Hydrogen bonding in crystals of the pyrrol-2-yl chloromethyl ketone derivatives and the methyl pyrrole-2-carboxylate

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Supplementary materials

Table S1. Selected geometrical parameters [Å, °] between atoms in non-hydrogen skeleton of molecules I-III.

	I	II	III
N1-C1	1.480(2)		
N1-C5	1.362(2)	1.359(3)	1.355(2)
N1-C2	1.393(2)	1.374(3)	1.371(2)
C2-C3	1.413(2)	1.393(3)	1.382(2)
C3-C4	1.408(2)	1.403(3)	1.403(2)
C4-C5	1.401(3)	1.381(3)	1.381(2)
C2-C6	1.451(2)	1.447(3)	1.454(2)
C6-O6	1.230(2)	1.227(3)	1.220(2)
C6-C7/O7	1.550(2)	1.518(3)	1.340(1)
C7-Cl8	1.772(2)	1.774(2)	-
C7-Cl9	1.796(2)	-	-
O7-C8	-	-	1.447(2)
C5-N1-C2	108.7(1)	109.2(2)	109.3(1)
N1-C2-C3	107.7(1)	107.5(2)	107.9(1)
N1-C2-C6	123.5(2)	120.8(2)	120.5(1)
C3-C2-C6	128.8(2)	131.7(2)	131.7(1)
C4-C3-C2	107.3(2)	107.5(2)	107.2(1)
C5-C4-C3	107.0(2)	107.2(2)	107.4(1)
N1-C5-C4	109.3(2)	108.7(2)	108.3(1)
O6-C6-C2	125.0(2)	122.3(2)	124.3(1)
O6-C6-C7/O7	120.3(2)	122.2(2)	124.1(1)
C2-C6-C7/O7	114.6(1)	115.5(2)	111.6(1)
C6-C7-Cl8	111.7(1)	112.0(2)	-
C6-C7-Cl9	107.7(1)	-	-
Cl8-C7-Cl9	109.5(1)	-	-
C6-O7-C8	-	-	116.4(1)

Table S2. Fingerprint plots of compound I-III showing the most important interactions occurring in crystals of I, II, and III taken from the Hirshfeld surface.

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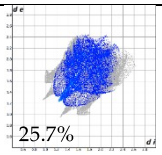
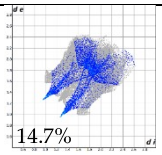
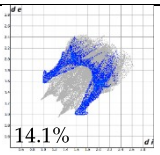
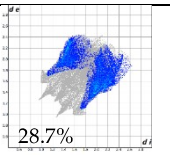
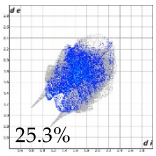
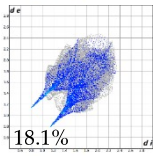
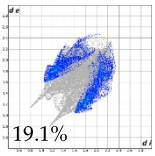
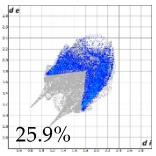
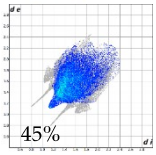
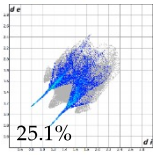
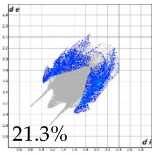
I	 25.7%	 14.7%	 14.1%	 28.7%
II	 25.3%	 18.1%	 19.1%	 25.9%
III	 45%	 25.1%	 21.3%	

