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Studies on the chemistry and biochemistry of gold(III) carboxamide pincer chelates Supplimentary Information



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By: Rufaro Razuwika

A thesis submitted to the Faculty of Science, University of the Witwatersrand, Johannesburg, in fulfilment of the requirements for the degree of Doctor of Philosophy.

[January 2024]

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Supplimentary infromation

S1. General characterisation

S1.1. IR instrumentation and spectra

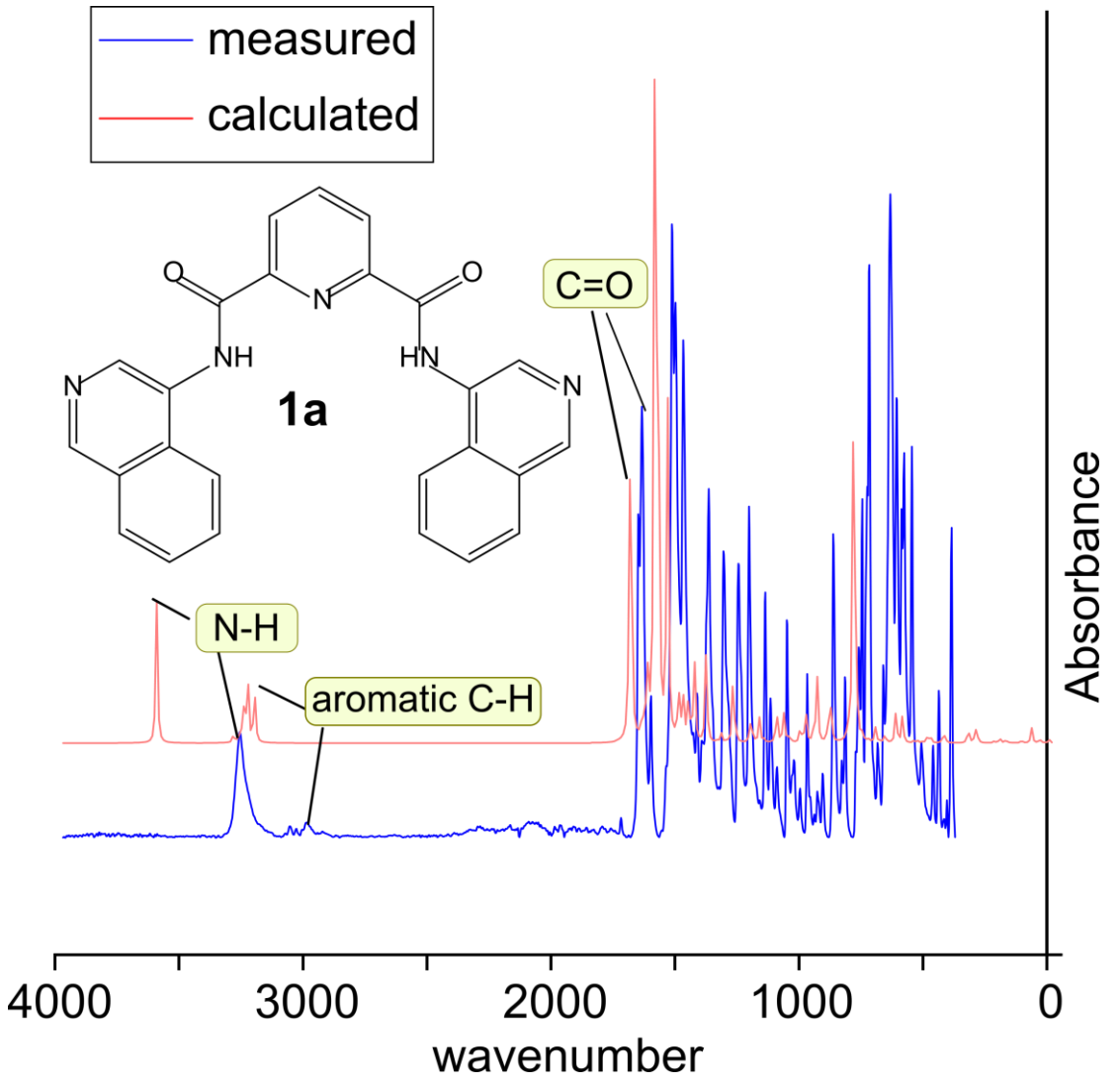


Figure S 1. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1a**.

