

Pharmaceutical Paroxetine-based organic salts of carboxylic acids with optimized properties. The identification and Characterization of a potential Novel API solid forms.

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Tabela S1. Crystal data and structural refinement parameters for the PRX organic salts.

	PRX-OXA	PRX-MAL	PRX-FUM	PRX-TART
Empirical formula	C ₄₀ H ₄₄ F ₂ N ₂ O ₁₁	C ₂₃ H ₂₄ FNO ₇	C ₂₃ H ₂₄ FNO ₇	C ₂₃ H ₂₇ FNO _{9.5}
Formula weight	766.78	445.43	445.43	488.45
Temperature (K)	298(2)	100(2)	100(2)	100(2)
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	<i>I</i> 2	<i>P</i> 1	<i>P</i> 1	<i>P</i> 2 ₁
a (Å)	18.960(3)	11.629(2)	7.2223(3)	14.3395(17)
b (Å)	6.7993(11)	11.649(2)	7.9950(10)	7.9557(9)
c (Å)	29.935(5)	17.584(5)	18.538(2)	19.608(2)
α (°)	90	77.740(4)	78.672(10)	90
β (°)	91.638(14)	77.333(4)	82.396(5)	97.036(2)
γ (°)	90	71.079(3)	85.860(7)	90
Volume (Å)³	3857.5(10)	2172.6(9)	1039.16(19)	2220.0(4)
Z / Z'	4, 2	1 / 4	1, 2	4 / 2
ρ_{calc} (g cm³)	1.317	1.362	1.424	1.461
μ (mm⁻¹)	0.102	0.106	0.111	0.119
F(000)	1608.0	932.0	468.0	1028.0
Crystal size/mm³	0.35×0.11×0.06	0.19×0.16×0.06	0.38× 0.27 × 0.2	0.10×0.06×0.03
2θ range for data collection/°	5.446 to 52.744	4.46 to 53.464	5.698 to 66.196	2.092 to 56.79
Index ranges	-23 ≤ h ≤ 23	-14 ≤ h ≤ 14	-11 ≤ h ≤ 11	-19 ≤ h ≤ 19
	-8 ≤ k ≤ 8	-14 ≤ k ≤ 14	-12 ≤ k ≤ 12	10 ≤ k ≤ 10
	-37 ≤ l ≤ 37	-21 ≤ l ≤ 21	-28 ≤ l ≤ 28	-26 ≤ l ≤ 26
Reflections collected	13051	44075	38812	55494
Independent reflections	7554 [R _{int} = 0.0663, R _{sigma} = 0.0903]	16775 [R _{int} = 0.0430, R _{sigma} = 0.0515]	15464 [R _{int} = 0.0383, R _{sigma} = 0.0412]	11054 [R _{int} = 0.0497, R _{sigma} = 0.0397]
	7554/73/505	16775/174/1148	15464/3/579	11054/1/631
Data/restraints/parameters				
R₁ [I ≥ 2σ(I)]	0.0774	0.0654	R ₁ = 0.0394,	0.0414
wR₂ [all data]	0.2645	0.1687	0.1061	0.1024
Goodness-of-fit on F²	1.021	1.040	1.048	1.037
Largest diff. peak/hole/e Å⁻³	0.29/-0.24	0.69/-0.34	0.40/-0.26	0.98/-0.33
Flack parameter	1.1(10)	0.1(4)	0.2(2)	0.4(2)

Table S2. H-bond and intermolecular interactions for the PRX organic salts.

PRX-OXA				
D-H...A	D...A	H...A	D-H...A	Symmetry code
N1B-H1BA...O2	2.693(3)	1.82	165	x,y,z
C1B-H1BD...O3A	3.414(4)	2.77	125	x,y,z
N1A-H1AA...O3	2.921(5)	2.21	136	$-x+1,+y,-z+1$
N1A-H1AA...O2	2.739(4)	1.98	143	$-x+1,+y,-z+1$
N1A-H1AB...O1	2.70(3)	1.82	172	$-x+1,+y+1,-z+1$
C5A-H5A...O3	3.628(4)	2.68	163	$-x+1,+y+1,-z+1$
N1B-H1BB...O1	2.736(4)	1.92	151	$x,+y+1,+z$
N1B-H1BB...O4	2.945(5)	2.34	125	$x,+y+1,+z$
C8A-H8A...OW2	3.457(4)	2.63	148	$x,+y+1,+z$
C1B-H1BC...O4	3.230(4)	2.70	115	$x,+y+1,+z$
C18A-H18A...O3B	3.418(5)	2.66	139	$-x+1/2+1,+y-1/2,-z+1/2+1$
C6B-H6BB...O2B	3.779(6)	2.86	159	$-x+1/2+1,+y-1/2,-z+1/2+1$
C2B-H2BA...O2	3.366(5)	2.78	120	$-x+1/2,+y+1/2,-z+1/2+1$
C2B-H2BA...O4	3.557(5)	2.63	159	$-x+1/2,+y+1/2,-z+1/2+1$
C8B-H8B...O3B	3.219(4)	2.59	125	$x,+y-1,+z$
-C9B-H9B...O2A	3.541(5)	2.90	127	$-x+1/2+1,+y+1/2,-z+1/2+1$
PRX-MAL				
N1A-H1AA...O7B	2.738(5)	1.86	162	x,y,z
N1A-H1AB...O4A	2.727(4)	1.88	153	x,y,z
O6A-H6A...O5A	2.437(3)	1.61	169	x,y,z
C2A-H2AA...O4C	3.400(6)	2.51	149	x,y,z
C2A-H2AB...O5A	3.372(5)	2.80	117	x,y,z
C5A-H5A...O6B	3.439(7)	2.55	148	x,y,z
C15A-H15A...O6B	3.692(10)	2.78	161	x,y,z
N1B-H1BB...O7A	2.774(6)	2.01	141	x,y,z
N1B-H1BB...O7C	3.324(5)	2.60	137	x,y,z
O6B-H6B...O5B	2.416(3)	1.58	170	x,y,z
C2B-H2BB...O7D	3.475(5)	2.57	152	x,y,z
C21B-H21B...O1D	3.436(8)	2.51	164	x,y,z
N1C-H1CB...O4C	2.715(5)	1.88	152	x,y,z
O6C-H6C...O5C	2.437(3)	1.61	170	x,y,z
C2C-H2CA...O4A	3.422(5)	2.52	151	x,y,z
C3C-H3CA...O7B	3.411(6)	2.63	136	x,y,z
C18C-H18C...O1D	3.573(5)	2.63	170	x,y,z
O6D-H6D...O5D	2.420(3)	1.58	168	x,y,z
C1D-H1DD...O4B	3.235(6)	2.34	149	x,y,z
C18D-H18D...O1C	3.697(5)	2.79	159	x,y,z
C1A-H1AC...O1B	3.655(6)	2.74	153	$x,+y-1,+z$
C1D-H1DC...O1C	3.526(5)	2.63	150	$x,+y-1,+z$
C12A-H12A...O6A	3.530(9)	2.69	147	$x,+y-1,+z$
C1A-H1AD...O7C	3.443(5)	2.47	167	$x,+y-1,+z$
C2D-H2DA...O3C	3.797(7)	2.85	161	$x,+y-1,+z$
C12D-H12D...O5C	3.476(9)	2.62	149	$x,+y-1,+z$
C2A-H2AB...O3B	3.671(6)	2.73	158	$x,+y-1,+z$
C21D-H21D...O1B	3.396(6)	2.47	163	$x,+y-1,+z$
N1C-H1CA...O7D	2.731(4)	1.85	162	$x-1,+y,+z$
C3A-H3AA...O7D	3.406(7)	2.64	134	$x-1,+y,+z$
C5C-H5C...O6D	3.413(5)	2.52	148	$x-1,+y,+z$
C12C-H12C...O6C	3.613(8)	2.74	154	$x-1,+y,+z$
C2D-H2DB...O7B	3.496(5)	2.57	156	$x-1,+y,+z$
C3D-H3DA...O4A	3.515(7)	2.74	135	$x-1,+y,+z$
C5D-H5D...O5D	3.454(7)	2.54	151	$x-1,+y,+z$
C1C-H1CD...O7A	3.444(5)	2.47	166	$x-1,+y,+z$
C19C-H19C...O6D	3.607(9)	2.73	154	$x-1,+y,+z$
C19D-H19D...O5D	3.674(10)	2.75	164	$x-1,+y,+z$
N1D-H1DA...O4D	2.741(5)	1.85	165	$x-1,+y,+z$

C9A-H9A...O2D	3.367(10)	2.46	160	$x, y, z+1$
N1D-H1DB...O7C	2.777(4)	2.02	139	$x-1, y-1, z$
C16A-H16A...O1B	3.637(5)	2.70	169	$x-1, y-1, z$
N1D-H1DB...O7A	3.296(5)	2.56	138	$x-1, y-1, z$
C22A-H22A...O1C	3.344(6)	2.41	164	$x+1, y, z$
C3B-H3BA...O4C	3.468(6)	2.71	133	$x+1, y, z$
N1B-H1BA...O5B	3.619(5)	2.84	144	$x+1, y+1, z$
N1B-H1BA...O4B	2.730(4)	1.84	164	$x+1, y+1, z$
C5B-H5B...O5B	3.439(5)	2.53	151	$x+1, y+1, z$
C12B-H12B...O5A	3.492(8)	2.64	149	$x, y+1, z$
C22C-H22C...O1A	3.316(8)	2.39	164	$x, y+1, z$
C2C-H2CB...O3D	3.703(5)	2.76	158	$x, y+1, z$
C1C-H1CC...O1D	3.609(6)	2.70	153	$x, y+1, z$
C1B-H1BC...O1A	3.599(6)	2.71	149	$x, y+1, z$
C2B-H2BA...O3A	3.663(5)	2.70	162	$x, y+1, z$
C1B-H1BD...O4D	3.228(5)	2.35	148	$x, y+1, z$
C9B-H9B...O2C	3.492(7)	2.74	137	$x+1, y, z+1$
C16C-H16C...O2B	3.323(8)	2.41	160	$x, y-1, z-1$
C16D-H16D...O2A	3.310(8)	2.42	156	$x-1, y+1, z-1$
PRX-FUM				
C1A-H1AD...O5B	3.283(4)	2.62	124	x, y, z
C5A-H5A...O6A	3.367(2)	2.49	146	x, y, z
N1A-H1AA...O4A	2.764(1)	1.90	156	$x, y+1, z$
C3A-H3AA...O4A	3.189(3)	2.49	127	$x, y+1, z$
O6A-H6A...O5A	2.558(3)	1.72	172	$x, y+1, z$
C5A-H5A...O4A	3.280(4)	2.58	127	$x, y+1, z$
C15A-H15A...O4A	3.605(4)	2.71	158	$x, y+1, z$
N1A-H1AB...O5A	2.808(1)	2.07	137	$x+1, y+1, z$
C21B-H21B...O7A	3.381(2)	2.48	158	$x+1, y, z$
C1A-H1AC...O6A	3.608(2)	2.79	140	$x+1, y, z$
C5B-H5B...O6B	3.520(2)	2.55	164	$x-1, y, z$
C8B-H8B...O3B	3.398(2)	2.62	140	$x-1, y, z$
C16B-H16B...O1B	3.321(3)	2.76	118	$x-1, y, z$
C8A-H8A...O3A	3.293(2)	2.43	150	$x-1, y, z$
C1B-H1BD...O7B	3.429(3)	2.70	130	$x-1, y, z$
C21A-H21A...O7B	3.334(2)	2.46	153	$x-1, y, z$
C9A-H9A...O2B	3.756(4)	2.83	165	$x, y-1, z+1$
N1B-H1BB...O7A	2.846(2)	2.33	116	$x, y-1, z$
O6B-H6B...O4B	3.189(4)	2.61	125	$x, y-1, z$
O6B-H6B...O5B	2.556(3)	1.73	170	$x, y-1, z$
N1B-H1BA...O5B	2.810(1)	1.91	167	$x-1, y-1, z$
C5B-H5B...O5B	3.586(4)	2.88	128	$x-1, y-1, z$
C3B-H3BA...O5B	3.516(3)	2.82	127	$x-1, y-1, z$
C3B-H3BB...O3B	3.605(3)	2.89	130	$x-1, y-1, z$
C9B-H9B...O2A	3.539(4)	2.63	161	$x-1, y+1, z-1$
PRX-TART				
O5-H5...O4	2.589(3)	2.09	119	x, y, z
O7-H7...O4	2.511(3)	1.69	173	x, y, z
O10-H10...O12	2.656(3)	2.20	115	x, y, z
N1A-H1AB...O6	2.969(3)	2.28	133	x, y, z
C2A-H2AA...O7	3.544(3)	2.68	148	x, y, z
C19A-H19A...O2B	3.483(3)	2.65	149	x, y, z
N1B-H1BA...O1	2.839(3)	2.38	112	x, y, z
C1B-H1BC...O1A	3.754(3)	2.84	157	x, y, z
C2B-H2BA...OW1	3.306(3)	2.54	135	x, y, z
OW1-HW1A...O1	2.913(3)	2.07	169	x, y, z
O5-H5...O6	3.059(3)	2.54	123	$-x+1, y+1/2, -z+1$
N1B-H1BA...O3	2.818(2)	1.98	155	$-x+1, y+1/2, -z+1$
O6-H6A...O3	2.816(2)	2.04	157	$-x+1, y+1/2, -z+1$
N1A-H1AA...O2	2.787(3)	1.92	163	$-x+1, y+1/2, -z+1$

