

Supporting Information for
Host-Guest Binding Selectivity of Ethylated Pillar[5]arene (EtP5A) towards Octane, 1,7-Octadiene, and 1,7-Octadiyne: A Computational Investigation

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Table S1. ω B97XD/6-311G* and B97D/6-311G* energies of the HOMO and LUMO (au), HOMO-LUMO gap and TDDFT gap (eV), and binding energy BE (kcal/mol) results for the inclusions complexes 1, 2, 3 in the implicit solvent phase (chloroform).

ω B97XD/B97D	Complex 1	Complex 2	Complex 3
HOMO (au)	-0.26066/-0.15817	-0.26234/-0.15911	-0.26331/-0.16006
LUMO (au)	0.04733/-0.03951	0.04573/-0.04071	0.04322/-0.04275
E _{gap} (eV)	8.38/3.23	8.38/3.22	8.34/3.19
TDDFT gap (eV)	4.57/3.39	4.58/3.27	4.54/3.34
BE (kcal/mol)	39.11/32.96	39.49/33.13	40.68/34.25

Table S2. ω B97XD/6-311G* and B97D/6-311G* energies of the HOMO and LUMO (au), HOMO-LUMO gap and TDDFT gap (eV), for the inclusions complexes 1, 2, 3 in the implicit solvent phase (chloroform).

ω B97XD/B97D	EtP5A	octane	1,7-octadiene	1,7-octadiyne
HOMO (au)	-0.25973/-0.15731	-0.38443/-0.26432	-0.33785/-0.22269	-0.35523/-0.23575
LUMO (au)	0.04654/-0.03980	0.12165/0.03237	0.08535/-0.01906	0.10789/0.00770
E _{gap} (eV)	8.33/3.20	13.77/8.07	11.52/5.54	12.60/6.62
TDDFT gap (eV)	4.54/3.35	9.77/8.15	7.47/6.93	8.85/6.93

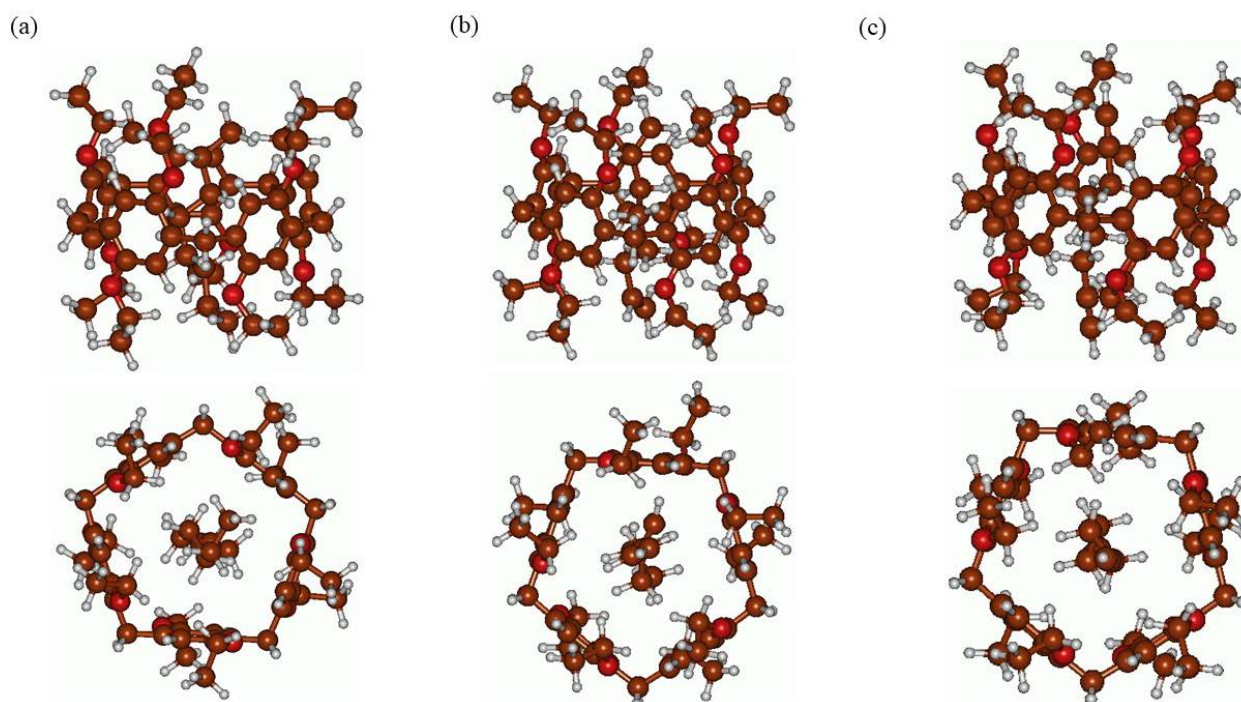


Figure S1. ω B97XD/6-311G* optimized geometry of the host-guest complexes 1 (a), 2 (b), 3 (b), in the implicit chloroform: side views (top row) and top views (bottom row).

