Supporting Information for:

Can Hydrogen Bonds Improve the Hole-Mobility in Amorphous Organic Semiconductors? Experimental and Theoretical Insights

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List of contents:

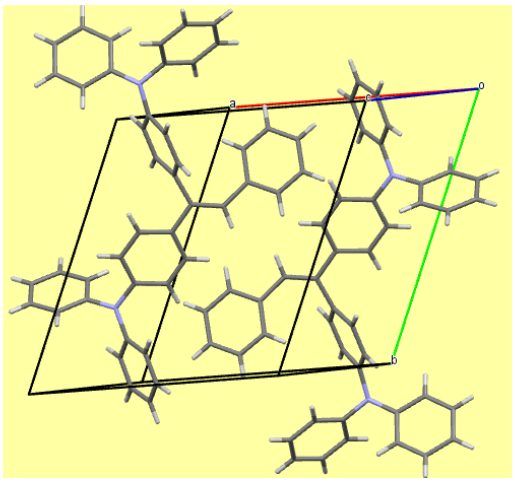
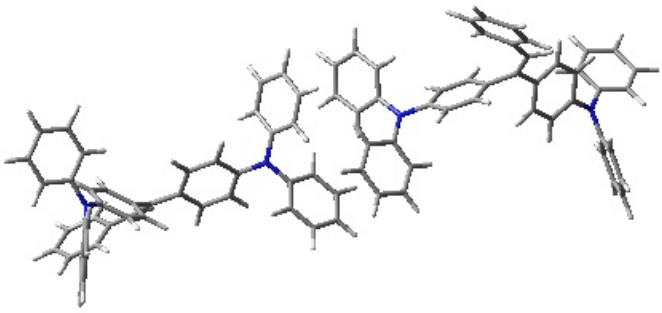
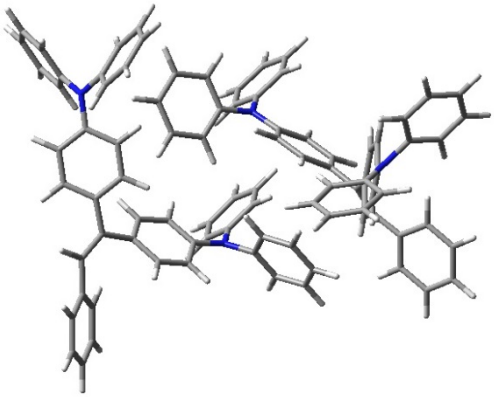


Fig. S1 Partial view of the unit cell corresponding to the crystal structure of compound 4.



Dimer type 1



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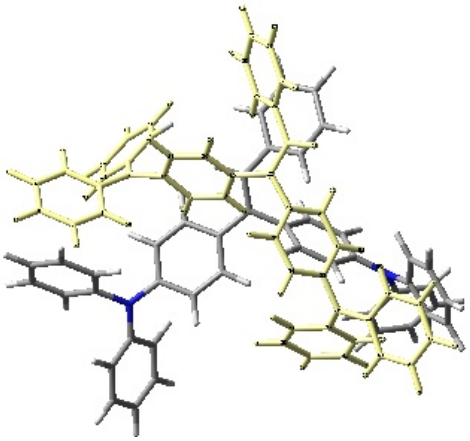

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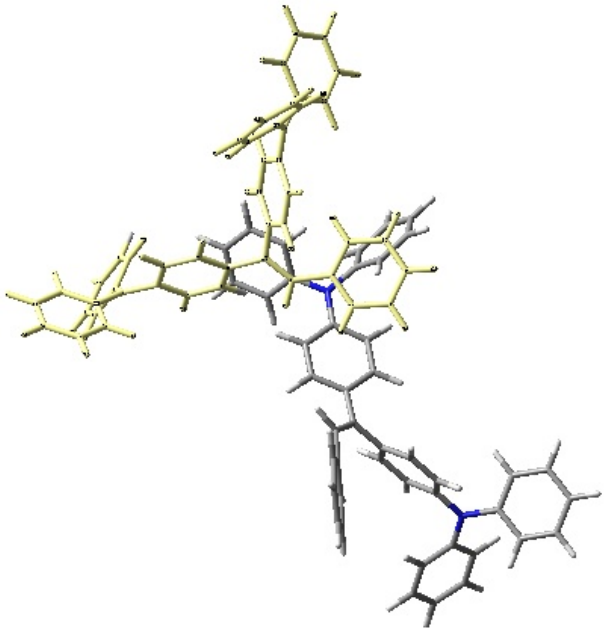
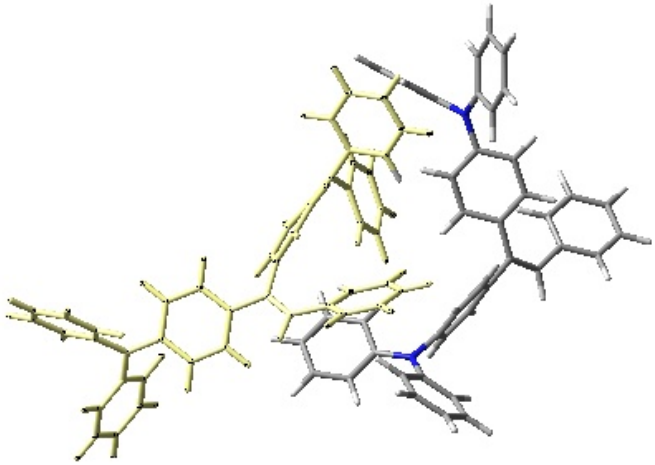
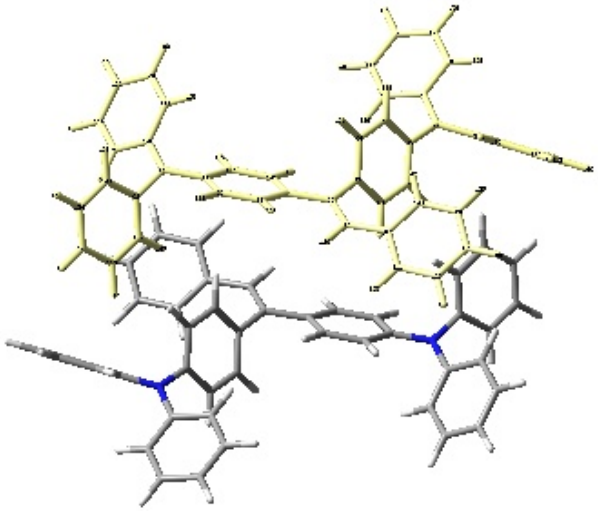


Dimer type 4



Dimer type 5



Dimer type 6

Fig. S2 Global view of the optimized geometry of some selected model dimers corresponding to compound 4. The dimer reported as “Dimer type 6” is similar to one of dimer-types extracted from the crystal structure (see Fig. S1) corresponding to the largest spatial overlap between adjacent molecules. In the case of methoxy- and methyl substituted compounds 5-7, identical dimer-types are considered by appropriate substitutions in the optimized geometries of compound 4. The comparison of the dissociation energies and of the average intermolecular distances across the series of compounds 4-7 is performed only between dimers of identical type.

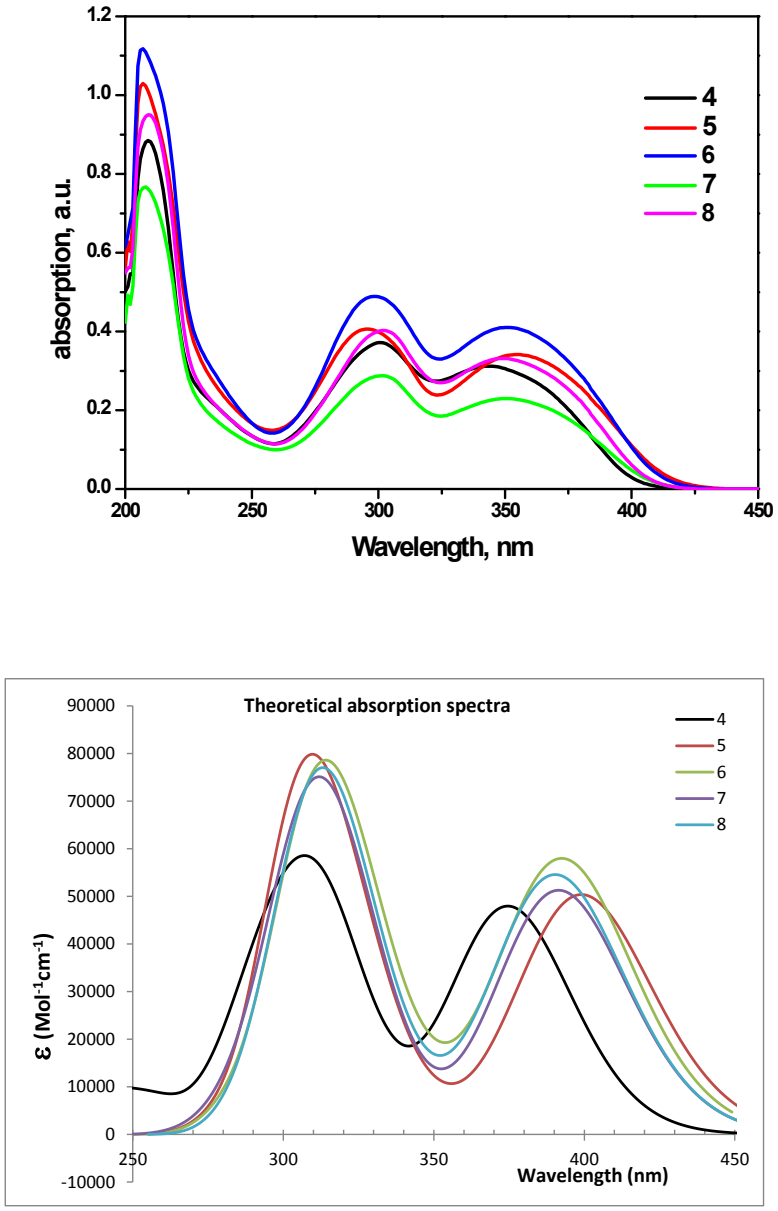


Fig. S3 Experimental (top) and theoretical (bottom) absorption spectra for the compounds 4-8. The theoretical spectra are obtained by mean of TDDFT calculations (gas phase). The absorption bands are obtained by considering peak half-widths at half height of 0.2 eV.

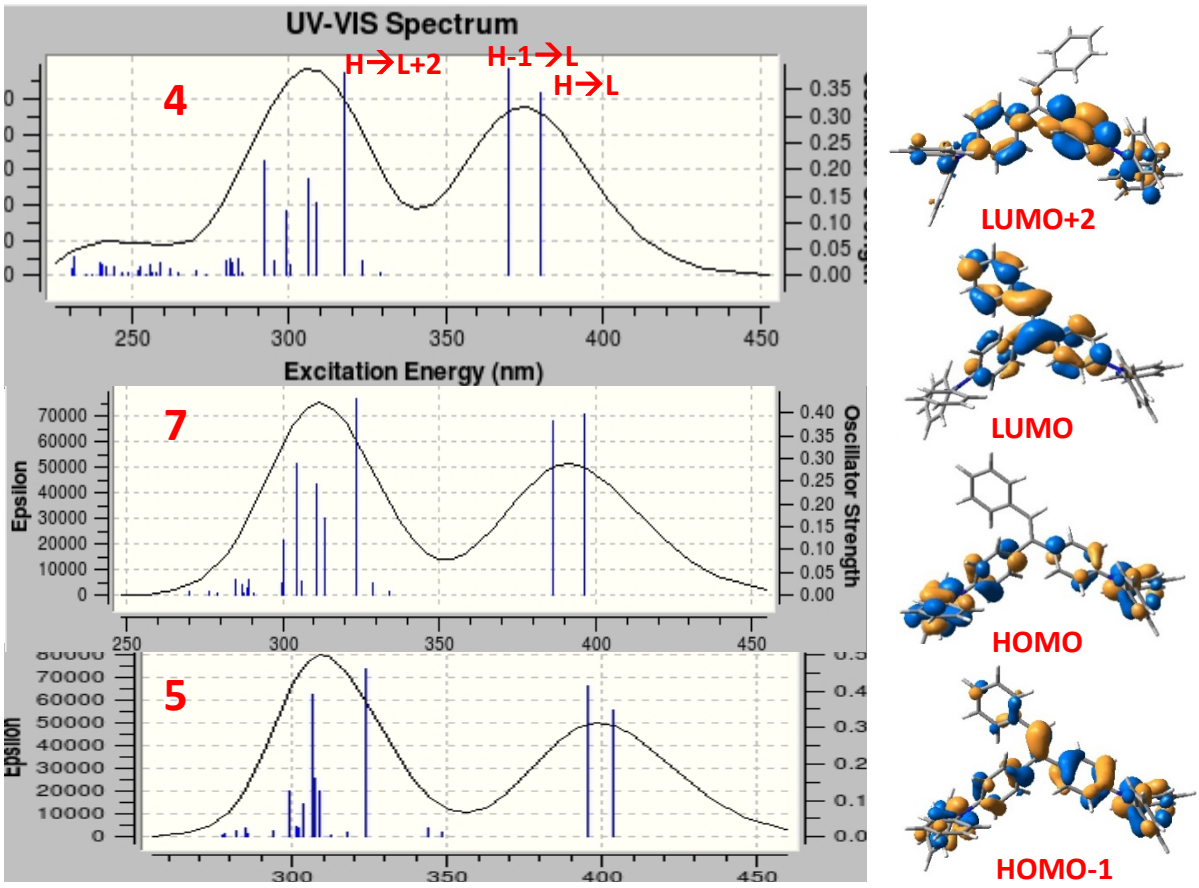
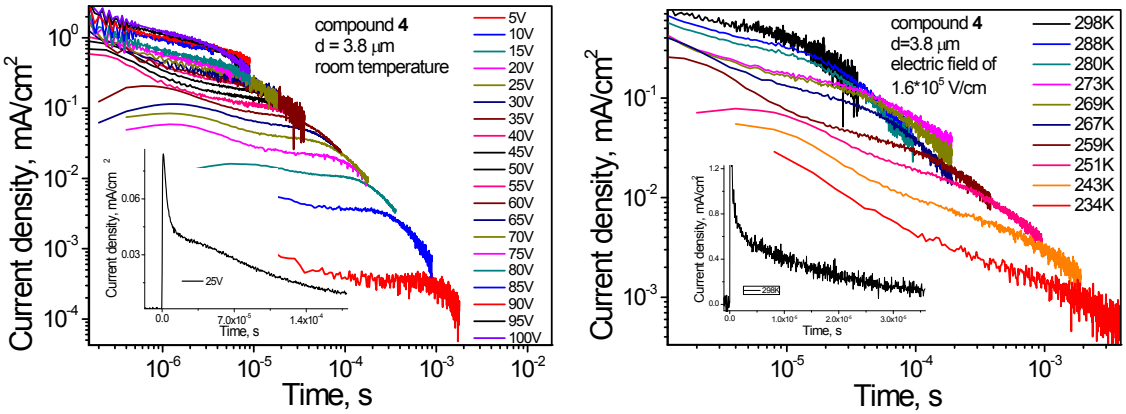
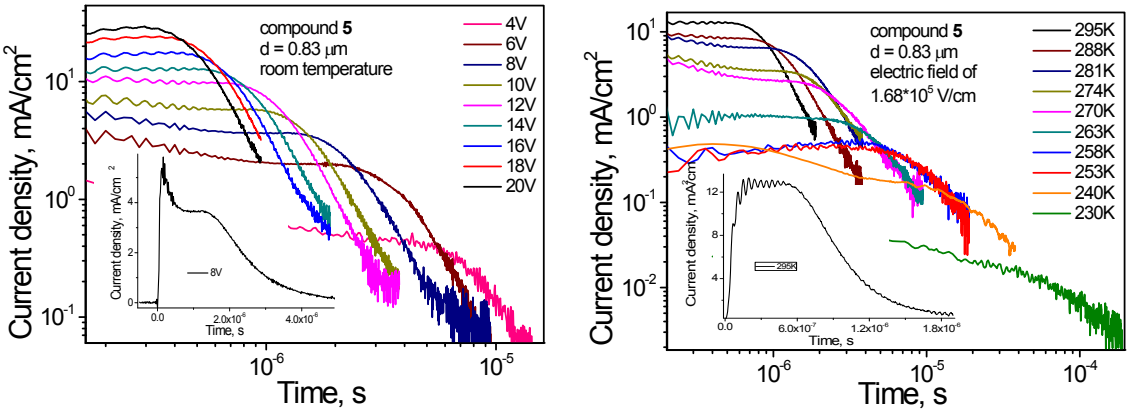


