Supporting Information

Synthesis, Characterization and Biological Evaluation of New Manganese Metal Carbonyl Compounds That Contain Sulfur and Selenium Ligands as a Promising New Class of CORMs

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[‡]Crystallographic information available free of charge at the Cambridge Crystallographic Data Centre as supplementary publication numbers CCDC 1894674, 1894675 and 1894677.

[§]Both authors contributed equally to this work.

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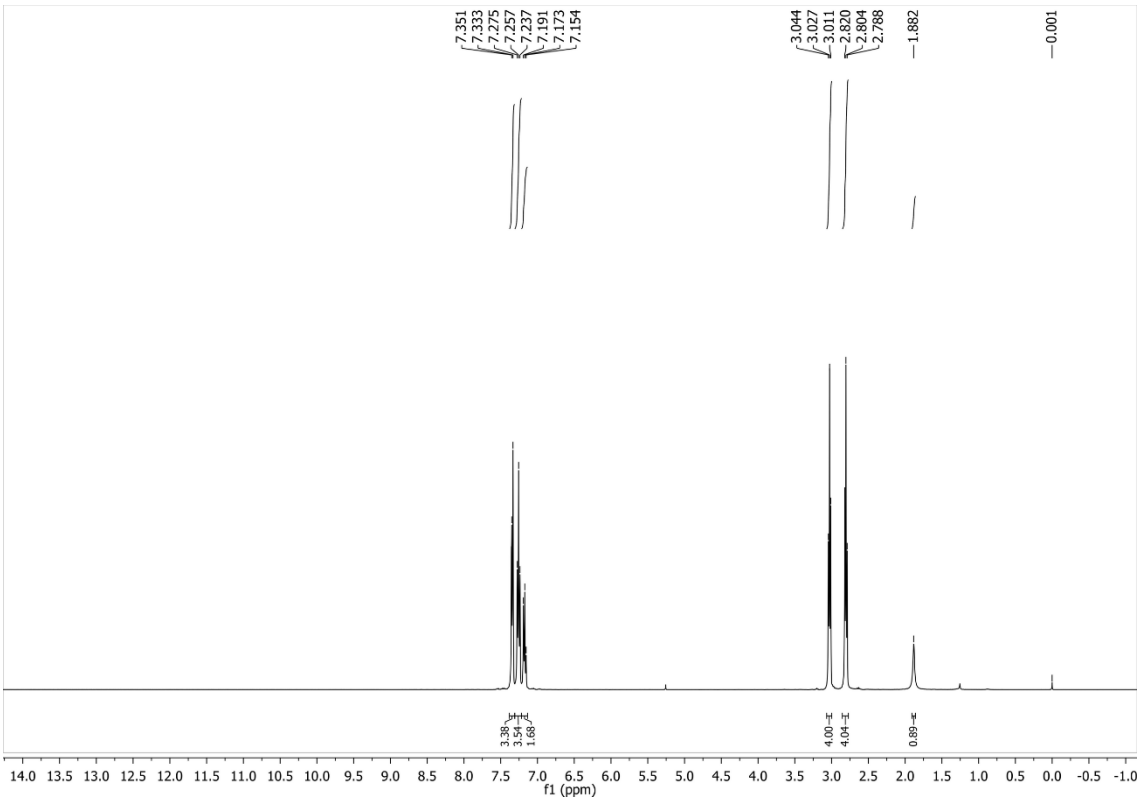

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1'**.

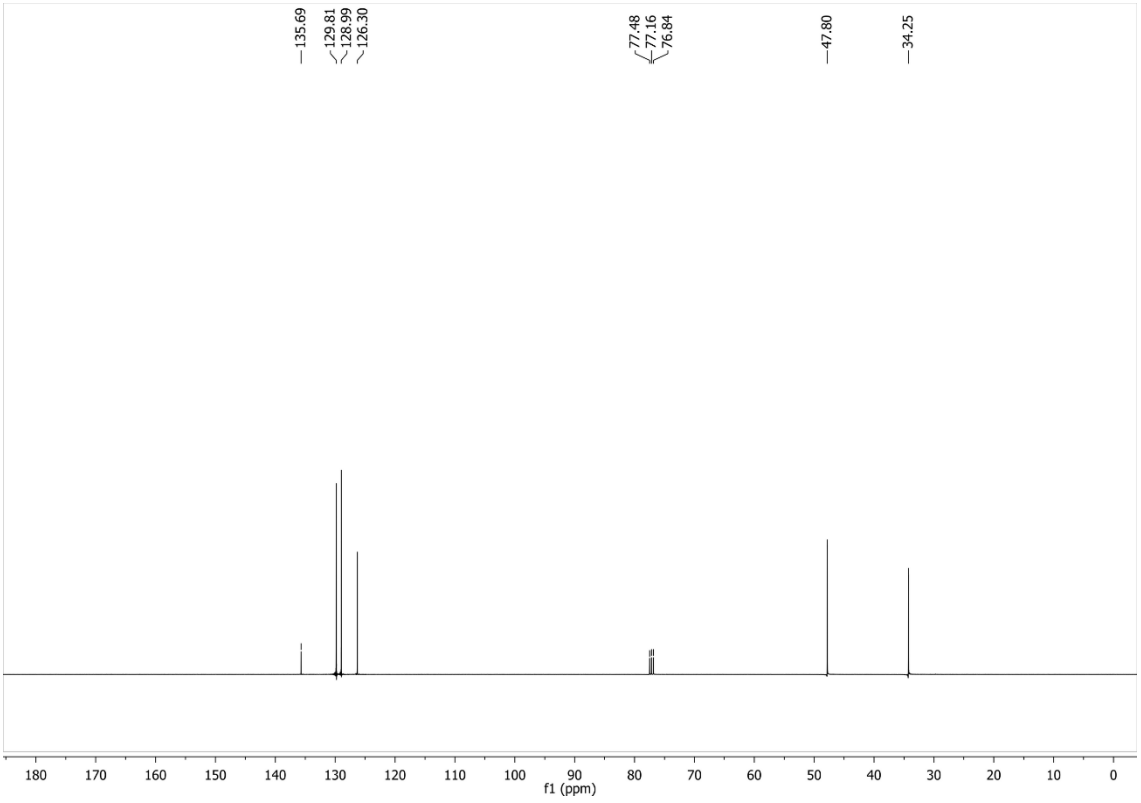

Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **1'**.

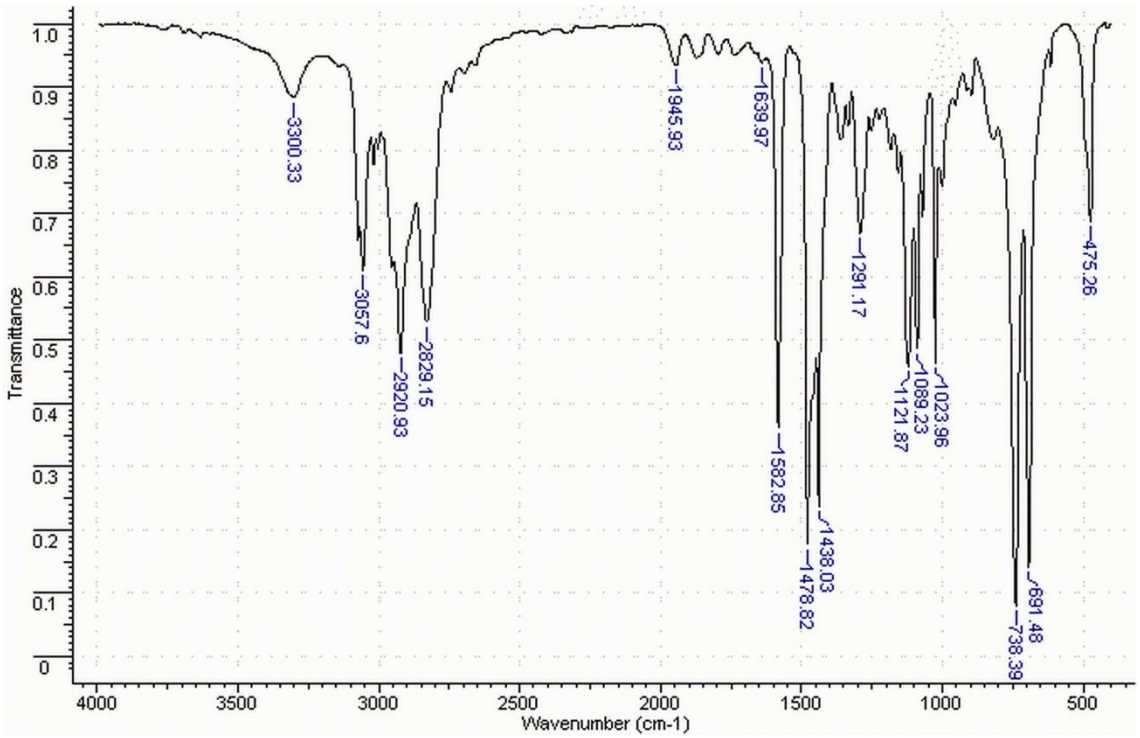

Figure S3. IR (KBr, cm^{-1}) spectrum of **1'**.

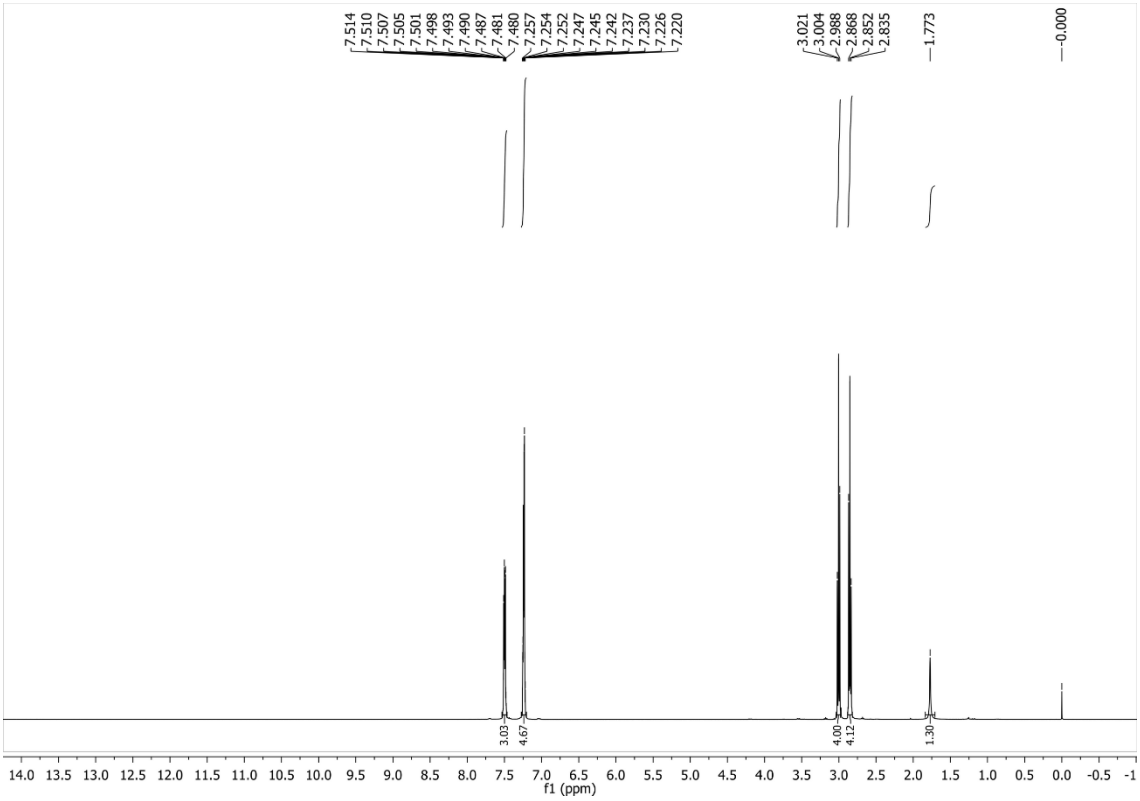

Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2'**.

