Towards a Black-Box for Biological EXAFS Data Analysis – II. Automatic BioXAS Refinement & Analysis (ABRA)

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Supplementary Material

Use of the Webinterface

Processing an EXAFS dataset with ABRA consists of several stages (see Fig. S1): An ABRA job is started via the web-interface (i) by uploading the dataset and providing a few basic parameters. This defines the pool of models (ii) sampling coordination space systematically. (iii) ABRA's first stage is executed, creating macros which are then directing DL_EXCURV (iv) during the refinement step. After constrained and an optional restrained refinement ABRA's second stage (v) is initiated, which analyses the results of the refinement, produces a total score and carries out an additional meta-analysis of the top-scoring models. Then, a notice is provided with the link to ABRA's final results: An HTML-page containing all information required for a publication and a publication-ready graph as well as an in-depth HTML-table containing all necessary information of *all* models which have been refined. In the next paragraphs these features implemented in ABRA will be explained roughly following this process sequence.

Web interface

On our web interface any user should be able to upload his dataset and start a successful ABRA run. For a typical Zn-EXAFS only the extracted fine structure has to be uploaded in ascii-format, and the usual personal information (name, email address) has to be entered. ABRA's default-values correspond to a standard biological Zn-EXAFS dataset.

In addition, experienced users can change variables to tailor the sampling of coordination space (and therefore the pool of models) to their demands:

List of the ligands: By default, ABRA will try to fit each dataset by a combination of the three ligands sulphur, histidine and oxygen. Additional scatterers can be added, e.g. a second metal ion, to model a metal-metal distance. For simplicity, these are treated as an additional ligand. Metal ions (e.g. Fe, Zn, …) added in this fashion will not affect the BVS, while non-metals will. Caution is advised though, since any increase of the total number of ligands potentially increases the pool of models (and thereby computation time) by

roughly an order of magnitude. This problem can be partially tackled by the introduction of restraints, see below.

We discourage users to switch off any of the first three ligands. Instead the range of coordination numbers for certain ligands can be limited. See below under *Restraining coordination space sampling*.

Range of coordination: In order to assure comparison of models with sufficiently different coordination numbers a range from 3 to 6 is fitted, which is a good choice for Zn, but different ranges could be necessary to fit other absorber atoms (e.g. Cu). This ranged should be defined rather generously, allowing ABRA to decide which models have to be rejected.

Number of independent metal centres per protein: Since EXAFS only measures the average occupancy of ligands non-integer coordination numbers are necessary for proteins containing more than one independent metal centre. When in doubt use the default value of 2 metal centres which will lead to a sampling of coordination space in 0.5 steps for all ligands. Typical numbers for this parameter are 2 or 3, balancing computational needs vs. sampling of the coordination space. We recommend using 2 metal centres even for mononuclear sites to ensure sufficient sampling of coordination space.

Oxidation state: In biological samples Zn is always present in oxidation state (II), but e.g. in the case of Fe typical oxidation states are (II) or (III). If the exact oxidation state is unknown, the user can give more than one oxidation state, ABRA will then try to determine the oxidation state using Bond-Valence-Sum (BVS) for every structural model independently.

Data range: The data range which should be taken into account for the refinement process can be entered in either energy- or k-space. A lower limit of k=3.0 $Å^{-1}$ is suggested, but can be adjusted down to k=2.0 $Å^{-1}$. The upper limit is currently k=16.5 $Å^{-1}$. Both limits can be autodetected, in this case ABRA will take the lowest/highest data point. By default the lower limit is 3.0 $Å^{-1}$ and the upper limit will be set automatically. There also exist several advanced options for experienced users; the most important ones are quickly highlighted.

Restraining coordination space sampling: The coordination number of any ligand can be restrained. For every ligand ABRA is expecting a lower and an upper limit of the coordination number, represented as a comma-separated string.

As mentioned above it might be useful to include additional ligands into the analysis, e.g. to model a metal-metal distance. In this case the metal should be introduced as an additional ligand. Since it must not be necessary to sample the whole coordination space for this ligand its coordination could be restrained to a fixed number (e.g. "0,6,0,6,0,6,1,1" would allow the first three ligands to be varied freely between 0 and 6, while the metal ligand at fourth position would be restrained to a coordination of 1). Note that ABRA will anyhow limit the total number of ligands as defined above.

In order to switch off the contribution of any of the first three ligands its upper limit should be set to 0 (e.g. to switch of the His-ligand use "0,6,0,0,0,6").

Treatment of Debye-Waller factors: ABRA follows the maxim to first try to fit the data with a model containing as few fit parameters (= degrees of freedom) as possible. Correspondingly all ligands of the first coordination sphere share the same Debye-Waller factor by default. This can be overridden, which is

advisable e.g. in the case of a ligand occupying a different coordination sphere than the standard ligands (metal-metal distances) or if the ligands have different vibrational properties (e.g. bridging sulphurs).

The Debye-Waller factors for the second and third coordination sphere of the histidine unit are approximated from the Debye-Waller of the histidine [0.,1.6,1.6,2.1,2.1] (Harvey)..

Multiple scattering & Restrained refinement: ABRA is always performing a multiple scattering simulation taking into account intra-ligand scattering; right now the only complex ligand requiring multiple scattering is histidine. The use of DL_Excurv's internal histidine-unit was abandoned in favor of a unit provided by M. Feiters (Feiters *et al.*, 2003).

This unit is kept rigid during the initial constrained refinement. An optional restrained refinement will be carried out based upon the initial constrained refinement and optimizes in addition the distances of the individual atoms of the histidine ring and their respective angles.

While this typically leads to an improvement of the fit index and optical fit quality the R-factor and reduced χ^2 are increased, which indicates that these additional degrees of freedom do not significantly improve the quality of the model. This is most probably caused by the rather small number of initial fit parameters (4 are typically sufficient for a constrained refinement, while another 8 variables have to be considered for restrained refinement, which is only partly compensated by the restrains introduced at the same time).

Additional references

Harvey, I. private communication.

Figure S1 Flowchart of ABRA's operation.

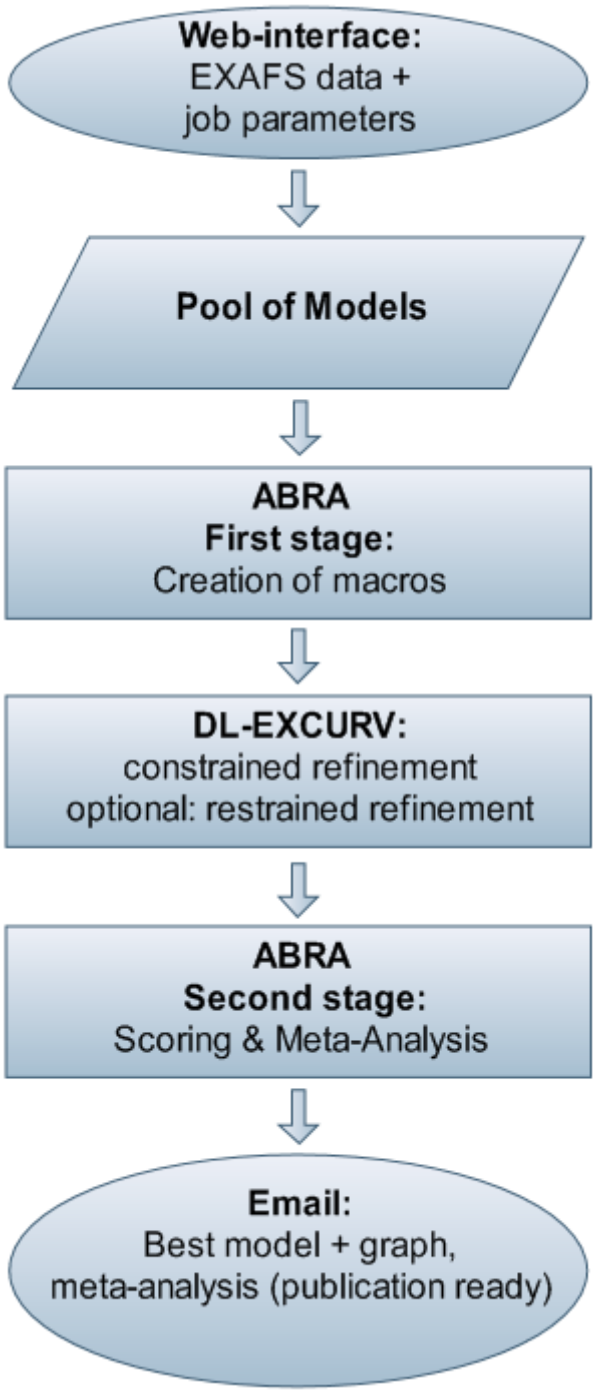

Table S1 Detailed results for HPV E7 The models included in the meta-analysis are given in bold. Their small number is indicative of the confidence in the presence of sulphur ligands. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S2.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.8739**	**[4.0, 0.0, 0.0]**	**0.907**	**2.334(1)**	**0.0(0)**	**0.0066(2)**	**-10.7(3)**	**2.0685**	**2**
2	**0.8671**	**[4.0, 0.0, 0.5]**	**0.944**	**2.335(1)**	**2.01(1)**	**0.0065(2)**	**-10.4(3)**	**2.2816**	**2**
3	**0.8614**	**[4.5, 0.0, 0.0]**	**0.844**	**2.336(1)**	**0.0(0)**	**0.0077(2)**	**-10.8(3)**	**2.3145**	**2**
4	**0.8564**	**[3.5, 0.0, 0.5]**	**1.152**	**2.335(1)**	**2.02(1)**	**0.0055(2)**	**-10.6(3)**	**2.0179**	**2**
5	0.8445	[4.0, 0.5, 0.0]	1.044	2.337(1)	2.05(2)	0.0066(2)	-10.9(3)	2.2864	2
6	0.8321	[4.5, 0.0, 0.5]	0.876	2.334(1)	1.95(1)	0.0077(2)	-10.3(2)	2.5843	2
7	0.8297	[3.5, 0.0, 0.0]	1.151	2.337(2)	0.0(0)	0.0055(2)	-11.3(3)	1.7953	2
8	0.8251	[4.0, 0.0, 1.0]	1.178	2.333(1)	1.979(6)	0.0068(2)	-9.9(3)	2.5497	2
9	0.8203	[5.0, 0.0, 0.0]	0.971	2.337(1)	0.0(0)	0.0089(2)	-10.7(3)	2.5648	2
10	0.8170	[3.5, 1.0, 0.0]	1.457	2.335(2)	2.068(9)	0.0054(2)	-10.6(4)	2.2520	2
11	0.8147	[4.0, 1.0, 0.0]	1.319	2.334(2)	2.046(9)	0.0068(2)	-9.9(3)	2.5428	2
12	0.8101	[4.0, 0.5, 0.5]	1.257	2.333(1)	1.993(7)	0.0067(2)	-10.1(3)	2.5767	2
13	0.8072	[4.5, 0.5, 0.0]	1.071	2.334(1)	1.98(1)	0.0077(2)	-10.3(3)	2.6105	2
14	0.8057	[3.5, 0.0, 1.0]	1.400	2.338(2)	2.039(7)	0.0057(2)	-10.9(3)	2.1949	2
15	0.7998	[3.0, 1.0, 0.0]	2.078	2.329(2)	2.032(9)	0.0045(2)	-9.5(4)	2.0651	2
16	0.7861	[3.0, 0.0, 0.5]	1.595	2.335(2)	2.04(1)	0.0042(2)	-11.1(4)	1.7488	2
17	0.7771	[4.5, 0.0, 1.0]	1.259	2.332(2)	1.981(7)	0.0078(2)	-9.3(3)	2.8127	2
18	0.7660	[3.5, 1.5, 0.0]	2.028	2.334(2)	2.059(7)	0.0055(2)	-9.7(4)	2.4968	2
19	0.7653	[3.5, 1.0, 0.5]	1.928	2.335(2)	2.053(7)	0.0056(2)	-10.2(4)	2.4652	2
20	0.7631	[5.0, 0.0, 0.5]	1.032	2.335(1)	1.94(1)	0.0088(2)	-10.3(2)	2.8429	2
21	0.7618	[3.0, 0.0, 0.0]	1.672	2.335(2)	0.0(0)	0.0042(2)	-11.4(4)	1.5472	2
22	0.7543	[3.5, 0.0, 1.5]	1.975	2.336(2)	2.027(6)	0.0059(2)	-10.7(4)	2.4268	2
23	0.7534	[4.5, 0.5, 0.5]	1.240	2.332(1)	1.97(8)	0.0079(2)	-9.7(3)	2.8746	2
24	0.7520	[5.5, 0.0, 0.0]	1.233	2.339(2)	0.0(0)	0.01(2)	-10.7(3)	2.8060	2
25	0.7508	[3.0, 1.0, 0.5]	2.548	2.329(2)	2.025(6)	0.0046(3)	-9.3(4)	2.2845	2
26	0.7427	[3.0, 1.5, 0.0]	2.641	2.328(2)	2.032(7)	0.0046(3)	-9.1(4)	2.3156	2
27	0.7407	[3.0, 0.0, 1.5]	2.476	2.335(2)	2.025(6)	0.0049(3)	-10.4(4)	2.1772	2
28	0.7405	[4.0, 0.0, 1.5]	1.769	2.332(2)	1.987(6)	0.007(2)	-9.6(3)	2.7778	2
29	0.7394	[4.5, 1.0, 0.0]	1.307	2.332(1)	1.984(8)	0.0077(2)	-9.6(3)	2.9005	2
30	0.7347	[4.0, 1.0, 0.5]	1.653	2.33(2)	1.989(6)	0.0067(2)	-9.1(3)	2.8757	2

