Electronic Supporting Information for

Ultrahigh binding affinity of a hydrocarbon guest inside cucurbit[7]uril enhanced by strong host-guest charge matching

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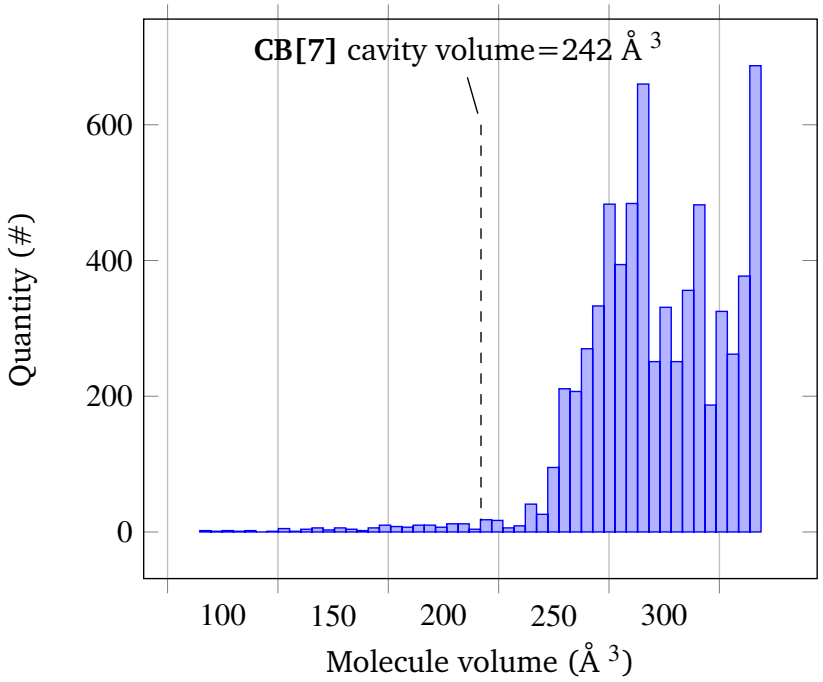

Figure S1 Volume distribution of the hydrocarbons from PubChem with 19 heavy atoms as computed by the RDKit using the `ComputeMolVolume` function. It can be seen that few reach a volume small enough to fit inside **CB[7]**

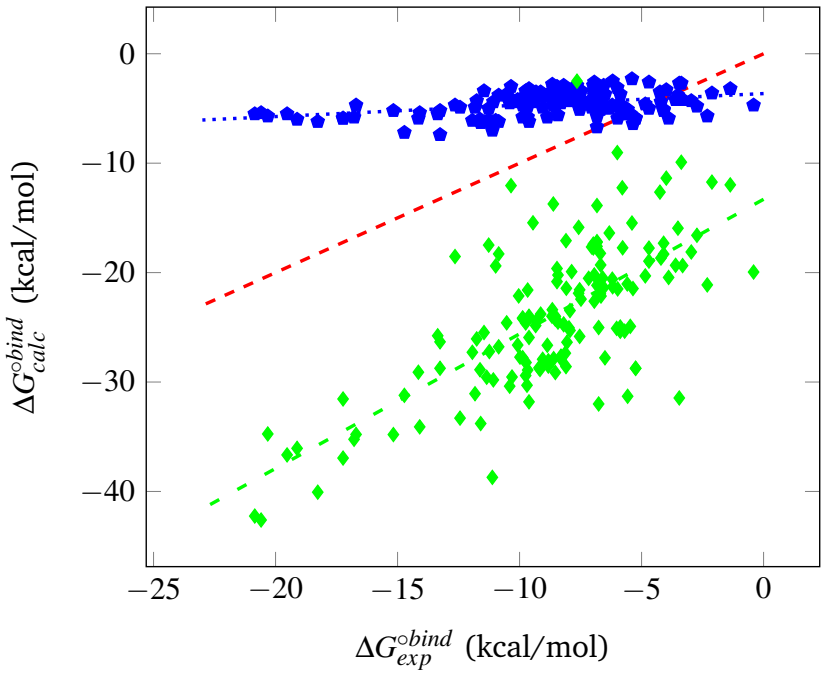

Figure S2 Benchmarking the binding affinities obtained using AutoDock Vina (blue ⬠ with blue dotted trendline) and using the present method (green ⋄ with green losely dashed trendline). The identity line corresponding to a correlation coefficient of 1 is represented by the red dashed line. The trendline are obtained using a linear regression. The linear regressions equations for the affinities estimated using AutoDock Vina ($f^{Vina}(x)$) is given by: $f^{Vina}(x) = 0.105\,x - 3.64 \quad (R^2 = 0.141)$ while in the case of the present method ($f^{GAFF}(x)$) the equation is given by: $f^{GAFF}(x) = 1.23\,x - 13.3 \quad (R^2 = 0.488)$. All guests are taken from the **CB[7]** section of the review paper [1] and $\Delta G^{\circ bind}_{exp}$ is computed as $\Delta G^{\circ bind}_{exp} = RTln(K)$ with the equilibrium constant K obtained from the reference paper. $\Delta G^{\circ bind}_{exp}$ is expressed in kcal/mol with R=8.3145 J/K/mol and T=300 K.

