Supporting Information

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NMR refined coordinates

Cimetidine (CIMETD03)

a = 10.7092, b = 18.8262 c = 6.8266 α = 90.0, β = 111.306, γ = 90.0

H1 H 0.37691 0.31269 -0.29632
H2 H 0.17699 0.27738 -0.20399
H3 H 0.12004 0.03622 0.38419
H4 H 0.14167 0.13476 -0.03176
H5 H 0.64168 0.26444 -0.14288
H6 H 0.57263 0.21321 -0.36333
H7 H 0.64811 0.17287 -0.136128
H8 H 0.39652 0.05110 -0.049987
H9 H 0.31799 0.15084 0.28294
H10 H 0.38586 0.10259 0.50901
H11 H 0.29745 -0.00286 0.30659
H12 H 0.24338 0.03913 0.08010
H13 H -0.09735 0.20273 -0.15490
H14 H -0.02294 0.17035 -0.32512
H15 H -0.13921 0.12031 -0.27283
H16 H 0.55568 0.08384 -0.01098
C1 C 0.26433 0.24625 -0.17620
C2 C 0.40725 0.16255 -0.07937
C3 C 0.46133 0.21270 -0.16582
C4 C 0.58825 0.21609 -0.20520
C5 C 0.46516 0.09381 0.01513
C6 C 0.35972 0.10138 0.34082
C7 C 0.25873 0.04428 0.23568
C8 C 0.02885 0.08971 0.11692
C9 C -0.06029 0.15706 -0.20794
C10 C -0.12642 0.04939 0.24915
N1 N 0.36740 0.26573 -0.22674
N2 N 0.28017 0.18441 -0.08948
N3 N 0.12908 0.05500 0.25444
N4 N 0.04556 0.12494 -0.04026

N5 N -0.09202 0.09238 0.13118
N6 N -0.16953 0.01282 0.34654
S1 S 0.51688 0.08869 0.30080

Histidine HCl H_2O (HISTCM01)

a = 15.301, b = 8.921 c = 6.846 α = 90.0, β = 90.0, γ = 90.0

H 0.28201 -0.89751 0.17445
H 0.36671 -0.50229 0.38175
H 0.35823 -1.01163 0.09545
H 0.30765 -1.03739 0.30818
H 0.39592 -0.66030 -0.18814
H 0.29723 -0.33307 0.13667
H 0.44547 -0.95462 0.36285
H 0.46592 -0.83225 0.05589
H 0.50708 -0.74252 0.25271
H 0.32448 -0.41232 -0.20287
H 0.10833 0.12103 0.29936
H 0.02726 0.14533 0.41451
C 0.36591 -0.80261 0.50210
C 0.40161 -0.87745 0.32025
C 0.44907 -0.77077 0.18363
C 0.40083 -0.63410 0.12580
C 0.34307 -0.47201 -0.07098
C 0.36766 -0.52196 0.23246
N 0.33225 -0.96113 0.21667
N 0.38479 -0.59889 -0.06372
N 0.33165 -0.42243 0.10683
O 0.28763 -0.81174 0.53938
O 0.42313 -0.73332 0.59934
O 0.08008 0.08847 0.40635
Cl 0.17438 0.22224 0.03165

Glycylglycine HCl H_2O (GLCICH01)

a = 8.813, b = 9.755 c = 9.788 α = 90.0, β = 104.10, γ = 90.0

H -0.44840 0.50385 0.34149
H -0.43247 0.63270 0.23787
H -0.28221 0.57640 0.35119
H -0.45994 0.41199 0.12319
H -0.30614 0.51042 0.10402
H -0.32030 0.22280 0.08702
H -0.12277 0.07022 0.12529
H -0.01687 0.16178 0.26009
H -0.10441 -0.14227 0.40543
H -0.04891 -0.31933 0.54501

H -0.22227 -0.28565 0.53316
C -0.35226 0.455321 0.17917
C -0.23456 0.34733 0.24847
C -0.13278 0.12490 0.21342
C -0.17496 0.02612 0.31727
N -0.38069 0.54926 0.28509
N -0.23898 0.23533 0.17403
O -0.14456 0.37112 0.36140
O -0.28605 0.04070 0.36890
O -0.07592 -0.07572 0.34388
O -0.14311 -0.28819 0.48543
Cl 0.44642 0.31098 0.41465

