

Supplementary information for:

Structural, antioxidant, and protein/DNA-binding properties of sulfate-coordinated Ni(II) complex with Pyridoxal-semicarbazone (PLSC) ligand

Table S1. Experimental and theoretical (functionals for Ni given below in conjunction with B3LYP/6-311++G(d,p)(H,C,N,O,S) level of theory) bond lengths of [Ni(PLSC)(SO₄)(H₂O)₂] (in Å)

Bond	Experimental	LanL2DZ	Def2-TZVP
Ni(1)-N(2)	2.0230(18)	2.164	2.143
Ni(1)-O(1)	2.0247(15)	2.079	2.076
Ni(1)-O(9)	2.0411(16)	1.990	2.232
Ni(1)-O(4)	2.0555(15)	2.010	2.006
Ni(1)-O(8)	2.0751(16)	2.220	1.987
Ni(1)-O(3)	2.0877(15)	2.172	2.174
S(1)-O(6)	1.4712(16)	1.462	1.463
S(1)-O(5)	1.4742(16)	1.487	1.487
S(1)-O(4)	1.4779(15)	1.553	1.554
S(1)-O(7)	1.4816(15)	1.606	1.605
O(1)-C(1)	1.295(3)	1.270	1.270
O(2)-C(9)	1.414(2)	1.420	1.420
O(3)-C(7)	1.249(3)	1.228	1.228
N(1)-C(2)	1.328(3)	1.339	1.339
N(1)-C(3)	1.354(3)	1.366	1.366
N(2)-C(6)	1.284(3)	1.293	1.293
N(2)-N(3)	1.368(2)	1.362	1.363
N(3)-C(7)	1.377(3)	1.402	1.401
N(4)-C(7)	1.332(3)	1.364	1.365
C(1)-C(5)	1.430(3)	1.442	1.442
C(1)-C(2)	1.432(3)	1.444	1.444
C(2)-C(8)	1.491(3)	1.487	1.487
C(3)-C(4)	1.375(3)	1.378	1.378
C(4)-C(5)	1.415(3)	1.424	1.423
C(4)-C(9)	1.520(3)	1.526	1.526
C(5)-C(6)	1.458(3)	1.455	1.455
R		0.988	0.984
MAE (Å)		0.036	0.039

Table S2. Experimental and theoretical (functionals for Ni given below in conjunction with B3LYP/6-311++G(d,p)(H,C,N,O,S) level of theory) bond lengths (in °) of [Ni(PLSC)(SO₄)(H₂O)₂]

Bond angle	Experimental	LanL2DZ	Def2-TZVP
N(2)-Ni(1)-O(1)	88.36(7)	81.18	81.61
N(2)-Ni(1)-O(9)	97.38(7)	100.16	99.59
O(1)-Ni(1)-O(9)	90.50(6)	80.79	80.61
N(2)-Ni(1)-O(4)	172.70(7)	177.31	176.33
O(1)-Ni(1)-O(4)	98.81(6)	98.02	97.58

