Electronic Supplementary Information Characterization of cisplatin/membrane interactions by QM/MM energy-decomposition analysis

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QM/MM Energy Decomposition Analysis (EDA) Based on Electron Deformation Densities

First, we will introduce the EDA equations for a purely quantum mechanical (QM) treatment and afterwards the particular case of QM/MM will be addressed. The mathematical derivation for QM is introduced elsewhere.[1,2] The readers are referred to these works to extend their knowledge on this EDA scheme. Consider an interacting quantum system formed

by two closed-shell fragments A and B. The interaction energy is defined as the difference between the AB complex energy and the energies of the A and B isolated fragments.

$$E_{\rm int} = E_{\rm AB} - (E_{\rm A}^{\rm AB} + E_{\rm B}^{\rm AB}) \tag{1}$$

In Eq (1), the superscript AB indicates that the fragment energies are calculated for the geometry of the fragments in the complex and the basis set of the complex. The latter is introduced to correct the basis set superposition error.[3] The AB complex energy may be written in terms of the one-electron and exchange-correlation densities, which are represented in Eq (2) by $\rho(\mathbf{r})$ and $\rho_{\rm XC}(\mathbf{r}_1, \mathbf{r}_2)$, respectively.

$$\begin{aligned} E_{\rm AB} = &-\frac{1}{2}\int \nabla^2 \rho(\mathbf{r}, \mathbf{r}')_{\mathbf{r}'=\mathbf{r}} d\mathbf{r} + \int \hat{\nu}_{\rm N}\rho(\mathbf{r})d\mathbf{r} + \frac{1}{2}\int\int \frac{\rho(\mathbf{r_1})\rho(\mathbf{r_2})}{|\mathbf{r}_2 - \mathbf{r}_1|} d\mathbf{r}_1 d\mathbf{r}_2 + \\ &+ \frac{1}{2}\int\int \frac{\rho_{\rm XC}(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_2 - \mathbf{r}_1|} d\mathbf{r}_1 d\mathbf{r}_2 + \sum_{I=1}^{N-1}\sum_{J>I}^{N} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} \end{aligned} \tag{2}$$

In Eq (2), the kinetic energy term is obtained from the one-electron density matrix, $\rho(\mathbf{r}, \mathbf{r}')_{\mathbf{r}'=\mathbf{r}}$, instead of the one-electron density, whereas the nuclei potential operator is represented by $\hat{\nu}_{\rm N}$. Operators and electron densities may be rewritten in terms of contributions from a hypothetical non-interacting system (unperturbed fragments) and those arising from the interaction (Eqs (3)-(6)). Thus, the nucleus-nucleus repulsion energy term is given by,

$$\sum_{I=1}^{N-1}\sum_{J>I}^{N} \frac{Z_I Z_J}{|\mathbf{R}_{IJ}|} = \sum_{I=1}^{N_{\rm A}-1}\sum_{J>I}^{N_{\rm A}} \frac{Z_I Z_J}{|\mathbf{R}_{IJ}|} + \sum_{I=N_{\rm A}+1}^{N-1}\sum_{J>I}^{N} \frac{Z_I Z_J}{|\mathbf{R}_{IJ}|} + \sum_{I=1}^{N_{\rm A}}\sum_{J=N_{\rm A}+1}^{N} \frac{Z_I Z_J}{|\mathbf{R}_{IJ}|} \tag{3}$$

where $N_{\rm A}$ represents the number of the nuclei belonging to fragment A and $\mathbf{R}_{IJ} = |\mathbf{R}_I - \mathbf{R}_J|$. On the other hand, the nuclei potential operator is,

$$\hat{\nu}_{\rm N} = \hat{\nu}_{\rm N_A} + \hat{\nu}_{\rm N_B} \tag{4}$$

and the one-electron and exchange-correlation densities are,

$$\rho(\mathbf{r}) = \rho_{\mathrm{A}}(\mathbf{r}) + \rho_{\mathrm{B}}(\mathbf{r}) + \Delta\rho_{\mathrm{Pau}}(\mathbf{r}) + \Delta\rho_{\mathrm{pol}}(\mathbf{r}) \tag{5}$$

$$\rho_{\mathrm{XC}}(\mathbf{r}_1, \mathbf{r}_2) = \rho_{\mathrm{XC,A}}(\mathbf{r}_1, \mathbf{r}_2) + \rho_{\mathrm{XC,B}}(\mathbf{r}_1, \mathbf{r}_2) + \rho_{\mathrm{X,AB}}(\mathbf{r}_1, \mathbf{r}_2) + \Delta\rho_{\mathrm{XC}}(\mathbf{r}_1, \mathbf{r}_2) \tag{6}$$

where the contributions from the Pauli repulsion and the electron polarization, $\Delta\rho_{\mathrm{Pau}}(\mathbf{r})$ and $\Delta\rho_{\mathrm{pol}}(\mathbf{r})$, have been included separately in Eq (5) as well as the interfragment exchange and polarization, $\rho_{\mathrm{X,AB}}(\mathbf{r}_1, \mathbf{r}_2)$ and $\Delta\rho_{\mathrm{XC}}(\mathbf{r}_1, \mathbf{r}_2)$, in Eq (6). The first two terms in Eqs (5) and (6) correspond, respectively, to the one-electron and exchange-correlation densities of the unperturbed fragments.

Additionally, the nuclei potential and the electron potential operators associated to each unperturbed fragment can be merged, giving rise to the unperturbed fragment potentials $\hat{\nu}_{\mathrm{A}}$ and $\hat{\nu}_{\mathrm{B}}$,

$$\hat{\nu}_{\mathrm{A}}(\mathbf{r}) = \hat{\nu}_{\mathrm{N_A}}(\mathbf{r}) + \int \frac{\rho_{\mathrm{A}}(\mathbf{r}_2)}{|\mathbf{r}_2 - \mathbf{r}_1|} d\mathbf{r}_2 \tag{7}$$

$$\hat{\nu}_{\mathrm{B}}(\mathbf{r}) = \hat{\nu}_{\mathrm{N_B}}(\mathbf{r}) + \int \frac{\rho_{\mathrm{B}}(\mathbf{r}_2)}{|\mathbf{r}_2 - \mathbf{r}_1|} d\mathbf{r}_2 \tag{8}$$

Introducing Eqs (3)-(8) into Eq (2) and removing the energies corresponding to the energies of each unperturbed fragment (Eq (1)), one gets the interaction energy decomposed into electrostatic (elec), exchange (exch), repulsion (rep) and polarization (pol) terms,

$$E_{\mathrm{int}} = E_{\mathrm{elec}} + E_{\mathrm{exch}} + E_{\mathrm{rep}} + E_{\mathrm{pol}} \tag{9}$$

whose corresponding expressions are given by Eqs (10)-(13).

$$E_{\rm elec} = \int \hat{\nu}_{\rm N_A}\rho_{\rm B}(\mathbf{r})d\mathbf{r} + \int \hat{\nu}_{\rm N_B}\rho_{\rm A}(\mathbf{r})d\mathbf{r} + \int\int \frac{\rho_{\rm A}(\mathbf{r}_1)\rho_{\rm B}(\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r}_1 d\mathbf{r}_2 + \\ + \sum_{I=1}^{N_{\rm A}}\sum_{J=N_{\rm A}+1}^{N}\frac{Z_I Z_J}{|\mathbf{R}_{IJ}|} \tag{10}$$

$$E_{\rm exch} = \frac{1}{2}\int\int \frac{\rho_{\rm X,AB}(\mathbf{r}_1,\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r}_1 d\mathbf{r}_2 \tag{11}$$

$$E_{\rm rep} = -\frac{1}{2}\int \nabla^2 \Delta\rho_{\rm Pau}(\mathbf{r},\mathbf{r}')_{\mathbf{r}'=\mathbf{r}}d\mathbf{r} + \int \hat{\nu}_{\rm A}\Delta\rho_{\rm Pau}(\mathbf{r})d\mathbf{r} + \int \hat{\nu}_{\rm B}\Delta\rho_{\rm Pau}(\mathbf{r})d\mathbf{r} + \\ + \frac{1}{2}\int\int \frac{\Delta\rho_{\rm Pau}(\mathbf{r}_1)\Delta\rho_{\rm Pau}(\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r_1} d\mathbf{r}_2 \tag{12}$$

$$E_{\rm pol} = -\frac{1}{2}\int \nabla^2 \Delta\rho_{\rm pol}(\mathbf{r},\mathbf{r}')_{\mathbf{r}'=\mathbf{r}}d\mathbf{r} + \int \hat{\nu}_{\rm A}\Delta\rho_{\rm pol}(\mathbf{r})d\mathbf{r} + \int \hat{\nu}_{\rm B}\Delta\rho_{\rm pol}(\mathbf{r})d\mathbf{r} + \\ + \frac{1}{2}\int\int \frac{\Delta\rho_{\rm pol}(\mathbf{r}_1)\Delta\rho_{\rm pol}(\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r}_1 d\mathbf{r}_2 + \int\int \frac{\Delta\rho_{\rm Pau}(\mathbf{r}_1)\Delta\rho_{\rm pol}(\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r}_1 d\mathbf{r}_2 + \\ + \frac{1}{2}\int\int \frac{\Delta\rho_{\rm XC}(\mathbf{r}_1,\mathbf{r}_2)}{|\mathbf{r}_2-\mathbf{r}_1|}d\mathbf{r}_1 d\mathbf{r}_2 \tag{13}$$

