

**USE OF CALIX[4]ARENES TO
RECOVER THE SELF-ASSEMBLY
ABILITY OF MUTATED p53
TETRAMERIZATION DOMAINS**

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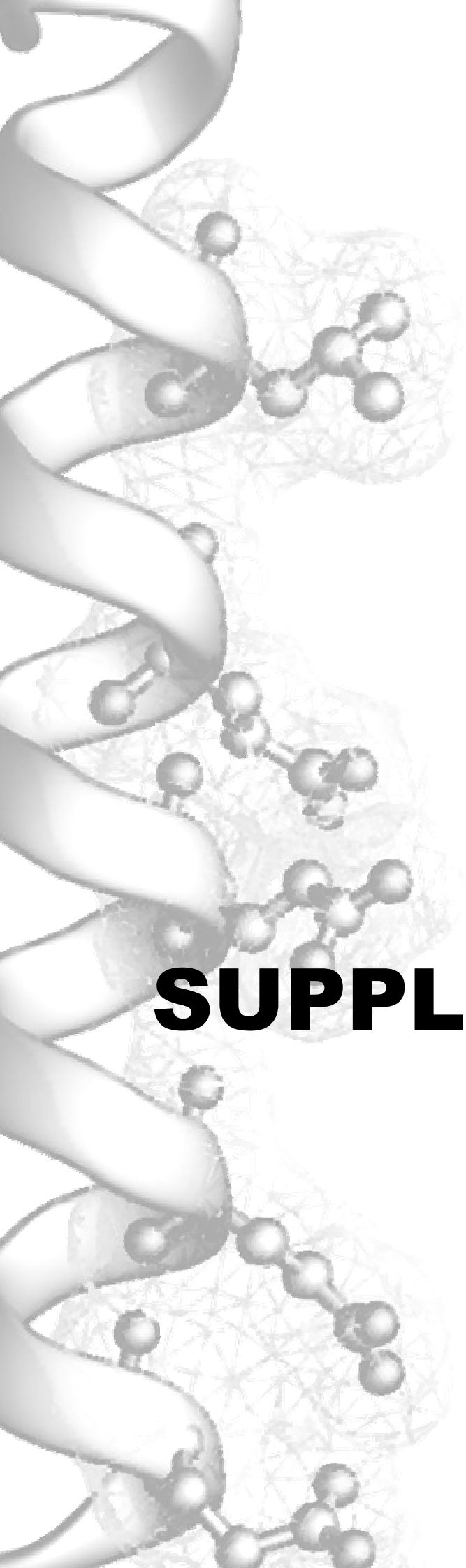
Universitat de Barcelona

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SUPPLEMENTARY

MATERIAL

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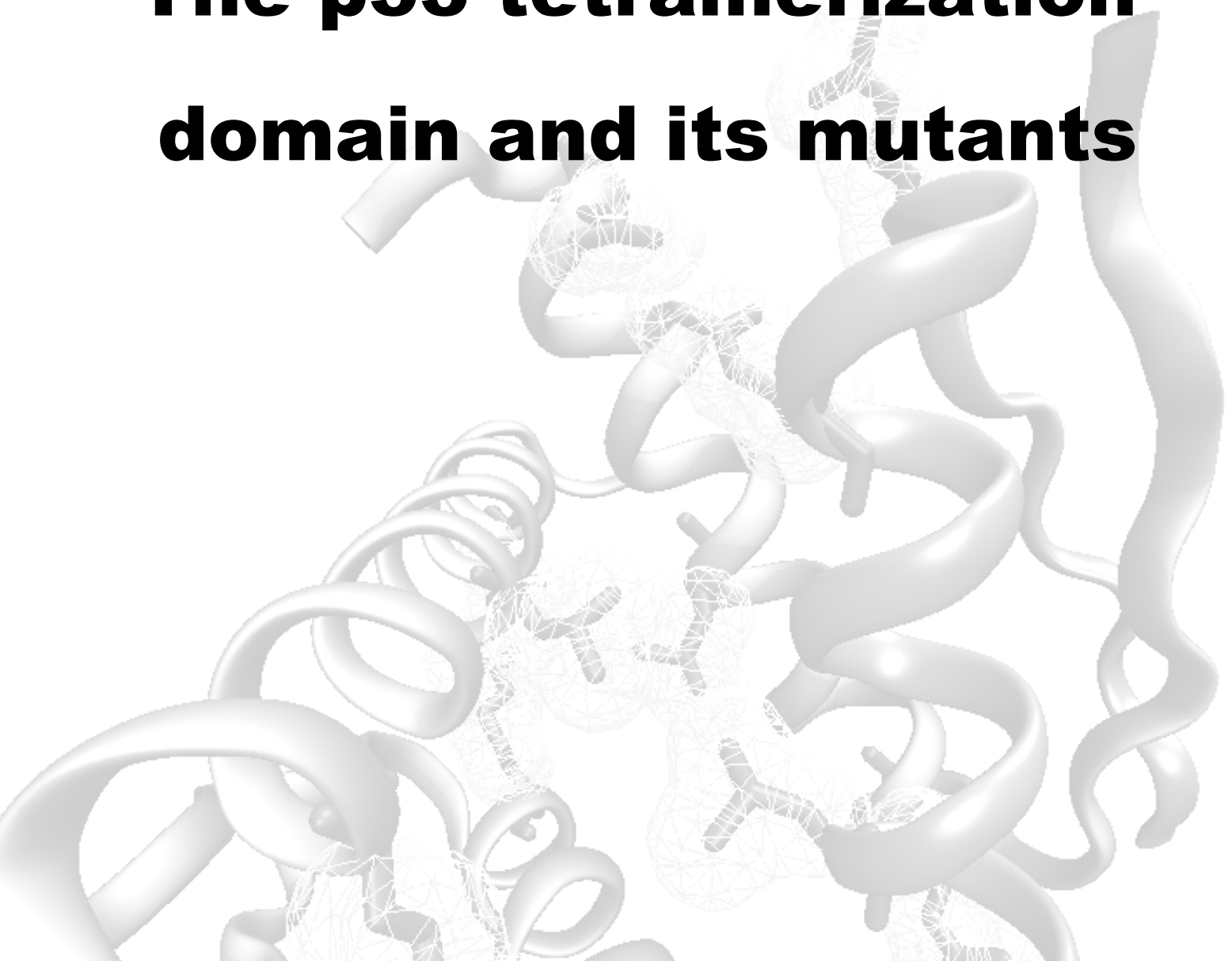
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The p53 tetramerization domain and its mutants



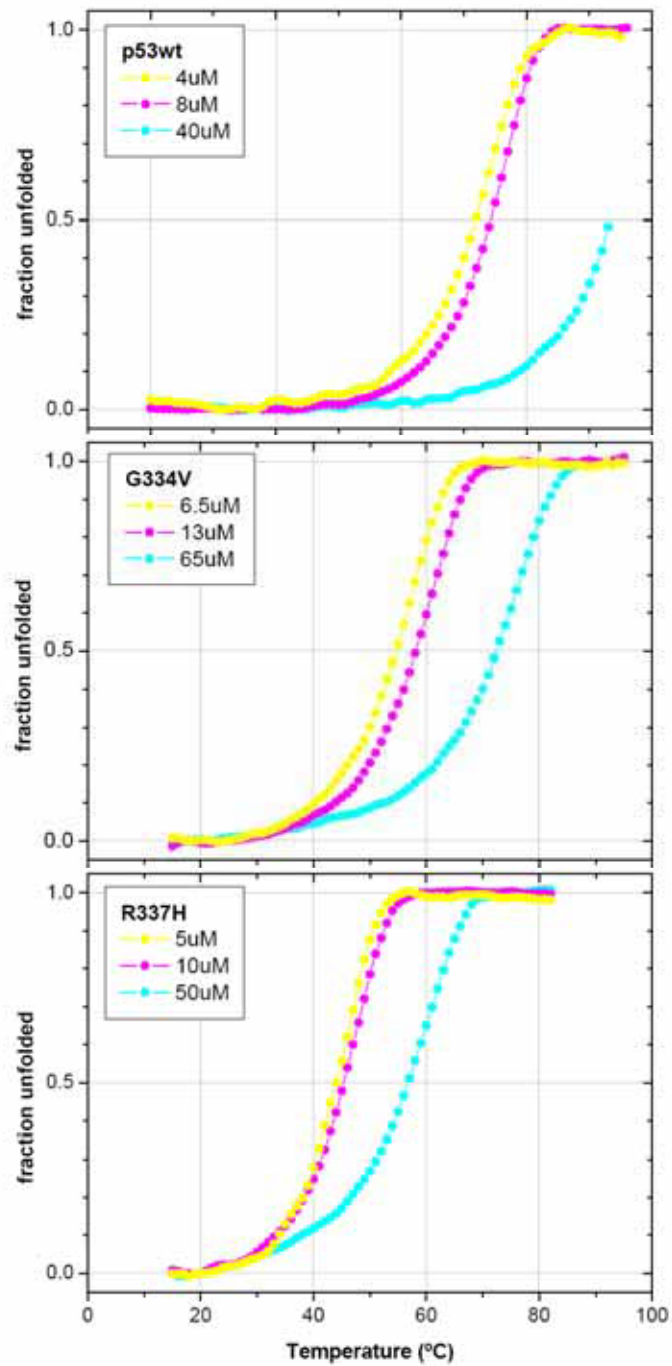
CD unfolding curves: concentration effects

Figure S1. CD unfolding curves in 25mM sodium phosphate buffer pH 7.0, 100mM NaCl, tracing θ at 220nm. Concentrations given as monomer.

G334V precipitation events in CD unfolding curves

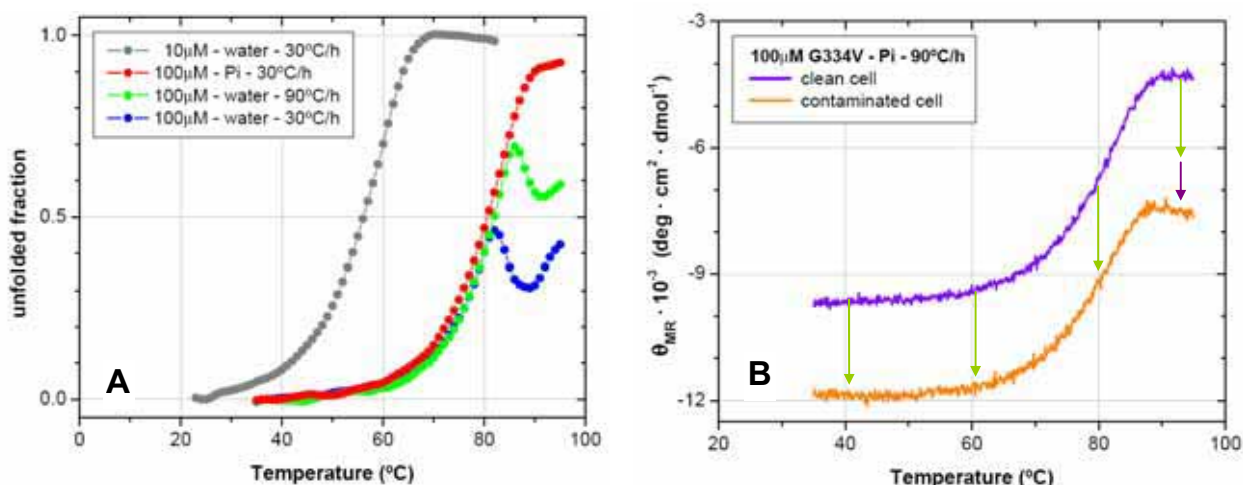


Figure S2. (A) Effects of concentration (10 μ M vs. 100 μ M monomer), buffer (water vs. 25mM phosphate, at pH 7) and heating rate (30 vs. 90°C/h). (B) G334V-aggregates contamination effects: the melting curve in orange was recorded in a cell where G334V had previously precipitated and was not cleaned with chromic mixture; the ellipticity was larger as a result of the protein that had been stuck onto the cell walls (green arrows). Said “contamination” also affected the unfolding pathway of the protein in solution (purple arrow).

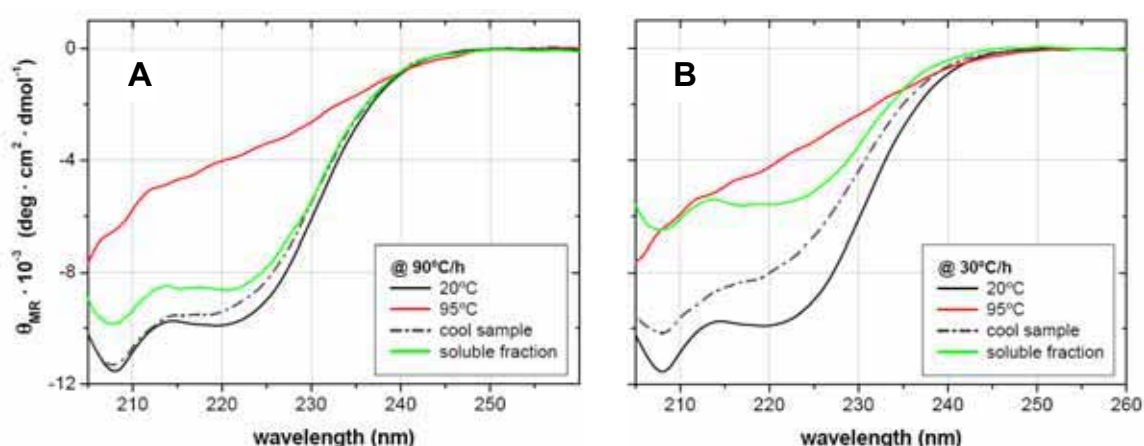


Figure S3. G334V precipitation and stacking onto the cell walls. In black, the CD spectrum for 100 μ M G334V (monomer) in water pH 7 at 20°C. In red, the unfolded profile at 95°C, after heating at (A) 90°C/h or (B) 30°C/h. The dashed grey line corresponds to the denatured samples cooled again, in the same cell. The spectrum for the soluble fraction of that sample is in green.

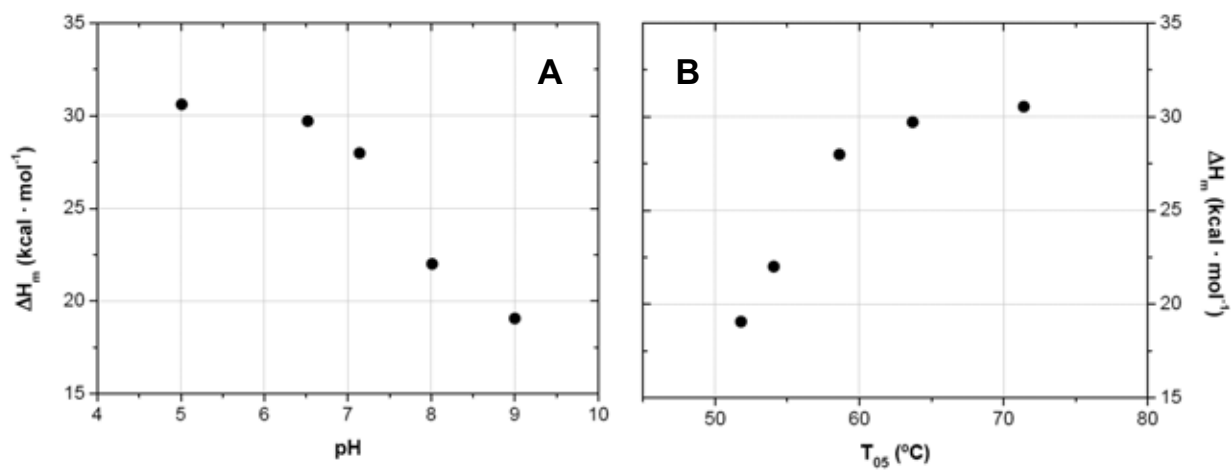
R337H DSC CURVES: effects of pH on ΔH_m 

Figure S4. Melting enthalpy for R337H plotted against (A) the pH and (B) the melting temperature (samples from Figure 1.25, main text).

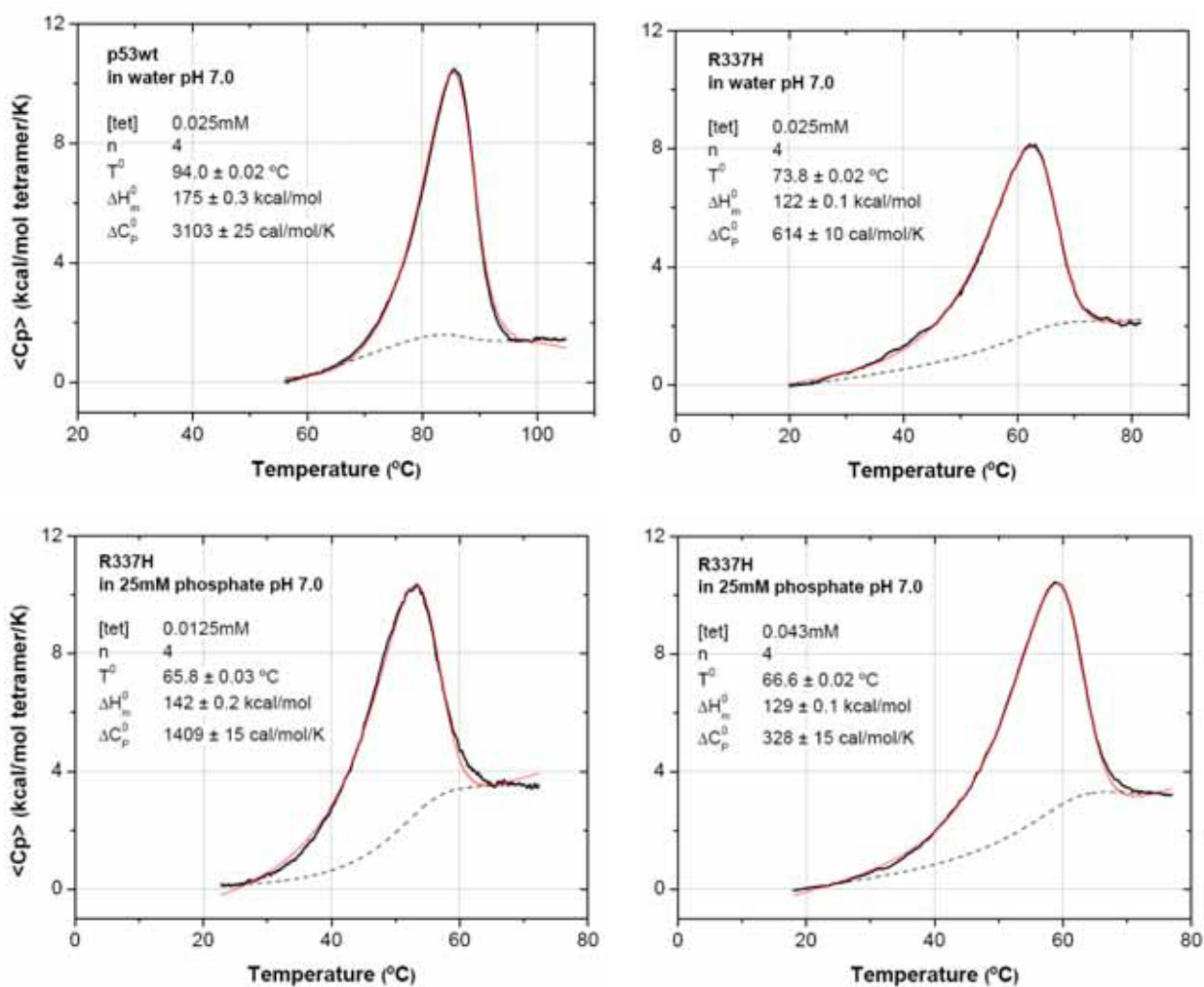
DSC CURVES. Mathematical adjustment to $N_4 \rightleftharpoons 4U$ 

Figure S5. Adjustment to the mathematical model of dissociation coupled to unfolding proposed by Freire *et al.* Values are given related to moles of tetramer.

**Calix4bridge:
a designed ligand for the
p53 tetramerization
domain**



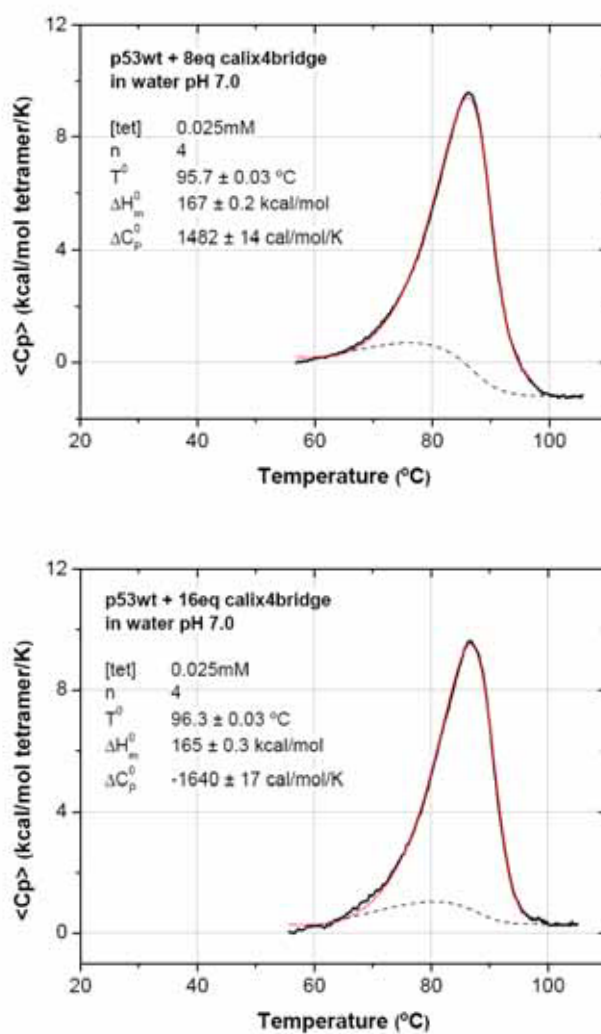
DSC CURVES of p53wt + calix4bridge.

