ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

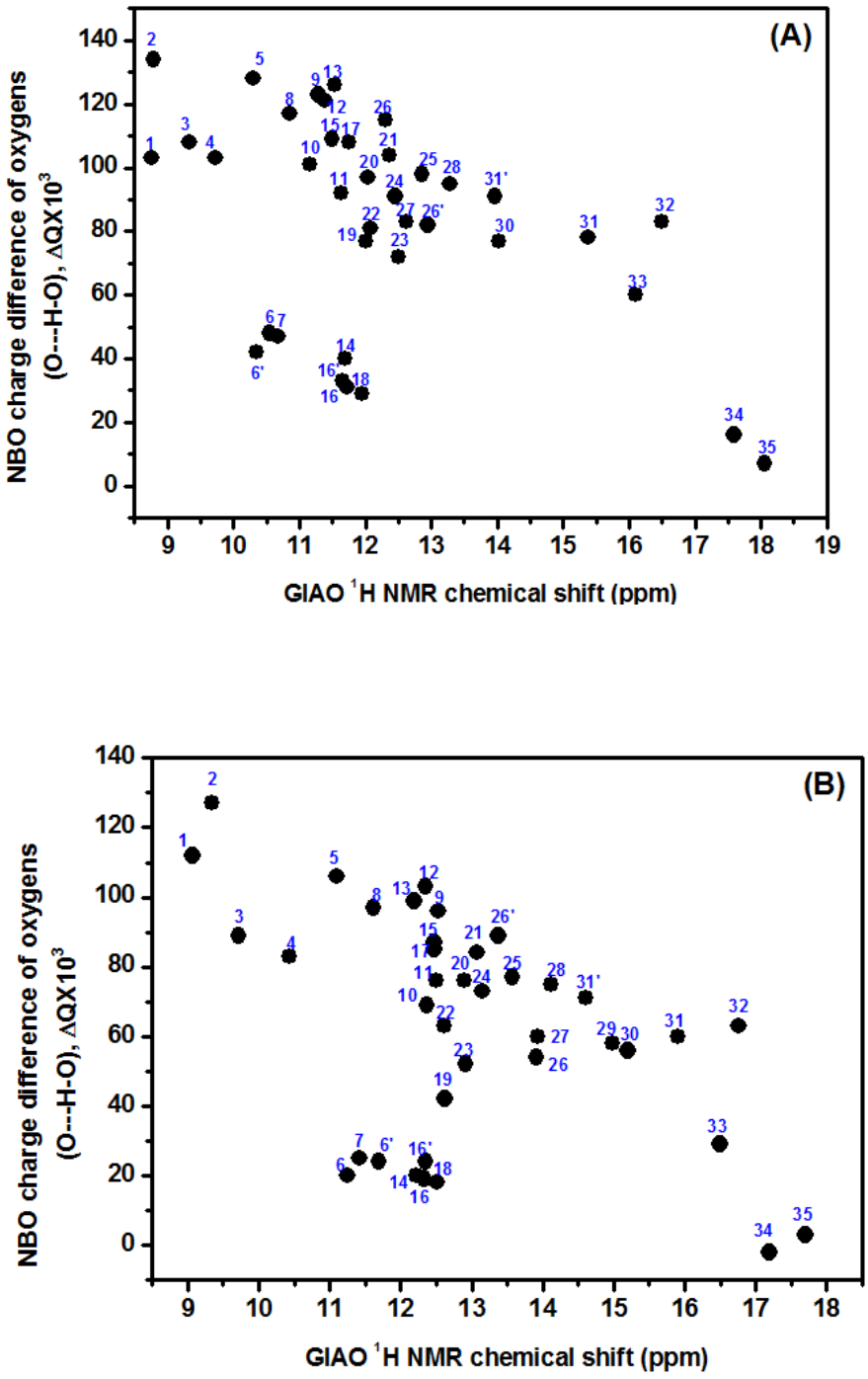


Fig. S1 Plot of the difference in the NBO charges, ΔQ × 10^3, of the two oxygens participating in the intramolecular O–H---O hydrogen bond of the compounds **1-35** of Scheme 1 *vs* GIAO calculated proton chemical shifts. The minimization of the structures and the NBO analysis were performed at the M06-2X/6-31+G(d)(A) and the B3LYP/6-31+G(d)(B) level of theory.

