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Supporting information

Proposal for Crystallization of 3-Amino-4-halo-5-methylisoxazoles: An Energetic and Topological Approach

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Table S1. QTAIM data and G_{AI} of dimers of compound **1**.

Dimer	Inter.	ρ_{INT}	$\nabla 2\rho$	G	V	BPL	Ellipticity	G_{AI}[b]
M1•••M2	N•••H-N	0.015326	+0.064098	+0.013455	-0.010885	4.251078	0.129167	-4.17
	N-H•••N	0.015326	+0.064098	+0.013455	-0.010885	4.251078	0.129167	-4.17
M1•••M3	O•••H-N	0.008197	+0.039956	+0.007819	-0.005649	4.527889	0.097784	-1.66
	O•••Cl	0.002279	+0.008790	+0.001713	-0.001228	7.221419	3.010133	-0.46
	N•••Cl	0.002483	+0.008521	+0.001649	-0.001169	7.300750	0.393319	-0.50
M1•••M4	C-H•••Cl	0.006021	+0.025268	+0.004847	-0.003378	5.416969	0.094680	-0.37
M1•••M5	Cl•••N	0.001028	+0.003606	+0.000668	-0.000435	8.429618	0.156814	-0.42
	C-H•••N	0.002989	+0.010214	+0.001997	-0.001441	5.870038	0.128641	-1.24
M1•••M6	C-H•••Cl	0.006020	+0.025265	+0.004847	-0.003377	5.417108	0.094694	-0.37
M1•••M7	O•••H-N	0.008197	+0.039958	+0.007819	-0.005649	4.527896	0.097793	-1.66
	O•••Cl	0.002279	+0.008790	+0.001713	-0.001228	7.221421	3.011512	-0.46
	N•••Cl	0.002483	+0.008521	+0.001649	-0.001169	7.300748	0.393299	-0.50
M1•••M8	C-H•••Cl	0.002202	+0.008392	+0.001518	-0.000938	6.764440	0.410496	-0.69
M1•••M9	C-H•••Cl	0.002203	+0.008393	+0.001518	-0.000938	6.764275	0.410382	-0.69
M1•••M10	C-H•••π	0.005263	+0.020647	+0.004021	-0.002881	6.836096	0.855462	-1.07
	C-H•••N	0.004368	+0.018990	+0.003719	-0.002691	5.734348	2.746002	-0.89
	Cl•••N	0.002123	+0.006810	+0.001306	-0.000910	7.605826	0.106768	-0.43
	Cl•••Cl	0.001739	+0.005592	+0.001044	-0.000691	8.081175	0.103875	-0.35
M1•••M11	C-H•••π	0.005263	+0.020647	+0.004021	-0.002881	6.836096	0.855462	-1.07
	C-H•••N	0.004368	+0.018990	+0.003719	-0.002691	5.734348	2.746002	-0.89
	Cl•••N	0.001739	+0.005592	+0.001044	-0.000691	8.081175	0.103875	-0.35
	Cl•••Cl	0.002123	+0.006810	+0.001306	-0.000910	7.605826	0.106768	-0.43
M1•••M12	Cl•••N	0.002518	+0.008267	+0.001572	-0.001078	7.357650	0.300825	-0.60
M1•••M13	N•••Cl	0.002518	+0.008267	+0.001572	-0.001078	7.357751	0.300809	-0.60
M1•••M14	N•••Cl	0.001028	+0.003606	+0.000668	-0.000435	8.429618	0.156814	-0.42
	N•••H-C	0.002989	+0.010214	+0.001997	-0.001441	5.870038	0.128641	-1.24
M1•••M15	C-H•••N	0.003899	+0.014744	+0.002846	-0.002006	5.959126	0.305849	-1.02
	N•••C	0.003618	+0.012906	+0.002485	-0.001744	7.006365	0.916383	-0.95
	C•••O	0.003681	+0.013956	+0.002744	-0.001999	6.685321	0.323654	-0.96
	O•••C	0.003681	+0.013956	+0.002744	-0.001999	6.685321	0.323654	-0.96
	N•••C	0.003618	+0.012906	+0.002485	-0.001744	7.006365	0.916383	-0.95
	N•••H-C	0.003899	+0.014744	+0.002846	-0.002006	5.959126	0.305849	-1.02

[a] Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal·mol^{-1}).