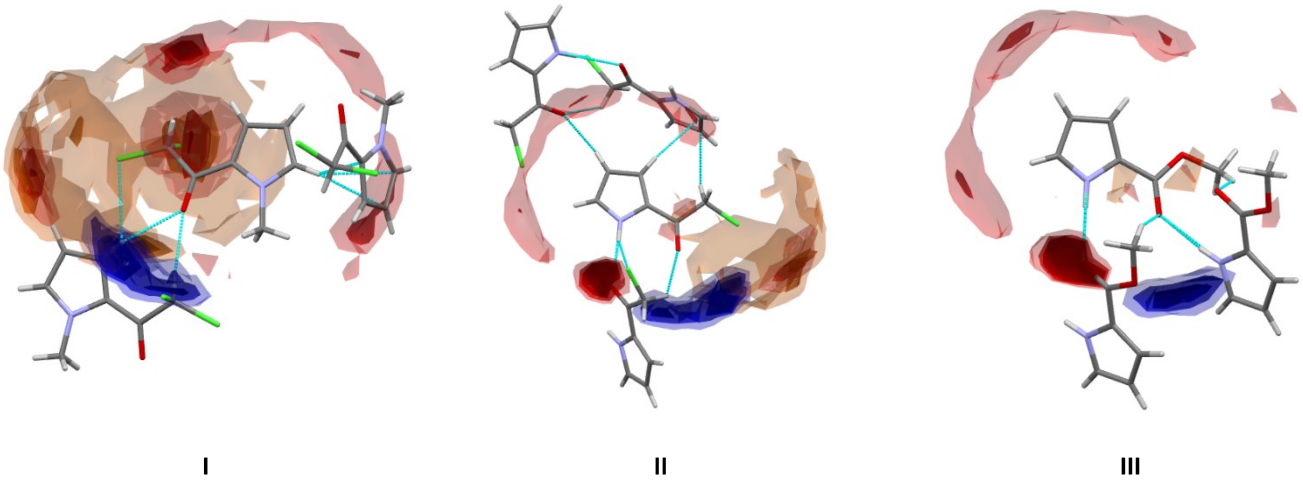
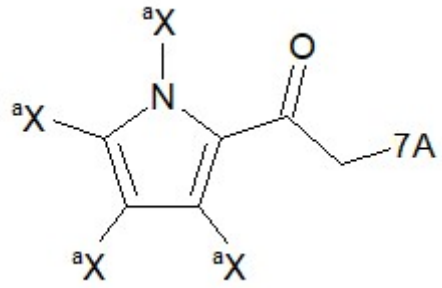
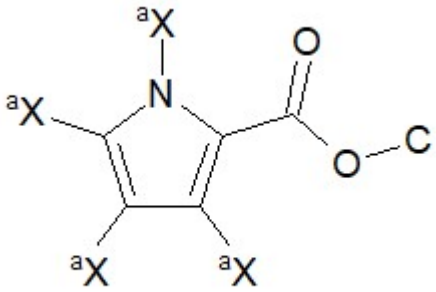


Figure S1. Full Interaction Maps for investigated structures I-III with interacting molecules.



Scheme S1. Scheme of searching fragment of pyrrol-2-yl ketone



Scheme S2. Scheme of the first searching fragment of molecule of ester, which give 100 hits. It was modifying by changing any-atoms X by H-atoms and C-atom from ester group becomes acyclic.

Table S3. Values of bond lengths [Å] in the structures of the pyrrol-2-yl ketones derivatives found in CSD