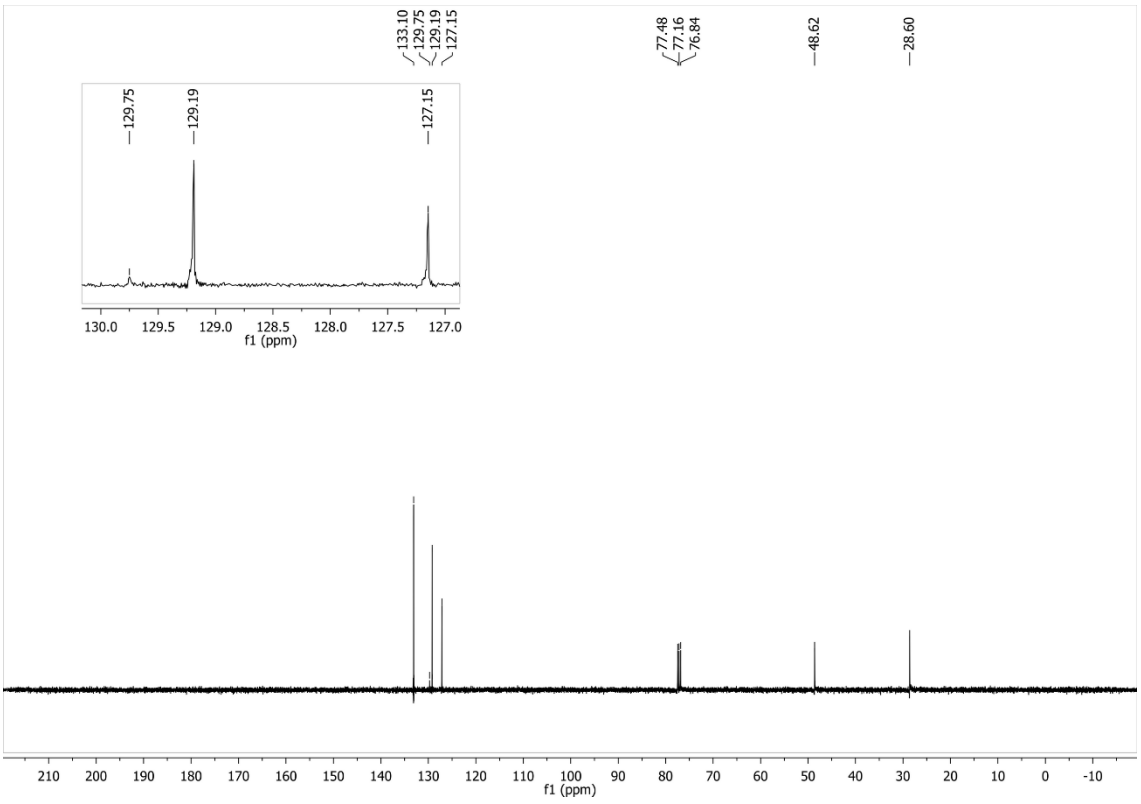

Figure S5. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **2'.**

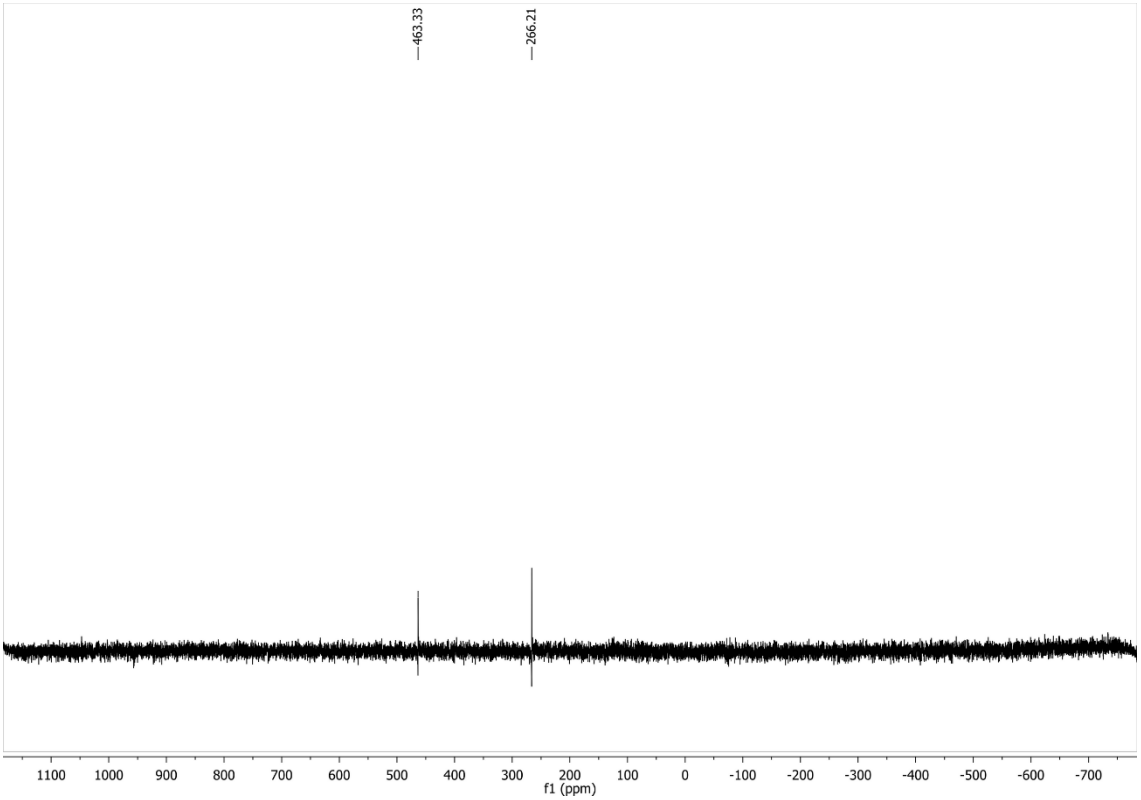

Figure S6. ^{77}Se NMR (38.14 MHz, $CDCl_3$) spectrum of **2'**

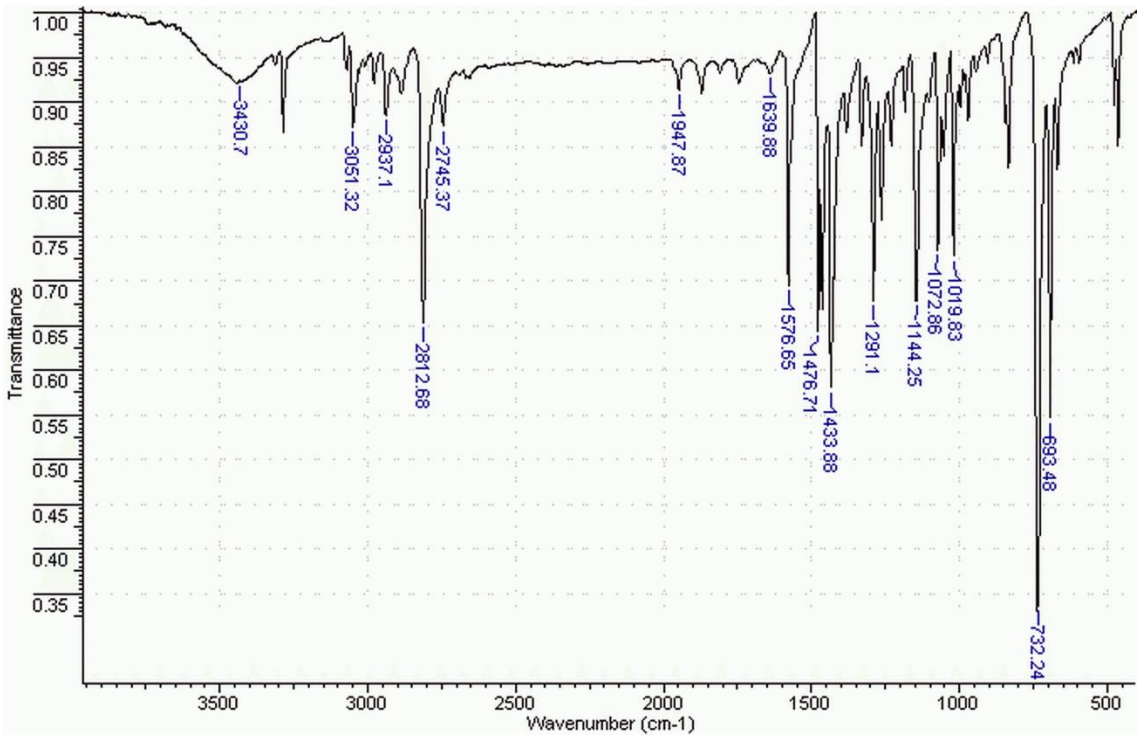

Figure S7. IR (KBr, cm^{-1}) spectrum of **2'**.

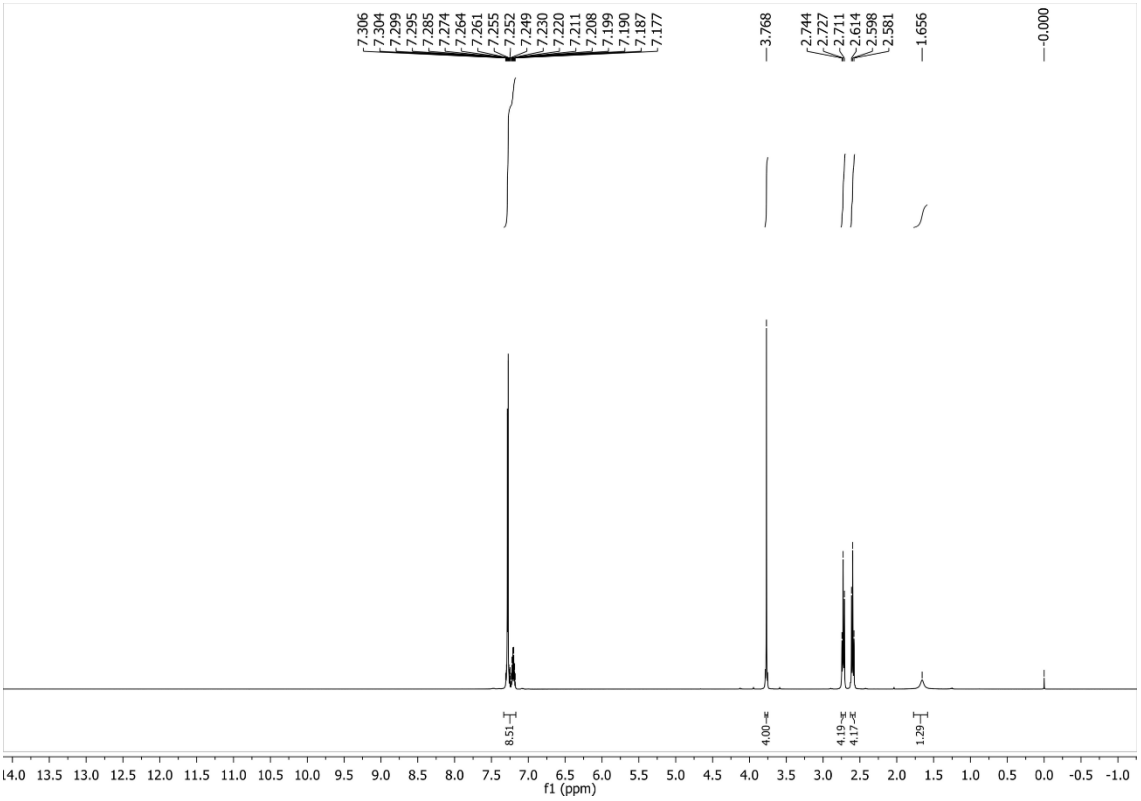

Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3'**.

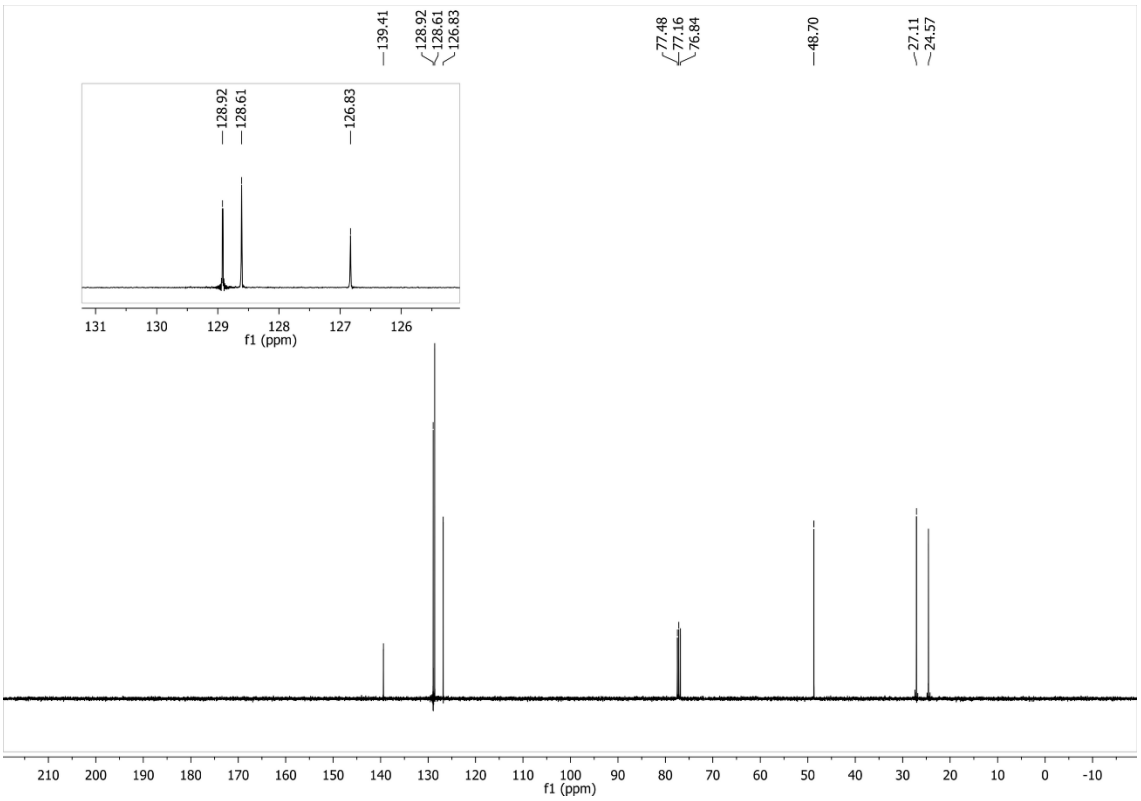

Figure S9. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3'**.

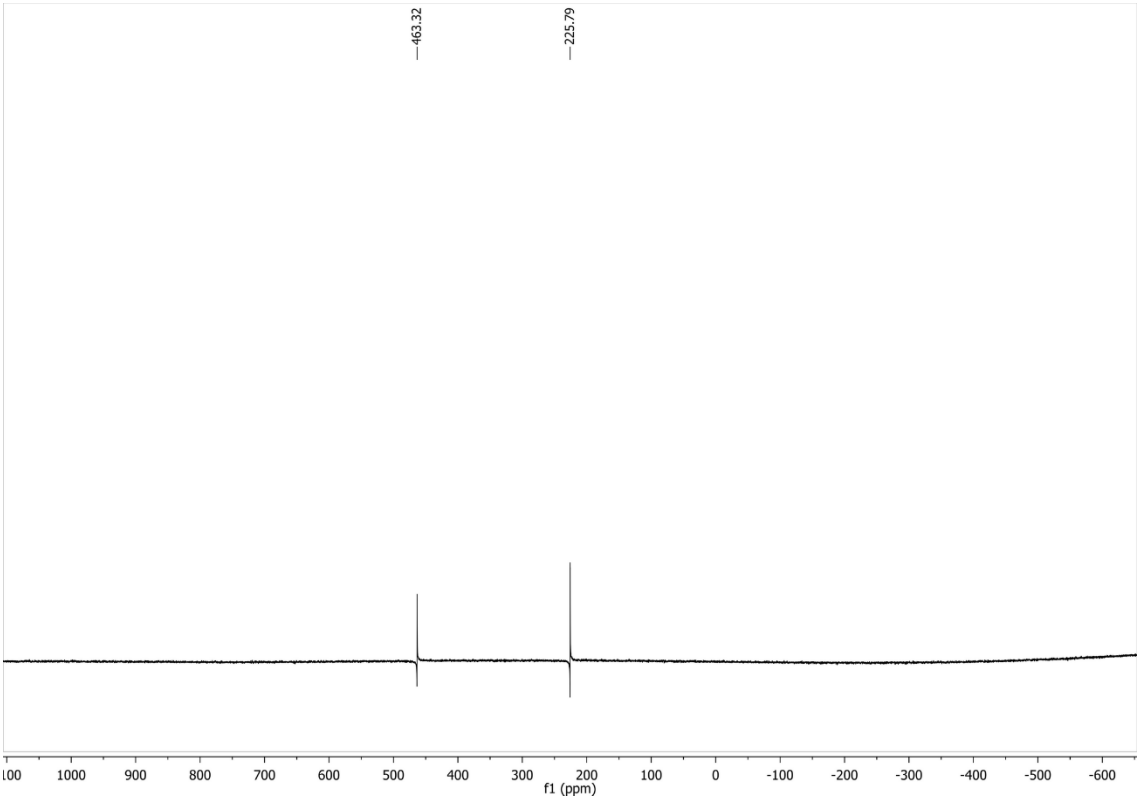

Figure S10. ^{77}Se NMR (38.14 MHz, $CDCl_3$) spectrum of **3'**.

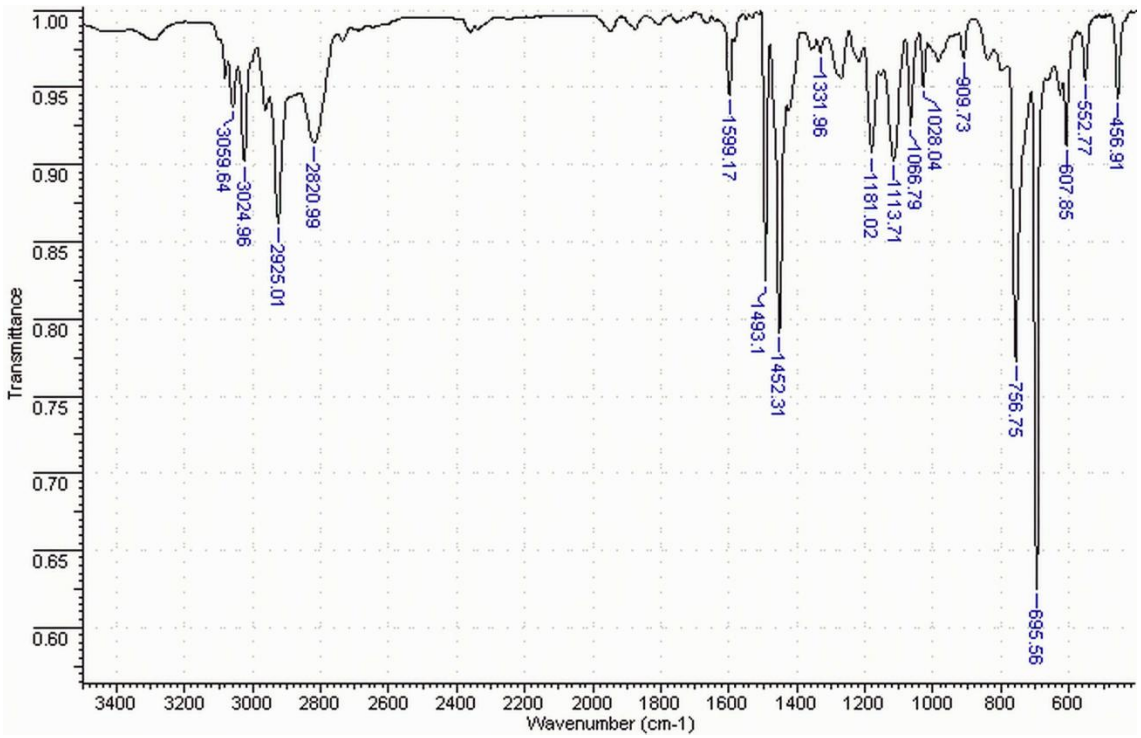

Figure S11. IR (KBr, cm^{-1}) spectrum of **3'**.