Table S2 Detailed results for GCM The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S3.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.8543**	**[3.0, 1.0, 0.0]**	**1.554**	**2.314(2)**	**2.028(8)**	**0.0051(2)**	**-8.7(4)**	**2.1355**	**2**
2	**0.8493**	**[3.0, 0.0, 1.0]**	**1.533**	**2.318(2)**	**2.011(7)**	**0.0052(2)**	**-9.4(4)**	**2.0561**	**2**
3	**0.8428**	**[3.0, 0.5, 0.5]**	**1.646**	**2.316(2)**	**2.019(8)**	**0.0052(2)**	**-9.1(4)**	**2.0972**	**2**
4	**0.8389**	**[3.0, 1.0, 0.5]**	**1.567**	**2.315(2)**	**2.021(5)**	**0.0054(2)**	**-8.5(4)**	**2.3528**	**2**
5	**0.8359**	**[3.0, 1.5, 0.0]**	**1.589**	**2.315(2)**	**2.03(6)**	**0.0053(2)**	**-8.3(4)**	**2.3760**	**2**
6	0.8311	[3.0, 0.0, 1.5]	1.671	2.319(2)	2.011(5)	0.0054(2)	-9.1(4)	2.2698	2
7	0.8303	[2.5, 0.0, 1.5]	1.781	2.317(2)	2.019(4)	0.004(2)	-9.2(4)	1.9939	2
8	0.8301	[3.5, 0.0, 0.5]	1.751	2.317(2)	2.0(2)	0.0069(3)	-9.3(4)	2.1197	2
9	0.8294	[3.5, 1.0, 0.0]	1.593	2.314(2)	2.014(9)	0.0068(2)	-8.3(4)	2.4276	2
10	0.8292	[3.5, 0.0, 1.0]	1.636	2.318(2)	2.0(8)	0.0069(3)	-9.0(4)	2.3393	2
11	0.8260	[3.0, 0.5, 1.0]	1.718	2.317(2)	2.017(5)	0.0053(2)	-8.9(4)	2.3100	2
12	0.8241	[3.0, 0.0, 0.5]	1.746	2.317(2)	2.01(1)	0.0053(2)	-9.6(5)	1.8430	2
13	0.8231	[3.5, 0.5, 0.0]	1.872	2.315(2)	2.02(2)	0.0069(3)	-8.9(5)	2.1597	2
14	0.8160	[3.0, 0.5, 0.0]	1.891	2.317(2)	2.03(2)	0.0053(3)	-9.4(5)	1.8720	2
15	0.8152	[3.5, 0.5, 0.5]	1.781	2.313(2)	1.991(9)	0.007(3)	-8.1(4)	2.4210	2
16	0.8058	[2.5, 2.0, 0.0]	1.996	2.314(2)	2.035(4)	0.004(3)	-8.0(4)	2.3418	2
17	0.8024	[2.5, 1.0, 1.0]	2.063	2.315(2)	2.026(4)	0.0041(3)	-8.5(4)	2.2804	2
18	0.7984	[3.5, 0.0, 0.0]	2.102	2.316(2)	0.0(0)	0.0072(3)	-9.4(5)	1.9002	2
19	0.7984	[4.0, 0.0, 0.5]	1.921	2.317(2)	1.99(2)	0.0085(3)	-9.0(4)	2.3966	2
20	0.7941	[4.0, 0.0, 0.0]	2.123	2.317(3)	0.0(0)	0.0087(3)	-9.4(5)	2.1658	2
21	0.7889	[4.0, 0.5, 0.0]	1.994	2.316(2)	2.01(2)	0.0084(3)	-8.9(5)	2.4330	2
22	0.7880	[3.5, 0.0, 1.5]	1.825	2.318(2)	2.001(6)	0.007(3)	-8.6(4)	2.5621	2
23	0.7846	[3.0, 2.0, 0.0]	1.780	2.314(2)	2.029(5)	0.0054(3)	-7.8(3)	2.6307	2
24	0.7844	[2.5, 0.0, 2.0]	2.290	2.318(2)	2.017(4)	0.0044(3)	-8.8(4)	2.2083	2
25	0.7844	[2.5, 0.5, 1.5]	2.279	2.316(2)	2.023(4)	0.0041(3)	-8.7(4)	2.2430	2
26	0.7844	[3.5, 1.5, 0.0]	1.669	2.314(2)	2.018(7)	0.0068(3)	-8.0(4)	2.6778	2
27	0.7842	[3.5, 1.0, 0.5]	1.693	2.313(2)	2.002(6)	0.0067(2)	-7.7(4)	2.6733	2
28	0.7832	[3.0, 1.0, 1.0]	1.900	2.316(2)	2.017(5)	0.0055(3)	-8.2(4)	2.5708	2
29	0.7799	[3.5, 0.5, 1.0]	1.845	2.317(2)	2.006(6)	0.0068(3)	-8.6(4)	2.6014	2
30	0.7795	[3.0, 1.5, 0.5]	1.889	2.315(2)	2.023(5)	0.0053(3)	-8.1(4)	2.6013	2

Table S3 Detailed results for ZnF-UBP The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S4.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.9121**	**[2.67, 1.0, 0.33]**	**0.919**	**2.308(2)**	**2.009(5)**	**0.0055(2)**	**-8.4(3)**	**2.1501**	**2**
2	**0.9107**	**[3.0, 1.0, 0.0]**	**0.883**	**2.31(2)**	**2.008(7)**	**0.0068(2)**	**-8.7(3)**	**2.1809**	**2**
3	**0.9103**	**[2.67, 1.0, 0.0]**	**0.972**	**2.309(2)**	**2.013(7)**	**0.0055(2)**	**-8.5(4)**	**1.9958**	**2**
4	**0.9096**	**[2.67, 1.33, 0.0]**	**0.936**	**2.308(2)**	**2.014(5)**	**0.0054(2)**	**-8.4(3)**	**2.1690**	**2**
5	**0.9020**	**[3.0, 1.0, 0.33]**	**0.853**	**2.309(2)**	**2.0(5)**	**0.0066(2)**	**-8.4(3)**	**2.3452**	**2**
6	**0.9016**	**[3.0, 0.0, 1.0]**	**0.950**	**2.312(2)**	**1.987(6)**	**0.0068(2)**	**-9.2(3)**	**2.1118**	**2**
7	**0.8990**	**[3.0, 1.33, 0.0]**	**0.866**	**2.309(2)**	**2.006(6)**	**0.0068(2)**	**-8.4(3)**	**2.3627**	**2**
8	**0.8976**	**[3.0, 0.33, 0.67]**	**1.015**	**2.311(2)**	**1.99(7)**	**0.0068(2)**	**-9.0(3)**	**2.1423**	**2**
9	**0.8973**	**[2.33, 1.0, 0.33]**	**1.093**	**2.309(2)**	**2.016(5)**	**0.0043(2)**	**-8.7(4)**	**1.9455**	**2**
10	**0.8963**	**[2.33, 1.33, 0.0]**	**1.119**	**2.308(2)**	**2.021(5)**	**0.0044(2)**	**-8.6(4)**	**1.9675**	**2**
11	**0.8939**	**[2.67, 1.0, 0.67]**	**1.011**	**2.309(2)**	**2.007(4)**	**0.0056(2)**	**-8.3(3)**	**2.2997**	**2**
12	**0.8939**	**[3.33, 1.0, 0.0]**	**0.883**	**2.31(2)**	**1.999(8)**	**0.0079(2)**	**-8.5(3)**	**2.3760**	**2**
13	**0.8930**	**[3.0, 0.0, 1.33]**	**0.999**	**2.313(2)**	**1.99(5)**	**0.0069(2)**	**-8.9(3)**	**2.2560**	**2**
14	**0.8930**	**[2.67, 0.0, 1.33]**	**1.029**	**2.313(2)**	**1.999(5)**	**0.0057(2)**	**-9.4(3)**	**2.0606**	**2**
15	**0.8928**	**[3.0, 0.0, 0.67]**	**1.054**	**2.313(2)**	**1.982(1)**	**0.0069(2)**	**-9.3(4)**	**1.9580**	**2**
16	**0.8928**	**[2.67, 1.33, 0.33]**	**1.014**	**2.31(2)**	**2.015(4)**	**0.0055(2)**	**-8.4(3)**	**2.3016**	**2**
17	**0.8924**	**[2.67, 0.33, 1.0]**	**1.066**	**2.312(2)**	**2.003(5)**	**0.0059(2)**	**-9.2(4)**	**2.0868**	**2**
18	**0.8918**	**[3.33, 0.0, 0.67]**	**1.048**	**2.312(2)**	**1.98(1)**	**0.008(2)**	**-9.2(4)**	**2.1453**	**2**
19	**0.8902**	**[3.33, 0.0, 1.0]**	**0.984**	**2.312(2)**	**1.98(7)**	**0.008(2)**	**-8.9(3)**	**2.3018**	**2**
20	**0.8899**	**[2.33, 1.33, 0.33]**	**1.193**	**2.309(2)**	**2.019(4)**	**0.0044(2)**	**-8.4(4)**	**2.1085**	**2**
21	**0.8898**	**[2.33, 1.0, 0.67]**	**1.188**	**2.309(2)**	**2.013(4)**	**0.0045(2)**	**-8.5(4)**	**2.0983**	**2**
22	**0.8896**	**[3.0, 0.67, 0.33]**	**1.085**	**2.311(2)**	**2.004(8)**	**0.0068(2)**	**-9.1(4)**	**2.1535**	**2**
23	0.8892	[2.67, 0.0, 1.0]	1.002	2.313(2)	1.998(6)	0.0056(2)	-9.7(4)	1.9131	2
24	0.8884	[2.67, 1.67, 0.0]	1.046	2.309(2)	2.018(5)	0.0054(2)	-8.2(3)	2.3316	2
25	0.8869	[3.0, 0.33, 1.0]	1.021	2.313(2)	1.997(5)	0.0068(2)	-9.1(3)	2.2737	2
26	0.8865	[2.33, 1.67, 0.0]	1.237	2.308(2)	2.024(4)	0.0043(3)	-8.2(4)	2.1332	2
27	0.8855	[2.67, 0.67, 0.67]	1.137	2.312(2)	2.01(5)	0.0056(2)	-9.2(4)	2.1086	2
28	0.8845	[3.33, 0.33, 0.67]	1.037	2.311(2)	1.989(8)	0.0079(2)	-8.8(3)	2.3252	2
29	0.8843	[2.67, 0.33, 0.67]	1.064	2.313(2)	2.006(7)	0.0056(2)	-9.7(4)	1.9320	2
30	0.8834	[2.33, 1.0, 0.0]	1.161	2.309(2)	2.028(7)	0.0042(2)	-8.8(4)	1.7871	2

