1.391 (3)	C80—C85	1.372 (4)
C32—C33	1.358 (4)	C81—C82	1.373 (4)
N34—C35	1.348 (3)	C82—C83	1.398 (5)
C36—C37	1.496 (3)	C83—C84	1.428 (5)
C36—C60	1.393 (4)	C83—C89	1.433 (5)
C37—O38	1.223 (3)	C84—C85	1.420 (5)
C37—N39	1.368 (4)	C84—C86	1.415 (5)
N39—S40	1.664 (2)	C86—C87	1.364 (6)
S40—O41	1.425 (2)	C87—C88	1.404 (8)
S40—O42	1.429 (2)	C88—C89	1.365 (7)
S40—C43	1.754 (3)	N90—C91	1.119 (11)
C43—C44	1.402 (4)	C91—C92	1.432 (10)
Cl1—C2—C3	119.5 (2)	S40—C43—C44	119.9 (2)
Cl1—C2—C7	118.4 (2)	S40—C43—C56	119.3 (2)
C3—C2—C7	122.1 (3)	C44—C43—C56	120.6 (2)
C2—C3—C4	118.9 (3)	C43—C44—C45	120.1 (3)
C3—C4—C5	120.9 (3)	C44—C45—C46	122.1 (3)
C4—C5—C6	119.0 (2)	C45—C46—N47	120.2 (2)
C4—C5—C8	120.4 (2)	C45—C46—C55	115.5 (2)
C6—C5—C8	120.5 (2)	N47—C46—C55	124.3 (2)
C5—C6—C7	120.7 (2)	C46—N47—C48	124.2 (2)
C6—C7—C2	118.5 (3)	N47—C48—C49	112.9 (2)
C5—C8—C9	123.2 (3)	C48—C49—C50	111.1 (2)
C5—C8—C13	114.1 (2)	C48—C49—C54	111.0 (2)
C9—C8—C13	122.7 (2)	C50—C49—C54	109.4 (2)
C8—C9—C10	121.7 (3)	C49—C50—C51	110.1 (2)
C8—C9—C16	122.7 (2)	C50—C51—O52	110.6 (2)
C10—C9—C16	115.5 (2)	C51—O52—C53	111.0 (2)
C9—C10—C11	113.0 (2)	O52—C53—C54	112.3 (3)

C10—C11—C12	111.9 (2)	C49—C54—C53	111.0 (2)
C11—C12—C13	107.7 (2)	C46—C55—C56	122.6 (2)
C11—C12—C14	110.0 (2)	C46—C55—N57	121.7 (2)
C13—C12—C14	109.5 (2)	C56—C55—N57	115.7 (2)
C11—C12—C15	110.8 (2)	C55—C56—C43	119.1 (2)
C13—C12—C15	110.3 (2)	C55—N57—O58	119.2 (2)
C14—C12—C15	108.6 (3)	C55—N57—O59	118.9 (2)
C12—C13—C8	115.0 (2)	O58—N57—O59	121.9 (2)
C9—C16—N17	112.4 (2)	C36—C60—C61	123.0 (2)
C16—N17—C18	112.25 (19)	C23—C61—C60	120.0 (2)
C16—N17—C22	110.5 (2)	O63—S62—O64	113.10 (12)
C18—N17—C22	108.0 (2)	O63—S62—O65	114.72 (12)
N17—C18—C19	110.3 (2)	O64—S62—O65	111.06 (12)
C18—C19—N20	113.0 (2)	O63—S62—C66	106.67 (13)
C19—N20—C21	116.8 (2)	O64—S62—C66	104.21 (12)
C19—N20—C23	115.8 (2)	O65—S62—C66	106.15 (13)
C21—N20—C23	116.3 (2)	S62—C66—C67	119.0 (2)
N20—C21—C22	112.3 (2)	S62—C66—C71	119.6 (2)
C21—C22—N17	111.7 (2)	C67—C66—C71	121.3 (3)
N20—C23—C24	120.7 (2)	C66—C67—C68	119.3 (3)
N20—C23—C61	121.3 (2)	C67—C68—C69	121.0 (3)
C24—C23—C61	118.0 (2)	C68—C69—C70	119.4 (3)
C23—C24—C25	120.7 (2)	C68—C69—C75	122.2 (3)
C24—C25—O26	121.1 (2)	C70—C69—C75	118.4 (3)
C24—C25—C36	122.1 (3)	C69—C70—C71	118.5 (3)
O26—C25—C36	116.7 (2)	C69—C70—C72	119.3 (3)
C25—O26—C27	118.6 (2)	C71—C70—C72	122.2 (3)
O26—C27—C28	118.7 (2)	C70—C71—C66	120.4 (3)
O26—C27—C35	119.0 (2)	C70—C72—C73	120.4 (3)
C28—C27—C35	122.2 (2)	C72—C73—C74	120.0 (3)
C27—C28—C29	117.6 (2)	C73—C74—C75	120.7 (3)

C28—C29—C30	117.9 (2)	C69—C75—C74	121.1 (3)
C28—C29—C33	136.7 (3)	O77—S76—O78	113.01 (13)
C30—C29—C33	105.4 (2)	O77—S76—O79	111.30 (12)
C29—C30—N31	110.0 (2)	O78—S76—O79	113.28 (15)
C29—C30—N34	122.6 (2)	O77—S76—C80	105.83 (13)
N31—C30—N34	127.3 (3)	O78—S76—C80	107.53 (14)
C30—N31—C32	107.0 (2)	O79—S76—C80	105.22 (13)
N31—C32—C33	110.7 (2)	S76—C80—C81	120.3 (2)
C29—C33—C32	106.8 (2)	S76—C80—C85	118.0 (2)
C30—N34—C35	119.4 (2)	C81—C80—C85	121.5 (3)
C27—C35—N34	120.2 (2)	C80—C81—C82	119.7 (3)
C25—C36—C37	126.6 (3)	C81—C82—C83	120.6 (3)
C25—C36—C60	116.2 (2)	C82—C83—C84	119.9 (3)
C37—C36—C60	117.1 (2)	C82—C83—C89	122.2 (3)
C36—C37—O38	120.6 (3)	C84—C83—C89	117.8 (4)
C36—C37—N39	118.4 (2)	C83—C84—C85	118.6 (3)
O38—C37—N39	120.9 (2)	C83—C84—C86	119.8 (3)
C37—N39—S40	122.43 (18)	C85—C84—C86	121.4 (3)
N39—S40—O41	103.34 (12)	C84—C85—C80	119.5 (3)
N39—S40—O42	109.04 (12)	C84—C86—C87	120.6 (4)
O41—S40—O42	120.08 (12)	C86—C87—C88	119.8 (4)
N39—S40—C43	107.24 (12)	C87—C88—C89	121.8 (4)
O41—S40—C43	108.56 (13)	C83—C89—C88	120.0 (4)
O42—S40—C43	107.90 (12)	N90—C91—C92	178.6 (9)

Table VIII: Hydrogen bond geometry (Å, °) of venetoclax napsylate acetonitrile hemisolvate

D—H···A	D—H	H···A	D···A	D—H···A
C6—H61···O52^{i}	0.92	2.49	3.336 (4)	152
C33—H331···O38^{ii}	0.94	2.44	3.27 (4)	146
N31—H311···O65^{iii}	0.858 (17)	1.968 (19)	2.767 (4)	155 (2)
N34—H341···O64^{iii}	0.861 (17)	1.79 (19)	2.628 (4)	164 (3)

C48—H481⋯O41^{iv}	0.96	2.57	3.432 (4)	150
N47—H471⋯O59	0.852 (17)	1.995 (18)	2.634 (4)	131 (16)
C56—H561⋯O78^{v}	0.92	2.42	3.288 (4)	156
N39—H391⋯O79^{v}	0.848 (17)	2.066 (18)	2.879 (4)	160.3 (18)
C19—H191⋯O78	0.97	2.41	3.347 (4)	163
N17—H171⋯O77	0.897 (17)	1.892 (18)	2.756 (4)	161.1 (19)
C4—H41⋯O63	0.92	2.43	3.123 (4)	132
C85—H851⋯O59^{vi}	0.95	2.54	3.427 (4)	155
C92—H921⋯O38^{vii}	0.95	2.55	3.422 (4)	152
C92—H921⋯O42^{vii}	0.95	2.43	3.175 (4)	135

Symmetry codes: (i) x+1, y+1, z+1; (ii) x, y+1, z; (iii) x−1, y+1, z; (iv) x, y−1, z; (v) x−1, y, z; (vi) x+1, y+1, z; (vii) x, y, z+1.

