

Electronic Supplementary Information

for

Physical properties and cytotoxicity of the Cu(II) and Zn(II) complexes with TMS-substituted indolo[2,3-*c*]quinoline-derived Schiff base

Christopher Wittmann,^a Iuliana Besleaga,^a Soheil Mahmoudi,^{a,b} Oleg Palamarciuc,^{c,d} Mihaela Balan-Porcarasu,^e Mihaela Dascalu,^c Sergiu Shova,^c Maria Cazacu,^c Mónika Kiricsi,^f Nóra Igaz,^f Orsolya Dömötör,^g Eva A. Enyedy,^{g,*} Dana Dvoranová,^h Peter Rapta,^{h,*} Vladimir B. Arion^{a,c,*}

^aUniversity of Vienna, Institute of Inorganic Chemistry, Währinger Strasse 42, 1090 Vienna, Austria

^bUniversity of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Strasse 42, 1090 Vienna, Austria

^cInorganic Polymers Department, “Petru Poni” Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41 A, Iasi 700487, Romania

^dPhysics of Semiconductors and Devices Laboratory, Faculty of Physics and Engineering and Institute of Applied Physics, Moldova State University, MD-2009 Chişinău, Republic of Moldova

^eNMR Laboratory, “Petru Poni” Institute of Macromolecular Chemistry, Aleea Gr. Ghica Voda 41 A, Iasi 700487, Romania

^fDepartment of Biochemistry and Molecular Biology, University of Szeged, Közép fasor 52, H-6726 Szeged, Hungary

^gDepartment of Molecular and Analytical Chemistry, Interdisciplinary Excellence Centre, University of Szeged, Dóm tér 7-8, H-6720 Szeged, Hungary

^hInstitute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, SK-81237 Bratislava, Slovakia

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NMR Numbering Scheme

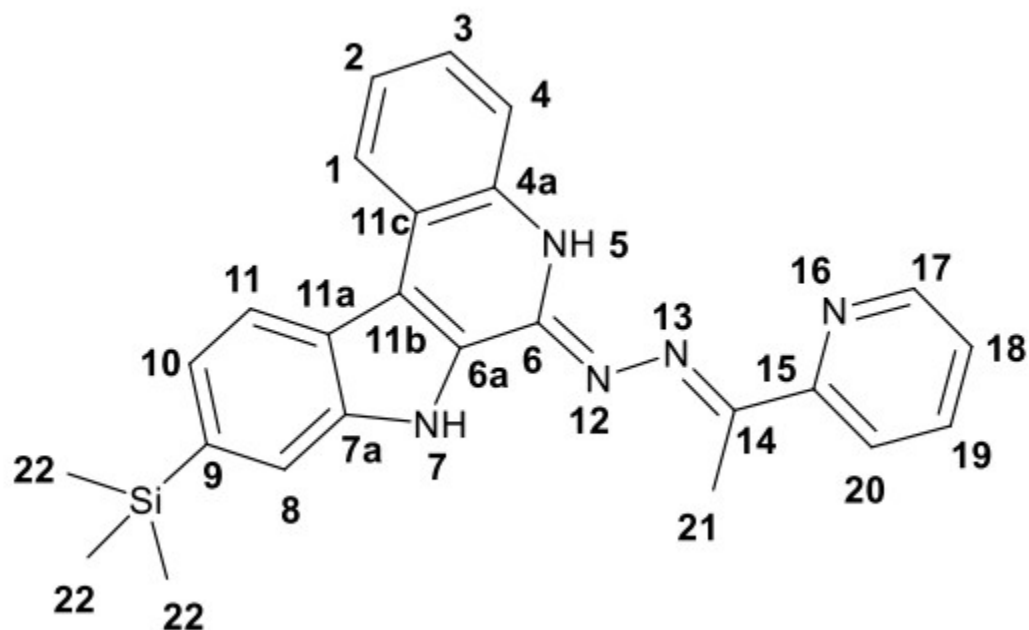


Figure S1. NMR atom numbering scheme for **HL^{TMS}**.

NMR data for organic compounds

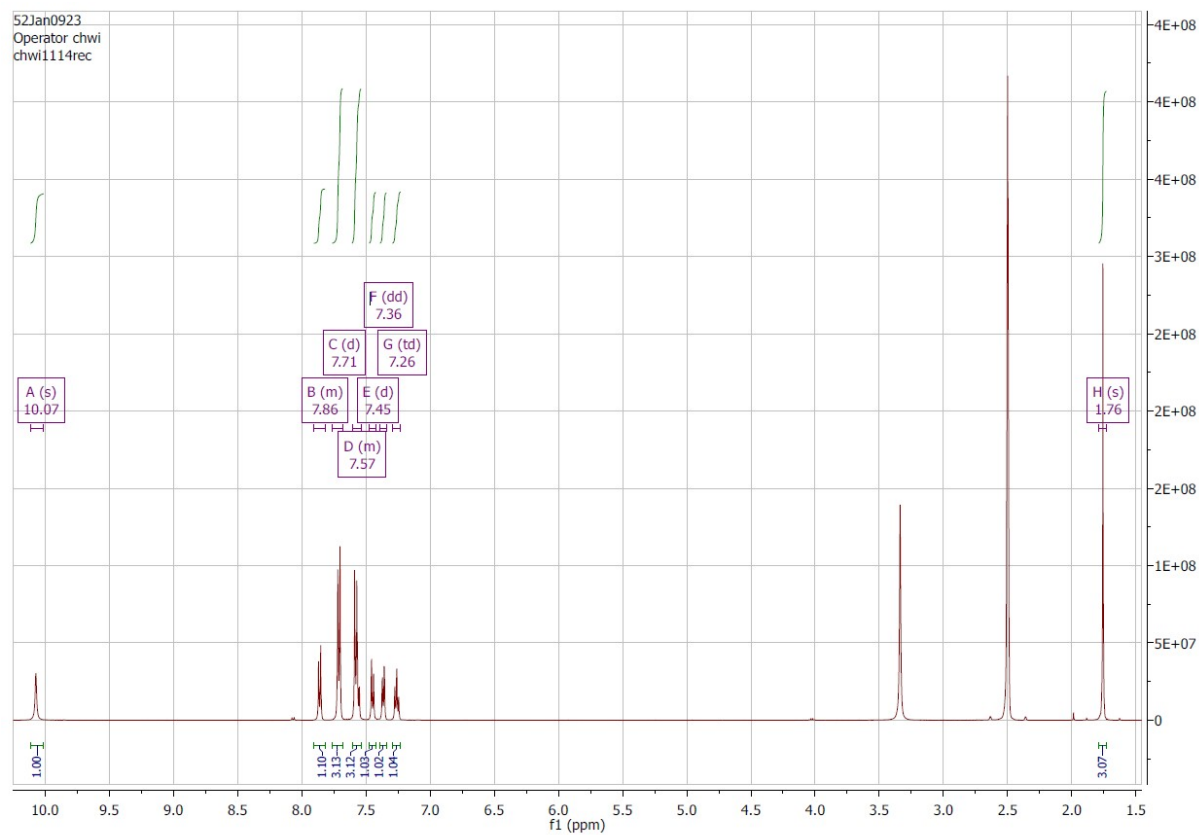


Figure S2. ^1H NMR spectrum of species A in $\text{DMSO}-d_6$.

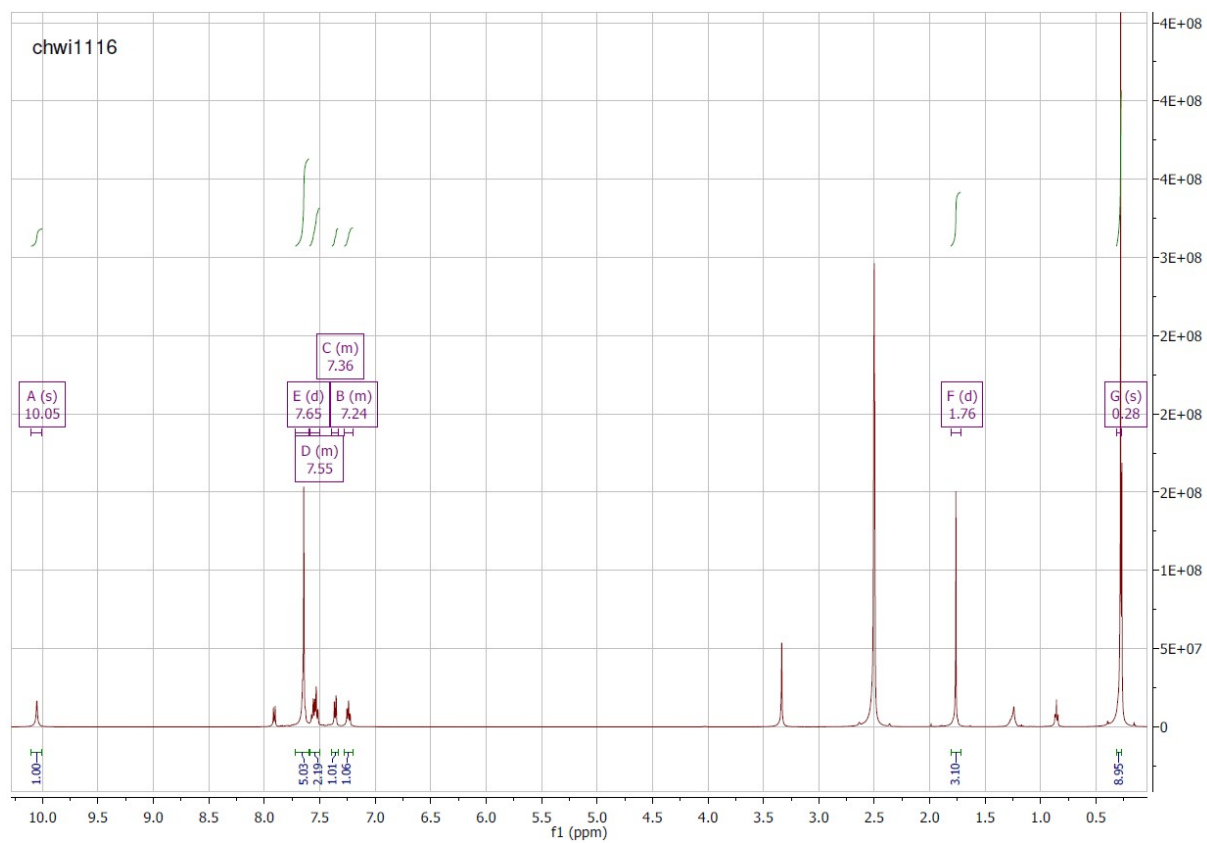


Figure S3. ^1H NMR spectrum of species **B** in $\text{DMSO}-d_6$.

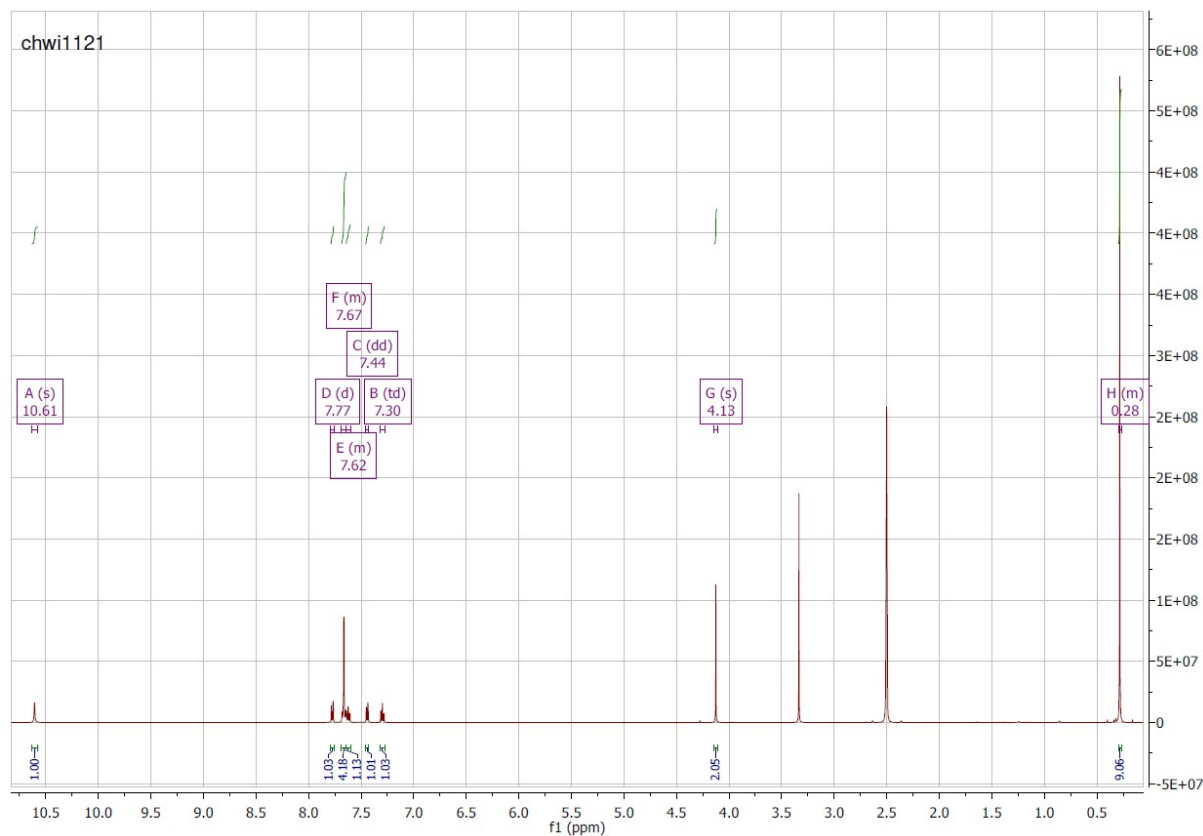


Figure S4. ^1H NMR spectrum of species **D** in $\text{DMSO-}d_6$.

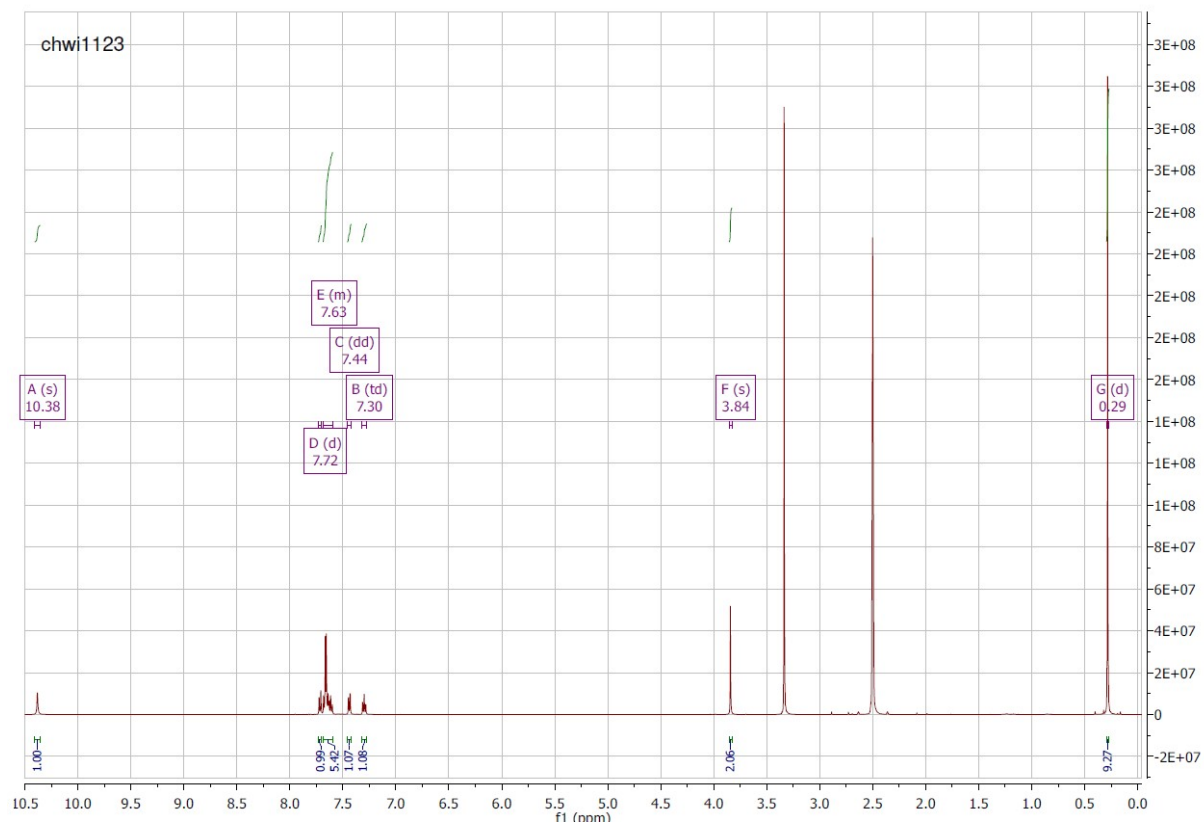


Figure S5. ^1H NMR spectrum of species E in $\text{DMSO}-d_6$.

