Supporting Information

Study of DNA interaction and cytotoxicity activity of oxidovanadium(V) complexes having ONO donor Schiff base ligands

Gurunath Sahu [1], Edward R. T. Tiekink [2] and Rupam Dinda [1,*]

[1] Department of Chemistry, National Institute of Technology, Rourkela, 769008 Odisha, India. E-mail: 518cy1003@nitrkl.ac.in

[2] Research Centre for Crystalline Materials, School of Medical and Life Sciences, Sunway University, 47500 Bandar Sunway, Selangor Darul Ehsan, Malaysia

* Correspondence: rupamdinda@nitrkl.ac.in

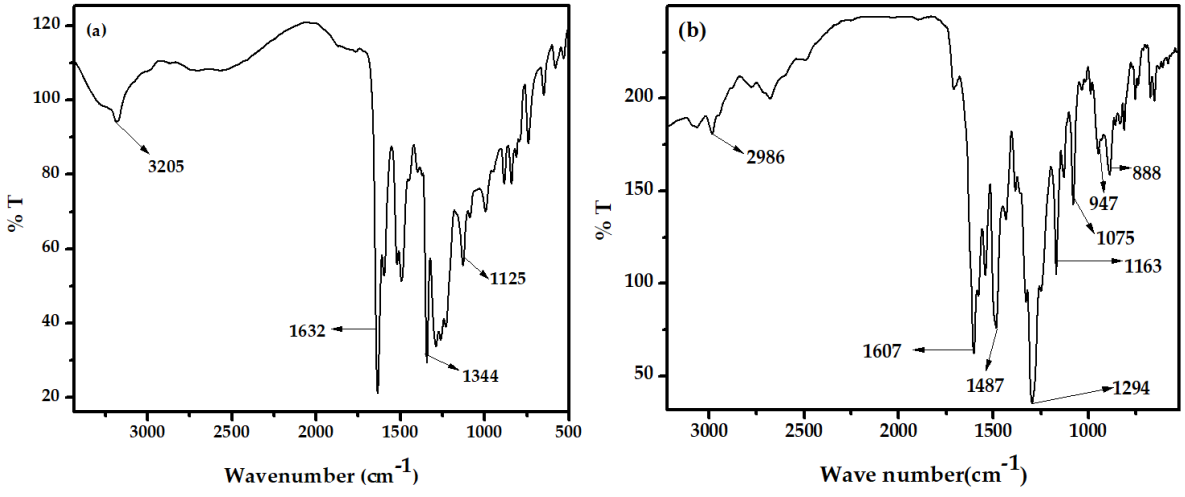

Figure S1. IR spectra of H_2L (a) and complex **1** (b)

