Lawsone – DAMN Based Colorimetric Chemosensor for Rapid Naked –
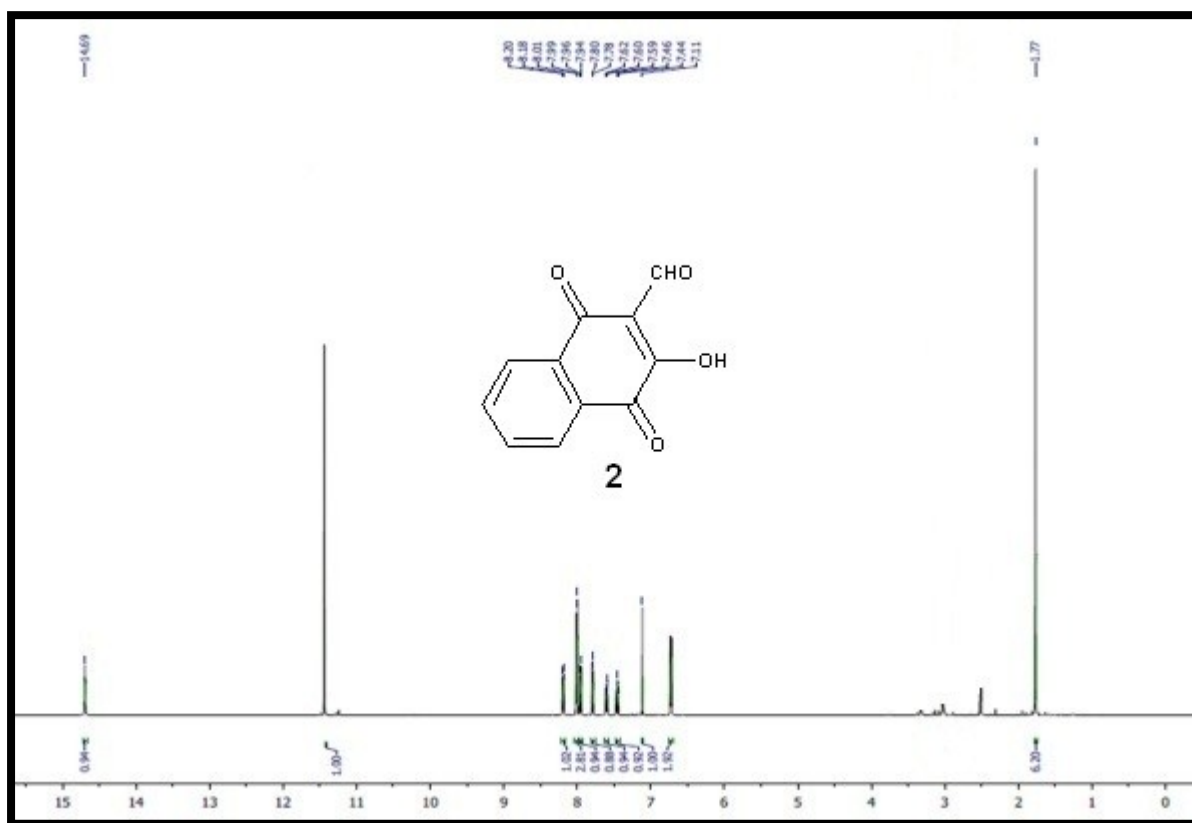
Eye Detection of Mercury (II)

