COMMUNICATION

The propensity of recrystallization solvents to form solvates

Michał Kaźmierczak,*[a] and Ewa Patyk-Kaźmierczak[a]

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

[a] *Faculty of Chemistry, Adam Mickiewicz University, Poznań. Uniwersytetu Poznańskiego 8 61-614 Poznań, Poland. E-mail: kax@amu.edu.pl*

Supporting Information

Table S1. Statistical parameters of the number of non-hydrogen atoms (N_{nH}) of the largest entity in the structure for entirety of the CSD, entirety of solvates deposited in CSD (all solvates) and for the crystals where one of the ten most commonly incorporated recrystallization solvents were used and is present in the final crystal.

	mean	median	standard deviation	coefficient of variation
CSD	41.17536	32	35.902462	0.87194
solvates	56.918001	48	37.248712	0.654428
dichloromethane	56.979104	51	30.126015	0.52872
water	38.507633	29	31.89262	0.828216
acetonitrile	61.788018	49	44.77383	0.724636
chloroform	61.564345	51	38.43149	0.624249
methanol	54.910707	44	38.761138	0.705894
tetrahydrofuran	57.260625	50	31.097178	0.543081
toluene	68.473496	58	38.476407	0.561917
benzene	58.406905	52	30.716771	0.52591
ether	62.203689	55	32.131499	0.516553
acetone	54.164778	46	33.442632	0.617424

Table S2. Statistical parameters of the number of non-hydrogen atoms (N_{nH}) of the largest entity in the structure for entirety of the CSD, entirety of cases with recrystallization solvent reported but where solvate was not formed (all *non-solvates*) and for the crystals where one of the ten most commonly incorporated recrystallization solvents were used and is not present in the final crystal.

	mean	median	standard deviation	coefficient of variation
CSD	41.17536	32	35.902462	0.87194
all *non-solvates*	37.696377	31	27.654569	0.733613
dichloromethane	38.700842	33	23.857872	0.616469
water	29.411825	23	31.34678	1.065788
acetonitrile	40.190988	32	37.141412	0.924123
chloroform	37.277436	29	28.412207	0.762182
methanol	36.737067	28	30.786331	0.838018
tetrahydrofuran	43.097823	38	27.044274	0.627509
toluene	42.003199	36	27.462929	0.653829
benzene	40.523351	35	28.719561	0.708716
ether	40.464731	34	29.088427	0.718859
acetone	32.557498	26	24.261138	0.745178