Both exchange and repulsion energies, Eqs (11) and (12), arise from the Pauli exclusion principle (Fermi hole) between same-spin electrons of different fragments, so that they are frequently merged into one term denoted as the Pauli energy, $E_{\rm Pau}$. On the other hand, the polarization term includes the induction and dispersion energies, which can be separated exactly at 2$^{\rm nd}$-order perturbation theory (PT) level.[4] Thus, the induction energy can be separated from $E_{\rm pol}$ if we combine the EDA scheme with 2$^{\rm nd}$-order PT.[2] At this level, the induction energy is given by[4]

$$E_{\rm ind} = \sum_{m\neq 0}\frac{[\int \hat{\nu}_{\rm A}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}]^2}{E_{\rm B}^m - E_{\rm B}^0} + \sum_{n\neq 0}\frac{[\int \hat{\nu}_{\rm B}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}]^2}{E_{\rm A}^n - E_{\rm A}^0} \tag{14}$$

where $\rho_{\rm A}^{n0}$ and $\rho_{\rm B}^{m0}$ are the induced transition one-electron densities within each fragment from the ground state configuration 0 to the excited state m or n. The denominators contain the corresponding energy differences.

Additionally, the 1st-order correction to the electron density,[2] the one required for the calculation of the 2nd-order energy, is given by,

$$\begin{aligned}\Delta\rho(\mathbf{r}) &= \Delta\rho_{\rm A}(\mathbf{r}) + \Delta\rho_{\rm B}(\mathbf{r}) \\ &= 2\sum_{n\neq 0}\frac{\int \hat{\nu}_{\rm B}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}}{E_{\rm A}^{n}-E_{\rm A}^{0}}\rho_{\rm A}^{n0} + 2\sum_{m\neq 0}\frac{\int \hat{\nu}_{\rm A}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}}{E_{\rm B}^{m}-E_{\rm B}^{0}}\rho_{\rm A}^{m0}\end{aligned} \tag{15}$$

which is naturally split into fragments A and B. It represents the polarization density at 1st-order, so that introducing Eq (15) into Eq (13) the induction energy may be obtained. However, it is easier to define and work with the charge-induction energy, $E_{\text{ch-ind}}$, which is the sum of the second and third terms of Eq (13).

$$E_{\text{ch-ind}} = \int \hat{\nu}_{\rm A}\Delta\rho_{\rm pol}(\mathbf{r})d\mathbf{r} + \int \hat{\nu}_{\rm B}\Delta\rho_{\rm pol}(\mathbf{r})d\mathbf{r} \tag{16}$$

Thus, introducing Eq (15) into Eq (16),

$$\begin{aligned}E_{\text{ch-ind}} =& 2\sum_{m\neq 0}\frac{[\int \hat{\nu}_{\rm A}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}]^2}{E_{\rm B}^{m}-E_{\rm B}^{0}} + 2\sum_{n\neq 0}\frac{[\int \hat{\nu}_{\rm B}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}]^2}{E_{\rm A}^{n}-E_{\rm A}^{0}} + \\ &+ 2\sum_{m\neq 0}\frac{\int \hat{\nu}_{\rm A}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}\int \hat{\nu}_{\rm B}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}}{E_{\rm B}^{m}-E_{\rm B}^{0}} + 2\sum_{n\neq 0}\frac{\int \hat{\nu}_{\rm B}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}\int \hat{\nu}_{\rm A}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}}{E_{\rm A}^{n}-E_{\rm A}^{0}}\end{aligned} \tag{17}$$

Identifying E_{ind} as one half of the first two terms of Eq (17) and reordering,

$$E_{\text{ind}} = \frac{1}{2}\left[E_{\text{ch-ind}} - 2\sum_{m\neq 0}\frac{\int \hat{\nu}_{\rm A}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}\int \hat{\nu}_{\rm B}\rho_{\rm B}^{m0}(\mathbf{r})d\mathbf{r}}{E_{\rm B}^{m}-E_{\rm B}^{0}} - 2\sum_{n\neq 0}\frac{\int \hat{\nu}_{\rm B}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}\int \hat{\nu}_{\rm A}\rho_{\rm A}^{n0}(\mathbf{r})d\mathbf{r}}{E_{\rm A}^{n}-E_{\rm A}^{0}}\right] \tag{18}$$

and, finally, replacing back the definition of 1st-order density (Eq 15), one obtains the following expression for E_{ind},

$$E_{\text{ind}} = \frac{1}{2}\left[E_{\text{ch-ind}} - \int \hat{\nu}_{\text{A}}\Delta\rho_{\text{A}}(\mathbf{r})d\mathbf{r} - \int \hat{\nu}_{\text{B}}\Delta\rho_{\text{B}}(\mathbf{r})d\mathbf{r}\right] \tag{19}$$

Which is one half of the charge-induction energy minus the intrafragment energies. This result may be rewritten as,

$$E_{\text{ind}} = \frac{1}{2}\left[\int \hat{\nu}_{\text{A}}\Delta\rho_{\text{B}}(\mathbf{r})d\mathbf{r} + \int \hat{\nu}_{\text{B}}\Delta\rho_{\text{A}}(\mathbf{r})d\mathbf{r}\right] \tag{20}$$

matching the well-known classical result for the induction energy, where half of the energy is employed in the induction process. Summarizing, the EDA based on electron deformation densities provides a partition of E_{int} into four terms with clear physical meaning: electrostatic (E_{elec}), Pauli (E_{Pau}), induction (E_{ind}) and dispersion plus higher order terms ($E_{\text{disp+res-pol}}$). In this last term, the pure 2nd-order dispersion energy represents by far most of the interaction. This interaction energy scheme can be easily extended to QM/MM methods where the MM region belongs to one of the fragments, the one representing the molecular environment. This environment may be a solvent or a macromolecular system, such as lipid membranes or DNA, among others. The interaction of the MM region with the molecular fragment A is introduced in the calculation of the different energy terms by adding the potential created by the MM force field, $\hat{\text{V}}_{\text{FF}}$, to the nuclei potential of fragment B,

$$\hat{\nu}_{N_{\text{B}}}^{\text{QM/MM}}(\mathbf{r}) = \hat{\nu}_{N_{\text{B}}}(\mathbf{r}) + \hat{\text{V}}_{\text{FF}} \tag{21}$$

Additionally, $\hat{\text{V}}_{\text{FF}}$ is also included in the calculation of the nucleus-nucleus interaction of the electrostatic energy (last term of Eq 10). In this work, we have employed for the MM region a simple electrostatic potential represented by atomic point charges.

Correlation Coefficients for Each Energy Component at the Min and at the Max Regions

As described in the main text, the correlation coefficients for each energy component were computed considering interatomic distances r between each cisplatin atom and each atom in the DOPC molecule. More precisely, for a given energy component, we computed the linear correlation coefficient of that component with respect to $1/r^n$, where n depends on the energy component, along the ensemble of geometries considered. Below the correlation coefficients computed for the Min region (Tables S1-S4) and for the Max region (Tables S5-S8) are reported. The rows are subdivided into the four residues of the DOPC molecule (choline, phosphate, glycerol and oleyl), and for each residue the correlation coefficients are displayed in decreasing order (in absolute value). Since there are six DOPC molecules in the QM region, there are also six atoms corresponding to the same atom type (or twelve, in the case of the oleyl tails); for each geometry, we considered the minimum distance between each cisplatin atom and each atom type of the DOPC molecule.