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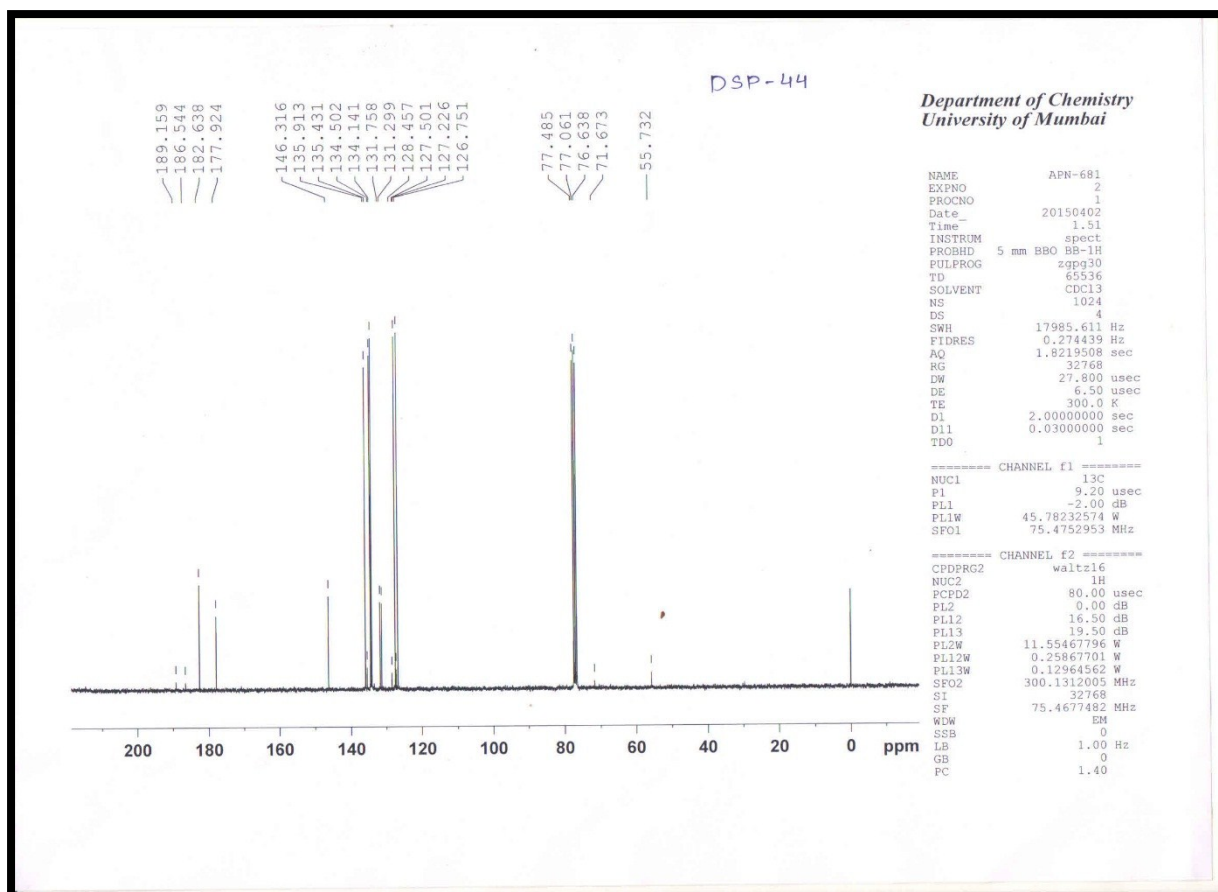
Marg, Matunga, Mumbai - 400 019 (India).

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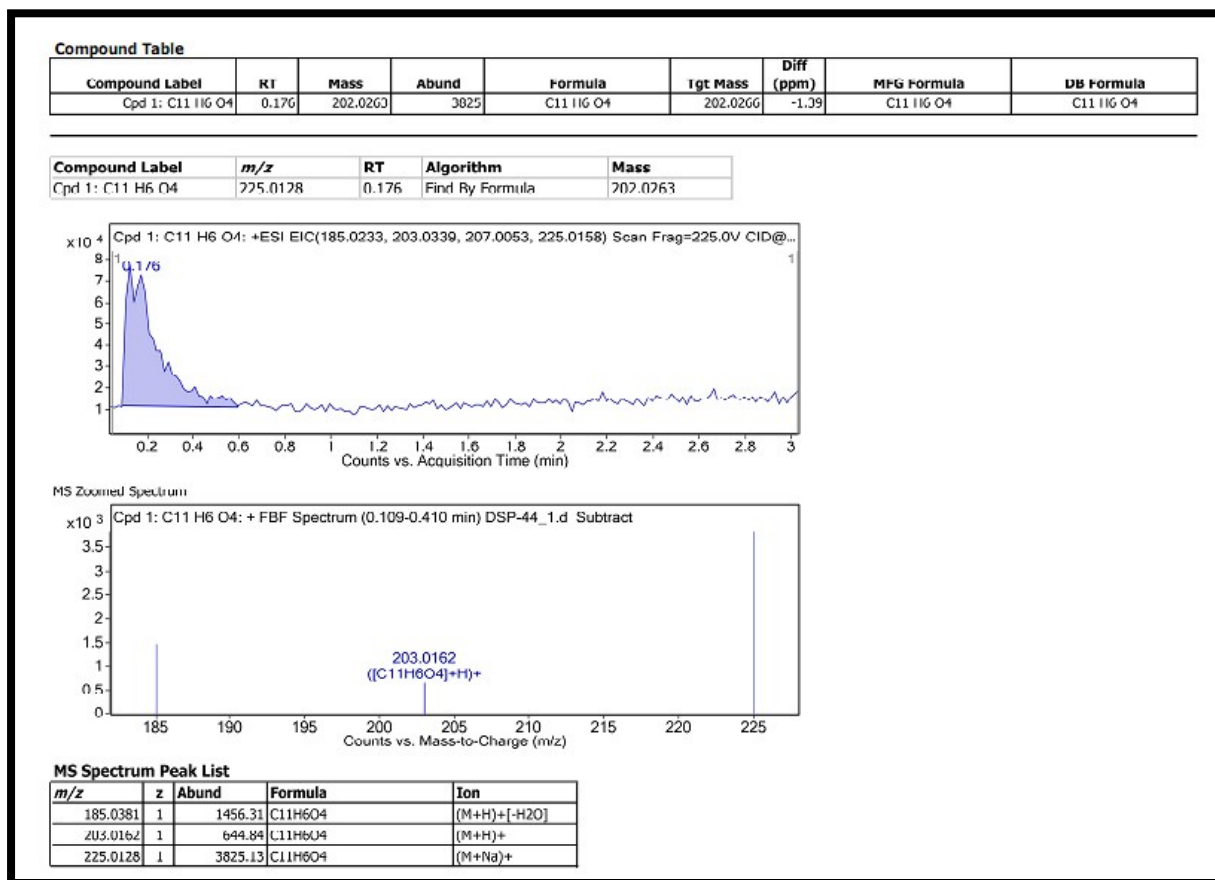

