Table S1. Crystallographic data of the test structure with a number of non-hydrogen atom in the asymmetric unit (N_{asym}) lower than 80 (small-size molecules). ID is the identification number in Crystallography Open Database or the reference number.

Name	ID	Space group	N_{asym}	Cell content
alley1	2104682	P -1	66	C_{112} H_{104} O_{16} Fe_4
alley	2225745	R 3c	54	C_{828} H_{720} N_{72} O_{36} Fe_{36}
allof	2230280	P 6_1	22	C_{78} H_{126} N_6 O_{48}
amide	(1)	P $bc2_1$	24	C_{56} H_{72} N_{24} O_{16}
apapa	(2)	P 4_12_12	69	C_{240} H_{296} N_{168} O_{128} P_{16}
av2pr	2103455	P 6_1	56	C_{205} H_{374} N_{48} O_{83}
ax118	(3)	P ccn	25	C_{152} H_{168} N_{16} O_{24} Cl_8
azet	(2)	P $ca2_1$	48	C_{168} H_{128} N_8 O_8 Cl_8
bats	2226585	P -42_1c	16	C_{120} H_{104} I_8
becker	2017537	P 6_3/m	40	C_{354} H_{432} N_{18} O_{60} P_{12} Cl_{30} C_6
bed	(2)	I 4	34	C_{208} H_{208} N_{32} O_{32}
blake	2016921	C 2/c	72	C_{300} H_{220} N_{60} O_{160} Cl_{40} Pb_{20}
bobby	(2)	P 2_13	5	C_{24} H_{24} N_4 O_{24} Na_4 Ca_4
butyl	2222707	R -3	22	C_{342} H_{342} N_{18} O_{36}
carbamato	2226134	I 2/a	59	C_{344} H_{320} N_{32} O_{48} P_{16} S_{16} Au_{16}
carbamide	2219630	P n	15	C_{24} H_{20} N_4 O_2
cephal	(3)	C 2	46	C_{144} H_{168} N_8 O_{32}
choror	2104300	P 3_221	54	C_{264} H_{180} N_{12} O_{48}
cime	(4)	C c	18	C_{40} H_{72} N_{24} O_4 S_4
cubane	2222097	I -42d	27.5	C_{316} H_{288} N_{32} O_{76} Zn_{16}
cuimid	(2)	P 3_221	12	C_{36} H_{48} N_{24} Cl_6 Cu_6
diam	(2)	P 4_2/n	15	C_{112} H_{160} O_8
diben	2228788	F dd2	32	C_{448} H_{448} O_{32} S_{32}
diole	(2)	I -42d	12.25	C_{160} H_{288} O_{36}
eg1scrat	(5)	C 12/c1	12	O_{60} Cs_8 Si_{24} Ti_4
ergo	(6)	P $2_12_12_1$	58	C_{224} H_{352} O_8
erica	(7)	P 2_1	43	C_{74} H_{86} O_8 P_2 Fe_2
euclor	(8)	C 2/c	21	O_{104} Na_8 S_{24} K_8 Cu_{24}
ewa	2017580	I mmm	6	Mg_{14} Zn_{50} Ce_{32}
fegas	(9)	P 6_3/mmc	0.75	S_{10} Fe_4 Ga_4
fisk	2017323	P 6_3/mmc	0.42	P_4 Ca_2 In_4
flubo	2017493	P -31c	2.17	B_4 O_{12} F_2 K_2 Zn_4 Cd_2
fnltk	(10)	I 2/c	44	C_{304} H_{192} N_{40} As_8
freies	(11)	P 2_1/a	6	S_{12} Ag_4 Sb_4 Pb_4
furan	2222612	P nma	4	C_{16} H_{12} O_{12} Cl_4
giac	(12)	P 2_1/c	21	C_{68} H_{32} N_4 O_8 S_4
gold	(2)	C c	56	C_{224} H_{128}
golen	2230759	I 4_1/a	44	C_{640} H_{704} N_{32} Cl_{32}
gra4	(3)	P -1	36	C_{60} H_{44} N_4 O_8
hexakis	2226269	C mca	28.5	C_{96} H_{400} N_{48} O_{232} V_{80}
hfac	2103750	I 4_1cd	33	C_{224} H_{96} N_{32} O_{64} F_{192} Cu_{16}