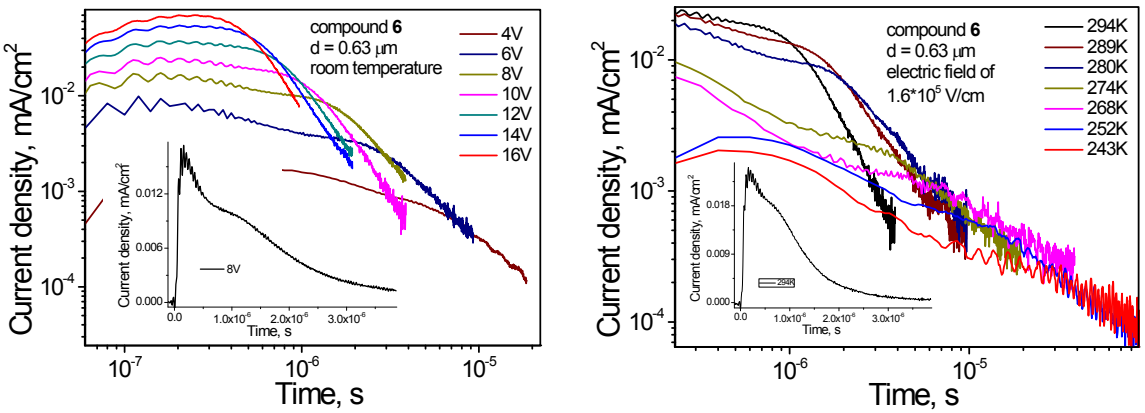
Fig. S4 Theoretical absorption spectra obtained by mean of TDDFT calculations (gas phase), for the compounds 4, 5 and 7. The absorption bands are obtained by considering peak half-widths at half height of 0.2 eV. Some relevant MOs are also presented.


compound 4
d = 3.8 μm
room temperature
5V
10V
15V
20V
25V
30V
35V
40V
45V
50V
55V
60V
65V
70V
75V
80V
85V
90V
95V
100V
Current density, mA/cm2
Time, s
25V
compound 4
d=3.8 μm
electric field of
1.6*10^5 V/cm
298K
288K
280K
273K
269K
267K
259K
251K
243K
234K

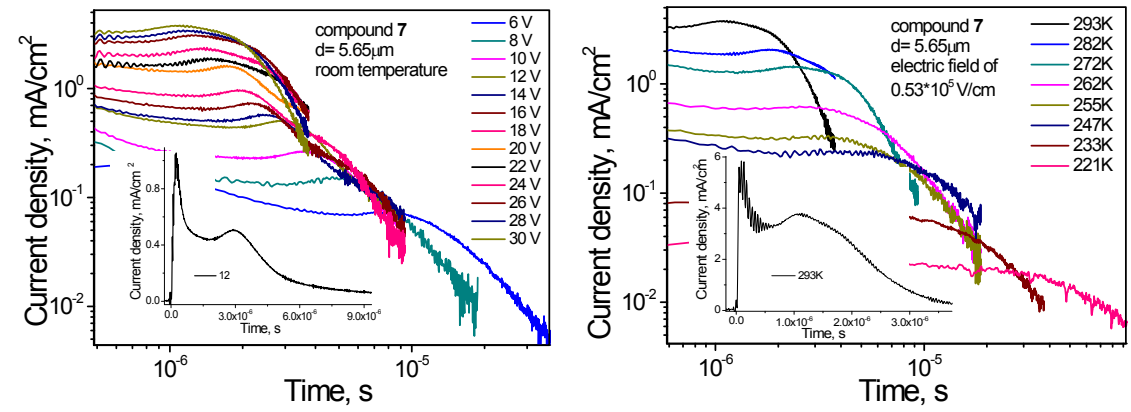
a)


compound 5
d = 0.83 μm
room temperature
4V
6V
8V
10V
12V
14V
16V
18V
20V
Current density, mA/cm2
Time, s
8V
compound 5
d = 0.83 μm
electric field of
1.68*10^5 V/cm
295K
288K
281K
274K
270K
263K
258K
253K
240K
230K

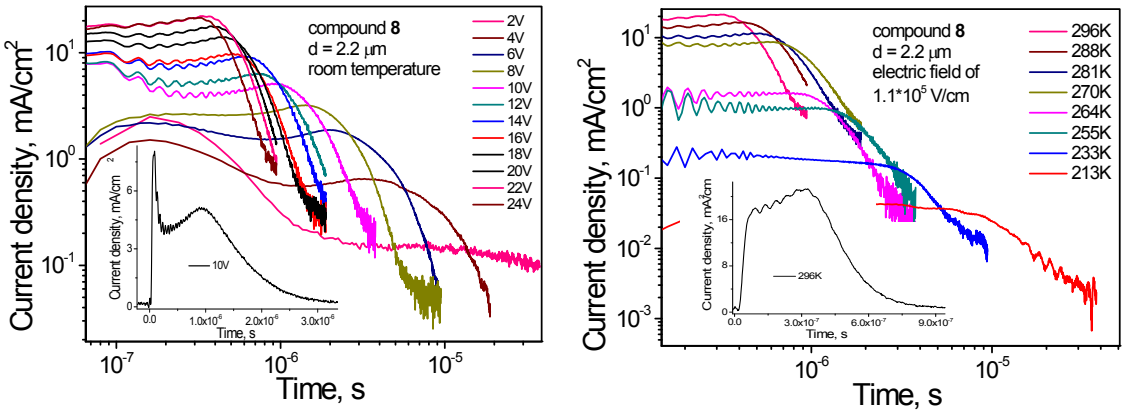
b)


compound 6
d = 0.63 μm
room temperature
4V
6V
8V
10V
12V
14V
16V
Current density, mA/cm2
Time, s
8V
compound 6
d = 0.63 μm
electric field of
1.6*10^5 V/cm
294K
289K
280K
274K
268K
252K
243K

c)

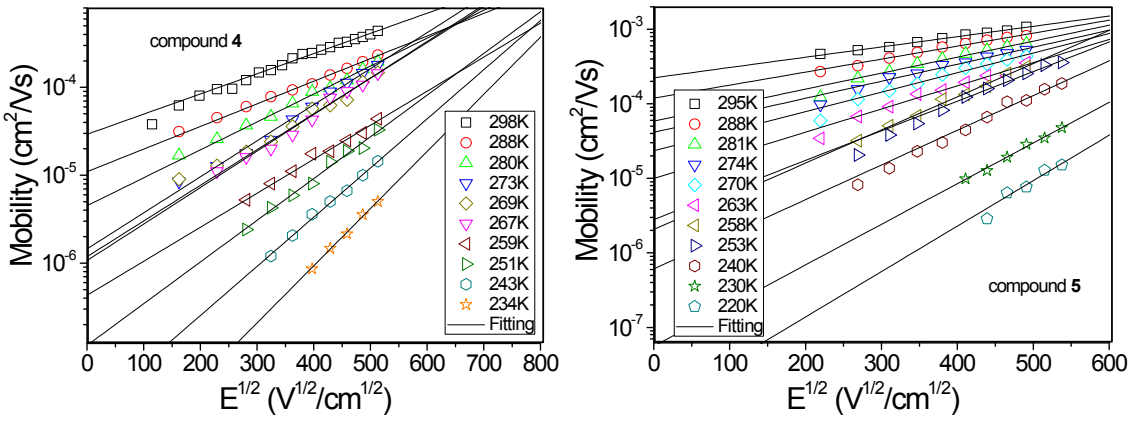


d)



e)

Fig. S5 Current transient pulses for the layers of the studied compounds 4-8, parametric in the electric field (the left) and temperature (the right) (a-e).



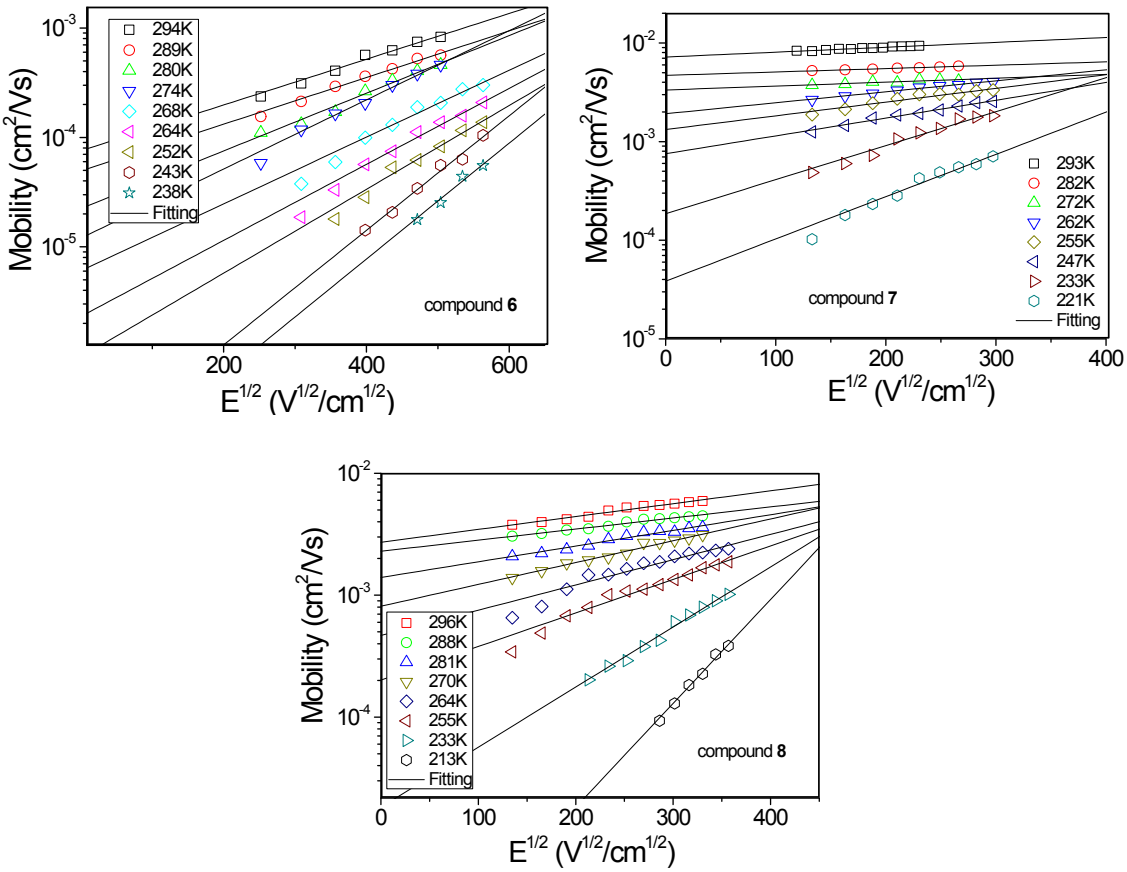


Fig. S6 Electric field dependencies of the mobility for the layers of the studied compounds at the different temperatures.

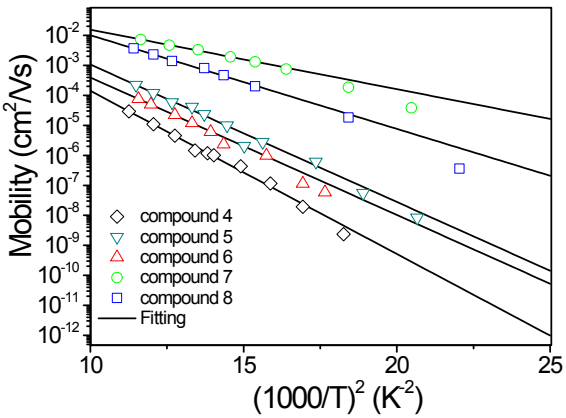


Fig. S7 The logarithm of the zero-field mobility vs $(1000/T)^2$. The zero-field mobility values were obtained by the fitting of the data in Fig. S6 as $\mu=\mu_0 \cdot exp(\beta \cdot E^{1/2})$ at the electric field E=0.