Supporting Information
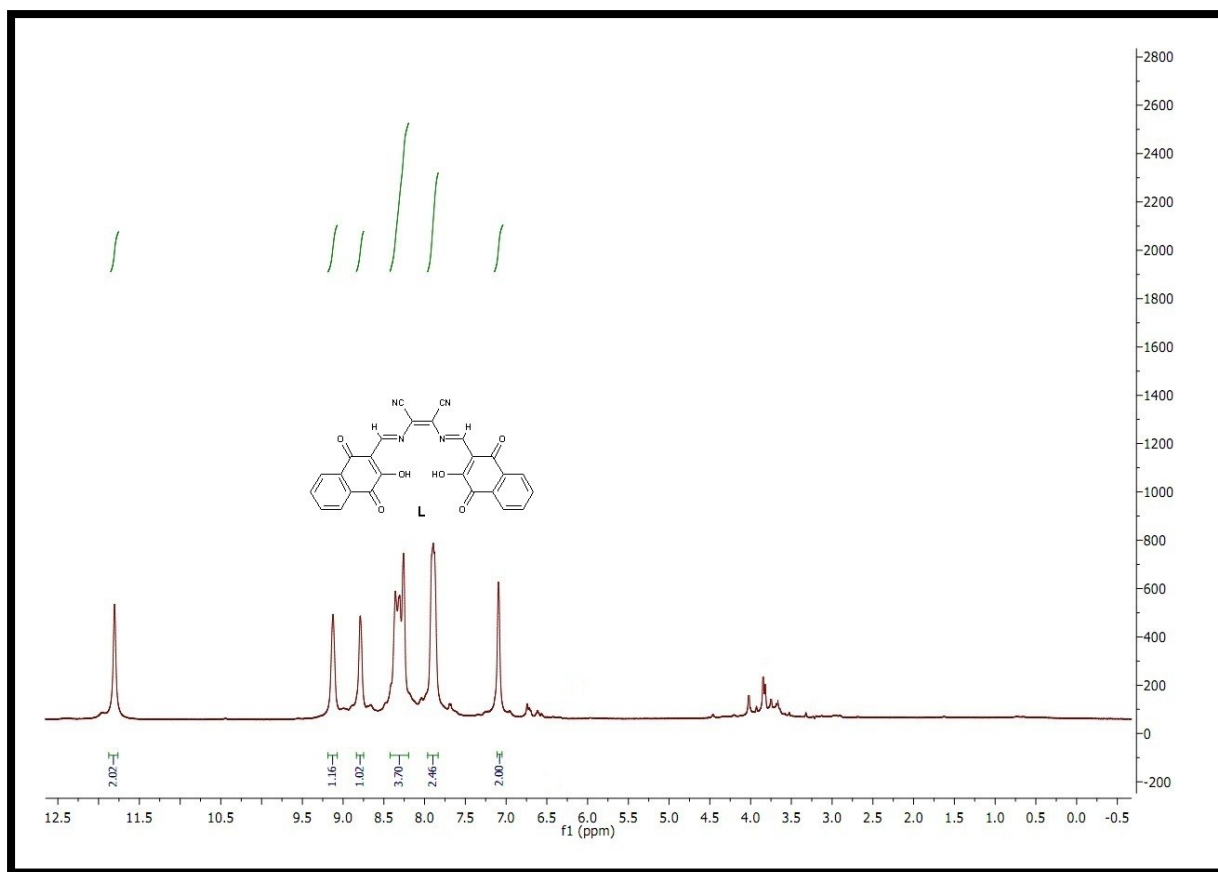
Figure S1. ^{1}H NMR spectra of *3-hydroxy-1, 4-dioxo-1, 4-dihydronaphthalene-2-carbaldehyde* **2** recorded in CDCl$_3$.

