Supporting Information for

Transport of anions across dialytic membrane induced by complexation towards dendritic receptors

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Spectral characterization of compounds

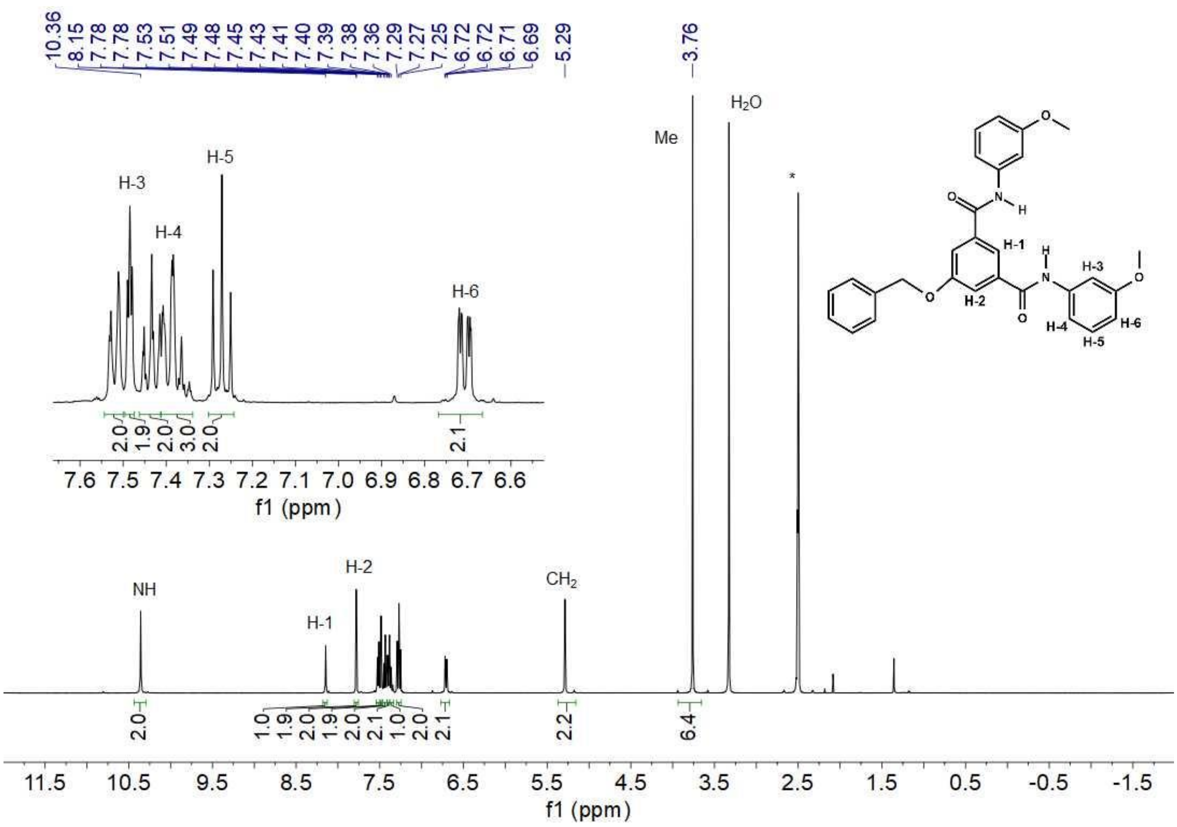

Figure S1. Receptor **M1** ^{1}H NMR (400 MHz), DMSO-d_6.

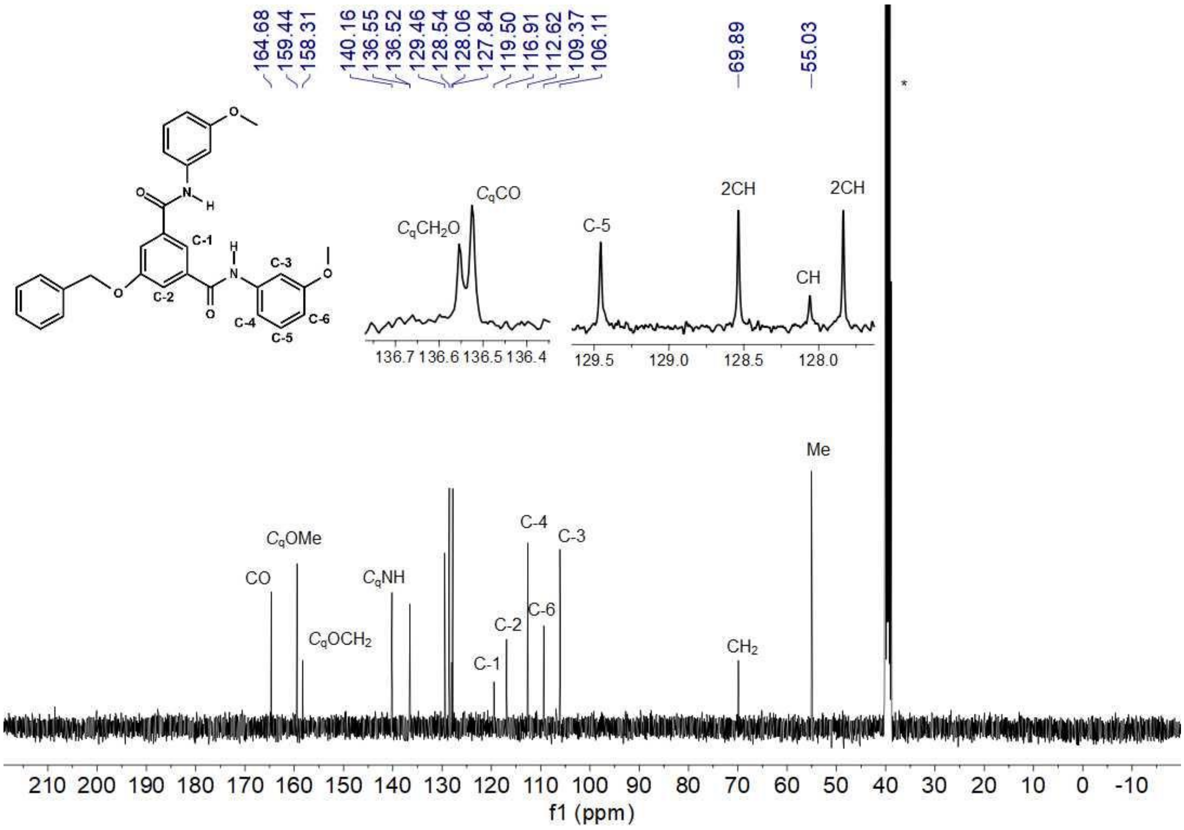

Figure S2. Receptor **M1** ^{13}C NMR (101 MHz), DMSO-d_6.

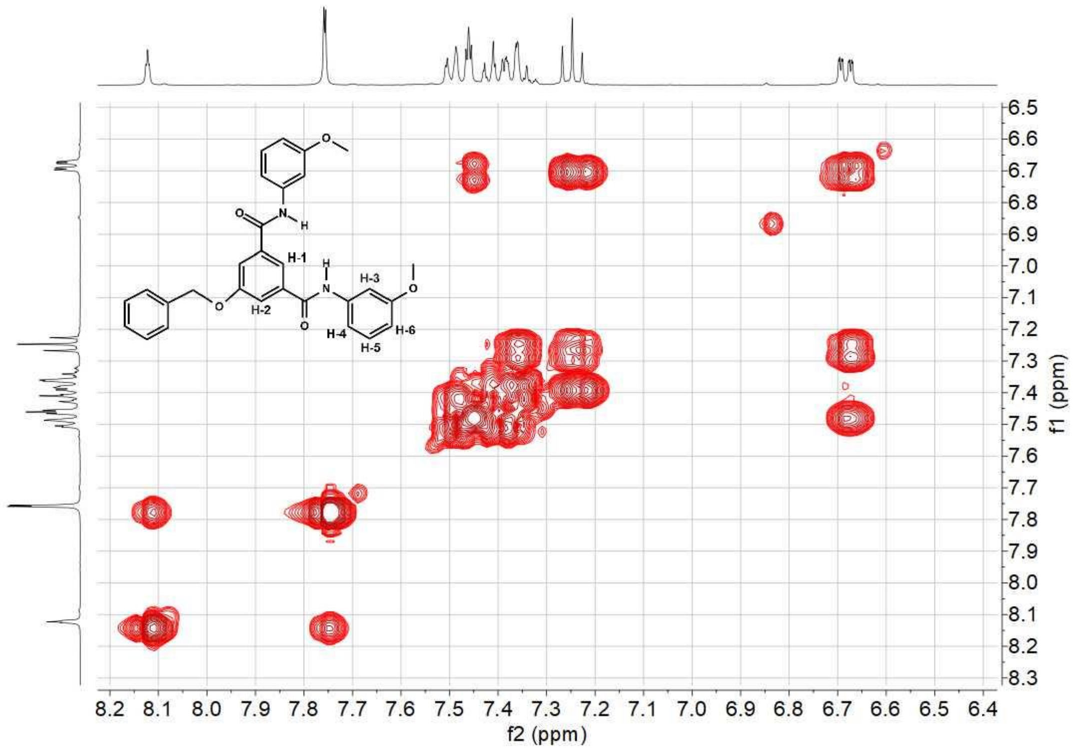

Figure S3. Receptor **M1** ^{1}H-^{1}H COSY (400 MHz), DMSO-*d$_6$*.

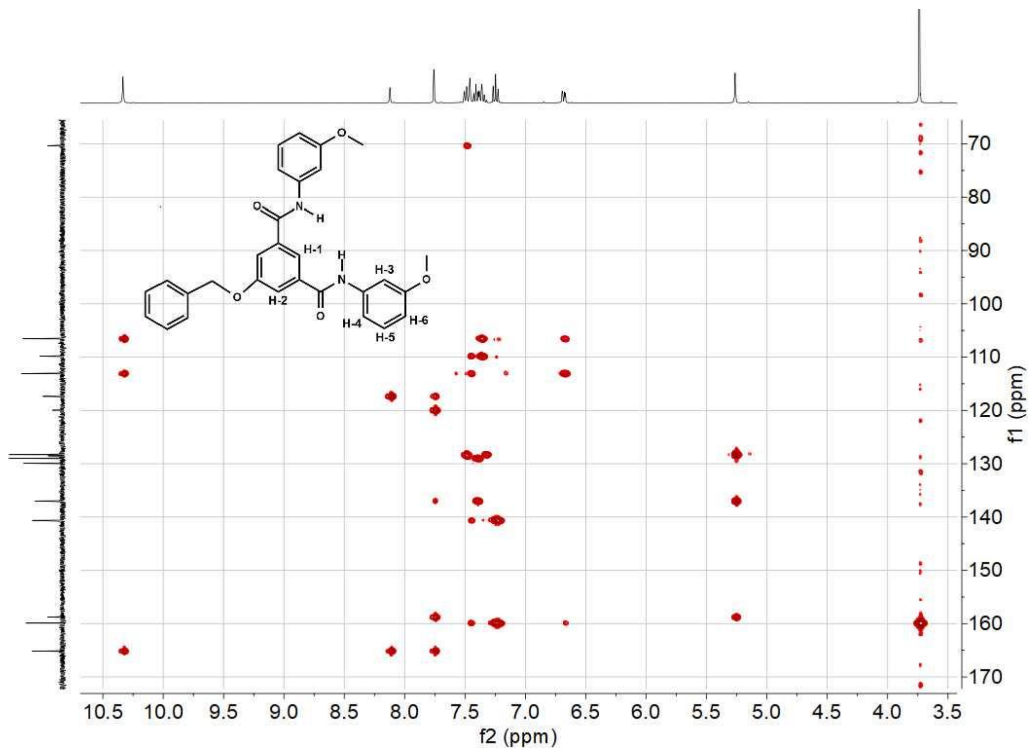

Figure S4. Receptor **M1** ^{1}H-^{13}C HMBC (400, 101 MHz), DMSO-*d$_6$*.

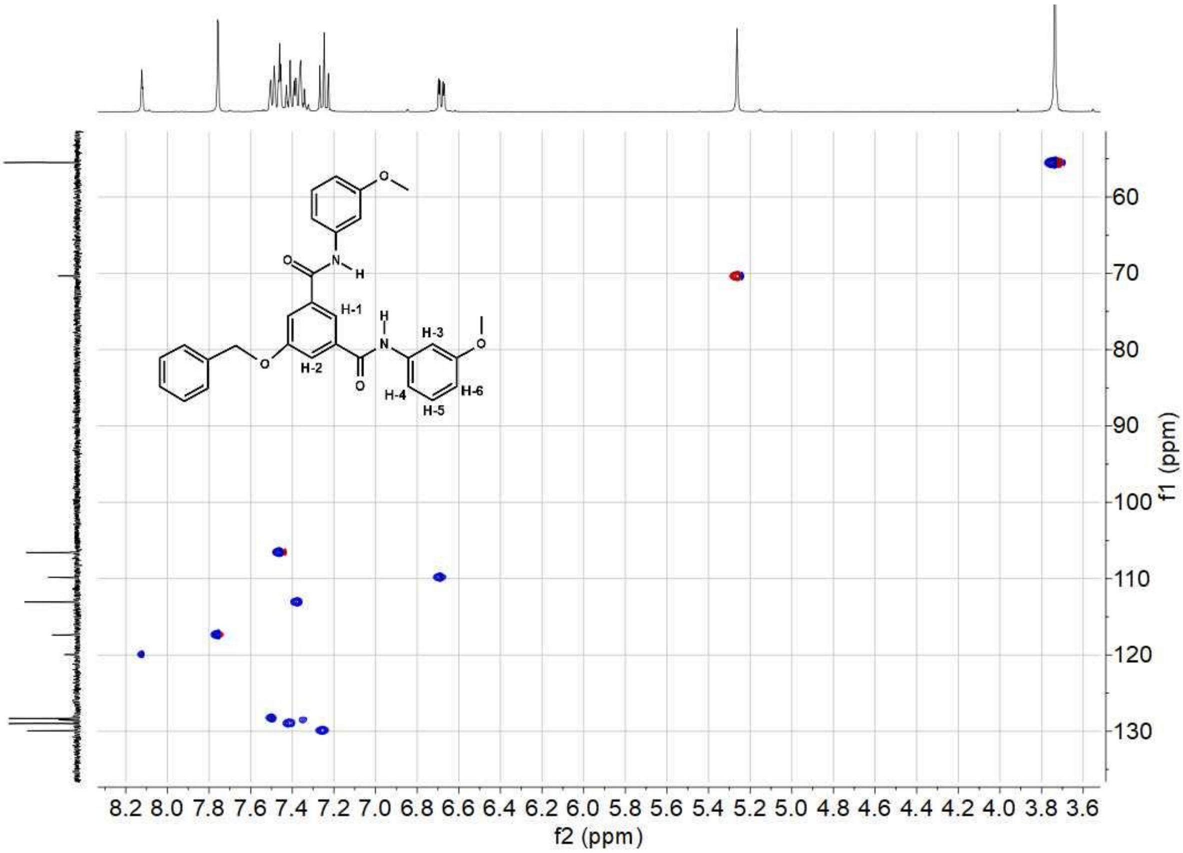

Figure S5. Receptor **M1** ^{1}H-^{13}C HSQC (400, 101 MHz), DMSO-*d₆*.

