Supplementary Materials

Table SM1 Most Relevant Bond Distances (Å) Valence Angles (^{o}) and Dihedral Angles (^{o}) for the most stable conformation for selected compounds **4k**, **4n** and **4o**, obtained by the different parametrizations.

Table SM2 Most Relevant Bond Distances (Å) Valence Angles (^{o}) and Dihedral Angles (^{o}) for the most stable conformation of compounds **4a-j, 4l, 4m, 4p-r** (AM1 calculations).

Figure SM1. Most stable conformations for compounds **4k, 4n** and **4o** calculated by different theoretical methods.

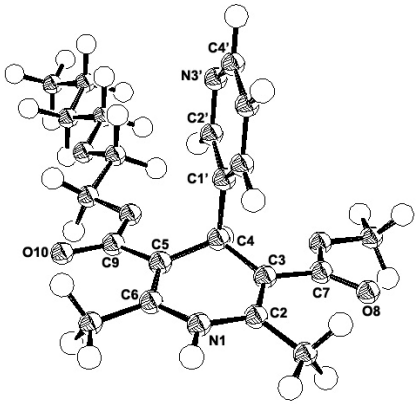
Figure SM2. Packing diagram projection of compound **4n**.

Table SM1 Most Relevant Bond Distances (Å) Valence Angles (^{o}) and Dihedral Angles (^{o}) for the most stable conformation for selected compounds **4k**, **4n** and **4o**, obtained by the different parametrizations

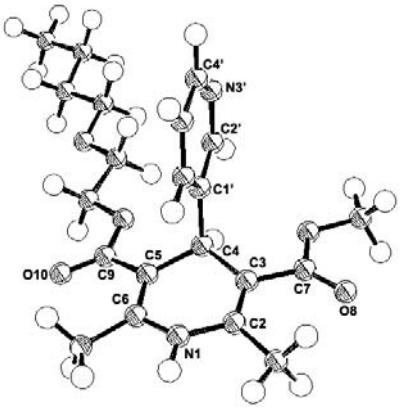
Compound	**4k** (AM1)	**4k** (HF/6-31G*)	**4k** (B3LYP/6-31G*)	**4n** (AM1)	**4n** (HF/6-31G*)	**4o** (AM1)	**4o** (HF/6-31G*)	**4o** (B3LYP/6-31G*)
Bond Distances								
N1-C2	1.39	1.39	1.39	1.394	1.380	1.39	1.38	1.38
C2-C3	1.37	1.34	1.36	1.372	1.341	1.37	1.34	1.36
C3-C4	1.50	1.51	1.53	1.500	1.525	1.50	1.52	1.53
C4-C5	1.50	1.52	1.53	1.502	1.525	1.50	1.52	1.53
C5-C6	1.37	1.34	1.36	1.372	1.341	1.37	1.34	1.36
C6-N1	1.39	1.38	1.39	1.394	1.380	1.39	1.38	1.38
C4-C1’	1.50	1..53	1.53	1.503	1.530	1.51	1.53	1.53
C7-O8	1.24	1.20	1.22	1.239	1.197	1.24	1.20	1.22
C9-O10	1.24	1.20	1.22	1.239	1.197	1.24	1.20	1.22
C2’-N3’ / C3’-N4’	1.34	1.32	1.34	1.345	1.321	1.35	1.32	1.34
N3’-C4’ / N4’-C5’	1.35	1.32	1.34	1.348	1.320	1.35	1.32	1.34
Bond Angles								
C6-N1-C2	120.5	123.4	123.9	120.1	123.4	120.5	123.3	123.9
C5-C9-O10	128.7	125.9	126.6	128.5	125.7	128.4	125.7	126.3
C3-C7-O8	128.6	126.0	126.7	128.4	125.7	128.5	125.7	126.3
C3-C4-C5	111.0	110.6	110.8	111.0	110.6	110.9	110.5	110.8
C2’-N3’-C4’ / C1’-N2’-C3’	117.4	117.8	117.2	117.4	117.8	117.0	116.9	116.4
Torsion Angles								
N1-C2-C3-C4	4.4	5.1	6.6	4.4	5.0	4.8	5.3	6.4
C2-C3-C4-C5	-20.9	-20.4	-22.3	-21.3	-20.6	-21.9	-21.6	-22.4
C3-C4-C5-C6	21.6	20.3	22.2	21.7	20.6	22.4	21.6	22.4
C4-C5-C6-N1	-5.1	-4.8	-6.3	-5.3	-5.0	-5.8	-5.3	-6.4
C5-C6 -N1-C2	-14.0	-13.8	-12.9	-14.2	-13.9	-14.0	-14.5	-13.0
C6-N1-C2-C3	14.4	13.6	12.7	14.7	13.9	14.5	14.5	13.0
$\Sigma\|\rho\|$	*80.4*	*78.0*	*83.0*	*81.6*	*79.0*	*83.4*	*82.8*	*83.6*
C3-C4-C1’-C2’	142.2	115.0	114.5	142.5	117.8	144.4	118.0	117.8
C2-C3-C4-C1’	102.3	104.7	102.8	101.9	104.3	101.0	103.0	102.3
C2-C3-C7-O8	-13.3	-4.5	-2.2	-13.3	-3.6	-12.3	-2.7	-2.0
C6-C5-C9-O10	8.6	1.9	1.1	9.7	3.6	10.7	2.7	2.0