Figure S6. Adjustment for samples of p53wt with calix4bridge to the mathematical model of dissociation coupled to unfolding proposed by Freire *et al.* Values are given related to moles of tetramer.

^1H -STD for NH_2 -calix4bridge

In order to confirm that STD results were not experimental artifacts, STD build-up curves were also traced for NH_2 -calix4bridge. Its affinity was considerably lower ($K_D \sim 0.8\text{mM}$), but still within the range for STD experiments. Lower temperature and lower ligand excess were used in order to improve the STD signals. Decreasing the ligand excess also decreases the observed STD, but it is balanced by the increase in the signal-to-noise ratio.³²

The quality for the STD experiment on NH_2 -calix4bridge was considerably lower than the achieved for calix4bridge, but high enough as to quantify the differences.

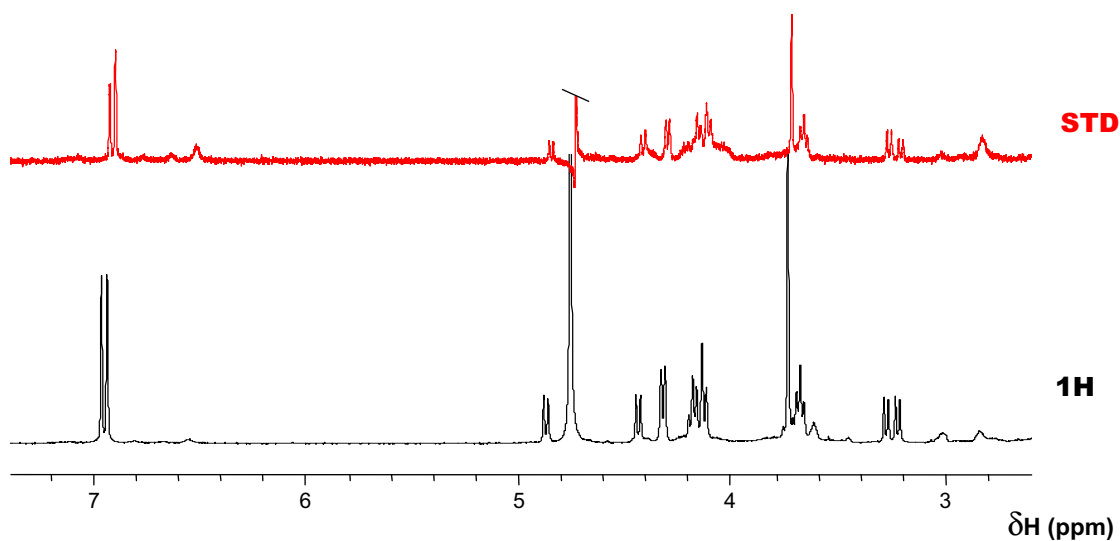


Figure S7. ^1H (black) and ^1H -STD (red) experiments on a 1mM NH_2 -calix4bridge sample in the presence of 16.25 μM tetrameric p53wt (600MHz, D_2O , 283K). STD experiment recorded with 1024 scans, using 50ms Gaussian shaped pulses during 3s for saturation at 0.72ppm and a 20ms spinlock.

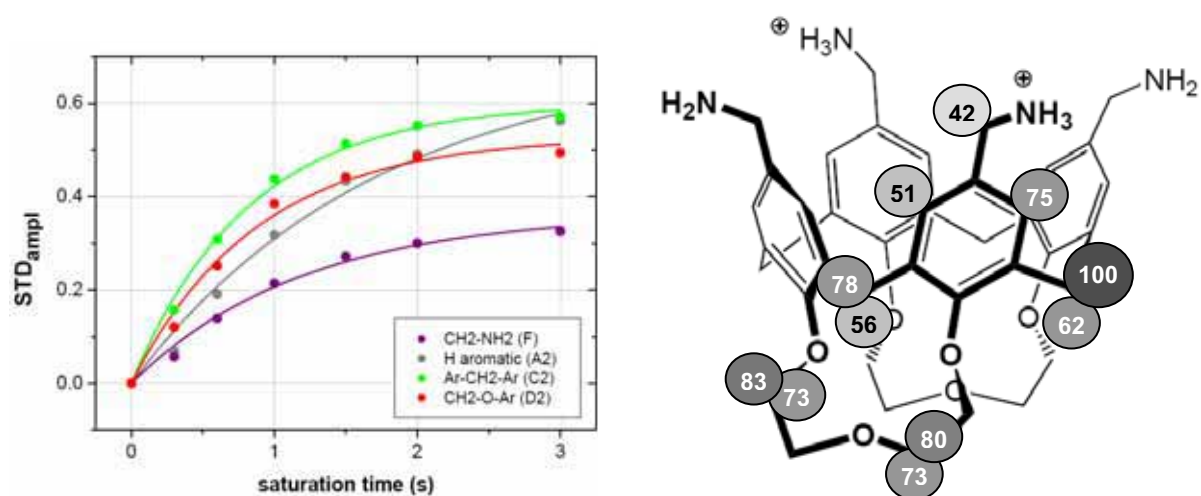


Figure S8. STD build-up curves for NH_2 -calix4bridge protons with different T1 and different saturation degrees (1mM ligand, 20 μM tetrameric p53wt, 600MHz, D_2O , 283K). STD results are represented on NH_2 -calix4bridge molecule (normalized to that of C2).

Table S1. Parameters for the mathematical adjustment of the STD built-up curves and saturation percentages for NH_2 -calix4bridge.

	$\text{STD}_{\text{max}}^{(a)}$	$k_{\text{sat}} (\text{s}^{-1})$	χ^2	$\nu_0 (\text{s}^{-1})$	% saturation
F	0.36 ± 0.02	0.84 ± 0.11	0.0002	0.30	42
A1	0.38 ± 0.04	1.00 ± 0.11	0.0010	0.38	51
A2	0.56 ± 0.07	0.97 ± 0.10	0.0020	0.55	75
B1	0.42 ± 0.04	0.98 ± 0.22	0.0009	0.41	56
B2	0.43 ± 0.02	1.33 ± 0.14	0.0003	0.57	78
C1	0.45 ± 0.02	1.02 ± 0.14	0.0004	0.46	62
C2	0.60 ± 0.02	1.22 ± 0.09	0.0002	0.73	100
D1	0.46 ± 0.02	1.15 ± 0.14	0.0004	0.53	73
D2	0.53 ± 0.02	1.14 ± 0.13	0.0005	0.60	83
E₁₋₃	0.41 ± 0.02	1.43 ± 0.19	0.0008	0.58	79
E₄₋₅	0.34 ± 0.02	1.55 ± 0.19	0.0007	0.53	73

^(a) The lower STD_{max} than for calix4bridge indicates of lower affinity.

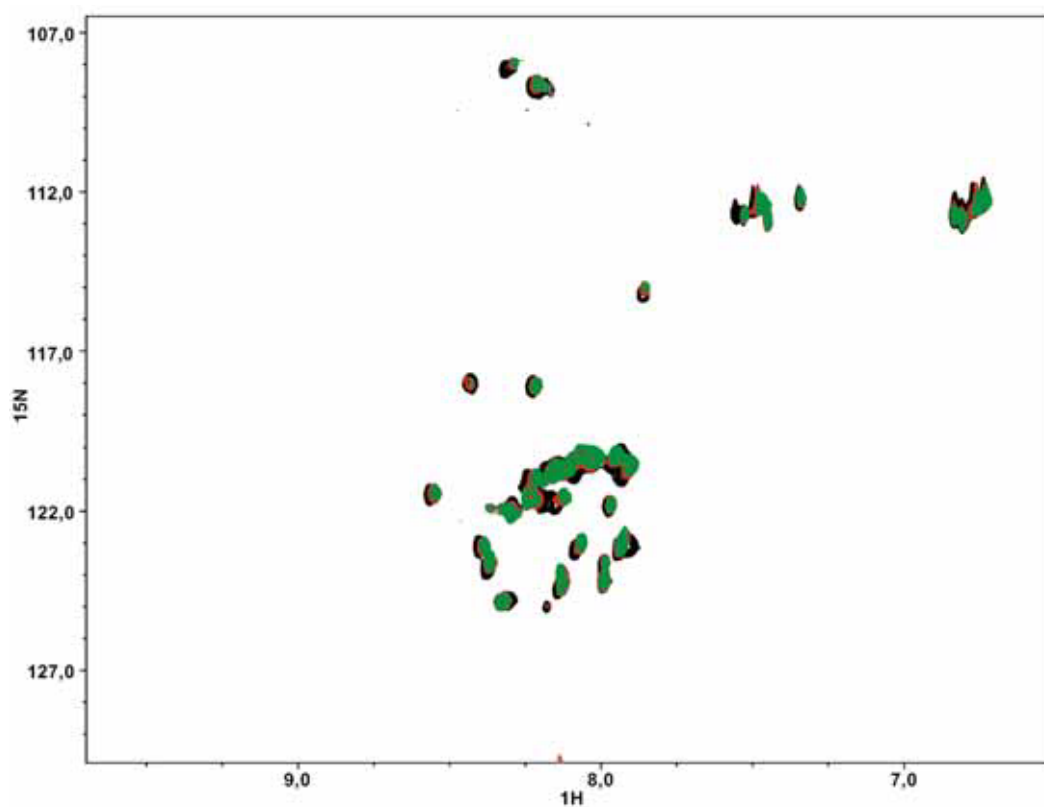
L344P negative control: HSQC

Figure S 9. HSQC spectra of 400 μ M 15 N-L344P in the absence (black) and the presence of 0.8mM (red) and 1.6mM (green) of calix4bridge. Upon addition of the ligand, the protein resonances experienced some minor perturbation, which suggested a non-specific interaction due to the large excess of ligand and the flexibility of the peptide.

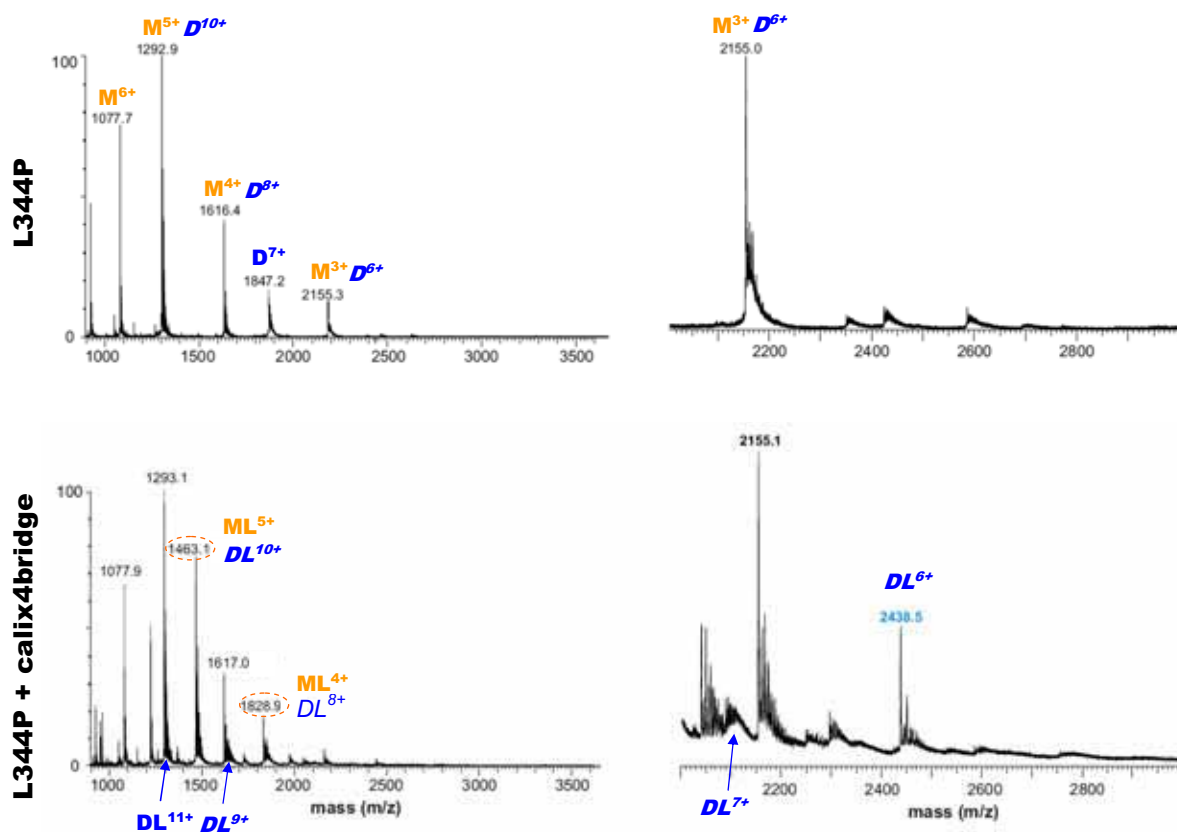
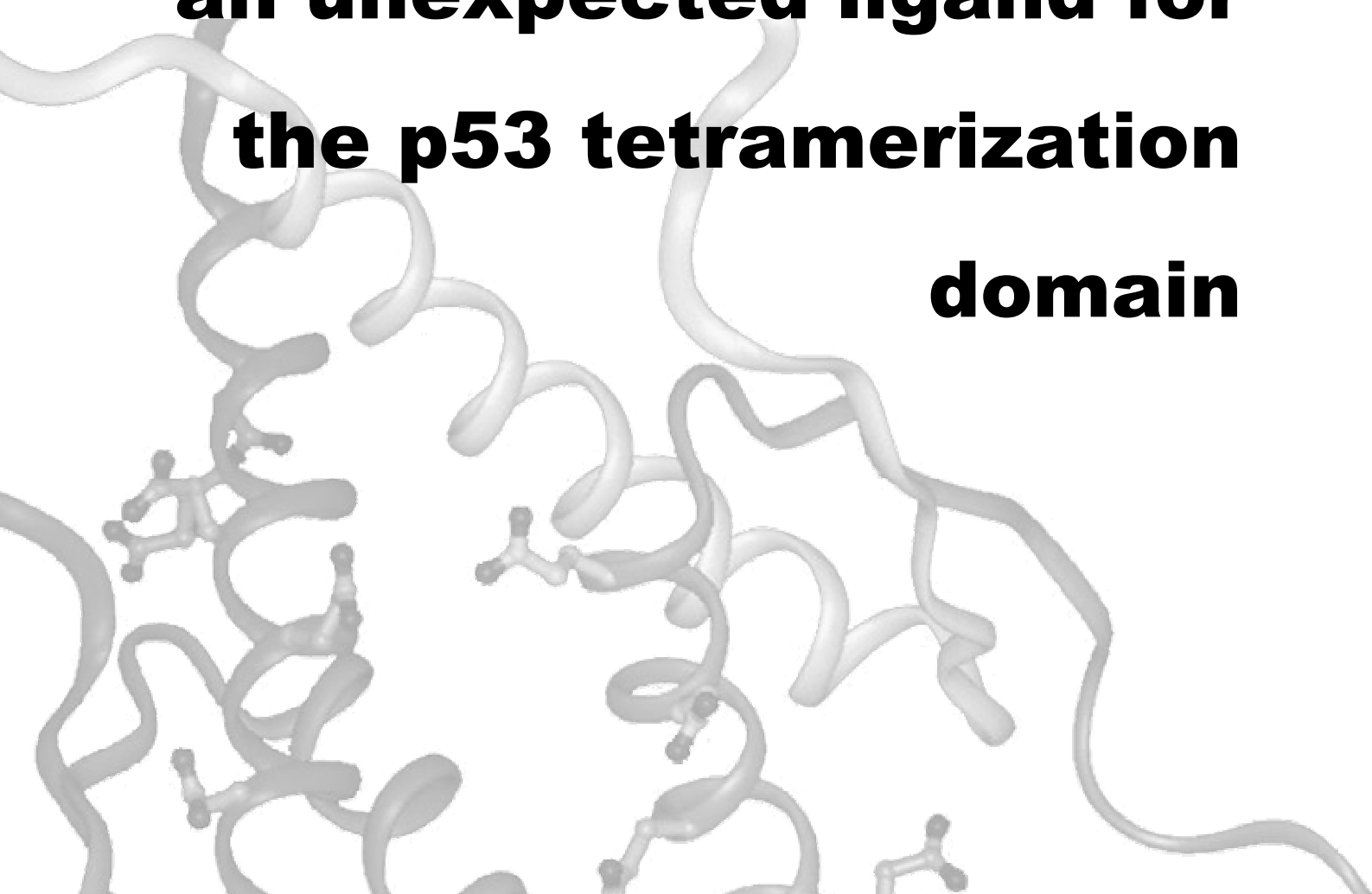
L344P negative control: ESI-MS

Figure S10. ESI-MS spectra of 50 μ M L344P in 10mM sodium acetate at pH 7, in the absence and the presence of 130 μ M calix4bridge (**M**, monomer; **D**, dimer).

**Calix4prop:
an unexpected ligand for
the p53 tetramerization
domain**



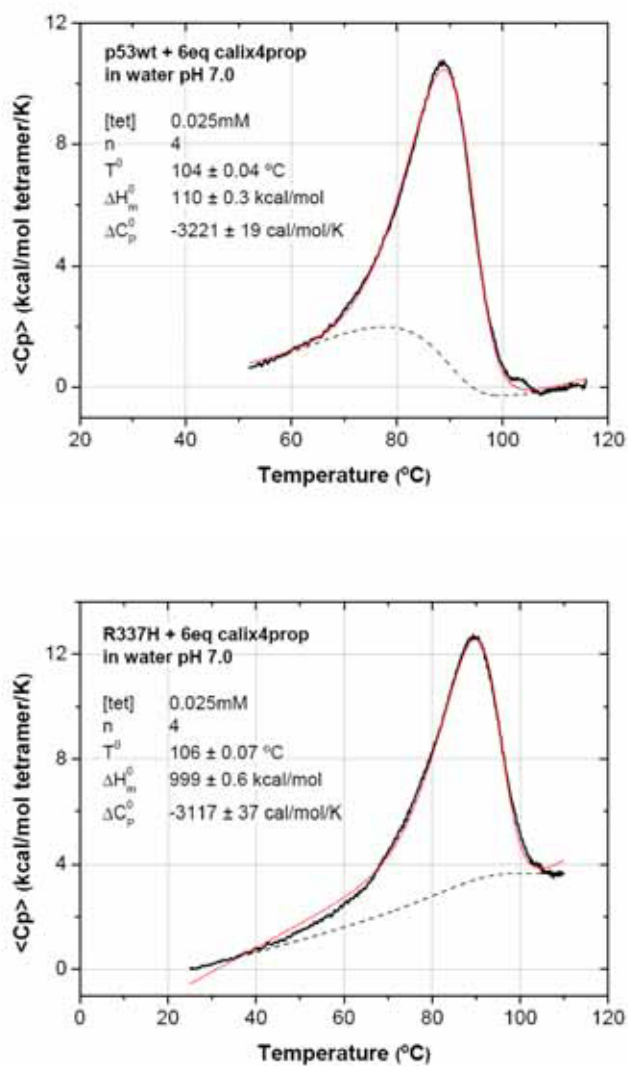
DSC CURVES of p53wt and R337H + 6eq calix4prop.

Figure S11. Adjustments for samples of p53wt and R337H with 6eq of calix4bridge to the mathematical model of dissociation coupled to unfolding proposed by Freire *et al.* Values are given related to moles of tetramer.