Table S1: Linear correlation coefficients of the electrostatic energy component (E_{ele}) with respect to $1/r$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Min region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	-0.63	-0.59	-0.58	-0.57
Choline	C31	-0.61	-0.56	-0.58	-0.55
Choline	H1A	-0.59	-0.53	-0.54	-0.53
Choline	H1B	-0.53	-0.46	-0.54	-0.49
Choline	C32	-0.50	-0.45	-0.49	-0.49
Choline	H2A	-0.49	-0.44	-0.46	-0.45
Choline	H2B	-0.46	-0.44	-0.46	-0.42
Choline	C33	-0.45	-0.43	-0.40	-0.38

Choline	H3A	-0.44	-0.42	-0.39	-0.35
Choline	H3B	-0.41	-0.41	-0.36	-0.35
Choline	H3C	-0.41	-0.40	-0.31	-0.31
Choline	C34	-0.38	-0.39	-0.31	-0.29
Choline	H4A	-0.37	-0.38	-0.29	-0.28
Choline	H4B	-0.32	-0.33	-0.27	-0.24
Choline	H4C	-0.28	-0.30	-0.23	-0.19
Choline	C35	-0.28	-0.30	-0.18	-0.16
Choline	H5A	-0.27	-0.29	-0.17	-0.15
Choline	H5B	-0.25	-0.27	-0.13	-0.11
Choline	H5C	-0.24	-0.23	-0.13	-0.10
Phosphate	O31	-0.37	-0.39	-0.28	-0.26
Phosphate	O32	-0.31	-0.34	-0.26	-0.25
Phosphate	O33	-0.27	-0.33	-0.19	-0.18
Phosphate	O34	-0.23	-0.24	-0.17	-0.15
Phosphate	P31	-0.08	-0.17	-0.02	-0.01
Glycerol	C3	0.37	0.33	0.36	0.36
Glycerol	HA	0.34	0.29	0.28	0.27
Glycerol	HB	0.28	0.28	0.27	0.26
Glycerol	C2	0.23	0.19	0.24	0.25
Glycerol	HX	0.19	0.18	0.18	0.18
Glycerol	C1	0.17	0.12	0.18	0.16
Glycerol	HR	0.05	0.01	0.04	0.04
Glycerol	HS	-0.02	-0.08	-0.03	-0.02
Glycerol	C11	-0.08	-0.13	-0.03	-0.03
Glycerol	O12	-0.08	-0.15	-0.05	-0.04
Glycerol	O11	-0.16	-0.16	-0.11	-0.10

Glycerol	C21	-0.19	-0.18	-0.11	-0.10
Glycerol	O22	-0.29	-0.28	-0.18	-0.16
Glycerol	O21	-0.34	-0.30	-0.23	-0.20
Oleyl	C12	0.22	0.25	-0.22	-0.23
Oleyl	H2R	0.21	0.23	-0.19	-0.20
Oleyl	H2S	0.21	0.23	-0.18	-0.18
Oleyl	C13	0.20	0.20	-0.18	-0.18
Oleyl	H3R	0.18	0.17	-0.18	-0.18
Oleyl	H3S	0.17	0.15	-0.18	-0.18
Oleyl	C14	0.16	0.13	-0.17	-0.18
Oleyl	H4R	0.16	0.13	-0.17	-0.18
Oleyl	H4S	0.14	0.11	-0.17	-0.18
Oleyl	C15	0.11	0.10	-0.17	-0.17
Oleyl	H5R	0.11	0.09	-0.17	-0.17
Oleyl	H5S	0.06	0.06	-0.16	-0.17
Oleyl	C16	-0.02	0.02	-0.16	-0.17
Oleyl	H6R	-0.03	-0.02	-0.16	-0.16
Oleyl	H6S	-0.04	-0.03	-0.16	-0.16
Oleyl	C17	-0.04	-0.03	-0.15	-0.16
Oleyl	H7R	-0.04	-0.03	-0.15	-0.16
Oleyl	H7S	-0.05	-0.04	-0.15	-0.15
Oleyl	C18	-0.07	-0.04	-0.15	-0.15
Oleyl	H8R	-0.07	-0.04	-0.15	-0.15
Oleyl	H8S	-0.07	-0.04	-0.14	-0.15
Oleyl	C19	-0.08	-0.05	-0.14	-0.15
Oleyl	H9R	-0.08	-0.05	-0.14	-0.15
Oleyl	C110	-0.08	-0.05	-0.13	-0.14

Oleyl	H10R	-0.09	-0.06	-0.13	-0.14
Oleyl	C111	-0.09	-0.06	-0.13	-0.14
Oleyl	H11R	-0.09	-0.07	-0.13	-0.13
Oleyl	H11S	-0.09	-0.07	-0.11	-0.11
Oleyl	C112	-0.11	-0.08	-0.10	-0.11
Oleyl	H12R	-0.12	-0.10	-0.10	-0.10
Oleyl	H12S	-0.13	-0.11	-0.09	-0.10
Oleyl	C113	-0.13	-0.11	-0.09	-0.09
Oleyl	H13R	-0.13	-0.11	-0.08	-0.08
Oleyl	H13S	-0.13	-0.12	-0.07	-0.08
Oleyl	C114	-0.15	-0.13	-0.06	-0.07
Oleyl	H14R	-0.15	-0.13	-0.04	-0.05
Oleyl	H14S	-0.15	-0.13	-0.01	0.02
Oleyl	C115	-0.15	-0.14	0.04	0.07
Oleyl	H15R	-0.15	-0.15	0.12	0.10
Oleyl	H15S	-0.16	-0.15	0.12	0.11
Oleyl	C116	-0.16	-0.15	0.12	0.11
Oleyl	H16R	-0.16	-0.15	0.12	0.12
Oleyl	H16S	-0.16	-0.16	0.13	0.12
Oleyl	C117	-0.17	-0.16	0.13	0.12
Oleyl	H17R	-0.17	-0.16	0.14	0.13
Oleyl	H17S	-0.17	-0.16	0.14	0.13
Oleyl	C118	-0.17	-0.16	0.14	0.14
Oleyl	H18R	-0.17	-0.16	0.15	0.14
Oleyl	H18S	-0.17	-0.16	0.15	0.14
Oleyl	H18T	-0.18	-0.17	0.17	0.16

Table S2: Linear correlation coefficients of the induction energy component (E_{ind}) with respect to $1/r^4$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Min region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	-0.69	-0.61	-0.59	-0.56
Choline	C31	-0.53	-0.45	-0.50	-0.49
Choline	H1A	-0.53	-0.42	-0.50	-0.45
Choline	H1B	-0.47	-0.38	-0.43	-0.42
Choline	C32	-0.43	-0.37	-0.38	-0.38
Choline	H2A	-0.37	-0.35	-0.36	-0.35
Choline	H2B	-0.36	-0.35	-0.36	-0.35
Choline	C33	-0.35	-0.30	-0.34	-0.32
Choline	H3A	-0.31	-0.25	-0.32	-0.32
Choline	H3B	-0.30	-0.24	-0.32	-0.31
Choline	H3C	-0.27	-0.23	-0.27	-0.28
Choline	C34	-0.22	-0.21	-0.26	-0.26
Choline	H4A	-0.21	-0.20	-0.26	-0.25
Choline	H4B	-0.21	-0.19	-0.17	-0.17
Choline	H4C	-0.21	-0.17	-0.13	-0.12
Choline	C35	-0.18	-0.16	-0.11	-0.08
Choline	H5A	-0.14	-0.16	-0.06	-0.04
Choline	H5B	-0.11	-0.09	-0.05	-0.02
Choline	H5C	-0.08	-0.06	-0.04	-0.02
Phosphate	O31	-0.32	-0.35	-0.25	-0.23
Phosphate	O32	-0.28	-0.34	-0.23	-0.22
Phosphate	O33	-0.24	-0.33	-0.20	-0.19
Phosphate	O34	-0.21	-0.19	-0.19	-0.19