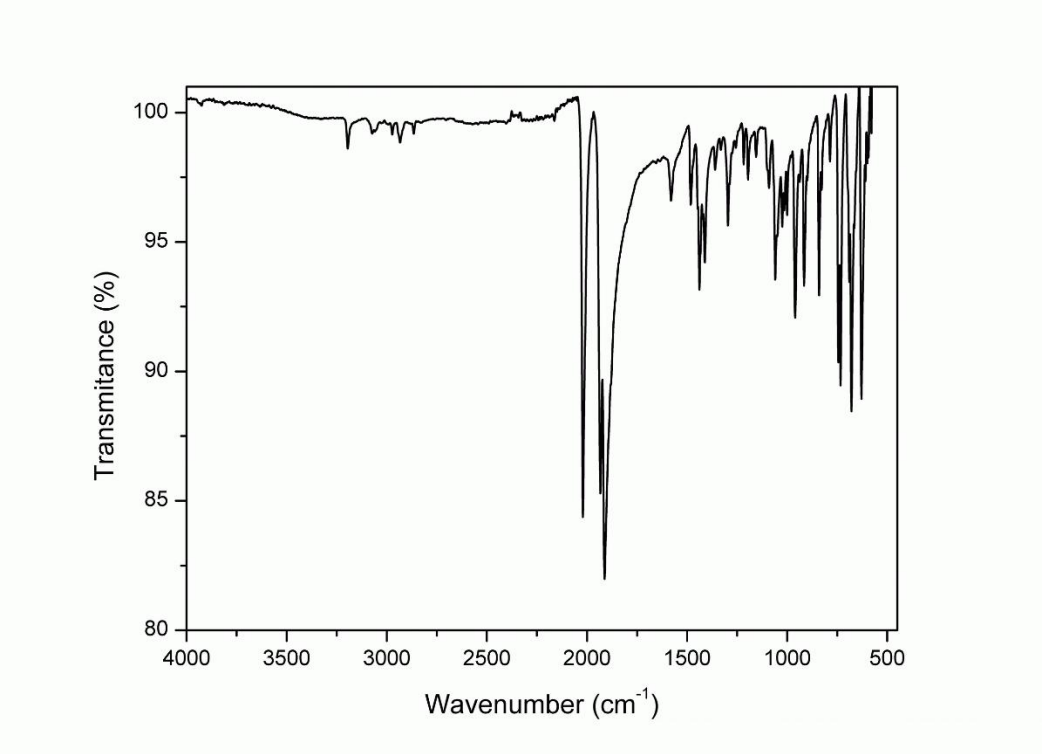

Figure S12. IR (ATR, cm^{-1}) spectrum of **1**.

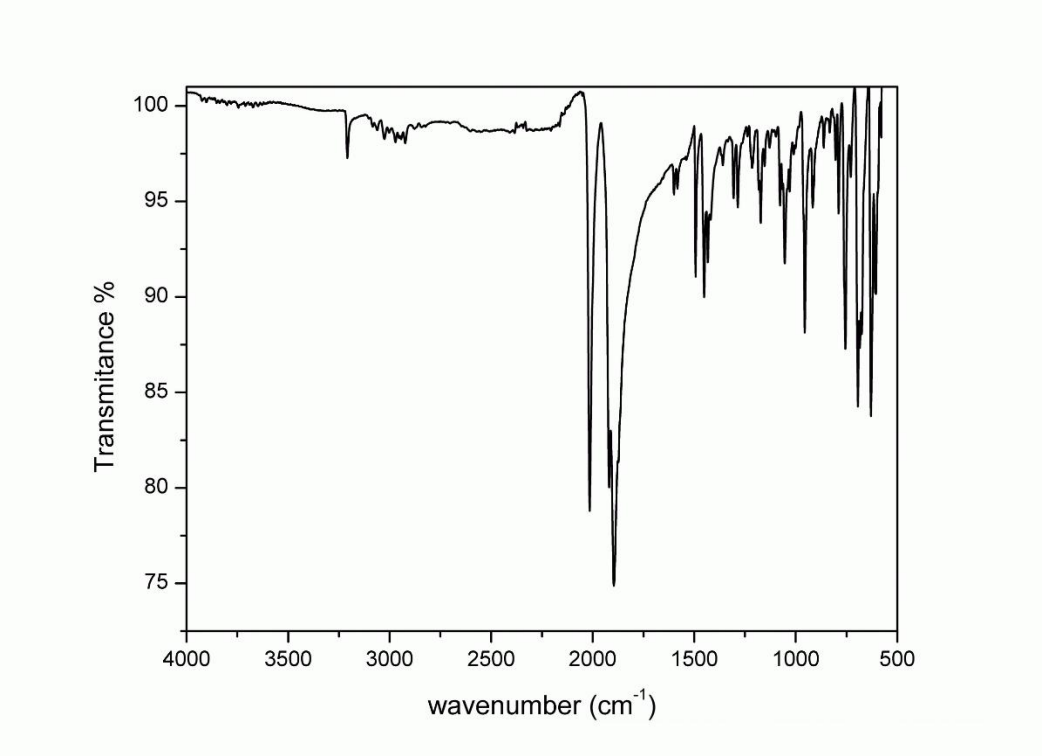

Figure S13. IR (ATR, cm^{-1}) spectrum of **2**.

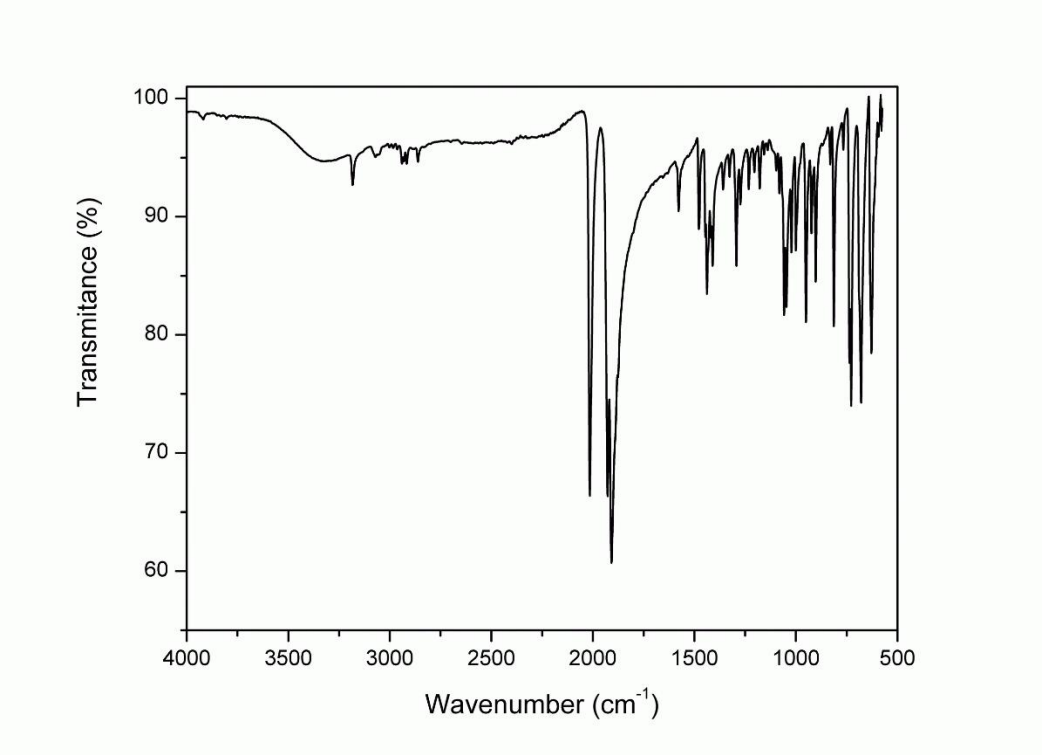

Figure S14. IR (ATR, cm^{-1}) spectrum of **3**.

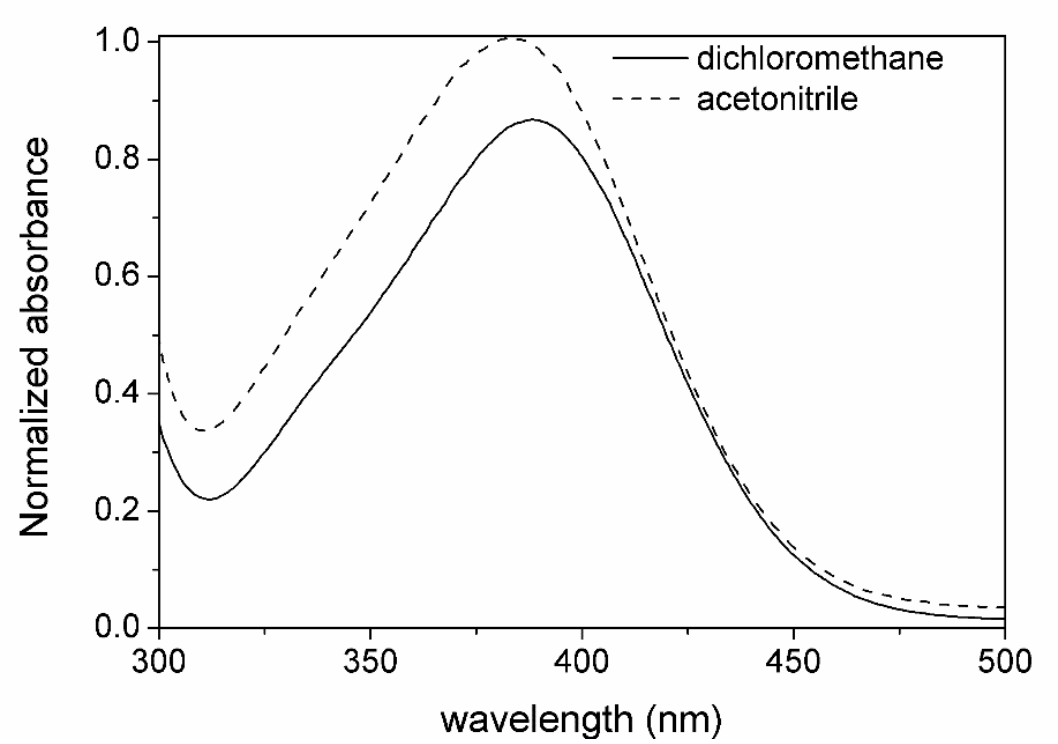

Figure S15. Changes in the UV-vis spectrum of **1** during an incubation period of 24 h in the dark in a dichloromethane solution (solid line) and 1:1 dichloromethane/acetonitrile solution (dashed line).

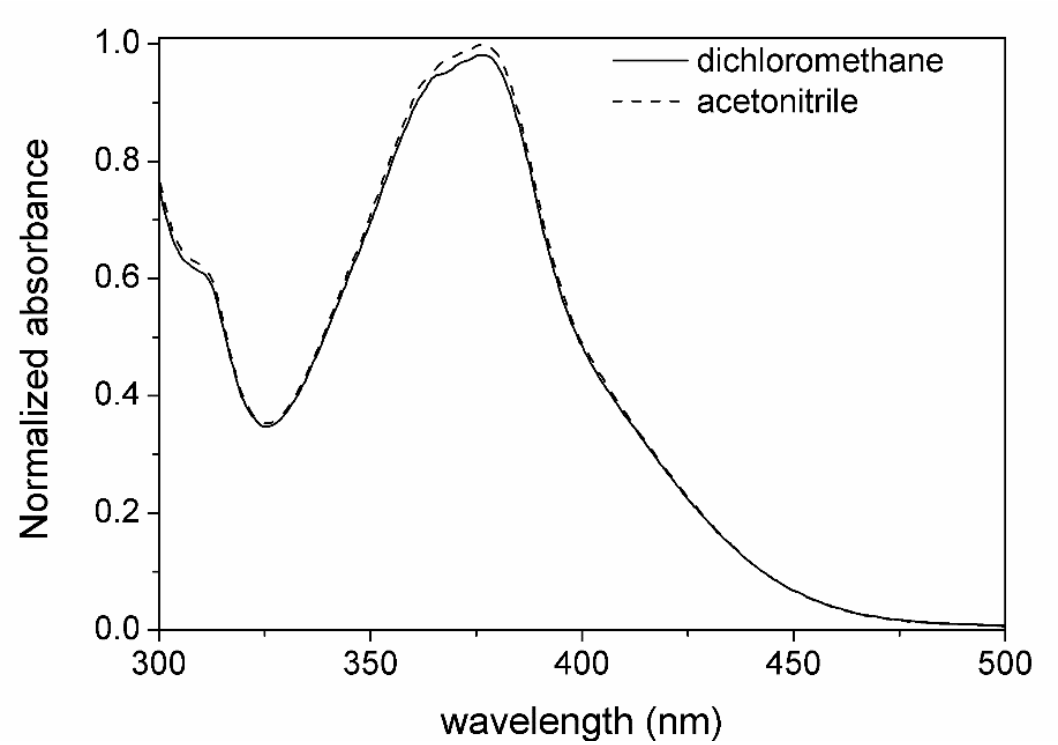

Figure S16. Changes in the UV-vis spectrum of **3** during an incubation period of 24 h in the dark in a dichloromethane solution (solid line) and 1:1 dichloromethane/acetonitrile solution (dashed line).

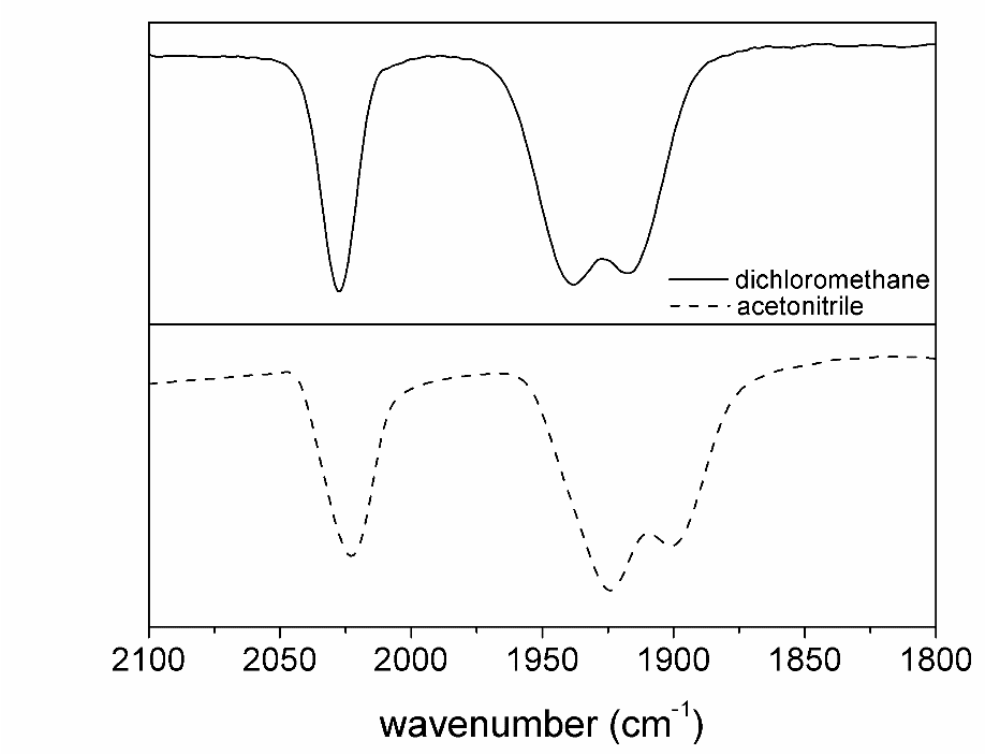

Figure S17. IR spectra of **1** after an incubation period of 24 h in the dark in: dichloromethane solution (solid line) and a 1:1 dichloromethane/acetonitrile solution (dashed line).

