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Supporting information for article:

The potential of dispersion-corrected density functional theory calculations for distinguishing between salts and cocrystals

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S1. Refcodes of structures used for the screening

S1.1. Refcodes of all structures experimentally determined as cocrystals used in the study (96)

ADARIH,AJAKEB,AJAKIF,AJIWIA,BARMIM,BUDZUV,BUFQAU,CIRXAD,DATQOF,DEHSIS10,DEXTOQ,DINSOK01,DITHUK,DITJAS,DITJEW,EKECOM01,GALBIF,GANXUP,GOBYOL,GUKWOZ,HONTAG,HONWAJ,HOZBOO,HUHQUW,HUSTOE,HUSVIA,HUSWIB,IFUQAC,JAZBES,JESMOK,KATBAJ,KURGOU,LUNMAI,LUNMEM,LUNMUC,LUNNAJ,LUNNEN,LUNNIR,LUNNOX,LUNNUD,LUNPEP,MEBRAN,MUPQET,NANQOJ,NOVSOG,NOVTAT,NUGZEV,NUGZOF,NUHBAU,NUQKOA,ODOHEV,OJENIA,PUJHUY,PUJNIS,RADGAF,RAPRIK,RESGOM,RIZWUS,ROLFUU,RONDAA,RONDEE,SEPLUV,SIYCIN,SOGXUH,SUVJEY,TETXUL,TEVWOH,TIFTAD,TIJKOM,TONMAL,UJORAM,ULAWAF,ULAWAF02,ULAWEJ,UNEBOE,UNECAR,VORCOV,VUZCIC,VUZCOI,WOPZUW,WOQBAF,WOQBEJ,WOQBIN,WUKREZ,WUKROJ,XAPWOA,XAQPEL,XAQPOV,XEBFOA,YECHAQ,YECHOE,YECHUK,YOCSIT,ZAJHOH,ZAJJEZ,ZUZDUT

S1.2. Refcodes of all structures experimentally determined as salts used in the study (173)

ABELUP,ADIJUT,AJEBIA,ALABEU,BEGVUF,BERCEG,BEXQUP,BOGVOJ,BOQXEK,BUDNUK,CAHKUS,CAHLED,CASCIJ,CASZIG,CAYJAO01,CINCAE,CIRVUV,CIRXEH,COCPOA,COLHER,CUKGUL,CUKHAS,CUQGOK,DAYVUV,DEHTAL10,DIBZAQ,DIBZAQ01,DINSAU10,DITJIA,DOTGID,DULGAT,DUNCOF,DUPFUQ,EDAVOU,EKELUB,EQUXUJ,EXALEU,FEMGAF,FEMGEJ,FIBCIC,FIBDEZ,FIJSUM,FIWJIF,FOBRAQ,FOVBUO,FOVROX,FOVRUD,FUWVAU,FUYSUN,GAMVIA,GEQBIN,GIFNAL,GIFNOZ,GIFRAO,GODNIW,GUHREG,GUTSET,GUTSIX,HAXFER,HAYZAJ,HAZHEV,HEWTAF,HEWWAI,HILMAR,HILSAX,HILSOL,HOFZEI,HOFZOS,HOXHEI,HUCXAF,HUHREH,HUSSIX,HUSSUJ,IMIPEZ,JAWWIO,JAWYAI,JEJNES,JOJJOH,KAPWAZ,KAPYIJ,KAXWOV,KEFZAX,KEQMAV,KEXYAN,KEZHAZ,KUFBUI,KUTXUT,LACBAS,LAPPAU,LAQGOA,LECCIF,LECCOL,LOCJUJ,LUJJAC,MELZAF,MEQNUR,MEQPED,MEQQOO,MIBYEB,MIPRIM,MIRYOC,MOYRIC,MOYRUO,MOYSAV,MOYSEZ,MUCMUT,NANNAS,NANNOG,NUQRAT,OCASEQ,ODAZID01,ODEJUD,PARNAX,PEBFIL,PEQGUO,PEZXIB,PIFGUH,POCVUY,POVZIK,PUJKOV,PUJWEX,PUJWIB,PUKJIP,PUMQAP01,PUMSEV,QIBSUP,QIQLIL,QIQLOR,QIQLUX,RADGEJ,REHFIU,RERFID,RESFUR,RESGEC,REZHAG,RIGMEA,RIGMIE,RIZXED,ROJJEG,SABPEQ,SAZGIJ01,SEGZUZ,SEMNAA,SIMGIF,SIMTEO,SLCADA10,SLCADB10,SUZZUI,SUZZUI01,TOYLOI,TUQKEW,ULAYAH,UNEBUK,VIGDIZ,VIGDUL,VUYWOC,WOCSEM,XESPEQ,XETLAK,XIBZUD,XILTAO,XINRUH,YAVRIW01,YETLOY,YEWRIB,YEXFUD,YUCQIX,YUCQOD,ZAJHUN,ZIVROL,ZIVRUR,ZOKSUN,ZUWMAF