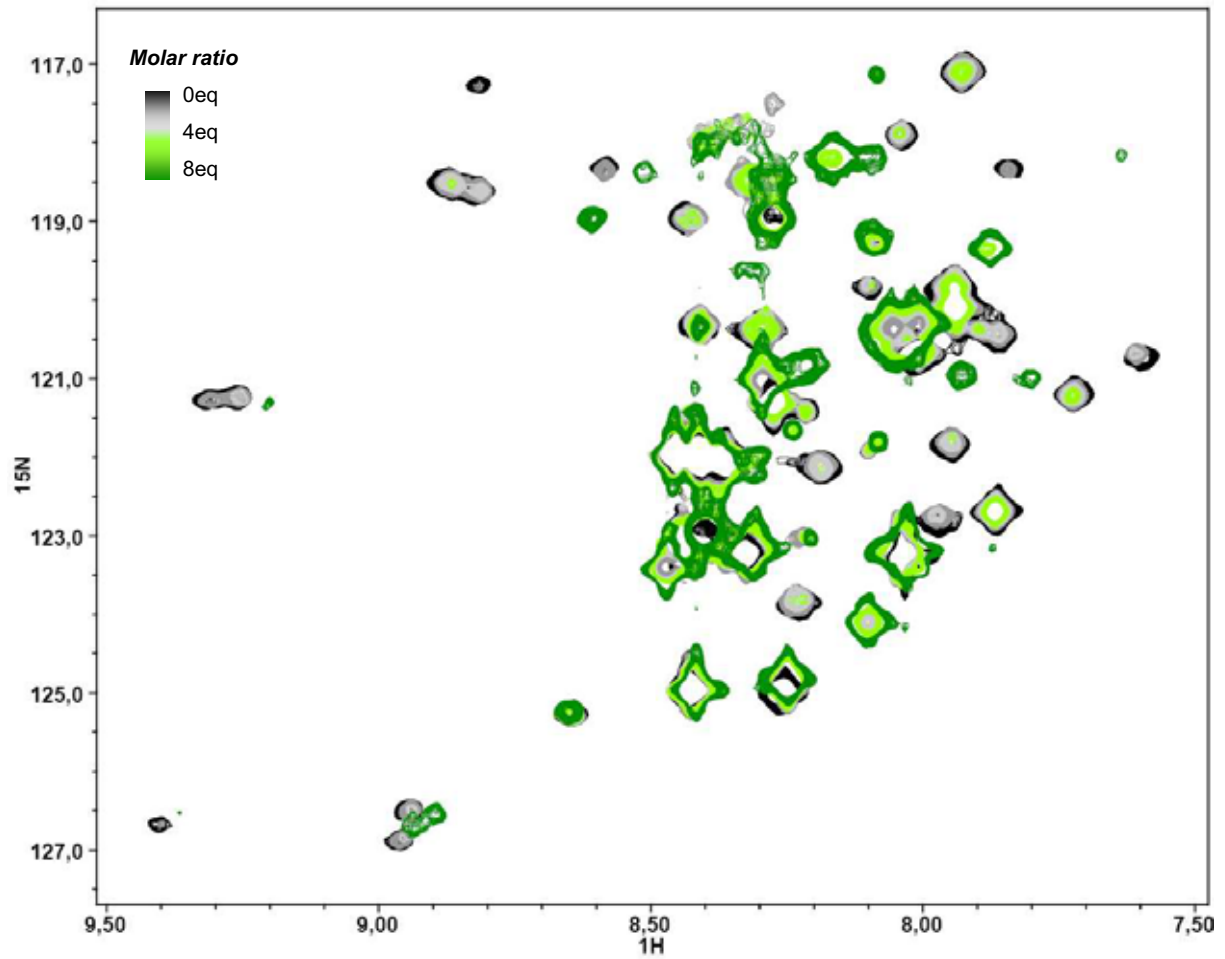
HSQC TITRATION OF p53wt + CALIX4PROP

Figure S12. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of p53wt with calix4prop (molar ratios relative to tetramer)

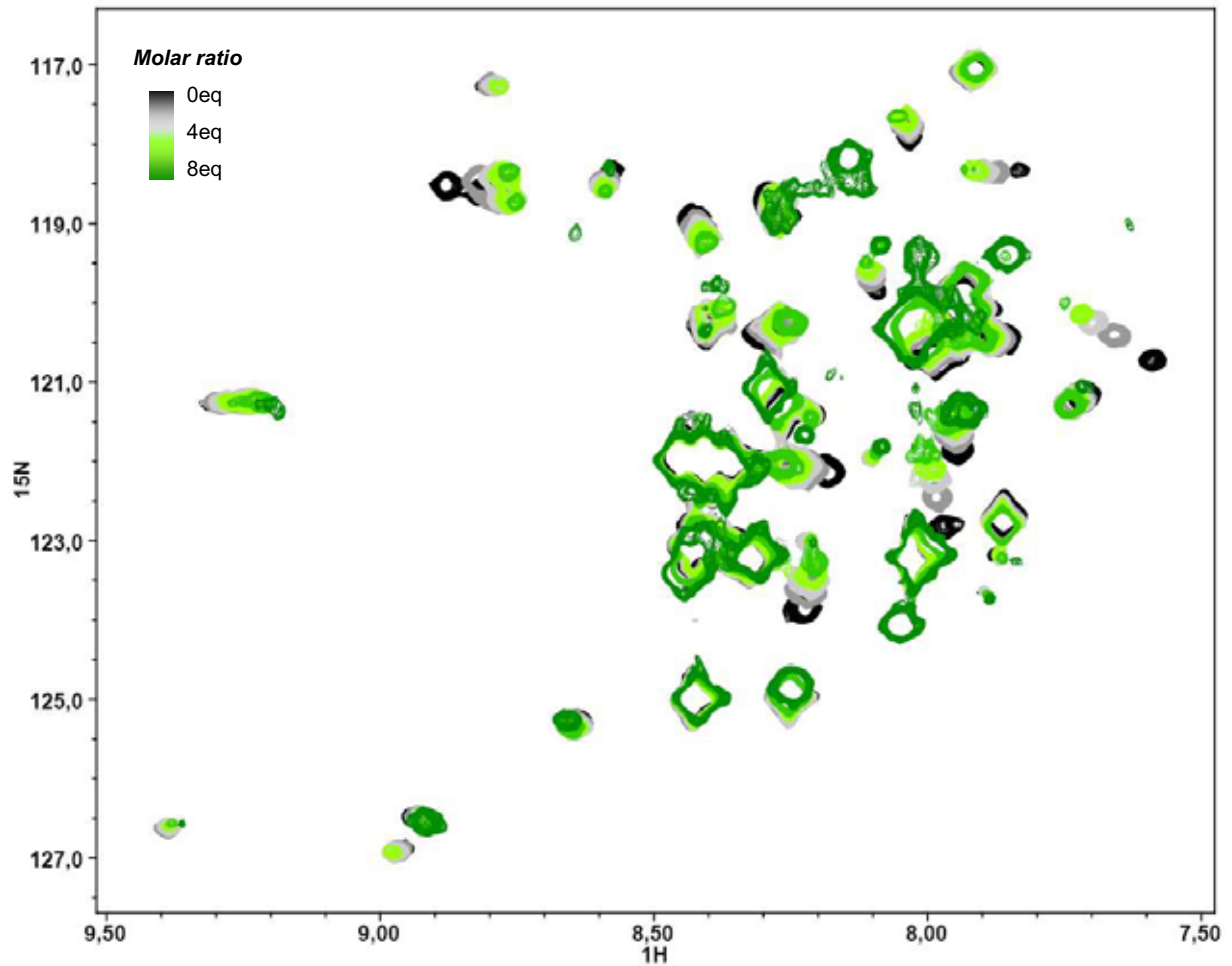
HSQC TITRATION OF p53wt + NH₂-CALIX4PROP

Figure S13. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of p53wt with NH₂-calix4prop (molar ratios relative to tetramer)

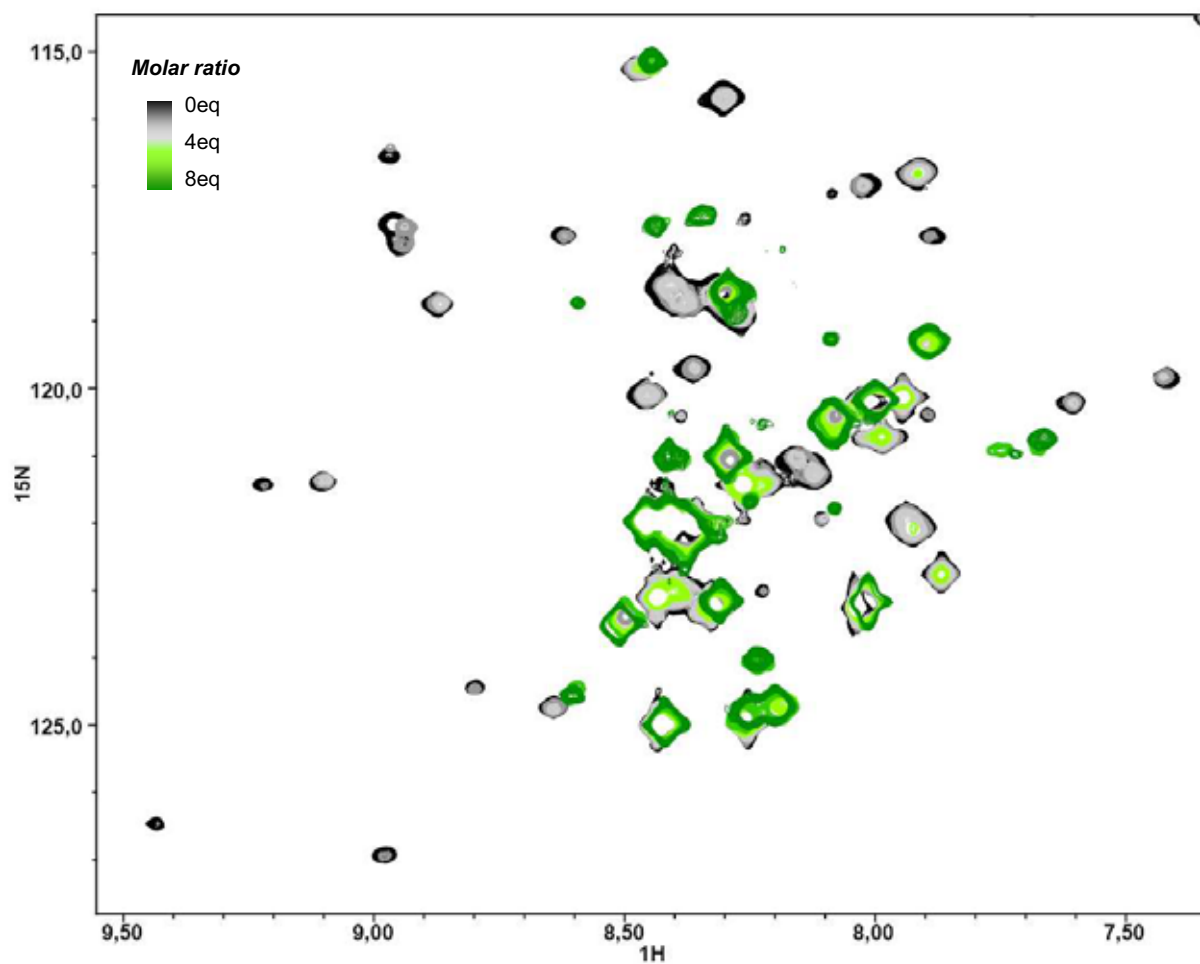
HSQC TITRATION OF R337H + CALIX4PROP (pH 7)

Figure S14. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of R337H with calix4prop (molar ratios relative to tetramer)

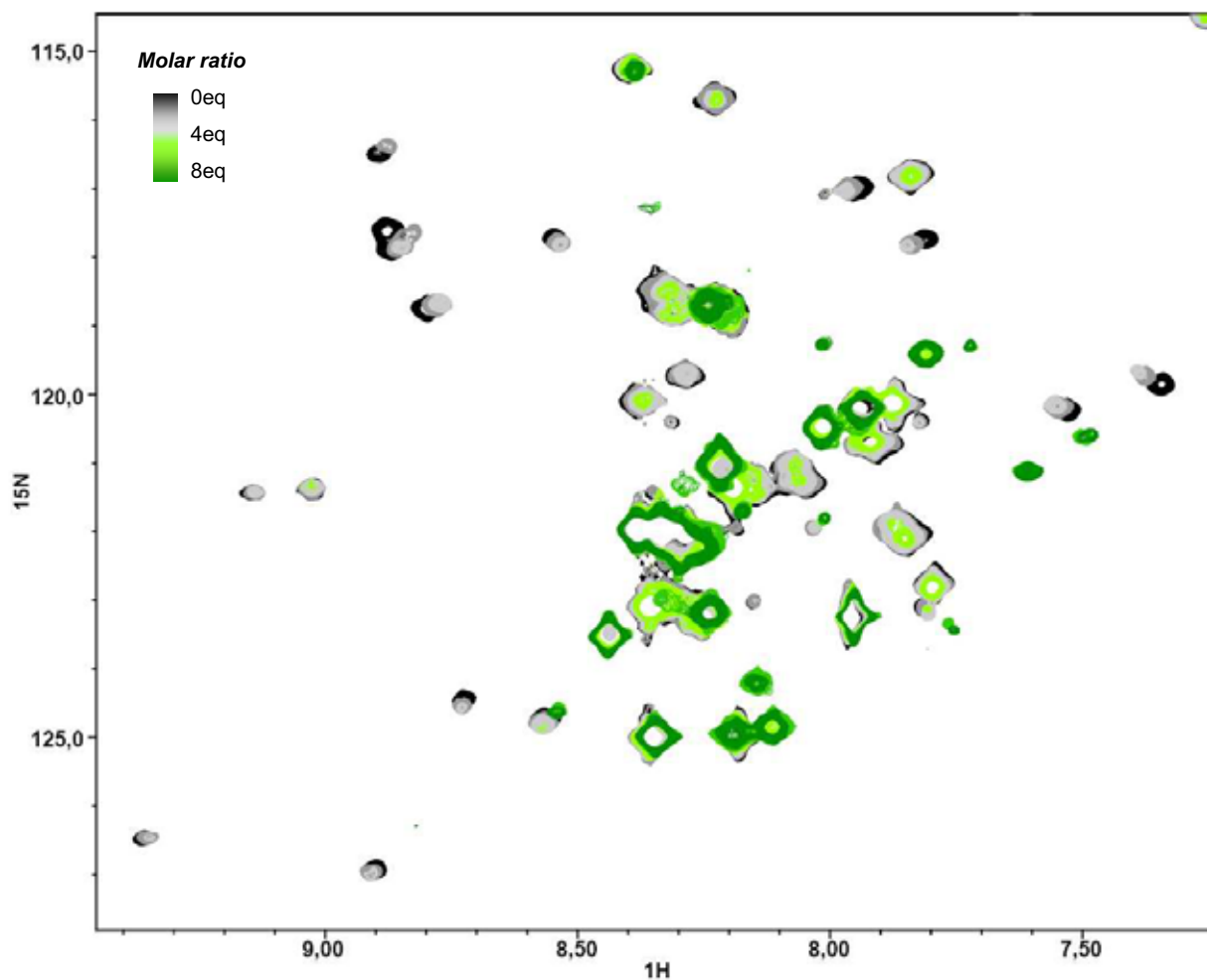
HSQC TITRATION OF R337H + NH₂-CALIX4PROP

Figure S15. Overlapped ¹⁵N-¹H-HSQC spectra of the titration of R337H with NH₂-calix4prop (molar ratios relative to tetramer)

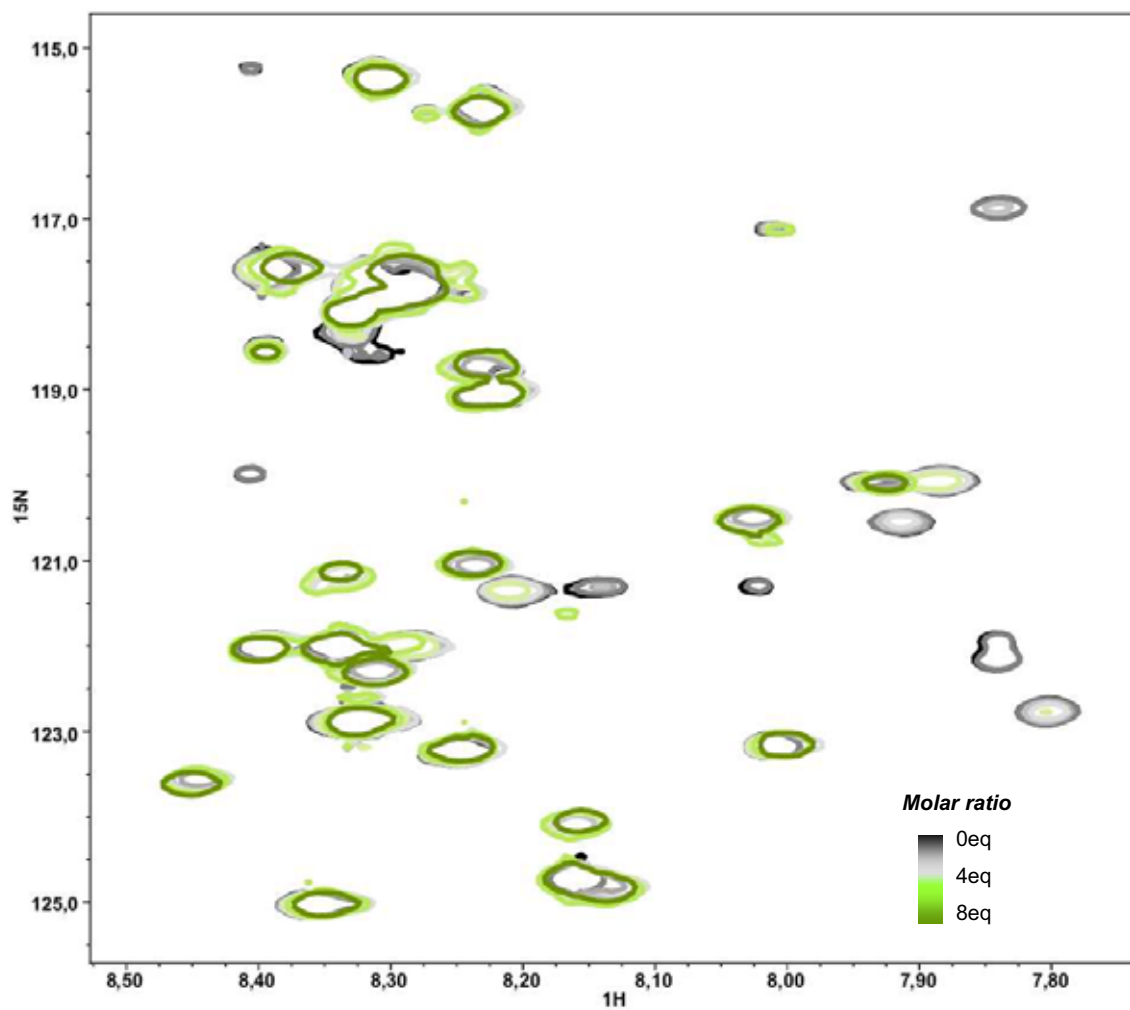
HSQC TITRATION OF R337H + CALIX4PROP pH 5

Figure S16. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of R337H with calix4prop in water at pH 5 (molar ratios relative to tetramer)

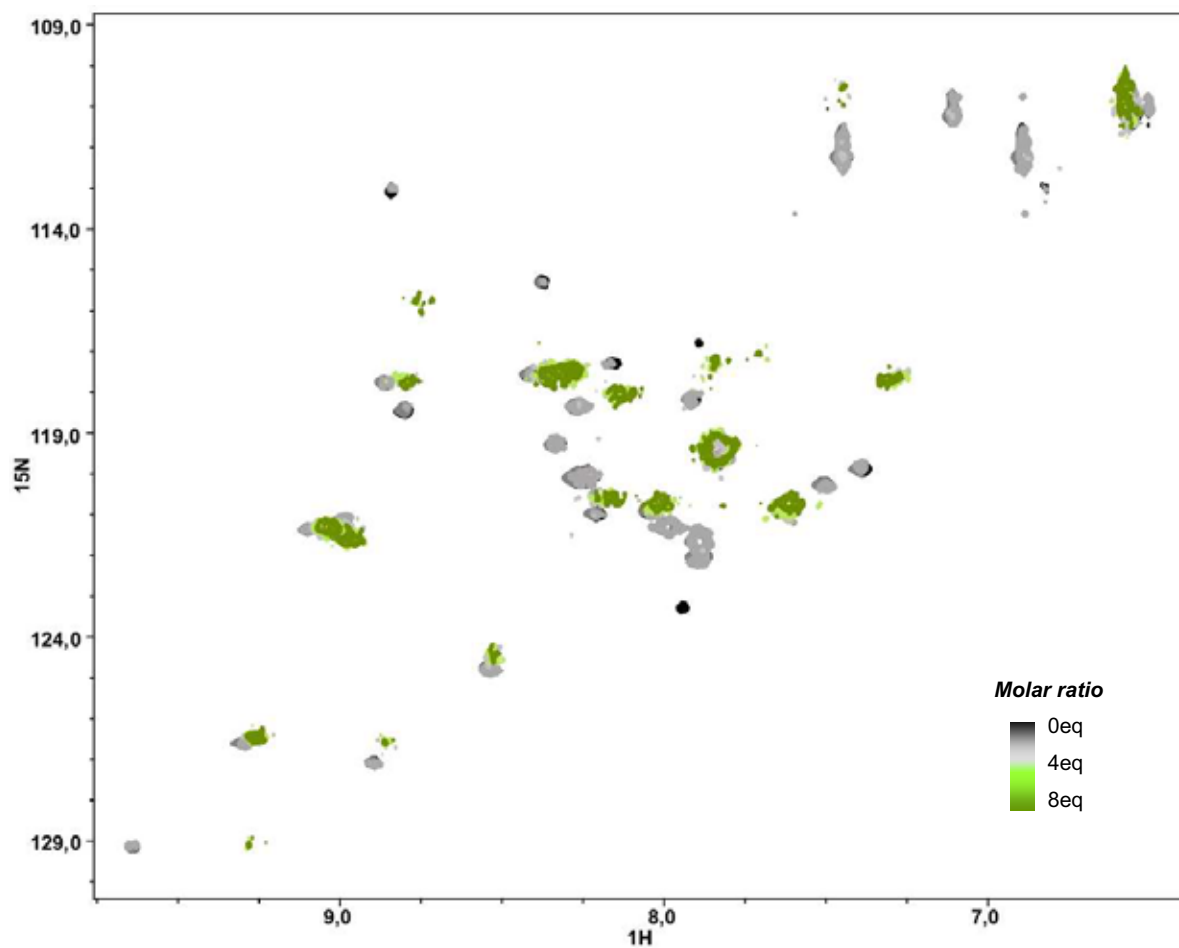
HSQC TITRATION OF R337H + CALIX4PROP pH 9