Refcode	N(1) – C(1)	N(1) – C(2)	C(2) – C(3)	C(3) – C(4)	C(4) – C(5)	C(5) – N(1)	C(2) – C(6)	C(6) – O(6)	C(6) – C(7	C(7) – Hal
AZEHAO	0.863	1.376	1.393	1.404	1.387	1.351	1.438	1.219	1.547	1.322
BETNOF	1.460	1.391	1.390	1.385	1.372	1.346	1.432	1.215	1.566	1.768
BETPAT	1.460	1.393	1.388	1.389	1.370	1.346	1.441	1.215	1.561	1.782
BETPEX	1.458	1.394	1.392	1.388	1.370	1.344	1.427	1.225	1.563	1.786
BETPIB	1.458	1.391	1.389	1.385	1.365	1.346	1.434	1.218	1.557	1.777
BETPOH	-	1.383	1.393	1.396	1.382	1.345	1.442	1.219	1.562	1.755
GOFQEZ	-	1.389	1.421	1.400	1.404	1.340	1.421	1.234	1.544	1.323
HUZBIN	1.465	1.393	1.371	1.394	1.372	1.332	1.457	1.199	1.557	1.768
JODHER	-	1.376	1.398	1.393	1.386	1.342	1.439	1.222	1.555	1.763
UCEKET	1.469	1.404	1.386	1.381	1.375	1.342	1.447	1.209	1.565	1.749
UHIQEJ	1.469	1.386	1.394	1.393	1.385	1.345	1.436	1.220	1.539	1.758
WEYYUV	1.476	1.391	1.386	1.377	1.352	1.340	1.444	1.209	1.563	1.767
WEYYUV01	1.472	1.400	1.405	1.400	1.385	1.356	1.445	1.223	1.581	1.788

Table S4. Values of bond angles [°] in the structures of the pyrrol-2-yl ketones derivatives found in CSD

Refcode	C(5) – N(1) – C(2)	C(2) – C(6) – O(6)	O(6) – C(6) – C(7)	C(6) – C(7) – Hal	N(1) – C(2) – C(3)	C(2) – C(3) – C(4)	C(3) – C(4) – C(5)	C(4) – C(5) – N(1)	N(1) – C(2) – C(6)	C(3) – C(2) – C(6)	C(2) – C(6) – C(7)
AZEHAO	108.45	124.67	117.75	110.87	108.09	107.26	106.54	109.65	119.68	132.21	117.55
BETNOF	108.11	125.59	118.92	110.15	106.99	108.01	107.00	109.88	122.56	130.45	115.48
BETPAT	108.02	123.50	116.15	109.22	107.18	107.79	107.12	109.89	121.09	131.71	120.34
BETPEX	108.37	124.41	116.04	107.93	106.54	108.22	106.85	110.01	122.23	131.18	119.54
BETPIB	107.90	123.66	116.01	112.07	106.94	108.02	106.97	110.16	121.51	131.38	120.21
BETPOH	109.56	122.39	118.35	110.76	107.23	106.99	107.92	108.29	118.57	134.15	119.23
GOFQEZ	110.38	124.24	115.46	110.85	106.70	106.74	107.93	108.23	115.82	137.47	120.27
HUZBIN	109.08	124.07	118.02	111.89	107.86	106.24	108.80	108.03	120.81	131.27	117.90
JODHER	110.05	123.14	117.83	110.62	107.52	106.19	108.67	107.57	117.73	134.73	119.02
UCEKET	107.42	125.29	117.51	110.45	107.74	107.17	107.94	109.73	120.97	131.28	117.20
UHIQEJ	108.84	125.25	120.09	111.68	107.20	107.64	107.04	109.25	123.59	129.17	114.60
WEYYUV	108.05	124.76	117.14	110.36	106.93	107.26	108.14	109.62	121.20	131.72	118.09
WEYYUV01	108.45	124.92	117.13	109.40	107.08	107.62	107.23	109.62	120.80	131.93	117.93

Table S5. Values of bond lengths [Å] in the structures of the pyrrol-2-carboxylate derivatives found in CSD

