Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2016

Supporting Information - Computational methods for the description of pharmacologically relevant Platinum complexes – Molecular structure and bond dissociation

Malte Kokoschka[a,b,*], Jakub Galgonek[c], Jiri Vondrasek[c] and Pavel Hobza[a,b]

[a]Gilead Sciences & IOCB Research Center, Department of Computational Chemistry, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, 166 10 Prague 6, Czech Republic.

[b]Department of Physical Chemistry, Palacky University, 771 46 Olomouc, Czech Republic.

[c] Bioinformatics Group, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, 166 10 Prague 6, Czech Republic.

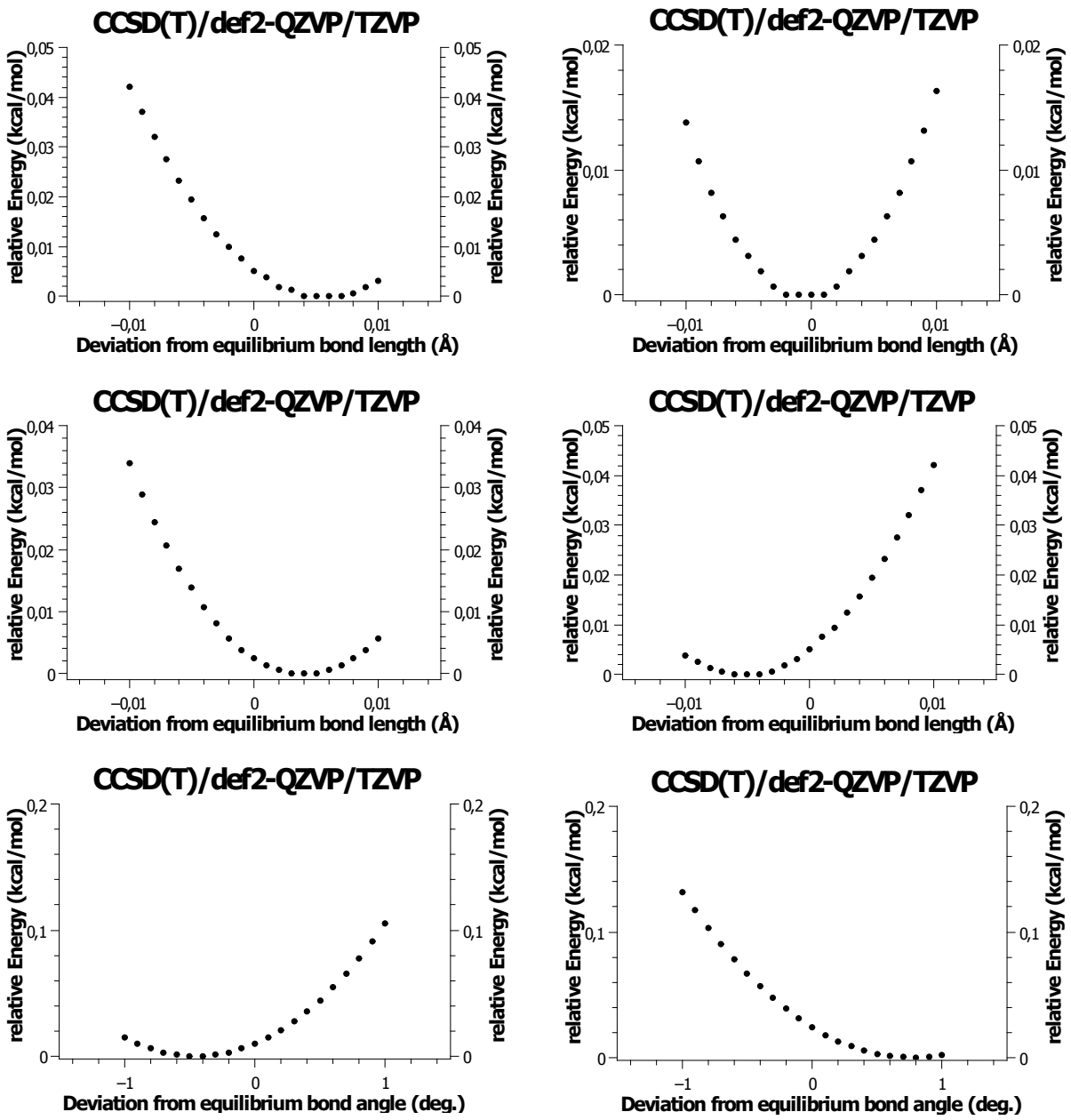

Figure S1: Bond length vs. energy scans of the Pt-Cl (left) and Pt-N (right) bond of Cisplatin (top) and Transplatin (middle). Bond angle vs. energy scan of Cl-Pt-Cl (left) and Cl-Pt-N (right) of Cisplatin (bottom)

Table S1: R34 set: RMSD comparison of all methods excluding spin-component-scaled methods against B2PLYP/def2-QZVPP (shell atoms, heavy atoms).