C3A-H3AA...O2	3.456(3)	2.77	128	$-x+1, +y+1/2, -z+1$
C5A-H5A...O2	3.397(3)	2.67	131	$-x+1, +y+1/2, -z+1$
O9-H9...OW1	2.989(3)	2.33	138	$-x+1, +y+1/2, -z+1$
O11-H11...O2	2.515(3)	1.70	170	$x-1, +y, +z$
N1B-H1BB...O8	2.806(2)	1.93	168	$-x+1, +y-1/2, -z+1$
C2A-H2AB...O5	3.403(3)	2.80	121	$-x+1, +y-1/2, -z+1$
C1A-H1AC...O5	3.275(3)	2.63	124	$-x+1, +y-1/2, -z+1$
C3-H3...O6	3.746(4)	2.81	160	$-x+1, +y-1/2, -z+1$
C8B-H8B...O5	3.481(3)	2.60	158	$-x+1, +y-1/2, -z+1$
C15B-H15B...O10	3.309(3)	2.47	150	$-x+1, +y-1/2, -z+1$
C2A-H2AB...O12	3.187(2)	2.52	125	$-x, +y-1/2, -z+1$
C9B-H9B...O12	3.388(3)	2.56	147	$-x, +y-1/2, -z+1$
C3A-H3AB...O9	3.440(3)	2.60	145	$-x, +y-1/2, -z+1$
C3A-H3AA...O11	3.657(3)	2.69	174	$-x, +y+1/2, -z+1$
C15A-H15A...O11	3.590(3)	2.79	145	$-x, +y+1/2, -z+1$
C15A-H15A...O12	3.341(3)	2.52	148	$-x, +y+1/2, -z+1$
C16A-H16A...O10	3.447(3)	2.68	140	$-x, +y+1/2, -z+1$
C12B-H12B...O3A	3.319(3)	2.59	136	$-x+1, +y-1/2, -z$
C9A-H9A...O3A	3.558(3)	2.88	131	$-x+1, +y-1/2, -z$
OW1-HW1B...O9	3.012(2)	2.19	162	$x+1, +y, +z$
C13A-H13B...O3B	3.166(2)	2.63	115	$-x+1, +y+1/2, -z$
C6B-H6BB...O2A	3.414(3)	2.65	135	$x, +y-1, +z$

Table S3. Molecular geometry data of the PRX salts. Bond in (Å) and angles and torsion angles in (°)

PRX-OXA			
A-B	Length/Å	A-B	Length/Å
O1-C20	1.212(11)	C18B-C19B	1.380(17)
O2-C21	1.252(10)	C18A-C19A	1.392(16)
O3-C20	1.253(10)	O1B-C6B	1.428(10)
O4-C21	1.241(9)	O1B-C7B	1.404(9)
O1A-C6A	1.411(10)	O2B-C10B	1.387(10)
O1A-C7A	1.383(8)	O2B-C13B	1.398(14)
O2A-C11A	1.373(10)	O3B-C11B	1.356(12)
O2A-C13A	1.429(10)	O3B-C13B	1.425(11)
O3A-C10A	1.367(9)	N1B-C1B	1.469(8)
O3A-C13A	1.388(13)	N1B-C2B	1.487(8)
N1A-C1A	1.473(9)	C1B-C5B	1.515(10)
N1A-C2A	1.468(10)	C2B-C3B	1.527(12)
C1A-C5A	1.497(12)	C3B-C4B	1.523(9)
C2A-C3A	1.497(12)	C4B-C5B	1.552(8)
C3A-C4A	1.541(9)	C4B-C14B	1.522(12)
C4A-C5A	1.545(9)	C5B-C6B	1.509(9)
C4A-C14A	1.517(12)	C7B-C8B	1.380(11)
C5A-C6A	1.511(9)	C7B-C12B	1.376(13)
C7A-C8A	1.368(10)	C8B-C9B	1.388(11)
C7A-C12A	1.389(11)	C9B-C10B	1.316(13)
C8A-C9A	1.412(10)	C10B-C11B	1.394(12)
C9A-C10A	1.376(13)	C11B-C12B	1.361(11)
C10A-C11A	1.367(11)	C14B-C15B	1.341(16)
C11A-C12A	1.360(9)	C14B-C19B	1.391(13)
C14A-C15A	1.375(15)	C15B-C16B	1.351(16)
C14A-C19A	1.358(11)	C16B-C17B	1.332(19)
C15A-C16A	1.384(14)	C17B-F1B	1.340(13)
C16A-C17A	1.339(15)	C20-C21	1.547(11)
C17A-C18A	1.346(17)		
C17A-F1A	1.331(12)		
C18B-C17B	1.35(2)		
A-B-C	Angle/°	A-B-C	Angle/°
C7A-O1A-C6A	117.3(6)	C1B-N1B-C2B	112.0(5)
C11A-O2A-C13A	104.5(7)	N1B-C1B-C5B	112.8(6)
C10A-O3A-C13A	104.4(7)	N1B-C2B-C3B	109.0(6)
C2A-N1A-C1A	111.2(6)	C4B-C3B-C2B	111.5(7)
N1A-C1A-C5A	112.7(7)	C3B-C4B-C5B	108.6(5)
N1A-C2A-C3A	109.4(8)	C14B-C4B-C3B	112.8(7)
C2A-C3A-C4A	112.8(7)	C14B-C4B-C5B	111.6(6)
C3A-C4A-C5A	107.4(6)	C1B-C5B-C4B	108.7(6)
C14A-C4A-C3A	112.9(7)	C6B-C5B-C1B	109.6(6)
C14A-C4A-C5A	112.8(6)	C6B-C5B-C4B	113.8(6)
C1A-C5A-C4A	108.8(6)	O1B-C6B-C5B	107.2(6)
C1A-C5A-C6A	109.3(7)	C8B-C7B-O1B	123.1(8)
C6A-C5A-C4A	114.5(6)	C12B-C7B-O1B	114.1(7)
O1A-C6A-C5A	107.7(6)	C12B-C7B-C8B	122.8(7)
O1A-C7A-C12A	114.8(6)	C7B-C8B-C9B	118.0(9)
C8A-C7A-O1A	123.3(8)	C10B-C9B-C8B	120.1(9)
C8A-C7A-C12A	121.9(6)	O2B-C10B-C11B	107.5(8)

C7A-C8A-C9A	120.5(8)	C9B-C10B-O2B	131.0(8)
C10A-C9A-C8A	117.0(7)	C9B-C10B-C11B	121.5(8)
O3A-C10A-C9A	127.8(7)	O3B-C11B-C10B	110.7(7)
O3A-C10A-C11A	111.2(8)	O3B-C11B-C12B	128.5(9)
C11A-C10A-C9A	120.9(7)	C12B-C11B-C10B	120.7(9)
C10A-C11A-O2A	108.7(6)	C11B-C12B-C7B	116.9(8)
C12A-C11A-O2A	128.0(7)	O2B-C13B-O3B	108.5(8)
C12A-C11A-C10A	123.2(8)	C15B-C14B-C4B	123.5(9)
C11A-C12A-C7A	116.5(7)	C15B-C14B-C19B	118.0(10)
O3A-C13A-O2A	109.6(8)	C19B-C14B-C4B	118.5(11)
C15A-C14A-C4A	122.5(7)	C14B-C15B-C16B	121.0(12)
C19A-C14A-C4A	120.4(10)	C17B-C16B-C15B	120.9(16)
C19A-C14A-C15A	117.1(10)	C16B-C17B-C18B	121.0(13)
C14A-C15A-C16A	122.7(9)	C16B-C17B-F1B	119.9(16)
C17A-C16A-C15A	118.3(12)	F1B-C17B-C18B	119.0(13)
C16A-C17A-C18A	120.8(11)	C18B-C19B-C14B	120.5(14)
F1A-C17A-C16A	120.3(12)	O1-C20-O3	127.2(8)
F1A-C17A-C18A	118.8(10)	O1-C20-C21	118.1(7)
C17B-C18B-C19B	118.5(13)	O3-C20-C21	114.6(8)
C17A-C18A-C19A	120.6(10)	O2-C21-C20	117.3(6)
C14A-C19A-C18A	120.3(11)	O4-C21-O2	125.2(8)
C7B-O1B-C6B	116.7(6)	O4-C21-C20	117.4(8)
C10B-O2B-C13B	107.3(7)		
C11B-O3B-C13B	105.9(8)		
A-B-C-D	Angle/°	A-B-C-D	Angle/°
O1-C20-C21-O2	-170.0(8)	F1A-C17A-C18A-C19A	-177.9(11)
O1-C20-C21-O4	6.5(11)	O1B-C7B-C8B-C9B	179.0(7)
O3-C20-C21-O2	12.3(11)	O1B-C7B-C12B-C11B	179.5(6)
O3-C20-C21-O4	-171.1(8)	O2B-C10B-C11B-O3B	0.1(9)
O1A-C7A-C8A-C9A	-179.2(7)	O2B-C10B-C11B-C12B	178.3(7)
O1A-C7A-C12A-C11A	-179.7(7)	O3B-C11B-C12B-C7B	-179.6(8)
O2A-C11A-C12A-C7A	-177.8(7)	C19A-C14A-C15A-C16A	-0.7(17)
O3A-C10A-C11A-O2A	1.4(9)	N1B-C1B-C5B-C4B	-57.0(8)
O3A-C10A-C11A-C12A	-176.5(7)	N1B-C1B-C5B-C6B	178.1(6)
N1A-C1A-C5A-C4A	-59.0(9)	N1B-C2B-C3B-C4B	58.2(9)
N1A-C1A-C5A-C6A	175.3(7)	C1B-N1B-C2B-C3B	-56.9(9)
N1A-C2A-C3A-C4A	57.7(11)	C1B-C5B-C6B-O1B	57.0(8)
C1A-N1A-C2A-C3A	-56.9(10)	C2B-N1B-C1B-C5B	58.3(9)
C1A-C5A-C6A-O1A	64.3(8)	C2B-C3B-C4B-C5B	-58.5(10)
C2A-N1A-C1A-C5A	59.8(10)	C2B-C3B-C4B-C14B	177.3(8)
C2A-C3A-C4A-C5A	-57.2(11)	C3B-C4B-C5B-C1B	56.2(9)
C2A-C3A-C4A-C14A	177.8(8)	C3B-C4B-C5B-C6B	178.6(8)
C3A-C4A-C5A-C1A	55.7(9)	C3B-C4B-C14B-C15B	65.8(11)
C3A-C4A-C5A-C6A	178.3(8)	C3B-C4B-C14B-C19B	-113.9(9)
C3A-C4A-C14A-C15A	35.5(12)	C4B-C5B-C6B-O1B	-64.9(8)
C3A-C4A-C14A-C19A	-142.1(9)	C4B-C14B-C15B-C16B	178.7(9)
C4A-C5A-C6A-O1A	-58.0(10)	C4B-C14B-C19B-C18B	179.5(9)
C4A-C14A-C15A-C16A	-178.4(10)	C5B-C4B-C14B-C15B	-56.8(11)
C4A-C14A-C19A-C18A	-179.5(9)	C5B-C4B-C14B-C19B	123.5(8)
C5A-C4A-C14A-C15A	-86.5(10)	C6B-O1B-C7B-C8B	-2.5(10)
C5A-C4A-C14A-C19A	95.9(9)	C6B-O1B-C7B-C12B	176.0(7)
C6A-O1A-C7A-C8A	-6.2(11)	C7B-O1B-C6B-C5B	-174.0(5)
C6A-O1A-C7A-C12A	174.1(7)	C7B-C8B-C9B-C10B	0.3(13)
C7A-O1A-C6A-C5A	-170.2(6)	C8B-C7B-C12B-C11B	-2.0(12)
C7A-C8A-C9A-C10A	-1.7(12)	C8B-C9B-C10B-O2B	-179.8(8)