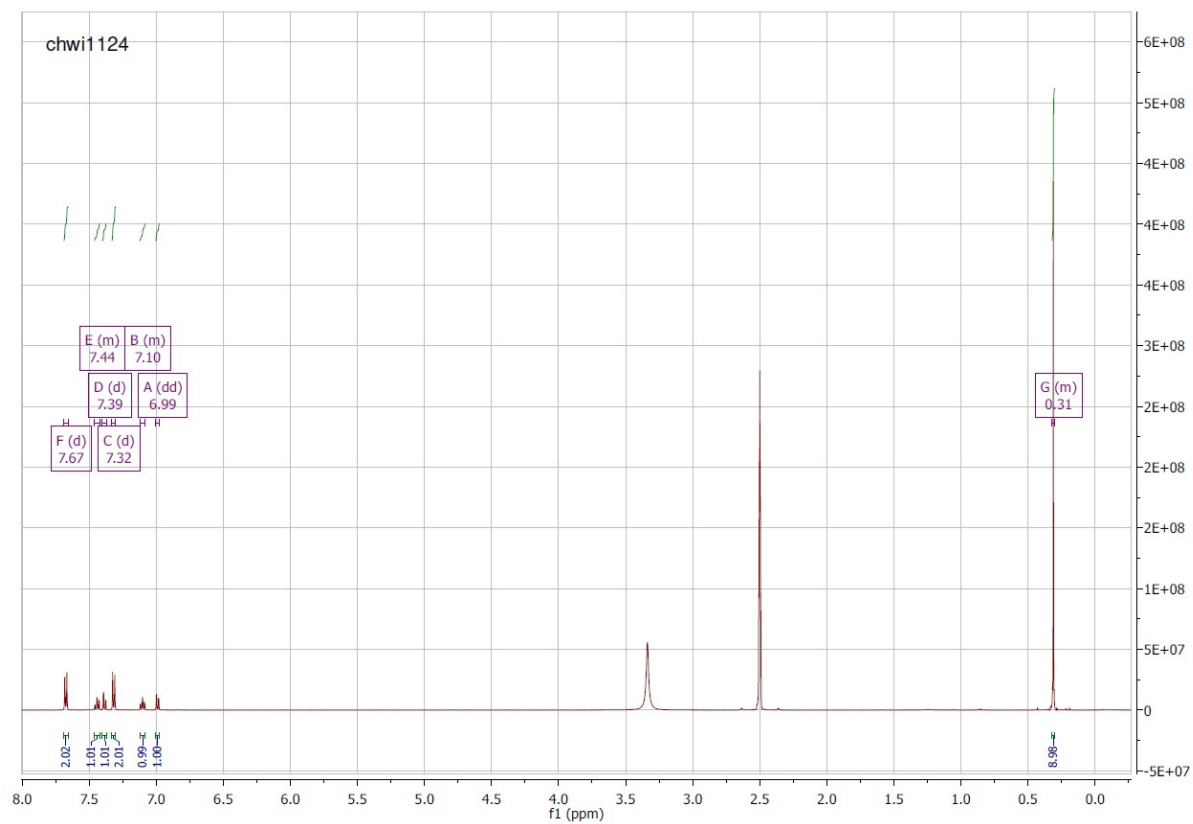


Figure S6. ^1H NMR spectrum of species **F** in $\text{DMSO}-d_6$.

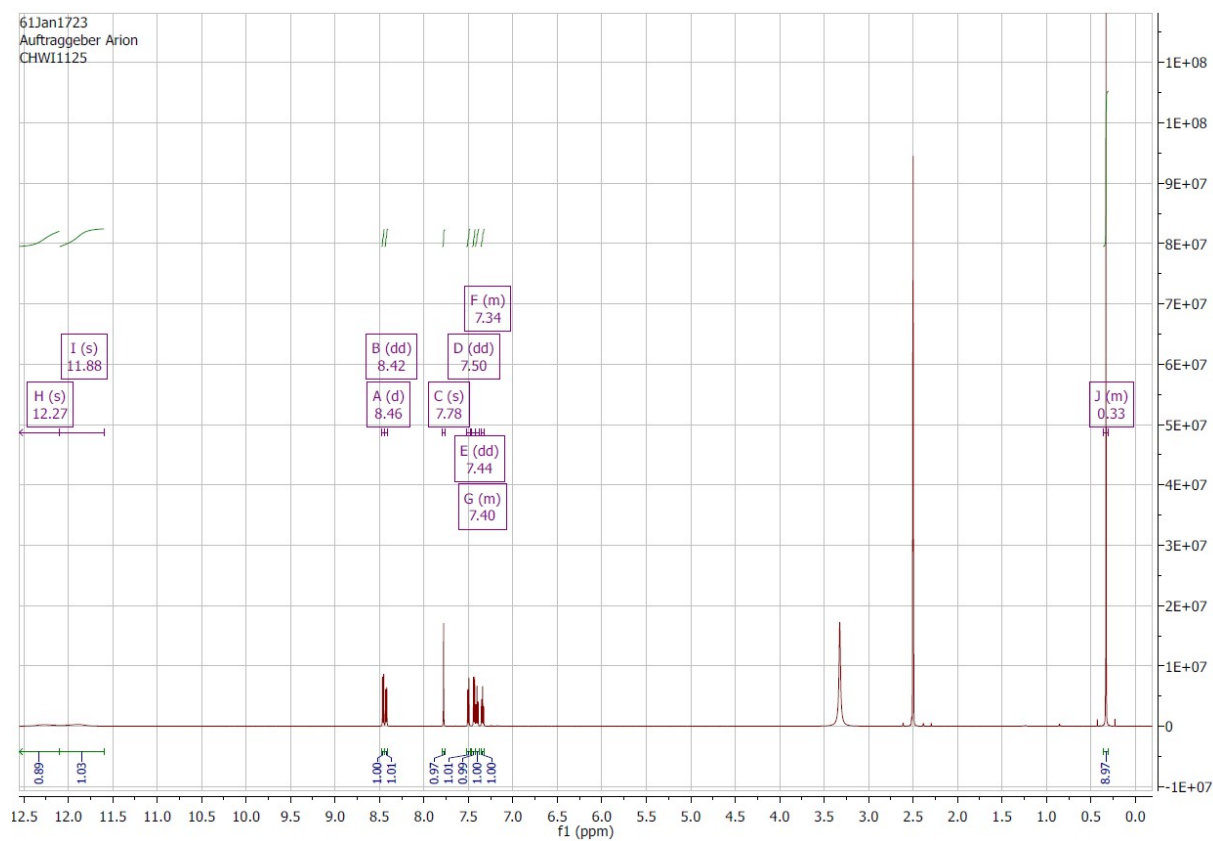


Figure S7. ^1H NMR spectrum of species **G** in $\text{DMSO-}d_6$.

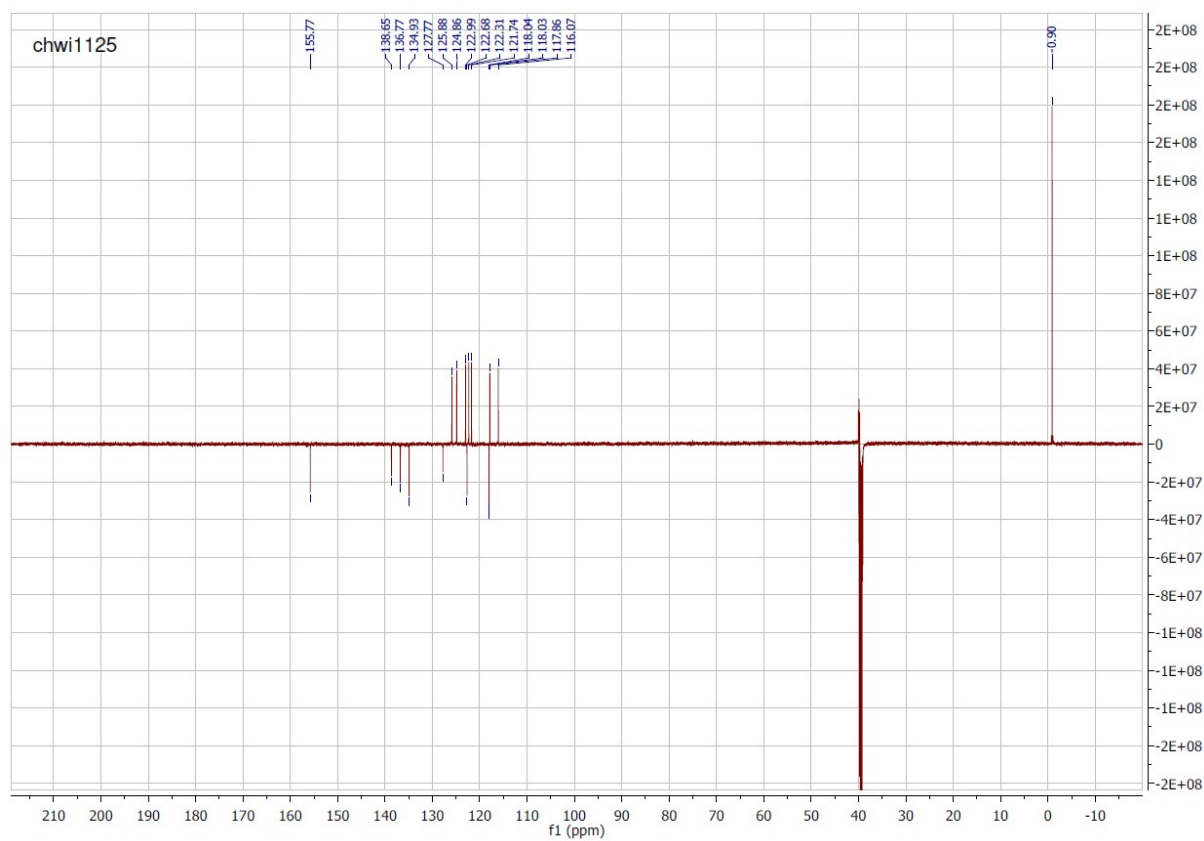


Figure S8. ^{13}C NMR spectrum of species **G** in $\text{DMSO-}d_6$.

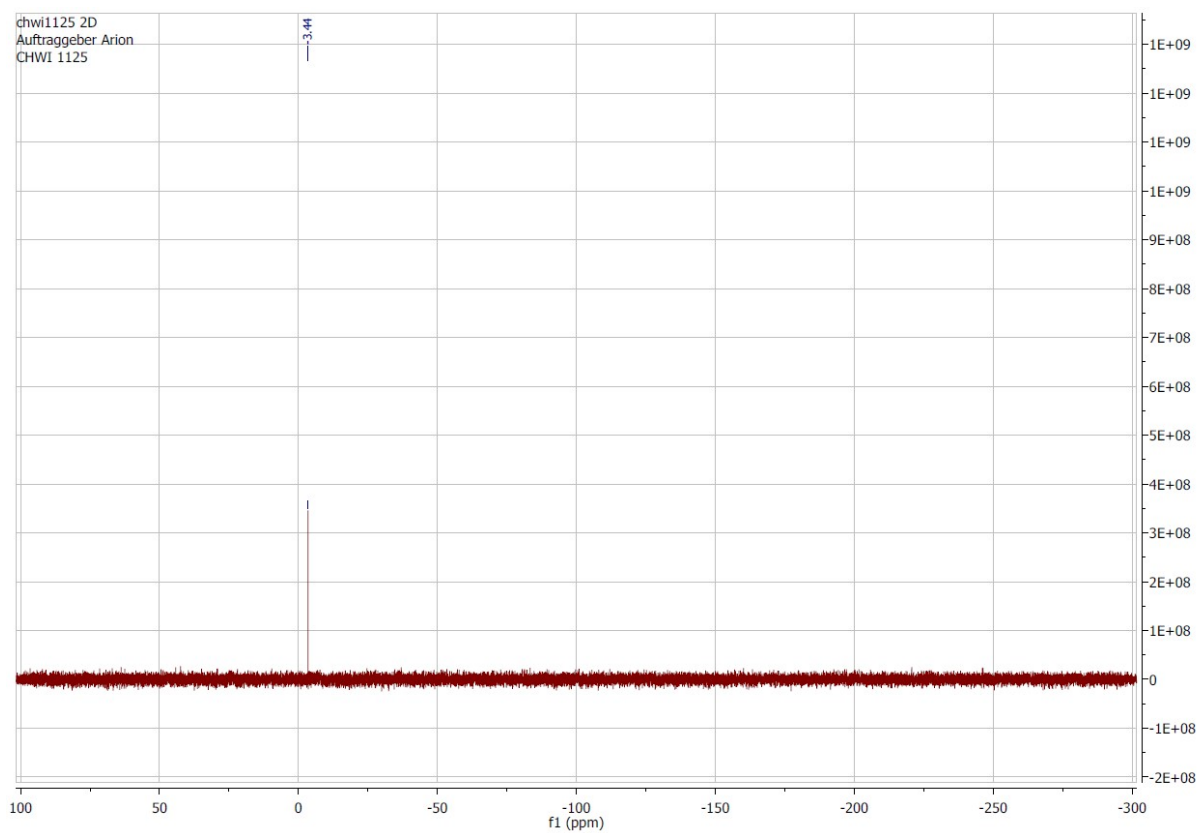


Figure S9. ^{29}Si NMR spectrum of species **G** in $\text{DMSO-}d_6$.

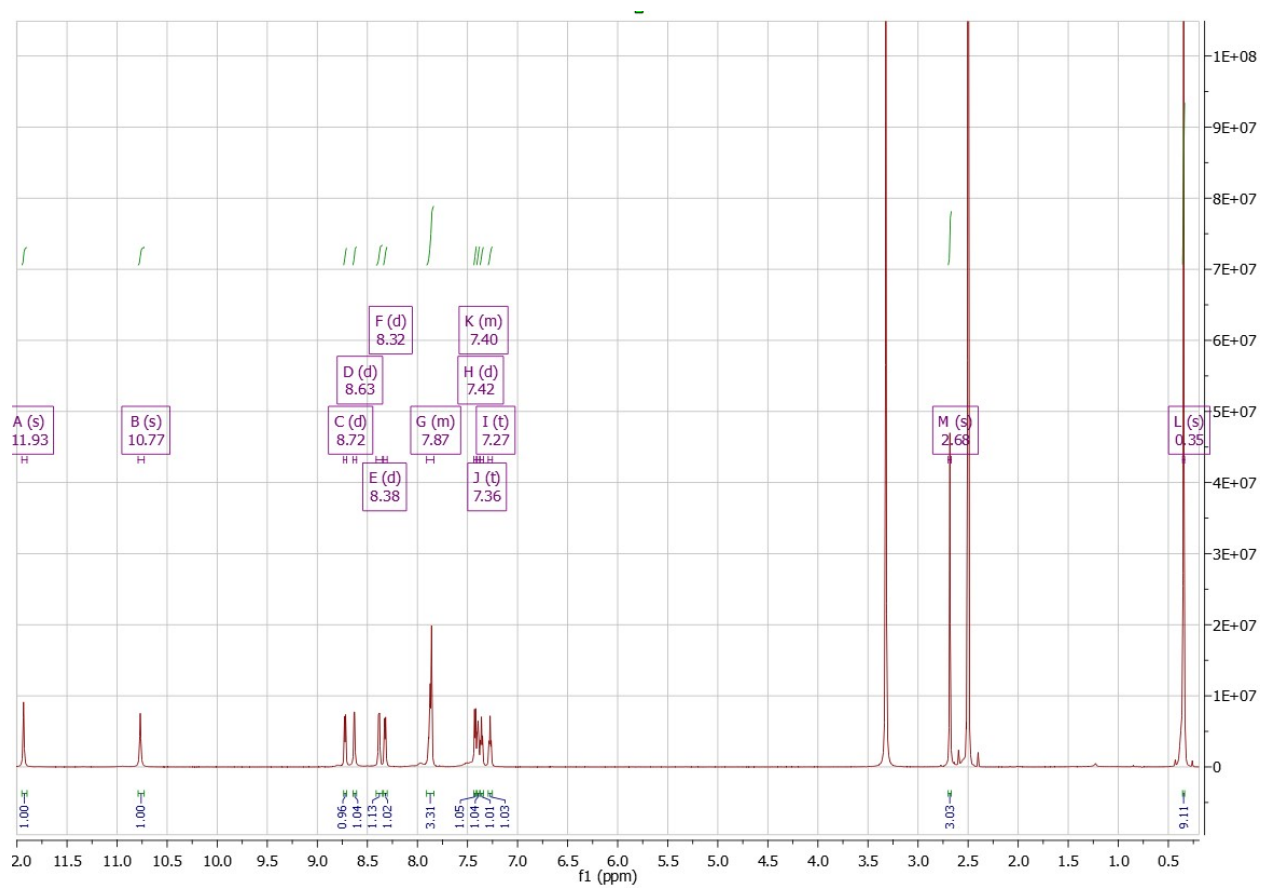


Figure S10. ¹H NMR spectrum of **HL^{TMS}** in DMSO-*d*₆.

