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# Comparison and evaluation of pair distribution functions, using a similarity measure based on cross-correlation functions - Supporting information

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Tables S1, S2, S3 and S4 provide an overview of structural changes as well as resulting $S_{12}^{\mathrm{PDF}}$, RMSCD and $R_{wp}^{\mathrm{PDF}}$ values for the four sets of 20 trial structures that deviate in only one lattice parameter.

Table S5 lists the similarity values $S_{12}^{\mathrm{PDF}}(l{=}0.5\ \text{Å})$ computed for different ranges of $r$ as well as the $S_{12}^{0,\mathrm{PDF}}$ (for the full range) of all trial structures of table 1 of the publication.

**Table S1**

Structural parameters and corresponding RMSCD, $S_{12}^{\mathrm{PDF}}$, $R_{wp}^{\mathrm{PDF}}$, $S_{12}^{0,\mathrm{PDF}}$ and $r_p$ values for the correct structure (R) and 20 trial structural models (A1-A20) of barbituric acid in space group $P\,2_1/c$ that exhibit the modification of the lattice parameter $a$.

| Structural model | $a$ / Å | $b$ / Å | $c$ / Å | $\beta$ / ° | RMSCD / Å | $R_{wp}^{\mathrm{PDF}}$ / % | $S_{12}^{\mathrm{PDF}}$ | $S_{12}^{0,\mathrm{PDF}}$ | $r_p$ |
|---|---|---|---|---|---|---|---|---|---|
| R | 4.8346 | 8.9153 | 12.4192 | 107.729 | 0.000 | 21.486 | 0.9990 | 0.9972 | 0.9769 |
| A1 | 4.9346 | 8.9153 | 12.4192 | 107.729 | 0.071 | 33.489 | 0.9966 | 0.9938 | 0.9438 |
| A2 | 5.0346 | 8.9153 | 12.4192 | 107.729 | 0.143 | 50.983 | 0.9911 | 0.9854 | 0.8696 |
| A3 | 5.1346 | 8.9153 | 12.4192 | 107.729 | 0.215 | 63.060 | 0.9847 | 0.9768 | 0.7990 |
| A4 | 5.2346 | 8.9153 | 12.4192 | 107.729 | 0.288 | 70.297 | 0.9795 | 0.9711 | 0.7460 |
| A5 | 5.3346 | 8.9153 | 12.4192 | 107.729 | 0.362 | 77.257 | 0.9751 | 0.9663 | 0.6887 |
| A6 | 5.4346 | 8.9153 | 12.4192 | 107.729 | 0.437 | 84.035 | 0.9708 | 0.9611 | 0.6291 |
| A7 | 5.5346 | 8.9153 | 12.4192 | 107.729 | 0.513 | 87.225 | 0.9678 | 0.9584 | 0.5966 |
| A8 | 5.6346 | 8.9153 | 12.4192 | 107.729 | 0.589 | 86.203 | 0.9671 | 0.9592 | 0.6003 |
| A9 | 5.7346 | 8.9153 | 12.4192 | 107.729 | 0.666 | 84.494 | 0.9665 | 0.9604 | 0.6135 |
| A10 | 5.8346 | 8.9153 | 12.4192 | 107.729 | 0.743 | 86.124 | 0.9642 | 0.9582 | 0.6012 |
| A11 | 5.9346 | 8.9153 | 12.4192 | 107.729 | 0.821 | 89.113 | 0.9610 | 0.9542 | 0.5785 |
| A12 | 6.0346 | 8.9153 | 12.4192 | 107.729 | 0.900 | 91.152 | 0.9583 | 0.9509 | 0.5593 |
| A13 | 6.1346 | 8.9153 | 12.4192 | 107.729 | 0.979 | 93.100 | 0.9556 | 0.9477 | 0.5361 |
| A14 | 6.2346 | 8.9153 | 12.4192 | 107.729 | 1.060 | 94.340 | 0.9534 | 0.9451 | 0.5206 |
| A15 | 6.3346 | 8.9153 | 12.4192 | 107.729 | 1.140 | 94.476 | 0.9518 | 0.9437 | 0.5186 |
| A16 | 6.4346 | 8.9153 | 12.4192 | 107.729 | 1.220 | 94.027 | 0.9505 | 0.9429 | 0.5246 |
| A17 | 6.5346 | 8.9153 | 12.4192 | 107.729 | 1.300 | 93.397 | 0.9496 | 0.9424 | 0.5324 |
| A18 | 6.6346 | 8.9153 | 12.4192 | 107.729 | 1.380 | 93.541 | 0.9512 | 0.9442 | 0.5308 |
| A19 | 6.7346 | 8.9153 | 12.4192 | 107.729 | 1.470 | 93.812 | 0.9539 | 0.9471 | 0.5286 |
| A20 | 6.8346 | 8.9153 | 12.4192 | 107.729 | 1.550 | 92.932 | 0.9558 | 0.9495 | 0.5420 |