Table IX: Selected geometric parameters (Å, °) of venetoclax tosylate

Cl1—C2	1.747 (3)	C36—C37	1.391 (4)
C2—C3	1.372 (5)	C37—N38	1.441 (4)
C2—C7	1.379 (5)	C37—C41	1.427 (4)
C3—C4	1.391 (5)	N38—O39	1.238 (4)
C4—C5	1.385 (5)	N38—O40	1.232 (4)
C5—C6	1.398 (5)	C41—N42	1.342 (4)
C5—C8	1.496 (4)	C41—C50	1.427 (4)
C6—C7	1.386 (5)	N42—C43	1.456 (4)
C8—C9	1.339 (5)	C43—C44	1.542 (4)
C8—C59	1.517 (5)	C44—C45	1.525 (4)
C9—C10	1.504 (4)	C44—C49	1.525 (4)
C9—C56	1.506 (4)	C45—C46	1.517 (5)
C10—N11	1.506 (4)	C46—O47	1.437 (4)
N11—C12	1.500 (4)	O47—C48	1.431 (4)
N11—C55	1.495 (4)	C48—C49	1.512 (5)
C12—C13	1.515 (4)	C50—C51	1.361 (4)
C13—N14	1.464 (4)	C52—C53	1.377 (4)
N14—C15	1.378 (4)	C54—C55	1.519 (4)

N14—C54	1.461 (4)	C56—C57	1.526 (5)
C15—C16	1.416 (4)	C57—C58	1.530 (5)
C15—C53	1.408 (4)	C58—C59	1.529 (5)
C16—C17	1.382 (4)	C58—C60	1.528 (5)
C17—O18	1.399 (4)	C58—C61	1.529 (6)
C17—C28	1.398 (4)	S62—O63	1.473 (2)
O18—C19	1.378 (3)	S62—O64	1.443 (2)
C19—C20	1.386 (4)	S62—O65	1.455 (2)
C19—C27	1.384 (4)	S62—C66	1.780 (3)
C20—C21	1.384 (4)	C66—C67	1.393 (5)
C21—C22	1.419 (4)	C66—C71	1.381 (5)
C21—C25	1.427 (4)	C67—C68	1.386 (5)
C22—N23	1.354 (4)	C68—C69	1.392 (6)
C22—N26	1.336 (4)	C69—C70	1.384 (6)
N23—C24	1.382 (4)	C69—C72	1.517 (5)
C24—C25	1.362 (5)	C70—C71	1.391 (5)
N26—C27	1.355 (4)	S73—O74	1.445 (2)
C28—C29	1.480 (4)	S73—O75	1.475 (2)
C28—C52	1.394 (4)	S73—O76	1.463 (2)
C29—O30	1.219 (4)	S73—C77	1.770 (4)
C29—N31	1.384 (4)	C77—C78	1.391 (5)
N31—S32	1.663 (3)	C77—C83	1.392 (5)
S32—O33	1.429 (2)	C78—C79	1.385 (5)
S32—O34	1.430 (2)	C79—C80	1.392 (6)
S32—C35	1.744 (3)	C80—C81	1.510 (6)
C35—C36	1.369 (4)	C80—C82	1.389 (6)
C35—C51	1.404 (4)	C82—C83	1.381 (6)
Cl1—C2—C3	120.2 (3)	C36—C37—C41	121.9 (3)
Cl1—C2—C7	118.3 (3)	N38—C37—C41	122.2 (3)
C3—C2—C7	121.5 (3)	C37—N38—O39	119.4 (3)

C2—C3—C4	119.7 (3)	C37—N38—O40	118.6 (3)
C3—C4—C5	120.6 (3)	O39—N38—O40	122.0 (3)
C4—C5—C6	118.2 (3)	C37—C41—N42	124.5 (3)
C4—C5—C8	121.7 (3)	C37—C41—C50	115.4 (3)
C6—C5—C8	120.0 (3)	N42—C41—C50	120.1 (3)
C5—C6—C7	121.7 (3)	C41—N42—C43	123.3 (3)
C6—C7—C2	118.3 (3)	N42—C43—C44	112.4 (3)
C5—C8—C9	124.3 (3)	C43—C44—C45	110.2 (3)
C5—C8—C59	113.9 (3)	C43—C44—C49	111.6 (3)
C9—C8—C59	121.7 (3)	C45—C44—C49	110.3 (3)
C8—C9—C10	121.6 (3)	C44—C45—C46	111.5 (3)
C8—C9—C56	122.8 (3)	C45—C46—O47	112.5 (3)
C10—C9—C56	115.3 (3)	C46—O47—C48	111.0 (2)
C9—C10—N11	114.2 (3)	O47—C48—C49	110.2 (3)
C10—N11—C12	112.6 (2)	C44—C49—C48	110.6 (3)
C10—N11—C55	109.5 (2)	C41—C50—C51	122.3 (3)
C12—N11—C55	109.8 (2)	C35—C51—C50	120.1 (3)
N11—C12—C13	110.4 (2)	C28—C52—C53	122.4 (3)
C12—C13—N14	111.2 (2)	C15—C53—C52	120.6 (3)
C13—N14—C15	120.6 (2)	N14—C54—C55	110.1 (3)
C13—N14—C54	112.4 (2)	C54—C55—N11	111.0 (2)
C15—N14—C54	118.5 (3)	C9—C56—C57	113.3 (3)
N14—C15—C16	120.6 (3)	C56—C57—C58	112.4 (3)
N14—C15—C53	121.7 (3)	C57—C58—C59	107.4 (3)
C16—C15—C53	117.6 (3)	C57—C58—C60	109.5 (3)
C15—C16—C17	120.0 (3)	C59—C58—C60	109.7 (3)
C16—C17—O18	116.3 (3)	C57—C58—C61	111.3 (3)
C16—C17—C28	122.5 (3)	C59—C58—C61	109.9 (3)
O18—C17—C28	120.8 (3)	C60—C58—C61	109.0 (3)
C17—O18—C19	119.0 (2)	C58—C59—C8	114.1 (3)
O18—C19—C20	124.9 (3)	O63—S62—O64	112.07 (14)

O18—C19—C27	113.9 (3)	O63—S62—O65	110.58 (14)
C20—C19—C27	121.2 (3)	O64—S62—O65	114.98 (14)
C19—C20—C21	118.3 (3)	O63—S62—C66	104.97 (14)
C20—C21—C22	118.3 (3)	O64—S62—C66	106.42 (15)
C20—C21—C25	136.4 (3)	O65—S62—C66	107.10 (15)
C22—C21—C25	105.3 (3)	S62—C66—C67	119.4 (3)
C21—C22—N23	109.7 (3)	S62—C66—C71	120.6 (3)
C21—C22—N26	122.3 (3)	C67—C66—C71	120.0 (3)
N23—C22—N26	128.0 (3)	C66—C67—C68	119.5 (3)
C22—N23—C24	107.4 (3)	C67—C68—C69	121.1 (3)
N23—C24—C25	110.4 (3)	C68—C69—C70	118.5 (3)
C21—C25—C24	107.2 (3)	C68—C69—C72	120.8 (4)
C22—N26—C27	119.3 (3)	C70—C69—C72	120.7 (4)
C19—C27—N26	120.6 (3)	C69—C70—C71	121.0 (4)
C17—C28—C29	127.4 (3)	C70—C71—C66	119.8 (3)
C17—C28—C52	116.7 (3)	O74—S73—O75	111.47 (15)
C29—C28—C52	115.9 (3)	O74—S73—O76	113.47 (14)
C28—C29—O30	122.8 (3)	O75—S73—O76	111.73 (14)
C28—C29—N31	116.3 (3)	O74—S73—C77	107.61 (15)
O30—C29—N31	120.9 (3)	O75—S73—C77	105.21 (15)
C29—N31—S32	122.7 (2)	O76—S73—C77	106.80 (16)
N31—S32—O33	110.62 (14)	S73—C77—C78	119.8 (3)
N31—S32—O34	103.48 (14)	S73—C77—C83	120.0 (3)
O33—S32—O34	119.51 (14)	C78—C77—C83	120.2 (3)
N31—S32—C35	101.91 (14)	C77—C78—C79	119.2 (3)
O33—S32—C35	108.81 (14)	C78—C79—C80	121.4 (4)
O34—S32—C35	111.01 (14)	C79—C80—C81	120.1 (4)
S32—C35—C36	120.2 (2)	C79—C80—C82	118.2 (4)
S32—C35—C51	119.2 (2)	C81—C80—C82	121.6 (4)
C36—C35—C51	120.3 (3)	C80—C82—C83	121.4 (4)
C35—C36—C37	119.9 (3)	C77—C83—C82	119.5 (4)

C36—C37—N38	115.9 (3)		

Table X: Hydrogen bond geometry (Å, °) of venetoclax tosylate

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H71···O64^{i}	0.95	2.49	3.428 (5)	171
C12—H122···O74	0.98	2.34	3.043 (5)	128
C24—H241···O74^{ii}	0.94	2.30	3.205 (5)	161
C45—H451···C16^{ii}	0.98	2.60	3.569 (5)	170
C53—H531···O33^{iii}	0.94	2.54	3.451 (5)	164
C54—H541···O33^{iii}	0.98	2.46	3.209 (5)	134
C55—H551···O65	0.99	2.44	3.121 (5)	126
N42—H421···O30^{iv}	0.859	2.205	2.915 (5)	139.9 (19)
N42—H421···O39	0.859	2.023	2.655 (5)	129.7 (17)
N31—H311···O47^{v}	0.852	2.061	2.837 (5)	151 (3)
N26—H261···O75^{vi}	0.867	1.755	2.617 (5)	173 (2)
N23—H231···O76^{vi}	0.859	2.055	2.851 (5)	154 (3)
N11—H111···O63	0.896	1.891	2.772 (5)	168 (2)

Symmetry codes: (i) −x+2, −y+1, −z+1; (ii) x−1, y, z; (iii) −x+1, −y+1, −z+2; (iv) −x, −y+1, −z+2; (v) x+1, y, z; (vi) −x+1, −y+2, −z+2.