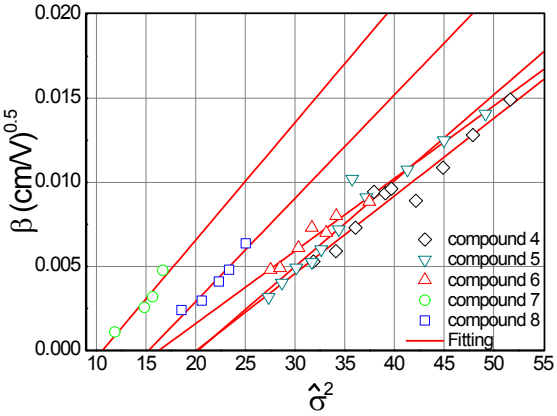


Fig. S8 The temperature dependence of the field dependencies of the mobility.

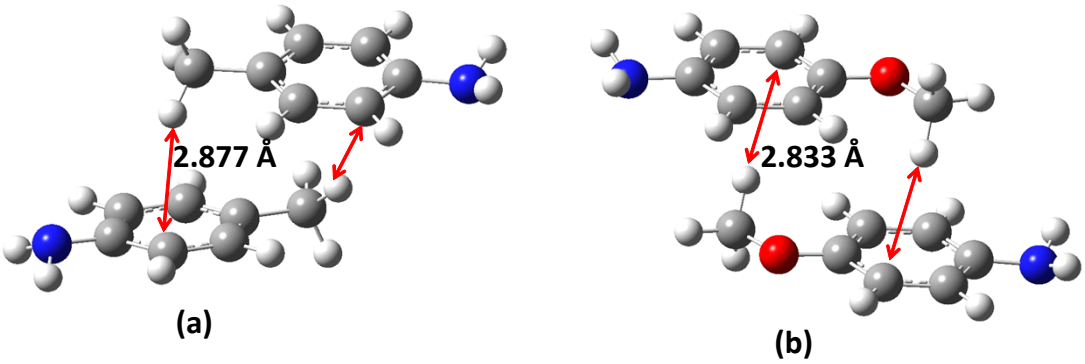
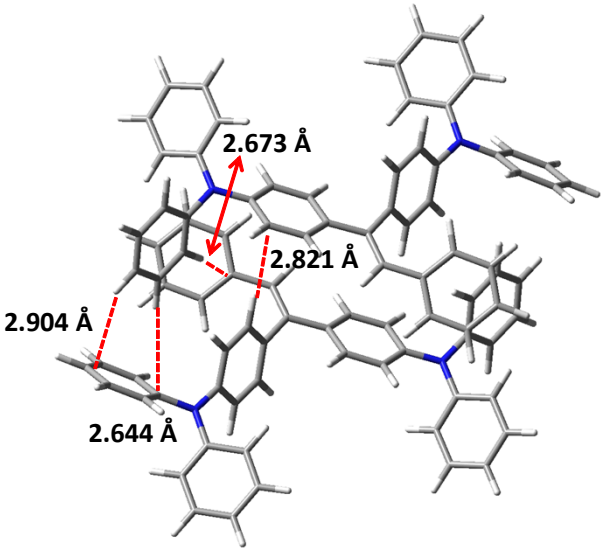
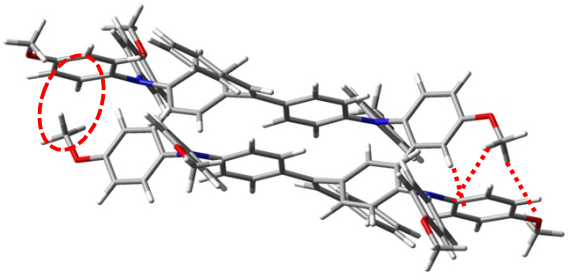


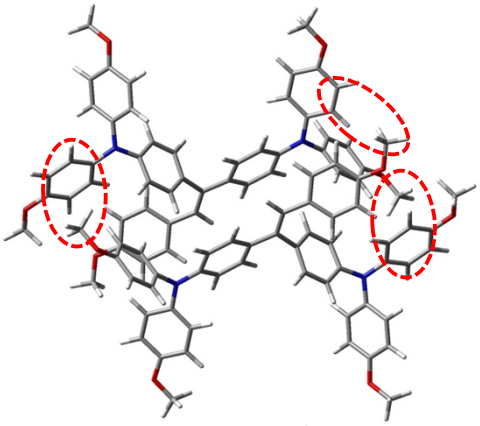
Fig. S9 Hypothetical dimers for (a) methyl- and (b) methoxy substituted anilines, optimized at the ωB97XD/6-31G(d,p) level.



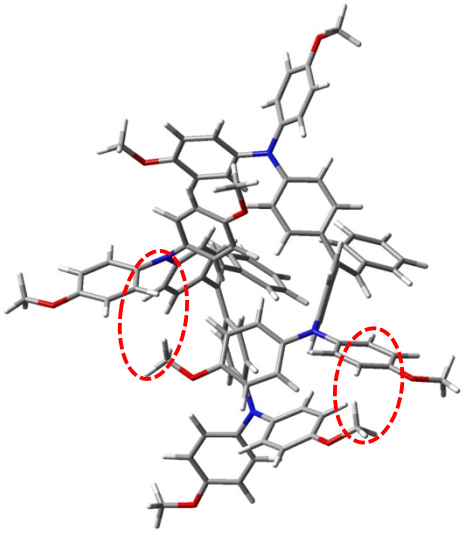
Compound 4- Dimer 6



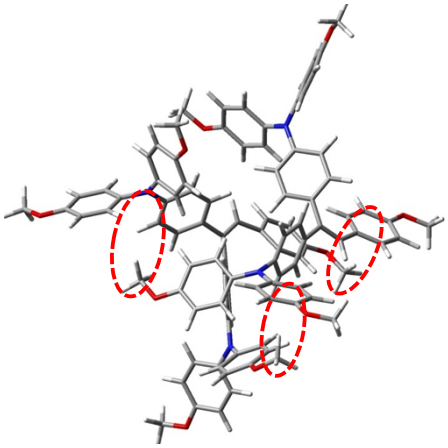
Compound 5- Dimer 6



Compound 6- Dimer 6



Compound 5- Dimer 5



Compound 6- Dimer 5

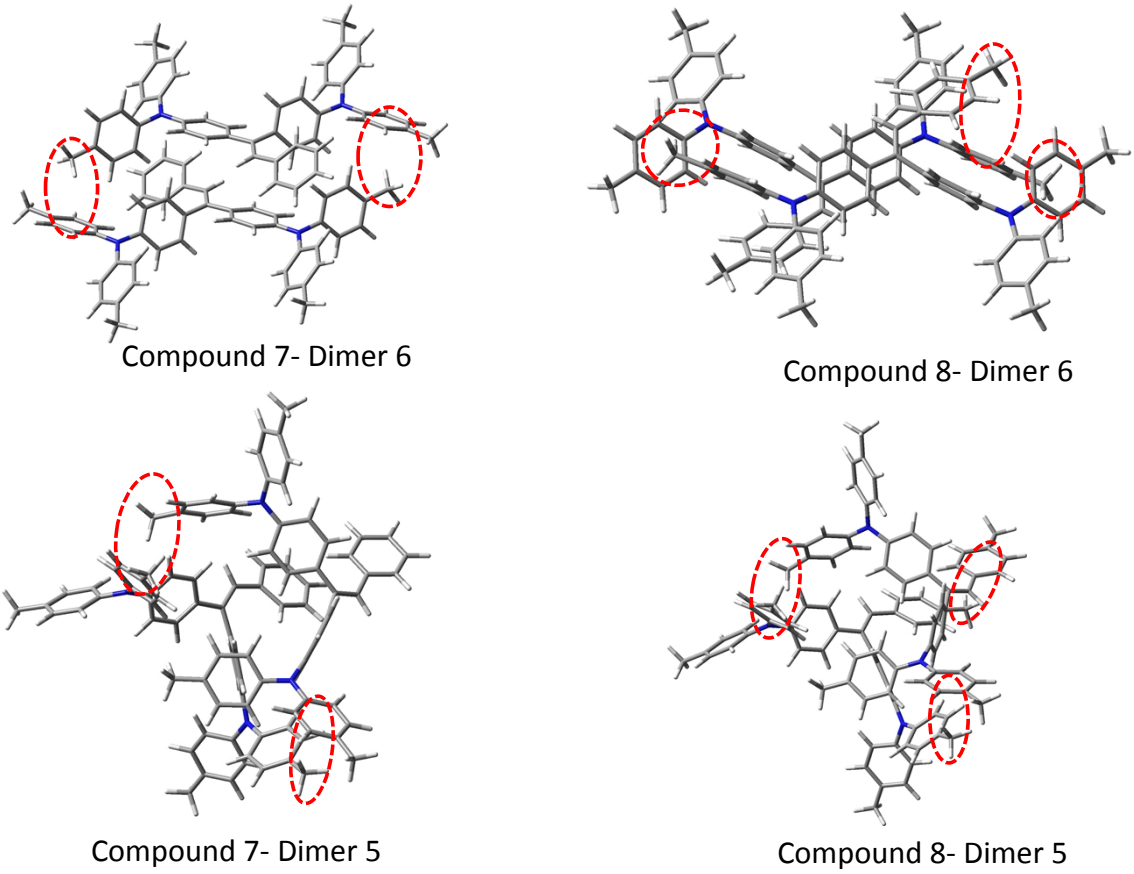


Fig. S10 Global view of the two most strongly interacting dimers for compounds 4-8. In each case, the moieties involved in short contacts are highlighted by dashed red circles. The C-H…..π short contacts in the highlighted regions vary in the range 2.6-3.1 Å.

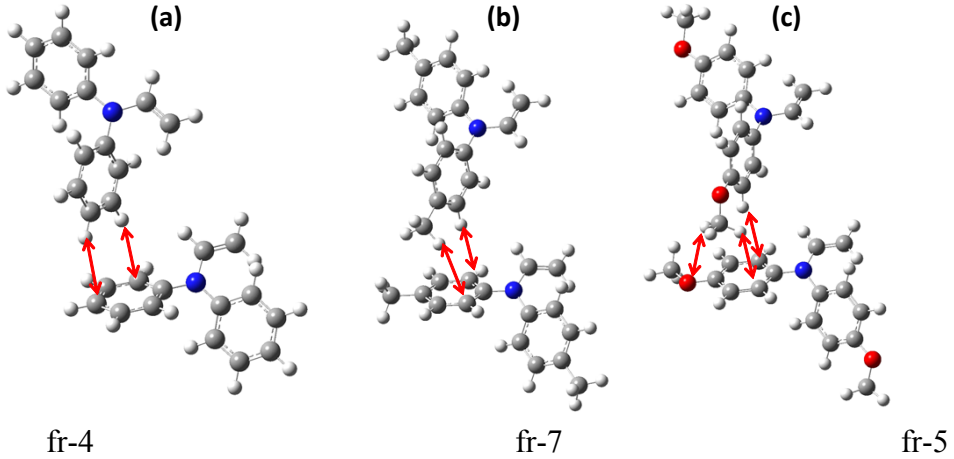


Fig. S11 Fragments fr-4, fr-7, and fr-5 extracted from Dimer-6 of compounds (a) 4, (b) 7, and (c) 5 involved in H-bonds. The short contacts are highlighted by the red arrows. In order to isolate only one Ph-Me or Ph-OMe moiety involved in H-bonds, only two phenyl groups out of the triphenylamine groups are retained, with the rest of the molecules being replaced by an ethylene fragment.

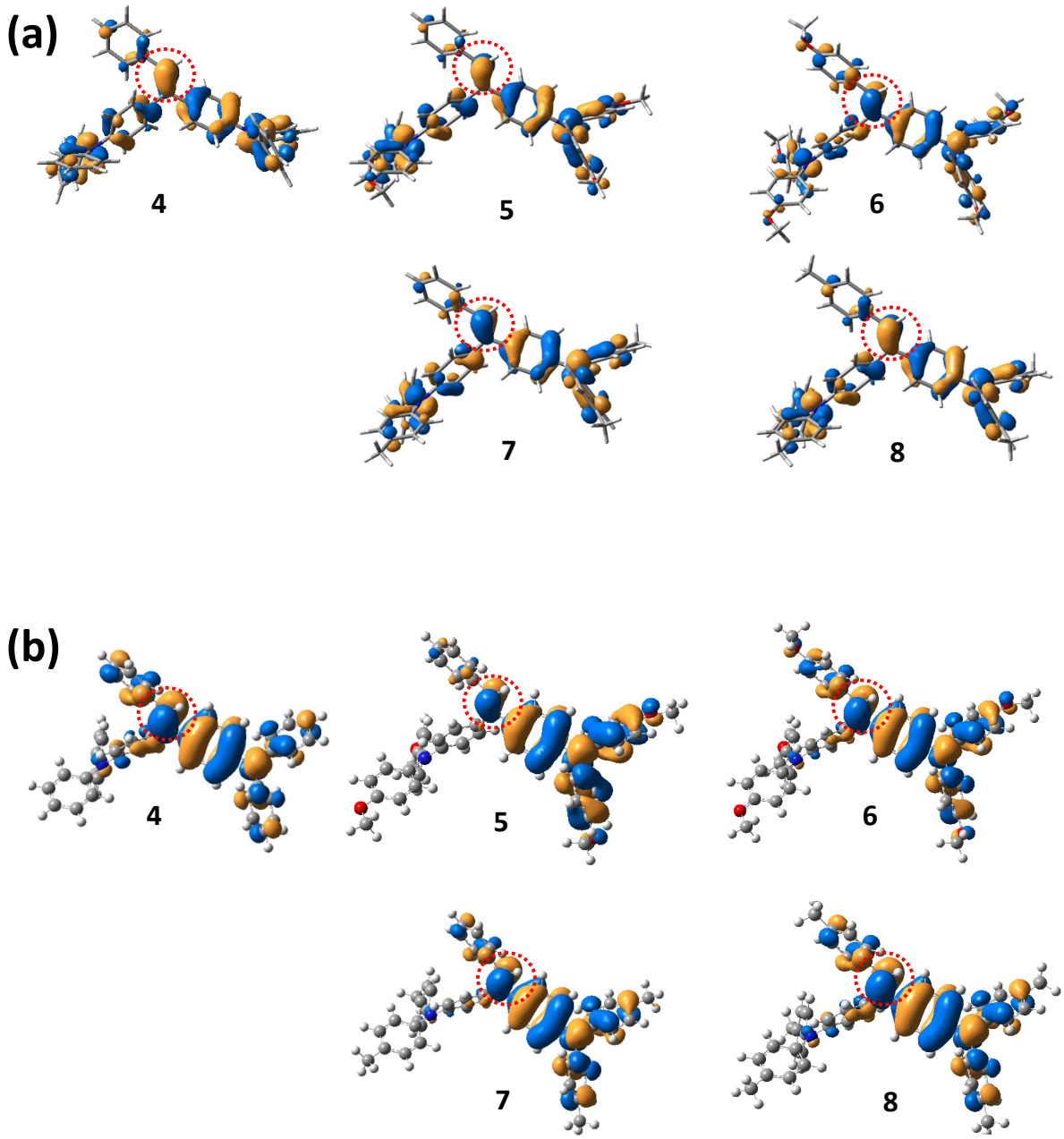


Fig. S12 HOMO pictograms of compound 4-8 obtained in (a) the neutral at the B3LYP/6-31G(d,p) level and (b) the cationic state at the LC-ωPBE/6-31G(d,p) level. The ethylenic moiety is highlighted by the red dashed circles. In all cases, HOMO is dominantly localized on the phenyl-ethenyl moiety and on only one of the TPA moieties.

