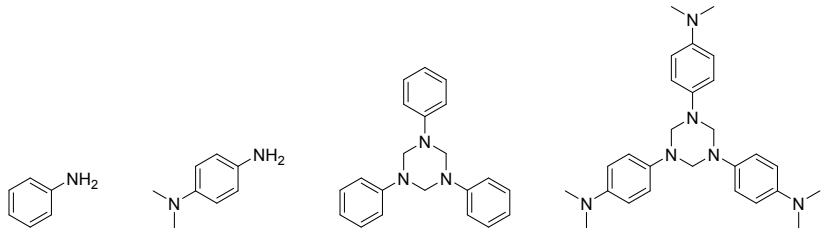
# Supporting Information

**Title**: Development of a portable and economical method of detecting trace metals from aqueous solution based on the coordination chemistry of 1,3,5-substituted hexahydrotriazines

**Authors:** Rudy J. Wojtecki, Alexander Y. Yuen, Gavin O. Jones, Thomas G. Zimmerman, Hans W. Horn, James L. Hedrick, and Jeannette M. García*

[a] *IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120 United States of America.*




**1A** **1B** **2A** **2B**

**Section (1) Materials & Methods.**

Reactions were performed in air and were stirred magnetically. *N,N*-Dimethyl-*p*-phenylenediamine (**1B**), 1,3,5-triphenyl-1,3,5-triazinane (**2A**), 4-nitroaniline and paraformaldehyde were purchased from Sigma-Aldrich and used as received. **1B** was opened and stored under an inert $N_2$ atmosphere. Acetone , methanol (MeOH), isopropanol (*i*-PrOH), diethyl ether ($Et_2O$), tetrahydrofuran (THF), and ethyl acetate (EtOAc) were purchased from J.T. Baker and used without further purification. Acetonitrile (MeCN) and dimethylsulfoxide (DMSO) were purchased from OmniSolv and used as received. $CDCl_3$, $d_4$-methanol, $d_3$-MeCN, $d_2$-DCM, $d_6$-DMSO, and $d_6$-acetone were purchased from Cambridge Isotope Laboratories (CIL) and used as received unless otherwise indicated. $CDCl_3$ was mixed and stored with $CaH_2$ and filtered with a 0.2um PTFE prior to usage.

**UV-Vis metal binding**

UV-Vis metal binding studies between **2A** and various metals were carried out with a Cary 5000 UV-VIS-IR spectrometer. Metal triflates (LiOTf, $Ca(OTf)_2$, $Eu(OTf)_3$, $Zn(OTf)_2$, and AgOTf) and **2A** were purchased from Sigma-Aldrich and used as received. GC/MS was performed on an Agilent 6890 Series GC system with a HP 5973 Mass Selective detector at 250°C for 30 min. TGA was performed with a temperature range from 30°C to 300°C and a ramp rate of 5°C/min with a TA Q-500. $^1$H NMR spectra were recorded on a Bruker Avance 400 spectrometer (400 MHz). Chemical shifts are

reported in ppm from tetramethylsilane with the solvent resonance as the internal standard [$d_6$-DMSO (2.50 ppm), $d_6$-acetone (2.05 ppm), $CDCl_3$ (7.26 ppm), $d_4$-methanol (3.31 ppm), $d_3$-MeCN (1.94 ppm), and $d_2$-DCM (5.32 ppm)]. $^1$H NMR peaks are reported in δ (ppm) as s (singlet), d (doublet), or t (triplet). $^{13}$C-NMR spectra were recorded at 100.6 MHz and was referenced to the solvent signal: $d_6$-DMSO (39.5 ppm).

Absorption spectra (200nm to 350 nm) were taken before and after each titration. The concentration of **2B** in the solvent system (80 vol % MeCN, 20 vol % DCM) was maintained at 25 µM. Metal titrations were performed over a range of 0:1 to ~2:1 (metal to hexahydrotriazine ratios). Metal triflates (LiOTf, $Ca(OTf)_2$, $Eu(OTf)_3$, $Zn(OTf)_2$, and AgOTf) were used in this study.

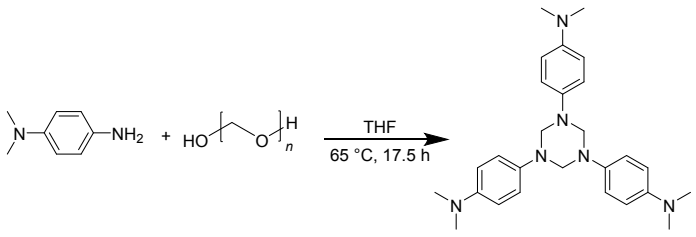
**$^1$H-NMR metal binding**

**2A** and **2B** were paired with triflate salts individually, and were studied using $^1$H-NMR spectroscopy. Same triflates salts were used from the UV-Vis studies. Samples were prepared at 10µM concentration of **2A** or **2B** in a solvent system composed of $d_3$-MeCN (80 vol. %) and $CD_2Cl_2$ (20 vol. %). Triflate salts (up to stoichiometric quantities) were introduced to the hexahydrotriazines and re-scanned with $^1$H-NMR analysis.

**Section (2) Synthesis of Triazines.**

**Synthesis of 4,4',4"-(1,3,5-triazinane-1,3,5-triyl)tris(N,N-dimethylaniline)**

**Scheme S1**. Representative procedure for the synthesis of 4,4',4"-(1,3,5-triazinane-1,3,5-triyl)tris(*N*,*N*-dimethylaniline) (**2B**).




**1B** **2B**

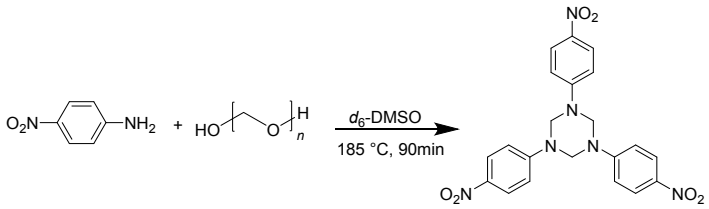
A 20-mL vial was charged with **1B** (1.36 g, 10.0 mmol), paraformaldehyde (0.30 g), and THF (20 mL). Reactions were heated in a sand bath set to 65 °C for 17.5 hours. Afterwards, the vial was removed from the hot sand and allowed to cool to room temperature. The solvent was then evaporated off using a rotary evaporator, the remaining solids were collected (1.48g, ≥95% purity by $^1$H NMR). The

solids were then washed with 200mL of diethyl ether and recollected (0.95g , ≥95% purity by $^1$H NMR). The products were then recrystallized by first dissolving products in hot EtOAc (50mL). Afterwards, diethyl ether (150mL) was added. The products were then allowed to recrystallize in a -20°C fridge overnight. 0.45g of crystals were isolated, pure (≥97% purity) by $^1$H NMR.

$^1$H-NMR: (400 MHz, $(CD_3)_2SO$) δ 6.97-6.95 (d, J = 8 Hz, 6H), 6.66-6.64 (d, J = 9Hz, 6H), 4.52 (s, 6H), 2.78 (s, 18H). $^{13}$C-NMR: (400 MHz, $(CD_3)_2SO$) δ 145.5, 139.7, 119.1, 113.9, 70.0, 40.95. IR (KBr): 2841(s), 2790(s), 1516(s), 1481(w), 1445(w), 1396(w), 1331(m), 1272(w), 1253(w), 1223(m), 1174(m), 972(m), 945(m), 886(w), 802(m). GC/MS: *m/z* 52, 60, 65, 77, 93, 106, 121, 131, 136, 147.

**Triazine synthesis with 4-nitroaniline**

**Scheme S2.** Representative procedure to synthesize a hexahydrotriazine with 4-nitroaniline.




The reaction was performed in an NMR tube and in ambient atmosphere. To prepare the reaction, 4-nitroaniline (13.8 mg, 10.0 µmol) was combined with paraformaldehyde (3.0 mg) and $d_6$-DMSO (0.7 mL). The NMR tube was then placed in a sand bath set to 185°C. $^1$H-NMR spectra were taken at t=0 min, 10 min, and 90 min. Attempts to synthesize HTs with electron deficient functional groups with 4-nitroaniline in Scheme S2 were unsuccessful and resulted in the formation multiple undesired side products. This was attributed to a diminishment in nucleophilicity of the electron-poor aniline towards formaldehyde.

**Table S1.** Conversion from starting amine to triazine as measured in a variety of solvent systems by 1H-NMR.

| Entry | Solvent | Conversion to **2B** (%)[a] |
|---|---|---|
| ***i*** | ***THF*** | ***>98*** |
| ii | MeCN | 80 |
| iii | EtOAc | 73 |
| iv | MeOH | 30 |
| v | *i*-PrOH | 29 |
| vi | Acetone | 23 |

[a]Calculated from crude $^1$H NMR spectroscopic analysis in $d_6$-DMSO (standard conditions were 0.5 M and 4 h at 65 °C).

## Section (3) Degradation Study.

Degradation studies with **2B**, **1B**, 4-nitroaniline, and **2A** were performed individually in various deuterated solvents, including $CDCl_3$, $d_4$-methanol, $d_3$-MeCN, $d_2$-DCM, $d_6$-DMSO, and $d_6$-acetone. Samples were prepared by pairing 5.0 mg of material (aniline or triazine) with 0.70 mL of a deuterated solvent in NMR tubes; each tube consisted of a unique material/deuterated solvent combination.

**Table S2.** Decomposition studies of hexahydrotriazines and starting materials in various solvents. Chemical change was determined by $^1$H NMR analysis.

| | | Deuterated solvent | | | | | |
|---|---|---|---|---|---|---|---|
| | | $d_6$-acetone | $CDCl_3$† | $d_6$-DMSO | $d_4$-methanol | $d_3$-MeCN | $d_2$-DCM† |
| Material | **2B** | Insoluble | Stable | Stable | Insoluble | Insoluble | Stable |
| | **2A** | Stable | Stable | Stable | Degrades | Stable | Stable |

† Solvents treated using base followed by syringe filtering before use.

**Table S3.** $^{1}$H NMR results on the titration of HTs 1B and 2B with stoichiometric quantities of metal triflates.

| | | | | Compound (**1B**) | | Compound (**2B**) | |
|---|---|---|---|---|---|---|---|
| Metal salt | classification | oxidation state | atomic radius (pm)[d] | $d_6$-DMSO | $d_3$-MeCN (80%) $d_2$-DCM (20%) | $d_6$-DMSO | $d_3$-MeCN (80%) $d_2$-DCM (20%) |
| AgOTf | soft[b] | +1 | 129 | No change | No change | Degradation | Degradation |
| $Zn(OTf)_2$ | borderline[b] | +2 | 74 | No change | Degradation | No change | Degradation |
| $Eu(OTf)_3$ | borderline[c] | +3 | 94.7 | No change | Degradation | Signal broadening | Degradation |
| $Ca(OTf)_2$ | hard[b] | +2 | 114 | No change | No change | No change | Signal broadening |
| LiOTf | hard[b] | +1 | 90 | No change | No change | No change | Signal broadening |

[a]Comparisons were made prior to and after adding metal salt (0.10 mM) in specified solvents. [b]Classified according tothat reported in Pearson, R. C. *J. Am. Chem. Soc.* 1963, **85**, 3533. cBruch, M. "NMR Spectroscopy Techniques" 2nd Ed. CRC Press, 1996 p. 263. [d]Crystal ionic radii, as reported in Shannon R, D. *Acta Cryst* 1976, **A32**, 751.