C8A–C7A–C12A–C11A	0.6(11)	C8B–C9B–C10B–C11B	0.2(13)
C8A–C9A–C10A–O3A	176.6(7)	C9B–C10B–C11B–O3B	-179.9(8)
C8A–C9A–C10A–C11A	2.0(12)	C9B–C10B–C11B–C12B	-1.7(12)
C9A–C10A–C11A–O2A	176.9(7)	C10B–O2B–C13B–O3B	-3.6(11)
C9A–C10A–C11A–C12A	-1.1(12)	C10B–C11B–C12B–C7B	2.5(12)
C10A–O3A–C13A–O2A	12.3(11)	C11B–O3B–C13B–O2B	3.6(11)
C10A–C11A–C12A–C7A	-0.3(11)	C12B–C7B–C8B–C9B	0.6(12)
C11A–O2A–C13A–O3A	-11.6(11)	C13B–O2B–C10B–C9B	-177.8(10)
C12A–C7A–C8A–C9A	0.4(12)	C13B–O2B–C10B–C11B	2.1(10)
C13A–O2A–C11A–C10A	6.1(9)	C13B–O3B–C11B–C10B	-2.3(10)
C13A–O2A–C11A–C12A	-176.0(9)	C13B–O3B–C11B–C12B	179.7(9)
C13A–O3A–C10A–C9A	176.4(9)	C14B–C4B–C5B–C1B	-178.9(7)
C13A–O3A–C10A–C11A	-8.5(10)	C14B–C4B–C5B–C6B	-56.5(10)
C14A–C4A–C5A–C1A	-179.2(7)	C14B–C15B–C16B–C17B	1.0(19)
C14A–C4A–C5A–C6A	-56.6(10)	C15B–C14B–C19B–C18B	-0.2(15)
C14A–C15A–C16A–C17A	-3(2)	C15B–C16B–C17B–C18B	1(2)
C15A–C14A–C19A–C18A	2.9(15)	C15B–C16B–C17B–F1B	177.6(11)
C15A–C16A–C17A–C18A	4(2)	C17B–C18B–C19B–C14B	2.5(18)
C15A–C16A–C17A–F1A	179.9(11)	C19B–C18B–C17B–C16B	-3(2)
C16A–C17A–C18A–C19A	-2(2)	C19B–C18B–C17B–F1B	-179.4(10)
C17A–C18A–C19A–C14A	-1.6(18)	C19B–C14B–C15B–C16B	-1.6(16)
C19A–C14A–C15A–C16A	-0.7(17)		

PRX-MAL

A–B	Length/Å	A–B	Length/Å
N1A–C1A	1.478(7)	N1C–C1C	1.488(7)
N1A–C2A	1.481(8)	N1C–C2C	1.494(8)
O1A–C6A	1.426(6)	O1C–C6C	1.424(7)
O1A–C7A	1.382(6)	O1C–C7C	1.373(7)
O2A–C10A	1.375(8)	O2C–C10C	1.384(9)
O2A–C13A	1.417(10)	O2C–C13C	1.434(12)
O3A–C11A	1.367(8)	O3C–C11C	1.374(8)
O3A–C13A	1.424(9)	O3C–C13C	1.426(10)
O4A–C20A	1.243(8)	O4C–C20C	1.246(8)
O5A–C20A	1.283(8)	O5C–C20C	1.276(8)
O6A–C23A	1.294(7)	O6C–C23C	1.277(7)
O7A–C23A	1.239(7)	O7C–C23C	1.238(7)
C1A–C5A	1.553(8)	C1C–C5C	1.518(8)
C2A–C3A	1.506(9)	C2C–C3C	1.512(9)
C3A–C4A	1.543(8)	C3C–C4C	1.527(8)
C4A–C5A	1.548(7)	C4C–C5C	1.550(8)
C4A–C14A	1.516(8)	C4C–C14C	1.517(8)
C5A–C6A	1.521(7)	C5C–C6C	1.529(7)
C7A–C8A	1.370(8)	C7C–C8C	1.375(9)
C7A–C12A	1.416(8)	C7C–C12C	1.414(8)
C8A–C9A	1.411(8)	C8C–C9C	1.400(9)
C9A–C10A	1.366(10)	C9C–C10C	1.376(11)
C10A–C11A	1.373(10)	C10C–C11C	1.369(11)
C11A–C12A	1.355(8)	C11C–C12C	1.366(9)
C14A–C15A	1.397(8)	C14C–C15C	1.378(10)
C14A–C19A	1.366(9)	C14C–C19C	1.394(9)
C15A–C16A	1.410(9)	C15C–C16C	1.395(11)
C16A–C17A	1.357(12)	C16C–C17C	1.373(11)
C17A–C18A	1.402(12)	C17C–C18C	1.355(11)
C17A–F1A	1.369(8)	C17C–F1C	1.369(8)
C18A–C19A	1.399(10)	C18C–C19C	1.402(9)

C20A–C21A	1.491(9)	C20C–C21C	1.497(8)
C21A–C22A	1.328(9)	C21C–C22C	1.351(9)
C22A–C23A	1.488(8)	C22C–C23C	1.499(8)
N1B–C1B	1.494(7)	N1D–C1D	1.496(8)
N1B–C2B	1.498(8)	N1D–C2D	1.506(8)
O1B–C6B	1.442(6)	O1D–C6D	1.424(7)
O1B–C7B	1.384(7)	O1D–C7D	1.387(7)
O2B–C10B	1.362(8)	O2D–C10D	1.382(9)
O2B–C13B	1.416(9)	O2D–C13D	1.439(9)
O3B–C11B	1.370(7)	O3D–C11D	1.366(8)
O3B–C13B	1.451(8)	O3D–C13D	1.435(8)
O4B–C20B	1.241(8)	O4D–C20D	1.256(8)
O5B–C20B	1.275(8)	O5D–C20D	1.260(8)
O6B–C23B	1.292(7)	O6D–C23D	1.280(7)
O7B–C23B	1.233(7)	O7D–C23D	1.243(7)
C1B–C5B	1.544(7)	C1D–C5D	1.516(8)
C2B–C3B	1.493(9)	C2D–C3D	1.500(9)
C3B–C4B	1.543(8)	C3D–C4D	1.549(8)
C4B–C5B	1.536(7)	C4D–C5D	1.530(7)
C4B–C14B	1.496(8)	C4D–C14D	1.511(8)
C5B–C6B	1.528(7)	C5D–C6D	1.530(8)
C7B–C8B	1.366(9)	C7D–C8D	1.388(9)
C7B–C12B	1.414(7)	C7D–C12D	1.388(8)
C8B–C9B	1.399(9)	C8D–C9D	1.409(9)
C9B–C10B	1.380(9)	C9D–C10D	1.360(10)
C10B–C11B	1.375(9)	C10D–C11D	1.375(9)
C11B–C12B	1.358(8)	C11D–C12D	1.375(8)
C14B–C15B	1.405(9)	C14D–C15D	1.388(10)
C14B–C19B	1.401(9)	C14D–C19D	1.401(9)
C15B–C16B	1.378(10)	C15D–C16D	1.376(12)
C16B–C17B	1.365(13)	C16D–C17D	1.378(13)
C17B–C18B	1.370(13)	C17D–C18D	1.359(12)
C17B–F1B	1.368(8)	C17D–F1D	1.385(8)
C18B–C19B	1.382(10)	C18D–C19D	1.385(10)
C20B–C21B	1.495(9)	C20D–C21D	1.512(8)
C21B–C22B	1.331(9)	C21D–C22D	1.349(9)
C22B–C23B	1.495(7)	C22D–C23D	1.501(8)
A–B–C	Angle/°	A–B–C	Angle/°
C1A–N1A–C2A	114.2(5)	C1C–N1C–C2C	112.4(5)
C7A–O1A–C6A	117.2(4)	C7C–O1C–C6C	117.3(4)
C10A–O2A–C13A	105.5(5)	C10C–O2C–C13C	105.1(6)
C11A–O3A–C13A	104.7(5)	C11C–O3C–C13C	104.9(6)
N1A–C1A–C5A	111.5(5)	N1C–C1C–C5C	111.9(4)
N1A–C2A–C3A	110.4(5)	N1C–C2C–C3C	110.8(5)
C2A–C3A–C4A	112.0(5)	C2C–C3C–C4C	112.0(5)
C3A–C4A–C5A	109.6(5)	C3C–C4C–C5C	110.3(5)
C14A–C4A–C3A	110.2(5)	C14C–C4C–C3C	111.4(5)
C14A–C4A–C5A	111.2(4)	C14C–C4C–C5C	110.8(5)
C4A–C5A–C1A	111.6(4)	C1C–C5C–C4C	112.9(5)
C6A–C5A–C1A	110.3(4)	C1C–C5C–C6C	109.4(4)
C6A–C5A–C4A	108.6(4)	C6C–C5C–C4C	108.1(4)
O1A–C6A–C5A	107.9(4)	O1C–C6C–C5C	109.3(4)
O1A–C7A–C12A	113.7(5)	O1C–C7C–C8C	124.8(5)
C8A–C7A–O1A	124.1(5)	O1C–C7C–C12C	113.9(5)
C8A–C7A–C12A	122.2(5)	C8C–C7C–C12C	121.3(5)