Refcode	N(1) – C(2)	C(2) – C(3)	C(3) – C(4)	C(4) – C(5)	C(5) – N(1)	C(2) – C(6)	C(6) – O(6)	C(6) – O(7)	O(7) – C(8)
CUHKUM	1.366	1.357	1.391	1.355	1.338	1.442	1.206	1.333	1.443
CUHLAT	1.366	1.370	1.384	1.356	1.341	1.439	1.209	1.331	1.445
CUHLEX	1.372	1.366	1.399	1.361	1.347	1.440	1.215	1.340	1.447
DUCYOQ	1.362	1.382	1.403	1.377	1.356	1.448	1.220	1.342	1.439
EHAZIW	1.380	1.380	1.416	1.377	1.355	1.453	1.211	1.351	1.462
EJALEH	1.369	1.373	1.394	1.365	1.350	1.444	1.214	1.331	1.447
GAQDEJ	1.366	1.373	1.392	1.370	1.348	1.438	1.219	1.346	1.447
PESNEH	1.375	1.373	1.401	1.373	1.350	1.448	1.218	1.346	1.445
PESNIL	1.372	1.368	1.401	1.351	1.347	1.441	1.210	1.334	1.437
SAZLAH	1.371	1.373	1.385	1.365	1.345	1.440	1.208	1.346	1.442
YICNOO	1.367	1.366	1.392	1.357	1.352	1.440	1.209	1.345	1.446

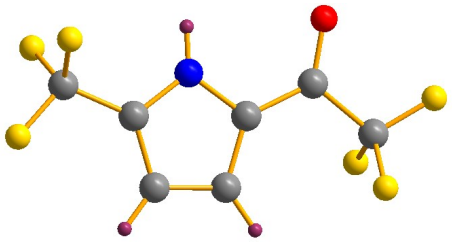
Table S6. Values of bond angles [°] in the structures of the pyrrol-2-carboxylate derivatives found in CSD

Refcode	C(5) – N(1) – C(2)	N(1) – C(2) – C(3)	C(2) – C(3) – C(4)	C(3) – C(4) – C(5)	C(4) – C(5) – N(1)	N(1) – C(2) – C(6)	C(3) – C(2) – C(6)	C(2) – C(6) – O(6)	O(6) – C(6)- O(7)	C(6) – O(7) – C(8)	C(2) – C(6) – O(7)
CUHKUM	109.69	107.13	107.52	107.68	107.98	120.91	131.85	124.62	123.42	117.15	111.95
CUHLAT	109.79	106.55	107.92	107.52	108.21	120.92	132.46	124.05	123.44	116.64	112.52
CUHLEX	108.97	107.60	107.44	107.28	108.71	120.07	132.29	124.99	122.39	115.98	112.61
DUCYOQ	109.8	107.7	107.2	107.4	108.0	120.9	131.4	124.1	123.9	116.6	123.9
EHAZIW	108.80	108.02	107.18	106.92	109.08	119.97	132.01	125.81	123.26	115.71	110.92
EJALEH	109.52	107.37	107.25	107.91	107.93	120.60	132.01	124.97	123.76	117.16	111.26
GAQDEJ	109.33	107.37	107.74	107.12	108.43	121.02	131.61	125.76	122.48	116.63	111.76
PESNEH	109.26	107.50	107.56	107.22	108.46	120.10	132.39	124.81	123.18	116.36	112.01
PESNIL	108.53	108.06	106.64	107.87	108.89	121.47	130.42	125.28	123.83	118.94	110.89
SAZLAH	109.05	107.05	108.00	107.16	108.73	123.66	129.26	124.73	122.99	118.39	112.28
YICNOO	108.64	107.25	108.31	106.57	109.23	123.21	129.34	125.92	122.23	117.05	111.84

Figure S2. Graphical representation of the structures of the pyrrol-2-yl ketones derivatives found in CSD

The colours describes: grey colour - C atom, blue colour - N atom, purple - H atom, red - O atom, green - Cl atom, yellow - F and olive - Br atoms