## Table S2

Structural parameters and corresponding RMSCD, $S_{12}^{\mathrm{PDF}}$ and $R_{wp}^{\mathrm{PDF}}$ values for the correct structure (R) and 20 trial structural models (B1-B20) of barbituric acid in space group $P\,2_1/c$ that exhibit the modification of the lattice parameter $b$.

| Structural model | $a$ / Å | $b$ / Å | $c$ / Å | $\beta$ / ° | RMSCD / Å | $R_{wp}^{\mathrm{PDF}}$ / % | $S_{12}^{\mathrm{PDF}}$ |
|---|---|---|---|---|---|---|---|
| R | 4.8346 | 8.9153 | 12.4192 | 107.729 | 0.000 | 21.486 | 0.998 |
| B1 | 4.8346 | 9.0153 | 12.4192 | 107.729 | 0.021 | 25.737 | 0.998 |
| B2 | 4.8346 | 9.1153 | 12.4192 | 107.729 | 0.043 | 35.301 | 0.996 |
| B3 | 4.8346 | 9.2153 | 12.4192 | 107.729 | 0.065 | 43.798 | 0.994 |
| B4 | 4.8346 | 9.3153 | 12.4192 | 107.729 | 0.086 | 50.083 | 0.992 |
| B5 | 4.8346 | 9.4153 | 12.4192 | 107.729 | 0.109 | 54.650 | 0.991 |
| B6 | 4.8346 | 9.5153 | 12.4192 | 107.729 | 0.130 | 57.923 | 0.990 |
| B7 | 4.8346 | 9.6153 | 12.4192 | 107.729 | 0.152 | 60.102 | 0.989 |
| B8 | 4.8346 | 9.7153 | 12.4192 | 107.729 | 0.174 | 61.950 | 0.988 |
| B9 | 4.8346 | 9.8153 | 12.4192 | 107.729 | 0.196 | 63.938 | 0.987 |
| B10 | 4.8346 | 9.9153 | 12.4192 | 107.729 | 0.218 | 65.590 | 0.986 |
| B11 | 4.8346 | 10.0153 | 12.4192 | 107.729 | 0.240 | 66.340 | 0.985 |
| B12 | 4.8346 | 10.1153 | 12.4192 | 107.729 | 0.262 | 66.707 | 0.985 |
| B13 | 4.8346 | 10.2153 | 12.4192 | 107.729 | 0.284 | 67.660 | 0.984 |
| B14 | 4.8346 | 10.3153 | 12.4192 | 107.729 | 0.307 | 69.262 | 0.984 |
| B15 | 4.8346 | 10.4153 | 12.4192 | 107.729 | 0.329 | 70.962 | 0.983 |
| B16 | 4.8346 | 10.5153 | 12.4192 | 107.729 | 0.351 | 72.422 | 0.982 |
| B17 | 4.8346 | 10.6153 | 12.4192 | 107.729 | 0.373 | 73.460 | 0.981 |
| B18 | 4.8346 | 10.7153 | 12.4192 | 107.729 | 0.396 | 73.857 | 0.981 |
| B19 | 4.8346 | 10.8153 | 12.4192 | 107.729 | 0.418 | 73.447 | 0.980 |
| B20 | 4.8346 | 10.9153 | 12.4192 | 107.729 | 0.441 | 72.560 | 0.980 |

