

Supplementary Information For

A LSER-based model to predict the solubilizing effect of drugs by inclusion with cucurbit[7]uril

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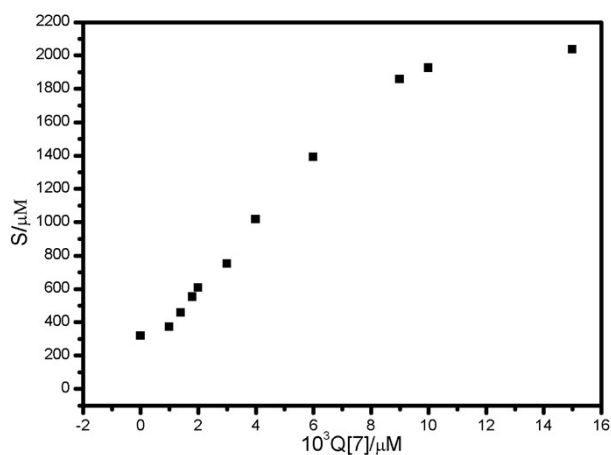


Fig. S1 Phase-solubility diagram of mixtures of VB₂ and cucurbit[7]uril in aqueous solvent (pH = 7).

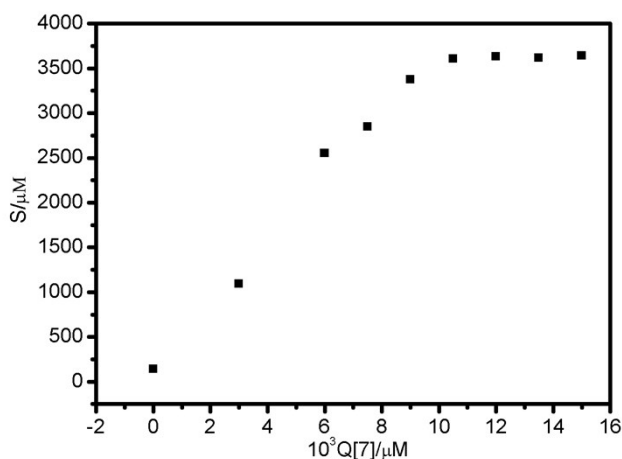


Fig. S2 Phase-solubility diagram of mixtures of triamterene and cucurbit[7]uril in aqueous solvent (pH = 7).

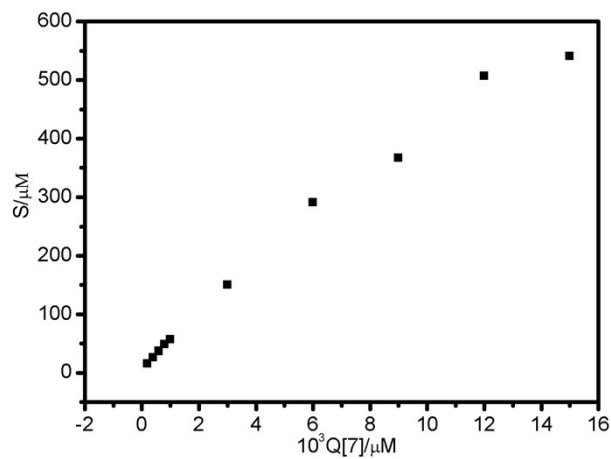


Fig. S3 Phase-solubility diagram of mixtures of guanine and cucurbit[7]uril in aqueous solvent (pH = 7).

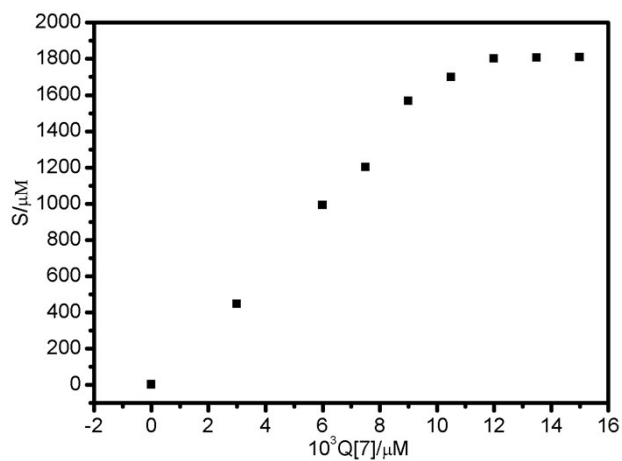


Fig. S4 Phase-solubility diagram of mixtures of 2-hydroxychalcone and cucurbit[7]uril in aqueous solvent (pH = 7).