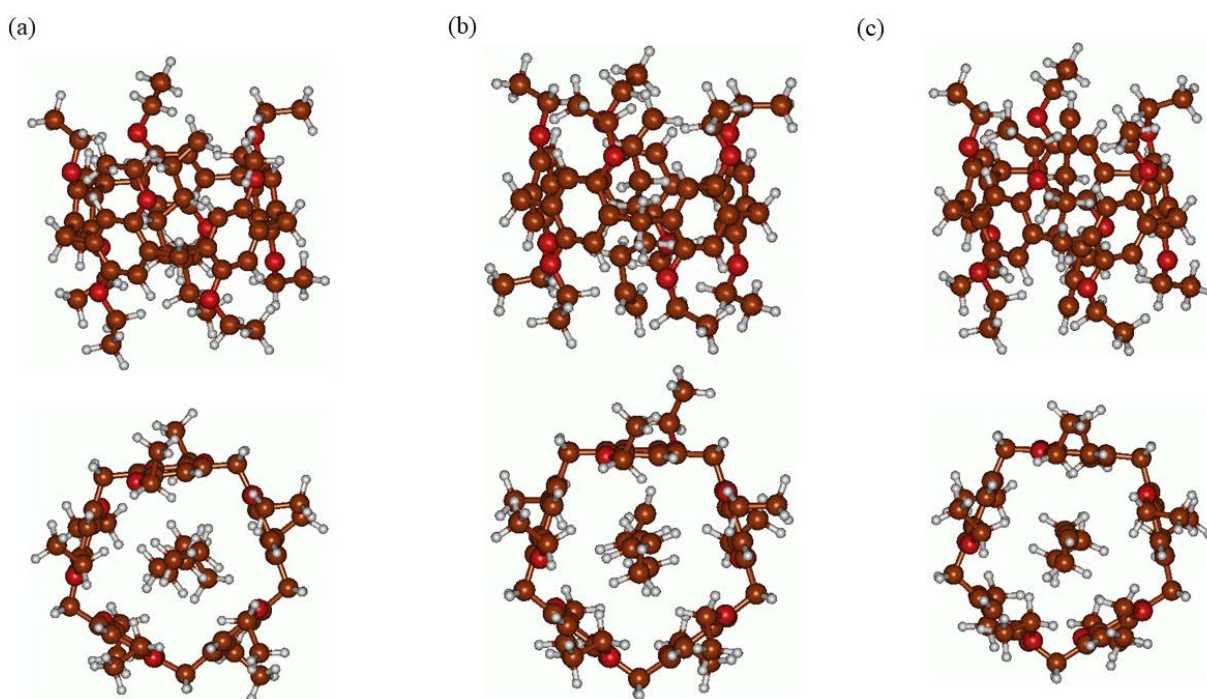


Figure S2. B97D/6-311G* optimized geometry of the host-guest complexes 1 (a), 2 (b), 3 (b), in the implicit chloroform: side views (top row) and top views (bottom row).

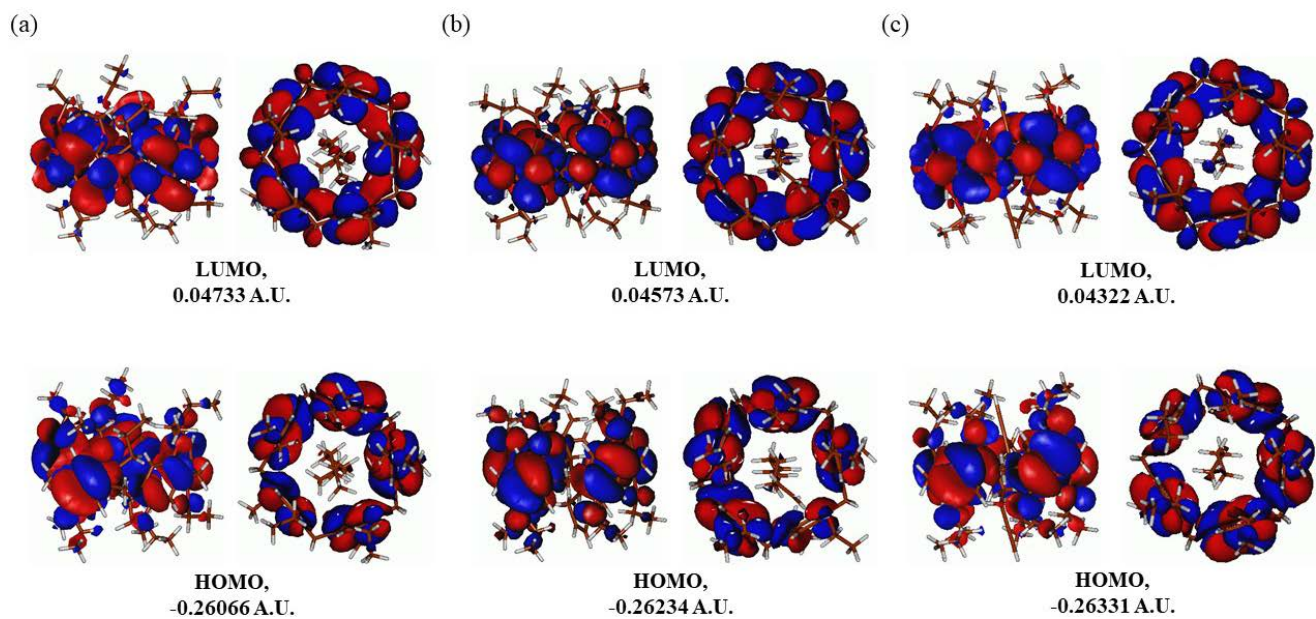


Figure S3. ω B97XD/6-311G* frontier MOs of the host-guest complexes 1 (a), 2 (b), 3 (b), in the implicit chloroform: HOMOs (top row) and LUMOs (bottom row), both side views and top views. Isosurface value 0.01 au.

