"Lp...synthon" interaction as a reason for the strong amplification of the synthon-forming hydrogen bonds

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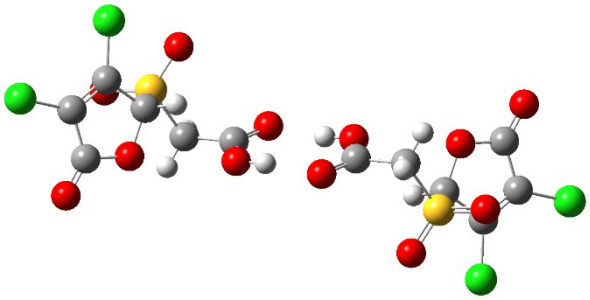
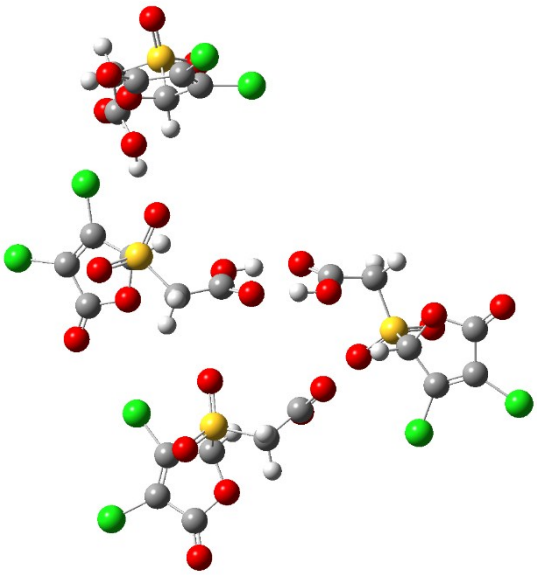
Supplemental Materials

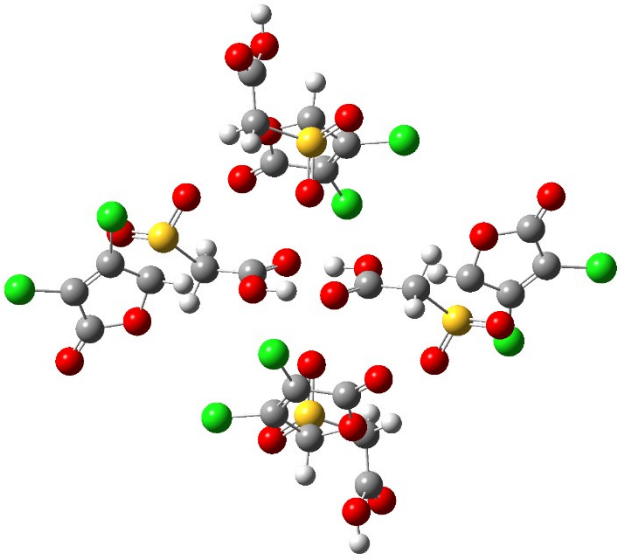
Figure S1 Optimized geometry of different types of associates.



H-bonded dimer



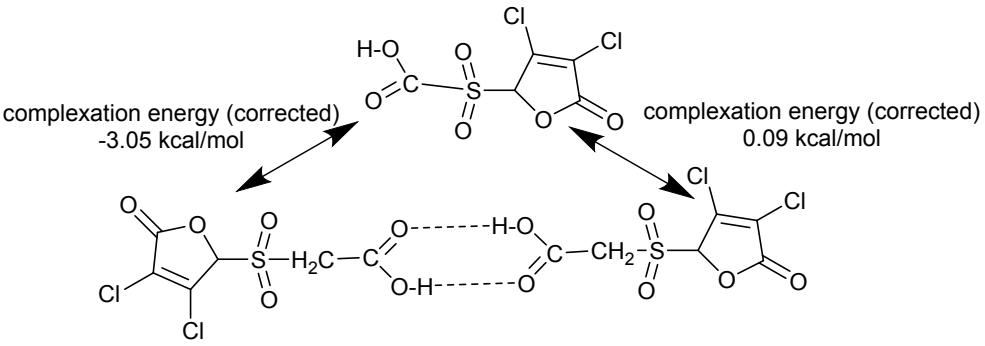
H-bonded tetramer which is realized in polymorph **1a**.



“Lp…synthon”-type tetramer conditionally separated in the crystalline structure of polymorph **1b**.

Figure S2. Single point DFT calculations.

