Arsenic sensor development based on modified with (*E*)-*N*′-(2-Nitrobenzylidine)-benzenesulfonohydrazide: A real sample analysis†

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Electronic supplementary materials (ESM)

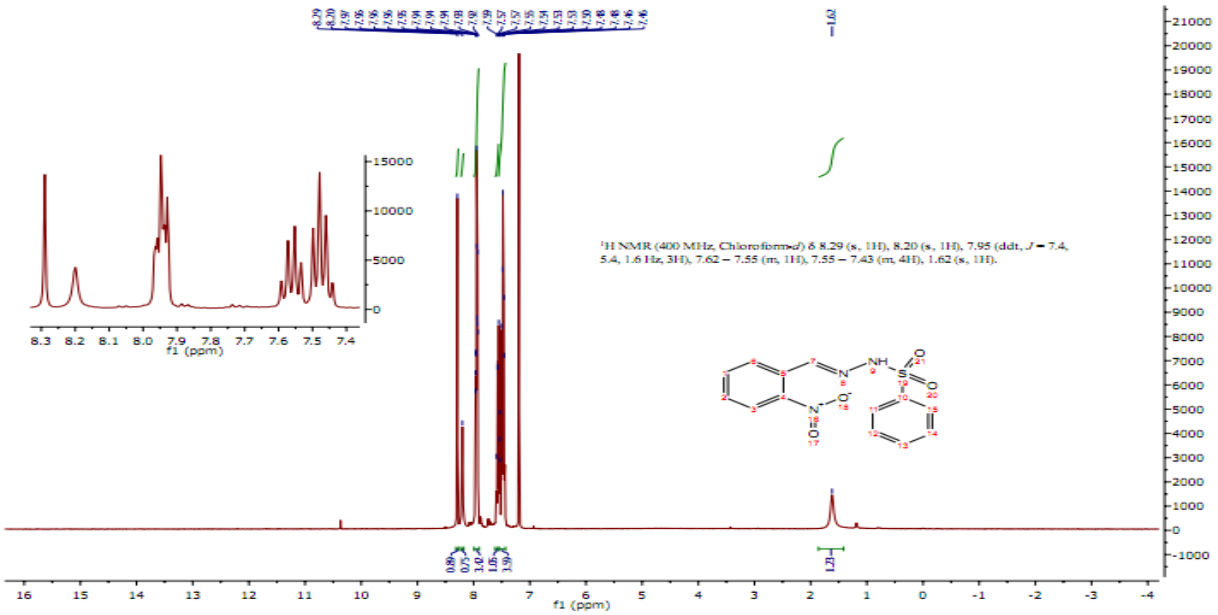

Fig. S1. [1]H-NMR of the compound NBBSH

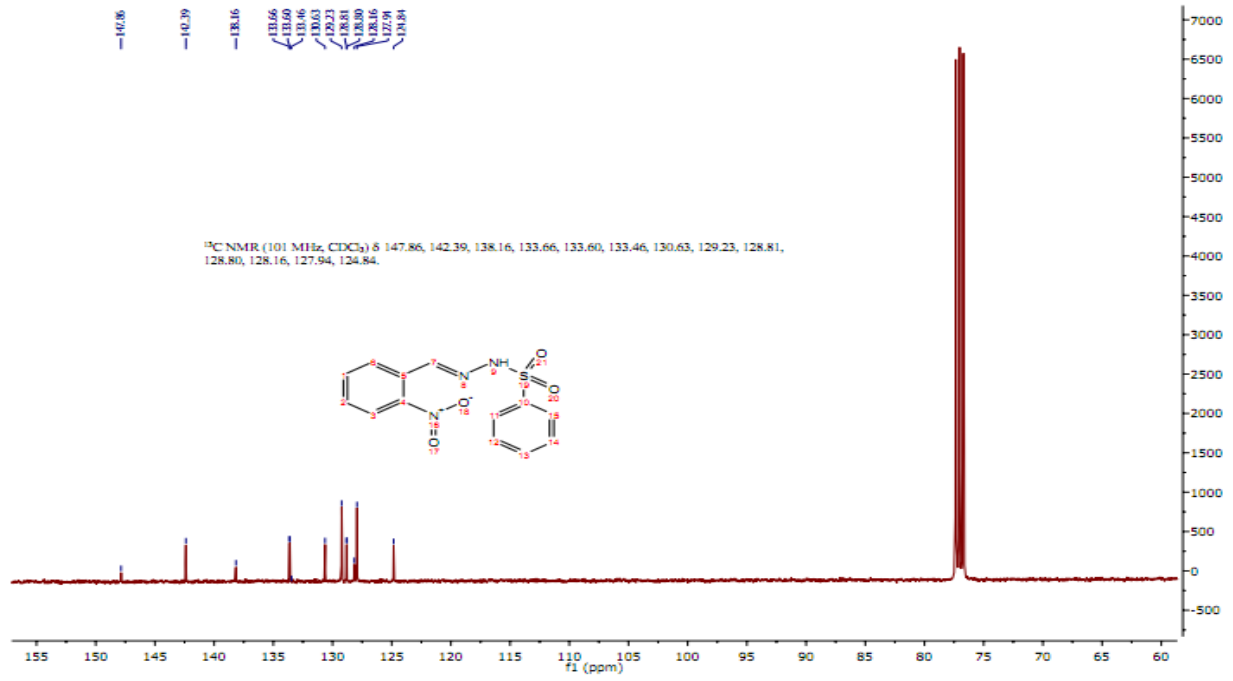

Fig. S2. ^{13}C-NMR of NBBSH molecule

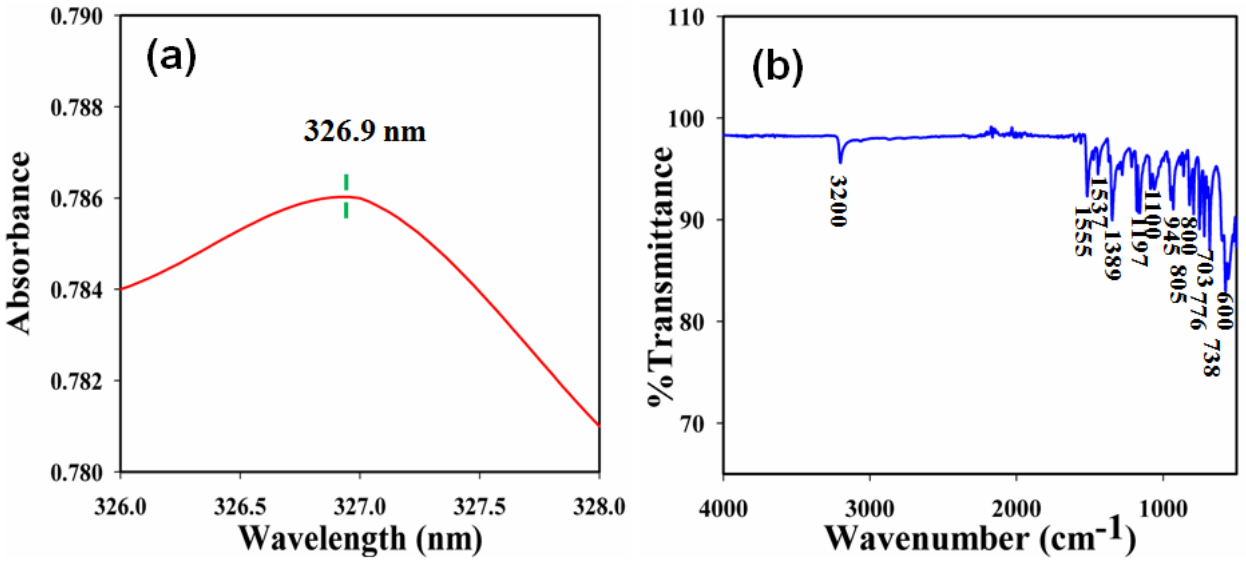

Fig. S3. (a) UV spectrum and (b) FTIR of compound NBBSH

Table S1: Crystal data and structure refinement for NBBSH

Parameters	**NBBSH**
Empirical formula	$C_{13}H_{11}N_3O_4S$
Formula weight	305.31
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.5720(3)
b/Å	23.2361(9)
c/Å	10.6070(4)
α/°	90
β/°	98.807(4)
γ/°	90
Volume/Å^3	1357.11(10)
Z	4
ρ_{calc}g/cm^3	1.494
μ/mm^{-1}	0.259
F(000)	632.0
Crystal size/mm^3	0.49 × 0.24 × 0.07
Radiation	MoKα (λ = 0.7107)
2Θ range for data collection/°	6.54 to 58.604
Index ranges	$-5 \leq h \leq 7$, $-29 \leq k \leq 31$, $-13 \leq l \leq 14$
Reflections collected	6309

