**Supplementary Material**

**Zn(II) complex for highly sensitive and selective detection of acetone at room temperature**

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***Crystal structure determination***

Single crystals of Zn complex were coated with a trace of Fomblin oil and quickly transferred to the goniometer head of a Bruker Quest diffractometer with a fixed chi angle, a sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator, a Photon100 CMOS area detector and an Oxford Cryosystems low-temperature device. Examination and data collection were performed with Mo Kα radiation (λ = 0.71073 Å) at 150 K.

Data were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX3 [1] [1]. The space groups were assigned, and the structures were solved by direct methods using XPREP within the SHELXTL suite of programs [2,3] and refined by full-matrix least squares against F2 with all reflections using Shelxl2018 [4,5] using the graphical interface Shelxle [6]. H atoms attached to carbon and nitrogen atoms as well as hydroxyl hydrogens were positioned geometrically and constrained to ride on their parent atoms. C-H bond distances were constrained to 0.95 Å for aromatic and alkene C-H moieties. N-H bond distances were constrained to 0.88 Å for planar (sp2 hybridized) N-H groups. Figures were drawn using ORTEP-3.3 [7] and MERCURY-4.1.0 [8].

**Computational methodology**

The full geometry optimizations have been carried out at DFT level of theory using the B3LYP functional [9–11] with the help of the Gaussian-09 program package [12]. The calculations were performed using 6-31G\* basis sets [13,14] for C, H, N, O, Cl atoms and def2-TZVP basis set for Zn atom. All the DFT calculations were performed with counter ions by employing the polarizable continuum model, CPCM (DMSO as solvent) [15–17]. No symmetry restrictions have been applied during geometry optimization. The Hessian matrix was calculated analytically for the optimized structures in order to prove the location of correct minima (no imaginary frequencies). The Cartesian atomic coordinates of the calculated optimized structures in DMSO are given in the ESI-material.

Table Ligands

Table S1. Crystallographic data of [Zn(bipy)2(H2O)](ClO4)2

Table S2. . Selected bond lengths [Å] and bond angles [°] of [Zn(bipy)2(H2O)](ClO4)2

**Table S1.**

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

CCDC No. CCDC 766185

Color White

Molecular formula C20H18N4OZn•2(ClO4)

Molecular weight 594.65

Crystal system P21/c

Space group Monoclinic

a (Å) 8.988 (3)

b (Å) 12.812 (4)

c (Å) 19.921 (5)

U (Å3) 2214.8 (12)

β = (°) 105.095 (12)

DX (Mg m−3) 1.783

Z 4

F (000) 1208

Crystal size/mm 0.30 × 0.25 × 0.20

μ(mm-1) 1.41

θ (°) 2.4–27.5

Index ranges -10 < h < 10; -15 < k < 14;

-15 < l < 23

No. of reflections collected 1115

No. of independent reflections (Rint) 3907 (0.055)

No. of observed [I > 2σ(I)] reflections 3218

No. of data/restraints/ parameters 3907/0/325

R[F2 > 2σ(F2)] 0.050

wR(F2) 0.129

Δρmax and Δρmin (e Å−3) 0.77 and -0.81

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**Table S2.**

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Zn—O1 2.028 (3) Zn—N2 2.061 (3)

Zn—N4 2.070 (3) Zn—N1 2.091 (3)

Zn—N3 2.104 (3)

O1—Zn—N2 118.99 (11) O1—Zn—N4 121.81 (12)

N2—Zn—N4 119.18 (12) O1—Zn—N1 89.67 (11)

N2—Zn—N1 79.03 (13) N4—Zn—N1 102.44 (13)

O1—Zn—N3 90.58 (10) N2—Zn—N3 99.86 (12)

N4—Zn—N3 78.39 (12) N1—Zn—N3 178.83 (13)

Zn—O1—H1A 121.2 Zn—O1—H1B 107.0

C12—N1—Zn 115.0 (3) C3—N2—C8 119.0 (3)

C3—N2—Zn 126.1 (2) C8—N2—Zn 114.9 (2)

C7—N3—C19 118.4 (3) C7—N3—Zn 114.7 (2)

C19—N3—Zn 126.3 (3) C9—N4—C6 118.8 (3)

C9—N4—Zn 125.7 (3) C6—N4—Zn 115.4 (2)

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**Fig. Legends.**

Scheme S1. Synthetic Scheme of Complex **1**

Fig S1.Thermal ellipsoidal presentation of the molecular structure of [Zn(bipy)2(H2O)](ClO4)2 with 30% probability factor.

Fig. S2. The 1H NMR spectrum of Complex **1**.

Fig. S3. The 13C NMR spectrum of Complex **1**.