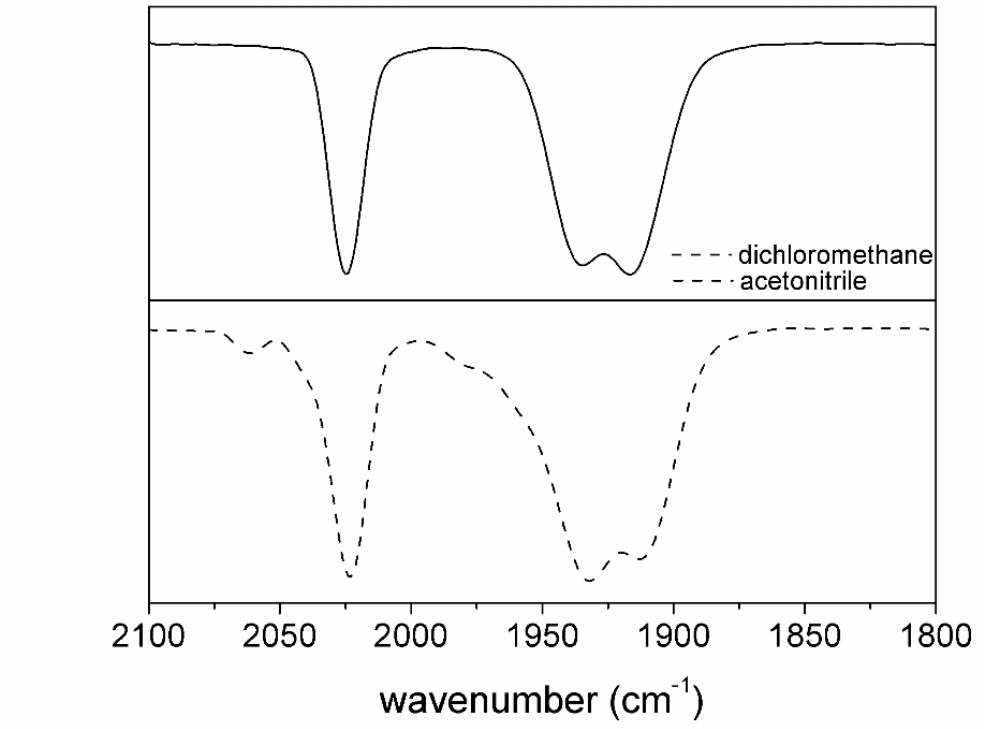

Figure S18. IR spectra of **3** after an incubation period of 24 h in the dark in: dichloromethane solution (solid line) and a 1:1 dichloromethane/acetonitrile solution (dashed line).

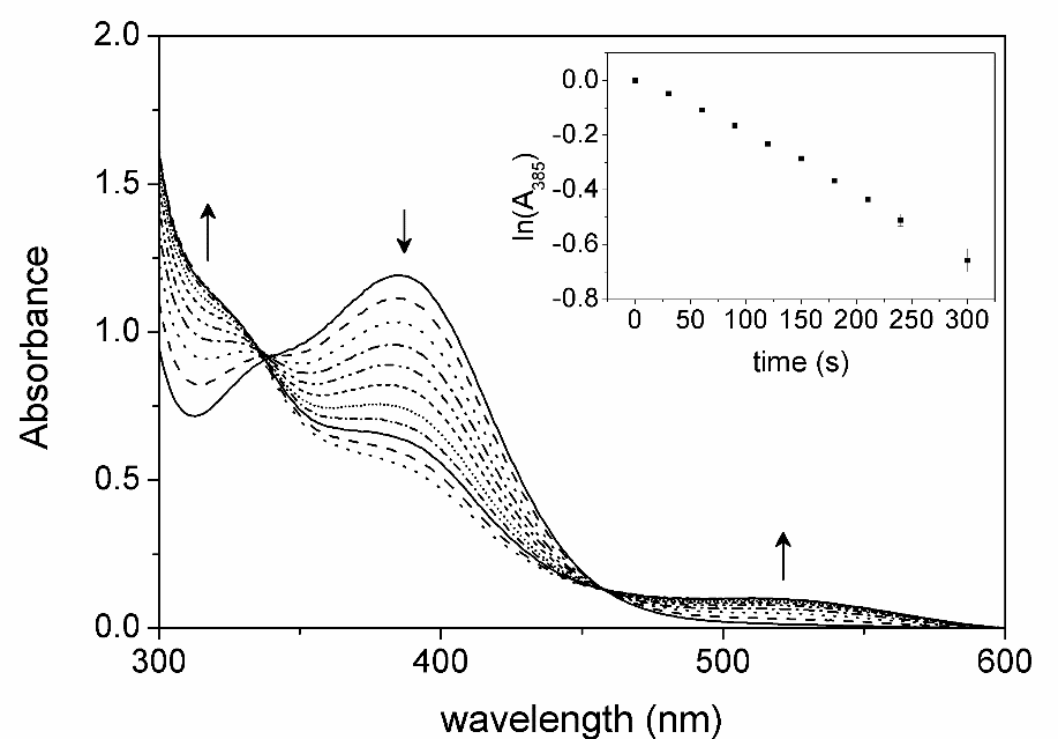

Figure S19. Changes in the UV spectra of **1** during excitation with a 380 ± 10 nm incident light in a dichloromethane solution.

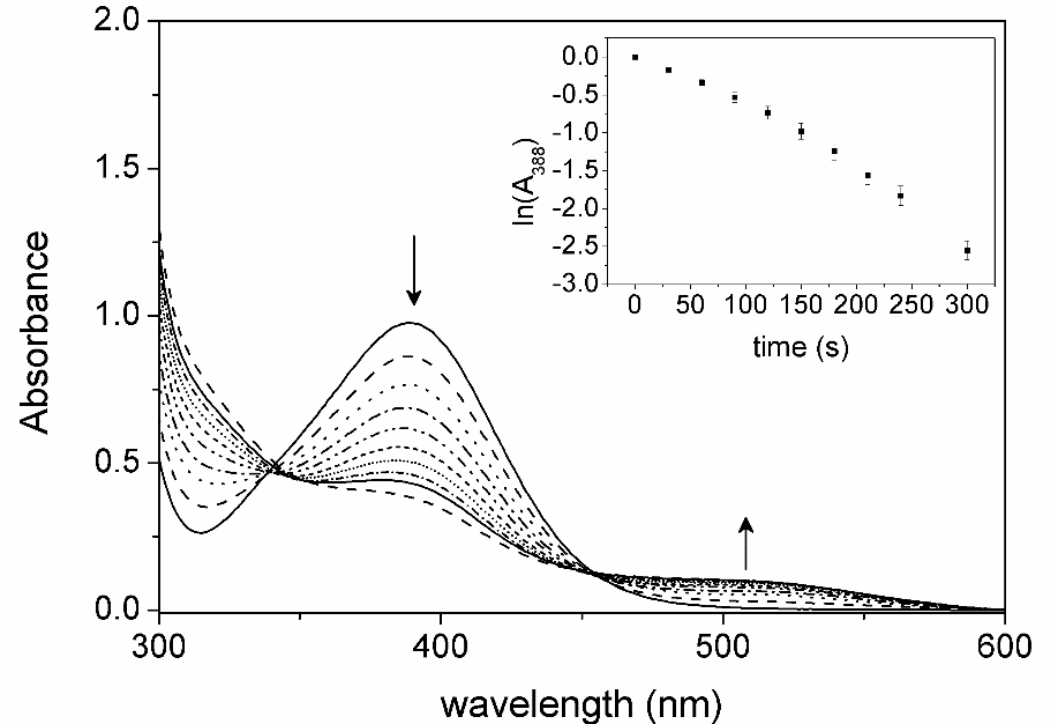

Figure S20. Changes in the UV spectra of **3** during excitation with a 380 ± 10 nm incident light in a dichloromethane solution.

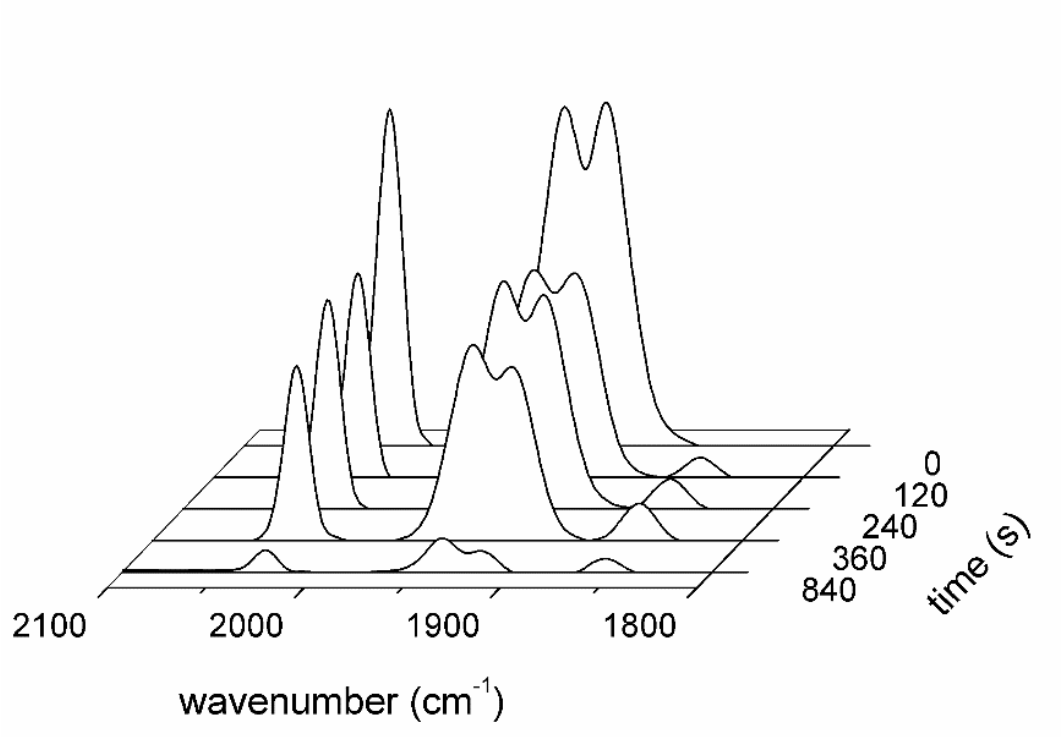

Figure S21. IR spectral changes of **1** during excitation with a 380 ± 10 nm incident light in a dichloromethane solution.

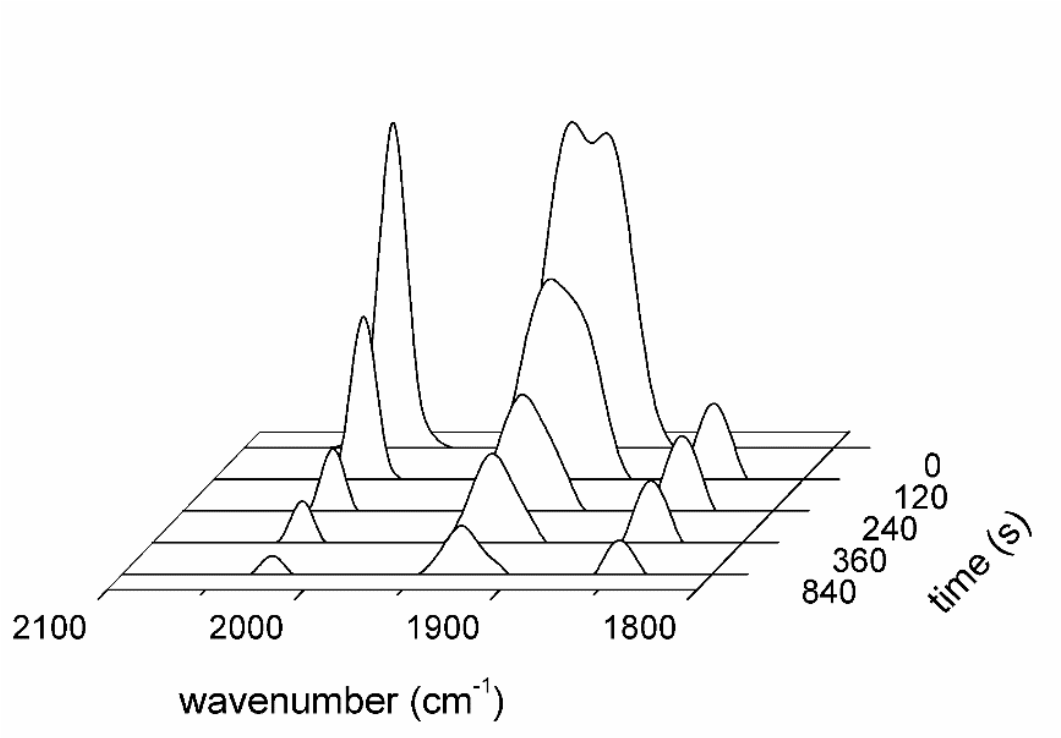

Figure S22. IR spectral changes of **3** during excitation with a 380 ± 10 nm incident light in a dichloromethane solution.

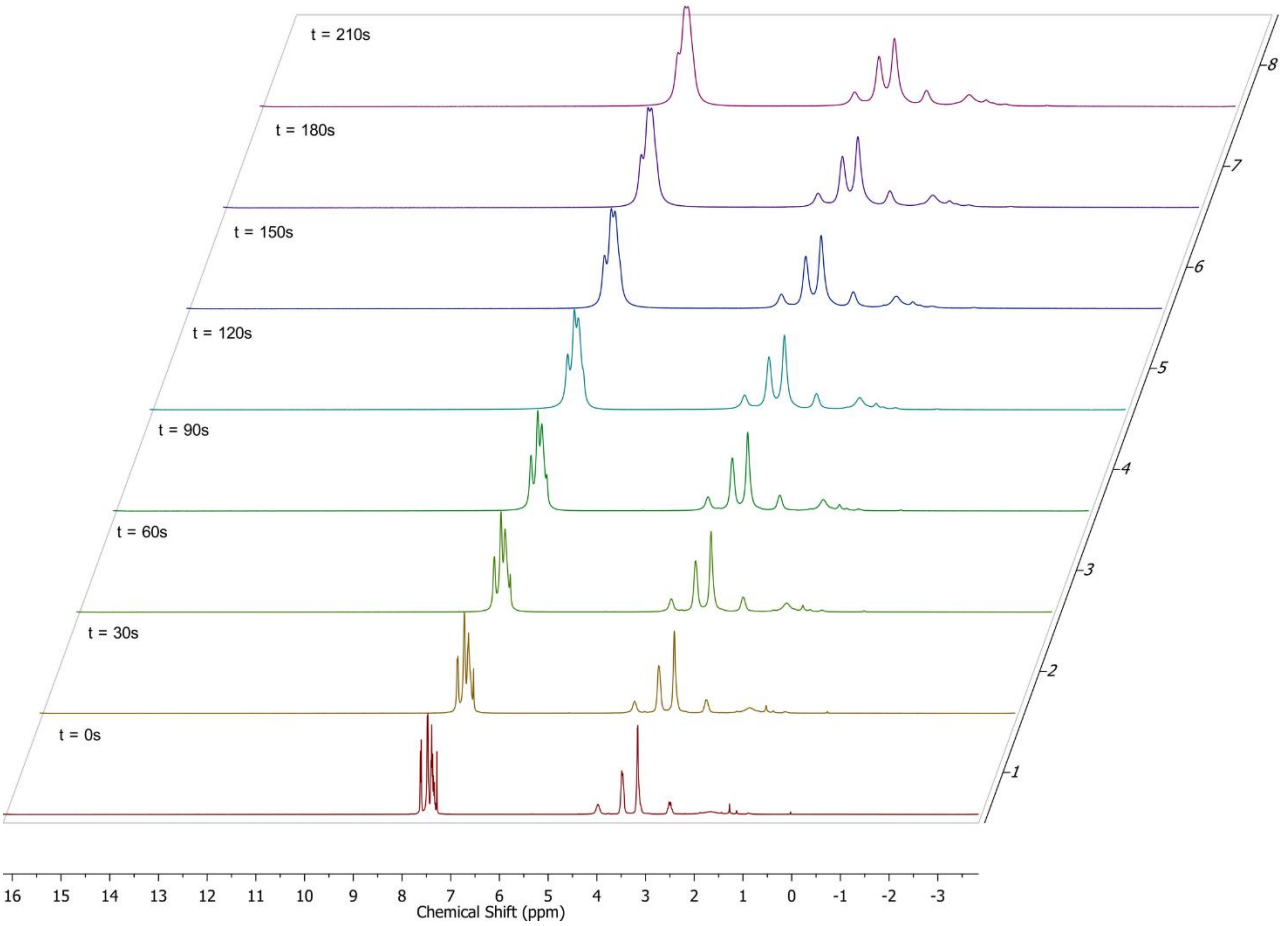

Figure S23. Changes in the **^{1}H** NMR spectra of **1** during excitation with a 380 ± 10 nm incident light in $CDCl_3$.