S1.3. Refcodes of experimentally determined cocrystals converging to slat from salt starting model (34)

AJAKEB,AJAKIF,AJIWIA,BUDZUV,BUFQAU,DINSOK01,DITHUK,DITJAS,DITJEW,GOBYOL,IFUQAC,KATBAJ,KURGOU,LUNNAJ,LUNPEP,NUGZEV,NUGZOF,NUHBAU,NUQKOA,PUJNIS,RADGAF,RIZWUS,SEPLUV,SIYCIN,SOGXUH,TETXUL,TIJKOM,UJORAM,ULAWAF,ULAWAF02,ULAWEJ,UNEBOE,VORCOV,XAQPOV

S1.4. Refcodes of experimentally determined cocrystals converging to cocrystals from cocrystal starting model (77)

ADARIH,AJAKIF,AJIWIA,BARMIM,BUDZUV,CIRXAD,DATQOF,DEHSIS10,DEXTOQ,DITHUK,DITJAS,EKECOM01,GALBIF,GANXUP,GOBYOL,GUKWOZ,HONTAG,HONWAJ,HOZBOO,HUHQUW,HUSTOE,HUSVIA,HUSWIB,IFUQAC,JAZBES,JESMOK,KATBAJ,LUNMAI,LUNMEM,LUNMUC,LUNNEN,LUNNIR,LUNNOX,LUNNUD,LUNPEP,MEBRAN,MUPQET,NANQOJ,NOVSOG,NOVTAT,NUGZEV,NUQKOA,OJENIA,PUJHUY,PUJNIS,RAPRIK,RESGOM,ROLFUU,RONDAA,RONDEE,SIYCIN,SOGXUH,SUVJEY,TEVWOH,TIFTAD,TIJKOM,TONMAL,UNECAR,VORCOV,VUZCIC,VUZCOI,WOPZUW,WOQBAF,WOQBEJ,WOQBIN,WUKREZ,WUKROJ,XAPWOA,XAQPEL,XEBFOA,YECHAQ,YECHOE,YECHUK,YOCSIT,ZAJHOH,ZAJJEZ,ZUZDUT

S1.5. Refcodes of experimentally determined cocrystals converging to cocrystals from both cocrystal and salt starting model (61)

ADARIH,BARMIM,CIRXAD,DATQOF,DEHSIS10,DEXTOQ,EKECOM01,GALBIF,GANXUP,GUKWOZ,HONTAG,HONWAJ,HOZBOO,HUHQUW,HUSTOE,HUSVIA,HUSWIB,JAZBES,JESMOK,LUNMAI,LUNMEM,LUNMUC,LUNNEN,LUNNIR,LUNNOX,LUNNUD,MEBRAN,MUPQET,NANQOJ,NOVSOG,NOVTAT,OJENIA,PUJHUY,RAPRIK,RESGOM,ROLFUU,RONDAA,RONDEE,SUVJEY,TEVWOH,TIFTAD,TONMAL,UNECAR,VUZCIC,VUZCOI,WOPZUW,WOQBAF,WOQBEJ,WOQBIN,WUKREZ,WUKROJ,XAPWOA,XAQPEL,XEBFOA,YECHAQ,YECHOE,YECHUK,YOCSIT,ZAJHOH,ZAJJEZ,ZUZDUT

S2. Detailed parameters of the DFT calculations setup

S2.1. PBE functional

Table S1 DFT calculation setup used for PBE functional calculations.