Phosphate	P31	-0.05	-0.12	-0.02	-0.01
Glycerol	C3	0.34	0.30	0.36	0.35
Glycerol	HA	0.32	0.29	0.27	0.27
Glycerol	HB	0.24	0.24	0.25	0.26
Glycerol	C2	0.20	0.14	0.22	0.19
Glycerol	HX	0.14	0.14	0.11	0.10
Glycerol	C1	0.11	0.07	0.07	0.04
Glycerol	HR	0.07	0.06	0.02	0.01
Glycerol	HS	0.01	-0.01	0.01	-0.00
Glycerol	C11	-0.06	-0.04	-0.03	-0.02
Glycerol	O12	-0.08	-0.06	-0.10	-0.10
Glycerol	O11	-0.09	-0.12	-0.12	-0.13
Glycerol	C21	-0.16	-0.14	-0.13	-0.13
Glycerol	O22	-0.24	-0.17	-0.18	-0.17
Glycerol	O21	-0.27	-0.19	-0.20	-0.19
Oleyl	C12	-0.22	-0.21	-0.22	-0.23
Oleyl	H2R	-0.21	-0.20	-0.22	-0.23
Oleyl	H2S	-0.21	-0.20	-0.22	-0.22
Oleyl	C13	-0.20	-0.19	-0.22	-0.22
Oleyl	H3R	-0.20	-0.19	-0.21	-0.22
Oleyl	H3S	-0.20	-0.19	-0.21	-0.21
Oleyl	C14	-0.19	-0.19	-0.21	-0.21
Oleyl	H4R	-0.19	-0.19	-0.20	-0.21
Oleyl	H4S	-0.18	-0.18	-0.20	-0.20
Oleyl	C15	-0.18	-0.17	-0.20	-0.20
Oleyl	H5R	-0.18	-0.17	-0.20	-0.20
Oleyl	H5S	-0.17	-0.17	-0.19	-0.20

Oleyl	C16	-0.17	-0.16	-0.19	-0.20
Oleyl	H6R	-0.17	-0.16	-0.19	-0.20
Oleyl	H6S	-0.16	-0.15	-0.18	-0.19
Oleyl	C17	-0.16	-0.15	-0.18	-0.19
Oleyl	H7R	-0.15	-0.13	-0.18	-0.18
Oleyl	H7S	-0.15	-0.13	-0.17	-0.18
Oleyl	C18	-0.15	-0.13	-0.16	-0.18
Oleyl	H8R	-0.15	-0.13	-0.16	-0.17
Oleyl	H8S	-0.14	-0.12	-0.16	-0.16
Oleyl	C19	-0.14	-0.11	-0.15	-0.16
Oleyl	H9R	-0.12	-0.11	-0.15	-0.16
Oleyl	C110	-0.11	-0.08	-0.15	-0.15
Oleyl	H10R	-0.09	-0.07	-0.14	-0.15
Oleyl	C111	-0.09	-0.07	-0.14	-0.15
Oleyl	H11R	-0.09	-0.07	-0.13	-0.14
Oleyl	H11S	-0.09	-0.06	-0.13	-0.13
Oleyl	C112	-0.08	-0.05	-0.12	-0.12
Oleyl	H12R	-0.08	-0.05	-0.11	-0.09
Oleyl	H12S	-0.08	-0.05	-0.07	-0.08
Oleyl	C113	-0.07	-0.05	-0.07	-0.07
Oleyl	H13R	-0.05	-0.04	-0.07	-0.06
Oleyl	H13S	-0.03	-0.03	-0.06	-0.05
Oleyl	C114	-0.03	-0.02	-0.03	-0.04
Oleyl	H14R	-0.02	-0.01	-0.03	-0.04
Oleyl	H14S	0.01	-0.01	-0.01	-0.01
Oleyl	C115	0.01	0.01	-0.01	-0.01
Oleyl	H15R	0.01	0.04	0.05	0.05

Oleyl	H15S	0.03	0.04	0.06	0.07
Oleyl	C116	0.04	0.07	0.07	0.08
Oleyl	H16R	0.09	0.09	0.08	0.08
Oleyl	H16S	0.10	0.10	0.08	0.08
Oleyl	C117	0.11	0.14	0.09	0.08
Oleyl	H17R	0.12	0.15	0.10	0.08
Oleyl	H17S	0.13	0.15	0.10	0.09
Oleyl	C118	0.16	0.17	0.11	0.10
Oleyl	H18R	0.16	0.19	0.11	0.11
Oleyl	H18S	0.19	0.19	0.13	0.11
Oleyl	H18T	0.19	0.19	0.15	0.12

Table S3: Linear correlation coefficients of the dispersion energy component (E_{dis}) with respect to $1/r^6$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Min region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	-0.49	-0.47	-0.43	-0.42
Choline	C31	-0.47	-0.45	-0.38	-0.37
Choline	H1A	-0.41	-0.40	-0.37	-0.31
Choline	H1B	-0.38	-0.36	-0.26	-0.27
Choline	C32	-0.26	-0.33	-0.24	-0.24
Choline	H2A	-0.24	-0.30	-0.23	-0.23
Choline	H2B	-0.23	-0.26	-0.22	-0.20
Choline	C33	-0.19	-0.23	-0.21	-0.20
Choline	H3A	-0.18	-0.19	-0.20	-0.19
Choline	H3B	-0.17	-0.18	-0.18	-0.17
Choline	H3C	-0.16	-0.18	-0.17	-0.17

Choline	C34	-0.15	-0.17	-0.12	-0.13
Choline	H4A	-0.15	-0.15	-0.12	-0.12
Choline	H4B	-0.13	-0.10	-0.11	-0.11
Choline	H4C	-0.13	-0.09	-0.11	-0.09
Choline	C35	-0.12	-0.06	-0.10	-0.08
Choline	H5A	-0.09	-0.04	-0.06	-0.06
Choline	H5B	-0.07	0.00	-0.06	-0.04
Choline	H5C	0.01	0.05	0.02	0.04
Phosphate	O31	-0.27	-0.45	-0.22	-0.21
Phosphate	O32	-0.27	-0.40	-0.21	-0.20
Phosphate	O33	-0.26	-0.32	-0.13	-0.10
Phosphate	O34	-0.22	-0.24	-0.10	-0.08
Phosphate	P31	-0.11	-0.17	-0.07	-0.06
Glycerol	C3	-0.36	-0.33	-0.31	-0.30
Glycerol	HA	-0.26	-0.28	-0.23	-0.23
Glycerol	HB	-0.26	-0.24	-0.22	-0.22
Glycerol	C2	-0.25	-0.21	-0.17	-0.16
Glycerol	HX	-0.22	-0.17	-0.14	-0.14
Glycerol	C1	-0.15	-0.16	-0.14	-0.14
Glycerol	HR	-0.15	-0.12	-0.13	-0.10
Glycerol	HS	-0.09	-0.10	-0.03	-0.05
Glycerol	C11	-0.02	-0.08	-0.03	-0.04
Glycerol	O12	-0.01	-0.06	0.01	0.00
Glycerol	O11	-0.00	-0.01	0.06	0.04
Glycerol	C21	0.05	0.03	0.11	0.11
Glycerol	O22	0.11	0.04	0.14	0.17
Glycerol	O21	0.16	0.14	0.22	0.22

Oleyl	C12	-0.32	-0.33	-0.31	-0.32
Oleyl	H2R	-0.31	-0.32	-0.31	-0.31
Oleyl	H2S	-0.30	-0.29	-0.30	-0.31
Oleyl	C13	-0.30	-0.29	-0.30	-0.30
Oleyl	H3R	-0.29	-0.29	-0.30	-0.30
Oleyl	H3S	-0.29	-0.28	-0.29	-0.28
Oleyl	C14	-0.27	-0.27	-0.27	-0.27
Oleyl	H4R	-0.27	-0.23	-0.25	-0.25
Oleyl	H4S	-0.26	-0.22	-0.25	-0.24
Oleyl	C15	-0.26	-0.19	-0.24	-0.24
Oleyl	H5R	-0.25	-0.18	-0.24	-0.24
Oleyl	H5S	-0.25	-0.17	-0.23	-0.23
Oleyl	C16	-0.24	-0.16	-0.22	-0.23
Oleyl	H6R	-0.22	-0.16	-0.19	-0.20
Oleyl	H6S	-0.21	-0.15	-0.18	-0.19
Oleyl	C17	-0.19	-0.13	-0.17	-0.17
Oleyl	H7R	-0.14	-0.13	-0.17	-0.17
Oleyl	H7S	-0.13	-0.12	-0.17	-0.16
Oleyl	C18	-0.13	-0.12	-0.16	-0.14
Oleyl	H8R	-0.12	-0.10	-0.15	-0.14
Oleyl	H8S	-0.11	-0.08	-0.15	-0.14
Oleyl	C19	-0.10	-0.07	-0.13	-0.14
Oleyl	H9R	-0.10	-0.07	-0.13	-0.13
Oleyl	C110	-0.09	-0.06	-0.13	-0.13
Oleyl	H10R	-0.08	-0.06	-0.12	-0.12
Oleyl	C111	-0.08	-0.05	-0.12	-0.12
Oleyl	H11R	-0.06	-0.05	-0.11	-0.12

