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Electronic Supplementary Information for:

^{1}H Isotropic Chemical Shift Metrics for NMR Crystallography of Powered Molecular Organics

Fatemeh Zakeri and Cory M. Widdifield*

Department of Chemistry and Biochemistry
University of Regina
3737 Wascana Parkway, Regina, Saskatchewan, Canada
S4S 0A2

*Author to whom correspondence is to be addressed. E-mail: cory.widdifield@uregina.ca

Tel.: +1 306-585-4550

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General Notes, and Equations Used to Calculate Statistical Parameters

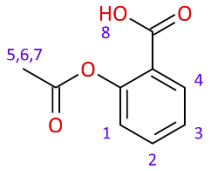
Notes: All experimentally determined ^{1}H isotropic chemical shifts can be found in the Excel files ('Summary_Outputs_1Param_Map.xlsx' and 'Summary_Outputs_2Param_Map.xlsx') included with this Electronic Supplementary Information. Additional details pertaining to the thymol computations are summarized in the Excel spreadsheets: 'Thymol_RMSDs_one-parameter_Final.xlsx' and 'Thymol_RMSDs_two-parameter_Final.xlsx'.

Although we used a standard equation to calculate the root-mean-squared deviation (RMSD) values reported in this account, we provide the equation used below as a convenience to the reader:

Root-Mean-Squared Deviation (RMSD)

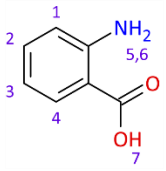
$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N}\left(\delta_{\text{iso,calc.}}^{i} - \delta_{\text{iso,expt.}}^{i}\right)^{2}}{N}}. \qquad [\mathbf{S1}]$$

In the above expression, $\delta_{\text{iso,calc.}}^{i}$ refers to the computationally predicted isotropic ^{1}H chemical shift value for the *i*-th hydrogen atom in a crystal structure, $\delta_{\text{iso,expt.}}^{i}$ is the experimentally measured isotropic ^{1}H chemical shift value that has been assigned to the *i*-th hydrogen atom, and where N crystallographically unique hydrogen atoms are being considered in a given crystal structure.



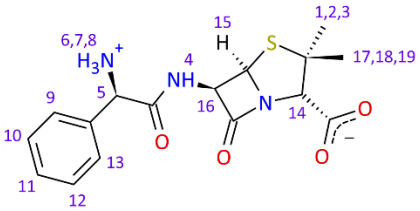
Aspirin

ACSALA07 (Form I)



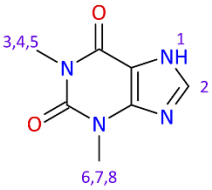
Anthranilic Acid

AMBACO10 (Form II)



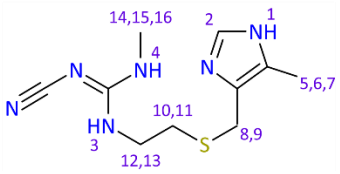
Ampicillin

AMCILL



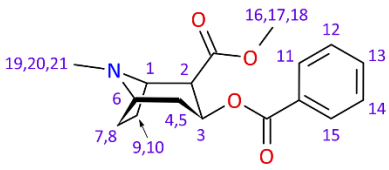
Theophylline

BAPLOT01 (Form II)



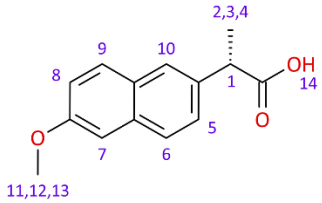
Cimetidine

CIMETD (Form A)



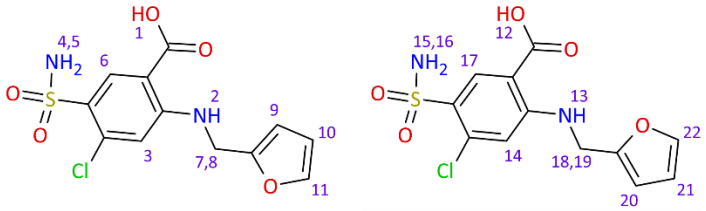
Cocaine

COCAIN10



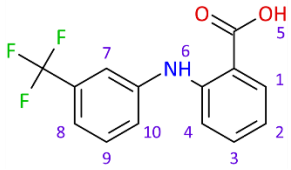
(S)-Naproxen

COYRUD13



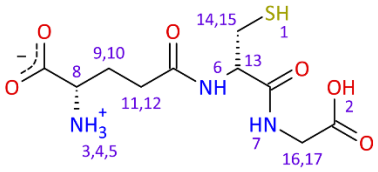
Furosemide

FURSEM01 (Form 1)