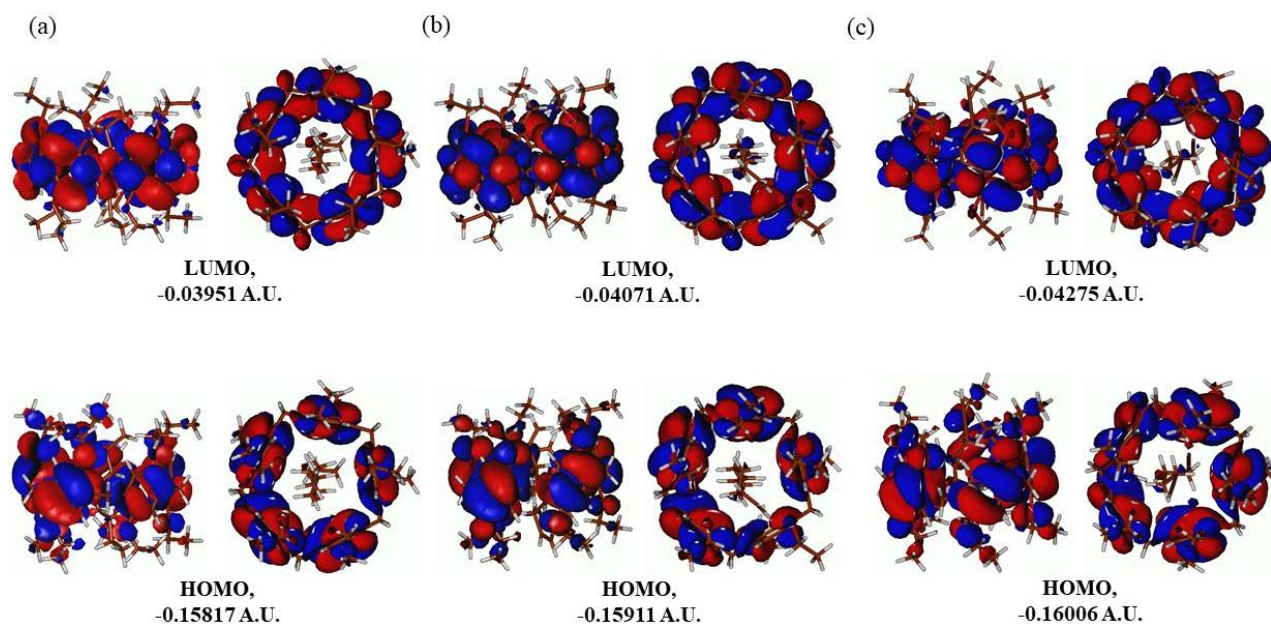


Figure S4. B97D/6-311G* frontier MOs of the host-guest complexes 1 (a), 2 (b), 3 (b), in the implicit chloroform: HOMOs (top row) and LUMOs (bottom row), both side views and top views. Isosurface value 0.01 au.

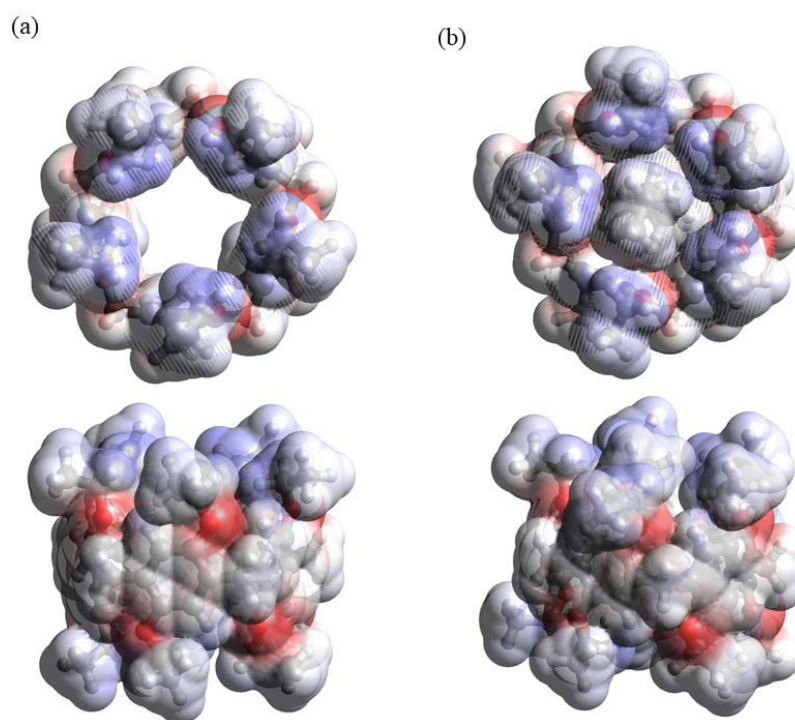


Figure S5. ω B97XD/6-311G* molecular electrostatic potential (MEP) plots for the host molecule (a) and the host-guest complex 1 (b), in the implicit chloroform: side views (bottom row) and top views (top row). Isosurface value 0.01 a.u.