Figure S2. ^{13}C NMR spectra of *3-hydroxy-1, 4-dioxo-1, 4-dihydronaphthalene-2-carbaldehyde*
2 recorded in CDCl$_3$.

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C11 H6 O4	0.176	202.0263	3825	C11 H6 O4	202.0266	-1.39	C11 H6 O4	C11 H6 O4

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C11 H6 O4	225.0128	0.176	Find By Formula	202.0263

x10 4 Cpd 1: C11 H6 O4: +ESI EIC(185.0233, 203.0339, 207.0053, 225.0158) Scan Frag=225.0V CID@...

Counts vs. Acquisition Time (min)

MS Zoomed Spectrum

x10 3 Cpd 1: C11 H6 O4: + FBF Spectrum (0.109-0.410 min) DSP-44_1.d Subtract

203.0162
([C11H6O4]+H)+

Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
185.0381	1	1456.31	C11H6O4	(M+H)+[-H2O]
203.0162	1	644.84	C11H6O4	(M+H)+
225.0128	1	3825.13	C11H6O4	(M+Na)+

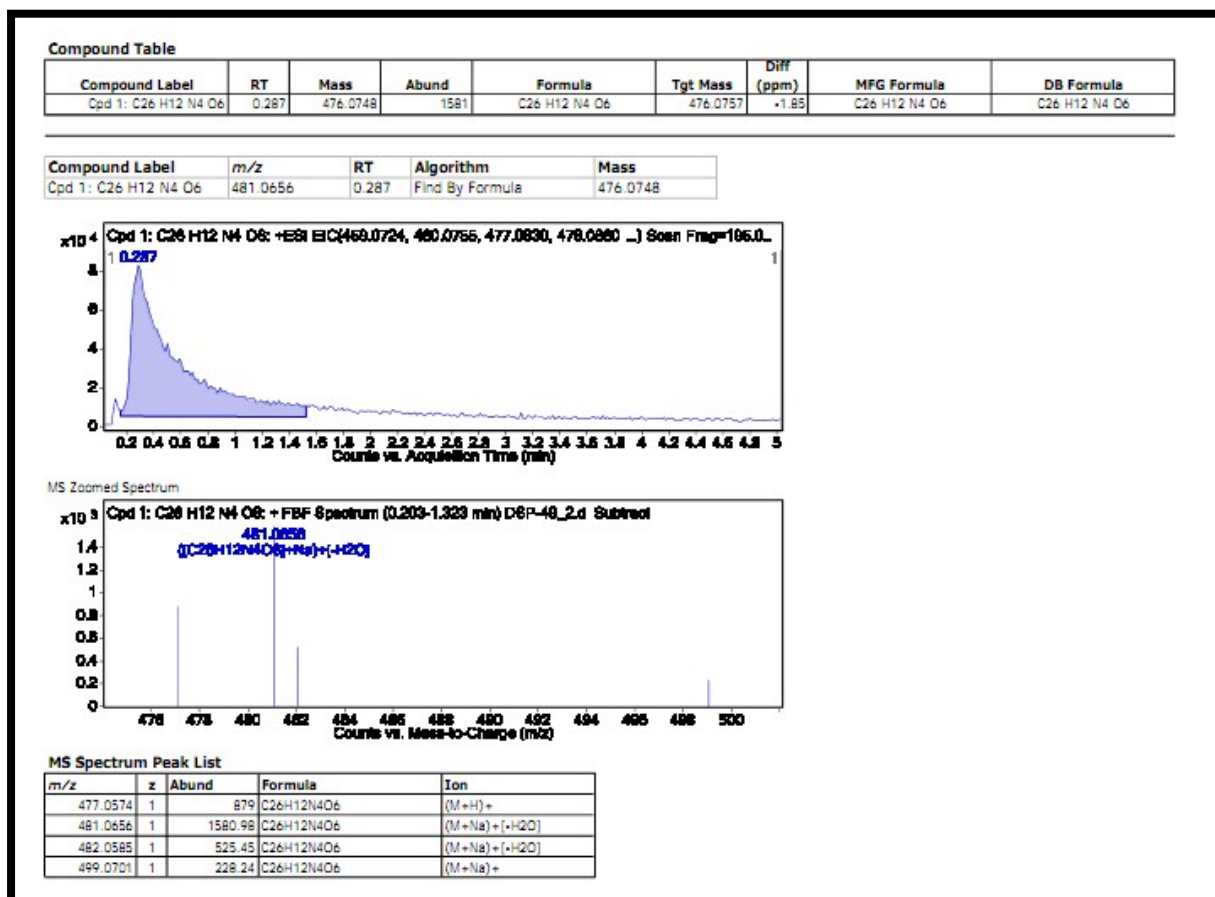**Figure S3**. *Mass spectra of 3-hydroxy-1, 4-dioxo-1, 4-dihydronaphthalene-2-carbaldehyde* **2**