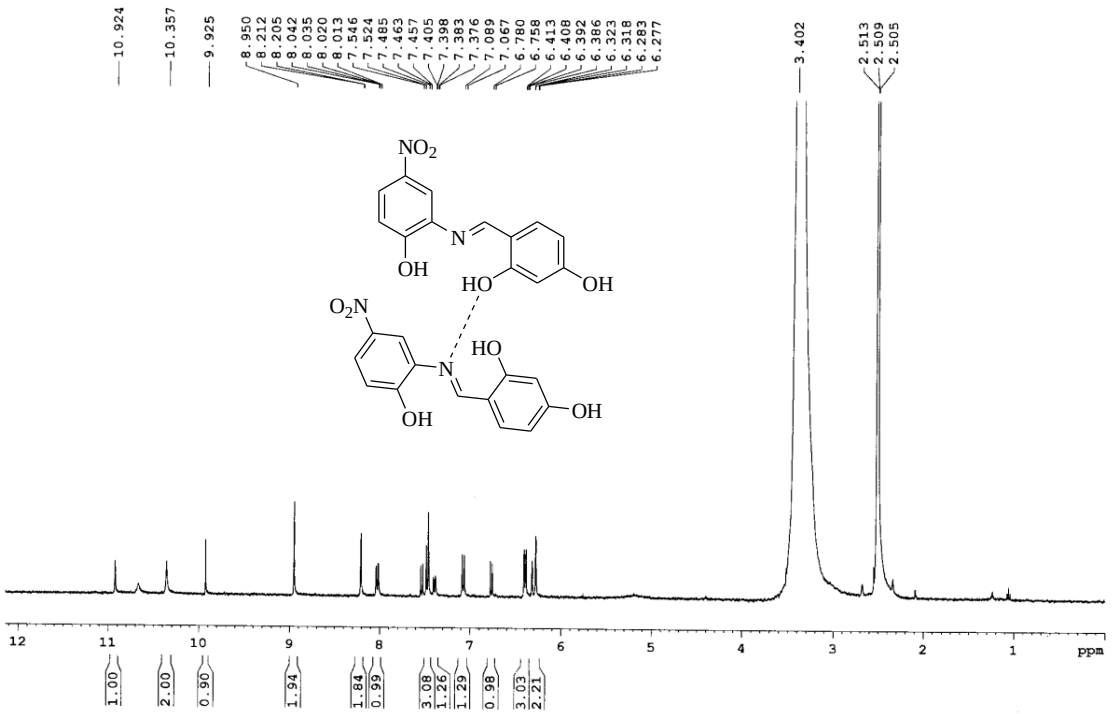

Figure S2. ^{1}H NMR of H_2L ligand in DMSO-d_6.