Table S2. QTAIM data and G_{AI} of dimers of compound **2**.

Dimer	Inter.[a]	ρ_{INT}	∇2ρ	G	V	BPL	Ellipticity	G_{AI}[b]
M1•••M2	N•••H-N	0.014235	+0.059791	+0.012428	-0.009908	4.304799	0.111969	-4.25
	N-H•••N	0.014235	+0.059791	+0.012428	-0.009908	4.304799	0.111969	-4.25
M1•••M3	C-Br•••O	0.001118	+0.005077	+0.000948	-0.000627	6.537782	0.106920	-1.53
M1•••M4	H•••H	0.002393	+0.009357	+0.001739	-0.001139	5.252885	0.220928	-0.81
M1•••M5	C-H•••Br	0.002415	+0.009191	+0.001646	-0.000995	7.074769	0.390169	-0.49
	H•••H	0.001549	+0.007183	+0.001230	-0.000665	6.814131	12.52159	-0.32
	C-H•••Br	0.002415	+0.009192	+0.001646	-0.000995	7.074641	0.390012	-0.49
M1•••M6	C-Br•••O	0.005928	+0.025483	+0.005003	-0.003635	6.247424	0.065919	-1.51
M1•••M7	N•••Br	0.003856	+0.014164	+0.002699	-0.001857	7.280892	0.529749	-0.47
	H•••H	0.006959	+0.028133	+0.005699	-0.004364	4.596268	0.682365	-0.85
	N•••Br	0.003856	+0.014162	+0.002699	-0.001857	7.280999	0.529563	-0.47
M1•••M8	C-H•••Br	0.003938	+0.013763	+0.002612	-0.001784	6.293995	0.079386	-1.12
	N-H•••O	0.001118	+0.005077	+0.000948	-0.000627	6.537782	0.106920	-0.32
M1•••M9	C-H•••Br	0.003938	+0.013764	+0.002612	-0.001784	6.294001	0.079421	-1.11
	N-H•••O	0.001119	+0.005078	+0.000948	-0.000627	6.537775	0.106939	-0.32
M1•••M10	C-H•••N	0.005617	+0.019871	+0.003919	-0.002870	5.267387	0.163343	-1.41
	Br•••N	0.003177	+0.010190	+0.001953	-0.001359	7.462650	0.292583	-0.79
M1•••M11	C-H•••N	0.005617	+0.019871	+0.003919	-0.002870	5.267387	0.163343	-1.41
	Br•••N	0.003177	+0.010190	+0.001953	-0.001359	7.462650	0.292583	-0.79
M1•••M12	Br•••Br	0.000982	+0.002613	+0.000472	-0.000290	9.314000	0.228472	-0.42
M1•••M13	Br•••Br	0.004107	+0.013920	+0.002644	-0.001807	7.448000	0.201361	-0.87
M1•••M14	C-H•••N	0.002839	+0.011958	+0.002235	-0.001480	6.590872	0.264485	-1.03
	C•••N	0.005018	+0.016430	+0.003198	-0.002289	7.586456	1.028788	-1.82
	N•••C	0.005018	+0.016430	+0.003198	-0.002289	7.586456	1.028788	-1.82
	C-H•••N	0.002839	+0.011958	+0.002235	-0.001480	6.590872	0.264485	-1.03
M1•••M15	C-H•••N	0.003340	+0.012825	+0.002462	-0.001718	5.838272	1.193427	-1.01
	Br•••π	0.003474	+0.012581	+0.002458	-0.001770	7.147323	0.653462	-1.05
	C•••C	0.003773	+0.011159	+0.002099	-0.001408	7.854917	1.573783	-1.14
	Br•••π	0.003474	+0.012581	+0.002458	-0.001770	7.147320	0.653497	-1.05
	C-H•••N	0.003341	+0.012827	+0.002463	-0.001718	5.838079	1.192675	-1.01

[a] Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal·mol^{-1}).

Table S3. QTAIM data and G_{AI} of dimers of compound **3**.