O(9)-Ni(1)-O(4)	83.98(6)	77.17	76.74
N(2)-Ni(1)-O(8)	88.24(7)	84.97	86.22
O(1)-Ni(1)-O(8)	94.03(6)	105.41	104.88
O(9)-Ni(1)-O(8)	172.88(7)	172.60	172.63
O(4)-Ni(1)-O(8)	89.89(6)	97.73	97.45
N(2)-Ni(1)-O(3)	79.30(7)	75.99	76.33
O(1)-Ni(1)-O(3)	167.51(6)	150.83	151.74
O(9)-Ni(1)-O(3)	89.15(6)	85.56	85.83
O(4)-Ni(1)-O(3)	93.57(6)	103.93	103.30
O(8)-Ni(1)-O(3)	87.61(6)	90.55	91.19
O(6)-S(1)-O(5)	108.85(9)	116.73	116.69
O(6)-S(1)-O(4)	108.37(9)	109.71	110.87
O(5)-S(1)-O(4)	109.58(9)	107.57	109.81
O(6)-S(1)-O(7)	110.23(9)	107.57	107.57
O(5)-S(1)-O(7)	109.91(9)	107.68	107.78
O(4)-S(1)-O(7)	109.87(9)	103.16	103.17
C(1)-O(1)-Ni(1)	128.17(13)	122.33	122.22
C(7)-O(3)-Ni(1)	111.82(13)	113.09	112.77
S(1)-O(4)-Ni(1)	134.84(9)	119.45	120.12
C(2)-N(1)-C(3)	124.93(18)	125.11	125.13
C(6)-N(2)-N(3)	117.82(17)	118.70	118.63
C(6)-N(2)-Ni(1)	130.30(15)	126.39	126.53
N(3)-N(2)-Ni(1)	111.64(13)	111.79	112.06
N(2)-N(3)-C(7)	116.46(17)	116.19	116.22
O(1)-C(1)-C(5)	126.15(19)	125.22	125.18
O(1)-C(1)-C(2)	117.43(19)	117.14	117.15
C(5)-C(1)-C(2)	116.42(19)	117.62	117.66
N(1)-C(2)-C(1)	119.72(19)	118.48	118.46
N(1)-C(2)-C(8)	118.4(2)	121.16	121.13
C(1)-C(2)-C(8)	121.9(2)	120.33	120.39
N(1)-C(3)-C(4)	119.01(19)	119.38	119.39
C(3)-C(4)-C(5)	119.58(19)	119.70	119.69
C(3)-C(4)-C(9)	118.16(19)	117.84	117.84
C(5)-C(4)-C(9)	122.25(18)	122.42	122.43
C(4)-C(5)-C(1)	120.34(18)	119.45	119.45
C(4)-C(5)-C(6)	116.94(18)	119.55	119.64
C(1)-C(5)-C(6)	122.64(19)	120.95	120.86
N(2)-C(6)-C(5)	123.91(19)	123.54	123.54
O(3)-C(7)-N(4)	124.07(19)	123.26	123.31
O(3)-C(7)-N(3)	120.39(18)	122.41	122.32
N(4)-C(7)-N(3)	115.50(18)	114.34	114.36
O(2)-C(9)-C(4)	111.71(17)	113.28	113.29

R	0.97	0.97
MAE (°)	3.45	3.33

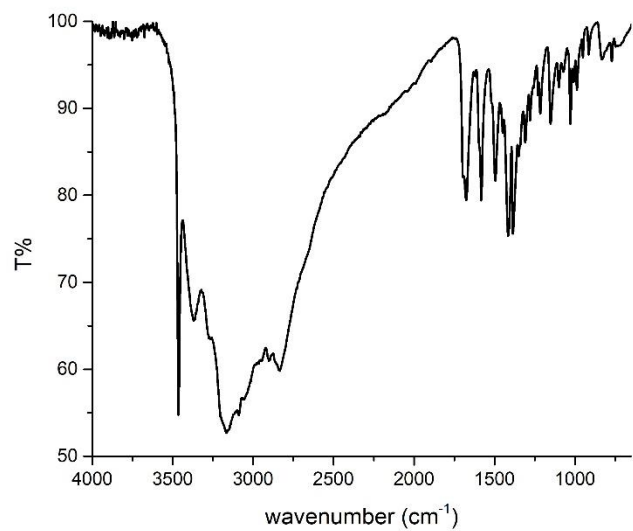


Figure S1. FTIR spectrum of PLSC ligand.

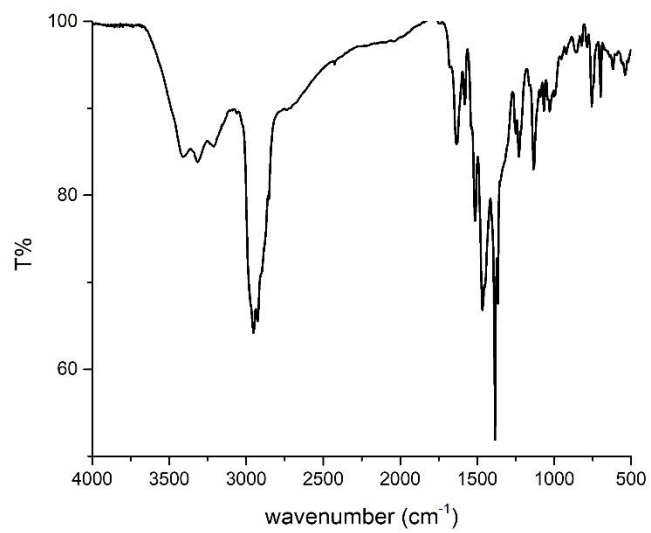


Figure S2. FTIR spectrum of [Ni(PLSC)(SO₄)(H₂O)₂].

