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Supporting information for article:

Weak intermolecular interactions in a series of biologically active 4′-methylthio-*trans*-stilbenes

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Tables 1 – 9. The details of the interactions for the pairs of molecules for which critical points were found. G_{cp}: kinetic energy density (kJ/mol/Bohr^3); V_{cp}: potential energy density (kJ/mol/Bohr^3); DEN: electron density at the BCP (e·Å^{-3}), LAP: laplacian at the BCP (e·Å^{-5}); distances in Å, angles in °, energies in kJ/mol.

Table 1. 1.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H21C	C5	-1+x,y,z	14.86	-12.49	2.6215	0.06599	0.633	3.573	2.61	147	-32.4	-32.9
C6'	H2'		7.53	-4.84	3.0878	0.02606	0.375	3.613	3.09	110		
H5'	C3'		7.63	-4.92	3.0652	0.02652	0.38	3.605	3.06	111		
S4'	H41C		6.87	-4.77	3.0878	0.02973	0.329	3.932	3.08	136		
C4	H41A	1/2-x, 1/2-y, 1-z	6.25	-4.45	2.9449	0.0295	0.296	3.976	2.93	160	-34.6	-34.1
C5	H3'		11.84	-8.89	2.717	0.04795	0.543	3.680	2.71	148		
C1'	H6		6.01	-4.31	3.0938	0.02924	0.283	4.129	3.09	160		
S4'	H5		9.79	-7.35	2.9782	0.0428	0.449	3.941	2.97	148		
O2	H41B	1/2-x, 3/2-y, 1-z	16.99	-11.75	2.5122	0.05068	0.816	3.343	2.50	133	-33.0	-31.4
H7	S4'		5.79	-4.08	3.1998	0.02758	0.275	4.199	3.19	154		
H5'	C6'		11.29	-8.84	2.7614	0.05005	0.505	3.793	2.76	159		
S4'	C8		2.57	-1.56	4.1898	0.0116	0.131	4.190				
H6'	S4'		11.02	-8.52	2.8912	0.04838	0.496	3.822	2.89	144		
H21B	H3	-x, 1/2+y, 1/2-z	10.54	-6.69	2.3735	0.03084	0.528	2.36			-3.2	-6.2
H21B	H4		10.61	-6.72	2.3632	0.03073	0.533	2.35				
C21	H41A	1/2-x, 1-y, -1/2+z	6.85	-4.06	3.0802	0.01906	0.354	3.779	3.07	123	-7.9	-6.4
H3	S4'		3.55	-2.39	3.3559	0.01865	0.173	4.396	3.35	161		
O2	H4	1-x, 1/2+y, 1/2-z	6.83	-4.6	2.9185	0.02757	0.333	3.860	2.91	145	-6.4	-9.0
H21A	H5		10.55	-7.62	2.2819	0.04155	0.495	2.27				
H41B	C4	3/2-x, 1-y, 1/2+z	8.47	-5.71	2.9203	0.03147	0.413	3.775	2.91	136	-5.1	-4.5