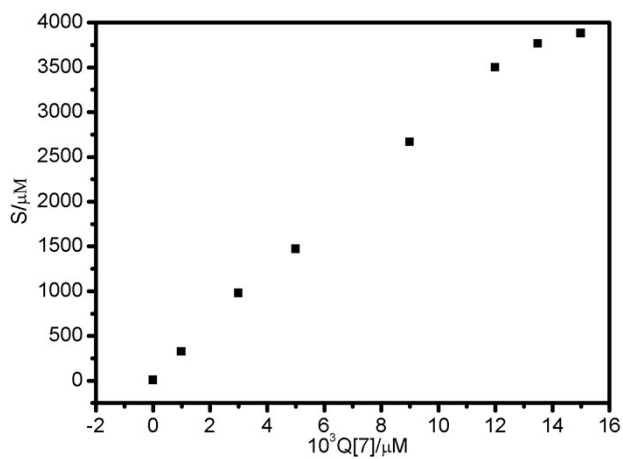


Fig. S5 Phase-solubility diagram of mixtures of gefitinib and cucurbit[7]uril in aqueous solvent (pH = 7).

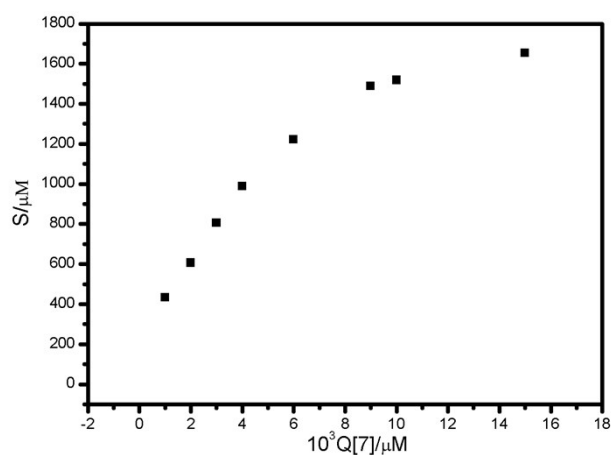
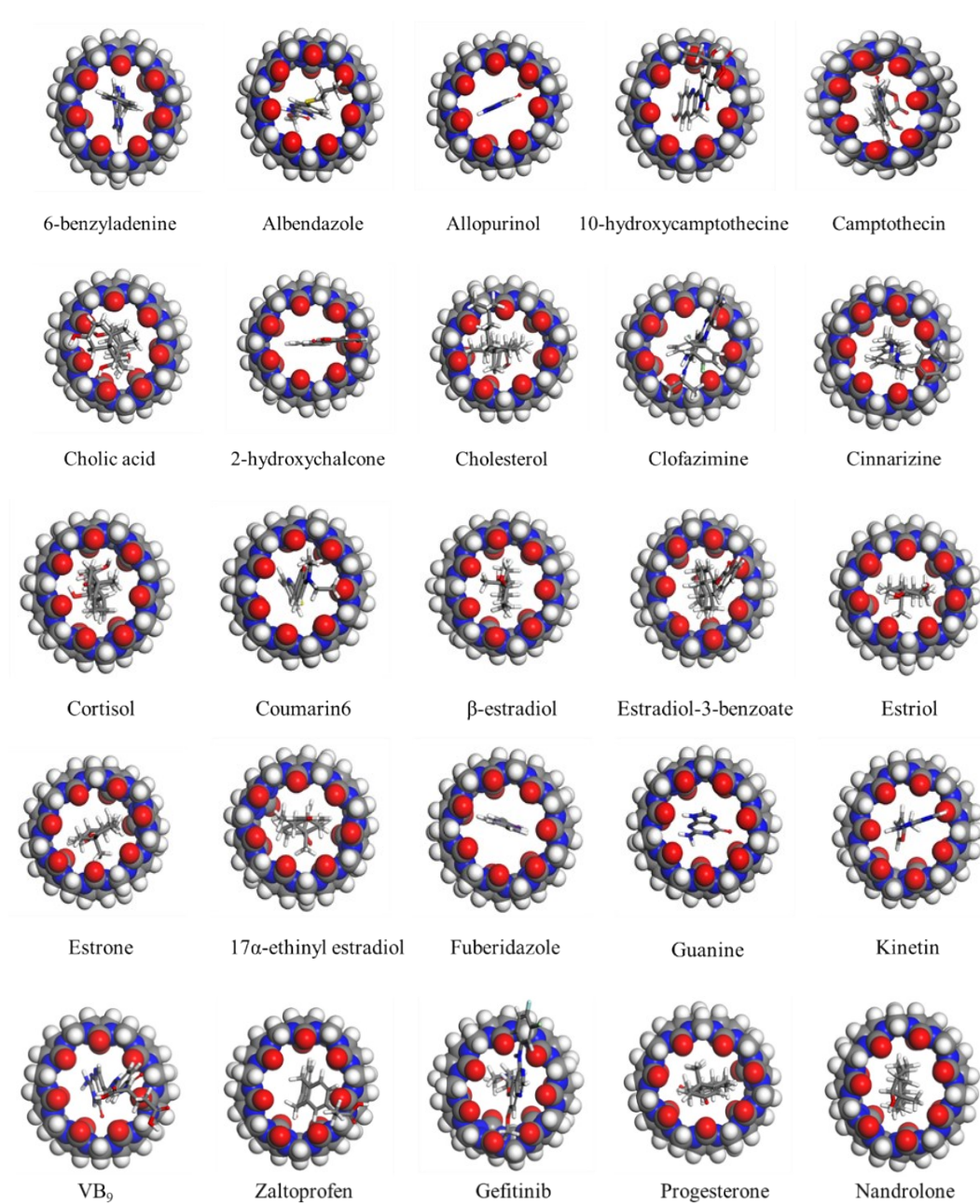