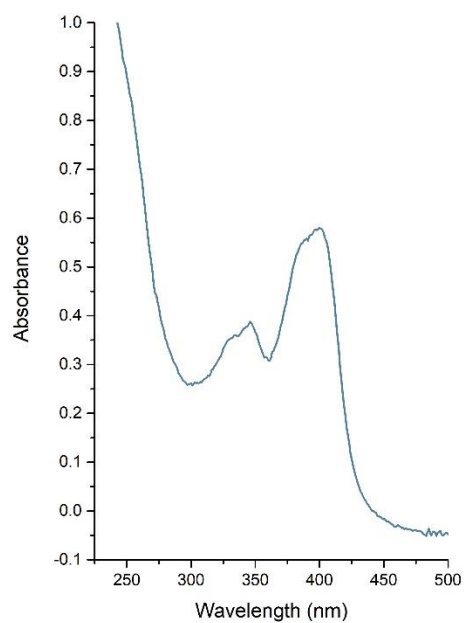


Figure S3. UV-VIS spectrum of [Ni(PLSC)(SO₄)(H₂O)₂]

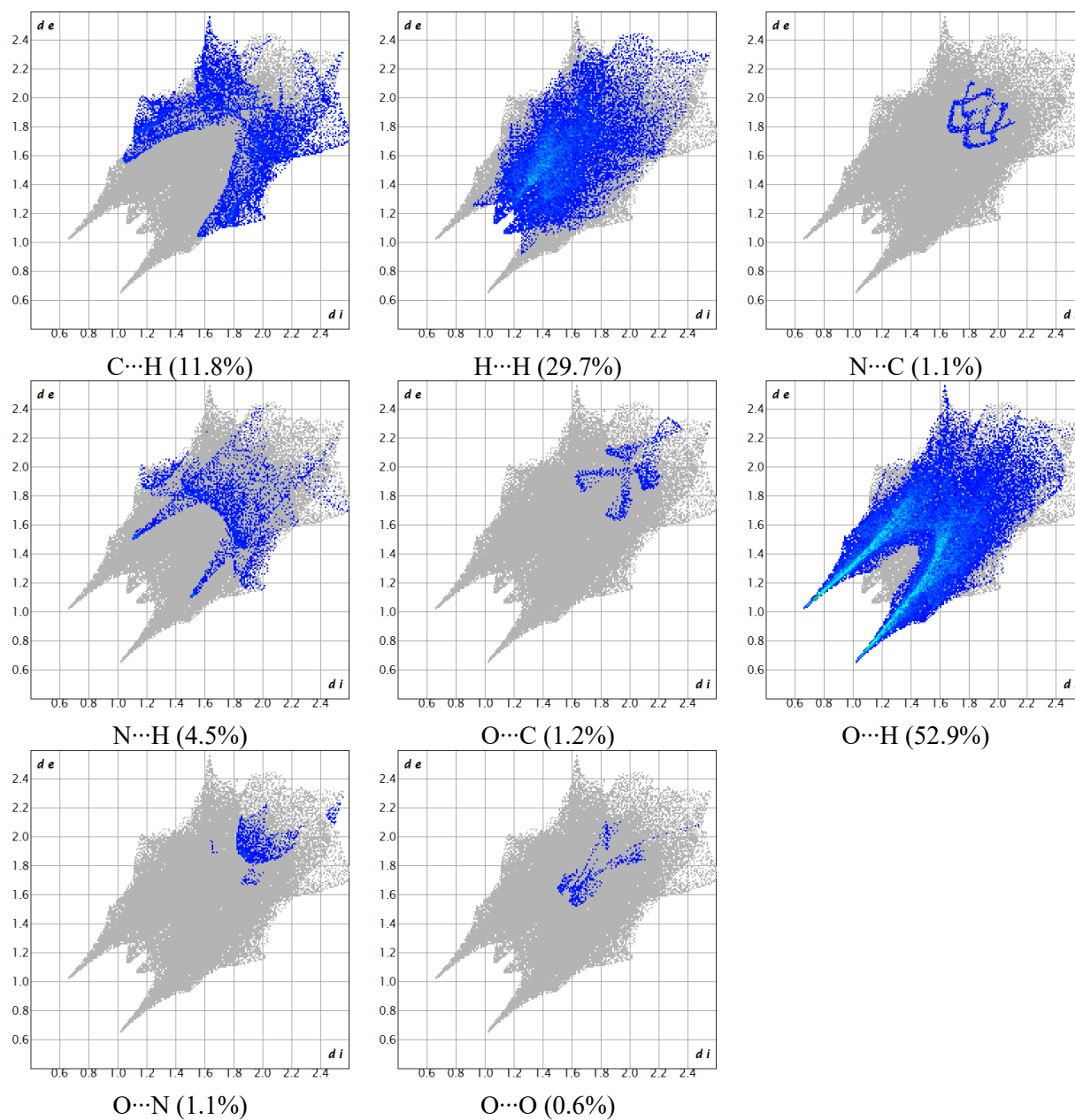


Figure S4. Fingerprint plots of the most numerous contacts within crystallographic structure of $[\text{Ni}(\text{PLSC})(\text{SO}_4)(\text{H}_2\text{O})_2]$

Table S3. The calculated Bond Critical Points (BCP) properties at the DFT/B3LYP-D3BJ/6-311+G(d,p)/LanL2DZ level of theory: the electron density ($\rho(r)$) and its Laplacian ($\nabla^2\rho(r)$); the Lagrangian kinetic electron density ($G(r)$) and the potential electron density ($V(r)$); the density of the total energy of electrons ($H(r)$) – Cremer-Kraka electronic energy density; the interatomic bond energy, E_{bond} ,

Bond	$\rho(r)$ [a.u.]	$\nabla^2\rho(r)$ [a.u.]	$G(r)$ [kJ mol ⁻¹]	$V(r)$ [kJ mol ⁻¹]	$H(r)$ [kJ mol ⁻¹]	$-G(r)/V(r)$	E_{bond} [kJ mol ⁻¹]
Ni–N2	0.051	0.331	200.9	-184.5	16.4	1.1	-92.2
Ni–O1	0.054	0.392	232.7	-208.2	24.5	1.1	-104.1
Ni–O3	0.045	0.295	171.1	-148.2	22.9	1.2	-74.1
Ni–O4	0.068	0.475	298.2	-284.5	13.7	1.0	-142.3
Ni–O8	0.075	0.499	320.0	-312.5	7.5	1.0	-156.3
Ni–O9	0.041	0.257	150.9	-133.1	17.8	1.1	-66.6
O5...H–CH ₂	0.017	0.053	33.9	-33.0	1.0	1.0	-16.5
O4...H–O9	0.022	0.094	57.1	-52.3	4.8	1.1	-26.2
O7...H–O8	0.280	-1.381	202.8	-1312.4	-1109.6	0.2	-656.2