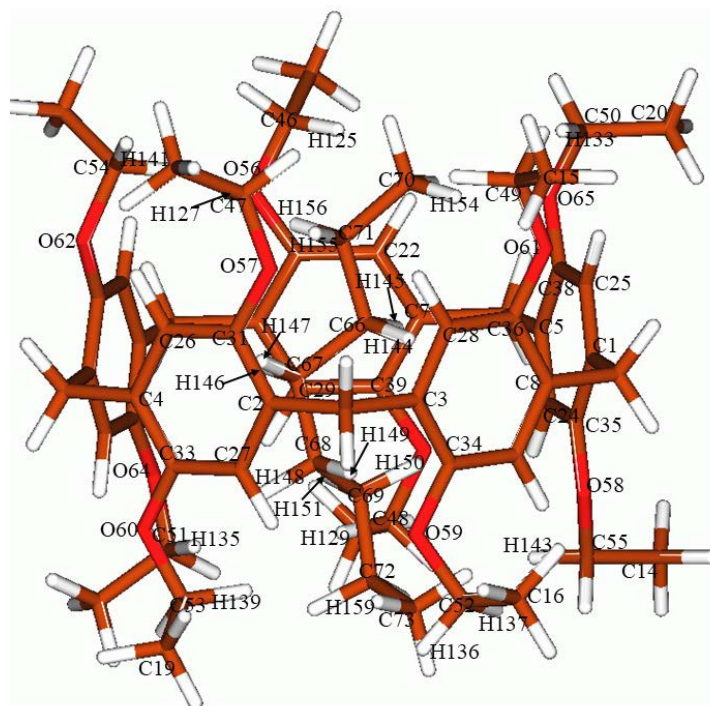


Figure S6. Labeled atoms within molecular structure of complex 1

Table S3. The NBO analysis results, ω B97XD/6-311G*, CHCl_3 .

Donor (i)	Type	Acceptor (j)	Type	$E^{(2)a}$	$E(j)-E(i)^b$	$F(i,j)^c$
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				kcal/mol ^{a,d}	a.u.	a.u.
Complex 1						
Host → guest						
C3-C34	π	C68-H149	σ^*	0.12	0.84	0.010
C5-C38	π	C66-H145	σ^*	0.12	0.84	0.010
C6-C32	π	C67-H146	σ^*	0.40	0.84	0.018
C7-C22	π	C66-H145	σ^*	0.20	0.84	0.012
C24-C35	π	C69-H150	σ^*	0.52	0.84	0.020
C26-C31	π	C67-H147	σ^*	0.28	0.85	0.015
C28-C36	π	C67-H144	σ^*	0.22	0.85	0.013
C29-C39	π	C69-H151	σ^*	0.43	0.83	0.018
C46-C125	σ	C70-H154	σ^*	0.14	1.13	0.011
C47-C127	σ	C71-H155	σ^*	0.15	1.12	0.011
C48-C129	σ	C69-H151	σ^*	0.12	1.13	0.010
C50-C133	σ	C70-C71	σ^*	0.11	1.11	0.010
C51-C135	σ	C68-H148	σ^*	0.13	1.13	0.011
C52-C137	σ	C72-C73	σ^*	0.18	1.09	0.012
C53-C139	σ	C73-H159	σ^*	0.12	1.12	0.010
O56	LP	C71-H156	σ^*	0.15	0.91	0.011
O58	LP	C73-H160	σ^*	0.46	0.90	0.019
O59	LP	C73-H159	σ^*	0.21	0.91	0.013
O60	LP	C68-H148	σ^*	0.18	0.91	0.012
O61	LP	C70-H154	σ^*	0.52	0.91	0.020
O65	LP	C70-H153	σ^*	0.81	0.91	0.025
Guest → host						
C68-H148	σ	C4-C33	π^*	0.23	0.64	0.012
C68-H148	σ	C19-C53	σ^*	0.12	1.01	0.010
C68-H148	σ	C51-H135	σ^*	0.29	1.03	0.015
C68-H149	σ	C2-C27	π^*	0.12	0.64	0.008
C68-H149	σ	C3-C34	π^*	0.12	0.64	0.009
C69-H151	σ	C48-H129	σ^*	0.12	1.03	0.010
C70-H153	σ	C5-C38	π^*	0.16	0.66	0.010
C70-H153	σ	C20-C50	σ^*	0.11	1.04	0.009
C70-H153	σ	C38-O65	σ^*	0.13	1.02	0.010
C70-H153	σ	C46-H125	σ^*	0.23	1.06	0.014
C70-H154	σ	C1-C25	π^*	0.12	0.67	0.009
C70-H154	σ	C15-C49	σ^*	0.19	1.03	0.013
C71-H155	σ	C47-H127	σ^*	0.14	1.03	0.011

C71-H156	σ	C54-H141	σ^*	0.19	1.03	0.013
C72-H157	σ	C55-H143	σ^*	0.15	1.04	0.011
C73-H159	σ	C16-C52	σ^*	0.12	1.04	0.010
C73-H159	σ	C53-H139	σ^*	0.17	1.06	0.012
C73-H160	σ	C14-C55	σ^*	0.20	1.04	0.013
C73-H160	σ	C52-H137	σ^*	0.10	1.06	0.009
C73-H160	σ	C55-O58	σ^*	0.10	0.96	0.009
Complex 2						
Host \rightarrow guest						
C3-C34	π	C68-H149	σ^*	0.10	0.83	0.009
C4-C26	π	C67-H147	σ^*	0.20	0.84	0.012
C5-C24	π	C66-H145	σ^*	0.18	0.83	0.012
C5-C24	π	C69-H150	σ^*	0.20	0.83	0.012
C6-C23	π	C67-H146	σ^*	0.26	0.84	0.014
C7-C22	π	C66-H145	σ^*	0.22	0.82	0.013
C8-C30	π	C66-H144	σ^*	0.12	0.83	0.010
C21-C32	π	C67-H146	σ^*	0.10	0.84	0.009
C29-C39	π	C69-H151	σ^*	0.41	0.82	0.018
C48-H129	σ	C72-C73	π^*	0.13	0.73	0.009
C50-H133	σ	C70-C71	π^*	0.38	0.74	0.015
C31	LP	C67-H147	σ^*	0.10	0.65	0.010
O56	LP	C71-H156	σ^*	0.26	0.94	0.014
O58	LP	C73-H157	σ^*	0.99	0.97	0.028
O60	LP	C68-H148	σ^*	0.16	0.91	0.011
O61	LP	C70-H154	σ^*	0.52	0.93	0.020
Guest \rightarrow host						
C67-H147	σ	C31	LP*	0.12	0.43	0.009
C68-H148	σ	C33	LP*	0.30	0.44	0.015
C68-H148	σ	C19-C53	σ^*	0.10	1.02	0.009
C68-H148	σ	C51-H135	σ^*	0.16	1.03	0.012
C68-H149	σ	C3-C34	π^*	0.21	0.65	0.012
C69-H150	σ	C5-C24	π^*	0.20	0.66	0.011
C70-C71	π	C20-C50	σ^*	0.10	0.81	0.008
C70-C71	π	C46-H125	σ^*	0.21	0.83	0.012
C70-C71	π	C47-H127	σ^*	0.31	0.83	0.014
C70-C71	π	C50-H133	σ^*	0.39	0.83	0.016
C71-H156	σ	C10-C37	π^*	0.13	0.68	0.009
C71-H156	σ	C54-H141	σ^*	0.11	1.06	0.010