Dimer	Inter.[a]	ρ_{INT}	∇2ρ	G	V	BPL	Ellipticity	G_{AI}[b]
M1•••M2	N•••H-N	0.014716	+0.055649	+0.011841	-0.009770	4.312185	0.089814	-4.36
	N-H•••N	0.014717	+0.055657	+0.011842	-0.009771	4.312157	0.089828	-4.37
M1•••M3	C-I•••O	0.008488	+0.031085	+0.006405	-0.005039	6.206098	0.071883	-2.27
M1•••M4	H•••H	0.002189	+0.008409	+0.001567	-0.001031	5.226553	0.127831	-0.72
M1•••M5	C-H•••I	0.002925	+0.009542	+0.001784	-0.001183	7.275435	0.375193	-0.56
	H•••H	0.001234	+0.004964	+0.000863	-0.000485	6.698287	1.060076	-0.24
	C-H•••I	0.002925	+0.009543	+0.001784	-0.001183	7.275380	0.375181	-0.56
M1•••M6	C-I•••O	0.008487	+0.031082	+0.006404	-0.005039	6.206134	0.071879	-2.25
M1•••M7	N•••I	0.004541	+0.014614	+0.002913	-0.002172	7.512974	0.570255	-0.43
	H•••H	0.005562	+0.020604	+0.004281	-0.003412	4.468403	0.436664	-0.53
	N•••I	0.004541	+0.014613	+0.002913	-0.002172	7.512914	0.570187	-0.43
M1•••M8	C-H•••I	0.002930	+0.008858	+0.001689	-0.001164	7.003455	0.126799	-1.22
M1•••M9	C-H•••I	0.002930	+0.008858	+0.001689	-0.001164	7.003430	0.126747	-1.19
M1•••M10	C-H•••N	0.004995	+0.016123	+0.003238	-0.002446	5.392469	0.141335	-1.23
	I•••N	0.003976	+0.010746	+0.002169	-0.001651	7.601744	0.291482	-0.98
M1•••M11	C-H•••N	0.004995	+0.016123	+0.003238	-0.002446	5.392469	0.141335	-1.23
	I•••N	0.003976	+0.010746	+0.002169	-0.001651	7.601744	0.291482	-0.98
M1•••M12	I•••I	0.002614	+0.006366	+0.001226	-0.000860	8.940000	0.207405	-0.82
M1•••M13	I•••I	0.005753	+0.014824	+0.003080	-0.002455	7.760000	0.204166	-1.26
M1•••M14	C-H•••N	0.003291	+0.012660	+0.002438	-0.001711	6.332219	0.183240	-1.27
	C•••N	0.004861	+0.015451	+0.003038	-0.002214	6.985906	2.004273	-1.88
	N•••C	0.004861	+0.015451	+0.003038	-0.002214	6.986396	2.005260	-1.88
	C-H•••N	0.003292	+0.012661	+0.002439	-0.001712	6.332049	0.183141	-1.27
M1•••M15	C-H•••N	0.002898	+0.010372	+0.002020	-0.001447	6.064290	1.983599	-0.95
	I•••π	0.004347	+0.013152	+0.002696	-0.002103	7.338056	1.337403	-1.42
	C•••C	0.003293	+0.009261	+0.001768	-0.001221	7.801040	5.714340	-1.08
	I•••π	0.004347	+0.013152	+0.002695	-0.002103	7.338067	1.338053	-1.42
	C-H•••N	0.002899	+0.010373	+0.002020	-0.001447	6.064046	1.980064	-0.95

[a] Atom···atom interaction. G_{AI} = Atom···atom interaction energy (kcal·mol^{-1}).

Table S4. Geometrical parameters of intermolecular interaction of compounds **1**–**3**.

Interaction type	$d_{(X...Y)}$ range (Å)	$Angle_{(X...Y)}$ range (°)
N-H···N	3.03-3.08	159-163
N-H···O	3.20	165
	3.96	131
C-H···N	3.64-4.08	110-170
C-H···X	3.56-4.15	92-135
	3.99-4.30	117-130
C-X···O	3.28-3.82	102-160
C-X···N	3.76-4.36	98-103
	3.85-4.01	95-117
X···X	4.27-4.73	102-120
	3.93-4.01	138-141
X···π	3.77-3.86	90-91
C-H···π	3.63	159
π···π	3.43-3.57	92-100
	3.52-4.66	126-127
CH···HC	4.17-4.30	-
	4.08-4.30	-
NH···HN	3.40-3.59	-

Table S5. Interaction energies[a] of the dimers present in the clusters of compounds **1**-**3**, with and without BSSE correction.