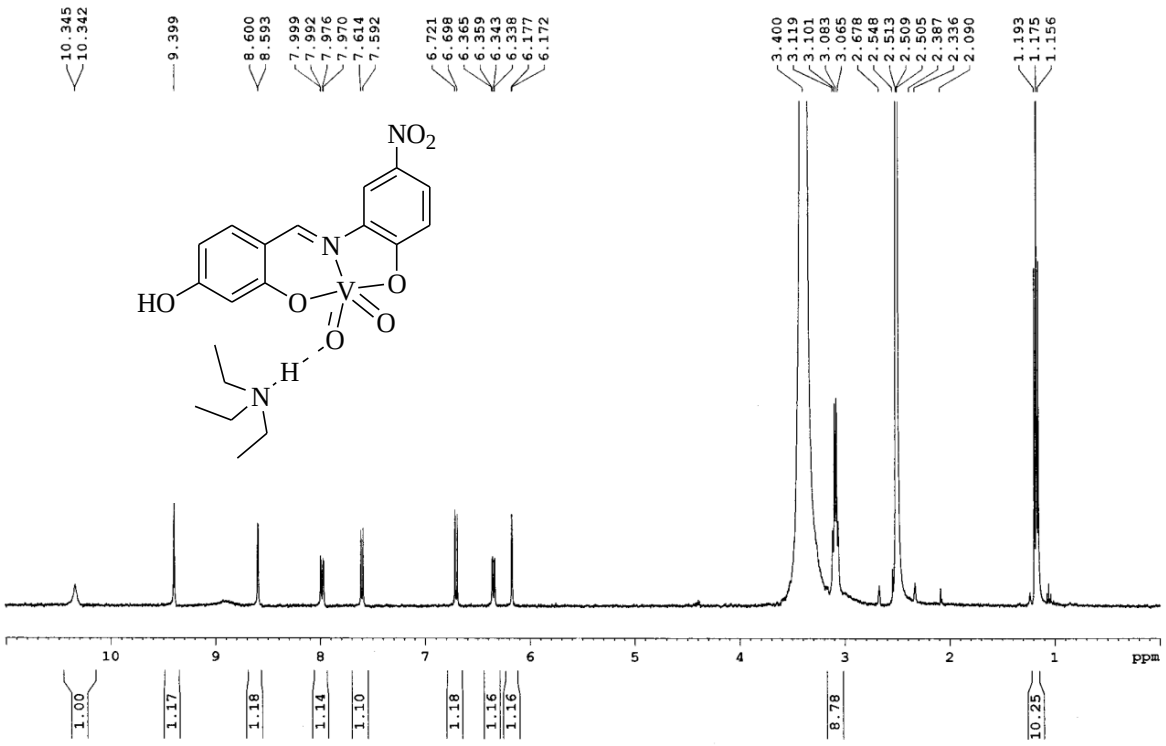

Figure S3. ^{1}H NMR spectra of **1** DMSO-d_6

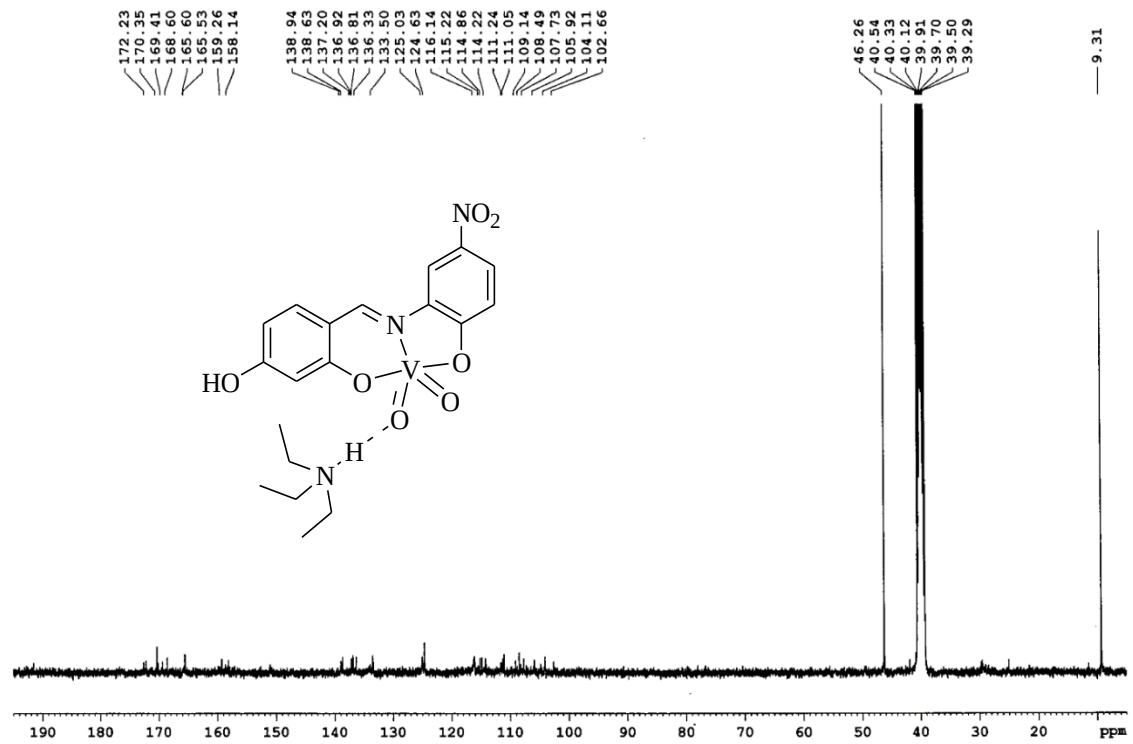