hkw0m	2016712	P n2_1m	7	C_4 H_{24} N_8 O_8 Na_4 Cl_4
hov1	(2)	C 2/m	15.5	Si_{36} Pr_{56} Ni_{32}
hwk3	2016711	I 2	7	C_4 H_{24} N_8 O_8 Na_4 Cl_4
indide	2225931	I 4/mcm	4.38	Ru_{41} In_{15} La_{84}
inos	(13)	P 2_1/n	26	C_{48} H_{112} O_{56}
jing	2230031	I 4	33.5	C_{192} H_{176} N_{24} O_{44} Cu_8
kirillov	2218097	F d-3m	2	C_{384} H_{768} N_{192} O_{192} P_{192} Cl_{192} Cu_{192}
kumar	2227526	P -42$_1$c	38.38	C_{268} H_{246} N_{16} O_{23}
lei	2225988	P bca	52	C_{304} H_{432} N_{48} O_{48} S_{16}
litho	(14)	P $2_12_12_1$	27	C_{96} H_{120} O_{12}
loganin	(2)	P $2_12_12_1$	27	C_{68} H_{104} O_{40}
mag255	(15)	P $2_12_12_1$	68	C_{224} H_{248} O_{24} N_{24}
mbh2	(2)	P 1	54	C_{45} H_{72} O_9
mema	2223241	R 3c	14.11	C_{216} H_{400} N_{18} O_2 Cl_{18}
mlx12b	2017265	I 4/m	2.38	O_{28} H_{16} P_4 V_4 Co_2
munic	(2)	C 2	40	C_{160} H_{128}
nabei_1	2016619	C c	67	B_8 C_{180} H_{124} N_{36} O_8 F_{32} Co_4
nabei_2	2016620	C 2/c	74	B_{24} C_{364} H_{260} N_{76} O_{24} F_{96} Co_8
newqb	(2)	P -1	62	C_{96} H_{80} N_8 O_{20}
no55	(2)	F dd2	24	C_{320} H_{384} N_{64}
pge2	(2)	P 1	25	C_{20} H_{32} O_5
photo	(16)	P $2_12_12_1$	17	C_{48} H_{52} N_4 O_{16}
picol	2217894	P 6_522	41.5	C_{288} H_{276} N_{48} O_{138} K_{12} Tb_{12}
pocro	(17)	B 112/m	3.5	K_2 Se_{16} Cr_{10}
pyrid	2219167	I 4_1/acd	10.5	C_{208} H_{144} N_{80} O_{32} Mn_{16}
quinol	(2)	R -3	24	C_{324} H_{324} O_{108}
quinone	2103571	P ccn	8	C_{40} H_{32} O_8 S_{16}
ramesh	2219800	R -3	40	C_{558} H_{612} N_{36} O_{126}
rauf4n	2229326	P 4_32_12	33	C_{240} H_{368} O_{24}
rc62	(3)	P 2_1	80	C_{136} O_{24}
rifolo	(18)	P 2_1	53	C_{78} H_{98} N_2 O_{26}
ringe	2016743	P 4/nmm	0.44	Cu_1 Sb_4 U_2
sahlberg	2016995	P 4/mbm	0.62	Mg_2 Sc_4 Ga_4
salex	(19)	P -3	15.83	H_{60} O_{69} Na_4 S_{12} K_4 Fe_6
schwarz	(20)	P 1	73	C_{46} H_{70} O_{27}
seidel	2228989	P 4_2/n	49	C_{320} H_{192} N_{64} Zn_8
selenid	(2)	P 2_1	25	C_{44} H_{56} O_4 Se_2
skn1	(21)	P 3_1	13	C_{21} H_{48} N_3 O_{12} Cl_3
sliva	2225554	P -43n	24.5	C_{336} H_{504} N_{72} O_{120} Na_6 P_{24} S_{24} Nd_6
solokha	2016696	F -43m	5	Mg_{76} Zn_{324} Ce_{80}
suoa	(2)	P $2_12_12_1$	47	C_{112} H_{152} O_{76}
sutovi	2016784	P 6_3/m	7	H_3 O_{41} Cl_7 As_{12} Cd_{24}
teoh	2226240	I -4	50	C_{336} H_{320} O_{48} Sn_{16}
tetrakis	2219750	I -43d	19.58	C_{672} H_{480} N_{192} O_{48} P_8 S_4 Ni_{16}
thiourea	2230193	I bca	18	C_{224} H_{304} N_{48} S_{16}
tiny3	(22)	P $2_12_12_1$	33	C_{88} H_{100} Cl_4 N_8 O_{32}
togr44	2017713	C 2/c	59	C_{392} H_{496} O_{32} Cl_{48}
totc	(2)	P 6_1	42.5	C_{219} H_{260} O_{36}
tpala	(2)	P 2_1	39	C_{56} H_{84} N_8 O_{14}
tph	(2)	B 22_12	39	C_{288} H_{240} N_{24}