Independent reflections	3211 [R_{int} = 0.0217, R_{sigma} = 0.0389]
Data/restraints/parameters	3211/0/193
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0441, wR_2 = 0.0973
Final R indexes [all data]	R_1 = 0.0665, wR_2 = 0.1106
Largest diff. peak/hole / e $Å^{-3}$	0.28/-0.37

Table S2: Bond Lengths for NBBSH

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.399(3)	C8	S1	1.7573(19)
C1	C6	1.393(3)	C9	C10	1.384(3)
C1	C7	1.468(3)	C10	C11	1.350(4)
C2	C3	1.391(3)	C11	C12	1.361(4)
C2	N1	1.465(3)	C12	C13	1.378(3)
C3	C4	1.375(3)	N1	O1	1.221(2)
C4	C5	1.379(3)	N1	O2	1.220(2)
C5	C6	1.376(3)	N2	N3	1.382(2)
C7	N2	1.274(2)	N3	S1	1.6336(17)
C8	C9	1.375(3)	O3	S1	1.4234(15)
C8	C13	1.371(3)	O4	S1	1.4304(14)

Table S3: Bond Angles for NBBSH

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C7	124.84(17)	C11	C10	C9	120.6(2)
C6	C1	C2	115.81(17)	C10	C11	C12	120.2(2)
C6	C1	C7	119.27(17)	C11	C12	C13	120.5(3)
C1	C2	N1	121.92(17)	C8	C13	C12	119.3(2)
C3	C2	C1	122.16(18)	O1	N1	C2	117.69(19)
C3	C2	N1	115.92(18)	O2	N1	C2	119.72(18)
C4	C3	C2	119.7(2)	O2	N1	O1	122.58(19)
C3	C4	C5	119.6(2)	C7	N2	N3	114.83(16)
C6	C5	C4	120.1(2)	N2	N3	S1	117.60(13)
C5	C6	C1	122.6(2)	N3	S1	C8	107.53(9)
N2	C7	C1	118.81(17)	O3	S1	C8	108.57(9)
C9	C8	S1	120.34(17)	O3	S1	N3	108.32(9)
C13	C8	C9	120.29(19)	O3	S1	O4	120.37(9)
C13	C8	S1	119.36(16)	O4	S1	C8	108.04(9)
C8	C9	C10	119.1(2)	O4	S1	N3	103.32(9)

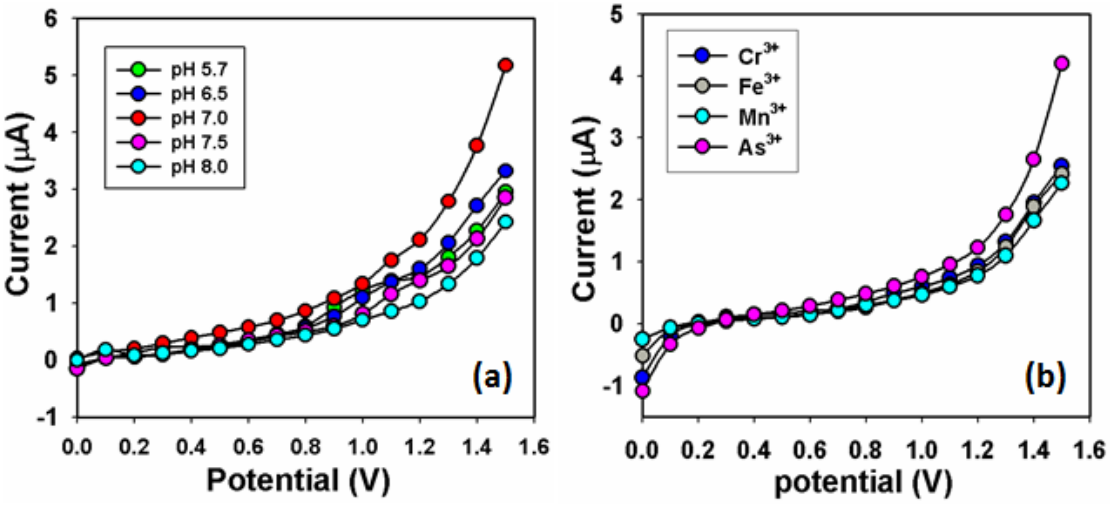

Fig. S4. (a) Optimization of pH and (b) Interference study