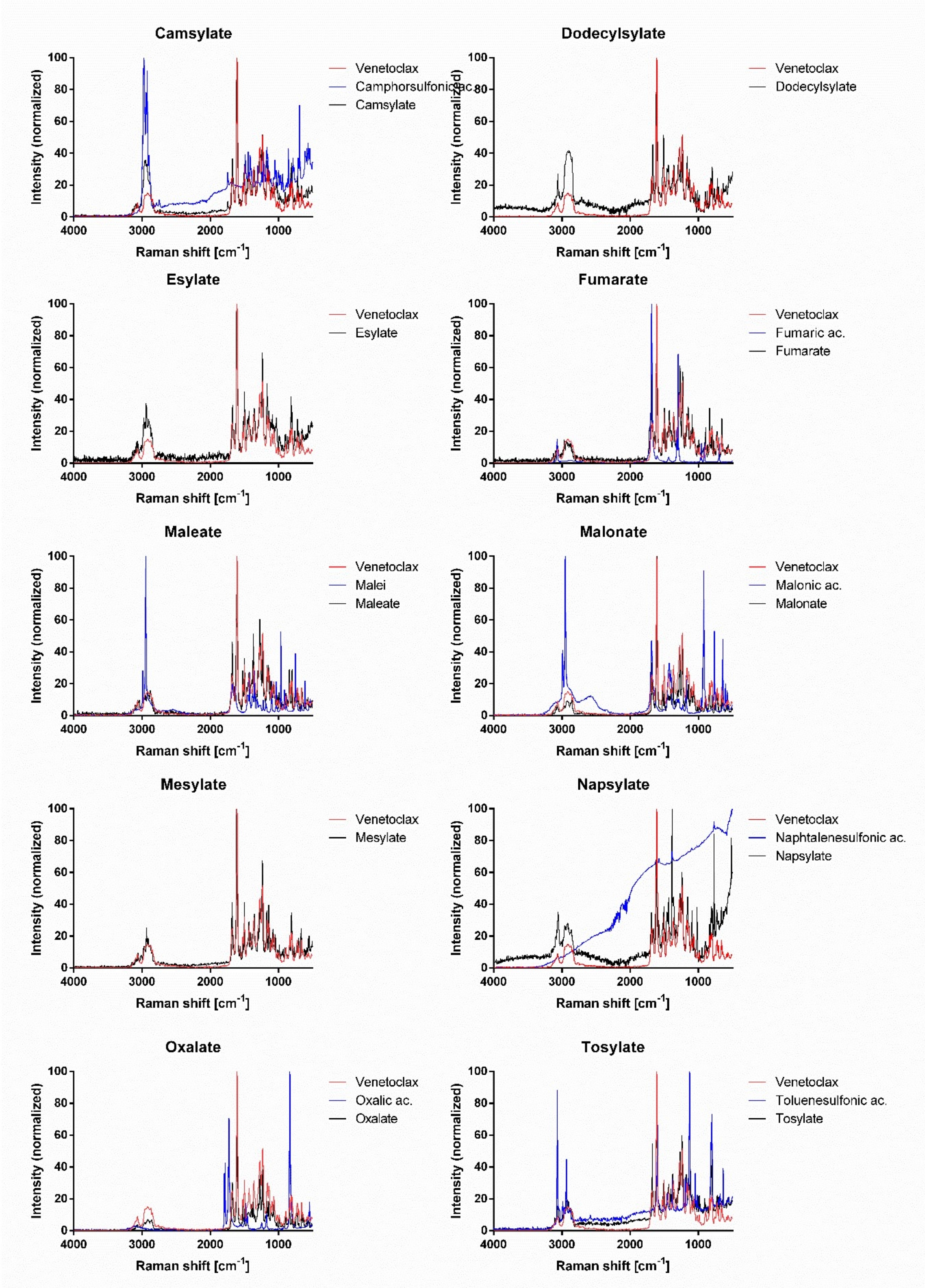

Fig. I: Normalized Raman spectra of novel salts

Nuclear magnetic resonance – transcript of spectra

Venetoclax camsylate

^{1}H NMR (500 MHz, DMSO) δ 11.77 (s, 1H), 11.70 (s, 1H), 9.17 (s, 1H), 8.64 (t, J = 6.1 Hz, 1H), 8.58 (d, J = 2.3 Hz, 1H), 8.06 (d, J = 2.7 Hz, 1H), 7.82 (dd, J = 9.4, 2.4 Hz, 1H), 7.60 – 7.50 (m, 3H), 7.41 (d, J = 8.0 Hz, 2H), 7.12 (dd, J = 23.7, 8.7 Hz, 3H), 6.74 (dd, J = 9.1, 2.4 Hz, 1H), 6.44 – 6.40 (m, 1H), 6.28 (d, J = 2.3 Hz, 1H), 4.30 (s, 10H), 3.86 (dd, J = 11.0, 4.3 Hz, 2H), 3.69 (d, J = 13.5 Hz, 2H), 3.60 (d, J = 4.8 Hz, 2H), 3.35 – 3.23 (m, 4H), 3.06 (t, J = 12.6 Hz, 2H), 2.90 (d, J = 14.7 Hz, 2H), 2.76 (d, J = 11.1 Hz, 2H), 2.66 (q, J = 10.4 Hz, 2H), 2.51 (d, J = 4.2 Hz, 7H), 2.41 (d, J = 14.7 Hz, 2H), 2.33 – 2.19 (m, 4H), 2.03 (s, 2H), 1.98 – 1.81 (m, 4H), 1.79 (s, 1H), 1.62 (d, J = 13.0 Hz, 2H), 1.47 (t, J = 6.5 Hz, 2H), 1.34 – 1.21 (m, 5H), 1.05 (s, 5H), 0.95 (s, 5H), 0.75 (s, 5H).

Venetoclax dodecylbesylate

^{1}H NMR (500 MHz, DMSO) δ 7.52 – 7.40 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.04 (ddd, *J* = 23.1, 9.0, 4.9 Hz, 3H), 5.12 (s, 2H), 3.78 (dd, *J* = 11.1, 4.3 Hz, 1H), 3.61 (d, *J* = 13.5 Hz, 1H), 3.27 – 3.15 (m, 2H), 2.96 (t, *J* = 12.7 Hz, 1H), 2.67 (d, *J* = 11.4 Hz, 1H), 2.43 (d, *J* = 4.2 Hz, 5H), 2.11 (s, 1H), 1.94 (s, 1H), 1.84 (s, 0H), 1.54 (d, *J* = 13.3 Hz, 1H), 1.49 (s, 1H), 1.44 – 1.33 (m, 3H), 1.24 – 1.06 (m, 10H), 0.93 (s, 1H), 0.86 (s, 2H), 0.73 (dq, *J* = 21.4, 6.5 Hz, 4H).

Venetoclax esylate

^{1}H NMR (500 MHz, DMSO) δ 11.78 (s, 1H), 11.70 (s, 1H), 9.21 (s, 1H), 8.64 (t, *J* = 6.0 Hz, 1H), 8.57 (d, *J* = 2.3 Hz, 1H), 8.07 (d, *J* = 2.5 Hz, 1H), 7.82 (dd, *J* = 9.3, 2.3 Hz, 1H), 7.59 (d, *J* = 2.6 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.43 – 7.37 (m, 2H), 7.14 (d, *J* = 9.3 Hz, 1H), 7.12 – 7.07 (m, 2H), 6.73 (dd, *J* = 9.0, 2.3 Hz, 1H), 6.42 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.28 (d, *J* = 2.4 Hz, 1H), 4.05 (s, 14H), 3.89 – 3.82 (m, 2H), 3.69 (d, *J* = 13.5 Hz, 2H), 3.59 (d, *J* = 4.5 Hz, 2H), 3.35 – 3.23 (m, 5H), 3.09 (s, 0H), 2.75 (d, *J* = 11.3 Hz, 2H), 2.45 (q, *J* = 7.4 Hz, 4H), 2.21 (d, *J* = 7.2 Hz, 2H), 2.02 (s, 2H), 1.89 (tt, *J* = 11.3, 3.0 Hz, 1H), 1.65 – 1.58 (m, 2H), 1.46 (t, *J* = 6.4 Hz, 2H), 1.26 (qd, *J* = 12.1, 4.5 Hz, 2H), 1.08 (t, *J* = 7.4 Hz, 5H), 0.95 (s, 5H).