Method	N	RMSD (mean) / Å		RMSD (min) / Å		RMSD (max) / Å	
RIJONX-B2PLYP/def2-QZVPP	34	0	0	0	0	0	0
RIJONX-B2PLYP/def2-QZVP	34	0.0011	0.0026	0.0004	0.0008	0.0022	0.0096
RIJONX-B2PLYP/def2-TZVPP	34	0.0032	0.0143	0.0007	0.0021	0.0153	0.0569
RIJONX-B2PLYP/def2-TZVP	34	0.0040	0.0152	0.0016	0.0036	0.0156	0.0768
RIJONX-B2PLYP/def2-SVP	34	0.0198	0.0940	0.0128	0.0180	0.0454	0.6436
RIJONX-B2PLYP/def2-SV(P)	34	0.0198	0.1062	0.0079	0.0294	0.0430	0.7967
RI-BP86/def2-TZVPP	34	0.0205	0.1446	0.0080	0.0167	0.0442	0.9780
RI-BP86/def2-SVP	34	0.0215	0.1473	0.0100	0.0241	0.0501	0.9802
RI-PBE/def2-QZVP	34	0.0221	0.1686	0.0100	0.0150	0.0463	1.1236
RI-BP86/def2-QZVP	34	0.0227	0.1693	0.0099	0.0168	0.0478	1.1265
RI-BP86/def2-TZVP	34	0.0239	0.1709	0.0111	0.0181	0.0776	1.1275
RI-B3LYP/def2-QZVP	34	0.0240	0.1768	0.0115	0.0228	0.0480	1.1243
RI-PBE-D3/def2-QZVP	34	0.0266	0.1778	0.0169	0.0154	0.0551	1.1219
RI-BP86/def2-SV(P)	34	0.0268	0.1795	0.0176	0.0352	0.0490	1.1379
RI-B3LYP-D3/def2-QZVP	34	0.0334	0.1825	0.0221	0.0218	0.0729	1.1275
RI-BP86-D3/def2-QZVP	34	0.0379	0.1843	0.0312	0.0182	0.0631	1.1240
RI-BLYP/def2-QZVP	34	0.0429	0.1874	0.0314	0.0393	0.0837	1.1438
RIJK-MP2/def2-SVP	34	0.0430	0.1955	0.0337	0.0166	0.0636	1.1061
RI-BLYP-D3/def2-QZVP	34	0.0437	0.1976	0.0362	0.0410	0.0602	1.1462
RIJK-MP2/def2-TZVPP	34	0.0444	0.2001	0.0317	0.0375	0.0846	1.1025
RIJK-MP2/def2-QZVPP	34	0.0463	0.2001	0.0352	0.0377	0.1000	1.0961
PM6-D3H4X	34	0.0505	0.2126	0.0104	0.0145	0.0956	0.9940
PM7	34	0.0552	0.2388	0.0148	0.0187	0.1866	1.1082

Table S2: R14 set: RMSD comparison of all methods including spin-component-scaled methods against B2PLYP/def2-QZVPP (shell atoms, heavy atoms).