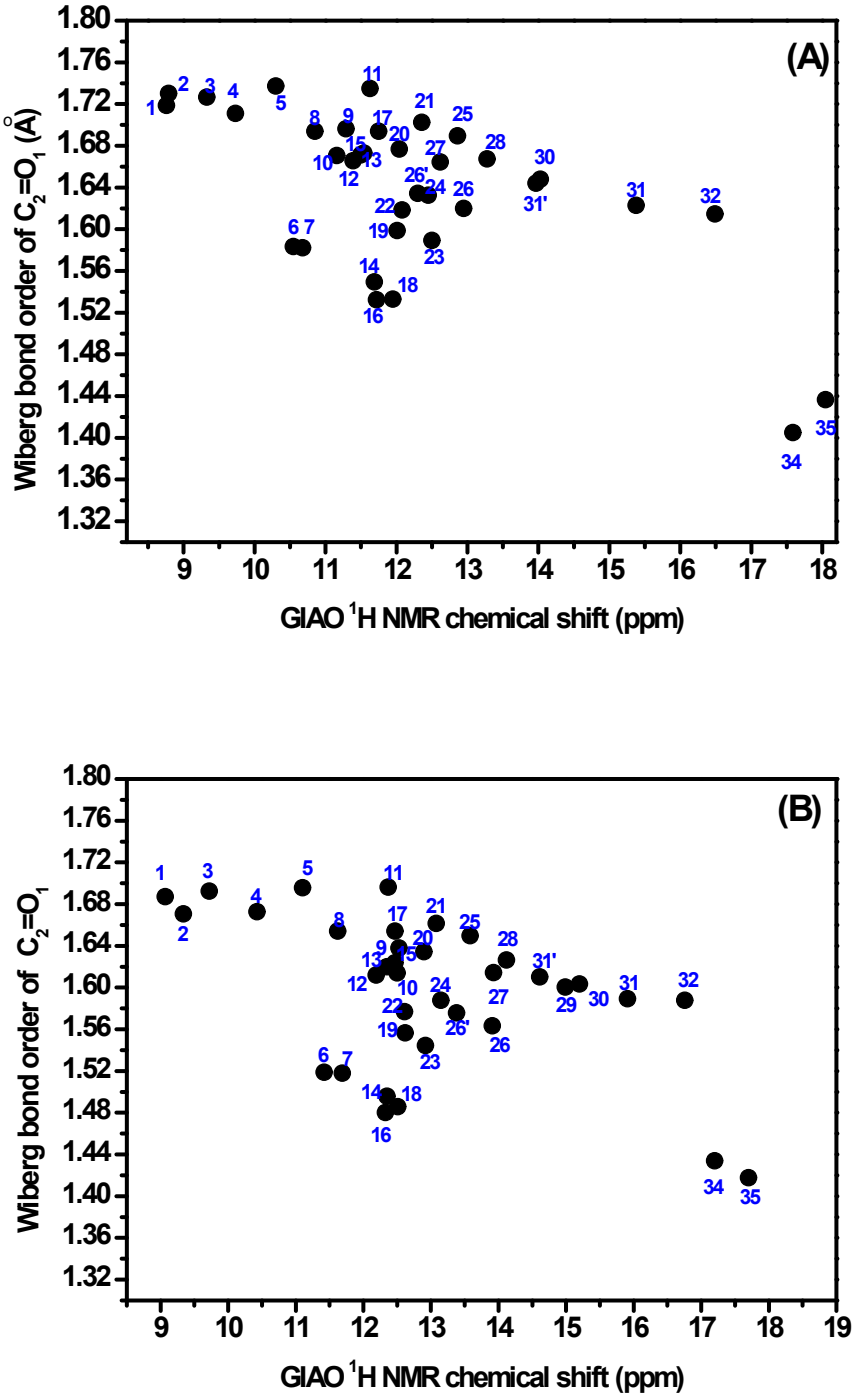


Fig. S2 Plot of calculated Wiberg bond order (Table 3) of the C_2=O_1 group of the intramolecular CO---H(O) hydrogen bond of the compounds **1-35** of Scheme 1 *vs* GIAO calculated proton chemical shifts. The minimization of the structures and the NBO analysis were performed at the M06-2X/6-31+G(d)(A) and the B3LYP/6-31+G(d)(B) level of theory.