Fig. S4. Thermogravimetric analysis of [Zn(bipy)2(H2O)](ClO4)2

Fig. S5. IR spectrum of [Zn(bipy)2(H2O)](ClO4)2

Fig. S6. UV-Vis Spectrum of Complex **1**.

Fig. S7. Change in the fluorescence intensity of [Zn(bipy)2(H2O)](ClO4)2 (dissolved in DMSO) upon titration with acetone.

**Fig. S8.** B3LYP/DFT optimized structures of the aggregate of Zn(II)-complex with the various used molecules for sensing. The d···d’ distance in angstrom represents the nearest distance between the carbon atoms of bipyridyl moiety of Zn(II)-complex and different solvents.

C:\Users\Mohammad Muddassir\Desktop\Bipyridyl\scheme.tif

Scheme S1

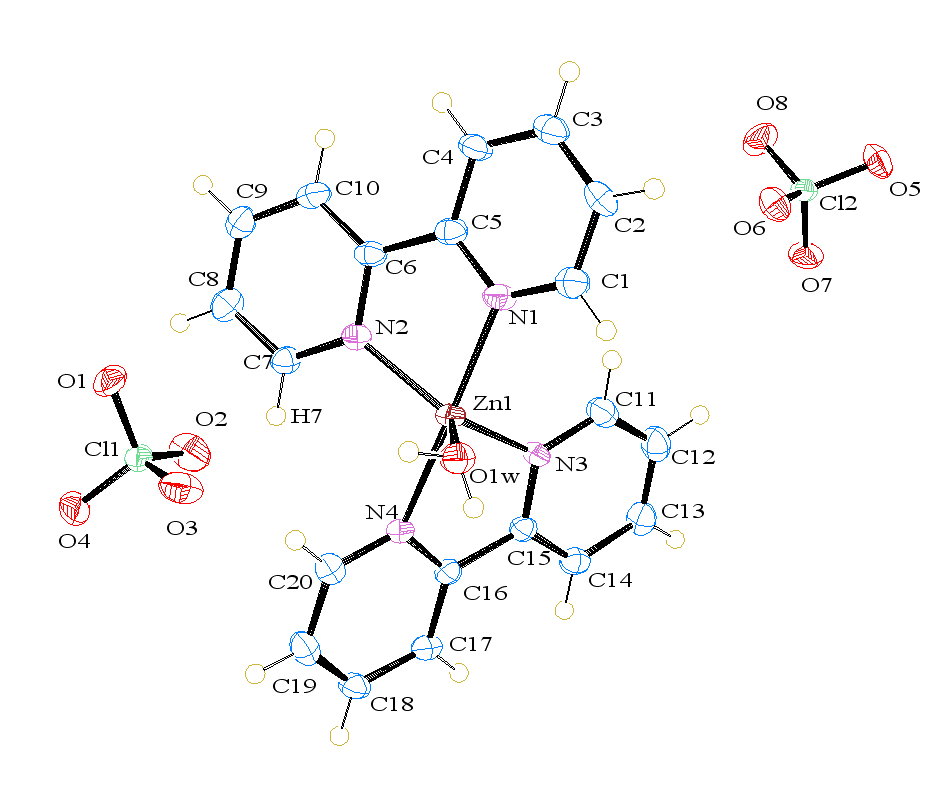


Fig. S1.