**Section (4): NMR spectra related to the synthesis and purification of 2B.**

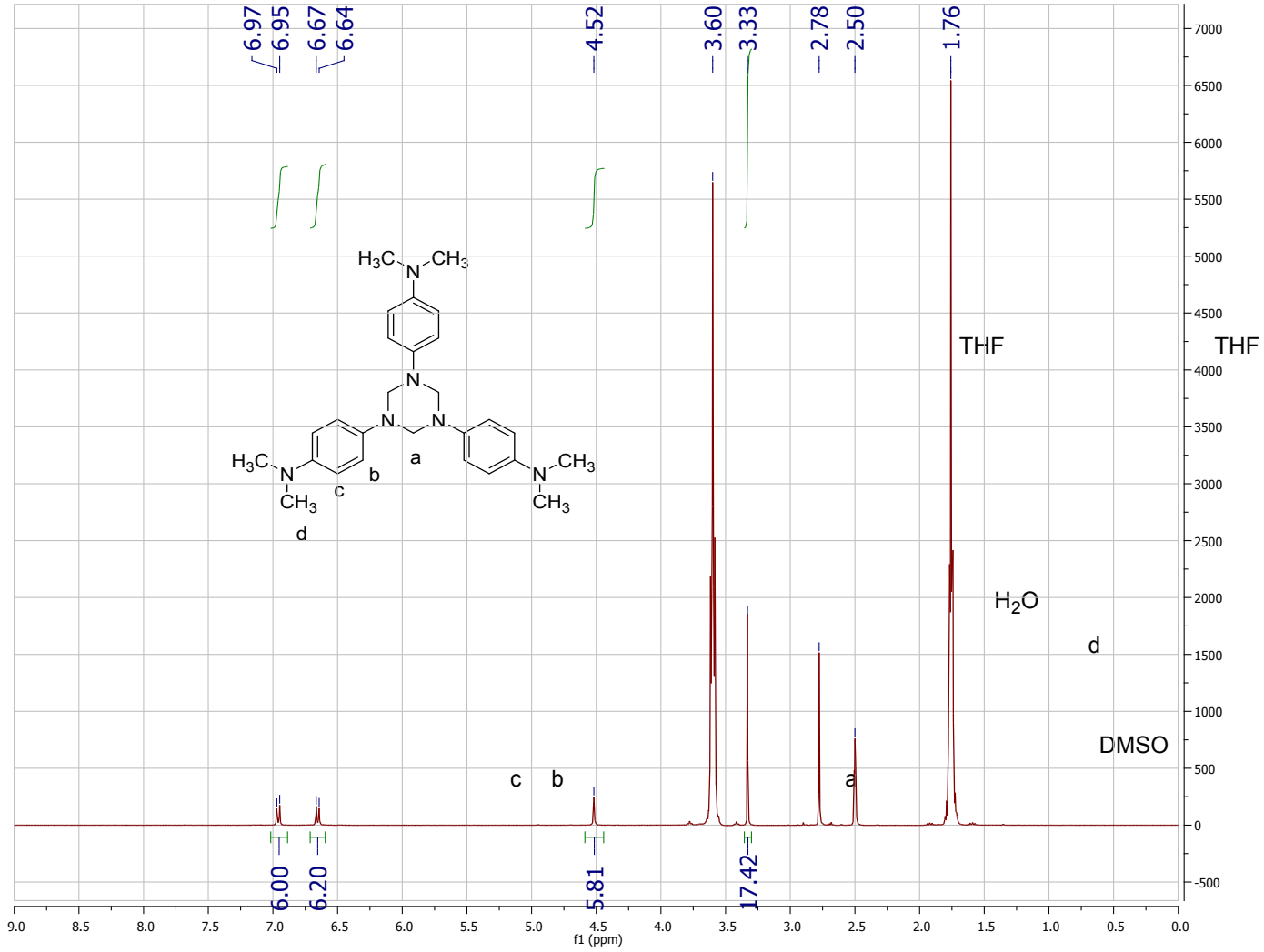



**Figure S1.** $^{1}$H NMR of **2B** in $d_6$-DMSO. Crude.

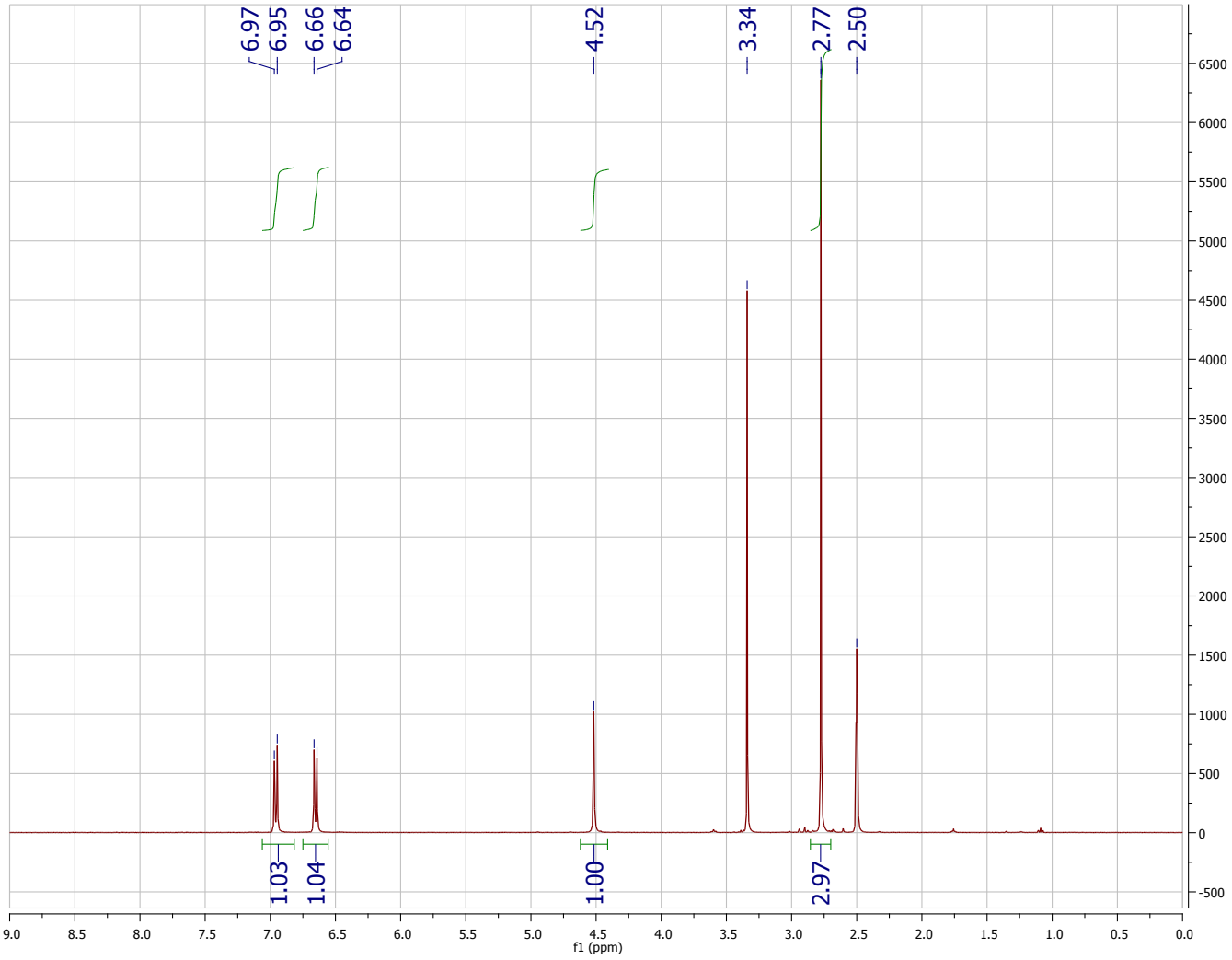



**Figure S2**. $^{1}$H NMR of **2B** in $d_6$-DMSO, after diethyl ether wash.

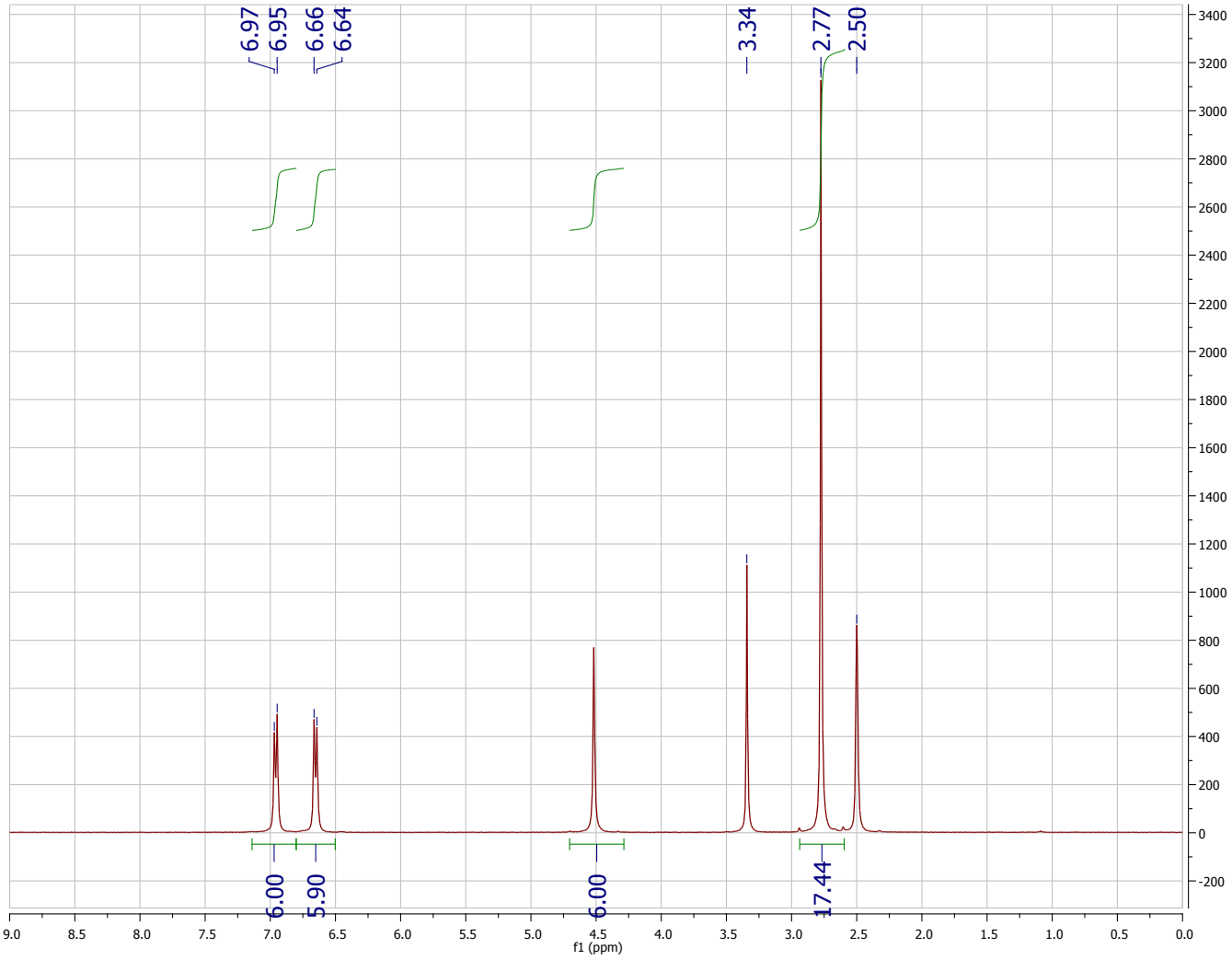



**Figure S3**. $^{1}$H NMR of **2B** after recrystallization.

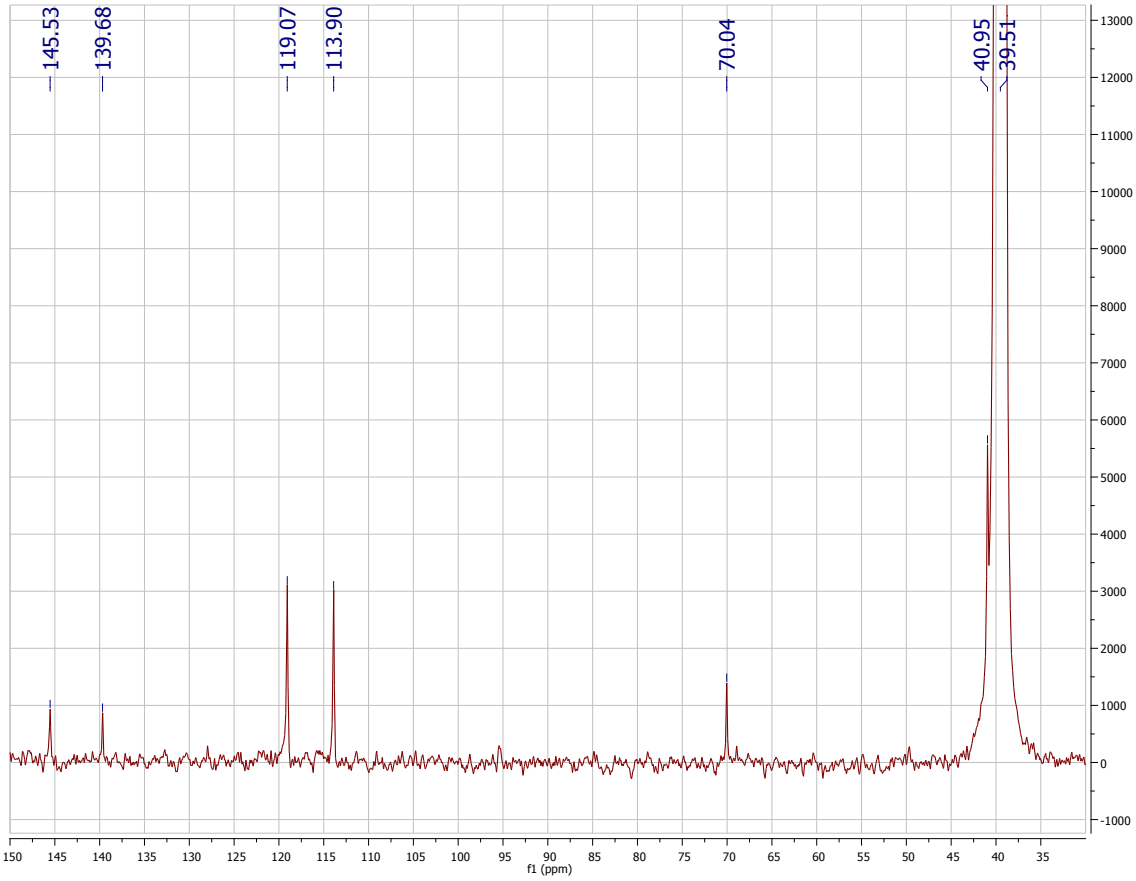



**Figure S4.** $^{13}$C-NMR (400 MHz) of **2B** in $d_6$-DMSO.

**Section (5): TGA of 2B.**

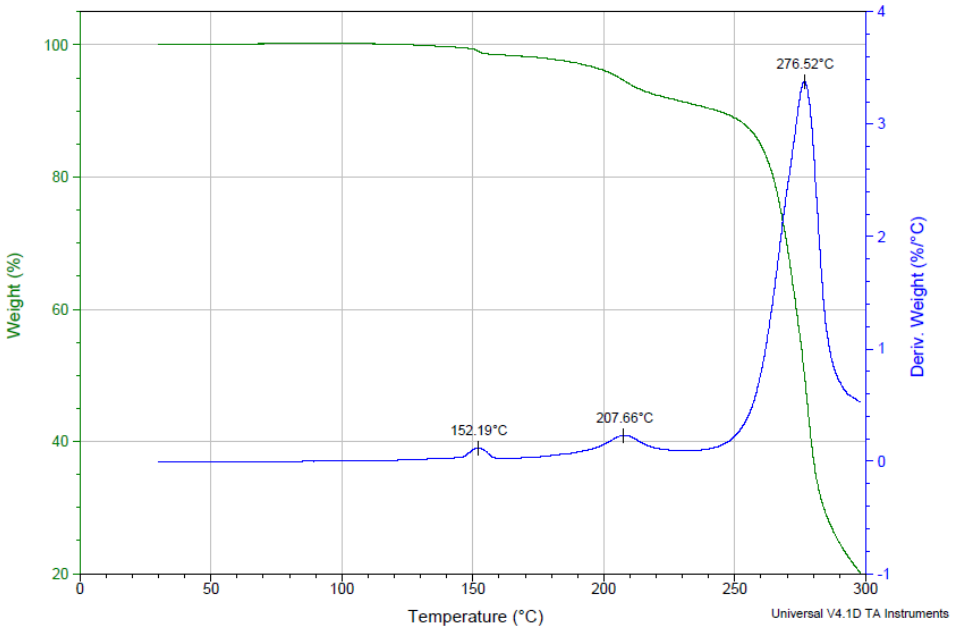



**Figure S5.** TGA of **2B**. Temperature range of 30°C-300°C, with ramp rate of 5°C/min.

**Section (6): NMR spectra related to the degradation study of nitroaniline.**

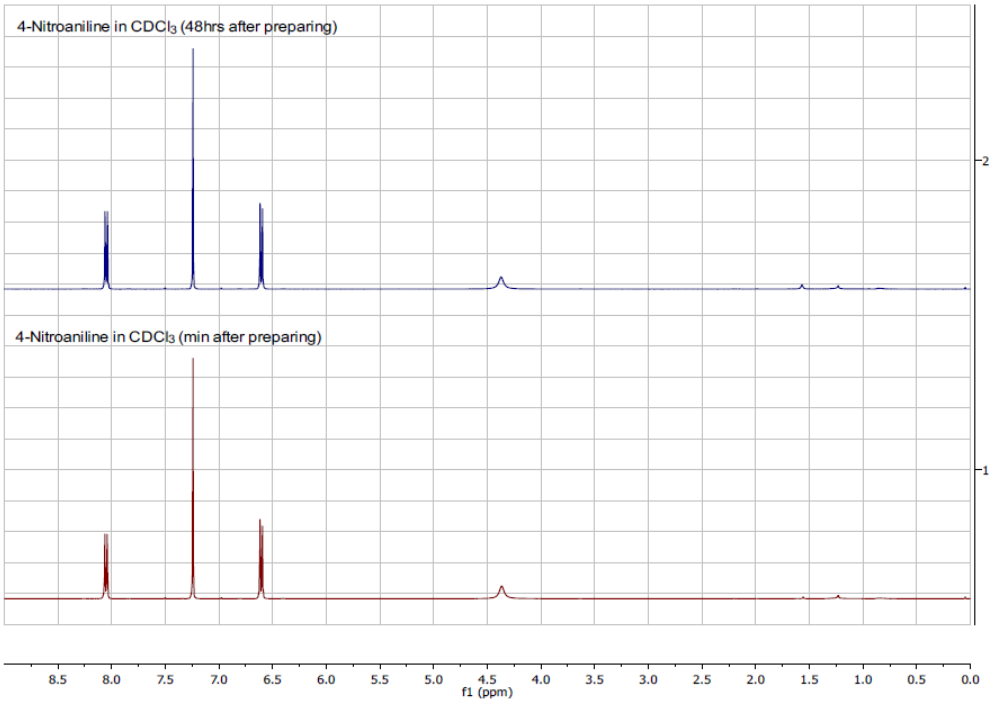



**Figure S6.** Degradation study of 4-Nitroaniline in $CDCl_3$.

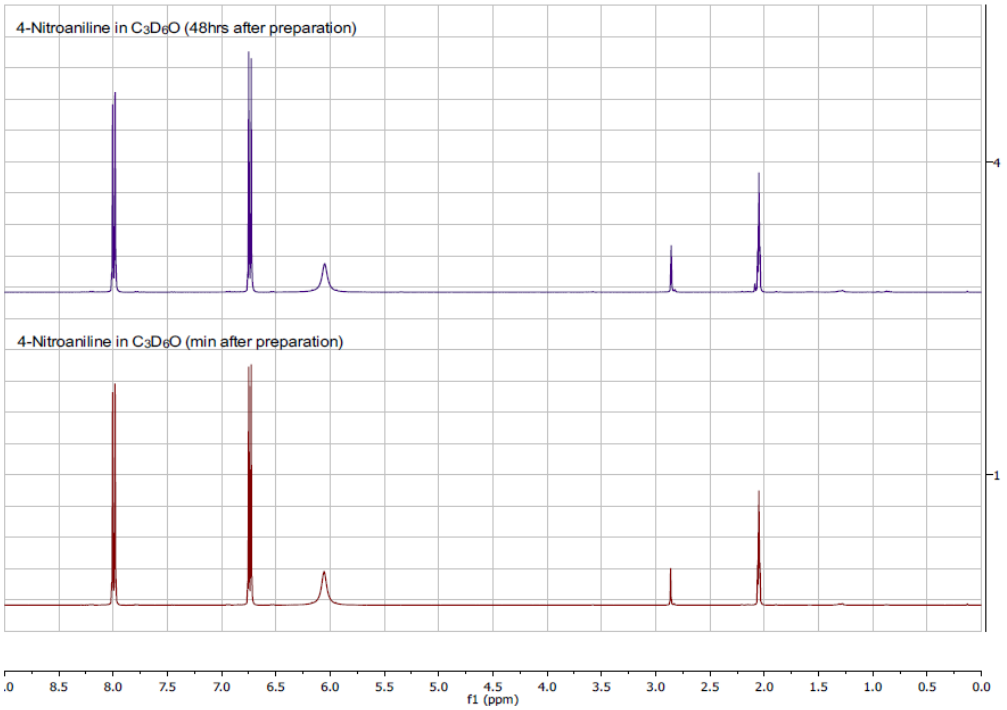



**Figure S7.** Degradation study of 4-Nitroaniline in $d_6$-acetone.

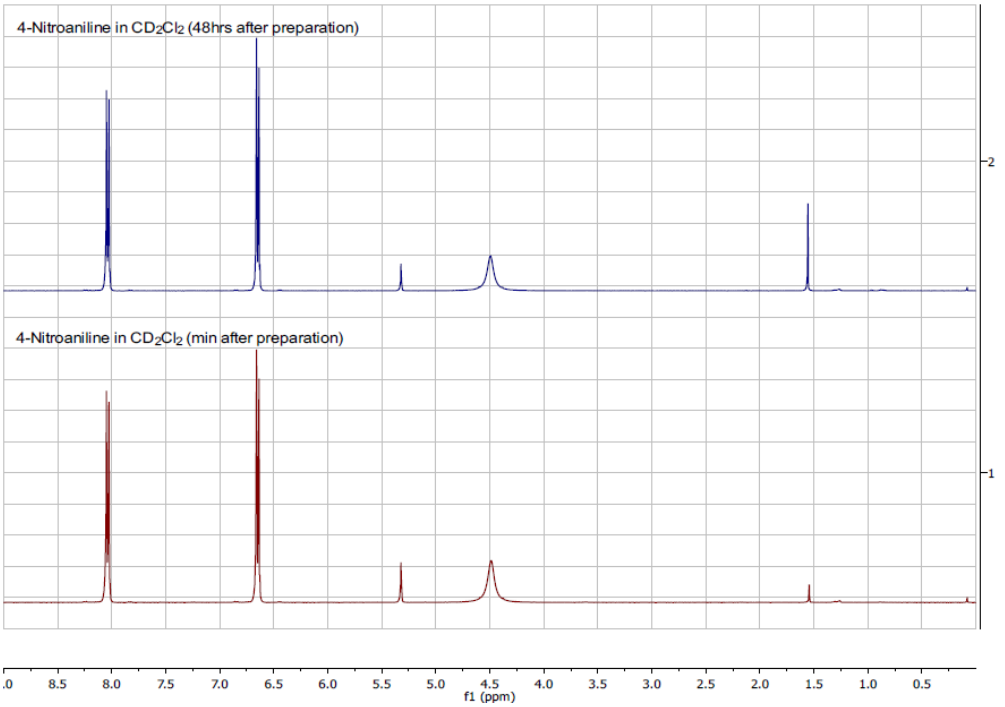



**Figure S8.** Degradation study of 4-Nitroaniline in $d_2$-DCM.

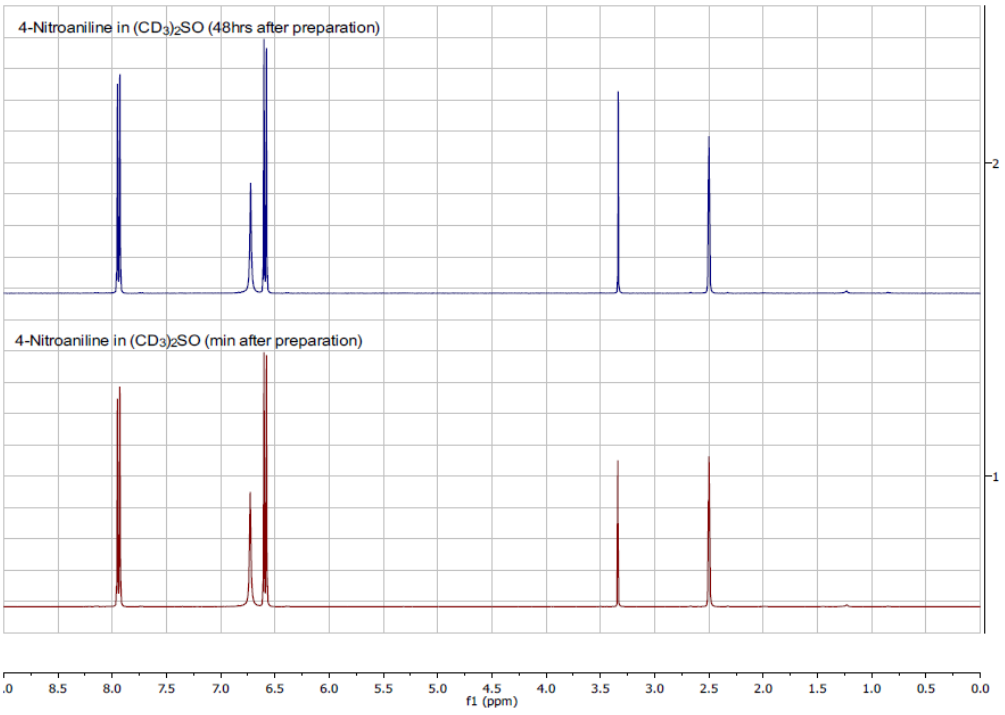