Venetoclax fumarate

^{1}H NMR (500 MHz, DMSO) δ 11.70 (d, *J* = 2.6 Hz, 1H), 8.62 (t, *J* = 6.0 Hz, 1H), 8.57 (d, *J* = 2.3 Hz, 1H), 8.05 (d, *J* = 2.6 Hz, 1H), 7.81 (dd, *J* = 9.2, 2.3 Hz, 1H), 7.57 – 7.47 (m, 3H), 7.38 – 7.32 (m, 2H), 7.12 (d, *J* = 9.4 Hz, 1H), 7.08 – 7.01 (m, 2H), 6.69 (dd, *J* = 9.1, 2.3 Hz, 1H), 6.64 (s, 4H), 6.40 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.20 (d, *J* = 2.3 Hz, 1H), 3.89 – 3.82 (m, 2H), 3.34 – 3.23 (m, 4H), 3.08 (d, *J* = 5.4 Hz, 4H), 2.77 (s, 2H), 2.44 (q, *J* = 7.3 Hz, 1H), 2.22 (s, 4H), 2.15 (s, 2H), 2.07 (s, 1H), 1.96 (s, 2H), 1.89 (ddd, *J* = 11.3, 7.5, 3.9 Hz, 1H), 1.62 (d, *J* = 12.3 Hz, 2H), 1.39 (t, *J* = 6.5 Hz, 2H), 1.26 (qd, *J* = 12.1, 4.5 Hz, 2H), 0.93 (s, 6H), 0.90 (d, *J* = 7.3 Hz, 1H).

Venetoclax malonate

^{1}H NMR (500 MHz, DMSO) δ 11.72 – 11.68 (m, 1H), 8.62 (t, *J* = 6.0 Hz, 1H), 8.57 (d, *J* = 2.3 Hz, 1H), 8.04 (d, *J* = 2.7 Hz, 1H), 7.81 (dd, *J* = 9.1, 2.3 Hz, 1H), 7.54 (d, *J* = 2.6 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.34 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.12 (d, *J* = 9.3 Hz, 1H), 7.07 – 7.01 (m, 2H), 6.68 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.39 (dt, *J* = 3.7, 1.8 Hz, 1H), 6.19 (d, *J* = 2.4 Hz, 1H), 3.88 – 3.81 (m, 2H), 3.35 (s, 5H), 3.33 – 3.21 (m, 4H), 3.08 (d, *J* = 5.6 Hz, 4H), 2.82 (s, 2H), 2.26 (s, 4H), 2.13 (d,

J = 6.6 Hz, 2H), 1.95 (s, 2H), 1.89 (ddd, J = 11.4, 6.4, 2.7 Hz, 0H), 1.64 – 1.57 (m, 2H), 1.38 (t, J = 6.4 Hz, 2H), 1.25 (qd, J = 10.3, 5.8 Hz, 2H), 0.91 (s, 4H).

Venetoclax maleate
^{1}H NMR (500 MHz, DMSO) δ 11.72 (t, J = 2.4 Hz, 1H), 8.64 (t, J = 6.0 Hz, 1H), 8.58 (d, J = 2.3 Hz, 1H), 8.05 (d, J = 2.6 Hz, 1H), 7.82 (dd, J = 9.3, 2.3 Hz, 1H), 7.58 – 7.49 (m, 3H), 7.42 – 7.35 (m, 2H), 7.14 (d, J = 9.4 Hz, 1H), 7.10 – 7.04 (m, 2H), 6.71 (dd, J = 9.1, 2.3 Hz, 1H), 6.41 (dd, J = 3.4, 1.8 Hz, 1H), 6.24 (d, J = 2.3 Hz, 1H), 6.13 (s, 2H), 3.86 (ddd, J = 11.4, 4.5, 1.9 Hz, 2H), 3.35 – 3.23 (m, 4H), 2.69 (s, 3H), 2.18 (t, J = 6.3 Hz, 2H), 2.00 (d, J = 2.8 Hz, 2H), 1.90 (ddp, J = 11.2, 7.6, 3.6 Hz, 1H), 1.62 (ddd, J = 12.8, 4.1, 2.0 Hz, 2H), 1.44 (t, J = 6.4 Hz, 2H), 1.32 – 1.14 (m, 2H), 0.94 (s, 5H).

Venetoclax mesylate
^{1}H NMR (500 MHz, DMSO) δ 11.76 (s, 1H), 11.69 (s, 1H), 9.14 (s, 1H), 8.63 (t, J = 6.1 Hz, 1H), 8.56 (d, J = 2.4 Hz, 1H), 8.05 (d, J = 2.6 Hz, 1H), 7.81 (dd, J = 9.3, 2.4 Hz, 1H), 7.57 (d, J = 2.7 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 9.3 Hz, 1H), 7.08 (d, J = 8.0 Hz, 2H), 6.72 (dd, J = 8.9, 2.3 Hz, 1H), 6.43 – 6.39 (m, 1H), 6.26 (d, J = 2.2 Hz, 1H), 4.06 (s, 11H), 3.85 (dd, J = 11.2, 4.3 Hz, 2H), 3.68 (d, J = 13.5 Hz, 2H), 3.58 (d, J = 4.6 Hz, 2H), 3.28 (dt, J = 22.4, 9.1 Hz, 6H), 3.04 (t, J = 12.8 Hz, 2H), 2.74 (d, J = 11.2 Hz, 2H), 2.50 (d, J = 4.5 Hz, 7H), 2.48 (s, 1H), 2.35 (s, 5H), 2.19 (d, J = 6.6 Hz, 2H), 2.02 (s, 2H), 1.89 (d, J = 12.8 Hz, 1H), 1.61 (d, J = 12.9 Hz, 2H), 1.46 (t, J = 6.4 Hz, 2H), 1.25 (qd, J = 12.1, 4.4 Hz, 2H), 0.94 (s, 5H).

Venetoclax napsylate
^{1}H NMR (500 MHz, DMSO) δ 11.77 (s, 1H), 11.70 (s, 1H), 9.08 (s, 1H), 8.64 (t, J = 6.0 Hz, 1H), 8.58 (d, J = 2.4 Hz, 1H), 8.15 (d, J = 1.6 Hz, 2H), 8.06 (d, J = 2.6 Hz, 1H), 7.97 (dt, J = 7.1, 3.6 Hz, 2H), 7.94 – 7.84 (m, 4H), 7.82 (dd, J = 9.2, 2.4 Hz, 1H), 7.71 (dd, J = 8.5, 1.7 Hz, 2H), 7.58 (d, J = 2.7 Hz, 1H), 7.53 (dq, J = 9.9, 3.3 Hz, 6H), 7.40 (d, J = 8.2 Hz, 2H), 7.14 (d, J = 9.4 Hz, 1H), 7.12 – 7.05 (m, 2H), 6.72 (dd, J = 9.0, 2.3 Hz, 1H), 6.42 (dd, J = 3.4, 1.9 Hz, 1H), 6.27 (d, J = 2.4 Hz, 1H), 5.58 (s, 5H), 3.89 – 3.82 (m, 2H), 3.68 (d, J = 13.5 Hz, 2H), 3.59 (d, J = 4.9 Hz, 2H), 3.34 – 3.22 (m, 6H), 3.02 (d, J = 12.6 Hz, 2H), 2.75 (d, J = 11.4 Hz, 2H), 2.18 (s, 2H), 2.01 (s, 2H), 1.89 (ddd, J = 11.4, 7.4, 3.8 Hz, 1H), 1.61 (d, J = 12.9 Hz, 2H), 1.43 (t, J = 6.4 Hz, 2H), 1.26 (qd, J = 12.0, 4.5 Hz, 2H), 0.93 (s, 6H).

Venetoclax oxalate
^{1}H NMR (500 MHz, DMSO) δ 11.72 (t, J = 2.4 Hz, 1H), 8.63 (t, J = 6.0 Hz, 1H), 8.58 (d, J = 2.3 Hz, 1H), 8.05 (d, J = 2.6 Hz, 1H), 7.82 (dd, J = 9.3, 2.3 Hz, 1H), 7.56 (d, J = 2.6 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.39 – 7.33 (m, 2H), 7.13 (d, J = 9.4 Hz, 1H), 7.09 – 7.03 (m, 2H), 6.70 (dd, J = 9.0, 2.4 Hz, 1H), 6.40 (dd, J = 3.4, 1.8 Hz, 1H), 6.21 (d, J = 2.3 Hz, 1H), 3.86 (ddd, J = 11.5, 4.6, 1.9 Hz, 2H), 3.34 – 3.23 (m, 4H), 3.16 (t, J = 4.9 Hz, 4H), 2.43 (s, 4H), 2.16 (t, J = 6.5 Hz, 2H), 1.97 (s, 2H), 1.89 (dqd, J = 11.0, 7.1, 3.3 Hz, 1H), 1.65 – 1.58 (m, 2H), 1.40 (t, J = 6.5 Hz, 2H), 1.26 (qd, J = 12.0, 4.5 Hz, 2H), 0.93 (s, 6H).