Parameter	Value	Units
CASTEP version	19.11	
Functional	PBE	
Dispersion correction	Tkatchenko-Scheffler	
Pseudopotential used	ultrasoft	
Energy cut-off	520	eV
total energy convergence tolerance	1.0 E-05	eV/atom
max ionic/ force tolerance	0.03	eV/Å

S2.2. PBE functional

Table S2 DFT calculation setup used for rSCAN functional calculations.

Parameter	Value	Units
CASTEP version	20.11	
functional	rSCAN	
Dispersion correction	none	
Pseudopotential used	on the fly ultrasoft	
Energy cut-off	571.4	eV
total energy convergence tolerance	2.0 E-05	eV/atom
max ionic/ force tolerance	0.05	eV/Å

S2.3. PBE0 functional

Table S3 DFT calculation setup used for PBE0 functional calculations.

Parameter	Value	Units
CASTEP version	19.11, 20.11	
functional	PBE0	
Dispersion correction	Tkatchenko-Scheffler	
Pseudopotential used	norm-conserving	
Energy cut-off	600	eV
total energy convergence tolerance	2.0 E-05	eV/atom
max ionic/ force tolerance	0.05	eV/Å

S2.4. PBE50 functional

Table S4 DFT calculation setup used for PBE50 functional calculations.

Parameter	Value	Units
CASTEP version	19.11	
functional	PBE50 (defined as custom XC: HF 0.5 PBE_X 0.5 PBE_C 1.0)	
Dispersion correction	none	
Pseudopotential used	norm conserving	
Energy cut-off	600	eV
total energy convergence tolerance	2.0 E-05	eV/atom
max ionic/ force tolerance	0.05	eV/Å

S3. Correlation between donor-acceptor distance and PBE calculation results for cocrystals

Table S5 Correlation between donor-acceptor distance and PBE calculation result for tranfers other than O-H…N

CSD code	Donor-acceptor distance (Å)	PBE calculation result	Transfer type
BARMIM	2.823	cocr.	N-H…N
JESMOK	2.812	cocr.	N-H…N
DEHSIS10	2.472	cocr.	F-H…N
MUPQET	2.825	cocr.	N-H…O
ZUZDUT	2.816	cocr.	O-H…O

Table S6 Correlation between donor-acceptor distance and PBE calculation result for potential O-H…N transfer

Table is ordered according to O…N distance

CSD code	Donor-acceptor distance (Å)	PBE calculation result
ULAWAF02	2.529	salt
XAQPOV	2.536	salt
LUNNAJ	2.538	salt
NUHBAU	2.539	salt
SEPLUV	2.539	salt
UJORAM	2.542	salt
ULAWEJ	2.546	salt
AJAKIF	2.548	cocr./salt
LUNPEP	2.548	cocr./salt
DINSOK01	2.552	salt
BUFQAU	2.559	salt
UNEBOE	2.562	salt
LUNNEN	2.563	cocr.
ULAWAF	2.564	salt
IFUQAC	2.566	cocr./salt
HUSTOE	2.567	cocr.
TETXUL	2.567	salt

VORCOV	2.575	cocr./salt
AJAKEB	2.577	salt
LUNNOX	2.578	cocr.
KATBAJ	2.578	cocr./salt
NUQKOA	2.579	cocr./salt
NUGZOF	2.580	salt
RIZWUS	2.582	salt
RADGAF	2.585	salt
TONMAL	2.586	cocr.
BUDZUV	2.587	cocr./salt
GUKWOZ	2.588	cocr.
DITJEW	2.588	salt
HOZBOO	2.599	cocr.
XEBFOA	2.602	cocr.
NOVSOG	2.603	cocr.
NUGZEV	2.603	cocr./salt
SOGXUH	2.603	cocr./salt
JAZBES	2.604	cocr.
DITJAS	2.605	cocr./salt
PUJHUY	2.608	cocr.
KURGOU	2.613	salt
ZAJHOH	2.614	cocr.
LUNNUD	2.614	cocr.
TIFTAD	2.621	cocr.
XAPWOA	2.622	cocr.
LUNMEM	2.624	cocr.
RONDAA	2.628	cocr.
HUHQUW	2.629	cocr.