Figure S4. ^{1}H NMR spectra of *2-((E)-((3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)methylene)amino)-3-((E)-((1-hydroxy-3,4-dioxo-3,4-dihydronaphthalen-2-yl)methylene)amino)malenonitrile* **L** recorded in CDCl$_3$.

S5
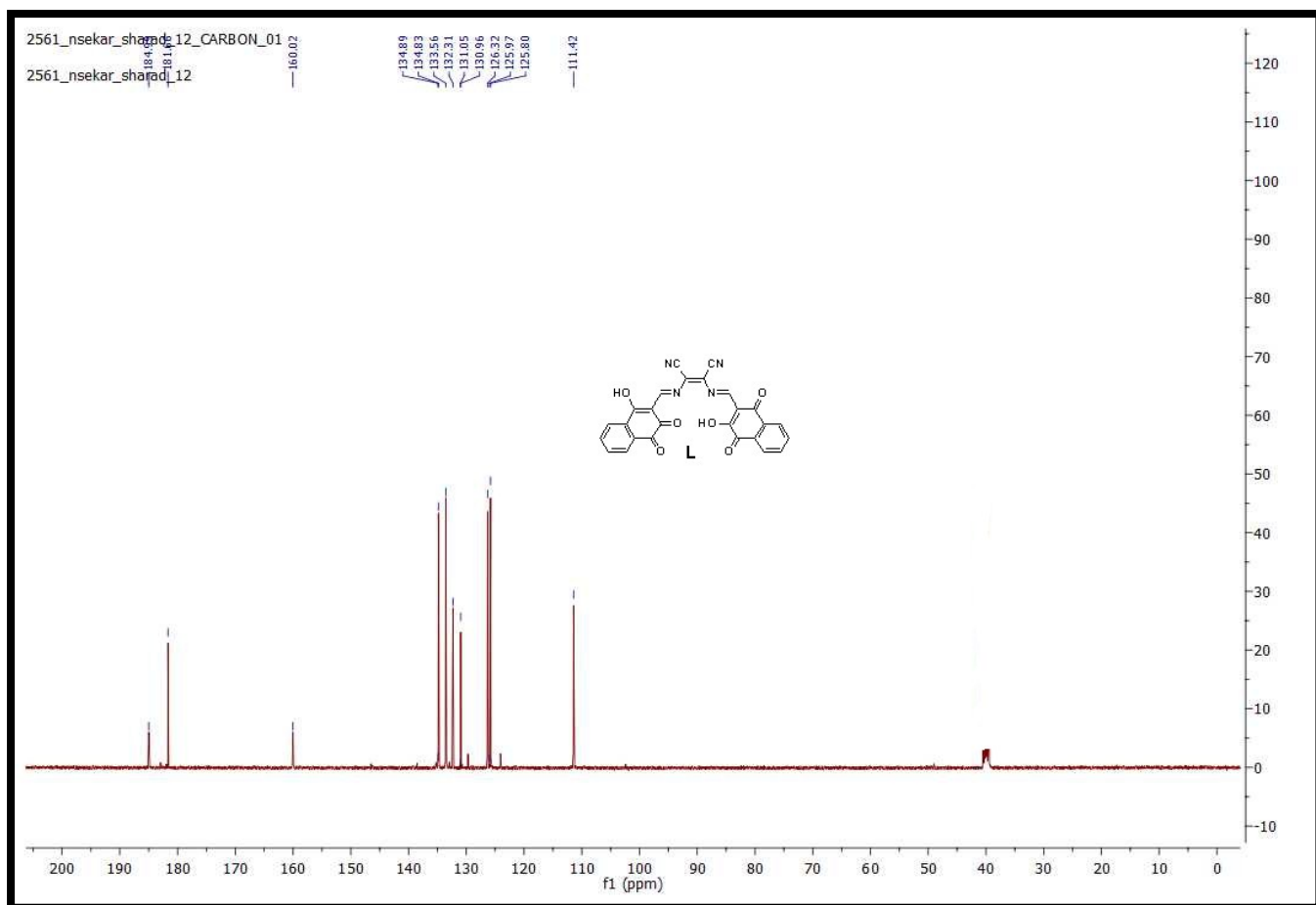
Figure S5. ^{13}C NMR spectra of 2-((E)-((3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2 yl)methylene)amino)-3-((E)-((1-hydroxy-3,4-dioxo-3,4-dihydronaphthalen-2 yl)methylene)amino)malenonitrile **L** recorded in CDCl$_3$.