triosic	2101410	C 222_1	43.5	C_{224} H_{308} N_{56} O_{56} S_8 Cl_4
tungsto	2218160	R 3	61.33	C_{324} H_{216} N_{54} O_{126} Fe_{12} W_{36}
tur10	(2)	P 6_322	17.33	C_{180} H_{288} O_{28}
wall26	2218446	P -43n	8	C_{128} H_{288} O_{32} Tl_{32}
xanthene	2220578	P $na2_1$	67	C_{220} H_{320} N_4 O_{44}
y75	(23)	P 21/n	34	C_{100} H_{136} N_{12} O_{24}
yah140	2230578	P 4/n	19.5	C_{96} H_{80} N_{32} O_{24} Mo_2 Tb_2
zhang	2222739	C 2/c	64.5	C_{304} H_{408} N_{48} O_{148} S_8 Mn_8

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Table S2. Crystallographic data of the test structure with a number of non-hydrogen atom in the asymmetric unit (N_{asym}) ranging from 81 to 400 (medium-size molecules). ID is the identification number in Crystallography Open Database, the Protein Data Bank code or the reference number. The 24 medium size structures used in the paper IV [Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Polidori, G. (2011). *J. Appl. Cryst*., **44**, 1143-1151] are highlighted in bold.

Name	ID	Space group	N_{asym}	Cell content
alley2	2104681	P bca	158	C_{960} H_{688} Na_{80} O_{184} Fe_{40}
amphisin	2012193	P $2_12_12_1$	102	C_{264} H_{464} N_{48} O_{96}
at119	2228715	P $2_12_12_1$	259	C_{764} H_{892} N_{48} O_{208} S_{16}
babu	2222265	C c	204	C_{528} H_{576} N_{96} O_{192}
bcdimp	(1)	P 2_1	96	C_{110} H_{152} N_8 O_{74}
bk53m	2228724	P -1	156	C_{216} H_{169} N_{56} O_{33} S_8
brock	2104241	B 2_1	208	C_{320} H_{768} N_{64} O_{416} Fe_{32}
budka	2229223	P 2_1/c	153	C_{564} H_{808} O_{40} Cl_8
bulged	1P79	P 42_12	138	C_{456} N_{168} O_{488} P_{48} K_{24}
c8new	(2)	P 2_1	130	C_{196} H_{272} N_{32} O_{32}
cah	(3)	P 2_1	155	C_{210} H_{260} N_{20} O_{30} F_{50}
carbru_1	2016443	P $2_12_12_1$	121	C_{428} H_{432} N_{16} O_{20} Cl_{16} Ru_4
carbru_2	2016444	P $2_12_12_1$	121	C_{428} H_{432} N_{16} O_{20} Cl_{16} Ru_4
cb3_pap	(4)	P 2_1/n	92	C_{304} H_{288} O_{64}
ceho1z	(5)	P 2_1	116	C_{128} H_{160} N_{16} O_{88}
ceho2z	(5)	P 2_1	232	C_{264} H_{304} N_{32} O_{168}
cemc1z	(6)	P 2_1	228	C_{248} H_{296} N_{32} O_{168} Cl_8
cemc2z	(6)	P 2_1	207	C_{210} H_{444} N_4 O_{200}
cephaibol_a	1OB4	P 2_12_12	113	C_{308} N_{72} O_{72}
cephaibol_c	1OB7	P $2_12_12_1$	112	C_{300} N_{72} O_{72}
cofi5a	2218002	P 2_1/c	107	C_{388} H_{520} O_{32} Cl_8
cyclo_bnz	2103881	P 2_1	206	C_{216} H_{224} N_8 O_{189}
cyclo_dba	2103880	P $2_12_12_1$	219	C_{508} H_{448} N_{16} O_{352}
dasco6	2200556	P 2_1	124	C_{162} H_{270} N_{38} O_{40} S_8
dext	(3)	P 2_1	94	C_{110} H_{152} O_{74} N_4
diene	2226177	P $2_12_12_1$	90	C_{264} H_{480} B_{12} F_{48} P_{24} Rh_{12}
dioxolan	2011222	P 2_1	141	C_{220} H_{252} N_{12} O_{48} Ru_2
dodeca	(7)	P $2_12_12_1$	200	C_{568} H_{912} N_{96} O_{136}
echino	2101407	p 65	89	C_{363} H_{486} N_{60} O_{102} S_{12}
ergop21	(8)	P 2_1	116	C224 H352 O8
gago	2227102	P 2_1/n	129	C_{240} H_{288} N_{48} O_{156} S_{24} Cl_{24} Mo_{24}
giorgi	(9)	P 2_1	88	C_{148} H_{220} N_4 O_{24}
glici2	(10)	C 2	139	C_{480} H_{760} O_{76}
gna	2WNA	C 222_1	146	C_{456} O_{384} N_{192} P_{96} Co_{16} Mg_{16} Br_8
guest	2202059	P $2_12_12_1$	105	C_{224} H_{440} O_{188} S_8
h104	(11)	P 2_1/c	84	C_{252} H_{384} N_{12} O_{60} Cl_{12}
hao	2226460	A ba2	84	C_{416} H_{496} N_{88} O_{144} S_{16} Gd_8
helix	1VRZ	C 2	164	C_{472} H_{736} N_{92} O_{92}
hepta	2103676	P $2_12_12_1$	109	C_{288} H_{550} O_{150}
hexa	2103675	P $2_12_12_1$	100	C_{252} H_{599} O_{149}