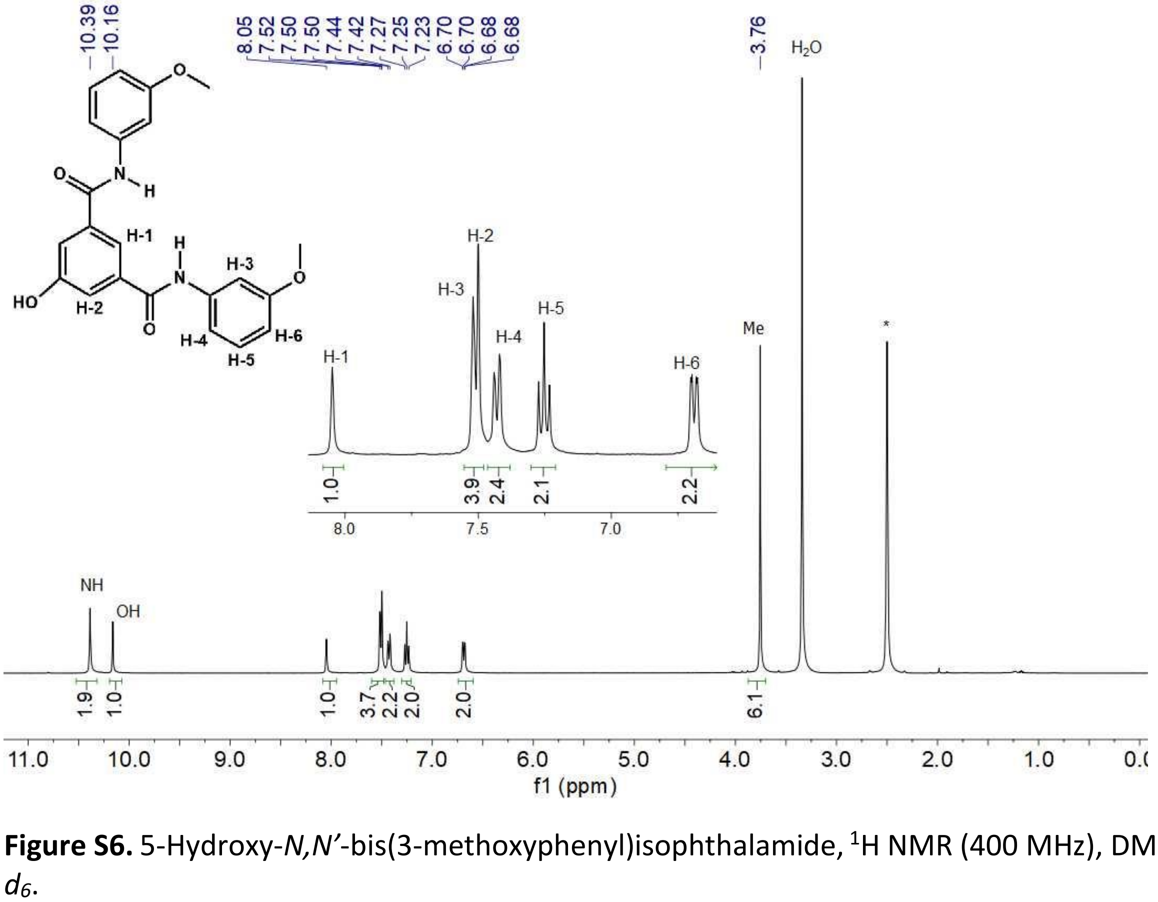

Figure S6. 5-Hydroxy-*N,N′*-bis(3-methoxyphenyl)isophthalamide, ^{1}H NMR (400 MHz), DMSO-*d₆*.

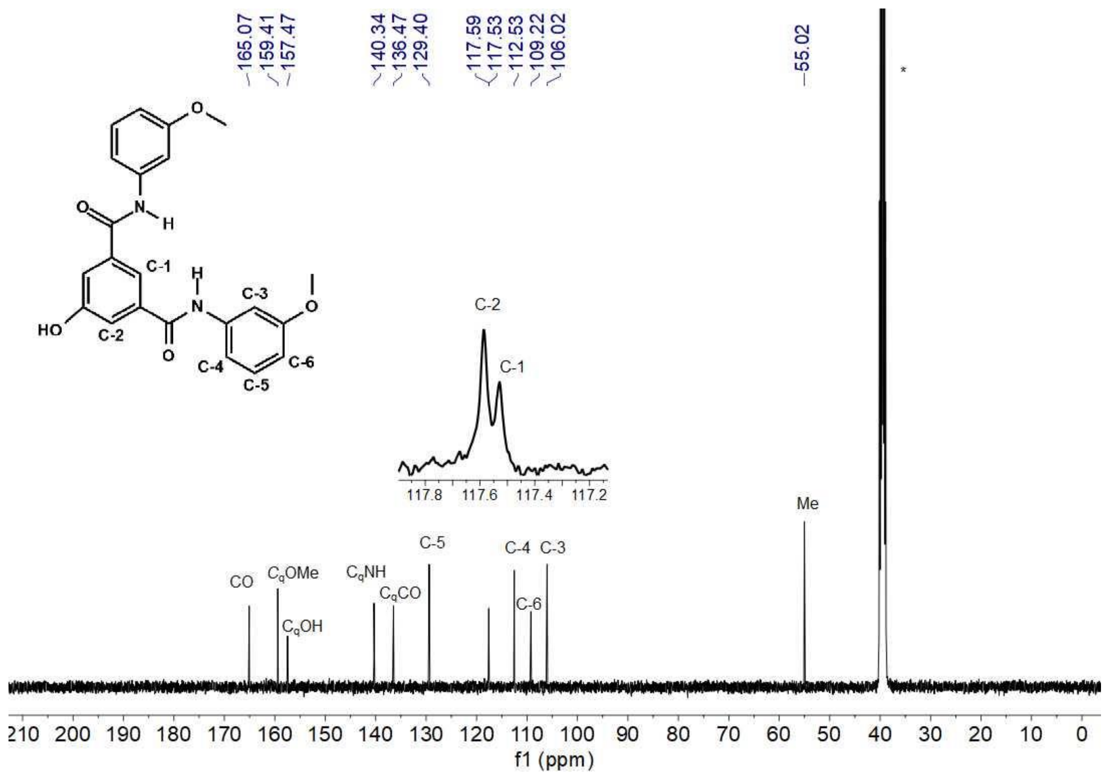

Figure S7. 5-Hydroxy-*N,N'*-bis(3-methoxyphenyl)isophthalamide, ^{13}C NMR (101 MHz), DMSO-d_6.

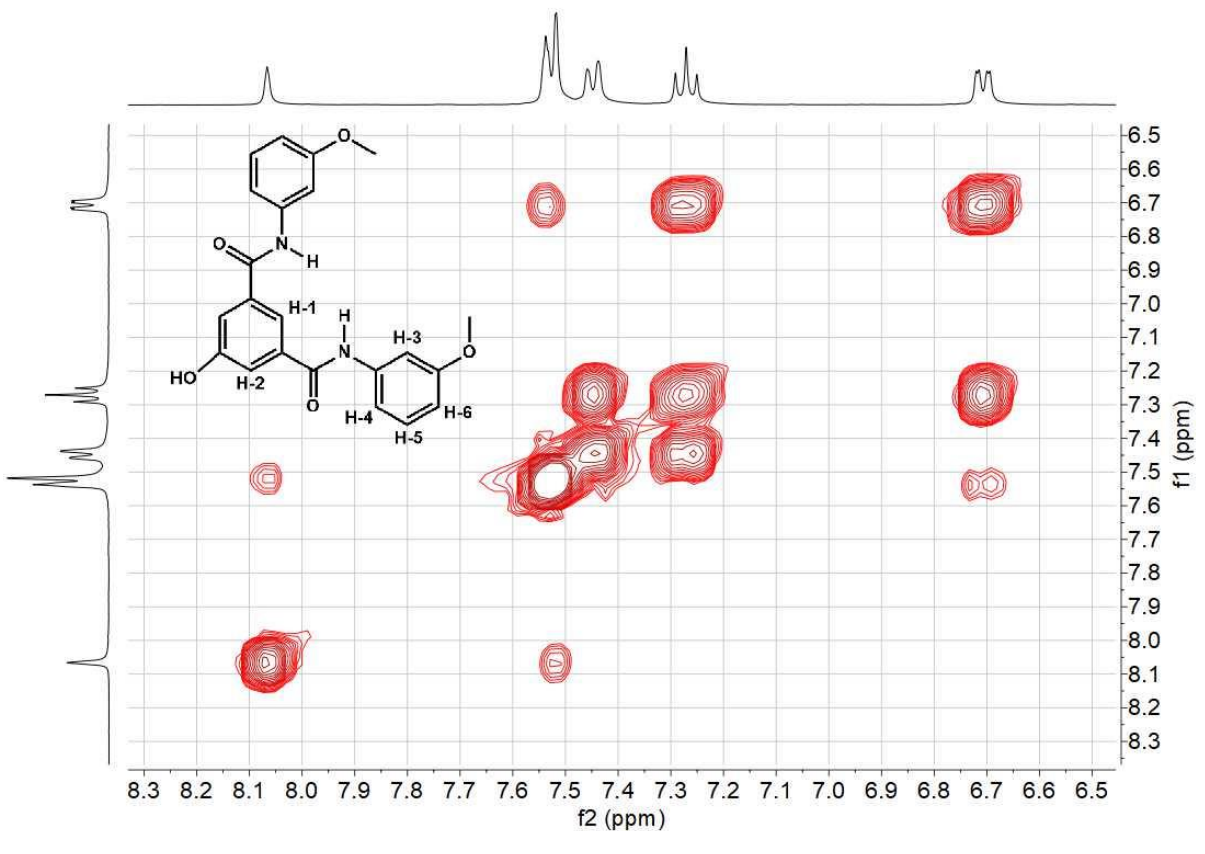

Figure S8. 5-Hydroxy-*N,N'*-bis(3-methoxyphenyl)isophthalamide, ^{1}H-^{1}H COSY (400 MHz), DMSO-d_6

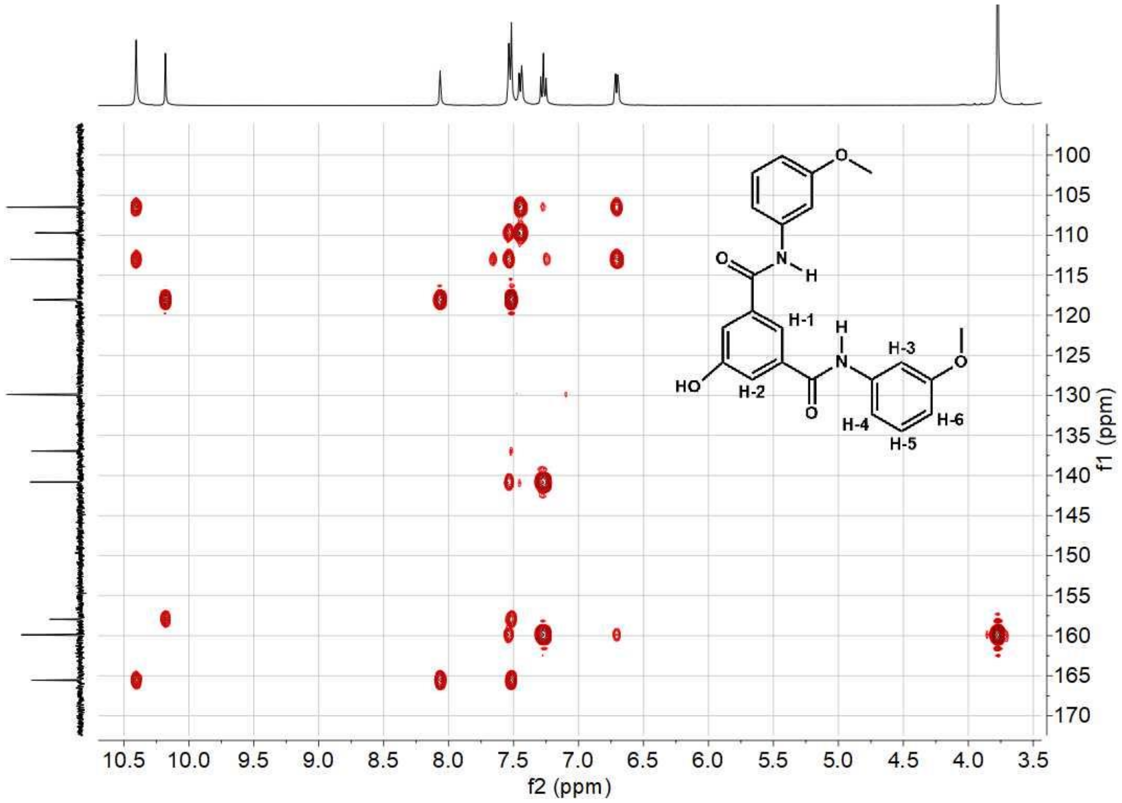

Figure S9. 5-Hydroxy-*N,N'*-bis(3-methoxyphenyl)isophthalamide, ^{1}H-^{13}C HMBC (400, 101 MHz), DMSO-d_6.