Venetoclax tosylate
^{1}H NMR (500 MHz, DMSO) δ 11.77 (s, 1H), 11.70 (s, 1H), 9.09 (s, 1H), 8.67 – 8.61 (m, 1H), 8.58 (d, J = 2.3 Hz, 1H), 8.07 (d, J = 2.7 Hz, 1H), 7.82 (dd, J = 9.3, 2.3 Hz, 1H), 7.61 – 7.46 (m, 6H), 7.41 (d, J = 8.0 Hz, 2H), 7.11 (dd, J = 16.4, 8.0 Hz, 6H), 6.76 – 6.70 (m, 1H), 6.45 – 6.40 (m, 1H),

6.28 (d, J = 2.3 Hz, 1H), 5.58 (s, 5H), 3.86 (dd, J = 11.2, 4.3 Hz, 2H), 3.69 (d, J = 13.5 Hz, 2H), 3.60 (d, J = 4.8 Hz, 2H), 3.29 (dt, J = 23.0, 8.9 Hz, 5H), 2.76 (d, J = 11.3 Hz, 2H), 2.51 (s, 2H), 2.30 (s, 5H), 2.19 (s, 2H), 2.02 (s, 2H), 1.89 (s, 1H), 1.62 (d, J = 13.0 Hz, 2H), 1.45 (t, J = 6.4 Hz, 2H), 1.27 (tt, J = 12.5, 6.3 Hz, 2H), 0.95 (s, 5H).

Venetoclax Acetonitrile solvate
^{1}H NMR (500 MHz, DMSO) δ 11.69 (t, *J* = 2.4 Hz, 1H), 8.60 (t, *J* = 6.0 Hz, 1H), 8.56 (d, *J* = 2.3 Hz, 1H), 8.04 (d, *J* = 2.6 Hz, 1H), 7.80 (dd, *J* = 9.3, 2.3 Hz, 1H), 7.54 (d, *J* = 2.6 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.37 – 7.31 (m, 2H), 7.11 (d, *J* = 9.4 Hz, 1H), 7.07 – 7.00 (m, 2H), 6.68 (dd, *J* = 9.0, 2.3 Hz, 1H), 6.39 (dd, *J* = 3.4, 1.9 Hz, 1H), 6.19 (d, *J* = 2.3 Hz, 1H), 3.85 (ddd, *J* = 11.5, 4.6, 1.9 Hz, 2H), 3.32 (s, 11H), 3.07 (d, *J* = 6.1 Hz, 3H), 2.76 (s, 1H), 2.22 – 2.18 (m, 2H), 2.13 (d, *J* = 6.9 Hz, 2H), 2.07 (s, 3H), 1.95 (s, 2H), 1.88 (ddt, *J* = 11.4, 7.9, 3.9 Hz, 1H), 1.65 – 1.57 (m, 2H), 1.38 (t, *J* = 6.5 Hz, 2H), 1.25 (qd, *J* = 12.1, 4.5 Hz, 2H), 0.92 (s, 5H).

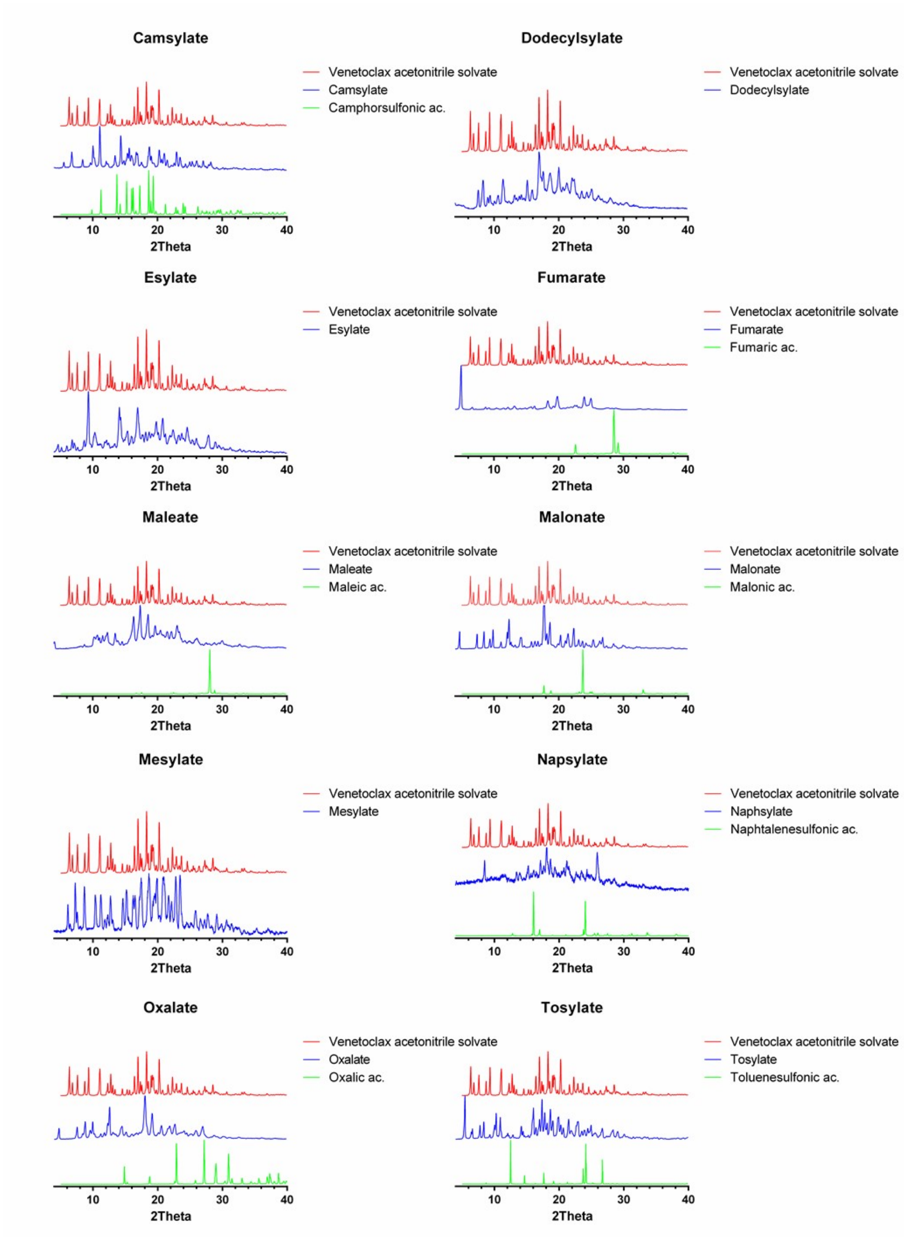

Fig. II: Normalized diffraction patterns of novel salts

	Temp. range [°C]	Mass loss [%]
Camsylate	25 – 50 50 – 100	-0.82 -0.80
Dodecylbesylate	25 – 50 50 – 100	-0.97 -0.43

Esylate	25 – 50 50 – 100	-0.29 -0.14
Fumarate	25 – 100 50 – 100	0.3 -0.3
Maleate	25 – 100 50 – 100	-0.20 -0.15
Malonate	25 – 50 50 – 100	-0.32 -0.03
Mesylate	25 – 50 50 – 100	-1.04 -0.47
Napsylate	25 – 50 50 – 100	-1.22 -0.55
Oxalate	25 – 50 50 – 100	-0.09 -0.45
Tosylate	25 – 50 50 – 100	-0.06 -0.07

Table XI: Mass loss calculated from TGA for the region of 25 – 100°C of all salts