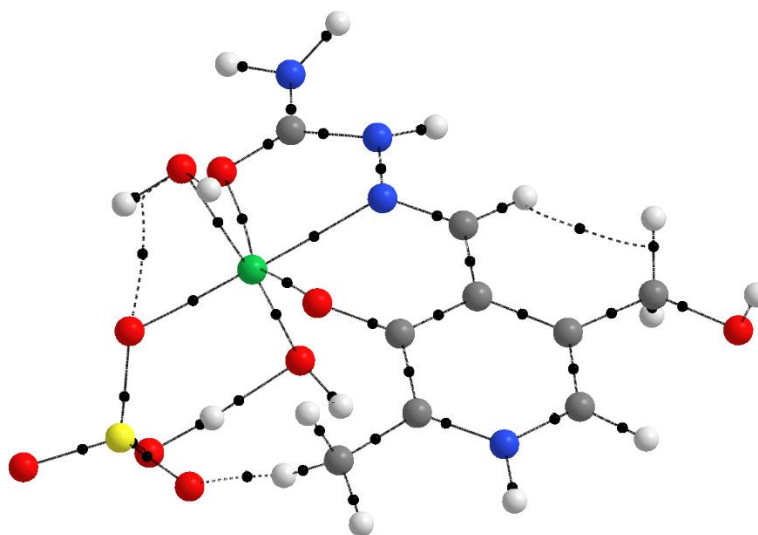
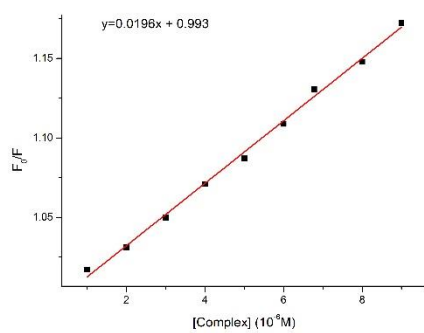
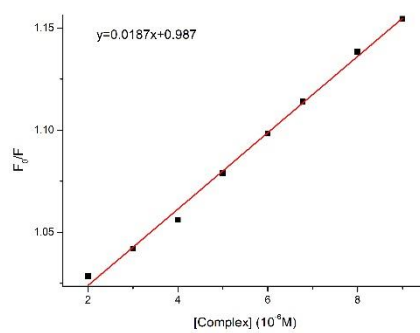


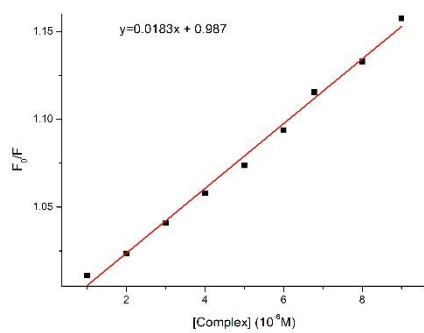
Figure S5. Bond Critical Points within structure of [Ni(PLSC)(SO₄)(H₂O)₂].



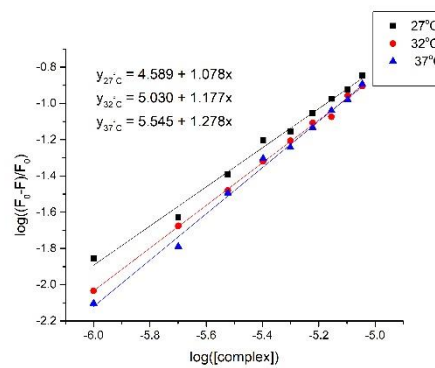
(a)



(b)



(c)



(d)

Figure S6. Stern-Volmer and double-log Stern-Volmer plots for the binding of $[Ni(PLSC)(SO_4)(H_2O)_2]$ to HSA.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MX25_24

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: MX25 24

Bond precision:	C-C = 0.0030 A	Wavelength=1.54184	
Cell:	a=8.9665 (1)	b=9.2874 (1)	c=17.6603 (3)
	alpha=90	beta=101.327 (2)	gamma=90
Temperature:	123 K		

	Calculated	Reported
Volume	1442.02 (3)	1442.02 (3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C9 H16 N4 Ni O9 S	C9 H16 N4 Ni O9 S
Sum formula	C9 H16 N4 Ni O9 S	C9 H16 N4 Ni O9 S
Mr	415.01	415.03
Dx, g cm ⁻³	1.912	1.912
Z	4	4
Mu (mm ⁻¹)	3.877	3.877
F000	856.0	856.0
F000'	848.07	
h, k, l _{max}	11, 11, 22	11, 11, 22
Nref	3158	3087
Tmin, Tmax	0.714, 0.922	0.636, 1.000
Tmin'	0.593	

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Correction method= # Reported T Limits: Tmin=0.636 Tmax=1.000
AbsCorr = GAUSSIAN
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Data completeness= 0.978 Theta (max)= 80.075

R(reflections)= 0.0350(2783)	wR2(reflections)= 0.1009(3087)
S = 1.063	Npar= 254

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.



Alert level C

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From O7 . 0.41 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 15 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 9 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Nil --N2 . 5.0 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Nil (II) . 2.10 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 9 Note
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 70 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
6 4 11,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.32 Note
Predicted wR2: Based on SigI**2 4.36 or SHELX Weight 9.91
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