## Table S3

Structural parameters and corresponding RMSCD, $S_{12}^{\mathrm{PDF}}$ and $R_{wp}^{\mathrm{PDF}}$ values for the correct structure (R) and 20 trial structural models (C1-C20) of barbituric acid in space group $P\,2_1/c$ that exhibit the modification of the lattice parameter $c$.

| Structural model | $a$ / Å | $b$ / Å | $c$ / Å | $\beta$ / ° | RMSCD / Å | $R_{wp}^{\mathrm{PDF}}$ / % | $S_{12}^{\mathrm{PDF}}$ |
|---|---|---|---|---|---|---|---|
| R | 4.8346 | 8.9153 | 12.4192 | 107.729 | 0.000 | 21.486 | 0.998 |
| C1 | 4.8346 | 8.9153 | 12.3192 | 107.729 | 0.035 | 24.552 | 0.998 |
| C2 | 4.8346 | 8.9153 | 12.2192 | 107.729 | 0.070 | 30.395 | 0.997 |
| C3 | 4.8346 | 8.9153 | 12.1192 | 107.729 | 0.105 | 36.735 | 0.995 |
| C4 | 4.8346 | 8.9153 | 12.0192 | 107.729 | 0.141 | 42.680 | 0.994 |
| C5 | 4.8346 | 8.9153 | 11.9192 | 107.729 | 0.176 | 47.957 | 0.992 |
| C6 | 4.8346 | 8.9153 | 11.8192 | 107.729 | 0.211 | 52.683 | 0.989 |
| C7 | 4.8346 | 8.9153 | 11.7192 | 107.729 | 0.246 | 57.067 | 0.987 |
| C8 | 4.8346 | 8.9153 | 11.6192 | 107.729 | 0.280 | 61.213 | 0.985 |
| C9 | 4.8346 | 8.9153 | 11.5192 | 107.729 | 0.315 | 65.089 | 0.983 |
| C10 | 4.8346 | 8.9153 | 11.4192 | 107.729 | 0.350 | 68.473 | 0.981 |
| C11 | 4.8346 | 8.9153 | 11.3192 | 107.729 | 0.385 | 70.994 | 0.980 |
| C12 | 4.8346 | 8.9153 | 11.2192 | 107.729 | 0.420 | 72.664 | 0.979 |
| C13 | 4.8346 | 8.9153 | 11.1192 | 107.729 | 0.454 | 73.947 | 0.978 |
| C14 | 4.8346 | 8.9153 | 11.0192 | 107.729 | 0.489 | 75.306 | 0.977 |
| C15 | 4.8346 | 8.9153 | 10.9192 | 107.729 | 0.523 | 76.854 | 0.977 |
| C16 | 4.8346 | 8.9153 | 10.8192 | 107.729 | 0.558 | 78.292 | 0.976 |
| C17 | 4.8346 | 8.9153 | 10.7192 | 107.729 | 0.592 | 79.237 | 0.975 |
| C18 | 4.8346 | 8.9153 | 10.6192 | 107.729 | 0.627 | 79.527 | 0.975 |
| C19 | 4.8346 | 8.9153 | 10.4192 | 107.729 | 0.661 | 79.318 | 0.975 |
| C20 | 4.8346 | 8.9153 | 10.4192 | 107.729 | 0.695 | 78.778 | 0.975 |