Thymine (THYMIN01)

a = 12.889, b = 6.852 c = 6.784 α = 90.0, β = 104.92, γ = 90.0

H 0.59900 0.28750 0.34797
H 0.59801 -0.29859 0.36181
H 0.77915 0.29178 0.53512
H 0.94215 0.14104 0.71051
H 0.92142 -0.06278 0.83304
H 0.95852 -0.08588 0.61794
C 0.58121 -0.00649 0.34094
C 0.74413 -0.18671 0.51579
C 0.79767 0.00089 0.56865
C 0.74363 0.15912 0.50392
C 0.91298 -0.00335 0.6899
N 0.63928 0.15965 0.39583
N 0.63952 -0.17179 0.40631
O 0.49068 -0.00994 0.24575
O 0.78669 -0.34579 0.56432

Acetaminophen (HXACAN26)

a = 12.88559, b = 9.38013 c = 7.10096 a = 90.0, b = 115.7002, g = 90.0

H 0.73434 0.04457 0.19004
H 0.48956 0.41110 -0.37030
H 0.65832 0.25609 -0.24597
H 0.57425 0.11652 0.22441
H 0.41082 0.27228 0.10324
H 0.19420 0.69453 -0.41842
H 0.10546 0.55723 -0.53697
H 0.16487 0.57552 -0.27060
H 0.30188 0.44410 -0.10573
C 0.43562 0.35021 -0.14603
C 0.50825 0.34560 -0.24423
C 0.60283 0.25566 -0.17348

C 0.62798 0.17241 -0.00096
C 0.55738 0.17744 0.10250
C 0.46246 0.26823 0.02806
C 0.28067 0.50143 -0.39125
C 0.17762 0.58939 -0.40418
N 0.33901 0.43798 -0.21500
O 0.71982 0.08514 0.06433
O 0.30360 0.50079 -0.54307

Glycine (GLYCIN18)

a = 7.037, b = 7.037 c = 5.478 a = 90.0, b = 90.0, g = 120.0

H -0.62430 -0.76730 -0.07797
H -0.42444 -0.81900 -0.08733
H -0.88373 -1.14479 -0.09046
H -0.67585 -1.19478 -0.11740
H -0.58699 -0.89645 0.14516
C -0.72578 -1.08266 -0.15918
C -0.72331 -1.05528 -0.43299
N -0.57897 -0.87691 -0.03507
O -0.87373 -1.21201 -0.54853
O -0.56985 -0.88325 -0.52526

L-Alanyl-glycyl-glycine monohydrate (AGG)
(New REFCODE)

a = 12.199, b = 5.37, c = 7.900, α = 90.0, β = 102.14, γ = 90.0

H 0.64962 0.12653 0.05189
H 0.56080 0.21747 0.16079
H 0.59903 0.40014 0.02333
H 0.80888 0.24969 0.48929
H 0.76905 0.01067 0.35051
H 0.67335 0.15468 0.44712
H 0.69218 0.53399 0.29028
H 0.89527 0.60134 0.37533
H 1.04139 0.74870 0.26142
H 0.99274 0.58437 0.07713
H 1.18968 0.49193 0.12606
H 1.23943 0.02227 0.27597
H 1.30985 0.24455 0.40524
H 1.47920 0.76478 0.34058
H 1.51614 0.62701 0.50631
C 0.71831 0.36395 0.24674
C 0.74380 0.18112 0.39337
C 0.82027 0.40420 0.16680
C 1.00518 0.57649 0.21142

C 1.08844 0.37025 0.27894
C 1.27072 0.20387 0.27700
C 1.35888 0.20190 0.16917
N 0.62554 0.27295 0.11124
N 0.89930 0.54460 0.25894
N 1.18080 0.37351 0.21507
O 0.82683 0.30350 0.03151
O 1.07116 0.21950 0.38623
O 1.44396 0.06786 0.22733
O 1.34378 0.31758 0.03016
O 1.50384 0.60949 0.38654