PUJNIS	2.629	cocr./salt
RESGOM	2.637	cocr.
XAQPEL	2.641	cocr.
LUNMAI	2.642	cocr.
GANXUP	2.643	cocr.
YOCSIT	2.644	cocr.
GOBYOL	2.647	cocr./salt
NANQOJ	2.647	cocr.
AJIWIA	2.648	cocr./salt
YECHUK	2.649	cocr.
WUKROJ	2.649	cocr.
TIJKOM	2.651	cocr./salt
RONDEE	2.652	cocr.
UNECAR	2.652	cocr.
LUNNIR	2.654	cocr.
VUZCOI	2.654	cocr.
YECHOE	2.658	cocr.
GALBIF	2.660	cocr.
ROLFUU	2.661	cocr.
CIRXAD	2.665	cocr.
ODOHEV	2.665	salt
LUNMUC	2.671	cocr.
NOVTAT	2.672	cocr.
RAPRIK	2.673	cocr.
DEXTOQ	2.674	cocr.
SUVJEY	2.679	cocr.
HUSWIB	2.684	cocr.
DITHUK	2.685	cocr./salt

EKECOM01	2.687	cocr.
DATQOF	2.688	cocr.
ZAJJEZ	2.688	cocr.
OJENIA	2.691	cocr.
HUSVIA	2.693	cocr.
SIYCIN	2.693	cocr./salt
HONTAG	2.703	cocr.
YECHAQ	2.710	cocr.
WOQBIN	2.716	cocr.
MEBRAN	2.722	cocr.
TEVWOH	2.723	cocr.
WUKREZ	2.724	cocr.
WOQBAF	2.736	cocr.
HONWAJ	2.736	cocr.
WOQBEJ	2.741	cocr.
WOPZUW	2.764	cocr.
VUZCIC	2.785	cocr.
ADARIH	2.816	cocr.

S4. Dual minima structures

Table S7 Energies of cocrystal and salt form for cocrystals with two energetic minima

CSD code	Cell enthalpy cocrystal (eV)	Cell enthalpy salt (eV)	Space group	Z used for calculation	Relative energy difference salt - cocrystal per one H-bond (kcal/mol)
AJAKIF	-17108.8934	-17108.8951	P-1	2	-0.0820
AJIWIA	-10703.2058	-10703.1657	P-1	2	1.9346
BUDZUV	-17108.9673	-17108.9744	P-1	2	-0.3425
DITHUK	-9851.8549	-9851.8056	P-1	2	2.3794

DITJAS	-19703.5545	-19703.6893	C2/c	4	-3.2516
GOBYOL	-19489.5902	-19489.5903	P21/n	4	-0.0024
IFUQAC	-11070.8469	-11070.8616	P21/n	4	-0.3546
KATBAJ	-11734.5635	-11734.5609	C2/c	4	0.0627
LUNPEP	-27016.8076	-27016.8168	P21/c	4	-0.2219
NUGZEV	-26919.6731	-26919.6729	P21/c	4	0.0048
NUQKOA	-19754.9366	-19754.9479	P-1	2	-0.5452
PUJNIS	-15448.2179	-15448.3126	P21/c	4	-2.2843
SIYCIN	-10090.7543	-10090.8009	P-1	2	-2.2481
SOGXUH	-21073.5752	-21073.5223	P21/c	4	1.2760
TIJKOM	-13888.4599	-13888.4285	P-1	2	1.5148
VORCOV	-9152.7865	-9152.9269	P21/c	4	-3.3862