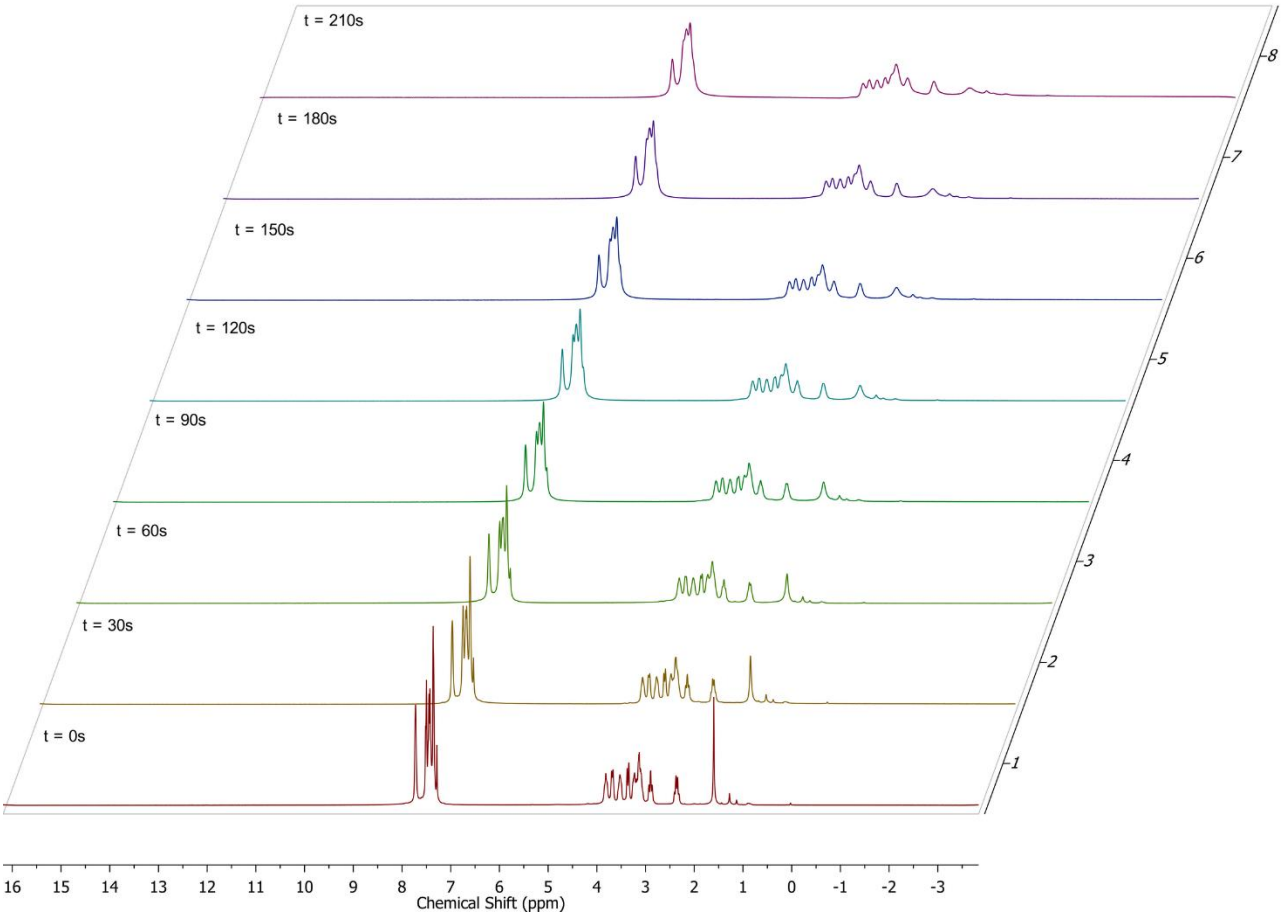

Figure S24. Changes in the **^{1}H** NMR spectra of **2** during excitation with a 380 ± 10 nm incident light in $CDCl_3$.

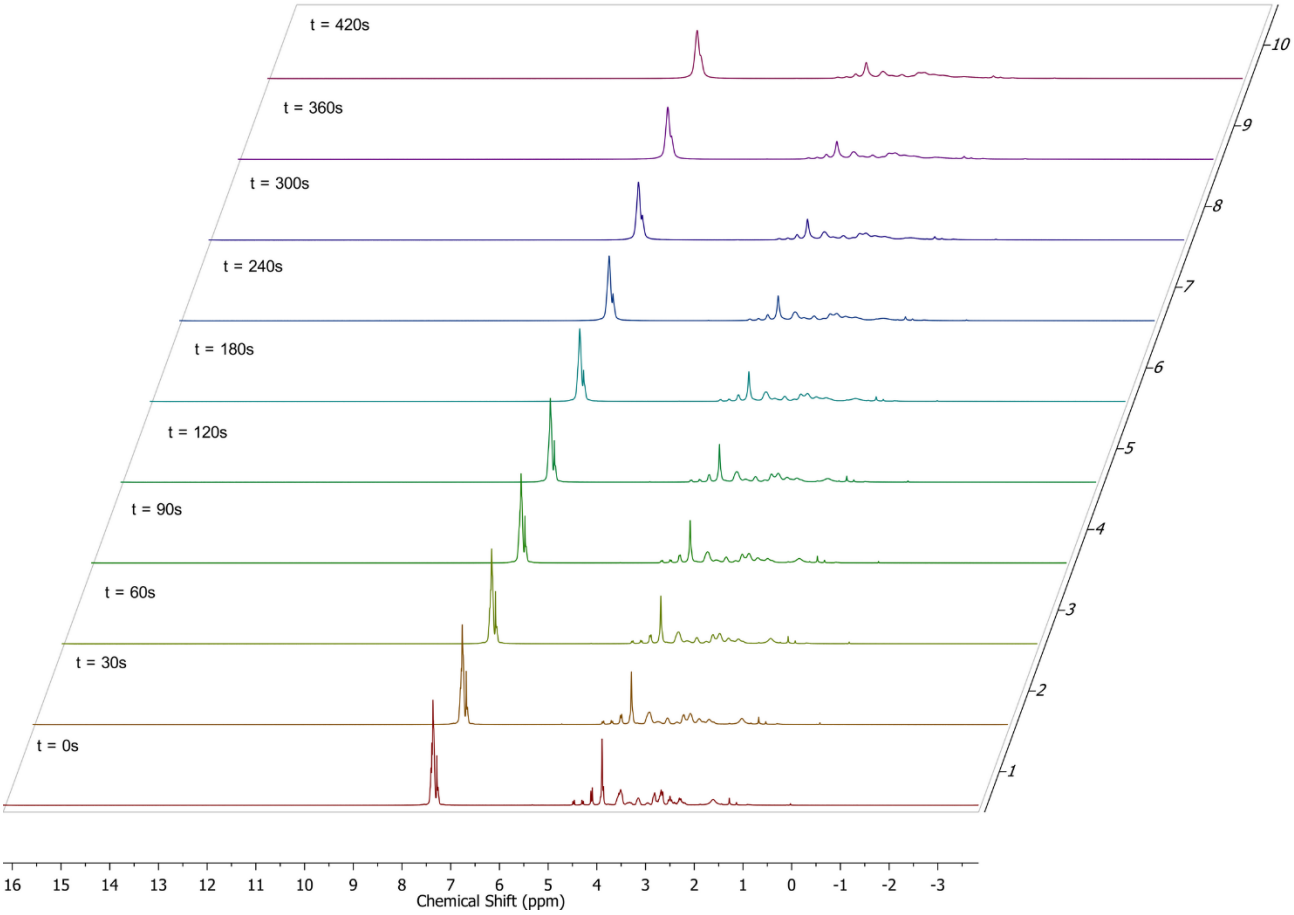

Figure S25. Changes in the **^{1}H** NMR spectra of **1** during excitation with a 380 ± 10 nm incident light in $CDCl_3$.

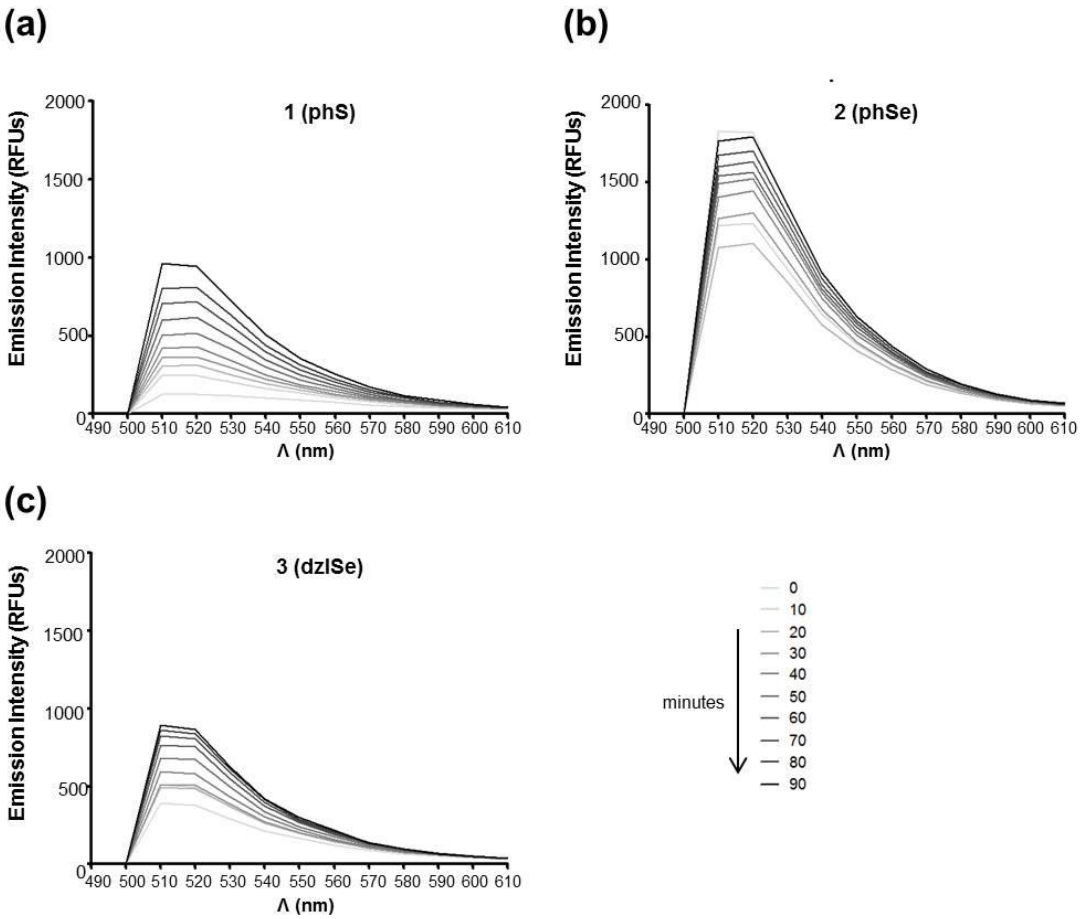

Figure S26. CO release photoemission spectra of **1-3** in aqueous solution. CO release was measured (using COP-1) from 490 to 650 nm (lex=475 nm). Photoemission spectra were taken at 0, 10, 20, 30, 40, 50, 60, 70, 80 and 90min after the addition of 1 μM COP-1 to 150μM of either $[MnBr(CO)_3(phS\text{-}\kappa^2\ S)]$ (**a**), $[MnBr(CO)_3(phSe\text{-}\kappa^2\ Se)]$ (**b**) or $[MnBr(CO)_3(bzlSe\text{-}\kappa^2\ Se)]$ (**c**) in PBS pH 7.4 at 37ºC.The results are shown as emission intensity in RFUs – relative fluorescent Units and represent mean of 3 independent experiments.

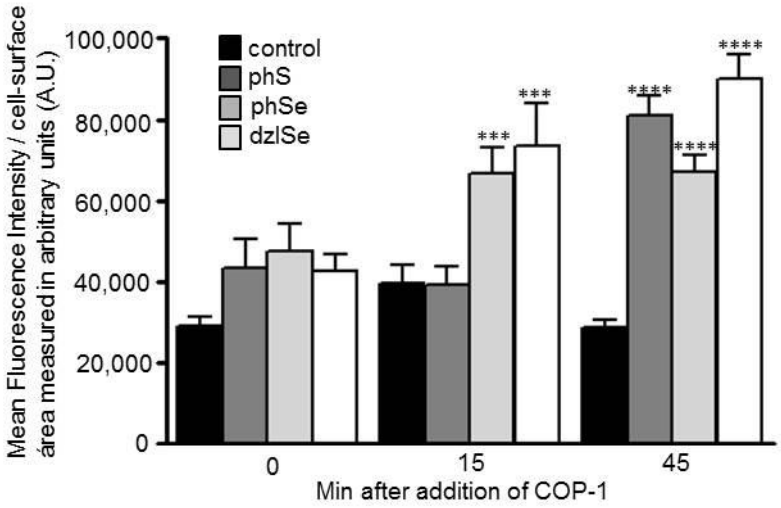

Figure S27. Quantification of CO release in live HeLa cells at 0, 15 and 30min after the addition of 1 µM COP-1 in PBS pH 7.4 (lem = 497-558nm ,lex = 488 nm). Cells were previously incubated with either phS, phSe or dzlSe at 150 µM. The results are shown as mean fluorescence intensity (arbitrary units) in relation to the cell-surface area. The compounds phS, phSe and dzlSe show a statistically significant increase in CO release compared to the control at 15min and at 30 min, determined by a Mann Whitney test (at T15min phS not significant, phSe p=0,0004 and dzlSe p=0,0001; at T30min phS p<0,0001, phSe p<0,0001 and dzlSe p<0,0001)