Glycyl-glycyl-L-valine dihydrate (GGV), CUWRUH

a = 5.786, b = 7.954, c = 14.420, a = 90.0, b = 93.85, g = 90.0

H -0.09923 0.12027 0.47593
H -0.05915 -0.04531 0.54113
H -0.29606 0.05468 0.54302
H -0.39113 -0.01706 0.38576
H -0.34980 -0.18949 0.45425
H -0.28666 -0.17803 0.25617
H -0.05044 -0.31537 0.17017
H 0.10691 -0.37898 0.26623
H 0.04050 0.04105 0.19946
H 0.46646 0.04698 0.11243
H 0.14959 0.32391 0.15459
H 0.17736 0.13085 -0.02030
H -0.04844 0.12708 0.04951
H 0.01090 0.30479 -0.00839
H 0.52492 0.32137 0.02359
H 0.53692 0.42798 0.12574
H 0.34070 0.48341 0.03907
H -0.09637 0.24835 0.32698
H 0.15681 0.23545 0.35359
H 0.49241 0.60286 0.31850
H 0.52129 0.427432 0.35327
C -0.26795 -0.08557 0.42604
C -0.07171 -0.14815 0.37142
C 0.03744 -0.27256 0.23106
C 0.23890 -0.16306 0.20624
C 0.36544 0.11245 0.15802
C 0.24790 0.26064 0.10674
C 0.08588 0.20104 0.02677
C 0.42504 0.38106 0.07195
C 0.52931 0.17707 0.23810
N -0.17306 0.02066 0.50213
N -0.12741 -0.19101 0.28482

N 0.19345 -0.00255 0.18886
O 0.12429 -0.16227 0.40878
O 0.42986 -0.22898 0.20013
O 0.73954 0.18500 0.22386
O 0.44132 0.22228 0.31158
O 0.52579 0.54099 0.37252
O 0.01374 0.26060 0.37824

Table 1. The ^{15}N Shift tensors for all benchmark compounds

Structure	Atom #	Exp.	DFT-D2*	NMR refined
Cimetidine	1	248.2	-29.7	-15.8
CIMETD03		176.2	63.9	65.5
		86.5	166.1	155.9
	3	312.2	-74.6	-76.1
		252.9	-14.3	-13.3
		4.0	236.1	236.5
	10	160.2	74.0	76.9
		64.4	173.3	171.5
		64.4	179.8	177.6
	12	157.7	90.8	84.0
		58.3	190.4	184.1
		33.3	197.4	196.8
	15	129.3	108.6	109.9
		81.3	155.7	158.2
		46.0	192.6	191.3
	17	410.3	-183.8	-164.1
		315.1	-82.8	-82.3
		32.9	217.9	207.3
Histidine HCl H_2O	Nd1	287.8	-47.3	-42.9
HISTCM01		217.5	15.8	20.1
		64.0	176.7	177.9
	Ne2	276.6	-39.4	-34.4
		195.1	34.0	41.8
		57.8	184.9	186.2
	NH_3^+	58.5	188.9	182.4
		45.3	198.9	194.3
		39.2	204.7	202.9
Glycylglycine HCl H_2O	NH_3^+	43.8	202.9	201.0
GLCICH01		37.6	208.93	207.6
		28.8	213.7	212.6
	NH (amide)	213.6	14.0	26.7
		66.0	173.1	175.7
		59.7	179.8	180.9
Thymine	N1	211.4	15.3	24.1
THYMIN01		115.1	105.9	113.3
		55.6	189.1	181.6
	N3	225.8	-2.5	10.1
		146.9	85.1	83.6
		98.5	145.2	135.8
Acetaminophen	N	240.5	-31.6	-12.1
HXACAN26		85.4	145.8	133.6
		85.3	162.6	149.4
Glycine (g-phase)	N	42.3	200.5	201.5
GLYCIN18		34.3	210.8	209.3
		23.7	221.0	219.9

Table 1. The ^{15}N Shift tensors for all benchmark compounds (continued).

AGG hydrate	NH (amide)	207	18.0	26.0
CALEX20		59	177.9	178.9
		48	189.5	188.8
GGV dihydrate	NH (amide)	218	10.5	16.0
CUWRUH		63	167.9	168.0
		53	185.0	181.9

Table 2. Data collection, refinement and other relevant crystallographic data for AGG.