Oleyl	H11S	-0.06	-0.04	-0.11	-0.11
Oleyl	C112	-0.04	-0.04	-0.10	-0.11
Oleyl	H12R	-0.04	-0.04	-0.10	-0.11
Oleyl	H12S	-0.03	-0.03	-0.09	-0.11
Oleyl	C113	-0.02	-0.03	-0.09	-0.10
Oleyl	H13R	-0.02	0.00	-0.08	-0.09
Oleyl	H13S	-0.01	0.01	-0.07	-0.09
Oleyl	C114	-0.01	0.01	-0.06	-0.09
Oleyl	H14R	-0.01	0.02	-0.05	-0.09
Oleyl	H14S	-0.00	0.02	-0.05	-0.08
Oleyl	C115	-0.00	0.02	-0.04	-0.06
Oleyl	H15R	0.01	0.03	-0.04	-0.05
Oleyl	H15S	0.01	0.04	-0.04	-0.04
Oleyl	C116	0.01	0.06	-0.03	-0.04
Oleyl	H16R	0.01	0.06	-0.02	-0.03
Oleyl	H16S	0.02	0.07	-0.02	-0.03
Oleyl	C117	0.03	0.07	-0.01	-0.03
Oleyl	H17R	0.05	0.08	0.00	-0.02
Oleyl	H17S	0.07	0.09	0.00	-0.01
Oleyl	C118	0.07	0.09	0.01	0.00
Oleyl	H18R	0.08	0.10	0.02	0.01
Oleyl	H18S	0.13	0.13	0.04	0.01
Oleyl	H18T	0.13	0.13	0.05	0.02

Table S4: Linear correlation coefficients of the Pauli energy component (E_{Pau}) with respect to $1/r^{12}$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Min region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	0.73	0.51	0.55	0.50
Choline	C31	0.50	0.31	0.48	0.48
Choline	H1A	0.46	0.28	0.39	0.37
Choline	H1B	0.35	0.25	0.32	0.30
Choline	C32	0.33	0.24	0.21	0.21
Choline	H2A	0.27	0.23	0.21	0.18
Choline	H2B	0.25	0.21	0.17	0.17
Choline	C33	0.23	0.17	0.16	0.15
Choline	H3A	0.20	0.17	0.15	0.14
Choline	H3B	0.19	0.17	0.13	0.13
Choline	H3C	0.18	0.16	0.12	0.12
Choline	C34	0.11	0.14	0.09	0.08
Choline	H4A	0.10	0.10	0.07	0.06
Choline	H4B	0.09	0.10	0.06	0.04
Choline	H4C	0.07	0.03	0.02	0.02
Choline	C35	0.06	0.02	0.02	0.01
Choline	H5A	0.04	0.02	0.01	-0.02
Choline	H5B	0.02	0.01	0.00	-0.02
Choline	H5C	-0.02	-0.03	-0.01	-0.04
Phosphate	O31	0.07	0.23	0.11	0.12
Phosphate	O32	0.07	0.19	0.07	0.07
Phosphate	O33	0.01	0.15	0.04	0.05
Phosphate	O34	-0.02	-0.01	0.04	0.03

Phosphate	P31	-0.03	-0.01	-0.03	-0.03
Glycerol	C3	0.20	0.22	-0.21	-0.18
Glycerol	HA	0.06	0.08	-0.19	-0.18
Glycerol	HB	0.06	0.08	-0.13	-0.17
Glycerol	C2	0.05	0.02	-0.10	-0.09
Glycerol	HX	0.04	0.02	-0.09	-0.07
Glycerol	C1	0.02	0.02	-0.07	-0.06
Glycerol	HR	-0.01	-0.00	-0.06	-0.05
Glycerol	HS	-0.04	-0.01	-0.04	-0.05
Glycerol	C11	-0.05	-0.02	-0.04	-0.03
Glycerol	O12	-0.06	-0.03	0.00	0.01
Glycerol	O11	-0.07	-0.03	0.02	0.01
Glycerol	C21	-0.13	-0.04	0.02	0.04
Glycerol	O22	-0.14	-0.05	0.03	0.06
Glycerol	O21	-0.17	-0.17	0.11	0.08
Oleyl	C12	0.29	0.22	0.31	0.31
Oleyl	H2R	0.23	0.22	0.26	0.25
Oleyl	H2S	0.23	0.20	0.21	0.19
Oleyl	C13	0.22	0.20	0.19	0.19
Oleyl	H3R	0.19	0.20	0.19	0.17
Oleyl	H3S	0.19	0.18	0.16	0.16
Oleyl	C14	0.18	0.17	0.15	0.15
Oleyl	H4R	0.17	0.17	0.15	0.15
Oleyl	H4S	0.16	0.17	0.14	0.15
Oleyl	C15	0.15	0.17	0.14	0.14
Oleyl	H5R	0.14	0.17	0.13	0.14
Oleyl	H5S	0.14	0.16	0.13	0.13

Oleyl	C16	0.13	0.14	0.12	0.12
Oleyl	H6R	0.13	0.13	0.11	0.11
Oleyl	H6S	0.12	0.12	0.11	0.10
Oleyl	C17	0.11	0.11	0.11	0.10
Oleyl	H7R	0.11	0.11	0.11	0.10
Oleyl	H7S	0.11	0.11	0.10	0.10
Oleyl	C18	0.10	0.10	0.09	0.09
Oleyl	H8R	0.10	0.10	0.09	0.08
Oleyl	H8S	0.08	0.09	0.08	0.08
Oleyl	C19	0.08	0.09	0.08	0.08
Oleyl	H9R	0.05	0.08	0.08	0.08
Oleyl	C110	0.05	0.06	0.08	0.08
Oleyl	H10R	0.05	0.06	0.07	0.08
Oleyl	C111	0.03	0.05	0.06	0.06
Oleyl	H11R	0.03	0.03	0.05	0.05
Oleyl	H11S	0.02	0.02	0.04	0.05
Oleyl	C112	0.00	0.02	0.04	0.04
Oleyl	H12R	0.00	0.02	0.03	0.04
Oleyl	H12S	-0.00	0.01	0.03	0.04
Oleyl	C113	-0.01	0.01	0.02	0.03
Oleyl	H13R	-0.01	0.00	0.00	0.03
Oleyl	H13S	-0.03	-0.00	0.00	0.02
Oleyl	C114	-0.03	-0.01	0.00	0.02
Oleyl	H14R	-0.03	-0.03	-0.01	0.00
Oleyl	H14S	-0.03	-0.03	-0.01	-0.01
Oleyl	C115	-0.03	-0.03	-0.02	-0.02
Oleyl	H15R	-0.03	-0.04	-0.03	-0.03

Oleyl	H15S	-0.03	-0.05	-0.03	-0.03
Oleyl	C116	-0.04	-0.06	-0.04	-0.03
Oleyl	H16R	-0.04	-0.07	-0.05	-0.04
Oleyl	H16S	-0.05	-0.07	-0.05	-0.05
Oleyl	C117	-0.05	-0.08	-0.05	-0.05
Oleyl	H17R	-0.05	-0.09	-0.05	-0.05
Oleyl	H17S	-0.07	-0.12	-0.05	-0.06
Oleyl	C118	-0.08	-0.12	-0.07	-0.06
Oleyl	H18R	-0.09	-0.12	-0.07	-0.06
Oleyl	H18S	-0.10	-0.12	-0.07	-0.07
Oleyl	H18T	-0.11	-0.15	-0.10	-0.08