C72-C73	π	C52-H137	σ^*	0.60	0.84	0.020
Complex 3						
Host \rightarrow guest						
C1-C25	π	C71-H152	σ^*	0.58	0.81	0.021
C3-C34	π	C70-H151	σ^*	0.12	0.80	0.010
C3-C34	π	C71-H153	σ^*	0.20	0.81	0.013
C4-C33	π	C70-H150	σ^*	0.19	0.80	0.012
C7-C22	π	C69-H149	σ^*	0.10	0.83	0.009
C9-C40	π	C69-H148	σ^*	0.32	0.83	0.016
C10-C37	π	C69-H149	σ^*	0.20	0.83	0.013
C21-C32	π	C70-H150	σ^*	0.13	0.81	0.010
C24-C35	π	C68-H146	σ^*	0.38	0.82	0.017
C28-C36	π	C67-C73	π^*	0.14	0.50	0.008
C28-C36	π	C69-C71	σ^*	0.14	0.78	0.010
C29-C39	π	C69-C70	σ^*	0.16	0.78	0.011
C29-C39	π	C68-H147	σ^*	0.20	0.83	0.013
C47-H127	σ	C67-C73	π^*	0.11	0.80	0.009
C48-H129	σ	C68-H147	σ^*	0.10	1.13	0.009
C51-H135	σ	C66-C72	π^*	0.17	0.79	0.010
C52-H137	σ	C66-C72	π^*	0.10	0.79	0.008
C53-H139	σ	C66-C72	π^*	0.13	0.80	0.009
C55-H143	σ	C68-H146	σ^*	0.11	1.12	0.010
O60	LP	C70-H150	σ^*	0.31	0.89	0.015
O64	LP	C68-H147	σ^*	0.21	0.91	0.013
Guest \rightarrow host						
C66-C72	π	C48-H129	σ^*	0.11	0.86	0.009
C66-C72	π	C55-H143	σ^*	0.11	0.86	0.009
C66-C72	π	C51-H135	σ^*	0.19	0.86	0.011
C66-C72	π	C52-H137	σ^*	0.18	0.86	0.011
C67-C73	π	C46-H125	σ^*	0.30	0.86	0.014
C67-C73	π	C49-H131	σ^*	0.36	0.86	0.016
C67-C73	π	C54-H141	σ^*	0.18	0.86	0.011
C67-C73	π	C47-H127	σ^*	0.33	0.86	0.015
C67-C73	π	C50-H133	σ^*	0.53	0.86	0.019
C67-C73	π	C54-H141	σ^*	0.13	0.86	0.009
C68-H146	σ	C29-C39	π^*	0.13	0.65	0.009
C68-H146	σ	C55-H143	σ^*	0.16	1.05	0.012
C68-H147	σ	C21-C32	π^*	0.15	0.65	0.010

C68-H147	σ	C29-C39	π^*	0.13	0.65	0.009
C68-H147	σ	C48-H129	σ^*	0.22	1.05	0.013
C70-H150	σ	C4-C33	π^*	0.33	0.67	0.015
C70-H150	σ	C33-O60	σ^*	0.14	1.03	0.011
C70-H151	σ	C3-C34	π^*	0.14	0.67	0.010

^a $E^{(2)}$ means energy of hyper-fconjugative interaction or stabilization energy (in kcal/mol).

^b Energy difference between donor and acceptor i and j NBO orbitals.

^c $F_{i,j}$ is the Fock matrix element between i and j NBO orbitals.

^d Only the stabilization energies equal to or higher than 0.1 kcal/mol are given.

Table S4. Representative values of the NBO analysis for the complex 1, ω B97XD/6-311G*, CHCl_3 .

Donor (i)	Type	Acceptor (j)	Type	$E^{(2)}$, kcal/mol ^{a,d}	$E(j)-E(i)$, ^b a.u.	$F(i,j)$, ^c a.u.
Host \rightarrow guest						
C6-C32	π	C67-H146	σ^*	0.40	0.84	0.018
C24-C35	π	C69-H150	σ^*	0.52	0.84	0.020
C26-C31	π	C67-H147	σ^*	0.28	0.85	0.015
C28-C36	π	C67-H144	σ^*	0.22	0.85	0.013
C29-C39	π	C69-H151	σ^*	0.43	0.83	0.018
O58	LP	C73-H160	σ^*	0.46	0.90	0.019
O59	LP	C73-H159	σ^*	0.21	0.91	0.013
O61	LP	C70-H154	σ^*	0.52	0.91	0.020
O65	LP	C70-H153	σ^*	0.81	0.91	0.025
Guest \rightarrow host						
C68-H148	σ	C4-C33	π^*	0.23	0.64	0.012
C68-H148	σ	C51-H135	σ^*	0.29	1.03	0.015
C70-H153	σ	C46-H125	σ^*	0.23	1.06	0.014

^a $E^{(2)}$ means energy of hyperconjugative interaction or stabilization energy (in kcal/mol).