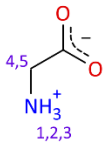
Flufenamic Acid

FPAMCA11 (Form I)



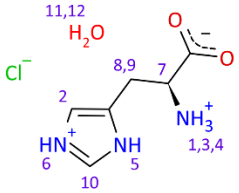
Glutathione

GLUTAS07 (Form I)



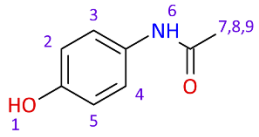
Glycine

GLYCIN28 (Form α)



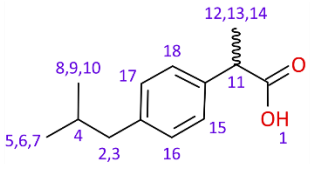
L-Histidine · HCl · H_2O

HISTCM01



Paracetamol

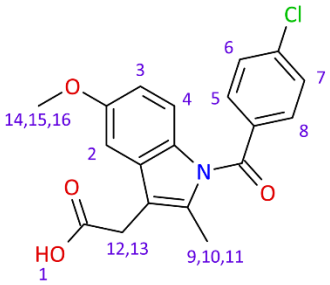
HXACAN35 (Form I)



Ibuprofen (R,S racemate)

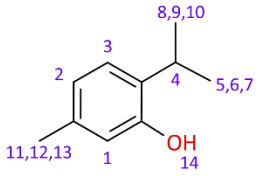
IBPRAC (Form 1)

Scheme S1. Building blocks, CSD refcodes, and numerical hydrogen labels for 14 of the 24 compounds considered in this study. For the remaining 10, please see **Scheme S2**.



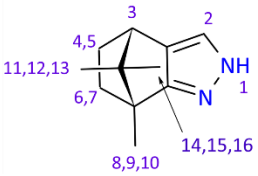
Indomethacin

INDMET (Form γ)



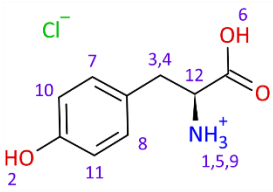
Thymol

IPMEPL



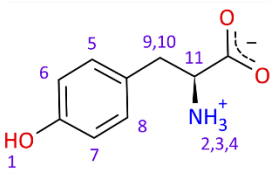
Campho(2,3-c)pyrazole

LABHEB



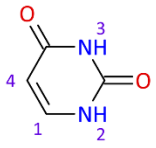
L-Tyrosine hydrochloride

LTYRHC10



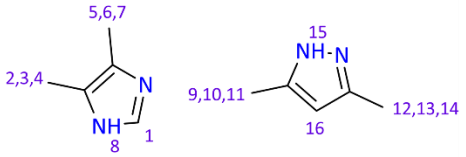
L-Tyrosine

LTYROS10



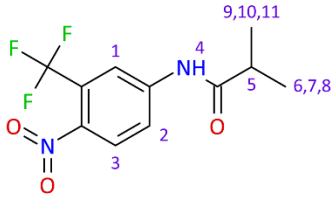
Uracil

URACIL



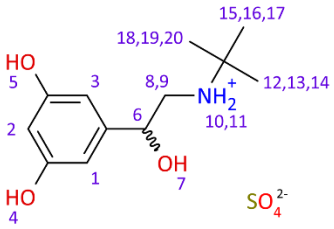
Dimethyl Pyrazole, Dimethyl Imidazole Co-Crystal

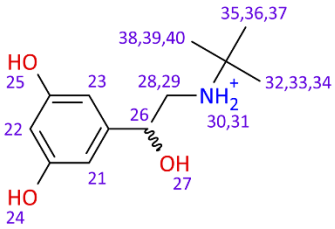
VOSREC



Flutamide

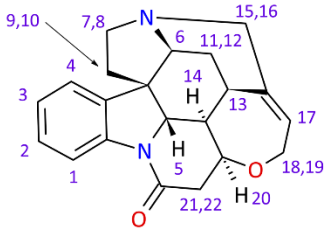
WEZCOT





Terbutaline hemisulfate (R,S Racemate)

ZIVKAQ (Form B)



Strychnine

ZZZUEE01

Scheme S2. Building blocks, CSD refcodes, and numerical hydrogen labels for 10 of the 24 compounds considered in this study. For the remaining 14, please see **Scheme S1**. **Note:** for LABHEB, the crystal structure is such that there are 6 crystallographically unique molecules (i.e., $Z' = 6$). For a more fulsome disclosure related to this crystal structure, please see the Excel spreadsheet (Summary_Outputs_1Param_Map.xlsx).