Figure S17. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of R337H with calix4prop in water at pH 9 (molar ratios relative to tetramer)

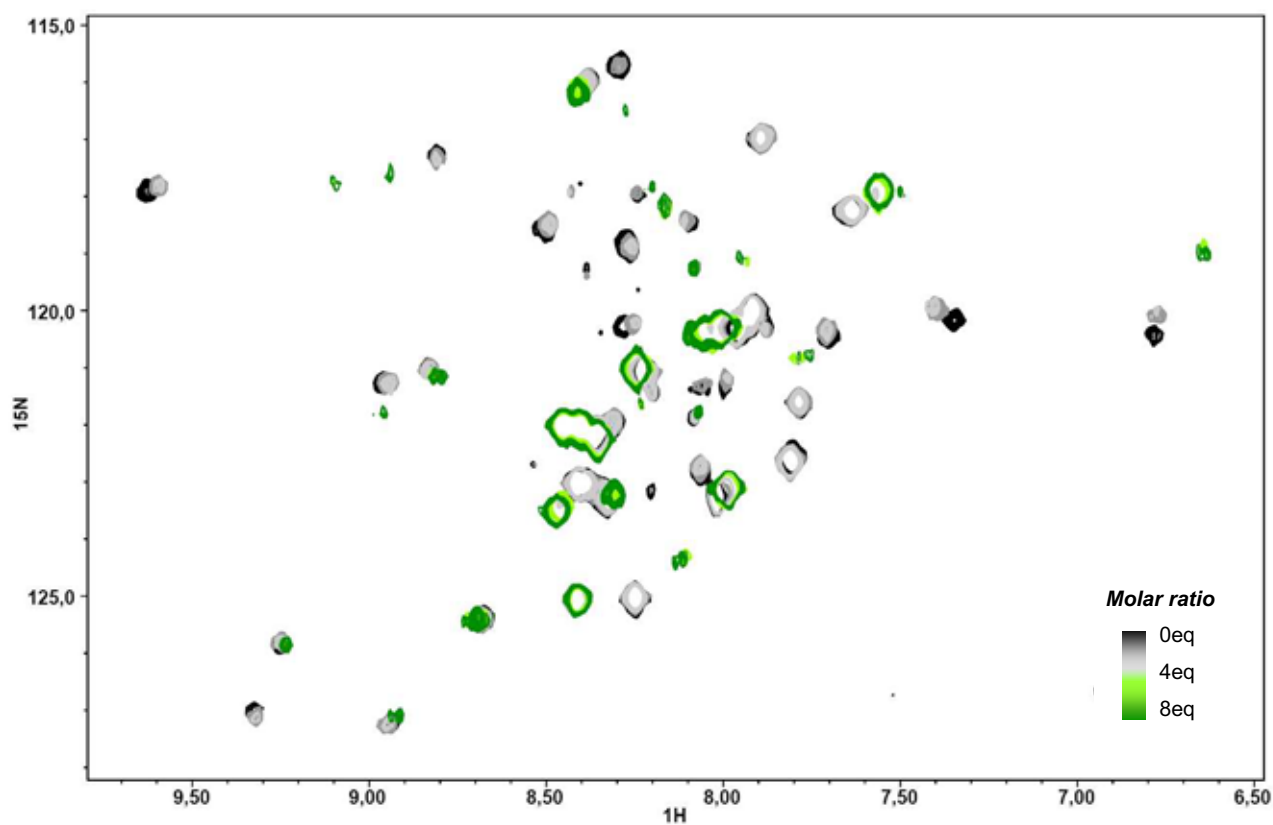
HSQC TITRATION OF G334V + CALIX4PROP

Figure S18. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of G334V with calix4prop (molar ratios relative to tetramer)

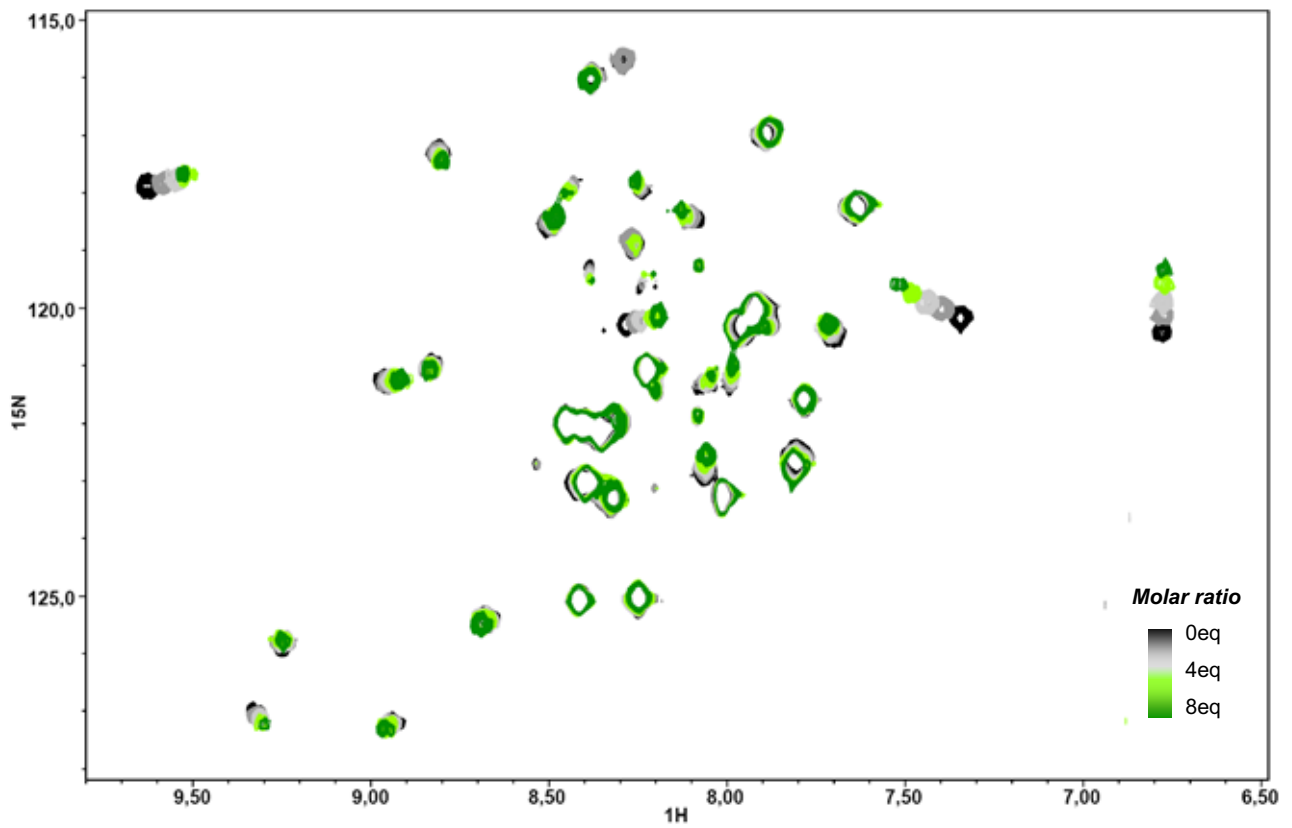
HSQC TITRATION OF G334V + NH₂-CALIX4PROP

Figure S19. Overlapped ¹⁵N-¹H-HSQC spectra of the titration of G334V with NH₂-calix4prop (molar ratios relative to tetramer)

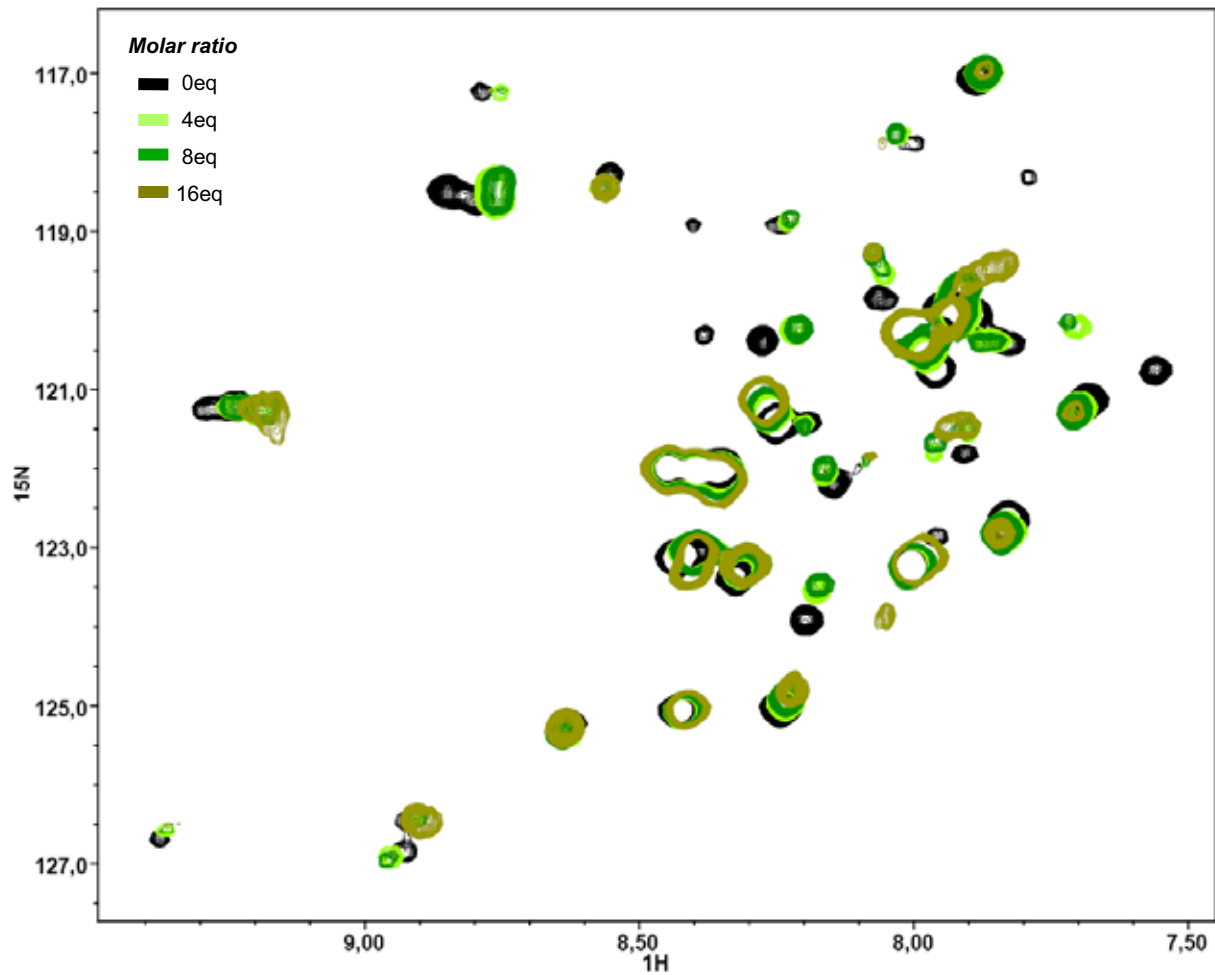
HSQC TITRATION OF p53wt + 4G4Pr-cone

Figure S20. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of p53wt with 4G4Pr-cone (molar ratios relative to tetramer)

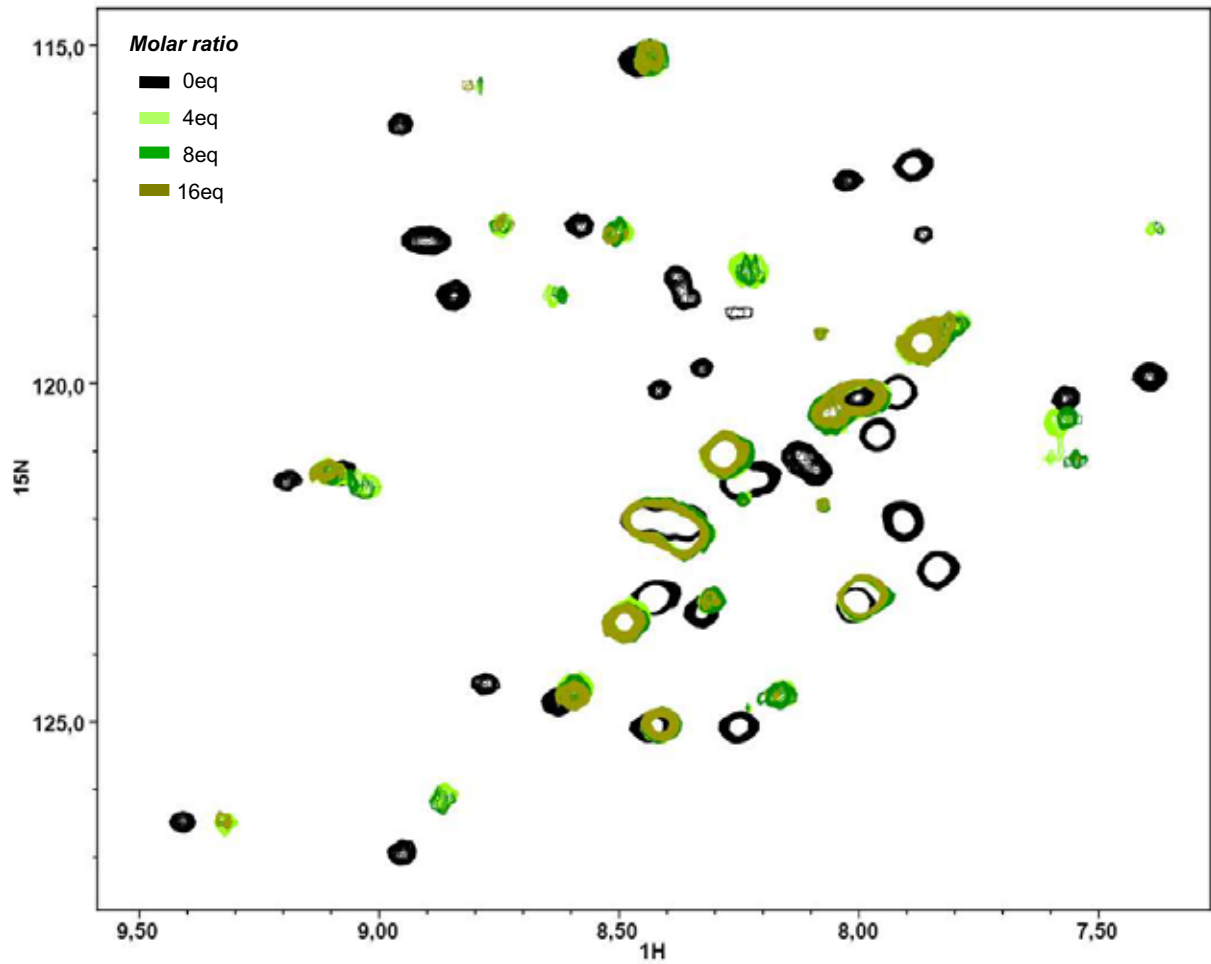
HSQC TITRATION OF R337H + 4G4Pr-cone

Figure S21. Overlapped ^{15}N - ^1H -HSQC spectra of the titration of R337H with 4G4Pr-cone (molar ratios relative to tetramer)

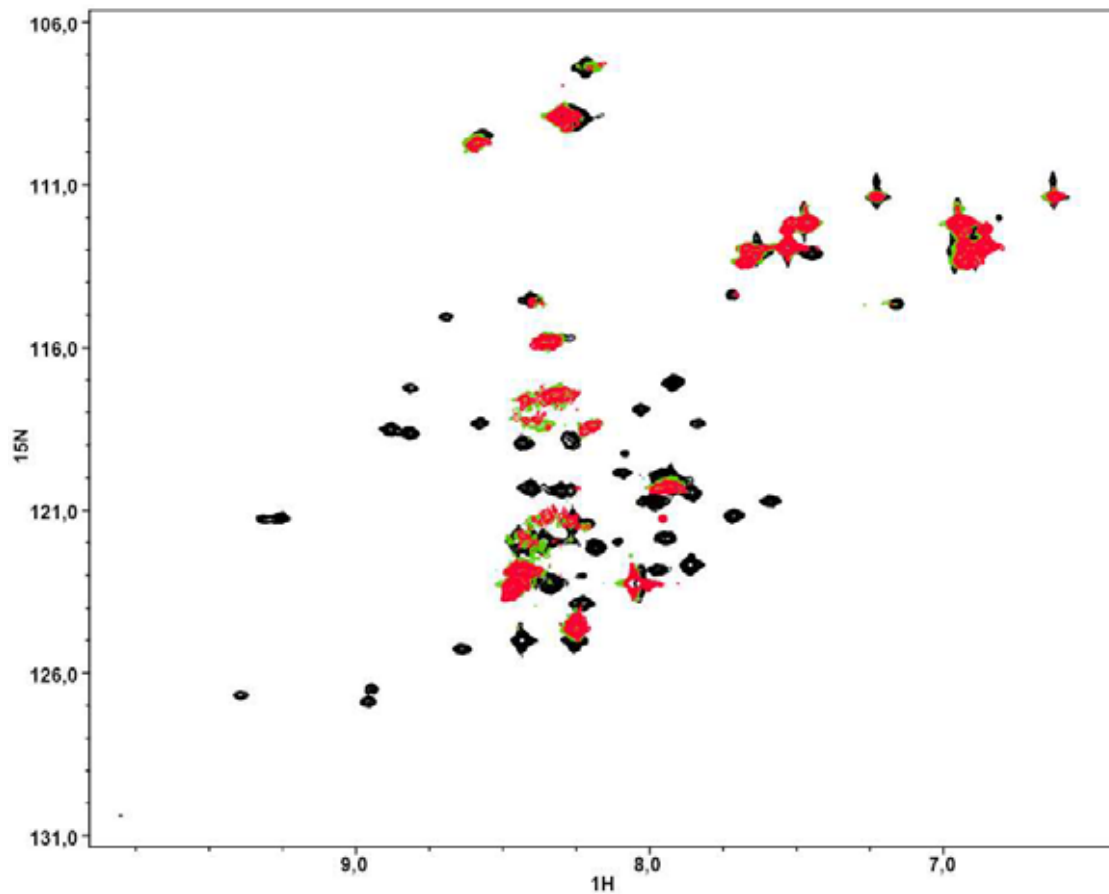
HSQC TITRATION OF p53wt + COOH-CALIX4PROP

Figure S22. 100 μM (tetramer) p53wt (black) with 4eq (green) and 8eq (red) of calix4prop, in water at pH 7. Protein precipitated in the presence of the calixarene.