Figure S4. ^{13}C NMR spectra of **1** DMSO-d_6

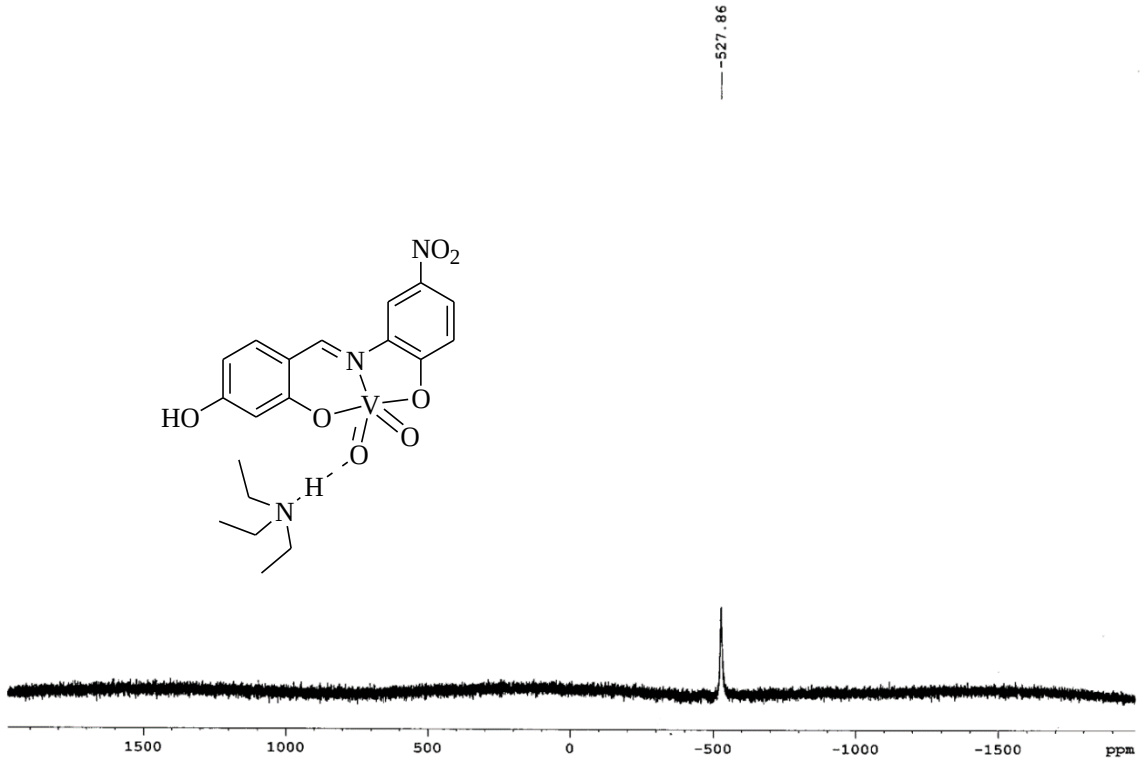

Figure S5. ^{51}V NMR spectra of **1** DMSO-d_6

