Table S1 Structural parameters of the BDE49-(D)LYS15 complex

	Bond length (Å)			Bond angle (°)	
	BDE49	BDE49-(D)LYS15		BDE49	BDE49-(D)LYS15
C(20)-N(44)		3.0890	Br(23)-C(22)-C(13)	120.2476	120.7109
C(20)-H(45)		3.8120	Br(23)-C(22)-C(20)	120.5343	119.2434
C(20)-H(46)		2.6570	C(13)-C(22)-C(20)	119.2129	119.6101
C(20)-H(47)		2.4770	H(21)-C(20)-C(22)	119.4751	118.7202
Br(23)-C(22)	1.8722	1.8963	H(21)-C(20)-C(18)	120.3365	120.5328
C(22)-C(13)	1.4209	1.4019	C(22)-C(20)-C(18)	120.1884	120.5599
C(22)-C(20)	1.3965	1.4019	H(19)-C(18)-C(20)	120.2939	120.2559
H(21)-C(20)	1.0842	1.0869	H(19)-C(18)-C(16)	119.7657	119.8822
C(20)-C(18)	1.3888	1.3963	C(20)-C(18)-C(16)	119.9344	119.5973
H(19)-C(18)	1.0842	1.087	Br(17)-C(16)-C(18)	119.1462	119.7109
C(18)-C(16)	1.4113	1.3909	Br(17)-C(16)-C(14)	119.7727	119.9169
Br(17)-C(16)	1.8837	1.8988	C(18)-C(16)-C(14)	121.0693	120.3716
C(16)-C(14)	1.3882	1.3929	H(15)-C(14)-C(16)	120.4072	120.3486
H(15)-C(14)	1.0828	1.0822	H(15)-C(14)-C(13)	120.8315	119.3136
C(14)-C(13)	1.3993	1.4027	C(16)-C(14)-C(13)	118.7003	120.337
C(13)-O(12)	1.3592	1.3771	O(12)-C(13)-C(22)	115.217	126.3598
O(12)-C(8)	1.3498	1.3764	O(12)-C(13)-C(14)	123.748	114.0693
Br(11)-C(3)	1.8735	1.8998	C(22)-C(13)-C(14)	120.8815	119.441
Br(10)-C(9)	1.8771	1.8975	C(8)-O(12)-C(13)	127.0508	119.5288
			Br(10)-C(9)-C(8)	119.8997	120.5569
			Br(10)-C(9)-C(1)	120.3963	119.596
			C(8)-C(9)-C(1)	119.7014	119.8157
			O(12)-C(8)-C(9)	115.4024	126.3484
			O(12)-C(8)-C(6)	124.1224	114.2224

Table S2 Structural parameters of the BDE108-(D)LYS15 complex

	Bond length (Å)		Bond angle (°)	
	BDE108	BDE108-	BDE108	BDE108-

		(D)LYS15			(D)LYS15
C(14)-N(44)		3.7390	H(23)-C(22)-C(13)	121.4887	121.1593
C(14)-H(47)		2.7470	H(23)-C(22)-C(20)	120.7377	119.5376
C(14)-H(46)		3.8580	C(13)-C(22)-C(20)	117.699	119.2939
C(14)-H(45)		4.2030	Br(21)-C(20)-C(22)	119.6274	119.7197
H(23)-C(22)	1.0831	1.0807	Br(21)-C(20)-C(18)	119.2347	119.5195
C(22)-C(13)	1.4034	1.3963	C(22)-C(20)-C(18)	121.1329	120.7603
C(22)-C(20)	1.3907	1.3947	H(19)-C(18)-C(20)	120.3169	120.3006
Br(21)-C(20)	1.891	1.8942	H(19)-C(18)-C(16)	120.2594	120.4272
C(20)-C(18)	1.4011	1.3944	C(20)-C(18)-C(16)	119.4156	119.27
H(19)-C(18)	1.0834	1.0836	Br(17)-C(16)-C(18)	119.0071	121.0612
C(18)-C(16)	1.405	1.394	Br(17)-C(16)-C(14)	119.9775	118.0858
Br(17)-C(16)	1.8873	1.9104	C(18)-C(16)-C(14)	121.0151	120.6655
C(16)-C(14)	1.3888	1.395	H(15)-C(14)-C(16)	121.9216	121.4157
H(15)-C(14)	1.0833	1.0861	H(15)-C(14)-C(13)	120.1817	119.0213
C(14)-C(13)	1.3994	1.3938	C(16)-C(14)-C(13)	117.8921	119.4419
C(13)-O(12)	1.3786	1.3772	O(12)-C(13)-C(22)	121.9663	122.2116
O(12)-C(7)	1.3401	1.3809	O(12)-C(13)-C(14)	115.0368	117.1687
C(8)-C(7)	1.4265	1.4057	C(22)-C(13)-C(14)	122.8136	120.5418
C(7)-C(5)	1.4142	1.3973	C(7)-O(12)-C(13)	124.9492	116.1242
C(5)-C(3)	1.3743	1.3912	Br(9)-C(8)-C(7)	118.4243	118.2229
			Br(9)-C(8)-C(1)	122.0012	122.0211
			C(7)-C(8)-C(1)	119.5666	119.7461
			O(12)-C(7)-C(8)	115.8809	119.9148
			O(12)-C(7)-C(5)	123.1227	119.3613