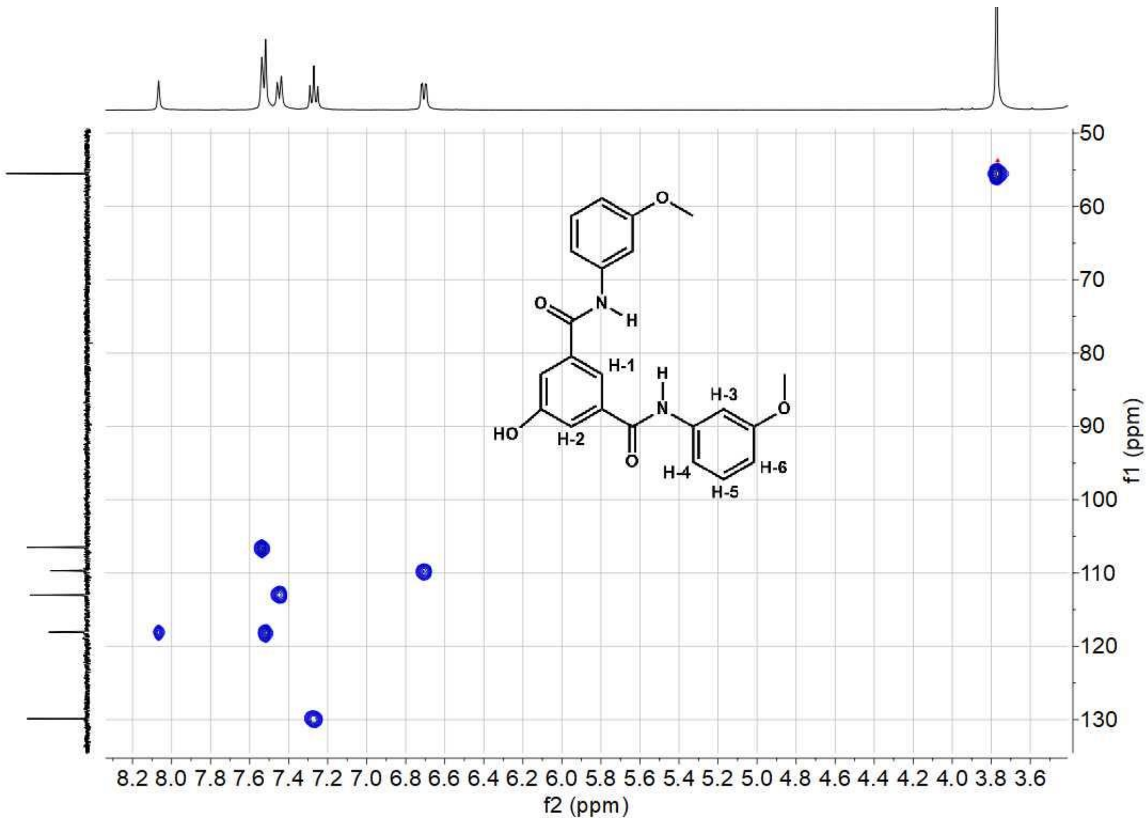

Figure S10. 5-Hydroxy-*N,N'*-bis(3-methoxyphenyl)isophthalamide, ^{1}H-^{13}C HSQC (400, 101 MHz), DMSO-d_6.

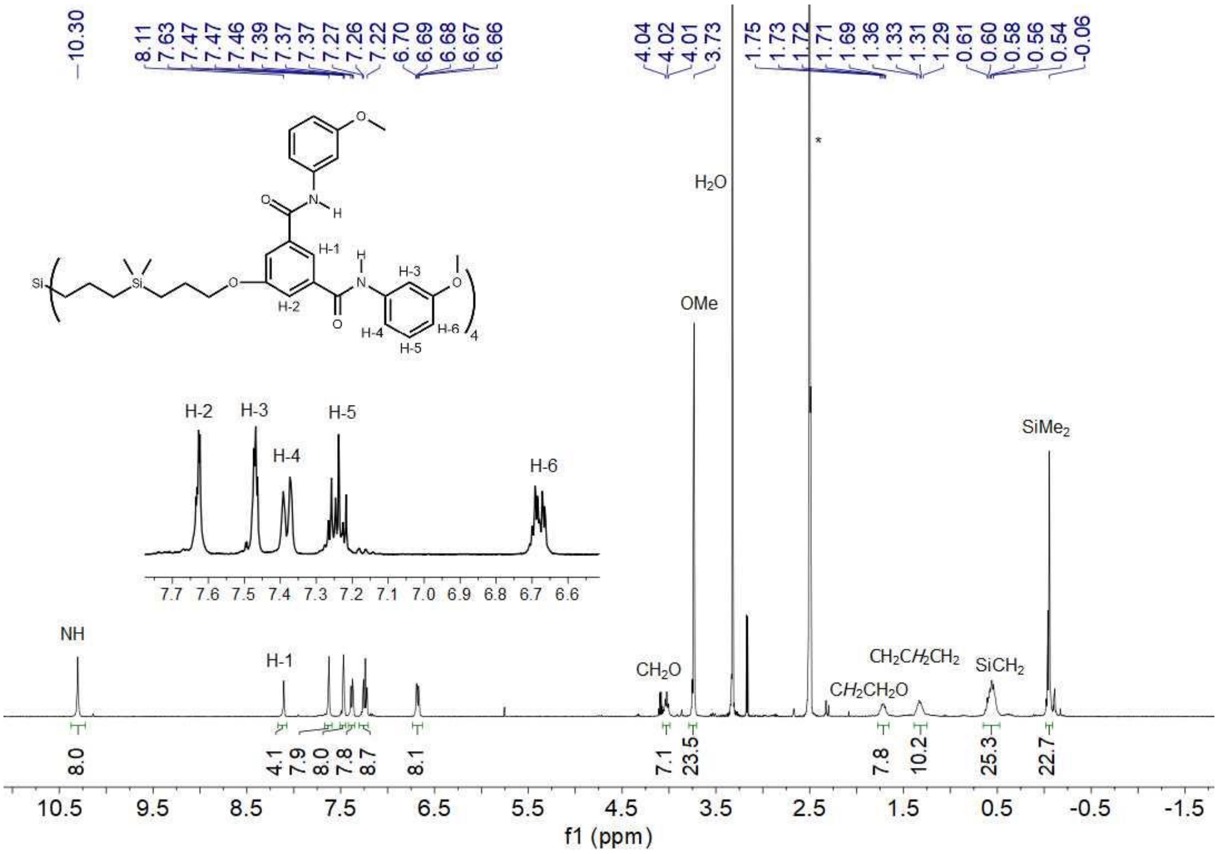

Figure S11. Receptor **Dm1** ^{1}H NMR (400 MHz), DMSO-*d$_6$*.

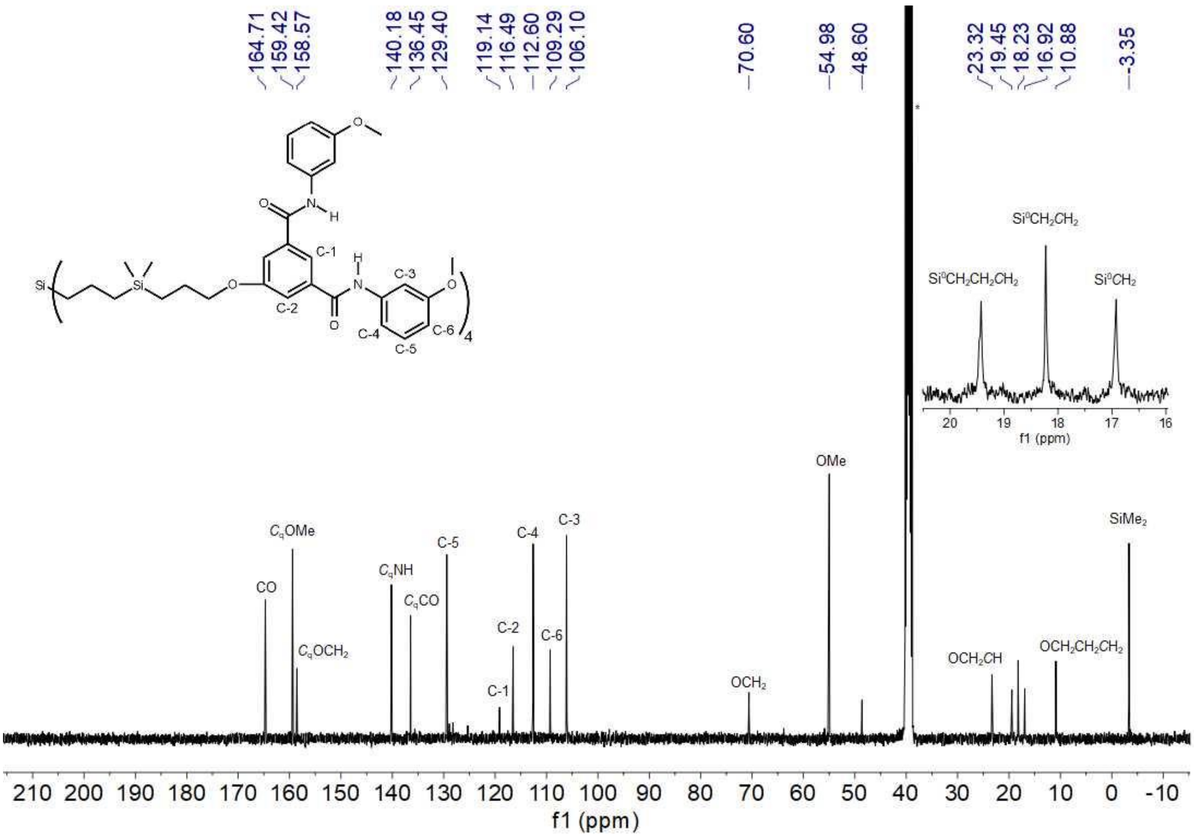

Figure S12. Receptor **Dm1** ^{13}C NMR (101 MHz), DMSO-*d$_6$*.

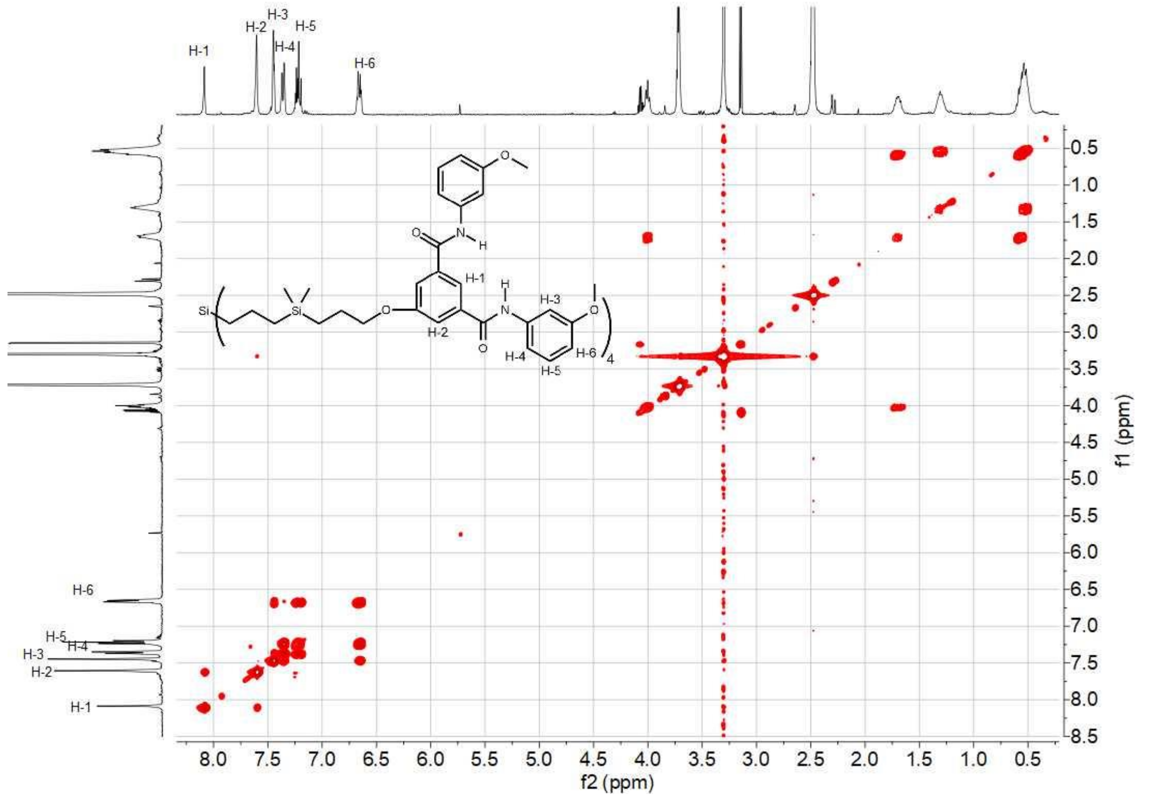

Figure S13. Receptor **Dm1** ^{1}H-^{1}H COSY (400 MHz), DMSO-d_6.