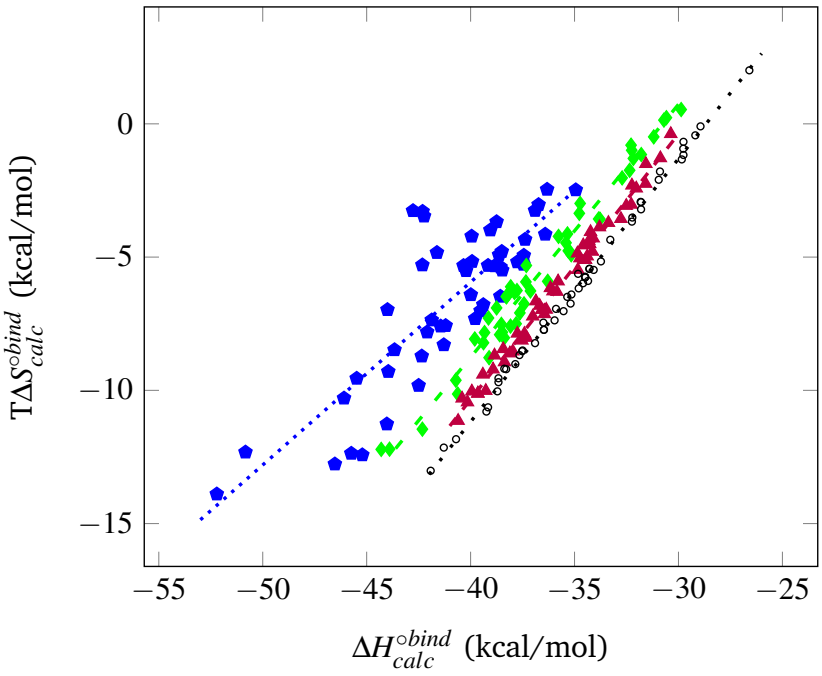

Figure S3 Binding enthalpy-entropy compensation for the 200 first guests using values computed with the GAFF model with GBSA-RRHO corrections. The first 50 guests are labelled with blue ⬠ with a blue dotted trend-line with equation $f^{1-50}(x) = 0.686\,x + 21.5 \quad (R^2 = 0.695)$. The guests ranked 51-100 are marked with green ⋄ with green loosely dashed trend-line of equation $f^{51-100}(x) = 0.949\,x + 29.2 \quad (R^2 = 0.969)$; the guests ranked 101-150 are marked with purple △ with purple dashed trend-line of equation $f^{101-150}(x) = 0.996\,x + 29.5 \quad (R^2 = 0.989)$; the guests ranked 151-200 are marked with black circles with a black loosely dotted trend-line of equation $f^{151-200}(x) = 0.987\,x + 28.3 \quad (R^2 = 0.997)$.