Table SM2. Most Relevant Bond Distances (Å) Valence Angles (°) and Dihedral Angles (°) for the most stable conformation of compounds **4a-j, 4l, 4m, 4p-r** (AM1 calculations).

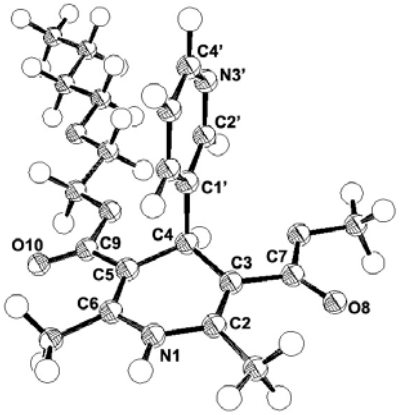
Compound	4a	4b	4c	4d	4e	4f	4g	4h	4i	4j	4l	4m	4p	4q	4r
Bond Distances															
N1-C2	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39
C2-C3	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37
C3-C4	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C4-C5	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50	1.50
C5-C6	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37	1.37
C6-N1	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39
C4-C1’	1.52	1.52	1.52	1.52	1.52	1.52	1.50	1.50	1.50	1.50	1.50	1.50	1.51	1.51	1.51
C7-O8	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24
C9-O10	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24	1.24
C1’-N2’/ C2’-N3’ / C3’-N4’	1.36	1.36	1.36	1.36	1.36	1.36	1.34	1.34	1.34	1.34	1.36	1.34	1.35	1.40	1.40
N2’-C3’/ N3’-C4’ / N4’-C5’	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.40	1.40
Bond Angles															
C6-N1-C2	121.2	121.2	121.2	121.2	121.2	121.2	120.5	120.5	120.6	120.5	120.6	120.5	120.6	120.5	120.6
C5-C9-O10	128.8	128.7	129.0	128.8	128.8	129.0	128.6	128.7	128.6	128.6	128.8	128.5	128.8	128.5	128.5
C3-C7-C8	128.8	128.8	128.8	128.6	128.6	128.7	128.5	128.4	128.8	128.7	128.5	128.4	128.7	128.5	128.9
C3-C4-C5	111.1	111.1	111.1	111.1	111.1	111.1	111.0	111.0	111.0	111.0	111.0	111.0	110.9	111.1	111.1
C1’-N2’-C3’	117.5	117.5	117.5	117.5	117.5	117.5	117.9	117.4	117.4	117.4	117.4	117.4	116.7	120.7	120.7
Torsion Angles															
N1-C2-C3-C4	8.8	8.8	9.6	8.8	9.3	9.5	5.3	4.4	4.6	4.4	4.5	4.4	4.5	5.5	5.9
C2-C3-C4-C5	-24.6	-24.7	-25.4	-24.8	-25.0	-25.2	-21.7	-21.2	-21.0	-20.9	-21.1	-21.3	-21.9	-21.8	-21.3
C3-C4-C5-C6	24.9	24.9	25.1	25.0	24.7	24.8	21.2	21.6	21.5	21.3	21.6	21.7	22.5	21.2	22.0
C4-C5-C6-N1	-9.3	-9.3	-9.0	-9.3	-8.8	-8.7	-4.5	-5.4	-5.5	-5.1	-5.5	-5.3	-6.1	-4.4	-4.5
C5-C6 -N1-C2	-9.4	-9.4	-9.8	-9.5	-9.7	-9.9	-14.5	-14.1	-13.6	-14.0	-13.7	-14.2	-13.6	-14.6	-13.6
C6-N1-C2-C3	9.6	9.6	9.4	9.7	9.5	9.5	14.1	14.5	14.1	14.4	14.2	14.7	14.2	14.0	14.3
$\Sigma\|\rho\|$	*86.6*	*86.7*	*88.3*	*87.1*	*87.0*	*87.6*	*82.3*	*81.2*	*80.3*	*80.1*	*80.6*	*81.6*	*82.8*	*76.0*	*75.7*
C3-C4-C1’-N2’/ C3-C4-C1’-C2’	-77.7	-77.7	-77.0	-78.1	-78.1	-80.4	142.2	141.9	142.1	142.2	142.6	142.4	144.7	93.3	94.0
C2-C3-C4-C1’	97.6	97.6	95.8	96.3	97.5	96.2	102.0	101.9	102.2	102.3	102.1	101.9	101.0	101.8	101.6
C2-C3-C7-O8	-6.7	-6.8	-6.1	-6.7	-6.8	-5.7	-13.1	-13.3	-11.5	-13.3	-11.5	-13.3	-10.8	-10.3	-11.3
C6-C5-C9-O10	6.4	6.5	6.7	6.8	6.7	7.1	9.7	9.87	10.4	8.6	10.2	9.7	10.9	11.1	10.6