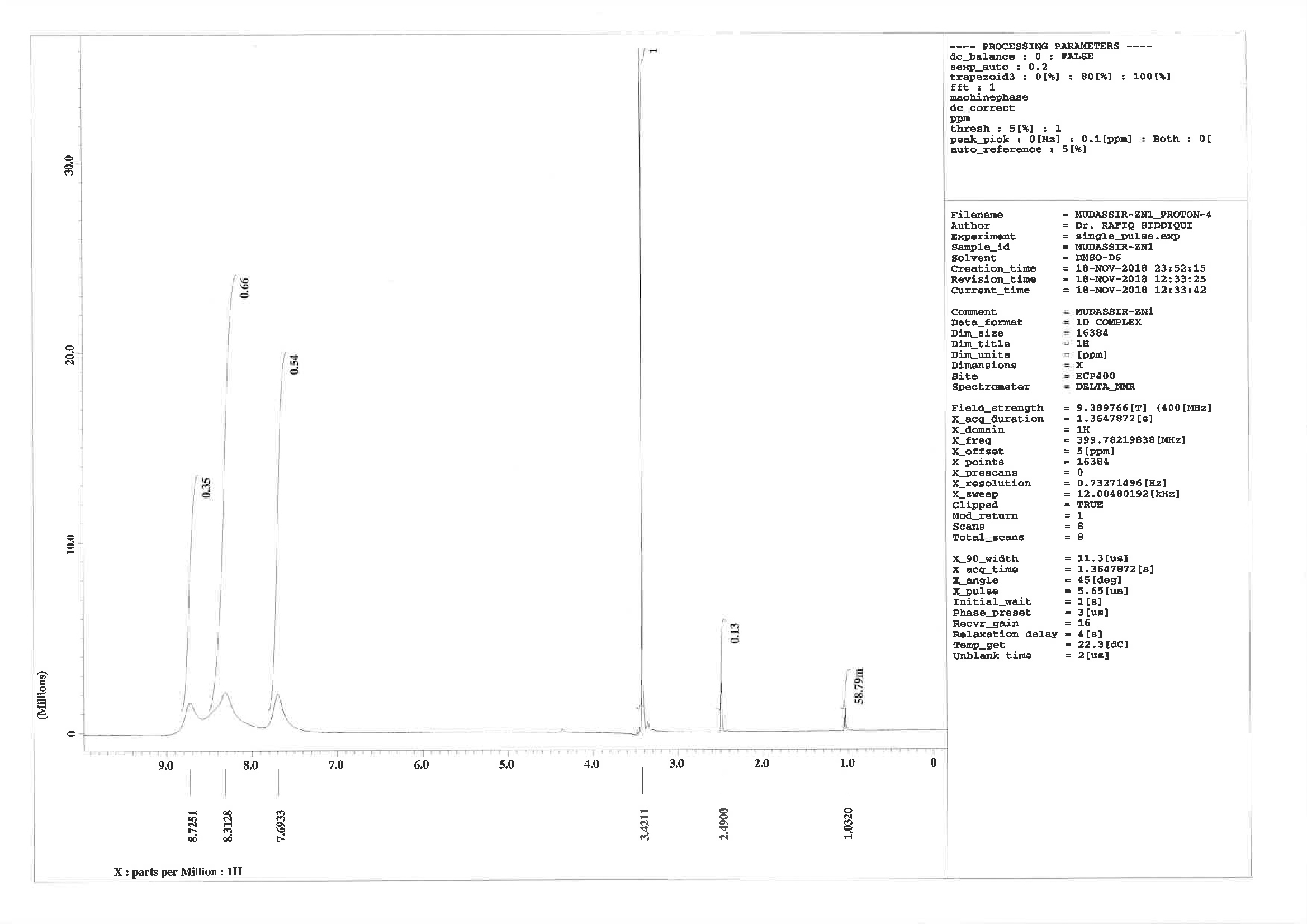


Fig. S2.