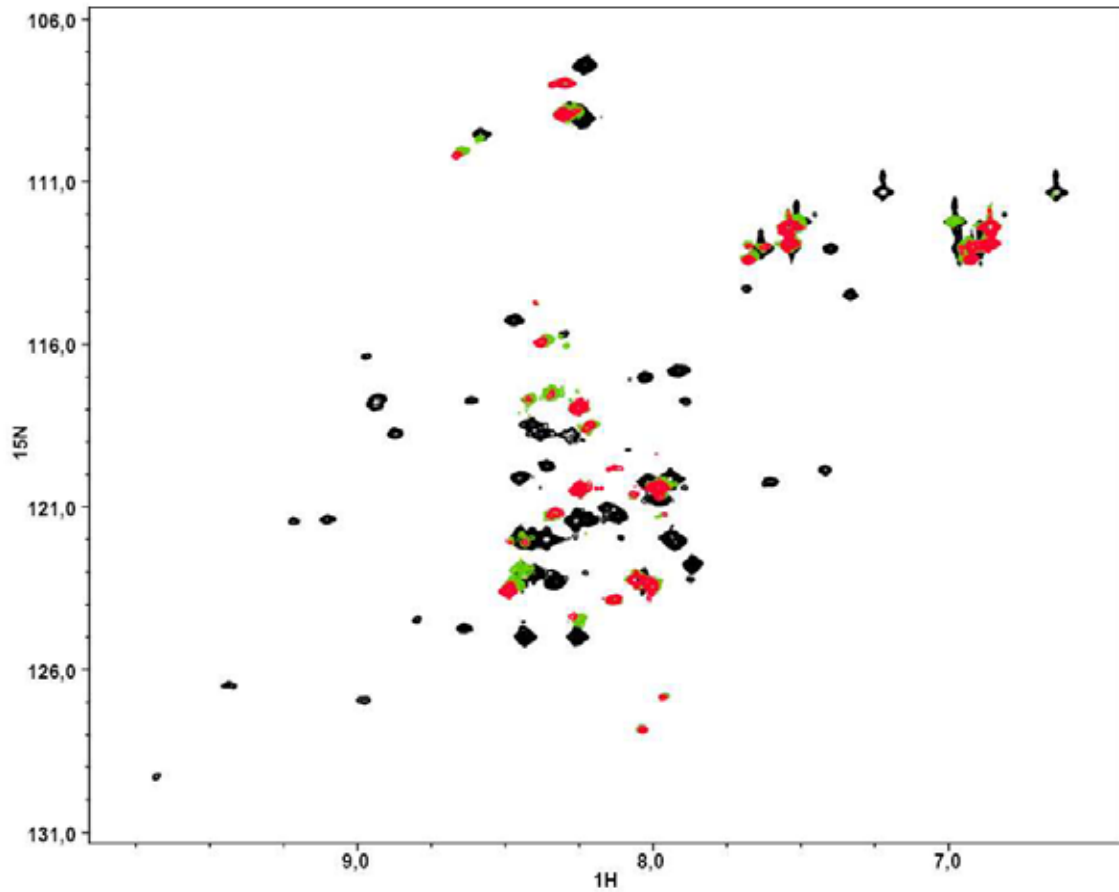
HSQC TITRATION OF R337H + COOH-CALIX4PROP

Figure S23. 100 μM (tetramer) p53wt (black) with 4eq (green) and 8eq (red) of calix4prop, in water at pH 7. The protein precipitated in the presence of the calixarene.

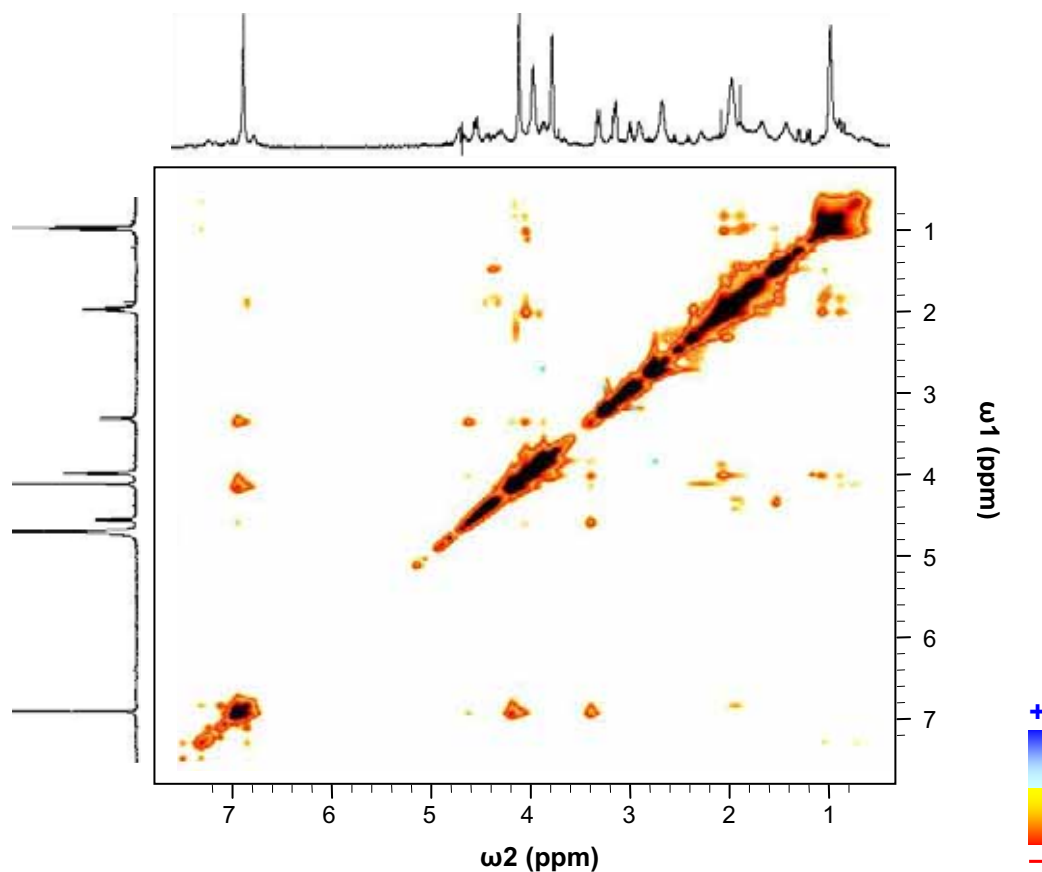
NOESY p53wt + 20eq CALIX4PROP

Figure S24. NOESY spectra of 500 μM calix4prop in the presence of 25 μM (tetramer) p53wt (in “99.99%” D_2O , at 308K, 500MHz, pulse with water suppression). The ^1H -spectrum shown in the top corresponds to the ligand-protein sample and the one at the left, to the free ligand.

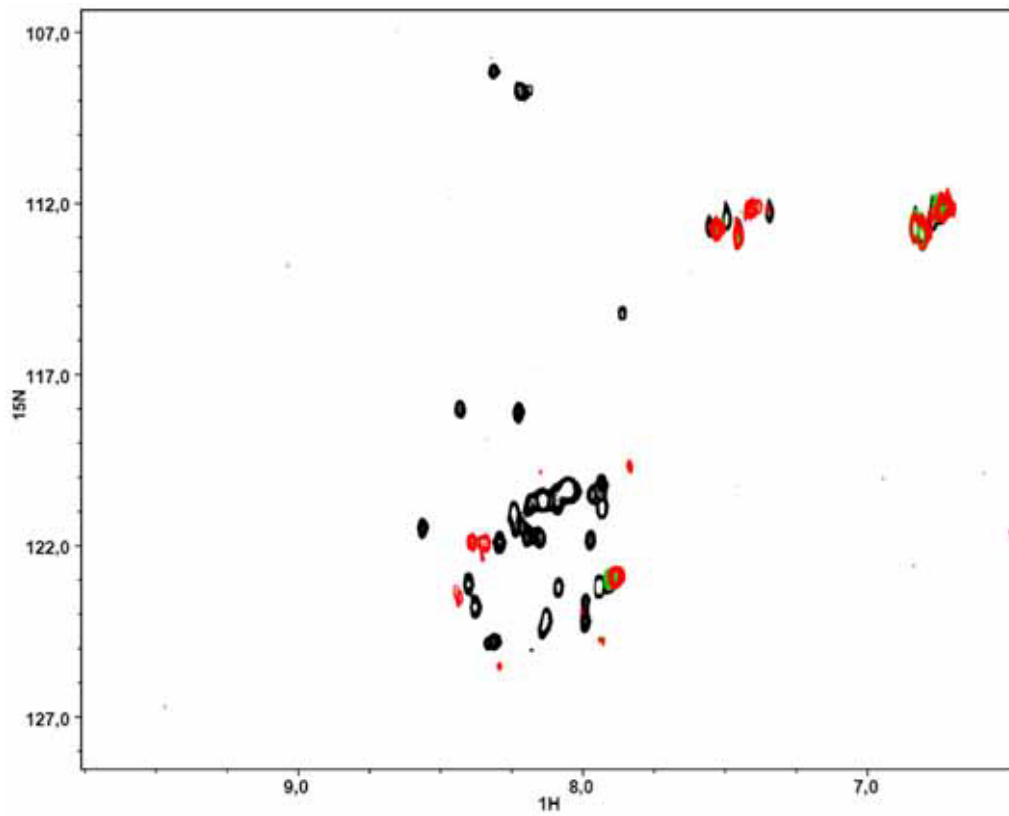
L344P negative control: HSQC

Figure S25. 400 μM L344P (black) with 1eq (green) and 2eq (red) of calix4prop, in water at pH 7. The protein precipitated when the calixarene was added.

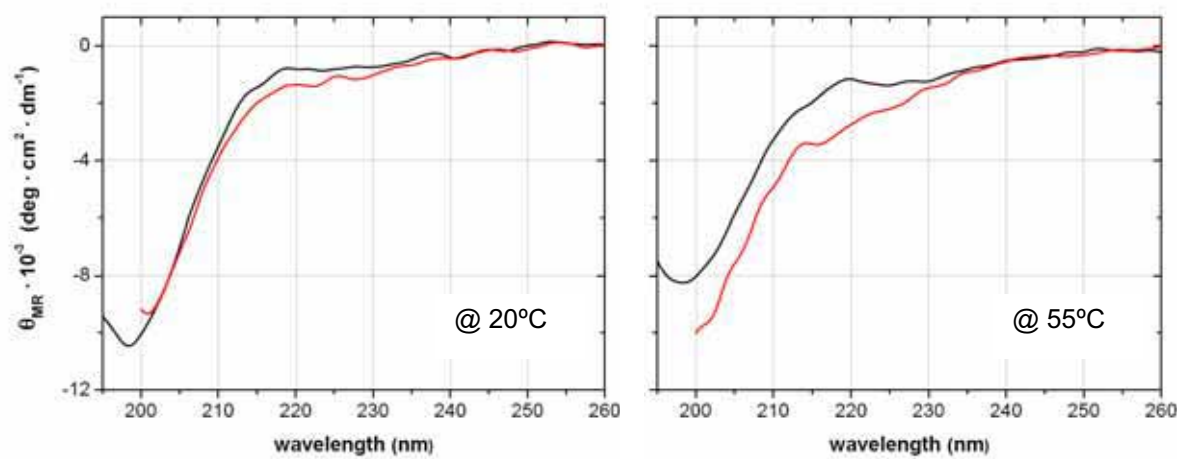
L344P negative control: CD

Figure S26. CD spectra of 30 μ M L344P (black) with 2eq of calix4prop, at 20°C (left) and 55°C (right), in water at pH 7.

L344P negative control: ESI-MS

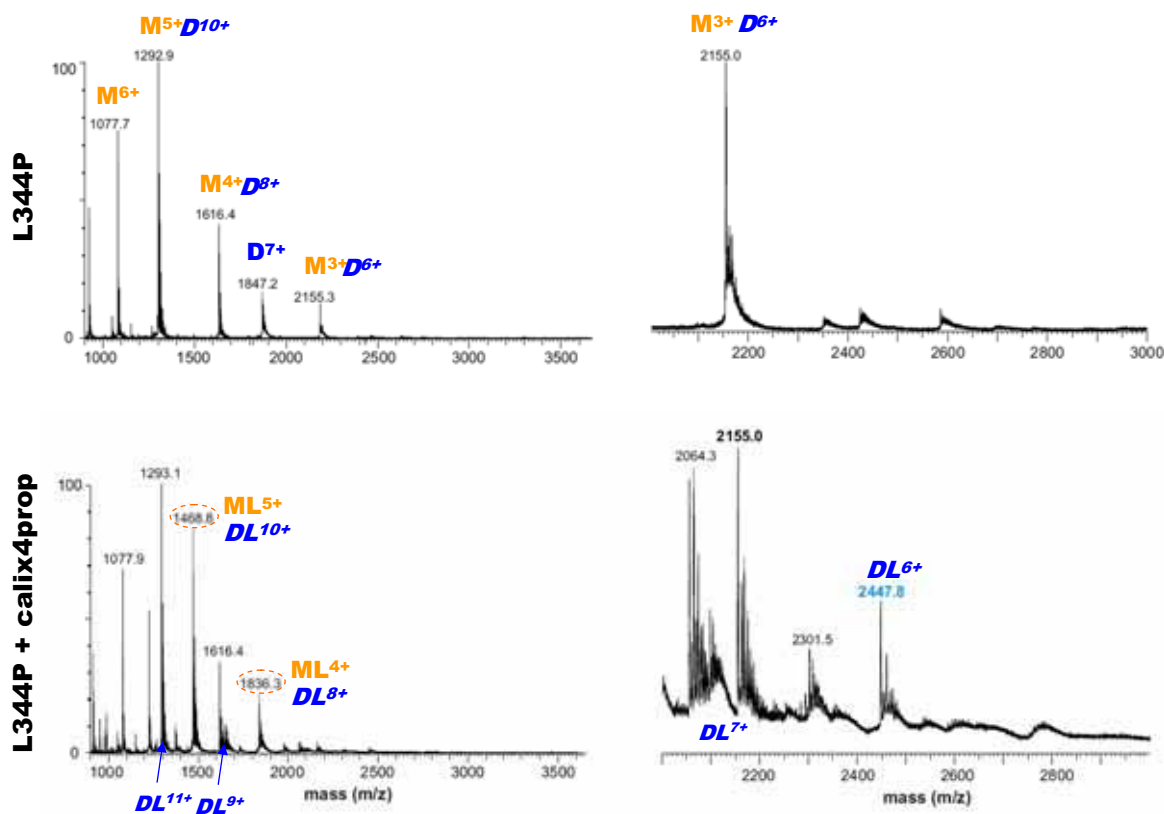


Figure S27. ESI-MS spectra of 50 μ M (monomer) R337H (upper panels) and L344P (lower panels) in the presence of 130 μ M calix4prop in 10mM ammonium acetate buffer pH 7. **T**: tetramer, **D**: dimer, **M**: monomer, **L**: ligand.

p53wt

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	6421.1	6552.3	12842.2	12973.4	13104.6	19263.3	19394.5	19525.7	19656.9	25684.4	25815.6	25946.8	26078.0	26209.2
1 H+	6422.1	6553.3	12843.2	12974.4	13105.6	19264.3	19395.5	19526.7	19657.9	25685.4	25816.6	25947.8	26079.0	26210.2
2 H+	3211.6	3277.2	6422.1	6487.7	6553.3	9632.7	9698.3	9763.9	9829.5	12843.2	12908.8	12974.4	13040.0	13105.6
3 H+	2141.4	2185.1	4281.7	4325.5	4369.2	6422.1	6465.8	6509.6	6553.3	8562.5	8606.2	8649.9	8693.7	8737.4
4 H+	1606.3	1639.1	3211.6	3244.4	3277.2	4816.8	4849.6	4882.4	4915.2	6422.1	6454.9	6487.7	6520.5	6553.3
5 H+	1285.2	1311.5	2569.4	2595.7	2621.9	3853.7	3879.9	3906.1	3932.4	5137.9	5164.1	5190.4	5216.6	5242.8
6 H+	1071.2	1093.1	2141.4	2163.2	2185.1	3211.6	3233.4	3255.3	3277.2	4281.7	4303.6	4325.5	4347.3	4369.2
7 H+	918.3	937.0	1835.6	1854.3	1873.1	2752.9	2771.6	2790.4	2809.1	3670.2	3688.9	3707.7	3726.4	3745.2
8 H+	803.6	820.0	1606.3	1622.7	1639.1	2408.9	2425.3	2441.7	2458.1	3211.6	3228.0	3244.4	3260.8	3277.2
9 H+	714.5	729.0	1427.9	1442.5	1457.1	2141.4	2155.9	2170.5	2185.1	2854.8	2869.4	2884.0	2898.6	2913.1
10 H+	643.1	656.2	1285.2	1298.3	1311.5	1927.3	1940.5	1953.6	1966.7	2569.4	2582.6	2595.7	2608.8	2621.9
11 H+	584.7	596.7	1168.5	1180.4	1192.3	1752.2	1764.1	1776.1	1788.0	2335.9	2347.9	2359.8	2371.7	2383.7
12 H+	536.1	547.0	1071.2	1082.1	1093.1	1606.3	1617.2	1628.1	1639.1	2141.4	2152.3	2163.2	2174.2	2185.1
13 H+	494.9	505.0	988.9	999.0	1009.0	1482.8	1492.9	1503.0	1513.1	1976.7	1986.8	1996.9	2007.0	2017.1
14 H+	459.7	469.0	918.3	927.7	937.0	1377.0	1386.3	1395.7	1405.1	1835.6	1845.0	1854.3	1863.7	1873.1
15 H+	429.1	437.8	857.1	865.9	874.6	1285.2	1294.0	1302.7	1311.5	1713.3	1722.0	1730.8	1739.5	1748.3
16 H+	402.3	410.5	803.6	811.8	820.0	1205.0	1213.2	1221.4	1229.6	1606.3	1614.5	1622.7	1630.9	1639.1
17 H+	378.7	386.4	756.4	764.1	771.9	1134.1	1141.9	1149.6	1157.3	1511.8	1519.6	1527.3	1535.0	1542.7
18 H+	357.7	365.0	714.5	721.7	729.0	1071.2	1078.5	1085.8	1093.1	1427.9	1435.2	1442.5	1449.8	1457.1
19 H+	339.0	345.9	676.9	683.8	690.7	1014.9	1021.8	1028.7	1035.6	1352.8	1359.7	1366.6	1373.5	1380.4
20 H+	322.1	328.6	643.1	649.7	656.2	964.2	970.7	977.3	983.8	1285.2	1291.8	1298.3	1304.9	1311.5
21 H+	306.8	313.0	612.5	618.8	625.0	918.3	924.5	930.8	937.0	1224.1	1230.3	1236.6	1242.8	1249.1
22 H+	292.9	298.8	584.7	590.7	596.7	876.6	882.6	888.5	894.5	1168.5	1174.4	1180.4	1186.4	1192.3
23 H+	280.2	285.9	559.4	565.1	570.8	838.5	844.2	849.9	855.6	1117.7	1123.4	1129.1	1134.8	1140.5

R337H

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	6402.0	6533.2	12804.0	12935.2	13066.4	19206.0	19337.2	19468.4	19599.6	25608.0	25739.2	25870.4	26001.6	26132.8
1 H+	6403.0	6534.2	12805.0	12936.2	13067.4	19207.0	19338.2	19469.4	19600.6	25609.0	25740.2	25871.4	26002.6	26133.8
2 H+	3202.0	3267.6	6403.0	6468.6	6534.2	9604.0	9669.6	9735.2	9800.8	12805.0	12870.6	12936.2	13001.8	13067.4
3 H+	2135.0	2178.7	4269.0	4312.7	4356.5	6403.0	6446.7	6490.5	6534.2	8537.0	8580.7	8624.5	8668.2	8711.9
4 H+	1601.5	1634.3	3202.0	3234.8	3267.6	4802.5	4835.3	4868.1	4900.9	6403.0	6435.8	6468.6	6501.4	6534.2
5 H+	1281.4	1307.6	2561.8	2588.0	2614.3	3842.2	3868.4	3894.7	3920.9	5122.6	5148.8	5175.1	5201.3	5227.6
6 H+	1068.0	1089.9	2135.0	2156.9	2178.7	3202.0	3223.9	3245.7	3267.6	4269.0	4290.9	4312.7	4334.6	4356.5
7 H+	915.6	934.3	1830.1	1848.9	1867.6	2744.7	2763.5	2782.2	2800.9	3659.3	3678.0	3696.8	3715.5	3734.3
8 H+	801.3	817.7	1601.5	1617.9	1634.3	2401.8	2418.2	2434.6	2451.0	3202.0	3218.4	3234.8	3251.2	3267.6
9 H+	712.3	726.9	1423.7	1438.2	1452.8	2135.0	2149.6	2164.2	2178.7	2846.3	2860.9	2875.5	2890.1	2904.6
10 H+	641.2	654.3	1281.4	1294.5	1307.6	1921.6	1934.7	1947.8	1961.0	2561.8	2574.9	2588.0	2601.2	2614.3
11 H+	583.0	594.9	1165.0	1176.9	1188.9	1747.0	1758.9	1770.9	1782.8	2329.0	2340.9	2352.9	2364.8	2376.7
12 H+	534.5	545.4	1068.0	1078.9	1089.9	1601.5	1612.4	1623.4	1634.3	2135.0	2145.9	2156.9	2167.8	2178.7
13 H+	493.5	503.6	985.9	996.0	1006.1	1478.4	1488.5	1498.6	1508.7	1970.8	1980.9	1991.0	2001.1	2011.2
14 H+	458.3	467.7	915.6	924.9	934.3	1372.9	1382.2	1391.6	1401.0	1830.1	1839.5	1848.9	1858.3	1867.6
15 H+	427.8	436.5	854.6	863.3	872.1	1281.4	1290.1	1298.9	1307.6	1708.2	1716.9	1725.7	1734.4	1743.2
16 H+	401.1	409.3	801.3	809.5	817.7	1201.4	1209.6	1217.8	1226.0	1601.5	1609.7	1617.9	1626.1	1634.3
17 H+	377.6	385.3	754.2	761.9	769.6	1130.8	1138.5	1146.2	1153.9	1507.4	1515.1	1522.8	1530.5	1538.2
18 H+	356.7	364.0	712.3	719.6	726.9	1068.0	1075.3	1082.6	1089.9	1423.7	1431.0	1438.2	1445.5	1452.8
19 H+	337.9	344.9	674.9	681.8	688.7	1011.8	1018.7	1025.7	1032.6	1348.8	1355.7	1362.6	1369.5	1376.4
20 H+	321.1	327.7	641.2	647.8	654.3	961.3	967.9	974.4	981.0	1281.4	1288.0	1294.5	1301.1	1307.6
21 H+	305.9	312.1	610.7	617.0	623.2	915.6	921.8	928.1	934.3	1220.4	1226.7	1232.9	1239.2	1245.4
22 H+	292.0	298.0	583.0	589.0	594.9	874.0	880.0	885.9	891.9	1165.0	1171.0	1176.9	1182.9	1188.9
23 H+	279.3	285.1	557.7	563.4	569.1	836.0	841.7	847.5	853.2	1114.4	1120.1	1125.8	1131.5	1137.2