C7A-C8A-C9A	119.6(6)	C7C-C8C-C9C	121.9(6)
C10A-C9A-C8A	117.4(6)	C10C-C9C-C8C	115.6(6)
C9A-C10A-O2A	128.6(6)	C9C-C10C-O2C	127.7(7)
C9A-C10A-C11A	122.2(6)	C11C-C10C-O2C	109.6(7)
C11A-C10A-O2A	109.1(6)	C11C-C10C-C9C	122.6(6)
O3A-C11A-C10A	110.7(6)	C10C-C11C-O3C	111.1(6)
C12A-C11A-O3A	127.1(6)	C12C-C11C-O3C	126.1(7)
C12A-C11A-C10A	122.1(6)	C12C-C11C-C10C	122.8(6)
C11A-C12A-C7A	116.4(5)	C11C-C12C-C7C	115.6(6)
O2A-C13A-O3A	108.6(5)	O3C-C13C-O2C	108.9(6)
C15A-C14A-C4A	119.7(5)	C15C-C14C-C4C	121.9(6)
C19A-C14A-C4A	121.6(5)	C15C-C14C-C19C	118.6(6)
C19A-C14A-C15A	118.7(6)	C19C-C14C-C4C	119.5(5)
C14A-C15A-C16A	120.2(6)	C14C-C15C-C16C	120.9(7)
C17A-C16A-C15A	118.5(6)	C17C-C16C-C15C	118.7(6)
C16A-C17A-C18A	123.3(6)	C18C-C17C-C16C	122.4(6)
C16A-C17A-F1A	119.6(7)	C18C-C17C-F1C	119.2(7)
F1A-C17A-C18A	116.8(7)	F1C-C17C-C16C	118.4(7)
C19A-C18A-C17A	115.9(7)	C17C-C18C-C19C	118.5(6)
C14A-C19A-C18A	123.2(7)	C14C-C19C-C18C	120.8(6)
O4A-C20A-O5A	122.9(6)	O4C-C20C-O5C	123.6(6)
O4A-C20A-C21A	117.1(5)	O4C-C20C-C21C	116.1(6)
O5A-C20A-C21A	120.0(6)	O5C-C20C-C21C	120.3(5)
C22A-C21A-C20A	131.4(6)	C22C-C21C-C20C	130.3(5)
C21A-C22A-C23A	129.9(6)	C21C-C22C-C23C	129.7(5)
O6A-C23A-C22A	120.8(5)	O6C-C23C-C22C	120.9(5)
O7A-C23A-O6A	121.1(5)	O7C-C23C-O6C	122.7(6)
O7A-C23A-C22A	118.1(5)	O7C-C23C-C22C	116.4(5)
C1B-N1B-C2B	113.1(4)	C1D-N1D-C2D	112.6(5)
C7B-O1B-C6B	117.3(4)	C7D-O1D-C6D	118.4(4)
C10B-O2B-C13B	106.7(5)	C10D-O2D-C13D	105.6(5)
C11B-O3B-C13B	105.4(5)	C11D-O3D-C13D	105.8(5)
N1B-C1B-C5B	110.8(5)	N1D-C1D-C5D	111.6(5)
C3B-C2B-N1B	110.0(5)	C3D-C2D-N1D	109.5(5)
C2B-C3B-C4B	112.0(5)	C2D-C3D-C4D	111.4(5)
C5B-C4B-C3B	109.9(5)	C5D-C4D-C3D	110.3(5)
C14B-C4B-C3B	110.4(5)	C14D-C4D-C3D	110.3(5)
C14B-C4B-C5B	112.2(4)	C14D-C4D-C5D	111.3(5)
C4B-C5B-C1B	111.5(4)	C1D-C5D-C4D	112.2(5)
C6B-C5B-C1B	109.8(4)	C1D-C5D-C6D	109.4(4)
C6B-C5B-C4B	109.4(4)	C4D-C5D-C6D	109.7(5)
O1B-C6B-C5B	107.8(4)	O1D-C6D-C5D	108.7(4)
O1B-C7B-C12B	113.6(5)	O1D-C7D-C8D	123.9(5)
C8B-C7B-O1B	124.8(5)	O1D-C7D-C12D	114.2(5)
C8B-C7B-C12B	121.5(5)	C8D-C7D-C12D	121.9(5)
C7B-C8B-C9B	120.9(6)	C7D-C8D-C9D	120.3(6)
C10B-C9B-C8B	117.6(6)	C10D-C9D-C8D	116.9(6)
O2B-C10B-C9B	129.4(6)	C9D-C10D-O2D	128.1(6)
O2B-C10B-C11B	110.1(6)	C9D-C10D-C11D	122.2(6)
C11B-C10B-C9B	120.5(6)	C11D-C10D-O2D	109.7(6)
O3B-C11B-C10B	109.7(5)	O3D-C11D-C10D	110.7(6)
C12B-C11B-O3B	126.8(5)	O3D-C11D-C12D	127.0(5)
C12B-C11B-C10B	123.4(6)	C12D-C11D-C10D	122.2(6)
C11B-C12B-C7B	116.0(5)	C11D-C12D-C7D	116.4(5)
O2B-C13B-O3B	107.1(5)	O3D-C13D-O2D	107.9(5)

C15B-C14B-C4B	121.0(5)	C15D-C14D-C4D	120.8(6)
C19B-C14B-C4B	120.5(5)	C15D-C14D-C19D	119.0(6)
C19B-C14B-C15B	118.5(6)	C19D-C14D-C4D	120.2(6)
C16B-C15B-C14B	121.2(7)	C16D-C15D-C14D	120.4(7)
C17B-C16B-C15B	118.2(7)	C15D-C16D-C17D	118.5(7)
C16B-C17B-C18B	122.9(7)	C16D-C17D-F1D	118.7(8)
C16B-C17B-F1B	118.9(8)	C18D-C17D-C16D	123.4(7)
F1B-C17B-C18B	118.2(8)	C18D-C17D-F1D	117.9(8)
C17B-C18B-C19B	119.3(7)	C17D-C18D-C19D	117.8(7)
C18B-C19B-C14B	119.9(7)	C18D-C19D-C14D	120.8(6)
O4B-C20B-O5B	123.3(6)	O4D-C20D-O5D	123.7(6)
O4B-C20B-C21B	116.9(5)	O4D-C20D-C21D	115.2(5)
O5B-C20B-C21B	119.9(6)	O5D-C20D-C21D	121.1(5)
C22B-C21B-C20B	130.8(6)	C22D-C21D-C20D	129.4(5)
C21B-C22B-C23B	130.3(6)	C21D-C22D-C23D	129.4(5)
O6B-C23B-C22B	120.0(5)	O6D-C23D-C22D	121.2(5)
O7B-C23B-O6B	122.5(5)	O7D-C23D-O6D	122.6(6)
O7B-C23B-C22B	117.5(5)	O7D-C23D-C22D	116.2(5)
A-B-C-D	Angle/°	A-B-C-D	Angle/°
N1A-C1A-C5A-C4A	-51.2(6)	N1C-C1C-C5C-C4C	-51.2(6)
N1A-C1A-C5A-C6A	-172.0(4)	N1C-C1C-C5C-C6C	-171.7(4)
N1A-C2A-C3A-C4A	57.3(6)	N1C-C2C-C3C-C4C	57.0(7)
O1A-C7A-C8A-C9A	-176.6(6)	O1C-C7C-C8C-C9C	-179.5(6)
O1A-C7A-C12A-C11A	176.1(5)	O1C-C7C-C12C-C11C	176.3(5)
O2A-C10A-C11A-O3A	-0.5(10)	O2C-C10C-C11C-O3C	1.0(10)
O2A-C10A-C11A-C12A	-177.3(7)	O2C-C10C-C11C-C12C	-179.5(7)
O3A-C11A-C12A-C7A	-175.0(7)	O3C-C11C-C12C-C7C	-176.4(6)
O4A-C20A-C21A-C22A	-177.2(6)	O4C-C20C-C21C-C22C	-177.2(6)
O5A-C20A-C21A-C22A	1.6(10)	O5C-C20C-C21C-C22C	2.3(10)
C1A-N1A-C2A-C3A	-57.0(7)	C1C-N1C-C2C-C3C	-57.7(6)
C1A-C5A-C6A-O1A	-70.0(5)	C1C-C5C-C6C-O1C	-68.4(6)
C2A-N1A-C1A-C5A	54.0(6)	C2C-N1C-C1C-C5C	54.9(6)
C2A-C3A-C4A-C5A	-55.4(6)	C2C-C3C-C4C-C5C	-52.9(7)
C2A-C3A-C4A-C14A	-178.2(5)	C2C-C3C-C4C-C14C	-176.4(5)
C3A-C4A-C5A-C1A	51.7(6)	C3C-C4C-C5C-C1C	50.0(6)
C3A-C4A-C5A-C6A	173.4(5)	C3C-C4C-C5C-C6C	171.2(5)
C3A-C4A-C14A-C15A	60.5(7)	C3C-C4C-C14C-C15C	-127.2(6)
C3A-C4A-C14A-C19A	-122.4(6)	C3C-C4C-C14C-C19C	55.8(7)
C4A-C5A-C6A-O1A	167.4(4)	C4C-C5C-C6C-O1C	168.3(4)
C4A-C14A-C15A-C16A	177.4(5)	C4C-C14C-C15C-C16C	-177.2(6)
C4A-C14A-C19A-C18A	-178.2(6)	C4C-C14C-C19C-C18C	177.7(5)
C5A-C4A-C14A-C15A	-61.3(6)	C5C-C4C-C14C-C15C	109.6(6)
C5A-C4A-C14A-C19A	115.7(6)	C5C-C4C-C14C-C19C	-67.3(6)
C6A-O1A-C7A-C8A	7.0(8)	C6C-O1C-C7C-C8C	4.7(8)
C6A-O1A-C7A-C12A	-171.8(5)	C6C-O1C-C7C-C12C	-174.6(5)
C7A-O1A-C6A-C5A	174.9(4)	C7C-O1C-C6C-C5C	178.7(4)
C7A-C8A-C9A-C10A	0.2(11)	C7C-C8C-C9C-C10C	2.5(11)
C8A-C7A-C12A-C11A	-2.8(9)	C8C-C7C-C12C-C11C	-3.0(9)
C8A-C9A-C10A-O2A	176.2(8)	C8C-C9C-C10C-O2C	175.6(8)
C8A-C9A-C10A-C11A	-1.8(12)	C8C-C9C-C10C-C11C	-1.4(12)
C9A-C10A-C11A-O3A	177.8(7)	C9C-C10C-C11C-O3C	178.5(8)
C9A-C10A-C11A-C12A	1.1(12)	C9C-C10C-C11C-C12C	-2.0(12)
C10A-O2A-C13A-O3A	10.9(10)	C10C-O2C-C13C-O3C	6.5(11)
C10A-C11A-C12A-C7A	1.2(10)	C10C-C11C-C12C-C7C	4.1(10)
C11A-O3A-C13A-O2A	-11.1(9)	C11C-O3C-C13C-O2C	-6.0(10)