Dimer	$G_{M1\cdots MN}$(kcal·mol^{-1})					
	With BSSE Correction			Without BSSE Correction		
	1	**2**	**3**	**1**	**2**	**3**
M1···M2	-8.33	-8.50	-8.73	-9,95	-10,06	-10,28
M1···M3	-2.63	-1.53	-2.27	-3,68	-2,21	-3,11
M1···M4	-0.37	-0.81	-0.72	-0,63	-1,04	-0,89
M1···M5	-1.66	-1.30	-1.35	-2,25	-1,81	-1,89
M1···M6	-0.37	-1.51	-2.25	-0,63	-2,20	-3,09
M1···M7	-2.63	-1.80	-1.40	-3,68	-3,52	-3,05
M1···M8	-0.69	-1.44	-1.22	-0,95	-2,15	-1,71
M1···M9	-0.69	-1.43	-1.19	-0,95	-2,14	-1,68
M1···M10	-1.66	-2.20	-2.21	-2,25	-3,17	-3,22
M1···M11	-0.60	-2.20	-2.21	-1,06	-3,17	-3,22
M1···M12	-0.60	-0.42	-0.82	-1,06	-0,50	-1,01
M1···M13	-2.75	-0.87	-1.26	-3,91	-1,16	-1,63
M1···M14	-2.75	-5.69	-6.29	-3,91	-8,43	-9,18
M1···M15	-5.87	-5.25	-5.81	-8,23	-7,64	-8,27
$G_{Cluster}$	-31.61	-34.94	-37.71	-43,15	-49,19	-52,22

[a] Calculated at the MP2/cc-pVTZ level of theory.

Figures

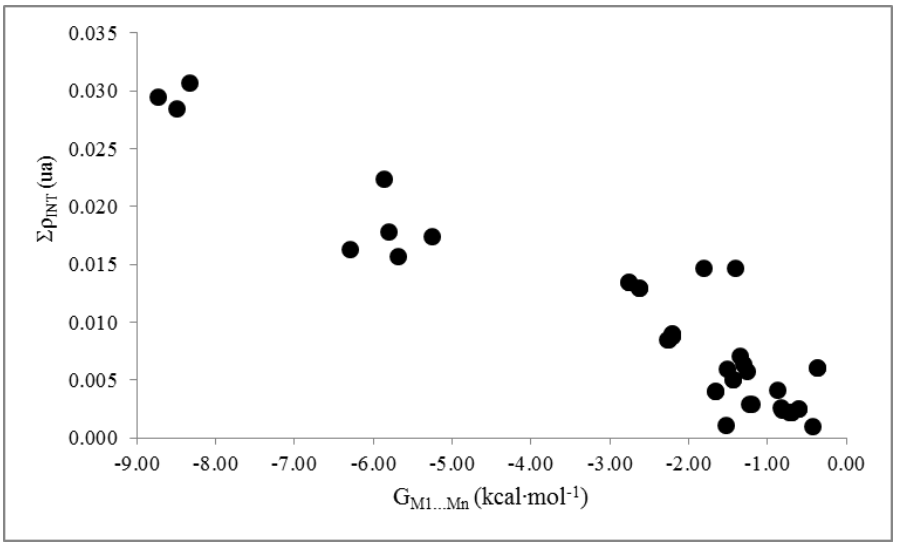


Figure S1. Correlation between the sum of the electron densities of all atoms···atom interactions and sum of energy dimers from the supramolecular cluster of compounds **1-3**.