Table 2. 2.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H31B	C4	-1+x,y,z	8,91	-6,72	2,8684	0,04075	0,408	3.928	2.87	164	-42.5	-41.0
H41A	C3'		13,66	-10,45	2,6978	0,054	0,619	3.532	2.70	133		
C6'	C8		5,14	-3,31	3,6992	0,02088	0,256	3.699				
H31A	O3	x-3/2, -y+1/2, 2-z	10,96	-6,96	2,8521	0,0316	0,549	3.341	2.85	107	-5.5	-7.5
C4	H4	x-3/2, -y+3/2, 2-z	10,9	-7,86	2,7523	0,04227	0,512	3.587	2.75	133	-13.4	-13.6
O3	H5		13,42	-8,84	2,6256	0,03927	0,661	3.409	2.63	128		
H2	S4'	-x, y-1/2, -z+3/2	9,16	-6,71	2,9506	0,0393	0,426	3.967	2.95	155	-29.6	-29.0
H31C	S4'		8,32	-6,26	2,9981	0,03892	0,381	3.867	3.00	137		
H7	S4'		2,65	-1,62	3,5627	0,01198	0,135	4.437	3.56	138		
H6'	C3'		9,56	-7,17	2,7479	0,04205	0,439	3.747	2.75	152		
C41'	C6		7,02	-4,51	3,5248	0,02495	0,35	3.525				
H41C	C7		7,21	-4,7	3,0461	0,02635	0,357	3.861	3.05	132		
H31A	S4'	-x+1/2, 1-y, z-1/2	11,52	-8,5	2,8898	0,04564	0,534	3.786	2.89	140	-6.8	-8.5
H6	H41C	1-x, y+1/2, -z+3/2	7,87	-5,09	2,4108	0,02717	0,391	2.41			-24.6	-24.4
H6	C5'		2,69	-1,73	3,3861	0,01423	0,133	4.467	3.39	172		
H8	C5'		2,34	-1,49	3,4857	0,01262	0,117	4.551	3.49	166		
H2'	C6'		7,78	-5,79	2,8629	0,03674	0,358	3.944	2.86	172		
H3'	C1		10,54	-8,43	2,7709	0,04981	0,464	3.786	2.77	155		

Table 3. 3.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H21B	H31A	x-1/2, -y+1/2, z-1/2	11,47	-7,25	2,3989	0,03198	0,576	2.39			-24.5	-31.7
H7	H31C		8,16	-6,87	2,2488	0,04618	0,347	2.23				
H6'	C4		12,62	-8,73	2,7805	0,04238	0,606	3.483	2.78	122		
H6'	H31C		12,4	-9,57	2,1404	0,05171	0,56	2.13				
H5'	C2		13,34	-10,15	2,6574	0,05271	0,607	3.619	2.65	148		
H41B	C7		8,67	-6,68	2,777	0,04163	0,391	3.832	2.77	166		
C2'	H5	x-1/2, -y+3/2, z-1/2	6,19	-4,39	3,0393	0,02908	0,294	4.033	3.03	153	-23.0	-26.3
S4'	H6		12,74	-10,54	2,8084	0,05883	0,548	3.834	2.80	158		
S4'	H8		12,32	-9,59	2,8411	0,05225	0,553	3.767	2.84	143		
S4'	H2'		3,44	-2,11	3,457	0,01414	0,175	4.242	3.45	131		
H41A	C2'		4,11	-2,54	3,2476	0,0162	0,209	4.081	3.24	135		
C5'	H3'	-x+1/2, y-1/2, -z+1/2	9,55	-7,02	2,8317	0,04051	0,444	3.814	2.83	151	-20.3	-11.1
S4'	H2'		6,48	-4,12	3,2744	0,02316	0,324	3.919	3.27	119		
O2	H21A	-x+1/2, y-1/2, -z+3/2	7,78	-5,53	2,7912	0,03358	0,368	3.865	2.78	175	-20.3	-19.6
H21B	C7		8,86	-6,63	2,8307	0,04008	0,407	3.608	2.82	132		
H21C	C6'		2,11	-1,25	3,5644	0,00927	0,109	4.401	3.56	136		
H31B	H5'		8,98	-6,61	2,4192	0,03921	0,416	2.41				
S4'	S4'	-x,1-y,-z	11,45	-9,16	3,5018	0,05235	0,505	3.502			-7.2	-9.8
H41C	C21	-x,1-y,1-z	5,55	-3,39	3,0524	0,01856	0,283	3.855	3.04	132	-7.8	-6.3
H31B	O3	1-x,-y,2-z	12,24	-7,76	2,7479	0,03361	0,614	3.281	2.74	110	-15.9	-22.0
C6	C3'	1-x,1-y,1-z	8	-5,39	3,4834	0,03038	0,39	3.483			-30.0	-29.4
H31A	C2	1-x,1-y,2-z	10,41	-8,39	2,8564	0,05004	0,456	3.930	2.84	175	-31.5	-34.3