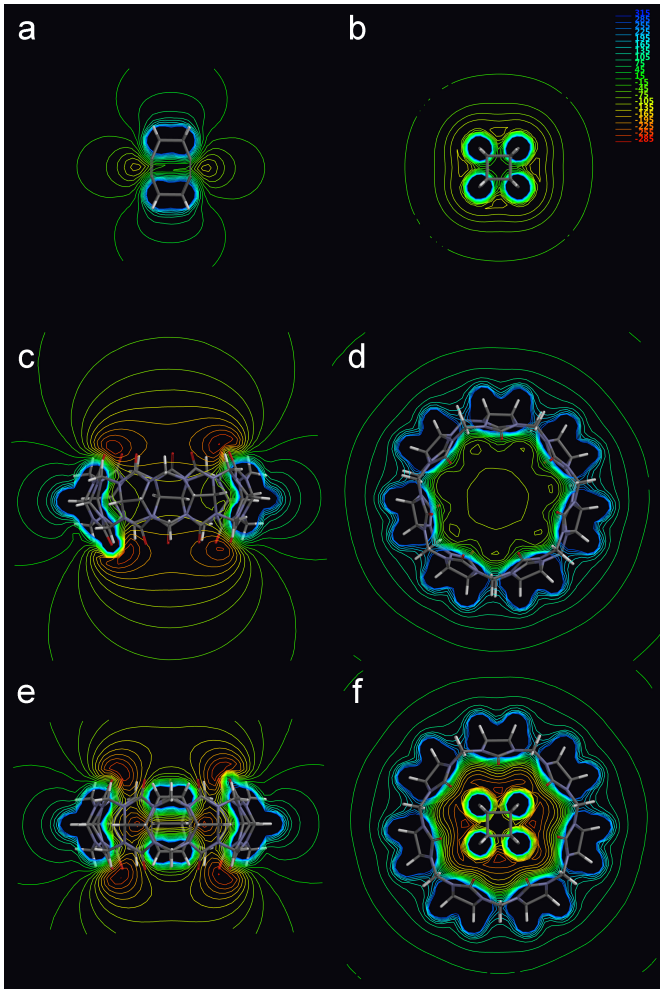

Figure S4 (a) Side and (b) top views of the electrostatic potential of **G38**,(c-d) those of **CB[7]** and (e-f) those of the corresponding host-guest complex. The guest **G38** has a large quadrupole moment θ_{zz} of +17.6962 B (along its long axis). The complex **G38 @CB[7]** has on the other hand a θ_{zz} of -172.0938 B, significantly lower than the θ_{zz} of -192.9825 B of free **CB[7]** suggesting a favourable matching of charge distribution.

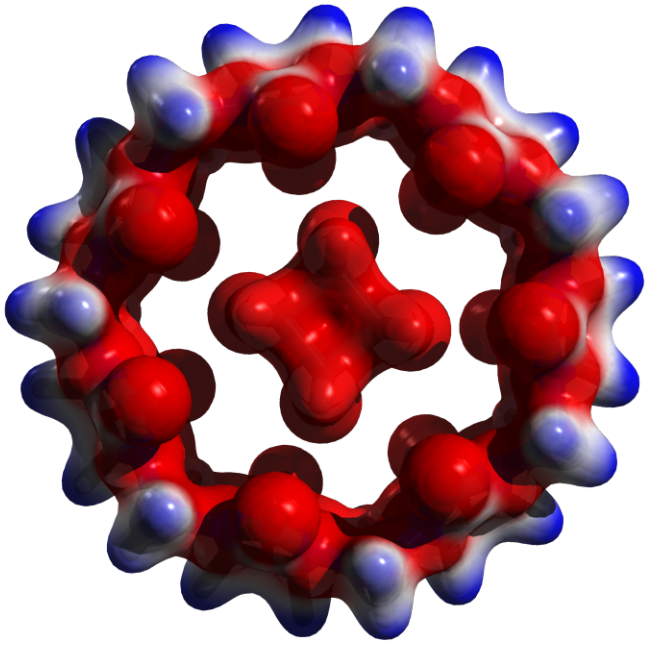

Figure S5 Electronic density ρ surface corresponding to 10% of the maximum density ρ_{max} of the **G38 @CB[7]** complex. The colour corresponds to the electrostatic potential with red indicating electron rich zones. As there is no visible electron density overlap between **CB[7]** and the guest **G38**, a chemical contribution to the binding enthalpy obtained using DFT is ruled out.

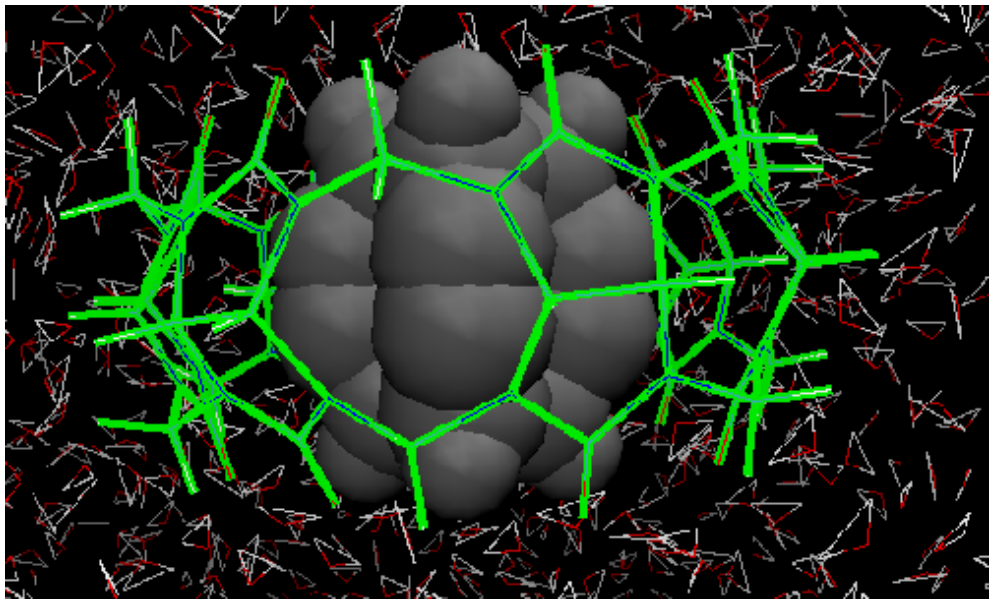

Figure S6 Snapshot of the solvated **G38 @CB[7]** complex at 1 bar and 298.15 K taken from a 500 ps trajectory.

Table S1 Top ranked 100 guests predicted using the GAFF model with GBSA-RRHO corrections labelled as their PubChem CID along with their canonical SMILES.