Table S5: Linear correlation coefficients of the electrostatic energy component (E_{ele}) with respect to $1/r$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Max region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	-0.34	-0.35	-0.32	-0.32
Choline	C31	-0.33	-0.34	-0.32	-0.31
Choline	H1A	-0.33	-0.34	-0.31	-0.31
Choline	H1B	-0.29	-0.30	-0.26	-0.25
Choline	C32	-0.28	-0.30	-0.25	-0.24
Choline	H2A	-0.28	-0.30	-0.25	-0.24
Choline	H2B	-0.27	-0.29	-0.24	-0.23
Choline	C33	-0.27	-0.29	-0.23	-0.23
Choline	H3A	-0.27	-0.29	-0.22	-0.21
Choline	H3B	-0.26	-0.29	-0.22	-0.21
Choline	H3C	-0.26	-0.29	-0.21	-0.20

Choline	C34	-0.26	-0.28	-0.21	-0.20
Choline	H4A	-0.24	-0.26	-0.20	-0.20
Choline	H4B	-0.23	-0.26	-0.20	-0.19
Choline	H4C	-0.23	-0.26	-0.19	-0.18
Choline	C35	-0.20	-0.24	-0.14	-0.13
Choline	H5A	-0.18	-0.23	-0.13	-0.12
Choline	H5B	-0.17	-0.23	-0.13	-0.12
Choline	H5C	-0.17	-0.21	-0.10	-0.09
Phosphate	O31	-0.41	-0.41	-0.40	-0.39
Phosphate	O32	-0.40	-0.41	-0.38	-0.38
Phosphate	O33	-0.40	-0.41	-0.38	-0.37
Phosphate	O34	-0.39	-0.39	-0.38	-0.37
Phosphate	P31	-0.38	-0.39	-0.36	-0.35
Glycerol	C3	-0.39	-0.38	-0.40	-0.40
Glycerol	HA	-0.39	-0.38	-0.39	-0.39
Glycerol	HB	-0.38	-0.38	-0.38	-0.38
Glycerol	C2	-0.38	-0.37	-0.38	-0.38
Glycerol	HX	-0.38	-0.36	-0.37	-0.37
Glycerol	C1	-0.35	-0.36	-0.34	-0.34
Glycerol	HR	-0.35	-0.35	-0.34	-0.34
Glycerol	HS	-0.32	-0.33	-0.31	-0.31
Glycerol	C11	-0.28	-0.30	-0.27	-0.27
Glycerol	O12	-0.28	-0.29	-0.27	-0.26
Glycerol	O11	-0.24	-0.26	-0.22	-0.22
Glycerol	C21	-0.19	-0.22	-0.15	-0.15
Glycerol	O22	-0.12	-0.17	-0.07	-0.06
Glycerol	O21	-0.11	-0.16	-0.07	-0.06

Oleyl	C12	-0.35	-0.34	-0.33	-0.33
Oleyl	H2R	-0.34	-0.33	-0.32	-0.32
Oleyl	H2S	-0.27	-0.29	-0.26	-0.26
Oleyl	C13	-0.23	-0.27	-0.20	-0.19
Oleyl	H3R	-0.20	-0.27	-0.16	-0.15
Oleyl	H3S	-0.19	-0.22	-0.15	-0.14
Oleyl	C14	-0.14	-0.22	-0.11	-0.11
Oleyl	H4R	-0.14	-0.21	-0.10	-0.10
Oleyl	H4S	-0.11	-0.15	-0.09	-0.10
Oleyl	C15	-0.10	-0.13	-0.09	-0.08
Oleyl	H5R	-0.10	-0.12	-0.08	-0.08
Oleyl	H5S	-0.10	-0.12	-0.08	-0.07
Oleyl	C16	-0.10	-0.11	-0.07	-0.06
Oleyl	H6R	-0.09	-0.11	-0.06	-0.06
Oleyl	H6S	-0.09	-0.11	-0.06	-0.05
Oleyl	C17	-0.09	-0.10	-0.06	-0.05
Oleyl	H7R	-0.08	-0.10	-0.05	-0.05
Oleyl	H7S	-0.07	-0.09	-0.05	-0.05
Oleyl	C18	-0.07	-0.09	-0.05	-0.04
Oleyl	H8R	-0.07	-0.08	-0.05	-0.04
Oleyl	H8S	-0.06	-0.07	-0.04	-0.04
Oleyl	C19	-0.06	-0.07	-0.03	-0.04
Oleyl	H9R	-0.06	-0.07	-0.03	-0.02
Oleyl	C110	-0.06	-0.06	-0.02	-0.01
Oleyl	H10R	-0.06	-0.06	-0.02	-0.01
Oleyl	C111	-0.06	-0.06	-0.02	-0.01
Oleyl	H11R	-0.05	-0.06	-0.02	-0.01

Oleyl	H11S	-0.05	-0.06	-0.01	-0.01
Oleyl	C112	-0.05	-0.06	-0.01	-0.01
Oleyl	H12R	-0.05	-0.06	-0.01	-0.01
Oleyl	H12S	-0.04	-0.06	-0.01	-0.01
Oleyl	C113	-0.04	-0.05	-0.01	0.00
Oleyl	H13R	-0.04	-0.05	-0.00	0.00
Oleyl	H13S	-0.02	-0.04	0.01	0.02
Oleyl	C114	-0.01	-0.03	0.01	0.02
Oleyl	H14R	-0.01	-0.03	0.02	0.02
Oleyl	H14S	-0.01	-0.03	0.03	0.04
Oleyl	C115	-0.00	-0.03	0.03	0.04
Oleyl	H15R	-0.00	-0.02	0.03	0.04
Oleyl	H15S	0.01	-0.02	0.04	0.04
Oleyl	C116	0.01	-0.02	0.05	0.06
Oleyl	H16R	0.01	-0.00	0.06	0.07
Oleyl	H16S	0.02	-0.00	0.07	0.07
Oleyl	C117	0.03	-0.00	0.07	0.07
Oleyl	H17R	0.04	0.00	0.07	0.07
Oleyl	H17S	0.04	0.01	0.08	0.08
Oleyl	C118	0.05	0.01	0.09	0.09
Oleyl	H18R	0.06	0.02	0.13	0.13
Oleyl	H18S	0.08	0.02	0.14	0.14
Oleyl	H18T	0.14	0.06	0.18	0.18

Table S6: Linear correlation coefficients of the induction energy component (E_{ind}) with respect to $1/r^4$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Max region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	-0.28	-0.23	-0.28	-0.28
Choline	C31	-0.23	-0.19	-0.25	-0.26
Choline	H1A	-0.22	-0.19	-0.23	-0.23
Choline	H1B	-0.13	-0.12	-0.14	-0.14
Choline	C32	-0.12	-0.08	-0.12	-0.13
Choline	H2A	-0.11	-0.07	-0.12	-0.12
Choline	H2B	-0.10	-0.06	-0.11	-0.12
Choline	C33	-0.09	-0.06	-0.11	-0.10
Choline	H3A	-0.07	-0.06	-0.10	-0.10
Choline	H3B	-0.07	-0.05	-0.10	-0.10
Choline	H3C	-0.07	-0.04	-0.08	-0.09
Choline	C34	-0.05	-0.03	-0.08	-0.08
Choline	H4A	-0.05	-0.03	-0.08	-0.08
Choline	H4B	-0.04	-0.03	-0.07	-0.08
Choline	H4C	-0.01	-0.02	-0.02	-0.02
Choline	C35	-0.01	-0.02	0.03	0.03
Choline	H5A	-0.01	-0.02	0.04	0.04
Choline	H5B	-0.00	-0.01	0.05	0.05
Choline	H5C	0.02	-0.01	0.07	0.08
Phosphate	O31	-0.32	-0.32	-0.32	-0.32
Phosphate	O32	-0.31	-0.29	-0.31	-0.31
Phosphate	O33	-0.30	-0.29	-0.29	-0.29
Phosphate	O34	-0.27	-0.26	-0.26	-0.25