C12A-C7A-C8A-C9A	2.2(10)	C12C-C7C-C8C-C9C	-0.3(10)
C13A-O2A-C10A-C9A	175.4(9)	C13C-O2C-C10C-C9C	178.1(9)
C13A-O2A-C10A-C11A	-6.5(10)	C13C-O2C-C10C-C11C	-4.6(10)
C13A-O3A-C11A-C10A	7.2(9)	C13C-O3C-C11C-C10C	3.1(9)
C13A-O3A-C11A-C12A	-176.3(8)	C13C-O3C-C11C-C12C	-176.3(7)
C14A-C4A-C5A-C1A	173.8(4)	C14C-C4C-C5C-C1C	173.8(5)
C14A-C4A-C5A-C6A	-64.4(6)	C14C-C4C-C5C-C6C	-64.9(6)
C14A-C15A-C16A-C17A	-1.9(9)	C14C-C15C-C16C-C17C	0.4(11)
C15A-C14A-C19A-C18A	-1.2(10)	C15C-C14C-C19C-C18C	0.6(9)
C15A-C16A-C17A-C18A	4.5(10)	C15C-C16C-C17C-C18C	-1.0(11)
C15A-C16A-C17A-F1A	178.4(6)	C15C-C16C-C17C-F1C	179.7(7)
C16A-C17A-C18A-C19A	-5.2(11)	C16C-C17C-C18C-C19C	1.4(10)
C17A-C18A-C19A-C14A	3.4(11)	C17C-C18C-C19C-C14C	-1.2(9)
C19A-C14A-C15A-C16A	0.3(8)	C19C-C14C-C15C-C16C	-0.2(10)
C20A-C21A-C22A-C23A	-4.7(11)	C20C-C21C-C22C-C23C	-7.1(10)
C21A-C22A-C23A-O6A	4.1(10)	C21C-C22C-C23C-O6C	7.0(10)
C21A-C22A-C23A-O7A	-174.6(6)	C21C-C22C-C23C-O7C	-173.5(6)
F1A-C17A-C18A-C19A	-179.3(6)	F1C-C17C-C18C-C19C	-179.3(6)
N1B-C1B-C5B-C4B	-53.0(6)	N1D-C1D-C5D-C4D	-52.1(6)
N1B-C1B-C5B-C6B	-174.4(4)	N1D-C1D-C5D-C6D	-174.0(5)
N1B-C2B-C3B-C4B	57.6(7)	N1D-C2D-C3D-C4D	58.0(6)
O1B-C7B-C8B-C9B	-176.4(6)	O1D-C7D-C8D-C9D	-177.2(6)
O1B-C7B-C12B-C11B	176.4(5)	O1D-C7D-C12D-C11D	177.2(5)
O2B-C10B-C11B-O3B	-0.7(9)	O2D-C10D-C11D-O3D	-0.1(9)
O2B-C10B-C11B-C12B	-177.8(7)	O2D-C10D-C11D-C12D	-177.3(7)
O3B-C11B-C12B-C7B	-175.8(6)	O3D-C11D-C12D-C7D	-176.7(6)
O4B-C20B-C21B-C22B	-179.4(6)	O4D-C20D-C21D-C22D	179.7(6)
O5B-C20B-C21B-C22B	1.1(10)	O5D-C20D-C21D-C22D	-1.2(10)
C1B-N1B-C2B-C3B	-58.0(7)	C1D-N1D-C2D-C3D	-58.5(6)
C1B-C5B-C6B-O1B	-68.9(6)	C1D-C5D-C6D-O1D	-67.9(6)
C2B-N1B-C1B-C5B	55.6(6)	C2D-N1D-C1D-C5D	55.5(6)
C2B-C3B-C4B-C5B	-55.9(6)	C2D-C3D-C4D-C5D	-55.5(7)
C2B-C3B-C4B-C14B	179.9(5)	C2D-C3D-C4D-C14D	-178.9(5)
C3B-C4B-C5B-C1B	52.7(6)	C3D-C4D-C5D-C1D	51.8(6)
C3B-C4B-C5B-C6B	174.4(4)	C3D-C4D-C5D-C6D	173.5(5)
C3B-C4B-C14B-C15B	-114.5(6)	C3D-C4D-C14D-C15D	-115.4(6)
C3B-C4B-C14B-C19B	66.9(7)	C3D-C4D-C14D-C19D	63.4(7)
C4B-C5B-C6B-O1B	168.4(4)	C4D-C5D-C6D-O1D	168.7(4)
C4B-C14B-C15B-C16B	-179.2(6)	C4D-C14D-C15D-C16D	-177.3(7)
C4B-C14B-C19B-C18B	178.2(6)	C4D-C14D-C19D-C18D	178.9(6)
C5B-C4B-C14B-C15B	122.6(6)	C5D-C4D-C14D-C15D	121.7(6)
C5B-C4B-C14B-C19B	-56.1(7)	C5D-C4D-C14D-C19D	-59.5(7)
C6B-O1B-C7B-C8B	6.9(8)	C6D-O1D-C7D-C8D	4.9(8)
C6B-O1B-C7B-C12B	-172.1(5)	C6D-O1D-C7D-C12D	-173.7(5)
C7B-O1B-C6B-C5B	174.7(4)	C7D-O1D-C6D-C5D	176.4(5)
C7B-C8B-C9B-C10B	-0.6(11)	C7D-C8D-C9D-C10D	0.2(11)
C8B-C7B-C12B-C11B	-2.6(8)	C8D-C7D-C12D-C11D	-1.5(9)
C8B-C9B-C10B-O2B	177.5(8)	C8D-C9D-C10D-O2D	177.0(8)
C8B-C9B-C10B-C11B	-1.1(12)	C8D-C9D-C10D-C11D	-1.6(12)
C9B-C10B-C11B-O3B	178.1(7)	C9D-C10D-C11D-O3D	178.7(7)
C9B-C10B-C11B-C12B	1.0(11)	C9D-C10D-C11D-C12D	1.5(12)
C10B-O2B-C13B-O3B	9.6(10)	C10D-O2D-C13D-O3D	5.2(10)
C10B-C11B-C12B-C7B	0.8(9)	C10D-C11D-C12D-C7D	0.1(10)
C11B-O3B-C13B-O2B	-10.0(9)	C11D-O3D-C13D-O2D	-5.3(9)
C12B-C7B-C8B-C9B	2.5(10)	C12D-C7D-C8D-C9D	1.3(10)

C13B–O2B–C10B–C9B	175.6(9)	C13D–O2D–C10D–C9D	178.1(9)
C13B–O2B–C10B–C11B	-5.7(10)	C13D–O2D–C10D–C11D	-3.2(10)
C13B–O3B–C11B–C10B	6.6(8)	C13D–O3D–C11D–C10D	3.4(8)
C13B–O3B–C11B–C12B	-176.4(6)	C13D–O3D–C11D–C12D	-179.5(7)
C14B–C4B–C5B–C1B	175.9(5)	C14D–C4D–C5D–C1D	174.6(5)
C14B–C4B–C5B–C6B	-62.4(6)	C14D–C4D–C5D–C6D	-63.6(6)
C14B–C15B–C16B–C17B	1.9(11)	C14D–C15D–C16D–C17D	-4.1(12)
C15B–C14B–C19B–C18B	-0.5(9)	C15D–C14D–C19D–C18D	-2.3(10)
C15B–C16B–C17B–C18B	-2.3(12)	C15D–C16D–C17D–C18D	2.9(13)
C15B–C16B–C17B–F1B	179.4(7)	C15D–C16D–C17D–F1D	-178.1(7)
C16B–C17B–C18B–C19B	1.3(11)	C16D–C17D–C18D–C19D	-1.3(11)
C17B–C18B–C19B–C14B	0.2(10)	C17D–C18D–C19D–C14D	1.0(10)
C19B–C14B–C15B–C16B	-0.6(10)	C19D–C14D–C15D–C16D	3.9(10)
C20B–C21B–C22B–C23B	-3.3(11)	C20D–C21D–C22D–C23D	-0.4(10)

PRX-FUM

A–B	Length/Å	A–B	Length/Å
O1A–C6A	1.427(2)	O1B–C6B	1.4283(19)
O1A–C7A	1.367(2)	O1B–C7B	1.3730(19)
O2A–C10A	1.377(2)	O2B–C10B	1.381(2)
O2A–C13A	1.427(2)	O2B–C13B	1.432(2)
O3A–C11A	1.366(2)	O3B–C11B	1.3706(19)
O3A–C13A	1.424(3)	O3B–C13B	1.436(2)
O4A–C20A	1.2392(17)	O4B–C20B	1.2312(18)
O5A–C20A	1.2755(17)	O5B–C20B	1.2845(17)
O7A–C23A	1.2158(18)	O6B–C23B	1.3142(17)
O6A–C23A	1.3156(17)	O7B–C23B	1.2199(18)
N1A–C1A	1.484(2)	N1B–C1B	1.487(2)
N1A–C2A	1.486(2)	N1B–C2B	1.488(2)
C1A–C5A	1.519(2)	C1B–C5B	1.522(2)
C2A–C3A	1.514(2)	C2B–C3B	1.515(2)
C3A–C4A	1.533(3)	C3B–C4B	1.534(2)
C4A–C5A	1.539(2)	C4B–C5B	1.540(2)
C4A–C14A	1.510(2)	C4B–C14B	1.505(2)
C5A–C6A	1.524(2)	C5B–C6B	1.520(2)
C7A–C8A	1.380(2)	C7B–C8B	1.383(2)
C7A–C12A	1.407(2)	C7B–C12B	1.403(2)
C8A–C9A	1.404(2)	C8B–C9B	1.408(2)
C9A–C10A	1.368(2)	C9B–C10B	1.370(2)
C10A–C11A	1.383(2)	C10B–C11B	1.382(2)
C11A–C12A	1.365(3)	C11B–C12B	1.369(2)
C14A–C15A	1.398(2)	C14B–C15B	1.398(2)
C14A–C19A	1.390(2)	C14B–C19B	1.393(2)
C15A–C16A	1.385(2)	C15B–C16B	1.388(2)
C16A–C17A	1.375(3)	C16B–C17B	1.373(3)
C17A–C18A	1.372(3)	C17B–C18B	1.372(3)
C17A–F1A	1.359(2)	C17B–F1B	1.357(2)
C18A–C19A	1.390(3)	C18B–C19B	1.393(2)
C20A–C21A	1.495(2)	C20B–C21B	1.499(2)
C21A–C22A	1.3266(19)	C21B–C22B	1.3293(19)
C22A–C23A	1.482(2)	C22B–C23B	1.486(2)
A–B–C	Angle/°	A–B–C	Angle/°

C7A-O1A-C6A	122.46(15)	C7B-O1B-C6B	119.90(13)
C10A-O2A-C13A	105.10(15)	C10B-O2B-C13B	104.32(13)
C11A-O3A-C13A	106.00(15)	C11B-O3B-C13B	104.55(13)
C1A-N1A-C2A	110.53(13)	C1B-N1B-C2B	112.30(12)
N1A-C1A-C5A	111.05(12)	N1B-C1B-C5B	111.13(11)
N1A-C2A-C3A	109.70(13)	N1B-C2B-C3B	110.09(12)
C2A-C3A-C4A	113.75(14)	C2B-C3B-C4B	111.25(13)
C3A-C4A-C5A	111.55(13)	C3B-C4B-C5B	109.56(12)
C14A-C4A-C3A	110.04(14)	C14B-C4B-C3B	111.78(12)
C14A-C4A-C5A	110.77(13)	C14B-C4B-C5B	111.78(12)
C1A-C5A-C4A	111.75(12)	C1B-C5B-C4B	110.87(12)
C1A-C5A-C6A	108.36(13)	C6B-C5B-C1B	109.41(12)
C6A-C5A-C4A	112.15(14)	C6B-C5B-C4B	112.84(12)
O1A-C6A-C5A	109.10(15)	O1B-C6B-C5B	107.00(12)
O1A-C7A-C8A	125.75(15)	O1B-C7B-C8B	124.06(14)
O1A-C7A-C12A	112.89(15)	O1B-C7B-C12B	113.92(14)
C8A-C7A-C12A	121.35(16)	C8B-C7B-C12B	121.80(14)
C7A-C8A-C9A	120.70(15)	C7B-C8B-C9B	120.61(14)
C10A-C9A-C8A	117.65(16)	C10B-C9B-C8B	117.02(15)
O2A-C10A-C11A	110.26(15)	O2B-C10B-C11B	109.64(14)
C9A-C10A-O2A	128.74(17)	C9B-C10B-O2B	128.63(15)
C9A-C10A-C11A	121.00(16)	C9B-C10B-C11B	121.70(15)
O3A-C11A-C10A	109.69(16)	O3B-C11B-C10B	109.84(14)
C12A-C11A-O3A	127.38(17)	C12B-C11B-O3B	127.57(15)
C12A-C11A-C10A	122.92(16)	C12B-C11B-C10B	122.58(14)
C11A-C12A-C7A	116.38(16)	C11B-C12B-C7B	116.20(15)
O3A-C13A-O2A	108.92(14)	O2B-C13B-O3B	107.40(13)
C15A-C14A-C4A	119.68(15)	C15B-C14B-C4B	121.06(14)
C19A-C14A-C4A	121.89(15)	C19B-C14B-C4B	120.48(14)
C19A-C14A-C15A	118.43(16)	C19B-C14B-C15B	118.43(15)
C16A-C15A-C14A	121.15(17)	C16B-C15B-C14B	120.85(16)
C17A-C16A-C15A	118.16(18)	C17B-C16B-C15B	118.48(17)
C18A-C17A-C16A	122.92(17)	C18B-C17B-C16B	123.00(16)
F1A-C17A-C16A	117.88(19)	F1B-C17B-C16B	118.31(18)
F1A-C17A-C18A	119.19(18)	F1B-C17B-C18B	118.68(18)
C17A-C18A-C19A	118.18(17)	C17B-C18B-C19B	117.94(17)
C18A-C19A-C14A	121.15(17)	C14B-C19B-C18B	121.28(16)
O4A-C20A-O5A	124.83(13)	O4B-C20B-O5B	124.37(14)
O4A-C20A-C21A	119.68(13)	O4B-C20B-C21B	120.11(13)
O5A-C20A-C21A	115.48(12)	O5B-C20B-C21B	115.52(13)
C22A-C21A-C20A	121.80(13)	C22B-C21B-C20B	121.55(13)
C21A-C22A-C23A	121.11(13)	C21B-C22B-C23B	121.22(13)
O7A-C23A-O6A	124.16(13)	O6B-C23B-C22B	112.75(12)
O7A-C23A-C22A	123.16(13)	O7B-C23B-O6B	124.07(13)
O6A-C23A-C22A	112.67(13)	O7B-C23B-C22B	123.17(13)
A-B-C-D	Angle/°	A-B-C-D	Angle/°
O1A-C7A-C8A-C9A	178.23(19)	O1B-C7B-C8B-C9B	-173.03(17)
O1A-C7A-C12A-C11A	-179.03(18)	O1B-C7B-C12B-C11B	171.85(15)
O2A-C10A-C11A-O3A	0.5(2)	O2B-C10B-C11B-O3B	0.2(2)
O2A-C10A-C11A-C12A	179.46(19)	O2B-C10B-C11B-C12B	179.26(17)