Label	PubChem CID	Canonical SMILES	Label	PubChem CID	Canonical SMILES
G1	**101803327**	C12(CC3CC(C1)CC(C2)C3)C#Cc1cc(ccc1)C=C	**G51**	**15931860**	C12(C(C(=C)C(C1)(CC2)C)(C)C)C
G2	**101803326**	C12(CC3CC(C1)CC(C2)C3)C#Cc1ccc(cc1)C=C	**G52**	**300774**	C12(CC3CC(C2)CC(C1)C3)c1ccc(cc1)C
G3	**144631**	C12(CC3CC(C1)CC(C2)C3)C#Cc1ccccc1	**G53**	**5368548**	C12(CC3CC(C2)CC(C1)C3)/C=C/C
G4	**15196674**	C\1(=C(#CC#C/C(=C(#CC#C1)/C#C)/C#C)/C#C)/C#C	**G54**	**141567**	C\1(=C/23CC4CC2CC(C3)C4)/C2CC3CC1CC(C2)C3
G5	**123461631**	C123C4C5CC(C1C1CC4CC(C3)C1)CC(C2)(C5)C	**G55**	**129813191**	C12/C(=C/34CC(C3)C=C4)/C3CC(C2)CC(C1)C3
G6	**86059398**	C12(CC3CC(C1)CC(C2)C3)C#CCC#CC(C)(C)C	**G56**	**522637**	C12(CC3CC(C1)CC(C2)C3)CC
G7	**145391**	C12(CC3CC(C1)CC(C2)C3)C#CC(C)(C)C	**G57**	**59986281**	C12(CC3CC(C2)CC(C1)C3)C[CH]
G8	**101005491**	C12(CC3CC(C1)CC(C2)C3)C#CC#C	**G58**	**57420426**	C12(CC3CC(C2)CC(C1)C3)C[CH2]
G9	**10752705**	C12(C3CC4CC1CC(C3)C4)[C@@H]1CCC[C@H]2C=CC1	**G59**	**90794527**	C(C(C)C)(C)(C)C#CC#CC(C)C
G10	**57857527**	C12(CCC(CC1)(CC2)C(C)(C)C)C(C)(C)C	**G60**	**18618115**	C1(C(C)(C)C)C2=C(CCCC2)C=C1
G11	**129805865**	C(C(C)(C)C#CC#CC(C(C)(C)C)(C)C)(C)(C)C	**G61**	**11829781**	[C@@]12(C(C(=C)[C@](C1)(CC2)C)(C)C)C
G12	**20680012**	C12(C3C(CC(C1)C3)(C)C)C1CC(C2)CC1	**G62**	**101698856**	C12C3CC(/C(=C\4/C5CC6C(C5)CC4C6)/C(C2)C3)C1
G13	**59413473**	c1(=C(C)C)c(c(c(=C(C)C)c(c1C)C)C)C	**G63**	**59886574**	C12(CCC(CC1)CC2)Cc1ccccc1
G14	**59265337**	C12(CCC(CC1)(CC2)C)Cc1ccc(cc1)CC	**G64**	**101002159**	C12(CC3CC(C1)CC(C2)C3)c1ccc(cc1)C#CC
G15	**12701266**	C12(CC3CC(C2)CC(C1)C3)/C=C/C(C)(C)C	**G65**	**51350035**	C123[C@@H](C4C[C@H](C1)C[C@H](C2)C4)CC(=C3)C
G16	**59498823**	C12(CCC(CC2)(CC1)C=C)Cc1ccc(cc1)CC	**G66**	**101452730**	C1CC(=Cc2c1cccc2)C#CC(C)(C)C
G17	**59265495**	C12(CCC(CC1)(CC2)Cc1ccc(cc1)CC)CC	**G67**	**12770181**	C12C3C(C1CC=CC3)CC2
G18	**123543605**	C12(CC3(CC(C1)CC(C2)C3)C)C(C)(C)C	**G68**	**15258388**	C12(CC3CC(C1)CC(C2)C3)C(=C)c1ccccc1
G19	**123862158**	C12(CC(C=C(C1)CCC2)C)C	**G69**	**67737864**	C1(CCCC1)C#Cc1cc2c(cc1)cccc2
G20	**102212342**	C12(CC3CC(C1)CC(C2)C3)C#CC1=CCCCC1	**G70**	**13227635**	C12(CCC(CC1)(CC2)C=C)C=C
G21	**71332814**	C1#CC#CC#CC#C1	**G71**	**100921744**	C12C3C4C(C5C1C(C4C#C5)C3)C2
G22	**101042791**	C1CC#CC#CCCCC#CC#CC1	**G72**	**129754847**	C12(C(C(CC1)(CC2)C#Cc1ccccc1)(C)C)C
G23	**57795934**	C12(CC3CC(C1)CC(C2)C3)c1cc(cc(c1)C=C)C=C	**G73**	**58341678**	C12C(C3CC(C2)CC(C1)C3)(C)C#C
G24	**18711338**	C12(C(C(CC1(C)C)CC2)(C)C)C	**G74**	**21014723**	C(C(C)(C)C#CC)(C)(C)C
G25	**16102301**	C12(CCC(CC2)(CC1)C#Cc1ccccc1)C	**G75**	**90894618**	C1(C(=CCC=C1)C#Cc1ccccc1)C