Table S3 Structural parameters of the BDE155-(D)LYS15 complex

	Bond length (Å)			Bond angle (°)	
	BDE155	BDE155-(D)LYS15		BDE155	BDE155-(D)LYS15
C(8)-N(44)		3.124	O(12)-C(13)-C(14)	124.838	125.3095
C(8)-H(47)		2.566	C(11)-O(12)-C(13)	127.7946	120.6247

C(8)-H(46)		2.625	O(12)-C(11)-C(10)	115.3054	116.1223
C(8)-H(45)		3.917	O(12)-C(11)-C(4)	124.8317	125.2142
C(13)-O(12)	1.3546	1.3771	C(10)-C(11)-C(4)	119.428	118.5339
O(12)-C(11)	1.3546	1.3775	Br(3)-C(10)-C(11)	119.2896	120.2977
C(11)-C(10)	1.4209	1.4087	Br(3)-C(10)-C(8)	120.1462	118.5343
C(11)-C(4)	1.4169	1.4047	C(11)-C(10)-C(8)	120.5478	121.168
C(10)-C(8)	1.3846	1.3966	H(9)-C(8)-C(10)	120.2774	117.577
C(10)-Br(3)	1.8793	1.8908	H(9)-C(8)-C(7)	120.6477	121.7588
H(9)-C(8)	1.083	1.0783	C(10)-C(8)-C(7)	119.0747	119.4056
C(8)-C(7)	1.4001	1.39	Br(2)-C(7)-C(8)	119.5746	119.6936
C(7)-Br(2)	1.875	1.9175	Br(2)-C(7)-C(5)	119.1192	119.8298
C(7)-C(5)	1.4054	1.3925	C(8)-C(7)-C(5)	121.3049	120.4647
H(6)-C(5)	1.0831	1.0827	H(6)-C(5)-C(7)	120.2169	120.5973
C(5)-C(4)	1.3841	1.4021	H(6)-C(5)-C(4)	119.9538	119.161
C(4)-Br(1)	1.8877	1.8983	C(7)-C(5)-C(4)	119.8228	120.2403
			Br(1)-C(4)-C(11)	121.504	126.6316
			Br(1)-C(4)-C(5)	118.5865	113.1384
			C(11)-C(4)-C(5)	119.7984	120.101

Table S4 The atomic charge distribution of BDE49 and BDE49-(D)LYS15 complex

Atomic number	BDE49	BDE49-(D)LYS15
C1	-0.08232	-0.10981
H2	0.17521	0.147928
C3	0.058108	0.065328
C4	-0.0783	-0.0976
H5	0.167936	0.136839
C6	-0.08851	-0.10848
H7	0.160726	0.126843
C8	0.335158	0.285401
C9	0.019216	0.049309
Br10	0.042514	-0.07608

Br11	0.051712	-0.07077
O12	-0.47839	-0.55849
C13	0.33126	0.324578
C14	-0.09894	-0.09614
H15	0.159269	0.145393
C16	0.037691	0.051046
Br17	0.012111	-0.05415
C18	-0.05409	-0.14832
H19	0.169276	0.138594
C20	-0.0823	-0.1777
H21	0.168896	0.13443
C22	0.020709	0.047948
Br23	0.053063	-0.05928
N44		-0.5404

Table S5 The atomic charge distribution of BDE108 and BDE108-(D)LYS15 complex

	BDE108	BDE108-(D)LYS15
O12	-0.47595	-0.55834
C13	0.308028	0.343113
C14	-0.089	-0.1839
H15	0.16611	0.107843
C16	0.038639	0.043022
Br17	0.002811	-0.10335
C18	-0.05481	-0.09832
H19	0.174278	0.14476
C20	0.037914	0.041761
Br21	-0.01075	-0.04644
C22	-0.09698	-0.11287
H23	0.156031	0.154165
N44		-0.54192