O3A-C11A-C12A-C7A	179.8(2)	O3B-C11B-C12B-C7B	-179.14(17)
O4A-C20A-C21A-C22A	-7.1(2)	O4B-C20B-C21B-C22B	1.2(2)
O5A-C20A-C21A-C22A	171.70(15)	O5B-C20B-C21B-C22B	-178.09(15)
N1A-C1A-C5A-C4A	-54.87(16)	N1B-C1B-C5B-C4B	-55.23(16)
N1A-C1A-C5A-C6A	-178.93(13)	N1B-C1B-C5B-C6B	179.68(12)
N1A-C2A-C3A-C4A	54.15(19)	N1B-C2B-C3B-C4B	57.46(17)
C1A-N1A-C2A-C3A	-61.01(18)	C1B-N1B-C2B-C3B	-58.01(17)
C1A-C5A-C6A-O1A	49.05(19)	C1B-C5B-C6B-O1B	56.10(17)
C2A-N1A-C1A-C5A	62.36(16)	C2B-N1B-C1B-C5B	57.27(16)
C2A-C3A-C4A-C5A	-47.44(18)	C2B-C3B-C4B-C5B	-55.98(16)
C2A-C3A-C4A-C14A	-170.79(14)	C2B-C3B-C4B-C14B	179.55(13)
C3A-C4A-C5A-C1A	46.93(17)	C3B-C4B-C5B-C1B	54.45(15)
C3A-C4A-C5A-C6A	168.84(13)	C3B-C4B-C5B-C6B	177.58(12)
C3A-C4A-C14A-C15A	58.3(2)	C3B-C4B-C14B-C15B	50.5(2)
C3A-C4A-C14A-C19A	-121.00(18)	C3B-C4B-C14B-C19B	-131.07(16)
C4A-C5A-C6A-O1A	-74.78(18)	C4B-C5B-C6B-O1B	-67.85(16)
C4A-C14A-C15A-C16A	-179.39(18)	C4B-C14B-C15B-C16B	179.94(16)
C4A-C14A-C19A-C18A	-179.84(18)	C4B-C14B-C19B-C18B	-179.04(16)
C5A-C4A-C14A-C15A	-65.6(2)	C5B-C4B-C14B-C15B	-72.72(19)
C5A-C4A-C14A-C19A	115.19(18)	C5B-C4B-C14B-C19B	105.71(17)
C6A-O1A-C7A-C8A	5.5(3)	C6B-O1B-C7B-C8B	-36.2(3)
C6A-O1A-C7A-C12A	-175.89(19)	C6B-O1B-C7B-C12B	149.16(16)
C7A-O1A-C6A-C5A	123.72(19)	C7B-O1B-C6B-C5B	160.55(15)
C7A-C8A-C9A-C10A	0.3(3)	C7B-C8B-C9B-C10B	1.6(3)
C8A-C7A-C12A-C11A	-0.4(3)	C8B-C7B-C12B-C11B	-2.9(3)
C8A-C9A-C10A-O2A	179.8(2)	C8B-C9B-C10B-O2B	179.28(17)
C8A-C9A-C10A-C11A	0.2(3)	C8B-C9B-C10B-C11B	-2.6(3)
C9A-C10A-C11A-O3A	-179.89(19)	C9B-C10B-C11B-O3B	-178.30(17)
C9A-C10A-C11A-C12A	-0.9(3)	C9B-C10B-C11B-C12B	0.8(3)
C10A-O2A-C13A-O3A	-1.4(2)	C10B-O2B-C13B-O3B	-19.95(19)
C10A-C11A-C12A-C7A	1.0(3)	C10B-C11B-C12B-C7B	2.0(3)
C11A-O3A-C13A-O2A	1.7(2)	C11B-O3B-C13B-O2B	20.12(19)
C12A-C7A-C8A-C9A	-0.2(3)	C12B-C7B-C8B-C9B	1.2(3)
C13A-O2A-C10A-C9A	-179.0(2)	C13B-O2B-C10B-C9B	-169.35(18)
C13A-O2A-C10A-C11A	0.6(2)	C13B-O2B-C10B-C11B	12.32(19)
C13A-O3A-C11A-C10A	-1.3(2)	C13B-O3B-C11B-C10B	-12.57(19)
C13A-O3A-C11A-C12A	179.8(2)	C13B-O3B-C11B-C12B	168.41(18)
C14A-C4A-C5A-C1A	169.87(13)	C14B-C4B-C5B-C1B	178.92(12)
C14A-C4A-C5A-C6A	-68.22(17)	C14B-C4B-C5B-C6B	-57.94(16)
C14A-C15A-C16A-C17A	-0.7(3)	C14B-C15B-C16B-C17B	-1.1(3)
C15A-C14A-C19A-C18A	0.9(3)	C15B-C14B-C19B-C18B	-0.6(3)
C15A-C16A-C17A-C18A	0.7(3)	C15B-C16B-C17B-C18B	-0.2(3)
C15A-C16A-C17A-F1A	-179.20(18)	C15B-C16B-C17B-F1B	179.71(17)
C16A-C17A-C18A-C19A	0.1(3)	C16B-C17B-C18B-C19B	1.0(3)
C17A-C18A-C19A-C14A	-0.9(3)	C17B-C18B-C19B-C14B	-0.7(3)
C19A-C14A-C15A-C16A	-0.1(3)	C19B-C14B-C15B-C16B	1.5(3)
C20A-C21A-C22A-C23A	178.03(13)	C20B-C21B-C22B-C23B	-178.34(14)
C21A-C22A-C23A-O7A	-8.9(2)	C21B-C22B-C23B-O6B	-173.39(14)
C21A-C22A-C23A-O6A	171.55(15)	C21B-C22B-C23B-O7B	5.9(2)
F1A-C17A-C18A-C19A	179.96(19)	F1B-C17B-C18B-C19B	-178.83(17)

PRX-TART			
A-B	Length/Å	A-B	Length/Å
O1-C4	1.230(3)	C10A-C11A	1.378(4)
O3-C1	1.242(3)	C11A-C12A	1.365(4)
O2-C4	1.278(3)	C14A-C15A	1.398(4)
O4-C1	1.259(3)	C14A-C19A	1.379(4)
O5-C2	1.416(3)	C15A-C16A	1.379(4)
O6-C3	1.411(3)	C16A-C17A	1.365(4)
O7-C5	1.303(4)	C17A-C18A	1.365(4)
O8-C5	1.208(4)	C17A-F1A	1.365(3)
O9-C6	1.397(4)	C18A-C19A	1.394(4)
O10-C7	1.395(4)	O1B-C6B	1.425(3)
O11-C8	1.293(4)	O1B-C7B	1.369(3)
O12-C8	1.209(4)	O2B-C10B	1.387(3)
C1-C2	1.535(4)	O2B-C13B	1.428(4)
C2-C3	1.534(4)	O3B-C11B	1.379(3)
C3-C4	1.529(4)	O3B-C13B	1.435(4)
C5-C6	1.526(4)	N1B-C1B	1.489(4)
C6-C7	1.543(4)	N1B-C2B	1.485(4)
C7-C8	1.522(4)	C1B-C5B	1.527(4)
O1A-C7A	1.368(3)	C2B-C3B	1.513(4)
O1A-C6A	1.428(3)	C3B-C4B	1.532(4)
O2A-C11A	1.371(3)	C4B-C5B	1.542(4)
O2A-C13A	1.430(4)	C4B-C14B	1.514(4)
O3A-C10A	1.380(3)	C5B-C6B	1.521(4)
O3A-C13A	1.423(4)	C7B-C8B	1.387(4)
N1A-C1A	1.494(3)	C7B-C12B	1.406(4)
N1A-C2A	1.501(4)	C8B-C9B	1.394(4)
C1A-C5A	1.518(4)	C9B-C10B	1.368(4)
C2A-C3A	1.521(4)	C10B-C11B	1.377(4)
C3A-C4A	1.537(4)	C11B-C12B	1.375(4)
C4A-C5A	1.536(4)	C14B-C15B	1.400(4)
C4A-C14A	1.510(4)	C14B-C19B	1.386(4)
C5A-C6A	1.519(4)	C15B-C16B	1.386(4)
C7A-C8A	1.378(4)	C16B-C17B	1.372(5)
C7A-C12A	1.407(4)	C17B-C18B	1.361(5)
C8A-C9A	1.403(4)	C17B-F1B	1.363(3)
C9A-C10A	1.365(4)	C18B-C19B	1.400(4)
A-B-C	Angle/°	A-B-C	Angle/°
O3-C1-O4	127.1(3)	O3A-C13A-O2A	108.6(2)
O3-C1-C2	117.6(2)	C15A-C14A-C4A	119.9(2)
O4-C1-C2	115.2(2)	C19A-C14A-C4A	121.7(2)
O5-C2-C1	111.0(2)	C19A-C14A-C15A	118.2(3)
O5-C2-C3	109.8(2)	C16A-C15A-C14A	121.5(3)
C3-C2-C1	110.2(2)	C17A-C16A-C15A	118.0(3)
O6-C3-C2	111.3(2)	C16A-C17A-F1A	118.6(3)
O6-C3-C4	113.0(2)	C18A-C17A-C16A	123.0(3)
C4-C3-C2	108.6(2)	C18A-C17A-F1A	118.4(3)
O1-C4-O2	126.1(2)	C17A-C18A-C19A	118.3(3)
O1-C4-C3	119.7(2)	C14A-C19A-C18A	120.9(3)
O2-C4-C3	114.2(2)	C7B-O1B-C6B	118.6(2)
O7-C5-C6	111.8(2)	C10B-O2B-C13B	104.1(2)
O8-C5-O7	126.1(3)	C11B-O3B-C13B	104.2(2)
O8-C5-C6	122.1(3)	C2B-N1B-C1B	113.5(2)
O9-C6-C5	112.3(3)	N1B-C1B-C5B	112.9(2)