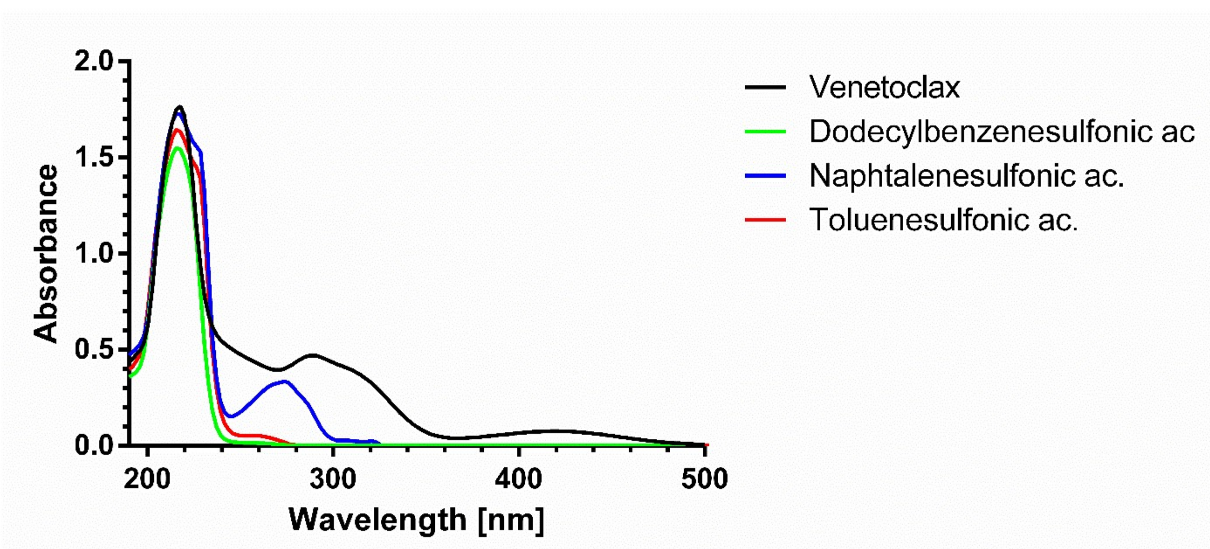

Fig. III: UV-Vis spectra of venetoclax and aromatic acids

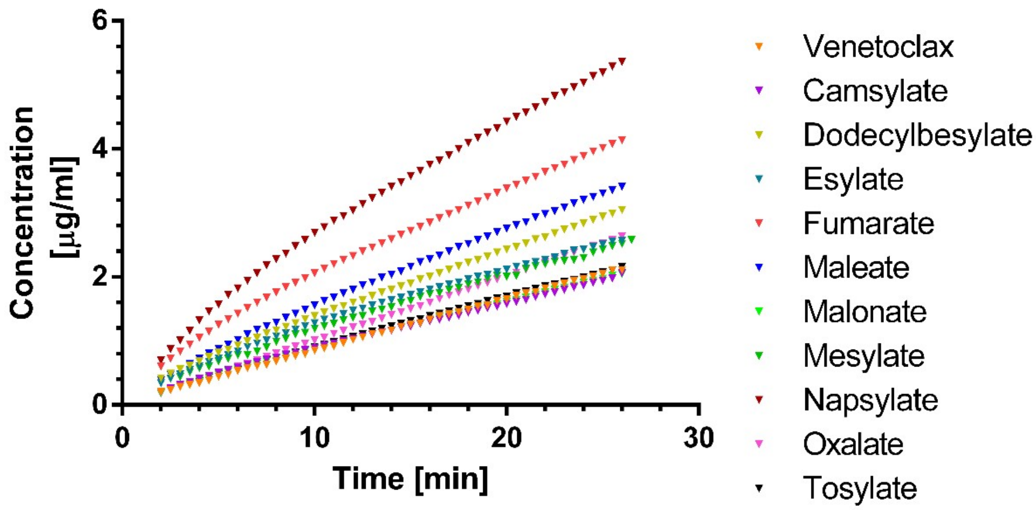

Fig. IV: average IDR curves of novel salts

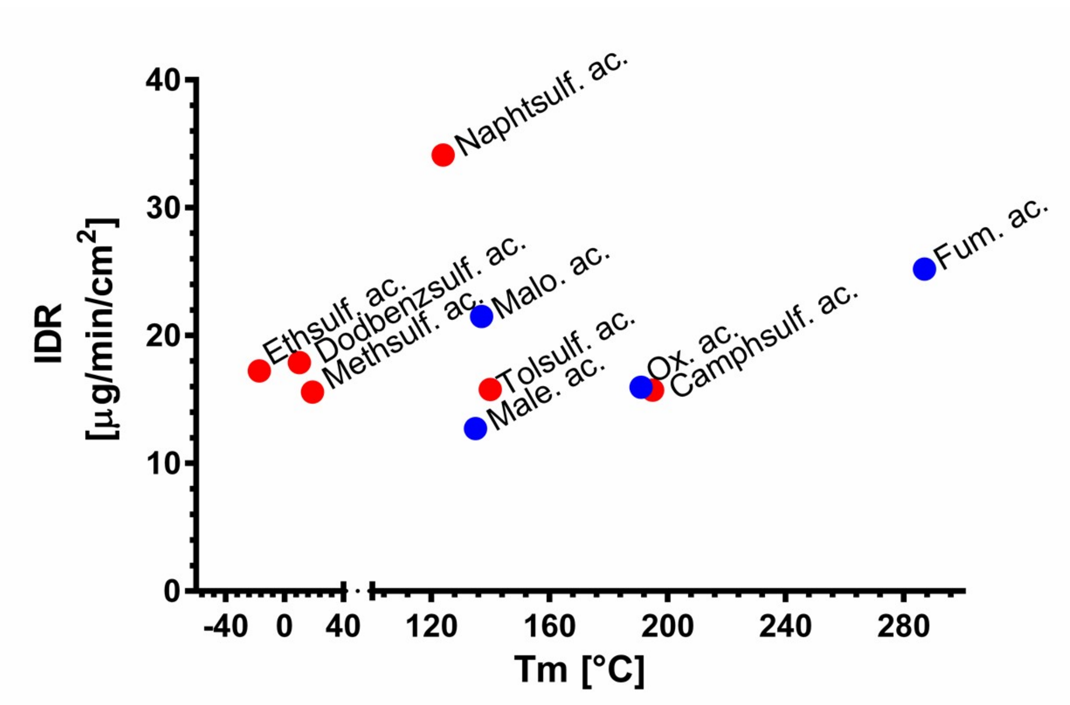

Fig. V: Correlation between IDR and Tm of the parent acids; sulfonic acids (red), dicarboxylic acids (blue)

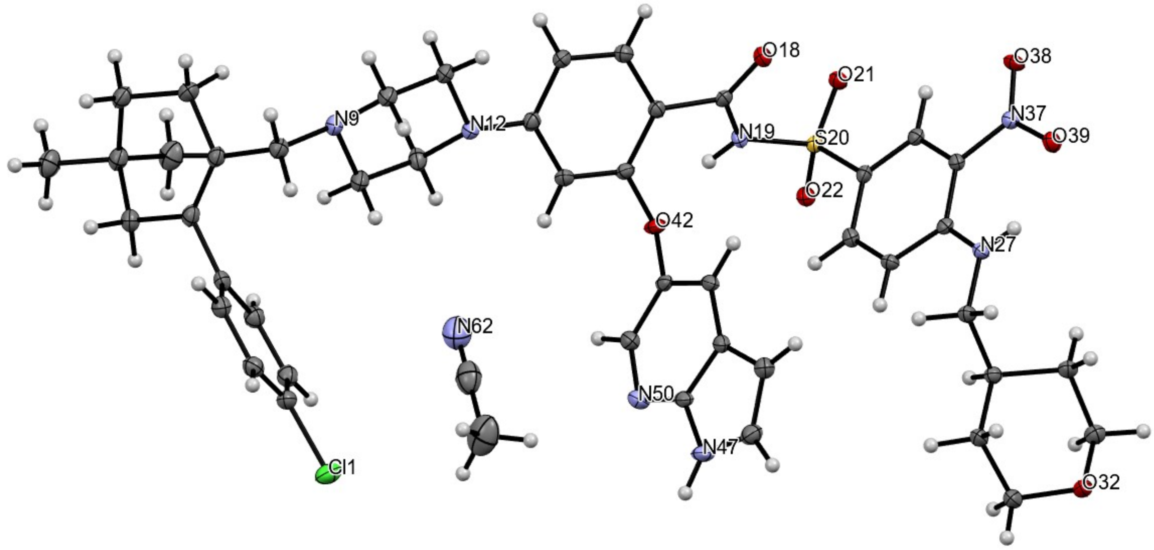

Fig. VI: The asymmetric unit of venetoclax acetonitrile solvate with thermal ellipsoids and numbering of non C/H atoms. The thermal ellipsoids are shown at the 50% probability level.

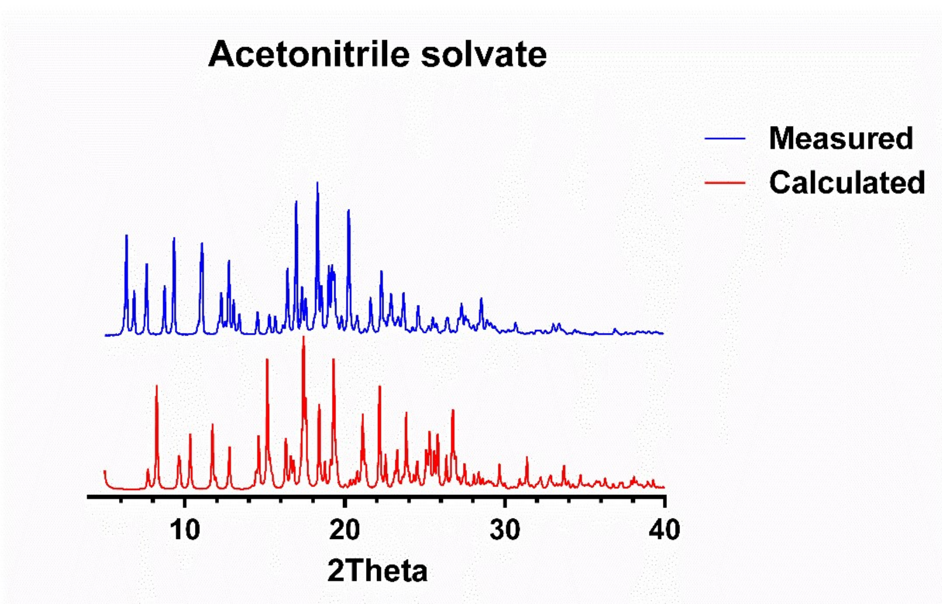

Fig VII: Comparison between calculated diffraction pattern and bulk powder of venetoclax acetonitrile solvate

