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**Chlorite dismutases – a heme enzyme family for use  
in bioremediation and generation of molecular oxygen**

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**Supplemental Table 1.** Overview of available crystal structures determined by X-ray diffraction (July 2013). a) No heme in crystal structure; b) no information about pH of crystallization condition; c) PDB-structure available, unpublished/Pubmed not available.

	<b>pdb-code</b>	<b>organism</b>	<b>heme ligand</b>	<b>subunits</b>	<b>pH</b>	<b>resolution (Å)</b>	<b>reference</b>
<i>chlorite dismutases</i>							
<b>AoCld</b>	2VXH	<i>Azospira oryzae</i> strain GR-1	SCN <sup>-</sup>	6	5.5	2.10	[32]
<b>DaCld</b>	3Q08	<i>Dechloromonas aromatica</i>	NO <sub>2</sub> <sup>-</sup>	5	6.5	3.05	[33]
<b>DaCld</b>	3Q09	<i>Dechloromonas aromatica</i>	NO <sub>2</sub> <sup>-</sup>	5	9.0	3.00	[33]
<b>NdCld</b>	3NN1	“ <i>Candidatus Nitrospira defluvii</i> ”	Imidazole	5	7.5	1.85	[12]
<b>NdCld</b>	3NN2	“ <i>Candidatus Nitrospira defluvii</i> ”	CN <sup>-</sup>	5	7.5	1.94	[12]
<b>NdCld R173A</b>	3NN3	<i>Candidatus “Nitrospira defluvii”</i>	H <sub>2</sub> O	5	4.6	2.60	[12]
<b>NdCld R173K</b>	3NN4	“ <i>Candidatus Nitrospira defluvii</i> ”	H <sub>2</sub> O	5	4.0	2.70	[12]
<b>NwCld</b>	3QPI	<i>Nitrobacter winogradskyi</i>	H <sub>2</sub> O	2	8.2	2.10	[11]
<i>putative chlorite dismutases</i>							
<b>GsCld</b>	1T0T	<i>Geobacillus stearothermophilus</i>	a)	5	b)	1.81	Chang et al. c)
<b>TaCld</b>	3DTZ	<i>Thermoplasma acidophilum</i>	a)	5	b)	1.75	Gilski et al. c)
<b>TtCld</b>	1VDH	<i>Thermus thermophilus</i>	a)	5	4.4	2.00	[34]

**Supplemental Table 2.** Sequence identities of characterized functional chlorite dismutases

(Clds) and chlorite dismutase-like enzymes, determined with the LALIGN server

([http://embnet.vital-it.ch/software/LALIGN\\_form.html](http://embnet.vital-it.ch/software/LALIGN_form.html)). Characterized Clds include AoCld, (chlorite dismutase from *Azospira oryzae*), DaCld (Cld from *Dechloromonas aromatica*), IdCld (Cld from *Ideonella dechloratans*), NdCld (Cld from “*Candidatus Nitrospira defluvii*”), NwCld (Cld from *Nitrobacter winogradskyi*) and PcCld (Cld from *Pseudomonas chloritidismutans*). Cld-like proteins include SaCld (Cld-like protein from *Staphylococcus aureus*) and TtCld (Cld-like protein from *Thermus thermophilus*).

%	AoCld	DaCld	IdCld	NdCld	NwCld	PcCld	SaCld	TtCld
AoCld	<b>100.0</b>	<b>94.3</b>	60.5	42.0	36.7	<b>95.4</b>	23.8	21.0
DaCld	<b>94.3</b>	<b>100.0</b>	63.5	42.0	36.7	<b>92.2</b>	23.8	21.0
IdCld	60.5	63.5	<b>100.0</b>	38.1	33.9	60.5	24.2	19.4
NdCld	42.0	42.0	38.1	<b>100.0</b>	31.5	42.3	23.8	22.1
NwCld	36.7	36.7	33.9	31.5	<b>100.0</b>	36.7	23.7	23.8
PcCld	<b>95.4</b>	<b>92.2</b>	60.5	42.3	36.7	<b>100.0</b>	24.8	22.6
SaCld	23.8	23.8	24.2	23.8	23.7	24.8	<b>100.0</b>	44.2
TtCld	21.0	21.0	19.4	22.1	23.8	22.6	44.2	<b>100.0</b>