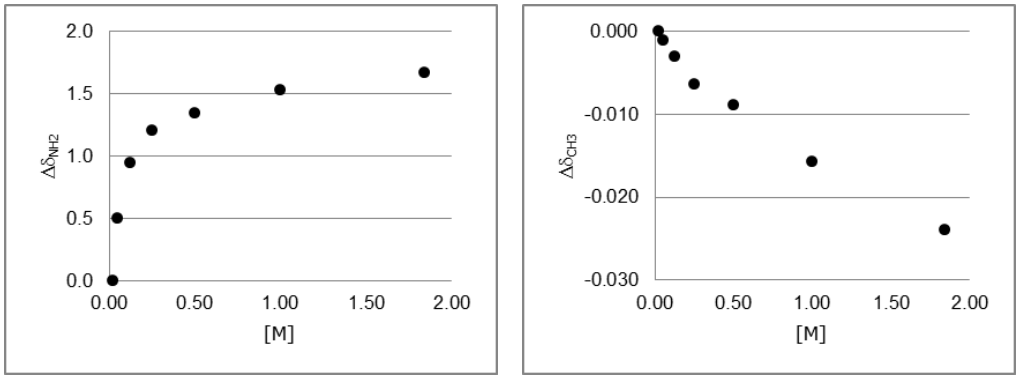


Figure S2.^{1}H NMR chemical shift changes of signals due to 3-NH_2 (K_{ass} = 8.0, $\Delta\delta_{dimer}$= 1.78) and 5-CH_3 (K_{ass} = 0.6, $\Delta\delta_{dimer}$= -0.03) of compound **1** in $CDCl_3$.

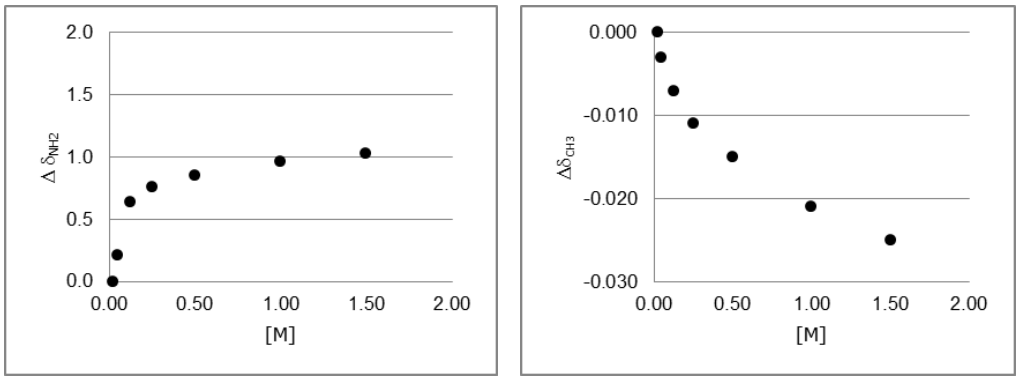
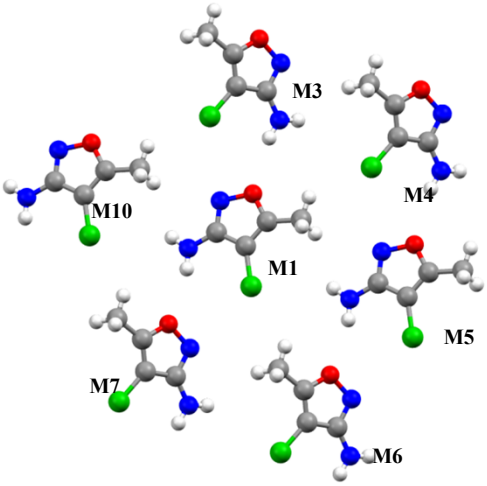
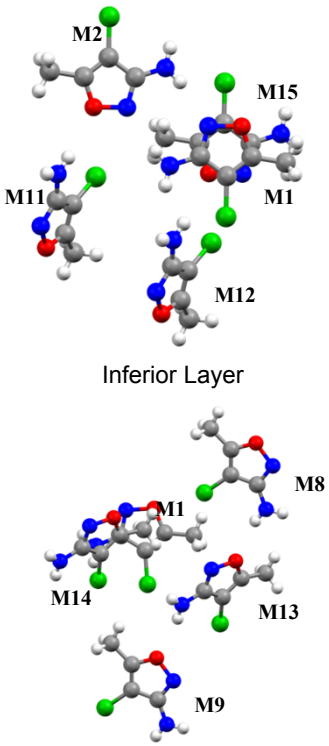


Figure S3.^{1}H NMR chemical shift changes of signals due to 3-NH_2 (K_{ass} = 12.8, $\Delta\delta_{dimer}$= 1.02) and 5-CH_3 (K_{ass} = 2.1, $\Delta\delta_{dimer}$= -0.03) of compound **3** in $CDCl_3$.

Figure S4. Supramolecular clusters showing central, superior, and inferior layer and each dimer separately for compound **1**.