G334V

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	6463.2	6594.4	12926.4	13057.6	13188.8	19389.6	19520.8	19652.0	19783.2	25852.8	25984.0	26115.2	26246.4	26377.6
1 H+	6464.2	6595.4	12927.4	13058.6	13189.8	19390.6	19521.8	19653.0	19784.2	25853.8	25985.0	26116.2	26247.4	26378.6
2 H+	3232.6	3298.2	6464.2	6529.8	6595.4	9695.8	9761.4	9827.0	9892.6	12927.4	12993.0	13058.6	13124.2	13189.8
3 H+	2155.4	2199.1	4309.8	4353.5	4397.3	6464.2	6507.9	6551.7	6595.4	8618.6	8662.3	8706.1	8749.8	8793.5
4 H+	1616.8	1649.6	3232.6	3265.4	3298.2	4848.4	4881.2	4914.0	4946.8	6464.2	6497.0	6529.8	6562.6	6595.4
5 H+	1293.6	1319.9	2586.3	2612.5	2638.8	3878.9	3905.2	3931.4	3957.6	5171.6	5197.8	5224.0	5250.3	5276.5
6 H+	1078.2	1100.1	2155.4	2177.3	2199.1	3232.6	3254.5	3276.3	3298.2	4309.8	4331.7	4353.5	4375.4	4397.3
7 H+	924.3	943.1	1847.6	1866.4	1885.1	2770.9	2789.7	2808.4	2827.2	3694.3	3713.0	3731.7	3750.5	3769.2
8 H+	808.9	825.3	1616.8	1633.2	1649.6	2424.7	2441.1	2457.5	2473.9	3232.6	3249.0	3265.4	3281.8	3298.2
9 H+	719.1	733.7	1437.3	1451.8	1466.4	2155.4	2170.0	2184.6	2199.1	2873.5	2888.1	2902.7	2917.3	2931.8
10 H+	647.3	660.4	1293.6	1306.8	1319.9	1940.0	1953.1	1966.2	1979.3	2586.3	2599.4	2612.5	2625.6	2638.8
11 H+	588.6	600.5	1176.1	1188.1	1200.0	1763.7	1775.6	1787.5	1799.5	2351.3	2363.2	2375.1	2387.0	2399.0
12 H+	539.6	550.5	1078.2	1089.1	1100.1	1616.8	1627.7	1638.7	1649.6	2155.4	2166.3	2177.3	2188.2	2199.1
13 H+	498.2	508.3	995.3	1005.4	1015.5	1492.5	1502.6	1512.7	1522.8	1989.7	1999.8	2009.9	2020.0	2030.0
14 H+	462.7	472.0	924.3	933.7	943.1	1386.0	1395.3	1404.7	1414.1	1847.6	1857.0	1866.4	1875.7	1885.1
15 H+	431.9	440.6	862.8	871.5	880.3	1293.6	1302.4	1311.1	1319.9	1724.5	1733.3	1742.0	1750.8	1759.5
16 H+	405.0	413.2	808.9	817.1	825.3	1212.9	1221.1	1229.3	1237.5	1616.8	1625.0	1633.2	1641.4	1649.6
17 H+	381.2	388.9	761.4	769.1	776.8	1141.6	1149.3	1157.0	1164.7	1521.8	1529.5	1537.2	1544.9	1552.6
18 H+	360.1	367.4	719.1	726.4	733.7	1078.2	1085.5	1092.8	1100.1	1437.3	1444.6	1451.8	1459.1	1466.4
19 H+	341.2	348.1	681.3	688.2	695.1	1021.5	1028.4	1035.3	1042.2	1361.7	1368.6	1375.5	1382.4	1389.3
20 H+	324.2	330.7	647.3	653.9	660.4	970.5	977.0	983.6	990.2	1293.6	1300.2	1306.8	1313.3	1319.9
21 H+	308.8	315.0	616.5	622.8	629.0	924.3	930.6	936.8	943.1	1232.1	1238.3	1244.6	1250.8	1257.1
22 H+	294.8	300.7	588.6	594.5	600.5	882.3	888.3	894.3	900.2	1176.1	1182.1	1188.1	1194.0	1200.0
23 H+	282.0	287.7	563.0	568.7	574.4	844.0	849.7	855.4	861.1	1125.0	1130.7	1136.4	1142.1	1147.9

L344P

	monomer	dimer	trimer	tetramer	pentamer	hexamer	heptamer	octamer
0 H+	6462.1	12924.2	19386.3	25848.4	32310.5	38772.6	45234.7	51696.8
1 H+	6463.1	12925.2	19387.3	25849.4	32311.5	38773.6	45235.7	51697.8
2 H+	3232.1	6463.1	9694.2	12925.2	16156.3	19387.3	22618.4	25849.4
3 H+	2155.0	4309.1	6463.1	8617.1	10771.2	12925.2	15079.2	17233.3
4 H+	1616.5	3232.1	4847.6	6463.1	8078.6	9694.2	11309.7	12925.2
5 H+	1293.4	2585.8	3878.3	5170.7	6463.1	7755.5	9047.9	10340.4
6 H+	1078.0	2155.0	3232.1	4309.1	5386.1	6463.1	7540.1	8617.1
7 H+	924.2	1847.3	2770.5	3693.6	4616.8	5539.9	6463.1	7386.3
8 H+	808.8	1616.5	2424.3	3232.1	4039.8	4847.6	5655.3	6463.1
9 H+	719.0	1437.0	2155.0	2873.0	3591.1	4309.1	5027.1	5745.1
10 H+	647.2	1293.4	1939.6	2585.8	3232.1	3878.3	4524.5	5170.7
11 H+	588.5	1175.9	1763.4	2350.9	2938.3	3525.8	4113.2	4700.7
12 H+	539.5	1078.0	1616.5	2155.0	2693.5	3232.1	3770.6	4309.1
13 H+	498.1	995.2	1492.3	1989.3	2486.4	2983.5	3480.6	3977.7
14 H+	462.6	924.2	1385.7	1847.3	2308.9	2770.5	3232.1	3693.6
15 H+	431.8	862.6	1293.4	1724.2	2155.0	2585.8	3016.6	3447.5
16 H+	404.9	808.8	1212.6	1616.5	2020.4	2424.3	2828.2	3232.1
17 H+	381.1	761.2	1141.4	1521.5	1901.6	2281.7	2661.9	3042.0
18 H+	360.0	719.0	1078.0	1437.0	1796.0	2155.0	2514.0	2873.0
19 H+	341.1	681.2	1021.3	1361.4	1701.6	2041.7	2381.8	2721.9
20 H+	324.1	647.2	970.3	1293.4	1616.5	1939.6	2262.7	2585.8
21 H+	308.7	616.4	924.2	1231.9	1539.6	1847.3	2155.0	2462.8
22 H+	294.7	588.5	882.2	1175.9	1469.7	1763.4	2057.1	2350.9
23 H+	282.0	562.9	843.9	1124.8	1405.8	1686.8	1967.7	2248.7

p53wt + 1 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7270.1	7401.3	13691.2	13822.4	13953.6	20112.3	20243.5	20374.7	20505.9	26533.4	26664.6	26795.8	26927.0	27058.2
1 H+	7271.1	7402.3	13692.2	13823.4	13954.6	20113.3	20244.5	20375.7	20506.9	26534.4	26665.6	26796.8	26928.0	27059.2
2 H+	3636.1	3701.7	6846.6	6912.2	6977.8	10057.2	10122.8	10188.4	10254.0	13267.7	13333.3	13398.9	13464.5	13530.1
3 H+	2424.4	2468.1	4564.7	4608.5	4652.2	6705.1	6748.8	6792.6	6836.3	8845.5	8889.2	8932.9	8976.7	9020.4
4 H+	1818.5	1851.3	3423.8	3456.6	3489.4	5029.1	5061.9	5094.7	5127.5	6634.4	6667.2	6700.0	6732.8	6765.6
5 H+	1455.0	1481.3	2739.2	2765.5	2791.7	4023.5	4049.7	4075.9	4102.2	5307.7	5333.9	5360.2	5386.4	5412.6
6 H+	1212.7	1234.6	2282.9	2304.7	2326.6	3353.1	3374.9	3396.8	3418.7	4423.2	4445.1	4467.0	4488.8	4510.7
7 H+	1039.6	1058.3	1956.9	1975.6	1994.4	2874.2	2892.9	2911.7	2930.4	3791.5	3810.2	3829.0	3847.7	3866.5
8 H+	909.8	926.2	1712.4	1728.8	1745.2	2515.0	2531.4	2547.8	2564.2	3317.7	3334.1	3350.5	3366.9	3383.3
9 H+	808.8	823.4	1522.2	1536.8	1551.4	2235.7	2250.3	2264.9	2279.4	2949.2	2963.7	2978.3	2992.9	3007.5
10 H+	728.0	741.1	1370.1	1383.2	1396.4	2012.2	2025.4	2038.5	2051.6	2654.3	2667.5	2680.6	2693.7	2706.8
11 H+	661.9	673.8	1245.7	1257.6	1269.5	1829.4	1841.3	1853.2	1865.2	2413.1	2425.1	2437.0	2448.9	2460.8
12 H+	606.8	617.8	1141.9	1152.9	1163.8	1677.0	1688.0	1698.9	1709.8	2212.1	2223.1	2234.0	2244.9	2255.9
13 H+	560.2	570.3	1054.2	1064.3	1074.4	1548.1	1558.2	1568.3	1578.4	2042.0	2052.1	2062.2	2072.3	2082.4
14 H+	520.3	529.7	978.9	988.3	997.7	1437.6	1447.0	1456.3	1465.7	1896.2	1905.6	1915.0	1924.4	1933.7
15 H+	485.7	494.4	913.7	922.5	931.2	1341.8	1350.6	1359.3	1368.1	1769.9	1778.6	1787.4	1796.1	1804.9
16 H+	455.4	463.6	856.7	864.9	873.1	1258.0	1266.2	1274.4	1282.6	1659.3	1667.5	1675.7	1683.9	1692.1
17 H+	428.7	436.4	806.4	814.1	821.8	1184.1	1191.8	1199.5	1207.2	1561.8	1569.5	1577.2	1584.9	1592.7
18 H+	404.9	412.2	761.6	768.9	776.2	1118.4	1125.6	1132.9	1140.2	1475.1	1482.4	1489.7	1496.9	1504.2
19 H+	383.6	390.5	721.6	728.5	735.4	1059.5	1066.4	1073.4	1080.3	1397.5	1404.4	1411.3	1418.2	1425.1
20 H+	364.5	371.1	685.6	692.1	698.7	1006.6	1013.2	1019.7	1026.3	1327.7	1334.2	1340.8	1347.4	1353.9
21 H+	347.2	353.4	653.0	659.2	665.5	958.7	965.0	971.2	977.5	1264.5	1270.7	1277.0	1283.2	1289.5
22 H+	331.5	337.4	623.3	629.3	635.3	915.2	921.2	927.1	933.1	1207.1	1213.0	1219.0	1225.0	1230.9
23 H+	317.1	322.8	596.3	602.0	607.7	875.4	881.2	886.9	892.6	1154.6	1160.3	1166.0	1171.7	1177.4

p53wt + 2 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	8119.1	8250.3	14540.2	14671.4	14802.6	20961.3	21092.5	21223.7	21354.9	27382.4	27513.6	27644.8	27776.0	27907.2
1 H+	8120.1	8251.3	14541.2	14672.4	14803.6	20962.3	21093.5	21224.7	21355.9	27383.4	27514.6	27645.8	27777.0	27908.2
2 H+	4060.6	4126.2	7271.1	7336.7	7402.3	10481.7	10547.3	10612.9	10678.5	13692.2	13757.8	13823.4	13889.0	13954.6
3 H+	2707.4	2751.1	4847.7	4891.5	4935.2	6988.1	7031.8	7075.6	7119.3	9128.5	9172.2	9215.9	9259.7	9303.4
4 H+	2030.8	2063.6	3636.1	3668.9	3701.7	5241.3	5274.1	5306.9	5339.7	6846.6	6879.4	6912.2	6945.0	6977.8
5 H+	1624.8	1651.1	2909.0	2935.3	2961.5	4193.3	4219.5	4245.7	4272.0	5477.5	5503.7	5530.0	5556.2	5582.4
6 H+	1354.2	1376.1	2424.4	2446.2	2468.1	3494.6	3516.4	3538.3	3560.2	4564.7	4586.6	4608.5	4630.3	4652.2
7 H+	1160.9	1179.6	2078.2	2096.9	2115.7	2995.5	3014.2	3033.0	3051.7	3912.8	3931.5	3950.3	3969.0	3987.7
8 H+	1015.9	1032.3	1818.5	1834.9	1851.3	2621.2	2637.6	2654.0	2670.4	3423.8	3440.2	3456.6	3473.0	3489.4
9 H+	903.1	917.7	1616.6	1631.2	1645.7	2330.0	2344.6	2359.2	2373.8	3043.5	3058.1	3072.6	3087.2	3101.8
10 H+	812.9	826.0	1455.0	1468.1	1481.3	2097.1	2110.3	2123.4	2136.5	2739.2	2752.4	2765.5	2778.6	2791.7
11 H+	739.1	751.0	1322.8	1334.8	1346.7	1906.6	1918.5	1930.4	1942.4	2490.3	2502.2	2514.2	2526.1	2538.0
12 H+	677.6	688.5	1212.7	1223.6	1234.6	1747.8	1758.7	1769.6	1780.6	2282.9	2293.8	2304.7	2315.7	2326.6
13 H+	625.5	635.6	1119.5	1129.6	1139.7	1613.4	1623.5	1633.6	1643.7	2107.3	2117.4	2127.5	2137.6	2147.7
14 H+	580.9	590.3	1039.6	1049.0	1058.3	1498.2	1507.6	1517.0	1526.4	1956.9	1966.3	1975.6	1985.0	1994.4
15 H+	542.3	551.0	970.3	979.1	987.8	1398.4	1407.2	1415.9	1424.7	1826.5	1835.2	1844.0	1852.7	1861.5
16 H+	508.4	516.6	909.8	918.0	926.2	1311.1	1319.3	1327.5	1335.7	1712.4	1720.6	1728.8	1737.0	1745.2
17 H+	478.6	486.3	856.3	864.0	871.7	1234.0	1241.7	1249.5	1257.2	1611.7	1619.4	1627.2	1634.9	1642.6
18 H+	452.1	459.4	808.8	816.1	823.4	1165.5	1172.8	1180.1	1187.4	1522.2	1529.5	1536.8	1544.1	1551.4
19 H+	428.3	435.2	766.3	773.2	780.1	1104.2	1111.1	1118.0	1124.9	1442.2	1449.1	1456.0	1462.9	1469.8
20 H+	407.0	413.5	728.0	734.6	741.1	1049.1	1055.6	1062.2	1068.7	1370.1	1376.7	1383.2	1389.8	1396.4
21 H+	387.6	393.9	693.4	699.6	705.9	999.2	1005.4	1011.7	1017.9	1304.9	1311.2	1317.4	1323.7	1329.9
22 H+	370.1	376.0	661.9	667.9	673.8	953.8	959.8	965.7	971.7	1245.7	1251.6	1257.6	1263.5	1269.5
23 H+	354.0	359.7	633.2	638.9	644.6	912.4	918.1	923.8	929.5	1191.5	1197.2	1202.9	1208.7	1214.4

R337H + 1 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7251.0	7382.2	13653.0	13784.2	13915.4	20055.0	20186.2	20317.4	20448.6	26457.0	26588.2	26719.4	26850.6	26981.8
1 H+	7252.0	7383.2	13654.0	13785.2	13916.4	20056.0	20187.2	20318.4	20449.6	26458.0	26589.2	26720.4	26851.6	26982.8
2 H+	3626.5	3692.1	6827.5	6893.1	6958.7	10028.5	10094.1	10159.7	10225.3	13229.5	13295.1	13360.7	13426.3	13491.9
3 H+	2418.0	2461.7	4552.0	4595.7	4639.5	6686.0	6729.7	6773.5	6817.2	8820.0	8863.7	8907.5	8951.2	8994.9
4 H+	1813.8	1846.6	3414.3	3447.1	3479.9	5014.8	5047.6	5080.4	5113.2	6615.3	6648.1	6680.9	6713.7	6746.5
5 H+	1451.2	1477.4	2731.6	2757.8	2784.1	4012.0	4038.2	4064.5	4090.7	5292.4	5318.6	5344.9	5371.1	5397.4
6 H+	1209.5	1231.4	2276.5	2298.4	2320.2	3343.5	3365.4	3387.2	3409.1	4410.5	4432.4	4454.2	4476.1	4498.0
7 H+	1036.9	1055.6	1951.4	1970.2	1988.9	2866.0	2884.7	2903.5	2922.2	3780.6	3799.3	3818.1	3836.8	3855.5
8 H+	907.4	923.8	1707.6	1724.0	1740.4	2507.9	2524.3	2540.7	2557.1	3308.1	3324.5	3340.9	3357.3	3373.7
9 H+	806.7	821.2	1518.0	1532.6	1547.2	2229.3	2243.9	2258.5	2273.1	2940.7	2955.2	2969.8	2984.4	2999.0
10 H+	726.1	739.2	1366.3	1379.4	1392.5	2006.5	2019.6	2032.7	2045.9	2646.7	2659.8	2672.9	2686.1	2699.2
11 H+	660.2	672.1	1242.2	1254.1	1266.0	1824.2	1836.1	1848.0	1860.0	2406.2	2418.1	2430.0	2442.0	2453.9
12 H+	605.3	616.2	1138.8	1149.7	1160.6	1672.3	1683.2	1694.1	1705.1	2205.8	2216.7	2227.6	2238.6	2249.5
13 H+	558.8	568.9	1051.2	1061.3	1071.4	1543.7	1553.8	1563.9	1574.0	2036.2	2046.2	2056.3	2066.4	2076.5
14 H+	518.9	528.3	976.2	985.6	995.0	1433.5	1442.9	1452.2	1461.6	1890.8	1900.2	1909.5	1918.9	1928.3
15 H+	484.4	493.1	911.2	919.9	928.7	1338.0	1346.7	1355.5	1364.2	1764.8	1773.5	1782.3	1791.0	1799.8
16 H+	454.2	462.4	854.3	862.5	870.7	1254.4	1262.6	1270.8	1279.0	1654.6	1662.8	1671.0	1679.2	1687.4
17 H+	427.5	435.2	804.1	811.8	819.6	1180.7	1188.4	1196.1	1203.9	1557.3	1565.0	1572.7	1580.4	1588.2
18 H+	403.8	411.1	759.5	766.8	774.1	1115.2	1122.5	1129.7	1137.0	1470.8	1478.1	1485.4	1492.7	1500.0
19 H+	382.6	389.5	719.6	726.5	733.4	1056.5	1063.4	1070.3	1077.2	1393.5	1400.4	1407.3	1414.2	1421.1
20 H+	363.6	370.1	683.7	690.2	696.8	1003.8	1010.3	1016.9	1023.4	1323.9	1330.4	1337.0	1343.5	1350.1
21 H+	346.3	352.5	651.1	657.4	663.6	956.0	962.2	968.5	974.7	1260.9	1267.1	1273.4	1279.6	1285.8
22 H+	330.6	336.6	621.6	627.6	633.5	912.6	918.6	924.5	930.5	1203.6	1209.6	1215.5	1221.5	1227.4
23 H+	316.3	322.0	594.6	600.3	606.0	873.0	878.7	884.4	890.1	1151.3	1157.0	1162.7	1168.4	1174.1