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C26 H12 N4 O6	0.287	476.0748	1581	C26 H12 N4 O6	476.0757	-1.85	C26 H12 N4 O6	C26 H12 N4 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C26 H12 N4 O6	481.0656	0.287	Find By Formula	476.0748

MS Zoomed Spectrum

MS Spectrum Peak List

| m/z	z	Abund	Formula	Ion
477.0574	1	879	C26H12N4O6	(M+H)+
481.0656	1	1580.98	C26H12N4O6	(M+Na)+[-H2O]
482.0585	1	525.45	C26H12N4O6	(M+Na)+[-H2O]
499.0701	1	228.24	C26H12N4O6	(M+Na)+

Figure S6. Mass spectra of 2-((E)-((3-hydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)methylene)amino)-3-((E)-((1-hydroxy-3,4-dioxo-3,4-dihydronaphthalen-2-yl)methylene)amino)malenonitrile **L.**
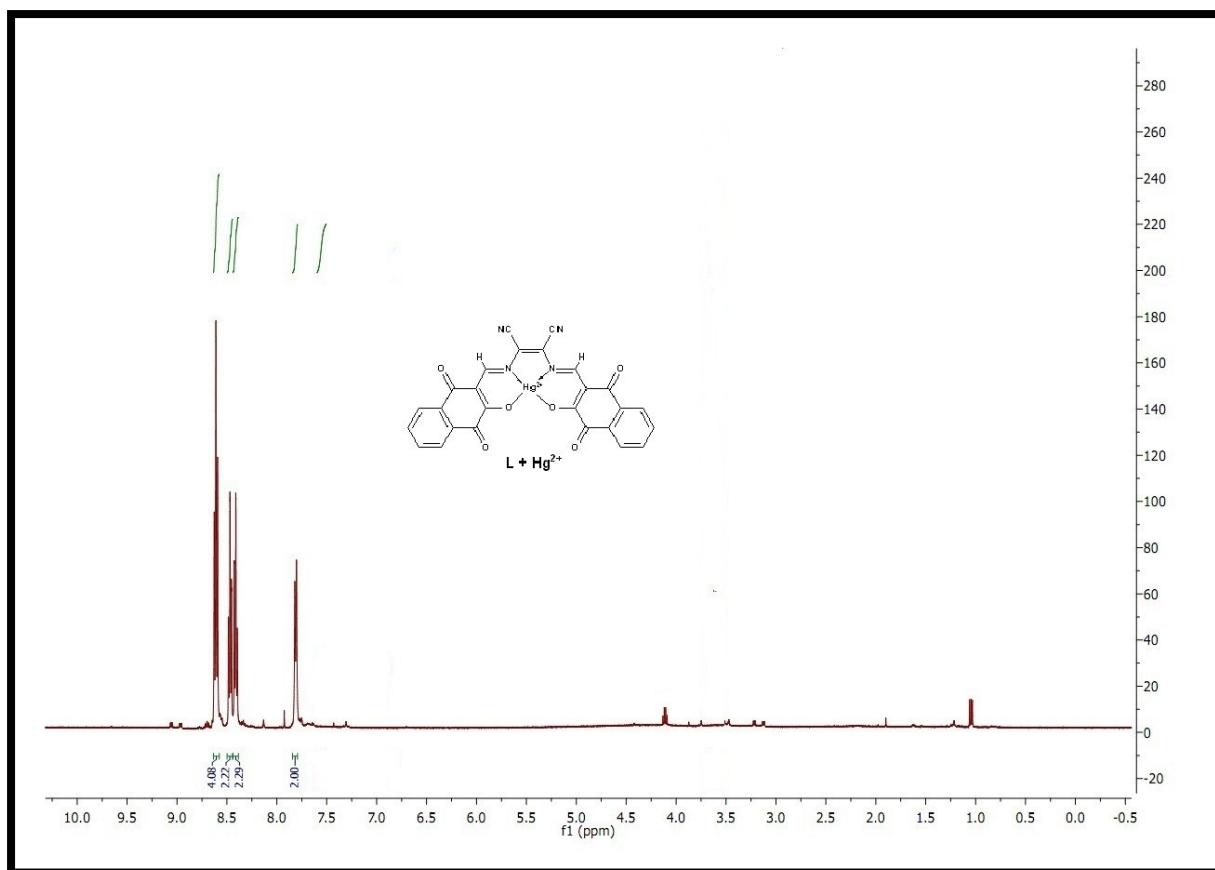
Figure S7. ^{1}H NMR spectra of **L+Hg^{2+}** complex recorded in CDCl$_3$.