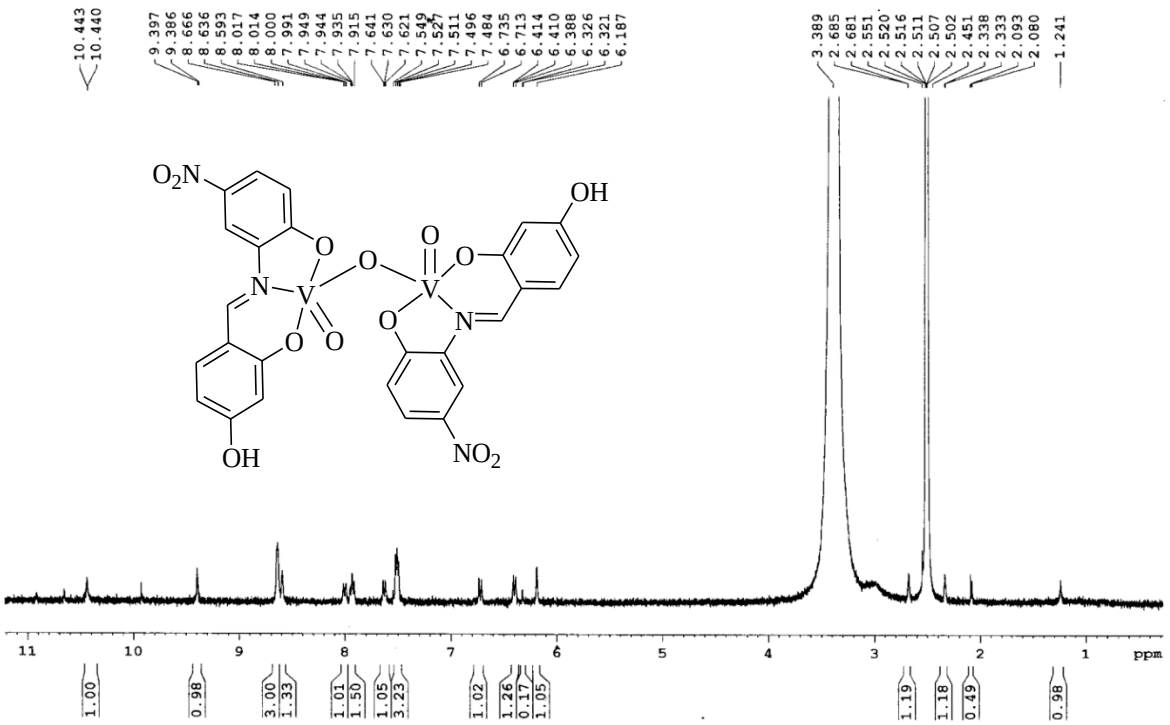

Figure S6. [1]H NMR spectra of **2** DMSO-d6

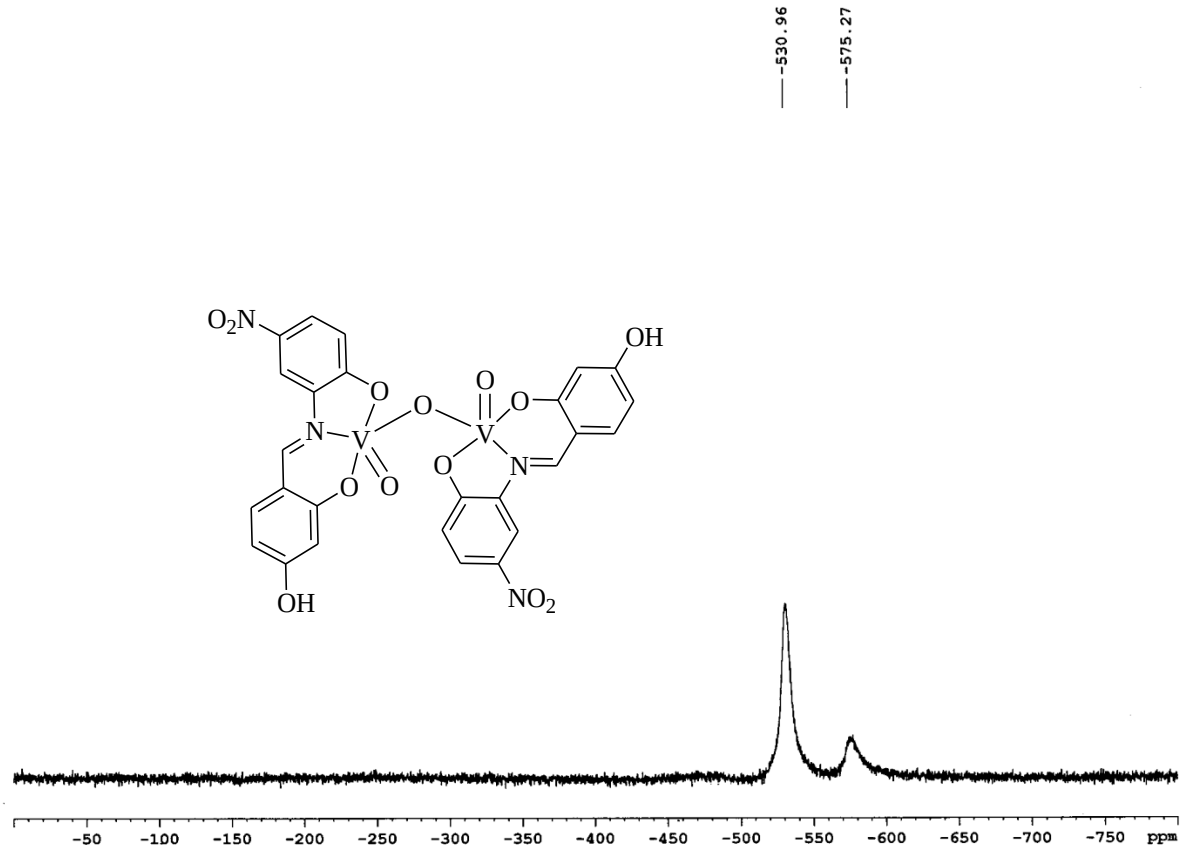

Figure S7. [51]V NMR spectra of **2** DMSO-d6