Table S1. $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD Values for 8 Different E_{cut} Values (2-param.)[a]

CSD Refcode	90 Ry[b]	55 Ry	45 Ry	35 Ry	25 Ry	15 Ry	10 Ry	5 Ry
ACSALA07	0.340	0.335	0.335	0.352	0.659	1.286	1.157	1.578
AMBACO10	0.400	0.401	0.398	0.403	0.446	0.651	0.589	0.445
AMCILL	0.127	0.128	0.128	0.125	0.151	0.562	0.493	1.829
BAPLOT01	0.207	0.206	0.198	0.204	0.294	0.371	0.176	0.277
CIMETD	0.536	0.536	0.537	0.538	0.531	0.595	0.814	1.785
COCAIN10	0.237	0.237	0.236	0.235	0.240	0.375	0.609	1.134
COYRUD13	0.344	0.342	0.343	0.355	0.485	0.587	1.146	0.940
FPAMCA11	0.163	0.161	0.160	0.156	0.207	0.635	0.385	1.085
FURSEM01	0.386	0.375	0.375	0.381	0.502	0.858	0.805	1.121
GLUTAS07	0.232	0.232	0.235	0.232	0.316	0.471	0.450	1.881
GLYCIN28	0.068	0.071	0.070	0.067	0.111	0.231	0.378	0.052
HISTCM01	0.147	0.142	0.141	0.176	0.561	1.207	0.308	1.147
HXACAN35	0.113	0.108	0.105	0.133	0.425	0.962	0.781	1.740
IBPRAC	0.213	0.209	0.209	0.230	0.472	1.130	1.104	1.729
INDMET	0.262	0.257	0.255	0.274	0.502	1.037	0.928	1.287
IPMEPL	0.082	0.086	0.088	0.083	0.409	0.900	0.346	1.285
LABHEB	0.231	0.231	0.231	0.231	0.245	0.265	0.345	1.822
LTYRHC10	0.236	0.235	0.238	0.248	0.443	1.052	1.056	0.696
LTYROS10	0.187	0.185	0.186	0.204	0.370	0.503	0.495	0.806
URACIL	0.094	0.093	0.094	0.088	0.052	0.265	0.290	1.821
VOSREC	0.348	0.347	0.347	0.347	0.368	0.419	0.373	2.302
WEZCOT	0.278	0.276	0.273	0.272	0.328	0.492	0.511	1.558
ZIVKAQ	0.472	0.471	0.470	0.468	0.632	1.069	1.017	1.398
ZZZUEE01	0.518	0.517	0.518	0.520	0.527	0.624	0.728	1.153
Avg. ^{1}H RMSD / ppm	0.259	0.258	0.257	0.263	0.386	0.689	0.637	1.286
***s*(^{1}H RMSD) / ppm**	0.134	0.134	0.134	0.133	0.160	0.321	0.306	0.558

[a] All numerical values in this Table correspond to $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD values, in ppm. Here, 'Structure-dependent' k-point grids were used. The k-point grids used for each crystal structure are provided in the Excel spreadsheet ('Summary_Outputs_2Param_Map.xlsx') that forms part of the Electronic Supplementary Information.

[b] Excepting the first column, in this row the E_{cut} value used is indicated.

Table S2. $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD Values for 8 Different E_{cut} Values (2-param., $1 \times 1 \times 1$ grid)[a]