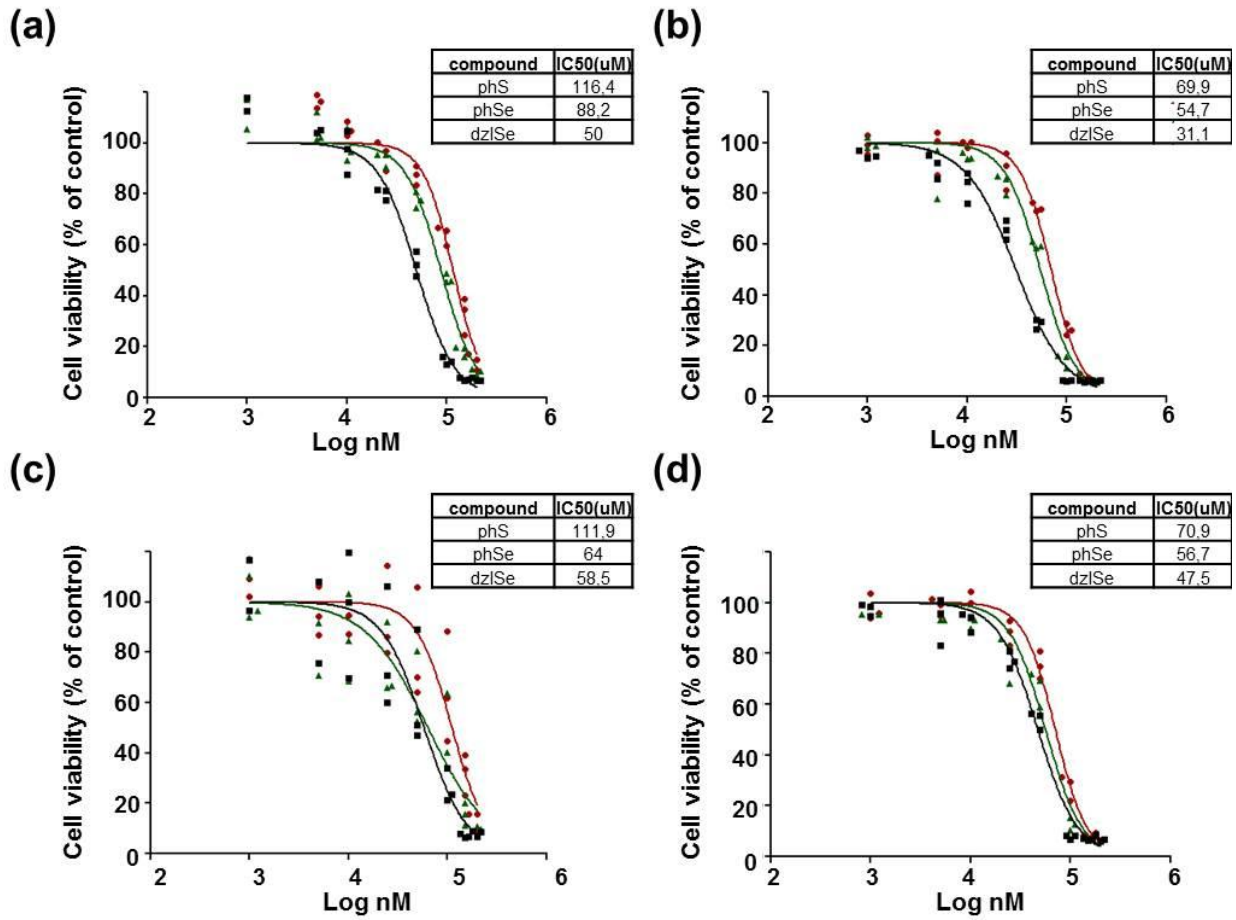

Figure S28. IC50s of compounds 1 (red line), 2 (green line) and 3 (black line) (a) HeLa after 24h incubation. (b) HeLa after 48h incubation. (c) HepG2 after 24h incubation. (d) HepG2 after 48h incubation. The IC50s were calculated with the help of GraphPad Prism5, with data from 3 independent experiments.

Table S1. Crystal data and structure refinement for **1**.

Deposition number	1894675	
Empirical formula	$C_{19}H_{19}BrMnNO_3S_2$	
Formula weight	508.32	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 7.9129(3) Å	□ = 90°.
	b = 20.3755(8) Å	□ = 94.8700(10)°.
	c = 13.0456(5) Å	□ = 90°.
Volume	2095.74(14) $Å^3$	
Z	4	
Density (calculated)	1.611 Mg/m^3	
Absorption coefficient	2.754 mm^{-1}	
F(000)	1024	
Crystal size	0.280 x 0.200 x 0.050 mm^3	
Theta range for data collection	1.858 to 31.163°.	
Index ranges	$-11 \le h \le 11$, $-23 \le k \le 29$, $-18 \le l \le 18$	
Reflections collected	27132	
Independent reflections	6757 [R(int) = 0.0394]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7462 and 0.6390	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6757 / 0 / 244	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.0788	
R indices (all data)	R1 = 0.0733, wR2 = 0.0884	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.584 and -0.493 $e.Å^{-3}$	

Table S2. Bond lengths (Å) and angles (°) for **1**.

Mn1-C3	1.795(3)
Mn1-C2	1.804(3)
Mn1-C1	1.810(3)
Mn1-N1	2.1255(19)
Mn1-S2	2.3748(6)
Mn1-Br1	2.5288(4)
C1-O1	1.142(3)
C2-O2	1.141(3)
C3-O3	1.143(3)
N1-C4	1.488(3)
N1-C6	1.490(3)
S2-C21	1.791(2)
S2-C7	1.812(2)
S1-C11	1.780(3)
S1-C5	1.815(3)
C4-C5	1.517(3)
C6-C7	1.509(3)
C11-C16	1.376(4)
C11-C12	1.377(4)
C12-C13	1.374(5)
C13-C14	1.325(6)
C14-C15	1.361(6)
C15-C16	1.428(6)
C21-C22	1.378(4)
C21-C26	1.391(3)
C22-C23	1.385(4)
C23-C24	1.374(5)
C24-C25	1.370(4)
C25-C26	1.377(4)
C3-Mn1-C2	90.67(11)
C3-Mn1-C1	91.21(12)
C2-Mn1-C1	88.43(12)
C3-Mn1-N1	92.16(9)

C2-Mn1-N1	95.06(10)
C1-Mn1-N1	175.13(9)
C3-Mn1-S2	97.70(8)
C2-Mn1-S2	171.63(9)
C1-Mn1-S2	91.01(9)
N1-Mn1-S2	85.05(5)
C3-Mn1-Br1	177.65(8)
C2-Mn1-Br1	87.73(8)
C1-Mn1-Br1	90.47(9)
N1-Mn1-Br1	86.27(5)
S2-Mn1-Br1	83.918(18)
O1-C1-Mn1	178.7(2)
O2-C2-Mn1	176.3(2)
O3-C3-Mn1	176.3(2)
C4-N1-C6	110.13(18)
C4-N1-Mn1	116.50(14)
C6-N1-Mn1	113.38(13)
C21-S2-C7	103.88(11)
C21-S2-Mn1	111.12(8)
C7-S2-Mn1	96.68(7)
C11-S1-C5	100.12(12)
N1-C4-C5	114.8(2)
C4-C5-S1	113.44(18)
N1-C6-C7	110.32(19)
C6-C7-S2	110.62(15)
C16-C11-C12	119.2(3)
C16-C11-S1	121.1(3)
C12-C11-S1	119.7(2)
C13-C12-C11	121.3(4)
C14-C13-C12	120.2(4)
C13-C14-C15	121.2(4)
C14-C15-C16	119.9(4)
C11-C16-C15	118.1(4)
C22-C21-C26	119.8(2)
C22-C21-S2	122.70(19)
C26-C21-S2	117.19(19)

C21-C22-C23	119.1(3)
C24-C23-C22	121.2(3)
C25-C24-C23	119.3(3)
C24-C25-C26	120.6(3)
C25-C26-C21	119.9(3)

Symmetry transformations used to generate equivalent atoms:

Table S3. Crystal data and structure refinement for **2**.

Deposition number	1894677	
Empirical formula	$C_{19}H_{19}BrMnNO_3Se_2$	
Formula weight	602.12	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.0565(2) Å	□ = 90°.
	b = 20.5626(5) Å	□ = 94.4920(10)°.
	c = 12.9929(3) Å	□ = 90°.
Volume	2145.83(9) $Å^3$	
Z	4	
Density (calculated)	1.864 Mg/m^3	
Absorption coefficient	5.888 mm^{-1}	
F(000)	1168	
Crystal size	0.360 x 0.280 x 0.040 mm^3	
Theta range for data collection	1.858 to 27.994°.	
Index ranges	$-8 \le h \le 10$, $-26 \le k \le 27$, $-17 \le l \le 17$	
Reflections collected	18943	
Independent reflections	5183 [R(int) = 0.0463]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.3812	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5183 / 0 / 244	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0812	
R indices (all data)	R1 = 0.0548, wR2 = 0.0881	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.891 and -0.857 $e.Å^{-3}$	

Table S4. Bond lengths (Å) and angles (°) for **2**.

Mn1-C3	1.790(4)
Mn1-C2	1.801(4)
Mn1-C1	1.803(4)
Mn1-N1	2.131(3)
Mn1-Se2	2.4758(7)
Mn1-Br1	2.5280(6)
C1-O1	1.145(5)
C2-O2	1.149(5)
C3-O3	1.148(5)
N1-C4	1.488(4)
N1-C6	1.494(5)
Se2-C21	1.932(4)
Se2-C7	1.949(4)
Se1-C11	1.913(4)
Se1-C5	1.955(4)
C4-C5	1.523(5)
C6-C7	1.505(5)
C11-C12	1.372(6)
C11-C16	1.388(6)
C12-C13	1.431(9)
C13-C14	1.362(10)
C14-C15	1.341(9)
C15-C16	1.367(7)
C21-C26	1.379(6)
C21-C22	1.384(5)
C22-C23	1.374(6)
C23-C24	1.367(8)
C24-C25	1.355(8)
C25-C26	1.394(6)
C3-Mn1-C2	90.70(18)
C3-Mn1-C1	90.73(18)
C2-Mn1-C1	88.39(19)
C3-Mn1-N1	92.36(14)

C2-Mn1-N1	94.81(15)
C1-Mn1-N1	175.52(16)
C3-Mn1-Se2	98.58(13)
C2-Mn1-Se2	170.66(12)
C1-Mn1-Se2	90.38(14)
N1-Mn1-Se2	85.96(8)
C3-Mn1-Br1	178.05(13)
C2-Mn1-Br1	88.27(13)
C1-Mn1-Br1	90.89(14)
N1-Mn1-Br1	86.08(8)
Se2-Mn1-Br1	82.49(2)
O1-C1-Mn1	178.3(4)
O2-C2-Mn1	176.8(4)
O3-C3-Mn1	177.0(4)
C4-N1-C6	110.1(3)
C4-N1-Mn1	115.9(2)
C6-N1-Mn1	114.7(2)
C21-Se2-C7	100.51(16)
C21-Se2-Mn1	109.80(11)
C7-Se2-Mn1	93.23(11)
C11-Se1-C5	97.16(17)
N1-C4-C5	115.0(3)
C4-C5-Se1	113.3(2)
N1-C6-C7	111.1(3)
C6-C7-Se2	110.6(2)
C12-C11-C16	119.5(5)
C12-C11-Se1	120.9(4)
C16-C11-Se1	119.5(3)
C11-C12-C13	117.9(6)
C14-C13-C12	120.2(5)
C15-C14-C13	121.2(6)
C14-C15-C16	119.8(6)
C15-C16-C11	121.4(5)
C26-C21-C22	120.0(4)
C26-C21-Se2	121.3(3)
C22-C21-Se2	118.4(3)

C23-C22-C21	120.2(4)
C24-C23-C22	120.1(5)
C25-C24-C23	119.9(4)
C24-C25-C26	121.4(5)
C21-C26-C25	118.3(5)

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for **3**.

Deposition number	1894674	
Empirical formula	$C_{21}H_{23}BrMnNO_3Se_2$	
Formula weight	630.17	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.5601(2) Å	□ = 103.0160(10)°.
	b = 12.4079(4) Å	□= 97.6530(10)°.
	c = 13.3682(5) Å	□ = 104.8100(10)°.
Volume	1156.72(7) $Å^3$	
Z	2	
Density (calculated)	1.809 Mg/m^3	
Absorption coefficient	5.466 mm^{-1}	
F(000)	616	
Crystal size	0.40 x 0.20 x 0.04 mm^3	
Theta range for data collection	1.597 to 26.999°.	
Index ranges	$-9 \le h \le 9$, $-15 \le k \le 15$, $-17 \le l \le 17$	
Reflections collected	21399	
Independent reflections	5046 [R(int) = 0.0368]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.4438	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5046 / 0 / 262	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.0892	
R indices (all data)	R1 = 0.0547, wR2 = 0.0968	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.696 and -0.763 $e.Å^{-3}$	

Table S6. Bond lengths (Å) and angles (°) for **3**.

Mn1-C3	1.788(5)
Mn1-C2	1.806(5)
Mn1-C1	1.817(5)
Mn1-N1	2.129(4)
Mn1-Se1	2.4625(8)
Mn1-Br1	2.5344(8)
C1-O1	1.140(6)
C2-O2	1.141(6)
C3-O3	1.138(6)
N1-C6	1.486(6)
N1-C4	1.491(6)
Se2-C5	1.952(6)
Se2-C10	1.965(6)
Se1-C7	1.954(5)
Se1-C20	1.986(5)
C4-C5	1.528(7)
C6-C7	1.499(7)
C10-C11	1.498(7)
C11-C12	1.386(7)
C11-C16	1.393(7)
C12-C13	1.383(8)
C13-C14	1.377(9)
C14-C15	1.366(9)
C15-C16	1.385(8)
C20-C21	1.501(7)
C21-C22	1.385(7)
C21-C26	1.385(8)
C22-C23	1.383(8)
C23-C24	1.354(9)
C24-C25	1.370(10)
C25-C26	1.373(9)
C3-Mn1-C2	92.1(2)
C3-Mn1-C1	92.2(2)

C2-Mn1-C1	88.0(2)
C3-Mn1-N1	90.56(19)
C2-Mn1-N1	95.13(18)
C1-Mn1-N1	175.76(18)
C3-Mn1-Se1	95.26(15)
C2-Mn1-Se1	172.65(15)
C1-Mn1-Se1	91.44(15)
N1-Mn1-Se1	85.11(11)
C3-Mn1-Br1	175.63(16)
C2-Mn1-Br1	90.21(15)
C1-Mn1-Br1	91.59(14)
N1-Mn1-Br1	85.54(11)
Se1-Mn1-Br1	82.47(3)
O1-C1-Mn1	177.6(4)
O2-C2-Mn1	177.1(4)
O3-C3-Mn1	178.9(5)
C6-N1-C4	110.5(4)
C6-N1-Mn1	112.9(3)
C4-N1-Mn1	115.9(3)
C5-Se2-C10	99.9(2)
C7-Se1-C20	100.7(2)
C7-Se1-Mn1	95.12(15)
C20-Se1-Mn1	110.73(16)
N1-C4-C5	114.8(4)
C4-C5-Se2	110.8(4)
N1-C6-C7	111.1(4)
C6-C7-Se1	111.7(3)
C11-C10-Se2	115.4(4)
C12-C11-C16	118.1(5)
C12-C11-C10	120.8(5)
C16-C11-C10	121.1(5)
C13-C12-C11	121.3(6)
C14-C13-C12	119.9(6)
C15-C14-C13	119.4(6)
C14-C15-C16	121.3(6)
C15-C16-C11	119.9(5)

C21-C20-Se1	106.8(3)
C22-C21-C26	117.8(5)
C22-C21-C20	120.8(5)
C26-C21-C20	121.2(5)
C23-C22-C21	120.7(6)
C24-C23-C22	120.4(6)
C23-C24-C25	119.7(6)
C24-C25-C26	120.5(6)
C25-C26-C21	120.8(6)

Symmetry transformations used to generate equivalent atoms:

Table S7. Cartesian coordinates of compounds **1-3** at BP86-D3/def2-SVP level of theory in the gas phase.