**Figure S9.** Degradation study of 4-Nitroaniline in $d_6$-DMSO.

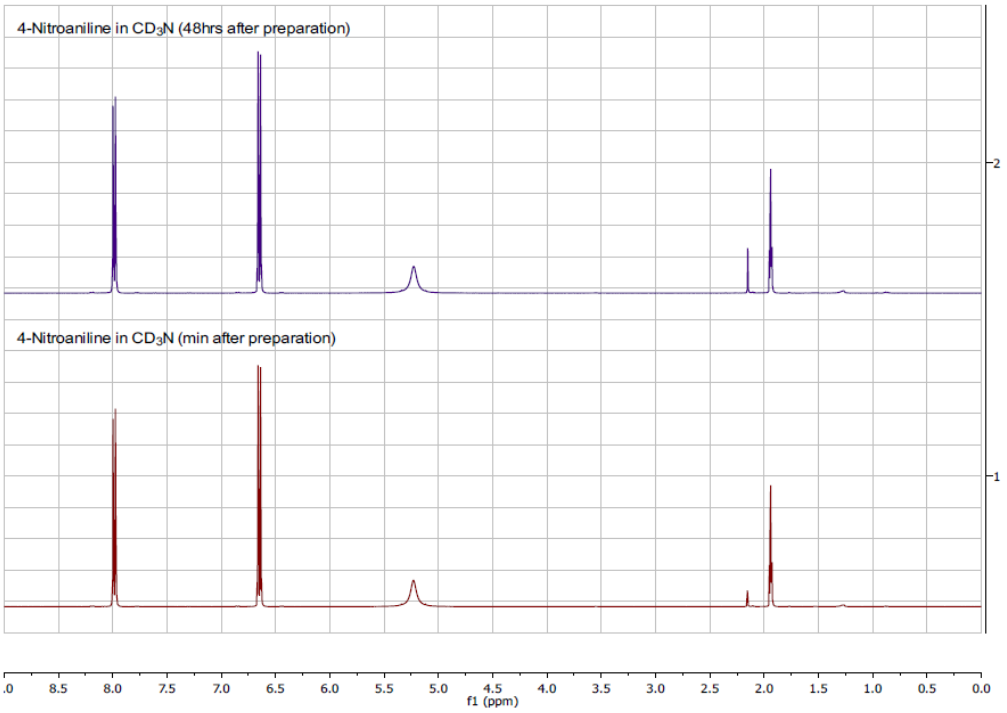



**Figure S10.** Degradation study of 4-Nitroaniline in $d_3$-MeCN.

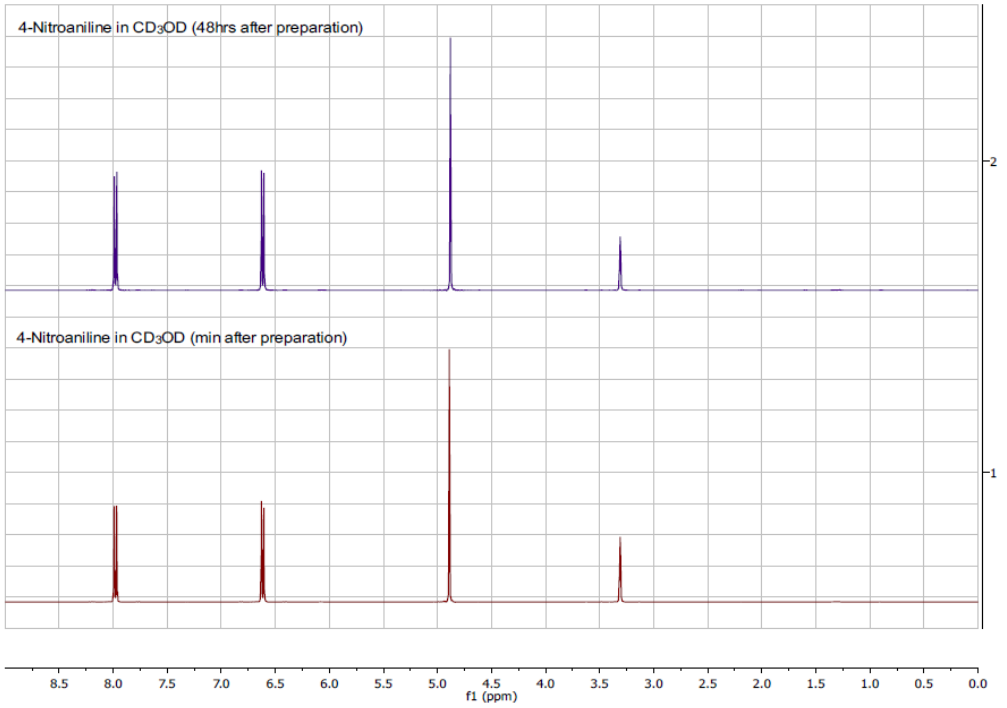



**Figure S11.** Degradation study of 4-Nitroaniline in $d_4$-methanol.

**Section (7): NMR spectra related to the degradation study of N,N-dimethyl-p-phenylenediamine.**

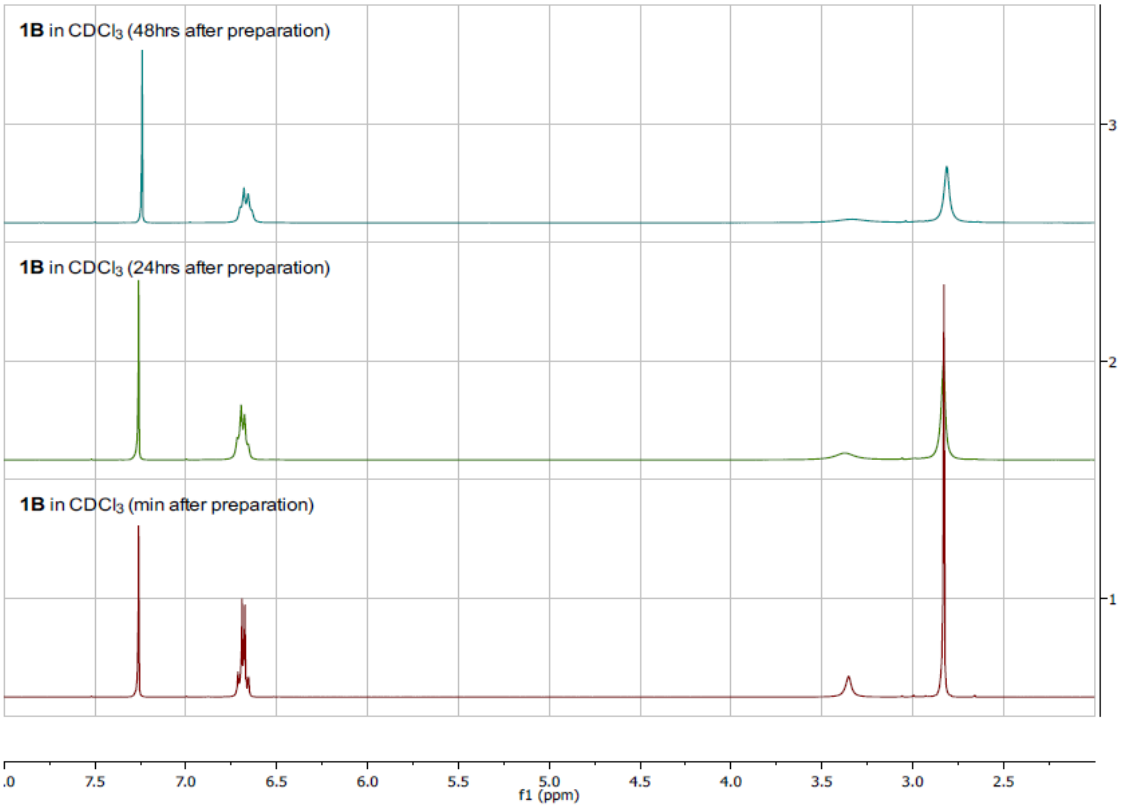



**Figure S12.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $CDCl_3$.

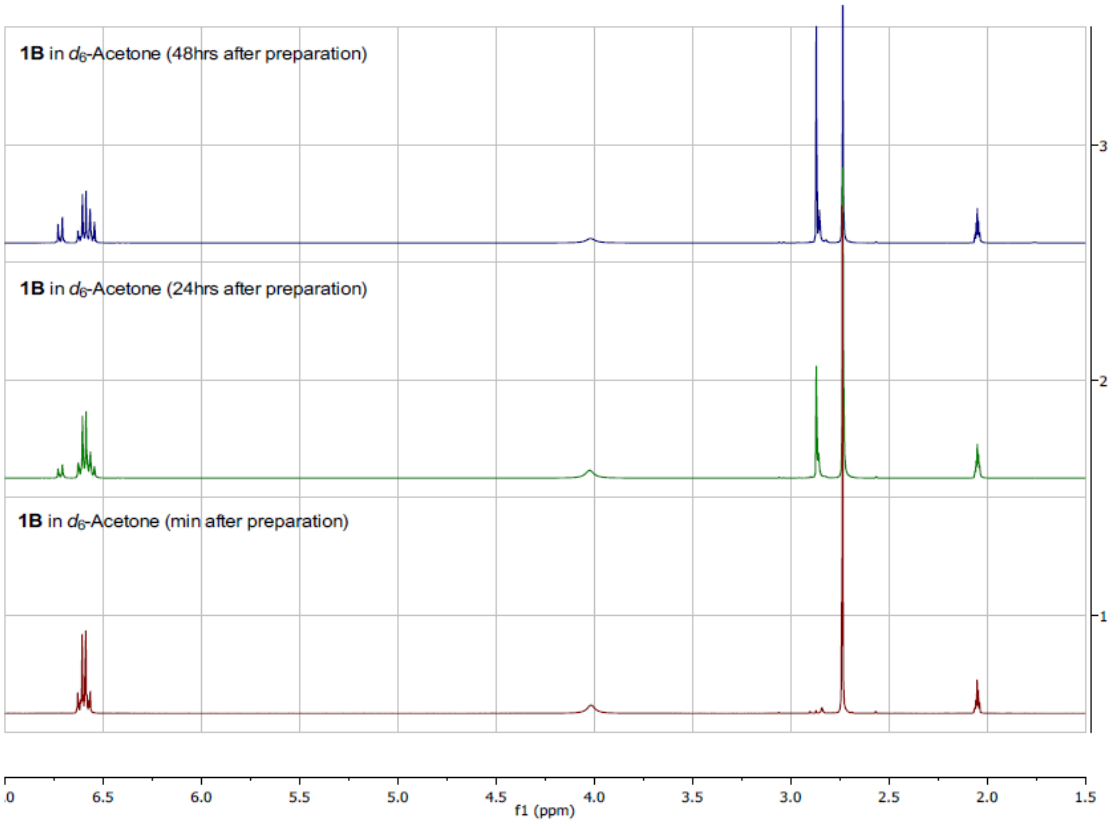



**Figure S13.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $d_6$-acetone.

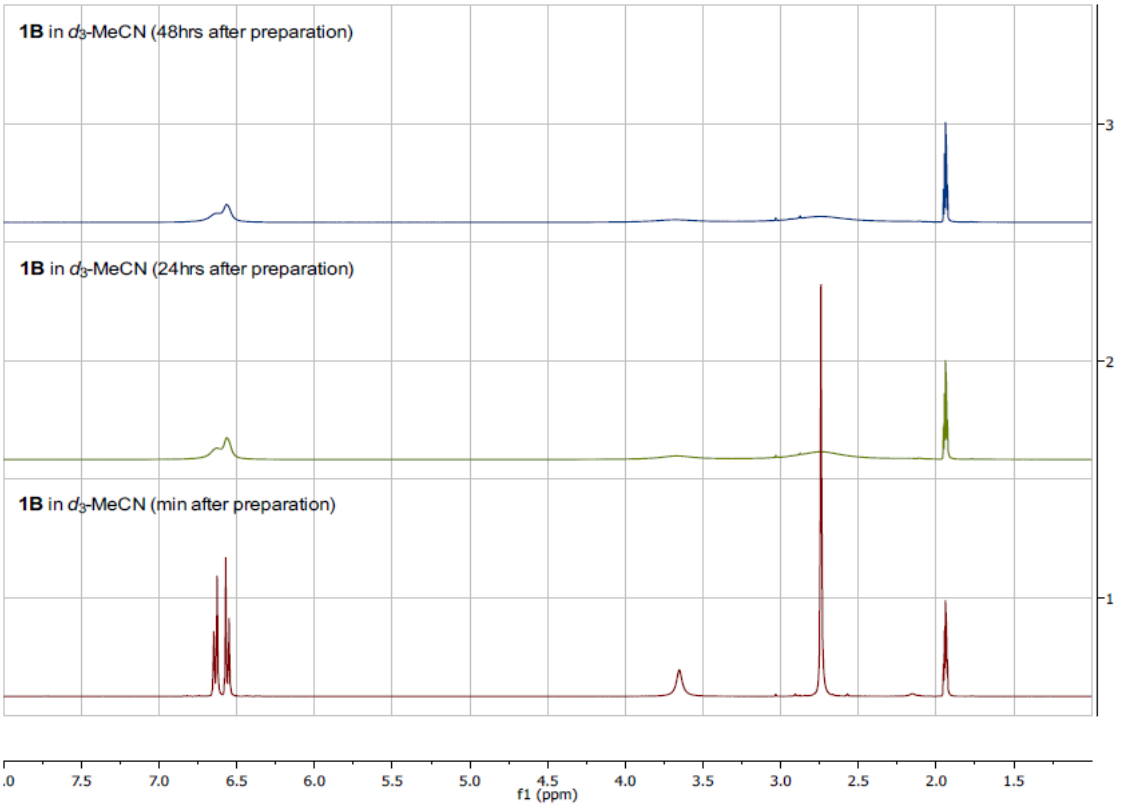



**Figure S14.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $d_3$-MeCN.

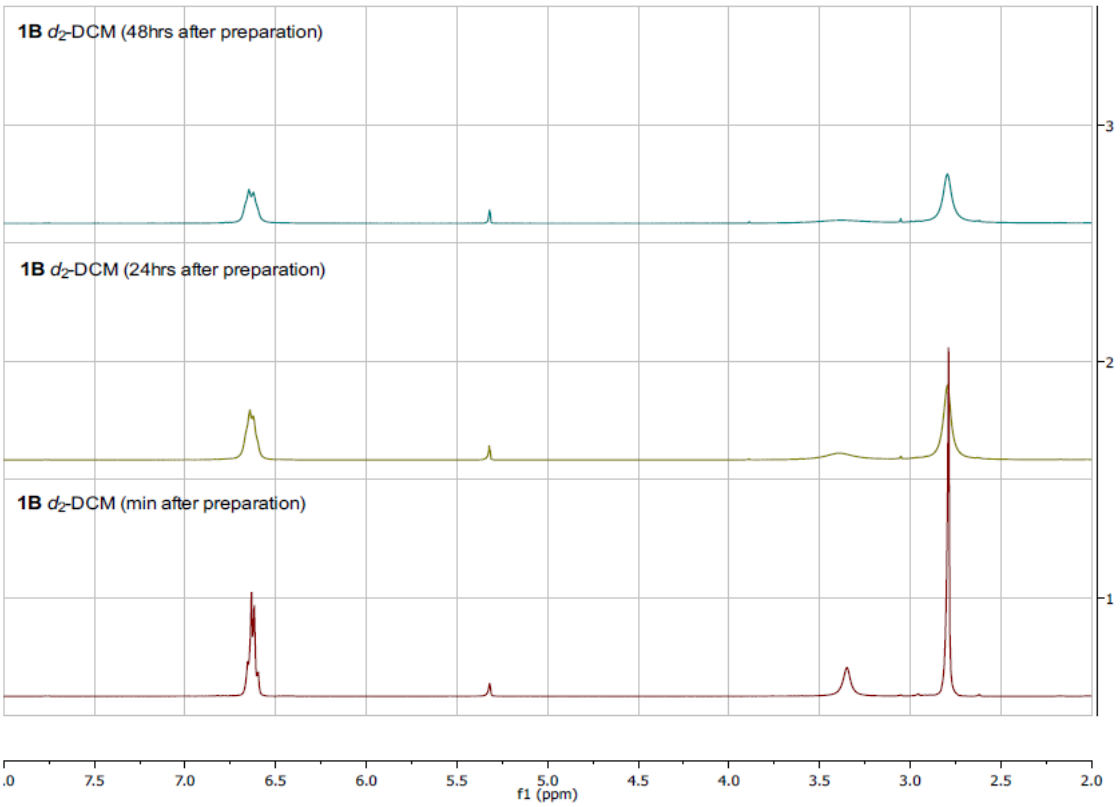



**Figure S15.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $d_2$-DCM.

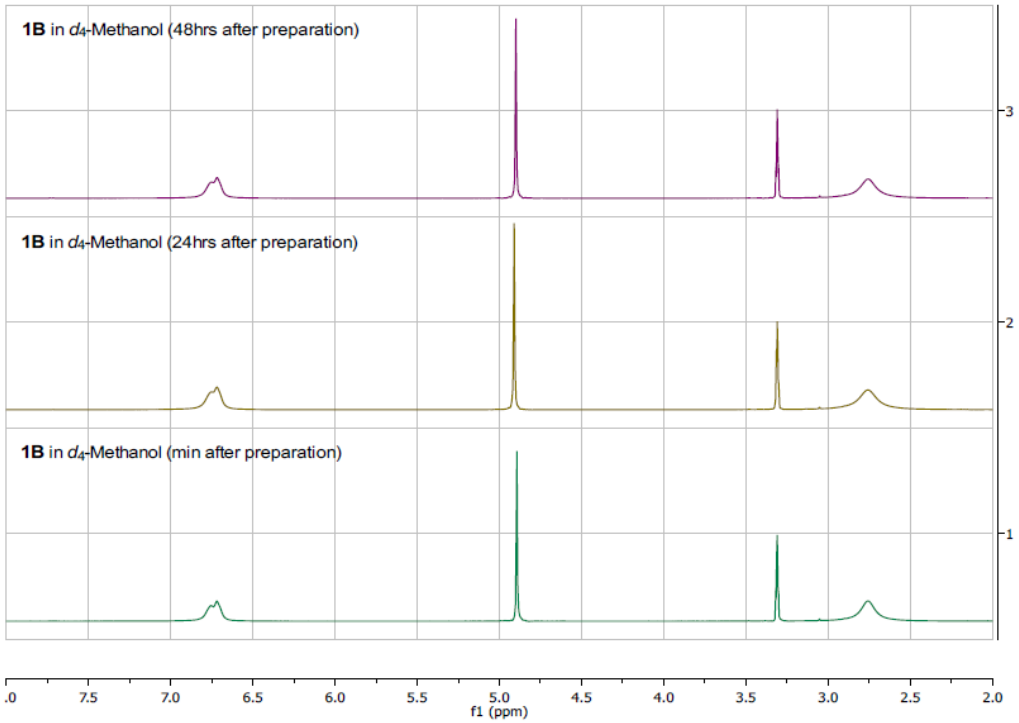



**Figure S16.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $d_4$-methanol.

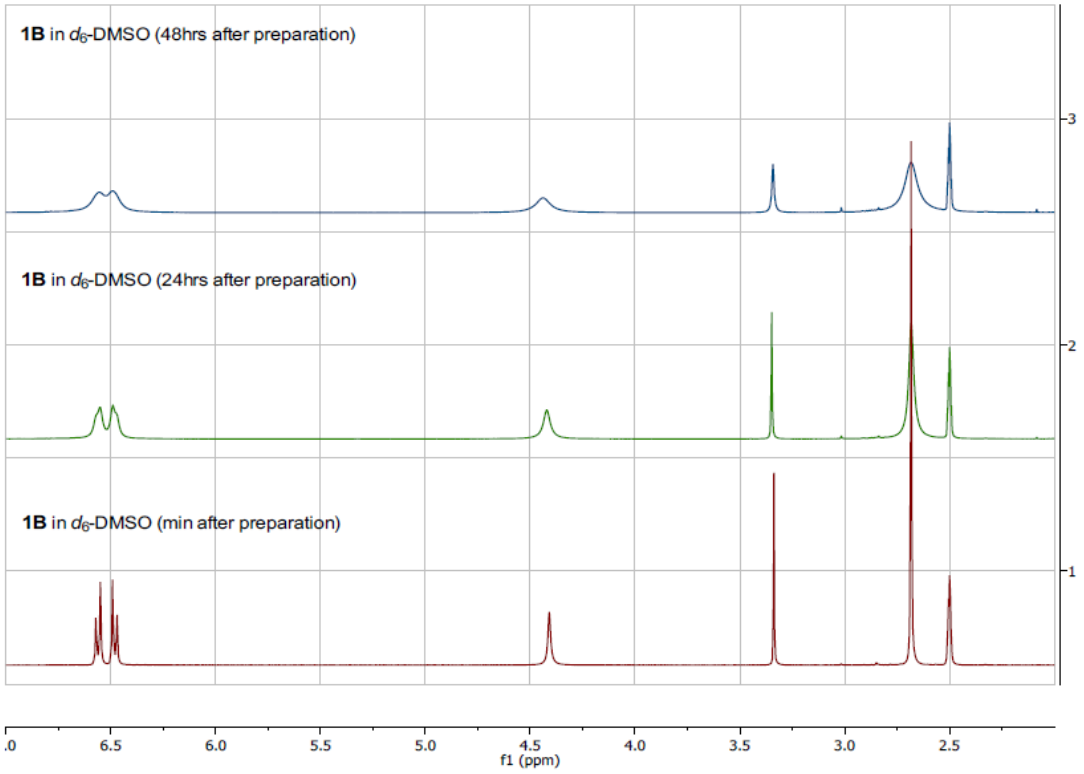