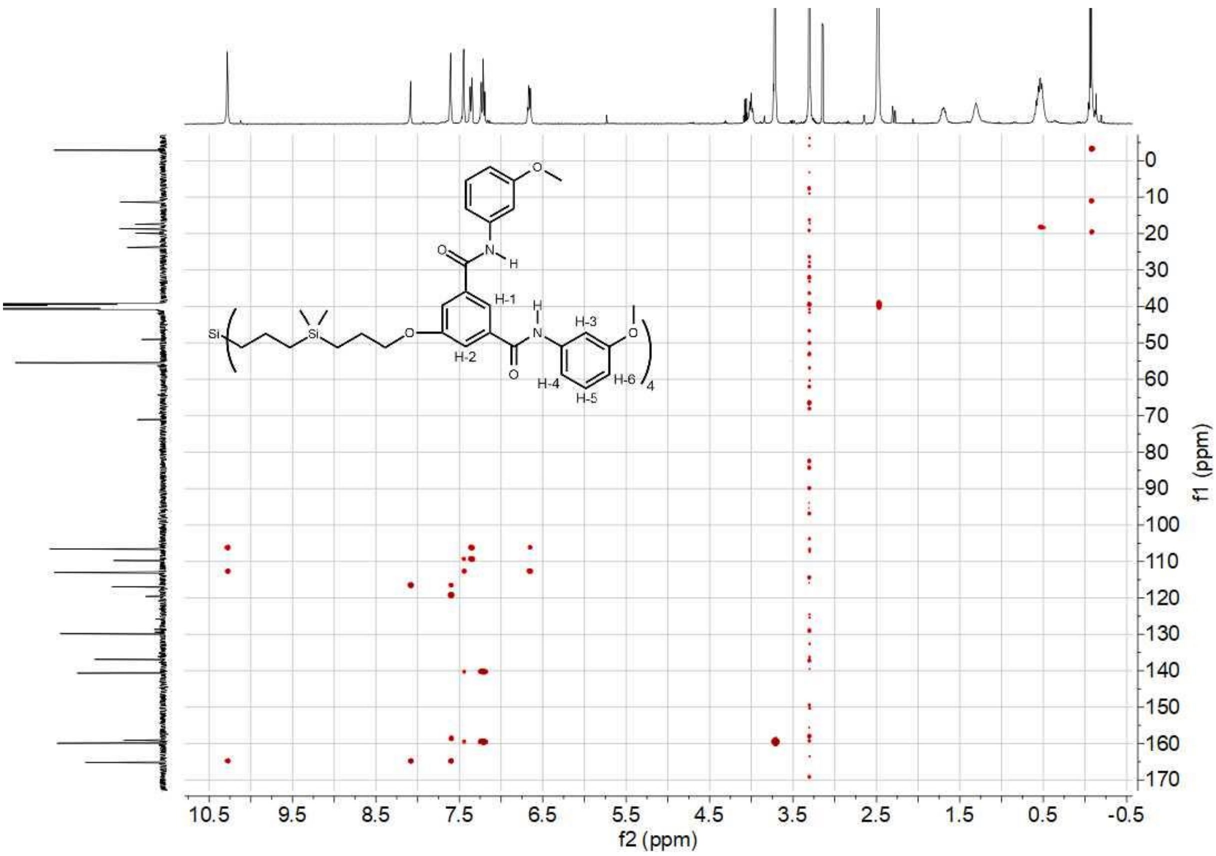

Figure S14. Receptor **Dm1** ^{1}H-^{13}C HMBC (400, 101 MHz), DMSO-d_6.

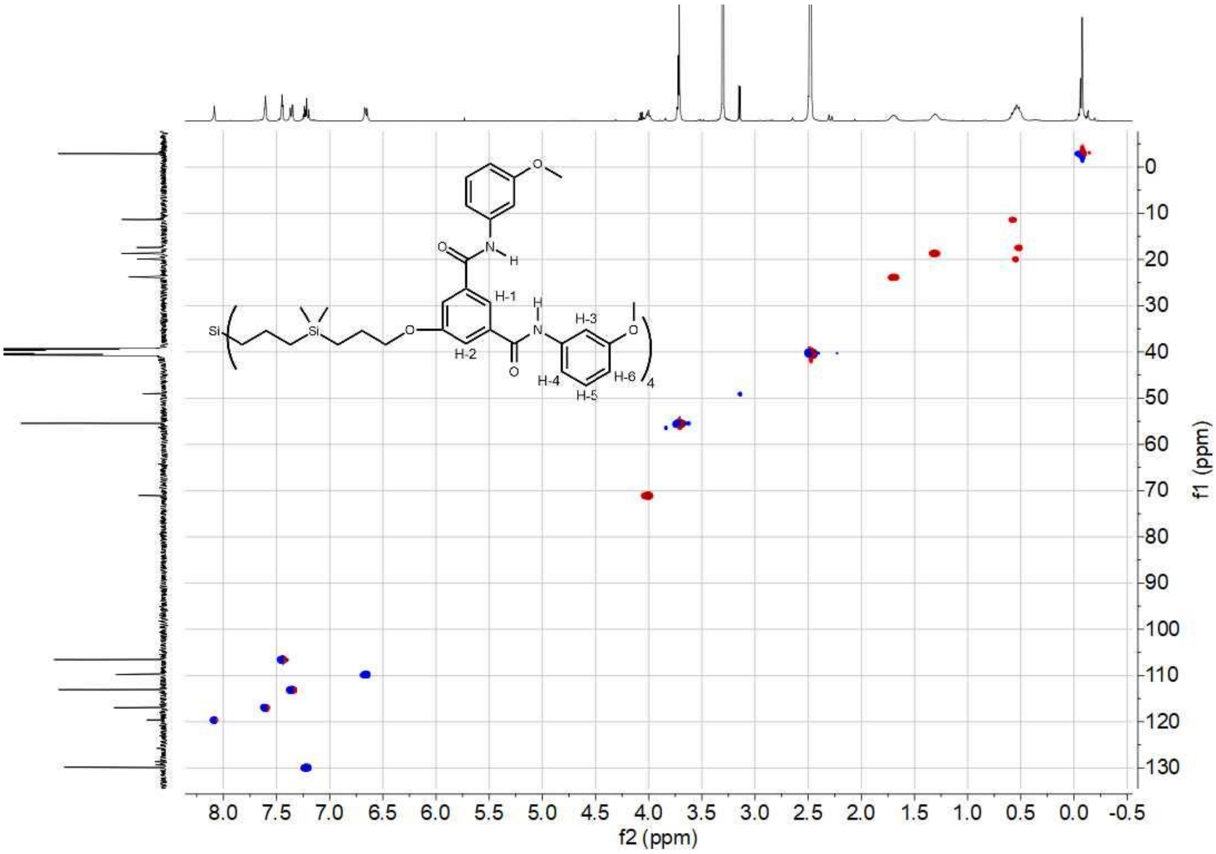

Figure S15. Receptor **Dm1** ^{1}H-^{13}C HSQC (400, 101 MHz), DMSO-d_6.

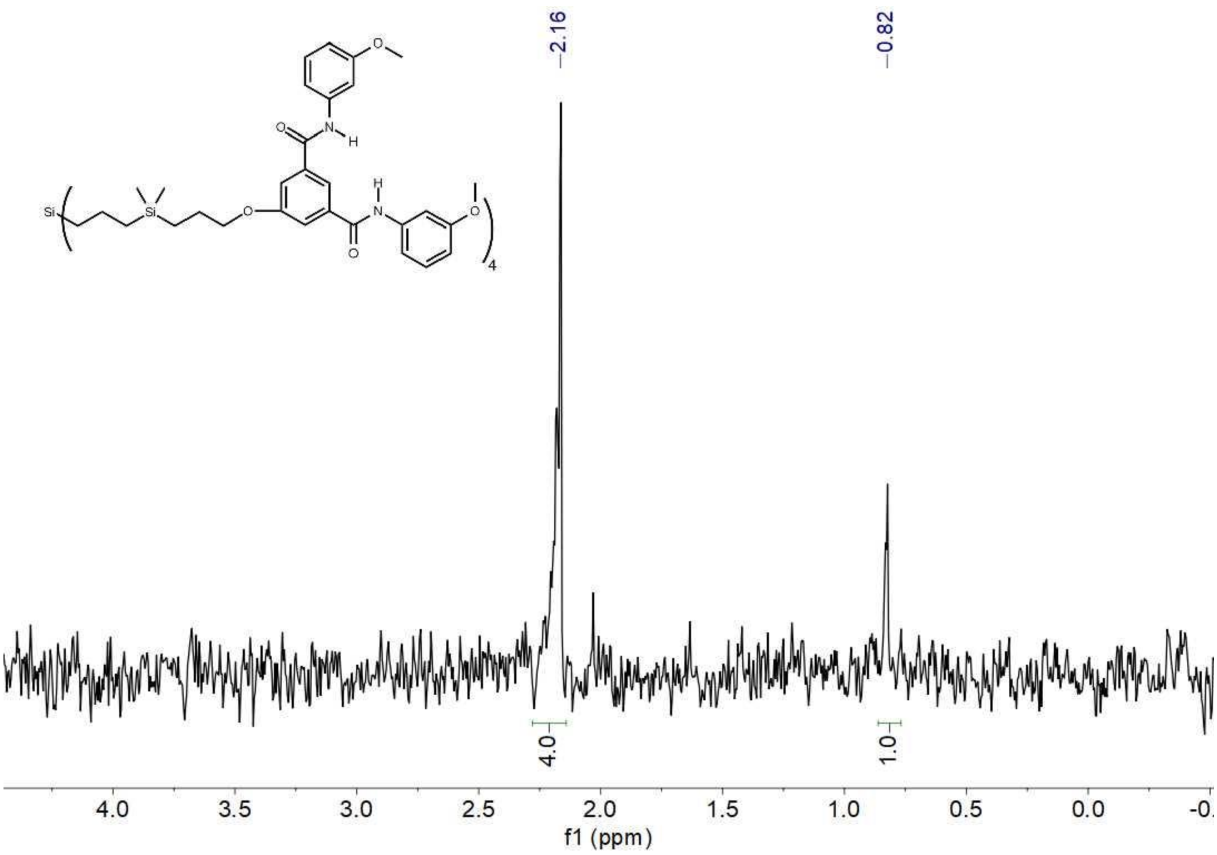

Figure S16. Receptor **Dm1** ^{29}Si NMR (80 MHz), DMSO-d_6.