Compound **1**

C	1.812734463000	-0.381432238000	0.405789335000
O	2.946504092000	-0.081353178000	0.484095889000
C	0.486177600000	-2.214574817000	1.269021127000
O	0.692217235000	-3.168412653000	1.925742293000
C	0.445234861000	-1.707783653000	-1.144924516000
O	0.634374145000	-2.289224407000	-2.159114490000
Mn	0.173130493000	-0.850546914000	0.288501289000
Br	-0.359431144000	0.519166397000	2.221576458000
S	0.239920377000	3.869047215000	-1.049095689000
S	-1.973579161000	-1.275661810000	0.408428401000
N	-0.318712676000	0.789475119000	-0.736888611000
C	2.902083230000	3.088247296000	1.910351256000
C	4.184385428000	3.489988650000	-0.099332947000
C	4.133714217000	3.170746646000	1.261191384000
C	1.718515294000	3.304490797000	1.202099835000
C	-3.372853201000	-3.374681425000	-2.852529453000
C	3.008145206000	3.725132024000	-0.809924877000
C	-2.917233703000	-4.657393520000	-2.549919557000
C	-2.391884452000	-2.537454963000	-0.813118919000
C	-2.202202160000	-4.878481584000	-1.369581890000
C	-3.111612599000	-2.308580352000	-1.986415671000
C	1.769758550000	3.615832895000	-0.161067236000
C	0.419405837000	2.597293333000	-2.356928996000

C	-2.682035672000	0.249683271000	-0.310085454000
C	-1.940352658000	-3.824607901000	-0.497093845000
C	-1.701630581000	0.776769938000	-1.328032370000
C	0.662570829000	1.200802376000	-1.794134583000
H	-0.320554132000	1.569835569000	-0.048700383000
H	0.635895639000	0.443760969000	-2.589573199000
H	1.656495238000	1.171120761000	-1.337004234000
H	1.256821200000	2.856918788000	-3.018311262000
H	-0.497357468000	2.672322198000	-2.957728443000
H	-1.973481993000	1.799354265000	-1.622908487000
H	-1.664314870000	0.138328689000	-2.221078963000
H	-2.779058949000	0.926816812000	0.548169561000
H	-3.676273843000	0.050078412000	-0.723453243000
H	-3.473038742000	-1.315636312000	-2.248216494000
H	-3.930672027000	-3.191992729000	-3.771730291000
H	-3.117516623000	-5.483842993000	-3.232143102000
H	-1.841193506000	-5.877493458000	-1.124070628000
H	-1.377029369000	-3.999252969000	0.420268162000
H	2.851878481000	2.820785237000	2.965956183000
H	0.754614130000	3.197498345000	1.697880790000
H	3.050109579000	3.993452184000	-1.866491797000
H	5.145574760000	3.559027316000	-0.610233792000
H	5.055337022000	2.976329343000	1.810074144000

Compound **2**

C	1.985998197000	-0.568022778000	0.488806126000
O	3.120759483000	-0.265888657000	0.558862917000

C	0.681894484000	-2.378988721000	1.414120525000
O	0.900643606000	-3.311998717000	2.097632376000
C	0.632857501000	-1.951033241000	-1.013205585000
O	0.837809168000	-2.557286901000	-2.010691715000
Se	-1.914178504000	-1.531380157000	0.579767561000
Se	0.319895782000	3.729598954000	-1.079018594000
Br	-0.202911605000	0.391504349000	2.266288763000
Mn	0.353884907000	-1.050945009000	0.391063703000
N	-0.163427300000	0.540303979000	-0.705095106000
C	0.837656280000	0.928103321000	-1.756219903000
C	-2.314037071000	-2.853859356000	-0.807853051000
C	0.582741944000	2.278966935000	-2.409130479000
C	1.970982148000	3.435224561000	-0.112768056000
C	-2.568198358000	0.108418479000	-0.312014037000
C	-1.530454151000	0.495505039000	-1.330416117000
C	-1.652023699000	-4.077598311000	-0.676500058000
C	-3.228200347000	-2.643581214000	-1.839421678000
C	-1.904053899000	-5.094098049000	-1.597188396000
C	3.202537505000	3.523861046000	-0.772878748000
C	-2.808414495000	-4.890567499000	-2.642580140000
C	1.917527859000	3.118230237000	1.246929712000
C	-3.469655766000	-3.667568111000	-2.761115098000
C	4.330825301000	2.939405264000	1.288777284000
C	4.379679458000	3.263584844000	-0.070259160000
C	3.102319177000	2.875822851000	1.946039099000
H	-3.760610268000	-1.698867237000	-1.944683320000
H	-4.177925904000	-3.501604524000	-3.573887710000

H	-2.996901494000	-5.685101069000	-3.365088279000
H	-1.380045519000	-6.045296759000	-1.500549785000
H	-0.932324542000	-4.235761196000	0.127652735000
H	3.242650803000	3.795706220000	-1.828606267000
H	5.338720706000	3.316369870000	-0.587193296000
H	5.252022827000	2.725017079000	1.830947446000
H	3.054381639000	2.603539088000	3.000583003000
H	0.956354623000	3.024361969000	1.750076276000
H	1.445231731000	2.537670832000	-3.034887727000
H	-0.308811387000	2.307797758000	-3.048197205000
H	0.854928841000	0.126794040000	-2.508133458000
H	1.817132218000	0.949213771000	-1.268562462000
H	-1.488947319000	-0.228096382000	-2.156770682000
H	-3.556513253000	-0.066994428000	-0.747181693000
H	-1.762401541000	1.491212661000	-1.733867733000
H	-2.648977992000	0.838763879000	0.502207864000
H	-0.191031127000	1.347183663000	-0.047411634000

Compound **3**

C	-1.436827137000	1.266062041000	-0.455193682000
O	-2.326430517000	1.940155180000	-0.076613153000
C	-0.705888431000	0.510317476000	-2.630852578000
O	-1.082949522000	0.673421906000	-3.729521171000
C	0.914033826000	1.590566067000	-1.094659886000
O	1.687266281000	2.494483272000	-1.111788768000
Br	-1.537680848000	-1.682356622000	-0.705834783000
Mn	-0.159249815000	0.293242450000	-1.020106227000

Se	1.325035148000	-1.317164531000	-1.780594540000
Se	-0.082483984000	1.999453489000	4.478457700000
N	0.465830047000	-0.136192204000	0.834610475000
C	0.348008002000	1.009336993000	1.813242048000
H	-0.674114517000	1.381590181000	1.718367725000
H	1.019696520000	1.807243414000	1.473984374000
C	0.620131384000	0.622588447000	3.258759324000
H	1.687391809000	0.555560505000	3.503328419000
H	0.132379234000	-0.326151721000	3.527269730000
C	-2.025132329000	1.672943207000	4.102843883000
H	-2.521105235000	2.177330591000	4.942228912000
H	-2.293136079000	2.187425560000	3.173140168000
C	-2.338733222000	0.212267667000	4.042735737000
C	-2.249395063000	-0.591567175000	5.191332483000
H	-1.967102330000	-0.133506949000	6.141353143000
C	-2.492931611000	-1.961745918000	5.119960404000
H	-2.424208372000	-2.571760924000	6.021963342000
C	-2.824424241000	-2.554804919000	3.895752688000
H	-3.012769668000	-3.627715510000	3.839716592000
C	-2.916584080000	-1.765758933000	2.748660650000
H	-3.170662231000	-2.211219209000	1.787150041000
C	-2.674788939000	-0.390382532000	2.821385377000
H	-2.766236484000	0.220973300000	1.921030524000
C	1.849721976000	-0.717073672000	0.931966373000
H	2.028224476000	-1.033870982000	1.969366506000
H	2.550910438000	0.094108380000	0.690987279000
C	2.009784680000	-1.884289511000	-0.005137912000

H	1.388009648000	-2.741313307000	0.281819007000
H	3.053180899000	-2.200747973000	-0.112490856000
C	2.978202247000	-0.385988783000	-2.462315794000
H	3.189680700000	0.460679140000	-1.801850356000
H	3.766263559000	-1.146601014000	-2.389176723000
C	2.703734224000	0.025974294000	-3.871796789000
C	2.351887996000	1.348650439000	-4.175506216000
H	2.314659482000	2.091846343000	-3.378985318000
C	2.039796808000	1.709040585000	-5.486832133000
H	1.759337300000	2.738983683000	-5.709342271000
C	2.072776847000	0.755987168000	-6.506381921000
H	1.820604805000	1.038965315000	-7.528972453000
C	2.424421564000	-0.564751319000	-6.212084515000
H	2.451582847000	-1.314197374000	-7.004033745000
C	2.734848549000	-0.927250263000	-4.902758343000
H	2.999410009000	-1.962030646000	-4.672665752000
H	-0.189201324000	-0.868387357000	1.170364882000

Table S8. Cartesian coordinates of compounds [$MnBr(CO)_3L$-κ^2 X] (in which L = phS, phSe or bzlSe and X = S or Se) at ωB97X-D3 level of theory with the SMD solvation model using dichloromethane as solvent.

[$MnBr(CO)_3$phS-κ^2 S]		
C	4.63897593839623	14.24969653180323	7.40231802761913
O	5.77337827298670	14.35476895174745	7.45379083304802
C	3.08289007607029	12.54256931111911	8.48364768690837
O	3.21942860045439	11.72376260268859	9.26522200081869
C	3.28926415975154	12.84392772988636	5.85115856357930
O	3.60680899999730	12.23010386862076	4.94103370624780
Mn	2.86813211255597	13.87373215986070	7.26460472133209
Br	2.17407565790237	15.41865094204763	9.22072907730838
S	3.22019732110012	18.69869913583378	6.46498151880832
S	0.46534747714594	13.43779878491897	7.04687015820490
N	2.38607435474893	15.60003354722108	5.97219390377937
C	6.44395441156441	17.31750224393508	8.51784315572776
C	7.25408734986364	18.87801537431389	6.86027486521157
C	7.50500441430961	17.96900627971306	7.89304652071764
C	5.13337450302239	17.54960213246297	8.09723321739722
C	-0.71840428081228	10.87282872824428	4.08145726968757
C	5.94696726085077	19.11674723160700	6.43982556539328
C	-0.20106293964119	9.66655091172745	4.54723593395280
C	0.23073394827955	12.03563925246719	5.97037379994969
C	0.55222352786627	9.64836625905113	5.72273957011201
C	-0.50088787660011	12.06094451976811	4.78280718592160
C	4.88211054801674	18.43813060210016	7.04670776783997
C	3.25239294781349	17.71611247173180	4.93732713615136
C	0.04348851843700	14.88449976911553	6.05419450097103
C	0.76114390556917	10.82535241761069	6.43378833093924

C	1.18099042297722	15.33599784377823	5.16480249677305
C	3.46091568622624	16.22597942781660	5.17702311815195
H	2.14658775590476	16.25836706675083	6.71653552958830
H	3.53910327113637	15.69639941278504	4.21593998260905
H	4.41853950054742	16.08396928419275	5.69547194649623
H	4.03882993544349	18.10114487264102	4.27411978987063
H	2.29135721764690	17.92379311320857	4.44374339544011
H	0.85664354379612	16.22928393805196	4.60673531297458
H	1.42951508828368	14.56209818728520	4.42265604044169
H	-0.19441580027147	15.65231191158766	6.80357390956412
H	-0.87625610726609	14.70471415324721	5.48404038572339
H	-0.91710892464303	12.98826974798208	4.38706600777129
H	-1.30034610510497	10.89903297300301	3.15670972996738
H	-0.38904110952327	8.74422056846529	3.99171023399665
H	0.97907822827181	8.71636960703392	6.10322555892258
H	1.33319568669182	10.79490341055160	7.36392496231032
H	6.63759947617827	16.60844187630113	9.32701255852637
H	4.30014855910582	17.02419516254464	8.57322378455889
H	5.74570073988309	19.82605877024283	5.63252294011952
H	8.07922377629516	19.40576574929683	6.37539119874297
H	8.52865063177144	17.76601565773773	8.22149639072386

[$MnBr(CO)_3phSe$-κ^2 Se]

C	5.02728059772332	13.19524477698313	7.14400639481062
O	6.16655845283237	13.17654104989916	7.18520797477939
C	3.26315803967645	11.61906758855124	8.07637266921982
O	3.32164063389487	10.65676430796238	8.68751036027250
C	3.25075778042680	12.22872118297103	5.55204629680478
O	3.32235716561432	11.63386017527373	4.57845496765326

Mn	3.21417282003798	13.15093702174963	7.10293287932210
Br	3.17889420178359	14.58405964688626	9.23982870507750
Se	3.23105758008773	18.35574787408478	5.73952175263633
Se	0.67110681714825	13.30619238115654	7.19594070483136
N	2.99005062305504	15.08828375403809	6.06776331440085
C	6.20800765688406	18.46776039413185	8.69882624154981
C	6.68238174070522	20.25662302466682	7.14251346503232
C	7.00757755685496	19.53789265511818	8.29405155480252
C	5.07616164186946	18.11646194255546	7.95915835483828
C	-1.59670635951487	11.25107864673909	4.28998803166320
C	5.56317748509696	19.89982637673810	6.39077561568961
C	-1.29326370464314	9.92353522826830	4.59013659572740
C	-0.07825010698322	11.99355080702952	6.01215948641765
C	-0.37143624631796	9.63199956322491	5.59882098065806
C	-0.99286522238807	12.29038980327369	5.00096788601012
C	4.76012597103575	18.82734745451146	6.79564065855090
C	4.03911812025405	16.93523110322074	4.66701668366640
C	0.55253583870634	14.93864402239059	6.14810648700551
C	0.23582039126278	10.66401649654875	6.30835228222056
C	1.76006052856545	15.13701090237277	5.25953819437501
C	4.19405869155308	15.59391198431639	5.37661163887288
H	2.84504151296445	15.70077499733373	6.87078985573591
H	4.52610637805897	14.84396953273617	4.64174966969080
H	4.98255090354704	15.67214073037867	6.13822027424048
H	5.02203957118065	17.28840531083071	4.32812380730188
H	3.40599771450925	16.85897947118808	3.77285249588198
H	1.64392172696648	16.10783719916570	4.75340262865167
H	1.81928324583053	14.36915979692622	4.47383079638817
H	0.47423432566014	15.73818130730335	6.89928290473216

H	-0.38139162678869	14.94582778888708	5.57408588712237
H	-1.26166287096905	13.31997760058650	4.75712294004458
H	-2.31528626913410	11.48977873136683	3.50183262335410
H	-1.77897889467561	9.11589064792418	4.03769058814286
H	-0.11816048811822	8.59817668372549	5.84999540467742
H	0.94335689620500	10.42467417997089	7.10639573661632
H	6.46816064821095	17.90343483567182	9.59833789386754
H	4.43915324057752	17.29072253455365	8.29367100037964
H	5.30945898697778	20.45808053566015	5.48639782218993
H	7.30652542925692	21.09391859669468	6.82005853466551
H	7.88472155751841	19.81974384853317	8.88223925032788

$[MnBr(CO)_3bzlSe\text{-}\kappa^2\ Se]$

C	4.14641254953731	14.52723666078435	7.10838613444536
O	5.19233594107699	14.77190041650628	7.49067201514059
C	2.61047604461394	12.51969499461528	7.43330907443184
O	2.70867208311103	11.55356063461858	8.03281533385812
C	3.21301315416233	13.32308561457483	5.04136945851759
O	3.70856406407969	12.81947191367508	4.14087136839035
Mn	2.49133381330852	14.07801968336646	6.50915596338662
Br	1.44646806284843	15.16054330264611	8.59961242031389
Se	1.61893909647248	19.21849141479436	6.21836224367769
Se	0.04980707019711	13.71967236435912	5.81246773766648
N	2.12656870994268	16.03059274878965	5.56579313476270
C	5.96157886570666	18.84403821768872	9.36285614668830
C	5.84265430036351	20.66991751928107	7.79177183594956
C	6.56255905520506	19.93655372446153	8.73587329121242
C	4.64442525916872	18.50193781427914	9.06155184768834
C	-2.41955363382960	9.46143580227777	4.76272292566120

C	4.52037421593385	20.33339623812931	7.50139309012011
C	-1.79676054958546	8.77437622849117	5.80477642138706
C	-0.68721769997179	11.15970741141574	4.81572297997011
C	-0.60790305653265	9.26847179257356	6.34225431154187
C	-1.87350884950137	10.65063757605850	4.27732862089291
C	3.89527137259561	19.25856203335890	8.14744527503103
C	2.91850932456254	18.38243536746360	5.03161658040769
C	-0.10242178880219	15.38593055003238	4.81915309562914
C	-0.05625291775491	10.44442715706963	5.84177337080751
C	1.24101248632815	15.92919689800218	4.39077585883333
C	3.27381500169312	16.92871271307167	5.34435633920167
H	1.58425646647327	16.45302431414380	6.32026022141647
H	3.88715235349426	16.51651984664192	4.52782959416340
H	3.89338194754937	16.90604295378359	6.25154103453848
H	3.84134422261836	18.97788755432857	5.04086116850607
H	2.46797856631587	18.50766309408207	4.03598409816263
H	1.07867567100459	16.91355430326678	3.92460561467139
H	1.72557038630977	15.28648712900078	3.63990983844109
H	-0.60668280322100	16.08624482771922	5.50008917026349
H	-0.76962293322046	15.21036284562918	3.96714310058933
H	-2.38065891517426	11.19353979068968	3.47510413158500
H	-3.34079139617512	9.06989600485525	4.32252992341168
H	-2.24058358978014	7.85925898356218	6.20585845202452
H	-0.10243878911232	8.73262522123049	7.14964294638619
H	0.87898824690847	10.82040621536996	6.26466181720256
H	6.52320155672625	18.25041405966890	10.08888402216066
H	4.18045505442434	17.64580072378704	9.56080776640837
H	3.96266436631502	20.92117204050265	6.76669396646607
H	6.31391852622267	21.51118254654837	7.27610015407395

H	7.58618081208701	20.22442376270625	8.99377698166950
C	2.43629645799738	18.91219633576765	7.95919224801365
H	2.24234073817442	17.87406819693755	8.26429761130490
H	1.81515735278388	19.53959152541323	8.61583905834889
C	-0.10604291684004	12.45735266129759	4.32129865652347
H	0.87937078399928	12.31738124770248	3.85736323759435
H	-0.76685719611064	12.93054993158007	3.58537078266036

Table S9. Cartesian coordinates of compounds $[Mn(CH_3CN)(CO)_3L\text{-}\kappa^2\ X]^+$ (in which L = phS, phSe or bzlSe and X = S or Se) at ωB97X-D3 level of theory with the SMD solvation model using acetonitrile as solvent.