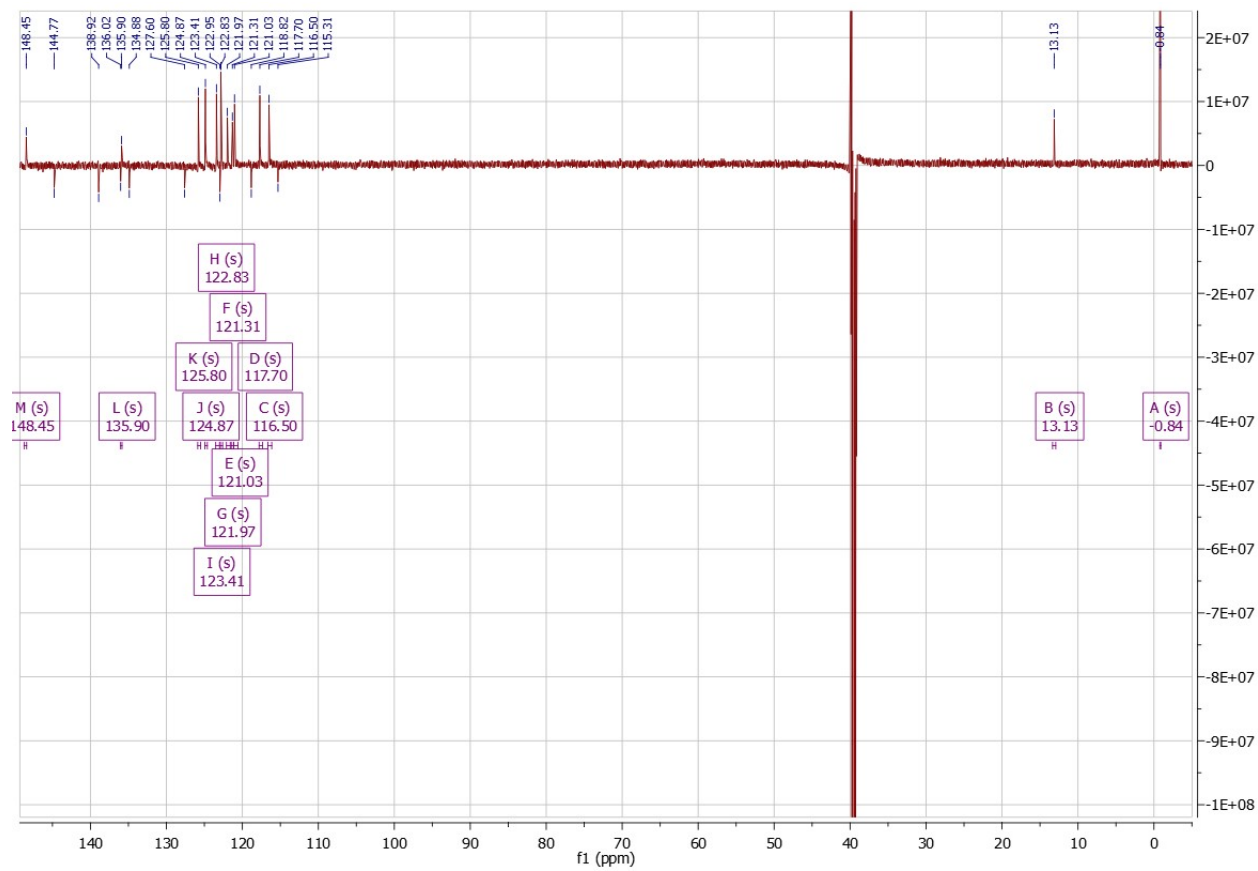


Figure S11. ^{13}C NMR spectrum of HL^{TMS} in $\text{DMSO-}d_6$.

ESI-MS for organic compounds

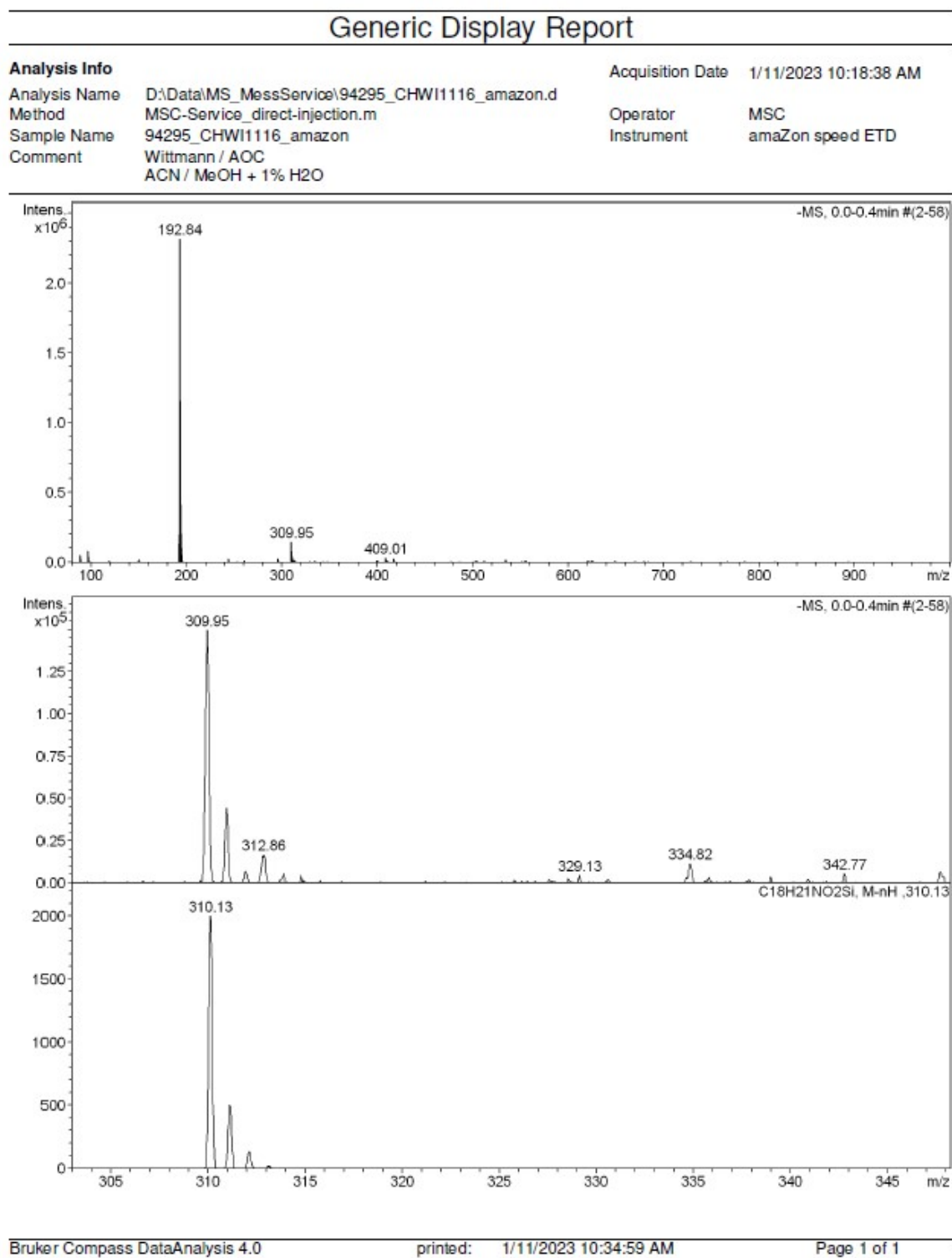


Figure S12. ESI(+) mass spectrum of **B**.

Generic Display Report

Analysis Info

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Method MSC-Service_direct-injection.m
Sample Name 94396_CHWI 1120_amazon
Comment Wittmann/ AOC
ACN / MeOH + 1% H₂O

Acquisition Date 1/12/2023 2:46:45 PM

Operator MSC
Instrument amaZon speed ETD

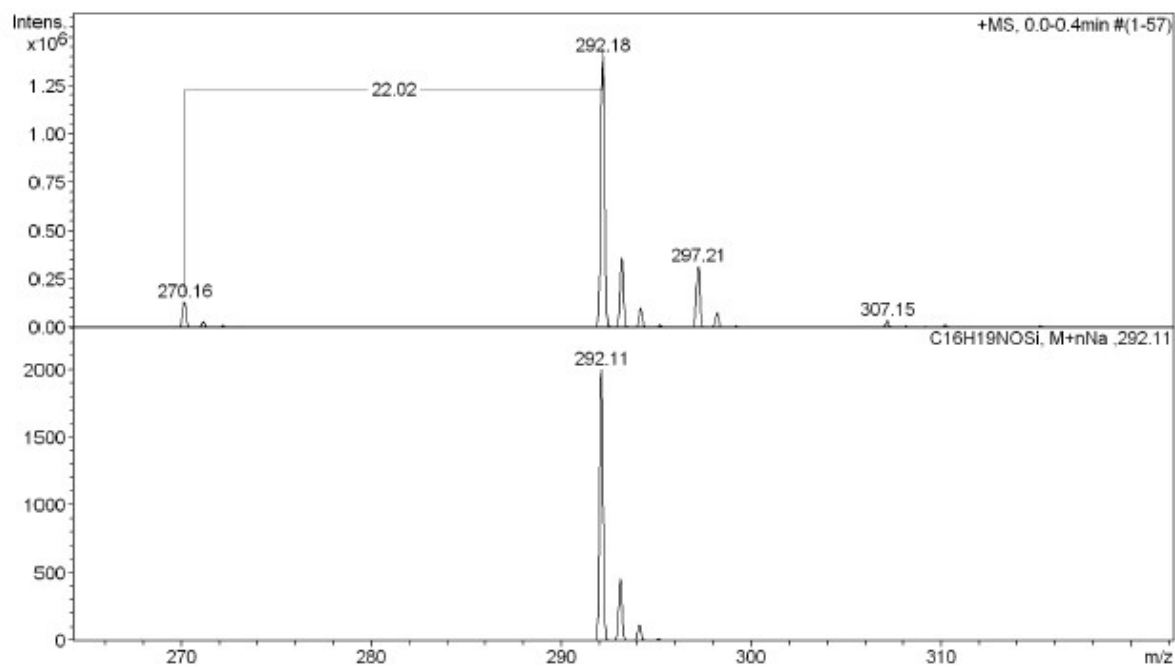
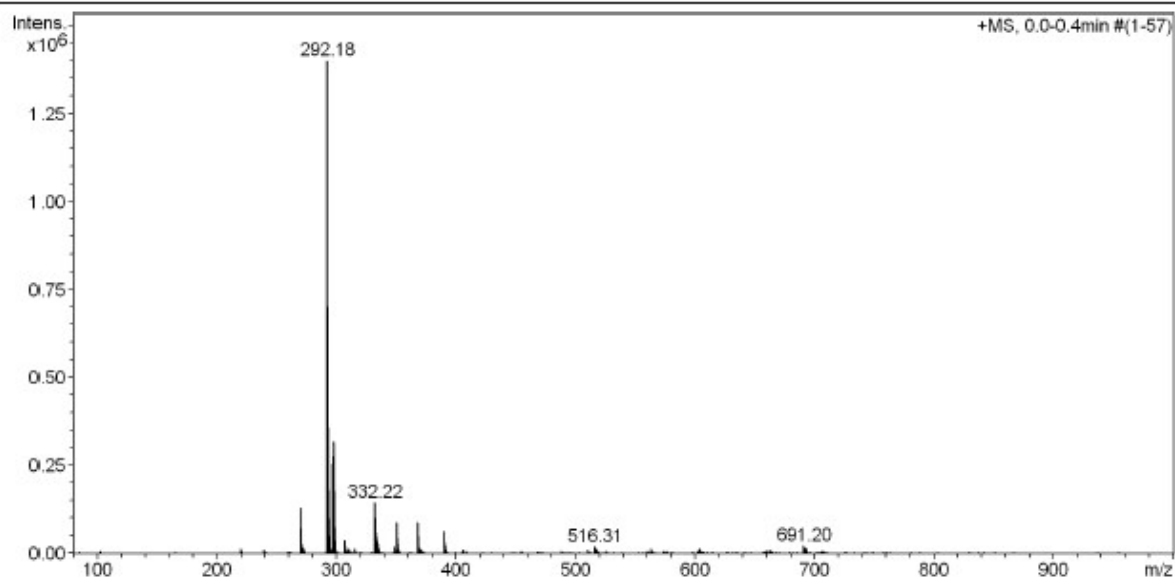


Figure S13. ESI(+) mass spectrum of C.

Generic Display Report

Analysis Info

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Sample Name 94424_CHWI1121_amazon
Comment Wittmann / Anorg.Chem.
ACN / MeOH + 1% H₂O

Acquisition Date 1/13/2023 11:11:30 AM

Operator MSC
Instrument amaZon speed ETD

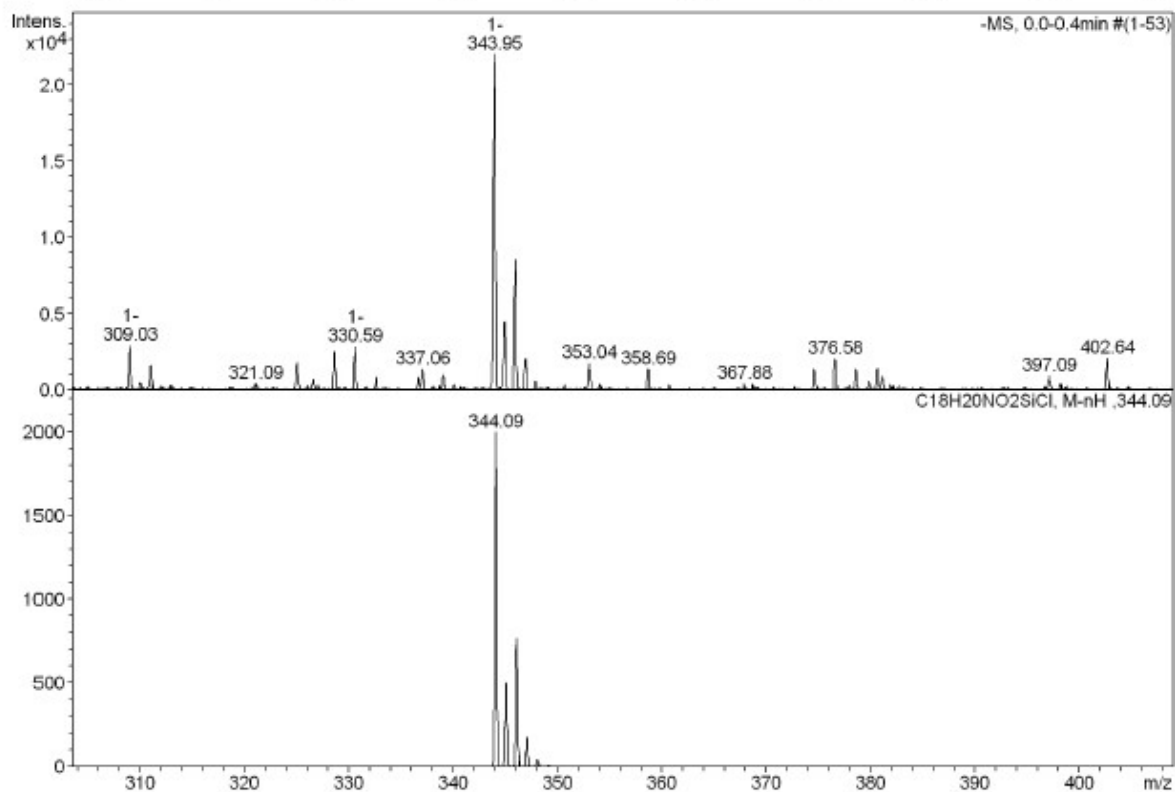
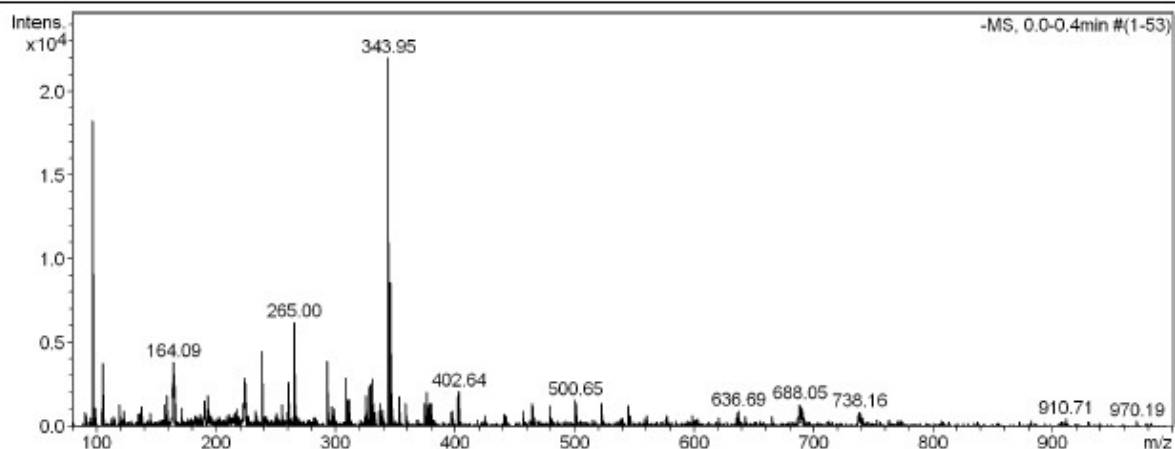


Figure S14. ESI(+) mass spectrum of **D**.