hsy115	2225069	P na2_1	120	C_{384} H_{480} N_{32} O_{64}
iak48bm	2225123	P 2_1/c	140	C_{416} H_{296} O_{96} P_8 As_{16} Ru_{24}
iled	(12)	P $2_12_12_1$	84	C_{240} H_{408} N_{24} O_{72}
inclu_rt	(13)	P 1	194	C_{97} H_{157} O_{97}
jamilas	(14)	P 1	100	C_{64} H_{68} O_{20} N_8 S_4 K_4
jebas	2220423	P 21/c	121.5	C_{342} H_{456} N_{32} O_{80} S_{32}
kemer	2015969	C 2/c	126	C_{648} H_{1056} N_{168} O_{96} S_{72} Cr_{12} Er_{12}
kfb44	2103879	P -1	368	C_{656} H_{576} N_{16} O_{32} Si_{32}
lasso	2NJW	P $2_12_12_1$	146	C_{608} N_{92} O_{104} S_8
macro	(15)	P $2_12_12_1$	123	C_{420} H_{432} O_{72}
mghex	(16)	P 3_1	95	C_{168} H_{240} N_{48} O_{60} Cl_6 Mg_3
mor59	(17)	P 2_1	126	C_{192} H_{328} N_{24} O_{36}
oe410	2204692	P 2_1/n	135	C_{432} H_{320} N_{48} O_{12} P_{16} Te_{16} Re_{16}
ohba	2202173	P 2_1	92	C_{162} H_{174} N_2 O_{20}
ohba_p1	2203226	P 1	188	C_{166} H_{158} N_2 O_{20}
pnib	1AKG	P $2_12_12_1$	114	C_{280} N_{72} O_{88} S_{16}
quail_a	2012678	P $2_12_12_1$	81	C_{220} H_{396} N_{36} O_{68}
quail_b	2012679	P $2_12_12_1$	83	C_{228} H_{412} N_{36} O_{68}
rac	2211608	P -1	93	C_{140} H_{138} N_{22} O_{16} Cl_4 Cu_4
rauf20	2220764	P 2_1/n	104	C_{232} H_{104} N_{32} O_{16} S_{16} Cl_{120}
shen	2230103	P c	90	C_{128} H_{184} N_8 O_{40} Co_4
so99	2016923	P -1	144	C_{224} H_{232} N_{32} O_{32}
sr166	(18)	P 2_1	112	C_{192} H_{192} O_{16} N_{16}
s6	(14)	P -1	89	C_{132} H_{141} N_{10} O_{24} S_{12}
ta	(19)	P 2_1	142	C_{170} H_{224} O_{114}
tato	(20)	P $2_12_12_1$	109	C_{224} H_{368} N_8 O_{204}
tb	(19)	P $2_12_12_1$	186	C_{520} H_{784} O_{224}
tb02rlm	(21)	P 1	197	C_{96} H_{224} O_{101}
tensin	2010528	P $2_12_12_1$	107	C_{284} H_{508} N_{48} O_{96}
theo	2227537	P $2_12_12_1$	110.8	C_{280} H_{500} N_{52} O_{111}
thebo	2008512	P 2_1/c	112	C_{360} H_{368} N_{48} O_{40}
thio2	2104680	P 2_1/c	144	C_{444} H_{288} N_{12} F_{72} P_{24} S_{12} Ag_{12}
tp	(19)	P 2_1	161	C_{210} H_{308} O_{112}
triazole	2221962	P -1	243	C_{378} H_{414} N_{72} S_{18} Cl_{18}
trip04e	2100208	P 2_1	223.5	C_{283} H_{295} O_{160} Cl_4
triostin_a	2101409	P $2_12_12_1$	94	C_{256} H_{360} N_{48} O_{64} S_8
triostin_c	2101408	P $2_12_12_1$	83.5	C_{219} H_{283} N_{48} O_{51} S_8 Cl_8
tval	(16)	P 1	156	C_{108} H_{180} N_{12} O_{36}
winter	(16)	P 2_1	88	C_{110} H_{178} N_{22} O_{32} Cl_{12}
x124	(22)	P 1	120	C_{92} H_{76} N_4 O_{12} S_4 Cl_8
y54	(23)	P $2_12_12_1$	100	C_{264} H_{344} N_{56} O_{80}
zaib	(24)	P -1	141	C_{193} H_{316} N_{36} O_{53}
zippercl	2WQ0	I 2_13	275	C_{4008} N_{1272} O_{1224} S_{24} Cl_{72}
zipperbr	2WQ1	I 2_13	275	C_{4008} N_{1272} O_{1224} S_{24} Br_{72}