G26	**58480260**	C12(CCC(CC2)(CC1)c1ccc(cc1)CC)CC	**G76**	**13525539**	C12(C(C(C(C1)(C)C)CC2)(C)C)C
G27	**101606130**	C12(C3C4C5(C(C14)C2C35)C#CCCC)C#CCCC	**G77**	**570934**	C12(CC3CC(C2)CC(C1)C3)C=C
G28	**129805870**	C(C(C)C)(C)(C)C#CC#CC(C(C)C)(C)C	**G78**	**101670766**	C1(=CC=CC=CC=C1)C#CC#CC1=CC=CC=CC=C1
G29	**12700932**	C12=C(C3CC4CC1CC(C3)C4)C1CC3CC2CC(C1)C3	**G79**	**102466237**	c12c(ccc(c1)C#CC1C=CC=C1)cccc2
G30	**57589448**	C12C3C4C5C(C1CC(C3)(C5)C#CC)CC(C4)(C2)C#CC	**G80**	**91416794**	c12c(cc(cc2)C#CC(C)C)ccc(c1)C
G31	**12859733**	C12(CC3CC(C1)CC(C2)C3)CC#C	**G81**	**59018499**	C12C3C4C5C(C1CC(C3)(C5)C=C)CC(C2)(C4)C=C
G32	**522511**	C12(CC3CC(C1)CC(C2)C3)c1cc(cc(c1)C)C	**G82**	**18326899**	C1(C2=C(C(C3=C1C(=CC3)C)(C)C)C(=CC2)C)(C)C
G33	**101726911**	[C@@]12(C([C@H](CC1(C)C)CC2)(C)C)C	**G83**	**607646**	C12CC3CC(C2)/C(=C/2=CC=C2)/C(C1)C3
G34	**129874833**	C\1=C#CC#C/C=C#CC#C1	**G84**	**97289314**	[C@@H]12C(/C(=C/C)/[C@@H](C1)CC2)(C)C
G35	**58944185**	C(C(C)(C)C#CC#CC)(C)(C)C	**G85**	**97289315**	[C@H]12C(/C(=C/C)/[C@H](C1)CC2)(C)C
G36	**584912**	C12(CC3CC(C2)CC(C1)C3)Cc1ccccc1	**G86**	**10888097**	C12(C3C4C5(C3C2C5C14)C#C)C#C
G37	**15442850**	C12(CC3CC(C1)CC(C2)C3)C1=CC(=C(C)C)C=C1	**G87**	**22717661**	C1(C2=C(C(C3=C1C(=C(C3)C)C)(C)C)C(=C(C2)C)C)(C)C
G38	**101402794**	C12C3C4C1C#CC1C(C(C1C#C4)C#C3)C#C2	**G88**	**71423428**	C12CCC(CC1)c1c2cc2c(c1)CCCC2
G39	**13528098**	C12(C3CC4CC2CC(C3)C4)C2CC3CC1CC(C2)C3	**G89**	**21675358**	C12(CCC(CC1)(CC2)c1ccccc1)C(C)C
G40	**10776723**	C12(C3CC4CC1CC(C3)C4)C1CCCC2CCC1	**G90**	**71425924**	C12CCC(CC1)c1c2cc2c(c1)CC=CC2
G41	**594781**	C12(CC3CC(C1)CC(C2)C3)C#C	**G91**	**101584199**	c\1(=C\2/C=CC=C2)/cc/c(=C/2=CC=CC=C2)/cc1
G42	**620000**	C12(CC3CC(C1)CC(C2)C3)c1ccc(cc1)C(C)(C)C	**G92**	**10080912**	[C@H]12C3[C@H](C1(C)C)[C@@H]1C[C@H]2CC(C3)C1
G43	**102162544**	C12(CC3CC(C1)CC(C2)C3)c1ccc(cc1)CCC	**G93**	**10773791**	C(c1ccc(cc1)C#CC#C)(C)(C)C
G44	**15562679**	C1(C(C)(C)C#CC#CC(C(C)(C)C#CC#C1)(C)C)(C)C	**G94**	**12654465**	C12C3CC(C1)CC(C2)CC3=C
G45	**13412836**	C12/C(=C/34CCC3CC4)/C3CC(C1)CC(C2)C3	**G95**	**13661808**	C12C(/C(=C/C)/C(C1)CC2)(C)C
G46	**91240295**	C(c1cc2CCC(=Cc2cc1)C#CCCC)(CC)C	**G96**	**4330444**	C12(CC3CC(C1)CCC(C2)C3)CC
G47	**603063**	C12(CC3CC(C2)CC(C1)C3)c1ccc(cc1)CC	**G97**	**138028**	C12(C34CC5CC(C3)CC(C4)C5)CC3CC(C1)CC(C2)C3
G48	**85680646**	C(C1=CCc2c1cc1c2ccccc1)(C)(C)C	**G98**	**85556200**	c12c(cccc1)C#CC=CC=CC#C2
G49	**15355856**	C12(CC3CC(C1)CC(C2)C3)c1ccc(cc1)C=C	**G99**	**19849413**	C12(CCC(CC1)(CC2)C)CC
G50	**59610346**	C12(CCC(CC1)(CC2)c1ccc(cc1)C(C)C)C(C)C	**G100**	**102594238**	c12c(cccc1)C#C/C=C=C/C#C2