Generic Display Report

Analysis Info

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Method MSC-Service_direct-injection.m
Sample Name 94472_CHWI1124_amazon
Comment Wittmann / Anorg.Chem.
ACN / MeOH + 1% H₂O

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Operator MSC
Instrument amaZon speed ETD

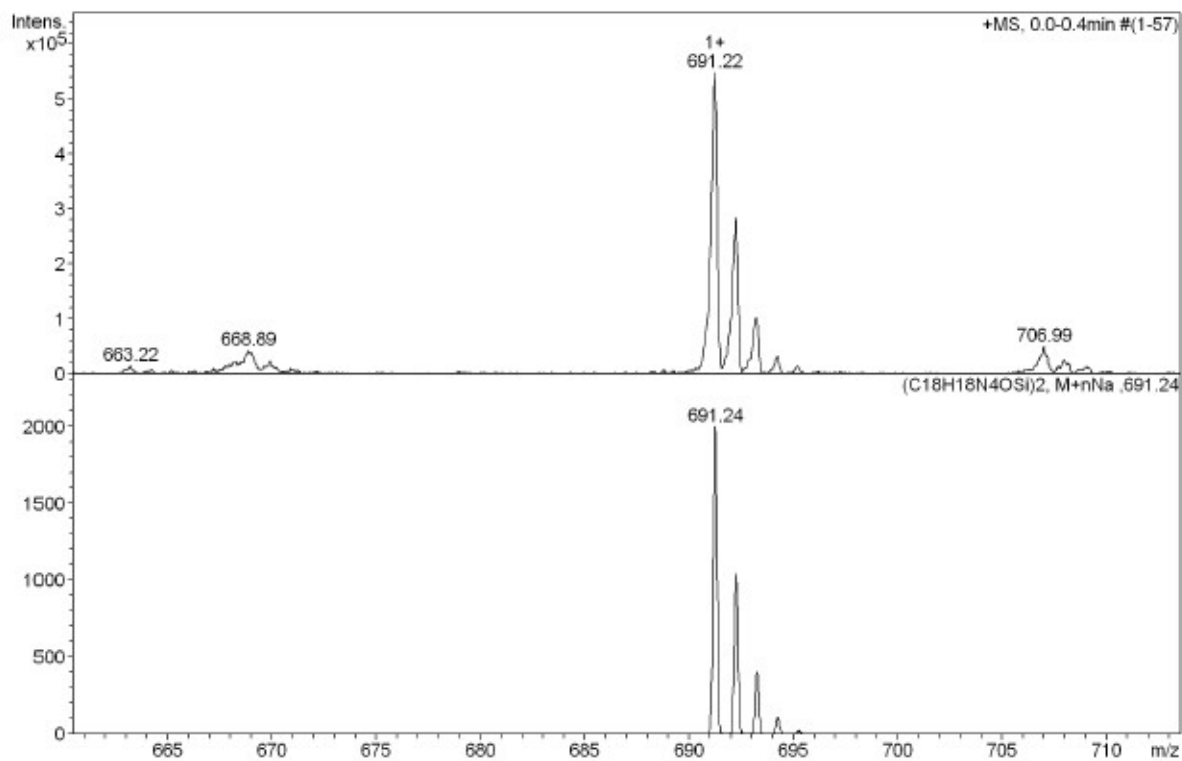
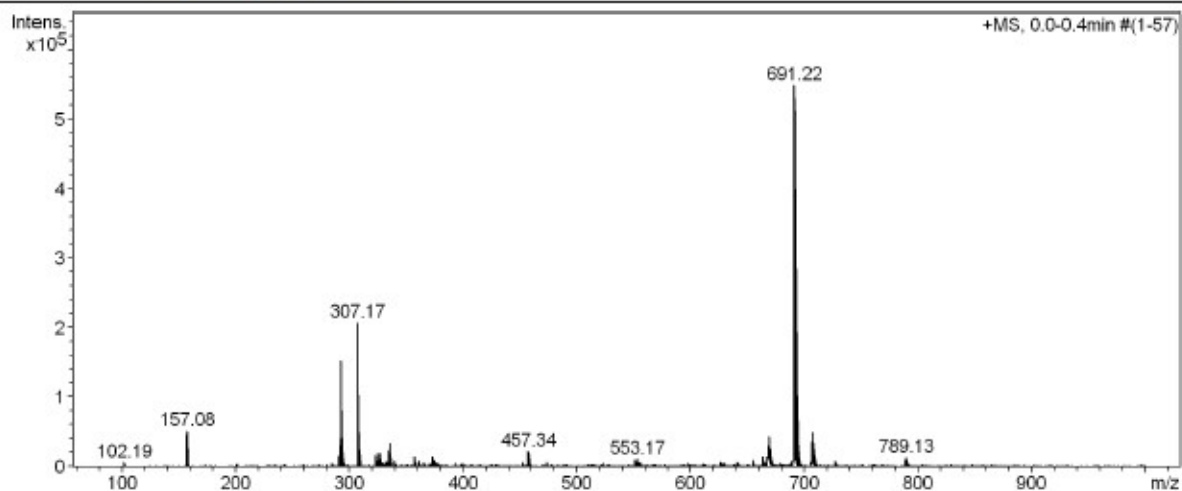


Figure S15. ESI(+) mass spectrum of **F**.

Generic Display Report

Analysis Info

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Sample Name CHWI 1122 22-30
Comment Wittmann / AOC
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ACN / MeOH + 1% H2O

Acquisition Date 1/16/2023 11:17:44 AM

Operator msc
Instrument maXis

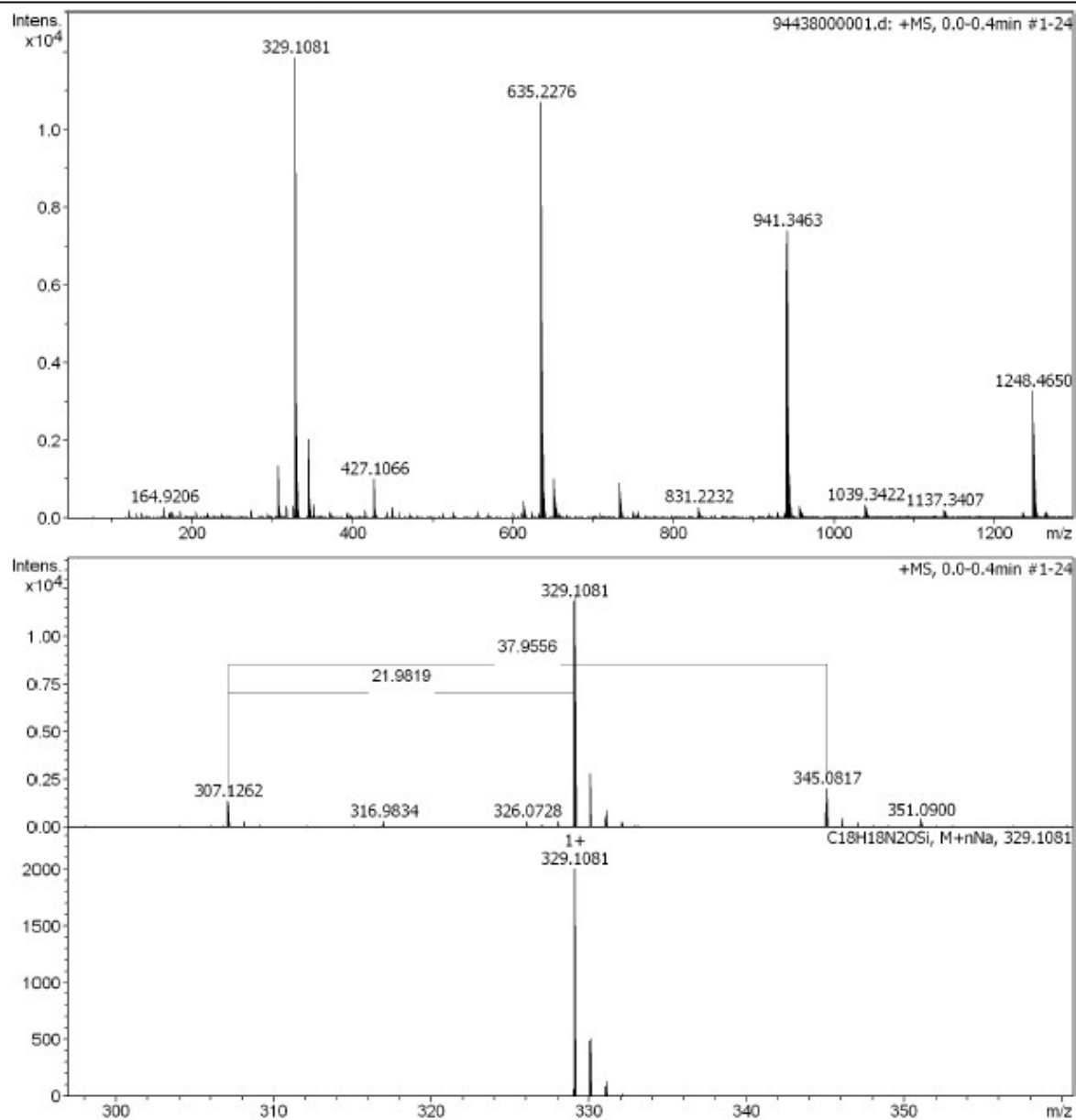


Figure S16. ESI(+) mass spectrum of G.

Generic Display Report

Analysis Info

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Method MSC-Service_direct-injection.m
Sample Name 95840_RINO3_amazon
Comment Noel / Anorg.Chem.
ACN / MeOH + 1% H₂O

Acquisition Date 3/22/2023 10:40:46 AM

Operator MSC
Instrument amaZon speed ETD

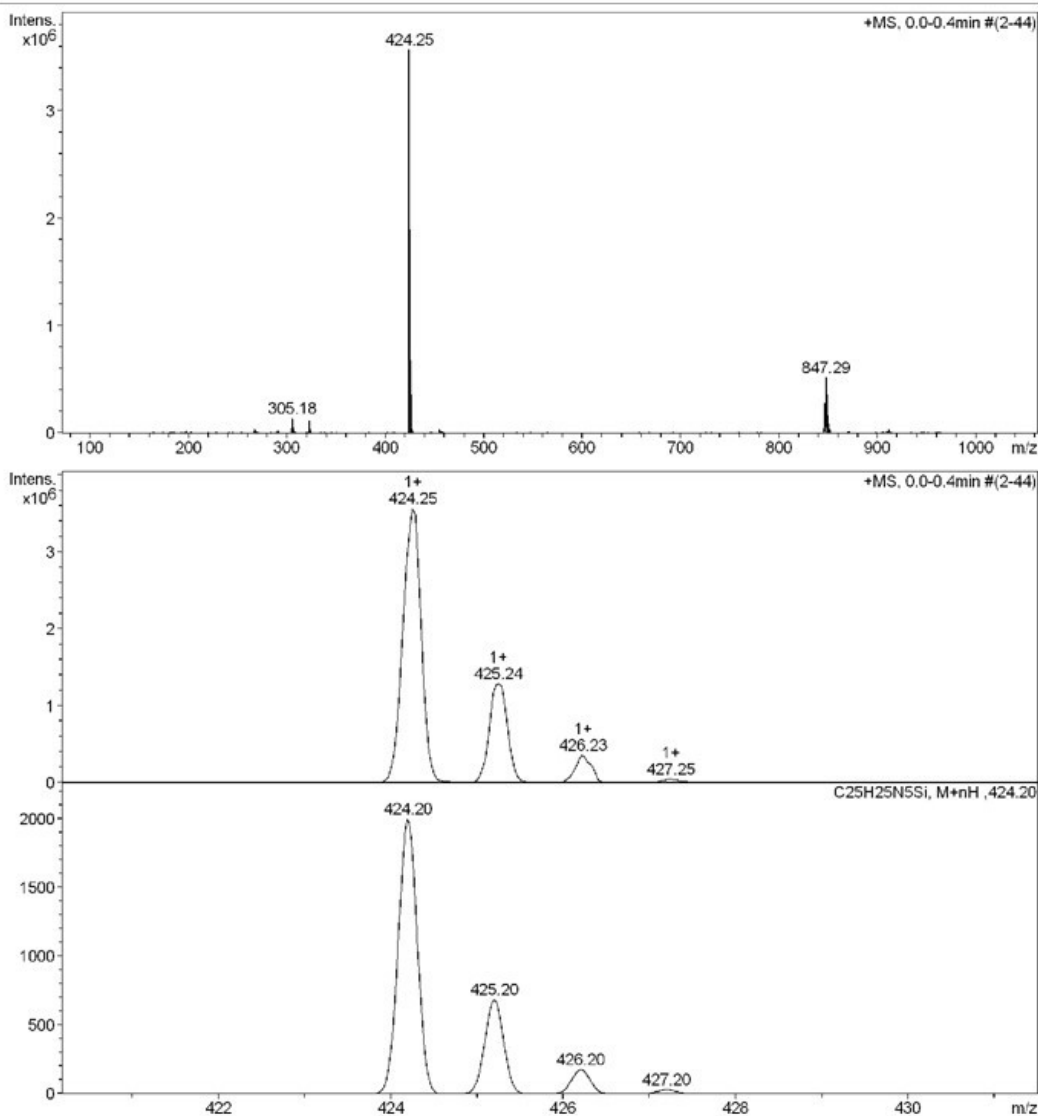


Figure S17. ESI(+) mass spectrum of **HL**^{TMS}.

Generic Display Report

Analysis Info

Analysis Name D:\Data\MS_MessService\95840_RINO3_amazon.d
Method MSC-Service_direct-injection.m
Sample Name 95840_RINO3_amazon
Comment Noel / Anorg.Chem.
ACN / MeOH + 1% H₂O

Acquisition Date 3/22/2023 10:40:46 AM

Operator MSC

Instrument amaZon speed ETD

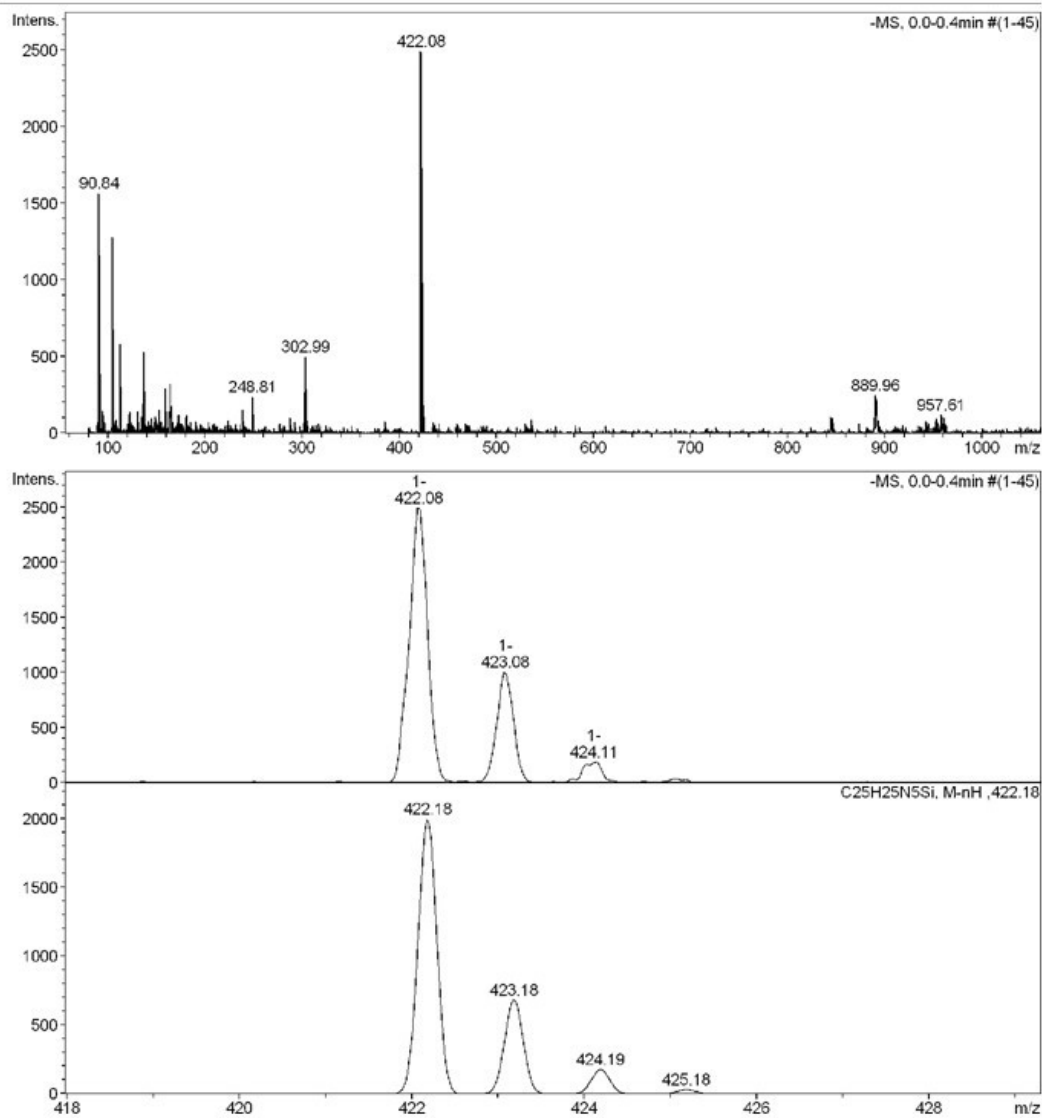


Figure S18. ESI(−) mass spectrum of **HL**^{TMS}.

NMR spectra of Zn(II) complex **2**

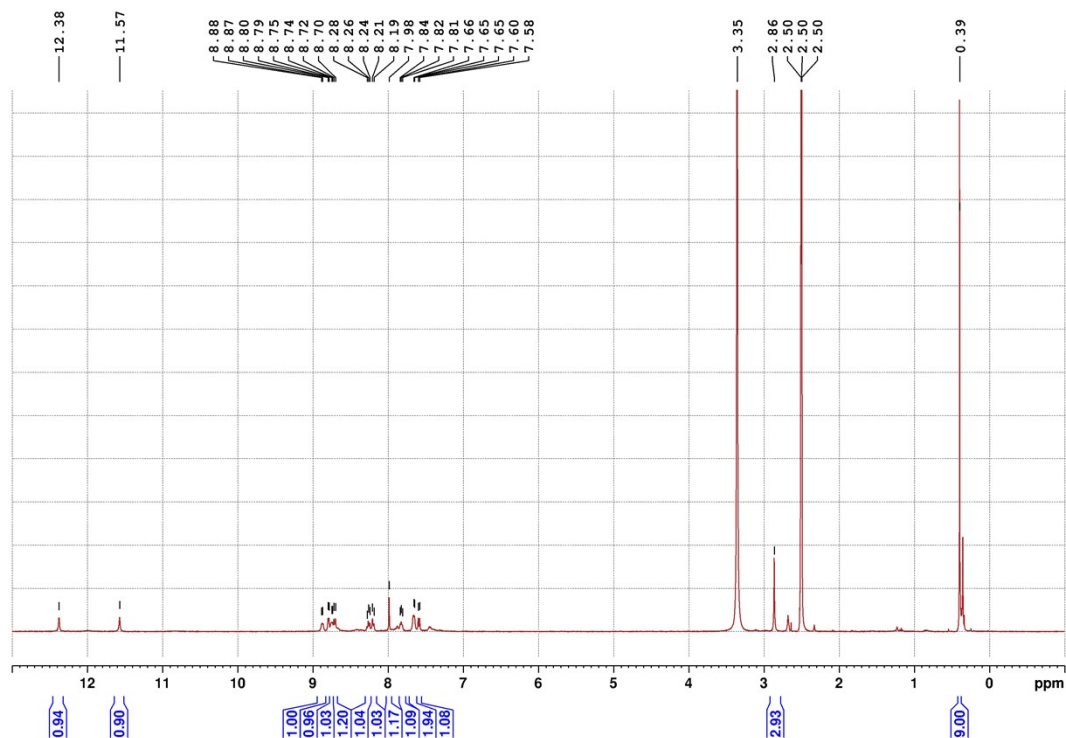


Figure S19. ^1H NMR spectrum of **2** in $\text{DMSO-}d_6$.

