SUPPORTING INFORMATION

Cytochrome c and Organic Molecules: the Solution Structure of the Para-Aminophenol Adduct[†]

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Table S1. Acquisition parameters for the NMR experiments

Experiments	Dimension of acquired data (nucleus)			Spectral width (ppm)			Ref
	t1	t2	t3	F1	F2	F3	
Water-LOGSY[a]	16384(^{1}H)	-	-	9.7	-	-	(*1*)
^{15}N-HSQC[b]	1024(^{1}H)	128(^{15}N)	-	15.0	40.0	-	(*2*)
^{15}N-NOESY-HSQC[c]	1024(^{1}H)	40(^{15}N)	256(^{1}H)	20.0	40.0	20.0	(*3*)

[a] Data acquired on a Bruker Avance 700 spectrometer equipped with a sample changer

[b] Data acquired on a Bruker Avance 900 and 800 spectrometers both equipped with a cryoprobe

[c] Data acquired on a Bruker Avance 800 spectrometer equipped with a cryoprobe

Table S2. Statistical analysis of the energy-minimized family of conformers and the mean structure of *S. cerevisiae* iso-1-cytochrome *c*

	REM[a] (35 structures)	<REM>[a] (mean)
RMS violations per meaningful distance restraint (Å)[b]		
intraresidue (438)	0.0099 ± 0.0016	0.0076
sequential (389)	0.0114 ± 0.0017	0.0093
medium-range (369)[c]	0.0068 ± 0.0017	0.0050
long-range (474)	0.0049 ± 0.0016	0.0056
total (1670)	0.0086 ± 0.0010	0.0070
RMS violations per meaningful dihedral angle restraints (deg)[b]		
ϕ (49)	0.00 ± 0.00	0.86
ψ (49)	0.00 ± 0.00	1.90
average number of restraints per residue	15	15
average number of violations per structure		
intraresidue (438)	7.5143 ± 1.4613	6
sequential (389)	8.2000 ± 1.9094	7
medium-range (369)[c]	4.1429 ± 1.6413	3
long-range (474)	3.1429 ± 1.6758	5
total (1670)	23.000 ± 3.7264	21
ϕ (49)	8.9714 ± 3.0283	12
ψ (49)	3.7714 ± 1.3541	4
average number of NOE violations larger than 0.3 Å	0.00 ± 0.00	0.00

	REM[a] (35 structures)	<REM>[a] (mean)
average number of NOE violations between 0.1 and 0.3 Å	2.3 ± 1.5	1
Average distance penalty function (kcal/mol)	8.145 ± 1.3	5.968
structural analysis[d]		
% of residues in most favorable regions	73.7	72.2
% of residues in allowed regions	23.5	25.6
% of residues in generously allowed regions	2.2	2.2
% of residues in disallowed regions	0.5	0.0

[a] REM indicates the energy-minimized family of 35 structures, and <REM> is the energy-minimized mean structure obtained from the coordinates of the individual REM structures.

[b] The number of meaningful restraints for each class is reported in parentheses.

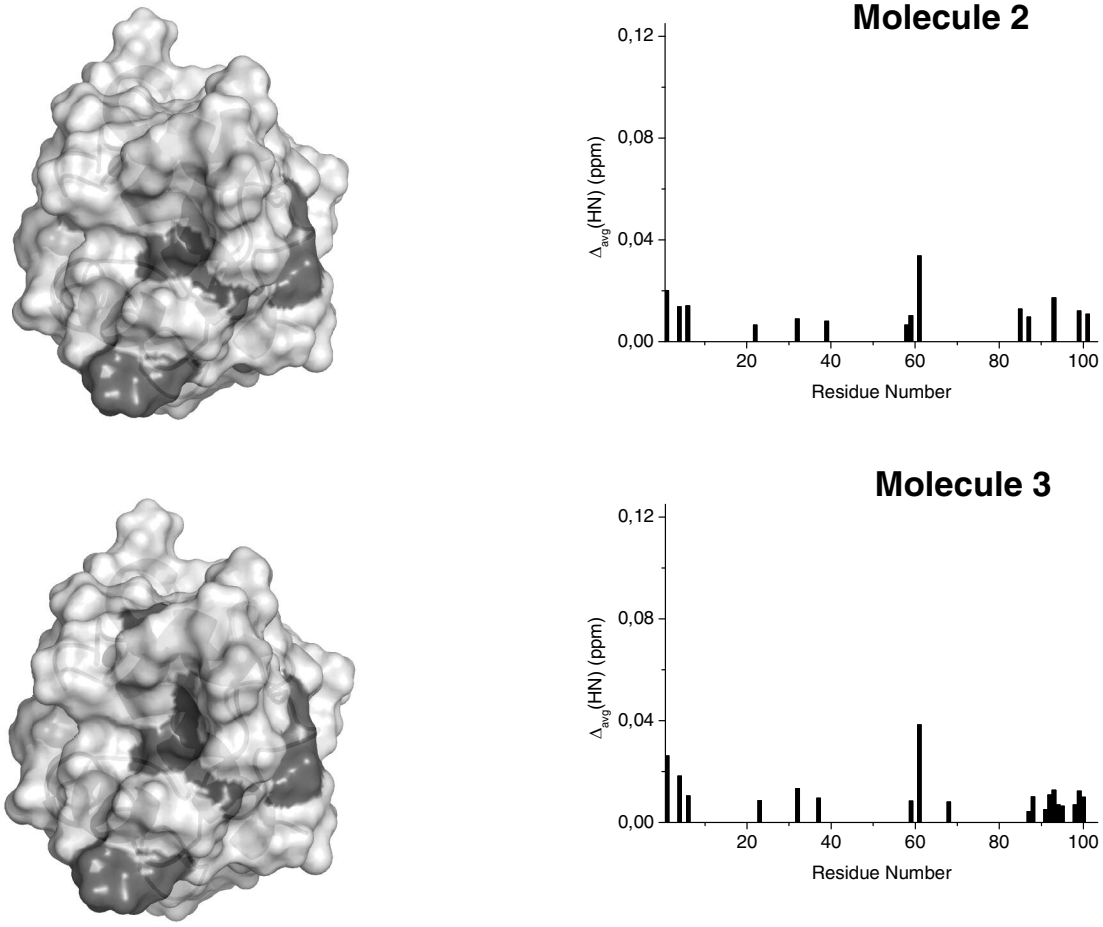
[c] Medium-range distance restraints are those between residues *i* and *i* + 2, *i* and *i* + 3, *i* and *i* + 4, and *i* and *i* + 5.

[d] As it results from the Ramachandran plot analysis.

Table S3. Number of intramolecular NOEs involving the side chains of residues in the p-aminophenol binding site, detected in the ^{15}N-NOESY-HSQC maps of bound and unbound cytochorme c. For unbound cytochrome c the total number of intramolecular NOEs involving the side chains of the same residues detected in all the NOESY maps acquired is provided in paranthesis.

Residue	unbound cyt c # of intramolecular NOEs	bound cyt c # of intramolecular NOEs
Glu61	5 (17)	5
Asn62	6 (6)	6
Asn63	27 (12)	12
Lys99	11 (9)	9

Fig. S1 Residues on cytochrome c surface experiencing CSP upon binding of molecules 2 (up), and 3 (down) are highlighted in grey. The plots of the observed CSP, extrapolated to 100% bound, as a function of the residue number are also reported.



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