Table S1 Structural data and calculated (δ, ppm) ^{1}H chemical shifts of selected compounds of Scheme 1. Minimization of the structures was performed at the B3LYP/6-311+G(2d,p) (black), M06-2X/6-31G+d (red) and MP2/6-31G+d (blue) level of theory

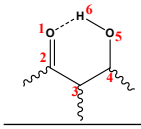
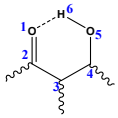
Compound 	O_1---O_5 (Å)	O_1---H_6 (Å)	C_2=O_1 (Å)	C_2-C_3 (Å)	C_3-C_4 (Å)	C_4-O_5 (Å)	O_5-H_6 (Å)	angle $O_1H_6O_5$ (°)	GIAO NMR (ppm)
3	2.82613	1.96789	1.23351	1.45430	1.40646	1.34954	0.98563	144.12	9.27
	2.84446	2.00225	1.22248	1.45986	1.39989	1.34343	0.97982	142.72	9.33
	2.86025	2.00125	1.24092	1.45986	1.40140	1.36052	0.98784	144.04	9.70.
									Exp 9.04
5	2.65650	1.78342	1.23460	1.45672	1.41919	1.34846	0.98868	145.29	11.1
A (56.5%)	2.67668	1.82655	1.22251	1.46320	1.40966	1.34489	0.98058	143.16	10.08
B (43.5 %)	2.69307	1.82467	1.24271	1.46120	1.41465	1.35972	0.98891	144.70	10.70
	2.65666	1.78486	1.23507	1.45441	1.41678	1.34749	0.98866	145.11	11.15
	2.67522	1.82531	1.22298	1.46074	1.40650	1.34362	0.98079	143.10	10.47
	2.69122	1.82293	1.24315	1.45899	1.41231	1.35864	0.98913	144.65	10.80
									Exp 0.60
8	2.65258	1.77701	1.23529	1.45417	1.42166	1.34430	0.98985	145.48	11.62
	2.67242	1.81916	1.22353	1.46039	1.41254	1.33983	0.98173	143.43	10.85
	2.69816	1.82467	1.24295	1.46021	1.41457	1.35654	0.98986	145.04	11.14
									Exp11.01
17	2.58490	1. 69790	1.24274	1.47236	1.42481	1.34321	0.99348	146.46	12.47
	2.60157	1.73631	1.23027	1.47738	1.41542	1.33896	0.98459	144.51	11.75
	2.61818	1.73758	1.24927	1.47659	1.41836	1.35576	0.99256	145.73	11.98
									Exp 12.26

Table S2 Wiberg charges within the intramolecular hydrogen bonded moiety of the compounds **1-35** of Scheme 1. Minimization of the structures and the NBO analysis were performed at the M06-2X/6-31G+Gd (blue) and 3LYP/6-31G+Gd (black) level of theory