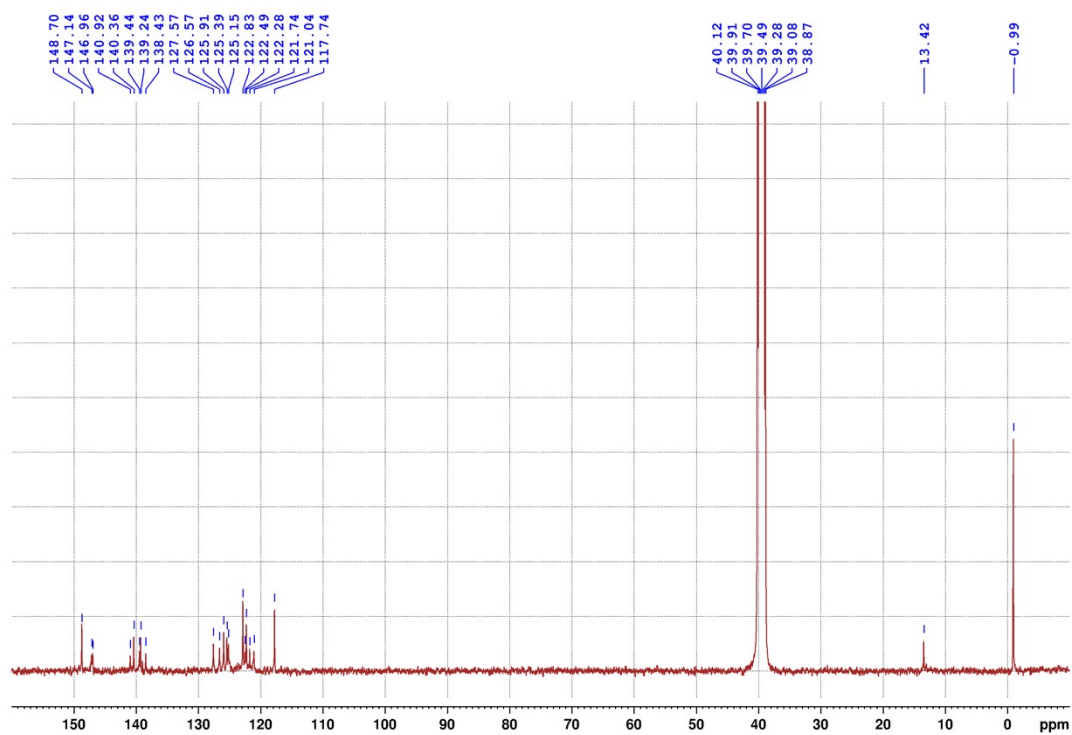


Figure S20. ¹³C NMR spectrum of **2** in DMSO-*d*₆.

ESI mass spectra of complexes 1 and 2

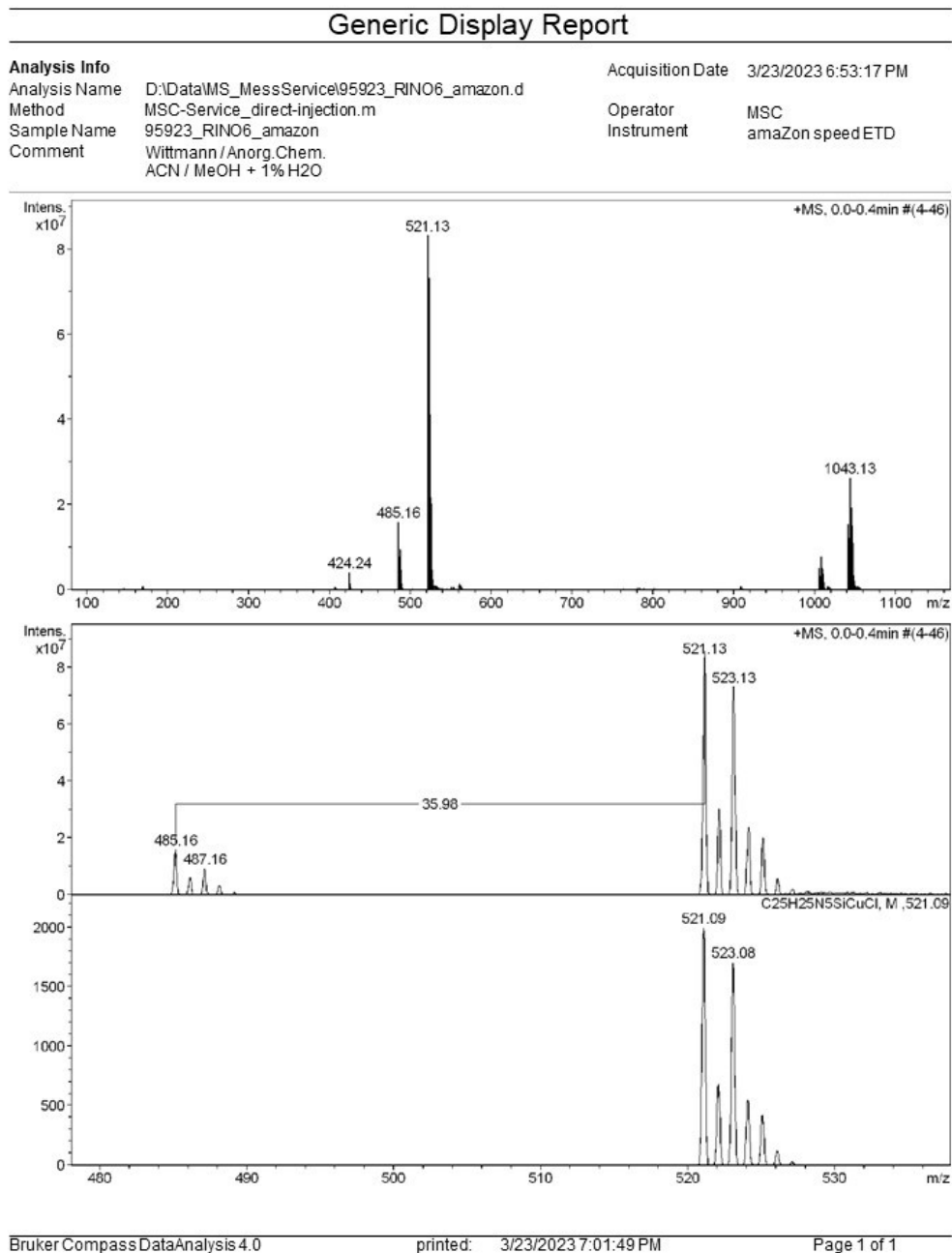


Figure S21. ESI(+) mass spectrum of **1**.

Generic Display Report

Analysis Info

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Method MSC-Service_direct-injection.m
Sample Name 95923_RINO6_amazon
Comment Wittmann / Anorg.Chem.
ACN / MeOH + 1% H₂O

Acquisition Date 3/23/2023 6:53:17 PM

Operator MSC

Instrument amaZon speed ETD

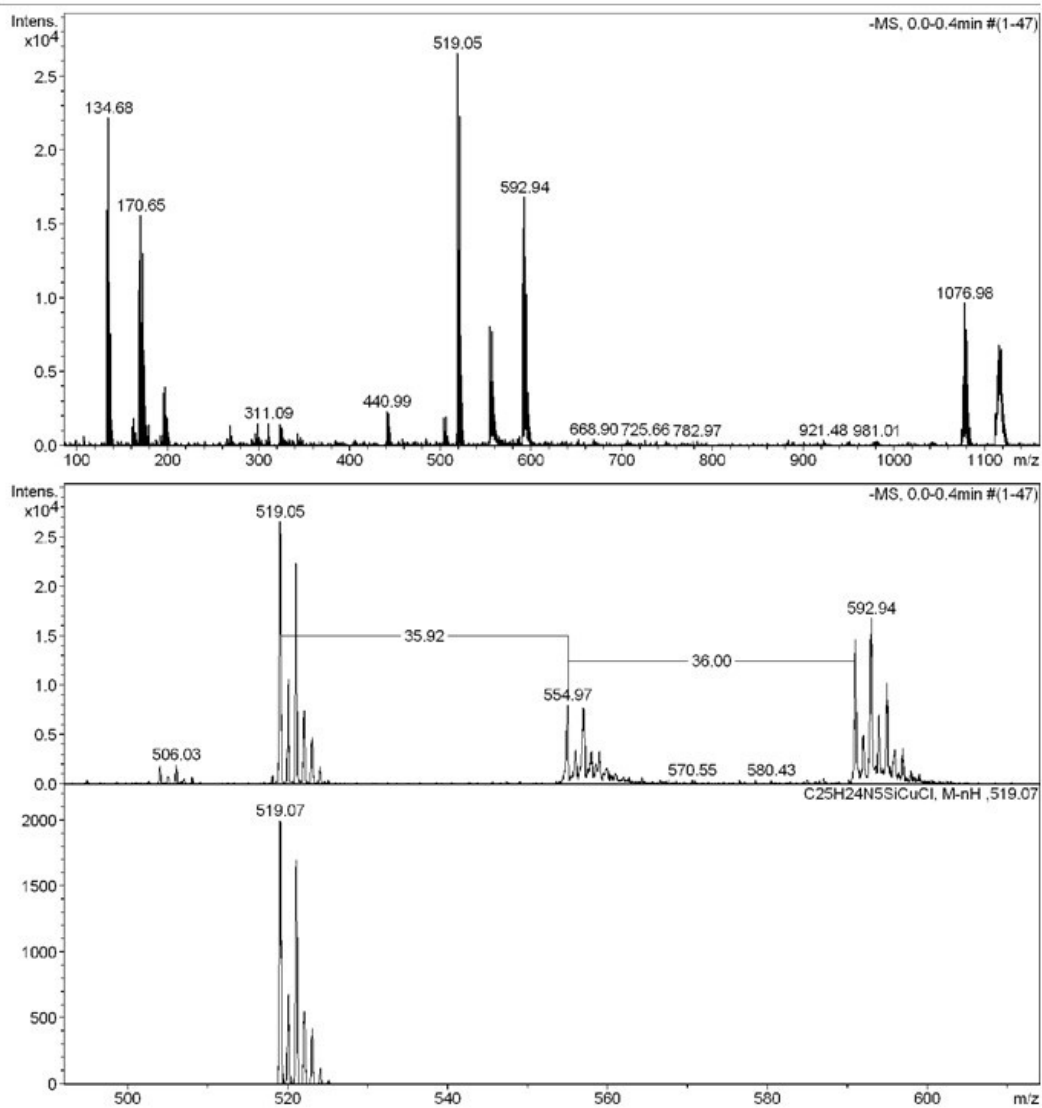


Figure S22. ESI(-) mass spectrum of **1**.

Generic Display Report

Analysis Info

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Method MSC-Service_direct-injection.m
Sample Name 96569_CHWI1157_amazon
Comment Wittmann / Anorg.Chem.
ACN / MeOH + 1% H₂O

Acquisition Date 4/26/2023 5:54:13 PM

Operator MSC

Instrument amaZon speed ETD

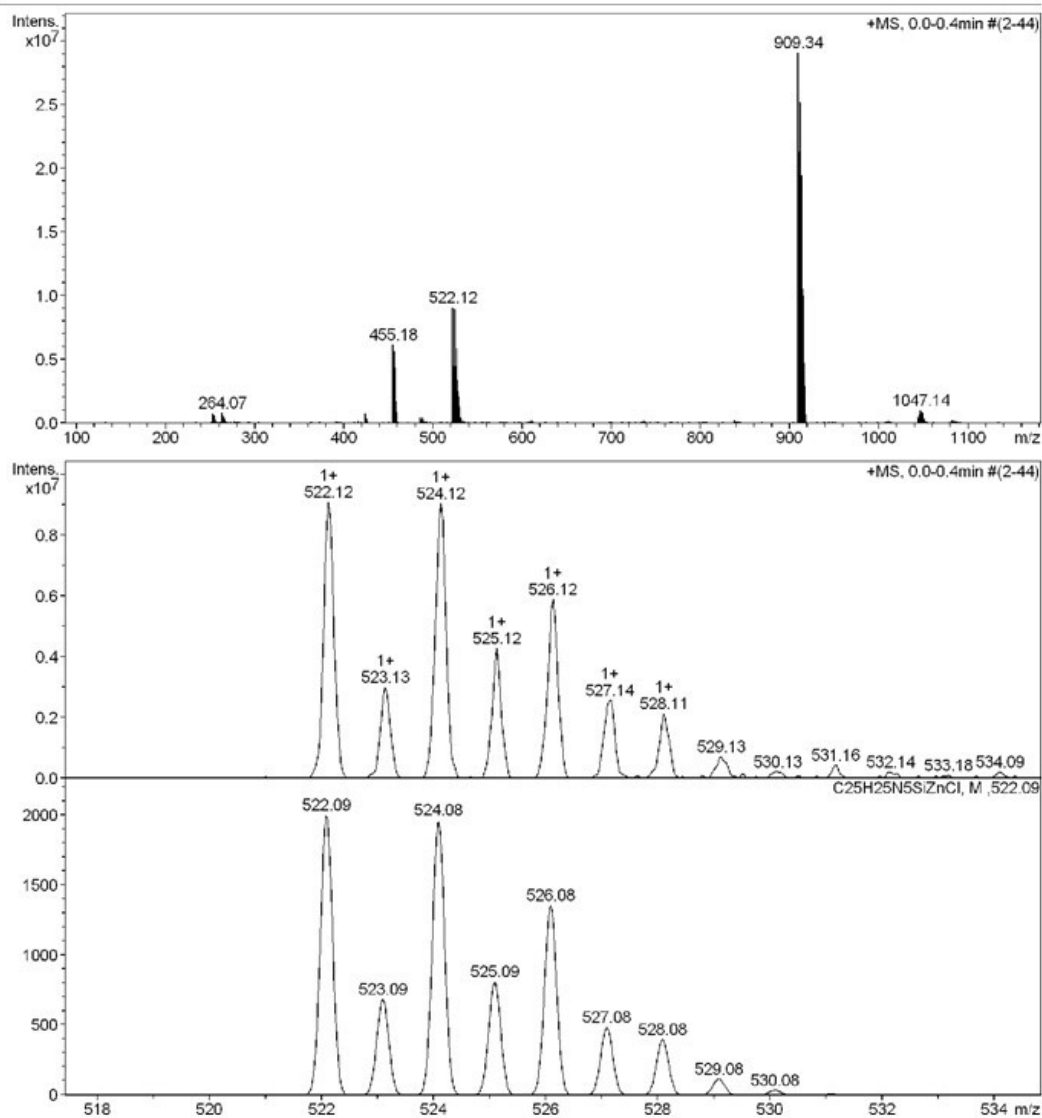


Figure S23. ESI(+) mass spectrum of **2**.

Generic Display Report

Analysis Info

Analysis Name D:\Data\MS_MessService\96569_CHWI1157_amazon.d
Method MSC-Service_direct-injection.m
Sample Name 96569_CHWI1157_amazon
Comment Wittmann / Anorg.Chem.
ACN / MeOH + 1% H2O

Acquisition Date 4/26/2023 5:54:13 PM

Operator MSC

Instrument amaZon speed ETD

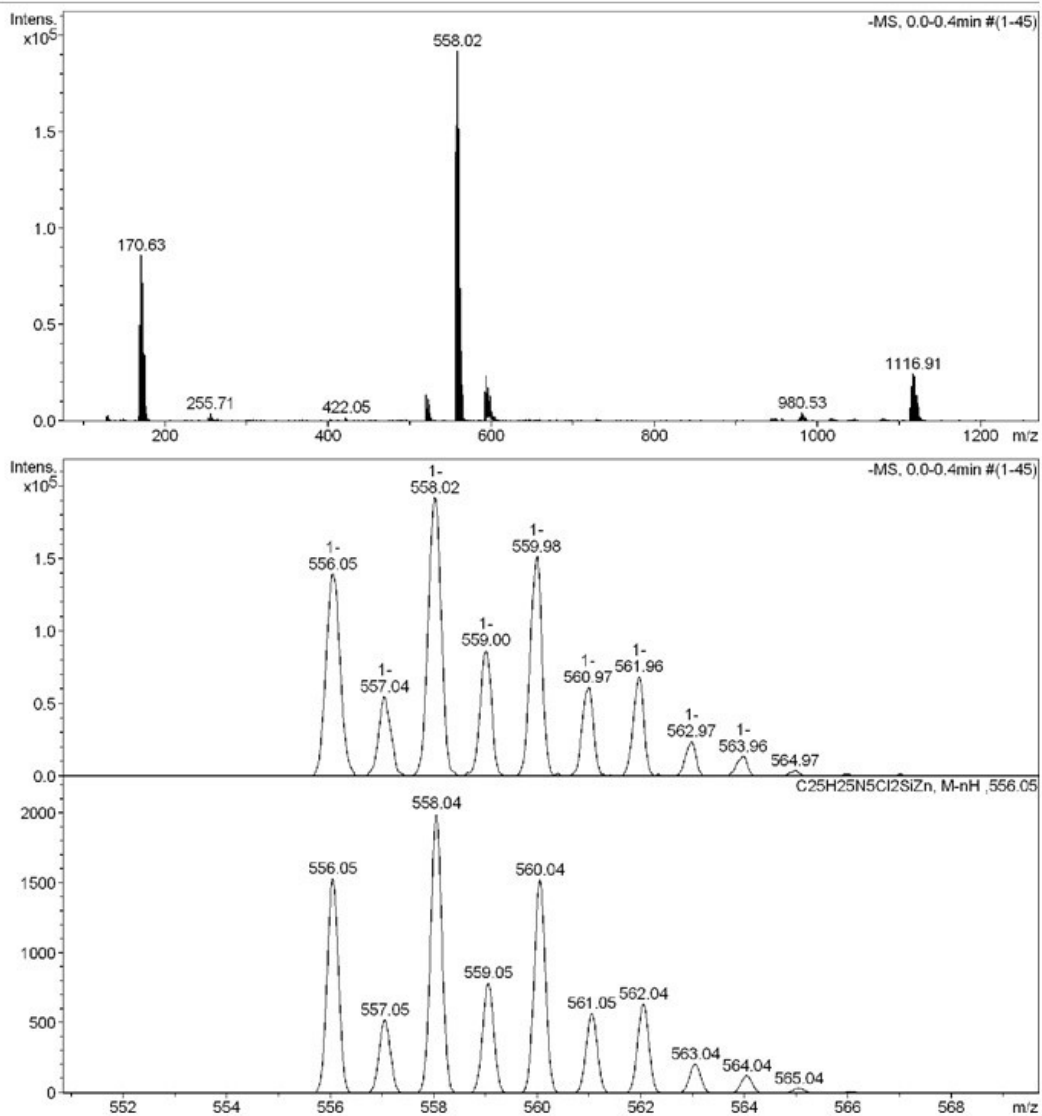


Figure S24. ESI(–) mass spectrum of **2**.