O9-C6-C7	109.2(2)	N1B-C2B-C3B	109.4(3)
C5-C6-C7	108.2(2)	C2B-C3B-C4B	111.9(2)
O10-C7-C6	110.9(2)	C3B-C4B-C5B	110.2(2)
O10-C7-C8	110.4(2)	C14B-C4B-C3B	110.8(2)
C8-C7-C6	109.0(3)	C14B-C4B-C5B	114.5(2)
O11-C8-C7	113.3(3)	O1A-C6B-C5A	106.7(2)
O12-C8-O11	125.5(3)	C1B-C5B-C4B	111.8(2)
O12-C8-C7	121.2(3)	C6B-C5B-C1B	107.8(2)
C7A-O1A-C6A	117.0(2)	C6B-C5B-C4B	109.7(2)
C11A-O2A-C13A	105.4(2)	O1B-C6B-C5B	107.8(2)
C10A-O3A-C13A	105.2(2)	O1B-C7B-C8B	115.2(2)
C1A-N1A-C2A	112.8(2)	O1B-C7B-C12B	123.7(3)
N1A-C1A-C5A	110.1(2)	C8B-C7B-C12B	121.1(3)
N1A-C2A-C3A	108.8(2)	C7B-C8B-C9B	121.8(3)
C2A-C3A-C4A	110.9(2)	C10B-C9B-C8B	116.5(3)
C5A-C4A-C3A	108.8(2)	C9B-C10B-O2B	128.5(3)
C14A-C4A-C3A	112.7(2)	C9B-C10B-C11B	121.8(3)
C14A-C4A-C5A	111.8(2)	C11B-C10B-O2B	109.7(2)
C1A-C5A-C4A	110.6(2)	C10B-C11B-O3B	109.8(2)
C1A-C5A-C6A	109.6(2)	C12B-C11B-O3B	127.1(3)
C6A-C5A-C4A	111.2(2)	C12B-C11B-C10B	123.1(3)
O1A-C7A-C8A	124.8(3)	C11B-C12B-C7B	115.6(3)
O1A-C7A-C12A	113.3(2)	O2B-C13B-O3B	107.7(2)
C8A-C7A-C12A	121.9(3)	C15B-C14B-C4B	120.5(2)
C7A-C8A-C9A	120.4(3)	C19B-C14B-C4B	121.1(3)
C10A-C9A-C8A	117.3(3)	C19B-C14B-C15B	118.3(3)
C9A-C10A-O3A	128.2(3)	C16B-C15B-C14B	121.0(3)
C9A-C10A-C11A	121.8(3)	C17B-C16B-C15B	118.5(3)
C11A-C10A-O3A	110.0(3)	C18B-C17B-C16B	122.9(3)
O2A-C11A-C10A	109.9(2)	C18B-C17B-F1B	118.6(3)
C12A-C11A-O2A	127.5(3)	F1B-C17B-C16B	118.5(3)
C12A-C11A-C10A	122.5(3)	C17B-C18B-C19B	118.3(3)
C11A-C12A-C7A	116.0(3)	C14B-C19B-C18B	121.1(3)
A-B-C-D	Angle/°	A-B-C-D	Angle/°
O3-C1-C2-O5	-174.4(2)	C14A-C4A-C5A-C1A	-177.5(2)
O3-C1-C2-C3	63.7(3)	C14A-C4A-C5A-C6A	-55.5(3)
O4-C1-C2-O5	5.8(3)	C14A-C15A-C16A-C17A	-0.1(5)
O4-C1-C2-C3	-116.0(3)	C15A-C14A-C19A-C18A	0.5(4)
O5-C2-C3-O6	-59.3(3)	C15A-C16A-C17A-C18A	0.7(5)
O5-C2-C3-C4	65.8(3)	C15A-C16A-C17A-F1A	179.3(3)
O6-C3-C4-O1	25.1(3)	C16A-C17A-C18A-C19A	-0.6(5)
O6-C3-C4-O2	-157.7(2)	C17A-C18A-C19A-C14A	0.0(4)
O7-C5-C6-O9	-166.7(2)	C19A-C14A-C15A-C16A	-0.4(4)
O7-C5-C6-C7	72.6(3)	F1A-C17A-C18A-C19A	-179.3(3)
O8-C5-C6-O9	14.2(4)	O1B-C7B-C8B-C9B	178.0(3)
O8-C5-C6-C7	-106.5(3)	O1B-C7B-C12B-C11B	-176.6(3)
O9-C6-C7-O10	-66.4(3)	O2B-C10B-C11B-O3B	0.1(3)
O9-C6-C7-C8	55.4(3)	O2B-C10B-C11B-C12B	-178.3(3)
O10-C7-C8-O11	-170.1(3)	O3B-C11B-C12B-C7B	179.7(3)
O10-C7-C8-O12	9.4(4)	N1B-C1B-C5B-C4B	-49.4(3)
C1-C2-C3-O6	63.3(3)	N1B-C1B-C5B-C6B	-170.1(2)
C1-C2-C3-C4	-171.6(2)	N1B-C2B-C3B-C4B	58.6(3)
C2-C3-C4-O1	-99.0(3)	C1B-N1B-C2B-C3B	-56.9(3)
C2-C3-C4-O2	78.2(3)	C1B-C5B-C6B-O1B	-55.9(3)
C5-C6-C7-O10	56.2(3)	C2B-N1B-C1B-C5B	53.3(3)

C5-C6-C7-C8	178.0(2)	C2B-C3B-C4B-C5B	-56.1(3)
C6-C7-C8-O11	67.8(3)	C2B-C3B-C4B-C14B	176.1(3)
C6-C7-C8-O12	-112.7(3)	C3B-C4B-C5B-C1B	50.6(3)
O1A-C7A-C8A-C9A	-176.7(3)	C3B-C4B-C5B-C6B	170.1(2)
O1A-C7A-C12A-C11A	176.4(2)	C3B-C4B-C14B-C15B	57.3(4)
O2A-C11A-C12A-C7A	-178.6(3)	C3B-C4B-C14B-C19B	-119.0(3)
O3A-C10A-C11A-O2A	-0.4(4)	C4B-C5B-C6B-O1B	-177.8(2)
O3A-C10A-C11A-C12A	179.9(3)	C4B-C14B-C15B-C16B	-174.5(3)
N1A-C1A-C5A-C4A	-56.9(3)	C4B-C14B-C19B-C18B	175.3(3)
N1A-C1A-C5A-C6A	-179.8(2)	C6A-O1A-C7A-C8A	2.3(4)
N1A-C2A-C3A-C4A	58.2(3)	C6A-O1A-C7A-C12A	-175.9(2)
C1A-N1A-C2A-C3A	-58.1(3)	C5B-C4B-C14B-C15B	-68.1(3)
C1A-C5A-C6A-O1A	-57.5(3)	C5B-C4B-C14B-C19B	115.6(3)
C2A-N1A-C1A-C5A	57.8(3)	C6B-O1B-C7B-C8B	-173.3(2)
C2A-C3A-C4A-C5A	-58.6(3)	C6B-O1B-C7B-C12B	5.4(4)
C2A-C3A-C4A-C14A	176.9(2)	C7B-O1B-C6B-C5B	167.7(2)
C3A-C4A-C5A-C1A	57.5(3)	C7B-C8B-C9B-C10B	-0.4(4)
C3A-C4A-C5A-C6A	179.5(2)	C8B-C7B-C12B-C11B	2.0(4)
C3A-C4A-C14A-C15A	69.4(3)	C8B-C9B-C10B-O2B	179.6(3)
C3A-C4A-C14A-C19A	-114.6(3)	C8B-C9B-C10B-C11B	0.1(4)
C4A-C5A-C6A-O1A	179.9(2)	C9B-C10B-C11B-O3B	179.6(3)
C4A-C14A-C15A-C16A	175.7(3)	C9B-C10B-C11B-C12B	1.3(5)
C4A-C14A-C19A-C18A	-175.6(3)	C10B-O2B-C13B-O3B	20.5(3)
C5A-C4A-C14A-C15A	-53.5(3)	C10B-C11B-C12B-C7B	-2.3(4)
C5A-C4A-C14A-C19A	122.5(3)	C11B-O3B-C13B-O2B	-20.5(3)
C7A-O1A-C6A-C5A	177.0(2)	C12B-C7B-C8B-C9B	-0.7(4)
C7A-C8A-C9A-C10A	0.0(5)	C13B-O2B-C10B-C9B	167.7(3)
C8A-C7A-C12A-C11A	-1.8(4)	C13B-O2B-C10B-C11B	-12.8(3)
C8A-C9A-C10A-O3A	179.6(3)	C13B-O3B-C11B-C10B	12.6(3)
C8A-C9A-C10A-C11A	-0.8(5)	C13B-O3B-C11B-C12B	-169.2(3)
C9A-C10A-C11A-O2A	179.9(3)	C14B-C4B-C5B-C1B	176.3(2)
C9A-C10A-C11A-C12A	0.2(5)	C14B-C4B-C5B-C6B	-64.2(3)
C10A-O3A-C13A-O2A	-9.8(3)	C14B-C15B-C16B-C17B	-1.1(4)
C10A-C11A-C12A-C7A	1.1(4)	C15B-C14B-C19B-C18B	-1.1(4)
C11A-O2A-C13A-O3A	9.6(3)	C15B-C16B-C17B-C18B	-0.7(5)
C12A-C7A-C8A-C9A	1.3(4)	C15B-C16B-C17B-F1B	179.9(3)
C13A-O2A-C11A-C10A	-5.6(3)	C16B-C17B-C18B-C19B	1.6(5)
C13A-O2A-C11A-C12A	174.0(3)	C17B-C18B-C19B-C14B	-0.6(4)
C13A-O3A-C10A-C9A	-174.1(3)	C19B-C14B-C15B-C16B	1.9(4)
C13A-O3A-C10A-C11A	6.3(3)	F1B-C17B-C18B-C19B	-179.1(3)

Table S4. pH values measured in different dissolution media before and after solubility studies.

Dissolution media	pH 2.0	pH 6.8	H ₂ O
pH (PRX-OXA solution)	2.08	6.71	3.40
pH (PRX-MAL solution)	2.10	6.70	4.0
pH (PRX-FUM solution)	2.14	6.80	3.1
pH (PRX-TART solution)	2.11	6.76	3.20

Table S5. pKa values and calculated ΔpK_a between PRX and acid coformers.

	pK_a	$pK_{a2} - pK_{a1}$	ΔpK_a
PRX	9.60	-	-
Oxalic acid	1.25; 4.25	3.00	8.35; 5.35
Maleic acid	1.94; 6.22	4.28	7.66; 3.38
Fumaric acid	3.03; 4.44	1.41	6.57; 5.16
L-Tartaric acid	2.96; 4.34	1.38	6.64; 5.26

Table S6. Principal FT-IR bands (cm⁻¹) for PRX and PRX salts.

PRX HCl	PRX-OXA	PRX-MAL	PRX-FUM	PRX-TART	Assignment
3397, 3395	-	-	3180	3215	v(NH)
2993	-	-	2980	2982	v(CH)
-	-	1650	1704	1717	v(COOH)
-	1600	1558	1551	1558	v _{as} (COO ⁻)
-	1470	1469	1468	1466	v _s (COO ⁻)
1182	1184	1186	1181	1185	v(C-F)

v = stretching, as = antisymmetric, s = symmetric.

Table S7. Solubility values (mg. mL⁻¹) obtained for the five compounds.