Table S1. Theoretical electronic and optical characteristics of compounds 4-8, obtained at the B3LYP/6-31G(d,p) level "in gas phase".

Compound	IP, eV [a]	ε_{HOMO} eV	ε_{LUMO} eV	*Gap* eV	$S_0 \rightarrow S_1$ [b] eV(nm)	α [c] bohr^3
4 (H,H)	5.68	-4.85	-1.25	3.60	3.26(380.1)	506 (504)
5 (H,OMe)	5.33	-4.52	-1.05	3.47	3.07(403.7)	587 (524)
6 (OMe,OMe)	5.22	-4.43	-0.91	3.52	3.11(398.1)	610 (532)
7 (H,Me)	5.53	-4.70	-1.16	3.54	3.13(396.3)	566 (516)
8 (Me,Me)	5.35	-4.66	-1.12	3.54	3.13(395.6)	582 (519)

[a] Adiabatic IP values. [b] Theoretical $S_0 \rightarrow S_1$ absorption wavelengths. [c] Static isotropic polarisabilities. In parentheses are shown isotropic polarisability of the core-compounds (corresponding to the same number of electrons for each compound), estimated by subtracting the contribution of the substituents (R=H, CH_3, OCH_3) from the total polarizability values.

Table S2. Electronic couplings (eV) between the monomer HOMOs for selected model dimers of compounds 4-8, obtained at the B3LYP/6-31G(d,p) level by using the dimer geometries optimized at the ωB97XD/6-31G(d,p). All calculations were performed "in gas phase".

	Dimer 1	Dimer 2	Dimer 3	Dimer 4	Dimer 5	Dimer 6	Average
4 (H,H)	0.020	-0.002	-0.020	-0.006	-0.011	-0.021	0.013
5 (H,OMe)	-0.010	0.006	-0.007	0.009	-0.017	0.037	0.014
6 (OMe,OMe)	0.009	0.005	-0.007	0.010	-0.018	0.042	0.015
7 (H,Me)	0.012	0.006	-0.001	0.004	0.001	0.003	0.004
8 (Me,Me)	0.012	0.006	-0.001	0.013	-0.002	-0.026	0.010

[a] Absolute values

Table S3. Dissociation energies (ZPE and BSSE corrected, kcal/mol) for selected model dimers of compounds 4-8, obtained at the the ωB97XD/6-31G(d,p). All calculations were performed "in gas phase". Dimer 6 corresponds to the geometry of a dimer extracted from the crystal structure of compound 4.

	Dimer 1	Dimer 2	Dimer 3	Dimer 4	Dimer 5	Dimer 6	Average
4 (H,H)	6.1	12.3	13.5	15.3	22.3	22.9	15.4
5 (H,OMe)	12.4	15.2	15.8	20.1	22.4	27.2	18.9
6 (OMe,OMe)	12.9	15.8	16.1	22.2	24.6	30.8	20.4
7 (H,Me)	10.2	13.0	15.8	20.8	21.8	24.0	17.6
8 (Me,Me)	10.7	13.8	16.0	22.7	23.5	27.0	19.0

Table S4. Intermolecular distance (Å) between monomers in selected model dimers of compounds 4-8, obtained at the the ωB97XD/6-31G(d,p). Each individual value for a given

compound and a given dimer corresponds to average of the shortest distances of each atom of one monomer with the atoms of the second monomer. All calculations were performed "in gas phase". The average values in parentheses are calculated by removing from each fragment the atoms corresponding to the methoxy or methyl groups.

	Dimer 1	Dimer 2	Dimer 3	Dimer 4	Dimer 5	Dimer 6	Average
4 (H,H)	3.82	3.99	4.12	3.84	3.88	3.89	3.92
5 (H,OMe)	3.73	3.77	3.83	3.88	3.97	3.84	3.84 (3.94)
6 (OMe,OMe)	3.73	3.79	3.80	3.88	3.93	3.86	3.83 (3.90)
7 (H,Me)	3.79	3.89	3.90	3.85	3.98	3.86	3.88 (3.92)
8 (Me,Me)	3.79	3.89	3.89	3.83	3.86	3.85	3.85 (3.91)

Table S5. Hole transport parameters for the layers of compounds 4-8.

Compound	σ , eV	μ_0 , cm^2/Vs	C, $(cm/V)^{1/2}$	Σ
4 (H,H)	0.145	39.2	0.00046	4.59
5 (H,OMe)	0.133	40.9	0.00043	4.05
6 (OMe,OMe)	0.133	15.3	0.00053	4.6
7 (H,Me)	0.087	1.5	0.0007	3.26
8 (Me,Me)	0.11	13.5	0.00061	3.91

Table S6. Intermolecular interaction energy (kcal/mol) and different contributions (induction, electrostatic, exchange, and dispersion) in the case of model dimers constituted by *para*-methyl and *para*-methoxy aniline. The values were calculated at the SAPT0/jun-cc-pvdz level (Annex II).

	Exchange	Dispersion	Exchange + Dispersion	Electrostatic	Induction	Interaction Energy	Disp./El.
CH_3	10.1	-7.6	2.4	-4.4	-1.3	-3.3	1.7
O-CH_3	12.4(+23%)	-8.6(+13%)	3.8	-6.6(+50%)	-1.7(+33%)	-4.5(+38%)	1.3
Difference	2.3	-1.0	1.4	-2.2	-0.4	-1.2	

Table S7. Variation of C-H bond-lengths (Å) involved in H-bonds in the Dimer-6 (Fig. S2 and main text) of compounds 4-8. The difference with respect to 4 is given in parentheses.

	4 (H,H)	5 (H,OMe)	6 (OMe,OMe)	7 (H,Me)	8 (Me,Me)
(methyl)C-H	-	-0.0006	-0.0014	-0.0001	-0.0003
(Ph)C-H	-0.0008	-0.0009 (-0.00007)	-0.0010 (-0.00012)	-0.0008 (0.0000)	-0.0004 (0.0004)
(Ph)C-H…..π	2.713	2.722 (0.010)	2.721 (0.009)	2.671 (-0.042)	2.731 (0.018)

Table S8. Intermolecular interaction energy and different contributions (induction, electrostatic, exchange, and dispersion) in the case of Dimer-6 of compounds 4-8. The values were calculated at the SAPT0/jun-cc-pvdz level (Annex II). Note that the ordering of the compounds follows that of the increasing interaction energy. All energy values are in kcal/mol.

	Exchange	Dispersion	Exchange + Dispersion	Electrostatic	Induction	Interaction Energy	Disp./ El.
4 (H,H)	48.6	-40.7	8.0	-20.9	-5.5	-18.4	1.95
7 (H,Me)	53.2	-44.8	8.4	-22.6	-6.3	-20.5(-2.1)	1.99
8 (Me,Me)	55.3	-47.1	8.2	-23.7	-6.2	-21.6(-3.2)	1.99
5 (H,OMe)	56.1	-47.5	8.6	-25.0	-7.1	-23.5(-5.1)	1.90
6 (OMe,OMe)	59.2	-50.0	9.2	-26.5	-7.7	-25.0(-6.6)	1.89

Table S9. Intermolecular interaction energy and different contributions (induction, electrostatic, exchange, and dispersion) in the case of Dimer-6 of compounds 4, 5, 7, and of fragments (fr-4, fr-5, fr-7) extracted from their dimers (Annex II and Fig. S11). The values were calculated at the SAPT0/jun-cc-pvdz level (Annex II). All energy values are in kcal/mol. In order to directly compare the values of the fragments (only one R=CH_3, OCH_3 involved in H-bonds) with those of the real compounds (two R=CH_3, OCH_3 involved in H-bonds), the values for the fragment are multiplied by two. The IE values in parentheses correspond to the percentage of IE of fragments fr-4, 7, 5 with respect to the IE of the corresponding reals compounds 4, 7, 5.

	dispersion+exchange			electrostatic			induction			Interaction Energy		
	H	CH_3	OCH_3	H	CH_3	OCH_3	H	CH_3	OCH_3	H	CH_3	OCH_3
absolute values												
fragments-4,7,5 [a]	2.5	2.8	3.1	-4.0	-5.4	-7.0	-1.4	-1.6	-2.0	-2.9(16%)	-4.2(20%)	-5.9(25%)
Full Comp. 4, 7, 5	8.0	8.4	8.6	-20.9	-22.6	-25.0	-5.5	-6.3	-7.1	-18.4	-20.5	-23.5
relative values with respect to R=H												
fragments-4,7,5 [a]	0.0	0.3	0.6	0.0	-1.4	-3.0	0.0	-0.2	-0.6	0.0	-1.3	-3.0
Full comp. 4, 7, 5	0.0	0.4	0.6	0.0	-1.7	-4.1	0.0	-0.7	-1.6	0.0	-2.0	-5.1
□*(Full-fragment)*	-	*0.1*	*0.0*	-	*-0.3*	*-1.1*	-	*-0.5*	*-1.0*	-	*-0.7*	*-2.0*

[a] Values multiplied by two.

Table S10. HOMO energies (eV) for each fragment of six dimer types of each compound 4-8. Each HOMO energy is calculated at the geometry of the corresponding dimer, and in the presence of the second fragment. These energies are calculated at the B3LYP/6-31(d,p) level during electronic coupling calculations (see experimental section for electronic coupling calculations). The difference between minimum and maximum values of each compound is given it the last line.

4	5	6	7	8
-4.994	-4.605	-4.519	-4.757	-4.739
-4.857	-4.561	-4.471	-4.696	-4.682
-4.787	-4.561	-4.471	-4.681	-4.671
-4.784	-4.525	-4.466	-4.657	-4.617
-4.783	-4.506	-4.403	-4.655	-4.616
-4.781	-4.494	-4.400	-4.647	-4.612
-4.775	-4.482	-4.399	-4.645	-4.603
-4.766	-4.477	-4.390	-4.628	-4.594
-4.761	-4.441	-4.378	-4.627	-4.589
-4.754	-4.432	-4.355	-4.617	-4.581
-4.753	-4.426	-4.342	-4.617	-4.581
-4.753	-4.420	-4.337	-4.604	-4.578
0.241	0.185	0.182	0.153	0.161

Annex I. Nature of intermolecular interactions

We suspect the hydrogen bonds established by means of methyl and methoxy groups to be the dominant factor explaining the stronger intermolecular interactions in 5-8 as compared to 4. In order to check for this assumption, we consider different hypothetical dimers.

1- Para methyl-aniline and para-methoxy aniline models. We firstly estimate the relative potential of methoxy and methyl groups for establishing efficient C-H….π hydrogen bonds, by considering dimers constituted by para-methyl and para-methoxy aniline. The dimer geometries optimized at the wB97XD/6-31G(d,p) level are shown in Figure S9. (Me)C-H….π(Ph) and (OMe)C-H….π(Ph) short contacts of 2.877 Å and 2.833 Å respectively were found. Following Nishio[1-3] and Hobza&Havlas[4], we consider these short contacts as improper (blue shifting) hydrogen bonds. One of the general characteristics of the improper H-bonds is the shortening

of the C-H bond-lengths (by 0.001-0.002 Å),[1-4] and increase of vibrational wavenumbers (blueshifting), as opposed to classical H-bonds, in which bond-length elongation and decrease of the vibrational wavenumbres (red shifting) were observed. In good agreement with these definitions and typical values, the C-H bond-lengths involved in H-bonds in para-substituted aniline dimer are shortened by 0.0003 Å and 0.0008 Å for methyl and methoxy cases respectively, as compared to the isolated monomers. Accordingly, increased (blue shifted) wavenumbers by 6 cm^{-1} and 17 cm^{-1} respectively were found. Note that bond-length shortenings correspond to averages over the three C-H bonds of a methyl group, so that that the exact shortenings of the C-H bonds really involved in H-bonds are even larger (by roughly 3 times).

The intermolecular interaction energies of each dimer were obtained by performing (SAPT)[6] calculations at the SAPT0/jun-cc-pvdz level, and the results are collected in Table S6. Both models exhibit efficient H-bonds of 3.3 kcal/mol and 4.5 kcal/mol (1.6 kcal/mol and 2.3 kcal/mol per individual H-bond) for methyl- and methoxy substituted anilines respectively. As expected, the C-H….π(Ph) H-bonds are substantially activated by the presence of oxygen atoms, exhibiting strong increase of the electrostatic contribution (by 50%, Table S6) as compared to the methyl substituted aniline. The dispersion-to-electrostatic ratios of 1.7 and 1.3 respectively for methyl and methoxy cases (Table S6) suggest a dominant dispersion contribution in both cases, but with increased contribution from the electrostatic interactions in the case of methoxy groups as compared to the methyl case. This trend (increasing of interaction strength with the increasing electrostatic contributions) is in line with the dominant electrostatic character indicated for the classical and stronger (red-shifting) H-bonds.

The pertinent information to retain from this example is that both methoxy and methyl groups have the potential to establish efficient C-H….π(Ph) H-bonds, with the strongest ones coming from the methoxy groups. We highlight additionally that the value of 1.6 kcal/mol

found here for the (Ph-H2)C-H…….π(Ph) H-bond is much larger than the 0.3 kcal/mol reported for H_3C-H….π(Ph) H-bonds,[1-4] indicating some activation effect due to the phenyl groups.

However, the models presented here correspond to an ideal geometrical orientation of the C-H bond with respect to π(Ph), which may not reach their equilibrium in the presence of other intermolecular interactions in more complex systems. This aspect will be addressed in the following.