**Figure S17.** Degradation study of *N*,*N*-dimethyl-*p*-phenylenediamine, **(1B)**, in $d_6$-DMSO.

**Section (8): NMR spectra related to the degradation study of 2A.**

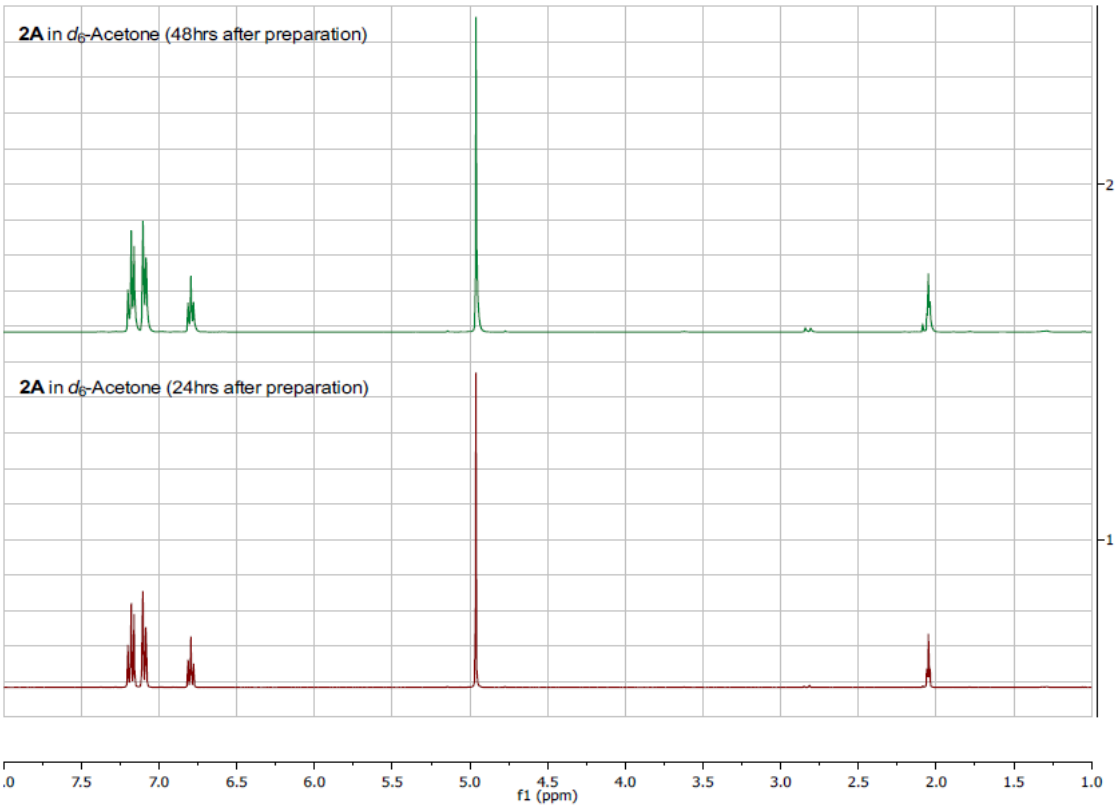



**Figure S18.** Degradation study of **2A** in $d_6$-acetone.

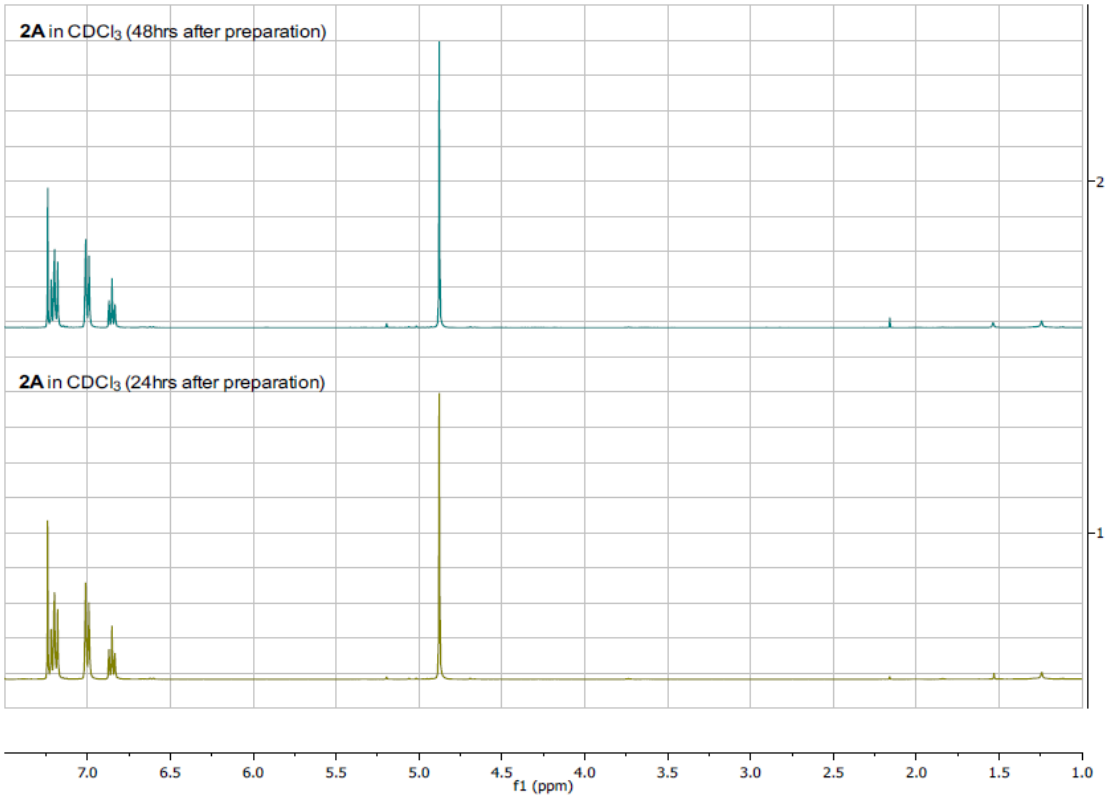



**Figure S19.** Degradation study of **2A** in $CDCl_3$.

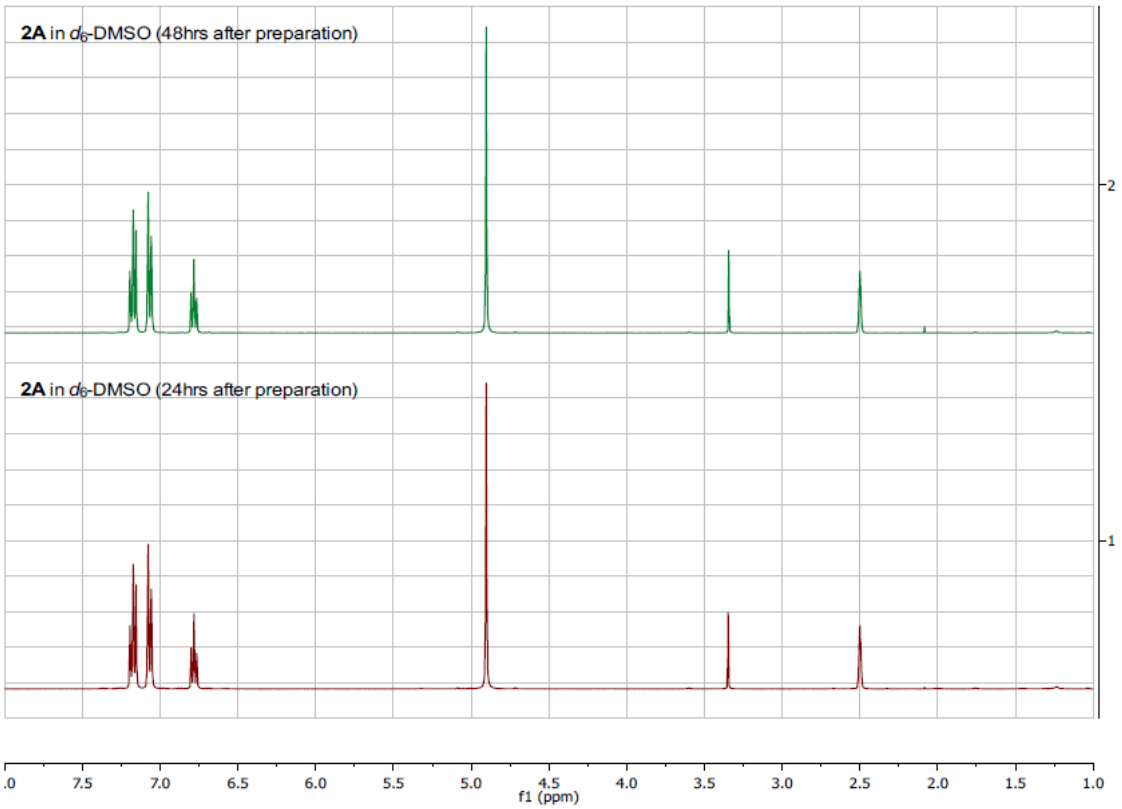



**Figure S20.** Degradation study of **2A** in $d_6$-DMSO.

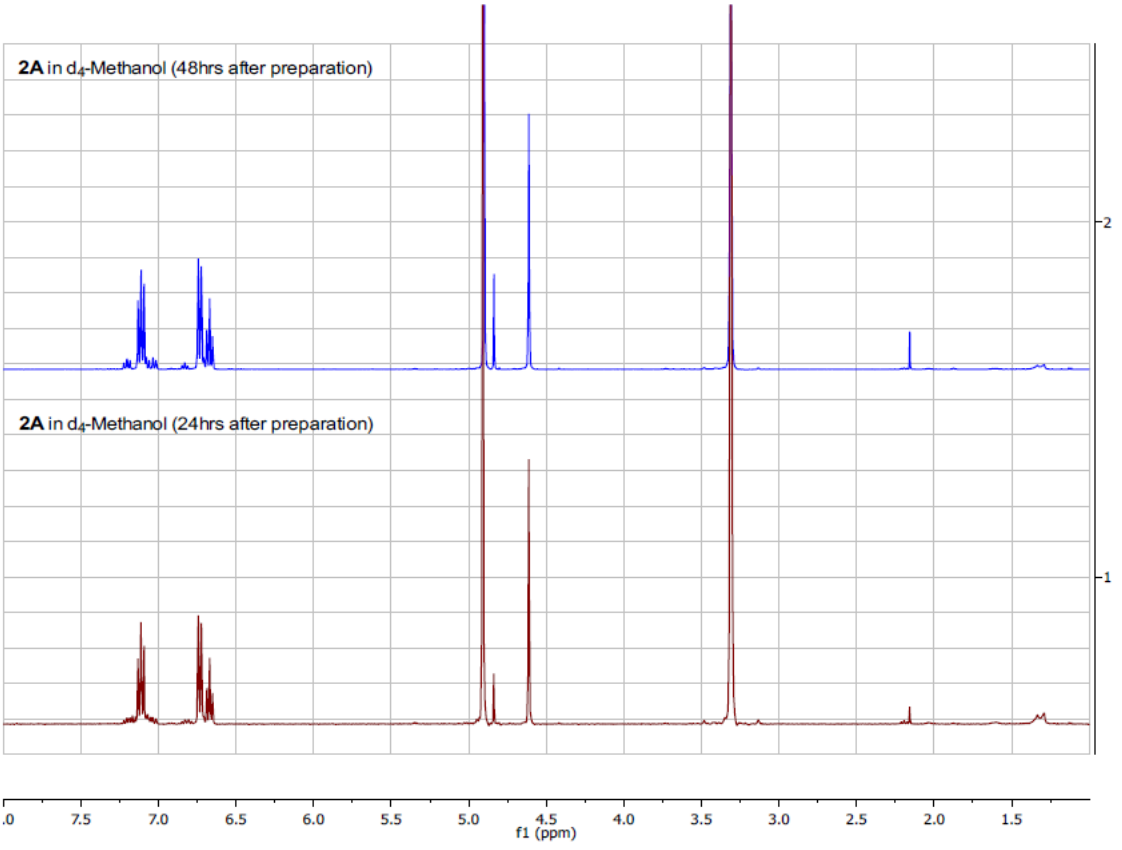



**Figure S21.** Degradation study of **2A** in $d_4$-methanol.

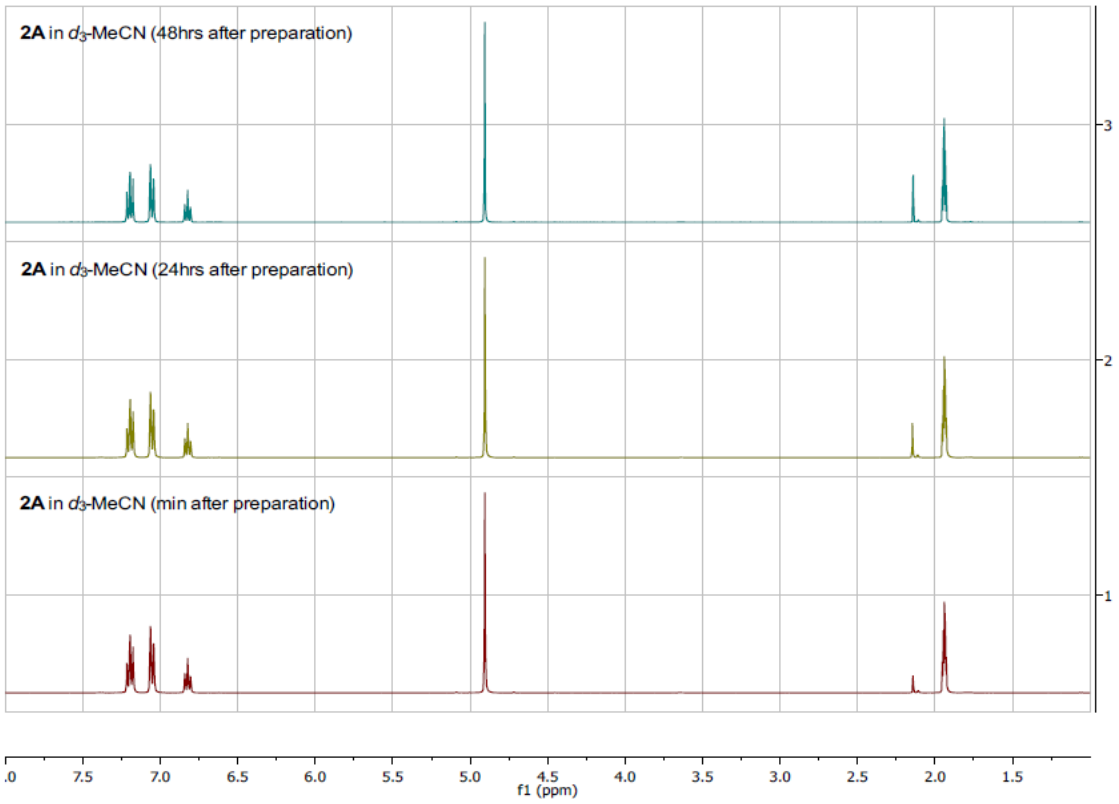



**Figure S22.** Degradation study of **2A** in $d_3$-MeCN.

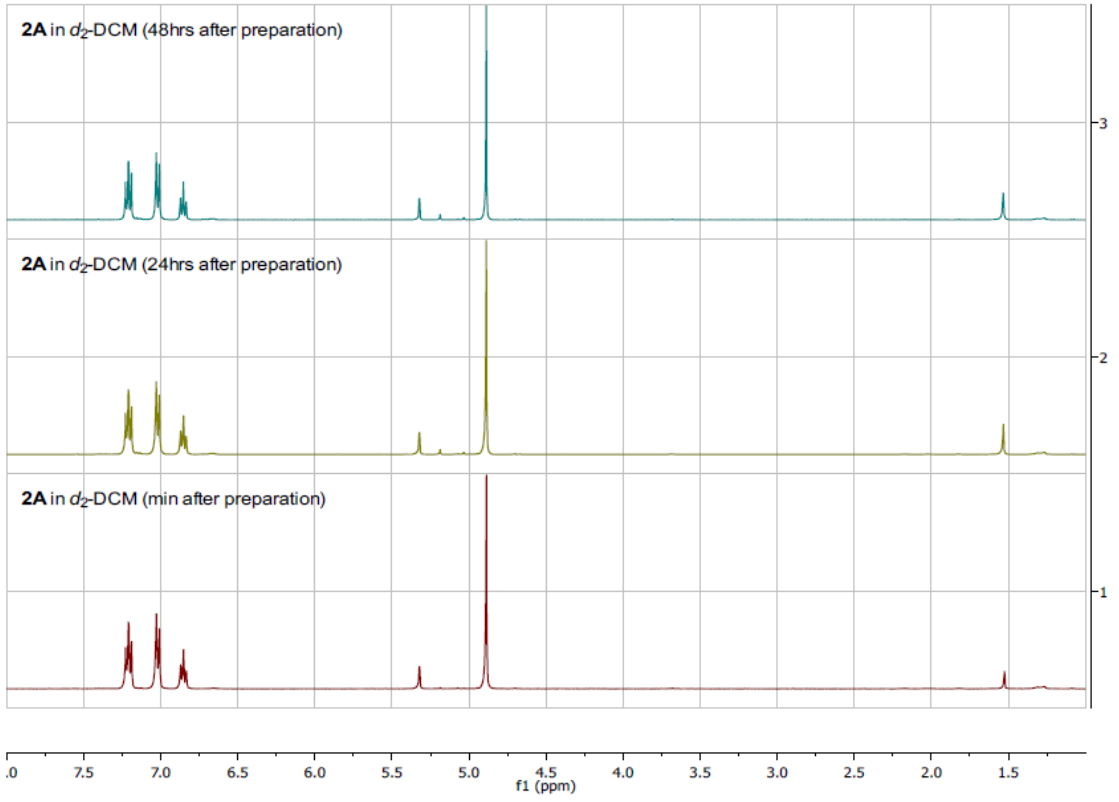



**Figure S23.** Degradation study of **2A** in $d_2$-DCM.

**Section (9): NMR spectra related to the degradation study of 2B.**

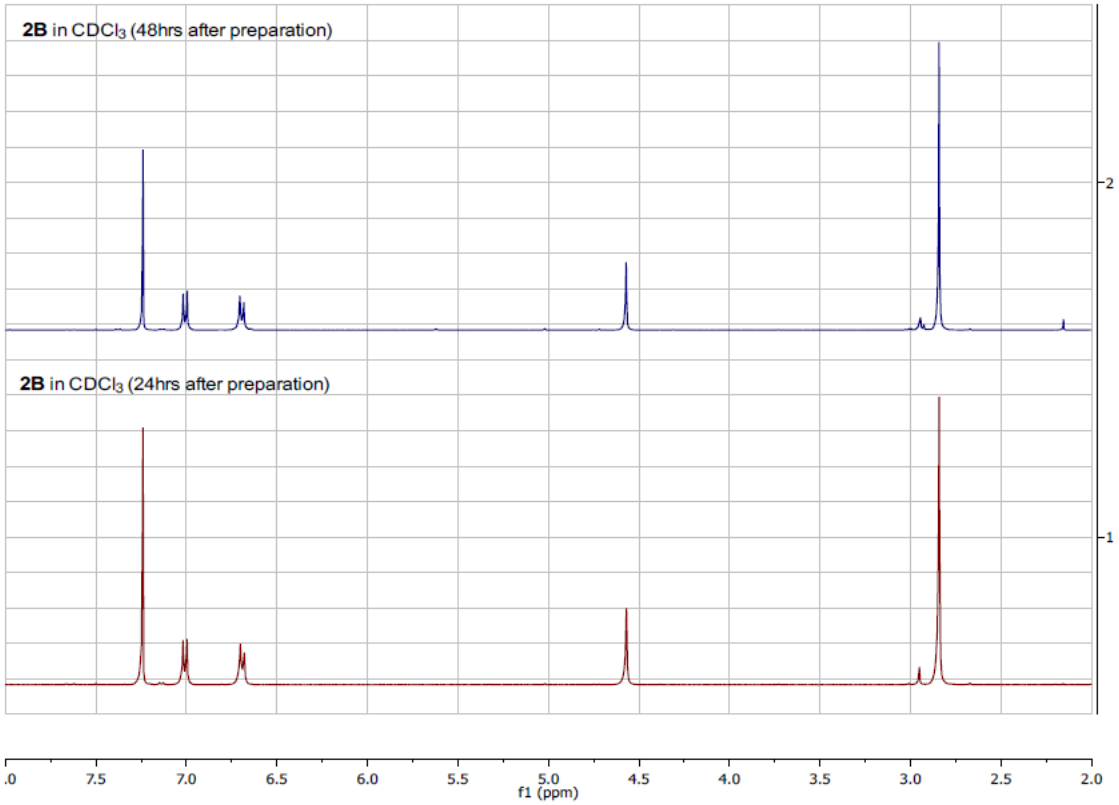



**Figure S24.** Degradation of **2B** in $CDCl_3$.

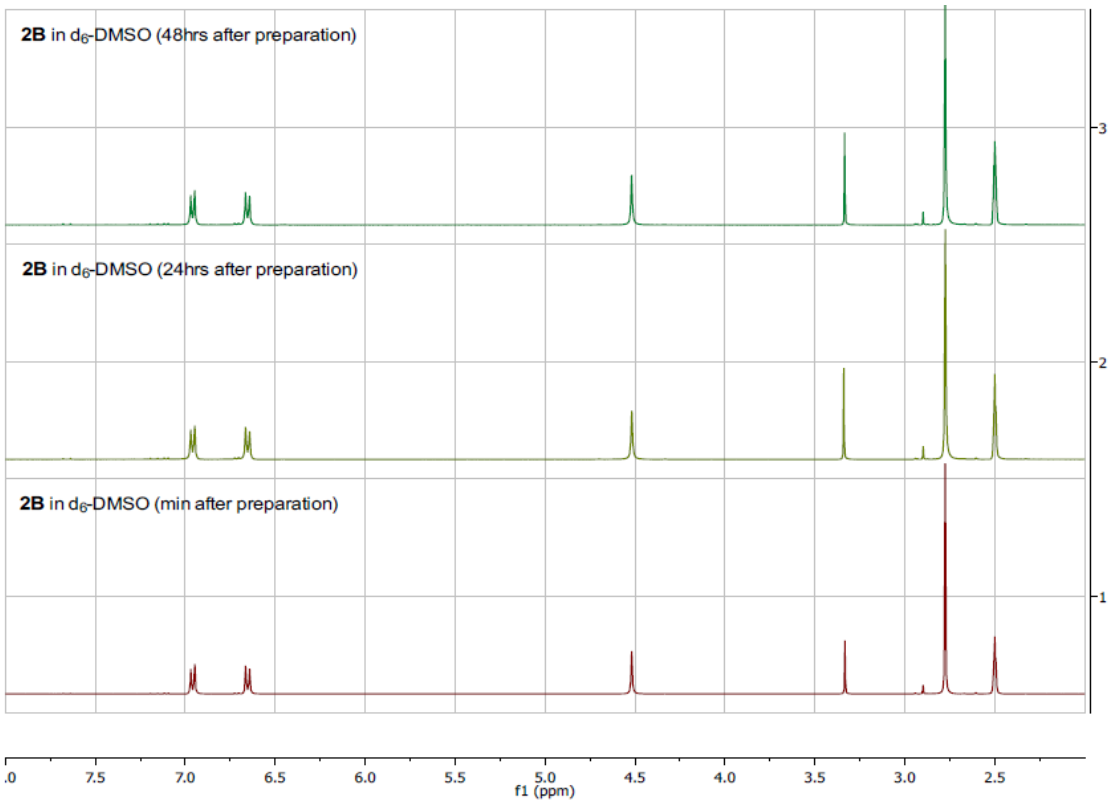



**Figure S25.** Degradation of **2B** in $d_6$-DMSO.

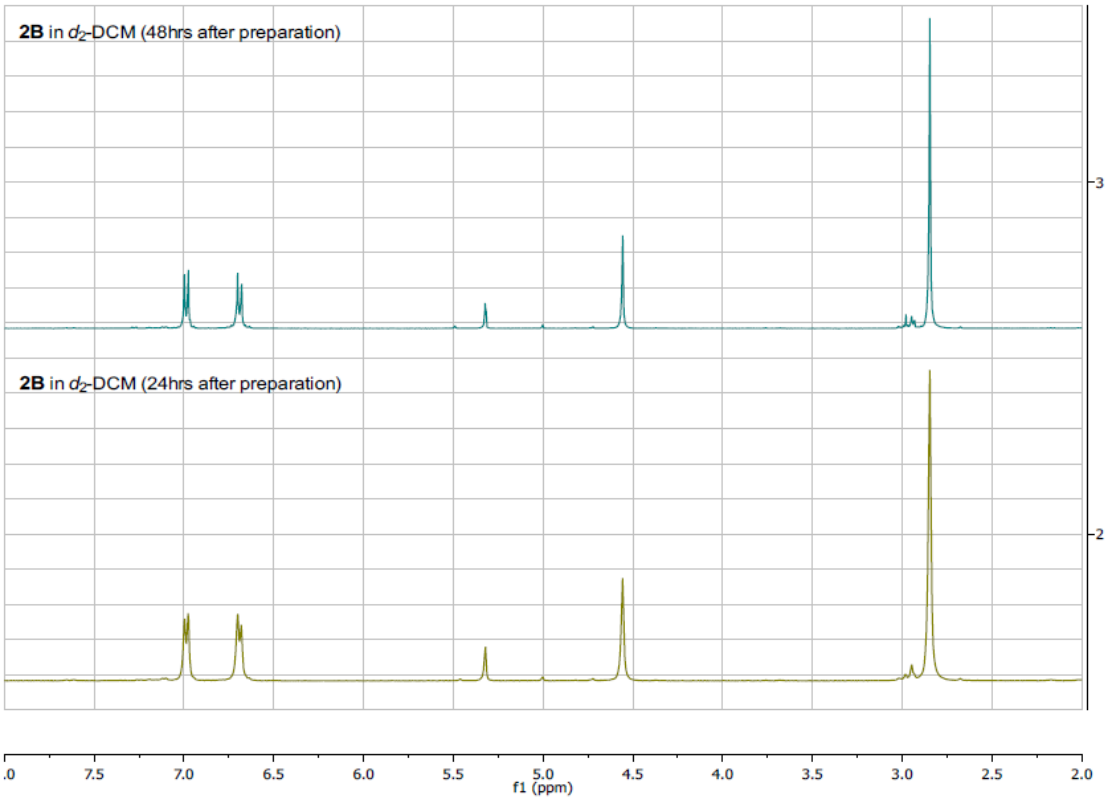



**Figure S26.** Degradation of **2B** in $d_2$-DCM.

**Section (10): 1H-NMR overlays of 2A with various metals.**

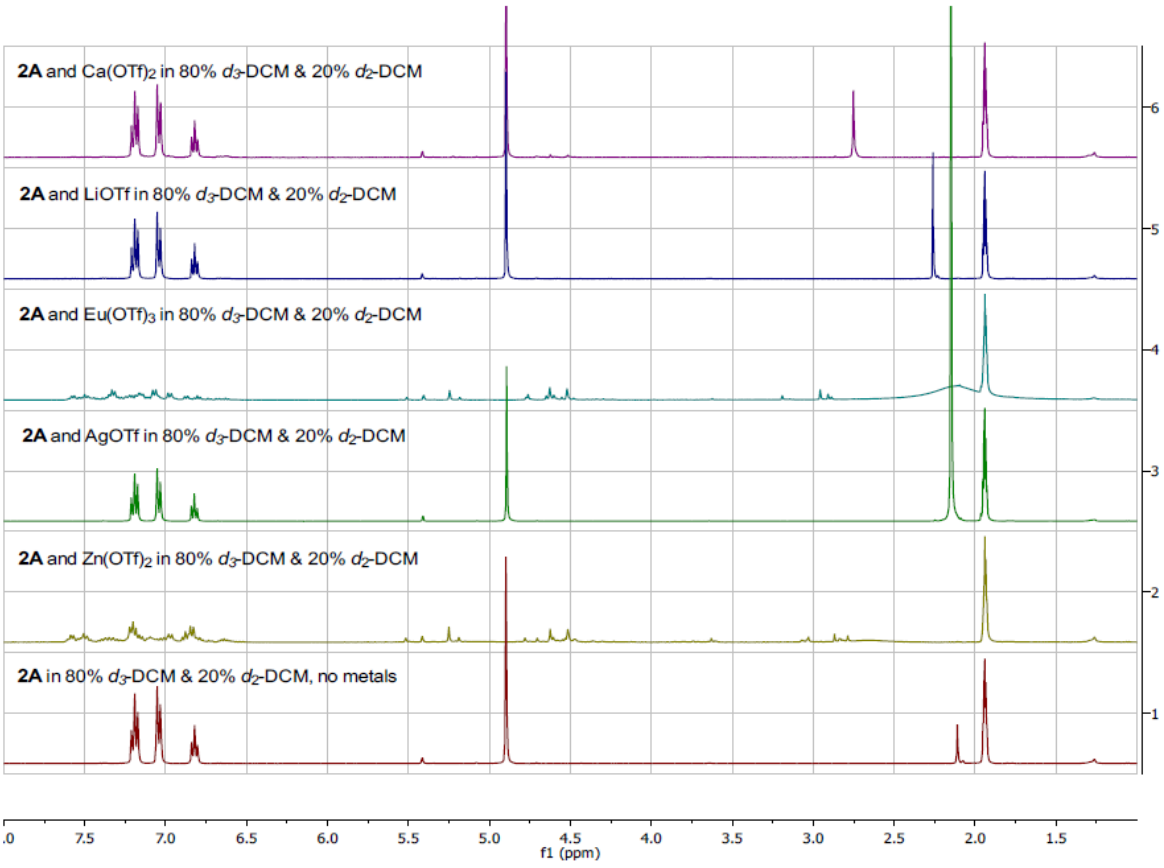