1) Single point molecule pair interaction energies (PBE0, 6-31G(d,p) level with BSSE corrections) for the molecular pair: “up” and “left” molecules, “up” and “right” molecules (see fig. 4)



2) Single point interaction energies (PBE0, 6-31G(d,p) level with BSSE corrections) for the model system: acetic acid dimer + DMSO.

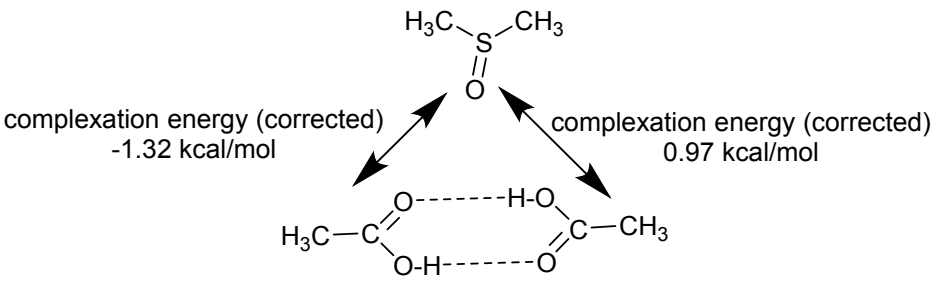


Table S1. The change in geometric parameters of hydrogen-bound fragments of the molecule in the series of calculated associates: dimer, H-bonded tetramer, tetramer “lp...synthon”-type.

	d, O-H, Å	d, H…O, Å	d, O…O, Å	d, C=O, Å	d, C-O, Å
Dimer	1.01	1.57	2.58	1.22	1.31
H-bonded tetramer	1.01	1.57	2.59	1.22	1.30
Tetramer «lp…synthon»	1.04	1.51	2.55	1.24	1.31

Table S2. CCDC search data.

Parameter Values for Query

Refcode	**∠X=O…Cg, °**	**H…O, Å**	**O…Cg, Å**	**X**
ACEDAC20	132,106	1,802	2,625	C
ACETUA	126,658	1,703	2,79	N
AKILAH	115,854	1,83	2,968	C
AMALOQ	123,833	1,921	2,885	C
BANPOW	116,005	1,743	2,906	Cl
BAQLUD	148,818	1,859	3,113	N
BIFQIR	137,757	1,564	2,758	C
BIPJUF	148,726	1,675	3,115	N
CUYKUC	150,3	1,752	2,938	N
DAWRUR	140,673	1,897	2,944	C
DUGBEN	173,773	1,74	2,844	C
EWELOH	158,635	1,794	3,193	C
FOBSUL	111,023	1,823	2,733	Cl
FUHDES	114,52	1,797	2,768	N
GAPPUK	125,509	1,864	2,909	N
GENMIW	149,563	1,729	2,877	C
GENMOC	154,111	1,564	2,833	C
GUGCUG	111,188	1,766	2,724	C
HAWKAR	124,357	1,786	2,957	Cl
HEWWIQ	118,173	1,842	2,83	N
HIBHIJ	156,497	1,675	2,847	N
HOQXER	129,033	1,701	2,777	C
HUFQUV01	126,668	1,825	2,686	Cl
ICOZOR01	171,179	1,851	2,883	N
IZALOK	124,354	1,825	3,149	N
JESYIS	146,078	1,777	2,81	C
JESYIS	148,301	1,804	2,821	C
KANCEI	124,187	1,764	2,701	S
KEHSIC	122,932	1,748	2,803	C
OFMAW01	110,513	1,837	2,99	S
LONKII	126,223	1,792	3,213	C

MALNAC02	128,605	1,722	2,747	C
NEDNOZ	131,749	1,573	2,845	C
NIPBAR	130,955	1,839	2,718	C
ODUSEM	149,621	1,816	3,018	C
OSETEN	130,899	1,836	2,856	C
POBTEF	128,948	1,45	2,801	N
POXZOS	123,233	1,731	2,927	C
REHMEW	159,185	1,424	3,109	N
RUFMOW	122,569	1,804	3,051	C
SAGZOR	136,956	1,729	2,739	N
SIGBEP	128,893	1,719	3,105	C
SIJKIG	120,974	1,83	2,777	C
SOZGEV	146,155	1,636	2,891	N
TIBGIV	119,998	1,843	2,861	N
UNEBOG	122,043	1,668	2,979	C
URILUD	134,125	1,778	2,835	N
VATLAE	144,784	1,741	2,991	C
VUWKUU	113,23	1,825	2,91	N
WUTJUR	133,631	1,734	2,868	S
XEGLOK	141,262	1,741	2,695	N
YUVMUY	110,04	1,817	3,038	C