Table S2 Top ranked 100 guests predicted using the GAFF model with GBSA-RRHO corrections along with their binding affinities broken down by contributions. All quantities are expressed in kcal/mol. T = 298.15 K

Label	$\Delta G^{\circ bind}$	$-T\Delta S^{\circ bind}$	$\Delta H^{\circ bind}$	ΔU_{val}	ΔU_{VDW}	ΔU_{Coul}	ΔW_{np}	ΔW_{elec}
G1	-39.51	3.26	-42.77	-0.06	-45.34	0.64	-1.38	3.37
G2	-39.02	3.29	-42.31	-0.04	-44.90	0.59	-1.34	3.38
G3	-38.78	3.46	-42.24	-0.05	-44.80	0.69	-1.34	3.27
G4	-38.51	12.32	-50.83	2.28	-55.30	3.94	-1.99	0.25
G5	-38.32	13.89	-52.21	-1.27	-55.28	-3.22	-1.04	8.62
G6	-37.03	6.97	-44.00	-0.08	-47.09	1.80	-1.45	2.83
G7	-37.02	5.29	-42.32	0.00	-45.48	1.24	-1.34	3.26
G8	-36.79	4.83	-41.62	0.02	-43.74	0.58	-1.27	2.81
G9	-35.93	9.55	-45.48	1.58	-50.88	-2.35	-1.33	7.50
G10	-35.80	10.29	-46.09	-1.66	-47.79	-1.51	-1.53	6.40
G11	-35.73	4.22	-39.95	0.10	-42.12	1.70	-1.56	1.94
G12	-35.18	8.48	-43.66	0.42	-47.14	-2.17	-1.30	6.55
G13	-35.07	3.68	-38.75	-0.92	-39.46	0.01	-1.18	2.79
G14	-35.06	3.99	-39.05	0.33	-42.35	-0.52	-1.78	5.28
G15	-35.02	5.32	-40.34	-0.04	-43.63	-0.21	-1.33	4.88
G16	-34.76	5.17	-39.93	0.22	-43.27	-0.20	-1.86	5.20
G17	-34.71	5.51	-40.22	0.38	-43.91	-0.43	-1.87	5.63
G18	-34.66	9.27	-43.96	1.35	-48.80	-2.07	-1.21	6.77
G19	-34.51	7.36	-41.87	-0.58	-44.16	-0.67	-1.14	4.69
G20	-34.27	7.82	-42.09	-0.14	-44.78	1.13	-1.31	3.03
G21	-33.86	2.46	-36.32	0.39	-36.22	0.49	-1.18	0.21
G22	-33.85	7.59	-41.44	3.00	-47.02	-0.87	-1.90	5.36
G23	-33.84	5.32	-39.16	0.51	-42.43	-0.84	-1.38	5.00
G24	-33.76	12.77	-46.53	-2.41	-47.14	-1.65	-1.15	5.85
G25	-33.71	4.92	-38.63	-0.05	-40.63	0.93	-1.63	2.76
G26	-33.71	4.79	-38.50	0.19	-41.55	-0.05	-1.81	4.74
G27	-33.70	3.03	-36.73	0.65	-39.83	3.36	-1.50	0.61
G28	-33.65	3.25	-36.90	0.69	-39.38	1.84	-1.56	1.52
G29	-33.63	8.72	-42.35	2.09	-48.29	-1.33	-1.20	6.39
G30	-33.63	7.57	-41.20	1.41	-45.37	-1.01	-1.21	5.02
G31	-33.58	6.42	-39.99	-0.38	-42.17	-0.50	-1.20	4.27
G32	-33.51	5.33	-38.84	0.41	-42.31	-0.41	-1.32	4.80