Table 4. 4.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H51C	H41B	x-1/2, -y+3/2, 1+z	6,9	-4,4	2,4636	0,02417	0,345	2.46			-8.3	-7.5
H51A	C4'		7,98	-5,8	2,9505	0,03563	0,373	3.901	2.95	146		
C1'	H21B	x,y,-1+z	6,68	-4,82	2,974	0,03157	0,313	3.942	2.97	148	-30.7	-29.3
C2'	C2		12,91	-9,61	3,2673	0,04972	0,595	3.267				
S4'	H6'		3,41	-2,13	3,4095	0,01487	0,172	4.306	3.41	140		
H21C	O5	x+1/2, -y+3/2, z	5,3	-3,5	2,9977	0,02264	0,261	4.034	3.00	159	-6.6	-5.3
H21A	C41'	x,1+y,1+z	4,07	-2,57	3,3271	0,0171	0,205	4.364	3.33	160	-5.9	-3.4
H6'	H21A	-x+3/2, y-1/2, z-1/2	7,99	-4,8	2,5029	0,02197	0,41	2.50			-14.3	-19.2
H5'	O2		12,56	-9,02	2,5998	0,0457	0,591	3.616	2.60	155		
H41B	H7		10,39	-6,86	2,347	0,03392	0,511	2.35				
H41A	C6'		9,05	-5,98	2,8623	0,03121	0,445	3.653	2.86	131		
H41B	O2		5,94	-3,63	2,9458	0,01937	0,303	3.787	2.95	134		
H21C	S4'	-x+3/2, y+1/2, z+3/2	11,11	-7,67	3,0469	0,03907	0,535	3.477	3.05	104	-4.9	-6.8
H41A	H51B	1-x, 1-y, z-3/2	7,24	-4,62	2,4397	0,02503	0,362	2.44			-7.0	-2.9
C4'	H6	1-x, 1-y, z-1/2	13,84	-10,99	2,6491	0,05794	0,613	3.624	2.65	149	-31.9	-29.0
C3'	C8		10,54	-7,58	3,3231	0,04129	0,495	3.323				
S4'	H8		7,35	-5,01	3,1133	0,02959	0,356	3.959	3.11	135		
H41C	O5		13,94	-10,35	2,516	0,05182	0,644	3.588	2.52	168		
C5'	O5		3,83	-2,25	3,7531	0,0129	0,199	3.753				
C1	H4	1-x, 2-y, z-1/2	13,76	-10,49	2,6919	0,05387	0,626	3.640	2.69	145	-26.7	-28.5
O5	H3		12,12	-8,89	2,6157	0,04655	0,564	3.654	2.62	159		
C7	H51C		6,45	-4,76	2,9793	0,03223	0,299	3.987	2.987	154		

Table 5. 5.