Method	N	RMSD (mean) / Å		RMSD (min) / Å		RMSD (max) / Å	
RIJONX-B2PLYP/def2-QZVPP	14	0	0	0	0	0	0
RIJONX-B2PLYP/def2-QZVP	14	0.0011	0.0027	0.0004	0.0008	0.0019	0.0096
RIJONX-B2PLYP/def2-TZVP	14	0.0028	0.0117	0.0019	0.0036	0.0041	0.0327
RIJONX-B2PLYP/def2-TZVPP	14	0.0037	0.0119	0.0026	0.0021	0.0056	0.0326
RIJONX-B2PLYP/def2-SVP	14	0.0188	0.0486	0.0131	0.0180	0.0400	0.2086
RIJONX-B2PLYP/def2-SV(P)	14	0.0192	0.0590	0.0115	0.0305	0.0347	0.2045
RI-BP86/def2-QZVP	14	0.0193	0.0880	0.0126	0.0168	0.0442	0.2906
RI-BP86/def2-TZVPP	14	0.0205	0.0903	0.0143	0.0167	0.0454	0.3091
RI-BP86/def2-TZVP	14	0.0206	0.0903	0.0137	0.0181	0.0463	0.3124
RI-PBE/def2-QZVP	14	0.0210	0.0907	0.0157	0.015	0.0371	0.3301
RI-BP86/def2-SVP	14	0.0216	0.0927	0.0154	0.0241	0.0478	0.2660
RI-PBE-D3/def2-QZVP	14	0.0228	0.0937	0.0171	0.0154	0.0480	0.3563
RI-B3LYP/def2-QZVP	14	0.0230	0.0961	0.0138	0.0228	0.0368	0.3298
RI-BP86-D3/def2-QZVP	14	0.0263	0.0971	0.0176	0.0182	0.0490	0.3938
RI-B3LYP-D3/def2-QZVP	14	0.0263	0.0991	0.0216	0.024	0.0346	0.4791
RIJK-SCS-MP2/def2-QZVPP	14	0.0287	0.1007	0.0219	0.0282	0.0411	0.3783
RI-BP86/def2-SV(P)	14	0.0333	0.1008	0.0241	0.0352	0.0484	0.2952
RIJK-LT-SOS-MP2/def2-QZVPP	14	0.0400	0.1009	0.0321	0.0198	0.0631	0.3766
RIJK-MP2/def2-SVP	14	0.0401	0.1047	0.0314	0.0166	0.0529	0.3747
RI-BLYP/def2-QZVP	14	0.0419	0.1072	0.0317	0.0393	0.0547	0.3132
RIJK-MP2/def2-TZVPP	14	0.0433	0.1117	0.0367	0.0375	0.0520	0.3752
RIJK-MP2/def2-QZVPP	14	0.0436	0.1119	0.0369	0.0377	0.0602	0.3733
RI-BLYP-D3/def2-QZVP	14	0.0464	0.1136	0.0352	0.0410	0.0601	0.4859
PM6-D3H4X	14	0.0550	0.1142	0.0145	0.0145	0.0956	0.3522

PM7	14	0.0679	0.1796	0.0215	0.0235	0.1866	0.5134

Table S3: Molecules contained in Benchmark set R34.

Compound
AJESEN
BEBBUG
BEBCAN
BONQOK
COQHEW
Cisplatin
DIBKIJ
DICTOY
FORJOL-cat
GALYAT
HAFDAU
HOJREE
IDAWEP
KABJUS
KEFKIQ
LALVAV
LECQUG
NUWFIV
OBIHAJ
OBOPEB
OJOLII
PRDPTB
QASJUQ
QASKEB
REJJEW
REMMIF
SENHOI
Transplatin
VEPROX
WIPNUE
XAKPOO
YEGFUL
ZUGSID
ZUZTIX

Table S4: Molecules contained in Benchmark set R14.

Compound
AJESEN
COQHEW
Cisplatin
DICTOY
FORJOL-cat
GALYAT
IDAWEP
NUWFIV
OBIHAJ
OBOPEB
QASJUQ
REJJEW
ZUGSID
ZUZTIX

Table S5: Molecules contained in Benchmark set R22, including information on the dissociated bond.

Compound	Bond type
CIRKOE	S-Pt
CIRKOE	Cl-Pt
COQHEW	N-Pt
CYTPTD10	N-Pt
Cisplatin	N-Pt
Cisplatin	Cl-Pt
DICTOY	N-Pt
DICTOY	N-Pt
FORJOL-cat	N-Pt
GALYAT	Cl-Pt
KABJUS	N-Pt
KABJUS	N-Pt
KABJUS	Cl-Pt
LALVAV	N-Pt
LALVAV	N-Pt
LALVAV	Cl-Pt
LECQUG	N-Pt
PRDPTB	N-Pt
Transplatin	N-Pt
Transplatin	Cl-Pt
VEPROX	N-Pt
ZUGSID	N-Pt