'Choose-a-size' approach in dynamic combinatorial chemistry: a single substrate dynamic combinatorial library of oligomacrocycles that adapts to the size and shape of carboxylates

Supporting Information

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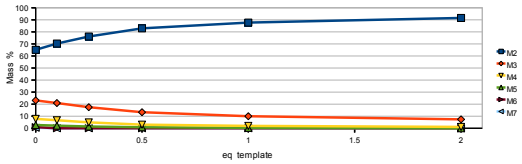
Contents

S1 Compositions of templated libraries

Template: A

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	70.32	76.13	82.85	87.71	91.57
	M3	23.07	20.93	17.49	13.28	9.98	7.33
	M4	7.82	6.6	4.91	3.04	1.98	1.1
	M5	2.67	2.15	1.48	0.83	0.33	0
	M6	0.93	0	0	0	0	0
	M7	0.38	0	0	0	0	0

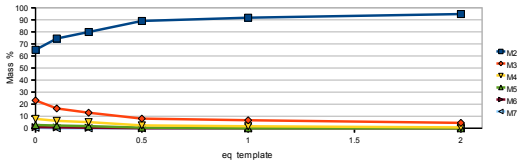
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.516E-03	3.806E-03	4.143E-03	4.385E-03	4.579E-03
	M3	7.691E-04	6.976E-04	5.829E-04	4.425E-04	3.326E-04	2.444E-04
	M4	1.955E-04	1.651E-04	1.226E-04	7.593E-05	4.949E-05	2.741E-05
	M5	5.341E-05	4.301E-05	2.961E-05	1.670E-05	6.632E-06	0.000E+00
	M6	1.551E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	M7	5.491E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00



Template: B

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	74.46	79.83	89.06	91.74	94.78
	M3	23.07	16.43	12.87	8.02	6.62	4.48
	M4	7.82	6.11	5.05	2.41	1.63	0.73
	M5	2.67	2.33	1.81	0.51	0.01	0.01
	M6	0.93	0.67	0.44	0	0	0
	M7	0.38	0	0	0	0	0

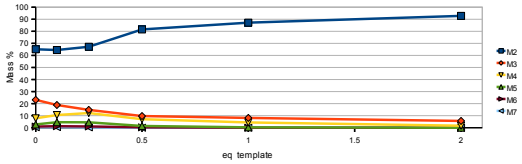
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.723E-03	3.992E-03	4.453E-03	4.587E-03	4.739E-03
	M3	7.691E-04	5.476E-04	4.290E-04	2.674E-04	2.206E-04	1.493E-04
	M4	1.955E-04	1.527E-04	1.263E-04	6.026E-05	4.075E-05	1.825E-05
	M5	5.341E-05	4.660E-05	3.620E-05	1.020E-05	2.000E-07	2.000E-07
	M6	1.551E-05	1.117E-05	7.333E-06	1.667E-08	1.666E-08	1.666E-10
	M7	5.491E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00



Template: C

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	64.39	67.12	81.49	87.19	92.78
	M3	23.07	18.87	14.8	9.7	8.1	5.61
	M4	7.82	10.47	12.19	7.02	4.38	1.62
	M5	2.67	4.54	4.5	1.48	0.33	0
	M6	0.93	1.21	1.05	0.3	0	0
	M7	0.38	0.51	0.34	0	0	0

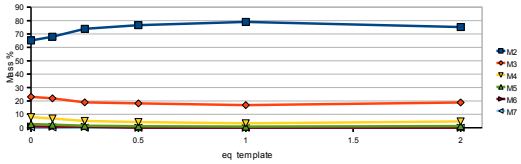
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.220E-03	3.356E-03	4.075E-03	4.359E-03	4.639E-03
	M3	7.691E-04	6.291E-04	4.934E-04	3.233E-04	2.700E-04	1.870E-04
	M4	1.955E-04	2.618E-04	3.047E-04	1.756E-04	1.095E-04	4.038E-05
	M5	5.341E-05	9.079E-05	9.000E-05	2.966E-05	6.658E-06	0.000E+00
	M6	1.551E-05	2.018E-05	1.754E-05	5.010E-06	0.000E+00	0.000E+00
	M7	5.491E-06	7.350E-06	4.868E-06	0.000E+00	0.000E+00	0.000E+00



Template: D

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	67.99	73.85	76.56	78.98	75.2
	M3	23.07	21.9	18.96	18.15	16.9	18.84
	M4	7.82	6.84	5.07	4.18	3.3	4.71
	M5	2.67	2.22	1.48	1.11	0.82	1.25
	M6	0.93	0.77	0.64	0	0	0
	M7	0.38	0.28	0	0	0	0

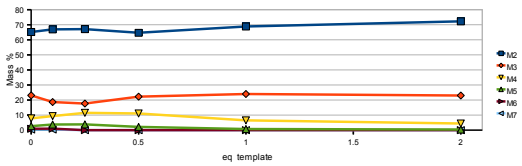
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.400E-03	3.693E-03	3.826E-03	3.949E-03	3.760E-03
	M3	7.691E-04	7.299E-04	6.320E-04	6.049E-04	5.632E-04	6.282E-04
	M4	1.955E-04	1.710E-04	1.268E-04	1.046E-04	8.259E-05	1.178E-04
	M5	5.341E-05	4.440E-05	2.960E-05	2.228E-05	1.631E-05	2.498E-05
	M6	1.551E-05	1.283E-05	1.067E-05	1.688E-08	1.699E-08	1.692E-10
	M7	5.491E-06	4.000E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00



Template: E

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	66.9	67.04	64.6	68.8	72.25
	M3	23.07	18.66	17.66	22.22	23.94	23
	M4	7.82	9.29	11.5	11.04	6.53	4.37
	M5	2.67	3.78	3.8	2.15	0.73	0.38
	M6	0.93	0.96	0	0	0	0
	M7	0.38	0.4	0	0	0	0

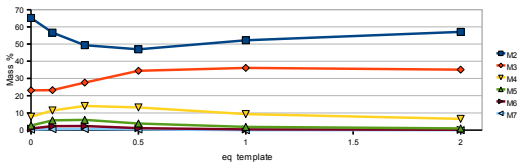
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.345E-03	3.352E-03	3.230E-03	3.440E-03	3.613E-03
	M3	7.691E-04	6.221E-04	5.887E-04	7.405E-04	7.979E-04	7.665E-04
	M4	1.955E-04	2.323E-04	2.875E-04	2.759E-04	1.632E-04	1.093E-04
	M5	5.341E-05	7.562E-05	7.605E-05	4.295E-05	1.460E-05	7.635E-06
	M6	1.551E-05	1.601E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	M7	5.491E-06	5.777E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00



Template: F

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	56.66	49.31	46.92	52.17	57.1
	M3	23.07	23.27	27.6	34.44	36.18	35.13
	M4	7.82	11.44	14.09	13.18	9.33	6.57
	M5	2.67	5.69	5.99	3.83	1.87	0.99
	M6	0.93	2.33	2.39	1.19	0.45	0.21
	M7	0.38	0.6	0.63	0.44	0	0

c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.833E-03	2.466E-03	2.346E-03	2.609E-03	2.855E-03
	M3	7.691E-04	7.758E-04	9.198E-04	1.148E-03	1.206E-03	1.171E-03
	M4	1.955E-04	2.860E-04	3.523E-04	3.295E-04	2.333E-04	1.643E-04
	M5	5.341E-05	1.137E-04	1.197E-04	7.669E-05	3.733E-05	1.980E-05
	M6	1.551E-05	3.891E-05	3.978E-05	1.982E-05	7.486E-06	3.500E-06
	M7	5.491E-06	8.625E-06	8.950E-06	6.228E-06	0.000E+00	0.000E+00



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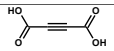
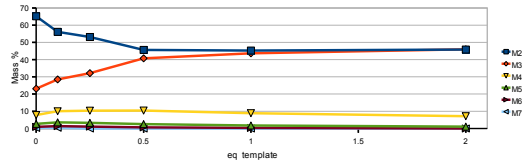
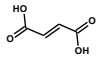


Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	56.14	53.1	45.64	45.29	45.82
	M3	23.07	28.51	32.14	40.74	43.68	45.99
	M4	7.82	10.02	10.34	10.43	8.89	7.13
	M5	2.67	3.54	3.3	2.57	1.76	1.07
	M6	0.93	1.34	1.12	0.62	0.37	0
	M7	0.38	0.45	0	0	0	0

c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.807E-03	2.655E-03	2.282E-03	2.265E-03	2.291E-03
	M3	7.691E-04	9.502E-04	1.071E-03	1.358E-03	1.456E-03	1.533E-03
	M4	1.955E-04	2.505E-04	2.585E-04	2.608E-04	2.223E-04	1.781E-04
	M5	5.341E-05	7.079E-05	6.599E-05	5.140E-05	3.529E-05	2.141E-05
	M6	1.551E-05	2.233E-05	1.866E-05	1.033E-05	6.182E-06	0.000E+00
	M7	5.491E-06	6.428E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00