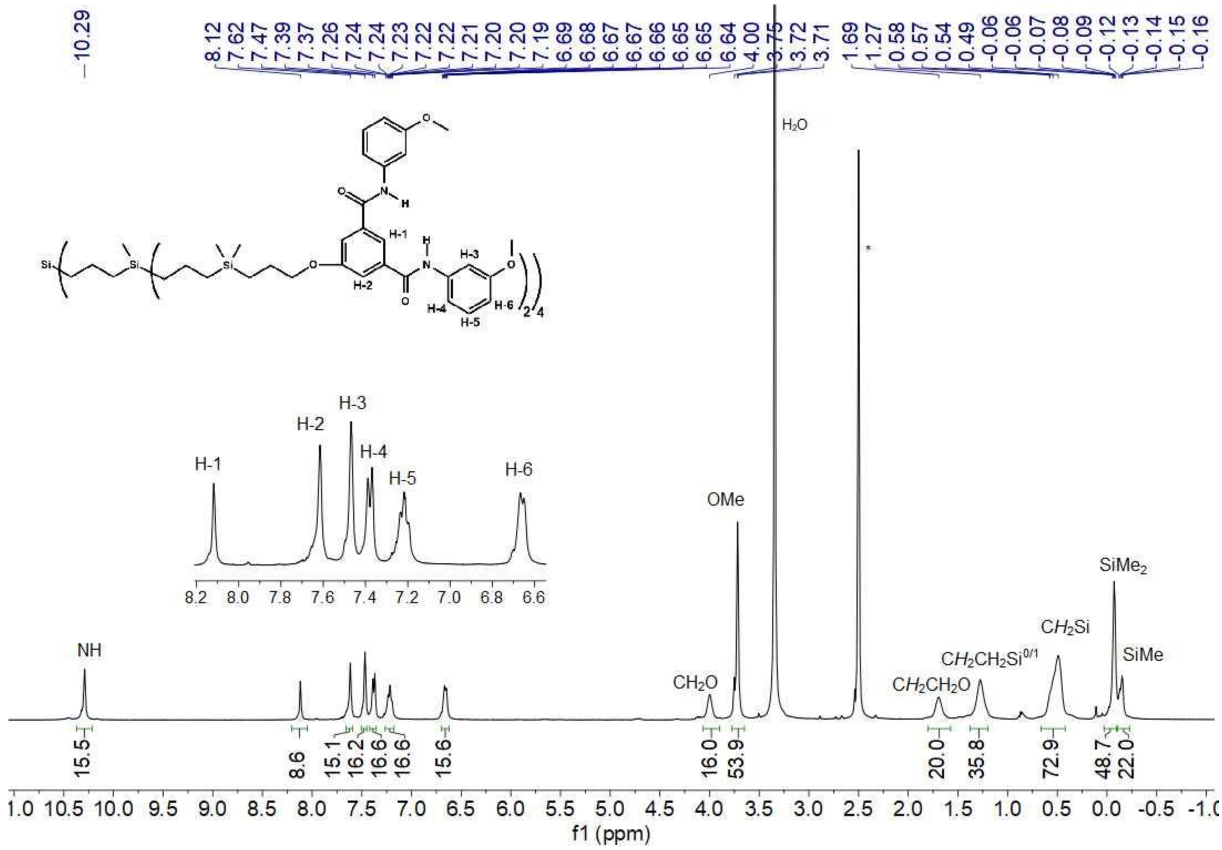

Figure S17. Receptor **Dm2** ^{1}H NMR (400 MHz), DMSO-*d$_6$.*

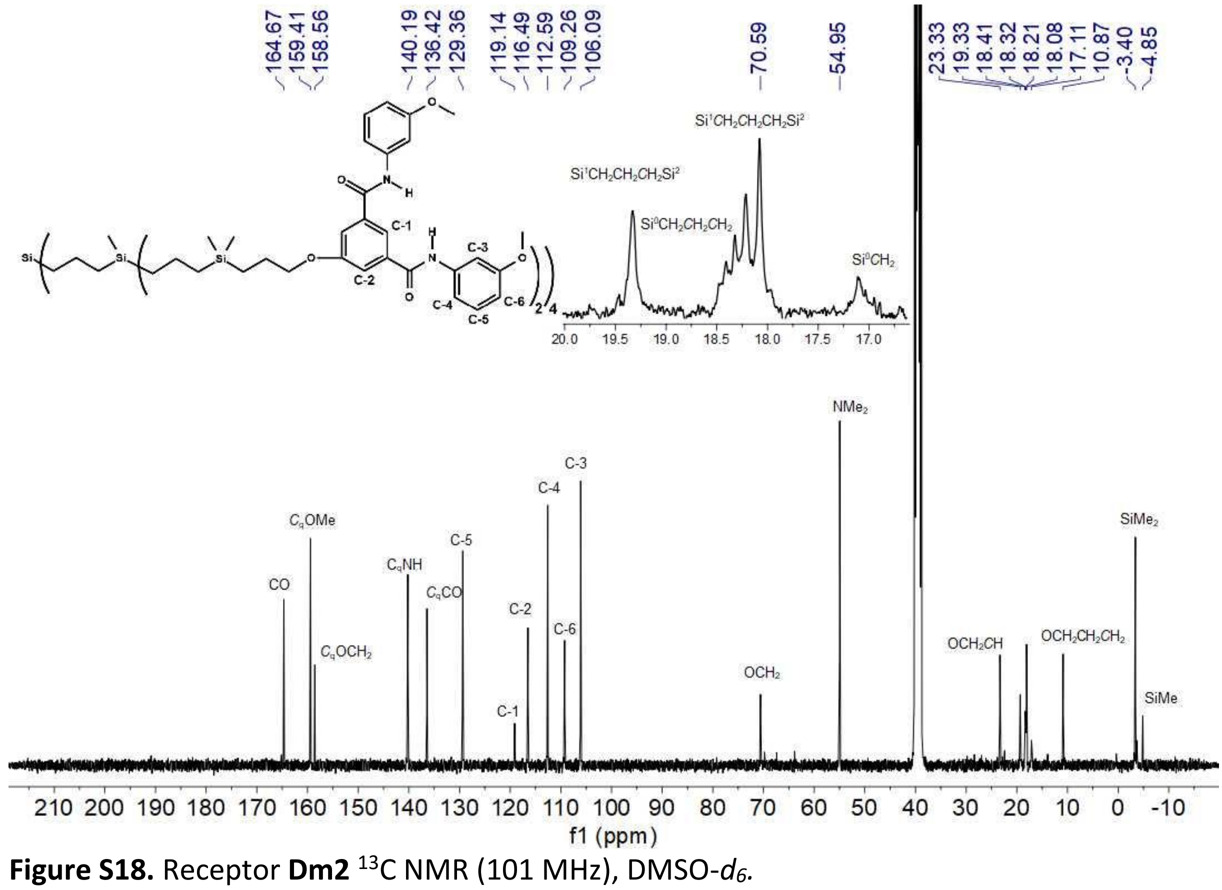

Figure S18. Receptor **Dm2** ^{13}C NMR (101 MHz), DMSO-*d$_6$.*

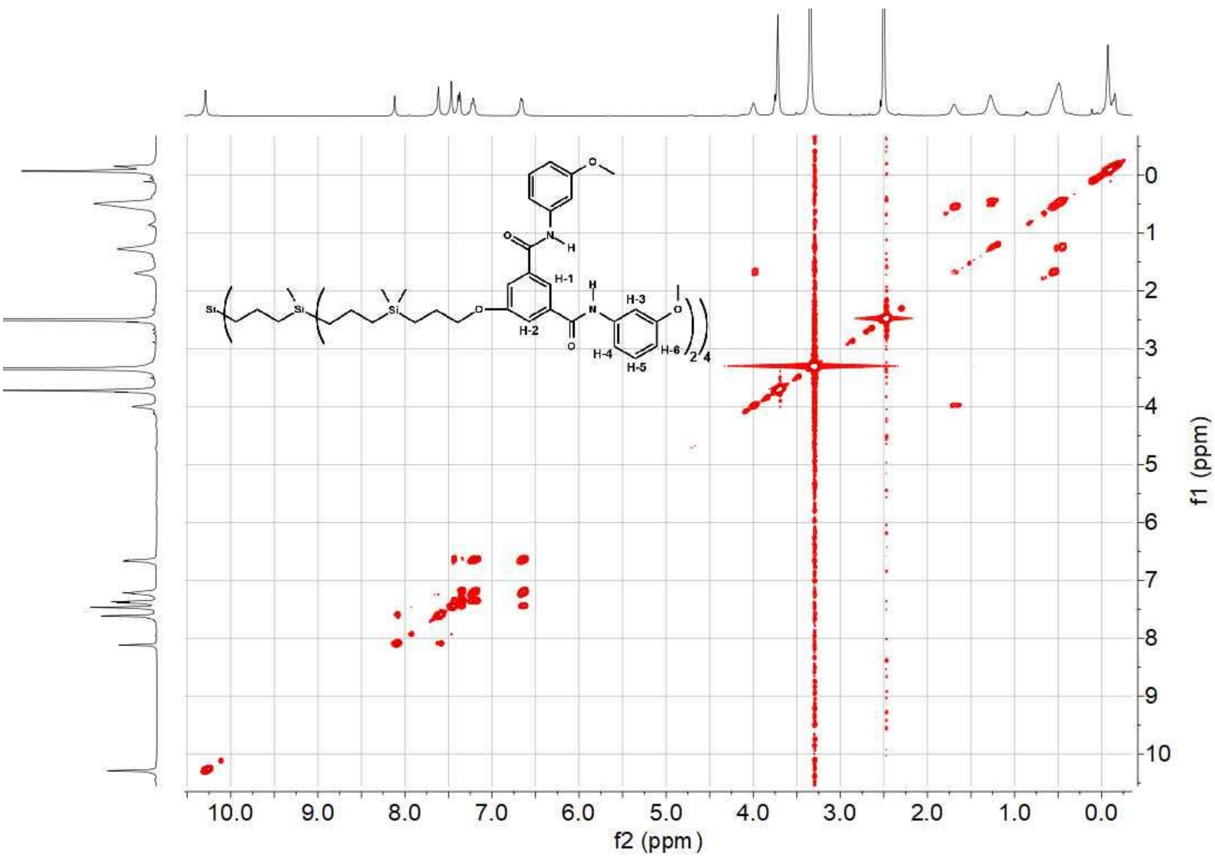

Figure S19. Receptor **Dm2** ^1H-^1H COSY (400 MHz), DMSO-d_6.

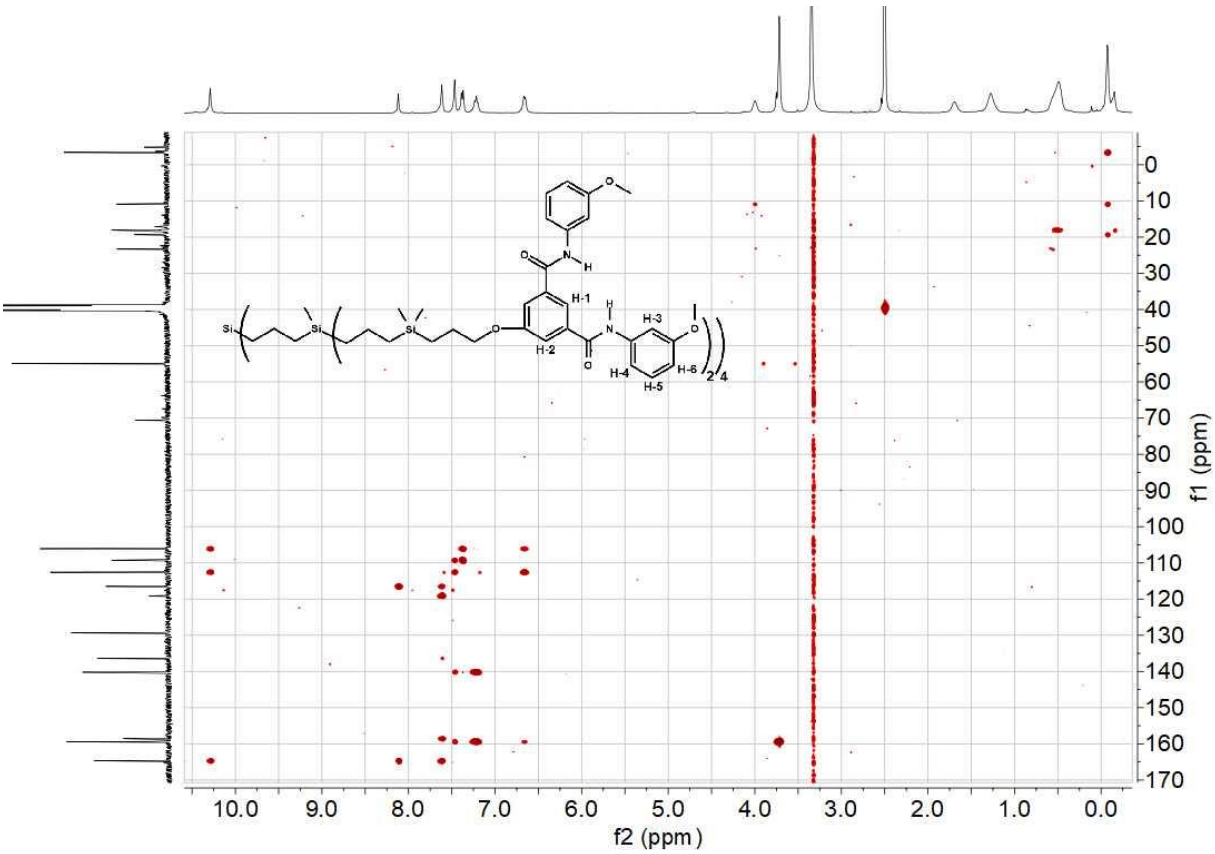

Figure S20. Receptor **Dm2** ^1H-^{13}C HMBC (400, 101 MHz), DMSO-d_6.

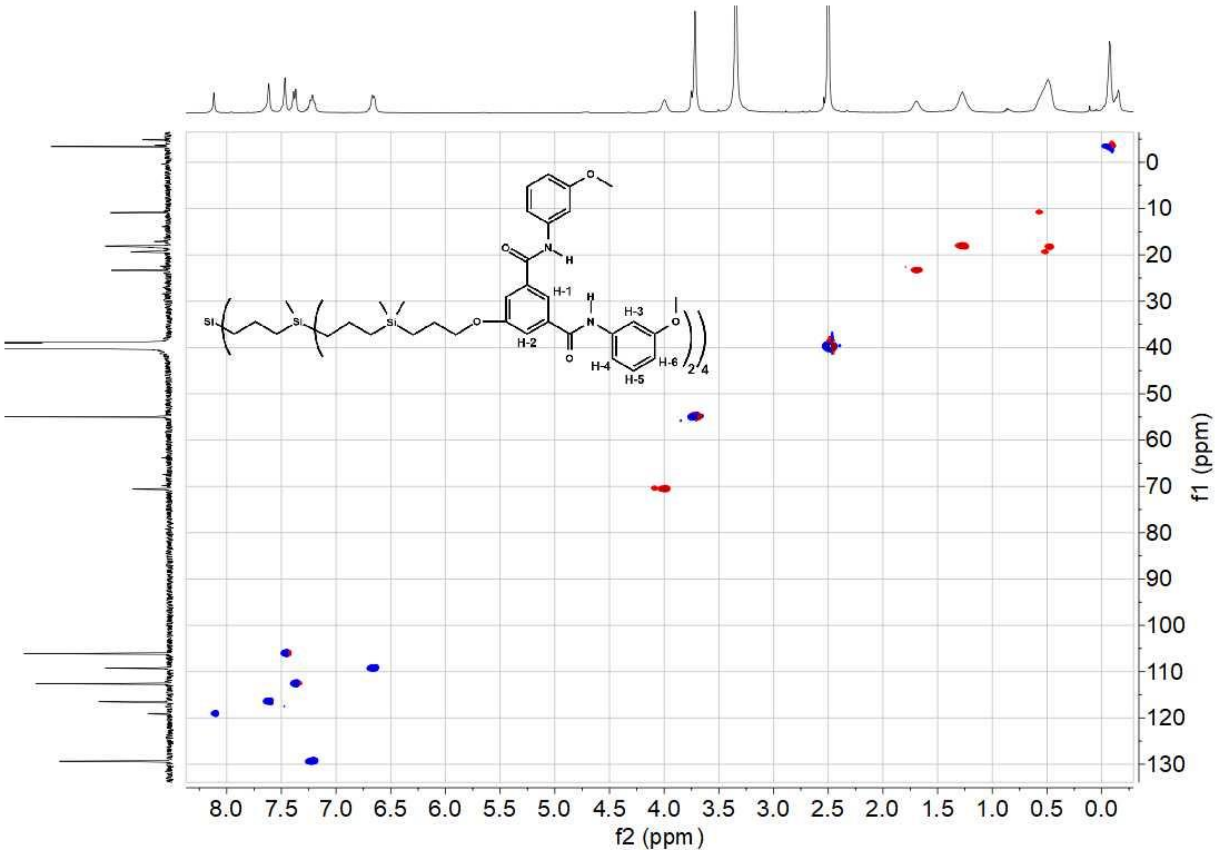

Figure S21. Receptor **Dm2** ^{1}H-^{13}C HSQC (400, 101 MHz), DMSO-*d*$_{6}$.

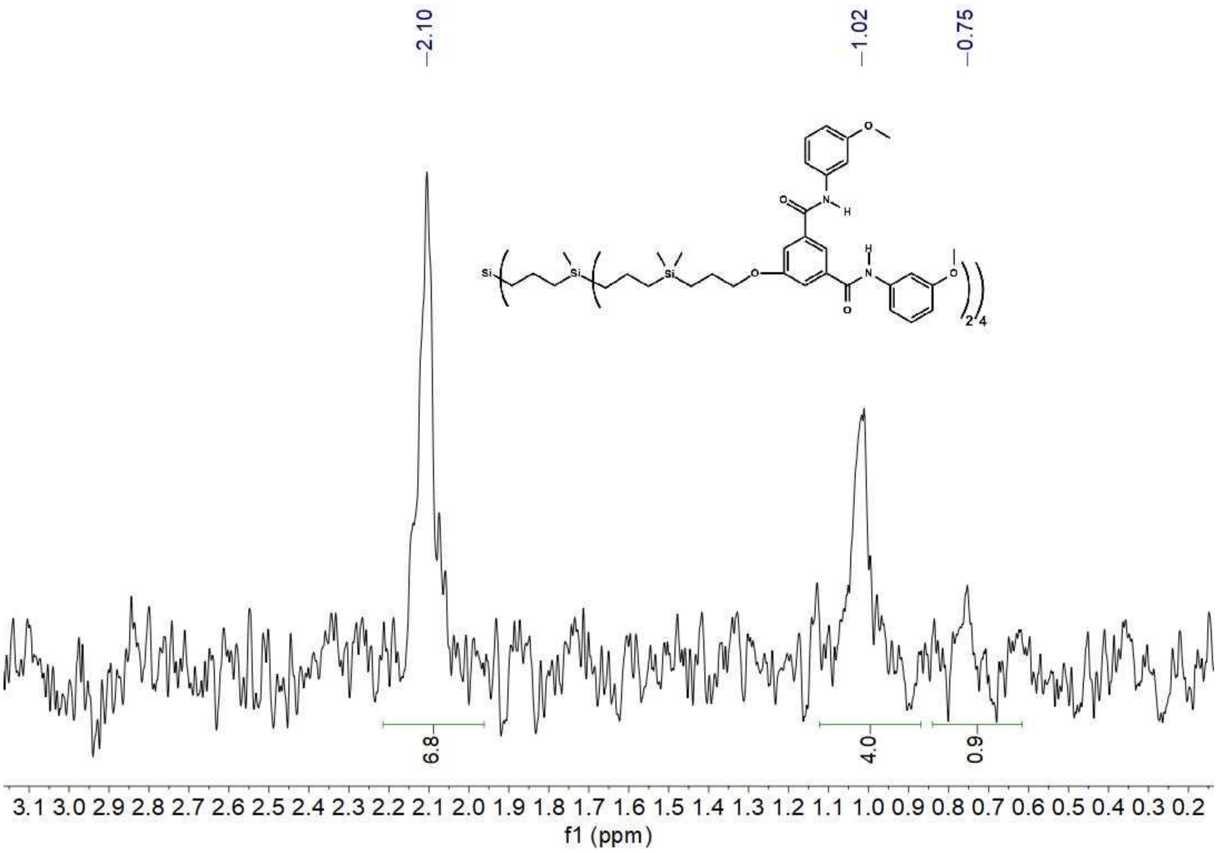

Figure S22. Receptor **Dm2** ^{29}Si NMR (80 MHz), DMSO-*d*$_{6}$.