2- H-bonds in the case of compounds 4-8. As a means to check for the presence of the H-bonds in the solid films of the real compounds (4-8), we firstly consider the model Dimer-6, corresponding to the strongest intermolecular interaction energy (Figure S2 and Table S3).

2.1-Geometrical insights. The geometry of this model dimer was extracted from the crystal structure of compound 4 (Figure S1), in which six (phenyl)C-H….π short contacts ranging between 3.02-3.15 Å were found. Starting from this geometry, and by adding methoxy- or methyl groups as appropriate, the same type of model dimer (Dimer-6) was simulated for compounds 5-8 (see Annex III in SI for the Cartesian coordinates of Dimer-6 of compounds 4-8).

We firstly focus on the evolution of the (phenyl)C-H….π interactions across the series, and compare the (methyl)C-H…….π distances in a second time. In the optimized geometry of the isolated ("gas phase") Dimer-6 of compound 4, the (phenyl)C-H….π distances roughly range between 2.64-2.90 Å. The C-H bond-lengths involved in H-bonds are shortened by 0.0004-0.0010 Å for compounds 4-8 (Table S7), as compared to the other C-H bond-lengths on the same phenyl groups which are not involved in H-bond interactions. *Non-negligible H-bonds by means of these (Ph)C-H….π interactions can thus be deduced for compound 4.*

We note that these (phenyl)C-H….π are present in all compounds 4-8. Interestingly, upon methoxy substitutions of compound 4, the additional shortening of the (Ph)C-H bonds in 5 and 6 as compared to the non-substituted compound 4 are very small (roughly -0.0001 Å, Table

S7), whereas the (Ph)C-H…..π distances slightly increase. These two opposite effects considered together, we deduce that the (Ph)C-H….π interaction strengths are not importantly modified upon methoxy substitutions. In the case of the methyl substituted compound 8, slightly shorter (Ph)C-H bond-length and longer (Ph)C-H…..π distances as compared to 4 were found, whereas for compound 7, no change in (Ph)C-H bond-length but shorter (Ph)C-H…..π distances were found. Again, opposite and slight geometrical modifications were observed for these compounds, supporting the hypothesis that the (Ph)C-H…..π interaction strengths are not importantly modified upon methoxy and methyl substitutions. This conclusion will be comforted by the numerical results presented in the following.

We suggest consequently that the increase in interaction energy upon methyl- and methoxy substitutions can, in great part, be attributed to the additional C-H….π short contacts established by means of methoxy[5] and methyl[1-4] groups. Figure S10 highlights different molecular moieties of Dimer-6 of compounds 5-8 involved in CH3….π or CH3…O short contacts, which C-H….π distances roughly range between 2.9-3.1 Å. C-H bond-length shortenings by 0.0001-0.001 Å were found in methyl- and methoxy groups involved in H-bonds as compared to those not involved in H-bonds, the shortening being more important in the case of methoxy substituted compound 6 (Table S7). We remember that these last values correspond to averages over the three C-H bonds of a methyl group, so that the exact shortenings of the C-H bonds really involved in H-bonds are even larger. Note that the change in the C-H bond-lengths of Dimer-6 of compounds 4-8 are less important than in the case of the substituted aniline model compounds, probably due to the out-of-equilibrium of the H-bond geometries in compounds 4-8.

All in all, it can be safely deduced that the additional H-bonds induced by the methoxy and methyl groups contribute significantly to additional strengthening of the intermolecular interactions. Moreover, as discussed above in the case of para-methyl and para-methoxy aniline

dimers, the methoxy groups in compounds 5-6 are expected to H-bind more strongly than the methyl groups in compounds 7-8.

Based on these considerations, and limiting the comparison to the only H-bond contributions, the intermolecular interaction energy is expected to increase in the order 4<7<8<5<6, in good agreement with the trend of the total interaction energies (Table 3).

We finally mention that similar arguments apply to the intermolecular interactions in other model dimers (Dimer-1 through Dimer-5), with the only difference being due to the number of short contacts.

2.1-Numerical insights. As a means to get more quantitative insight on these intermolecular interactions, symmetry adapted perturbation theory (SAPT)[6] calculations at the SAPT0/jun-cc-pvdz level were conducted for the Dimer-6 of compounds 4-8, and the results are collected in Table S8. We note that the trend of the SAPT0 interaction energies across compounds 4-8 is identical to the trend obtained by the calculations at the DFT level (Table S3).

While giving insighting information, the SAPT0 calculations shown in Table S8 does not allow to distinguish explicitly between, on the one hand, the contributions to the intermolecular interactions coming from the additional H-bonds established upon methyl and methoxy substitutions, and on the other hand, the contributions due to the strengthening of other interactions.

In order to explicitly estimate these two individual effects, from the optimized geometries of Dimer-6 in different compounds we have extracted the appropriate fragments directly involved in (Me,OMe)C-H….π H-bonds. We limit this comparison to compounds 4, 5, and 7. We remember that in Dimer-6 of compounds 5 and 7, there are only two OMe or Me groups involved in new H-bonds (Figure S10). For each of these compounds, we consider consequently fragments containing only one methyl or methoxy group, out of the two groups involved in H-bonds. The isolated fragments will be reported as fr-4, fr-5, and fr-7 (Figure S11). The missing atoms for each compound are replaced by one ethenyl fragment. Note that preserving the real

phenyl group instead of –C2H3 in fragments fr-4, 5, 7 (Figure S11) would induce one additional (Ph)C-H….π(Ph) H-bond (the short contact of 2.821 Å in Dimer-6 of compound 4, Figure S10), which would blur the conclusions on the specific role of the (Me,OMe)C-H….π H-bonds.

In the Table S9 are collected the SAPT0 results for fr-4 (R=H), fr-5 (R=OCH_3), fr-7 (R=CH_3), along with the results for compounds 4, 5, and 7. The contribution of the additional (Me,OMe)C-H….π H-bonds to the total *IE* of each compound is highlighted by the (vertical) comparison between the absolute values. The comparison for instance, between the intermolecular *IE* in fr-5 (-5.9 kcal/mol) and the corresponding value of the real compound 5 (-23.5 kcal/mol) allows to deduce that, out of the total *IE* of -23.5 kcal/mol, -5.9 kcal/mol (25%) are due to the two (Me,OMe)C-H….π H-bonds, whereas -23.5+5.9=-17.6 kcal/mol (75%) are due to other interactions (probably stemming from the dispersion and electrostatic contributions in π-π stacked moieties and the (Ph)C-H….π H-bonds already present in the un-substituted compound 4). However, the pertinent information is that 25% of the total intermolecular *IE* comes specifically from the two methoxy groups involved in the two new H-bonds, which constitutes a quite important contribution to the intermolecular binding energy in this compound. As expected, the contribution of these H-bonds decreases to 20% in the case of methyl substituted compound 7 (Table S9).

Now we focus on the contribution of the (Me,OMe)C-H….π H-bonds to the evolution of intermolecular *IE* across the series 4-8. In Table S9, this is highlighted by the comparison between the relative values with respect to compound 4. In the following, the increase in intermolecular interaction energy between a substituted species and the non-substituted one will be reported as Δ*IE(fragment)* and Δ*IE(real)*, depending respectively if fragments or real compounds are compared. In the case of methoxy substitutions for instance, the intermolecular *IE* increases by Δ*IE(fragment)*= -3 kcal/mol (from -2.9 to -5.9 kcal/mol), which is roughly 60% of Δ*IE(real)*= -5.1 kcal/mol (from -18.4 to -23.5 kcal/mol, Table S9). This result is very

important, as it means that, when considering the increase in intermolecular *IE* upon methoxy substitution of compound 4, the main contribution (60%) stems from the new H-bonds established by means of methoxy groups. The difference $\Delta IE(real) - \Delta IE(fragment) =$ -2 kcal/mol seems to be due to the electrostatic (-1.1 kcal/mol) and the induction (-1 kcal/mol) terms (Table S9), roughly related to the enhancement of these contributions in the π- π stacked moieties and in the H-bonds already present in the un-substituted compound 4. This last result additionally confirms our assumption (see above) that the (Ph)C-H….π interaction strengths are not importantly modified upon methoxy and methyl substitutions.

A similar comparison in the case of R=CH3 results in $\Delta IE(fragment) =$ -1.3 kcal/mol and $\Delta IE(real) =$ -2 kcal/mol (Table S9), indicating that 66% of the increase in *IE* upon methyl substitutions comes from the -CH3….π(Ph) H-bonds. The remaining 33% seems to be mainly related to the increase in induction energy.

We finally note that the fragmentation proposed in this study (Figure S11) is source of some errors coming from the truncation of the molecular backbone. However, while the numerical values given here should be considered as qualitative ones, the trends and the general conclusions remain pertinent. This is comforted by our additional test calculations (-NH2 moiety instead of –N(Ph)(C2H3) one in fr-4, 5, 7, Figure S11): going from more truncation (-NH2 moiety) to less truncation (–N(Ph)(C2H3) moiety) in these models, results in increased H-bond strength from -2.3 kcal/mol to -3 kcal/mol respectively. Consequently, our conclusion on the dominant role of the new H-bonds becomes more pertinent in the frame of a more realistic (less truncated) fragment model.

Based on these geometrical and energy observations, we conclude that the increase in the intermolecular interaction energy of compounds 5-8 as compared to 4 is principally due to the new H-bonds established by means of methyl and methoxy groups.

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Annex II. Temperature dependent TOF results and analysis

To better understand the effect of molecular-polarity modifications on the charge transport properties, we explored the field and temperature dependencies of the mobility in vapor deposited triphenylamine twin compounds containing methoxy- and methyl groups, using the time-of-flight (TOF) method [1]. We analyzed the experimental results within the Gaussian disorder model [2]. The Gaussian disorder model predicts the field and temperature dependencies of the mobility given as:

$$\mu = \mu_0 \exp[-(\frac{2\hat{\sigma}}{3})^2]\exp[C(\hat{\sigma}^2 - \Sigma^2)E^{1/2}] \quad (1)$$

Here, σ is the energy width of the hopping site manifold, and Σ is the positional disorder due to a distribution of intersite distances; C is a constant and $\hat{\sigma} = \sigma/kT$.

Figure S5 shows a set of TOF signals for the layers of the studied compounds, parametric in the electric field and temperature. A Poole−Frenkel-like field dependencies of the mobility μ of the studied compounds at the different temperatures are plotted in Figure S5. To determine the values of σ for the studied compounds using Eq. (1), the temperature dependencies of the zero-field mobility ($\mu_{(E=0)}$) were plotted semilogarithmically versus $1000/T^2$ (Figure S6). The zero-field mobility values were obtained by the extrapolation of the data to the electric field E = 0 as illustrated in Figure S5. Using Eq. (1), σ can be determined from the slope of a plot of

log $\mu_{(E=0)}$ versus T^{-2}. Figure S7 shows the field dependencies of the mobilities at the different temperatures. The results are plotted as $\beta = d\ ln\mu/dE^{0.5}$ versus $\hat{\sigma}^2$. The values of Σ and C can be determined from the slope and intercept of a plot of β versus $\hat{\sigma}^2$ (Figure S7). Hole transport parameters for the layers of compounds 4-8 are presented in Table S5.

In view of the limited window of temperature measurements (constrained by the glass transition temperatures and the temperatures at which the hole transport becomes dispersive), and the resulting graphical uncertainties (Figure S8), the absolute values of C and Σ might contain errors, and should be considered with care. However, their trends across the series 4-8 can be reliably discussed. In order to check for the reliability of the large μ_0 values (Table S5), we have re-considered compound 5, presenting the clearer TOF signals (Figure S5b). Once removing some points from the plots in Figure S6 (258 °C and below), a μ_0 value of roughly 20 cm^2/Vs is still obtained, comforting the reliability of the globally large μ_0 values across the series. Finally, we note that the dispersive-like signals obtained in the case of compound 4 suggest that the mobility value for this compound should be even smaller and the σ value even larger, which does not modify the analysis and conclusions drawn in the main text.

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Annex III. Cartesian coordinates (Å) of Dimer-6 for compounds 4-8, optimized at the ωB97XD/6-31G(d,p) level in gas phase

Compound 4

N	24.09683000	13.12272600	8.56818700
N	21.60187100	6.19866400	15.03924400
C	20.45291200	9.16999800	12.26334900
C	20.10735200	9.27962400	13.61236600
C	20.49696900	8.31182200	14.52779500
C	21.23722100	7.20519200	14.10756200
C	18.67602500	10.42812700	11.08235700
C	20.79055600	11.67763800	9.40304500
C	21.04145700	10.97844700	10.59235200
C	20.58984700	5.61347000	15.83422400
C	22.94517600	5.77908800	15.13626700
C	23.74935500	14.34571600	7.92530800

C	23.09708300	12.40220100	9.24342500
C	21.23146100	8.08103800	11.85850300
C	19.98917400	10.20049000	11.29194300
C	21.78674400	12.38014000	8.74510800
C	17.51138700	9.66073500	11.56000600
C	21.60911700	7.09950900	12.76462100
C	23.98486400	6.69345600	14.92878600
C	16.39242200	7.63426900	12.29623100
C	22.35605800	11.00584500	11.07548600
C	19.35904000	5.27505500	15.26259500
C	24.08159200	14.55373000	6.58607200
C	25.46287400	12.77678900	8.66740800
C	23.36441100	11.69332900	10.41865100
C	20.79678400	5.37621900	17.19719900
C	26.43163300	13.77327500	8.82833700
C	17.53785900	8.28836000	11.85938400
C	23.08684700	15.34213000	8.63938300
C	18.35249200	4.71863100	16.04356000
C	16.28363800	10.32763400	11.66869400
C	18.56349800	4.47411000	17.39785500
C	22.74698200	16.53455200	8.01415300
C	27.77735500	13.43407200	8.90582400
C	25.30828500	6.27857300	15.00729600
C	19.79216300	4.80269700	17.96650800
C	28.17786500	12.10275900	8.83955300
C	23.26131200	4.44718300	15.42986500
C	25.62144800	4.95685500	15.31122400
C	24.58873700	4.04847200	15.52558700
C	25.86845200	11.44001500	8.58289200
C	15.19294600	8.32687200	12.44505700
C	23.07062100	16.74605100	6.67682200
C	23.74552900	15.75419400	5.96829400
C	15.14099800	9.67883900	12.12097000
C	27.21426300	11.11006900	8.68080900
H	19.52727100	10.13651200	13.94119900
H	20.21815600	8.40259400	15.57258100
H	18.40902100	11.29503300	10.48202900
H	19.80357900	11.64385100	8.95350200
H	21.52071900	7.99191400	10.81572700
H	21.56000800	12.90143700	7.82119200
H	22.19358000	6.24446000	12.44077000
H	23.74815400	7.72813700	14.70530900
H	16.43845300	6.57383600	12.52498000
H	22.59845100	10.48261400	11.99430800
H	19.19776900	5.45805300	14.20482400
H	24.60256400	13.77276300	6.04142300
H	24.36938600	11.69049900	10.82508100
H	21.74877900	5.64250200	17.64407500
H	26.11887500	14.80980900	8.89544300
H	18.45797500	7.72802600	11.74485900
H	22.85037900	15.17956400	9.68435700
H	17.40019200	4.46837900	15.58654400
H	16.23746600	11.37990100	11.40993100
H	17.77947300	4.03163200	18.00338100
H	22.23504000	17.30491700	8.57996300
H	28.51686600	14.21926300	9.02940200