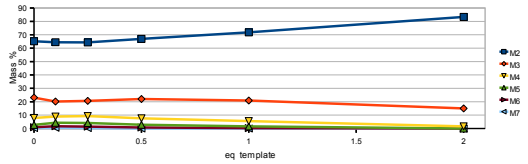


Template: H



Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	64.45	64.28	66.91	71.77	83.38
	M3	23.07	20.11	20.59	22.03	20.86	15
	M4	7.82	8.92	9.27	7.54	5.54	1.63
	M5	2.67	4.29	4.08	2.8	1.55	0
	M6	0.93	1.68	1.41	0.72	0.27	0
	M7	0.38	0.54	0.37	0	0	0

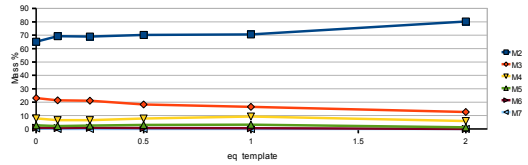
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.223E-03	3.214E-03	3.346E-03	3.589E-03	4.169E-03
	M3	7.691E-04	6.702E-04	6.863E-04	7.344E-04	6.955E-04	4.999E-04
	M4	1.955E-04	2.231E-04	2.318E-04	1.885E-04	1.384E-04	4.063E-05
	M5	5.341E-05	8.584E-05	8.160E-05	5.593E-05	3.110E-05	0.000E+00
	M6	1.551E-05	2.808E-05	2.350E-05	1.203E-05	4.514E-06	0.000E+00
	M7	5.491E-06	7.736E-06	5.286E-06	0.000E+00	0.000E+00	0.000E+00



Template: I

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	69.26	68.96	70.23	70.59	80.2
	M3	23.07	21.37	21.09	18.29	16.52	12.63
	M4	7.82	6.57	6.54	7.8	9.23	5.91
	M5	2.67	2.12	2.54	3	3.13	1.25
	M6	0.93	0.69	0.87	0.69	0.53	0
	M7	0.38	0	0	0	0	0

c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.463E-03	3.448E-03	3.511E-03	3.529E-03	4.010E-03
	M3	7.691E-04	7.122E-04	7.030E-04	6.096E-04	5.505E-04	4.210E-04
	M4	1.955E-04	1.642E-04	1.635E-04	1.949E-04	2.308E-04	1.479E-04
	M5	5.341E-05	4.237E-05	5.075E-05	6.006E-05	6.266E-05	2.503E-05
	M6	1.551E-05	1.155E-05	1.449E-05	1.148E-05	8.818E-06	0.000E+00
	M7	5.491E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00



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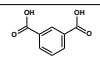
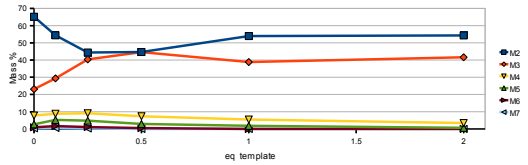


Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	54.35	44.36	44.69	53.93	54.31
	M3	23.07	29.37	40.34	44.58	38.81	41.59
	M4	7.82	8.83	9.08	7.33	5.47	3.45
	M5	2.67	5.22	4.81	2.93	1.79	0.65
	M6	0.93	1.67	1.12	0.47	0	0
	M7	0.38	0.56	0.29	0	0	0

c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.718E-03	2.218E-03	2.235E-03	2.696E-03	2.716E-03
	M3	7.691E-04	9.790E-04	1.345E-03	1.486E-03	1.294E-03	1.386E-03
	M4	1.955E-04	2.208E-04	2.270E-04	1.832E-04	1.368E-04	8.620E-05
	M5	5.341E-05	1.044E-04	9.620E-05	5.855E-05	3.580E-05	1.303E-05
	M6	1.551E-05	2.776E-05	1.867E-05	7.853E-06	0.000E+00	0.000E+00
	M7	5.491E-06	8.027E-06	4.143E-06	0.000E+00	0.000E+00	0.000E+00



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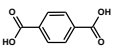
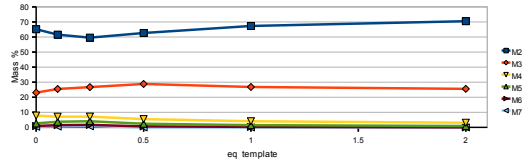


Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	61.59	59.55	62.6	67.27	70.48
	M3	23.07	25.49	26.76	28.84	26.81	25.56
	M4	7.82	7.1	7.16	5.47	4.11	3.04
	M5	2.67	3.75	4.12	2.43	1.48	0.92
	M6	0.93	1.49	1.68	0.66	0.33	0
	M7	0.38	0.58	0.73	0	0	0

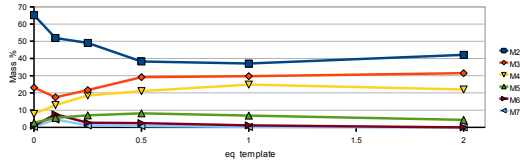
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	3.079E-03	2.977E-03	3.130E-03	3.363E-03	3.524E-03
	M3	7.691E-04	8.498E-04	8.921E-04	9.613E-04	8.938E-04	8.519E-04
	M4	1.955E-04	1.775E-04	1.791E-04	1.368E-04	1.028E-04	7.599E-05
	M5	5.341E-05	7.501E-05	8.244E-05	4.860E-05	2.960E-05	1.840E-05
	M6	1.551E-05	2.484E-05	2.795E-05	1.100E-05	5.501E-06	0.000E+00
	M7	5.491E-06	8.287E-06	1.039E-05	0.000E+00	0.000E+00	0.000E+00



Template: L

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	51.9	49.08	38.28	37.1	42.16
	M3	23.07	17.48	21.64	29.18	29.75	31.45
	M4	7.82	12.93	18.49	21.07	24.87	22.02
	M5	2.67	5.51	6.97	8.19	6.84	4.37
	M6	0.93	7.58	2.65	2.47	1.15	0
	M7	0.38	4.59	1.17	0.82	0.27	0

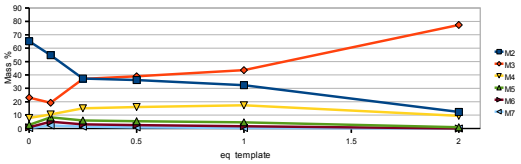
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.595E-03	2.454E-03	1.914E-03	1.855E-03	2.108E-03
	M3	7.691E-04	5.828E-04	7.213E-04	9.727E-04	9.918E-04	1.048E-03
	M4	1.955E-04	3.233E-04	4.624E-04	5.266E-04	6.218E-04	5.506E-04
	M5	5.341E-05	1.102E-04	1.393E-04	1.637E-04	1.369E-04	8.736E-05
	M6	1.551E-05	1.264E-04	4.423E-05	4.113E-05	1.923E-05	0.000E+00
	M7	5.491E-06	6.551E-05	1.666E-05	1.175E-05	3.905E-06	0.000E+00



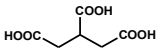
Template: M

Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	54.73	37.35	36.15	32.36	12.33
	M3	23.07	19.17	37.05	38.99	43.62	77.31
	M4	7.82	10.5	15.09	16.04	17.3	9.41
	M5	2.67	8.37	6.02	5.47	4.62	0.95
	M6	0.93	5.02	3.09	2.55	1.7	0
	M7	0.38	2.21	1.41	0.8	0.39	0

c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.737E-03	1.867E-03	1.808E-03	1.618E-03	6.163E-04
	M3	7.691E-04	6.391E-04	1.235E-03	1.300E-03	1.454E-03	2.577E-03
	M4	1.955E-04	2.626E-04	3.773E-04	4.010E-04	4.325E-04	2.354E-04
	M5	5.341E-05	1.674E-04	1.203E-04	1.094E-04	9.241E-05	1.907E-05
	M6	1.551E-05	8.365E-05	5.155E-05	4.250E-05	2.834E-05	0.000E+00
	M7	5.491E-06	3.151E-05	2.008E-05	1.143E-05	5.572E-06	0.000E+00

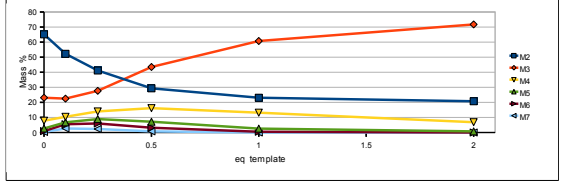


Template: N



Mass %	eq:	0	0.1	0.25	0.5	1	2
	M2	65.12	52.24	41.11	29.33	23.05	20.78
	M3	23.07	22.46	27.66	43.48	60.7	71.71
	M4	7.82	10.4	13.94	16.19	13.12	6.78
	M5	2.67	6.75	8.94	7.12	2.6	0.73
	M6	0.93	5.49	6	3.12	0.52	0
	M7	0.38	2.67	2.34	0.77	0.01	0