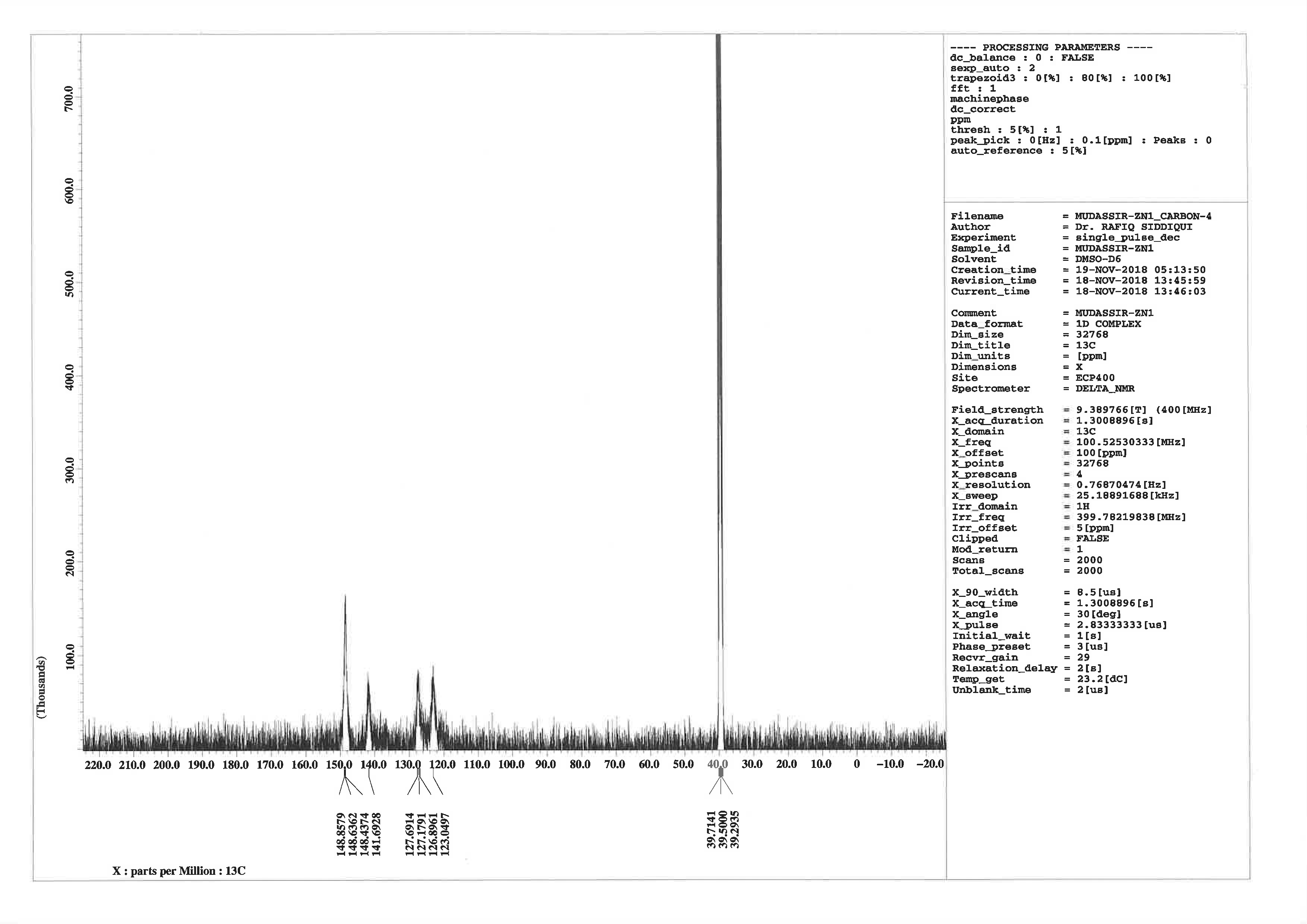


Fig. S3.

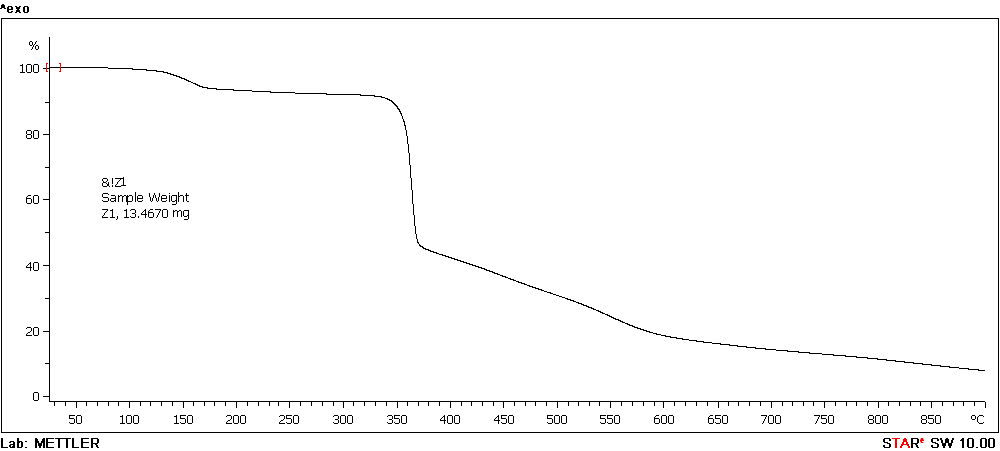


Fig. S4.

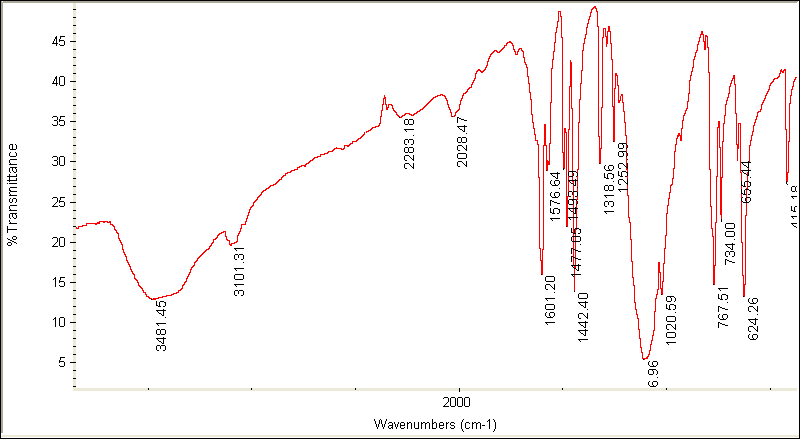


Fig. S5.



Fig. S6.



Fig. S7.

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**Fig. S8.**

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