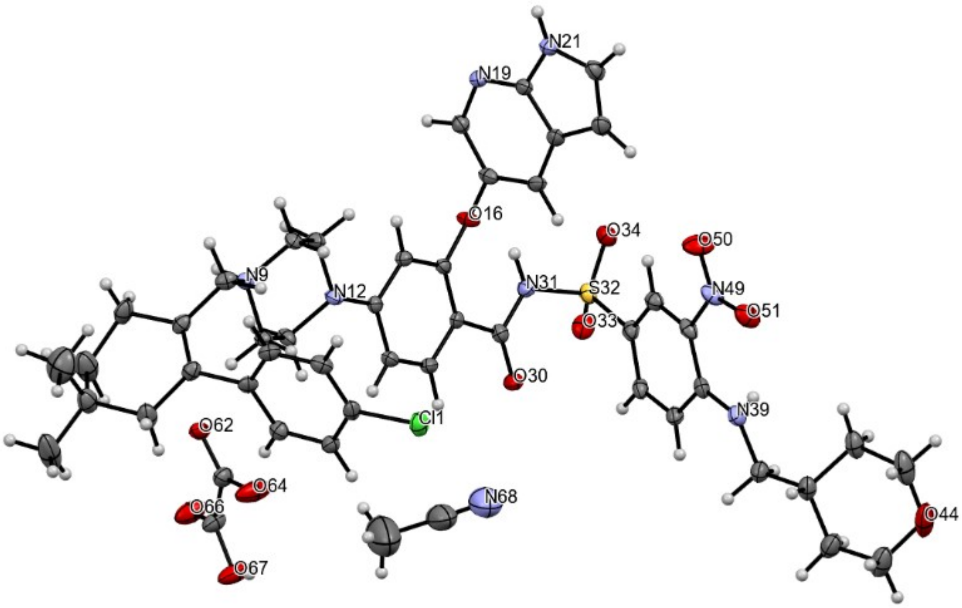

Fig. VIII: The asymmetric unit of venetoclax oxalate acetonitrile solvate with thermal ellipsoids and numbering of non C/H atoms.

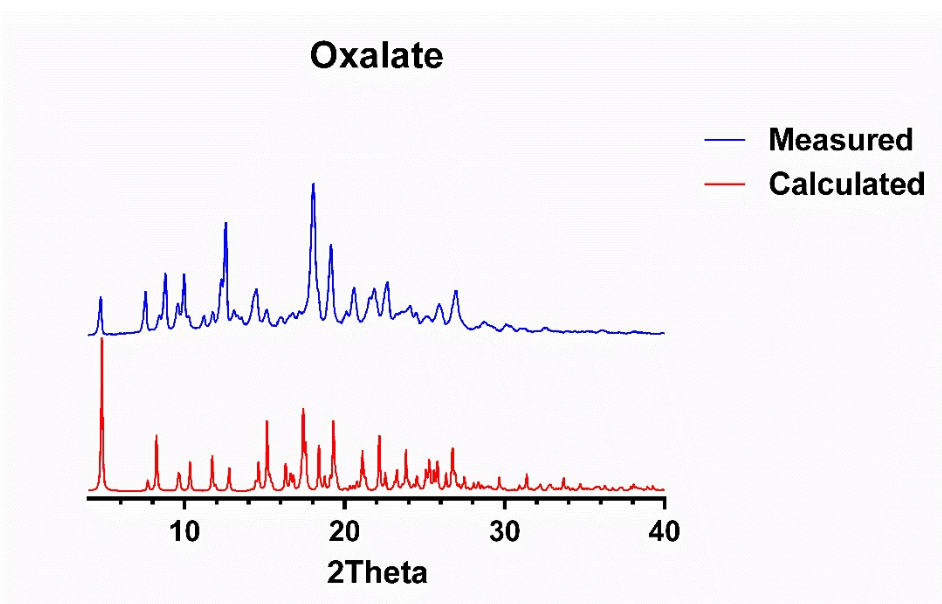

Fig IX: Comparison between calculated theoretical diffraction pattern of solvated venetoclax oxalate and measured desolvated bulk powder

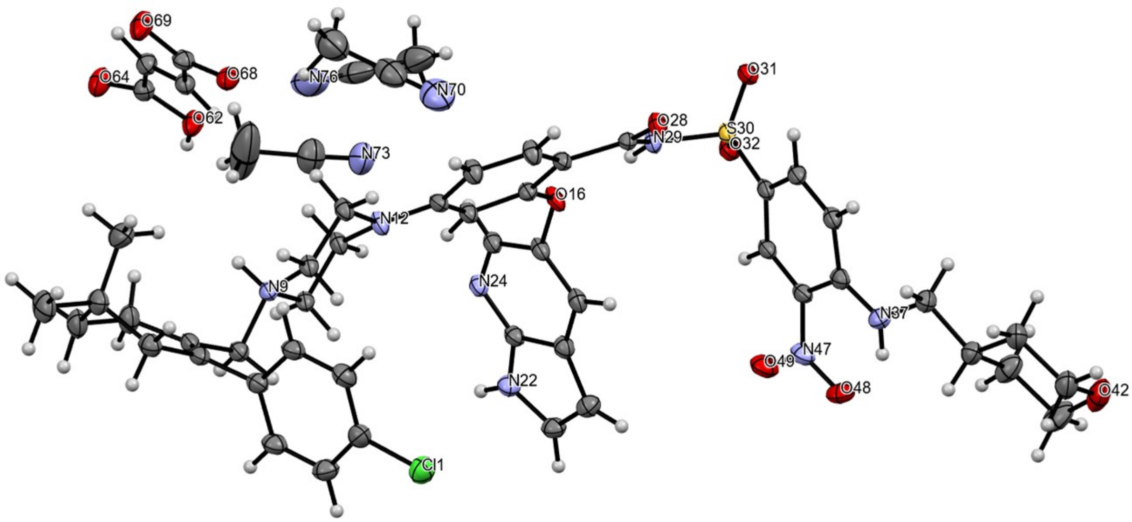

Fig. X: The asymmetric unit of venetoclax fumarate acetonitrile solvate with thermal ellipsoids and numbering of non C/H atoms. The thermal ellipsoids are shown at the 50% probability level.

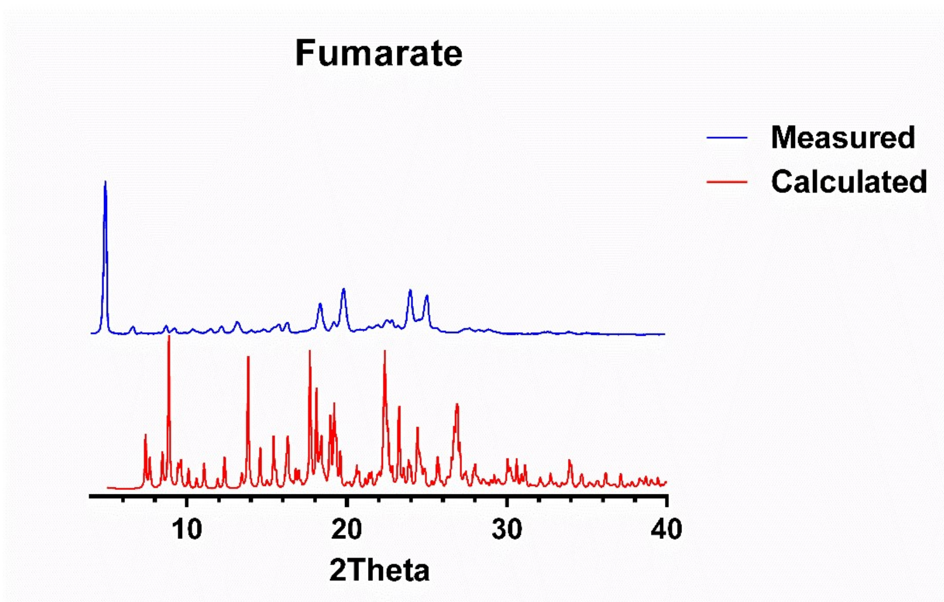

Fig XI: Comparison between calculated theoretical diffraction pattern of solvated venetoclax fumarate and measured desolvated bulk powder

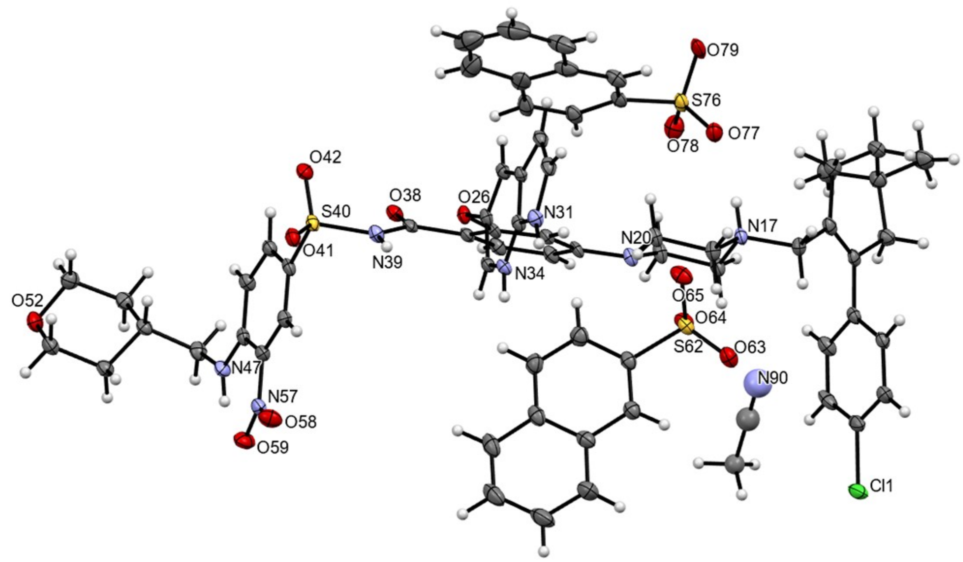

Fig. XII: The asymmetric unit of venetoclax napsylate 1:2 acetonitrile hemisolvate with thermal ellipsoids and numbering of non C/H atoms. The thermal ellipsoids are shown at the 50% probability level.