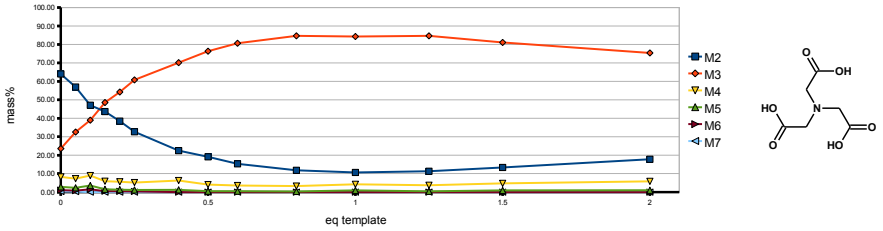
c[mol/L]	eq:	0	0.1	0.25	0.5	1	2
	M2	3.256E-03	2.612E-03	2.056E-03	1.466E-03	1.152E-03	1.039E-03
	M3	7.691E-04	7.486E-04	9.222E-04	1.449E-03	2.023E-03	2.390E-03
	M4	1.955E-04	2.601E-04	3.486E-04	4.047E-04	3.281E-04	1.695E-04
	M5	5.341E-05	1.351E-04	1.787E-04	1.423E-04	5.197E-05	1.460E-05
	M6	1.551E-05	9.142E-05	1.001E-04	5.195E-05	8.695E-06	0.000E+00
	M7	5.491E-06	3.809E-05	3.339E-05	1.103E-05	1.433E-07	0.000E+00



Template: O

%mas	eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
	M2	64.01	56.88	47.05	43.63	38.47	32.64	-	22.44	19.11	15.32	11.81	10.60	11.26	13.35	17.77
	M3	23.53	32.53	38.97	48.52	54.23	60.78	-	70.14	76.37	80.68	84.65	84.30	84.63	81.08	75.40
	M4	8.22	7.25	8.93	5.89	5.58	5.15	-	6.21	4.03	3.55	3.24	4.18	3.71	4.68	5.82
	M5	2.84	2.29	3.63	1.50	1.31	1.11	-	1.22	0.49	0.46	0.30	0.92	0.39	0.90	1.01
	M6	1.05	0.79	1.51	0.46	0.40	0.32	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	M7	0.34	0.25	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

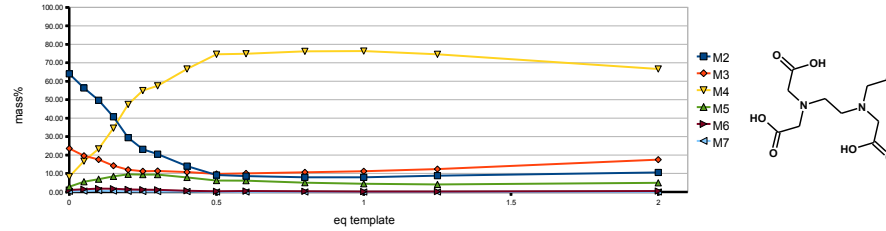
c [mol/L]	eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
	M2	3.201E-03	2.844E-03	2.353E-03	2.181E-03	1.924E-03	1.632E-03	-	1.122E-03	9.556E-04	7.659E-04	5.903E-04	5.298E-04	5.632E-04	6.673E-04	8.884E-04
	M3	7.845E-04	1.084E-03	1.299E-03	1.617E-03	1.808E-03	2.026E-03	-	2.338E-03	2.546E-03	2.689E-03	2.822E-03	2.810E-03	2.821E-03	2.703E-03	2.513E-03
	M4	2.056E-04	1.813E-04	2.233E-04	1.473E-04	1.396E-04	1.287E-04	-	1.551E-04	1.007E-04	8.871E-05	8.111E-05	1.045E-04	9.277E-05	1.169E-04	1.455E-04
	M5	5.676E-05	4.579E-05	7.068E-05	2.993E-05	2.615E-05	2.221E-05	-	2.435E-05	9.860E-06	9.157E-06	6.076E-06	1.839E-05	7.835E-06	1.791E-05	2.021E-05
	M6	1.744E-05	1.318E-05	2.518E-05	7.741E-06	6.746E-06	5.362E-06	-	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	M7	4.883E-06	3.568E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00



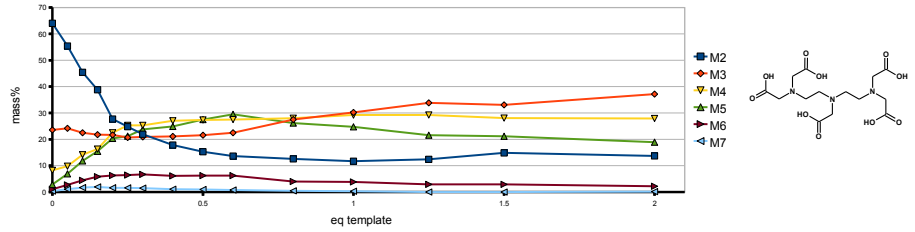
Template: P

%mas	eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
	M2	64.01	56.30	49.71	40.67	29.36	23.09	20.48	13.96	9.14	8.59	7.89	7.89	8.82	-	10.54
	M3	23.53	19.61	17.54	14.17	12.02	11.19	11.32	10.76	9.75	10.00	10.62	11.17	12.37	-	17.46
	M4	8.22	16.70	23.35	34.54	47.41	54.91	57.49	66.63	74.62	74.84	76.18	76.35	74.58	-	66.63
	M5	2.84	5.48	6.90	8.44	9.56	9.38	9.36	7.83	6.18	6.13	4.98	4.41	4.04	-	4.90
	M6	1.05	1.42	1.79	1.74	1.34	1.20	1.15	0.65	0.31	0.44	0.34	0.17	0.19	-	0.48
	M7	0.34	0.48	0.70	0.44	0.30	0.22	0.20	0.17	0.00	0.00	0.00	0.00	0.00	-	0.00

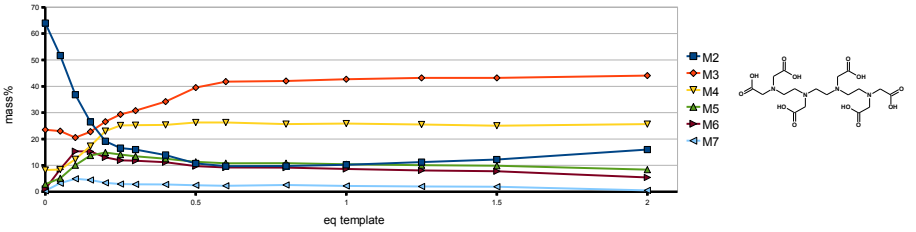
c [mol/L]	eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
	M2	3.201E-03	2.815E-03	2.486E-03	2.034E-03	1.468E-03	1.155E-03	1.024E-03	6.978E-04	4.572E-04	4.293E-04	3.943E-04	3.946E-04	4.409E-04	-	5.269E-04
	M3	7.845E-04	6.538E-04	5.847E-04	4.723E-04	4.007E-04	3.730E-04	3.772E-04	3.587E-04	3.249E-04	3.332E-04	3.539E-04	3.724E-04	4.122E-04	-	5.819E-04
	M4	2.056E-04	4.175E-04	5.838E-04	8.634E-04	1.185E-03	1.373E-03	1.437E-03	1.666E-03	1.865E-03	1.871E-03	1.904E-03	1.909E-03	1.865E-03	-	1.666E-03
	M5	5.676E-05	1.096E-04	1.381E-04	1.688E-04	1.911E-04	1.876E-04	1.871E-04	1.566E-04	1.237E-04	1.227E-04	9.965E-05	8.823E-05	8.083E-05	-	9.799E-05
	M6	1.744E-05	2.369E-05	2.986E-05	2.897E-05	2.239E-05	2.008E-05	1.922E-05	1.089E-05	5.103E-06	7.326E-06	5.604E-06	2.867E-06	3.192E-06	-	8.029E-06
	M7	4.883E-06	6.817E-06	9.978E-06	6.353E-06	4.329E-06	3.209E-06	2.915E-06	2.479E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	-	0.000E+00



Template:	Q														
eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
M2	64.01	55.39	45.44	38.79	27.69	24.79	21.91	17.83	15.28	13.62	12.56	11.71	12.43	14.84	13.71
M3	23.53	24.18	22.49	21.76	21.65	20.68	20.88	21.08	21.56	22.46	27.46	30.21	33.84	33.05	37.14
M4	8.22	9.80	14.15	16.27	22.46	25.30	25.31	27.03	27.35	27.51	27.99	29.21	29.24	28.07	27.91
M5	2.84	6.89	11.80	15.45	20.31	21.23	23.76	24.87	27.50	29.46	26.17	24.75	21.56	21.15	18.89
M6	1.05	2.68	4.44	5.82	6.29	6.45	6.68	6.10	6.21	6.21	3.95	3.82	2.93	2.90	2.21
M7	0.34	1.06	1.68	1.92	1.60	1.56	1.46	1.04	0.97	0.74	0.43	0.30	0.00	0.00	0.14
eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
M2	3.201E-03	2.769E-03	2.272E-03	1.939E-03	1.384E-03	1.239E-03	1.096E-03	9.103E-04	7.727E-04	6.812E-04	6.370E-04	5.856E-04	6.215E-04	7.418E-04	6.855E-04
M3	7.845E-04	8.059E-04	7.497E-04	7.252E-04	7.216E-04	6.892E-04	6.961E-04	7.172E-04	7.270E-04	7.485E-04	9.292E-04	1.007E-03	1.128E-03	1.102E-03	1.238E-03
M4	2.056E-04	2.450E-04	3.538E-04	4.067E-04	5.616E-04	6.325E-04	6.328E-04	6.899E-04	6.915E-04	6.877E-04	7.098E-04	7.302E-04	7.311E-04	7.016E-04	6.977E-04
M5	5.676E-05	1.378E-04	2.360E-04	3.090E-04	4.062E-04	4.246E-04	4.751E-04	5.078E-04	5.563E-04	5.893E-04	5.309E-04	4.950E-04	4.311E-04	4.230E-04	3.778E-04
M6	1.744E-05	4.474E-05	7.403E-05	9.704E-05	1.048E-04	1.075E-04	1.113E-04	1.038E-04	1.046E-04	1.035E-04	6.688E-05	6.361E-05	4.879E-05	4.830E-05	3.676E-05
M7	4.883E-06	1.514E-05	2.394E-05	2.739E-05	2.286E-05	2.225E-05	2.090E-05	1.513E-05	1.407E-05	1.052E-05	6.188E-06	4.339E-06	0.000E+00	0.000E+00	2.071E-06