**Figure S27. 2A** and metal binding study in $^{1}$H NMR in 80%d-MeCN 20%d-DCM.

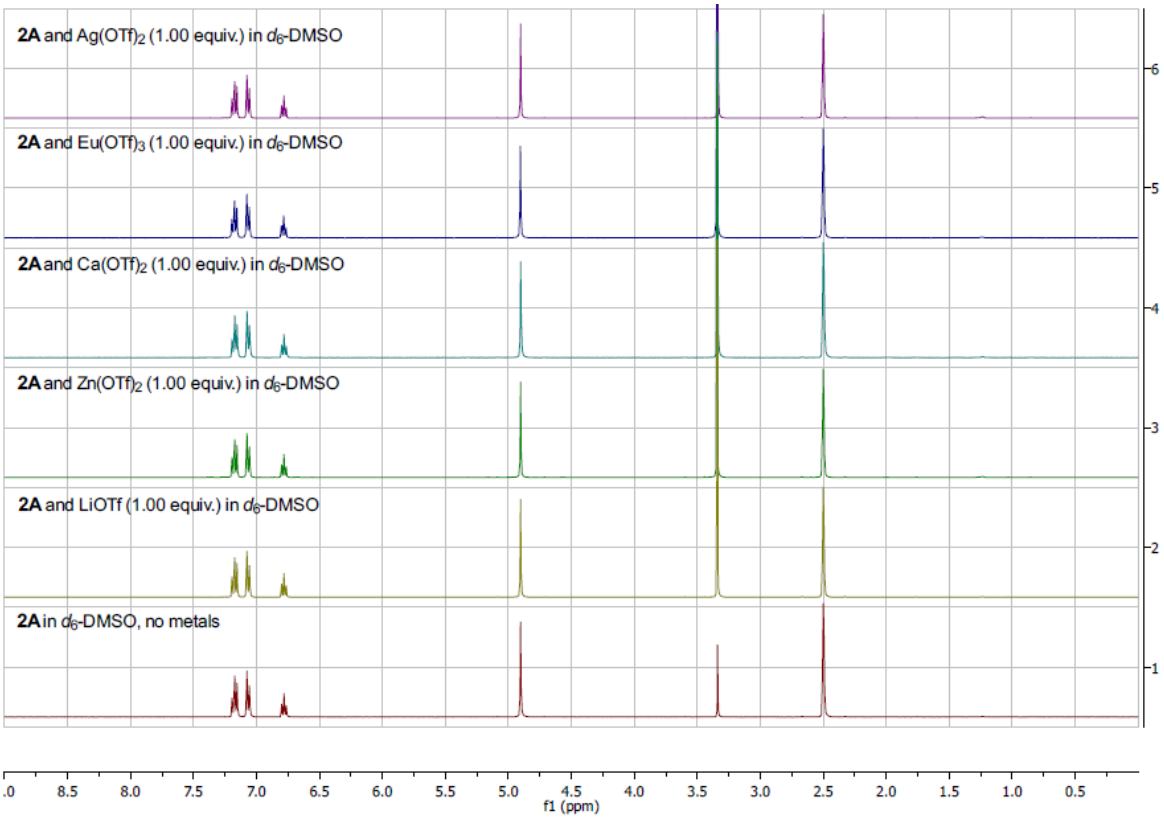



**Figure S28. 2A** and metal binding study in $d_6$-DMSO with $^1$H NMR.

**Section (11): 1H-NMR overlays of 2B with various metals.**

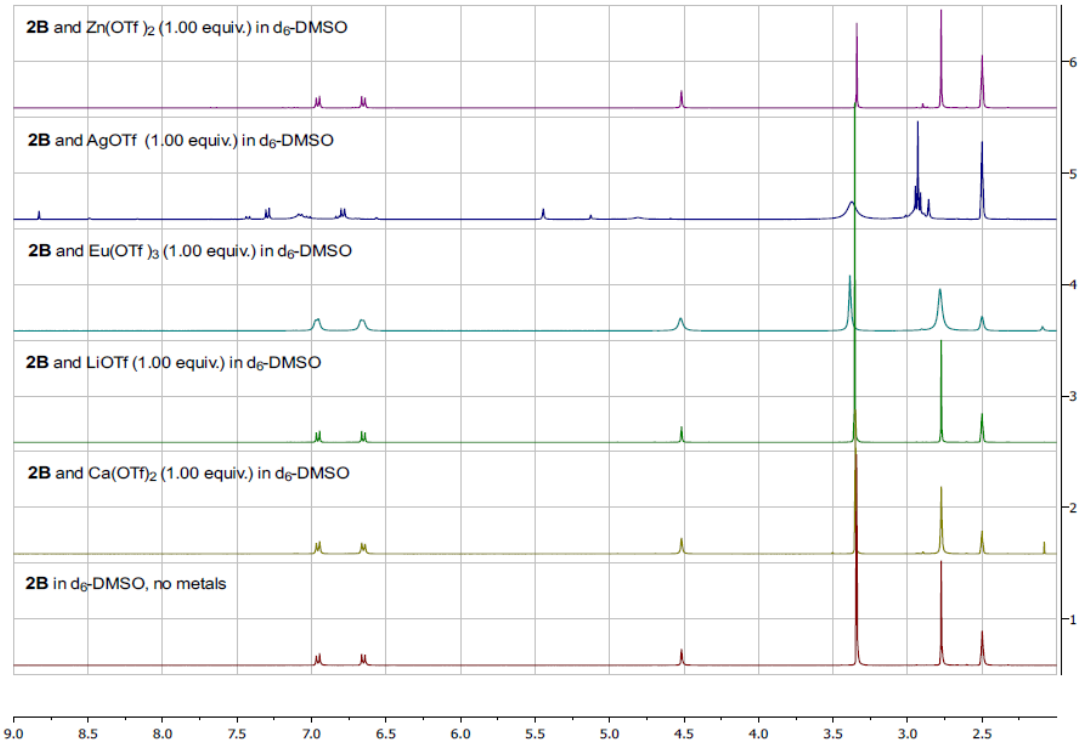



**Figure S29. 2B** and metal binding study in $d_6$-DMSO with $^1$H NMR.

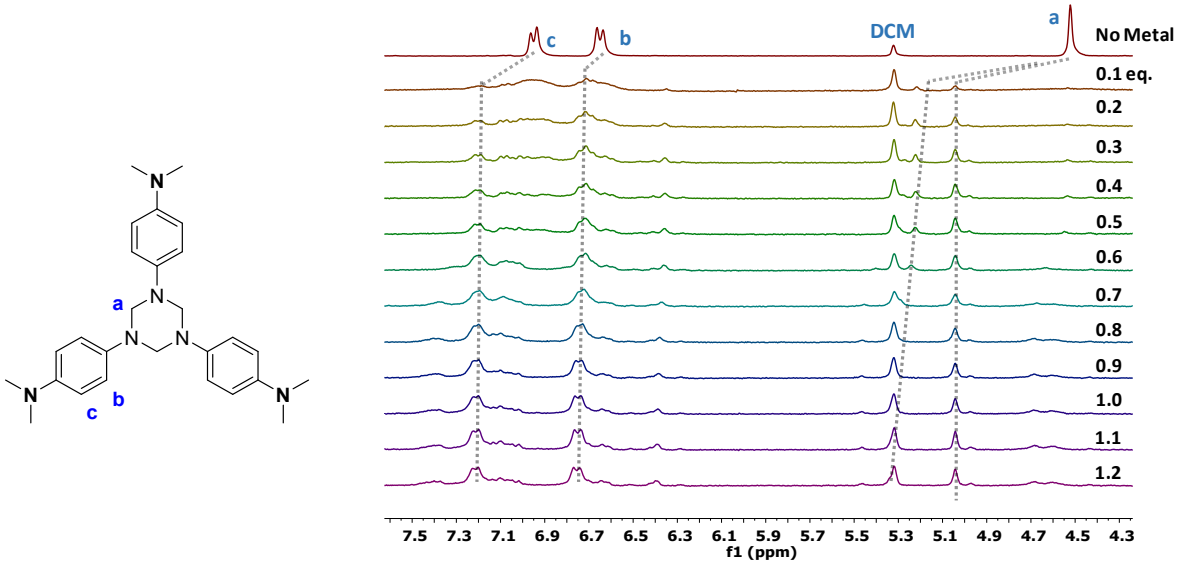



**Figure S30.** $^1$H-NMR titration of **2B** using increasing equivalents of $Zn(OTf)_2$ in 20% $d_3$-MeCN and 80% $d_2$-DCM.

**Section (12): 1H-NMR overlays of 2B with Zn(OTf)2 and subsequent metal removal.**

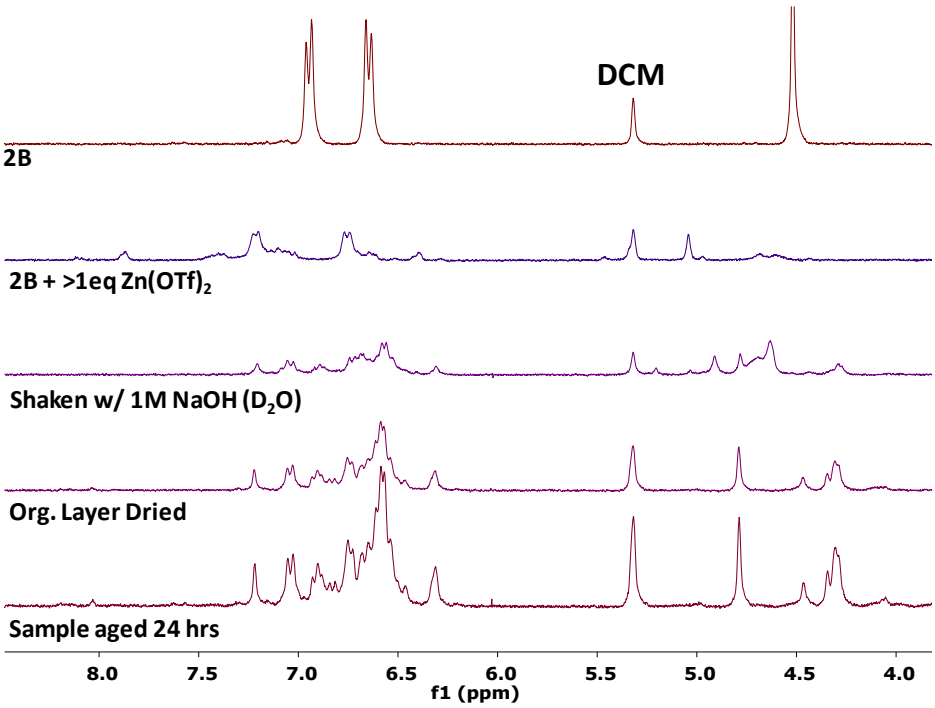



**Figure S31.** 1H-NMR spectra of **2B** stacked with additional spectra of **2B** and excess Zn(OTf)2, after shaking the sample with 1M NaOH to remove the Zn(OTf)2, the same NMR sample in which the organic layer was dried and redissolved in the same solvent system and the sample aged for a period of 24hrs. These spectra were taken in a solution of 80% CD2Cl2 and 20% *MeCN* (D3).