Atom1	Atom2	Symcode	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
O3B	H51B	x,y,z	23,43	-19,56	2,4	0,08591	1,002	3.463	2.40	165	-11.0	13.2
H4A	C31B		6,94	-5,03	3,2143	0,03261	0,325	4.004	3.22	132		
H2'A	C5'B	1-x, -1/2+y, 1-z	20,94	-19,11	2,5772	0,09102	0,836	3.611	2.58	174	-37.9	-35.8
H8A	S4'B		11,07	-8,94	3,0326	0,05204	0,485	3.984	3.03	146		
H6A	S4'B		9,43	-7,22	3,1891	0,04332	0,427	3.743	3.19	112		
H41B	H6B		6,08	-4,38	2,8102	0,02968	0,286	2.81				
H41B	C8B		5,49	-3,81	3,2863	0,02587	0,263	4.247	3.29	148		
H51C	O3A	1-x,1-y,1-z	20,01	-15,98	2,5036	0,07294	0,883	3.252	2.50	125	-12.2	-16.4
H4A	H4A		8,27	-6,54	2,5213	0,0422	0,367	2.52				
H41A	H2A	x, -y+1/2, z-1/2	12,71	-11,21	2,2878	0,0644	0,522	2.29			-25.0	-23.7
O5A	H41C		12,38	-9,05	2,7173	0,04692	0,577	3.499	2.72	128		
H6A	S4'A		17,78	-16,24	2,7405	0,08255	0,71	3.732	2.74	151		
H41C	H31C		7,95	-5,94	2,7576	0,03736	0,366	2.94				
H3'A	H7A		4,84	-3,39	2,8473	0,0245	0,231	2.85				
H2'A	C5'A		13,91	-11,39	2,8617	0,06099	0,603	3.498	2.86	117		
H5'A	C3'B	2-x,1-y,1-z	17,93	-15,77	2,6477	0,07888	0,738	3.592	2.65	145	-51.8	-39.6
H31C	C4B		17,12	-14,96	2,6438	0,07606	0,707	3.533	2.65	138		
C4A	H31E		13,36	-10,91	2,8549	0,05928	0,58	3.585	2.86	124		
H6'A	C1'B		10,01	-7,73	2,9474	0,04548	0,452	3.743	2.95	130		
H7A	C7B		3,76	-2,45	3,4604	0,01779	0,186	4.192	3.46			
C5'A	H2'B	2-x, 1/2+y, 1/2-z	19,72	-17,71	2,6192	0,08593	0,798	3.658	2.62	159	-37.1	-36.0
S4'A	H51E		14,09	-12,15	2,8633	0,06637	0,589	3.928	2.86	165		
S4'A	H8B		10,73	-8,64	3,0327	0,05079	0,471	3.987	3.03	147		
C6A	H41E		7,41	-5,49	3,1287	0,03527	0,343	4.071	3.13	145		
H31A	C1B	1-x,1-y,1-z	12,64	-10,18	2,9227	0,05615	0,554	3.984	2.92	165	-50.7	-42.1

C1'A	H6'B		9,88	-7,57	3,0352	0,04452	0,448	3.637	3.03	115		
H5'B	C3'A		18,36	-16,16	2,6827	0,08011	0,754	3.717	2.68	158		
H31D	C4A		15,48	-13,31	2,6733	0,06995	0,648	3.702	2.67	157		
H4B	O5B	2-x,1-y,-z	15,53	-11,88	2,5679	0,0583	0,704	3.618	2.57	162	-12.3	-10.8
H41D	H7B	x, -y+3/2, z+1/2	9,29	-7,57	2,4539	0,04748	0,404	2.45			-24.3	-20.9
H3'B	H6'B		8,9	-6,8	2,6753	0,04164	0,404	2.67				
C41B	H2B		10,18	-8,09	2,9807	0,0482	0,451	4.054	2.98	168		
H8B	S4'B		4,53	-3,08	3,4858	0,02216	0,219	4.370	3.49	139		

Table 6. 6.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
C5	H21A	-1+x, y, z	11.75	-9.75	2.7448	0.05625	0.505	3.711	2.75	148	-38.5	-35.7
H41B	H3		4.83	-3.17	2.656	0.02102	0.238	2.66				
C2'	C6'		5.75	-3.63	3.6897	0.02114	0.289	3.690				
C3'	C5'		5.66	-3.58	3.6897	0.02094	0.284	3.690				
S4'	H41E		7.02	-4.85	3.0846	0.02978	0.337	3.909	3.09	133		
H5	C1'	x+1/2, -y+3/2, 1-z	9.64	-7.32	2.8103	0.04326	0.439	3.836	2.81	157	-35.4	-35.0
H41A	C5'		6.44	-4.79	3.0949	0.03272	0.297	4.138	3.09	161		
H6	C1		5.57	-3.85	3.0793	0.02593	0.267	4.057	3.08	150		
H8	C6		3.45	-2.33	3.2671	0.0185	0.168	4.330	3.27	165		
H2'	C5		10.07	-7.66	2.7822	0.0445	0.458	3.845	2.78	165		
H3'	H41A		6.18	-3.59	2.5968	0.01646	0.322	2.60				
C1'	H41F	x-1/2, -y+1/2, 1-z	12.22	-9.89	2.6816	0.05543	0.534	3.750	2.68	167	-26.8	-24.6
S4'	H6'		8.73	-6.26	3.0254	0.03657	0.412	3.905	3.03	138		
H41D	H21C		12.19	-9.89	2.0937	0.05552	0.532	2.09				
C5'	H5'		7.66	-5.58	2.9152	0.03487	0.358	3.813	2.92	140		
H21B	H41C	1-x, y+1/2, -z+1/2	13.18	-8.43	2.318	0.03595	0.658	2.32			-6.3	-6.6
S4'	H3	-x+1/2, 1-y, z-1/2	10.04	-7.79	2.9124	0.04596	0.451	3.921	2.91	154	-15.5	-16.4
S4'	H21B		6.84	-4.7	3.166	0.02892	0.33	3.995	3.17	134		
H41D	O4		9.6	-5.95	2.7987	0.02721	0.486	3.479	2.80	120		
H21C	O4	-x, y-1/2, -z+1/2	8.85	-6.19	2.7519	0.03502	0.423	3.736	2.75	150	-4.9	-6.0