AZEHAO



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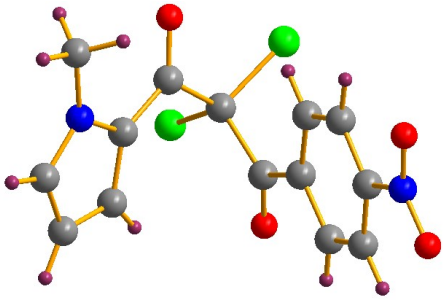
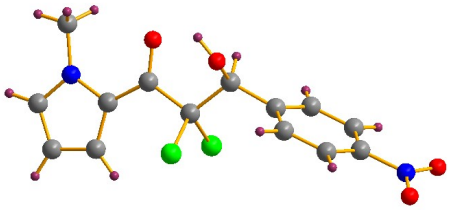
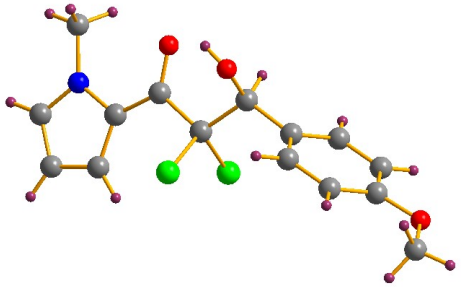


BETPAT



BETPEX



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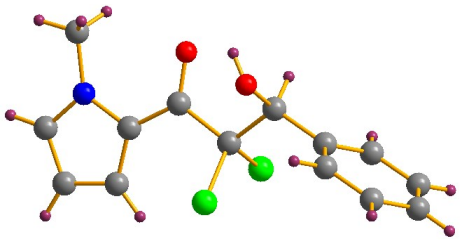
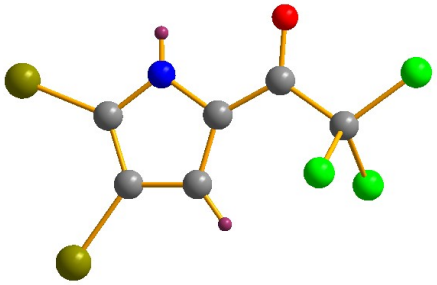


BETPOH



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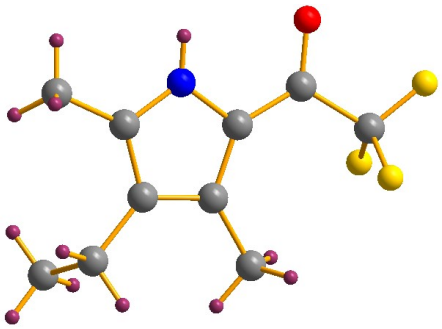
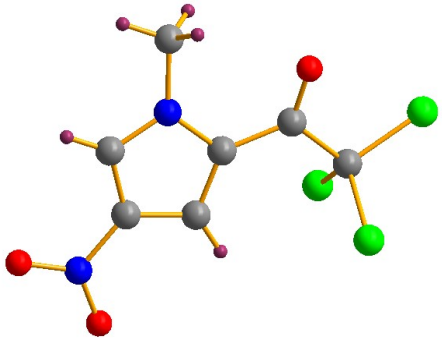
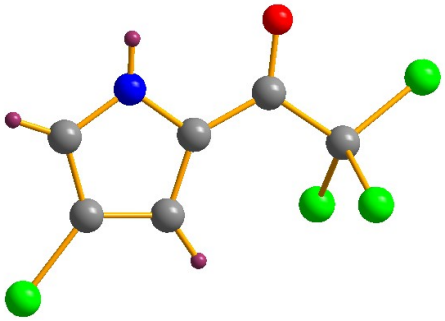


HUZBIN



JODHER



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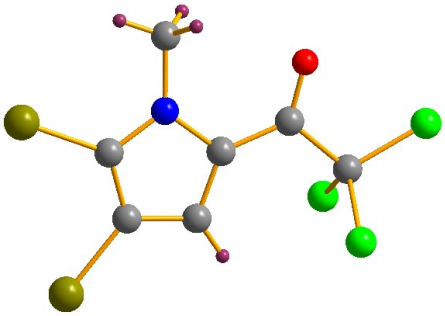