Table S6 The atomic charge distribution of BDE155 and BDE155-(D)LYS15 complex

Atomic number	BDE155	BDE155-(D)LYS15
Br1	0.005811	-0.02032
Br2	0.049	-0.05945
Br3	0.037301	-0.04041
C4	0.067605	0.055092
C5	-0.08754	-0.10097
H6	0.174597	0.156163
C7	0.059965	0.050132
C8	-0.0841	-0.1585
H9	0.174903	0.091831
C10	0.024552	0.032679
C11	0.318088	0.331029
O12	-0.48049	-0.54455
C13	0.31819	0.265851
C14	0.06756	0.056747
Br15	0.005867	-0.0705
C16	-0.08753	-0.10431
H17	0.174599	0.147618
C18	0.059972	0.066714
Br19	0.049028	-0.06054
C20	-0.0841	-0.09819
H21	0.174906	0.148335
C22	0.024485	0.037268
Br23	0.037346	-0.0624
N44		-0.55342

Table S7 The atomic coordinates of BDE49-(D)LYS15 complex

Atom	X(Å)	Y(Å)	Z(Å)
C(1)	13.8650	-45.8250	42.9720

H(2)	13.3628	-44.9415	42.5982
C(3)	13.3620	-47.0960	42.6970
C(4)	13.9950	-48.2310	43.1950
H(5)	13.5865	-49.2153	42.9986
C(6)	15.1540	-48.0890	43.9580
H(7)	15.6409	-48.9610	44.3819
C(8)	15.6970	-46.8200	44.2100
C(9)	15.0270	-45.6820	43.7420
Br(10)	15.7111	-43.9474	44.0931
Br(11)	11.7903	-47.2684	41.6446
O(12)	16.8330	-46.8360	44.9870
C(13)	18.0640	-46.6680	44.3930
C(14)	18.3390	-47.5930	43.3750
H(15)	17.6054	-48.3514	43.1366
C(16)	19.5410	-47.5310	42.6740
Br(17)	19.9146	-48.8087	41.3208
C(18)	20.4740	-46.5410	42.9640
H(19)	21.3736	-46.4519	42.3614
C(20)	20.1900	-45.5930	43.9490
H(21)	20.8642	-44.7594	44.1239
C(22)	18.9810	-45.6410	44.6570
Br(23)	18.7072	-44.4461	46.1034
N(24)	19.0690	-52.6360	46.3190
H(25)	19.0365	-53.5369	46.7895
H(26)	18.4584	-52.7188	45.5067
C(27)	18.4990	-51.5980	47.1970
H(28)	18.8617	-51.7619	48.2200
C(29)	16.9700	-51.6720	47.1980
H(30)	16.4271	-51.4123	48.1297
O(31)	16.3630	-51.9600	46.1710

C(32)	18.9060	-50.1920	46.7420
H(33)	18.2967	-49.4529	47.2834
H(34)	18.6219	-50.0976	45.6852
C(35)	20.3700	-49.8500	46.9110
H(36)	20.9687	-50.5965	46.3752
H(37)	20.6525	-49.9213	47.9702
C(38)	20.6540	-48.4620	46.3850
H(39)	20.0924	-47.7043	46.9472
H(40)	20.3016	-48.4060	45.3470
C(41)	22.1380	-48.1350	46.4080
H(42)	22.7200	-48.9365	45.9451
H(43)	22.5233	-47.9754	47.4182
N(44)	22.4340	-46.9000	45.6220
H(45)	23.4392	-46.7383	45.5053
H(46)	22.0299	-46.0716	46.0746
H(47)	21.9828	-46.9415	44.6913

Table S8 The atomic coordinates of BDE108-(D)LYS15 complex

Atom	X(Å)	Y(Å)	Z(Å)
C(1)	15.4680	-44.3920	42.7170
C(2)	14.9730	-45.4860	43.4520
C(3)	15.8410	-46.4780	43.9230
H(4)	15.4363	-47.3069	44.4919
C(5)	17.2050	-46.3980	43.6610
H(6)	17.8771	-47.1679	44.0235
C(7)	17.7060	-45.3280	42.9150
C(8)	16.8500	-44.3110	42.4580
Br(9)	17.6041	-42.8812	41.4771
Br(10)	14.3047	-43.0471	42.0901
Br(11)	13.1275	-45.6658	43.8404