Fig. S6 Phase-solubility diagram of mixtures of VB₉ and cucurbit[7]uril in aqueous solvent (pH = 7).



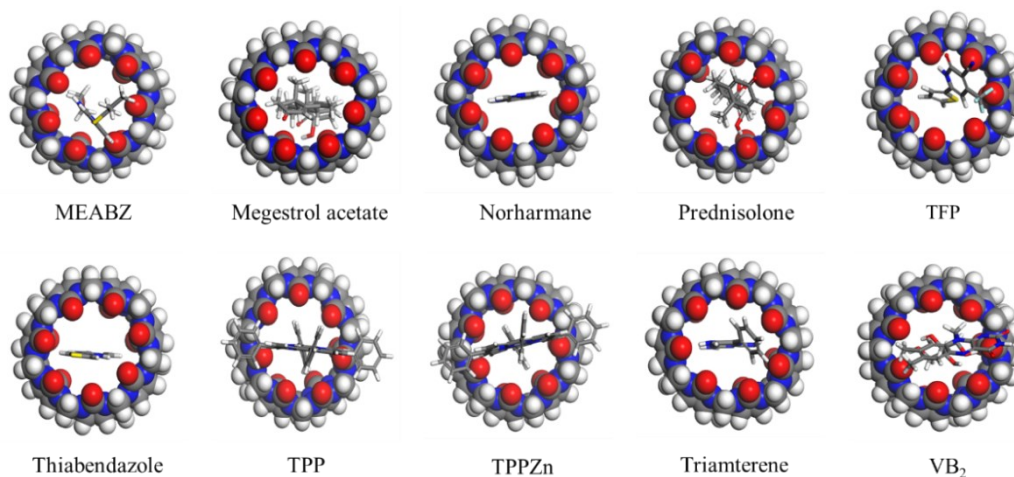


Fig. S7 Optimized inclusion structures at the DFT / B3LYP / 6-311G* level.

Table S1. The molecular parameters of 35 drug-cucurbit[7]uril inclusions.