	Over all	Inner Shell	Outer Shell
Low resolution limit	4.90	4.90	0.61
High resolution limit	0.58	1.83	0.58
Rmerge	0.116	0.066	0.112
Rpim (all I+ & I-)	0.063	0.041	0.103
Total number of observations	5298	147	287
Total number unique	1815	61	171
Mean((I)/sd(I))	9.6	9.4	6.1
Completeness	66.2	66.5	44.1
Multiplicity	2.9	2.4	1.7
R1(F^2)	0.0529		

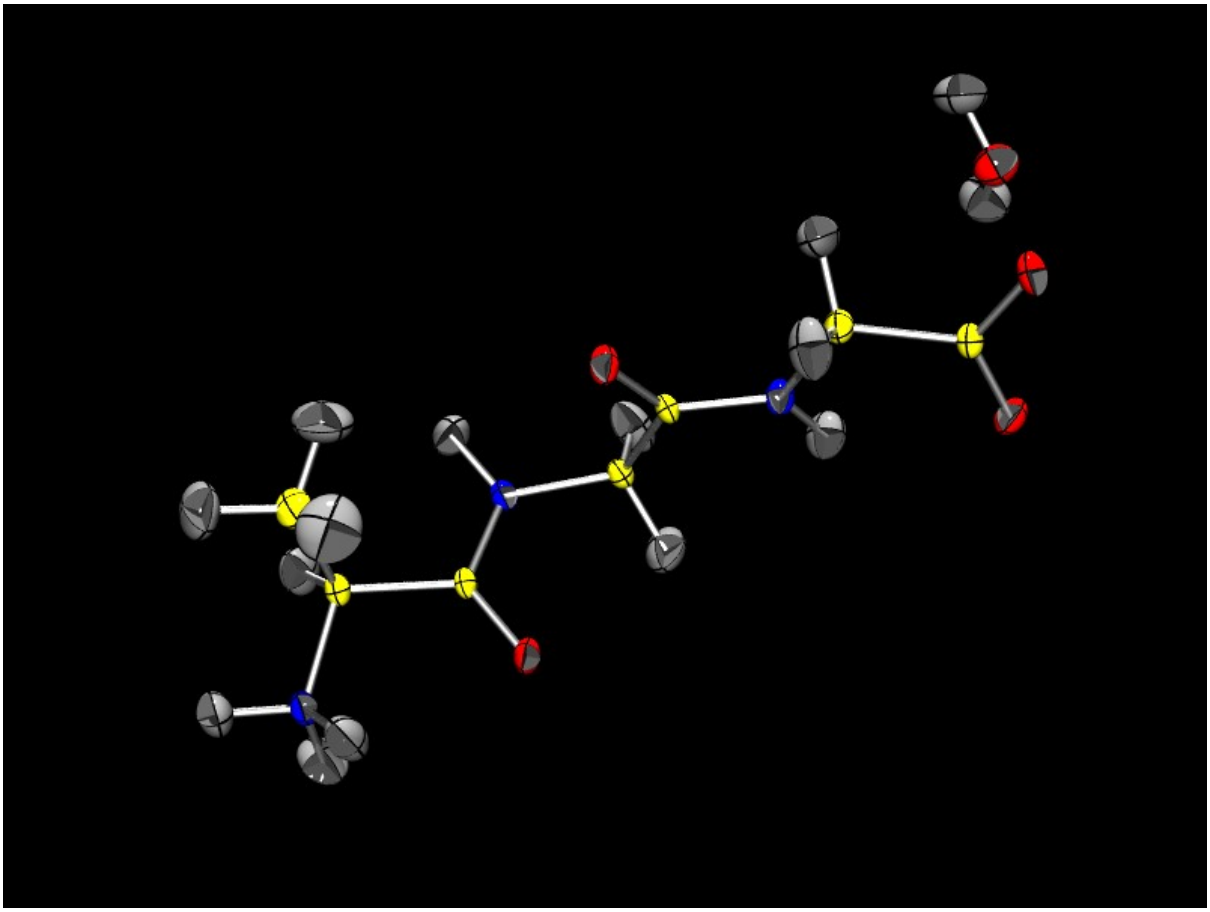

Figure 1. An ellipsoidal plot of the final structure of AGG obtained from the single crystal neutron analysis at 150 K (Ortep 3.2 for Windows (version 2.02)).