R337H + 2 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	8100.0	8231.2	14502.0	14633.2	14764.4	20904.0	21035.2	21166.4	21297.6	27306.0	27437.2	27568.4	27699.6	27830.8
1 H+	8101.0	8232.2	14503.0	14634.2	14765.4	20905.0	21036.2	21167.4	21298.6	27307.0	27438.2	27569.4	27700.6	27831.8
2 H+	4051.0	4116.6	7252.0	7317.6	7383.2	10453.0	10518.6	10584.2	10649.8	13654.0	13719.6	13785.2	13850.8	13916.4
3 H+	2701.0	2744.7	4835.0	4878.7	4922.5	6969.0	7012.7	7056.5	7100.2	9103.0	9146.7	9190.5	9234.2	9277.9
4 H+	2026.0	2058.8	3626.5	3659.3	3692.1	5227.0	5259.8	5292.6	5325.4	6827.5	6860.3	6893.1	6925.9	6958.7
5 H+	1621.0	1647.2	2901.4	2927.6	2953.9	4181.8	4208.0	4234.3	4260.5	5462.2	5488.4	5514.7	5540.9	5567.2
6 H+	1351.0	1372.9	2418.0	2439.9	2461.7	3485.0	3506.9	3528.7	3550.6	4552.0	4573.9	4595.7	4617.6	4639.5
7 H+	1158.1	1176.9	2072.7	2091.5	2110.2	2987.3	3006.0	3024.8	3043.5	3901.9	3920.6	3939.3	3958.1	3976.8
8 H+	1013.5	1029.9	1813.8	1830.2	1846.6	2614.0	2630.4	2646.8	2663.2	3414.3	3430.7	3447.1	3463.5	3479.9
9 H+	901.0	915.6	1612.3	1626.9	1641.5	2323.7	2338.2	2352.8	2367.4	3035.0	3049.6	3064.2	3078.7	3093.3
10 H+	811.0	824.1	1451.2	1464.3	1477.4	2091.4	2104.5	2117.6	2130.8	2731.6	2744.7	2757.8	2771.0	2784.1
11 H+	737.4	749.3	1319.4	1331.3	1343.2	1901.4	1913.3	1925.2	1937.1	2483.4	2495.3	2507.2	2519.1	2531.1
12 H+	676.0	686.9	1209.5	1220.4	1231.4	1743.0	1753.9	1764.9	1775.8	2276.5	2287.4	2298.4	2309.3	2320.2
13 H+	624.1	634.2	1116.5	1126.6	1136.7	1609.0	1619.1	1629.2	1639.3	2101.5	2111.6	2121.6	2131.7	2141.8
14 H+	579.6	588.9	1036.9	1046.2	1055.6	1494.1	1503.5	1512.9	1522.3	1951.4	1960.8	1970.2	1979.5	1988.9
15 H+	541.0	549.7	967.8	976.5	985.3	1394.6	1403.3	1412.1	1420.8	1821.4	1830.1	1838.9	1847.6	1856.4
16 H+	507.3	515.5	907.4	915.6	923.8	1307.5	1315.7	1323.9	1332.1	1707.6	1715.8	1724.0	1732.2	1740.4
17 H+	477.5	485.2	854.1	861.8	869.5	1230.6	1238.4	1246.1	1253.8	1607.2	1615.0	1622.7	1630.4	1638.1
18 H+	451.0	458.3	806.7	814.0	821.2	1162.3	1169.6	1176.9	1184.2	1518.0	1525.3	1532.6	1539.9	1547.2
19 H+	427.3	434.2	764.3	771.2	778.1	1101.2	1108.1	1115.0	1121.9	1438.2	1445.1	1452.0	1458.9	1465.8
20 H+	406.0	412.6	726.1	732.7	739.2	1046.2	1052.8	1059.3	1065.9	1366.3	1372.9	1379.4	1386.0	1392.5
21 H+	386.7	393.0	691.6	697.8	704.1	996.4	1002.7	1008.9	1015.2	1301.3	1307.5	1313.8	1320.0	1326.3
22 H+	369.2	375.1	660.2	666.1	672.1	951.2	957.1	963.1	969.1	1242.2	1248.1	1254.1	1260.1	1266.0
23 H+	353.2	358.9	631.5	637.2	642.9	909.9	915.6	921.3	927.0	1188.2	1193.9	1199.6	1205.3	1211.0

G334V + 1 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7312.2	7443.4	13775.4	13906.6	14037.8	20238.6	20369.8	20501.0	20632.2	26701.8	26833.0	26964.2	27095.4	27226.6
1 H+	7313.2	7444.4	13776.4	13907.6	14038.8	20239.6	20370.8	20502.0	20633.2	26702.8	26834.0	26965.2	27096.4	27227.6
2 H+	3657.1	3722.7	6888.7	6954.3	7019.9	10120.3	10185.9	10251.5	10317.1	13351.9	13417.5	13483.1	13548.7	13614.3
3 H+	2438.4	2482.1	4592.8	4636.5	4680.3	6747.2	6790.9	6834.7	6878.4	8901.6	8945.3	8989.1	9032.8	9076.5
4 H+	1829.1	1861.9	3444.9	3477.7	3510.5	5060.7	5093.5	5126.3	5159.1	6676.5	6709.3	6742.1	6774.9	6807.7
5 H+	1463.4	1489.7	2756.1	2782.3	2808.6	4048.7	4075.0	4101.2	4127.4	5341.4	5367.6	5393.8	5420.1	5446.3
6 H+	1219.7	1241.6	2296.9	2318.8	2340.6	3374.1	3396.0	3417.8	3439.7	4451.3	4473.2	4495.0	4516.9	4538.8
7 H+	1045.6	1064.3	1968.9	1987.7	2006.4	2892.2	2911.0	2929.7	2948.5	3815.5	3834.3	3853.0	3871.8	3890.5
8 H+	915.0	931.4	1722.9	1739.3	1755.7	2530.8	2547.2	2563.6	2580.0	3338.7	3355.1	3371.5	3387.9	3404.3
9 H+	813.5	828.0	1531.6	1546.2	1560.8	2249.7	2264.3	2278.9	2293.5	2967.9	2982.4	2997.0	3011.6	3026.2
10 H+	732.2	745.3	1378.5	1391.7	1404.8	2024.9	2038.0	2051.1	2064.2	2671.2	2684.3	2697.4	2710.5	2723.7
11 H+	665.7	677.7	1253.3	1265.2	1277.2	1840.9	1852.8	1864.7	1876.7	2428.4	2440.4	2452.3	2464.2	2476.1
12 H+	610.4	621.3	1149.0	1159.9	1170.8	1687.6	1698.5	1709.4	1720.4	2226.2	2237.1	2248.0	2259.0	2269.9
13 H+	563.5	573.6	1060.6	1070.7	1080.8	1557.8	1567.9	1578.0	1588.1	2055.0	2065.1	2075.2	2085.3	2095.4
14 H+	523.3	532.7	985.0	994.3	1003.7	1446.6	1456.0	1465.4	1474.7	1908.3	1917.6	1927.0	1936.4	1945.8
15 H+	488.5	497.2	919.4	928.1	936.9	1350.2	1359.0	1367.7	1376.5	1781.1	1789.9	1798.6	1807.4	1816.1
16 H+	458.0	466.2	862.0	870.2	878.4	1265.9	1274.1	1282.3	1290.5	1669.9	1678.1	1686.3	1694.5	1702.7
17 H+	431.1	438.8	811.3	819.0	826.8	1191.5	1199.2	1206.9	1214.7	1571.7	1579.4	1587.1	1594.8	1602.6
18 H+	407.2	414.5	766.3	773.6	780.9	1125.4	1132.7	1139.9	1147.2	1484.4	1491.7	1499.0	1506.3	1513.6
19 H+	385.9	392.8	726.0	732.9	739.8	1066.2	1073.1	1080.0	1086.9	1406.4	1413.3	1420.2	1427.1	1434.0
20 H+	366.6	373.2	689.8	696.3	702.9	1012.9	1019.5	1026.1	1032.6	1336.1	1342.7	1349.2	1355.8	1362.3
21 H+	349.2	355.4	657.0	663.2	669.5	964.7	971.0	977.2	983.5	1272.5	1278.8	1285.0	1291.3	1297.5
22 H+	333.4	339.3	627.2	633.1	639.1	920.9	926.9	932.9	938.8	1214.7	1220.7	1226.6	1232.6	1238.6
23 H+	318.9	324.6	599.9	605.6	611.3	880.9	886.6	892.3	898.1	1161.9	1167.7	1173.4	1179.1	1184.8

G334V + 2 calix4bridge

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	8161.2	8292.4	14624.4	14755.6	14886.8	21087.6	21218.8	21350.0	21481.2	27550.8	27682.0	27813.2	27944.4	28075.6
1 H+	8162.2	8293.4	14625.4	14756.6	14887.8	21088.6	21219.8	21351.0	21482.2	27551.8	27683.0	27814.2	27945.4	28076.6
2 H+	4081.6	4147.2	7313.2	7378.8	7444.4	10544.8	10610.4	10676.0	10741.6	13776.4	13842.0	13907.6	13973.2	14038.8
3 H+	2721.4	2765.1	4875.8	4919.5	4963.3	7030.2	7073.9	7117.7	7161.4	9184.6	9228.3	9272.1	9315.8	9359.5
4 H+	2041.3	2074.1	3657.1	3689.9	3722.7	5272.9	5305.7	5338.5	5371.3	6888.7	6921.5	6954.3	6987.1	7019.9
5 H+	1633.2	1659.5	2925.9	2952.1	2978.4	4218.5	4244.8	4271.0	4297.2	5511.2	5537.4	5563.6	5589.9	5616.1
6 H+	1361.2	1383.1	2438.4	2460.3	2482.1	3515.6	3537.5	3559.3	3581.2	4592.8	4614.7	4636.5	4658.4	4680.3
7 H+	1166.9	1185.6	2090.2	2108.9	2127.7	3013.5	3032.3	3051.0	3069.7	3936.8	3955.6	3974.3	3993.1	4011.8
8 H+	1021.2	1037.6	1829.1	1845.5	1861.9	2637.0	2653.4	2669.8	2686.2	3444.9	3461.3	3477.7	3494.1	3510.5
9 H+	907.8	922.4	1625.9	1640.5	1655.1	2344.1	2358.6	2373.2	2387.8	3062.2	3076.8	3091.4	3105.9	3120.5
10 H+	817.1	830.2	1463.4	1476.6	1489.7	2109.8	2122.9	2136.0	2149.1	2756.1	2769.2	2782.3	2795.4	2808.6
11 H+	742.9	754.9	1330.5	1342.4	1354.3	1918.1	1930.0	1941.9	1953.8	2505.6	2517.5	2529.5	2541.4	2553.3
12 H+	681.1	692.0	1219.7	1230.6	1241.6	1758.3	1769.2	1780.2	1791.1	2296.9	2307.8	2318.8	2329.7	2340.6
13 H+	628.8	638.9	1126.0	1136.0	1146.1	1623.1	1633.2	1643.3	1653.4	2120.3	2130.4	2140.5	2150.6	2160.7
14 H+	583.9	593.3	1045.6	1055.0	1064.3	1507.3	1516.6	1526.0	1535.4	1968.9	1978.3	1987.7	1997.0	2006.4
15 H+	545.1	553.8	976.0	984.7	993.5	1406.8	1415.6	1424.3	1433.1	1837.7	1846.5	1855.2	1864.0	1872.7
16 H+	511.1	519.3	915.0	923.2	931.4	1319.0	1327.2	1335.4	1343.6	1722.9	1731.1	1739.3	1747.5	1755.7
17 H+	481.1	488.8	861.3	869.0	876.7	1241.4	1249.2	1256.9	1264.6	1621.6	1629.4	1637.1	1644.8	1652.5
18 H+	454.4	461.7	813.5	820.8	828.0	1172.5	1179.8	1187.1	1194.4	1531.6	1538.9	1546.2	1553.5	1560.8
19 H+	430.5	437.4	770.7	777.6	784.5	1110.9	1117.8	1124.7	1131.6	1451.0	1457.9	1464.9	1471.8	1478.7
20 H+	409.1	415.6	732.2	738.8	745.3	1055.4	1061.9	1068.5	1075.1	1378.5	1385.1	1391.7	1398.2	1404.8
21 H+	389.6	395.9	697.4	703.6	709.9	1005.2	1011.4	1017.7	1023.9	1312.9	1319.2	1325.4	1331.7	1337.9
22 H+	372.0	377.9	665.7	671.7	677.7	959.5	965.5	971.5	977.4	1253.3	1259.3	1265.2	1271.2	1277.2
23 H+	355.8	361.5	636.8	642.5	648.3	917.9	923.6	929.3	935.0	1198.9	1204.6	1210.3	1216.0	1221.7

L344P + 1 calix4bridge

	monomer	dimer	trimer	tetramer	pentamer	hexamer	heptamer	octamer
0 H+	7311.1	14622.2	21933.3	29244.4	36555.5	43866.6	51177.7	58488.8
1 H+	7312.1	14623.2	21934.3	29245.4	36556.5	43867.6	51178.7	58489.8
2 H+	3656.6	7312.1	10967.7	14623.2	18278.8	21934.3	25589.9	29245.4
3 H+	2438.0	4875.1	7312.1	9749.1	12186.2	14623.2	17060.2	19497.3
4 H+	1828.8	3656.6	5484.3	7312.1	9139.9	10967.7	12795.4	14623.2
5 H+	1463.2	2925.4	4387.7	5849.9	7312.1	8774.3	10236.5	11698.8
6 H+	1219.5	2438.0	3656.6	4875.1	6093.6	7312.1	8530.6	9749.1
7 H+	1045.4	2089.9	3134.3	4178.8	5223.2	6267.7	7312.1	8356.5
8 H+	914.9	1828.8	2742.7	3656.6	4570.4	5484.3	6398.2	7312.1
9 H+	813.3	1625.7	2438.0	3250.4	4062.7	4875.1	5687.4	6499.8
10 H+	732.1	1463.2	2194.3	2925.4	3656.6	4387.7	5118.8	5849.9
11 H+	665.6	1330.3	1994.9	2659.6	3324.2	3988.9	4653.5	5318.2
12 H+	610.3	1219.5	1828.8	2438.0	3047.3	3656.6	4265.8	4875.1
13 H+	563.4	1125.8	1688.2	2250.6	2813.0	3375.4	3937.7	4500.1
14 H+	523.2	1045.4	1567.7	2089.9	2612.1	3134.3	3656.6	4178.8
15 H+	488.4	975.8	1463.2	1950.6	2438.0	2925.4	3412.8	3900.3
16 H+	457.9	914.9	1371.8	1828.8	2285.7	2742.7	3199.6	3656.6
17 H+	431.1	861.1	1291.2	1721.3	2151.3	2581.4	3011.5	3441.5
18 H+	407.2	813.3	1219.5	1625.7	2031.9	2438.0	2844.2	3250.4
19 H+	385.8	770.6	1155.4	1540.2	1925.0	2309.8	2694.6	3079.4
20 H+	366.6	732.1	1097.7	1463.2	1828.8	2194.3	2559.9	2925.4
21 H+	349.1	697.3	1045.4	1393.6	1741.7	2089.9	2438.0	2786.2
22 H+	333.3	665.6	998.0	1330.3	1662.6	1994.9	2327.3	2659.6
23 H+	318.9	636.7	954.6	1272.5	1590.4	1908.2	2226.1	2544.0

p53wt + 1 calix4prop

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7298.2	7429.4	13719.3	13850.5	13981.7	20140.4	20271.6	20402.8	20534.0	26561.5	26692.7	26823.9	26955.1	27086.3
1 H+	7299.2	7430.4	13720.3	13851.5	13982.7	20141.4	20272.6	20403.8	20535.0	26562.5	26693.7	26824.9	26956.1	27087.3
2 H+	3650.1	3715.7	6860.7	6926.3	6991.9	10071.2	10136.8	10202.4	10268.0	13281.8	13347.4	13413.0	13478.6	13544.2
3 H+	2433.7	2477.5	4574.1	4617.8	4661.6	6714.5	6758.2	6801.9	6845.7	8854.8	8898.6	8942.3	8986.0	9029.8
4 H+	1825.6	1858.4	3430.8	3463.6	3496.4	5036.1	5068.9	5101.7	5134.5	6641.4	6674.2	6707.0	6739.8	6772.6
5 H+	1460.6	1486.9	2744.9	2771.1	2797.3	4029.1	4055.3	4081.6	4107.8	5313.3	5339.5	5365.8	5392.0	5418.3
6 H+	1217.4	1239.2	2287.6	2309.4	2331.3	3357.7	3379.6	3401.5	3423.3	4427.9	4449.8	4471.7	4493.5	4515.4
7 H+	1043.6	1062.3	1960.9	1979.6	1998.4	2878.2	2896.9	2915.7	2934.4	3795.5	3814.2	3833.0	3851.7	3870.5
8 H+	913.3	929.7	1715.9	1732.3	1748.7	2518.6	2535.0	2551.4	2567.8	3321.2	3337.6	3354.0	3370.4	3386.8
9 H+	811.9	826.5	1525.4	1539.9	1554.5	2238.8	2253.4	2268.0	2282.6	2952.3	2966.9	2981.4	2996.0	3010.6
10 H+	730.8	743.9	1372.9	1386.1	1399.2	2015.0	2028.2	2041.3	2054.4	2657.2	2670.3	2683.4	2696.5	2709.6
11 H+	664.5	676.4	1248.2	1260.1	1272.1	1831.9	1843.9	1855.8	1867.7	2415.7	2427.6	2439.5	2451.5	2463.4
12 H+	609.2	620.1	1144.3	1155.2	1166.1	1679.4	1690.3	1701.2	1712.2	2214.5	2225.4	2236.3	2247.3	2258.2
13 H+	562.4	572.5	1056.3	1066.4	1076.5	1550.3	1560.4	1570.4	1580.5	2044.2	2054.3	2064.4	2074.5	2084.6
14 H+	522.3	531.7	981.0	990.3	999.7	1439.6	1449.0	1458.3	1467.7	1898.3	1907.6	1917.0	1926.4	1935.7
15 H+	487.5	496.3	915.6	924.4	933.1	1343.7	1352.4	1361.2	1369.9	1771.8	1780.5	1789.3	1798.0	1806.8
16 H+	457.1	465.3	858.5	866.7	874.9	1259.8	1268.0	1276.2	1284.4	1661.1	1669.3	1677.5	1685.7	1693.9
17 H+	430.3	438.0	808.0	815.7	823.5	1185.7	1193.4	1201.2	1208.9	1563.4	1571.2	1578.9	1586.6	1594.3
18 H+	406.5	413.7	763.2	770.5	777.8	1119.9	1127.2	1134.5	1141.8	1476.6	1483.9	1491.2	1498.5	1505.8
19 H+	385.1	392.0	723.1	730.0	736.9	1061.0	1067.9	1074.8	1081.7	1399.0	1405.9	1412.8	1419.7	1426.6
20 H+	365.9	372.5	687.0	693.5	700.1	1008.0	1014.6	1021.1	1027.7	1329.1	1335.6	1342.2	1348.8	1355.3
21 H+	348.5	354.8	654.3	660.5	666.8	960.1	966.3	972.6	978.8	1265.8	1272.1	1278.3	1284.6	1290.8
22 H+	332.7	338.7	624.6	630.6	636.5	916.5	922.4	928.4	934.4	1208.3	1214.3	1220.3	1226.2	1232.2
23 H+	318.3	324.0	597.5	603.2	608.9	876.7	882.4	888.1	893.8	1155.8	1161.6	1167.3	1173.0	1178.7

p53wt + 2 calix4prop

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	8175.3	8306.5	14596.4	14727.6	14858.8	21017.5	21148.7	21279.9	21411.1	27438.6	27569.8	27701.0	27832.2	27963.4
1 H+	8176.3	8307.5	14597.4	14728.6	14859.8	21018.5	21149.7	21280.9	21412.1	27439.6	27570.8	27702.0	27833.2	27964.4
2 H+	4088.7	4154.3	7299.2	7364.8	7430.4	10509.8	10575.4	10641.0	10706.6	13720.3	13785.9	13851.5	13917.1	13982.7
3 H+	2726.1	2769.8	4866.5	4910.2	4953.9	7006.8	7050.6	7094.3	7138.0	9147.2	9190.9	9234.7	9278.4	9322.1
4 H+	2044.8	2077.6	3650.1	3682.9	3715.7	5255.4	5288.2	5321.0	5353.8	6860.7	6893.5	6926.3	6959.1	6991.9
5 H+	1636.1	1662.3	2920.3	2946.5	2972.8	4204.5	4230.7	4257.0	4283.2	5488.7	5515.0	5541.2	5567.4	5593.7
6 H+	1363.6	1385.4	2433.7	2455.6	2477.5	3503.9	3525.8	3547.7	3569.5	4574.1	4596.0	4617.8	4639.7	4661.6
7 H+	1168.9	1187.6	2086.2	2104.9	2123.7	3003.5	3022.2	3041.0	3059.7	3920.8	3939.5	3958.3	3977.0	3995.8
8 H+	1022.9	1039.3	1825.6	1842.0	1858.4	2628.2	2644.6	2661.0	2677.4	3430.8	3447.2	3463.6	3480.0	3496.4
9 H+	909.4	923.9	1622.8	1637.4	1652.0	2336.3	2350.9	2365.4	2380.0	3049.7	3064.3	3078.9	3093.5	3108.0
10 H+	818.5	831.7	1460.6	1473.8	1486.9	2102.8	2115.9	2129.0	2142.1	2744.9	2758.0	2771.1	2784.2	2797.3
11 H+	744.2	756.1	1327.9	1339.9	1351.8	1911.7	1923.6	1935.5	1947.5	2495.4	2507.3	2519.3	2531.2	2543.1
12 H+	682.3	693.2	1217.4	1228.3	1239.2	1752.5	1763.4	1774.3	1785.3	2287.6	2298.5	2309.4	2320.4	2331.3
13 H+	629.9	640.0	1123.8	1133.9	1144.0	1617.7	1627.8	1637.9	1648.0	2111.7	2121.8	2131.8	2141.9	2152.0
14 H+	585.0	594.3	1043.6	1053.0	1062.3	1502.3	1511.6	1521.0	1530.4	1960.9	1970.3	1979.6	1989.0	1998.4
15 H+	546.0	554.8	974.1	982.8	991.6	1402.2	1410.9	1419.7	1428.4	1830.2	1839.0	1847.7	1856.5	1865.2
16 H+	512.0	520.2	913.3	921.5	929.7	1314.6	1322.8	1331.0	1339.2	1715.9	1724.1	1732.3	1740.5	1748.7
17 H+	481.9	489.6	859.6	867.3	875.0	1237.3	1245.0	1252.8	1260.5	1615.0	1622.8	1630.5	1638.2	1645.9
18 H+	455.2	462.5	811.9	819.2	826.5	1168.6	1175.9	1183.2	1190.5	1525.4	1532.7	1539.9	1547.2	1554.5
19 H+	431.3	438.2	769.2	776.1	783.0	1107.2	1114.1	1121.0	1127.9	1445.1	1452.0	1458.9	1465.9	1472.8
20 H+	409.8	416.3	730.8	737.4	743.9	1051.9	1058.4	1065.0	1071.6	1372.9	1379.5	1386.1	1392.6	1399.2
21 H+	390.3	396.5	696.1	702.3	708.6	1001.8	1008.1	1014.3	1020.6	1307.6	1313.8	1320.1	1326.3	1332.6
22 H+	372.6	378.6	664.5	670.4	676.4	956.3	962.3	968.3	974.2	1248.2	1254.2	1260.1	1266.1	1272.1
23 H+	356.4	362.2	635.6	641.3	647.0	914.8	920.5	926.2	931.9	1194.0	1199.7	1205.4	1211.1	1216.8