NMR titration data

Compound **M1**

c **M1** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0021	0	0
0.0021	0.0010	509.9
0.0021	0.0020	1042.2
0.0021	0.0029	1146.0
0.0021	0.0047	1170.3
0.0021	0.0064	1185.0
0.0021	0.0087	1195.5
0.0021	0.0120	1200.8
0.0021	0.0149	1205.3
0.0021	0.0196	1207.5
0.0021	0.0522	1229.4

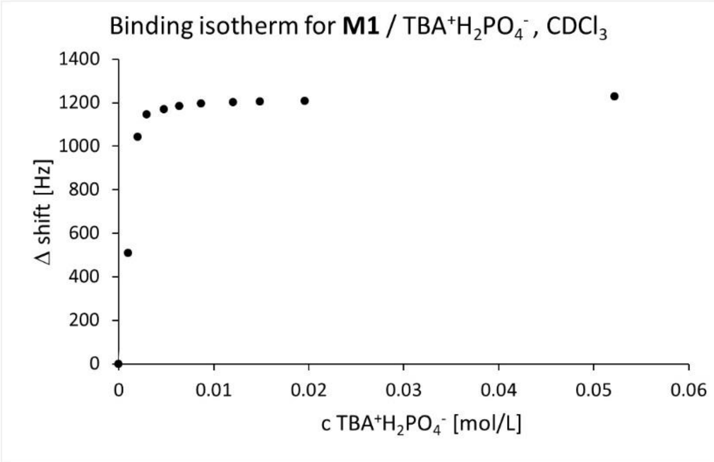

Figure S23. ^{1}H NMR titration of **M1** by $TBA^+H_2PO_4^-$ in $CDCl_3$

c **M1** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0105	0	0
0.0105	0.0021	79.4
0.0105	0.0059	225.6
0.0105	0.0095	302.0
0.0105	0.0128	352.8
0.0105	0.0174	406.0
0.0105	0.0242	452.4
0.0105	0.0299	478.9
0.0105	0.0392	510.0
0.0105	0.0465	532.0
0.0105	0.1047	608.0

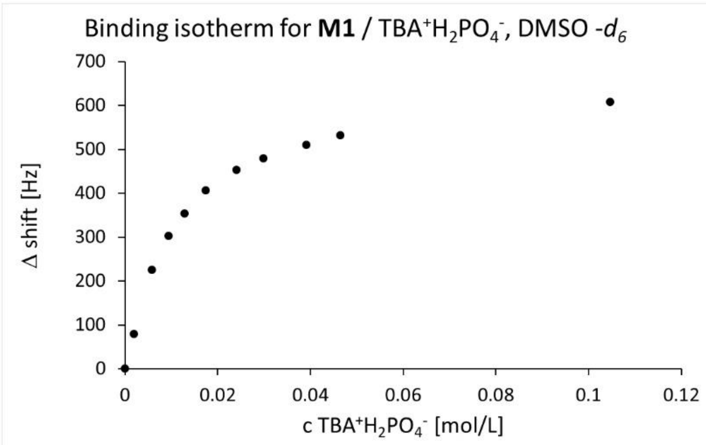

Figure S24. ^{1}H NMR titration of **M1** by $TBA^+H_2PO_4^-$ in DMSO-d_6.

c **M1** [mol/L]	c TBA$^+$Cl$^-$ [mol/L]	Δ shift [Hz]
0.0052	0	0
0.0052	0.0025	578.8
0.0052	0.0049	1025.1
0.0052	0.0072	1078.6
0.0052	0.0116	1094.6
0.0052	0.0157	1103.8
0.0052	0.0213	1109.1
0.0052	0.0295	1111.3
0.0052	0.0365	1112.0
0.0052	0.0479	1116.4

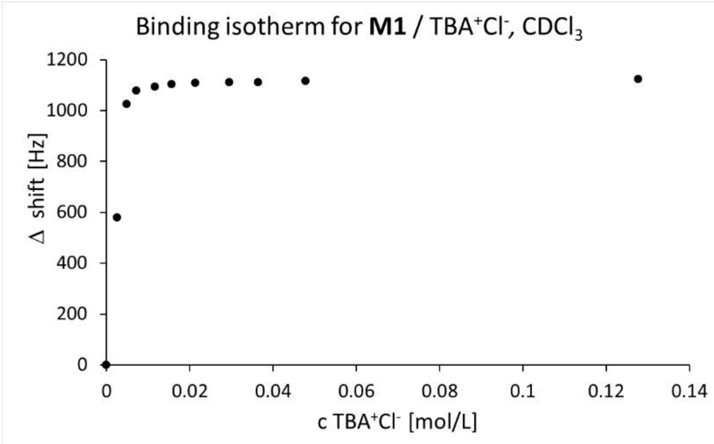

Figure S25. ^{1}H NMR titration of **M1** by TBA$^+$Cl$^-$ in $CDCl_3$.

c **M1** [mol/L]	c TBA$^+$Cl$^-$ [mol/L]	Δ shift [Hz]
0.0111	0	0
0.0111	0.0032	31.6
0.0111	0.0062	59.6
0.0111	0.0091	82.0
0.0111	0.0147	110.2
0.0111	0.0198	128.6
0.0111	0.0269	145.6
0.0111	0.0372	173.0
0.0111	0.0461	198.0
0.0111	0.0605	215.9
0.0111	0.1613	276.1

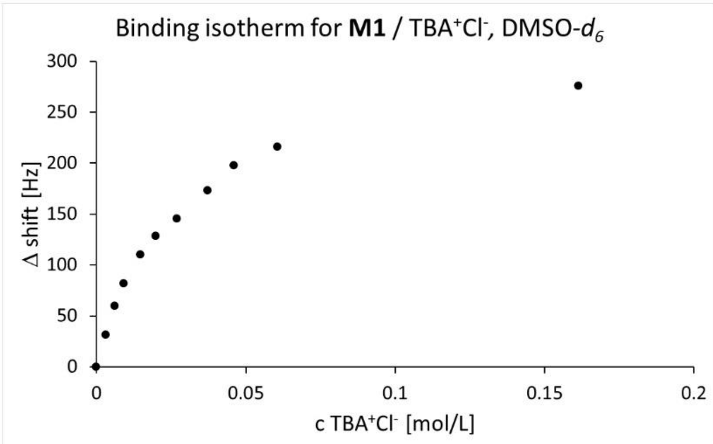

Figure S26. ^{1}H NMR titration of **M1** by TBA$^+$Cl$^-$ in DMSO-d_6.

c **M1** [mol/L]	c TBA⁺Br⁻ [mol/L]	Δ shift [Hz]
0.0063	0	0
0.0063	0.0022	284.0
0.0063	0.0042	685.7
0.0063	0.0062	861.2
0.0063	0.0100	923.9
0.0063	0.0135	960.7
0.0063	0.0184	983.6
0.0063	0.0254	994.0
0.0063	0.0315	1003.4
0.0063	0.0413	1006.9
0.0063	0.1102	1016.3

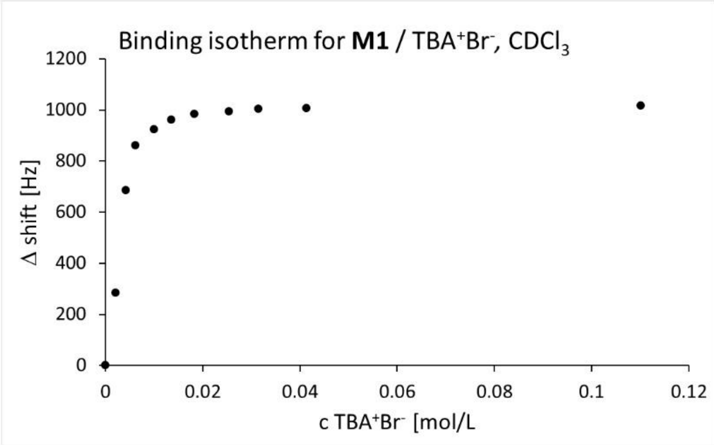

Figure S27. ^{1}H NMR titration of **M1** by TBA$^+$Br$^-$ in CDCl$_3$.

c **M1** [mol/L]	c TBA⁺Br⁻ [mol/L]	Δ shift [Hz]
0.0122	0	0
0.0122	0.0025	1.0
0.0122	0.0071	2.8
0.0122	0.0114	2.8
0.0122	0.0154	5.6
0.0122	0.0210	7.6
0.0122	0.0290	10.4
0.0122	0.0359	12.6
0.0122	0.0472	16.3
0.0122	0.0559	18.0
0.0122	0.1258	35.9

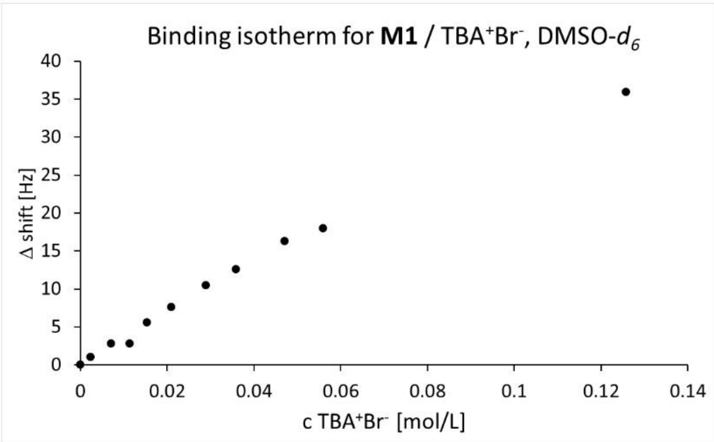

Figure S28. ^{1}H NMR titration of **M1** by TBA$^+$Br$^-$ in DMSO-d_6.

c **M1** [mol/L]	c TBA⁺AcO⁻ [mol/L]	Δ shift [Hz]
0.0052	0	0
0.0052	0.0016	277.7
0.0052	0.0032	676.4
0.0052	0.0047	924.9
0.0052	0.0076	1092.6
0.0052	0.0102	1149.7
0.0052	0.0139	1158.4
0.0052	0.0192	1173.5
0.0052	0.0238	1186.7
0.0052	0.0312	1191.8
0.0052	0.0832	1216.1

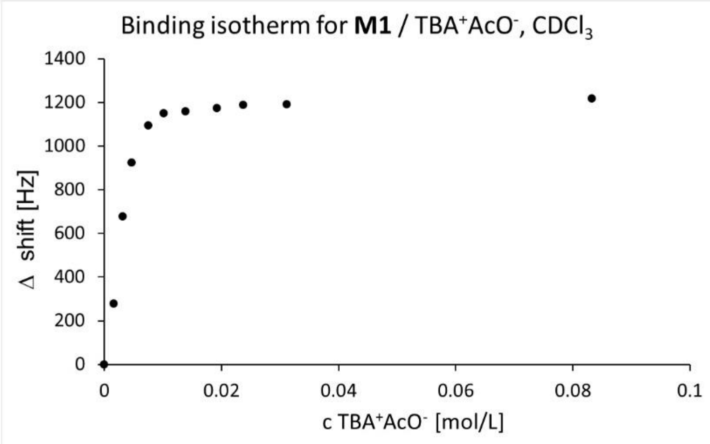

Figure S29. ^{1}H NMR titration of **M1** by TBA^+AcO^- in $CDCl_3$.

c **M1** [mol/L]	c TBA⁺AcO⁻ [mol/L]	Δ shift [Hz]
0.0117	0	0
0.0117	0.0015	53.8
0.0117	0.0043	143.2
0.0117	0.0069	211.2
0.0117	0.0093	262.3
0.0117	0.0126	319.2
0.0117	0.0175	381.8
0.0117	0.0217	419.7
0.0117	0.0284	463.4
0.0117	0.0337	482.5
0.0117	0.0758	612.7

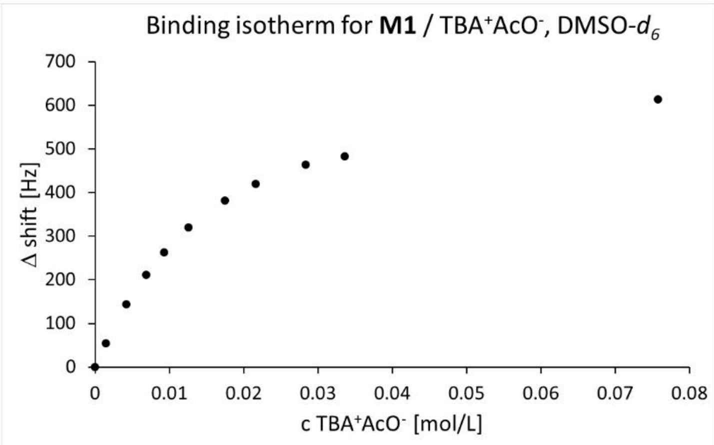

Figure S30. ^{1}H NMR titration of **M1** by TBA^+AcO^- in DMSO-d_6.

c **M1** [mol/L]	c TBA⁺BzO⁻ [mol/L]	Δ shift [Hz]
0.0088	0	0
0.0088	0.0024	398.4
0.0088	0.0047	721.3
0.0088	0.0070	959.0
0.0088	0.0112	1306.6
0.0088	0.0151	1356.6
0.0088	0.0205	1362.8
0.0088	0.0284	1383.2
0.0088	0.0352	1382.6
0.0088	0.0462	1383.2
0.0088	0.1231	1381.2