H	26.10096300	7.00166700	14.84196800
H	19.96727800	4.62456600	19.02283000
H	29.22862400	11.84148400	8.90703800
H	22.46332100	3.72860600	15.58223600
H	26.65627000	4.63874700	15.37934300
H	24.81491300	3.01193400	15.75577700
H	25.12198700	10.66519400	8.44375400
H	14.30536300	7.81425300	12.80199800
H	22.79548000	17.68031300	6.19740300
H	24.00291900	15.90931500	4.92515300
H	14.21346500	10.23245900	12.22794400
H	27.51188600	10.06809000	8.61627600
N	15.96940200	11.61432000	15.33108800
N	18.46436500	18.53836000	8.86002100
C	19.61333100	15.56704100	11.63592800
C	19.95889400	15.45741000	10.28691300
C	19.56927500	16.42520800	9.37148000
C	18.82901800	17.53183800	9.79170800
C	21.39021400	14.30891400	12.81692800
C	19.27567900	13.05940200	14.49623500
C	19.02478100	13.75859500	13.30692800
C	19.47638900	19.12356000	8.06504400
C	17.12105700	18.95792700	8.76299300
C	16.31687200	10.39132900	15.97396800
C	16.96915100	12.33484300	14.65585200
C	18.83477900	16.65600000	12.04077000
C	20.07706500	14.53655000	12.60733800
C	18.27949000	12.35690200	15.15417100
C	22.55485200	15.07630600	12.33927800
C	18.45712200	17.63752500	11.13464800
C	16.08137300	18.04355300	8.97047800
C	23.67382000	17.10277100	11.60305200
C	17.71018000	13.73119900	12.82379300
C	20.70718800	19.46198900	8.63667900
C	15.98462100	10.18331100	17.31320000
C	14.60335900	11.96026200	15.23186500
C	16.70182500	13.04371500	13.48062600
C	19.26945800	19.36080100	6.70206500
C	13.63459800	10.96377900	15.07092800
C	22.52838200	16.44868100	12.03990000
C	16.97938900	9.39491800	15.25989800
C	21.71373600	20.01841900	7.85571600
C	23.78260100	14.40940500	12.23058800
C	21.50273600	20.26293000	6.50141900
C	17.31925200	8.20249600	15.88512900
C	12.28887800	11.30298700	14.99343700
C	14.75795100	18.45842900	8.89196800
C	20.27407900	19.93432700	5.93276000
C	11.88837200	12.63430100	15.05971100
C	16.80491200	20.28982900	8.46938900
C	14.44477900	19.78014400	8.58803600
C	15.47748400	20.68853200	8.37366700
C	14.19778600	13.29703600	15.31638400
C	24.87329400	16.41016600	11.45422400
C	16.99559900	7.99099300	17.22245700
C	16.32068000	8.98284600	17.93097900

C	24.92524100	15.05819900	11.77831100
C	12.85197700	13.62698700	15.21846200
H	20.53897800	14.60052300	9.95808300
H	19.84808800	16.33443200	8.32669400
H	21.65721700	13.44201100	13.41725800
H	20.26265600	13.09318700	14.94577800
H	18.54552000	16.74512700	13.08354500
H	18.50622400	11.83560400	16.07808600
H	17.87265600	18.49257400	11.45849500
H	16.31809000	17.00887500	9.19396000
H	23.62779000	18.16320300	11.37430400
H	17.46778900	14.25443100	11.90497200
H	20.86845500	19.27899800	9.69445100
H	15.46364100	10.96427500	17.85784600
H	15.69685100	13.04654800	13.07419600
H	18.31746800	19.09450600	6.25518500
H	13.94735400	9.92724500	15.00382100
H	21.60826600	17.00901600	12.15442600
H	17.21586800	9.55748700	14.21492700
H	22.66603100	20.26868300	8.31273700
H	23.82877000	13.35713700	12.48934800
H	22.28676000	20.70541300	5.89589600
H	17.83120300	7.43213400	15.31932200
H	11.54936500	10.51779800	14.86985400
H	13.96527700	17.73533100	9.05729900
H	20.09896900	20.11245000	4.87643600
H	10.83761400	12.89557900	14.99222200
H	17.60289800	21.00841100	8.31701500
H	13.40995500	20.09824600	8.51991700
H	15.25130200	21.72506800	8.14347500
H	14.94425300	14.07185400	15.45552700
H	25.76087800	16.92278400	11.09728300
H	17.27073900	7.05673200	17.70187700
H	16.06327900	8.82772200	18.97411700
H	25.85277300	14.50457700	11.67133500
H	12.55435600	14.66896700	15.28299700

Compound 5

C	13.04649900	13.43857800	14.81548100
C	12.12248600	12.39639000	14.87092000
C	12.58254800	11.08044500	14.97593700
C	13.93935200	10.81219500	15.00383200
C	14.87773300	11.85028100	14.94009300
C	14.41126800	13.16131700	14.86682100
N	16.26171500	11.54515700	15.00350600
C	17.22359100	12.25685800	14.28096200
C	18.54720300	12.35112600	14.73881000
C	19.48993200	13.09065600	14.04241500
C	19.17587200	13.76287000	12.85468700
C	17.86140700	13.63108700	12.38759500
C	16.90653100	12.90245900	13.07625000
C	20.13618900	14.65211300	12.16081200
C	21.46846700	14.59192600	12.36872200
C	22.52197700	15.52269900	11.91772000

C	22.31008600	16.88313900	11.63051200
C	23.35933600	17.70113800	11.22855800
C	24.65225500	17.19454600	11.11432100
C	24.88768600	15.86137500	11.43376600
C	23.83704600	15.04405600	11.83384000
C	16.67124200	10.62176000	16.01514900
C	16.62536400	10.99531500	17.36169800
C	17.01108600	10.10720700	18.34915900
C	17.44945100	8.82204300	18.00568800
C	17.48572100	8.43755800	16.66365200
C	17.09720400	9.34323100	15.67722200
C	19.56459300	15.66447900	11.22993100
C	19.92048700	15.65111400	9.87953000
C	19.53014600	16.67582100	9.03227800
C	18.79171200	17.75403500	9.52611900
C	18.36739600	17.73776900	10.85745700
C	18.73681100	16.69068000	11.69208200
N	18.52418300	18.86465400	8.68538600
C	17.26653600	19.51311100	8.80246800
C	16.09273500	18.76044400	8.67033500
C	14.85265600	19.35699700	8.80355200
C	14.75147900	20.73063600	9.04929200
C	15.91326600	21.49086700	9.17276000
C	17.15986000	20.87639600	9.06344600
C	19.61664300	19.54127500	8.09414300
C	20.89790000	19.48333000	8.64430800
C	21.97263500	20.13821700	8.04547100
C	21.77461600	20.89074200	6.88984600
C	20.49102300	20.96698100	6.33970400
C	19.43292000	20.29294000	6.92367500
H	20.53760400	14.84100500	9.50643100
H	19.83583900	16.66910300	7.99107700
H	21.84670900	13.75497000	12.95051300
H	20.48331200	13.18401700	14.46929500
H	18.43022500	16.69843800	12.73378700
H	18.82505500	11.87645300	15.67331000
H	17.77268400	18.56106400	11.23919200
H	16.16744500	17.69692900	8.46806000
H	23.16509400	18.74983800	11.01985400
H	17.57321700	14.12136600	11.46349100
H	21.07366300	18.90226900	9.54297000
H	16.28179200	11.99167400	17.62182500
H	15.89677900	12.84732900	12.68595300
H	18.44603800	20.34879600	6.47682600
H	14.28939300	9.78851400	15.07970400
H	21.32050900	17.31118100	11.73329300
H	17.12423400	9.05002500	14.63368100
H	22.95279400	20.04654800	8.49873300
H	24.03141300	14.00490000	12.07546800
O	22.75291200	21.55587900	6.21779400
H	17.80659100	7.44478100	16.36962900
H	11.85398500	10.27871300	15.02810500
H	13.94034000	18.77918100	8.70516700
H	20.34816900	21.54763200	5.43485600
O	10.77192300	12.55316900	14.83425500
H	18.05994400	21.47192500	9.17478500

O	13.48828500	21.22286800	9.14784400
H	15.86957200	22.55559000	9.36804500
H	15.12001400	13.98205400	14.84074400
H	25.46849300	17.83623100	10.79778900
O	17.81382900	8.03092200	19.04292000
H	16.98541700	10.38241100	19.39767000
H	25.88887500	15.44834600	11.36517900
H	12.72514500	14.47114400	14.74946500
C	13.33746800	22.60093900	9.39833800
H	12.26413000	22.78722200	9.43780400
H	13.78795100	22.89040400	10.35640500
H	13.77848900	23.20880700	8.59794300
C	10.26615000	13.86440200	14.74276000
H	9.18010000	13.77130300	14.72464100
H	10.55999600	14.47374200	15.60710400
H	10.59918800	14.36432500	13.82403300
C	18.20769600	6.70648300	18.75105100
H	18.47512300	6.24892900	19.70326000
H	17.38940400	6.13698600	18.29598400
H	19.07465700	6.67205800	18.08020500
C	24.06590800	21.46995200	6.72224800
H	24.69132300	22.05026500	6.04393500
H	24.14098700	21.89334000	7.73194600
H	24.42434100	20.43229300	6.74279600
C	16.70689500	7.03590700	12.67071100
C	17.75614500	7.85390700	12.26875800
C	17.54425400	9.21434800	11.98155700
C	16.22918500	9.69299200	12.06544300
C	15.17854600	8.87567300	12.46551800
C	15.41397700	7.54250000	12.78495500
C	18.59776300	10.14512300	11.53055600
C	19.93004200	10.08493400	11.73846400
C	20.89035900	10.97417800	11.04459100
C	20.57630200	11.64639100	9.85686100
C	21.51903300	12.38591900	9.16046700
C	22.84264400	12.48018700	9.61831800
C	23.15970100	11.83458900	10.82303200
C	22.20482300	11.10596100	11.51168500
N	23.80452100	13.19188600	8.89577400
C	25.18850300	12.88676200	8.95919400
C	26.12688500	13.92484700	8.89545700
C	27.48368800	13.65659600	8.92336100
C	27.94375000	12.34065200	9.02838400
C	27.01973500	11.29846400	9.08381900
C	25.65496700	11.57572600	9.03247000
C	23.39499900	14.11528300	7.88413100
C	23.44087900	13.74172800	6.53758100
C	23.05516300	14.62983900	5.55012000
C	22.61680200	15.91500400	5.89359000
C	22.58052900	16.29948800	7.23562600
C	22.96903900	15.39381300	8.22205700
C	20.50163900	9.07256300	12.66933800
C	20.14575300	9.08592400	14.01974200
C	20.53609600	8.06121200	14.86698700
C	21.27452200	6.98299600	14.37313800
C	21.69882800	6.99926500	13.04179800

C	21.32941400	8.04635900	12.20717900
N	21.54205200	5.87237400	15.21386600
C	22.79969400	5.22390900	15.09677400
C	23.97350100	5.97657300	15.22887400
C	25.21357400	5.38001200	15.09564800
C	25.31474100	4.00636800	14.84993200
C	24.15294900	3.24614000	14.72649600
C	22.90635900	3.86061900	14.83581800
C	20.44959200	5.19576000	15.80511800
C	19.16833300	5.25371000	15.25496000
C	18.09359800	4.59882900	15.85380400
C	18.29161900	3.84630700	17.00943000
C	19.57521500	3.77006500	17.55956600
C	20.63331700	4.44409900	16.97558800
H	19.52864200	9.89603400	14.39284800
H	20.23041000	8.06792900	15.90819000
H	18.21952100	10.98208200	10.94877000
H	19.58292300	11.55303000	9.42997900
H	21.63599300	8.03860400	11.16547100
H	21.24118300	12.86059000	8.22596600
H	22.29353400	6.17596900	12.66005500
H	23.89880000	7.04009200	15.43113100
H	16.90113700	5.98720600	12.87940900
H	22.49301100	10.61568300	12.43579100
H	18.99256800	5.83476900	14.35629600
H	23.78444800	12.74536900	6.27745400
H	24.16945200	11.88971900	11.21333000
H	21.62020100	4.38824000	17.42243200
H	25.77684500	14.94852800	8.81958200
H	18.74572100	7.42586400	12.16597200
H	22.94200700	15.68701900	9.26559800
H	17.11343600	4.69050300	15.40054700
H	16.03481800	10.73214900	11.82382100
O	17.31332300	3.18117600	17.68148800
H	22.25966100	17.29226600	7.52964900
H	28.21225300	14.45832800	8.87119600
H	26.12589500	5.95782500	15.19400700
H	19.71806900	3.18941600	18.46441500
O	29.29431200	12.18387200	9.06505900
H	22.00627100	3.26509200	14.72450400
O	26.57793100	3.51412800	14.75136900
H	24.19663500	2.18141400	14.53123000
H	24.94622100	10.75498900	9.05854400
H	14.59774000	6.90081400	13.10148600
O	22.25243200	16.70612800	4.85635800
H	23.08083500	14.35463500	4.50160900
H	14.17735800	9.28870300	12.53411000
H	27.34108900	10.26589800	9.14984000
C	21.85856400	18.03056700	5.14822600
H	21.59114600	18.48812300	4.19601500
H	20.99159800	18.06499200	5.81906500
H	22.67685300	18.60006200	5.60330000
C	29.80008400	10.87264000	9.15656300
H	30.88613400	10.96573800	9.17468900
H	29.46704000	10.37272100	10.07529000
H	29.50624300	10.26329600	8.29222000