^b Energy difference between donor and acceptor i and j NBO orbitals.

^c $F_{i,j}$ is the Fock matrix element between i and j NBO orbitals.

^d Only the stabilization energies higher than 0.20 kcal/mol are given.

Table S5. Representative values of the NBO analysis for the complex 2, ω B97XD/6-311G*, CHCl₃.

Donor (i)	Type	Acceptor (j)	Type	$E^{(2)}$, kcal/mol ^{a,d}	E(j)-E(i), ^b a.u.	F(i,j), ^c a.u.
Host → guest						
C6-C23	π	C67-H146	σ^*	0.26	0.84	0.014
C7-C22	π	C66-H145	σ^*	0.22	0.82	0.013
C29-C39	π	C69-H151	σ^*	0.41	0.82	0.018
C50-H133	σ	C70-C71	π^*	0.38	0.74	0.015
O56	LP	C71-H156	σ^*	0.26	0.94	0.014
O58	LP	C73-H157	σ^*	0.99	0.97	0.028
O61	LP	C70-H154	σ^*	0.52	0.93	0.020
Guest → host						
C68-H148	σ	C33	LP*	0.30	0.44	0.015
C68-H149	σ	C3-C34	π^*	0.21	0.65	0.012
C70-C71	π	C46-H125	σ^*	0.21	0.83	0.012
C70-C71	π	C47-H127	σ^*	0.31	0.83	0.014
C70-C71	π	C50-H133	σ^*	0.39	0.83	0.016
C72-C73	π	C52-H137	σ^*	0.60	0.84	0.020

^a $E^{(2)}$ means energy of hyperconjugative interaction or stabilization energy (in kcal/mol).

^b Energy difference between donor and acceptor i and j NBO orbitals.

^c $F_{i,j}$ is the Fock matrix element between i and j NBO orbitals.

^d Only the stabilization energies higher than 0.20 kcal/mol are given.

Table S6. Representative values of the NBO analysis for the complex 3, ω B97XD/6-311G*, CHCl₃.

Donor (i)	Type	Acceptor (j)	Type	$E^{(2)}$, kcal/mol ^{a,d}	E(j)-E(i), ^b a.u.	F(i,j), ^c a.u.
Host → guest						
C1-C25	π	C71-H152	σ^*	0.58	0.81	0.021
C9-C40	π	C69-H148	σ^*	0.32	0.83	0.016
C10-C37	π	C69-H149	σ^*	0.20	0.83	0.013
C24-C35	π	C68-H146	σ^*	0.38	0.82	0.017
O60	LP	C70-H150	σ^*	0.31	0.89	0.015
O64	LP	C68-H147	σ^*	0.21	0.91	0.013
Guest → host						
C67-C73	π	C46-H125	σ^*	0.30	0.86	0.014
C67-C73	π	C49-H131	σ^*	0.36	0.86	0.016
C67-C73	π	C47-H127	σ^*	0.33	0.86	0.015

C67-C73	π	C50-H133	σ^*	0.53	0.86	0.019
C68-H147	σ	C48-H129	σ^*	0.22	1.05	0.013
C70-H150	σ	C4-C33	π^*	0.33	0.67	0.015

^a $E^{(2)}$ means energy of hyperconjugative interaction or stabilization energy (in kcal/mol).

^b Energy difference between donor and acceptor i and j NBO orbitals.

^c F_{ij} is the Fock matrix element between i and j NBO orbitals.

^d Only the stabilization energies higher than 0.20 kcal/mol are given.

xyz coordinates of the optimized complexes 1-3

Complex 1, wB97XD/6-311G*, CHCl₃

C	-3.842828774937	1.821046772061	-0.007421050154
C	2.967055532029	3.041194050445	0.304110490444
C	0.677177435280	4.060695424757	0.259422759175
C	4.414821602419	0.641053442953	0.169252410530
C	-4.189384411351	-0.965136712996	-0.037371851586
C	2.146294704998	-3.826645335556	0.017434186808
C	-2.893963760700	-3.093037765565	-0.064934558202
C	-2.092157323078	3.595209746425	0.125812896188
C	4.117219333812	-1.826081248473	0.091118803613
C	-0.328391529062	-4.231516524903	-0.011664549250
C	4.293271626084	2.336400118188	4.526292678255
C	-2.439108658635	-4.814265715426	-4.085013116290
C	3.360358153408	-3.323610155741	-4.342413304876
C	-5.339839423608	1.097797020702	-3.853602485468
C	-1.515849977797	5.055992041177	4.138220085692
C	-0.073370881971	6.261164432687	-2.948578271500
C	3.769898087992	-3.234702425225	4.433178659905
C	-1.779681567705	-4.808545522200	4.084968541102
C	4.825189412144	2.349866697822	-3.909798148105
C	-6.227464028843	0.195815256507	3.490535417880
C	3.610961669954	-2.286859797594	-1.119567339631
C	-2.236354082353	-3.317541797681	1.141128161364
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C	-3.967633552128	-0.258790372015	-1.214196647525
C	-4.081767450199	1.116194548289	1.166981895180
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C	-0.978191973343	-3.988168036020	-1.216257231321
C	-1.338021648185	3.770655166811	-1.027120180103
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C	0.032925121674	4.000921716862	-0.974934960275
C	-3.800456363755	1.120161834328	-1.215022401344
C	-1.441906285778	3.635072675266	1.364931363597
C	-0.957719755718	-3.864008474784	1.181184910737
C	-4.259522411406	-0.263087470345	1.166291954620
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C	2.162804745653	4.320150810242	0.350770554091
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C	5.121549557339	-0.694915202430	0.115546580771
C	-3.574813849903	3.308150793430	0.034945893584
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O	0.809008903526	4.143169716283	-2.098018889138
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O	-2.224920607282	3.418965799235	2.464573784843
O	4.117665532727	-1.853721014380	2.443981900872
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C	-0.315379621790	-0.048704726154	-3.834780688473
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Complex 2, wB97XD/6-311G*, CHCl₃