G33	-33.37	12.37	-45.74	-2.86	-45.83	-1.50	-1.17	5.63
G34	-33.18	5.38	-38.56	2.26	-42.35	0.92	-1.69	2.31
G35	-33.04	4.34	-37.38	-0.11	-38.76	1.60	-1.42	1.31
G36	-33.00	8.29	-41.29	-0.09	-44.32	-0.83	-1.38	5.36
G37	-32.99	5.49	-38.48	0.21	-41.55	-0.56	-1.28	4.72
G38	-32.79	12.42	-45.21	-0.20	-50.21	-3.30	-0.71	9.22
G39	-32.76	11.27	-44.03	2.53	-50.29	-2.56	-1.28	7.57
G40	-32.68	9.82	-42.50	2.88	-48.71	-2.58	-1.41	7.32
G41	-32.60	6.79	-39.39	-0.04	-41.85	0.45	-1.13	3.19
G42	-32.57	5.18	-37.75	0.43	-41.18	-0.58	-1.27	4.84
G43	-32.50	4.94	-37.44	0.46	-40.78	-0.62	-1.25	4.76
G44	-32.50	7.02	-39.52	0.40	-41.85	1.58	-1.64	1.98
G45	-32.47	7.31	-39.78	0.88	-44.20	-0.01	-1.29	4.85
G46	-32.46	2.48	-34.94	2.06	-40.28	1.82	-1.87	3.33
G47	-32.31	5.19	-37.50	0.45	-40.83	-0.61	-1.27	4.75
G48	-32.26	4.15	-36.41	-0.04	-37.08	-1.69	-1.46	3.87
G49	-32.19	5.27	-37.46	0.45	-40.65	-0.81	-1.26	4.81
G50	-32.09	6.47	-38.57	0.52	-42.43	-0.55	-1.84	5.74
G51	-32.08	12.22	-44.30	-1.84	-44.78	-2.11	-1.14	5.58
G52	-32.01	5.32	-37.32	0.46	-40.58	-0.61	-1.26	4.66
G53	-31.96	6.11	-38.07	0.37	-41.37	-0.26	-1.22	4.42
G54	-31.85	7.29	-39.14	1.77	-44.89	-0.25	-1.31	5.56
G55	-31.84	6.91	-38.75	0.15	-42.14	-0.27	-1.28	4.79
G56	-31.81	6.46	-38.27	-0.33	-40.82	-0.68	-1.11	4.68
G57	-31.80	6.47	-38.27	-0.32	-40.81	-0.70	-1.11	4.68
G58	-31.79	6.49	-38.28	-0.33	-40.81	-0.70	-1.11	4.68
G59	-31.74	2.99	-34.73	1.23	-37.43	1.68	-1.44	1.24
G60	-31.73	8.07	-39.80	0.89	-43.56	-1.30	-1.46	5.64
G61	-31.69	12.21	-43.90	-1.74	-44.49	-2.08	-1.14	5.56
G62	-31.56	6.33	-37.89	0.51	-41.69	-0.17	-1.33	4.80
G63	-31.55	4.22	-35.77	0.34	-38.46	-0.57	-1.58	4.51
G64	-31.52	6.25	-37.77	0.43	-40.76	-1.22	-1.26	5.05
G65	-31.50	7.83	-39.33	-0.08	-42.26	-0.80	-1.13	4.96
G66	-31.48	0.80	-32.28	1.85	-36.58	1.65	-1.75	2.57
G67	-31.41	3.36	-34.77	-8.29	-28.36	-0.45	-1.15	3.50
G68	-31.41	5.93	-37.34	1.70	-42.35	-0.66	-1.36	5.33
G69	-31.26	0.99	-32.25	0.20	-33.65	0.75	-1.61	2.08
G70	-31.21	4.13	-35.34	-0.08	-37.42	0.02	-1.53	3.66