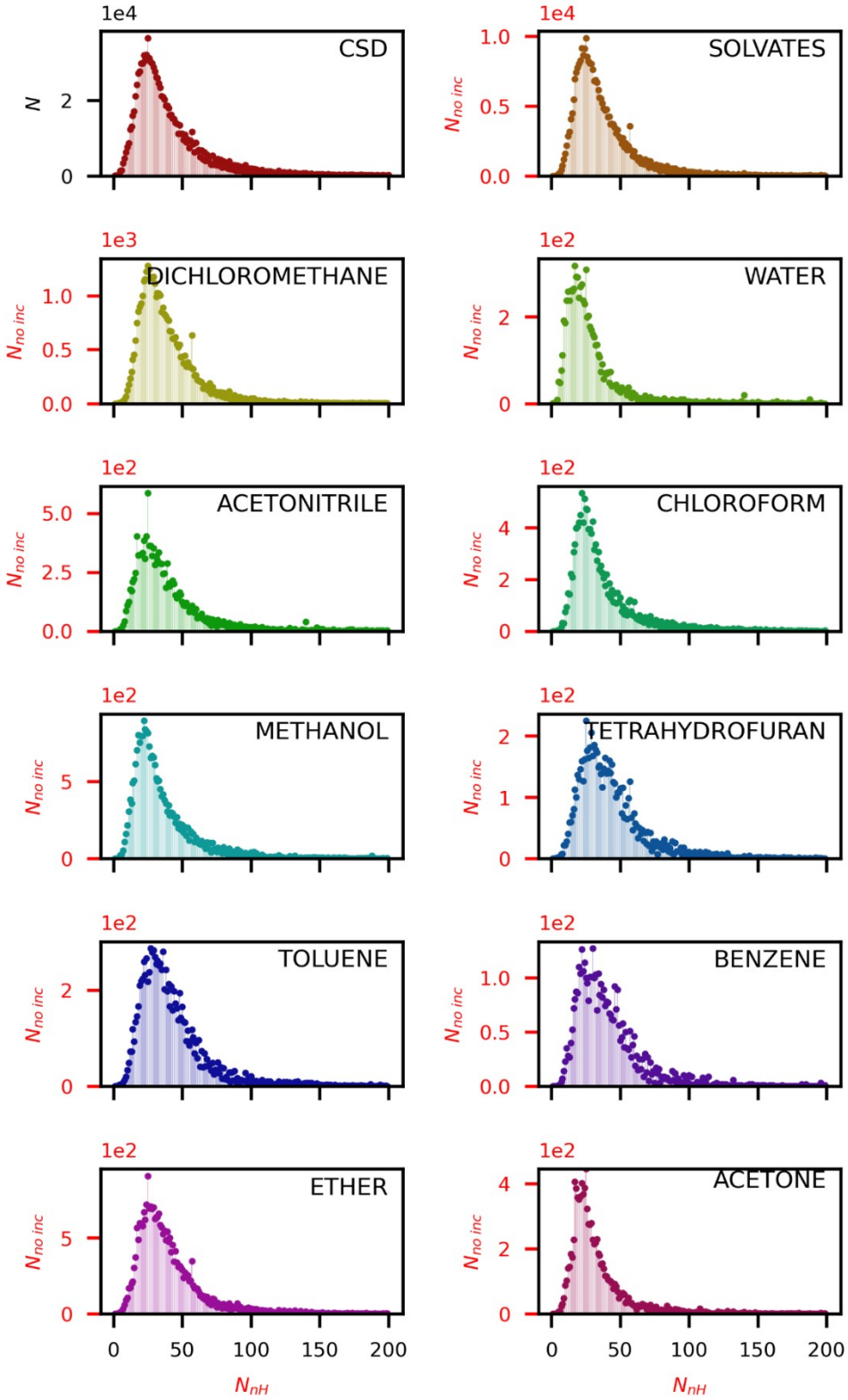

Figure S1. Distributions of the number of non-hydrogen atoms (^{nH} of the largest entity in the structure for entirety of the CSD, entirety of solvates deposited in the CSD (and non-solvates-where recrystallization solvent was reported but solvate was not formed), and for crystals where one of the ten most commonly incorporated recrystallization solvents was used and solvate was not formed. For clarity axes for all titles of plots were provided only on left, right and bottom of the figure.

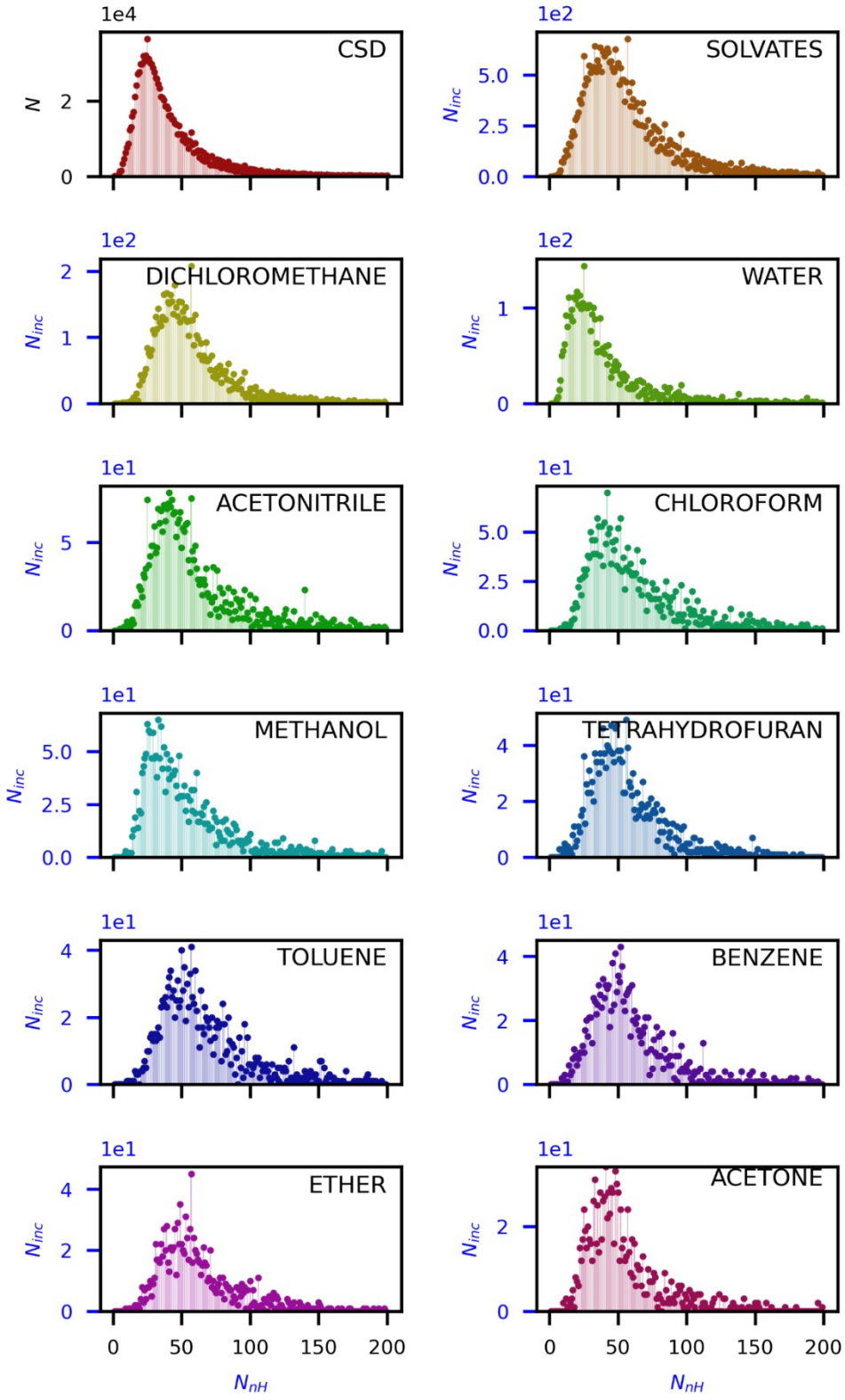

Figure S1. Distributions of the number of non-hydrogen atoms (nH of the largest entity in the structure for entirety of the CSD, entirety of solvates deposited in the CSD (and non-solvates-where recrystallization solvent was reported but solvate was not formed), and for crystals where one of the ten most commonly incorporated recrystallization solvents was used and it is present in the final crystal. For clarity axes for all titles of plots were provided only on left, right and bottom of the figure.