Table S4 Detailed results for *Ec* ZiPD The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S5.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.9021**	**[0.0,3.0,1.5]**	**0.916**	**0.0(0)**	**1.993(3)**	**0.012(5)**	**-7.6(4)**	**2.3289**	**2**
2	**0.9013**	**[0.0,3.5,1.0]**	**0.882**	**0.0(0)**	**1.995(3)**	**0.0117(5)**	**-7.5(3)**	**2.3608**	**2**
3	**0.9003**	**[0.0,3.0,1.0]**	**1.119**	**0.0(0)**	**1.994(3)**	**0.0098(5)**	**-7.6(4)**	**2.0942**	**2**
4	**0.8980**	**[0.0,4.0,0.0]**	**1.127**	**0.0(0)**	**2.003(3)**	**0.0094(5)**	**-7.4(3)**	**2.1309**	**2**
5	**0.8966**	**[0.0,4.5,0.0]**	**0.771**	**0.0(0)**	**1.998(2)**	**0.0107(4)**	**-6.8(3)**	**2.4299**	**2**
6	**0.8955**	**[0.0,3.5,0.5]**	**1.155**	**0.0(0)**	**2.004(3)**	**0.0095(5)**	**-8.2(4)**	**2.0818**	**2**
7	**0.8948**	**[0.0,4.0,0.5]**	**0.801**	**0.0(0)**	**1.993(2)**	**0.0108(4)**	**-6.5(3)**	**2.4183**	**2**
8	**0.8928**	**[0.0,2.5,1.5]**	**1.205**	**0.0(0)**	**1.988(3)**	**0.0097(5)**	**-7.3(4)**	**2.0832**	**2**
9	**0.8863**	**[0.0,2.0,2.0]**	**1.276**	**0.0(0)**	**1.982(4)**	**0.01(6)**	**-6.8(5)**	**2.0712**	**2**
10	**0.8829**	**[0.0,2.5,2.0]**	**1.167**	**0.0(0)**	**1.991(3)**	**0.0125(6)**	**-7.9(4)**	**2.2965**	**2**
11	0.8786	[0.0,2.0,2.5]	1.264	0.0(0)	1.991(4)	0.0123(6)	-7.8(4)	2.2516	2
12	0.8768	[0.0,4.0,1.0]	0.711	0.0(0)	1.998(3)	0.0135(4)	-7.5(3)	2.6117	2
13	0.8760	[0.0,3.5,0.0]	1.333	0.0(0)	1.998(3)	0.007(5)	-7.2(4)	1.8899	2
14	0.8736	[0.0,4.5,0.5]	0.695	0.0(0)	2.001(3)	0.0132(4)	-7.5(3)	2.6344	2
15	0.8721	[0.5,3.0,0.5]	1.146	2.276(9)	1.985(3)	0.0065(5)	-6.6(4)	2.2143	2
16	0.8705	[0.0,3.5,1.5]	0.851	0.0(0)	1.996(3)	0.0139(5)	-7.8(3)	2.5815	2
17	0.8688	[0.5,3.5,0.5]	1.011	2.29(1)	1.99(3)	0.0088(5)	-6.8(4)	2.4533	2
18	0.8651	[0.0,3.0,0.5]	1.463	0.0(0)	2.0(3)	0.0075(6)	-8.2(4)	1.8359	2
19	0.8649	[0.0,3.0,2.0]	0.959	0.0(0)	1.992(3)	0.0143(5)	-7.6(4)	2.5647	2
20	0.8635	[0.0,1.5,2.5]	1.503	0.0(0)	1.991(4)	0.0111(7)	-8.5(5)	1.9764	2
21	0.8624	[0.0,1.5,3.0]	1.468	0.0(0)	1.989(4)	0.0132(7)	-8.0(5)	2.2186	2
22	0.8600	[0.0,1.0,3.0]	1.572	0.0(0)	1.985(4)	0.0114(7)	-8.1(5)	1.9631	2
23	0.8584	[0.0,5.0,0.0]	0.751	0.0(0)	2.001(2)	0.0128(4)	-6.9(3)	2.6781	2
24	0.8568	[0.0,2.5,1.0]	1.555	0.0(0)	1.994(4)	0.0079(6)	-8.1(5)	1.8213	2
25	0.8566	[0.0,1.0,3.5]	1.540	0.0(0)	1.98(4)	0.0136(7)	-7.5(5)	2.2269	2
26	0.8541	[0.5,2.0,1.0]	1.490	2.273(9)	1.98(4)	0.0043(6)	-7.0(5)	1.9130	2
27	0.8537	[0.0,2.0,1.5]	1.573	0.0(0)	1.99(4)	0.0084(6)	-8.1(5)	1.7960	2
28	0.8513	[0.5,3.5,0.0]	0.970	2.257(9)	1.984(3)	0.0066(5)	-6.1(3)	2.2812	2
29	0.8483	[0.0,2.5,2.5]	1.220	0.0(0)	1.99(4)	0.0141(6)	-7.6(4)	2.5336	2
30	0.8471	[0.5,2.0,2.0]	1.348	2.29(1)	1.975(4)	0.0096(6)	-6.5(5)	2.4019	2

Table S5 Detailed results for *At* Glx2-2 The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S6.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.8625**	**[0.0,4.0,0.5,1.0]**	**1.291**	**0.0(0)**	**1.998(4)**	**0.0142(5)**	**-3.5(4)**	**2.3858**	**2**
2	**0.8611**	**[0.0,3.0,1.5,1.0]**	**1.381**	**0.0(0)**	**1.992(4)**	**0.01419(5)**	**-3.6(5)**	**2.3352**	**2**
3	**0.8509**	**[0.0,3.5,1.0,1.0]**	**1.526**	**0.0(0)**	**2.003(5)**	**0.0155(8)**	**-4.8(6)**	**2.3103**	**2**
4	**0.8478**	**[0.0,3.0,1.0,1.0]**	**1.716**	**0.0(0)**	**1.996(5)**	**0.0132(9)**	**-3.7(6)**	**2.0829**	**2**
5	**0.8476**	**[0.0,4.5,0.0,1.0]**	**1.491**	**0.0(0)**	**2.007(4)**	**0.01429(6)**	**-4.2(5)**	**2.3715**	**2**
6	**0.8476**	**[0.0,4.0,0.0,1.0]**	**1.706**	**0.0(0)**	**2.005(5)**	**0.0132(8)**	**-4.0(5)**	**2.1195**	**2**
7	**0.8476**	**[0.0,3.5,0.5,1.0]**	**1.716**	**0.0(0)**	**2.002(5)**	**0.0131(9)**	**-4.2(6)**	**2.0931**	**2**
8	**0.8454**	**[0.0,2.5,1.5,1.0]**	**1.751**	**0.0(0)**	**1.993(5)**	**0.0139(9)**	**-4.2(7)**	**2.0552**	**2**
9	**0.8437**	**[0.0,2.0,2.0,1.0]**	**1.772**	**0.0(0)**	**1.987(5)**	**0.0137(9)**	**-3.6(7)**	**2.0434**	**2**
10	0.8377	[0.0,2.0,2.5,1.0]	1.712	0.0(0)	1.987(5)	0.0143(7)	-3.8(6)	2.2760	2
11	0.8345	[0.5,4.0,0.0,1.0]	1.497	2.33(1)	1.997(4)	0.0123(8)	-3.7(4)	2.4272	2
12	0.8337	[0.5,3.5,0.5,1.0]	1.529	2.33(2)	1.992(4)	0.0121(8)	-3.7(5)	2.4118	2
13	0.8325	[0.0,1.0,3.0,1.0]	1.900	0.0(0)	1.978(6)	0.01429(6)	-3.7(7)	2.0005	2
14	0.8312	[0.0,2.5,2.0,1.0]	1.816	0.0(0)	2.0(5)	0.0127(7)	-4.6(6)	2.2413	2
15	0.8301	[0.0,3.5,1.5,1.0]	1.398	0.0(0)	2.0(5)	0.0181(8)	-4.4(5)	2.5537	2
16	0.8301	[0.5,3.0,1.0,1.0]	1.568	2.33(2)	1.986(4)	0.0123(8)	-3.3(5)	2.4014	2
17	0.8297	[0.5,3.5,0.0,1.0]	1.732	2.32(1)	1.993(5)	0.0097(8)	-3.7(5)	2.1842	2
18	0.8293	[0.0,2.0,1.5,1.0]	1.873	0.0(0)	1.985(5)	0.0108(8)	-3.7(7)	1.8205	2
19	0.8280	[0.5,3.0,0.5,1.0]	1.748	2.31(1)	1.987(5)	0.0099(8)	-3.3(5)	2.1774	2
20	0.8277	[0.5,2.5,1.5,1.0]	1.668	2.33(2)	1.983(5)	0.0128(9)	-3.6(6)	2.3729	2
21	0.8273	[0.5,2.0,1.5,1.0]	1.834	2.31(2)	1.978(5)	0.0106(8)	-3.3(7)	2.1311	2
22	0.8254	[0.5,2.5,1.0,1.0]	1.832	2.31(1)	1.983(5)	0.01(9)	-3.5(7)	2.1522	2
23	0.8230	[0.5,2.0,2.0,1.0]	1.735	2.32(2)	1.978(5)	0.0131(9)	-3.1(6)	2.3622	2
24	0.8208	[0.0,1.5,3.0,1.0]	1.938	0.0(0)	1.986(5)	0.0142(5)	-4.2(7)	2.2366	2
25	0.8192	[0.0,3.0,0.5,1.0]	2.001	0.0(0)	2.001(5)	0.011(9)	-4.2(6)	1.8309	2
26	0.8191	[0.0,3.5,0.0,1.0]	2.007	0.0(0)	2.008(5)	0.011(9)	-4.7(6)	1.8395	2
27	0.8189	[0.0,3.0,2.0,1.0]	1.550	0.0(0)	1.995(0)	0.01857(0)	-4.2(0)	2.5436	2
28	0.8170	[0.0,2.5,1.0,1.0]	2.005	0.0(0)	1.999(6)	0.0112(9)	-4.8(7)	1.7969	2
29	0.8168	[0.0,4.0,1.0,1.0]	1.438	0.0(0)	1.998(4)	0.0143(7)	-3.5(4)	2.6117	2
30	0.8164	[0.5,1.0,2.5,1.0]	1.999	2.31(2)	1.968(6)	0.012(1)	-3.2(8)	2.0863	2

Table S6 Detailed results for *Bc* bla The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S7.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.7935**	**[0.0, 3.0, 1.0]**	**2.314**	**0.0(0)**	**1.993(4)**	**0.0091(7)**	**-5.9(6)**	**2.0999**	**2**
2	**0.7925**	**[0.0, 3.5, 0.5]**	**2.319**	**0.0(0)**	**1.998(4)**	**0.009(7)**	**-6.2(6)**	**2.1158**	**2**
3	**0.7899**	**[0.0, 4.0, 0.0]**	**2.307**	**0.0(0)**	**2.0(4)**	**0.009(7)**	**-6.0(5)**	**2.1483**	**2**
4	**0.7841**	**[0.0, 2.5, 1.5]**	**2.432**	**0.0(0)**	**1.991(5)**	**0.0094(7)**	**-6.4(7)**	**2.0663**	**2**
5	**0.7828**	**[0.5, 3.5, 0.0]**	**2.282**	**2.3(1)**	**1.995(4)**	**0.0063(6)**	**-6.1(5)**	**2.1888**	**2**
6	**0.7797**	**[0.0, 2.0, 2.0]**	**2.457**	**0.0(0)**	**1.981(5)**	**0.0095(7)**	**-5.6(7)**	**2.0768**	**2**
7	**0.7791**	**[0.0, 4.5, 0.0]**	**2.162**	**0.0(0)**	**1.999(4)**	**0.0108(7)**	**-5.7(5)**	**2.4234**	**2**
8	**0.7783**	**[0.0, 4.0, 0.5]**	**2.149**	**0.0(0)**	**1.993(4)**	**0.011(7)**	**-5.5(5)**	**2.4183**	**2**
9	**0.7766**	**[0.0, 3.0, 1.5]**	**2.236**	**0.0(0)**	**1.985(4)**	**0.011(7)**	**-5.3(6)**	**2.3798**	**2**
10	**0.7742**	**[0.5, 2.0, 1.5]**	**2.432**	**2.3(1)**	**1.979(4)**	**0.0072(7)**	**-5.8(6)**	**2.1337**	**2**
11	0.7721	[0.0, 3.5, 1.0]	2.227	0.0(0)	1.988(4)	0.0107(7)	-5.5(6)	2.4059	2
12	0.7715	[0.0, 2.5, 2.0]	2.398	0.0(0)	1.985(5)	0.0118(8)	-5.8(7)	2.3341	2
13	0.7708	[0.0, 2.0, 2.5]	2.430	0.0(0)	1.981(5)	0.0122(8)	-5.6(7)	2.3133	2
14	0.7706	[0.5, 3.0, 0.5]	2.282	2.28(1)	1.985(4)	0.0071(6)	-5.4(5)	2.2110	2
15	0.7669	[0.5, 4.0, 0.0]	2.108	2.3(1)	1.993(4)	0.0086(6)	-5.8(4)	2.4728	2
16	0.7669	[0.5, 3.5, 0.5]	2.132	2.3(1)	1.988(4)	0.0084(6)	-5.7(5)	2.4572	2
17	0.7650	[0.5, 2.5, 1.0]	2.382	2.28(1)	1.98(4)	0.007(7)	-5.5(6)	2.1907	2
18	0.7650	[0.0, 3.0, 0.5]	2.559	0.0(0)	1.992(4)	0.0075(7)	-5.6(6)	1.8760	2
19	0.7647	[0.5, 3.0, 1.0]	2.170	2.29(1)	1.983(4)	0.0088(7)	-5.5(5)	2.4486	2
20	0.7644	[0.5, 2.5, 0.5]	2.596	2.29(1)	1.992(4)	0.0047(6)	-6.6(7)	1.8928	2
21	0.7643	[0.0, 1.5, 2.5]	2.658	0.0(0)	1.986(5)	0.0106(8)	-6.8(8)	2.0033	2
22	0.7643	[0.0, 2.0, 1.5]	2.593	0.0(0)	1.984(5)	0.0077(7)	-6.0(7)	1.8254	2
23	0.7631	[0.0, 2.5, 1.0]	2.608	0.0(0)	1.989(5)	0.0075(7)	-6.0(7)	1.8461	2
24	0.7614	[0.0, 3.5, 0.0]	2.592	0.0(0)	1.997(4)	0.0074(7)	-5.9(6)	1.8951	2
25	0.7613	[0.5, 2.5, 1.5]	2.343	2.3(1)	1.981(5)	0.009(7)	-5.6(6)	2.4064	2
26	0.7612	[0.0, 1.0, 3.0]	2.691	0.0(0)	1.983(6)	0.011(8)	-6.6(8)	1.9737	2
27	0.7606	[0.5, 2.0, 1.0]	2.628	2.29(1)	1.985(4)	0.005(6)	-6.2(7)	1.8777	2
28	0.7567	[0.5, 2.0, 2.0]	2.408	2.29(2)	1.976(5)	0.0094(7)	-5.4(6)	2.3962	2
29	0.7549	[0.0, 1.5, 3.0]	2.659	0.0(0)	1.982(6)	0.0127(9)	-6.2(8)	2.2610	2
30	0.7532	[0.0, 4.0, 1.0]	2.105	0.0(0)	1.993(4)	0.0129(7)	-5.6(5)	2.6472	2