Table S2 (Continued) Top ranked 100 guests predicted using the GAFF model with GBSA-RRHO corrections along with their binding affinities broken down by contributions. All quantities are expressed in kcal/mol. T = 298.15 K

Label	$\Delta G^{\circ bind}$	$-T\Delta S^{\circ bind}$	$\Delta H^{\circ bind}$	ΔU_{val}	ΔU_{VDW}	ΔU_{Coul}	ΔW_{np}	ΔW_{elec}
G70	-31.21	4.13	-35.34	-0.08	-37.42	0.02	-1.53	3.66
G71	-31.17	8.21	-39.38	0.44	-41.98	-0.01	-0.70	2.87
G72	-31.09	9.62	-40.71	-0.13	-42.79	-0.04	-1.52	3.79
G73	-31.00	7.52	-38.52	0.31	-41.43	-0.49	-1.19	4.30
G74	-30.95	4.46	-35.41	-0.13	-37.20	0.83	-1.32	2.42
G75	-30.87	1.30	-32.17	1.43	-35.20	1.15	-1.52	1.98
G76	-30.86	11.46	-42.32	-0.96	-44.22	-1.45	-1.22	5.55
G77	-30.85	6.27	-37.12	0.36	-40.20	-0.42	-1.13	4.28
G78	-30.84	-0.14	-30.70	0.75	-31.91	0.90	-1.57	1.13
G79	-30.81	-0.23	-30.58	1.66	-34.81	2.20	-1.77	2.16
G80	-30.70	0.49	-31.19	1.93	-35.83	1.92	-1.65	2.45
G81	-30.69	7.91	-38.60	1.48	-43.76	-2.79	-1.12	7.60
G82	-30.68	2.03	-32.71	-5.95	-27.98	0.55	-0.93	1.60
G83	-30.67	6.76	-37.43	0.35	-40.25	-0.23	-1.26	3.99
G84	-30.67	7.82	-38.49	-1.01	-39.88	-0.38	-1.17	3.96
G85	-30.66	7.82	-38.48	-1.00	-39.88	-0.38	-1.17	3.96
G86	-30.64	1.15	-31.79	0.26	-33.70	2.11	-0.97	0.53
G87	-30.61	1.74	-32.35	-3.86	-28.80	-1.59	-0.47	2.40
G88	-30.54	4.76	-35.30	1.37	-39.56	0.07	-1.33	4.17
G89	-30.54	7.09	-37.63	0.50	-41.14	-0.79	-1.83	5.63
G90	-30.49	4.76	-35.26	1.35	-39.24	-0.26	-1.33	4.21
G91	-30.49	7.59	-38.08	-4.64	-34.75	-0.76	-1.59	3.66
G92	-30.48	10.14	-40.62	-0.23	-43.72	-0.94	-1.07	5.35
G93	-30.41	-0.54	-29.87	0.63	-31.81	-0.34	-1.44	3.1
G94	-30.38	5.91	-36.29	-0.01	-38.66	-0.06	-1.07	3.52
G95	-30.35	8.03	-38.38	-0.89	-39.88	-0.41	-1.18	4.00
G96	-30.34	8.77	-39.11	-0.27	-41.74	-1.23	-1.16	5.29
G97	-30.31	7.50	-37.81	1.76	-43.33	-1.77	-1.32	6.86
G98	-30.27	3.57	-33.84	1.87	-37.45	0.50	-1.55	2.81
G99	-30.25	4.91	-35.16	-0.09	-37.41	-0.37	-1.41	4.14
G100	-30.20	3.58	-33.78	1.92	-37.43	0.54	-1.56	2.77

Table S3 DFT ωB97XD/6-31G* binding affinity (ΔE) of the top ranked 50 guests obtained from the GAFF model with GBSA-RRHO corrections. All quantities are expressed in kcal/mol. Guests are sorted by decreasing magnitude of DFT binding energy.

Label	ΔE	Label	ΔE
G38	-62.78	**G50**	-44.73
G5	-54.34	**G26**	-44.68
G21	-53.05	**G20**	-44.65
G39	-49.47	**G12**	-44.60
G6	-49.18	**G49**	-44.40
G22	-49.16	**G47**	-44.40
G45	-48.80	**G31**	-44.10
G18	-48.76	**G37**	-43.98
G17	-48.68	**G19**	-43.91
G36	-48.64	**G43**	-43.70
G9	-48.41	**G7**	-43.60
G23	-47.33	**G40**	-41.75
G15	-47.11	**G41**	-41.65
G24	-46.78	**G25**	-41.35
G33	-46.78	**G11**	-41.00
G14	-46.76	**G8**	-40.76
G1	-46.58	**G44**	-37.60
G29	-46.14	**G28**	-36.96
G16	-45.96	**G46**	-36.52
G32	-45.80	**G27**	-35.33
G10	-45.77	**G48**	-34.88
G2	-45.74	**G35**	-34.72
G3	-45.11	**G4**	-26.17
G42	-45.10	**G13**	-22.20
G30	-44.81	**G34**	-11.02

Table S4 Ten selected guests within the 50 highest ranked guests obtained from GAFF model with GBSA-RRHO corrections, along with their SAPT energy decomposition in kcal/mol. Guests are sorted by decreasing magnitude of their total SAPT interaction energy. The contributions to the SAPT energy decomposition include the electrostatic energy (E_{elst}), the exchange energy (E_{exch}), the induction energy (E_{ind}) and the dispersion energy (E_{disp}). The sum of all contribution is termed E_{tot}

Label	PubChem CID	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{tot}
G38	**101402794**	-42.82	39.49	-15.81	-53.05	-72.19
G5	**123461631**	-21.33	62.07	-7.38	-69.93	-36.57
G1	**101803327**	-11.72	35.76	-6.28	-52.83	-35.08
G9	**10752705**	-29.045	75.62	-8.61	-72.91	-34.95
G39	**13528098**	-29.65	79.98	-9.29	-75.25	-34.22
G24	**18711338**	-17.03	46.01	-5.53	-55.22	-31.78
G10	**57857527**	-14.71	43.84	-6.14	-54.26	-31.26
G11	**129805865**	-9.37	34.74	-5.57	-48.84	-29.03
G30	**57589448**	-8.08	43.61	-5.74	-57.35	-27.55
G27	**101606130**	-7.06	28.38	-4.99	-42.49	-26.16

References

[1] S. J. Barrow, S. Kasera, M. J. Rowland, J. del Barrio and O. A. Scherman, *Chem. Rev*, 2015, **115**, 12320–12406.