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H	-3.555046117961	-0.636932595353	4.181229648202
H	-2.709669724955	0.727723465323	3.448857816016
H	4.832264022137	-0.414224649630	-4.243943762012
H	4.919810267308	1.185319466994	-3.500397095873
H	1.154482620084	-0.676250811035	0.557651474395
H	0.922206910108	1.046382556300	0.273985315127
H	-1.530419573139	0.708643893620	0.022660500645
H	-1.349422819213	-1.003776898594	0.344705363270
H	-1.625515090398	-0.584825702405	-2.036343626681
H	-0.069778588275	-1.329248293356	-1.718859448310
H	1.053981932084	0.905928044139	-1.927280801463
H	-0.515098969329	1.663422911815	-2.133979276476
H	1.281059061897	0.145265707333	-5.546111690521
H	0.428855084914	-0.058997008756	4.171705142323
H	1.437652725865	-1.049733357452	2.969971089199
H	-0.807961821279	0.446293643701	-4.342379342882
H	-0.593041077693	1.157667594130	2.323412636526
H	2.232903461489	0.353258889112	-3.965226460893

Complex 3, wB97XD/6-311G*, CHCl₃

C	0.884216948938	4.139197566381	-0.507415304265
C	3.721197091773	-1.999176527760	0.179160016249
C	4.243512691628	0.408572469174	-0.169619910727
C	1.620195873213	-3.838153626352	0.470284996598
C	-1.897072876104	3.828726060586	-0.286614122305
C	-3.314957270293	-2.750919218508	0.533980894046
C	-3.777253122522	2.212562706971	-0.014936527909
C	3.065346883936	2.939747649648	-0.441111301550
C	-0.858270408917	-4.115259416265	0.620187372815
C	-4.382825250977	-0.507131964205	0.338016847658
C	3.747581225279	-2.974389121164	4.487212722232
C	-4.899432072398	0.794500822876	-4.205962758733
C	-2.919219990536	-4.500700758177	-3.552610128879
C	-0.589275937707	3.895049969218	-4.854933069582
C	4.914230931415	3.068448082903	3.575452900041
C	4.431636418700	1.215480848607	-4.546102656307
C	-1.851963220644	-3.232004584566	5.073364501505
C	-4.020462409249	1.170043269815	4.644505052334
C	3.193996594365	-4.693588903453	-3.544156505692
C	-0.634775843645	5.332581644763	3.771819486311
C	-1.493705966858	-3.861962051408	-0.593941862326
C	-3.866097774489	1.658843771325	1.256177421944
C	-2.678303248419	-3.006484207264	1.740733356638
C	-1.264063379588	3.748128226579	-1.521326463036
C	0.253308224227	4.206750619977	0.731941595526
C	2.156733212874	-3.184520740806	1.575870450675
C	3.179128596191	-2.646088818769	-0.925480506179
C	4.050118859971	1.228468799455	0.937003331233
C	-4.320060798787	0.053235487949	-0.934420459364
C	3.260160241157	2.120905873459	-1.548929742566
C	3.190461385033	-2.262371755065	1.445651464389
C	-2.696781146771	-3.167177313786	-0.650780295081
C	2.127151910563	-3.546537971764	-0.797044468496
C	3.829588514029	0.858462447464	-1.426410944991
C	0.115656403950	3.875893341922	-1.642386427353
C	3.447885832524	2.477257926036	0.819636865257
C	-4.136221445461	0.308134613633	1.443624255604
C	-1.120434538644	4.027821711502	0.858627410837
C	-3.984933171140	1.388685863265	-1.123609191010