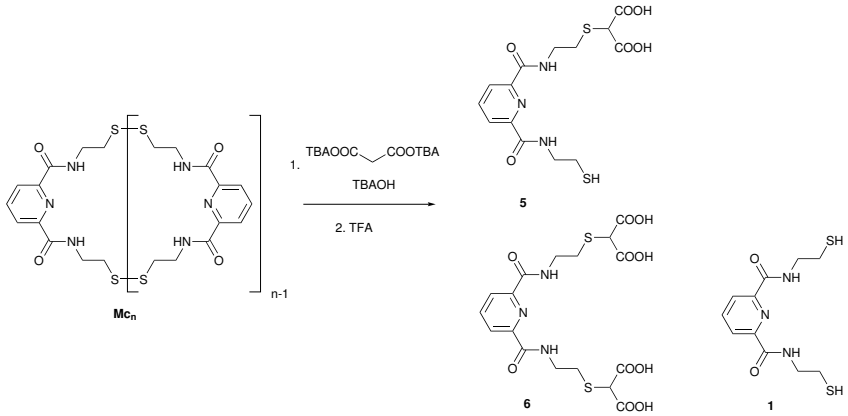


Template:	R														
eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
M2	64.01	51.66	36.82	26.46	19.17	16.57	15.99	13.92	10.75	9.70	9.76	10.25	11.22	12.23	15.98
M3	23.53	22.99	20.52	22.77	26.59	29.36	30.76	34.21	39.50	41.79	42.01	42.66	43.19	43.17	44.06
M4	8.22	8.44	12.34	17.31	22.97	25.14	25.26	25.36	26.26	26.26	25.68	25.84	25.48	25.07	25.66
M5	2.84	5.12	10.05	13.75	14.86	14.12	13.42	12.53	11.32	10.81	10.84	10.43	10.04	9.85	8.38
M6	1.05	8.55	15.35	15.29	13.04	11.91	11.76	11.21	9.72	9.19	9.15	8.64	8.07	7.77	5.41
M7	0.34	3.24	4.92	4.43	3.36	2.90	2.81	2.77	2.46	2.26	2.57	2.18	2.00	1.91	0.51
eq:	0	0.05	0.1	0.15	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1	1.25	1.5	2
M2	3.201E-03	2.583E-03	1.841E-03	1.323E-03	9.586E-04	8.287E-04	7.996E-04	6.961E-04	5.374E-04	4.850E-04	4.879E-04	5.123E-04	5.610E-04	6.117E-04	7.991E-04
M3	7.845E-04	7.664E-04	6.841E-04	7.591E-04	8.863E-04	9.786E-04	1.025E-03	1.140E-03	1.317E-03	1.393E-03	1.400E-03	1.422E-03	1.440E-03	1.439E-03	1.469E-03
M4	2.056E-04	2.110E-04	3.084E-04	4.326E-04	5.744E-04	6.286E-04	6.314E-04	6.341E-04	6.564E-04	6.564E-04	6.419E-04	6.461E-04	6.370E-04	6.267E-04	6.414E-04
M5	5.676E-05	1.023E-04	2.010E-04	2.751E-04	2.973E-04	2.824E-04	2.684E-04	2.506E-04	2.265E-04	2.162E-04	2.168E-04	2.087E-04	2.009E-04	1.970E-04	1.675E-04
M6	1.744E-05	1.425E-04	2.559E-04	2.548E-04	2.174E-04	1.985E-04	1.960E-04	1.868E-04	1.619E-04	1.531E-04	1.525E-04	1.439E-04	1.344E-04	1.295E-04	9.022E-05
M7	4.883E-06	4.632E-05	7.028E-05	6.322E-05	4.801E-05	4.137E-05	4.021E-05	3.951E-05	3.509E-05	3.225E-05	3.667E-05	3.110E-05	2.854E-05	2.725E-05	7.350E-06



S2 Reaction of a library with malonate

Templation of a library **Mc**$_n$ with an excess of malonate diTBA salt resulted in disapperance of the macrocylces. We suggest the following reaction to proceed:



In the reaction mixture we identified compounds **1** and **5** by the means of MS.

S3 HPLC-HRMS analysis

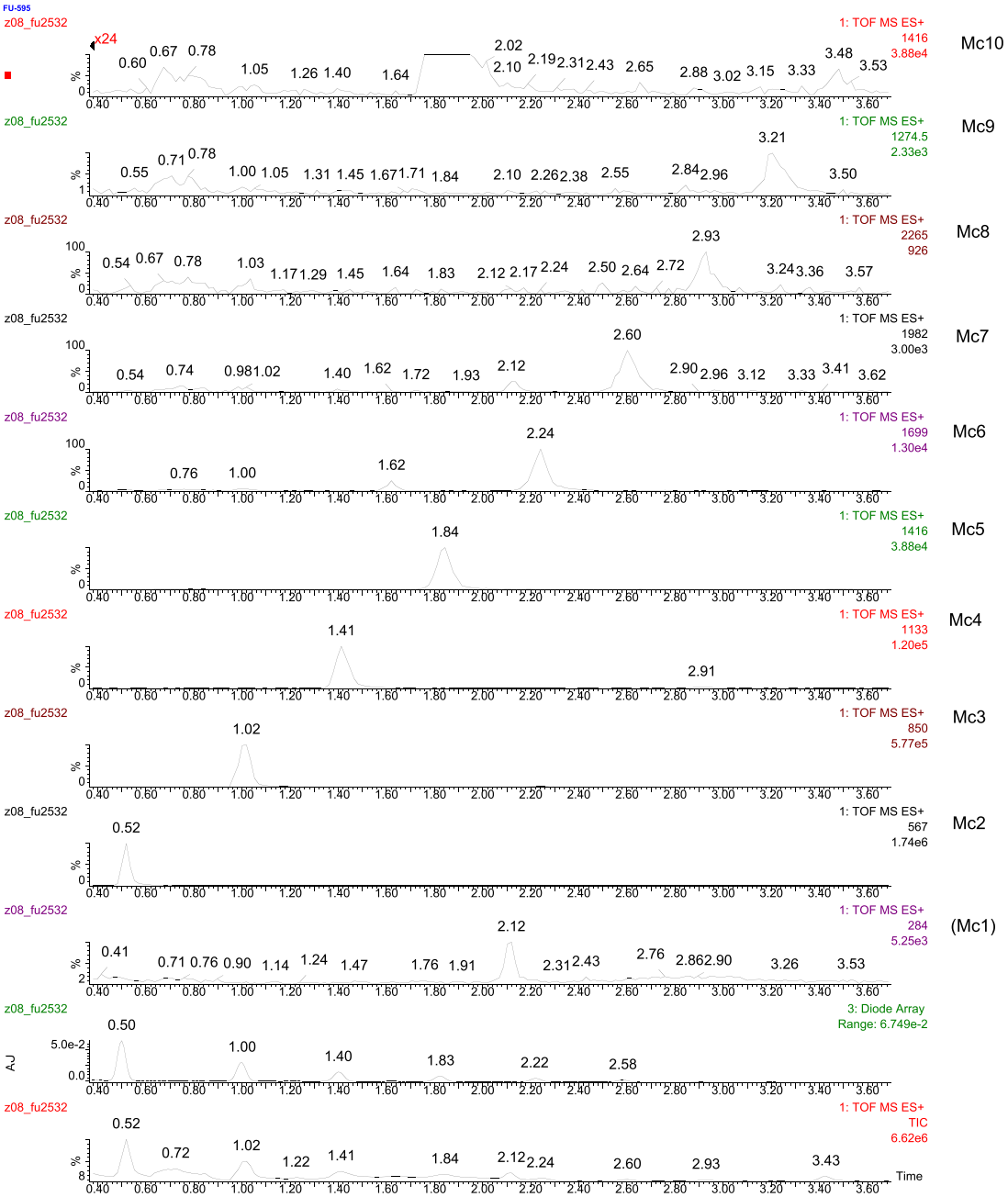


Figure S1: LC-MS analysis of the library. Total ion current, UV (220 nm), and extracted ion chromatograms for **Mc**$_1$-**Mc**$_{10}$