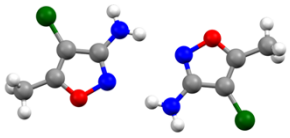


Central Layer

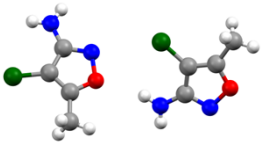


Inferior Layer

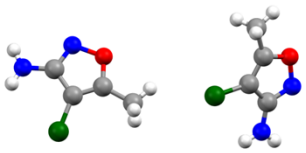
Superior Layer



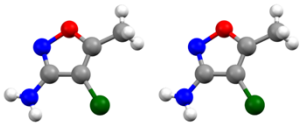
M1···M2



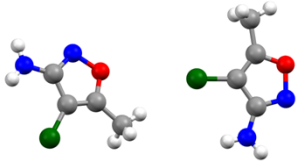
M1···M3 and M1···M7



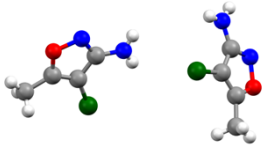
M1···M4 and M1···M6



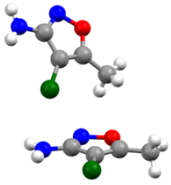
M1···M5 and M1···M10



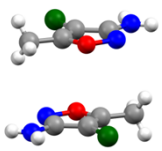
M1···M8 and M1···M9



M1···M11 and M1···M12

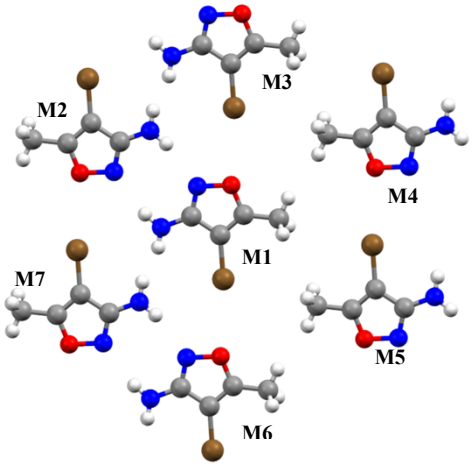


M1···M13 and M1···M14

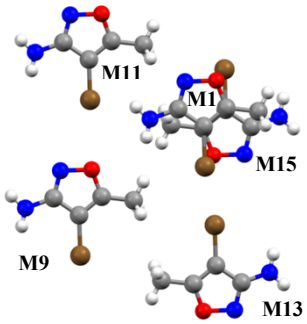


M1···M15

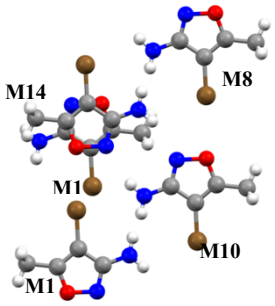
Figure S5. Supramolecular clusters showing central, superior, and inferior layer and each dimer separately for compound **2**.