Table 7. 7.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H21A	H41D	x-3/2, -y+1/2, 1-z	4.8	-3.08	2.6363	0.0198	0.239	2.64			-2.9	-1.3
C2	H51C	x-1,y,z	12.83	-9.91	2.7828	0.05289	0.578	3.761	2.78	149	-51.2	-53.8
H21C	C5		15.87	-13.21	2.6549	0.06766	0.681	3.671	2.66	155		
H41A	O5		9.91	-7.07	2.6882	0.0391	0.468	3.709	2.69	156		
H7	H8		2.18	-1.22	2.9888	0.00718	0.115	2.99				
C6'	C2'		6.52	-4.24	3.6025	0.02458	0.324	3.602				
C5'	C3'		6.18	-4.01	3.6066	0.02374	0.307	3.607				
S4'	H41F		9.65	-6.92	2.953	0.03894	0.454	3.750	2.95	130		
C6	H41E	x-1/2, -y+3/2, 1-z	7.21	-4.97	2.9075	0.03005	0.347	3.848	2.91	145	-31.7	-26.8
H51A	C41'		2.86	-1.76	3.3992	0.01282	0.145	4.426	3.40	158		
C8	H3'		6.61	-4.41	2.9541	0.02649	0.324	3.836	2.95	138		
C2'	H2'		7.84	-5.74	2.89	0.03575	0.365	3.789	2.89	139		
S4'	H51A		7.23	-4.75	3.1264	0.02694	0.356	3.860	3.13	125		
H21B	H51B	1+x, -1+y, z	10.28	-6.62	2.3565	0.03156	0.512	2.36			-3.2	-5.0
O2	S4'	x+1/2, -y+1/2, 1-z	8.64	-5.87	3.4446	0.03252	0.419	3.445			-31.8	-26.6
H5'	C6'		8.64	-6.45	2.8486	0.03927	0.398	3.873	2.85	157		
H6'	S4'		8.24	-6.1	3.0196	0.03765	0.381	3.969	3.02	146		
H41C	C21	2-x, y-1/2, -z+1/2	13.2	-8.49	2.8079	0.03659	0.657	3.374	2.81	112	-2.2	-3.8
O4	H21B	1-x, y-1/2, -z+1/2	15.6	-12.11	2.4954	0.05999	0.701	3.528	2.50	158	-22.4	-30.9
O4	H3		10.78	-6.91	2.7711	0.03204	0.538	3.389	2.77	116		
H41C	C2		7.9	-5.34	2.9743	0.03038	0.384	3.388	2.97	141		
O5	H41B		19.66	-14.77	2.4398	0.06504	0.902	3.328	2.44	138		
H51B	C41	-x, y-1/2, -z+1/2	11.86	-8.83	2.7407	0.04724	0.547	3.800	2.74	164.1	-5.7	-4.1