**Section (13): UV-Vis spectra of 2A w/ various metals.**

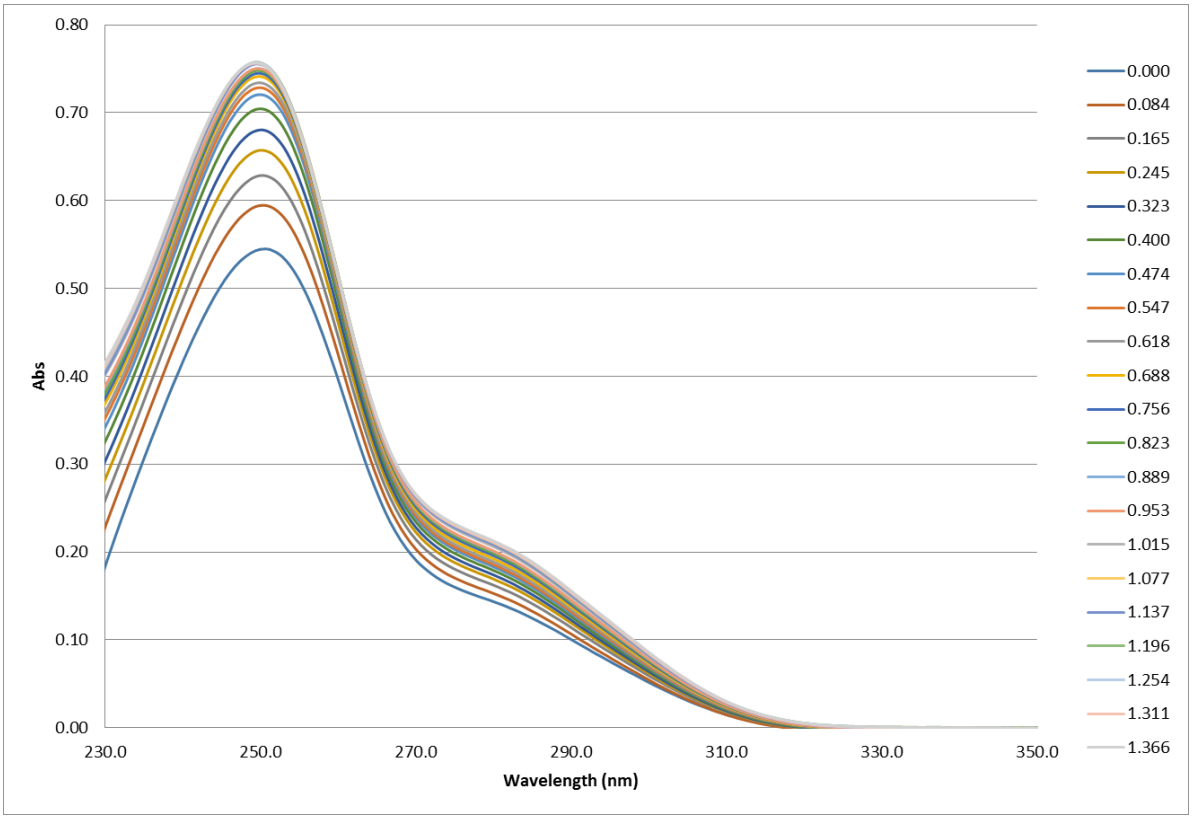



**Figure S32.** UV-VIS Absorption Spectroscopy, **2A** and LiOTf titration in 80% Acetonitrile and 20% DCM.

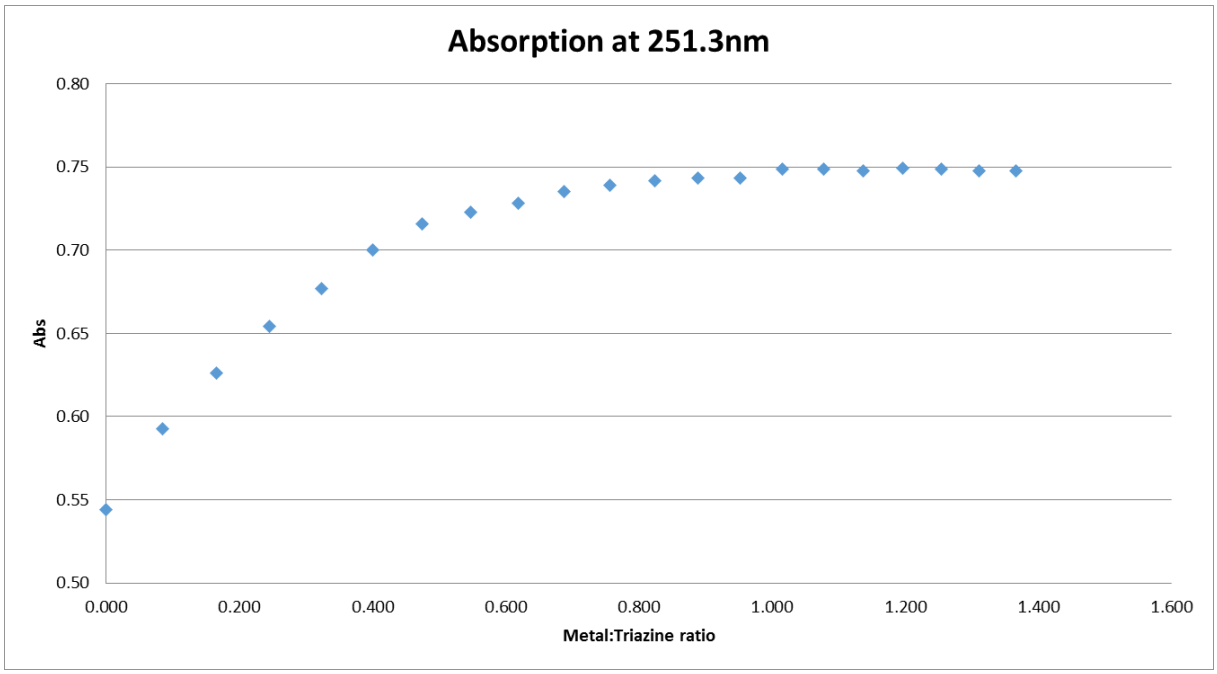



**Figure S33.** UV-VIS Absorption Spectroscopy, **2A** and LiOTf titration in 80% Acetonitrile and 20% DCM.

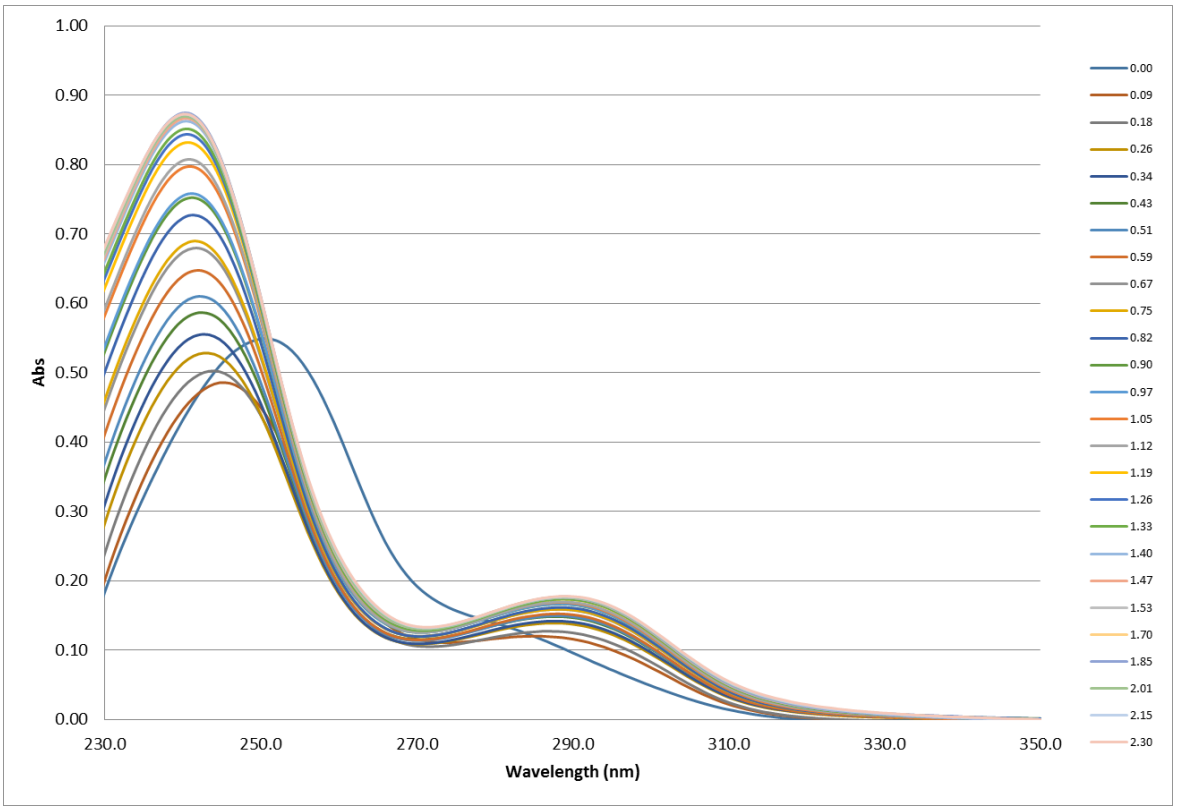



**Figure S34.** UV-VIS Absorption Spectroscopy, **2A** and $Ca(OTf)_2$ titration in 80% Acetonitrile and 20% DCM.

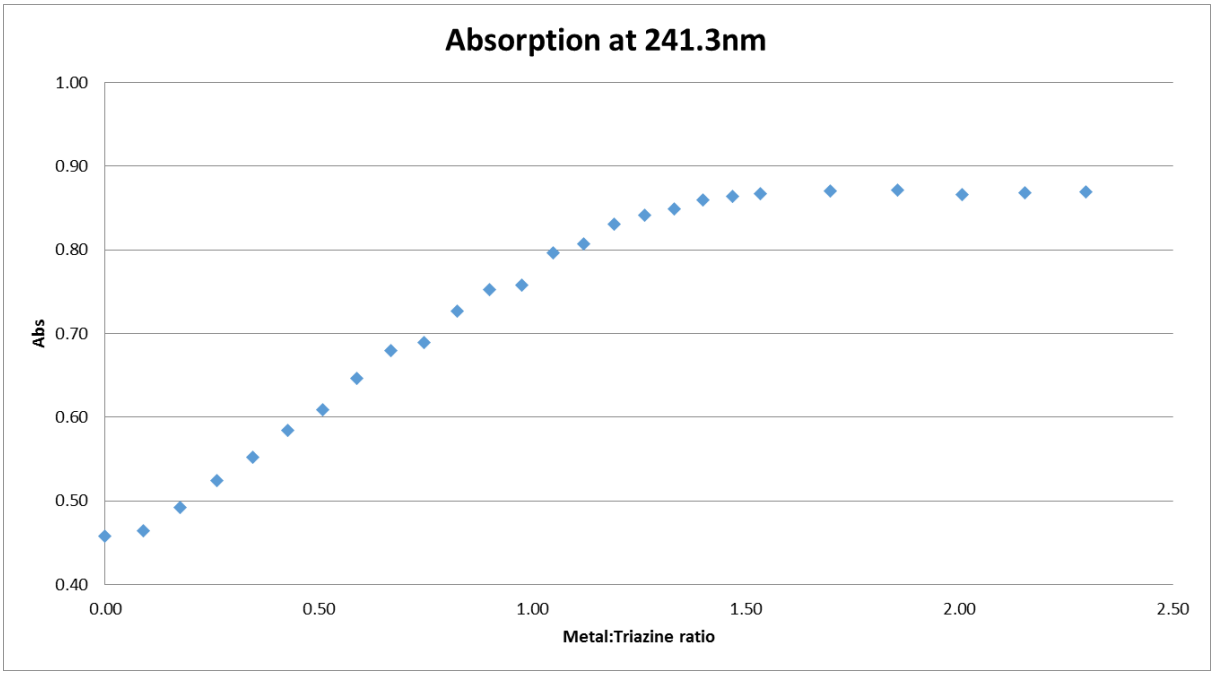



**Figure S35.** UV-VIS Absorption Spectroscopy, **2A** and $Ca(OTf)_2$ titration in 80% Acetonitrile and 20% DCM.

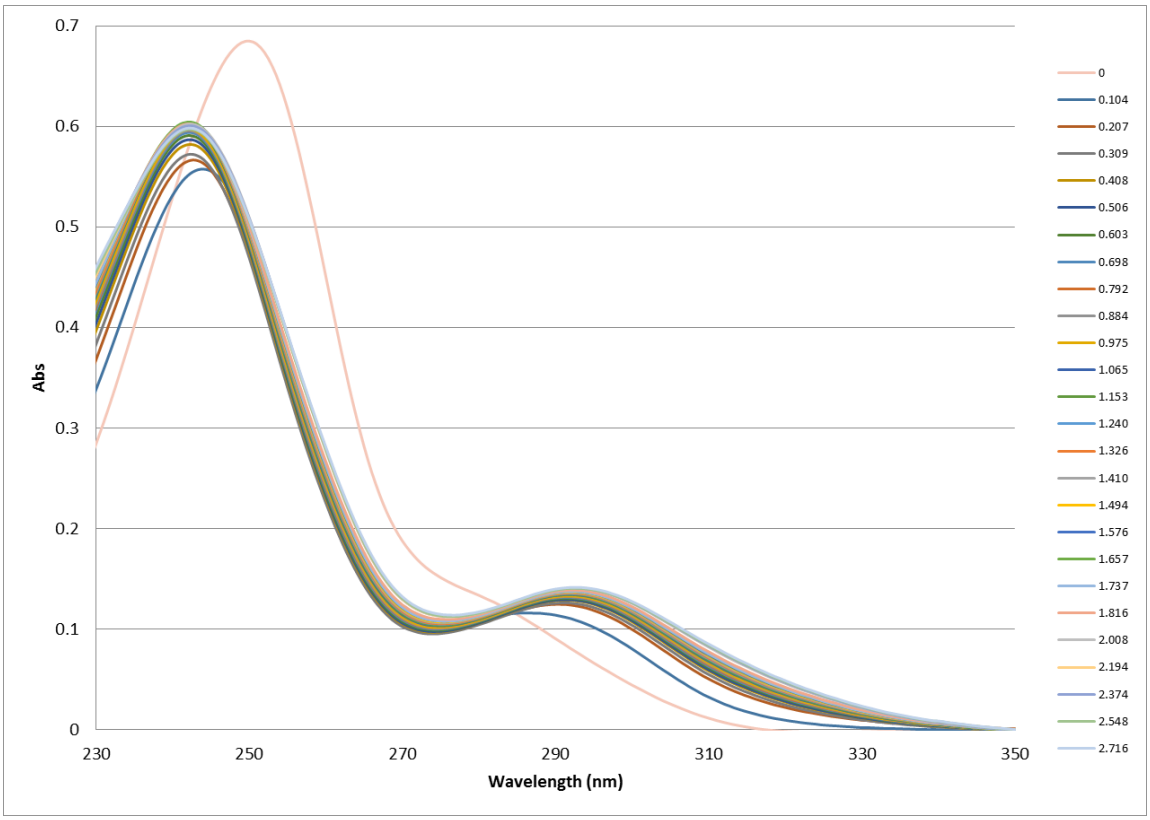



**Figure S36.** UV-VIS Absorption Spectroscopy, **2A** and AgOTf titration in 80% Acetonitrile and 20% DCM.

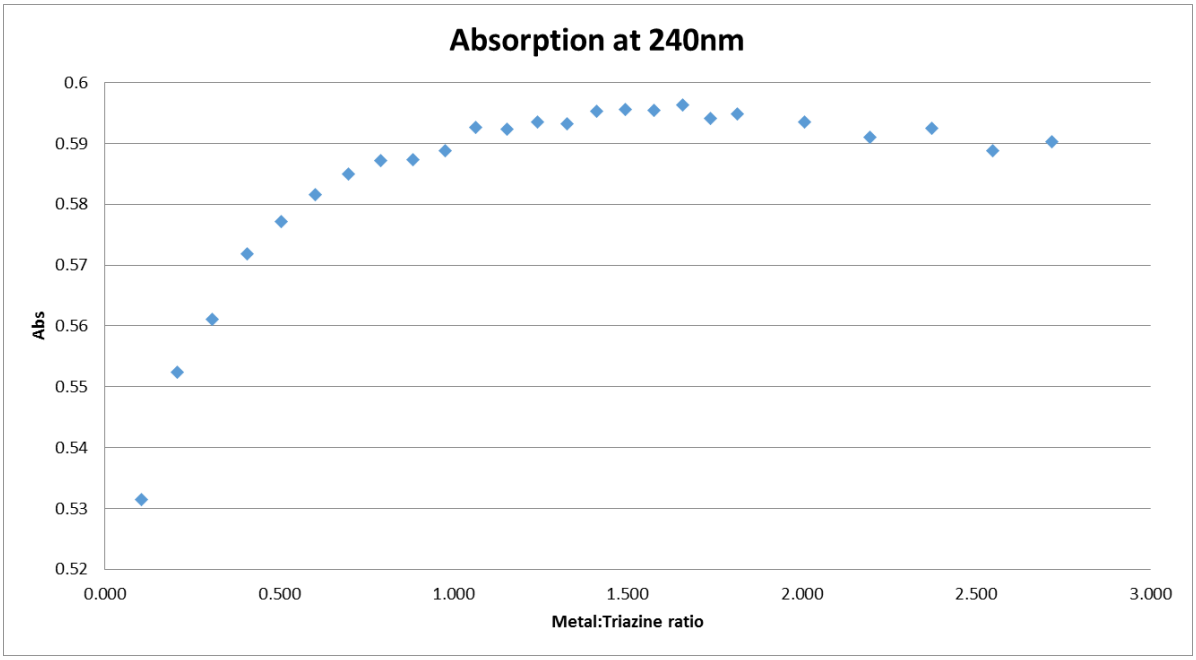



**Figure S37.** UV-VIS Absorption Spectroscopy, **2A** and AgOTf titration in 80% Acetonitrile and 20% DCM.

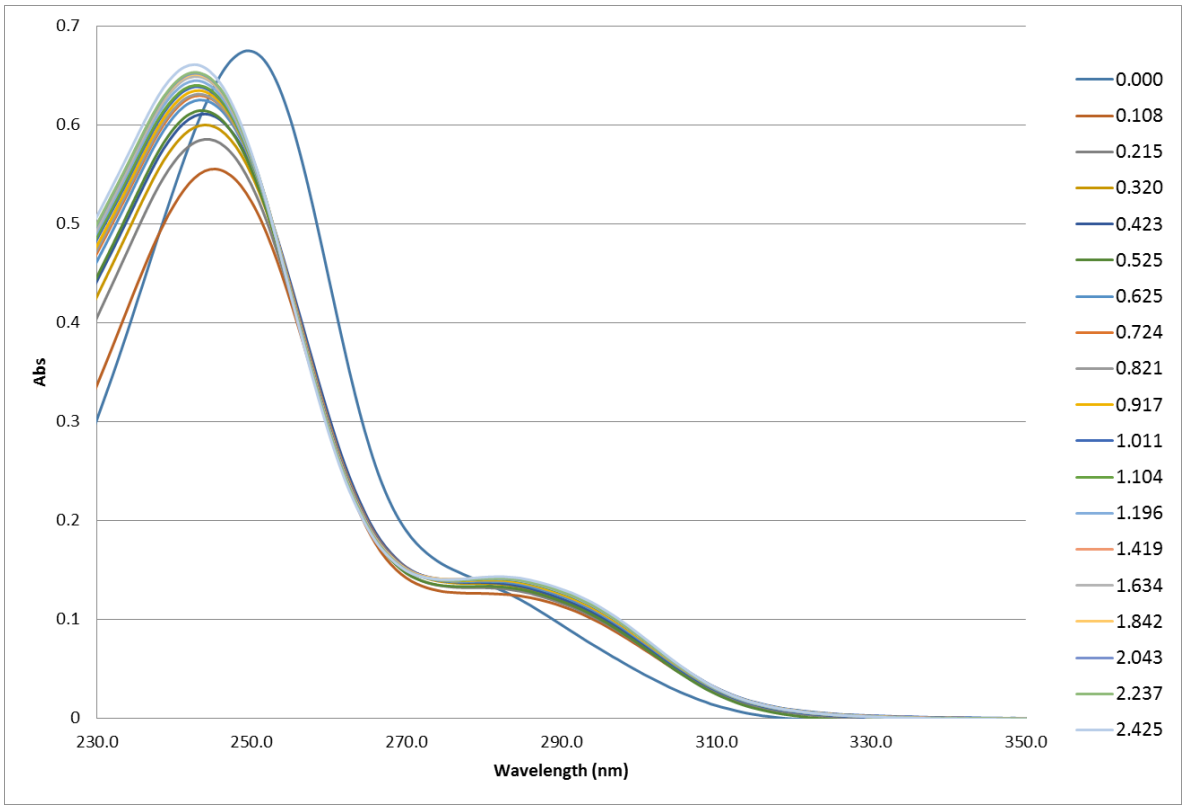



**Figure S38.** UV-VIS Absorption Spectroscopy, **2A** and $Zn(OTf)_2$ titration in 80% Acetonitrile and 20% DCM.

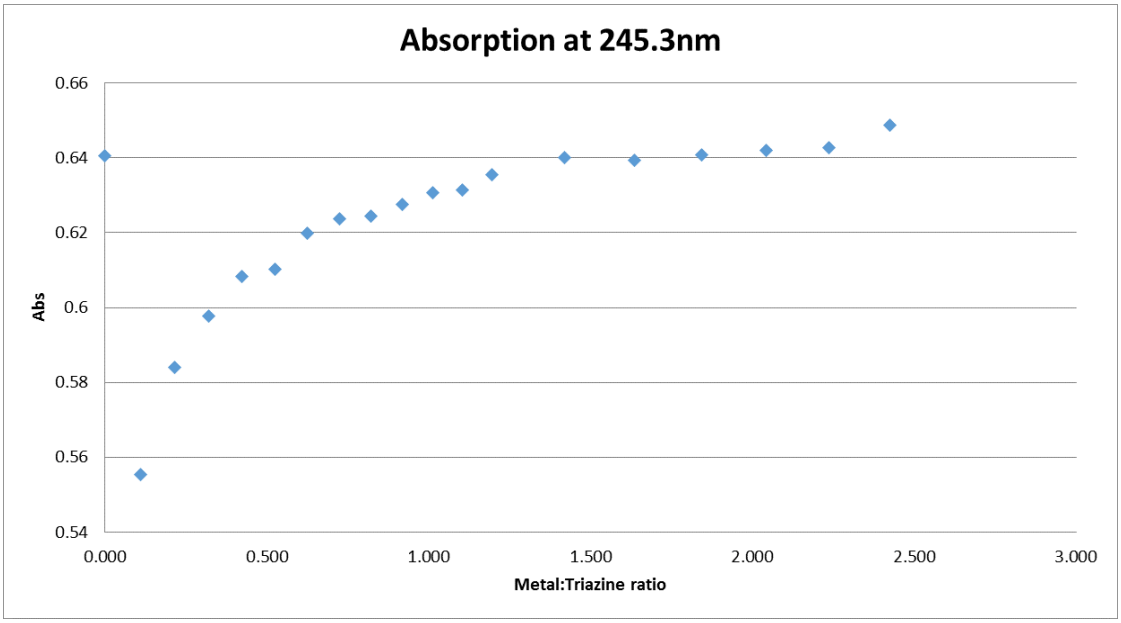



**Figure S39.** UV-VIS Absorption Spectroscopy, **2A** and $Zn(OTf)_2$ titration in 80% Acetonitrile and 20% DCM.

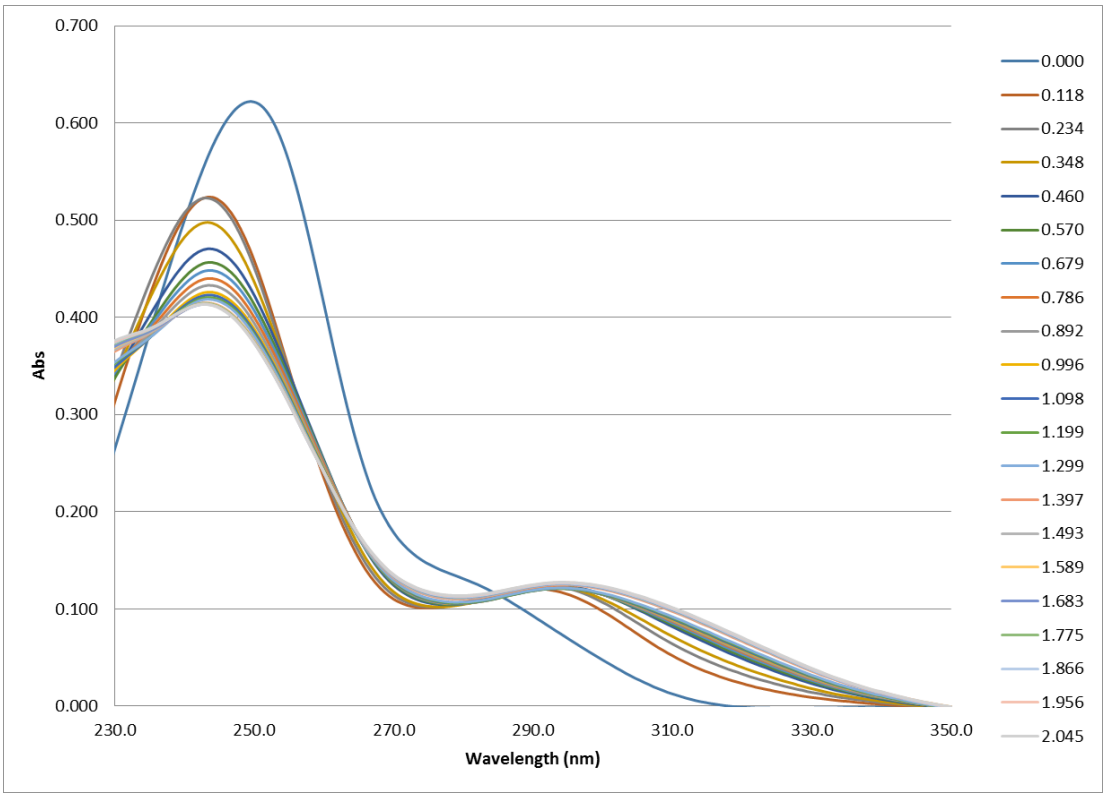



**Figure S40.** UV-VIS Absorption Spectroscopy, **2A** and $Eu(OTf)_3$ titration in 80% Acetonitrile and 20% DCM.

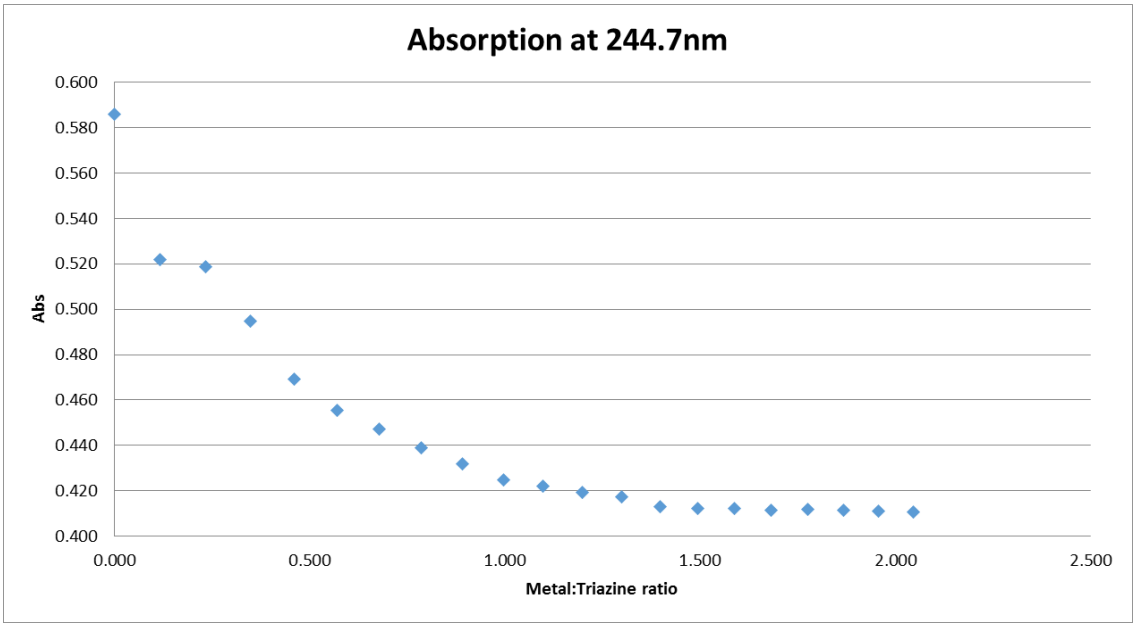



**Figure S41.** UV-VIS Absorption Spectroscopy, **2A** and $Eu(OTf)_3$ titration in 80% Acetonitrile and 20% DCM.

**Section (14): Cartisian coordinates for optimized structures of 2A with metal chlorides.**

**Cartesian coordinates for optimized structures: Part 1 – Coordination of group I metal chlorides to phenyltriazine (2A)**

All calculations were performed with the GAMESS-US[1–3] suite of packages using the dispersion–corrected B3LYP-D3 density functional theory (DFT) method. Geometry optimizations were performed with the 6-31+G(d) basis set for first and second row atoms and with the SBKJC basis set and ECP for atoms in the third row and higher. Geometry optimizations were followed by single point energy calculations with the aug-cc-pVTZ[10,11] basis set for first and second row atoms and with the SBKJC basis set and ECP for atoms in the third row and higher. A continuum dielectric with the IEF-cPCM[12–14] method was utilized to represent reaction conditions and all reported stationary points were optimized in implicit MeCN solvent. Reported energies are free energies in kcal/mol. Only vibrational free energy corrections to the electronic energy at 298 K were used in accordance with recommendations for molecules optimized in implicit solvent.[15] Normal modes of all structures were examined to verify that equilibrium structures possess no imaginary frequencies and that one imaginary frequency corresponding to bond formation or bond breaking was obtained for transition state structures. Intrinsic reaction coordinate (IRC) calculations were also performed to verify that transition states are connected to reactant complexes and intermediates on the potential energy surfaces of reactions.

The following settings were used in GAMESS-US.

$dft  nrad=126  nleb=770 $end

$tescav ntsall=240 $end

$force temp=298  $end

Gradient tolerance [a.u.]:  0.00003 for minima and saddle points

agcl
E [6-311+G(2d,p); Hartrees] = -161.2707161199
E [aug-cc-pVTZ; Hartrees] = -161.2707309778
Gvib [kcal/mol] = .209
Ag 0.00000000 0.00000000 1.17047556
Cl 0.00000000 0.00000000 -1.25825196

cacl2
E [aug-cc-pVTZ; Hartrees] = -30.7330820895
Gvib [kcal/mol] = .217
Ca 0.07409295 0.13420856 0.53682711
Cl -0.39583013 1.35847452 -1.59043435
Cl 0.54324293 -1.08817749 2.66536951

kcl
E [6-311+G(2d,p); Hartrees] = -15.2044407364
E [aug-cc-pVTZ; Hartrees] = -15.2044619143
Gvib [kcal/mol] = .000
K 0.00000000 0.00000000 1.52423287
Cl 0.00000000 0.00000000 -1.61200927

licl
E [6-311+G(2d,p); Hartrees] = -22.5557424743
E [aug-cc-pVTZ; Hartrees] = -22.5602765579
Gvib [kcal/mol] = .635
Li 0.00000000 0.00000000 1.04291393
Cl 0.00000000 0.00000000 -1.13069033

mgcl2
E [6-311+G(2d,p); Hartrees] = -30.8505587622
E [aug-cc-pVTZ; Hartrees] = -30.8501493851
Gvib [kcal/mol] = .689
MG 0.07382529 0.13485940 0.53727118
CL -0.36037984 1.26613631 -1.43061873
CL 0.50806030 -0.99649009 2.50510980

nacl
E [6-311+G(2d,p); Hartrees] = -15.2308973180
E [aug-cc-pVTZ; Hartrees] = -15.2309281304
Gvib [kcal/mol] = .000
Na 0.00000000 0.00000000 1.28770723
Cl 0.00000000 0.00000000 -1.37548363

phtriazn3eq_agcl

E [6-311+G(2d,p); Hartrees] = -1138.5130583624
E [aug-cc-pVTZ; Hartrees] = -1138.8387622787
Gvib [kcal/mol] = 228.992

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| N | 0.28648334 | -0.35280693 | 1.28708569 |
| N | 0.63273951 | 1.06890998 | -0.57076800 |
| C | -0.37957075 | -1.34637650 | 0.44219980 |
| C | 1.31919579 | 0.37097439 | 0.52295578 |
| C | -0.02338520 | 0.09308031 | -1.46592977 |
| C | -2.01911943 | -1.36665396 | -1.37714764 |
| C | -1.84003966 | -1.78959095 | -2.70198795 |
| C | -2.85597129 | -2.50023803 | -3.35413880 |
| C | -4.04385804 | -2.81200514 | -2.68899775 |
| C | -4.21953168 | -2.39528189 | -1.36241249 |
| C | -3.22069650 | -1.66901584 | -0.71435869 |
| C | 0.68616722 | -0.76994956 | 2.59875690 |
| C | 0.84908388 | -2.11794189 | 2.94918110 |
| C | 1.20789701 | -2.46279408 | 4.25876816 |
| C | 1.42682902 | -1.47300816 | 5.21958867 |
| C | 1.27170709 | -0.12534672 | 4.86699483 |
| C | 0.89349817 | 0.22361661 | 3.57086863 |
| C | 1.36702206 | 2.10197221 | -1.24593390 |
| C | 2.76519345 | 2.19165387 | -1.19993028 |
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| C | 2.69431671 | 4.20073165 | -2.56421539 |
| C | 1.29699754 | 4.10500278 | -2.61773891 |
| C | 0.63713025 | 3.07012417 | -1.95554854 |
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| H | -1.13893116 | -1.86275393 | 1.02835191 |
| H | 2.07907292 | -0.33723262 | 0.14635735 |
| H | 1.80198960 | 1.10417124 | 1.16774255 |
| H | 0.73020478 | -0.59502411 | -1.88906012 |
| H | -0.52002958 | 0.62223786 | -2.27853932 |
| H | -0.91746547 | -1.58093049 | -3.23446315 |
| H | -2.70577479 | -2.81725767 | -4.38322559 |
| H | -4.82720840 | -3.36852041 | -3.19694128 |
| H | -5.14445420 | -2.61975538 | -0.83698044 |
| H | -3.37597564 | -1.31552761 | 0.30237523 |
| H | 0.70814147 | -2.90557908 | 2.21572472 |
| H | 1.32515559 | -3.51198078 | 4.51836967 |
| H | 1.70993605 | -1.74473877 | 6.23318321 |
| H | 1.42531869 | 0.65513513 | 5.60801580 |
| H | 0.73563197 | 1.26758765 | 3.31091799 |
| H | 3.35439569 | 1.44988961 | -0.67030459 |
| H | 4.50512771 | 3.30686767 | -1.80042198 |
| H | 3.20794336 | 5.01436620 | -3.06966921 |
| H | 0.71823648 | 4.84904833 | -3.15922268 |
| H | -0.44913572 | 3.01891063 | -1.96796557 |
| Ag | -1.52113098 | 1.50589039 | 0.77787483 |
| Cl | -3.15553953 | 3.07635141 | 1.73674021 |

phtriazn3eq_cacl2
E [6-311+G(2d,p); Hartrees] = -1007.9722046519
E [aug-cc-pVTZ; Hartrees] = -1008.3276432613
Gvib [kcal/mol] = 229.489

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|---|---|---|---|
| N | 0.90186708 | -1.30172472 | 0.59995674 |
| N | 0.59834608 | 0.19734117 | -1.20267956 |
| N | 0.87591551 | 1.02777139 | 1.00363375 |
| C | 0.17032040 | -1.11333249 | -0.67725531 |
| C | 0.16334941 | 1.27027143 | -0.26516342 |
| C | 0.46529805 | -0.28138951 | 1.57400290 |
| C | 0.88359220 | -2.67072998 | 1.06889551 |
| C | 0.04423886 | -3.10632637 | 2.10066356 |
| C | 0.08260861 | -4.44570044 | 2.50829811 |
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| C | 1.76975316 | -4.91667882 | 0.84043735 |
| C | 1.74878202 | -3.57924526 | 0.44419593 |
| C | 0.22811825 | 0.47264060 | -2.57706555 |
| C | -0.82524002 | -0.18863787 | -3.22056159 |
| C | -1.12729050 | 0.11875008 | -4.55332143 |
| C | -0.39911900 | 1.09400064 | -5.23904439 |
| C | 0.64744702 | 1.75922082 | -4.58810620 |
| C | 0.96557603 | 1.44602591 | -3.26609934 |
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| C | 0.03951108 | 4.18449522 | 2.88313650 |
| C | 1.04689237 | 4.17703254 | 3.85115274 |
| C | 1.97668481 | 3.12975165 | 3.87352869 |
| C | 1.90270972 | 2.10642463 | 2.92895783 |
| H | -0.91804987 | -1.16534843 | -0.50741344 |
| H | 0.46420374 | -1.89377511 | -1.38058399 |
| H | -0.93188362 | 1.25008508 | -0.14183541 |
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| H | -0.64115217 | -2.42275254 | 2.59141833 |
| H | -0.56707579 | -4.77511074 | 3.31500481 |
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| H | 2.44604357 | -5.61183740 | 0.35001902 |
| H | 2.41185841 | -3.23580855 | -0.34694744 |
| H | -1.41925738 | -0.93711083 | -2.70642522 |
| H | -1.94220489 | -0.40389877 | -5.04751237 |
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| H | 1.22715294 | 2.51452868 | -5.11263215 |
| H | 1.79438931 | 1.94382716 | -2.76910810 |
| H | -0.85333295 | 3.16962242 | 1.21041918 |
| H | -0.68702072 | 4.99249384 | 2.85813651 |
| H | 1.11097835 | 4.98023009 | 4.58049382 |
| H | 2.76979245 | 3.11551264 | 4.61664121 |
| H | 2.63786425 | 1.30397559 | 2.93507646 |
| Ca | 2.86888574 | 0.11388684 | -0.07350341 |

| | | | |
|---|---|---|---|
| Cl | 4.40294075 | -0.79352308 | 1.94339362 |
| Cl | 4.09121789 | 2.20123546 | -1.24825179 |

phtriazn3eq
E [6-311+G(2d,p); Hartrees] = -977.1879611020
E [aug-cc-pVTZ; Hartrees] = -977.5151170523
Gvib [kcal/mol] = 230.153