#	$\chi_1/\text{a.u.}$	$\log p_{1w}/\text{a.u.}$	$I_3/\text{a.u.}$	$E_{3LUMO}/\text{a.u.}$	A_3/Bohr^2
Cinnarizine	2.544E-01	5.524E+00	3.979E-02	-4.170E-03	4.124E+03
Allopurinol	2.961E-01	-7.547E-01	4.203E-02	-3.710E-03	3.176E+03
MEABZ	2.479E-01	3.302E+00	4.063E-02	-8.390E-03	3.839E+03
Albendazole	2.481E-01	3.433E+00	4.344E-02	-2.340E-03	3.531E+03
Thiabendazole	2.762E-01	4.078E+00	4.361E-02	-2.230E-03	3.341E+03
6-benzyladenine	2.476E-01	2.146E+00	4.390E-02	-3.280E-03	3.355E+03
Gefitinib	2.636E-01	4.203E+00	4.066E-02	-1.415E-02	3.925E+03
Kinetin	2.624E-01	1.264E+00	4.401E-02	-1.194E-02	3.483E+03
Nandrolone	2.875E-01	3.267E+00	4.414E-02	-8.430E-03	3.162E+03
Norharmane	2.701E-01	2.173E+00	4.398E-02	-5.570E-03	3.344E+03
Triamterene	2.674E-01	1.279E+00	4.228E-02	-6.600E-03	3.302E+03
2-hydroxychalcone	3.270E-01	3.460E+00	4.131E-02	-4.671E-02	3.606E+03
VB ₉	2.933E-01	-2.311E-01	3.818E-02	-3.927E-02	3.967E+03
Fuberidazole	2.608E-01	4.125E+00	4.394E-02	-5.410E-03	3.423E+03
10-hydroxycamptothecine	3.100E-01	1.504E+00	3.939E-02	-4.160E-02	3.649E+03
Prednisolone	2.958E-01	1.260E+00	4.077E-02	-1.247E-02	3.326E+03
Clofazimine	2.844E-01	7.137E+00	3.682E-02	-5.383E-02	4.312E+03
β -estradiol	2.850E-01	3.838E+00	4.177E-02	-5.860E-03	3.470E+03
VB ₂	3.549E-01	-6.020E-02	3.982E-02	-7.024E-02	3.661E+03
TFP	3.642E-01	1.892E+00	4.165E-02	-5.538E-02	3.435E+03
Progesterone	2.908E-01	3.860E+00	4.054E-02	-1.015E-02	3.308E+03
Cholic acid	2.525E-01	2.913E+00	3.815E-02	-6.500E-03	3.840E+03
Cortisol	3.091E-01	1.284E+00	4.199E-02	-1.031E-02	3.125E+03
TPP	2.792E-01	8.690E+00	3.483E-02	-6.332E-02	4.862E+03
Guanine	2.334E-01	-1.288E+00	4.245E-02	-7.080E-03	3.061E+03
Estriol	2.322E-01	2.871E+00	4.189E-02	-6.220E-03	3.501E+03
Estrone	2.449E-01	3.939E+00	4.193E-02	-6.660E-03	3.455E+03
TPPZn	2.751E-01	9.531E+00	3.433E-02	-6.020E-02	4.860E+03

Camptothecin	3.208E-01	1.746E+00	3.884E-02	-4.140E-02	3.339E+03
Coumarin6	2.817E-01	5.382E+00	3.933E-02	-3.409E-02	3.731E+03
Megestrol acetate	3.049E-01	3.127E+00	3.889E-02	-2.401E-02	3.306E+03
Zaltoprofen	2.991E-01	3.541E+00	3.891E-02	-2.315E-02	3.408E+03
Cholesterol	2.269E-01	7.376E+00	3.694E-02	-5.920E-03	3.637E+03
Estradiol-3-benzoate	2.314E-01	5.512E+00	3.923E-02	-3.514E-02	3.617E+03
17 -ethinyl estradiol	2.339E-01	4.887E+00	4.254E-02	-6.340E-03	3.093E+03
#	V_1/Bohr^3	$\Delta E_{12}/\text{a.u.}$	$\Delta G_{3w}/\text{a.u.}$	$E_{1max}/\text{a.u.}$	$E_{1min}/\text{a.u.}$
Cinnarizine	3.430E+03	-1.799E-02	-2.321E-01	2.368E-02	-4.457E-02
Allopurinol	9.968E+02	-3.385E-02	-2.243E-01	8.059E-02	-6.020E-02
MEABZ	2.592E+03	-2.912E-02	-2.283E-01	7.078E-02	-5.482E-02
Albendazole	2.195E+03	-3.085E-02	-2.270E-01	6.956E-02	-5.520E-02
Thiabendazole	1.575E+03	-2.335E-02	-2.227E-01	6.603E-02	-5.750E-02
6-benzyladenine	1.861E+03	-3.171E-02	-2.297E-01	7.971E-02	-5.423E-02
Gefitinib	3.525E+03	-3.670E-02	-1.051E-02	8.872E-02	-5.602E-02
Kinetin	1.689E+03	-3.409E-02	-2.384E-01	9.553E-02	-8.059E-02
Nandrolone	2.491E+03	-3.179E-02	-2.314E-01	7.203E-02	-6.759E-02
Norharmane	1.426E+03	-2.214E-02	-2.253E-01	8.059E-02	-6.382E-02
Triamterene	2.000E+03	-3.689E-02	-2.365E-01	5.864E-02	-7.902E-02
2-hydroxychalcone	1.936E+03	-2.037E-02	-2.204E-01	4.664E-02	-5.037E-02
VB ₉	3.334E+03	-6.687E-02	-2.558E-01	1.032E-01	-6.912E-02
Fuberidazole	1.512E+03	-1.876E-02	-2.258E-01	7.431E-02	-6.150E-02
10-hydroxycamptothecin	2.759E+03	-3.549E-02	-2.356E-01	9.962E-02	-6.150E-02
Prednisolone	2.992E+03	-5.718E-02	-2.245E-01	9.706E-02	-7.051E-02
Clofazimine	3.825E+03	-1.571E-02	-2.342E-01	4.122E-02	-4.963E-02
β -estradiol	2.439E+03	-2.875E-02	-2.286E-01	8.129E-02	-5.716E-02
VB ₂	2.851E+03	-3.901E-02	-2.497E-01	9.301E-02	-6.987E-02
TFP	1.807E+03	-4.083E-02	-2.136E-01	9.022E-02	-6.847E-02
Progesterone	2.881E+03	-4.303E-02	-2.201E-01	3.087E-02	-6.595E-02
Cholic acid	3.615E+03	-3.896E-02	-2.418E-01	7.697E-02	-6.243E-02
Cortisol	3.032E+03	-6.272E-02	-2.232E-01	7.905E-02	-6.470E-02
TPP	5.166E+03	-1.208E-02	-2.338E-01	2.402E-02	-4.491E-02
Guanine	1.102E+03	-4.942E-02	-2.314E-01	8.716E-02	-8.245E-02
Estriol	2.504E+03	-2.935E-02	-2.355E-01	8.162E-02	-5.791E-02
Estrone	2.390E+03	-3.157E-02	-2.244E-01	8.302E-02	-5.955E-02
TPPZn	5.185E+03	-1.152E-02	-2.536E-01	6.329E-02	-2.798E-02
Camptothecin	2.696E+03	-4.175E-02	-2.304E-01	4.634E-02	-5.997E-02
Coumarin6	2.867E+03	-2.959E-02	-2.309E-01	4.230E-02	-8.913E-02
Megestrol acetate	3.025E+03	-3.641E-02	-2.181E-01	4.037E-02	-6.820E-02
Zaltoprofen	2.354E+03	-3.785E-02	-2.211E-01	7.840E-02	-5.844E-02
Cholesterol	3.851E+03	-3.898E-02	-2.114E-01	6.732E-02	-6.062E-02
Estradiol-3-benzoate	3.272E+03	-3.326E-02	-2.263E-01	6.931E-02	-6.126E-02
17 -ethinyl estradiol	2.637E+03	-4.312E-02	-2.218E-01	8.107E-02	-5.232E-02