$[MnBr(CO)_3phS\text{-}\kappa^2\ S]$			
C	4.78232860234880	14.40925685457304	7.26228441589034
O	5.91032502625926	14.54541103476406	7.21920404270096
C	3.37292241494448	12.67016038846707	8.47702510077156
O	3.64517743362730	11.88523676584486	9.25445513255139
C	3.42584282955521	12.81151852365993	5.88463313001331
O	3.72731650661520	12.07766794873144	5.06886455693941
Mn	3.00642452087089	13.96331987880349	7.23790063014211
N	2.36369999387972	15.23590367860806	8.71813932441119
S	3.10365553469650	18.65406373518967	6.91676939727419
S	0.57116345602709	13.49090078133410	7.07264195741284
N	2.41977619468730	15.66552099239169	5.95318344085679
C	6.44918602141469	17.26345013901861	8.75803506851302
C	7.16319801353021	18.78275723800670	7.02361408254579
C	7.47393996082640	17.89159183652650	8.05567442954397
C	5.11871218369616	17.50453140212860	8.41473900359000
C	-0.94215689882812	10.85451351457978	4.34826080625467
C	5.83502828391158	19.03407100100306	6.68520874815248
C	-0.45980488980715	9.64616992990007	4.84618752174193
C	0.23012192215805	12.05205173654023	6.08286055191083
C	0.39245486307825	9.64499032166062	5.95336420769965
C	-0.59425574206025	12.06182059035656	4.95665147783908
C	4.80334086878391	18.37929674417278	7.37142812572763
C	3.09276438386024	17.95266518773916	5.24006370515392
C	0.11318002447521	14.89519032365759	6.03565695502957
C	0.73525526749380	10.84361062109519	6.57320915002801

C	1.23869244951200	15.34065406489734	5.13078683615036
C	3.41339053575571	16.46171493765793	5.20068826404260
H	2.10808222653905	16.28519596296968	6.70014937044148
H	3.43681689169248	16.10376180288851	4.16150793443367
H	4.41520109793356	16.29797435128924	5.61980742253305
H	3.79649809935758	18.50908163505535	4.60721509246378
H	2.08493153182901	18.16526772985551	4.85108125665851
H	0.90082533337099	16.21401020766685	4.55014273947651
H	1.52173507517451	14.55503497321192	4.41434666949957
H	-0.14743638851555	15.68923099698626	6.75010851309615
H	-0.80482251253411	14.67429882615608	5.47905519109885
H	-0.99167147628683	12.98911145670698	4.54349925454934
H	-1.59891694634948	10.86750228381763	3.47471489214463
H	-0.75418783759088	8.70898553714929	4.36648109457176
H	0.79229412648573	8.70923718895016	6.35265349752395
H	1.38073042275817	10.83319584746751	7.45590597318835
H	6.68281635331452	16.56037455205459	9.56110141021622
H	4.32254886791945	16.98849609380336	8.95218305690667
H	5.59861393181325	19.73367153835019	5.87867272474470
H	7.96094059915059	19.28954209073317	6.47502596592351
H	8.51477214217313	17.68068346734592	8.31781006817145
C	1.92163849045750	15.97633324640556	9.47295921799215
C	1.36307446852940	16.94348783975732	10.39296624452400
H	2.17299312387149	17.45746375210503	10.92856391295028
H	0.71412620959922	16.42278484470108	11.10990842109530
H	0.77571729259473	17.67297977936468	9.81832655170841

[$MnBr(CO)_3phSe$-κ^2 Se]

C	4.78451040264213	14.41945876732116	7.31668712141662

O	5.91284895922414	14.55982482354016	7.27962009759520
C	3.39197017145105	12.68387690640927	8.54737784736009
O	3.67149993543383	11.89993893059919	9.32412217220431
C	3.41690063340208	12.79717066614173	5.96225365502475
O	3.70684565347995	12.05229551559842	5.15124104186982
Mn	3.01332460033060	13.96405154905266	7.30237023632643
N	2.38648043489188	15.26474802827267	8.76281333214542
Se	3.02495114492076	18.74765324874427	6.97620391832566
Se	0.49486057446227	13.44375496756820	7.19009418499319
N	2.40890566145396	15.63839254395021	5.98855381979735
C	6.55683107639008	17.32484306174309	8.74245972468023
C	7.21394589953992	18.88668680359119	7.02163143025373
C	7.55724195743063	17.98091289217403	8.02998431151247
C	5.21553473313006	17.55930752449027	8.43734108007759
C	-1.01883402937886	10.80573602027951	4.28502824340509
C	5.87477162927307	19.13137393512439	6.72090027241200
C	-0.53357491917292	9.57958060649737	4.73688316590228
C	0.16061643641103	11.93392094693593	6.05934604856185
C	0.32459058460116	9.53570297935942	5.83838898338362
C	-0.67038973088156	11.98809244021372	4.93979907477269
C	4.86853305908949	18.45681375913108	7.42389225838314
C	3.06760293193214	17.91112809643383	5.20912597744392
C	0.07373983802615	14.91971453850387	6.00207524678668
C	0.67156581032233	10.71117179018126	6.50104675455979
C	1.24782632018159	15.31140380460593	5.13721437466698
C	3.41822492235544	16.42987817884450	5.25032862246783
H	2.07487453812908	16.26674582599339	6.71902134346658
H	3.50030186239776	16.02664676224206	4.23035974291310
H	4.40165558590387	16.30637695454966	5.72245252199551

H	3.78490347071907	18.45869367253278	4.58522401300469
H	2.06759330752153	18.09557952706519	4.78960208362743
H	0.95432934303313	16.17506399659084	4.51901606972642
H	1.53865237463824	14.50047818800346	4.45249374635364
H	-0.21571332109361	15.73809670504154	6.67654125727190
H	-0.81511731882033	14.67232787167158	5.41096456913264
H	-1.07215805234078	12.93177067692129	4.56820482557047
H	-1.68079573750600	10.85119865883873	3.41637047464335
H	-0.83061525671634	8.66068270543490	4.22469915250433
H	0.72396197008801	8.58515236330866	6.20188085703100
H	1.32432159174766	10.66829998251781	7.37802159007686
H	6.81893241731970	16.60881998785776	9.52498313393947
H	4.43827192230372	17.02214520310553	8.98315357277455
H	5.61239517092626	19.84290242625974	5.93291931423915
H	7.99399436698115	19.40965057694881	6.46288119862954
H	8.60634546454540	17.77972895765416	8.26536271774779
C	1.95077189677389	16.02554179034102	9.50123324672402
C	1.39226588312160	17.01143919826584	10.40230355740611
H	2.20138068091703	17.54671257558453	10.91781502009901
H	0.75438243099653	16.50313330362721	11.13791712900819
H	0.79274160207098	17.72112494043633	9.81551240458537

[$MnBr(CO)_3bzlSe\text{-}\kappa^2$ Se]

C	3.44773067590435	15.08096117005137	7.16925374494897
O	4.49530010333536	15.33643986451276	7.53470916650340
C	1.89239921516707	13.04737715322200	7.51397232242378
O	1.98858336878860	12.08052369570091	8.10543867802426
C	2.56181818993989	13.82923778741530	5.12015412560408
O	3.08948434147406	13.34922212761204	4.23151758570587

Mn	1.78697548962205	14.61532873657820	6.57415845146650
N	0.87411712374001	15.63218777920160	8.12230732034905
Se	1.25283801083131	19.73242962200655	6.29614843180289
Se	-0.59926421279794	14.19312070427616	5.84686284651234
N	1.44277809263978	16.52492380677308	5.48676094770176
C	5.81047398660034	19.18333675010250	9.16868914754889
C	5.67218602308906	20.94934408792440	7.53169368329109
C	6.41198711255301	20.23371297761257	8.47312848901653
C	4.47444728688856	18.86877769163245	8.93491231231933
C	-0.52526436756998	9.74098164444115	6.65200561925268
C	4.32968854640774	20.63802117401476	7.30694761297612
C	0.60191208515913	9.08112181492281	6.15857463973982
C	-0.21678488465359	11.51204636798210	5.02111013893797
C	1.30391022843257	9.62254042962949	5.08253725523743
C	-0.93296434191064	10.94715015802609	6.08657894807877
C	3.70856089289408	19.60607215356642	8.01921001694674
C	2.29660767937124	18.83633860433207	4.91390822524603
C	-0.77433380391303	15.78529057188072	4.74618591954132
C	0.89829984125037	10.83218622921866	4.52025248188325
C	0.56767611797219	16.32693267883314	4.30983682407113
C	2.61643873485589	17.36894503691205	5.17879814061497
H	0.89536989178469	17.05922242501696	6.16175152794941
H	3.12938500859705	16.93667307635540	4.30627552294167
H	3.32000151117135	17.30795496073046	6.02070308495703
H	3.23672334109084	19.38252954853132	4.76047331115604
H	1.68924930665727	18.98179566931505	4.00909428398604
H	0.40351900393344	17.27565988546637	3.77592569935385
H	1.07709098488211	15.64500365486968	3.61297580247754
H	-1.31844638964090	16.51552643502138	5.36142829910568

H	-1.41131663289286	15.53035797325728	3.89030039085810
H	-1.81213730931981	11.46104432101619	6.48860791367198
H	-1.09233784359770	9.31311936220125	7.48280878592892
H	0.93632457381257	8.14561621818422	6.61515979496603
H	2.17259382713302	9.10185095780521	4.67193369983611
H	1.45375033035427	11.25622693670329	3.67991806675452
H	6.38549296550376	18.60391260864780	9.89553558614946
H	4.00960300866757	18.04833543446603	9.48979454862688
H	3.75655250382002	21.21532687206230	6.57628227242864
H	6.14318222323532	21.75834644827923	6.96688875623067
H	7.45256980611661	20.50267104114327	8.67791082133175
C	2.23745765325350	19.27002599281965	7.90889688712677
H	2.09153169201392	18.20142391215680	8.12231047454690
H	1.67347564406482	19.81594259507961	8.68167705141153
C	-0.61227882868180	12.84179513593865	4.44004866532346
H	0.07068218198724	13.15295731366021	3.64035225439126
H	-1.63665817855205	12.83822782547383	4.04319506562832
C	0.38157759055429	16.31442978173109	8.90083880325199
C	-0.21553902354715	17.22663164847887	9.85467592072658
H	0.57585798632150	17.72049238890500	10.43546560368427
H	-0.87327714196768	16.66604186262808	10.53226277424084
H	-0.80272560002670	17.97666089847380	9.30619909031277

Table S10. Wiberg bond orders (W_{XY}), Natural Population Analysis, NPA, of compounds **1-3** at BP86/def2-SVP level of theory.

Interaction	W_{XY}	NPA	
		group/atom	charge
Compound **1**			
$Mn_{(1)}$-$C_{(1)}O_{(1)}$	0.699	$Mn_{(1)}$	-0.078
$Mn_{(1)}$-$C_{(2)}O_{(2)}$	0.677	$C_{(1)}O_{(1)}$	0.031
$Mn_{(1)}$-$C_{(3)}O_{(3)}$	0.707	$C_{(1)}$	0.479
$Mn_{(1)}$-$Br_{(1)}$	0.273	$O_{(1)}$	-0.448
$Mn_{(1)}$-$N_{(1)}$	0.236	$C_{(2)}O_{(2)}$	0.038
$Mn_{(1)}$-$S_{(2)}$	0.337	$C_{(2)}$	0.479
		$O_{(2)}$	-0.441
		$C_{(3)}O_{(3)}$	-0.036
		$C_{(3)}$	0.422
		$O_{(3)}$	-0.458
		$Br_{(1)}$	-0.462
		$N_{(1)}$	-0.693
		$S_{(2)}$	0.414
Compound **2**			
$Mn_{(1)}$-$C_{(1)}O_{(1)}$	1.083	$Mn_{(1)}$	-0.072
$Mn_{(1)}$-$C_{(2)}O_{(2)}$	1.026	$C_{(1)}O_{(1)}$	0.020
$Mn_{(1)}$-$C_{(3)}O_{(3)}$	1.130	$C_{(1)}$	0.468
$Mn_{(1)}$-$Br_{(1)}$	0.360	$O_{(1)}$	-0.448
$Mn_{(1)}$-$N_{(1)}$	0.277	$C_{(2)}O_{(2)}$	0.025
$Mn_{(1)}$-$Se_{(2)}$	0.399	$C_{(2)}$	0.469
		$O_{(2)}$	-0.444
		$C_{(3)}O_{(3)}$	-0.042
		$C_{(3)}$	0.419
		$O_{(3)}$	-0.461
		$Br_{(1)}$	-0.454
		$N_{(1)}$	-0.694
		$Se_{(2)}$	0.564
Compound **3**			
$Mn_{(1)}$-$C_{(1)}O_{(1)}$	1.052	$Mn_{(1)}$	-0.074
$Mn_{(1)}$-$C_{(2)}O_{(2)}$	1.029	$C_{(1)}O_{(1)}$	0.047
$Mn_{(1)}$-$C_{(3)}O_{(3)}$	1.159	$C_{(1)}$	0.479
$Mn_{(1)}$-$Br_{(1)}$	0.359	$O_{(1)}$	-0.432
$Mn_{(1)}$-$N_{(1)}$	0.279	$C_{(2)}O_{(2)}$	0,012
$Mn_{(1)}$-$Se_{(1)}$	0.417	$C_{(2)}$	0.466
		$O_{(2)}$	-0.454
		$C_{(3)}O_{(3)}$	-0.071
		$C_{(3)}$	0.412

	$O_{(3)}$	-0.483
	$Br_{(1)}$	-0.448
	$N_{(1)}$	-0.674
	$Se_{(2)}$	0.513