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WEYYUV

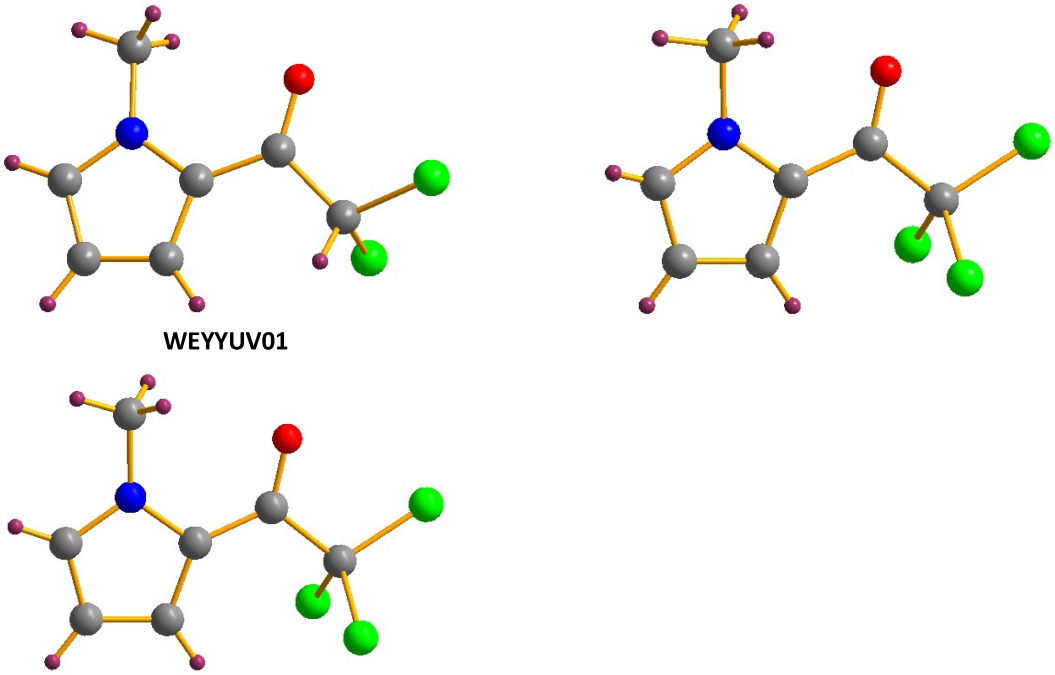
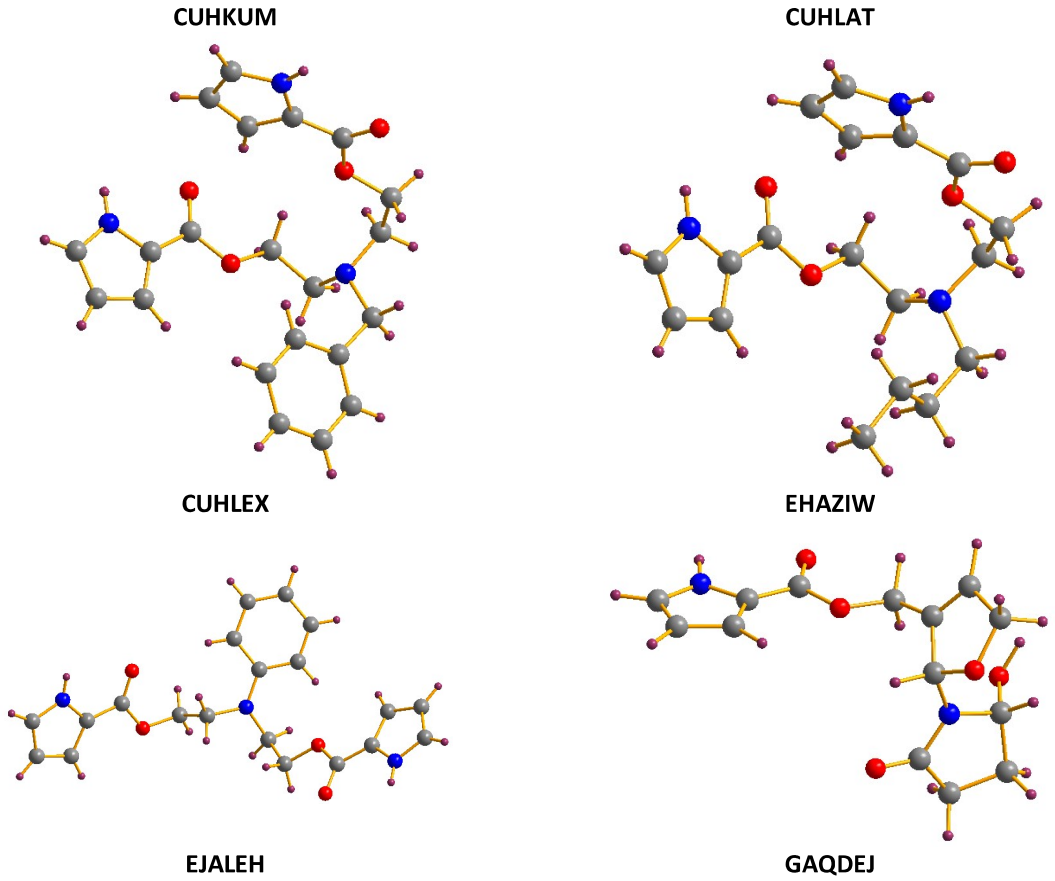
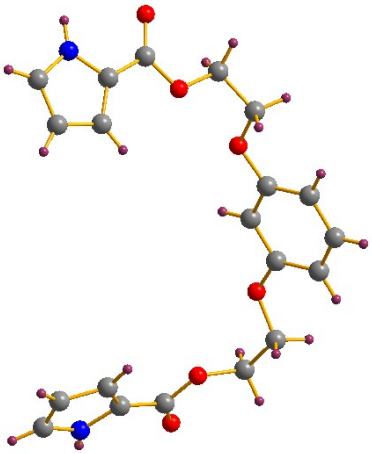