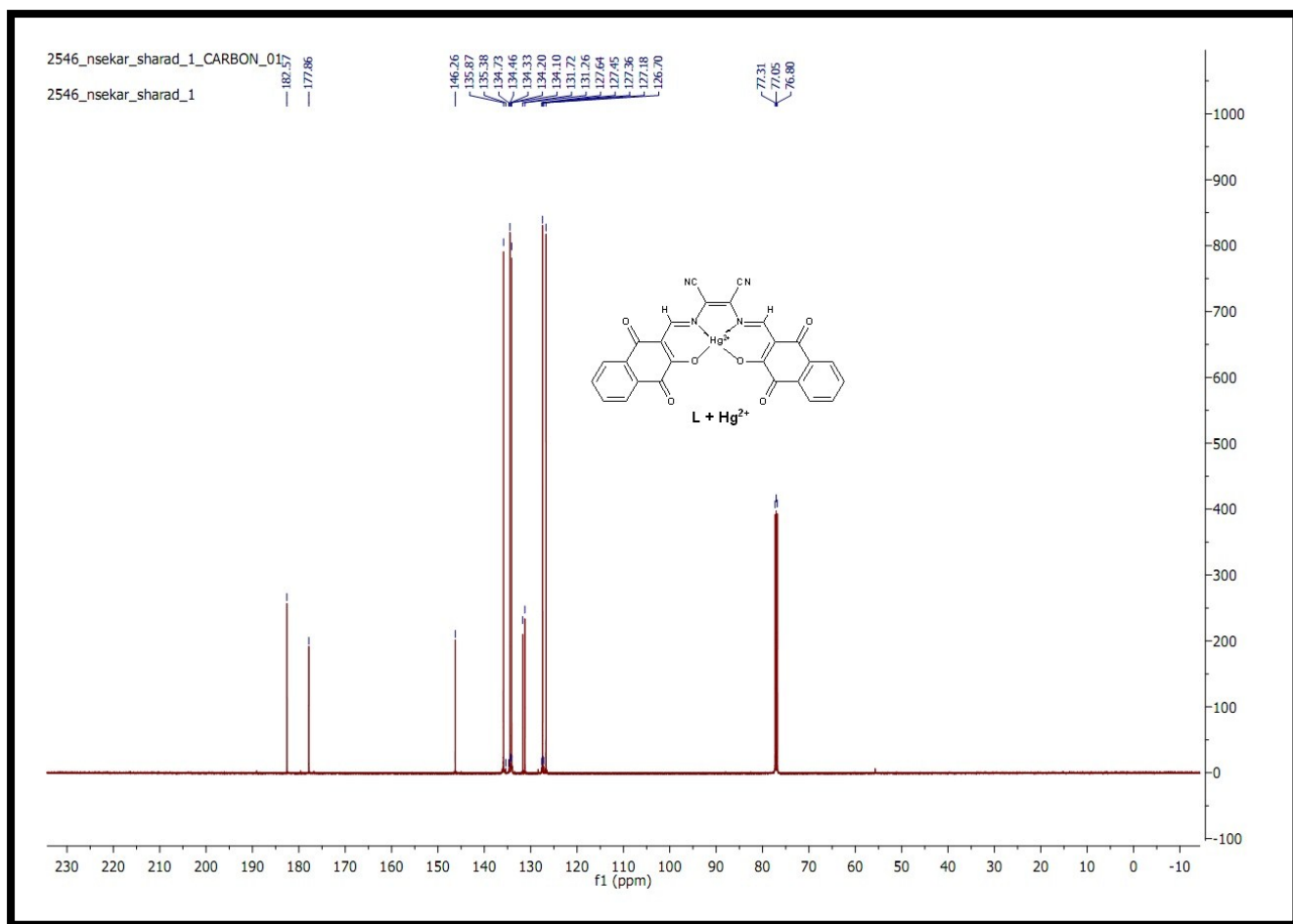
Figure S8. ^{13}C NMR spectra of **L+Hg^{2+}** complex recorded in CDCl$_3$.
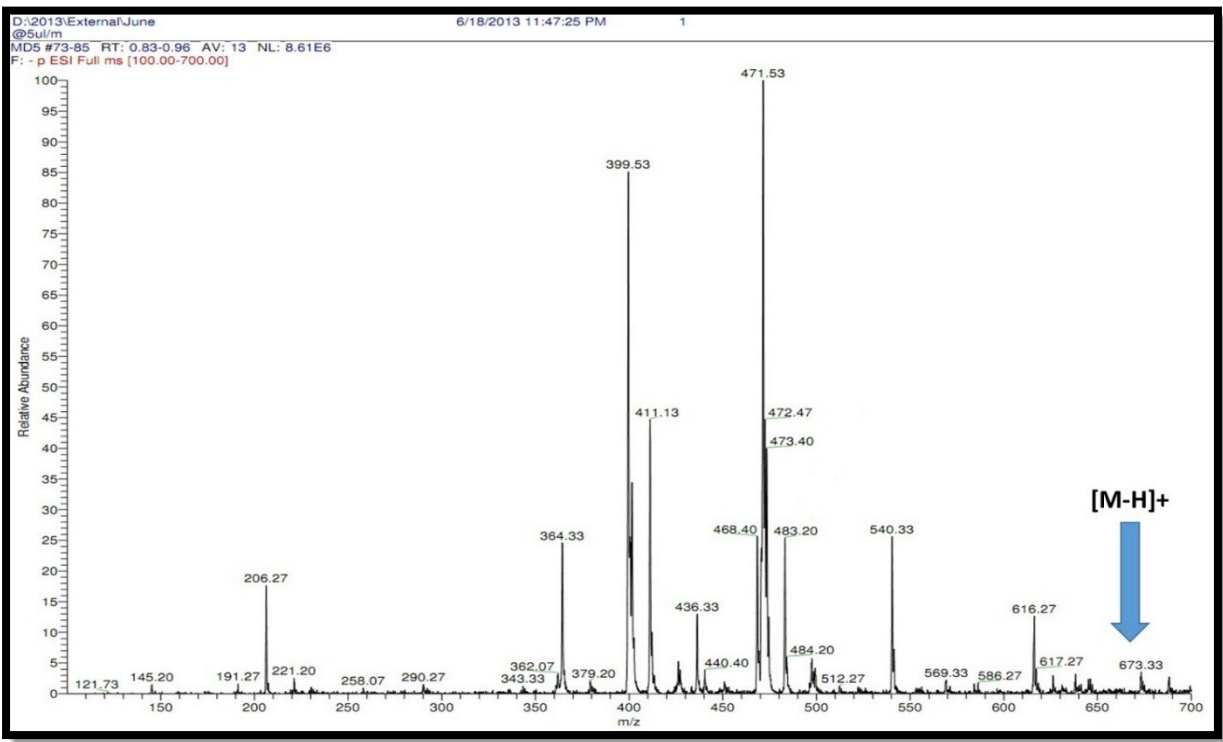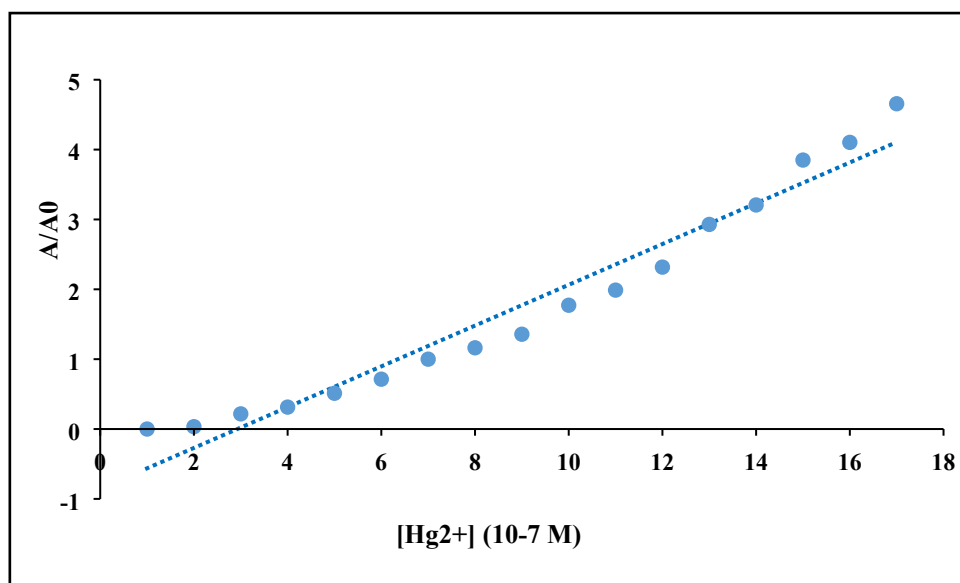
Figure S9. Mass spectra of **L+Hg²⁺** complex.

Figure 10. Ratiometric calibration curve A_{595}/A_{481} as a function of the concentration of Hg^{2+}.