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Table S3. Crystallographic data of the protein test structure with a number of non-hydrogen atom in the asymmetric unit (N_{asym}) ranging from 200 to about 2000. HA indicates the number and species of the heavy atoms ($Z \geq 16$) in the asymmetric unit. Data at atomic resolution (up to 1.2 Å).

PDB code	Space group	N_{asym}	HA
1AA5	$P\ 4_3 2_1 2$	200	8Cl
1SH0	$P\ 4_3 2_1 2$	207	8Cl
1HHY	$P\ 6_3 22$	208	4Cl
1P9I	$C\ 222_1$	213	None
1ICK	$P\ 2_1 2_1 2_1$	250	None
1A0M	I 4	255	10S
2BF9	C 2	305	1Zn
2ERL	C 2	305	7S
1A7Z	$P\ 2_1 2_1 2_1$	307	2Cl
1ALZ	$P\ 2_1 2_1 2_1$	313	None
1CBN	$P\ 2_1$	330	6S
1HHZ	$P\ 3_2 21$	354	6Cl
1BX7	$P\ 4_3 2_1 2$	365	11S
2FDN	$P\ 4_3 2_1 2$	373	16S 8Fe
8RXN	$P\ 2_1$	392	6S 1Fe
1IRO	R 3	411	5S 1Fe
1IRN	R 3	411	5S 1Zn
1NKD	C 2	439	4S
1IGD	$P\ 2_1 2_1 2_1$	468	1 S
1C75	$P\ 2_1 2_1 2_1$	528	3S 1Fe
1B0Y	P 222	593	9S 4Fe
1CTJ	R 3	672	3S 1Fe
2PVB	$P\ 2_1 2_1 2_1$	814	3S 2Ca
1A6N	$P\ 2_1$	892	3S 1Fe

1D4T	P 2_1	911	3S
3PYP	P 6_3	983	6S
1MFM	P $2_12_12_1$	1106	2S 2Cl 1Cu 1Zn 4Cd
1A6G	P 2_1	1224	3S 1Fe
1CKU	P $2_12_12_1$	1229	18S 8Fe
1SWZ	P 3_221	1254	2Cl 3Rb
1I76	P $2_12_12_1$	1315	3S 2Ca 2Zn
1JM1	P 6_1	1496	10 S 2Fe
1FY2	C 2	1685	12S 1Cl 1Cd
1NLS	I 222	1810	2S 1Ca 1 Mn
1GY0	P 3_1	2006	26S 4 Fe