Table 8. 8.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
C41A	H6B	-1/2+x,-1/2-y, -1/2+z	3,03	-1,9	3,3096	0,01404	0,153	3.22	4.218	172	-25.4	-22.2
H31B	H41F		3,76	-2,16	2,7711	0,01163	0,197	2.76				
H41B	H2'B		4,58	-3,08	2,513	0,0216	0,224	2.50				
H7A	S4'B		4,71	-3,17	3,239	0,02203	0,23	3.23	4.189	147		
H41A	C51B		5,07	-3,1	3,1804	0,0177	0,259	3.17	4.122	146		
H2A	S4'B		6,27	-4,55	3,0816	0,03076	0,293	3.08	4.109	159		
H41B	H8B		7,49	-4,91	2,4007	0,02727	0,37	2.39				
H5'A	C2'B		10,05	-6,69	2,9798	0,03384	0,493	2.98	3.497	110		
C6'A	C3'B		10,72	-7,29	3,4501	0,03708	0,519		3.450			
H31D	H51D	-1+x, y, z	6,63	-4,24	2,5796	0,02384	0,331	2.57			-2.8	-1.7
H31C	H51B		9,75	-6,94	2,2727	0,03851	0,462	2.26			-1.5	-1.4
C41B	H6A	x-1/2,-y+1/2,z+1/2	3,45	-2,16	3,2987	0,01511	0,174	3.29	4.367	169	-23.7	-22.5
H7B	S4'A		3,5	-2,25	3,4122	0,01653	0,174	3.41	4.305	141		
H41D	H8A		4,27	-2,93	2,5218	0,02176	0,206	2.51				
C31B	S4'A		6,74	-4,45	3,8074	0,02616	0,331	3.807				
C5'B	H2'A		7,29	-4,59	3,0735	0,02409	0,367	3.07	3.669	115		
H6'B	C3'A		8,08	-5,18	3,0551	0,02708	0,403	3.05	3.613	113		
H2B	S4'A		10,81	-8,29	2,8472	0,04711	0,49	2.84	3.885	160		
H41F	H51C		12,92	-8,77	2,296	0,04128	0,627	2.28				
O3A	H42D	x,1+y,z	12,81	-8,96	2,6036	0,04384	0,611	2.60	3.496	140	-11.0	-9.0
O4A	H42D		13,53	-8,76	2,6996	0,03779	0,672	2.70	3.297	114		
H31A	S4'A	-x+1/2, y-1/2, -z+1/2	6,03	-4,31	3,1602	0,0292	0,284	3.15	4.175	157	-46.4	-45.5
H6'A	C3'A		7,94	-5,7	2,9735	0,03464	0,374	2.97	3.974	154		
C2A	S4'A		9,05	-6,49	3,5614	0,03745	0,426	3.561				
H41C	C7A		9,32	-7,24	2,8293	0,0441	0,418	2.82	3.858	160		