Table S7 Detailed results for Bis(acetato)bis(imidazol)zinc(II) The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S8.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.8732**	**[0.0,2.0,2.0]**	**1.429**	**0.0(0)**	**1.983(3)**	**0.0047(4)**	**-7.5(4)**	**2.0656**	**2**
2	**0.8698**	**[0.0,2.5,1.5]**	**1.442**	**0.0(0)**	**1.986(3)**	**0.0044(4)**	**-7.5(4)**	**2.0944**	**2**
3	**0.8682**	**[0.0,2.0,2.5]**	**1.320**	**0.0(0)**	**1.981(3)**	**0.0067(4)**	**-7.2(4)**	**2.3133**	**2**
4	**0.8660**	**[0.0,2.5,2.0]**	**1.303**	**0.0(0)**	**1.984(3)**	**0.0064(4)**	**-7.2(3)**	**2.3404**	**2**
5	**0.8654**	**[0.0,3.0,1.5]**	**1.280**	**0.0(0)**	**1.988(2)**	**0.0062(4)**	**-7.5(3)**	**2.3605**	**2**
6	**0.8611**	**[0.0,3.5,1.0]**	**1.221**	**0.0(0)**	**1.989(2)**	**0.0058(4)**	**-7.0(3)**	**2.3994**	**2**
7	**0.8589**	**[0.0,3.0,1.0]**	**1.480**	**0.0(0)**	**1.987(3)**	**0.0045(4)**	**-7.1(3)**	**2.1342**	**2**
8	**0.8549**	**[0.0,1.5,2.5]**	**1.639**	**0.0(0)**	**1.981(3)**	**0.0052(5)**	**-7.9(4)**	**2.0306**	**2**
9	**0.8549**	**[0.0,1.0,3.0]**	**1.647**	**0.0(0)**	**1.976(3)**	**0.0055(5)**	**-7.7(4)**	**2.0114**	**2**
10	**0.8523**	**[0.0,3.5,0.5]**	**1.518**	**0.0(0)**	**1.991(3)**	**0.0043(4)**	**-7.2(3)**	**2.1562**	**2**
11	0.8506	[0.0,1.0,3.5]	1.591	0.0(0)	1.978(3)	0.0076(5)	-7.9(4)	2.2390	2
12	0.8501	[0.0,1.5,3.0]	1.569	0.0(0)	1.98(3)	0.0071(5)	-7.8(4)	2.2732	2
13	0.8436	[0.0,3.0,2.0]	1.134	0.0(0)	1.987(2)	0.0082(4)	-7.5(3)	2.5996	2
14	0.8405	[0.0,4.0,0.5]	1.353	0.0(0)	1.991(2)	0.0063(4)	-6.7(3)	2.4314	2
15	0.8401	[0.0,3.5,1.5]	1.115	0.0(0)	1.99(2)	0.0079(4)	-7.5(3)	2.6237	2
16	0.8375	[0.0,2.0,1.5]	1.750	0.0(0)	1.982(3)	0.0027(5)	-7.4(4)	1.8353	2
17	0.8345	[0.0,4.5,0.0]	1.384	0.0(0)	1.995(2)	0.0062(4)	-6.9(3)	2.4497	2
18	0.8326	[0.0,2.0,3.0]	1.401	0.0(0)	1.983(3)	0.0091(4)	-7.7(3)	2.5360	2
19	0.8313	[0.0,2.5,1.0]	1.800	0.0(0)	1.986(3)	0.0024(5)	-7.4(4)	1.8611	2
20	0.8308	[0.0,2.5,2.5]	1.359	0.0(0)	1.985(2)	0.0086(4)	-7.7(3)	2.5680	2
21	0.8289	[0.0,1.0,2.5]	1.818	0.0(0)	1.979(3)	0.0032(5)	-8.2(5)	1.7574	2
22	0.8280	[0.0,1.5,2.0]	1.868	0.0(0)	1.98(3)	0.0028(5)	-7.9(5)	1.7989	2
23	0.8239	[0.0,4.5,0.5]	1.145	0.0(0)	1.995(2)	0.0072(4)	-7.4(3)	2.6774	2
24	0.8212	[0.0,0.0,4.5]	1.951	0.0(0)	1.977(3)	0.0089(6)	-8.4(5)	2.1517	2
25	0.8210	[0.0,0.0,4.0]	1.962	0.0(0)	1.976(3)	0.007(6)	-8.6(5)	1.9178	2
26	0.8208	[0.0,0.5,3.5]	1.989	0.0(0)	1.978(3)	0.0066(6)	-8.4(5)	1.9540	2
27	0.8204	[0.0,0.5,4.0]	1.948	0.0(0)	1.977(3)	0.0088(6)	-8.2(4)	2.1983	2
28	0.8190	[0.0,4.0,0.0]	1.826	0.0(0)	1.994(3)	0.0049(5)	-6.7(3)	2.1834	2
29	0.8184	[0.0,4.0,1.0]	1.129	0.0(0)	1.988(2)	0.0081(4)	-6.7(3)	2.6832	2
30	0.8177	[0.0,1.0,4.0]	1.680	0.0(0)	1.978(3)	0.0099(5)	-7.7(4)	2.4774	2

Table S8 Detailed results for Tetrakis(imidazole)zinc(II)-perchlorate The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S9.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.6383**	**[0.0,3.5,0.5]**	**3.54**	**0.0(0)**	**1.98(3)**	**0.0021(6)**	**-7.0(5)**	**2.2213**	**2**
2	**0.6293**	**[0.0,4.5,0.0]**	**3.11**	**0.0(0)**	**1.981(3)**	**0.0029(5)**	**-6.6(4)**	**2.5442**	**2**
3	**0.6235**	**[0.0,4.0,0.5]**	**3.23**	**0.0(0)**	**1.977(3)**	**0.0031(5)**	**-6.4(4)**	**2.5251**	**2**
4	0.6159	[0.0,4.0,0.0]	3.52	0.0(0)	1.98(3)	0.0023(5)	-6.8(4)	2.2676	2
5	0.5989	[0.0,3.5,1.0]	3.59	0.0(0)	1.973(3)	0.0032(5)	-6.2(5)	2.5054	2
6	0.5893	[0.0,3.0,1.5]	3.81	0.0(0)	1.97(3)	0.0034(6)	-6.1(5)	2.4782	2
7	0.5884	[0.0,5.0,0.0]	3.08	0.0(0)	1.981(3)	0.004(4)	-6.6(4)	2.8269	2
8	0.5865	[0.0,4.0,1.0]	3.33	0.0(0)	1.975(3)	0.0037(5)	-6.3(4)	2.7792	2
9	0.5841	[0.0,4.5,0.5]	3.18	0.0(0)	1.977(3)	0.0038(5)	-6.2(4)	2.8109	2
10	0.5699	[0.0,3.0,1.0]	4.20	0.0(0)	1.972(4)	0.0036(7)	-6.3(6)	2.2225	2
11	0.5682	[0.0,3.5,0.0]	4.40	0.0(0)	1.985(4)	0.0022(7)	-7.3(6)	1.9575	2
12	0.5541	[0.5,4.0,0.5]	3.78	2.38(1)	1.981(3)	0.0022(5)	-7.1(4)	2.7263	2
13	0.5534	[0.5,4.0,0.0]	4.08	2.39(1)	1.986(3)	0.002(5)	-7.3(4)	2.4534	2
14	0.5534	[0.0,2.5,1.5]	4.35	0.0(0)	1.966(4)	0.0021(6)	-6.2(6)	2.2108	2
15	0.5500	[0.5,4.5,0.0]	3.62	2.4(1)	1.986(3)	0.0029(5)	-7.1(4)	2.7263	2
16	0.5461	[0.0,3.5,1.5]	3.88	0.0(0)	1.971(3)	0.0039(6)	-5.9(5)	2.7620	2
17	0.5443	[0.5,3.5,0.5]	4.31	2.38(1)	1.981(4)	0.002(6)	-7.1(5)	2.4436	2
18	0.5428	[0.0,3.0,2.0]	4.13	0.0(0)	1.97(3)	0.0039(6)	-6.0(5)	2.7219	2
19	0.5353	[0.5,3.5,1.0]	4.16	2.38(1)	1.979(3)	0.0022(6)	-6.9(5)	2.6934	2
20	0.5325	[0.0,5.5,0.0]	3.18	0.0(0)	1.982(3)	0.0051(5)	-6.1(4)	3.1012	2
21	0.5310	[0.0,2.0,2.0]	4.62	0.0(0)	1.961(4)	0.0021(6)	-5.7(7)	2.1921	2
22	0.5287	[0.0,5.0,0.5]	3.33	0.0(0)	1.979(3)	0.0053(5)	-5.9(4)	3.0800	2
23	0.5224	[0.5,3.0,1.5]	4.44	2.37(1)	1.975(3)	0.002(6)	-7.0(5)	2.6795	2
24	0.5149	[0.0,4.5,1.0]	3.62	0.0(0)	1.976(3)	0.005(5)	-5.9(4)	3.0582	2
25	0.5104	[0.0,2.5,2.0]	4.75	0.0(0)	1.965(4)	0.0039(7)	-5.8(6)	2.4637	2
26	0.5092	[0.5,3.0,1.0]	4.39	2.41(1)	1.976(4)	0.002(6)	-7.0(5)	2.4092	2
27	0.5045	[0.0,4.0,1.5]	3.86	0.0(0)	1.973(3)	0.0052(5)	-5.7(5)	3.0359	2
28	0.4935	[0.0,2.0,2.5]	5.03	0.0(0)	1.962(4)	0.0042(7)	-5.7(7)	2.4352	2
29	0.4904	[0.5,4.5,0.5]	3.58	2.43(1)	1.984(3)	0.0041(5)	-7.0(4)	2.9577	2
30	0.4895	[0.5,5.0,0.0]	3.86	2.34(1)	1.981(3)	0.0035(5)	-6.3(4)	3.0813	2