C	-1.451319914667	-3.660828613774	1.796339320785
C	4.821721546774	-0.977855860062	-0.000706517355
C	-3.396123344475	3.663701500522	-0.187984298417
C	-4.622225447080	-1.990244619570	0.505239737578
C	0.480456335374	-4.816439628291	0.645083002607
C	2.386381517621	4.279813022697	-0.603558861759
C	-3.304306468841	0.231166482183	3.690701106093
C	3.221971418424	-1.729704449674	3.793714537526
C	-3.607666231120	1.151857065934	-3.493162810739
C	3.456714510343	2.870425698392	3.196780144843
C	-1.057709240291	3.965142100938	3.264618882037
C	-2.702406985342	-3.081896892199	-3.057994892198
C	3.498565387475	0.318580883199	-3.752371967622
C	1.951765620789	-3.900948605912	-3.178184325574
C	-0.842319868298	-2.905993955728	3.987904698056
C	0.194294499881	3.024162196741	-3.889578014543
O	-4.166208814548	-0.280438904929	2.678613895680
O	3.744922463610	-1.571395996763	2.483546740839
O	0.783542213113	3.770933884486	-2.831454755943
O	4.008786008447	-0.008984301059	-2.467689924081
O	1.507400952776	-4.158584521577	-1.853079731870
O	3.174936701212	3.302663361615	1.873047909567
O	-0.791339062018	-3.903331460535	2.972368052991
O	-3.825384499797	1.969933044602	-2.350260467073
O	-3.337152495444	-2.836132411742	-1.810353478925
O	-1.789953629498	4.036939472827	2.048251027943
C	-0.125650837222	-0.635489237526	-4.680786285394
C	0.557442051731	0.582886982803	3.437013958930
C	-0.835874854087	-0.141506359549	-1.257003601288
C	-0.656999890629	-0.257840604844	0.251453729481
C	0.308195379231	-0.772813106466	-2.057414523902
C	0.568163476585	0.500627540512	0.777561347970
C	0.084071111815	-0.702829555288	-3.498925301308
C	0.588207309875	0.552087336591	2.235206572229
H	4.838580810872	-2.949355668564	4.534852477768
H	3.451834003434	-3.888816439940	3.969343087962
H	3.360940330062	-3.024030315380	5.508916709021
H	-5.554097888488	0.180035659209	-3.584567256753
H	-4.678923417000	0.239205023910	-5.122062995711
H	-5.444001429568	1.701440884776	-4.478591354566
H	-2.498582548704	-5.239783860716	-2.867864017733
H	-2.443720974234	-4.631384785126	-4.528502858755
H	-3.986527319164	-4.706337905962	-3.660499266581
H	-1.450525637781	4.368554061862	-4.379275925065
H	-0.952029795064	3.289436491811	-5.690515686049
H	0.050189311038	4.683884114714	-5.257550066542
H	5.068986719374	2.794382032486	4.622666158607
H	5.197319298777	4.116101897720	3.450263889579
H	5.582911766512	2.460465046766	2.962757162829
H	4.571942947442	2.186896411692	-4.067893409532
H	4.021347172779	1.384599395451	-5.545490993059
H	5.411457804678	0.744499193047	-4.652764957842
H	-1.639546821191	-4.211566504496	5.507558121230
H	-2.876286584001	-3.247215585173	4.695291120431
H	-1.795326746974	-2.486203642245	5.871683216850
H	-4.883544706392	0.671551167547	5.091674710261
H	-4.374813798376	2.073825008053	4.144687434677
H	-3.343761599223	1.469988875909	5.449793291478
H	4.054302927854	-4.413334365592	-2.933085345451
H	3.450350409752	-4.518846594970	-4.592490416369
H	3.013658001449	-5.762246254739	-3.408333360896
H	-0.140244755747	5.233349761642	4.741954596988
H	-1.508000076231	5.976641408507	3.897992580694

H	0.055862029765	5.829361367825	3.087832189615
H	-0.995801668662	-4.199222994645	-1.493907084102
H	-3.668789552167	2.307460667477	2.100354597485
H	-3.158189194692	-2.659349647948	2.646915596140
H	-1.885610364200	3.560398444566	-2.387291945650
H	0.881030491149	4.365927006085	1.599218965244
H	1.729188339013	-3.414988080193	2.543171561447
H	3.586723894511	-2.395668054466	-1.895586654550
H	4.347922217471	0.838089819587	1.901054858887
H	-4.480819113597	-0.606000594455	-1.777501935763
H	2.930223709141	2.499252438581	-2.507464231756
H	5.417170939871	-1.238545331520	-0.877277809883
H	5.485156887443	-0.991653829322	0.865163856250
H	-3.861058575358	4.063008348404	-1.090407031654
H	-3.772591690414	4.239142677206	0.658840536194
H	-5.164429670404	-2.175401659026	1.433440736998
H	-5.242300362580	-2.352506118733	-0.316470362416
H	0.599998077537	-5.340253528126	1.593889568978
H	0.513990535285	-5.561567613461	-0.150756019173
H	2.735296467781	4.966201589532	0.169025466579
H	2.654460414489	4.707442590110	-1.570529266959
H	-2.949984120224	-0.646666741716	4.237821637426
H	-2.431127254353	0.705727452659	3.230848276229
H	3.548925351224	-0.834469646853	4.326409999046
H	2.128886558431	-1.701309613949	3.763132355148
H	-2.971438914646	1.752239198760	-4.148736424993
H	-3.036240304022	0.261032124462	-3.215223288059
H	2.816299803084	3.491620689745	3.826399085321
H	3.131532175871	1.833867647426	3.328205734021
H	-1.748325310076	3.501567436056	3.973221494753
H	-0.207425702213	3.286141159688	3.148373211624
H	-3.159646233955	-2.367441132945	-3.745879839953
H	-1.639127031424	-2.830736624593	-2.997031230845
H	3.380870826285	-0.643715539574	-4.254535696753
H	2.498273239145	0.753240120071	-3.661504752183
H	1.111676632045	-4.199620015793	-3.807690321320
H	2.097473041610	-2.825578582905	-3.327099892448
H	0.161706706033	-2.879101779241	4.421756886267
H	-1.025829443142	-1.927644897554	3.532431607015
H	1.033934661098	2.556280344263	-4.410096417621
H	-0.419835727921	2.215478038401	-3.481774156722
H	-0.301716266648	-0.575419737611	-5.729891046529
H	0.548271026941	0.616907397403	4.501481140372
H	-0.950660691866	0.912616884478	-1.533518703637
H	-1.769086381083	-0.639863954061	-1.527232997259
H	-0.583824258796	-1.311252383176	0.539370671264
H	-1.555808631266	0.138256670138	0.729451815169
H	0.413414782875	-1.821918843947	-1.762526740534
H	1.264603153004	-0.293248315717	-1.822982656714
H	0.571241953748	1.525677667266	0.390699424290
H	1.498137844809	0.036727258095	0.433263138516