**Table S4**

Structural parameters and corresponding RMSCD, $S_{12}^{\mathrm{PDF}}$ and $R_{wp}^{\mathrm{PDF}}$ values for the correct structure (R) and 20 trial structural models (Beta1-Beta20) of barbituric acid in space group $P\,2_1/c$ that exhibit the modification of the lattice parameter $\beta$.

| Structural model | $a$ / Å | $b$ / Å | $c$ / Å | $\beta$ / ° | RMSCD / Å | $R_{wp}^{\mathrm{PDF}}$ / % | $S_{12}^{\mathrm{PDF}}$ |
|---|---|---|---|---|---|---|---|
| R | 4.8346 | 8.9153 | 12.4192 | 107.729 | 0.000 | 21.486 | 0.998 |
| Beta1 | 4.8346 | 8.9153 | 12.4192 | 108.229 | 0.028 | 24.464 | 0.998 |
| Beta2 | 4.8346 | 8.9153 | 12.4192 | 108.729 | 0.057 | 30.162 | 0.997 |
| Beta3 | 4.8346 | 8.9153 | 12.4192 | 109.229 | 0.085 | 36.468 | 0.996 |
| Beta4 | 4.8346 | 8.9153 | 12.4192 | 109.729 | 0.114 | 42.180 | 0.994 |
| Beta5 | 4.8346 | 8.9153 | 12.4192 | 110.229 | 0.142 | 47.096 | 0.992 |
| Beta6 | 4.8346 | 8.9153 | 12.4192 | 110.729 | 0.171 | 51.354 | 0.990 |
| Beta7 | 4.8346 | 8.9153 | 12.4192 | 111.229 | 0.199 | 55.162 | 0.989 |
| Beta8 | 4.8346 | 8.9153 | 12.4192 | 111.729 | 0.227 | 58.563 | 0.987 |
| Beta9 | 4.8346 | 8.9153 | 12.4192 | 112.229 | 0.256 | 61.533 | 0.986 |
| Beta10 | 4.8346 | 8.9153 | 12.4192 | 112.729 | 0.284 | 64.060 | 0.985 |
| Beta11 | 4.8346 | 8.9153 | 12.4192 | 113.229 | 0.312 | 66.146 | 0.984 |
| Beta12 | 4.8346 | 8.9153 | 12.4192 | 113.729 | 0.340 | 67.783 | 0.983 |
| Beta13 | 4.8346 | 8.9153 | 12.4192 | 114.229 | 0.368 | 68.993 | 0.982 |
| Beta14 | 4.8346 | 8.9153 | 12.4192 | 114.729 | 0.397 | 69.972 | 0.981 |
| Beta15 | 4.8346 | 8.9153 | 12.4192 | 115.229 | 0.425 | 71.009 | 0.981 |
| Beta16 | 4.8346 | 8.9153 | 12.4192 | 115.729 | 0.452 | 72.296 | 0.980 |
| Beta17 | 4.8346 | 8.9153 | 12.4192 | 116.229 | 0.480 | 73.920 | 0.979 |
| Beta18 | 4.8346 | 8.9153 | 12.4192 | 116.729 | 0.508 | 75.888 | 0.978 |
| Beta19 | 4.8346 | 8.9153 | 12.4192 | 117.229 | 0.523 | 78.039 | 0.977 |
| Beta20 | 4.8346 | 8.9153 | 12.4192 | 117.729 | 0.564 | 80.066 | 0.975 |

**Table S5**

Comparison of the structural models of the tables 1 and 2 of the publication to the experimental PDF of barbituric acid: Similarity values $S_{12}^{PDF}(l=0.5\ Å)$ computed for different ranges of $r$ and $S_{12}^{0,PDF}$ for the full range.