Table S2. Standardized residuals and leverage of the model.

#	Standardized residual	Leverage
Cinnarizine	0.583	0.252
Allopurinol	1.314	0.154
MEABZ	1.189	0.088
Albendazole	1.037	0.085
Thiabendazole	0.683	0.122
6-benzyladenine	1.055	0.101
Gefitinib	-0.430	0.077
Kinetin	-0.532	0.157
Nandrolone	1.087	0.118
Norharmane	-0.110	0.069
Triamterene	1.703	0.079
2-hydroxychalcone	0.577	0.175
VB ₉	-0.880	0.371
Fuberidazole	-0.932	0.105
10-hydroxycamptothecin	0.525	0.111
Prednisolone	-0.414	0.067
Clofazimine	1.509	0.135
β -estradiol	-1.479	0.091
VB ₂	0.158	0.519
TFP	-1.056	0.391
Progesterone	0.206	0.100
Cholic acid	-1.193	0.211
Cortisol	-1.342	0.094
TPP	-0.601	0.300
Guanine	1.248	0.424
Estriol	-0.639	0.114
Estrone	-0.503	0.043
TPPZn	-0.398	0.311
Camptothecin	1.148	0.176
Coumarin6	0.197	0.043
Megestrol acetate	0.820	0.134
Zaltoprofen	-0.211	0.096
Cholesterol	0.092	0.360
Estradiol-3-benzoate	0.298	0.366
17 -ethinyl estradiol	-1.449	0.236

Table S3. The molecular parameters of MEABZ by inclusion with cucurbit[n]uril (n=6,7,8).

	MEABZ-cucurbit[6]uril	MEABZ-cucurbit[7]uril	MEABZ-cucurbit[8]uril
$\chi_1/a.u.$	2.479E-01	2.479E-01	2.479E-01
$\log p_{1w}/a.u.$	3.302E+00	3.302E+00	3.302E+00
$I_3/a.u.$	3.808E-02	4.063E-02	4.020E-02

$E_{3LUMO}/\text{a.u.}$	-6.970E-03	-8.390E-03	-1.114E-02
A_3/Bohr^2	3.141E+03	3.839E+03	4.396E+03