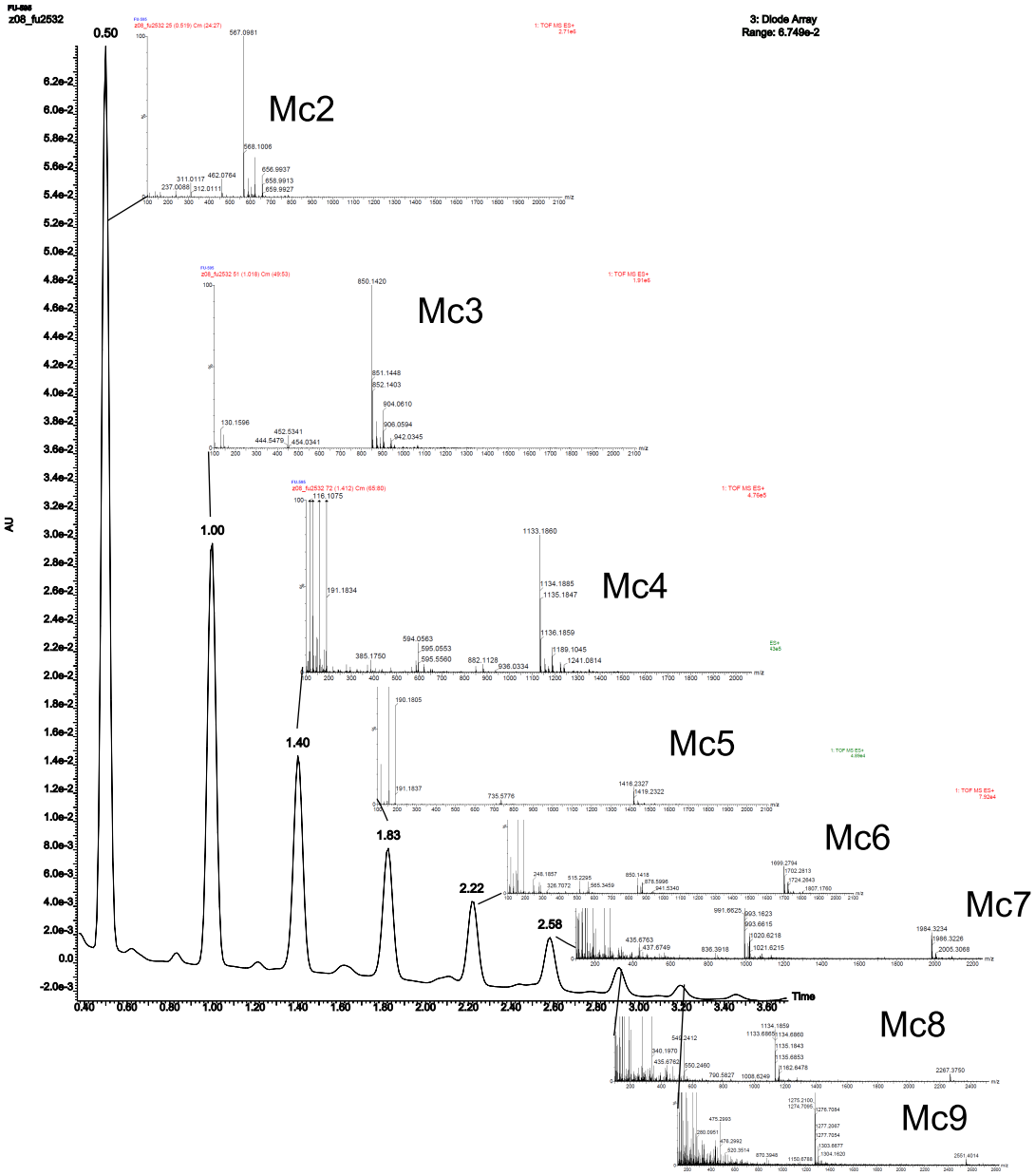


Figure S2: UV trace of LCMS analysis and MS spectra for each peak

HRMS results for oligomers:

Mc$_2$	Calc. for $C_{22}H_{27}N_6O_4S_4$ $(M+H^+)$:	567.0971
	found:	567.0981
Mc$_3$	Calc. for $C_{33}H_{40}N_9O_6S_6$ $(M+H^+)$:	850.1420
	found:	850.1420
Mc$_4$	Calc. for $C_{44}H_{53}N_{12}O_8S_8$ $(M+H^+)$:	1133.1869
	found:	1133.1860
Mc$_5$	Calc. for $C_{55}H_{66}N_{15}O_{10}S_{10}$ $(M+H^+)$:	1416.2318
	found:	1416.2327
Mc$_6$	Calc. for $C_{66}H_{79}N_{18}O_{12}S_{12}$ $(M+H^+)$:	1699.276
	found:	1699.279
Mc$_7$	Calc. for $C_{77}H_{92}N_{21}O_{14}S_{14}$ $(M+H^+)$:	1982.321
	found:	1982.327

S4 Preparative HPLC

The libraries were prepared as described above (typically 5 mL, 0.02 mmol, 28 mg) and were templated with appropriate template at its optimal concentration:

	isolated yields [%]			
Template	**Mc**$_2$	**Mc**$_3$	**Mc**$_4$	**Mc**$_5$
A, 2 eq	70	0	0	0
O, 1 eq	15	60	5	0
P, 0.75 eq	25	20	40	4
Q, 0.6 eq	10	18	22	25

Preparative isolation of oligomeric macrocyles was performed with HPLC column (Poligroprep C18 12um i.d. 20 mm l 300 mm) with gradient elution:

	eluent composition [%]	
time [min]	DMF	H_2O
0	60	40
5	60	40
20	73	27
40	80	20

UV detector was set to $\lambda = 285$ nm.

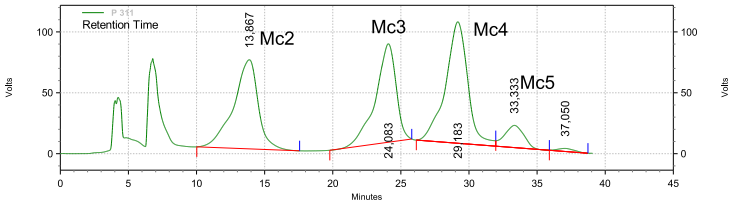


Figure S3: An example of preparative resolution of library members. DCC templated with EDTA (**P**).

S5 DCLfit analyses

S5.1 Analysis of untemplated libraly

Since monomeric macrocycle does not form upon oxidation of **1** it is treated as virtual molecule which is used to calculate formation constants of higher oligomers. The first formation constant K_2 corresponds to the reaction:

$$\mathrm{Mc}_1 + \mathrm{Mc}_1 \rightleftharpoons \mathrm{Mc}_2 \tag{1}$$

$$K_2 = \frac{[\mathrm{Mc}_2]}{[\mathrm{Mc}_1]^2} \tag{2}$$

This formation constant is arbitrary set to $\log(K_2) = 1$, and this defines the concentration of virtual **Mc**$_1$. Other macrocylces are in equilibrium according to following equations:

$$\mathrm{Mc}_{n-1} + \mathrm{Mc}_1 \rightleftharpoons \mathrm{Mc}_n \tag{3}$$

$$K_n = \frac{[\mathrm{Mc}_n]}{[\mathrm{Mc}_{n-1}] \cdot [\mathrm{Mc}_1]} \tag{4}$$

The association constants K_3-K_6 were fitted for a series of libraries with various total concentrations. The fitted values are as follows:

$$\log(K_2) \stackrel{\mathrm{def}}{=} 1.00$$
$$\log(K_3) = 1.13$$
$$\log(K_4) = 1.19$$
$$\log(K_5) = 1.21$$
$$\log(K_6) = 1.20$$

K_3 is slightly lower then following values which indicates that $\mathbf{Mc}_2$ is more stable. K_4-K_6 being nearly equal indicate simple polymerisation model for higher oligomers with a single formation constant K_n.
The values obtained in this set of experiments were used in analyses of templated libraries.