Compound	Aqueous medium	pH 2.0	pH 6.8
PRX-OXA	4,598 ± 0,071	19,817 ± 0,043	0,914 ± 0.055
PRX-MAL	1,857 ± 0,093	0,941 ± 0,013	0,235 ± 0.018
PRX-FUM	0,174 ± 0,035	0,521 ± 0,064	0,197 ± 0.026
PRX-TART	0,468 ± 0,028	0,783 ± 0,024	0,366 ± 0.032

Fig. S1. Overlapping the independent molecule conformations of PRX-OXA (blue), PRX-MAL (green), PRX-FUM (red) and PRX-TART (yellow) salts, obtained from SCXRD analysis.

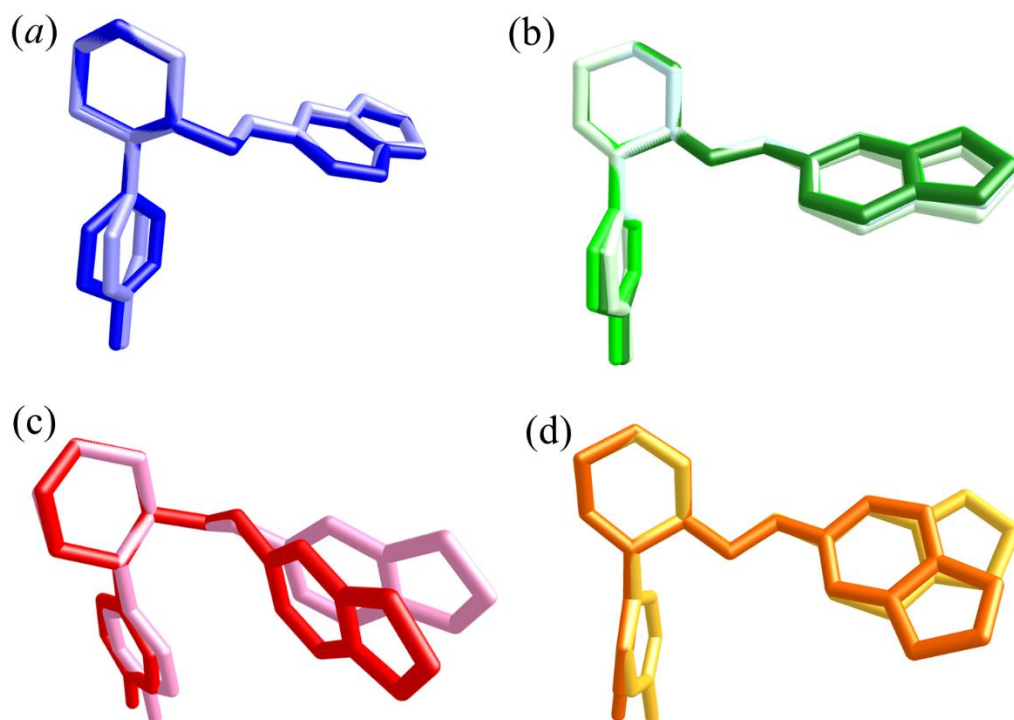


Fig. S2. PXRD data of the undissolved solid from the equilibrium solubility studies of the PRX salts in aqueous medium. In all cases the experimental PXRD patterns are in good agreement with the simulated ones obtained from the SCXRD data. Similar results were also founded for the solid residues of the PRX salts from the equilibrium solubility studies in buffered media (pH 2.0 and pH 6.8).

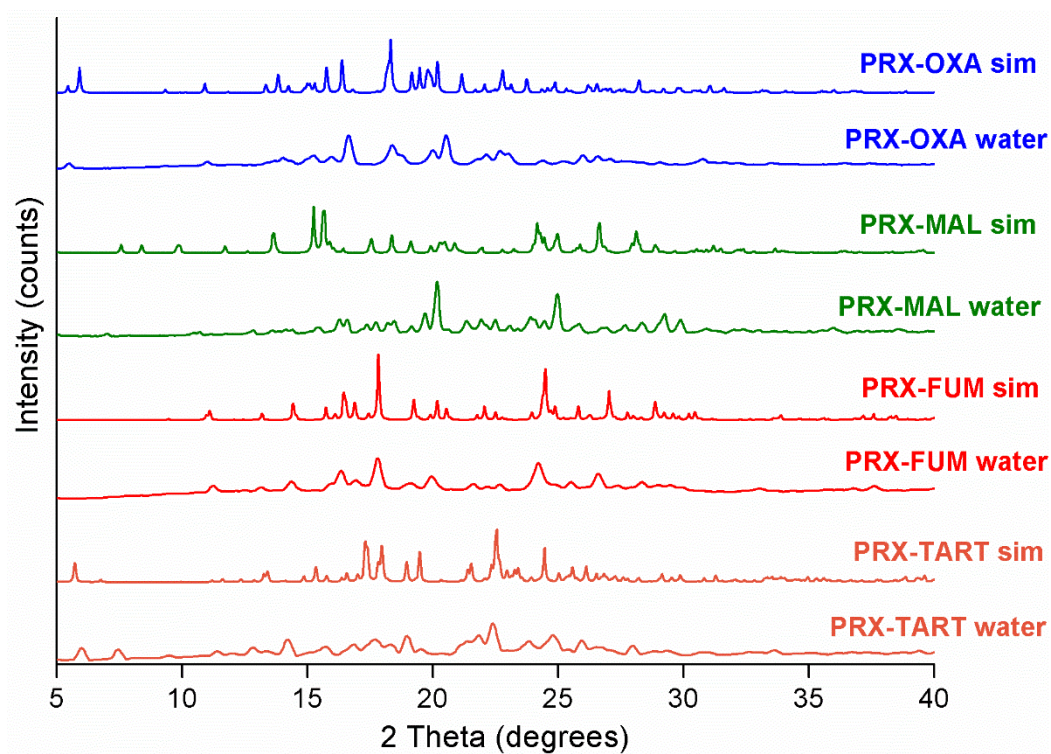


Fig. S3. Indexing by Le Bail of PRX-MAL salt.

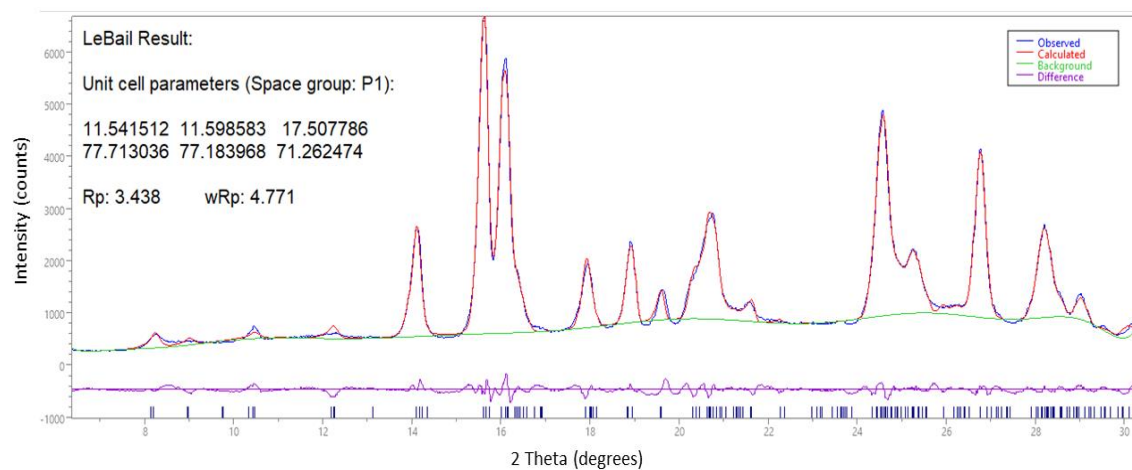


Fig. S4. Indexing by Le Bail of PRX-FUM salt.

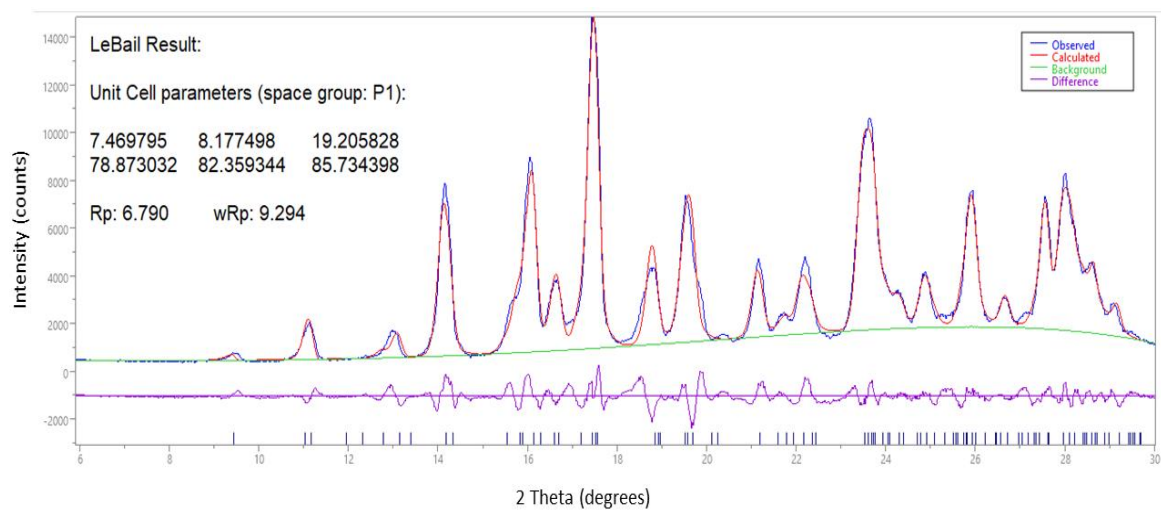


Fig. S5. Indexing by Le Bail of PRX-TART salt.

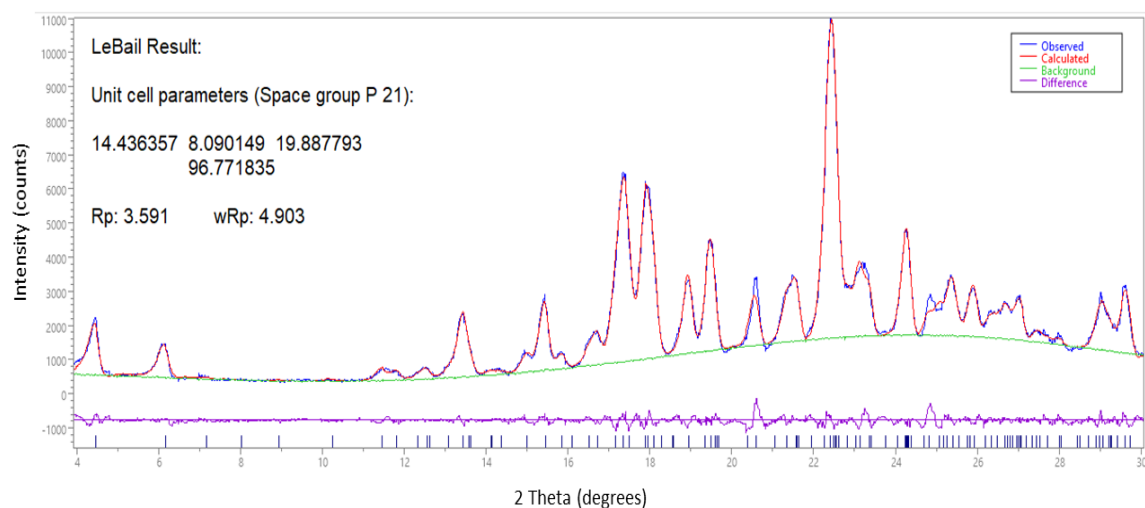


Fig. S6. Comparison between the PRX-OXA and sodium oxalate PXRD patterns showing that the peaks at 17.1° and 25.8° in 2θ (represented by the blue arrows) correspond to the sodium oxalate crystalline phase.