Figure S3. Graphical representation of the structures of the pyrrol-2-carboxylate derivatives found in CSD

The colours describes: grey colour - C atom, blue colour - N atom, purple - H atom, red - O atom, green - Cl atom.





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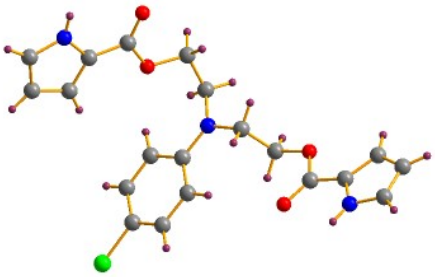

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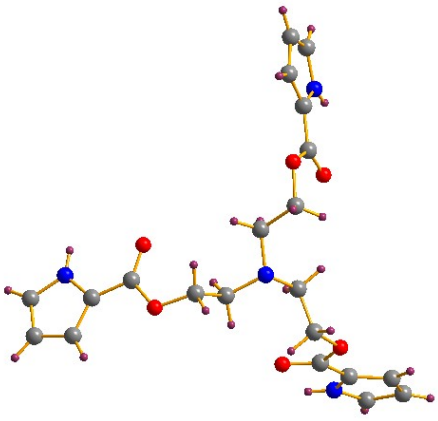
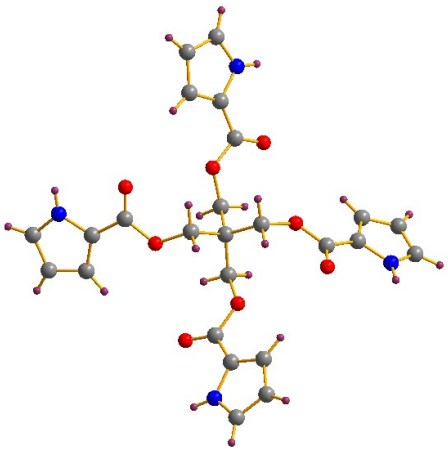


SAZLAH



YICNOO