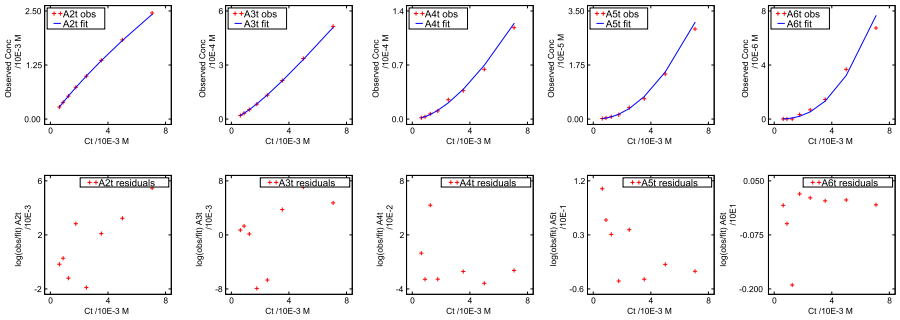


Figure S4: Concentrations of components of untemplated libraries at various total concentrations fitted with DCLfit software

S5.2 Analyses of templated libraries

Association constants fitted in the experiments were defined as follows:

$$K(\mathrm{Mc}_n - \mathrm{T}_m) \quad = \quad \frac{[\mathrm{Mc}_n\mathrm{T}_m]}{[\mathrm{Mc}_n\mathrm{T}_{m-1}] \cdot [\mathrm{T}]} \tag{5}$$

$$\mathrm{Mc_nT_{m-1}} + \mathrm{T} \quad <=> \quad \mathrm{Mc_nT_m} \tag{6}$$

Template A Applied model includes following species (**T** stands for template) : $\mathbf{Mc}_2$; $\mathbf{Mc}_3$; $\mathbf{Mc}_4$; $\mathbf{Mc}_5$; $\mathbf{Mc}_2$-**T**; $\mathbf{Mc}_3$-**T**; $\mathbf{Mc}_3$-$\mathbf{T}_2$; $\mathbf{Mc}_4$-**T**; $\mathbf{Mc}_4$-$\mathbf{T}_2$; $\mathbf{Mc}_5$-**T**; $\mathbf{Mc}_5$-$\mathbf{T}_2$.
Values obtained:

$$\log(K(M_2T)) = 2.78$$
$$\log(K(M_3T)) = 2.55$$
$$\log(K(M_4T)) = 2.67$$
$$\log(K(M_5T)) = 2.85$$
$$\log(K(M_3T_2)) = 0.85$$
$$\log(K(M_4T_2)) = 1.02$$
$$\log(K(M_5T_2)) = 1.61$$

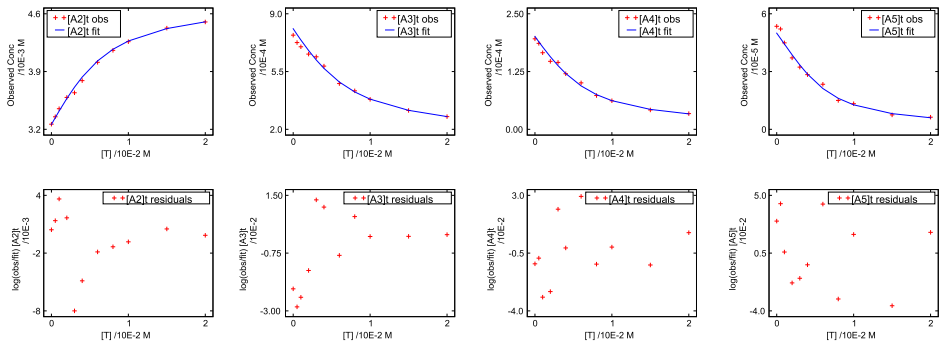


Figure S5: Templation effects of anion **A** fitted with DCLfit

Template O Applied model includes following species (**T** stands for template) : **Mc**$_2$; **Mc**$_3$; **Mc**$_4$; **Mc**$_5$; **Mc**$_2$-**T**; **Mc**$_3$-**T**; **Mc**$_3$-**T**$_2$; **Mc**$_4$-**T**; **Mc**$_4$-**T**$_2$; **Mc**$_5$-**T**; **Mc**$_5$-**T**$_2$.
Values obtained:

$$\log\left(K\left(Mc_2T\right)\right) = 1.99$$
$$\log\left(K\left(Mc_3T\right)\right) = 4.06$$
$$\log\left(K\left(Mc_4T\right)\right) = 3.50$$
$$\log\left(K\left(Mc_5T\right)\right) = 3.58$$
$$\log\left(K\left(Mc_3T_2\right)\right) = 0.00$$
$$\log\left(K\left(Mc_4T_2\right)\right) = 1.93$$
$$\log\left(K\left(Mc_5T_2\right)\right) = 2.00$$

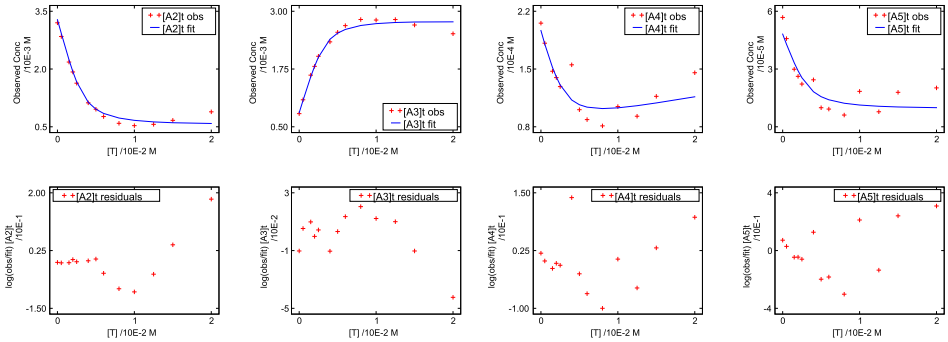


Figure S6: Templation effects of anion **O** fitted with DCLfit

Template P Applied model includes following species (**T** stands for template) : **Mc**$_2$; **Mc**$_3$; **Mc**$_4$; **Mc**$_5$; **Mc**$_2$-**T**; **Mc**$_3$-**T**; **Mc**$_3$-**T**$_2$; **Mc**$_4$-**T**; **Mc**$_4$-**T**$_2$; **Mc**$_5$-**T**; **Mc**$_5$-**T**$_2$.
Values obtained:

$$\log\left(K\left(Mc_2T\right)\right) = 1.64$$
$$\log\left(K\left(Mc_3T\right)\right) = 3.33$$
$$\log\left(K\left(Mc_4T\right)\right) = 5.10$$
$$\log\left(K\left(Mc_5T\right)\right) = 4.97$$
$$\log\left(K\left(Mc_3T_2\right)\right) = 0.00$$
$$\log\left(K\left(Mc_4T_2\right)\right) = 1.86$$
$$\log\left(K\left(Mc_5T_2\right)\right) = 0.00$$

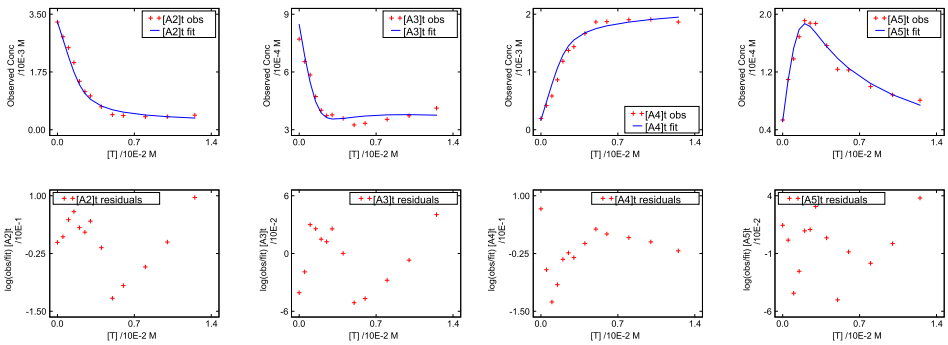


Figure S7: Templation effects of anion **P** fitted with DCLfit

Template Q Applied model includes following species (**T** stands for template) : **Mc**$_2$; **Mc**$_3$; **Mc**$_4$; **Mc**$_5$; **Mc**$_2$-**T**; **Mc**$_3$-**T**; **Mc**$_3$-**T**$_2$; **Mc**$_4$-**T**; **Mc**$_4$-**T**$_2$; **Mc**$_5$-**T**; **Mc**$_5$-**T**$_2$; **Mc**$_6$-**T**; **Mc**$_6$-**T**$_2$.
Values obtained:

$$\log(K(Mc_2T)) = 1.85$$
$$\log(K(Mc_3T)) = 3.38$$
$$\log(K(Mc_4T)) = 4.24$$
$$\log(K(Mc_5T)) = 4.84$$
$$\log(K(Mc_6T)) = 6.21$$
$$\log(K(Mc_3T_2)) = 1.43$$
$$\log(K(Mc_4T_2)) = 1.33$$
$$\log(K(Mc_5T_2)) = 2.04$$
$$\log(K(Mc_6T_2)) = 1.84$$