H5'A	C8A		10,41	-7,2	2,825	0,03784	0,5	2.82	3.665	134		
C1A	H41B		10,73	-7,3	2,8551	0,03702	0,52	2.85	3.515	119		
C2'B	H5'B	-x+1/2, y+1/2, -z+3/2	6,45	-4,51	3,0277	0,029	0,308	3.02	3.991	148	-34.1	-36.8
C8B	H41E		7,86	-5,75	2,8933	0,03574	0,366	2.88	3.847	148		
S4'B	H7B		9,64	-6,67	3,0297	0,0361	0,463	3.03	3.797	128		
S4'B	H6'B		11,8	-9,35	2,8728	0,05249	0,523	2.87	3.874	154		
H42C	O4B	x,y,z	8,97	-6,07	2,746	0,03291	0,436	2.74	3.664	143	-12.1	-11.9
H31A	C2B	-x,-y,1-z	4,74	-2,86	3,2185	0,01617	0,243	3.21	3.883	121	-13.4	-14.3
C31A	H31F		8	-5,58	2,9495	0,03279	0,383	2.94	3.948	154		
H42C	H31D	-x,1-y,1-z	5,6	-4,05	2,4714	0,02852	0,262	2.45			-17.3	-18.6
C2A	H31E		9,07	-6,2	2,9233	0,03385	0,438	2.91	3.836	143		
H31B	H31E		13,68	-9,12	2,2387	0,04093	0,669	2.23				
O4B	H31D	-x, 1-y, 1-z	14,03	-9,19	2,6458	0,03981	0,693	2.64	3.335	121	-14.4	-19.4
S4'A	S4'B	1-x,-y,1-z	4,58	-2,93	4,0583	0,01902	0,229	4.058			-44.2	-42.8
H51A	C6B		9,21	-6,27	2,88	0,03387	0,446	2.87	3.573	122		
C8A	H2'B		10,7	-7,47	2,7865	0,03914	0,511	2.78	3.594	131		
C4A	H51E		11,35	-8,75	2,7605	0,04895	0,512	2.75	3.718	148		
C5'A	H3'B		13,45	-10,91	2,6989	0,0589	0,587	2.69	3.749	163		
H42B	O5A	1-x, -y, 1-z	14,63	-11,43	2,5148	0,0583	0,655	2.50	3.580	170	-14.1	-18.7
C42A	C42A		6,98	-4,18	3,5642	0,02009	0,359	3.564				
H51F	C5A	1-x,1-y,1-z	5,68	-3,96	3,0399	0,02672	0,272	3.03	3.942	142	-47.8	-22.5
H3'A	S4'B		9,3	-6,28	3,0776	0,03341	0,453	3.07	3.828	127		
H3'A	C4'B		9,36	-6,29	2,9998	0,03321	0,456	3.00	3.548	112		
H42E	H51B		9,59	-6,68	2,308	0,03655	0,459	2.29				
H42A	O5B		10,47	-7,43	2,6986	0,04002	0,496	2.69	3.686	152		
H51C	C6B		11,05	-8,89	2,7576	0,05167	0,485	2.75	3.734	150		
H2'A	C6'B		11,24	-8,61	2,738	0,04814	0,51	2.73	3.733	153		

H51D	O4B	1-x,1-y,1-z	8,81	-6,34	2,7466	0,03711	0,414	2.74	3.804	167	-12.1	-21.5
H51D	O5B		9,92	-6,51	2,7253	0,03252	0,489	2.72	3.556	134		

Table 9. 9.

Atom1	Atom2	Symmetry operation	Gcp	Vcp	D	Rho	Lap	A···B	H···B	A-H···B	Pixel	CrystExp
H41B	S4'	x-1/2, -y+1/2, z+1/2	5.22	-3.61	3.212	0.02501	0.251	4.195	3.21	151	-6.5	-5.3
H61A	S4'	-x+1/2, y-3/2, -z+1/2	6.24	-3.88	3.235	0.02114	0.316	3.880	3.23	119	-4.6	-6.5
H5	C7	x, y-1, z	1.94	-1.08	3.7516	0.00658	0.103	4.324	3.75	115	-46.8	-46.5
H41C	O2		11.29	-7.64	2.7093	0.03781	0.548	3.484	2.71	128		
H61C	C1'		11.88	-9.32	2.6976	0.05179	0.53	3.638	2.70	144		
C8	H41F		12.1	-9.2	2.6791	0.04971	0.55	3.655	2.68	149		
H8	H3'	-x+1/2, y-1/2, -z+1/2	5.84	-3.8	2.4473	0.02306	0.289	2.45			-13.9	-12.1
H2'	C3'		6.47	-4.58	2.925	0.02987	0.307	3.942	2.93	155		
H61A	H2'		10.54	-7.6	2.2752	0.04152	0.494	2.28				
O4	H21C	-x+1/2, y-1/2, -z+3/2	9.45	-5.77	2.8212	0.02555	0.482	3.419	2.82	114	-5.5	-9.8
H3	H21B		13.87	-10.1	2.1774	0.04977	0.648	2.18				
C41	H5	-x,-1-y,1-z	2.67	-1.59	3.3347	0.01095	0.138	4.422	3.34	177	-9.3	-5.1
C41	C41		4.52	-2.58	3.9472	0.01258	0.237	3.947				
H41B	C61		5.54	-3.34	3.1507	0.01787	0.284	3.987	3.15	134		
C5	C5	-x, -y, 1-z	5.41	-3.64	3.6194	0.02391	0.264	3.619			-44.2	-45.8
C1	H41A		9.47	-7.56	2.8304	0.04657	0.418	3.905	2.83	169		
C3	H61B		10.48	-8.48	2.7535	0.0505	0.458	3.804	2.75	162		
C6'	C6'	1-x, 1-y, 1-z	2.95	-1.68	4.1201	0.00979	0.155	4.120			-61.4	-53.8
O2	C4'		5.62	-3.57	3.6469	0.02112	0.281	3.647				
S4'	H21C		8.59	-6.47	3.0255	0.03975	0.393	3.962	3.03	144		
H41E	C3		13.12	-10.02	2.7156	0.05256	0.596	3.570	2.72	135		
H5'	H5'	1-x,2-y,1-z	7.34	-5.28	2.2879	0.03318	0.345	2.29			-9.8	-20.7
H6'	H41F		9.7	-6.68	2.3581	0.03589	0.467	2.36				
H21B	H41D		13.53	-9.97	2.1327	0.0502	0.627	2.13				