Phosphate	P31	-0.27	-0.26	-0.25	-0.25
Glycerol	C3	-0.42	-0.40	-0.40	-0.39
Glycerol	HA	-0.42	-0.39	-0.40	-0.38
Glycerol	HB	-0.40	-0.36	-0.35	-0.33
Glycerol	C2	-0.35	-0.33	-0.34	-0.33
Glycerol	HX	-0.34	-0.33	-0.33	-0.31
Glycerol	C1	-0.33	-0.33	-0.31	-0.30
Glycerol	HR	-0.29	-0.28	-0.30	-0.30
Glycerol	HS	-0.25	-0.26	-0.23	-0.23
Glycerol	C11	-0.24	-0.21	-0.23	-0.22
Glycerol	O12	-0.22	-0.20	-0.21	-0.21
Glycerol	O11	-0.14	-0.13	-0.13	-0.13
Glycerol	C21	-0.11	-0.09	-0.11	-0.11
Glycerol	O22	-0.07	-0.06	-0.07	-0.06
Glycerol	O21	-0.06	-0.06	-0.05	-0.05
Oleyl	C12	-0.37	-0.36	-0.37	-0.36
Oleyl	H2R	-0.35	-0.31	-0.37	-0.35
Oleyl	H2S	-0.28	-0.26	-0.24	-0.24
Oleyl	C13	-0.25	-0.24	-0.22	-0.20
Oleyl	H3R	-0.25	-0.23	-0.21	-0.19
Oleyl	H3S	-0.24	-0.23	-0.18	-0.17
Oleyl	C14	-0.23	-0.22	-0.18	-0.16
Oleyl	H4R	-0.23	-0.22	-0.17	-0.15
Oleyl	H4S	-0.23	-0.22	-0.17	-0.15
Oleyl	C15	-0.20	-0.21	-0.17	-0.15
Oleyl	H5R	-0.20	-0.19	-0.16	-0.14
Oleyl	H5S	-0.20	-0.17	-0.16	-0.14

Oleyl	C16	-0.19	-0.17	-0.15	-0.14
Oleyl	H6R	-0.19	-0.16	-0.15	-0.14
Oleyl	H6S	-0.19	-0.15	-0.14	-0.14
Oleyl	C17	-0.18	-0.14	-0.14	-0.13
Oleyl	H7R	-0.17	-0.14	-0.14	-0.13
Oleyl	H7S	-0.17	-0.13	-0.14	-0.13
Oleyl	C18	-0.17	-0.13	-0.13	-0.13
Oleyl	H8R	-0.16	-0.12	-0.13	-0.12
Oleyl	H8S	-0.15	-0.12	-0.12	-0.12
Oleyl	C19	-0.15	-0.12	-0.12	-0.12
Oleyl	H9R	-0.15	-0.12	-0.12	-0.12
Oleyl	C110	-0.14	-0.11	-0.11	-0.11
Oleyl	H10R	-0.13	-0.11	-0.11	-0.10
Oleyl	C111	-0.13	-0.10	-0.11	-0.10
Oleyl	H11R	-0.13	-0.10	-0.10	-0.10
Oleyl	H11S	-0.12	-0.10	-0.10	-0.09
Oleyl	C112	-0.12	-0.09	-0.10	-0.09
Oleyl	H12R	-0.12	-0.09	-0.09	-0.09
Oleyl	H12S	-0.11	-0.08	-0.09	-0.09
Oleyl	C113	-0.11	-0.08	-0.09	-0.08
Oleyl	H13R	-0.11	-0.08	-0.09	-0.08
Oleyl	H13S	-0.10	-0.08	-0.08	-0.08
Oleyl	C114	-0.10	-0.07	-0.08	-0.08
Oleyl	H14R	-0.09	-0.07	-0.08	-0.08
Oleyl	H14S	-0.09	-0.07	-0.08	-0.07
Oleyl	C115	-0.09	-0.06	-0.07	-0.06
Oleyl	H15R	-0.08	-0.06	-0.07	-0.06

Oleyl	H15S	-0.08	-0.06	-0.06	-0.05
Oleyl	C116	-0.08	-0.05	-0.05	-0.04
Oleyl	H16R	-0.07	-0.05	-0.05	-0.04
Oleyl	H16S	-0.07	-0.04	-0.05	-0.03
Oleyl	C117	-0.07	-0.04	-0.05	-0.03
Oleyl	H17R	-0.06	-0.03	-0.04	-0.02
Oleyl	H17S	-0.05	-0.03	-0.03	-0.02
Oleyl	C118	-0.05	-0.03	-0.02	-0.02
Oleyl	H18R	-0.04	-0.02	-0.01	-0.01
Oleyl	H18S	-0.03	0.02	-0.01	-0.00
Oleyl	H18T	0.01	0.04	0.03	0.04

Table S7: Linear correlation coefficients of the dispersion energy component (E_{dis}) with respect to $1/r^6$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Max region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	0.10	0.09	-0.09	-0.09
Choline	C31	0.09	0.09	-0.06	-0.06
Choline	H1A	0.08	0.06	-0.04	-0.04
Choline	H1B	0.07	0.05	-0.02	-0.03
Choline	C32	0.07	0.03	-0.02	-0.02
Choline	H2A	0.06	0.03	-0.02	-0.02
Choline	H2B	0.04	0.03	-0.01	-0.01
Choline	C33	0.03	0.03	0.01	-0.00
Choline	H3A	0.02	0.01	0.01	-0.00
Choline	H3B	0.02	-0.00	0.01	0.00
Choline	H3C	0.01	-0.02	0.02	0.01

Choline	C34	0.00	-0.02	0.02	0.03
Choline	H4A	-0.00	-0.02	0.04	0.04
Choline	H4B	-0.01	-0.02	0.04	0.04
Choline	H4C	-0.01	-0.02	0.04	0.04
Choline	C35	-0.01	-0.02	0.04	0.04
Choline	H5A	-0.02	-0.02	0.05	0.05
Choline	H5B	-0.04	-0.03	0.06	0.06
Choline	H5C	-0.05	-0.05	0.07	0.06
Phosphate	O31	-0.03	-0.03	-0.02	-0.02
Phosphate	O32	-0.00	0.00	-0.01	-0.02
Phosphate	O33	-0.00	0.00	-0.01	-0.01
Phosphate	O34	0.00	0.01	0.00	0.00
Phosphate	P31	0.02	0.03	0.01	0.01
Glycerol	C3	-0.24	-0.23	-0.20	-0.17
Glycerol	HA	-0.20	-0.21	-0.16	-0.14
Glycerol	HB	-0.17	-0.14	-0.12	-0.11
Glycerol	C2	-0.10	-0.10	-0.09	-0.09
Glycerol	HX	-0.08	-0.07	-0.06	-0.06
Glycerol	C1	-0.06	-0.06	-0.06	-0.06
Glycerol	HR	-0.05	-0.05	-0.06	-0.06
Glycerol	HS	-0.05	-0.04	-0.05	-0.05
Glycerol	C11	-0.04	-0.03	-0.05	-0.05
Glycerol	O12	-0.03	-0.02	-0.05	-0.05
Glycerol	O11	-0.03	0.01	-0.05	-0.05
Glycerol	C21	-0.03	0.01	-0.05	-0.05
Glycerol	O22	-0.02	0.04	-0.03	-0.03
Glycerol	O21	-0.00	0.06	-0.03	-0.02

Oleyl	C12	-0.37	-0.28	-0.30	-0.27
Oleyl	H2R	-0.31	-0.27	-0.28	-0.26
Oleyl	H2S	-0.31	-0.26	-0.27	-0.26
Oleyl	C13	-0.30	-0.26	-0.25	-0.25
Oleyl	H3R	-0.29	-0.23	-0.25	-0.25
Oleyl	H3S	-0.29	-0.22	-0.25	-0.23
Oleyl	C14	-0.29	-0.22	-0.24	-0.22
Oleyl	H4R	-0.25	-0.21	-0.23	-0.21
Oleyl	H4S	-0.25	-0.21	-0.23	-0.20
Oleyl	C15	-0.24	-0.20	-0.22	-0.19
Oleyl	H5R	-0.24	-0.19	-0.21	-0.19
Oleyl	H5S	-0.24	-0.19	-0.21	-0.19
Oleyl	C16	-0.23	-0.19	-0.21	-0.19
Oleyl	H6R	-0.21	-0.18	-0.20	-0.19
Oleyl	H6S	-0.21	-0.18	-0.19	-0.19
Oleyl	C17	-0.20	-0.17	-0.19	-0.18
Oleyl	H7R	-0.20	-0.17	-0.19	-0.18
Oleyl	H7S	-0.20	-0.17	-0.19	-0.18
Oleyl	C18	-0.19	-0.16	-0.19	-0.18
Oleyl	H8R	-0.18	-0.16	-0.19	-0.18
Oleyl	H8S	-0.18	-0.16	-0.18	-0.17
Oleyl	C19	-0.18	-0.16	-0.18	-0.17
Oleyl	H9R	-0.18	-0.15	-0.17	-0.17
Oleyl	C110	-0.18	-0.15	-0.17	-0.16
Oleyl	H10R	-0.17	-0.15	-0.16	-0.16
Oleyl	C111	-0.16	-0.13	-0.16	-0.15
Oleyl	H11R	-0.15	-0.13	-0.16	-0.15