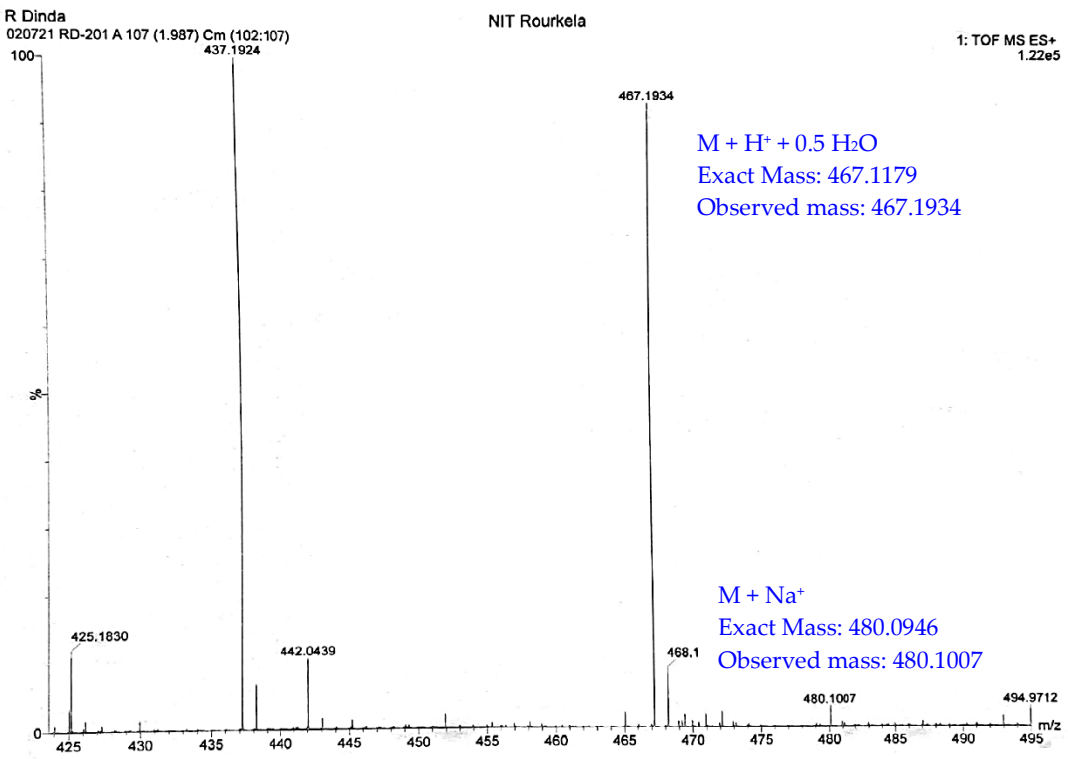

Figure S8. ESI–MS of **1** (100 pmol/μL) in MeCN (recorded in the positive ion mode).