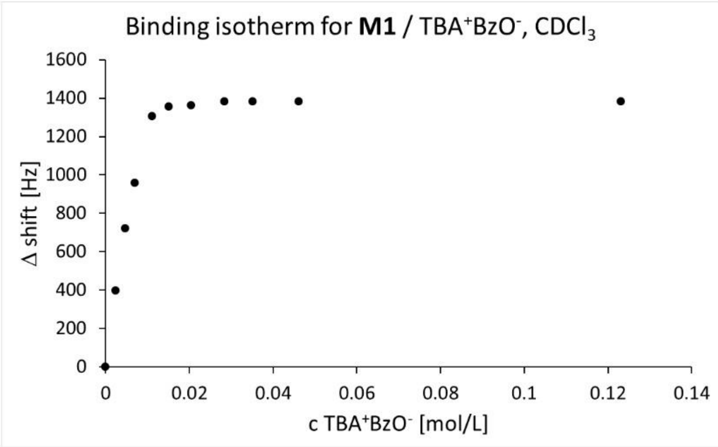

Figure S31. ^{1}H NMR titration of **M1** by TBA^+BzO^- in $CDCl_3$.

c **M1** [mol/L]	c TBA⁺BzO⁻ [mol/L]	Δ shift [Hz]
0.0046	0	0
0.0046	0.0011	71.4
0.0046	0.0021	117.1
0.0046	0.0031	166.2
0.0046	0.0051	246.6
0.0046	0.0068	286.6
0.0046	0.0093	338.8
0.0046	0.0129	390.2
0.0046	0.0159	425.1
0.0046	0.0209	478.3
0.0046	0.0558	577.9

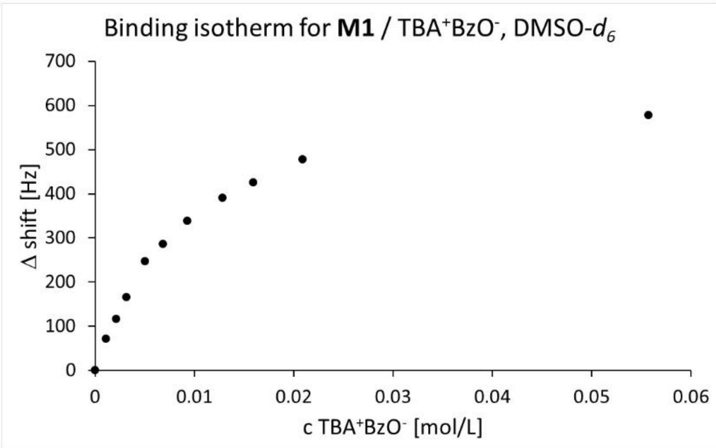

Figure S32. ^{1}H NMR titration of **M1** by TBA^+BzO^- in DMSO-d_6.

c **M1** [mol/L]	c DMSO [mol/L]	Δ shift [Hz]
0.0105	0	0
0.0105	0.0034	15.8
0.0105	0.0097	42.7
0.0105	0.0156	67.5
0.0105	0.0211	86.8
0.0105	0.0287	110.5
0.0105	0.0397	142.6
0.0105	0.0492	165.4
0.0105	0.0645	194.8
0.0105	0.0765	221.2
0.0105	0.1721	336.7

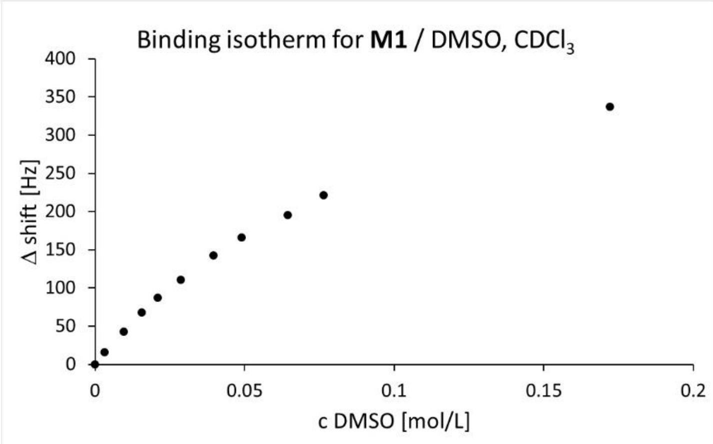

Figure S33. [1]H NMR titration of **M1** by DMSO in $CDCl_3$.

Compound **Dm1**

c **Dm1** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0092	0	0
0.0092	0.0027	2.1
0.0092	0.0077	35.7
0.0092	0.0124	66.5
0.0092	0.0168	103.7
0.0092	0.0228	199.7
0.0092	0.0316	719.7
0.0092	0.0391	1011.5
0.0092	0.0513	1068.3
0.0092	0.0608	1085.7
0.0092	0.1367	1145.4

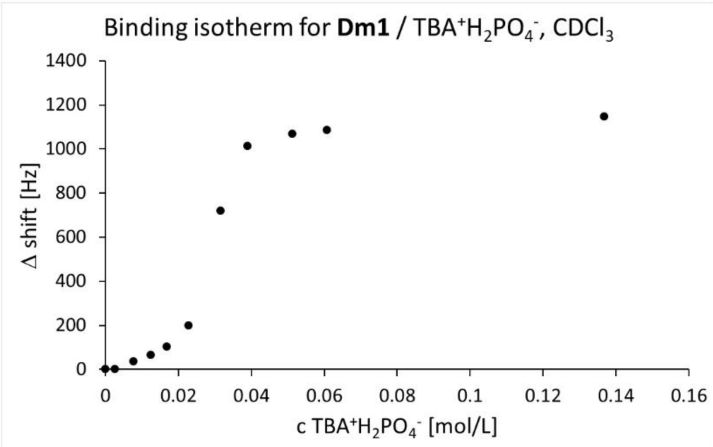

Figure S34. [1]H NMR titration of **Dm1** by $TBA^+H_2PO_4^-$ in $CDCl_3$.

Dm1, mole fraction	Δ shift [Hz]*mole fraction of **Dm1**
1	0
0.7747	1.6
0.5436	19.4
0.4259	28.3
0.3544	36.8
0.2880	57.5
0.2261	162.7
0.1909	193.2
0.1524	162.8
0.1317	143.0
0.0631	72.4

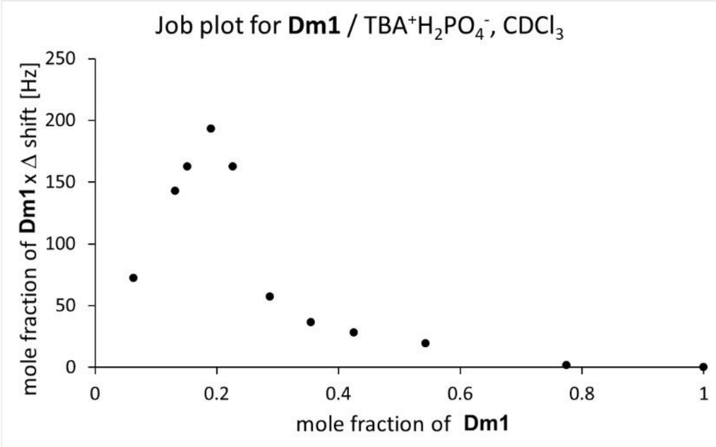

Figure S35. Job plot of the system **Dm1** / $TBA^+H_2PO_4^-$ in $CDCl_3$.

c **Dm1** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0098	0	0
0.0098	0.0025	12.6
0.0098	0.0049	74.4
0.0098	0.0073	128.6
0.0098	0.0117	178.3
0.0098	0.0158	222.5
0.0098	0.0214	274.5
0.0098	0.0297	305.9
0.0098	0.0367	351.1
0.0098	0.0482	376.7
0.0098	0.1285	564.4

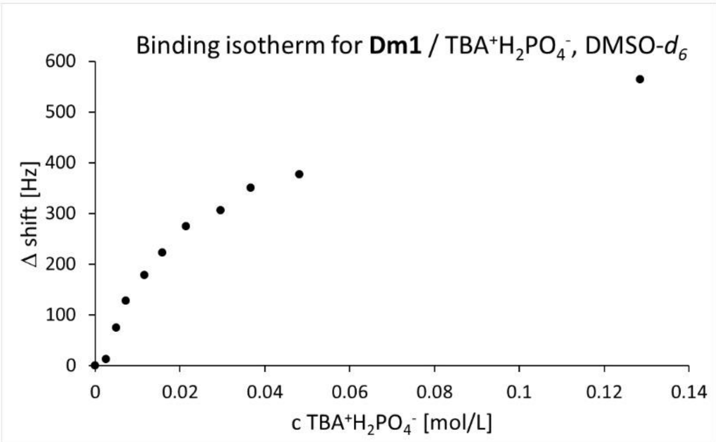

Figure S36. ^{1}H NMR titration of **Dm1** by $TBA^+H_2PO_4^-$ in DMSO-d_6.

Dm1, mole fraction	Δ shift [Hz]*mole fraction of **Dm1**
1	0
0.7945	10.0
0.6637	49.4
0.5728	73.6
0.4550	81.1
0.3819	85.0
0.3129	85.9
0.2475	75.7
0.2099	73.7
0.1683	63.4
0.0705	39.8

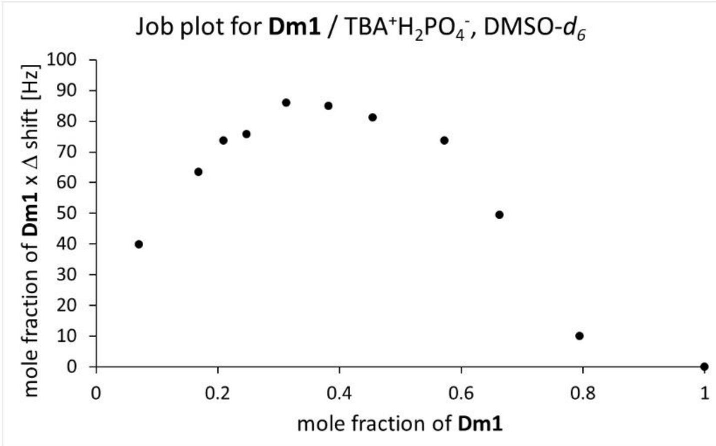

Figure S37. Job plot of the system **Dm1** / $TBA^+H_2PO_4^-$ in DMSO-d_6.

Compound **Dm2**

c **Dm2** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0055	0	0
0.0055	0.0024	12.2
0.0055	0.0068	44.0
0.0055	0.0110	88.3
0.0055	0.0148	180.4
0.0055	0.0201	308.2
0.0055	0.0279	528.3
0.0055	0.0345	704.0
0.0055	0.0453	928.5
0.0055	0.0537	1000.1
0.0055	0.0806	1090.3
0.0055	0.1209	1164.0

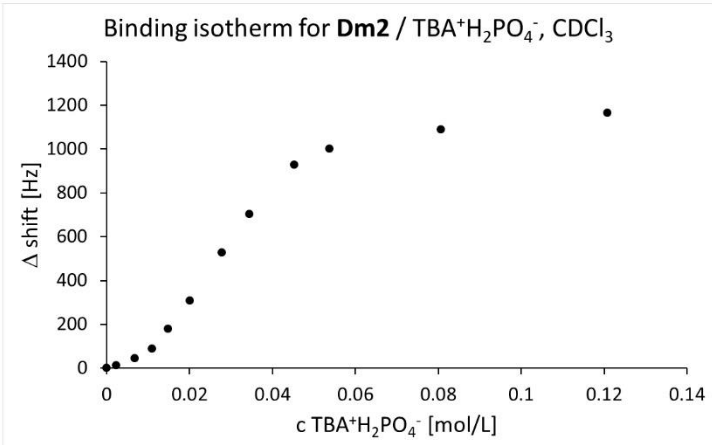

Figure S38. ^{1}H NMR titration of **Dm2** by $TBA^+H_2PO_4^-$ in $CDCl_3$.

Dm2, mole fraction	Δ shift [Hz]*mole fraction of **Dm2**
1	0
0.7002	8.4
0.4473	19.7
0.3350	29.5
0.2716	48.9
0.2156	66.4
0.1656	87.4
0.1382	97.3
0.1088	101.0
0.0934	93.4
0.0642	70.1
0.0438	51.0

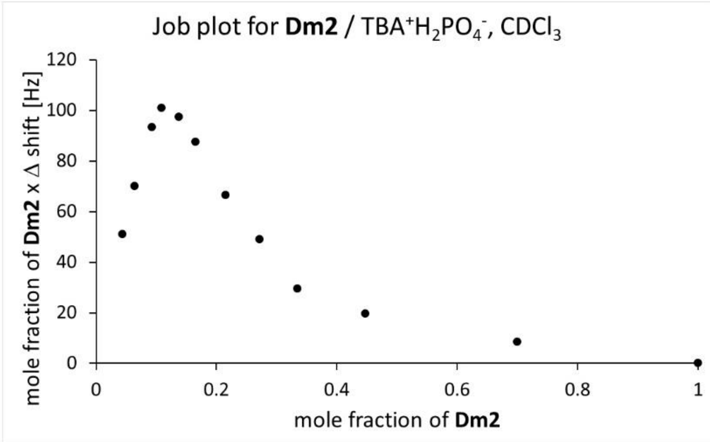

Figure S39. Job plot of the system **Dm2** / $TBA^+H_2PO_4^-$ in $CDCl_3$.

c **Dm2** [mol/L]	c $TBA^+H_2PO_4^-$ [mol/L]	Δ shift [Hz]
0.0051	0	0
0.0051	0.0025	8.1
0.0051	0.0071	44.5
0.0051	0.0114	68.2
0.0051	0.0154	120.0
0.0051	0.0209	180.1
0.0051	0.0289	235.9
0.0051	0.0358	276.0
0.0051	0.0469	316.1
0.0051	0.0556	348.1
0.0051	0.1252	540.2

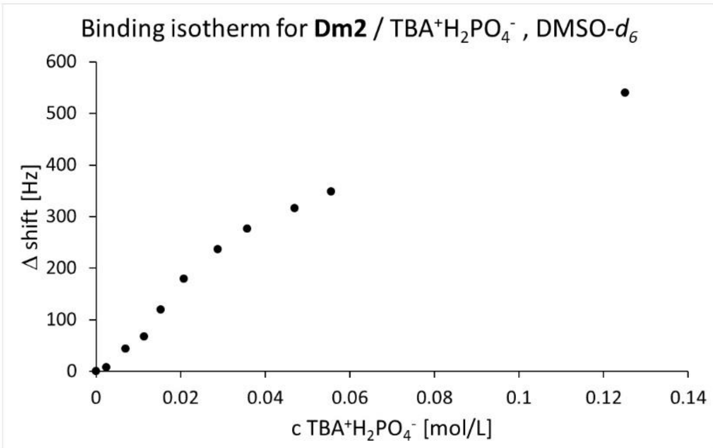

Figure S40. ^{1}H NMR titration of **Dm2** by $TBA^+H_2PO_4^-$ in DMSO-d_6.