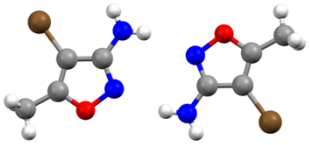
Central layer



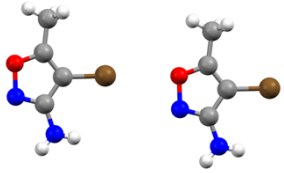
Inferior layer



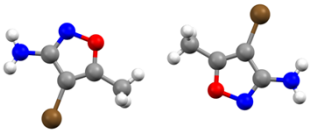
Superior layer



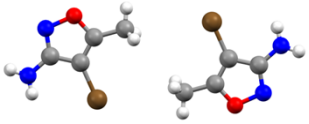
M1···M2



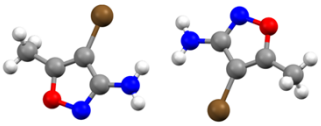
M1···M3 and M1···M6



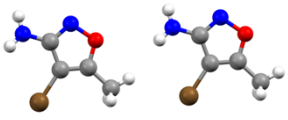
M1···M4



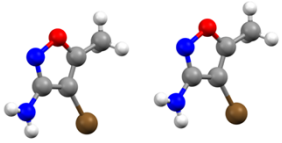
M1···M5



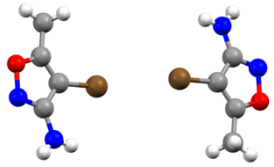
M1···M7



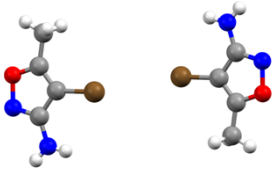
M1···M8 and M1···M9



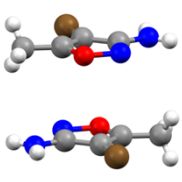
M1···M10 and M1···M11



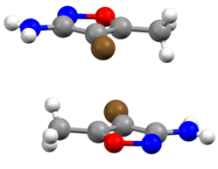
M1···M12



M1···M13

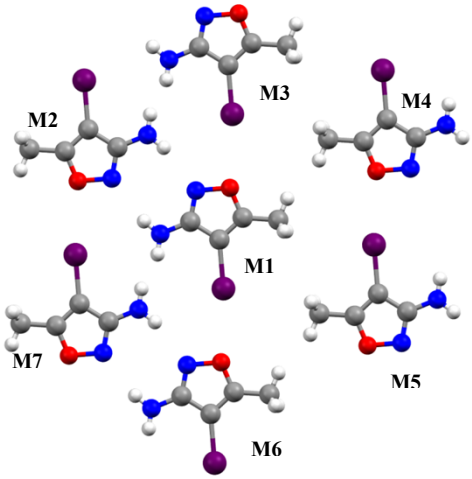


M1···M14

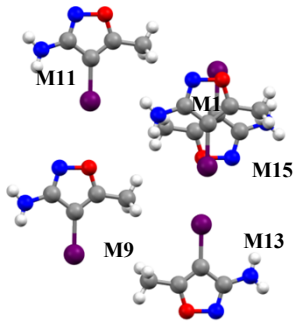


M1···M15

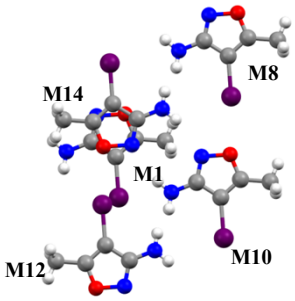
Figure S6. Supramolecular clusters showing central, superior, and inferior layer and each dimer separately for compound **3**.



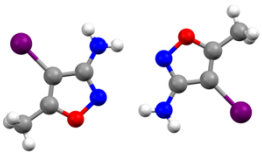
Central Layer



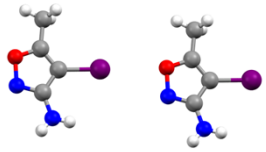
Inferior Layer



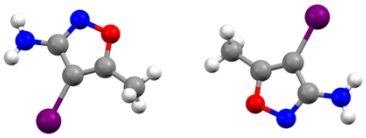
Superior Layer



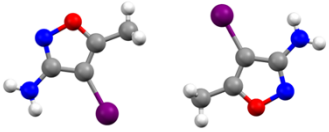
M1···M2



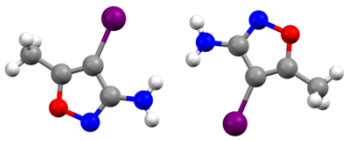
M1···M3 and M1···M6



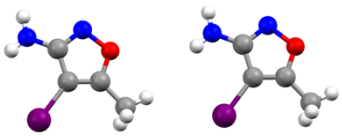
M1···M4



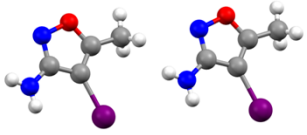
M1···M5



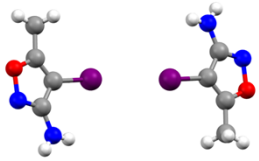
M1···M7



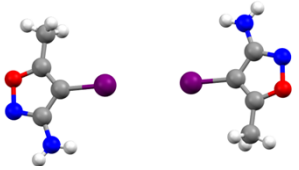
M1···M8 and M1···M9



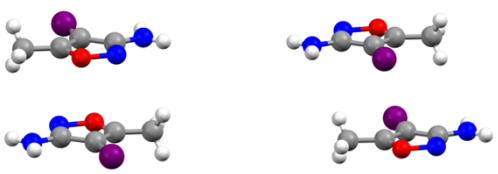
M1···M10 and M1···M11



M1···M12



M1···M13



M1···M14 M1···M15