| Structural model | $S_{12}^{PDF}$ | $S_{12}^{PDF}$ | $S_{12}^{PDF}$ | $S_{12}^{PDF}$ | $S_{12}^{0,PDF}$ |
|---|---|---|---|---|---|
| Range: | 1.1-3.3 Å | 3.3-6 Å | 6-30 Å | 1.1-30 Å | 1.1-30 Å |
| R | 0.9972 | 0.9992 | 0.9995 | 0.9990 | 0.9972 |
| A1 | 0.9971 | 0.9992 | 0.9967 | 0.9966 | 0.9938 |
| A5 | 0.9932 | 0.9719 | 0.9756 | 0.9751 | 0.9663 |
| A10 | 0.9898 | 0.9253 | 0.9713 | 0.9642 | 0.9582 |
| A15 | 0.9870 | 0.8786 | 0.9656 | 0.9518 | 0.9437 |
| A20 | 0.9854 | 0.8697 | 0.9727 | 0.9558 | 0.9495 |
| B1 | 0.9972 | 0.9990 | 0.9987 | 0.9983 | 0.9962 |
| B5 | 0.9972 | 0.9943 | 0.9909 | 0.9914 | 0.9849 |
| B10 | 0.9963 | 0.9873 | 0.9862 | 0.9866 | 0.9794 |
| B15 | 0.9945 | 0.9837 | 0.9828 | 0.9831 | 0.9763 |
| B20 | 0.9933 | 0.9794 | 0.9813 | 0.9810 | 0.9749 |
| C1 | 0.9969 | 0.9992 | 0.9988 | 0.9984 | 0.9962 |
| C5 | 0.9979 | 0.9986 | 0.9910 | 0.9921 | 0.9879 |
| C10 | 0.9975 | 0.9976 | 0.9784 | 0.9818 | 0.9764 |
| C15 | 0.9962 | 0.9953 | 0.9731 | 0.9770 | 0.9710 |
| C20 | 0.9948 | 0.9929 | 0.9721 | 0.9759 | 0.9696 |
| Beta1 | 0.9971 | 0.9989 | 0.9990 | 0.9986 | 0.9964 |
| Beta5 | 0.9961 | 0.9966 | 0.9923 | 0.9927 | 0.9876 |
| Beta10 | 0.9962 | 0.9930 | 0.9835 | 0.9851 | 0.9789 |
| Beta15 | 0.9951 | 0.9934 | 0.9790 | 0.9813 | 0.9761 |
| Beta20 | 0.9962 | 0.9926 | 0.9722 | 0.9758 | 0.9702 |
| P1 | 0.9978 | 0.9776 | 0.9898 | 0.9882 | 0.9830 |
| P2 | 0.9963 | 0.9721 | 0.9861 | 0.9841 | 0.9787 |
| P3 | 0.9788 | 0.9890 | 0.9831 | 0.9796 | 0.9718 |
| P4 | 0.9640 | 0.9830 | 0.9740 | 0.9620 | 0.9550 |
| P5 | 0.9526 | 0.9844 | 0.9633 | 0.9428 | 0.9380 |
| O1 | 0.9949 | 0.9779 | 0.9901 | 0.9881 | 0.9818 |
| O2 | 0.9978 | 0.9743 | 0.9862 | 0.9848 | 0.9776 |
| O3 | 0.9885 | 0.9712 | 0.9799 | 0.9773 | 0.9711 |
| O4 | 0.9884 | 0.9648 | 0.9755 | 0.9725 | 0.9658 |
| O5 | 0.9894 | 0.9581 | 0.9706 | 0.9671 | 0.9596 |
| PO1 | 0.9926 | 0.9823 | 0.9912 | 0.9905 | 0.9857 |
| PO2 | 0.9837 | 0.9957 | 0.9711 | 0.9804 | 0.9733 |
| PO3 | 0.9813 | 0.9939 | 0.9831 | 0.9644 | 0.9548 |
| PO4 | 0.9856 | 0.9708 | 0.9630 | 0.9544 | 0.9434 |
| PO5 | 0.9897 | 0.9442 | 0.9458 | 0.9331 | 0.9181 |
| W | 0.9794 | 0.8419 | 0.9393 | 0.8947 | 0.8818 |