Compound 	O1	C2	C3	C4	O5	H6
1	-0.578	+ 0.546	-0.207	+0.407	-0.690	+0.533
	-0.572	+0.571	-0.227	+0.413	-0.706	+0.541
2	-0.588	+ 0.550	-0.207	+0.405	-0.691	+0.533
	-0.579	+0.567	-0.212	+0.390	-0.7006	+0.541
3	-0.604	+ 0.562	-0.241	+0.383	-0.693	+0.533
	-0.601	-0.584	-0.255	+0.392	-0.709	+0.543
4	-0.612	+ 0.581	-0.234	+0.425	-0.695	+0.537
	-0.608	+0.604	-0.255	+0.433	-0.711	+0.547
	-0.614	+ 0.578	-0.240	+0.424	-0.696	+0.537
	-0.610	+-0.608	-0.250	+0.434	-0.712	+0.547
5	-0.593	+0.390	-0.239	+0.361	-0.699	+0.533
	-0.595	+0.387	-0.241	+0.366	-0.697	+0.533
	-0.590	+0.410	-0.251	+0.362	-0.718	+0.544
	-0.592	+0.408	-0.254	+0.368	-0.716	+0.545
6	-0.672	+0.554	-0.224	+0.381	-0.696	+0.536
	-0.672	+0.554	-0.225	+0.392	-0.692	+0.538
	-0.667	+0587	-0.242	+0.387	-0.714	+0.547
	-0.667	+0587	-0.242	+0.400	-0.710	+0.549
7	-0.673	+ 0.556	-0.224	+0.380	-0.698	+0.536
	-0.668	+0.588	-0.241	+0.387	-0.716	+0.547
8	-0.596	+ 0.389	-0.259	+0.386	-0.693	+0.534
	-0.595	+0.409	-0.274	+0.392	-0.712	+0.546
9	-0582	+ 0.461	-0.238	+0.414	-0.678	+0.536
	-0.576	+0.489	-0.260	+0.423	-0.699	+0.548
10	-0.617	+ 0.555	-0.227	+0.394	-0.693	+0.537
	-0.611	-0.582	-0.241	+0.399	-0.712	+0.548
11	-0.588	+ 0.389	-0.255	+0.434	-0.657	+0.534
	-0.587	-0.409	-0.269	+0.438	-0.679	+0.549
12	-0.591	+ 0.501	-0.216	+0.394	-0.690	+0.536
	-0.589	+0.530	-0.233	+0.401	-0.710	+0.548
13	-0.586	+ 0.504	-0.208	+0.385	-0.689	+0.536
	-0.584	+0.533	-0.223	+0.390	-0.710	+0.548
14	-0.666	+ 0.548	-0.205	+0.390	-0.690	+0.538
	-0.669	+0.583	-0.218	+0.405	-0.709	+0.549
15	-0.611	+ 0.555	-0.234	+0.384	-0.698	+0.535
	-0.608	+0.581	-0.248	+0.390	-0.717	+0.548
16	-0.674,	+ 0.541	-0.217	+0.394	-0.694	+0.538
	-0.674	+ 0.541	-0.213	+0.402	-0.693	+0.538
	-0.678	+0.582	-0.237	+0.401	-0.709	+0.549
	-0.678	+0.582	-0.242	+0.429	-0.711	+0.549
17	-0.610	+ 0.561	-0.245	+0.385	-0.698	+0.534
	-0.609	+0.582	-0.257	+0.391	-0.717	+0.547
18	-0.679	+ 0.553	-0.224	+0.389	-0.697	+0.536
	-0.685	+-0.591	-0.242	+0.406	-0.714	+0.548
19	-0.637	+ 0.487	-0.249	+0.383	-0.699	+0.536
	-0.639	+0.518	-0.268	+0.394	-0.716	+0.549
20	-0.624	+ 0.582	-0.245	+0.394	-0.700	+0.535
	-0.621	-0.606	-0.261	+0.402	-0.718	+0.548
21	-0.608	+ 0.487	-0.249	+0.383	-0.692	+0.538
	-0.607	+0.405	-0.292	+0.447	-0.711	+0.552
22	-0.631	+ 0.524	-0.271	+0.390	-0.694	+0.535
	-0.631	+0.555	-0.290	+0.401	-0.712	+0.548
23	-0.647	+ 0.484	-0.280	+0.401	-0.699	+0.535
	-0.644	+0.515	-0.294	+0.415	-0.716	+0.549
24	-0.627	+ 0.558	-0.231	+0.399	-0.700	+0.534
	-0.626	+0.587	-0.248	+0.408	-0.717	+0.547
25	-0.610	+ 0.381	-0.254	+0.408	-0.687	+0.535
	-0.610	+0.402	-0.271	+0.418	-0.708	+0.549
26	-0.622	+ 0.548	-0.197	+0.350	-0.676	+0.536

	-0.617	+0.582	-0.211	+0.351	-0.699	+0.549
	-0.610	+ 0.528	-0.214	+0.399	-0.701	+0.537
	-0.606	+0.563	-0.233	+0.405	-0.721	+0.551
27	-0.629	+ 0.555	-0.236	+0.405	-0.689	+0.536
	-0.627	+0.580	-0.251	+0.412	-0.710	+0.550
28	-0.621	+ 0.556	-0.259	+0.436	-0.696	+0.538
	-0.621	+0.579	-0.276	+0.446	-0.716	+0.553
29	-0.634	+ 0.553	-0.245	+0.447	-0.692	+0.539
30	-0.630	+ 0.555	-0.251	+0.452	-0.686	+0.539
	-0.631	+0.579	-0.270	+0.463	-0.708	+0.555
31	-0.629	+ 0.565	-0.309	+0.441	-0.689	+0.538
	-0.632	+0.587	-0.330	+0.456	-0.710	+0.553
	-0.630	+ 0.557	-0.313	+ 0.464	-0.701	+0.539
	-0.634	+0.582	-0.336	+0.478	-0.725	+0.555
32	-0.629	+ 0.567	-0.318	+0.481	-0.692	+0.540
	-0.635	+0.589	-0.343	+0.499	-0.717	+0.556
33	-0.640	+ 0.544	-0.381	+0.527	-0.669	+0.538
	-0.642	+0.585	-0.399	+0.510	-0.702	+0.554
34	-0.693	+0.620	0.036	0.583	-0.696	+0.542
			-0.340(N)	-0.030		
	-0.707	+0.649	0.023	0.605	-0.723	+0.557
			-0.324(N)	-0.057		
35	-0.703	+ 0.545	-0.248	+0.612	-0.701	+0.542
			-0.067	-0.273		
	-0.722	+0.676	-0.271	+0.638	-0.729	+0.557
			-0.052	-0.298		