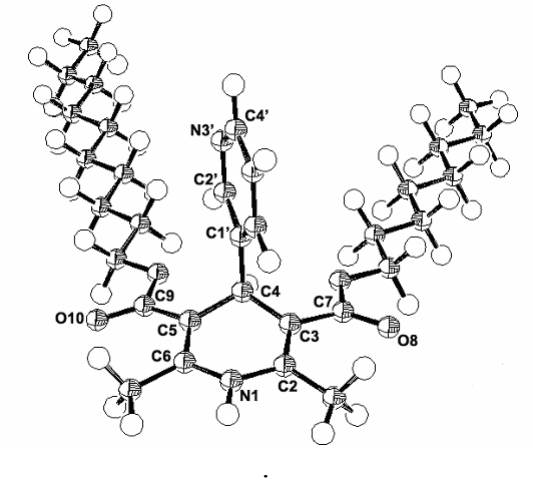
4k (AM1)



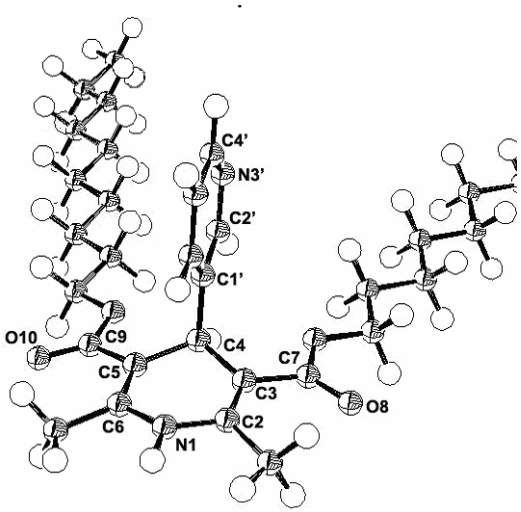
4k (HF/6-31G*)



4k (B3LYP/6-31G*)



4n (AM1)