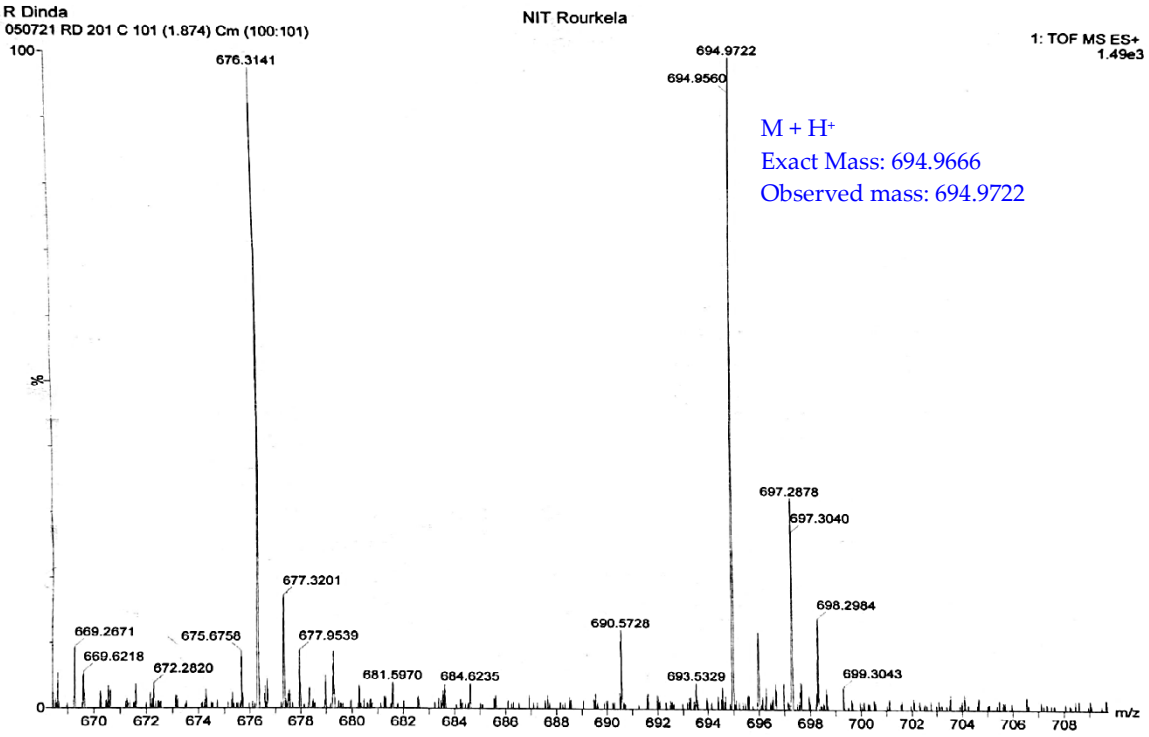

Figure S9. ESI–MS of **2** (100 pmol/μL) in MeCN (recorded in the positive ion mode).

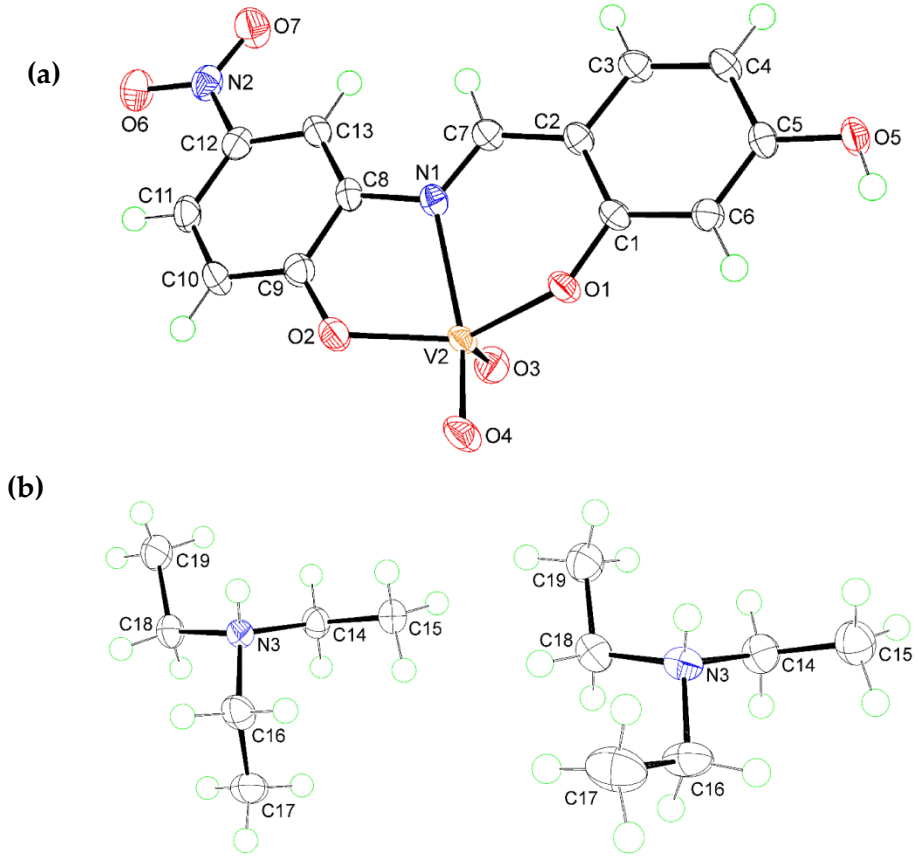

Figure S10. Molecular structures of (a) the second independent complex anion and (b) the two independent cations of salt **1** showing atom labelling scheme and displacement ellipsoids at the 70% probability level.