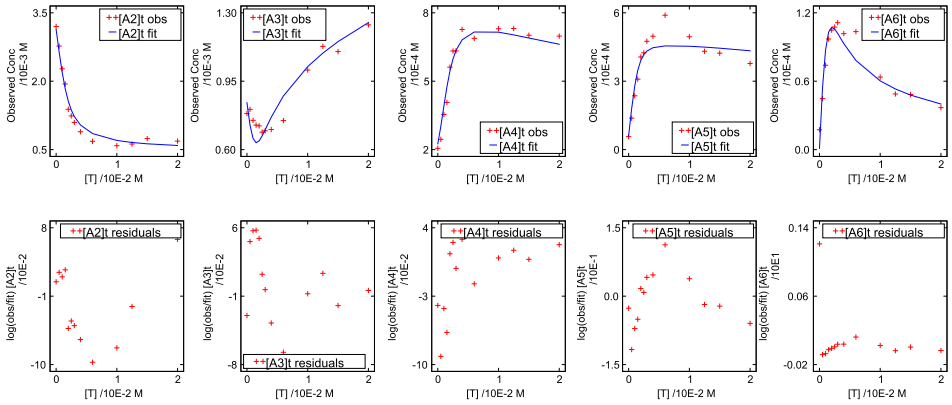


Figure S8: Templation effects of anion **Q** fitted with DCLfit

Template R Applied model includes following species (**T** stands for template) : **Mc**$_2$; **Mc**$_3$; **Mc**$_4$; **Mc**$_5$; **Mc**$_2$-**T**; **Mc**$_3$-**T**; **Mc**$_3$-**T**$_2$; **Mc**$_4$-**T**; **Mc**$_4$-**T**$_2$; **Mc**$_5$-**T**; **Mc**$_5$-**T**$_2$; **Mc**$_6$-**T**; **Mc**$_6$-**T**$_2$.
Values obtained:

$$\log(K(Mc_2T)) = 2.49$$
$$\log(K(Mc_3T)) = 4.30$$
$$\log(K(Mc_4T)) = 5.05$$
$$\log(K(Mc_5T)) = 5.58$$
$$\log(K(Mc_6T)) = 7.51$$
$$\log(K(Mc_3T_2)) = 1.21$$
$$\log(K(Mc_4T_2)) = 1.51$$
$$\log(K(Mc_5T_2)) = 2.60$$
$$\log(K(Mc_6T_2)) = 3.13$$

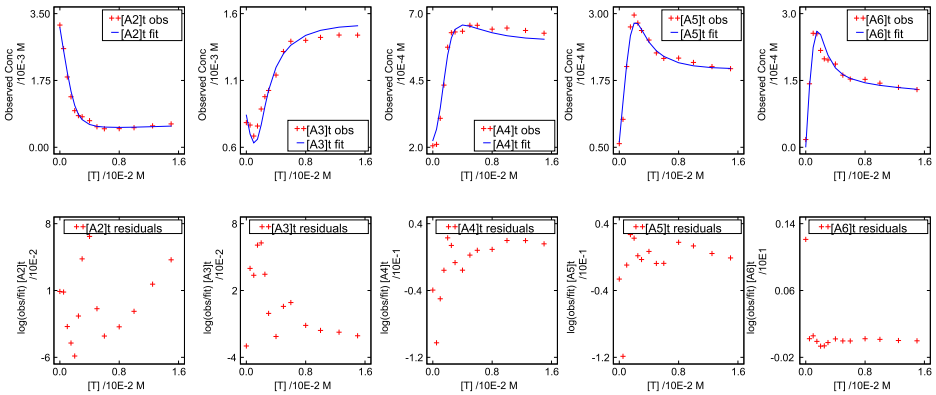


Figure S9: Templation effects of anion **R** fitted with DCLfit

S6 Competitive ^{1}H NMR titration

Separte stock solutions of pure $\mathbf{Mc}_2$-$\mathbf{Mc}_5$ were prepared in DMSO-d_6, c=10 mM. In the competitive experiments 50 uL of these solutions were mixed in an NMR tube and diluted with 0.3 mL to obtain a final concentration of 1 mM of each macrocylce. The solutions were titrated with solutions of appropriate TBA salt (**O**, **P**, and **Q**) in DMSO-d_6 (c=33 mM) added in portions of 5 uL (1/3 eq of each macrocylcle). Additional titrations of pure $\mathbf{Mc}_3$ and $\mathbf{Mc}_4$ hosts were performed for unambiguous signals assignment.

The titrations are presented herein:

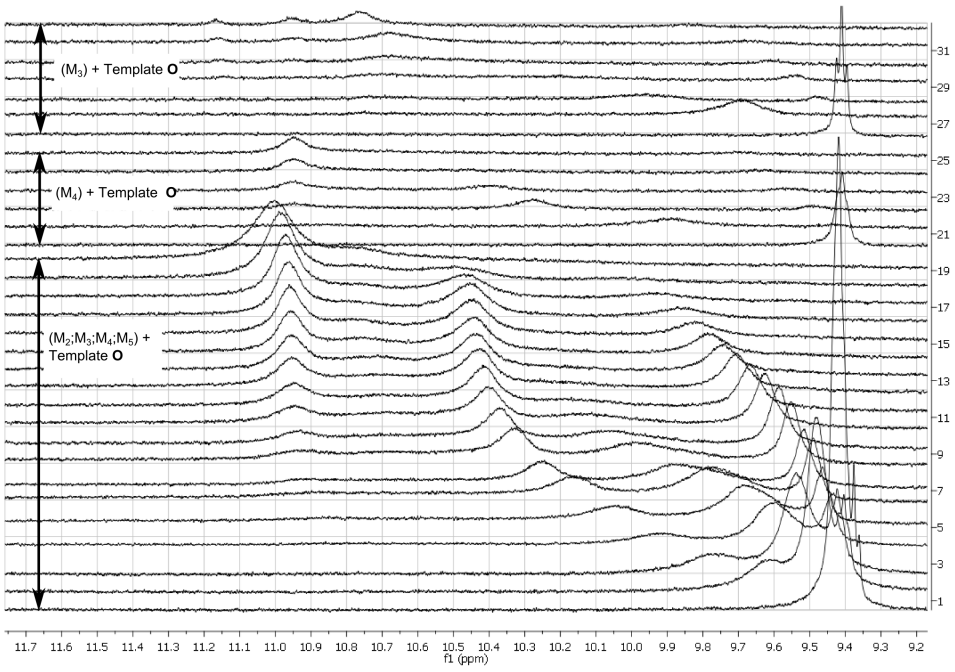


Figure S10: Competitive titration with template **O** (NTA anion)

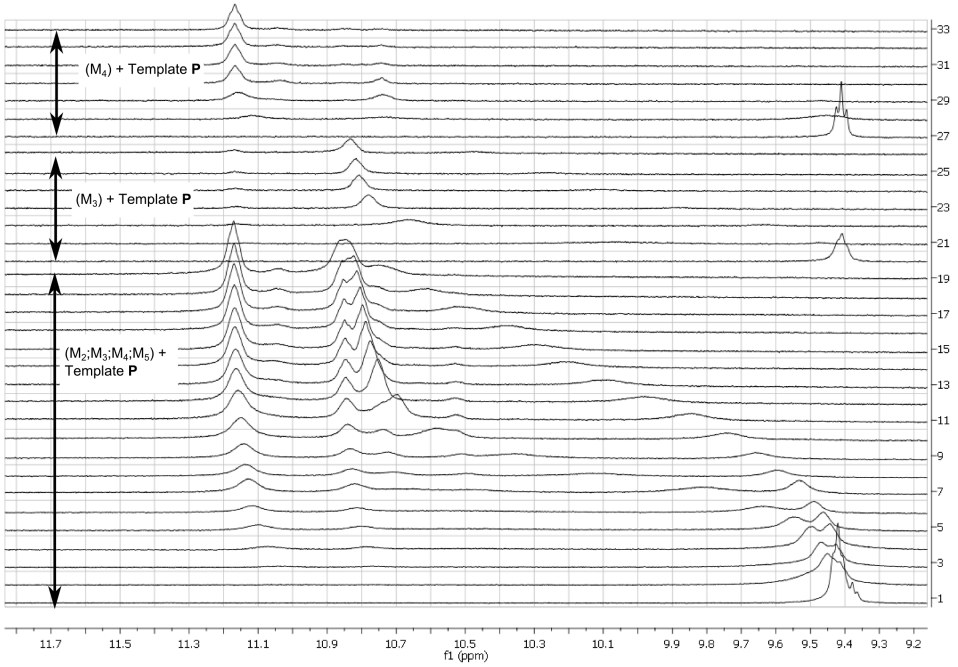


Figure S11: Competitive titration with template **P** (EDTA anion)

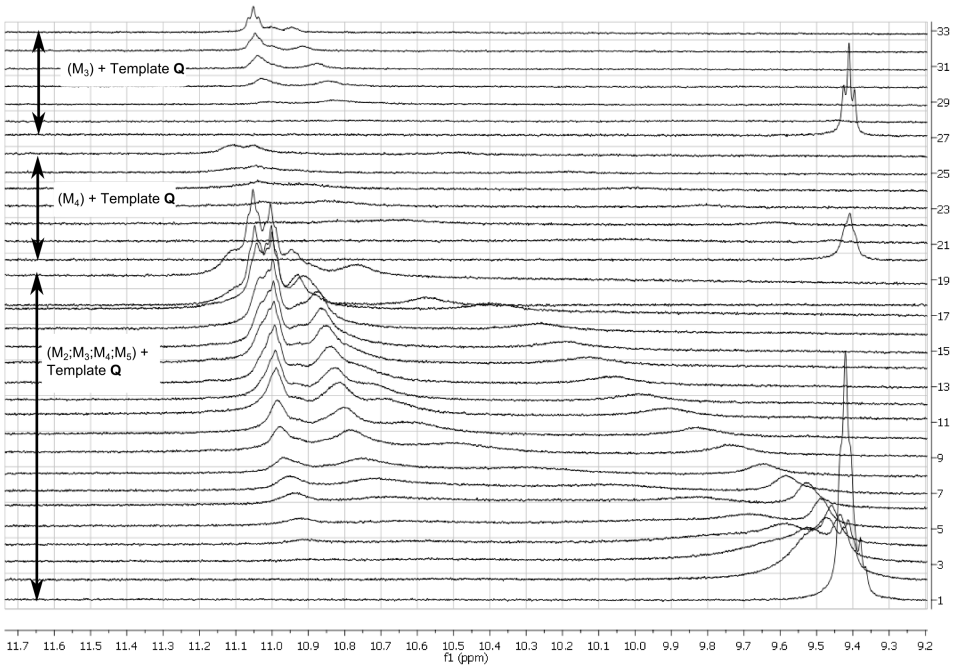


Figure S12: Competitive titration with template **Q** (DTPA anion)