R337H + 1 calix4prop

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7279.1	7410.3	13681.1	13812.3	13943.5	20083.1	20214.3	20345.5	20476.7	26485.1	26616.3	26747.5	26878.7	27009.9
1 H+	7280.1	7411.3	13682.1	13813.3	13944.5	20084.1	20215.3	20346.5	20477.7	26486.1	26617.3	26748.5	26879.7	27010.9
2 H+	3640.6	3706.2	6841.6	6907.2	6972.8	10042.6	10108.2	10173.8	10239.4	13243.6	13309.2	13374.8	13440.4	13506.0
3 H+	2427.4	2471.1	4561.4	4605.1	4648.8	6695.4	6739.1	6782.8	6826.6	8829.4	8873.1	8916.8	8960.6	9004.3
4 H+	1820.8	1853.6	3421.3	3454.1	3486.9	5021.8	5054.6	5087.4	5120.2	6622.3	6655.1	6687.9	6720.7	6753.5
5 H+	1456.8	1483.1	2737.2	2763.5	2789.7	4017.6	4043.9	4070.1	4096.3	5298.0	5324.3	5350.5	5376.7	5403.0
6 H+	1214.2	1236.1	2281.2	2303.1	2324.9	3348.2	3370.1	3391.9	3413.8	4415.2	4437.1	4458.9	4480.8	4502.7
7 H+	1040.9	1059.6	1955.4	1974.2	1992.9	2870.0	2888.8	2907.5	2926.2	3784.6	3803.3	3822.1	3840.8	3859.6
8 H+	910.9	927.3	1711.1	1727.5	1743.9	2511.4	2527.8	2544.2	2560.6	3311.6	3328.0	3344.4	3360.8	3377.2
9 H+	809.8	824.4	1521.1	1535.7	1550.3	2232.5	2247.0	2261.6	2276.2	2943.8	2958.4	2972.9	2987.5	3002.1
10 H+	728.9	742.0	1369.1	1382.2	1395.4	2009.3	2022.4	2035.6	2048.7	2649.5	2662.6	2675.8	2688.9	2702.0
11 H+	662.7	674.7	1244.7	1256.7	1268.6	1826.7	1838.7	1850.6	1862.5	2408.7	2420.7	2432.6	2444.5	2456.4
12 H+	607.6	618.5	1141.1	1152.0	1163.0	1674.6	1685.5	1696.5	1707.4	2208.1	2219.0	2230.0	2240.9	2251.8
13 H+	560.9	571.0	1053.4	1063.5	1073.6	1545.9	1555.9	1566.0	1576.1	2038.3	2048.4	2058.5	2068.6	2078.7
14 H+	520.9	530.3	978.2	987.6	997.0	1435.5	1444.9	1454.3	1463.6	1892.8	1902.2	1911.5	1920.9	1930.3
15 H+	486.3	495.0	913.1	921.8	930.6	1339.9	1348.6	1357.4	1366.1	1766.7	1775.4	1784.2	1792.9	1801.7
16 H+	455.9	464.1	856.1	864.3	872.5	1256.2	1264.4	1272.6	1280.8	1656.3	1664.5	1672.7	1680.9	1689.1
17 H+	429.2	436.9	805.8	813.5	821.2	1182.4	1190.1	1197.8	1205.5	1558.9	1566.7	1574.4	1582.1	1589.8
18 H+	405.4	412.7	761.1	768.4	775.6	1116.7	1124.0	1131.3	1138.6	1472.4	1479.7	1487.0	1494.3	1501.6
19 H+	384.1	391.0	721.1	728.0	734.9	1058.0	1064.9	1071.8	1078.7	1395.0	1401.9	1408.8	1415.7	1422.6
20 H+	365.0	371.5	685.1	691.6	698.2	1005.2	1011.7	1018.3	1024.8	1325.3	1331.8	1338.4	1344.9	1351.5
21 H+	347.6	353.9	652.5	658.7	665.0	957.3	963.6	969.8	976.1	1262.2	1268.4	1274.7	1280.9	1287.2
22 H+	331.9	337.8	622.9	628.8	634.8	913.9	919.8	925.8	931.8	1204.9	1210.8	1216.8	1222.8	1228.7
23 H+	317.5	323.2	595.8	601.5	607.2	874.2	879.9	885.6	891.3	1152.5	1158.2	1163.9	1169.6	1175.3

R337H + 2 calix4prop

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	8156.2	8287.4	14558.2	14689.4	14820.6	20960.2	21091.4	21222.6	21353.8	27362.2	27493.4	27624.6	27755.8	27887.0
1 H+	8157.2	8288.4	14559.2	14690.4	14821.6	20961.2	21092.4	21223.6	21354.8	27363.2	27494.4	27625.6	27756.8	27888.0
2 H+	4079.1	4144.7	7280.1	7345.7	7411.3	10481.1	10546.7	10612.3	10677.9	13682.1	13747.7	13813.3	13878.9	13944.5
3 H+	2719.7	2763.5	4853.7	4897.5	4941.2	6987.7	7031.5	7075.2	7118.9	9121.7	9165.5	9209.2	9252.9	9296.7
4 H+	2040.1	2072.9	3640.6	3673.4	3706.2	5241.1	5273.9	5306.7	5339.5	6841.6	6874.4	6907.2	6940.0	6972.8
5 H+	1632.2	1658.5	2912.6	2938.9	2965.1	4193.0	4219.3	4245.5	4271.8	5473.4	5499.7	5525.9	5552.2	5578.4
6 H+	1360.4	1382.2	2427.4	2449.2	2471.1	3494.4	3516.2	3538.1	3560.0	4561.4	4583.2	4605.1	4627.0	4648.8
7 H+	1166.2	1184.9	2080.7	2099.5	2118.2	2995.3	3014.1	3032.8	3051.5	3909.9	3928.6	3947.4	3966.1	3984.9
8 H+	1020.5	1036.9	1820.8	1837.2	1853.6	2621.0	2637.4	2653.8	2670.2	3421.3	3437.7	3454.1	3470.5	3486.9
9 H+	907.2	921.8	1618.6	1633.2	1647.7	2329.9	2344.5	2359.1	2373.6	3041.2	3055.8	3070.4	3085.0	3099.6
10 H+	816.6	829.7	1456.8	1469.9	1483.1	2097.0	2110.1	2123.3	2136.4	2737.2	2750.3	2763.5	2776.6	2789.7
11 H+	742.5	754.4	1324.5	1336.4	1348.3	1906.5	1918.4	1930.3	1942.3	2488.5	2500.4	2512.3	2524.3	2536.2
12 H+	680.7	691.6	1214.2	1225.1	1236.1	1747.7	1758.6	1769.6	1780.5	2281.2	2292.1	2303.1	2314.0	2324.9
13 H+	628.4	638.5	1120.9	1131.0	1141.0	1613.3	1623.4	1633.5	1643.6	2105.8	2115.9	2126.0	2136.1	2146.2
14 H+	583.6	593.0	1040.9	1050.2	1059.6	1498.2	1507.5	1516.9	1526.3	1955.4	1964.8	1974.2	1983.6	1992.9
15 H+	544.7	553.5	971.5	980.3	989.0	1398.3	1407.1	1415.8	1424.6	1825.1	1833.9	1842.6	1851.4	1860.1
16 H+	510.8	519.0	910.9	919.1	927.3	1311.0	1319.2	1327.4	1335.6	1711.1	1719.3	1727.5	1735.7	1743.9
17 H+	480.8	488.5	857.4	865.1	872.8	1234.0	1241.7	1249.4	1257.1	1610.5	1618.3	1626.0	1633.7	1641.4
18 H+	454.1	461.4	809.8	817.1	824.4	1165.5	1172.7	1180.0	1187.3	1521.1	1528.4	1535.7	1543.0	1550.3
19 H+	430.3	437.2	767.2	774.1	781.0	1104.2	1111.1	1118.0	1124.9	1441.1	1448.0	1454.9	1461.8	1468.7
20 H+	408.8	415.4	728.9	735.5	742.0	1049.0	1055.6	1062.1	1068.7	1369.1	1375.7	1382.2	1388.8	1395.4
21 H+	389.4	395.6	694.2	700.5	706.7	999.1	1005.4	1011.6	1017.8	1304.0	1310.2	1316.5	1322.7	1329.0
22 H+	371.7	377.7	662.7	668.7	674.7	953.7	959.7	965.7	971.6	1244.7	1250.7	1256.7	1262.6	1268.6
23 H+	355.6	361.3	634.0	639.7	645.4	912.3	918.0	923.7	929.4	1190.7	1196.4	1202.1	1207.8	1213.5

G334V + 1 calix4prop

	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	7340.3	7471.5	13803.5	13934.7	14065.9	20266.7	20397.9	20529.1	20660.3	26729.9	26861.1	26992.3	27123.5	27254.7
1 H+	7341.3	7472.5	13804.5	13935.7	14066.9	20267.7	20398.9	20530.1	20661.3	26730.9	26862.1	26993.3	27124.5	27255.7
2 H+	3671.2	3736.8	6902.8	6968.4	7034.0	10134.4	10200.0	10265.6	10331.2	13366.0	13431.6	13497.2	13562.8	13628.4
3 H+	2447.8	2491.5	4602.2	4645.9	4689.6	6756.6	6800.3	6844.0	6887.8	8911.0	8954.7	8998.4	9042.2	9085.9
4 H+	1836.1	1868.9	3451.9	3484.7	3517.5	5067.7	5100.5	5133.3	5166.1	6683.5	6716.3	6749.1	6781.9	6814.7
5 H+	1469.1	1495.3	2761.7	2787.9	2814.2	4054.3	4080.6	4106.8	4133.1	5347.0	5373.2	5399.5	5425.7	5451.9
6 H+	1224.4	1246.3	2301.6	2323.5	2345.3	3378.8	3400.7	3422.5	3444.4	4456.0	4477.9	4499.7	4521.6	4543.5
7 H+	1049.6	1068.4	1972.9	1991.7	2010.4	2896.2	2915.0	2933.7	2952.5	3819.6	3838.3	3857.0	3875.8	3894.5
8 H+	918.5	934.9	1726.4	1742.8	1759.2	2534.3	2550.7	2567.1	2583.5	3342.2	3358.6	3375.0	3391.4	3407.8
9 H+	816.6	831.2	1534.7	1549.3	1563.9	2252.9	2267.4	2282.0	2296.6	2971.0	2985.6	3000.1	3014.7	3029.3
10 H+	735.0	748.2	1381.4	1394.5	1407.6	2027.7	2040.8	2053.9	2067.0	2674.0	2687.1	2700.2	2713.4	2726.5
11 H+	668.3	680.2	1255.9	1267.8	1279.7	1843.4	1855.4	1867.3	1879.2	2431.0	2442.9	2454.8	2466.8	2478.7
12 H+	612.7	623.6	1151.3	1162.2	1173.2	1689.9	1700.8	1711.8	1722.7	2228.5	2239.4	2250.4	2261.3	2272.2
13 H+	565.6	575.7	1062.8	1072.9	1083.0	1560.0	1570.1	1580.2	1590.3	2057.1	2067.2	2077.3	2087.4	2097.5
14 H+	525.3	534.7	987.0	996.3	1005.7	1448.6	1458.0	1467.4	1476.7	1910.3	1919.7	1929.0	1938.4	1947.8
15 H+	490.4	499.1	921.2	930.0	938.7	1352.1	1360.9	1369.6	1378.4	1783.0	1791.7	1800.5	1809.2	1818.0
16 H+	459.8	468.0	863.7	871.9	880.1	1267.7	1275.9	1284.1	1292.3	1671.6	1679.8	1688.0	1696.2	1704.4
17 H+	432.8	440.5	813.0	820.7	828.4	1193.2	1200.9	1208.6	1216.3	1573.3	1581.1	1588.8	1596.5	1604.2
18 H+	408.8	416.1	767.9	775.2	782.4	1126.9	1134.2	1141.5	1148.8	1486.0	1493.3	1500.6	1507.9	1515.2
19 H+	387.3	394.2	727.5	734.4	741.3	1067.7	1074.6	1081.5	1088.4	1407.8	1414.7	1421.6	1428.6	1435.5
20 H+	368.0	374.6	691.2	697.7	704.3	1014.3	1020.9	1027.5	1034.0	1337.5	1344.1	1350.6	1357.2	1363.7
21 H+	350.5	356.8	658.3	664.6	670.8	966.1	972.3	978.6	984.8	1273.9	1280.1	1286.3	1292.6	1298.8
22 H+	334.7	340.6	628.4	634.4	640.4	922.2	928.2	934.1	940.1	1216.0	1222.0	1227.9	1233.9	1239.9
23 H+	320.1	325.8	601.2	606.9	612.6	882.2	887.9	893.6	899.3	1163.2	1168.9	1174.6	1180.3	1186.0

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	monomer		dimer			trimer				tetramer				
w/o Met	1	0	2	1	0	3	2	1	0	4	3	2	1	0
w/ Met	0	1	0	1	2	0	1	2	3	0	1	2	3	4
0 H+	2817.4	8348.6	14680.6	14811.8	14943.0	21143.8	21275.0	21406.2	21537.4	27607.0	27738.2	27869.4	28000.6	28131.8
1 H+	8218.4	8349.6	14681.6	14812.8	14944.0	21144.8	21276.0	21407.2	21538.4	27608.0	27739.2	27870.4	28001.6	28132.8
2 H+	4109.7	4175.3	7341.3	7406.9	7472.5	10572.9	10638.5	10704.1	10769.7	13804.5	13870.1	13935.7	14001.3	14066.9
3 H+	2740.1	2783.9	4894.5	4938.3	4982.0	7048.9	7092.7	7136.4	7180.1	9203.3	9247.1	9290.8	9334.5	9378.3
4 H+	2055.4	2088.2	3671.2	3704.0	3736.8	5287.0	5319.8	5352.6	5385.4	6902.8	6935.6	6968.4	7001.2	7034.0
5 H+	1644.5	1670.7	2937.1	2963.4	2989.6	4229.8	4256.0	4282.2	4308.5	5522.4	5548.6	5574.9	5601.1	5627.4
6 H+	1370.6	1392.4	2447.8	2469.6	2491.5	3525.0	3546.8	3568.7	3590.6	4602.2	4624.0	4645.9	4667.8	4689.6
7 H+	1174.9	1193.7	2098.2	2117.0	2135.7	3021.5	3040.3	3059.0	3077.8	3944.9	3963.6	3982.3	4001.1	4019.8
8 H+	1028.2	1044.6	1836.1	1852.5	1868.9	2644.0	2660.4	2676.8	2693.2	3451.9	3468.3	3484.7	3501.1	3517.5
9 H+	914.0	928.6	1632.2	1646.8	1661.3	2350.3	2364.9	2379.5	2394.0	3068.4	3083.0	3097.6	3112.2	3126.8
10 H+	822.7	835.9	1469.1	1482.2	1495.3	2115.4	2128.5	2141.6	2154.7	2761.7	2774.8	2787.9	2801.1	2814.2
11 H+	748.0	760.0	1335.6	1347.5	1359.5	1923.2	1935.1	1947.0	1958.9	2510.7	2522.7	2534.6	2546.5	2558.4
12 H+	685.8	696.7	1224.4	1235.3	1246.3	1763.0	1773.9	1784.9	1795.8	2301.6	2312.5	2323.5	2334.4	2345.3
13 H+	633.1	643.2	1130.3	1140.4	1150.5	1627.4	1637.5	1647.6	1657.7	2124.6	2134.7	2144.8	2154.9	2165.0
14 H+	588.0	597.3	1049.6	1059.0	1068.4	1511.3	1520.6	1530.0	1539.4	1972.9	1982.3	1991.7	2001.0	2010.4
15 H+	548.8	557.6	979.7	988.5	997.2	1410.6	1419.3	1428.1	1436.8	1841.5	1850.2	1859.0	1867.7	1876.5
16 H+	514.6	522.8	918.5	926.7	934.9	1322.5	1330.7	1338.9	1347.1	1726.4	1734.6	1742.8	1751.0	1759.2
17 H+	484.4	492.1	864.6	872.3	880.0	1244.8	1252.5	1260.2	1267.9	1624.9	1632.7	1640.4	1648.1	1655.8
18 H+	457.5	464.8	816.6	823.9	831.2	1175.7	1182.9	1190.2	1197.5	1534.7	1542.0	1549.3	1556.6	1563.9
19 H+	433.5	440.4	773.7	780.6	787.5	1113.8	1120.7	1127.6	1134.5	1454.0	1460.9	1467.8	1474.7	1481.6
20 H+	411.9	418.4	735.0	741.6	748.2	1058.2	1064.8	1071.3	1077.9	1381.4	1387.9	1394.5	1401.0	1407.6
21 H+	392.3	398.6	700.1	706.3	712.6	1007.8	1014.1	1020.3	1026.6	1315.6	1321.9	1328.1	1334.4	1340.6
22 H+	374.5	380.5	668.3	674.3	680.2	962.1	968.0	974.0	980.0	1255.9	1261.8	1267.8	1273.8	1279.7
23 H+	358.3	364.0	639.3	645.0	650.7	920.3	926.0	931.7	937.4	1201.3	1207.0	1212.7	1218.4	1224.1

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	monomer	dimer	trimer	tetramer	pentamer	hexamer	heptamer	octamer
0 H+	7339.2	14678.4	22017.6	29356.8	36696	44035.2	51374.4	58713.6
1 H+	7340.2	14679.4	22018.6	29357.8	36697.0	44036.2	51375.4	58714.6
2 H+	3670.6	7340.2	11009.8	14679.4	18349.0	22018.6	25688.2	29357.8
3 H+	2447.4	4893.8	7340.2	9786.6	12233.0	14679.4	17125.8	19572.2
4 H+	1835.8	3670.6	5505.4	7340.2	9175.0	11009.8	12844.6	14679.4
5 H+	1468.8	2936.7	4404.5	5872.4	7340.2	8808.0	10275.9	11743.7
6 H+	1224.2	2447.4	3670.6	4893.8	6117.0	7340.2	8563.4	9786.6
7 H+	1049.5	2097.9	3146.4	4194.8	5243.3	6291.7	7340.2	8388.7
8 H+	918.4	1835.8	2753.2	3670.6	4588.0	5505.4	6422.8	7340.2
9 H+	816.5	1631.9	2447.4	3262.9	4078.3	4893.8	5709.3	6524.7
10 H+	734.9	1468.8	2202.8	2936.7	3670.6	4404.5	5138.4	5872.4
11 H+	668.2	1335.4	2002.6	2669.8	3337.0	4004.2	4671.4	5338.6
12 H+	612.6	1224.2	1835.8	2447.4	3059.0	3670.6	4282.2	4893.8
13 H+	565.6	1130.1	1694.7	2259.2	2823.8	3388.3	3952.9	4517.4
14 H+	525.2	1049.5	1573.7	2097.9	2622.1	3146.4	3670.6	4194.8
15 H+	490.3	979.6	1468.8	1958.1	2447.4	2936.7	3426.0	3915.2
16 H+	459.7	918.4	1377.1	1835.8	2294.5	2753.2	3211.9	3670.6
17 H+	432.7	864.4	1296.2	1727.9	2159.6	2591.3	3023.0	3454.7
18 H+	408.7	816.5	1224.2	1631.9	2039.7	2447.4	2855.1	3262.9
19 H+	387.3	773.5	1159.8	1546.1	1932.4	2318.6	2704.9	3091.2
20 H+	368.0	734.9	1101.9	1468.8	1835.8	2202.8	2569.7	2936.7
21 H+	350.5	700.0	1049.5	1398.9	1748.4	2097.9	2447.4	2796.9
22 H+	334.6	668.2	1001.8	1335.4	1669.0	2002.6	2336.2	2669.8
23 H+	320.1	639.2	958.3	1277.4	1596.5	1915.6	2234.7	2553.8