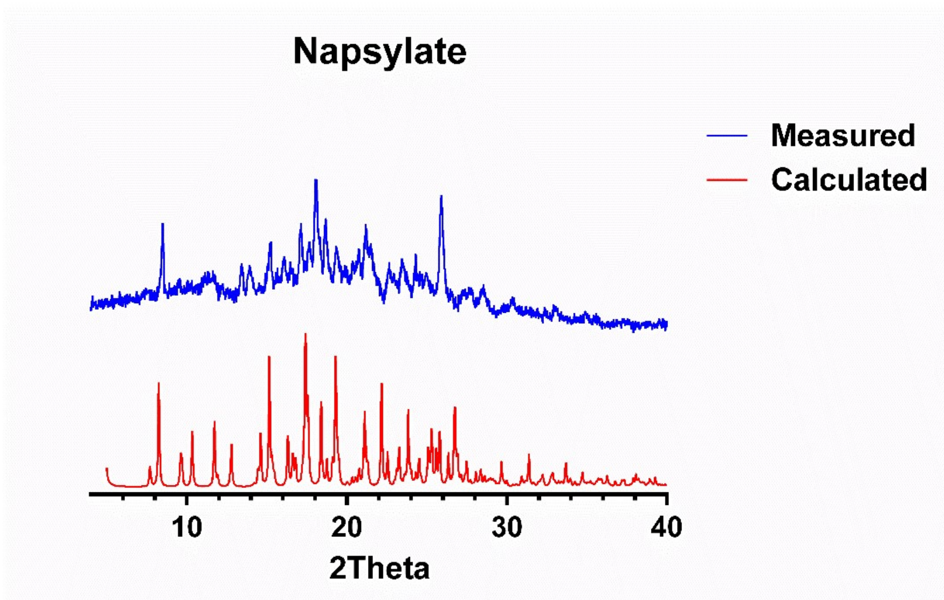

Fig XIII: Comparison between calculated theoretical diffraction pattern of solvated venetoclax napsylate and measured desolvated bulk powder

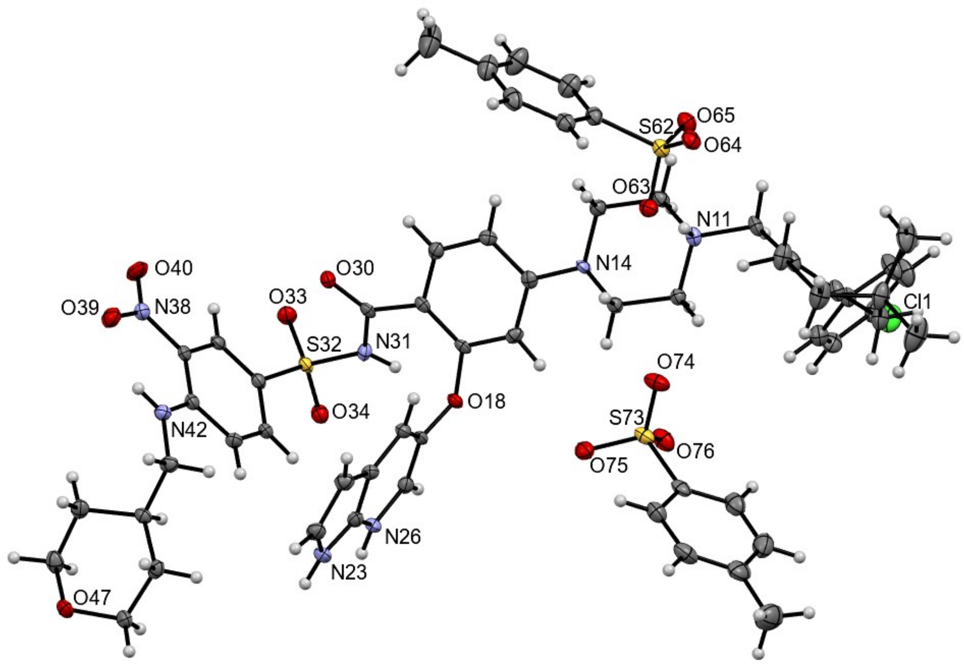

Fig. XIV: The asymmetric unit of venetoclax tosylate 1:2 with thermal ellipsoids and numbering of non C/H atoms. The thermal ellipsoids are shown at the 50% probability level.

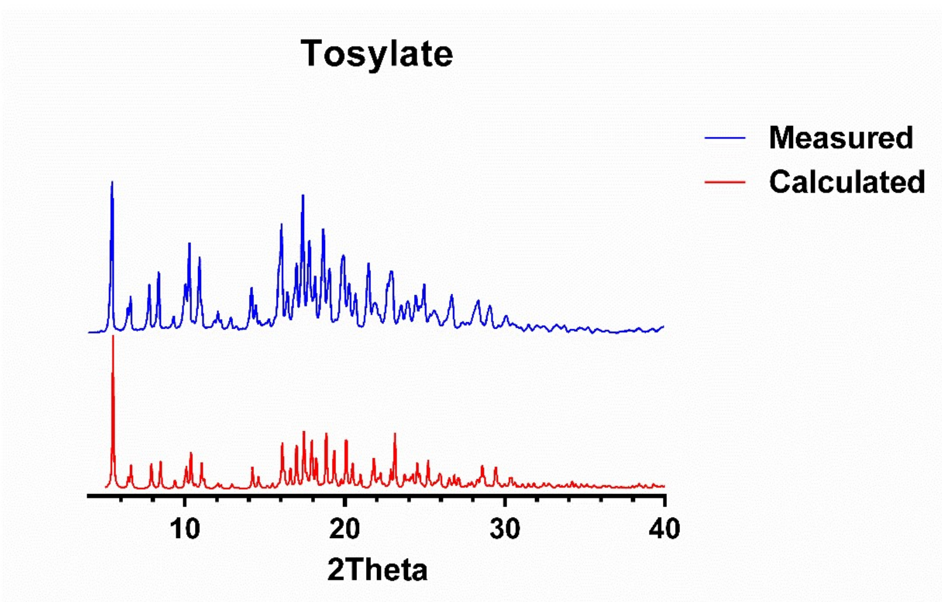

Fig XV: Comparison between calculated theoretical diffraction pattern of venetoclax tosylate and measured bulk powder

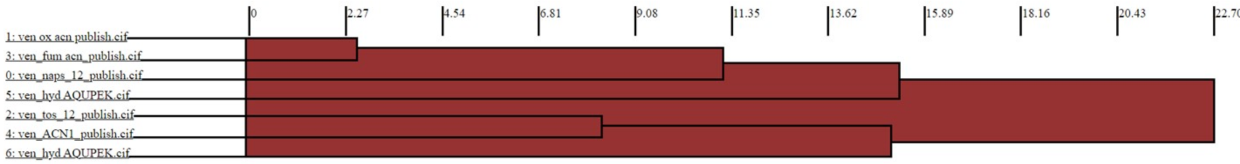

Fig. XVI: Similarity dendrogram - conformation of venetoclax

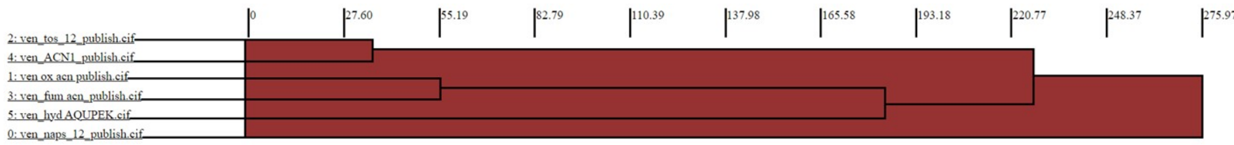

Fig XVII: Similarity dendrogram - packing of venetoclax