CSD Refcode	90 Ry[b]	55 Ry	45 Ry	35 Ry	25 Ry	15 Ry	10 Ry	5 Ry
ACSALA07	0.310	0.308	0.308	0.321	0.591	1.182	1.259	1.568
AMBACO10	0.473	0.474	0.471	0.474	0.503	0.555	0.431	0.342
AMCILL	0.266	0.266	0.266	0.265	0.306	0.629	0.528	2.379
BAPLOT01	0.316	0.313	0.312	0.311	0.388	0.516	0.586	1.160
CIMETD	0.568	0.570	0.569	0.569	0.568	0.612	0.944	1.854
COCAIN10	0.246	0.244	0.245	0.244	0.251	0.445	0.756	1.395
COYRUD13	0.386	0.383	0.383	0.391	0.463	0.548	0.865	1.993
FPAMCA11	0.162	0.163	0.161	0.160	0.211	0.578	0.443	1.128
FURSEM01	0.390	0.387	0.383	0.386	0.509	0.853	0.756	1.152
GLUTAS07	0.562	0.563	0.564	0.563	0.610	0.688	1.070	1.990
GLYCIN28	0.028	0.032	0.028	0.026	0.025	0.055	0.031	0.695
HISTCM01	0.207	0.204	0.202	0.230	0.585	1.225	0.498	0.510
HXACAN35	0.449	0.445	0.443	0.471	0.764	1.232	1.182	1.792
IBPRAC	0.241	0.238	0.238	0.258	0.506	1.192	1.168	1.777
INDMET	0.275	0.272	0.269	0.286	0.531	1.060	1.074	1.554
IPMEPL	0.096	0.095	0.094	0.102	0.424	0.955	0.377	1.597
LABHEB	0.228	0.229	0.229	0.229	0.241	0.264	0.347	1.805
LTYRHC10	0.823	0.826	0.827	0.818	0.801	1.225	1.634	2.531
LTYROS10	0.406	0.406	0.407	0.414	0.505	0.715	1.302	1.681
URACIL	0.041	0.038	0.039	0.052	0.128	0.350	1.225	2.145
VOSREC	0.331	0.326	0.324	0.329	0.384	0.590	0.639	2.320
WEZCOT	0.223	0.221	0.222	0.216	0.200	0.290	0.479	1.389
ZIVKAQ	0.464	0.462	0.462	0.462	0.642	1.095	1.308	1.439
ZZZUEE01	0.512	0.513	0.512	0.514	0.520	0.614	0.716	1.271
Avg. ^{1}H RMSD / ppm	0.333	0.332	0.332	0.337	0.444	0.728	0.817	1.561
***s*(^{1}H RMSD) / ppm**	0.183	0.183	0.184	0.182	0.195	0.346	0.398	0.558

[a] All numerical values in this Table correspond to $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD values, in ppm. Here, $1 \times 1 \times 1$ k-point grids were used.
[b] Excepting the first column, in this row the E_{cut} value used is indicated.

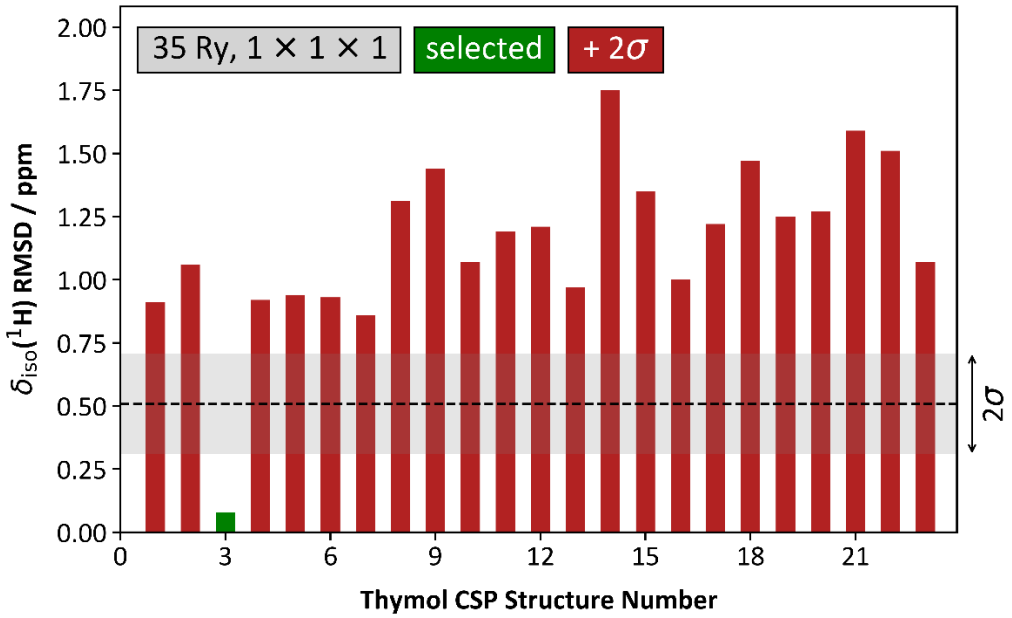


Figure S1. Structure selection process for 23 CSP-generated crystal structures of thymol using a one-parameter linear mapping, a 1 × 1 × 1 k-point grid, and $E_{\mathrm{cut}} = 35$ Ry. The $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD metric is provided as a 'grey band' and conforms to the average values and standard deviations provided in **Table 3**. The coloring scheme of the bars is unchanged from the main paper.