Table S9 Detailed results for *Ss* ABCE1 The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S10.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.7007**	**[4.0,0.0,0.0]**	**4.245**	**2.29(3)**	**0.0(0)**	**0.0093(5)**	**-5.7(5)**	**2.8149**	**3**
2	**0.6922**	**[4.5,0.0,0.0]**	**4.380**	**2.29(3)**	**0.0(0)**	**0.0106(5)**	**-5.5(5)**	**3.1668**	**3**
3	0.6737	[3.0,0.0,0.0]	4.675	2.291(3)	0.0(0)	0.0066(4)	-6.5(6)	2.1055	2
4	0.6691	[2.5,0.0,1.0]	4.334	2.302(3)	2.08(1)	0.0053(5)	-8.4(6)	2.0957	2
5	0.6669	[3.0,0.0,0.5]	4.420	2.296(3)	2.08(3)	0.0067(5)	-7.2(6)	2.2735	2
6	0.6531	[2.5,0.0,0.5]	4.820	2.295(3)	2.08(3)	0.0051(5)	-7.4(7)	1.9320	2
7	0.6501	[3.5,0.0,0.0]	4.326	2.291(3)	0.0(0)	0.0079(4)	-6.0(5)	2.4564	2
8	0.6484	[3.5,0.0,0.5]	4.293	2.293(3)	2.09(4)	0.0084(5)	-6.6(5)	2.6342	3
9	0.6115	[2.5,0.5,0.5]	4.274	2.302(3)	2.09(2)	0.005(5)	-8.4(6)	2.1628	2
10	0.6104	[5.0,0.0,0.0]	4.681	2.29(3)	0.0(0)	0.012(5)	-5.2(5)	3.5187	3
11	0.6101	[3.0,0.0,1.0]	4.216	2.298(3)	2.09(2)	0.0073(5)	-7.8(6)	2.4481	2
12	0.5914	[2.5,0.0,1.5]	4.157	2.305(3)	2.09(1)	0.0058(6)	-9.1(6)	2.2625	2
13	0.5854	[3.0,0.5,0.0]	4.352	2.294(3)	2.1(4)	0.0067(6)	-7.1(6)	2.3499	2
14	0.5769	[2.5,0.5,0.0]	4.773	2.297(3)	2.1(4)	0.005(6)	-7.6(7)	1.9877	2
15	0.5384	[1.5,0.0,2.0]	5.782	2.297(5)	2.079(8)	0.0041(9)	-8.5(7)	1.8230	2
16	0.5319	[3.5,0.5,0.0]	4.172	2.294(3)	2.12(5)	0.0083(5)	-6.8(5)	2.6842	3
17	0.5225	[2.5,1.0,0.0]	4.376	2.299(3)	2.1(2)	0.0049(6)	-7.7(6)	2.2398	2
18	0.5107	[1.5,0.5,1.5]	6.523	2.298(6)	2.067(9)	0.005(1)	-8.2(8)	1.9286	2
19	0.4934	[2.5,0.5,1.0]	4.023	2.307(3)	2.1(1)	0.0056(6)	-9.5(6)	2.3136	2
20	0.4853	[3.0,0.5,0.5]	5.066	2.299(3)	2.1(2)	0.007(5)	-7.8(6)	2.5078	3
21	0.4821	[2.5,1.0,0.5]	4.105	2.303(3)	2.1(1)	0.0054(6)	-8.5(6)	2.4073	2
22	0.4803	[5.5,0.0,0.0]	5.124	2.29(3)	0.0(0)	0.0133(5)	-5.1(5)	3.8706	3
23	0.4689	[4.0,0.0,0.5]	4.293	2.291(4)	2.15(4)	0.0099(5)	-6.4(5)	2.9698	3
24	0.4668	[3.0,0.0,1.5]	4.159	2.3(4)	2.11(1)	0.0081(5)	-8.8(5)	2.5979	3
25	0.4639	[3.0,1.0,0.0]	4.135	2.297(3)	2.11(2)	0.0071(5)	-7.4(6)	2.5805	3
26	0.4603	[4.0,0.5,0.0]	5.212	2.292(3)	2.13(4)	0.0097(5)	-6.3(5)	3.0408	3
27	0.4584	[1.5,0.0,1.5]	5.496	2.3(5)	2.09(1)	0.004(9)	-9.6(8)	1.6006	2
28	0.4383	[2.0,0.0,2.0]	4.083	2.315(3)	2.098(7)	0.004(6)	-10.9(6)	2.0633	2
29	0.4355	[3.5,0.0,1.0]	4.201	2.294(4)	2.13(2)	0.009(4)	-7.5(5)	2.7795	3
30	0.4267	[3.5,0.5,0.5]	5.051	2.296(4)	2.12(2)	0.0089(5)	-7.5(5)	2.8472	3

Table S10 Detailed results for *Pa* RM2-4$_{ox}$ The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S11.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.7957**	**[4.0,0.0,0.0]**	**2.991**	**2.285(3)**	**0.0(0)**	**0.0078(3)**	**-13.3(5)**	**2.8532**	**3**
2	**0.7819**	**[4.5,0.0,0.0]**	**3.092**	**2.285(3)**	**0.0(0)**	**0.0093(4)**	**-13.1(5)**	**3.2099**	**3**
3	0.7623	[3.0,0.0,0.0]	3.490	2.289(3)	0.0(0)	0.0054(4)	-14.7(7)	2.1169	2
4	0.7557	[3.0,0.0,0.5]	3.180	2.289(3)	2.04(2)	0.005(4)	-14.7(7)	2.3356	2
5	0.7203	[3.5,0.0,0.0]	3.147	2.284(3)	0.0(0)	0.0065(3)	-13.2(5)	2.5033	3
6	0.7150	[3.5,0.0,0.5]	2.971	2.291(3)	2.09(3)	0.0068(4)	-15.0(6)	2.6475	3
7	0.6911	[4.0,0.5,0.5]	4.098	2.291(3)	2.05(2)	0.008(4)	-14.3(6)	3.3194	3
8	0.6849	[3.0,0.5,0.0]	3.658	2.283(3)	2.0(3)	0.0051(4)	-13.3(7)	2.4940	2
9	0.6814	[5.0,0.0,0.0]	3.442	2.285(3)	0.0(0)	0.011(4)	-12.8(5)	3.5666	3
10	0.6570	[3.0,1.0,0.0]	3.087	2.291(3)	2.08(2)	0.0052(4)	-14.8(7)	2.6573	3
11	0.6403	[3.5,0.0,1.0]	4.005	2.281(3)	1.99(1)	0.0063(4)	-11.9(6)	3.0244	3
12	0.6338	[3.0,0.0,1.0]	2.861	2.298(3)	2.09(1)	0.0056(4)	-16.6(6)	2.4481	2
13	0.6124	[3.5,0.5,0.0]	3.018	2.291(3)	2.1(4)	0.0066(4)	-14.8(6)	2.7178	3
14	0.6019	[2.0,1.0,0.5]	5.053	2.284(4)	2.07(1)	0.0043(7)	-13.3(0)	2.1990	2
15	0.5706	[3.0,1.0,0.5]	2.974	2.3(3)	2.09(1)	0.0056(4)	-16.5(6)	2.7830	3
16	0.5462	[2.0,1.0,1.0]	5.570	2.291(5)	2.07(1)	0.0051(8)	-13.3(9)	2.3739	2
17	0.5315	[3.5,1.0,0.0]	2.974	2.294(3)	2.1(2)	0.007(4)	-15.3(6)	2.9593	3
18	0.5288	[5.5,0.0,0.0]	3.894	2.284(3)	0.0(0)	0.0121(4)	-12.3(5)	3.9338	3
19	0.4985	[3.0,0.5,0.5]	2.940	2.298(3)	2.1(2)	0.0056(4)	-16.5(6)	2.5134	3
20	0.4759	[2.5,0.0,1.5]	2.749	2.308(3)	2.095(9)	0.0041(4)	-18.7(6)	2.2412	2
21	0.4704	[3.0,0.0,1.5]	2.789	2.304(3)	2.1(1)	0.0064(4)	-18.0(6)	2.5906	3
22	0.4500	[4.0,0.0,0.5]	3.048	2.286(4)	2.14(4)	0.0085(4)	-14.2(5)	3.0124	3
23	0.4460	[3.5,0.5,0.5]	3.544	2.297(3)	2.11(2)	0.0073(4)	-16.5(6)	2.8523	3
24	0.3988	[1.5,1.5,1.0]	7.163	2.318(7)	2.072(9)	0.0041(1)	-16.5(0)	2.2256	2
25	0.3891	[1.5,0.0,2.0]	7.815	2.283(7)	2.04(1)	0.004(1)	-13.0(0)	1.9505	2
26	0.3478	[3.0,0.5,1.0]	2.834	2.303(3)	2.11(1)	0.0061(4)	-17.7(6)	2.6547	3
27	0.3187	[1.5,2.0,0.5]	8.209	2.287(6)	2.056(9)	0.004(1)	-12.7(9)	2.4511	2
28	0.3075	[3.0,1.5,0.0]	3.066	2.299(3)	2.11(1)	0.0061(5)	-16.4(6)	2.8237	3
29	0.2779	[2.5,1.0,1.0]	2.988	2.309(3)	2.105(8)	0.0045(5)	-18.4(6)	2.5539	3
30	0.2773	[3.5,1.0,0.5]	2.978	2.299(3)	2.12(1)	0.0079(4)	-16.8(5)	3.0753	3

Table S11 Detailed results for *Pa* RM2-4$_{red}$ The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S12.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.9121**	**[3.5,0.0,0.0]**	**1.043**	**2.327(1)**	**0.0(0)**	**0.0053(2)**	**-13.8(3)**	**2.2287**	**2**
2	**0.9006**	**[4.5,0.0,0.0]**	**1.231**	**2.329(2)**	**0.0(0)**	**0.0077(2)**	**-13.5(3)**	**2.8500**	**3**
3	0.8848	[4.5,0.5,0.0]	1.513	2.326(2)	2.0(2)	0.0078(2)	-13.1(3)	3.2157	3
4	0.8763	[5.0,0.0,0.0]	1.656	2.328(2)	0.0(0)	0.009(2)	-13.0(3)	3.1752	3
5	0.8619	[4.0,0.0,0.0]	1.022	2.327(1)	0.0(0)	0.0065(2)	-13.7(3)	2.5471	3
6	0.7975	[4.5,1.0,0.0]	1.967	2.327(2)	2.04(1)	0.0077(2)	-13.0(4)	3.4802	3
7	0.7970	[5.0,0.0,0.5]	2.269	2.328(2)	2.07(3)	0.0093(3)	-12.5(4)	3.3769	3
8	0.7959	[4.0,1.0,0.0]	1.573	2.328(2)	2.08(1)	0.0066(2)	-13.3(4)	3.0920	3
9	0.7753	[4.0,1.0,0.5]	2.167	2.332(2)	2.071(9)	0.0067(3)	-13.6(4)	3.2794	3
10	0.7703	[5.5,0.0,0.0]	2.294	2.327(2)	0.0(0)	0.0104(3)	-12.3(4)	3.5022	3
11	0.7504	[3.5,0.0,0.5]	0.970	2.33(1)	2.1(1)	0.0054(2)	-14.5(3)	2.3966	2
12	0.7381	[4.0,1.5,0.0]	2.174	2.331(2)	2.073(9)	0.0065(3)	-13.5(4)	3.3632	3
13	0.6833	[4.5,1.0,0.5]	2.695	2.33(2)	2.05(1)	0.0079(3)	-13.3(4)	3.6535	3
14	0.6812	[5.0,0.0,1.0]	3.056	2.328(3)	2.05(2)	0.0094(3)	-12.2(5)	3.6009	3
15	0.6710	[5.5,0.0,0.5]	2.700	2.33(2)	2.06(3)	0.0107(3)	-13.4(4)	3.6811	3
16	0.6509	[3.5,1.0,1.0]	2.637	2.334(2)	2.084(7)	0.0054(3)	-13.5(5)	3.1211	3
17	0.6442	[4.0,2.0,0.0]	3.166	2.327(3)	2.061(8)	0.0067(3)	-12.4(4)	3.7088	3
18	0.6436	[4.5,1.5,0.0]	2.752	2.326(2)	2.04(1)	0.0078(3)	-12.4(4)	3.7954	3
19	0.6420	[3.0,1.0,1.5]	3.553	2.334(3)	2.079(6)	0.0043(4)	-13.4(5)	3.0182	3
20	0.6379	[5.5,0.5,0.0]	2.599	2.327(2)	2.02(3)	0.0104(3)	-12.8(4)	3.8267	3
21	0.6350	[3.5,1.0,0.5]	1.702	2.332(2)	2.092(8)	0.0054(2)	-14.0(4)	2.9230	3
22	0.6334	[6.0,0.0,0.0]	2.725	2.327(2)	0.0(0)	0.0115(3)	-13.0(4)	3.8206	3
23	0.6328	[5.0,0.5,0.0]	2.379	2.326(2)	1.96(2)	0.0091(3)	-13.1(3)	3.5740	3
24	0.6316	[5.0,1.0,0.0]	2.710	2.325(2)	2.03(2)	0.0091(3)	-11.7(4)	3.8327	3
25	0.6301	[4.0,1.5,0.5]	3.256	2.331(3)	2.073(8)	0.0064(3)	-12.6(5)	3.5632	3
26	0.6225	[4.0,1.0,1.0]	3.135	2.333(3)	2.08(8)	0.0069(3)	-13.1(5)	3.4504	3
27	0.6197	[3.5,2.0,0.0]	2.869	2.33(2)	2.081(7)	0.0053(3)	-12.4(4)	3.3113	3
28	0.5991	[3.5,2.0,0.5]	3.949	2.332(3)	2.07(7)	0.0058(4)	-12.6(5)	3.5342	3
29	0.5790	[3.5,1.5,1.0]	3.897	2.333(3)	2.078(7)	0.0054(4)	-12.8(5)	3.4197	3