O(12)	19.0660	-45.2340	42.6950
C(13)	19.6620	-46.3270	42.1060
C(14)	21.0510	-46.4130	42.1830
H(15)	21.6034	-45.6067	42.6566
C(16)	21.7060	-47.4870	41.5800
Br(17)	23.5894	-47.6586	41.8506
C(18)	20.9870	-48.4610	40.8890
H(19)	21.4984	-49.3010	40.4339
C(20)	19.6000	-48.3490	40.7990
Br(21)	18.6180	-49.6574	39.8441
C(22)	18.9300	-47.2830	41.3990
H(23)	17.8575	-47.2011	41.2944
N(24)	19.0690	-52.6360	46.3190
H(25)	19.0393	-53.5371	46.7925
H(26)	18.4537	-52.7229	45.5089
C(27)	18.4990	-51.5980	47.1970
H(28)	18.8640	-51.7626	48.2195
C(29)	16.9700	-51.6720	47.1980
H(30)	16.4262	-51.4126	48.1295
O(31)	16.3630	-51.9600	46.1710
C(32)	18.9060	-50.1920	46.7420
H(33)	18.2972	-49.4543	47.2884
H(34)	18.6199	-50.0968	45.6846
C(35)	20.3700	-49.8500	46.9110
H(36)	20.9694	-50.5964	46.3749
H(37)	20.6542	-49.9175	47.9706
C(38)	20.6540	-48.4620	46.3850
H(39)	20.0990	-47.7083	46.9614
H(40)	20.2949	-48.3950	45.3465

C(41)	22.1380	-48.1350	46.4080
H(42)	22.7335	-48.9311	45.9531
H(43)	22.5100	-47.9637	47.4218
N(44)	22.4340	-46.9000	45.6220
H(45)	23.4143	-46.6051	45.7146
H(46)	21.8452	-46.1103	45.9160
H(47)	22.2667	-47.0443	44.6108

Table S9 The atomic coordinates of BDE155-(D)LYS15 complex

BDE49-(D)LYS108 complex			
Atom	X(Å)	Y(Å)	Z(Å)
Br(1)	15.4568	-44.3405	44.9361
Br(2)	20.8481	-44.0187	46.4080
Br(3)	19.4841	-47.4190	42.0620
C(4)	17.2130	-44.9360	44.5300
C(5)	18.1880	-44.3980	45.3820
H(6)	17.8887	-43.6940	46.1482
C(7)	19.5220	-44.7740	45.2470
C(8)	19.9040	-45.6740	44.2590
H(9)	20.9380	-45.8117	43.9858
C(10)	18.9340	-46.2160	43.4130
C(11)	17.5730	-45.8820	43.5560
O(12)	16.7080	-46.4630	42.6550
C(13)	15.5680	-45.8040	42.2520
C(14)	15.5380	-44.6400	41.4690
Br(15)	17.1644	-43.8923	40.8416
C(16)	14.3120	-44.0450	41.1370
H(17)	14.3038	-43.1597	40.5128
C(18)	13.1210	-44.5870	41.6110
Br(19)	11.4717	-43.7675	41.1540

C(20)	13.1310	-45.7120	42.4260
H(21)	12.2081	-46.1235	42.8158
C(22)	14.3520	-46.3100	42.7510
Br(23)	14.3648	-47.7928	43.9276
N(24)	19.0690	-52.6360	46.3190
H(25)	19.0211	-53.5400	46.7857
H(26)	18.4624	-52.7101	45.5011
C(27)	18.4990	-51.5980	47.1970
H(28)	18.8642	-51.7638	48.2193
C(29)	16.9700	-51.6720	47.1980
H(30)	16.4261	-51.4110	48.1293
O(31)	16.3630	-51.9600	46.1710
C(32)	18.9060	-50.1920	46.7420
H(33)	18.2979	-49.4545	47.2891
H(34)	18.6180	-50.0937	45.6858
C(35)	20.3700	-49.8500	46.9110
H(36)	20.9695	-50.5965	46.3748
H(37)	20.6541	-49.9201	47.9707
C(38)	20.6540	-48.4620	46.3850
H(39)	20.0982	-47.7049	46.9537
H(40)	20.2935	-48.3998	45.3473
C(41)	22.1380	-48.1350	46.4080
H(42)	22.7293	-48.9365	45.9561
H(43)	22.5128	-47.9640	47.4209
N(44)	22.4340	-46.9000	45.6220
H(45)	23.4404	-46.6923	45.6099
H(46)	21.9572	-46.0558	46.0014
H(47)	22.1348	-47.0211	44.6503