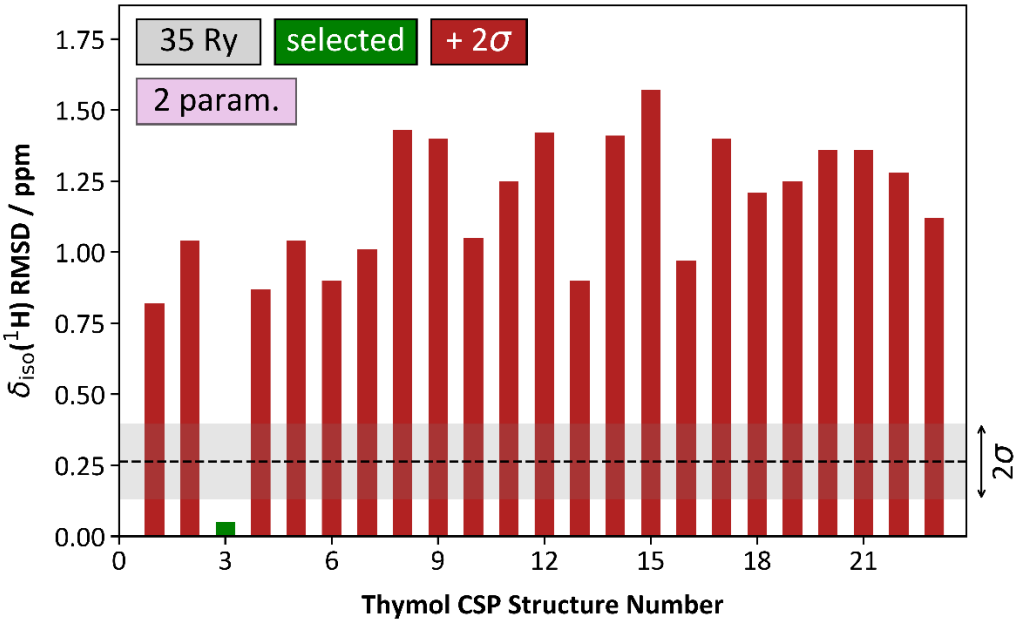


Figure S2. Structure selection process for 23 CSP-generated crystal structures of thymol using a two-parameter linear mapping, 'structure-dependent' k-point grids, and $E_{\mathrm{cut}} = 35$ Ry. The $\delta_{\mathrm{iso}}(^1\mathrm{H})$ RMSD metric is provided as a 'grey band' and conforms to the average values and standard deviations provided in **Table S1**. The coloring scheme of the bars is unchanged from the main paper.

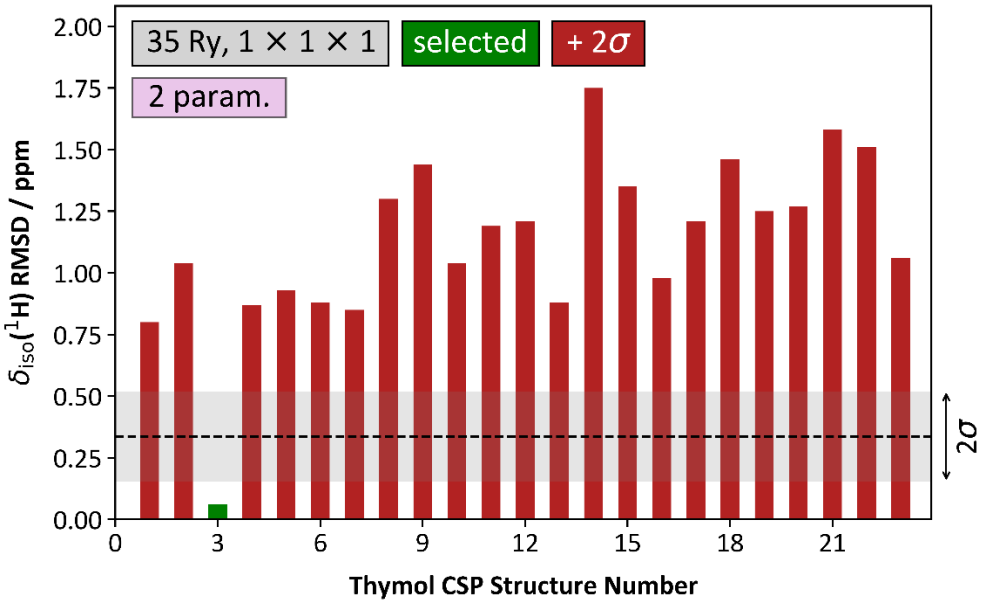


Figure S3. Structure selection process for 23 CSP-generated crystal structures of thymol using a two-parameter linear mapping, a 1 × 1 × 1 k-point grid, and $E_{\mathrm{cut}} = 35$ Ry. The $\delta_{\mathrm{iso}}(^{1}\mathrm{H})$ RMSD metric is provided as a 'grey band' and conforms to the average values and standard deviations provided in **Table S2**. The coloring scheme of the bars is unchanged from the main paper.