**Supporting information for:**

**Insights into the Catalytic Mechanism of the Chlorothalonil Dehalogenase from *Pseudomonas* sp. CTN-3**

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**Table S1.** EasySpin parameters for BN-A.

|  |  |
| --- | --- |
| Sys.g | 2.615 2.615 2.610 |
| Sys.S | 1.5 |
| Sys.Nucs | 59Co |
| Sys.A (MHz) | -10 -287 -180 |
| Sys.D (MHz) | 1000000 166000 |
| Sys.lw (mT) | 1 |
| Sys.gStrain | 0.75 0.22 0.45 |
| Sys.AStrain (MHz) | 30 60 20 |
| Sys.gAStrainCorr | -1 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.468 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| pepper | (Sys,Exp) |

**Table S2.** EasySpin parameters for BN-B.

|  |  |
| --- | --- |
| Sys.g | 2.690 2.690 2.300 |
| Sys.S | 1.5 |
| Sys.Nucs | 59Co |
| Sys.A (MHz) | -10 -375 -100 |
| Sys.D (MHz) | 1000000 333000 |
| Sys.lw (mT) | 1 |
| Sys.gStrain | 0.75 0.10 0.65 |
| Sys.AStrain (MHz) | 10 10 10 |
| Sys.gAStrainCorr | -1 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.468 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| pepper | (Sys,Exp) |

**Table S3.** EasySpin parameters for TCPN.

|  |  |
| --- | --- |
| Sys.g | 2.625 2.625 2.590 |
| Sys.S | 1.5 |
| Sys.Nucs | 59Co |
| Sys.A (MHz) | -10 -287 -180 |
| Sys.D (MHz) | 1000000 164000 |
| Sys.lw (mT) | 1 |
| Sys.gStrain | 0.75 0.22 0.45 |
| Sys.AStrain (MHz) | 30 60 20 |
| Sys.gAStrainCorr | -1 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.468 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| pepper | (Sys,Exp) |

**Table S4.** EasySpin parameters for TCTPN-A.

|  |  |
| --- | --- |
| Sys.g | 2.625 2.625 2.590 |
| Sys.S | 1.5 |
| Sys.Nucs | 59Co |
| Sys.A (MHz) | -10 -287 -180 |
| Sys.D (MHz) | 1000000 164000 |
| Sys.lw (mT) | 1 |
| Sys.gStrain | 0.75 0.22 0.45 |
| Sys.AStrain (MHz) | 30 60 20 |
| Sys.gAStrainCorr | -1 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.468 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| pepper | (Sys,Exp) |

**Table S5.** EasySpin parameters for TCTPN-B.

|  |  |
| --- | --- |
| Sys.g | 2.625 2.625 2.590 |
| Sys.S | 3 |
| Sys.Nucs | 59Co, 59Co |
| Sys.A (MHz) | 10 250 180; 10 250 180 |
| Sys.D (MHz) | 2000000 32700 |
| Sys.lw (mT) | 1 |
| Sys.DStrain (MHz) | 120000 10000 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.648 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| Opt.Method | hybrid |
| Opt.nKnots | 10 4 |
| pepper | (Sys,Exp,Opt) |

**Table S6.** EasySpin parameters for ACN.

|  |  |
| --- | --- |
| Sys.g | 2.49 2.49 2.63 |
| Sys.S | 1.5 |
| Sys.Nucs | 59Co |
| Sys.A (MHz) | -10 -250 -180 |
| Sys.D (MHz) | 1000000 141000 |
| Sys.lw (mT) | 1 |
| Sys.gStrain | 0.46 0.15 0.35 |
| Sys.AStrain (MHz) | 30 10 10 |
| Sys.gAStrainCorr | -1 |
| Exp.Temperature (K) | 10 |
| Exp.mwFreq (GHz) | 9.468 |
| Exp.Range (mT) | 5 505 |
| Exp.nPoints | 4166 |
| pepper | (Sys,Exp) |