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| N | -0.74914396 | -1.15210090 | -0.25126936 |
| N | -0.61729266 | 1.22982123 | -0.24674904 |
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| C | -1.39180122 | 0.08446216 | 0.21184016 |
| C | 0.76836083 | 1.16227560 | 0.23590241 |
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| C | 4.97214636 | 0.60587353 | 0.60071408 |
| C | 5.60610388 | -0.43722330 | -0.07707006 |
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| C | -1.55161250 | -2.32066232 | -0.14636667 |
| C | -1.16733327 | -3.44264770 | 0.61103294 |
| C | -1.97440453 | -4.58709465 | 0.64582796 |
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| C | -2.76851351 | -2.37706626 | -0.85755737 |
| C | -1.23221174 | 2.50643610 | -0.14440096 |
| C | -2.42601806 | 2.71966187 | 0.56992740 |
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| C | -2.43120985 | 5.06907276 | -0.05755892 |
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| H | 0.64772773 | -1.27890035 | 1.35117852 |
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| H | 1.33301841 | 2.00392015 | -0.16180497 |
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| H | 5.55892078 | 1.32935683 | 1.16216422 |
| H | 6.68866817 | -0.53249025 | -0.05646301 |
| H | 5.30023480 | -2.16906949 | -1.33636792 |
| H | 2.85287673 | -1.92950030 | -1.42197837 |
| H | -0.24840895 | -3.43695155 | 1.18762340 |
| H | -1.65285033 | -5.44252788 | 1.23557995 |
| H | -3.80861549 | -5.51857585 | -0.01858255 |
| H | -4.50655837 | -3.53229645 | -1.36322721 |
| H | -3.06979754 | -1.53578651 | -1.47622946 |
| H | -2.89940675 | 1.91160229 | 1.11734944 |
| H | -3.94472527 | 4.12382986 | 1.15731747 |
| H | -2.89212932 | 6.05290514 | -0.02585427 |
| H | -0.76922965 | 5.69174809 | -1.29353340 |

| | | | |
|---|---|---|---|
| H | 0.25339980 | 3.45729780 | -1.40263159 |

phtriazn3eq_kcl
E [6-311+G(2d,p); Hartrees] = -992.4235556458
E [aug-cc-pVTZ; Hartrees] = -992.7504887470
Gvib [kcal/mol] = 228.189

| | | | |
|---|---|---|---|
| N | -0.98362905 | -0.66435343 | -0.67913381 |
| N | 0.34117672 | -0.38875216 | 1.27248776 |
| N | 0.68971290 | 1.01683457 | -0.60970241 |
| C | -0.33430386 | -1.37864838 | 0.43444755 |
| C | 1.36282379 | 0.33551535 | 0.49558904 |
| C | 0.01249584 | 0.04261605 | -1.48381583 |
| C | -1.98661350 | -1.40241913 | -1.37782538 |
| C | -1.88724561 | -1.71434131 | -2.74374474 |
| C | -2.92948648 | -2.38982419 | -3.39177522 |
| C | -4.07076111 | -2.78188751 | -2.68900569 |
| C | -4.16833418 | -2.48352528 | -1.32326623 |
| C | -3.14297358 | -1.79495872 | -0.67604291 |
| C | 0.74004106 | -0.79880407 | 2.58025437 |
| C | 0.77304588 | -2.14562040 | 2.97745558 |
| C | 1.11081445 | -2.48539497 | 4.29385590 |
| C | 1.43920494 | -1.49674580 | 5.22372391 |
| C | 1.42061469 | -0.15252906 | 4.82769795 |
| C | 1.06772780 | 0.19423408 | 3.52400497 |
| C | 1.40464353 | 2.05727017 | -1.27442235 |
| C | 2.78137561 | 2.26797861 | -1.09047008 |
| C | 3.42075207 | 3.34845134 | -1.71161955 |
| C | 2.70869266 | 4.21872577 | -2.53939566 |
| C | 1.33831671 | 4.00344351 | -2.73807923 |
| C | 0.69097100 | 2.94108972 | -2.10797809 |
| H | 0.37397772 | -2.13249365 | 0.03614522 |
| H | -1.09033601 | -1.89304872 | 1.02727922 |
| H | 2.13422804 | -0.37283880 | 0.13292179 |
| H | 1.84360316 | 1.07732168 | 1.13215033 |
| H | 0.75754028 | -0.65166733 | -1.92088296 |
| H | -0.49127309 | 0.56658584 | -2.29568269 |
| H | -1.00387856 | -1.44531170 | -3.31372901 |
| H | -2.83523555 | -2.61618116 | -4.45108872 |
| H | -4.87494482 | -3.30947999 | -3.19513026 |
| H | -5.05328968 | -2.77253565 | -0.76166671 |
| H | -3.24894788 | -1.54836742 | 0.37781914 |
| H | 0.54733887 | -2.93980641 | 2.27332462 |
| H | 1.12489369 | -3.53344256 | 4.58320864 |
| H | 1.70360881 | -1.76520697 | 6.24313625 |
| H | 1.66448816 | 0.63104152 | 5.54085896 |
| H | 1.03366313 | 1.24389526 | 3.24138167 |
| H | 3.36956463 | 1.59676965 | -0.47347787 |
| H | 4.48572763 | 3.49600329 | -1.54933767 |
| H | 3.20989603 | 5.05376398 | -3.02171744 |
| H | 0.76608257 | 4.67527316 | -3.37311293 |

| | | | |
|---|---|---|---|
| H | -0.37807458 | 2.80748641 | -2.25598438 |
| K | -1.79249729 | 1.78691860 | 0.97258698 |
| Cl | -4.04519750 | 3.69696625 | 1.83469391 |

phtriazn3eq_licl
E [6-311+G(2d,p); Hartrees] = -999.7932664870
E [aug-cc-pVTZ; Hartrees] = -1000.1209368467
Gvib [kcal/mol] = 231.292

| | | | |
|---|---|---|---|
| N | 1.36074970 | -0.04874705 | -0.07449547 |
| N | -0.66803977 | -0.83222658 | 0.84151738 |
| N | -0.69937949 | 0.67679542 | -0.96914023 |
| C | 0.70110753 | -0.43230198 | 1.19393760 |
| C | -1.40149316 | 0.31949984 | 0.27050331 |
| C | 0.68065032 | 1.11462404 | -0.66010466 |
| C | 2.79547289 | 0.00633749 | -0.00235560 |
| C | 3.50874650 | 1.21190105 | -0.05707226 |
| C | 4.90825516 | 1.20029456 | 0.00057660 |
| C | 5.60309558 | -0.00456976 | 0.12952818 |
| C | 4.88905287 | -1.20868625 | 0.19115765 |
| C | 3.49612851 | -1.20527932 | 0.11637581 |
| C | -1.40193920 | -1.57975256 | 1.82550074 |
| C | -1.04775424 | -1.59233975 | 3.18167450 |
| C | -1.78414067 | -2.36252073 | 4.09095092 |
| C | -2.88482283 | -3.10740623 | 3.66160772 |
| C | -3.24396746 | -3.08734569 | 2.30724787 |
| C | -2.50321591 | -2.33756273 | 1.39340199 |
| C | -1.39791420 | 1.52941446 | -1.89089525 |
| C | -2.48720357 | 2.32438873 | -1.50804228 |
| C | -3.14214465 | 3.11931063 | -2.45765631 |
| C | -2.70741515 | 3.14329337 | -3.78473735 |
| C | -1.61378503 | 2.35401231 | -4.16518987 |
| C | -0.96929158 | 1.54561996 | -3.22869733 |
| H | 0.72180733 | 0.41137842 | 1.90797592 |
| H | 1.22358366 | -1.28295550 | 1.63169090 |
| H | -1.42982230 | 1.15454946 | 0.99401597 |
| H | -2.42157846 | 0.01880816 | 0.03148220 |
| H | 0.66140181 | 1.98021697 | 0.02718997 |
| H | 1.18717520 | 1.40239723 | -1.58133806 |
| H | 2.99149593 | 2.16295275 | -0.13568693 |
| H | 5.45045140 | 2.14148159 | -0.04613142 |
| H | 6.68889534 | -0.00871830 | 0.17856288 |
| H | 5.41834732 | -2.15410961 | 0.28009267 |
| H | 2.94737788 | -2.14374418 | 0.13362864 |
| H | -0.20942913 | -1.00612445 | 3.54424637 |
| H | -1.49495144 | -2.36792525 | 5.13893013 |
| H | -3.45601780 | -3.70077871 | 4.37081519 |
| H | -4.09213168 | -3.67098424 | 1.95833013 |
| H | -2.76749176 | -2.35162549 | 0.33884976 |
| H | -2.83182874 | 2.34112817 | -0.47896365 |
| H | -3.98886557 | 3.72704631 | -2.14816817 |

| | | | |
|---|---|---|---|
| H | -3.21492717 | 3.76564492 | -4.51719821 |
| H | -1.27170183 | 2.35420371 | -5.19710792 |
| H | -0.14124341 | 0.91195646 | -3.53707575 |
| Li | 0.00762692 | -1.37281300 | -1.13416435 |
| Cl | 0.03107433 | -3.05873865 | -2.53785858 |

phtriazn3eq_mgcl2
E [6-311+G(2d,p); Hartrees] = -1008.1153301576
E [aug-cc-pVTZ; Hartrees] = -1008.4461829225
Gvib [kcal/mol] = 230.871

| | | | |
|---|---|---|---|
| N | 0.85203247 | -1.27835862 | 0.60856980 |
| N | 0.55837334 | 0.20951394 | -1.18464210 |
| N | 0.86095172 | 1.03603250 | 1.00725561 |
| C | 0.11643468 | -1.09536975 | -0.66155932 |
| C | 0.13770321 | 1.29092266 | -0.25606966 |
| C | 0.42775817 | -0.26320795 | 1.58876359 |
| C | 0.87391311 | -2.64675717 | 1.07355148 |
| C | 0.05515777 | -3.09762511 | 2.11487732 |
| C | 0.12273000 | -4.43625693 | 2.52154407 |
| C | 0.98759220 | -5.32698744 | 1.88079199 |
| C | 1.79754708 | -4.87327688 | 0.83151755 |
| C | 1.74763817 | -3.53650814 | 0.43514500 |
| C | 0.22996322 | 0.47690768 | -2.56948254 |
| C | -0.75714795 | -0.24143140 | -3.25666092 |
| C | -1.02091386 | 0.04839952 | -4.60155338 |
| C | -0.31920086 | 1.06055140 | -5.26031850 |
| C | 0.65884208 | 1.78357642 | -4.56609763 |
| C | 0.93750180 | 1.49105277 | -3.23057842 |
| C | 0.90344589 | 2.12342641 | 1.96318526 |
| C | -0.04019198 | 3.15589021 | 1.97276915 |
| C | 0.07021962 | 4.18439913 | 2.91744628 |
| C | 1.10345304 | 4.17547807 | 3.85788597 |
| C | 2.04064259 | 3.13442210 | 3.84773161 |
| C | 1.94676695 | 2.11564771 | 2.89954913 |
| H | -0.97200233 | -1.13748312 | -0.49325825 |
| H | 0.40719391 | -1.87988846 | -1.35935869 |
| H | -0.95497803 | 1.28691420 | -0.12186890 |
| H | 0.45942227 | 2.25188388 | -0.65533673 |
| H | -0.65828666 | -0.26418285 | 1.76694101 |
| H | 0.96099463 | -0.43156757 | 2.52347550 |
| H | -0.63728415 | -2.42587126 | 2.61250691 |
| H | -0.51166122 | -4.77867255 | 3.33502650 |
| H | 1.03387084 | -6.36604236 | 2.19644682 |
| H | 2.48071387 | -5.55591344 | 0.33277358 |
| H | 2.39719359 | -3.17443936 | -0.35720105 |
| H | -1.33190453 | -1.02117886 | -2.76801083 |
| H | -1.78514325 | -0.51911992 | -5.12636488 |
| H | -0.52937826 | 1.28399074 | -6.30304047 |
| H | 1.21848219 | 2.56944308 | -5.06724750 |
| H | 1.72007534 | 2.02548692 | -2.70232125 |

| | | | |
|---|---|---|---|
| H | -0.86057860 | 3.17396369 | 1.26236519 |
| H | -0.66158328 | 4.98799488 | 2.91725026 |
| H | 1.18193570 | 4.97382482 | 4.59118621 |
| H | 2.85359282 | 3.12144679 | 4.56911347 |
| H | 2.68593726 | 1.31813581 | 2.87153941 |
| Mg | 2.64175472 | 0.13279900 | -0.00079703 |
| Cl | 4.09819115 | -0.86932011 | 1.57597028 |
| Cl | 3.82205550 | 1.87614712 | -1.07473203 |

phtriazn3eq_nacl
E [6-311+G(2d,p); Hartrees] = -992.4597505032
Gvib [kcal/mol] = 229.458

| | | | |
|---|---|---|---|
| N | 1.98323313 | -0.06871760 | 0.62032455 |
| C | 1.31356951 | -1.34823421 | 0.31343151 |
| N | 0.17924009 | -1.04748548 | -0.56712437 |
| C | -0.77906248 | -0.15987283 | 0.12444440 |
| N | -0.07595774 | 1.08942374 | 0.43371270 |
| C | 1.06562570 | 0.82347374 | 1.33394933 |
| C | 3.31684575 | -0.18199752 | 1.13151528 |
| C | 3.66913707 | 0.22368832 | 2.42732158 |
| C | 5.00233910 | 0.14450662 | 2.85044967 |
| C | 5.98979333 | -0.35783426 | 2.00020776 |
| C | 5.63692983 | -0.77640133 | 0.71017475 |
| C | 4.31500081 | -0.68215209 | 0.27586759 |
| C | -0.42473408 | -2.15703720 | -1.24526540 |
| C | -0.23451819 | -3.48813316 | -0.84483158 |
| C | -0.82439878 | -4.53151888 | -1.57032893 |
| C | -1.62192531 | -4.26154197 | -2.68452597 |
| C | -1.81894501 | -2.93206223 | -3.08117451 |
| C | -1.21901056 | -1.89001569 | -2.37464247 |
| C | -0.88365168 | 2.21341786 | 0.80944062 |
| C | -2.21663765 | 2.08534073 | 1.22736098 |
| C | -2.96793250 | 3.22578443 | 1.54020002 |
| C | -2.39711575 | 4.49772537 | 1.45842917 |
| C | -1.06288328 | 4.62662992 | 1.05002762 |
| C | -0.31506444 | 3.49678265 | 0.71979523 |
| H | 0.99124170 | -1.83864833 | 1.25170579 |
| H | 2.00671255 | -2.00840478 | -0.20816444 |
| H | -1.16311184 | -0.65582417 | 1.03629364 |
| H | -1.61686624 | 0.05721206 | -0.53836540 |
| H | 0.70542659 | 0.37875228 | 2.28125942 |
| H | 1.57726021 | 1.75963738 | 1.55791542 |
| H | 2.91966635 | 0.59859236 | 3.11699829 |
| H | 5.26024085 | 0.47098324 | 3.85494398 |
| H | 7.02253663 | -0.41929052 | 2.33342819 |
| H | 6.39604272 | -1.15933043 | 0.03260013 |
| H | 4.05879408 | -0.97784484 | -0.73898686 |
| H | 0.36161192 | -3.72829743 | 0.02967618 |
| H | -0.66291060 | -5.55790357 | -1.24987849 |
| H | -2.08139089 | -5.07411773 | -3.24130411 |

| | | | |
|---|---|---|---|
| H | -2.42733586 | -2.70514489 | -3.95313302 |
| H | -1.35203251 | -0.86426958 | -2.71075870 |
| H | -2.68017304 | 1.10846215 | 1.31953969 |
| H | -4.00148319 | 3.10954327 | 1.85709984 |
| H | -2.98245852 | 5.37978729 | 1.70454382 |
| H | -0.60808388 | 5.61080946 | 0.97020240 |
| H | 0.71036424 | 3.61308518 | 0.37607038 |
| NA | 1.40103864 | 0.97306225 | -1.63307476 |
| CL | 2.25818438 | 2.08263903 | -3.82220951 |

phtriazn3eq_zncl2
E [6-311+G(2d,p); Hartrees] = -1233.3315561157
E [aug-cc-pVTZ; Hartrees] = -1233.6587897920
Gvib [kcal/mol] = 229.810

| | | | |
|---|---|---|---|
| N | 0.86538712 | -1.24522846 | 0.59823202 |
| N | 0.42729206 | 0.24608635 | -1.17442938 |
| N | 0.89621735 | 1.05732672 | 1.00905261 |
| C | 0.07900278 | -1.06778365 | -0.65627317 |
| C | 0.11717706 | 1.31743693 | -0.22666993 |
| C | 0.45391166 | -0.23586718 | 1.59652243 |
| C | 0.90092628 | -2.62094203 | 1.05592452 |
| C | 0.04224381 | -3.09996232 | 2.05021310 |
| C | 0.12349485 | -4.44151913 | 2.44357735 |
| C | 1.04302140 | -5.30161903 | 1.83694296 |
| C | 1.89431544 | -4.81659844 | 0.83575654 |
| C | 1.82877290 | -3.47689318 | 0.45149427 |
| C | 0.14588145 | 0.52030161 | -2.54765865 |
| C | -0.76082834 | -0.25057427 | -3.29103490 |
| C | -0.98052682 | 0.03376496 | -4.64480879 |
| C | -0.31902039 | 1.09693879 | -5.26339824 |
| C | 0.57956514 | 1.87207251 | -4.51807452 |
| C | 0.82095408 | 1.58163934 | -3.17547407 |
| C | 0.92529125 | 2.15155418 | 1.96602568 |
| C | -0.02010542 | 3.18461328 | 1.95637785 |
| C | 0.06974299 | 4.21564377 | 2.90012857 |
| C | 1.08470841 | 4.21383324 | 3.85983166 |
| C | 2.02278059 | 3.17431809 | 3.86913076 |
| C | 1.94852638 | 2.15141470 | 2.92348872 |
| H | -0.99554462 | -1.18540567 | -0.43725001 |
| H | 0.39187124 | -1.83163893 | -1.36784131 |
| H | -0.96301289 | 1.34911026 | -0.00846448 |
| H | 0.43070118 | 2.27494822 | -0.63854176 |
| H | -0.62978607 | -0.23280235 | 1.77900324 |
| H | 0.99292570 | -0.41738453 | 2.52520902 |
| H | -0.68934560 | -2.44892995 | 2.51882440 |
| H | -0.54088374 | -4.81077787 | 3.22036800 |
| H | 1.10034213 | -6.34259465 | 2.14414750 |
| H | 2.61966313 | -5.47561207 | 0.36599315 |
| H | 2.50512796 | -3.08521216 | -0.30434758 |
| H | -1.31065112 | -1.06513793 | -2.82980020 |

| | | | |
|---|---|---|---|
| H | -1.68350777 | -0.57555319 | -5.20754025 |
| H | -0.49741313 | 1.31942720 | -6.31222994 |
| H | 1.11268227 | 2.69451507 | -4.98880752 |
| H | 1.55772622 | 2.15373623 | -2.62083191 |
| H | -0.82932315 | 3.20542759 | 1.23459341 |
| H | -0.66484490 | 5.01655260 | 2.88304069 |
| H | 1.14735884 | 5.01468109 | 4.59196115 |
| H | 2.82229494 | 3.16374026 | 4.60553066 |
| H | 2.68587328 | 1.35509445 | 2.91580210 |
| Zn | 2.70104786 | -0.06117405 | 0.19097717 |
| Cl | 3.99346490 | -0.75963937 | 1.94989845 |
| Cl | 3.90432727 | 0.55346512 | -1.60589247 |

zncl2
E [6-311+G(2d,p); Hartrees] = -256.0817919116
E [aug-cc-pVTZ; Hartrees] = -256.0817919150
Gvib [kcal/mol] = .539

| | | | |
|---|---|---|---|
| Zn | 0.07385506 | 0.13478736 | 0.53720902 |
| Cl | -0.32748629 | 1.18044007 | -1.28170057 |
| Cl | 0.47513698 | -0.91072183 | 2.35625383 |

**Section 15: Detector Results:**

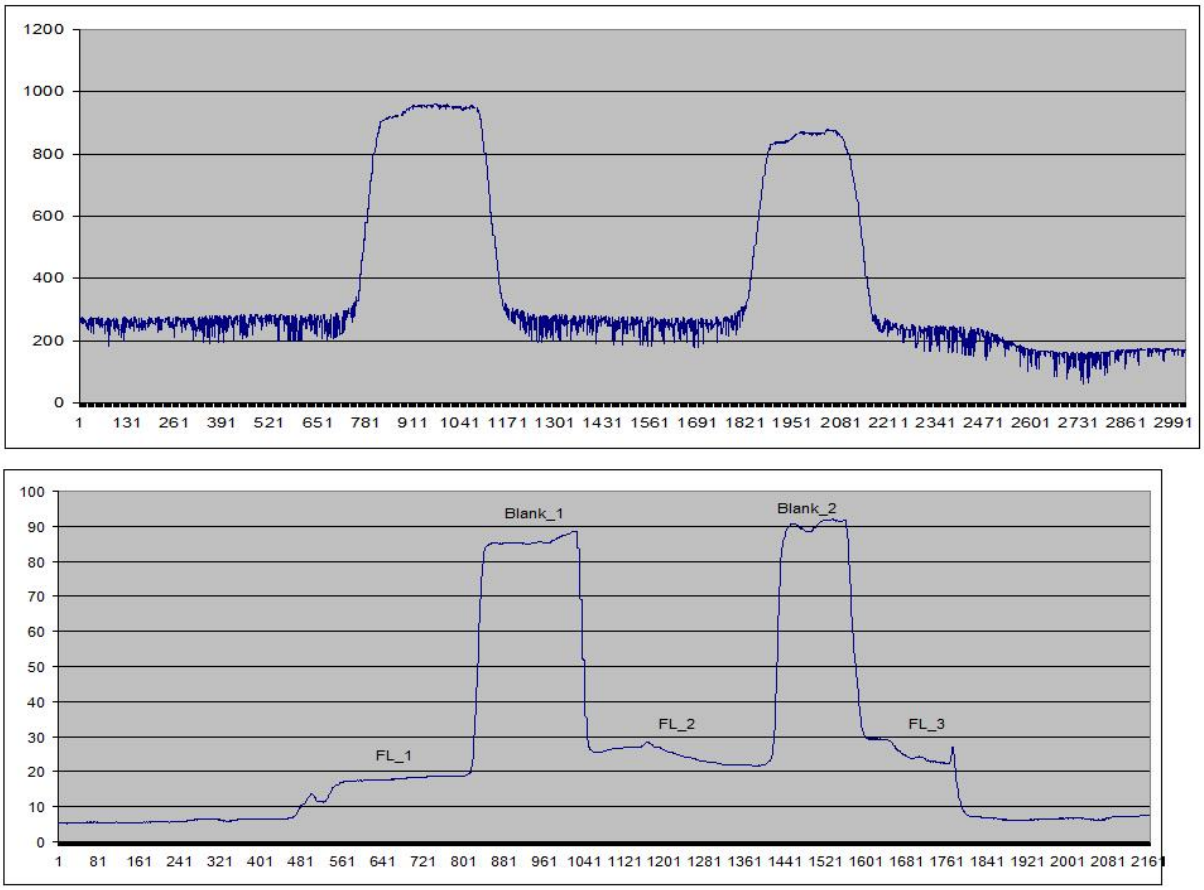


**Figure S42:** Comparison of two different light sources for fluorometer detection system. Y-axis transmission in arbitrary units. X-axis position of test strip. For comparison areas of high transmission (two peaks in top and bottom spectra) are areas where silica was removed from PET strips. (Top) use of low pressure mercury light source. (Bottom) use of LED light source.