S5. Results of RMSCD calculations

S5.1. RMSCD without hydrogen atoms

Table S8 The RMSCD values calculated with hydrogen atoms excluded

The data are ordered from highest RMSCD

CSD code	Experimentally determined as salt of cocrystal	RMSCD hydrogen atoms excluded	RMSCD explanation
DIBZAQ	salt	0.151	Water molecule significantly changed its position (O7)
JOJJOH	salt	0.1419	Water molecule significantly changed its position (O11)
FIJSUM	salt	0.1287	Structure is not solved correctly - incorrect water and carbon-hydrogen positions leads probably to incorrect heavy atom positions as well.
CIRXEH	salt	0.1096	Slight re-adjustment of all heavy atoms
FEMGAF	salt	0.1095	Cycle C1-C6 adjusted its position
DINSAU10	salt	0.1066	All oxygen atoms adjusted theirs position

EQUXUJ	salt	0.0987	Some N, C and O atoms slightly adjusted their position
PIFGUH	salt	0.097	N1, C7, C8 and O1 and O2 adjusted their position
CASCIJ	salt	0.0968	O and N atoms adjusted their position
GUTSET	salt	0.0904	C11-C13 and oxygen atoms moved a little
CAYJAO01	salt	0.0857	All oxygen atoms adjusted their position a little
QIQLUX	salt	0.0856	Oxygen atoms on N2-N4 adjusted their position
FOVROX	salt	0.0843	Almost all oxygen atoms adjusted their position a little
ZUZDUT	cocr.	0.0834	Nonsense N1, H45, H46 (NH2 group) experimental structure geometry
ZAJJEZ	cocr.	0.083	O1 and N4 adjusted their position a little
SUVJEY	cocr.	0.0827	O1, N1, N2 and C5 moved a little
HAYZAJ	salt	0.0791	O1 and O6 adjusted their position a little
MIRYOC	salt	0.0779	C14 and oxygen atoms moved a little
UJORAM	cocr.	0.0754	O5 adjusted its position
ALABEU	salt	0.0749	O1 adjusted its position

S5.2. RMSCD with hydrogen atoms included

Table S9 The RMSCD values calculated with hydrogen atoms included in the calculation

The data are ordered from highest RMSCD

CSD code	Experimentally determined as salt of cocrystal	RMSCD hydrogen included	RMSCD explanation
JOJJOH	salt	0.3363	O11 on water molecule adjusted to position forming H-bond
ZUZDUT	cocrystal	0.2535	Nonsense N1, H45, H46 (NH_2 group) experimental structure geometry
RIZWUS	cocrystal	0.2389	H30 formation salt from cocrystal, in original structure C4, H3 and H4 nonsense geometry
FIJSUM	salt	0.2199	Water molecule (O5) adjusted position forming H-bond

FEMGEJ	salt	0.2189	Little movement of almost all hydrogen atoms
FEMGAF	salt	0.2186	Little movement of almost all hydrogen atoms
QIQLUX	salt	0.2084	Water molecule adjusted in position forming H-bond
KURGOU	cocrystal	0.1983	Formation of salt from cocrystal, little movement of other hydrogen atoms
ROJJEG	salt	0.1833	Methyl hydrogen atoms on C9 adjusted theirs position
BARMIM	cocrystal	0.1815	Movement of all hydrogen atoms, especially H13 and H14 on C9 significantly adjusted theirs position
DIBZAQ	salt	0.1801	Water molecule adjusted (O7) to position forming H-bond
ZOKSUN	salt	0.1737	All hydrogen atoms adjusted their position
FUWVAU	salt	0.1662	Nonsense H16 position in original cif
CASCIJ	salt	0.1656	Water (O6) molecule and all hydrogen atoms adjusted their position
TETXUL	cocrystal	1.632	H1 formation of salt from cocrystal, little movement of other hydrogen atoms
DINSOK01	cocrystal	0.1598	H5 formation of salt from cocrystal, other hydrogen atoms also slightly changed their position
ODOHEV	cocrystal	0.1577	The original structure is not solved right
MIRYOC	salt	0.1574	All hydrogen atoms adjusted their position
DINSAU10	salt	0.1565	All hydrogen atoms adjusted their position, most significantly H1
VUYWOC	salt	0.1556	All hydrogen atoms adjusted their position, most significantly methyl hydrogen atoms H9,H10 and H11 on C14