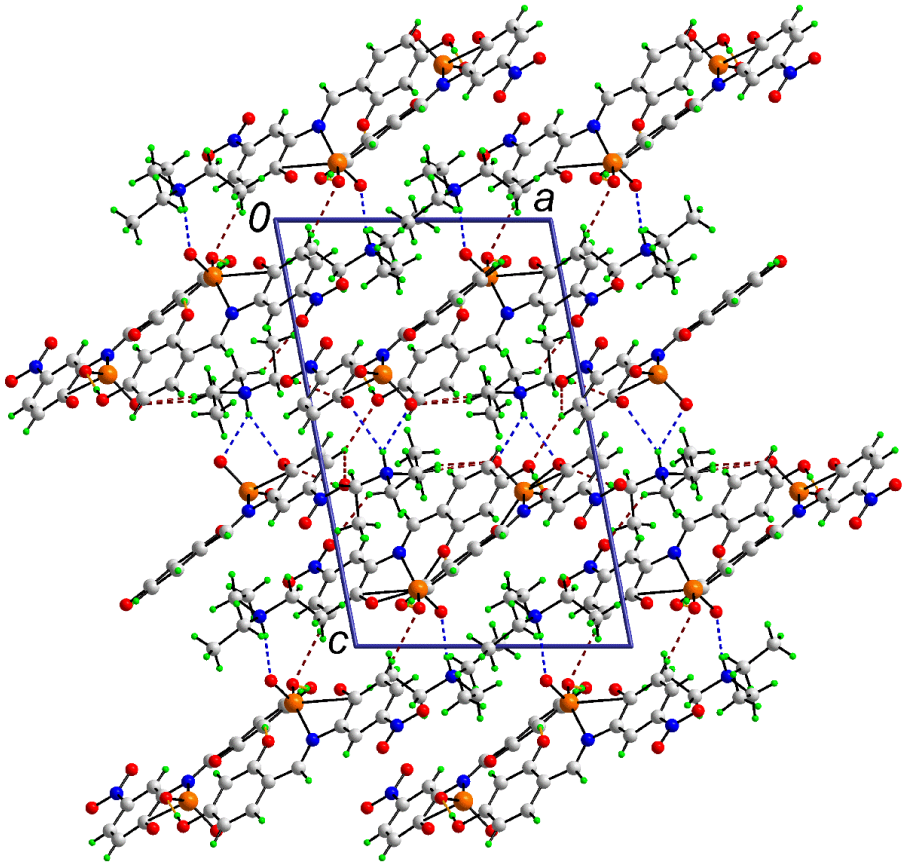

Figure S11. A view in projection down the *b*-axis of the unit-cell contents for salt **1**. The O–H···O, N–H···O and C–H···O interactions are indicated by orange, blue and brown dashed lines, respectively.

Table S1. Geometric parameters (Å, °) characterizing identified intermolecular contacts in salt **1**

A	H	B	H···B	A···B	A–H···B	symmetry operation
C6a	H6a	O1b	2.48	3.4151(16)	170	*x*, *y*, *z*
C6b	H6b	O1a	2.60	3.4842(16)	155	*x*, *y*, *z*
C10b	H10b	O4b	2.39	3.1704(17)	140	-*x*, -*y*, 2-*z*
C11a	H11a	O5b	2.46	3.1509(17)	130	2-*x*, 1-*y*, 1-*z*
C14a	H14a	O3a	2.49	3.4377(17)	159	1-*x*, 1-*y*, 1-*z*
C16a	H16b	O2a	2.56	3.5241(17)	165	2-*x*, 1-*y*, 1-*z*
C18a	H18a	O7b	2.53	3.2637(18)	131	1-*x*, -*y*, 1-*z*

C19a	H19c	O3a	2.55	3.5338(19)	179	1-*x*, 1-*y*, 1-*z*