Table S1. Comparison of the relevant geometrical parameters found in the crystal structures of **6**, **8** and **9**, and in the appropriate molecules docked at the active sites

	6	**6_1A2**	**6_1B1**	**8**	**8_1A2**	**8_1B1**	**9**	**9_1A2**	**9_1B1**
C1-C7	1.465(5)	1.449	1.478	1.471(2) 1.465(2)	1.440	1.460	1.466(2)	1.452	1.483
C7-C8	1.311(5)	1.346	1.351	1.331(3) 1.330(3)	1.344	1.347	1.323(2)	1.339	1.351
C8-C1’	1.463(5)	1.453	1.470	1.466(2) 1.473(3)	1.442	1.465	1.460(2)	1.455	1.459
C4’-S4’	1.759(4)	1.748	1.776	1.7581(18) 1.7594(17)	1.733	1.753	1.7611(18)	1.744	1.772
S4’-C41’	1.758(5)	1.800	1.805	1.7998(19) 1.794(2)	1.799	1.797	1.780(2)	1.796	1.802
C3’-C4’-C5’	117.5(3)	121.04	119.78	118.73(16) 118.83(16)	121.78	120.65	117.56(17)	121.18	119.95
C4’-S4’-C41’	104.5(2)	95.43	98.92	103.71(19) 103.20(9)	94.93	97.47	103.71(10)	94.37	97.12
C1-C7-C8-C1’	178.1(3)	177.20	178.48	173.35(18) 175.50(18)	179.40	178.30	179.9(2)	174.36	177.92
C7=C8···S4’-C41’	17.8	-86.75	136.43	12.4 -5.3	94.93	-89.16	10.4	89.60	157.62
A/B	7.3(6)	37.15	14.76	13.98(11) 10.08(12)	36.09	27.02	2.99(19)	40.81	21.01
B/A’	2.4(5)	26.66	19.39	12.9(2) 14.5(2)	31.08	6.96	7.10(18)	28.55	38.87
A/A’	9.4(2)	10.69	5.11	26.84(5) 24.49(6)	5.62	20.11	4.24(9)	12.26	17.89
A/OMe	2.2(4) 14.5(6)	8.45 53.55	13.91 33.07	5.73(9) *80.93(14)* 5.81(9) 9.46(15	5.74 10.60 59.30	38.57 51.83 73.63	0.6(2) 4.20(13) 2.0(2)	1.90 14.92 57.91	14.65 45.58 77.96
A’/SMe	14.7(4)	60.82	62.74	20.9(8) 7.16(14)	63.24	82.02	2.93(11)	64.09	60.28