Crystallographic data

Table S1. Crystallographic data and refinement details for complexes studied.

Compound	1	2
empirical formula	C ₂₅ H ₂₅ Cl ₂ CuN ₅ Si	C ₂₅ H ₂₅ Cl ₂ N ₅ SiZn
fw	558.03	559.86
space group	monoclinic, <i>P</i> 2 ₁ / <i>c</i>	triclinic, <i>P</i> ¹
<i>a</i> , Å	13.1421(7)	7.2600(14)
<i>b</i> , Å	14.3009(7)	12.210(2)
<i>c</i> , Å	14.7259(9)	15.930(3)
α , °		72.75(3)
β , °	94.735(5)	81.99(3)
γ , °		85.37(3)
<i>V</i> [Å ³]	2758.2(3)	1334.3(5)
<i>Z</i>	4	2
λ [Å]	0.71073	0.02508
ρ_{calcd} , g cm ⁻³	1.344	1.393
cryst size, mm ³	0.10 × 0.07 × 0.02	0.005 × 0.0013 × 0.0005
<i>T</i> [K]	100(2)	294(2)
μ , mm ⁻¹	1.051	
<i>R</i> ₁ ^a	0.0854	0.2068
<i>wR</i> ₂ ^b	0.2770	0.4689
GOF ^c	0.894	1.382
CCDC no.	2378782	2378723

^a $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. ^b $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. ^c GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where *n* is the number of reflections and *p* is the total number of parameters refined.

Stability in solution

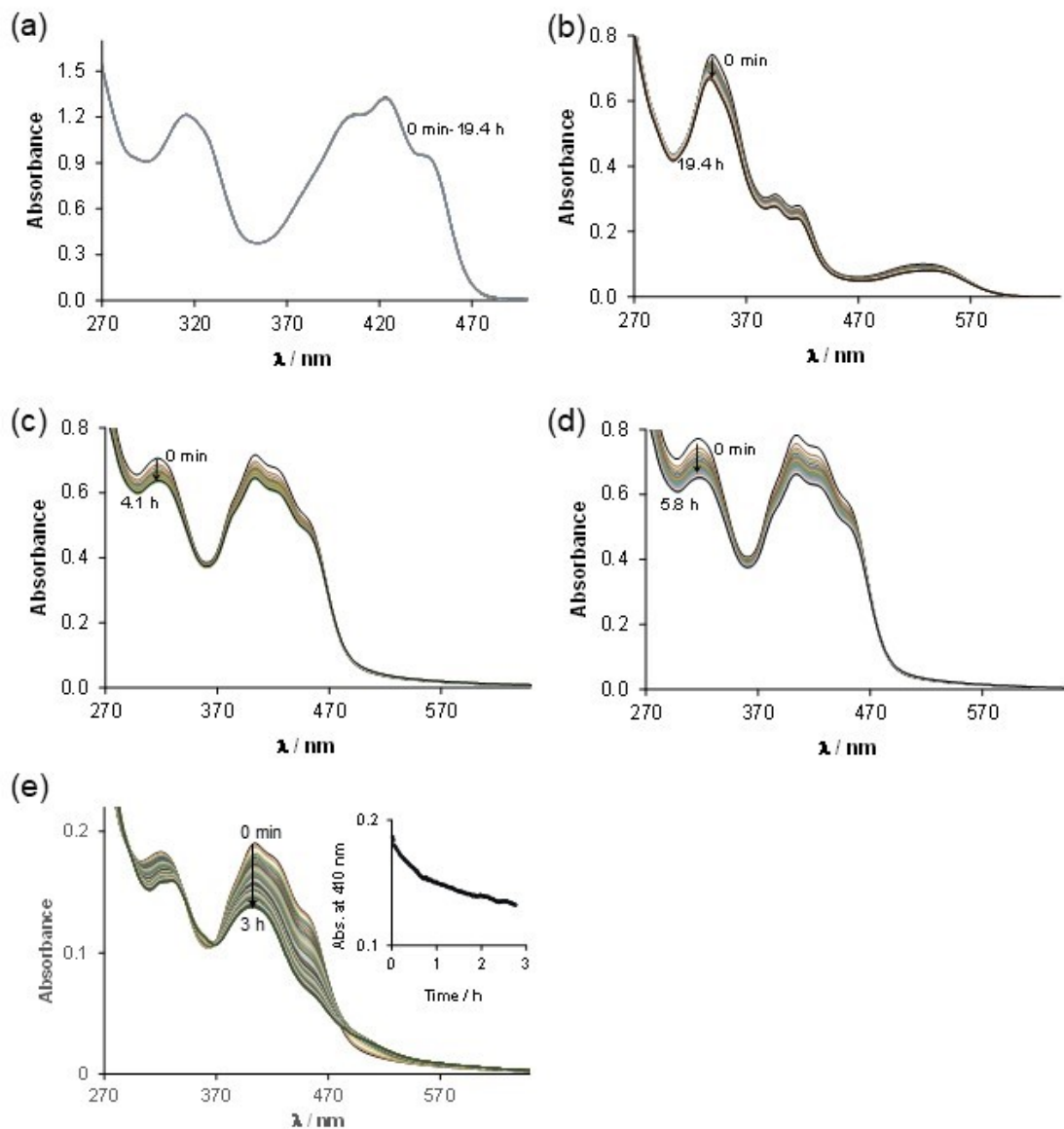


Figure S25. UV-vis absorption spectra recorded over time for HL^{TMS} in (a) DMSO, at pH (b) 2.0, (c) 7.4 (d) 11.7 and (e) at pH 7.4 under constant broad-band irradiation with a diode array photometer (D_2 + W lamp); $\{c = 50 \mu\text{M}$ (a-d) $12 \mu\text{M}$ (e); $\ell = 1 \text{ cm}$; $T = 25.0 \text{ }^\circ\text{C}\}$.

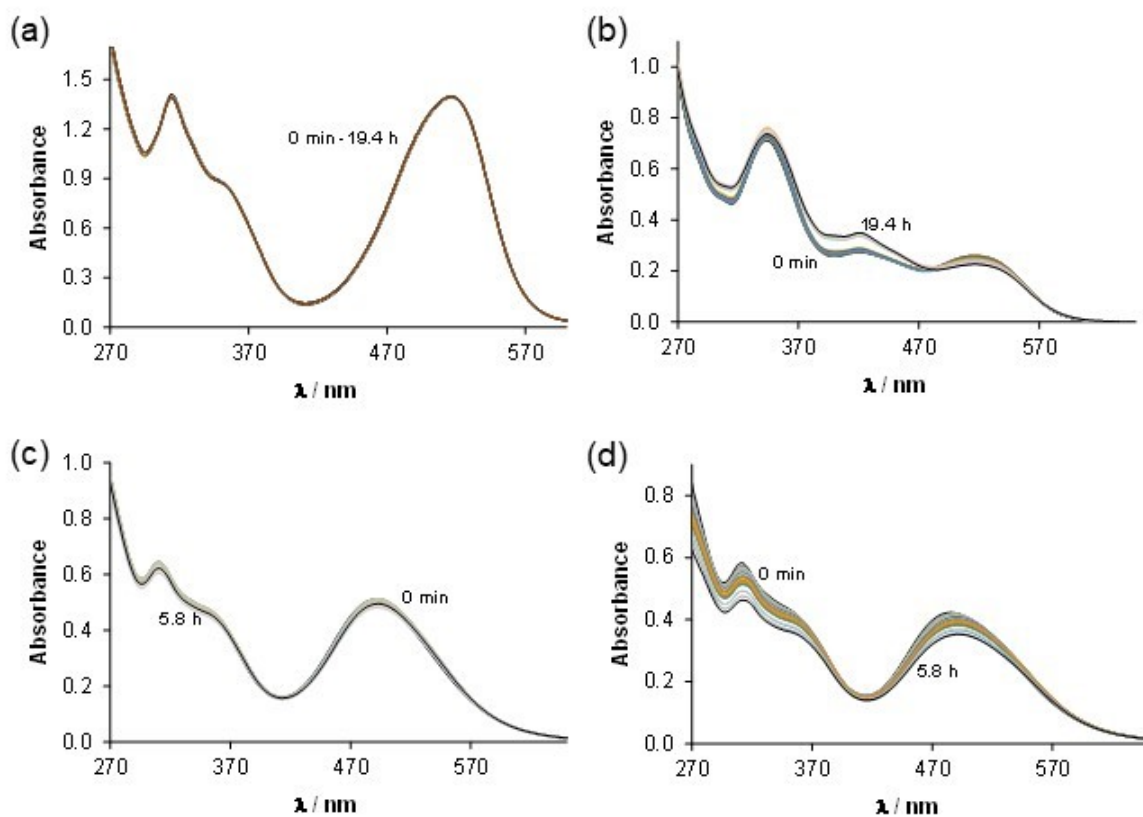


Figure S26. UV-vis absorption spectra recorded for **1** in a) DMSO, at pH b) 2.0, c) 7.4 and d) 11.7 over time; $\{c = 50 \text{ } \mu\text{M}; \ell = 1 \text{ cm}; T = 25.0 \text{ } ^\circ\text{C}\}$.

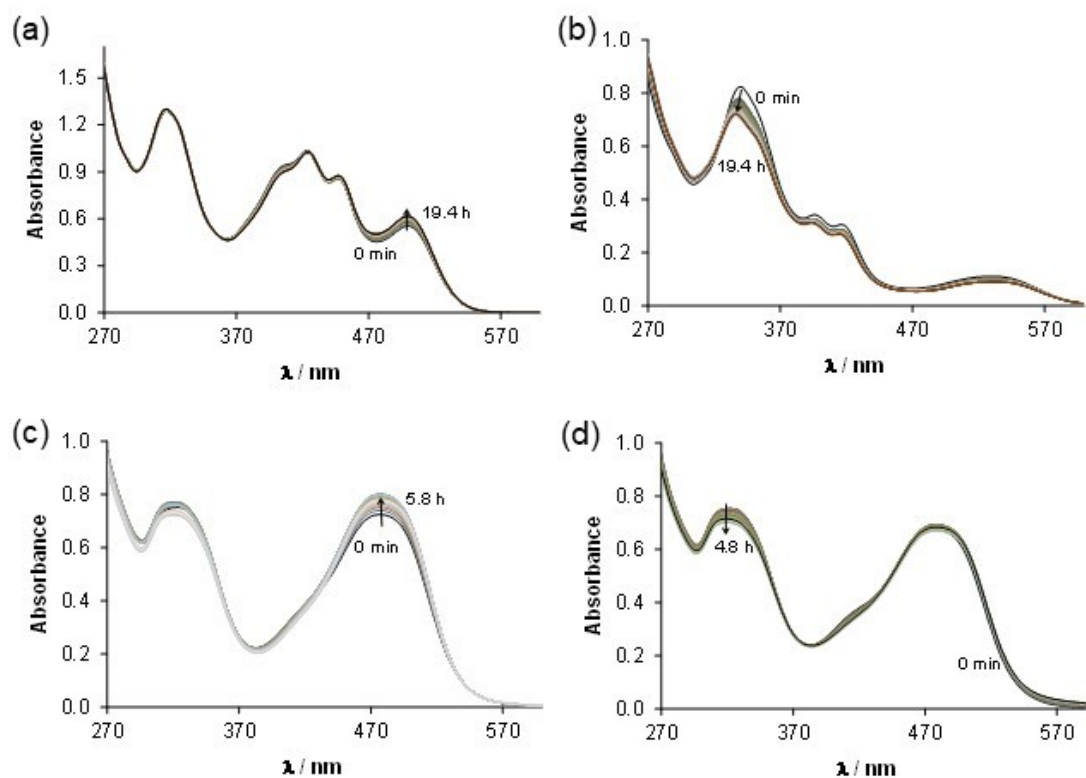


Figure S27. UV-vis absorption spectra recorded for **2** in (a) DMSO, at pH (b) 2.0, (c) 7.4 and (d) 11.7 over time; $\{c = 50 \text{ } \mu\text{M}; \ell = 1 \text{ cm}; T = 25.0 \text{ } ^\circ\text{C}\}$.

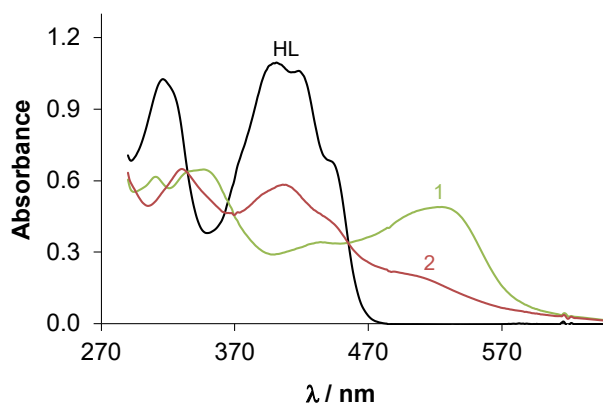


Figure S28. UV-vis absorption spectra recorded for the ligand **HL**^{TMS} and its complexes after dissolution in tetrahydrofuran; $\{c = 50 \text{ } \mu\text{M}; \ell = 1 \text{ cm}; T = 25.0 \text{ } ^\circ\text{C}\}$.

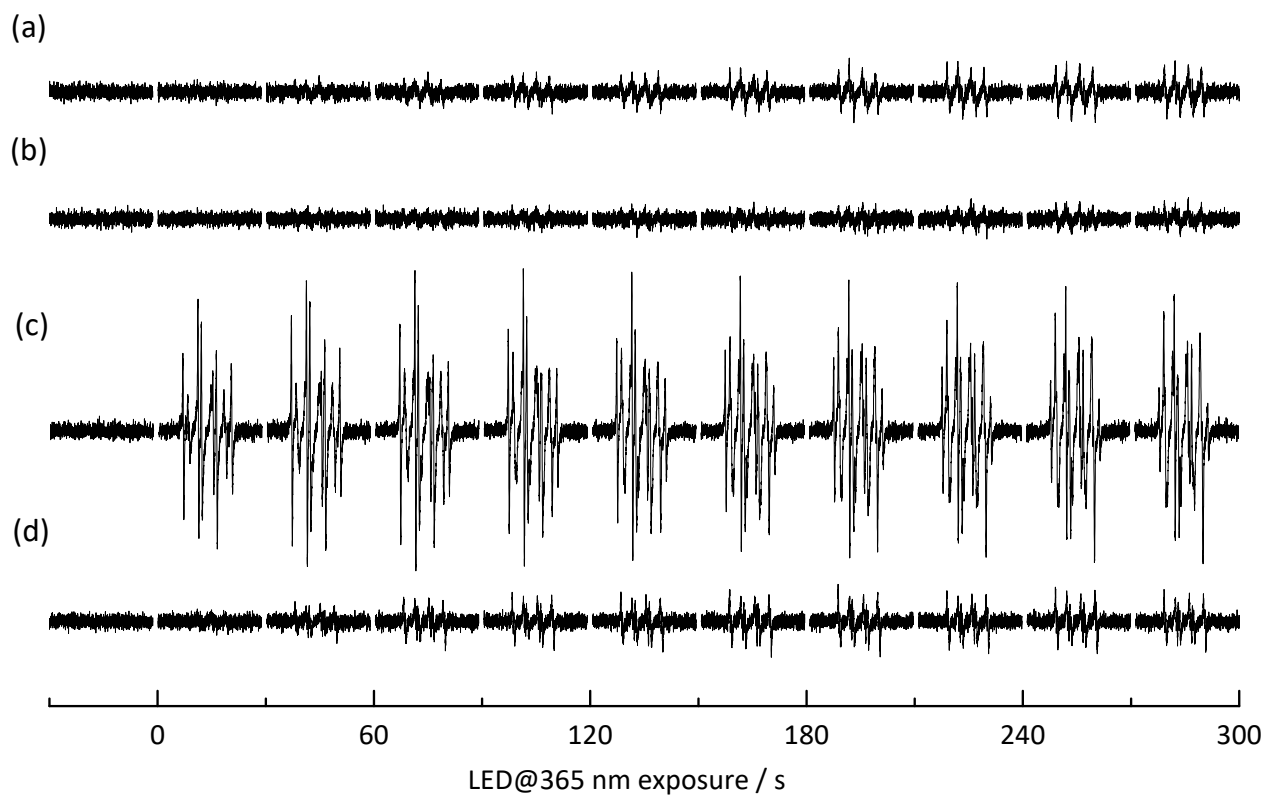


Figure S29. The time-courses of EPR spectra (SW = 10 mT) monitored upon LED@365 nm exposure (irradiance 18 mW cm^{-2}) of aerated (a) **HL**^{TMS}, (b) **1**, (c) **2** in the DMSO and (d) **2** in the 50% (v/v) DMSO:H₂O solutions containing spin trap DMPO. Initial concentrations: $c(\text{sample}) = 33 \text{ }\mu\text{M}$ and $c(\text{DMPO}) = 35 \text{ mM}$.