Oleyl	H11S	-0.15	-0.13	-0.16	-0.15
Oleyl	C112	-0.15	-0.13	-0.16	-0.15
Oleyl	H12R	-0.15	-0.12	-0.15	-0.15
Oleyl	H12S	-0.15	-0.12	-0.15	-0.15
Oleyl	C113	-0.15	-0.12	-0.14	-0.15
Oleyl	H13R	-0.14	-0.11	-0.13	-0.13
Oleyl	H13S	-0.13	-0.10	-0.13	-0.13
Oleyl	C114	-0.13	-0.07	-0.12	-0.12
Oleyl	H14R	-0.12	-0.07	-0.11	-0.11
Oleyl	H14S	-0.11	-0.07	-0.11	-0.10
Oleyl	C115	-0.10	-0.07	-0.10	-0.10
Oleyl	H15R	-0.10	-0.06	-0.10	-0.10
Oleyl	H15S	-0.09	-0.06	-0.10	-0.10
Oleyl	C116	-0.09	-0.05	-0.10	-0.09
Oleyl	H16R	-0.09	-0.03	-0.09	-0.08
Oleyl	H16S	-0.09	-0.03	-0.09	-0.07
Oleyl	C117	-0.08	-0.01	-0.06	-0.05
Oleyl	H17R	-0.07	-0.01	-0.06	-0.04
Oleyl	H17S	-0.05	-0.00	-0.05	-0.03
Oleyl	C118	-0.05	0.01	-0.02	-0.01
Oleyl	H18R	-0.04	0.02	-0.01	-0.00
Oleyl	H18S	-0.03	0.05	-0.00	0.00
Oleyl	H18T	0.05	0.06	0.07	0.09

Table S8: Linear correlation coefficients of the Pauli energy component (E_{Pau}) with respect to $1/r^{12}$, where r is the interatomic distance between each cisplatin atom type (Pt, Cl, N, H) and each atom of the DOPC molecule at the Max region.

Lip.Res.	Lip.Atom.	Pt	Cl	N	H
Choline	N31	0.10	0.09	0.09	0.08
Choline	C31	0.05	0.03	0.06	0.06
Choline	H1A	0.03	0.03	0.06	0.05
Choline	H1B	0.03	0.03	0.04	0.03
Choline	C32	0.03	0.03	0.03	0.03
Choline	H2A	0.03	0.03	0.02	0.02
Choline	H2B	0.02	0.03	0.02	0.02
Choline	C33	0.02	0.03	0.02	0.01
Choline	H3A	0.01	0.02	0.01	0.01
Choline	H3B	0.01	0.01	-0.01	0.00
Choline	H3C	0.00	0.01	-0.01	-0.00
Choline	C34	-0.01	0.01	-0.01	-0.00
Choline	H4A	-0.02	0.01	-0.01	-0.01
Choline	H4B	-0.03	-0.01	-0.02	-0.01
Choline	H4C	-0.05	-0.02	-0.02	-0.02
Choline	C35	-0.05	-0.03	-0.03	-0.03
Choline	H5A	-0.07	-0.03	-0.04	-0.04
Choline	H5B	-0.08	-0.05	-0.04	-0.04
Choline	H5C	-0.09	-0.05	-0.05	-0.05
Phosphate	O31	0.13	0.14	0.10	0.10
Phosphate	O32	0.11	0.11	0.10	0.09
Phosphate	O33	0.11	0.11	0.09	0.08
Phosphate	O34	0.10	0.10	0.09	0.08

Phosphate	P31	0.09	0.05	0.07	0.06
Glycerol	C3	0.35	0.36	0.23	0.18
Glycerol	HA	0.34	0.35	0.21	0.16
Glycerol	HB	0.28	0.30	0.17	0.14
Glycerol	C2	0.24	0.17	0.14	0.14
Glycerol	HX	0.14	0.15	0.14	0.13
Glycerol	C1	0.13	0.14	0.12	0.11
Glycerol	HR	0.11	0.13	0.09	0.07
Glycerol	HS	0.09	0.13	0.07	0.06
Glycerol	C11	0.09	0.11	0.06	0.06
Glycerol	O12	0.09	0.11	0.06	0.06
Glycerol	O11	0.08	0.04	0.06	0.06
Glycerol	C21	0.06	0.02	0.06	0.06
Glycerol	O22	0.05	0.01	0.06	0.06
Glycerol	O21	0.03	0.00	0.05	0.05
Oleyl	C12	0.41	0.36	0.41	0.38
Oleyl	H2R	0.40	0.35	0.39	0.38
Oleyl	H2S	0.38	0.34	0.37	0.36
Oleyl	C13	0.37	0.29	0.36	0.29
Oleyl	H3R	0.37	0.29	0.35	0.29
Oleyl	H3S	0.35	0.28	0.35	0.27
Oleyl	C14	0.35	0.27	0.28	0.24
Oleyl	H4R	0.33	0.25	0.21	0.21
Oleyl	H4S	0.28	0.18	0.21	0.21
Oleyl	C15	0.24	0.17	0.20	0.17
Oleyl	H5R	0.24	0.17	0.19	0.17
Oleyl	H5S	0.22	0.14	0.19	0.16

Oleyl	C16	0.22	0.14	0.19	0.16
Oleyl	H6R	0.21	0.13	0.18	0.15
Oleyl	H6S	0.18	0.13	0.15	0.15
Oleyl	C17	0.18	0.13	0.15	0.14
Oleyl	H7R	0.18	0.13	0.14	0.14
Oleyl	H7S	0.18	0.13	0.13	0.13
Oleyl	C18	0.17	0.13	0.13	0.12
Oleyl	H8R	0.17	0.12	0.12	0.11
Oleyl	H8S	0.15	0.10	0.12	0.11
Oleyl	C19	0.15	0.10	0.12	0.10
Oleyl	H9R	0.14	0.10	0.11	0.09
Oleyl	C110	0.14	0.08	0.10	0.08
Oleyl	H10R	0.13	0.08	0.10	0.08
Oleyl	C111	0.13	0.08	0.10	0.08
Oleyl	H11R	0.11	0.07	0.10	0.07
Oleyl	H11S	0.10	0.07	0.09	0.07
Oleyl	C112	0.10	0.06	0.09	0.07
Oleyl	H12R	0.10	0.05	0.09	0.07
Oleyl	H12S	0.10	0.03	0.09	0.07
Oleyl	C113	0.09	0.03	0.07	0.06
Oleyl	H13R	0.09	0.03	0.06	0.06
Oleyl	H13S	0.09	0.03	0.06	0.05
Oleyl	C114	0.09	0.02	0.05	0.05
Oleyl	H14R	0.08	0.02	0.05	0.04
Oleyl	H14S	0.08	0.02	0.04	0.04
Oleyl	C115	0.07	0.00	0.04	0.04
Oleyl	H15R	0.07	-0.00	0.04	0.04

Oleyl	H15S	0.05	-0.00	0.03	0.04
Oleyl	C116	0.05	-0.01	0.03	0.03
Oleyl	H16R	0.04	-0.01	0.02	0.02
Oleyl	H16S	0.03	-0.02	0.02	0.02
Oleyl	C117	0.02	-0.03	0.02	0.02
Oleyl	H17R	0.01	-0.04	0.01	0.01
Oleyl	H17S	0.01	-0.04	0.01	0.00
Oleyl	C118	0.00	-0.05	0.01	-0.01
Oleyl	H18R	-0.01	-0.07	-0.00	-0.01
Oleyl	H18S	-0.03	-0.07	-0.03	-0.03
Oleyl	H18T	-0.04	-0.10	-0.05	-0.07

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