Table S12 Detailed results for *Hs* TH1$_{nat}$ The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S13.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.6600**	**[0.0,0.5,4.5]**	**3.648**	**0.0(0)**	**2.066(6)**	**0.0121(9)**	**0.0(8)**	**2.121**	**2**
2	**0.6436**	**[0.0,0.5,4.0]**	**3.271**	**0.0(0)**	**2.07(6)**	**0.0121(1)**	**0.3(8)**	**1.897**	**2**
3	0.6433	[1.0,0.0,3.0]	2.745	2.33(1)	2.074(9)	0.011(1)	0.4(9)	1.829	2
4	0.6287	[0.0,0.0,5.5]	4.411	0.0(0)	2.065(6)	0.0122(9)	-0.5(8)	2.248	2
5	0.6285	[1.0,0.0,3.5]	2.647	2.34(1)	2.079(8)	0.013(1)	-0.4(8)	1.992	2
6	0.6242	[1.5,0.0,3.0]	2.836	2.328(9)	2.076(9)	0.012(1)	0.5(8)	2.143	2
7	0.6212	[1.0,0.0,2.5]	2.939	2.323(1)	2.065(9)	0.008(1)	0.8(0)	1.666	2
8	0.6209	[0.0,0.5,5.0]	4.351	0.0(0)	2.065(6)	0.0121(9)	-0.5(7)	2.331	2
9	0.6142	[0.0,0.0,5.0]	3.780	0.0(0)	2.064(6)	0.0123(9)	0.6(8)	2.049	2
10	0.6133	[1.5,0.5,2.5]	2.749	2.327(8)	2.069(9)	0.012(1)	1.0(8)	2.250	2
11	0.6086	[1.0,0.5,2.5]	2.723	2.32(1)	2.072(8)	0.01(1)	1.0(9)	1.934	2
12	0.6081	[0.0,1.0,3.5]	3.103	0.0(0)	2.071(6)	0.012(1)	0.7(8)	1.973	2
13	0.6060	[1.5,0.0,3.5]	2.981	2.342(9)	2.067(8)	0.013(1)	0.3(8)	2.340	2
14	0.6023	[0.5,0.0,4.0]	3.069	2.28(3)	2.07(9)	0.013(1)	1.1(9)	1.975	2
15	0.6000	[1.0,0.5,2.0]	3.729	2.32(1)	2.073(1)	0.009(1)	0.0(0)	1.730	2
16	0.5989	[0.5,0.0,4.5]	3.475	2.34(3)	2.062(6)	0.012(1)	0.8(8)	2.162	2
17	0.5903	[0.0,1.5,4.5]	4.907	0.0(0)	2.064(6)	0.0122(9)	-0.3(7)	2.709	3
18	0.5891	[0.0,1.0,5.0]	4.923	0.0(0)	2.064(6)	0.0122(9)	-0.4(8)	2.626	3
19	0.5875	[0.0,0.5,5.5]	5.325	0.0(0)	2.066(6)	0.0122(9)	-1.5(7)	2.529	3
20	0.5857	[0.0,1.5,3.0]	3.167	0.0(0)	2.071(6)	0.0121(1)	0.8(8)	2.055	2
21	0.5835	[1.5,0.0,4.0]	3.409	2.35(1)	2.066(8)	0.013(1)	-0.5(8)	2.528	3
22	0.5832	[0.0,2.0,4.0]	4.532	0.0(0)	2.064(6)	0.0123(9)	0.3(7)	2.792	3
23	0.5826	[0.0,1.0,4.5]	3.986	0.0(0)	2.065(6)	0.0122(9)	0.3(7)	2.414	2
24	0.5800	[1.0,0.5,3.0]	2.567	2.34(1)	2.081(7)	0.012(1)	-0.3(8)	2.064	2
25	0.5780	[1.0,1.0,2.0]	2.544	2.32(1)	2.074(8)	0.01(1)	1.1(8)	2.008	2
26	0.5755	[0.5,0.5,4.5]	4.069	2.34(3)	2.061(6)	0.012(1)	0.2(8)	2.457	3
27	0.5740	[0.0,0.0,6.0]	5.372	0.0(0)	2.067(6)	0.0123(9)	-1.6(8)	2.439	3
28	0.5625	[2.0,1.5,1.5]	2.933	2.328(6)	2.063(9)	0.011(1)	1.6(7)	2.753	3
29	0.5615	[0.0,1.0,4.0]	3.473	0.0(0)	2.066(6)	0.0122(9)	1.3(8)	2.204	2
30	0.5550	[1.5,1.0,2.5]	2.587	2.337(9)	2.071(8)	0.013(1)	1.0(7)	2.501	3

Table S13 Detailed results for *Hs* TH1$_{ox}$ The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S14.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.9141**	**[0.0,2.5,3.5]**	**1.314**	**0.0(0)**	**2.051(4)**	**0.0218(8)**	**-7.1(3)**	**2.9778**	**3**
2	**0.9135**	**[0.0,3.5,2.0]**	**1.348**	**0.0(0)**	**2.056(4)**	**0.0184(8)**	**-7.1(4)**	**2.8984**	**3**
3	**0.9085**	**[0.0,2.0,4.0]**	**1.428**	**0.0(0)**	**2.048(5)**	**0.0218(9)**	**-7.1(4)**	**2.9152**	**3**
4	**0.9065**	**[0.0,2.5,3.0]**	**1.353**	**0.0(0)**	**2.051(4)**	**0.0193(8)**	**-7.3(4)**	**2.7655**	**3**
5	**0.9052**	**[0.0,3.0,2.5]**	**1.455**	**0.0(0)**	**2.051(4)**	**0.0186(8)**	**-7.0(4)**	**2.8517**	**3**
6	**0.8981**	**[0.0,1.5,4.5]**	**1.590**	**0.0(0)**	**2.042(5)**	**0.0222(9)**	**-6.9(4)**	**2.8747**	**3**
7	**0.8960**	**[0.0,1.5,2.5]**	**1.607**	**0.0(0)**	**2.049(5)**	**0.0134(9)**	**-7.7(4)**	**1.9671**	**2**
8	**0.8955**	**[1.0,2.5,1.5]**	**1.631**	**2.317(9)**	**2.023(5)**	**0.01418(5)**	**-4.7(5)**	**2.9503**	**3**
9	**0.8952**	**[0.5,3.5,1.0]**	**1.599**	**2.33(2)**	**2.036(4)**	**0.01423(6)**	**-5.3(4)**	**2.9330**	**3**
10	**0.8949**	**[0.0,0.5,4.0]**	**1.616**	**0.0(0)**	**2.038(4)**	**0.0132(7)**	**-7.2(4)**	**2.0679**	**2**
11	**0.8925**	**[0.5,2.5,2.0]**	**1.506**	**2.33(2)**	**2.033(4)**	**0.0136(8)**	**-5.7(4)**	**2.7735**	**3**
12	0.8912	[0.0,2.0,3.5]	1.517	0.0(0)	2.047(5)	0.0197(9)	-7.0(4)	2.7086	3
13	0.8891	[0.0,0.0,4.5]	1.725	0.0(0)	2.037(4)	0.0136(7)	-7.4(4)	1.9841	2
14	0.8890	[0.0,1.0,5.0]	1.717	0.0(0)	2.04(5)	0.0226(9)	-6.8(4)	2.8015	3
15	0.8867	[0.0,1.0,3.0]	1.710	0.0(0)	2.045(5)	0.0139(9)	-7.6(5)	1.9010	2
16	0.8861	[1.0,2.0,2.0]	1.758	2.323(1)	2.017(5)	0.0132(1)	-4.5(5)	2.8829	3
17	0.8853	[0.0,0.5,3.5]	1.601	0.0(0)	2.043(4)	0.0127(8)	-7.8(4)	1.8233	2
18	0.8840	[0.0,3.5,1.5]	1.658	0.0(0)	2.043(4)	0.01404(5)	-5.8(4)	2.7851	3
19	0.8838	[0.0,4.5,0.5]	1.767	0.0(0)	2.051(4)	0.015(8)	-5.8(4)	2.8978	3
20	0.8833	[1.0,3.5,0.5]	1.719	2.314(9)	2.026(5)	0.014(1)	-4.2(5)	3.1214	3
21	0.8824	[0.0,0.5,5.5]	1.737	0.0(0)	2.042(5)	0.0236(9)	-7.1(4)	2.6982	3
22	0.8820	[0.0,2.5,4.0]	1.370	0.0(0)	2.052(4)	0.024(9)	-7.1(3)	3.1815	3
23	0.8819	[0.0,1.0,3.5]	1.701	0.0(0)	2.037(4)	0.0129(7)	-6.8(4)	2.1630	2
24	0.8813	[0.0,2.0,4.5]	1.463	0.0(0)	2.047(5)	0.024(9)	-6.9(4)	3.1377	3
25	0.8808	[0.0,1.5,4.0]	1.636	0.0(0)	2.04(4)	0.0186(8)	-6.7(4)	2.6716	3
26	0.8803	[0.0,4.0,1.0]	1.663	0.0(0)	2.056(4)	0.0153(8)	-6.5(4)	2.7739	3
27	0.8800	[0.0,5.0,0.5]	1.691	0.0(0)	2.054(4)	0.0168(8)	-5.7(4)	3.1703	3
28	0.8793	[1.0,3.0,1.0]	1.806	2.309(9)	2.019(5)	0.01406(5)	-3.7(5)	3.0835	3
29	0.8790	[0.5,3.0,2.0]	1.728	2.32(2)	2.031(4)	0.0143(9)	-5.0(4)	3.1105	3
30	0.8785	[0.0,1.5,3.0]	1.608	0.0(0)	2.04(4)	0.0125(7)	-6.7(4)	2.2342	2