Dm2, mole fraction	Δ shift [Hz]*mole fraction of **Dm2**
1	0
0.6745	5.4
0.4179	18.4
0.3089	21.0
0.2486	29.8
0.1960	35.3
0.1497	35.3
0.1245	34.4
0.0978	30.9
0.0838	29.2
0.0390	21.1

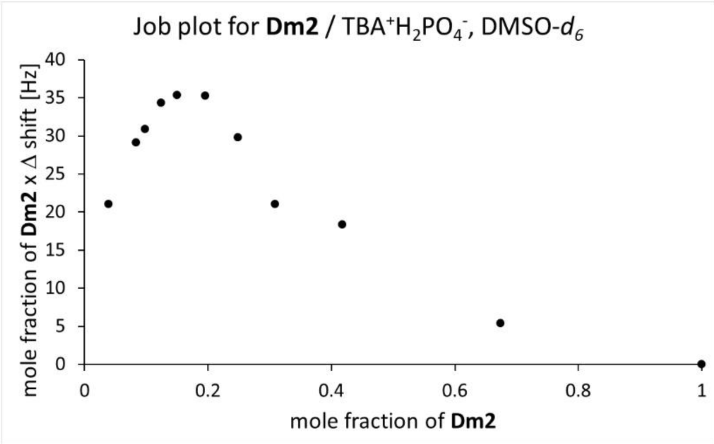

Figure S41. Job plot of the system **Dm2** / $TBA^+H_2PO_4^-$ in DMSO-d_6.

Detailed description of dialytic experiments

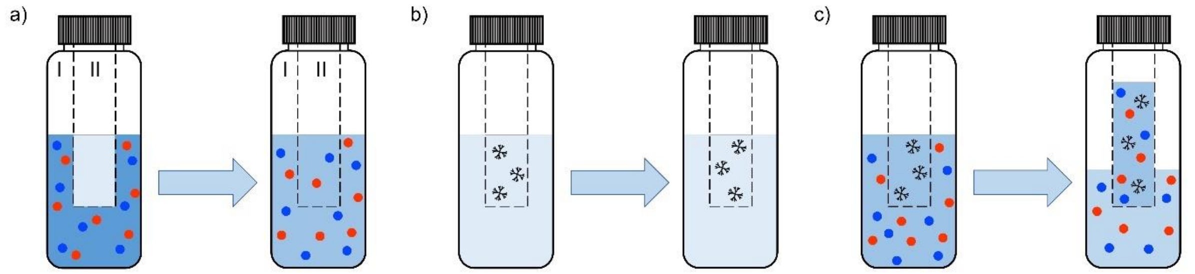

Figure S42. Schematic depiction of preliminary experiments; a) ions in comp. I and no receptor in comp. II, b) no ions in comp. I and receptor in comp. II, and c) ions in comp. I and receptor in comp. II.

Table S1. Setting of the preliminary experiments, corresponding to Figure S43.

Setting	Time [h]	V_I [mL]	V_{II} [mL]	c_{Dm1} [mol/L]	$c_{P\text{-}I}$ [mol/L]	$c_{P\text{-}II}$ [mol/L]	$n_{transfI}$ [mmol]
a)	0	3.00	0.50	0	0.0100	0	0
	24	3.00	0.50	0	0.0086	0.0080	0.0040
b)	0	3.00	0.50	0.0100	0	0	0
	24	3.00	0.50	0.0100	0	0	0
c)	0	3.00	0.50	0.0100	0.0100	0	0
	24	2.85	0.65	0.0077	0.0080	0.0100	0.0065
c)	0	3.00	0.50	0.0100	0.0230	0	0
	24	2.10	1.40	0.0036	0.0185	0.0230	0.0322

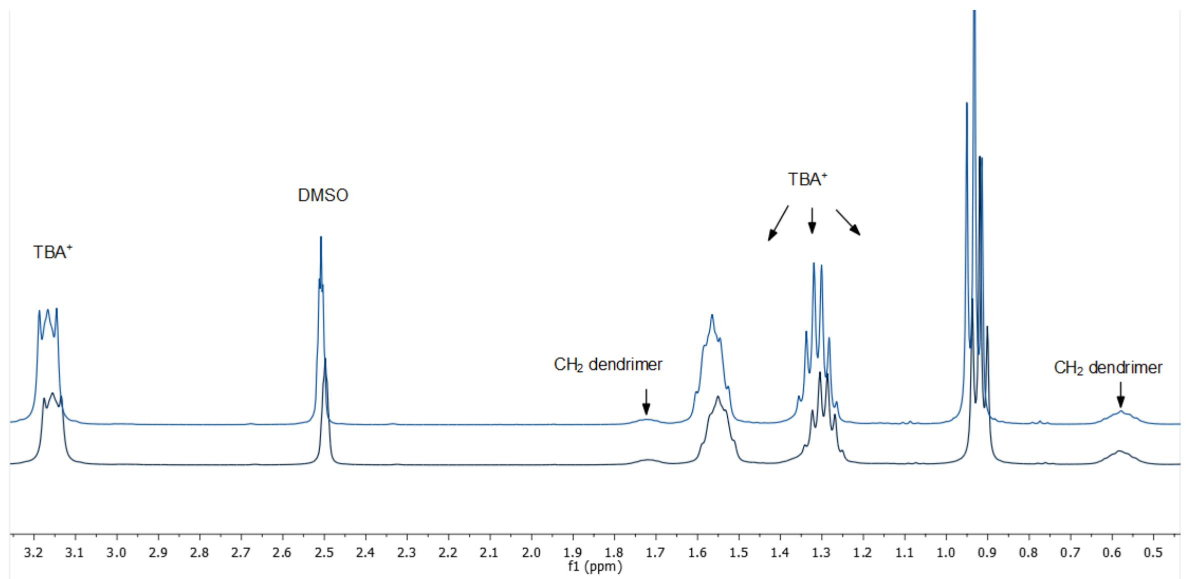

Figure S43. Comparison of ^{1}H NMR spectra of compartment II taken in time 0 (dark blue) and in 24h (light blue) and the indication of the signals used for integration.

Details for the final dialytic experiments

Table S2. Detailed description of dialytic experiments

Entry	Receptor ID n_{Dm}: n_P	Time [h]	V_I [mL]	V_{II} [mL]	c_{P-I} [mol/L]	c_{P-II} [mol/L]	Δc_P [mol/L]	n_{P-I} [mmol]	n_{P-II} [mmol]	Σn [mmol]	c_{Dm-II} [mol/L]	n_{Dm-II} [mmol]	n_{transf} [mmol]
1	**Dm1**	0	3.10	0.50	0.0101	0.0101	0	0.0312	0.0050	0.0362	0.0084	0.0042	0
	1:1	24	2.75	0.85	0.0097	0.0108	0.0011	0.0266	0.0091	0.0357	0.0050	0.0038	0.0041
2	**Dm1**	0	3.10	0.50	0.0258	0.0258	0	0.0776	0.0128	0.0904	0.0091	0.0045	0
	1:3	24	2.55	0.96	0.0230	0.0311	0.0081	0.0587	0.0297	0.0885	0.0047	0.0041	0.0169
3	**Dm1**	0	3.10	0.50	0.0504	0.0504	0	0.1505	0.0250	0.1755	0.0091	0.0045	0
	1:5.5	24	2.68	0.80	0.0483	0.0556	0.0073	0.1294	0.0446	0.1741	0.0056	0.0041	0.0197
4	**Dm1**	0	3.10	0.50	0.0818	0.0818	0	0.2464	0.0408	0.2872	0.0071	0.0035	0
	1:11.5	24	2.61	0.90	0.0797	0.0834	0.0037	0.2080	0.0752	0.2832	0.0039	0.0032	0.0344
5	**Dm1**	0	3.10	0.50	0.0493	0.0493	0	0.1479	0.0246	0.1725	0.0049	0.0025	0
	1:10	24	2.73	0.77	0.0478	0.0504	0.0026	0.1302	0.0389	0.1692	0.0032	0.0022	0.0143
6	**Dm2**	0	3.10	0.50	0.0247	0.0247	0	0.0783	0.0124	0.0907	0.0084	0.0042	0
	1:3	24	2.72	0.95	0.0224	0.0257	0.0033	0.0608	0.0244	0.0852	0.0045	0.0038	0.0120
7	**Dm2**	0	3.10	0.50	0.0253	0.0253	0	0.0765	0.0126	0.0892	0.0044	0.0022	0
	1:6	24	2.77	0.75	0.0247	0.0284	0.0038	0.0682	0.0214	0.0896	0.0029	0.0020	0.0088
8	**Dm2**	0	3.10	0.50	0.0496	0.0496	0	0.1574	0.0258	0.1832	0.0037	0.0019	0
	1:13	24	2.93	0.76	0.0471	0.0569	0.0098	0.1381	0.0432	0.1812	0.0026	0.0017	0.0173
9	**Dm2**	0	3.10	0.50	0.0495	0.0495	0	0.1485	0.0248	0.1733	0.0025	0.0012	0
	1:20	24	2.63	0.87	0.0465	0.0530	0.0065	0.1225	0.0458	0.1684	0.0014	0.0011	0.0211
10	**Dm2**	0	3.10	0.50	0.0914	0.0914	0	0.2833	0.0457	0.3289	0.0029	0.0015	0
	1:30	24	2.41	1.19	0.0876	0.0946	0.0070	0.2114	0.1123	0.3237	0.0012	0.0013	0.0666

Abbreviations used in **Table S1** and **Table S2**:

n_A amount of substance of $TBA^+H_2PO_4^-$ [mmol]

n_{Dm} amount of substance of respective dendrimer [mmol]

V_I volume contained in compartment I [mL]

V_{II} volume contained in compartment II [mL]

c_{A-I} molar concentration of $TBA^+H_2PO_4^-$ in compartment I [mol/L]

c_{A-II} molar concentration of $TBA^+H_2PO_4^-$ in compartment II [mol/L]

c_{Dm} molar concentration of respective dendrimer in compartment II [mol/L]

n_{A-I} amount of substance of $TBA^+H_2PO_4^-$ in compartment I [mmol]

n_{A-II} amount of substance of $TBA^+H_2PO_4^-$ in compartment II [mmol]

n_{transf} amount of substance of $TBA^+H_2PO_4^-$ transferred over the membrane [mmol].

Computer Modelling

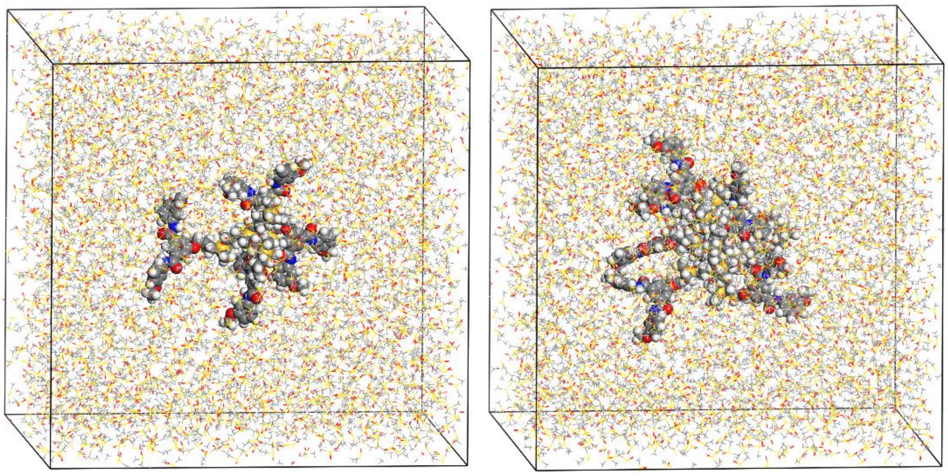

Figure S44. Visualization of the simulated systems i.e. dendrimers **Dm1** (left), **Dm2** (right) surrounded by 3000 DMSO molecules in simulation box.

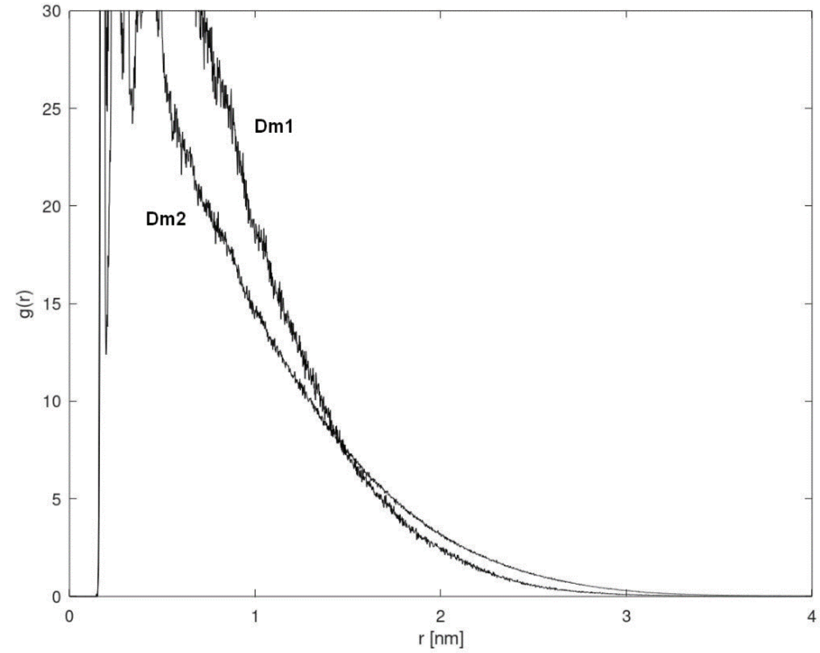

Figure S45. Selected part of the radial distribution functions of the dendrimers hydrogen atoms in case of **Dm1** and **Dm2**. The *r* value, where the *g(r)* is approaching zero determines the largest dendrimer dimension.