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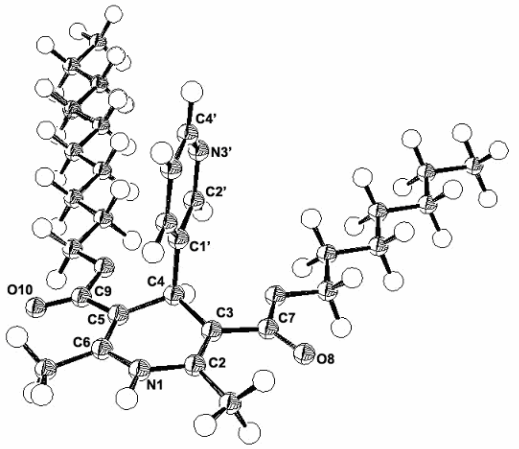
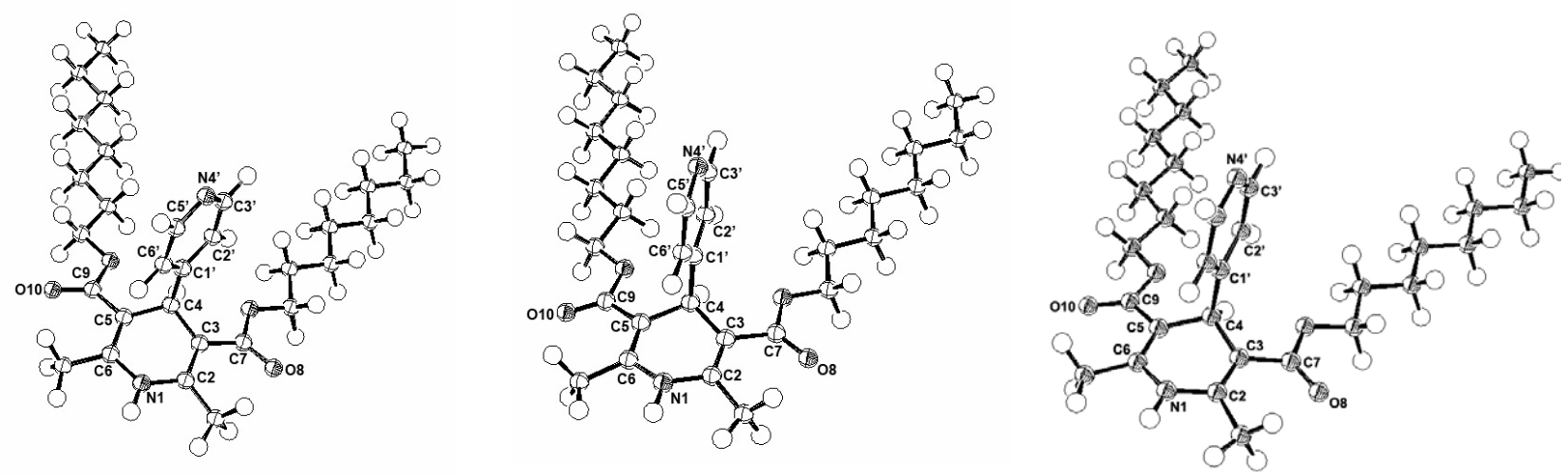


4n (B3LYP/6-31G*)



4o (AM1) **4o (HF/6-31G*)** **4o (B3LYP/6-31G*)**

Figure SM1. Most stable conformations for compounds **4k, 4n** and **4o** calculated by different theoretical methods.

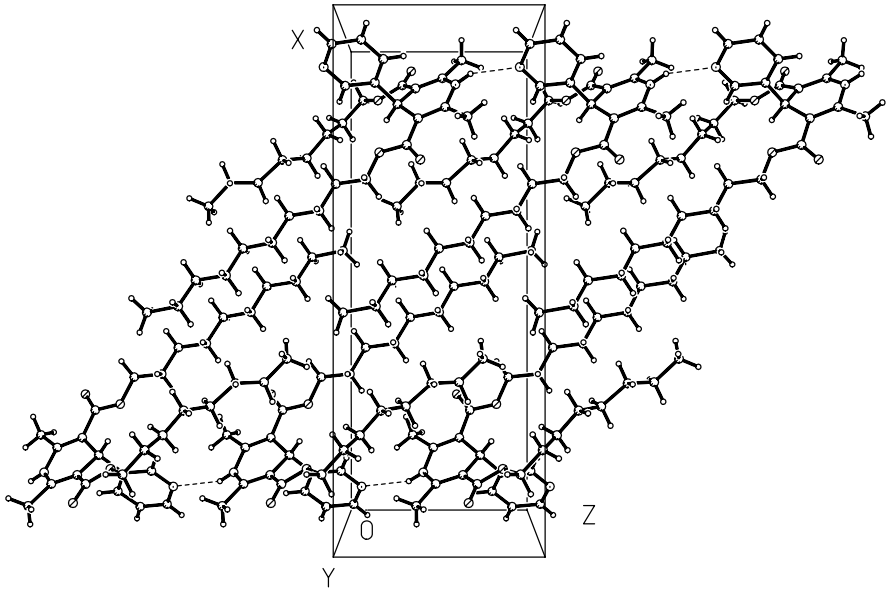


Figure SM2. Packing diagram projection of compound **4n**. The hydrogen bond present in the crystal structure is denoted by dashed lines.