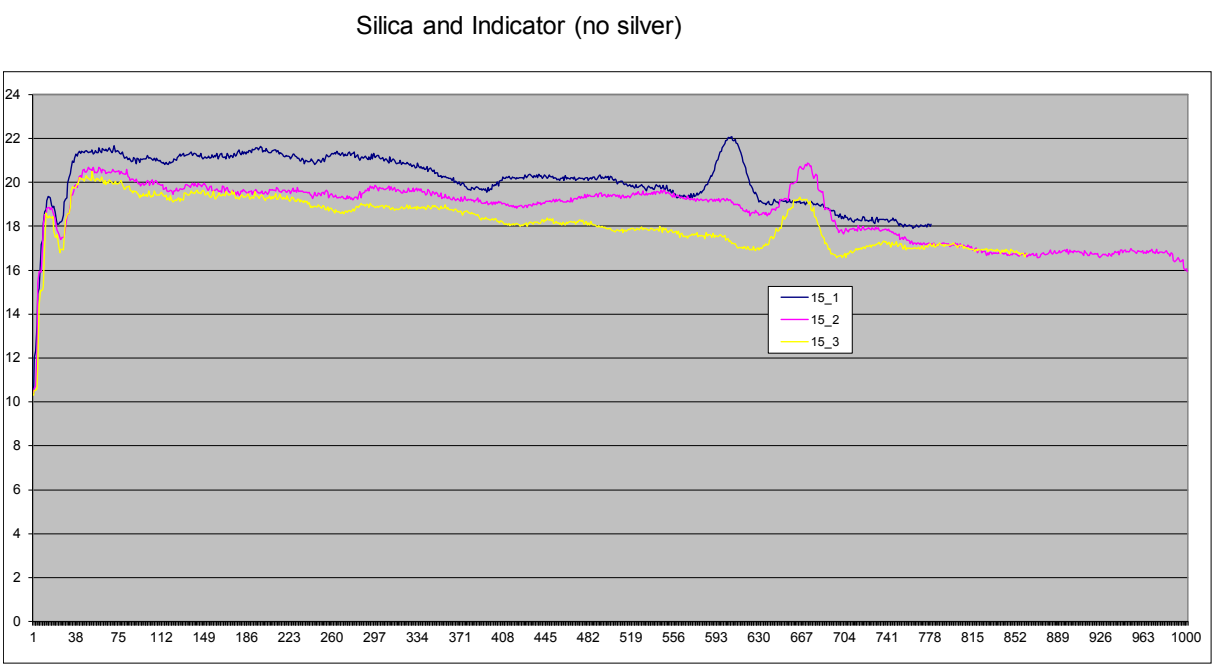


**Figure S43:** Baseline measurements of test strips containing silica, fluorescent indicator and triazine 2B. No metal was exposed to these test strips.

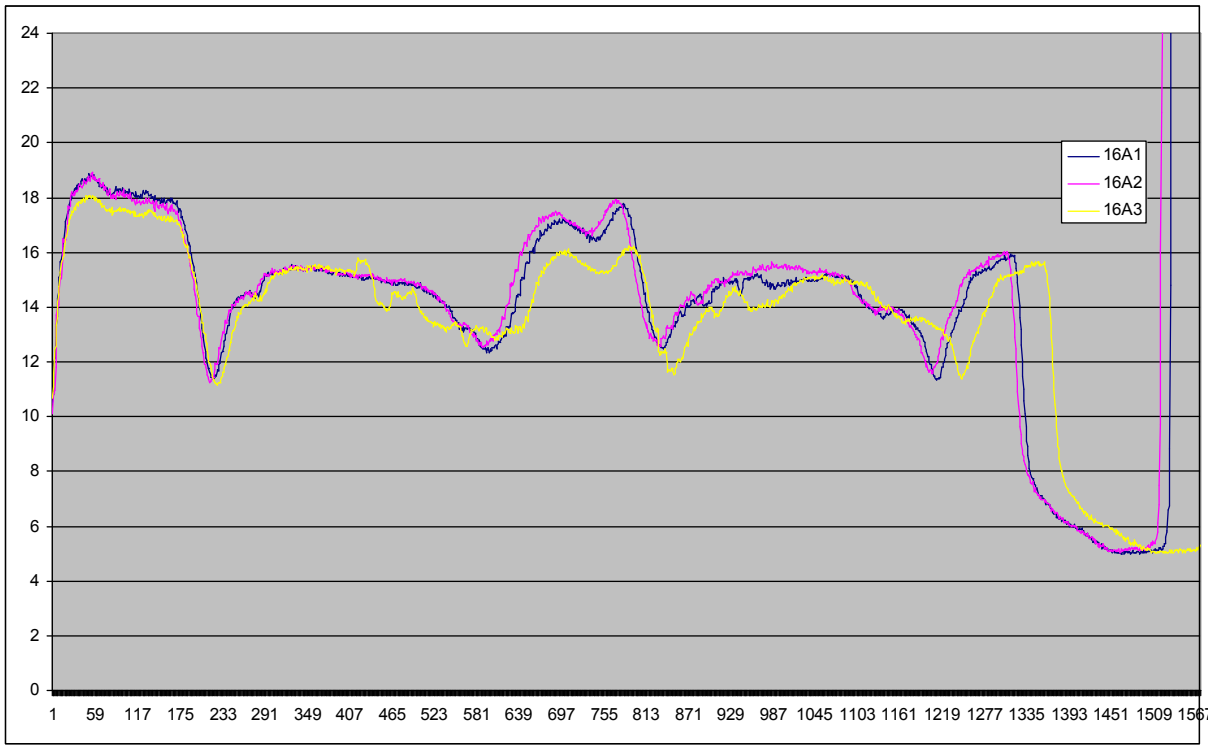


**Figure S44:** Results of test strip exposed to a low concentration (6.25 ug/L) of Ag(OTf). Y-axis corresponds with transmission % and x-axis corresponds with position of the test strip in arbitrary units. Reduction in transmission at position ca. 233 to ca. 581 and 871 to 1219 correspond with areas of the test strip exposed to Ag(OTf). The same sample was run three separate times showing the reproducibility of this method.

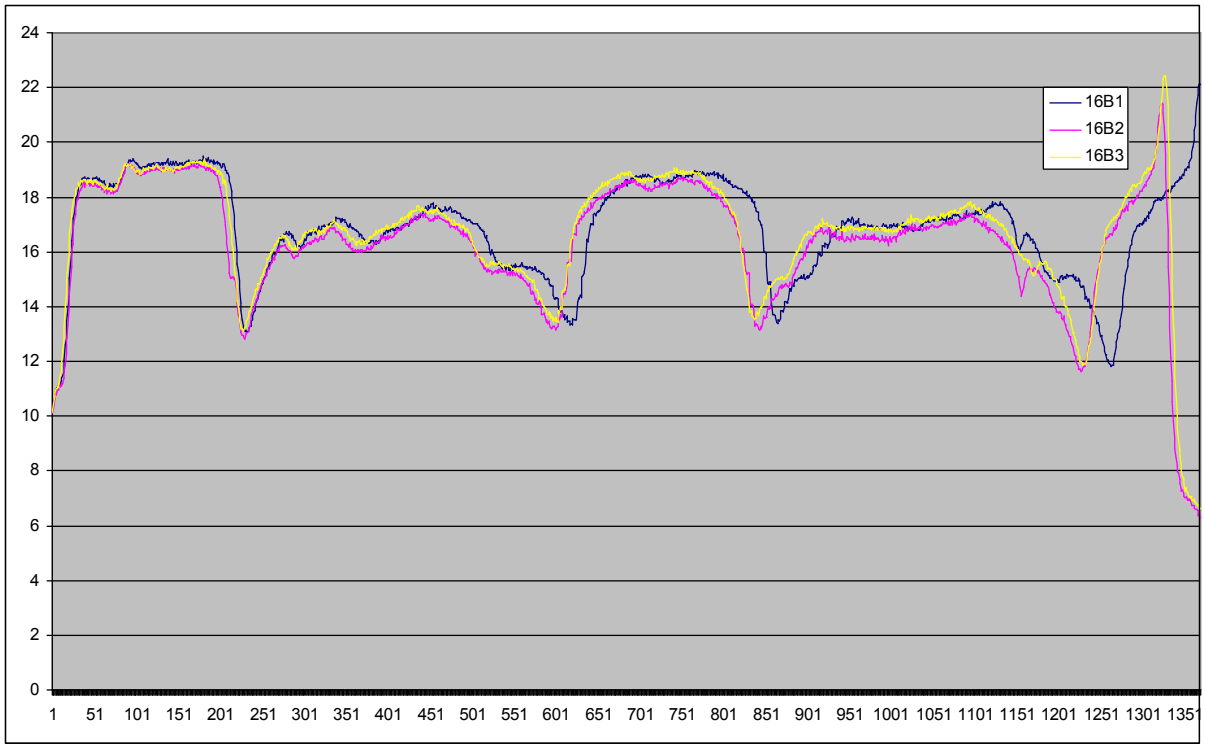


**Figure S45:** Results of 2nd test strip exposed to a low concentration (6.25 ug/L) of Ag(OTf). Y-axis corresponds with transmission % and x-axis corresponds with position of the test strip in arbitrary units. Reduction in transmission at position ca. 251 to ca. 601 and 851 to 1201 correspond with areas of the test strip exposed to Ag(OTf). The same sample was run three separate times showing the reproducibility of this method.

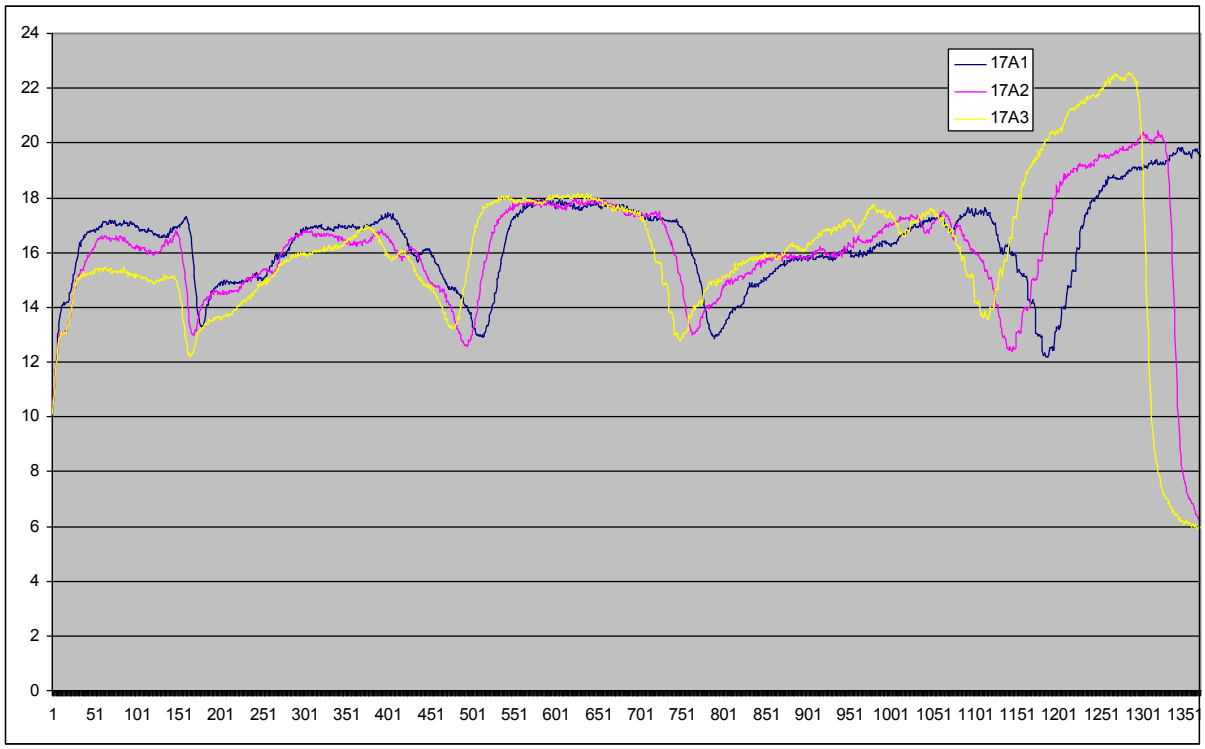


**Figure S46:** Results of test strip exposed to a 2x safety threshold (12.5 ug/L) of Ag(OTf). Y-axis corresponds with transmission % and x-axis corresponds with position of the test strip in arbitrary units. Reduction in transmission at position ca. 201 to ca. 501 and 801 to 1201

correspond with areas of the test strip exposed to Ag(OTf). The same sample was run three separate times showing the reproducibility of this method.

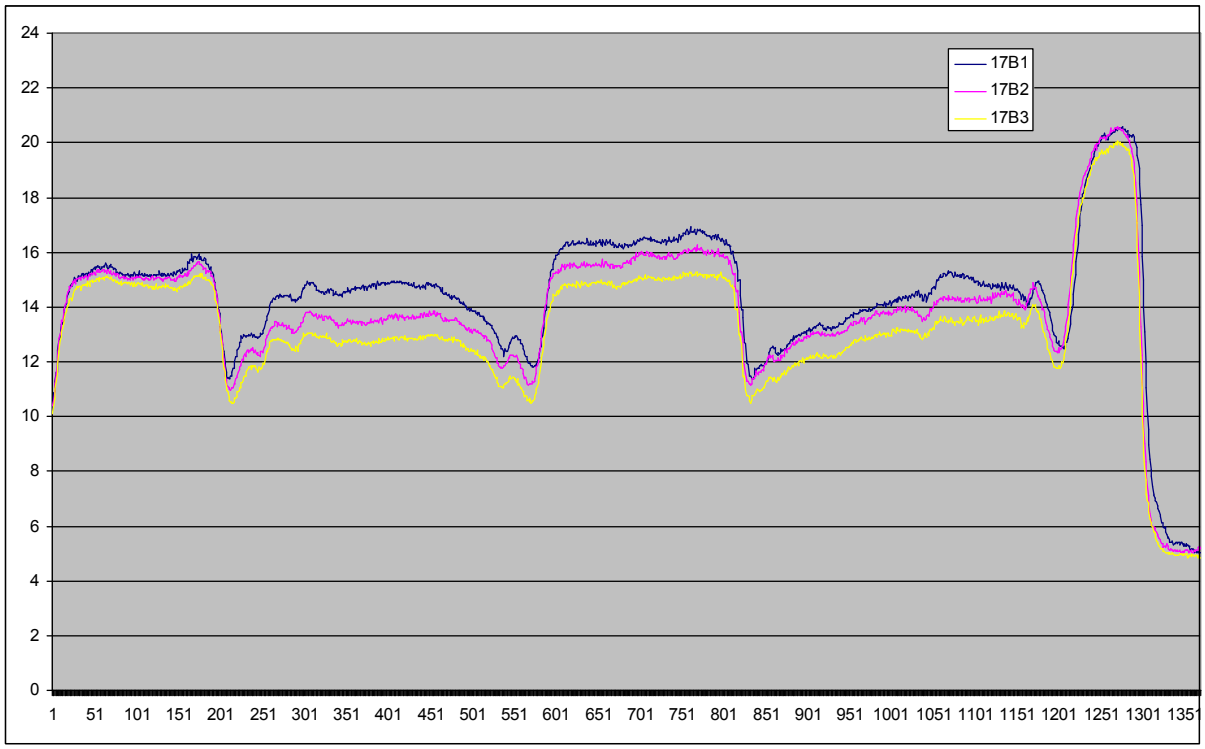


**Figure S47:** Results of 2nd test strip exposed to a 2x safety threshold (12.5 ug/L) of Ag(OTf). Y-axis corresponds with transmission % and x-axis corresponds with position of the test strip in arbitrary units. Reduction in transmission at position ca. 201 to ca. 551 and 801 to 1201 correspond with areas of the test strip exposed to Ag(OTf). The same sample was run three separate times showing the reproducibility of this method.

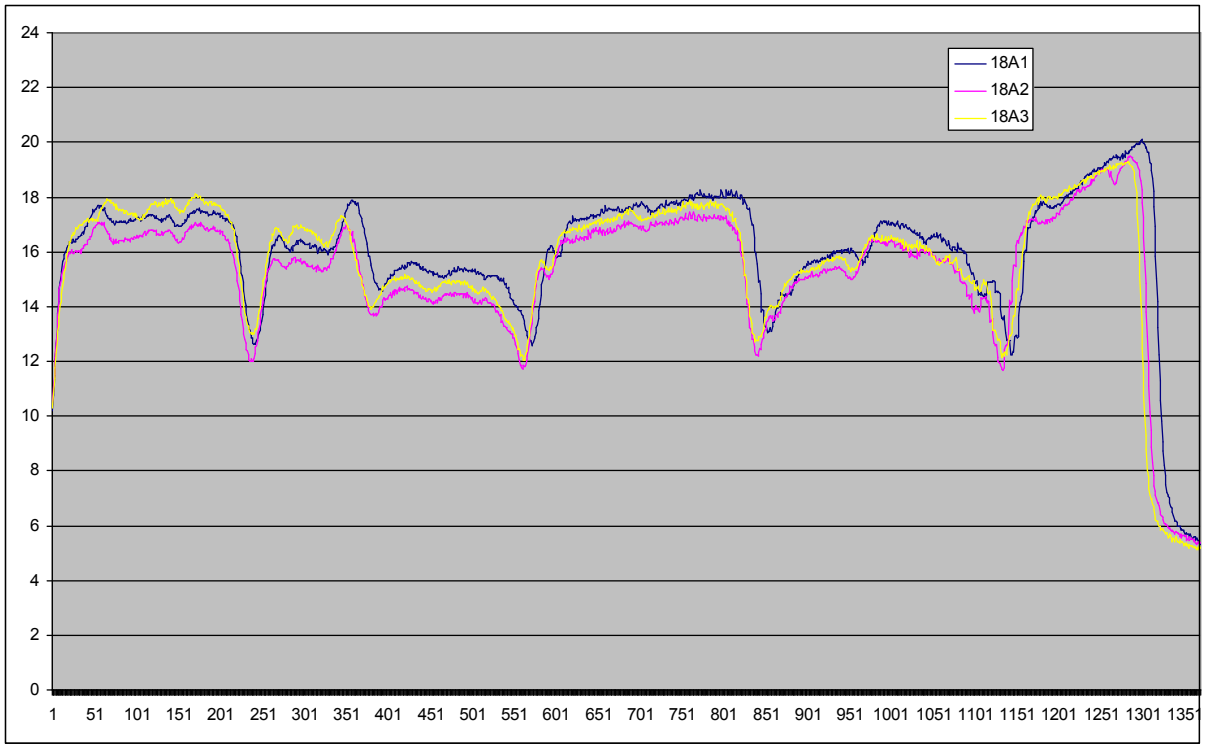


**Figure S48:** Results of test strip exposed to a 3x safety threshold (25 ug/L) of Ag(OTf). Y-axis corresponds with transmission % and x-axis corresponds with position of the test strip in arbitrary units. Reduction in transmission at position ca. 351 to ca. 551 and 851 to 1151 correspond with areas of the test strip exposed to Ag(OTf). The same sample was run three separate times showing the reproducibility of this method.

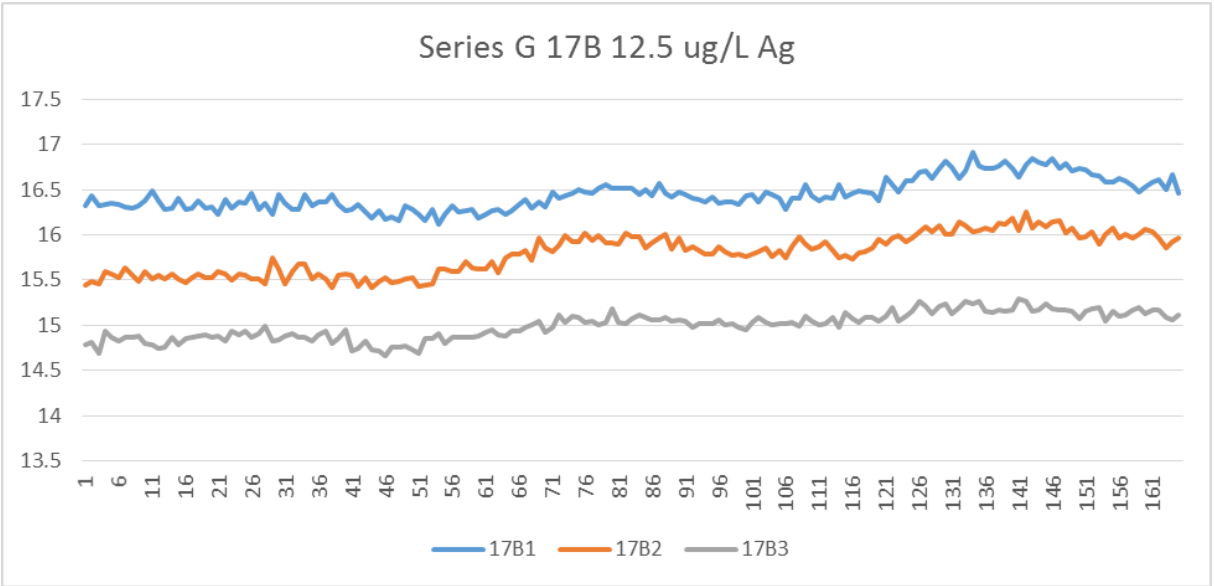


**Figure S49.** Three subsequent reads of a strip coated with indicator and a silver concentration of 12.5 ug/L. The exposure to the UV light exposes the indicator, decreasing the transmission with each exposure.