C	26.72873600	2.13605000	14.50090400
H	27.80207300	1.94976000	14.46142400
H	26.28772500	1.52820400	15.30132100
H	26.27823600	1.84656500	13.54285200
C	16.00032500	3.26711000	17.17704100
H	15.37491100	2.68680200	17.85535900
H	15.64189700	4.30477000	17.15649300
H	15.92523700	2.84372000	16.16734400

Compound 6

C	20.47134400	4.40654800	16.90845600
C	20.36247900	5.21695600	15.76811600
C	19.10360800	5.36061500	15.18375100
C	17.97657600	4.74281800	15.72185400
C	18.09993100	3.93443500	16.84948200
C	19.36126100	3.76473500	17.43037400
N	21.50164500	5.87408600	15.24266500
C	22.73642100	5.18098000	15.13707500
C	23.93284700	5.88744600	15.31371100
C	25.15394300	5.25057800	15.19212500
C	25.21225300	3.88084900	14.91300200
C	24.02756600	3.16627300	14.74401600
C	22.80108700	3.82189300	14.84233400
O	26.45948500	3.34629700	14.82973500
C	26.56730800	1.97049100	14.54706000
O	17.06584900	3.30115300	17.46642600
C	15.77617900	3.48520900	16.92657400
C	21.29031700	6.99987700	14.40320700
C	20.57764900	8.09727200	14.89166900
C	20.20129800	9.12138500	14.03708100
C	20.55183400	9.08985800	12.68544400
C	21.37303700	8.05362600	12.23360700
C	21.72432900	7.00514300	13.07511400
C	19.96796200	10.08520800	11.74280400
C	20.91492200	10.97720200	11.03512000
C	20.59556100	11.61887000	9.83213300
C	21.52865400	12.36235000	9.12678500
C	22.84697800	12.49271100	9.59063300
C	23.16789100	11.87887400	10.81039800
C	22.22299900	11.14405800	11.50714100
N	23.79487700	13.21257600	8.85407800
C	23.36122600	14.12469400	7.84172800
C	23.42557800	13.75265000	6.49571800
C	23.03487000	14.63488200	5.50473500
C	22.57563500	15.91354100	5.84479700
C	22.51767900	16.29516000	7.18691800
C	22.90693100	15.39433300	8.17686300
O	22.21327000	16.70255100	4.80581600
C	21.80823300	18.02462600	5.09678800
C	18.63413800	10.12227300	11.53839800
C	17.60374700	9.17842600	12.01293900
C	17.84046900	7.81717300	12.28599300
C	16.82910500	6.98288400	12.72765000
C	15.53202700	7.47259000	12.91153600

C	15.25640100	8.80071600	12.59314500
C	16.28626300	9.62480200	12.14599800
C	25.18780900	12.96942100	8.93502900
C	26.08311500	14.03611000	8.77304700
C	27.45027700	13.83226300	8.82090500
C	27.96927900	12.55342000	9.04262900
C	27.09080800	11.48150300	9.18874300
C	25.71469300	11.69166900	9.11759000
O	29.32564400	12.46109400	9.09141700
C	29.88869000	11.18548200	9.29079800
H	19.59338900	9.94183900	14.40335900
H	20.26896500	8.11294000	15.93181100
H	18.23982700	10.94498100	10.94646200
H	19.60669700	11.49712200	9.40179100
H	21.67976200	8.03393700	11.19200800
H	21.24723700	12.81414700	8.18205500
H	22.30372400	6.16865800	12.69830800
H	23.89062100	6.94749800	15.54195100
H	17.02007900	5.93210800	12.92137700
H	22.51421500	10.67712600	12.44249200
H	18.98386800	5.98808800	14.30867700
H	23.78972800	12.76285700	6.23865900
H	24.17163400	11.96325100	11.21035600
H	21.43894900	4.27977300	17.38232800
H	25.68865200	15.03106200	8.59837200
H	18.82912800	7.39885800	12.14103800
H	22.86088700	15.68579700	9.22027500
H	17.01669000	4.91345400	15.24722200
H	16.05751700	10.65865600	11.91284800
H	22.18260700	17.28343500	7.47872200
H	28.14257600	14.65735200	8.68929800
H	26.08358100	5.79272400	15.32536600
H	19.44596500	3.13922200	18.31242800
H	21.88360300	3.26183000	14.69515200
H	24.03790100	2.10605400	14.52150000
H	25.04586600	10.84332100	9.21189400
O	14.62241700	6.58178900	13.38850400
H	23.07544900	14.36065000	4.45644600
H	14.26265300	9.21674500	12.70459800
H	27.45606200	10.47296900	9.34124300
H	21.54081000	18.47946600	4.14325500
H	20.93854300	18.05192100	5.76416800
H	22.62012900	18.60019500	5.55495000
H	30.96955200	11.32739800	9.29855000
H	29.57658700	10.74983300	10.24875400
H	29.62291100	10.49399900	8.48093800
H	27.63401200	1.74661000	14.52756700
H	26.08585600	1.35893900	15.32092900
H	26.12999800	1.72154700	13.57164800
H	15.09681500	2.91767900	17.56262100
H	15.48092700	4.54252200	16.93552900
H	15.70909600	3.10703100	15.89877600
C	13.29323100	7.02657300	13.54595000
H	12.73076400	6.17566800	13.93077000
H	13.22474300	7.85694700	14.25961300
H	12.85830000	7.34456100	12.59045600

C	20.70513100	20.97245600	6.46914600
C	21.96645900	20.80265900	7.05001300
C	22.08978600	19.99421400	8.17760000
C	20.96272800	19.37644700	8.71568300
C	19.70385800	19.52019600	8.13133700
C	19.59502000	20.33067300	6.99104400
N	18.56466700	18.86308500	8.65675800
C	17.32992500	19.55624400	8.76240100
C	16.13346400	18.84985500	8.58569400
C	14.91240000	19.48677400	8.70733000
C	14.85415900	20.85648100	8.98657800
C	16.03888200	21.57098200	9.15563600
C	17.26532800	20.91530800	9.05726400
O	13.60695500	21.39108900	9.06988800
C	13.49920000	22.76687500	9.35269300
O	23.00056700	21.43591500	6.43308700
C	24.29023600	21.25175500	6.97290800
C	18.77595200	17.73723700	9.49614800
C	19.48860300	16.63985500	9.00762800
C	19.86493100	15.61568800	9.86216000
C	19.51438300	15.64714100	11.21379600
C	18.69318600	16.68335600	11.66568400
C	18.34192200	17.73189600	10.82423600
C	20.09823500	14.65173700	12.15638800
C	21.43205800	14.61462100	12.36078900
C	22.46247200	15.55846600	11.88629100
C	22.22577800	16.91974100	11.61332800
C	23.23715500	17.75403500	11.17170800
C	24.53421800	17.26430700	10.98776800
C	24.80981700	15.93615400	11.30607100
C	23.77994200	15.11206500	11.75318200
C	19.15125300	13.75974600	12.86404400
C	19.47056200	13.11813000	14.06707100
C	18.53744400	12.37465900	14.77239700
C	17.21914900	12.24425400	14.30848000
C	16.89829100	12.85803900	13.08867300
C	17.84320600	13.59285200	12.39195700
N	16.27122600	11.52439800	15.04501400
C	16.70485400	10.61232800	16.05741800
C	16.64039100	10.98440700	17.40341300
C	17.03109400	10.10222800	18.39444600
C	17.49044100	8.82359300	18.05444800
C	17.54850800	8.44193900	16.71234100
C	17.15925400	9.34271000	15.72234600
O	17.85279900	8.03464000	19.09347500
C	18.25795000	6.71258600	18.80256800
C	14.87829200	11.76751800	14.96399200
C	13.98300200	10.70082200	15.12602100
C	12.61583800	10.90463700	15.07809700
C	12.09681700	12.18345200	14.85625600
C	12.97526900	13.25537600	14.71009300
C	14.35138600	13.04524500	14.78131500
O	10.74045100	12.27574400	14.80740800
C	10.17738500	13.55132800	14.60790900
H	20.47283500	14.79524800	9.49584200
H	19.79729800	16.62424200	7.96748900

H	21.82634400	13.79187300	12.95268700
H	20.45940000	13.23991800	14.49746100
H	18.38644800	16.70298600	12.70727900
H	18.81881800	11.92290600	15.71716000
H	17.76253700	18.56836900	11.20108600
H	16.17563900	17.78982100	8.35735800
H	23.04620300	18.80482700	10.97805100
H	17.55203300	14.05974900	11.45657500
H	21.08244500	18.74892100	9.59072300
H	16.27616000	11.97418400	17.66042000
H	15.89457300	12.77362400	12.68865800
H	18.62741600	20.45752200	6.51719000
H	14.37747900	9.70589100	15.30078400
H	21.23713100	17.33807100	11.75832500
H	17.20538100	9.05122100	14.67894500
H	23.04966800	19.82350600	8.65221400
H	24.00866500	14.07819000	11.98626400
H	17.88366800	7.45368000	16.42058600
H	11.92355200	10.07954300	15.20974100
H	13.98273500	18.94468900	8.57403500
H	20.62044900	21.59801500	5.58712300
H	18.18284100	21.47530900	9.20450100
H	16.02860000	22.63118100	9.37824800
H	15.02019800	13.89360100	14.68697600
O	25.44384100	18.15511700	10.51083900
H	16.99043000	10.37648700	19.44272400
H	25.80355300	15.52010900	11.19457800
H	12.60999900	14.26389000	14.55750200
H	12.43250700	22.99080800	9.37220200
H	13.93651700	23.01570300	10.32813000
H	13.98068700	23.37847500	8.57888400
H	9.09652600	13.40938800	14.60012700
H	10.44311800	14.24287900	15.41772600
H	10.48951400	13.98691100	13.64993100
H	18.52532100	6.25778800	19.75613600
H	17.44613500	6.13695300	18.34434800
H	19.12770100	6.68533500	18.13526400
H	24.96962300	21.81927400	6.33687600
H	24.35735900	21.62987700	8.00072300
H	24.58542300	20.19442400	6.96389600
C	26.77300800	17.71030600	10.35331500
H	27.33548500	18.56122100	9.96853400
H	27.20796400	17.39223800	11.30877100
H	26.84144500	16.87998000	9.63959100

Compound 7

C	16.48864200	7.37640400	12.53044600
C	17.59621900	8.09400100	12.09532700
C	17.49330100	9.46161300	11.78696600
C	16.22576200	10.05303100	11.87927000
C	15.11880400	9.33873000	12.32136300
C	15.24777200	7.99588800	12.66153000
C	18.61615400	10.29577500	11.31898100
C	19.93964400	10.13335800	11.52663800

C	20.95867800	10.95123700	10.82609400
C	20.68245700	11.64327300	9.63935600
C	21.66194000	12.34475800	8.95511500
C	22.98432900	12.37535700	9.42333800
C	23.27038800	11.69356600	10.61324500
C	22.27854600	11.00619000	11.29332200
N	23.97452100	13.06406700	8.71118000
C	25.34583700	12.73095200	8.79524800
C	26.30990000	13.74279200	8.81349400
C	27.66111500	13.42445700	8.86586800
C	28.09727100	12.09962000	8.91617500
C	27.12532900	11.09713800	8.89031400
C	25.77199500	11.39905400	8.81854600
C	23.60349600	14.16147000	7.87803800
C	23.80465800	14.09844500	6.50095200
C	23.43650000	15.17148400	5.69578600
C	22.85991400	16.32011400	6.24178100
C	22.67578200	16.37018800	7.62625500
C	23.04330200	15.30713100	8.43887400
C	20.44443900	9.10511700	12.47964500
C	20.10606900	9.18283700	13.83239500
C	20.48566400	8.18515000	14.71839800
C	21.20164400	7.07679100	14.26309800
C	21.58601200	7.01392000	12.92103100
C	21.22380300	8.02876800	12.04546300
N	21.51113600	6.01906400	15.15757100
C	22.81773700	5.47658700	15.15545200
C	23.92333600	6.33120900	15.10473900
C	25.21045900	5.81278300	15.07690300
C	25.44345300	4.43634400	15.12088500
C	24.33246900	3.59368900	15.17567600
C	23.03724500	4.09666500	15.18193500
C	20.45658000	5.37194600	15.83836500
C	19.18915700	5.25711300	15.26092100
C	18.15875600	4.61884700	15.94421000
C	18.35611700	4.05834000	17.20442700
C	19.62914900	4.17483400	17.77129500
C	20.66030100	4.82934600	17.11391500
H	19.52575500	10.03058400	14.18208500
H	20.20593900	8.24650300	15.76500000
H	18.30465400	11.15309000	10.72661400
H	19.68829600	11.59927100	9.20665900
H	21.51152100	7.96751800	11.00022400
H	21.41304100	12.84682700	8.02647000
H	22.15760800	6.16083600	12.57022800
H	23.76461600	7.40431200	15.07911400
H	16.59657100	6.32142300	12.76516400
H	22.54048700	10.49455500	12.21341600
H	19.00861300	5.67608700	14.27624500
H	24.24597100	13.20574200	6.06899600
H	24.28095000	11.69891000	11.00521800
H	21.63633000	4.91706800	17.57937500
H	25.99050700	14.77912200	8.78415100
H	18.54656900	7.58531400	11.98971600
H	22.89834900	15.35688300	9.51113300
H	17.18009900	4.55293600	15.47590300