NCI-60 One-Dose Screening

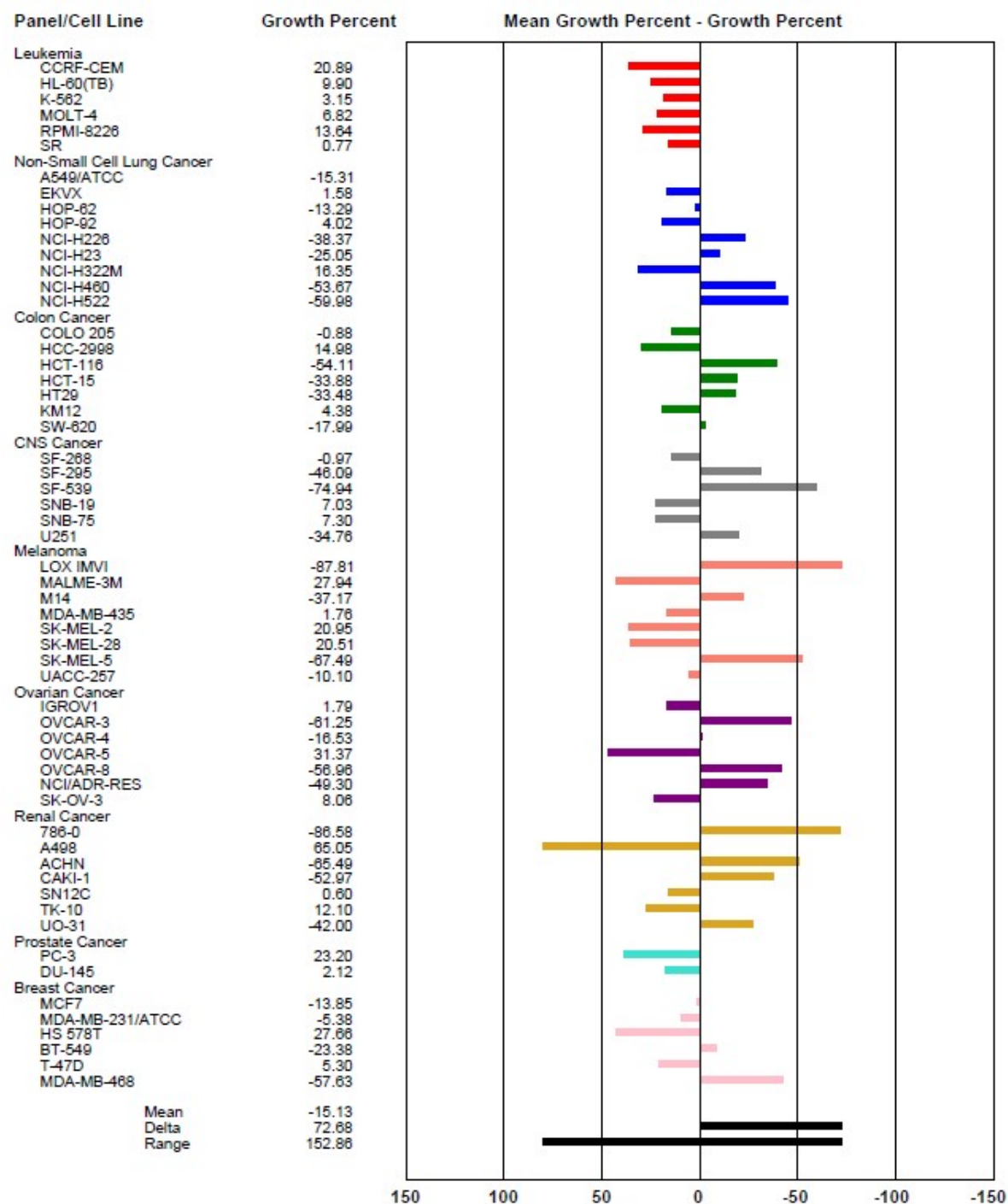


Figure S30. One-dose mean graph for HL^{TMS}.

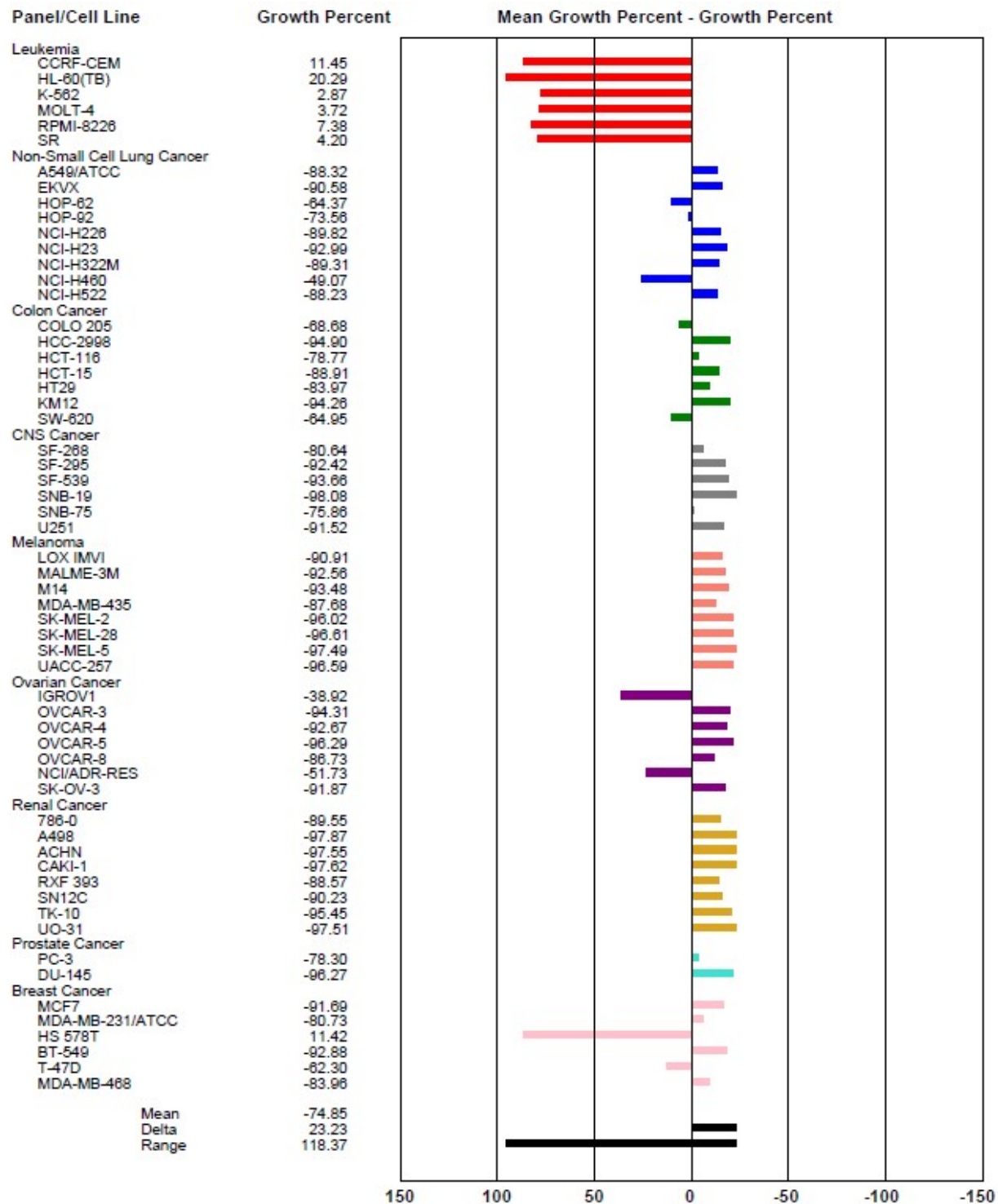


Figure S31. One-dose mean graph for 1.

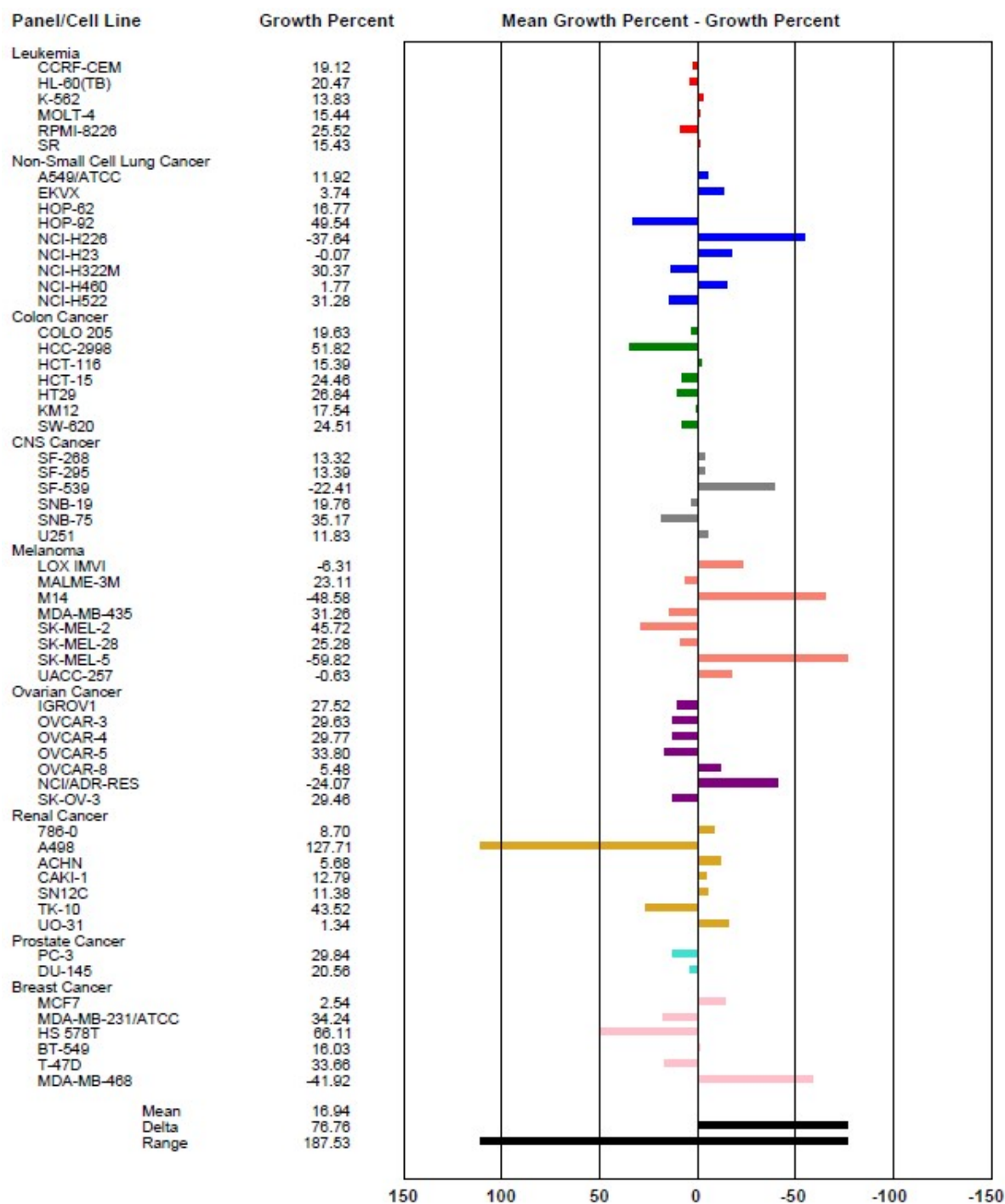


Figure S32. One-dose mean graph for 2.

NCI-60 Five-Dose Screening

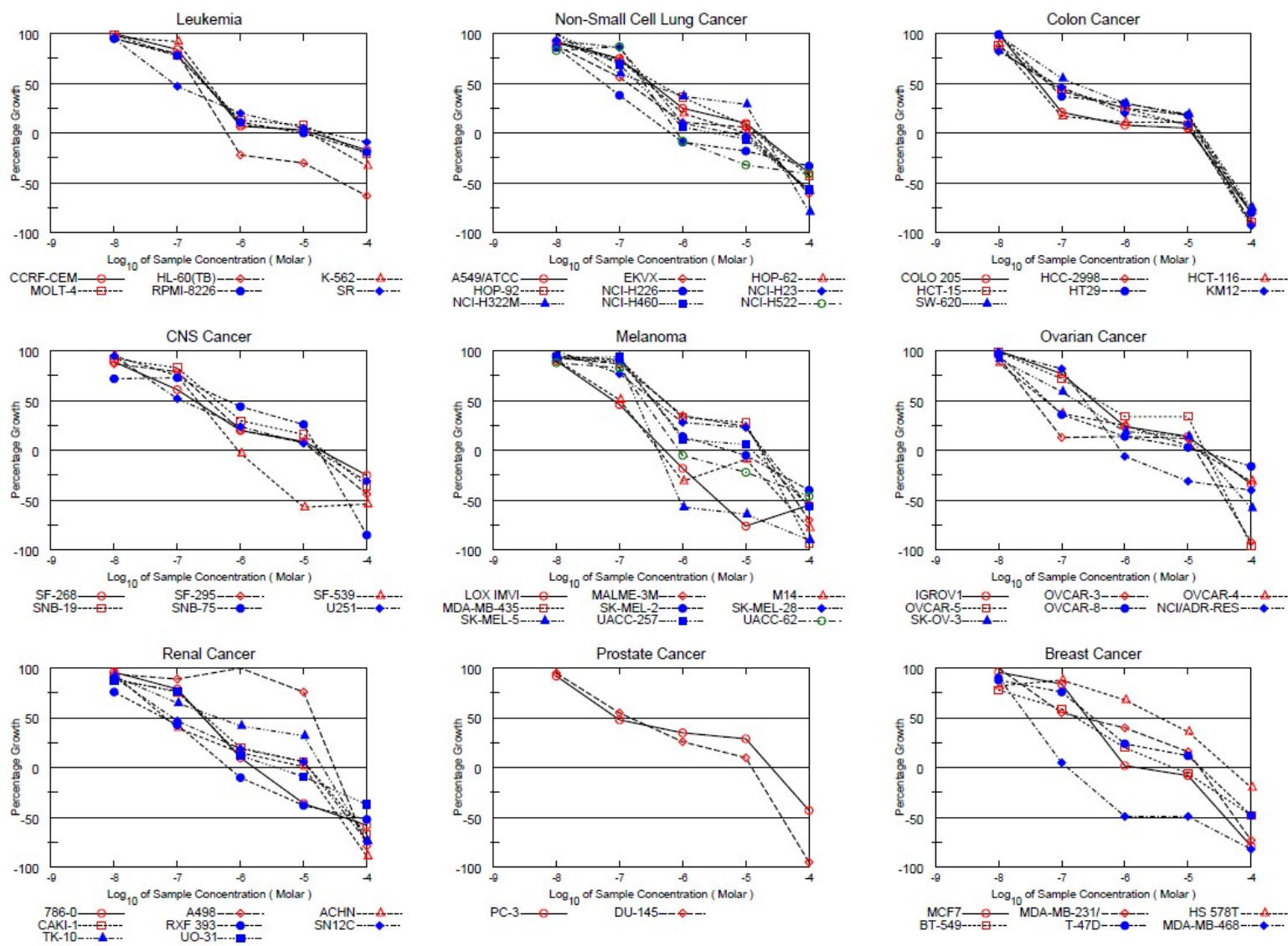


Figure S33. Dose response curves for HL^{TMS}.