S7 NMR spectra of new compounds

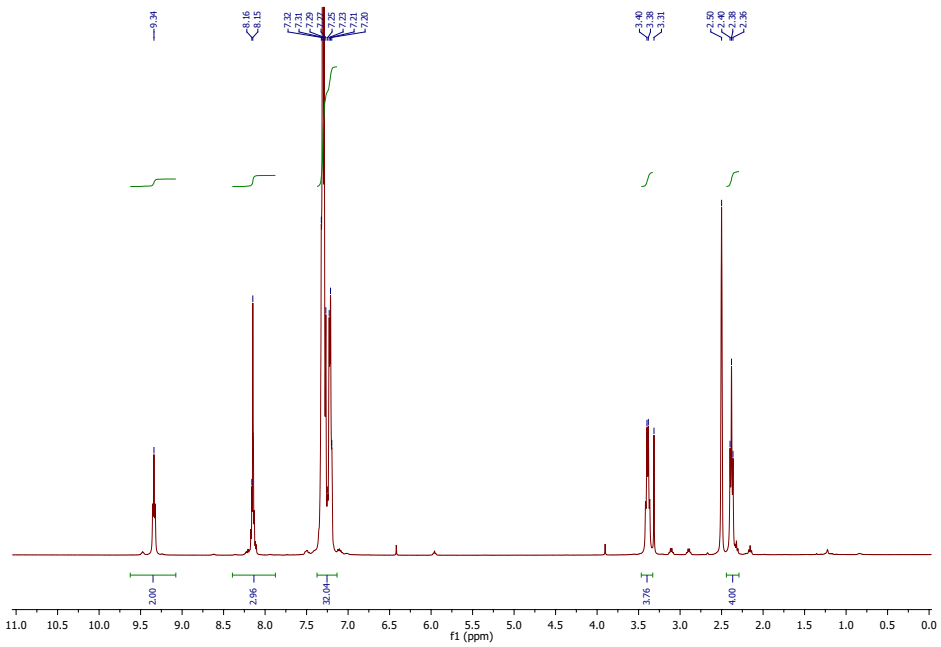


Figure S13: ^{1}H NMR spectrum of **4c** in $CDCl_3$

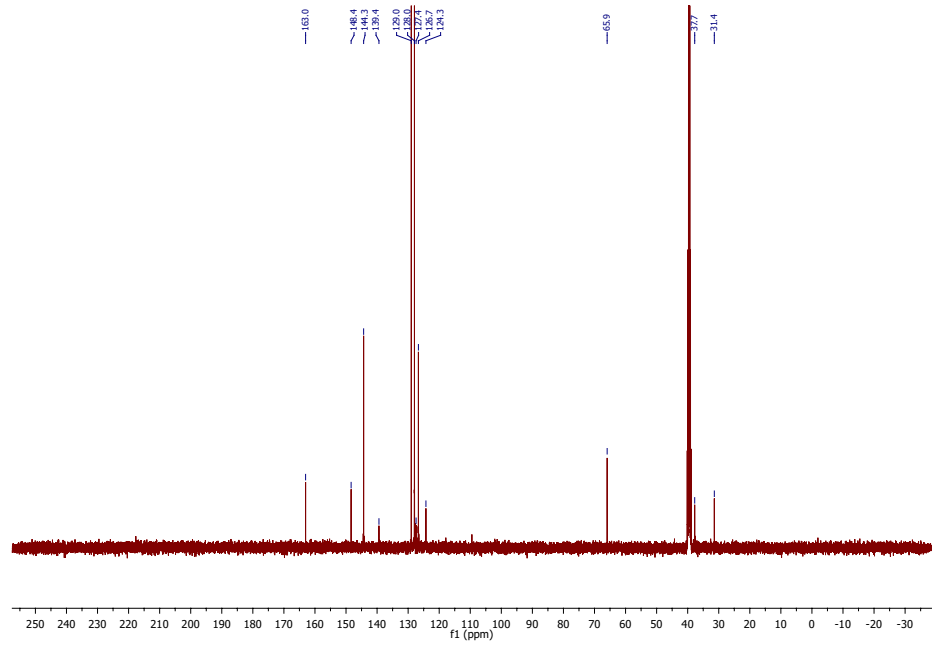


Figure S14: ^{13}C NMR spectrum of **4c** in $CDCl_3$

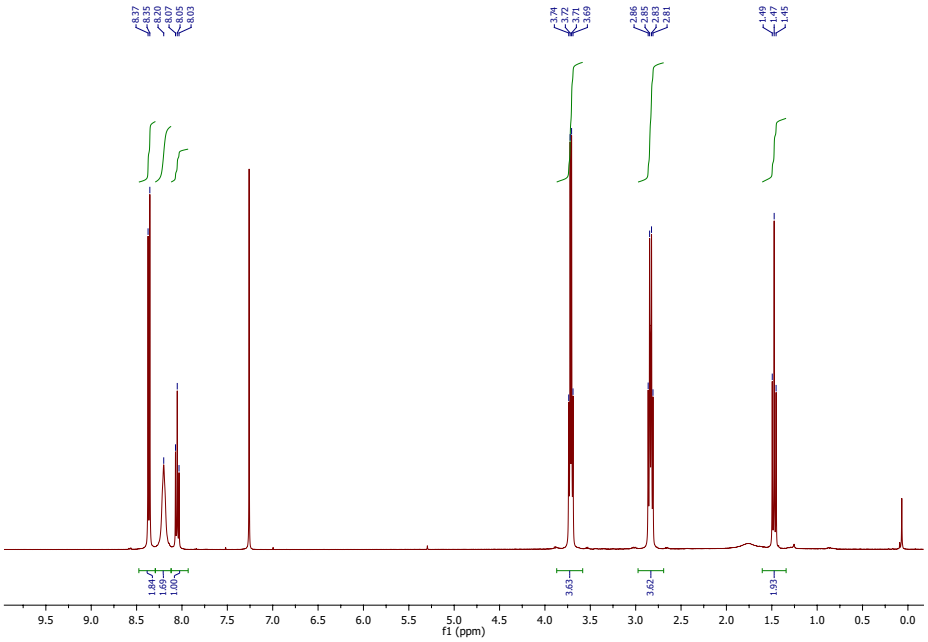


Figure S15: ^{1}H NMR spectrum of **1** in DMSO−d_6

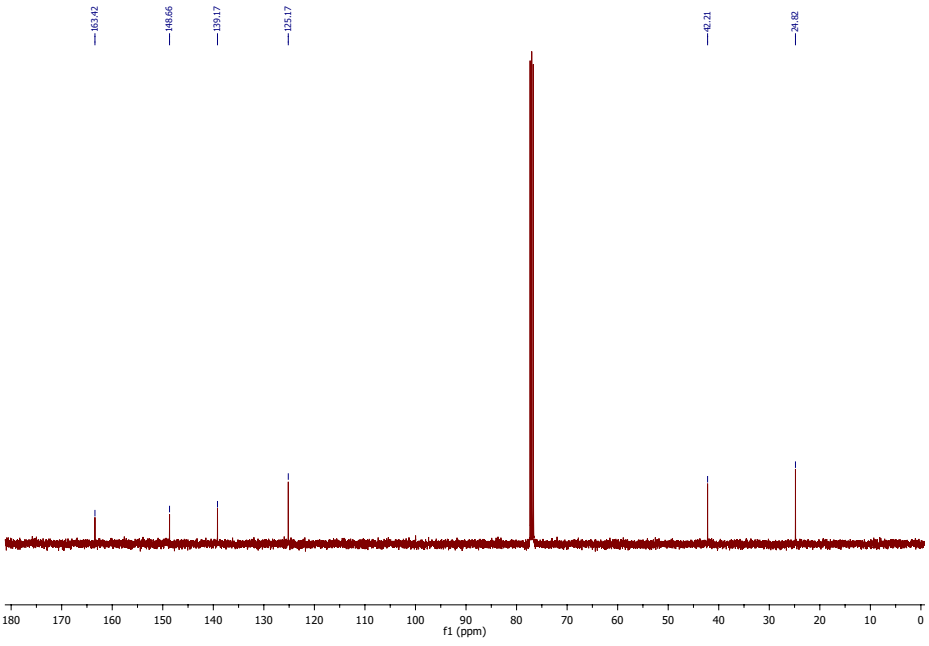


Figure S16: ^{13}C NMR spectrum of **1** in DMSO−d_6