Table S14 Detailed results for Fe-Pvd The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S15.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.8083**	**[0.0,1.0,5.0]**	**2.763**	**0.0(0)**	**2.013(3)**	**0.0092(4)**	**-7.6(4)**	**3.0136**	**3**
2	**0.8021**	**[0.0,1.0,4.5]**	**2.967**	**0.0(0)**	**2.013(3)**	**0.0078(4)**	**-7.6(4)**	**2.7784**	**3**
3	**0.7959**	**[0.0,0.5,5.5]**	**2.841**	**0.0(0)**	**2.01(3)**	**0.0092(5)**	**-7.4(4)**	**2.9419**	**3**
4	**0.7907**	**[0.0,0.0,6.0]**	**2.646**	**0.0(0)**	**2.008(3)**	**0.0093(4)**	**-7.5(4)**	**2.8611**	**3**
5	**0.7899**	**[0.0,0.5,5.0]**	**2.970**	**0.0(0)**	**2.011(3)**	**0.008(5)**	**-7.8(4)**	**2.6975**	**3**
6	0.7865	[0.0,0.0,5.5]	2.763	0.0(0)	2.01(3)	0.0083(4)	-7.7(4)	2.6086	3
7	0.7861	[0.0,1.5,4.0]	3.218	0.0(0)	2.014(3)	0.0079(5)	-7.5(4)	2.8660	3
8	0.7842	[0.0,1.5,4.5]	2.984	0.0(0)	2.014(3)	0.0088(5)	-7.5(4)	3.1006	3
9	0.7743	[0.0,2.0,3.5]	3.362	0.0(0)	2.015(3)	0.0076(5)	-7.4(4)	2.9532	3
10	0.7698	[0.0,2.0,4.0]	3.048	0.0(0)	2.016(3)	0.0086(5)	-7.5(4)	3.1786	3
11	0.7629	[0.0,1.0,5.5]	2.705	0.0(0)	2.012(3)	0.0103(5)	-7.2(4)	3.2576	3
12	0.7625	[0.0,0.0,6.5]	2.649	0.0(0)	2.008(3)	0.0106(5)	-7.1(3)	3.0996	3
13	0.7596	[0.0,0.5,6.0]	2.817	0.0(0)	2.01(3)	0.0104(5)	-7.2(3)	3.1791	3
14	0.7571	[0.5,1.5,3.5]	3.559	2.3(1)	2.011(3)	0.0064(5)	-7.2(4)	2.9954	3
15	0.7519	[0.0,2.5,3.0]	3.630	0.0(0)	2.018(3)	0.0077(5)	-7.5(4)	3.0235	3
16	0.7499	[0.0,0.0,4.5]	3.362	0.0(0)	2.011(3)	0.0063(5)	-8.3(5)	2.1285	2
17	0.7462	[0.0,1.0,4.0]	3.315	0.0(0)	2.01(3)	0.0068(5)	-7.5(4)	2.5638	3
18	0.7438	[0.5,1.0,4.5]	3.116	2.32(1)	2.007(3)	0.008(5)	-6.9(4)	3.1483	3
19	0.7420	[0.0,0.0,5.0]	2.990	0.0(0)	2.01(3)	0.0073(4)	-7.9(4)	2.3714	2
20	0.7414	[0.0,1.5,3.5]	3.595	0.0(0)	2.013(3)	0.0068(5)	-7.5(5)	2.6386	3
21	0.7391	[0.0,2.5,3.5]	3.296	0.0(0)	2.017(3)	0.0085(5)	-7.4(4)	3.2644	3
22	0.7383	[0.5,2.0,3.0]	3.743	2.3(1)	2.012(3)	0.0064(5)	-7.0(5)	3.0839	3
23	0.7376	[0.5,1.0,4.0]	3.319	2.29(1)	2.005(3)	0.0066(5)	-6.8(4)	2.9506	3
24	0.7328	[0.0,2.0,3.0]	3.818	0.0(0)	2.015(3)	0.0067(5)	-7.5(5)	2.7193	3
25	0.7320	[0.5,1.5,4.0]	3.300	2.3(1)	2.009(3)	0.0078(5)	-7.0(4)	3.2475	3
26	0.7320	[0.0,0.5,4.5]	3.240	0.0(0)	2.011(3)	0.0072(5)	-7.9(4)	2.4610	3
27	0.7307	[0.5,1.0,3.5]	3.712	2.31(1)	2.01(3)	0.0055(4)	-7.7(5)	2.6601	3
28	0.7293	[0.0,1.5,5.0]	2.910	0.0(0)	2.012(3)	0.0105(5)	-7.1(4)	3.3533	3
29	0.7287	[0.5,0.5,4.5]	3.330	2.31(1)	2.005(3)	0.0071(5)	-7.1(4)	2.8346	3
30	0.7278	[0.5,0.0,5.0]	3.133	2.32(1)	2.005(3)	0.0072(4)	-7.3(4)	2.7282	3

Table S15 Detailed results for ALAD (Dent et al.) The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S16.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.6949**	**[2.0,0.0,1.5]**	**3.168**	**2.277(4)**	**2.03(1)**	**0.0045(8)**	**-8.7(9)**	**1.828**	**2**
2	**0.6929**	**[2.0,0.5,1.5]**	**3.380**	**2.276(4)**	**2.023(1)**	**0.0048(8)**	**-7.7(8)**	**2.095**	**2**
3	**0.6927**	**[2.5,0.0,1.5]**	**3.179**	**2.268(4)**	**2.01(1)**	**0.007(8)**	**-6.9(8)**	**2.201**	**2**
4	**0.6873**	**[2.0,0.5,1.0]**	**3.383**	**2.274(4)**	**2.03(1)**	**0.0045(8)**	**-8.2(9)**	**1.878**	**2**
5	**0.6866**	**[2.0,0.0,2.0]**	**3.085**	**2.282(4)**	**2.037(9)**	**0.0058(8)**	**-9.4(8)**	**2.003**	**2**
6	**0.6806**	**[2.0,1.0,0.5]**	**3.442**	**2.271(4)**	**2.03(1)**	**0.0041(8)**	**-7.3(9)**	**1.929**	**2**
7	**0.6780**	**[2.5,0.5,1.0]**	**3.302**	**2.267(4)**	**2.02(1)**	**0.0068(8)**	**-6.7(8)**	**2.230**	**2**
8	0.6767	[2.5,1.0,0.5]	3.258	2.266(4)	2.02(1)	0.0065(8)	-6.2(8)	2.275	2
9	0.6759	[2.0,1.5,0.5]	3.469	2.271(4)	2.025(1)	0.004(8)	-6.7(8)	2.189	2
10	0.6706	[2.5,0.0,2.0]	3.271	2.271(5)	2.03(1)	0.0087(8)	-7.5(8)	2.361	2
11	0.6702	[2.5,0.5,1.5]	3.336	2.271(4)	2.03(1)	0.0082(8)	-7.3(8)	2.402	2
12	0.6672	[2.0,1.5,0.0]	3.594	2.271(4)	2.04(1)	0.0042(9)	-7.2(9)	1.949	2
13	0.6650	[2.5,1.5,0.0]	3.344	2.265(4)	2.03(2)	0.0065(8)	-6.1(9)	2.301	2
14	0.6626	[2.5,0.0,1.0]	3.350	2.262(5)	2.0(2)	0.006(7)	-6.0(9)	2.020	2
15	0.6562	[2.5,0.5,0.5]	3.526	2.265(4)	2.03(2)	0.0065(8)	-6.6(9)	2.013	2
16	0.6559	[3.0,0.0,1.5]	3.172	2.266(4)	2.03(1)	0.01(7)	-6.9(7)	2.486	2
17	0.6541	[2.0,2.0,0.5]	3.651	2.277(4)	2.04(9)	0.0054(9)	-7.3(7)	2.372	2
18	0.6533	[3.0,0.0,1.0]	3.248	2.261(4)	2.01(2)	0.0087(7)	-5.7(8)	2.327	2
19	0.6525	[2.0,0.5,2.0]	3.732	2.277(5)	2.024(8)	0.0058(9)	-7.6(7)	2.300	2
20	0.6512	[2.5,1.0,1.0]	3.387	2.267(4)	2.02(1)	0.0068(8)	-6.0(8)	2.484	2
21	0.6497	[2.0,1.0,1.5]	3.703	2.275(5)	2.023(9)	0.0057(9)	-6.8(8)	2.351	2
22	0.6479	[2.5,2.0,0.0]	3.385	2.267(4)	2.04(1)	0.0076(8)	-6.2(7)	2.514	2
23	0.6476	[3.0,0.5,1.0]	3.263	2.265(4)	2.03(2)	0.0099(7)	-6.7(8)	2.531	2
24	0.6469	[2.5,1.5,0.5]	3.408	2.268(4)	2.02(1)	0.0067(8)	-6.2(8)	2.521	2
25	0.6439	[2.0,2.5,0.0]	3.727	2.276(4)	2.044(9)	0.0054(9)	-7.1(7)	2.402	2
26	0.6437	[3.0,0.5,0.5]	3.346	2.261(4)	2.03(2)	0.009(8)	-5.9(8)	2.345	2
27	0.6409	[2.0,1.5,1.0]	3.761	2.275(5)	2.023(8)	0.0047(8)	-6.7(7)	2.392	2
28	0.6345	[3.0,1.0,0.5]	3.246	2.263(4)	2.02(2)	0.009(8)	-5.6(8)	2.601	2
29	0.6226	[2.5,1.5,1.0]	3.422	2.273(5)	2.06(1)	0.0096(8)	-8.2(7)	2.592	2
30	0.6218	[2.5,2.0,0.5]	3.558	2.272(5)	2.05(1)	0.0092(9)	-6.8(7)	2.663	2

Table S16 Detailed results for GAL4 (Povey et al.) The models included in the meta-analysis are given in bold. The best model together with the experimental data and the corresponding Fourier transforms are given in Fig. S17.

Rank	ABRA Score	Model [S, His, O]	χ^2	$R_{Sulphur}$	$R_{light\_ligands}$	$2\sigma^2$	Fermi-energy	BVS	Ox. State
1	**0.9218**	**[2.5,0.0,1.0,1.0]**	**0.869**	**2.3(3)**	**1.984(9)**	**0.0096(4)**	**-6.3(5)**	**1.8864**	**2**
2	**0.9203**	**[3.0,0.0,0.5,1.0]**	**0.871**	**2.293(3)**	**1.95(2)**	**0.012(4)**	**-5.3(5)**	**1.9904**	**2**
3	**0.9193**	**[3.0,0.0,1.0,1.0]**	**0.843**	**2.298(3)**	**1.965(1)**	**0.0122(4)**	**-5.6(4)**	**2.2038**	**2**
4	**0.9189**	**[2.5,0.5,0.5,1.0]**	**0.911**	**2.3(3)**	**2.0(1)**	**0.0096(4)**	**-6.3(5)**	**1.9105**	**2**
5	**0.9145**	**[3.5,0.0,0.0,1.0]**	**0.975**	**2.292(3)**	**0.0(0)**	**0.01429(6)**	**-5.4(5)**	**2.0275**	**2**
6	**0.9138**	**[2.5,1.0,0.0,1.0]**	**0.906**	**2.294(3)**	**1.99(1)**	**0.0093(4)**	**-5.2(5)**	**1.9922**	**2**
7	**0.9122**	**[2.5,1.0,0.5,1.0]**	**0.962**	**2.303(3)**	**2.01(8)**	**0.0101(5)**	**-6.3(5)**	**2.1472**	**2**
8	**0.9112**	**[2.5,0.5,1.0,1.0]**	**1.002**	**2.308(3)**	**2.013(9)**	**0.0105(5)**	**-7.2(5)**	**2.0800**	**2**
9	**0.9107**	**[2.5,0.0,1.5,1.0]**	**1.013**	**2.307(4)**	**2.003(8)**	**0.0107(5)**	**-7.0(5)**	**2.0592**	**2**
10	**0.9101**	**[3.0,0.5,0.0,1.0]**	**0.917**	**2.294(3)**	**1.98(2)**	**0.0119(4)**	**-5.5(5)**	**2.0120**	**2**
11	**0.9093**	**[2.5,1.5,0.0,1.0]**	**0.958**	**2.3(3)**	**2.009(8)**	**0.0097(4)**	**-5.7(5)**	**2.2035**	**2**
12	**0.9089**	**[3.0,0.5,0.5,1.0]**	**0.854**	**2.297(3)**	**1.97(1)**	**0.012(4)**	**-5.7(5)**	**2.2494**	**2**
13	0.8970	[2.0,1.0,0.5,1.0]	1.126	2.304(4)	2.023(8)	0.0072(5)	-6.6(6)	1.8374	2
14	0.8958	[2.0,1.5,0.0,1.0]	1.153	2.304(4)	2.032(9)	0.0073(5)	-6.6(6)	1.8605	2
15	0.8945	[3.5,0.0,0.5,1.0]	0.854	2.293(3)	1.93(2)	0.01427(6)	-5.1(4)	2.2935	2
16	0.8937	[2.5,0.0,0.5,1.0]	1.019	2.296(3)	1.97(2)	0.0096(4)	-6.1(6)	1.6763	2
17	0.8912	[2.0,0.0,1.5,1.0]	1.066	2.312(4)	2.022(7)	0.0079(5)	-8.1(6)	1.7327	2
18	0.8894	[3.0,0.0,0.0,1.0]	1.135	2.292(3)	0.0(0)	0.0122(4)	-5.6(5)	1.7379	2
19	0.8892	[2.0,0.5,1.0,1.0]	1.074	2.313(4)	2.036(8)	0.0078(5)	-8.4(6)	1.7460	2
20	0.8878	[2.5,0.5,0.0,1.0]	1.115	2.295(4)	2.0(2)	0.0096(4)	-5.9(7)	1.7051	2
21	0.8872	[4.0,0.0,0.0,1.0]	1.123	2.295(3)	0.0(0)	0.01429(6)	-5.5(4)	2.2985	2
22	0.8839	[3.0,0.0,1.5,1.0]	1.070	2.305(4)	1.989(9)	0.0133(5)	-6.4(5)	2.3722	2
23	0.8837	[3.0,0.5,1.0,1.0]	1.037	2.305(4)	1.999(1)	0.0131(5)	-6.5(5)	2.3977	2
24	0.8827	[3.5,0.5,0.0,1.0]	1.077	2.294(3)	1.98(2)	0.0143(4)	-5.4(5)	2.3000	2
25	0.8797	[2.0,1.0,0.0,1.0]	1.176	2.295(4)	2.01(1)	0.0067(4)	-5.5(6)	1.6720	2
26	0.8794	[3.0,1.0,0.5,1.0]	0.950	2.3(3)	1.991(9)	0.0125(5)	-5.5(5)	2.4812	2
27	0.8787	[2.0,0.0,1.0,1.0]	1.016	2.306(3)	2.01(9)	0.007(4)	-7.6(6)	1.5529	2
28	0.8778	[3.0,1.0,0.0,1.0]	0.816	2.29(3)	1.97(1)	0.0117(4)	-4.4(4)	2.3297	2
29	0.8763	[2.5,0.5,1.5,1.0]	1.298	2.313(4)	2.026(9)	0.0122(7)	-7.6(6)	2.2469	2
30	0.8761	[2.0,1.5,0.5,1.0]	1.272	2.318(4)	2.057(8)	0.009(7)	-8.5(6)	1.9631	2