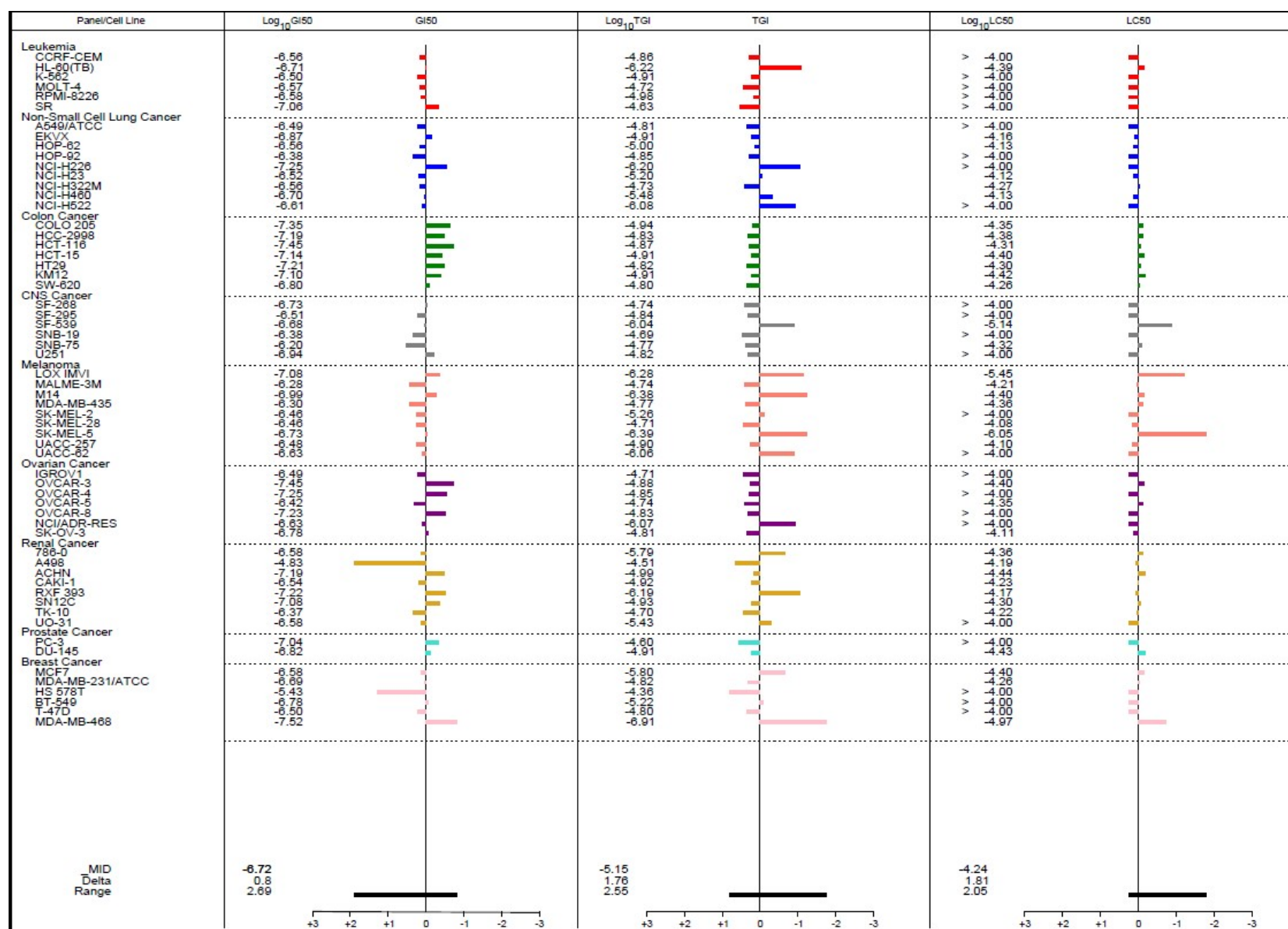


Figure S34. Five-dose mean graph for HL^{TMS}.

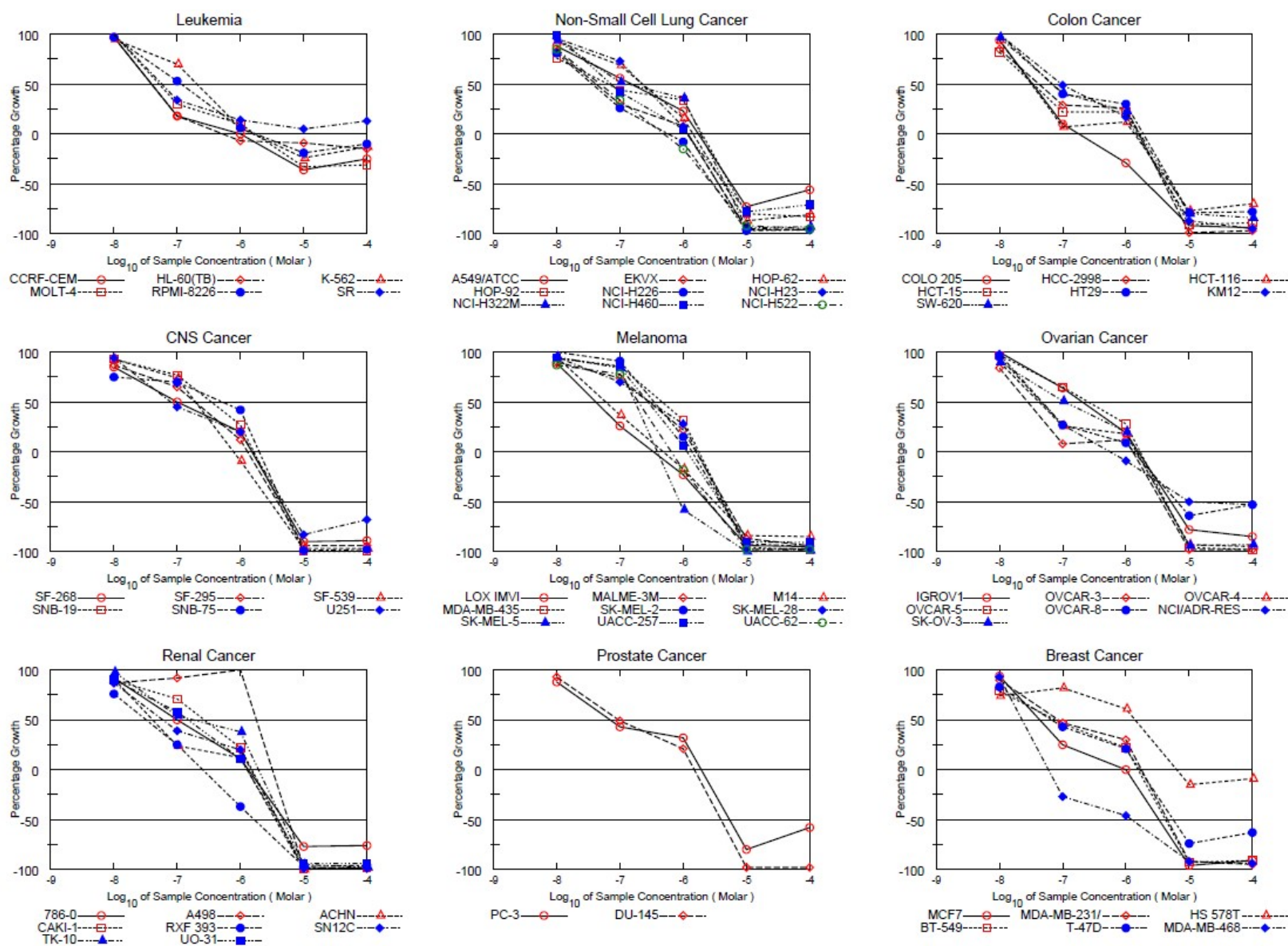


Figure S35. Dose response curves for 1.

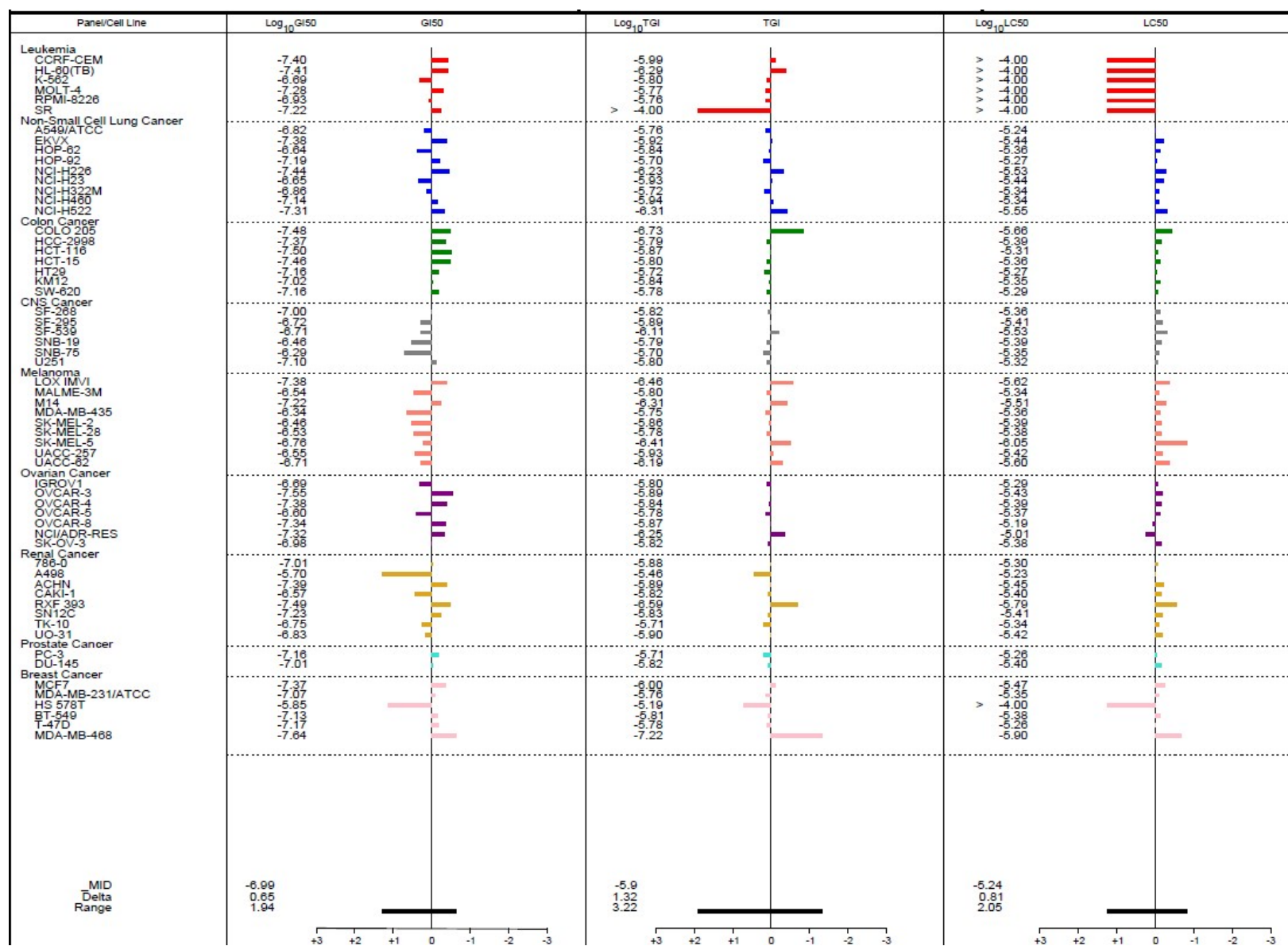


Figure S36. Five-dose mean graph for 1.

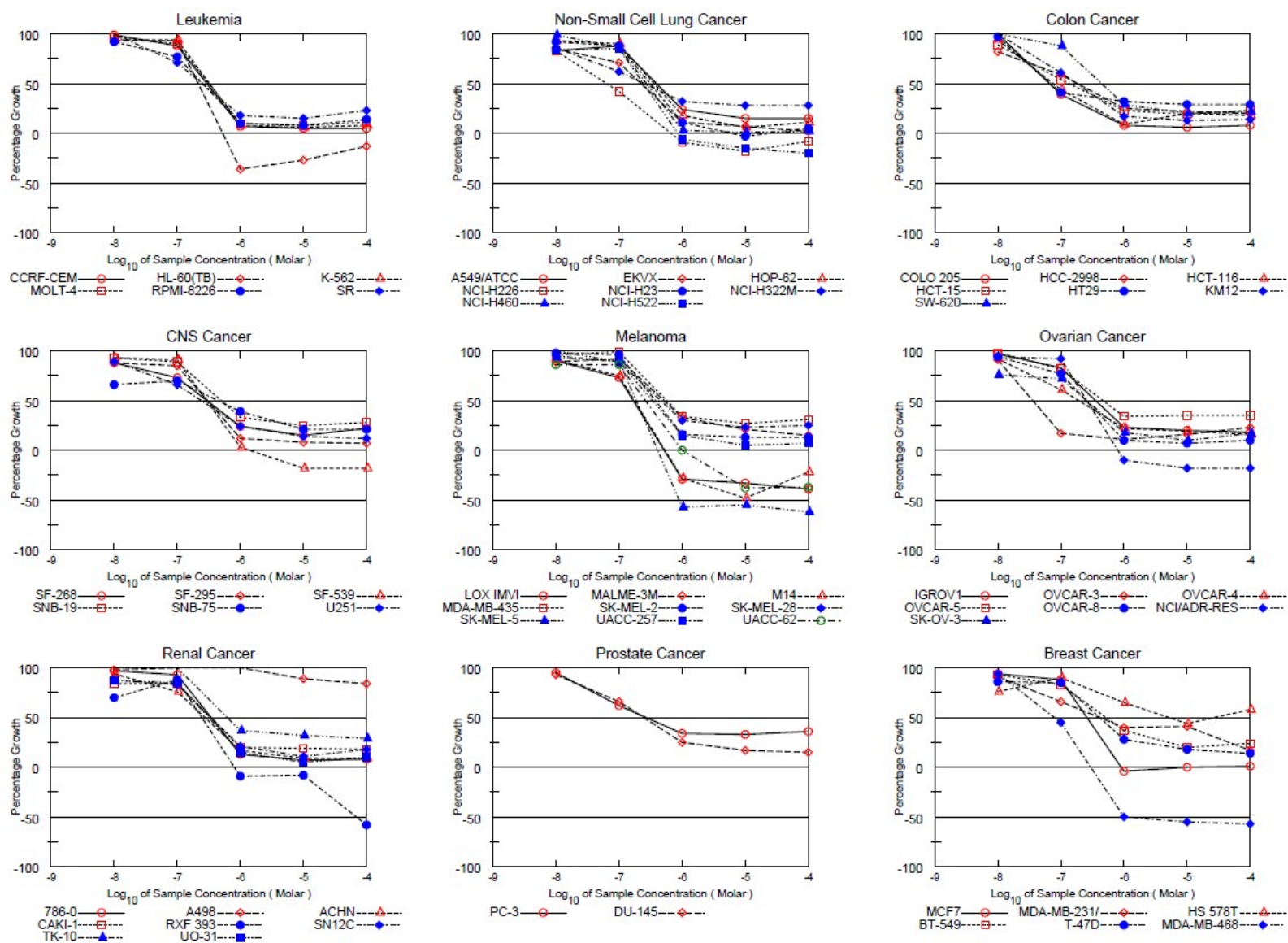
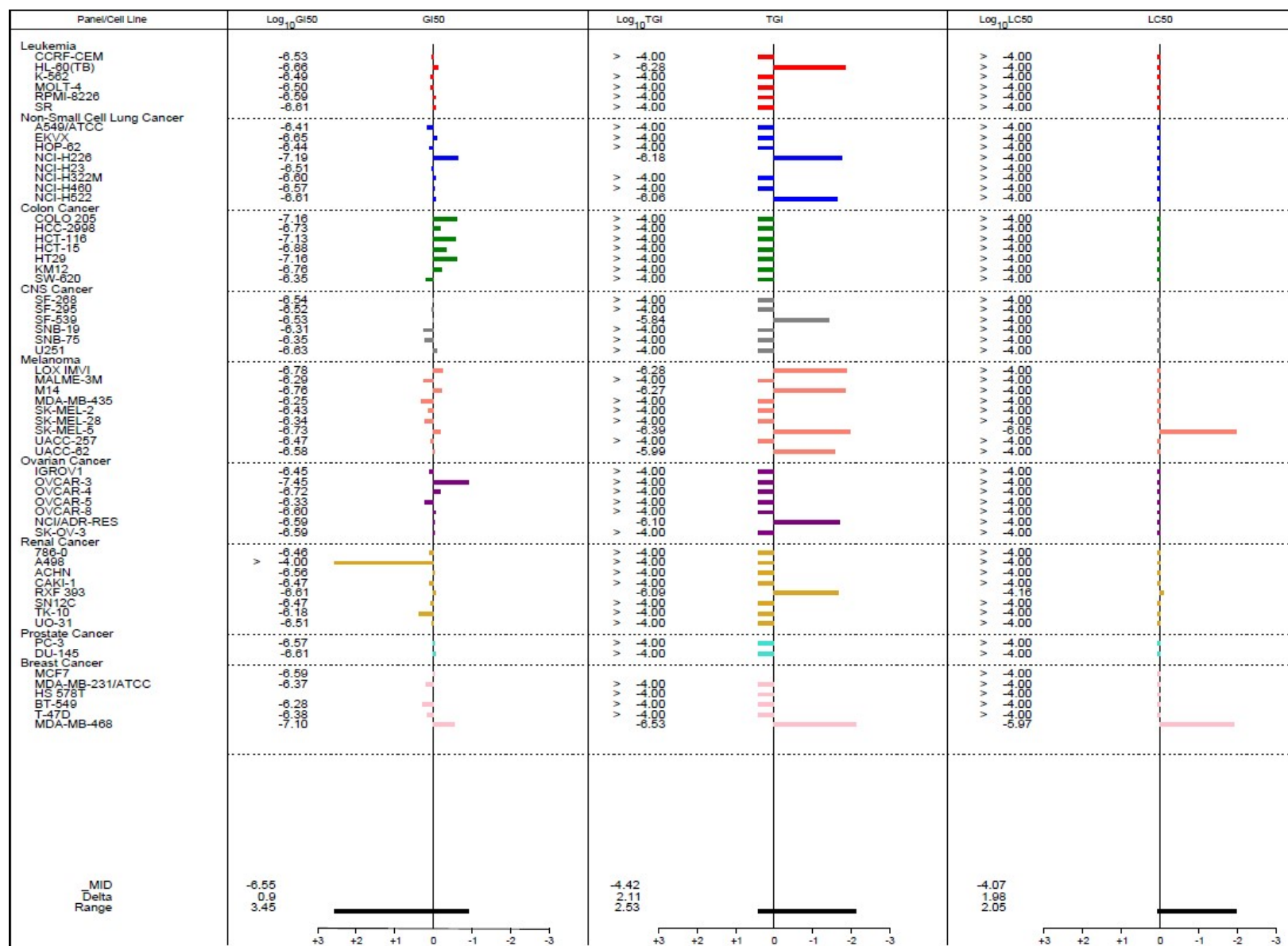


Figure S37. Dose response curves for 2.



Figure

S38.

Five-dose

mean

graph

for

2.

S40