H	16.11855400	11.09971200	11.61675200
C	17.24050400	3.37141400	17.94892300
H	22.24234900	17.25843500	8.07641800
H	28.39245800	14.22863500	8.87473000
H	26.05415400	6.49653900	15.03172100
H	19.81324200	3.76003300	18.75907900
C	29.56267300	11.76118100	9.01709000
H	22.19068200	3.41886900	15.20656200
C	26.84581600	3.88376500	15.13574100
H	24.47941000	2.51692000	15.19676900
H	25.03779600	10.60138400	8.77936500
H	14.38857400	7.43376100	13.01338100
C	22.45950600	17.48716300	5.37687400
H	23.58939900	15.10862800	4.62165700
H	14.15900800	9.83764000	12.40986800
H	27.43269800	10.05462400	8.90828700
H	17.01736900	3.88724400	18.88931900
H	16.32249600	3.34738600	17.35630400
H	17.50486700	2.33909800	18.19991200
H	26.87900200	2.87054000	14.72599500
H	27.52603900	4.50758100	14.54911900
H	27.24139700	3.83841400	16.15674000
H	29.78972500	10.81926000	8.50973300
H	30.18378100	12.54282700	8.57125700
H	29.87182800	11.65242800	10.06289400
H	22.38828000	17.19857500	4.32476700
H	21.49619100	17.90069900	5.68907800
H	23.19212500	18.29831400	5.45301300
C	12.94090700	13.63990800	15.00897300
C	11.96896100	12.63742900	14.98311300
C	12.40511200	11.31259100	15.03341500
C	13.75632700	10.99425000	15.08578400
C	14.72039300	12.00608700	15.10402900
C	14.29423900	13.33798800	15.08073500
N	16.09171000	11.67296900	15.18809300
C	17.08190100	12.36167900	14.47593300
C	18.40429200	12.39227300	14.94415300
C	19.38377500	13.09375800	14.25991000
C	19.10755200	13.78579500	13.07317300
C	17.78768300	13.73084700	12.60595000
C	16.79584000	13.04347200	13.28602700
C	20.12658500	14.60367400	12.37262800
C	21.45007500	14.44126000	12.58028600
C	22.57292500	15.27542400	12.11230100
C	22.47000500	16.64303500	11.80393700
C	23.57758000	17.36063500	11.36882000
C	24.81845300	16.74115400	11.23773900
C	24.94742300	15.39831200	11.57790700
C	23.84046600	14.68400900	12.01999900
C	16.46273500	10.57556400	16.02123200
C	16.26157300	10.63858500	17.39831800
C	16.62973400	9.56554500	18.20348100
C	17.20632100	8.41691800	17.65748400
C	17.39045100	8.36684600	16.27301000
C	17.02292900	9.42990400	15.46039300
C	19.62178900	15.63191200	11.41962000

C	19.96016200	15.55419300	10.06687100
C	19.58056800	16.55188000	9.18086800
C	18.86458300	17.66023700	9.63616700
C	18.48021000	17.72310600	10.97823300
C	18.84242000	16.70825800	11.85380100
N	18.55509500	18.71796600	8.74169300
C	17.24849800	19.26045400	8.74381900
C	16.14289200	18.40583900	8.79452500
C	14.85577300	18.92427300	8.82236200
C	14.62278800	20.30071500	8.77838900
C	15.73377800	21.14336200	8.72360500
C	17.02899800	20.64037700	8.71734500
C	19.60965700	19.36508600	8.06090800
C	20.87707700	19.47991500	8.63835800
C	21.90748300	20.11817800	7.95507500
C	21.71013000	20.67868900	6.69485800
C	20.43709900	20.56220200	6.12798500
C	19.40594200	19.90769000	6.78535800
H	20.54047900	14.70644900	9.71718300
H	19.86029600	16.49052800	8.13426700
H	21.76157700	13.58394700	13.17265300
H	20.37793600	13.13775500	14.69260500
H	18.55469800	16.76950700	12.89903900
H	18.65319000	11.89020100	15.87279700
H	17.90861000	18.57618700	11.32903500
H	16.30160600	17.33273600	8.82014200
H	23.46964900	18.41561500	11.13410200
H	17.52574000	14.24248400	11.68585700
H	21.05761600	19.06093900	9.62303300
H	15.82025800	11.53128600	17.83027600
H	15.78527700	13.03813100	12.89405700
H	18.42991500	19.81997200	6.31989500
H	14.07571800	9.95791900	15.11512600
H	21.51965300	17.15172000	11.90954700
H	17.16788100	9.38015500	14.38813300
H	22.88613800	20.18408500	8.42338500
H	23.94767500	13.63732900	12.28251900
C	22.82574800	21.36560900	5.95036600
H	17.82388600	7.47860200	15.82284400
H	11.67376700	10.50841500	15.02455400
H	14.01207400	18.24052200	8.86753800
H	20.25301100	20.97700700	5.14020100
C	10.50356100	12.97587600	14.88220500
H	17.87556600	21.31817000	8.69272300
C	13.22042900	20.85330200	8.76353300
H	15.58684400	22.22013200	8.70251900
H	15.02844300	14.13565500	15.11991400
H	25.67765000	17.30328200	10.88588900
C	17.60673400	7.24986700	18.52238700
H	16.47683500	9.62839800	19.27761000
H	25.90722000	14.89940300	11.48940400
H	12.63354100	14.68242300	14.99100400
H	13.18725000	21.86652800	9.17327800
H	12.82484700	20.89865400	7.74253500
H	12.54020300	20.22949200	9.35015800
H	23.04890400	20.84976100	5.00998500

H	22.56138000	22.39791800	5.69935100
H	23.74374600	21.38966100	6.54300000
H	10.27649600	13.91773900	15.38966600
H	10.19442900	13.08475100	13.83640700
H	9.88244500	12.19417800	15.32793400
H	17.67794600	7.53844900	19.57449700
H	16.87412500	6.43870700	18.44623600
H	18.57005700	6.83634500	18.21019000

Compound 8

C	12.85799000	13.64958200	15.20309200
C	11.88911300	12.64520900	15.14624400
C	12.32852100	11.32097700	15.18019200
C	13.67972600	11.00595900	15.24672800
C	14.64109400	12.01951400	15.29653200
C	14.21099400	13.35022800	15.28912200
N	16.01399100	11.69498900	15.38638800
C	16.99322400	12.39052100	14.66040100
C	18.31443800	12.44961100	15.12772700
C	19.28651100	13.13924800	14.42145200
C	19.00051100	13.79121700	13.21376000
C	17.67761200	13.72275200	12.75839100
C	16.69384200	13.04569200	13.46099000
C	20.01769900	14.56927000	12.46720100
C	21.34276100	14.40521700	12.66276300
C	22.46057100	15.18926600	12.10623400
C	22.37588000	16.53948400	11.72475700
C	23.46389900	17.19040900	11.16254900
C	24.68120100	16.53412600	10.95678600
C	24.79193400	15.21813000	11.40278600
C	23.70731700	14.56720600	11.97813500
C	16.38645000	10.55249000	16.15031500
C	16.03501100	10.46367500	17.49635400
C	16.38186700	9.33655500	18.23284100
C	17.09001700	8.28243500	17.65243700
C	17.43453700	8.38776000	16.30204600
C	17.08875200	9.50544900	15.55554400
C	19.51519500	15.56101900	11.47469400
C	19.84596000	15.43010300	10.12364500
C	19.49428900	16.41346300	9.20928200
C	18.81089400	17.55321500	9.63474300
C	18.42167500	17.66262000	10.97140300
C	18.75991700	16.66618900	11.87707700
N	18.54685800	18.60625400	8.71546900
C	17.23735300	19.14265900	8.66788600
C	16.14159200	18.27464600	8.63157300
C	14.84814900	18.77682400	8.61427600
C	14.59975600	20.15149500	8.61123500
C	15.70080300	21.00767000	8.64539800
C	17.00160900	20.51978500	8.68471300
C	19.64165500	19.30339300	8.16014800
C	20.86975800	19.37131900	8.82417900
C	21.94061700	20.05726800	8.25886600
C	21.82368900	20.71490400	7.03693300

C	20.59027300	20.64276800	6.38129100
C	19.52137600	19.94082500	6.91734200
H	20.40555700	14.55784300	9.79925900
H	19.77369300	16.31947100	8.16501700
H	21.65805000	13.57925800	13.29677800
H	20.28227200	13.20282300	14.84810400
H	18.47677400	16.76545000	12.92061500
H	18.56914600	11.97047000	16.06689800
H	17.87172600	18.54053700	11.29480800
H	16.31383400	17.20327700	8.62531300
H	23.36175700	18.23063700	10.86171600
H	17.40862200	14.20835500	11.82623100
H	20.99127000	18.87727800	9.78246700
H	15.48767400	11.27952700	17.95780700
H	15.68200100	13.01766700	13.07309700
H	18.58000300	19.88763900	6.38089000
H	13.99960700	9.96974400	15.26707900
H	21.45116300	17.08594800	11.86652400
H	17.35750900	9.57030200	14.50755300
H	22.88779800	20.08161500	8.79188500
H	23.81550700	13.53991000	12.30855000
C	22.97963300	21.46448200	6.42646000
H	17.97227600	7.57552200	15.82183800
H	11.60039000	10.51444500	15.14638700
H	14.01215000	18.08256900	8.59150700
H	20.46960100	21.12980700	5.41692800
C	10.42450300	12.98195900	15.02998500
H	17.83862500	21.20817400	8.72984100
C	13.19242500	20.68768100	8.54724300
H	15.54111700	22.08274100	8.65908800
H	14.94328600	14.14846100	15.34897900
C	25.80966000	17.21669100	10.23138200
C	17.45944600	7.05529900	18.44423100
H	16.10653800	9.28203400	19.28280400
H	25.73010500	14.68445600	11.27813500
H	12.54797600	14.69143300	15.19750200
H	23.18322500	21.11675200	5.40813600
H	22.77202800	22.53822400	6.36762800
H	23.89243000	21.33356600	7.01331700
H	13.13052900	21.69511900	8.96765500
H	12.83700600	20.74087400	7.51197200
H	12.49719800	20.04842900	9.09875100
H	10.18430200	13.90480700	15.56559300
H	10.13440700	13.12635300	13.98305100
H	9.79842200	12.18316700	15.43665000
H	17.46728900	7.26150900	19.51807600
H	16.74411900	6.24463200	18.26555200
H	18.44432500	6.67813700	18.15586700
H	26.75615400	16.68828400	10.37423600
H	25.59996800	17.24685500	9.15511900
H	25.94049900	18.24944300	10.56859500
C	16.60243200	7.54648600	12.73678700
C	17.69042800	8.19742200	12.17454900
C	17.60569100	9.54762000	11.79301000
C	16.35892200	10.16964100	11.92107800
C	15.27432700	9.51870600	12.49645600

C	15.38510700	8.20273600	12.94252000
C	18.72347200	10.33168600	11.23644500
C	20.04854100	10.16768900	11.43200500
C	21.06570500	10.94574900	10.68541900
C	20.77966000	11.59777000	9.47776500
C	21.75171200	12.28741100	8.77146600
C	23.07295300	12.34645200	9.23872400
C	23.37238000	11.69123200	10.43809600
C	22.38862800	11.01417200	11.14072200
N	24.05216200	13.04198600	8.51270900
C	25.42506200	12.71745500	8.60252200
C	26.38643200	13.73100400	8.65236600
C	27.73763900	13.41597600	8.71885900
C	28.17704200	12.09174100	8.75272200
C	27.20816000	11.08737400	8.69583500
C	25.85515700	11.38673800	8.60984900
C	23.67969500	14.18453300	7.74885700
C	24.03105100	14.27339200	6.40280100
C	23.68419400	15.40055900	5.66638500
C	22.97612700	16.45468400	6.24688300
C	22.63169400	16.34931500	7.59729200
C	22.97747600	15.23157800	8.34372100
C	20.55107000	9.17598800	12.42454900
C	20.22030900	9.30695700	13.77559400
C	20.57198500	8.32363400	14.68999400
C	21.25538400	7.18386800	14.26457600
C	21.64460200	7.07441400	12.92792000
C	21.30635100	8.07080600	12.02220800
N	21.51942500	6.13086400	15.18388900
C	22.82893600	5.59448000	15.23151400
C	23.92468800	6.46250400	15.26777200
C	25.21813700	5.96033900	15.28510500
C	25.46654400	4.58567300	15.28823800
C	24.36550300	3.72948400	15.25412700
C	23.06469400	4.21735300	15.21477700
C	20.42463000	5.43374700	15.73924000
C	19.19653400	5.36577600	15.07520100
C	18.12567200	4.67985900	15.64054500
C	18.24259100	4.02229700	16.86251900
C	19.47599900	4.09447700	17.51816900
C	20.54490000	4.79639000	16.98208500
H	19.66070700	10.17922600	14.09994700
H	20.29257900	8.41766300	15.73425600
H	18.40814500	11.15760700	10.60239900
H	19.78387700	11.53424000	9.05115900
H	21.58948900	7.97150400	10.97867200
H	21.49696600	12.76659400	7.83232600
H	22.19455500	6.19648600	12.60454900
H	23.75243700	7.53387300	15.27395900
H	16.70461000	6.50627500	13.03766700
H	22.65765700	10.52853700	12.07285400
H	19.07502700	5.85976600	14.11688500
H	24.57832400	13.45753800	5.94127700
H	24.38424100	11.71922200	10.82594100
H	21.48626600	4.84961500	17.51854600
H	26.06655500	14.76722100	8.63208200

H	18.61516500	7.65098400	12.03280900
H	22.70878300	15.16668900	9.39172600
H	17.17849400	4.65548100	15.10752200
H	16.25069500	11.19691700	11.59061200
C	17.08664800	3.27273300	17.47301400
H	22.09402100	17.16155600	8.07757200
H	28.46577400	14.22250400	8.75269700
H	26.05412800	6.65460400	15.30782900
H	19.59666200	3.60750200	18.48256500
C	29.64165100	11.75497100	8.86892800
H	22.22768500	3.52895400	15.16969000
C	26.87387300	4.04948900	15.35228300
H	24.52520100	2.65441400	15.24050600
H	25.12285800	10.58851300	8.54996200
C	14.25667300	7.52016600	13.66795900
C	22.60669600	17.68187000	5.45516800
H	23.95945500	15.45511500	4.61640700
H	14.33613700	10.05235200	12.62107900
H	27.51817100	10.04552200	8.70136000
H	16.88326900	3.62026100	18.49144800
H	16.17377300	3.40389700	16.88633300
H	17.29412400	2.19895000	17.53156900
H	26.93587000	3.04222400	14.93146900
H	27.56919400	4.68898100	14.80117300
H	27.22909000	3.99587200	16.38760100
H	29.88188200	10.83229300	8.33303800
H	30.26773800	12.55389700	8.46253600
H	29.93171000	11.61024800	9.91582700
H	22.59878200	17.47571000	4.38131300
H	21.62184600	18.05905400	5.74360700
H	23.32206100	18.49250400	5.63384300
H	13.31015800	8.04852300	13.52506800
H	14.12588100	6.48738800	13.33080800
H	14.46636200	7.49007600	14.74422500