Figure S2 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for *HPV* E7

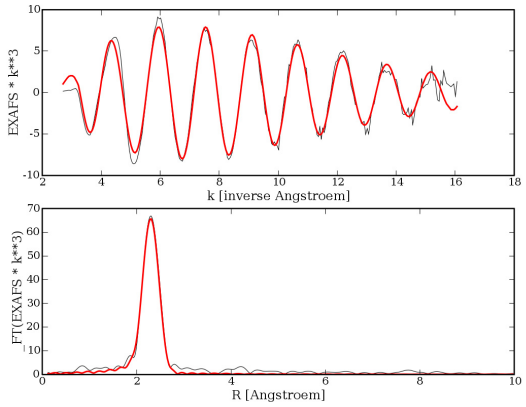

Figure S3 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for GCM

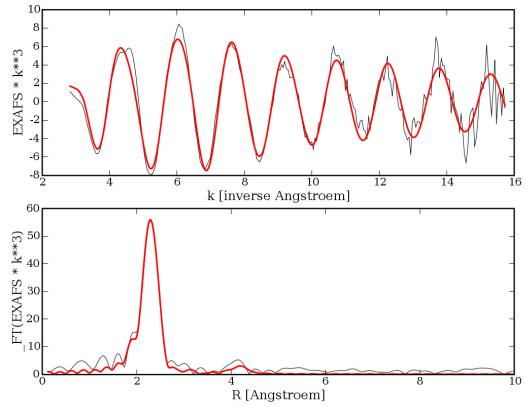

Figure S4 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for ZnF-UBP

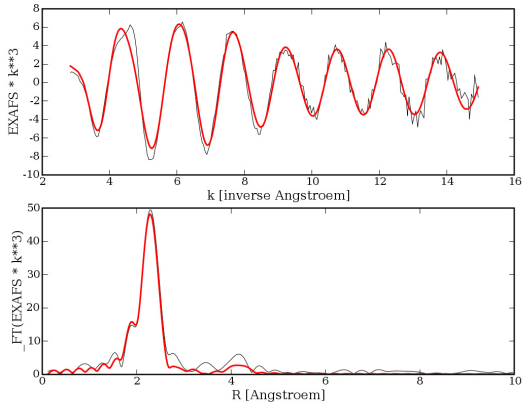

Figure S5 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for *Ec* ZiPD

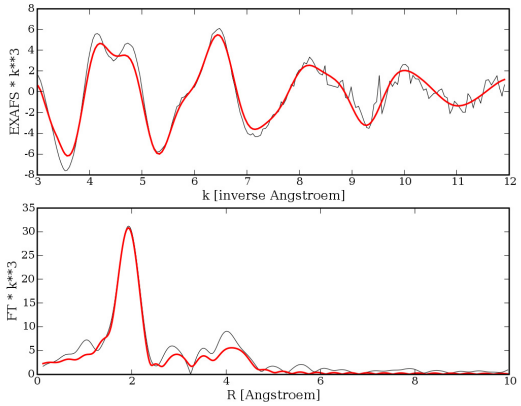

Figure S6 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for *At* Glx2-2

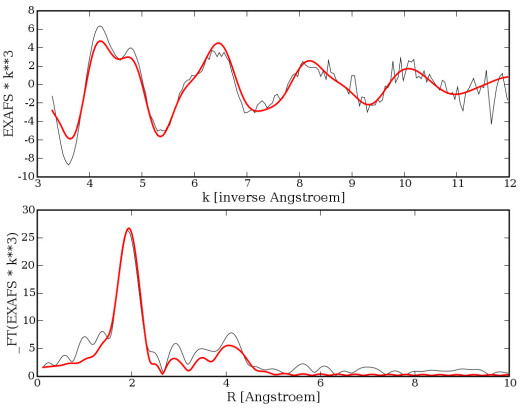

Figure S7 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for *Bc* bla

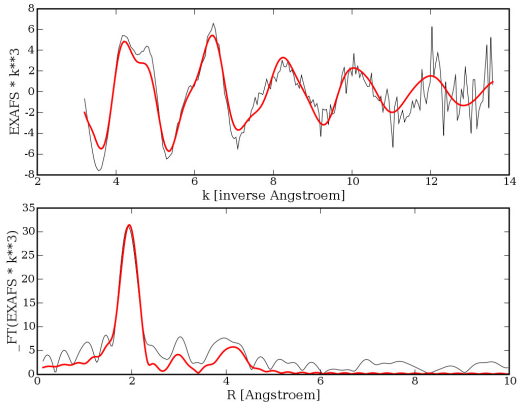

Figure S8 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Bis(acetato)bis(imidazol)zinc(II)

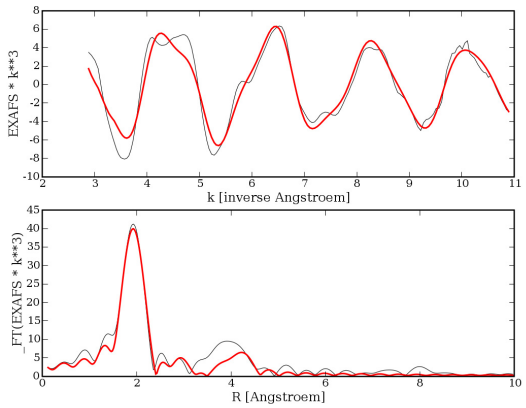

Figure S9 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Tetrakis(imidazole)zinc(II)-perchlorate

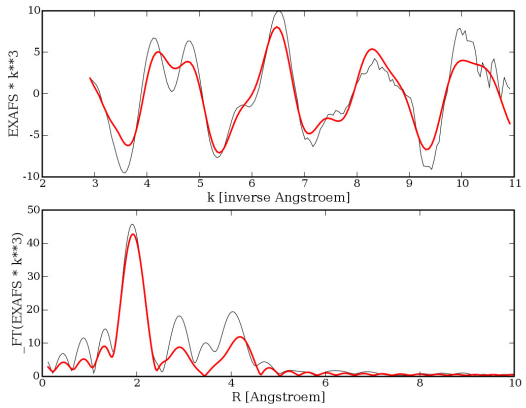

Figure S10 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Ss ABCE1

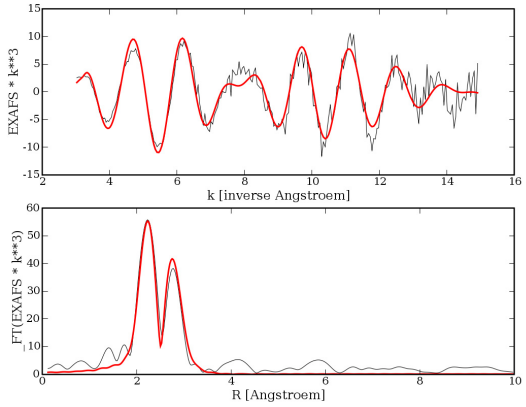

Figure S11 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Pa RM2-4ox

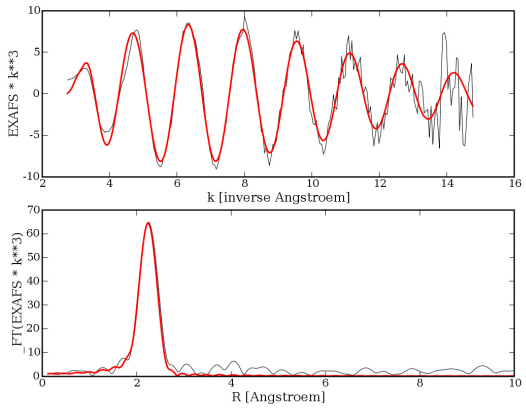

Figure S12 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Pa RM2-4red

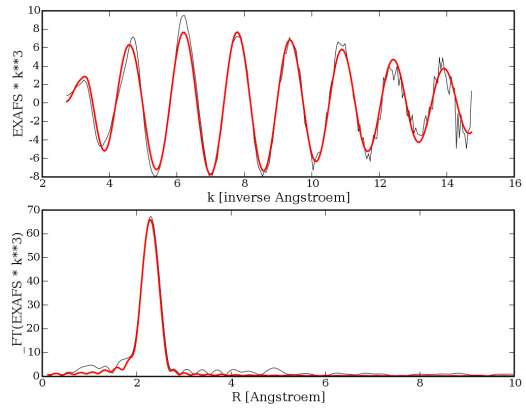

Figure S13 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Hs $TH1_{nat}$

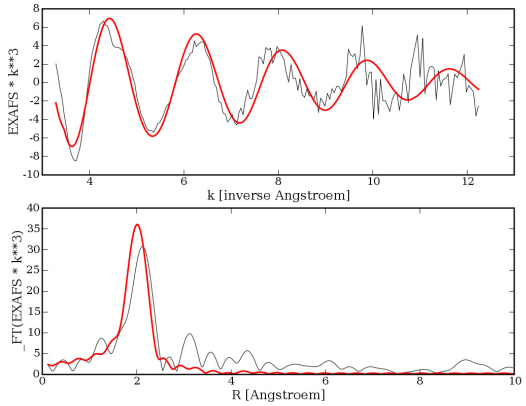

Figure S14 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Hs $TH1_{ox}$

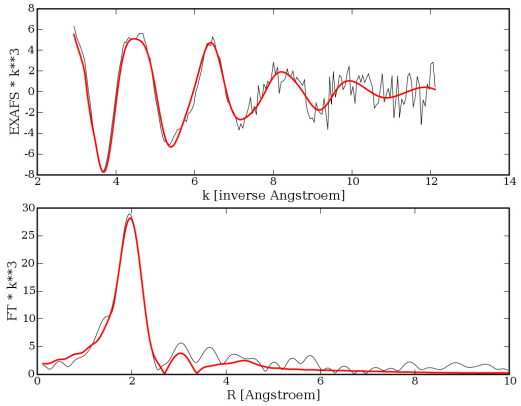

Figure S15 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for Fe-Pvd

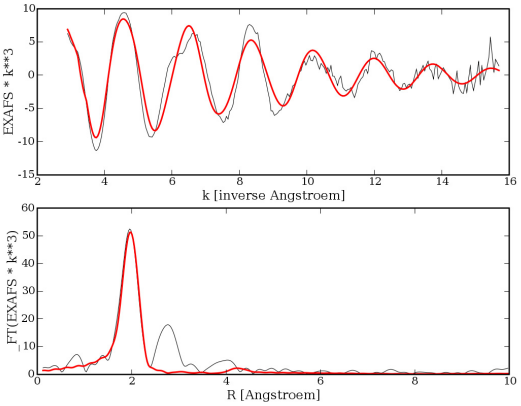

Figure S16 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for ALAD (Dent et. al)

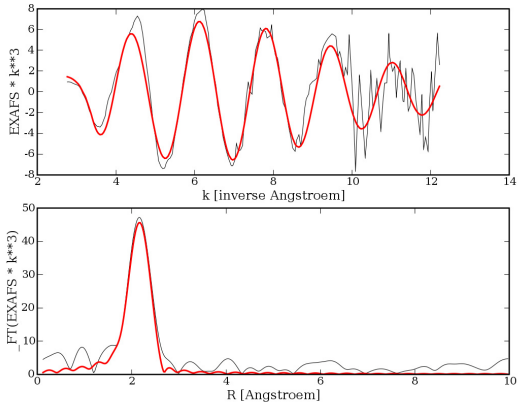

Figure S17 Best fit (red line) vs. original data (black line) in k-space (above) and backtransformed into R-space (below) for GAL4 (Povey et al.)