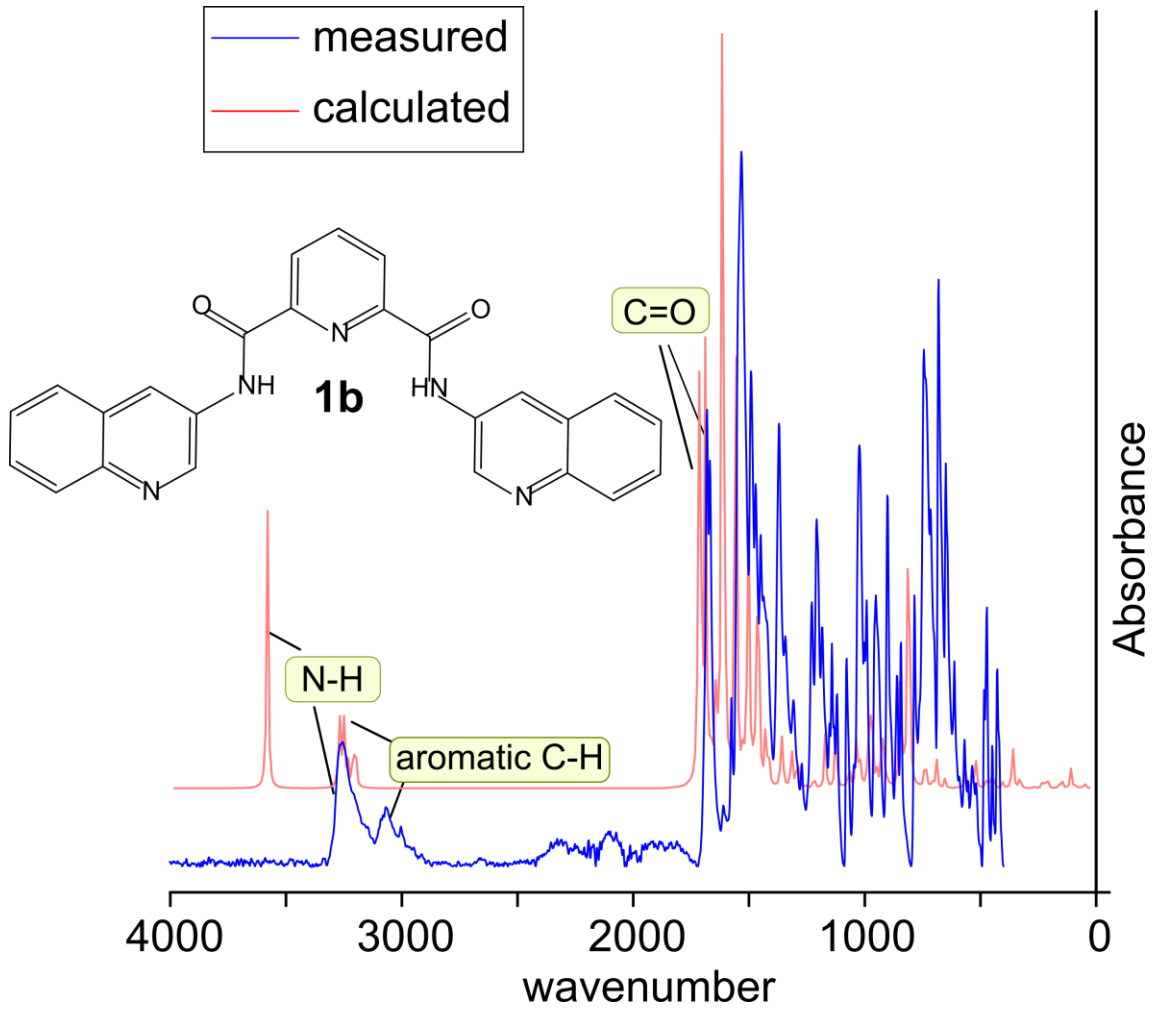


Figure S 2. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1b**.

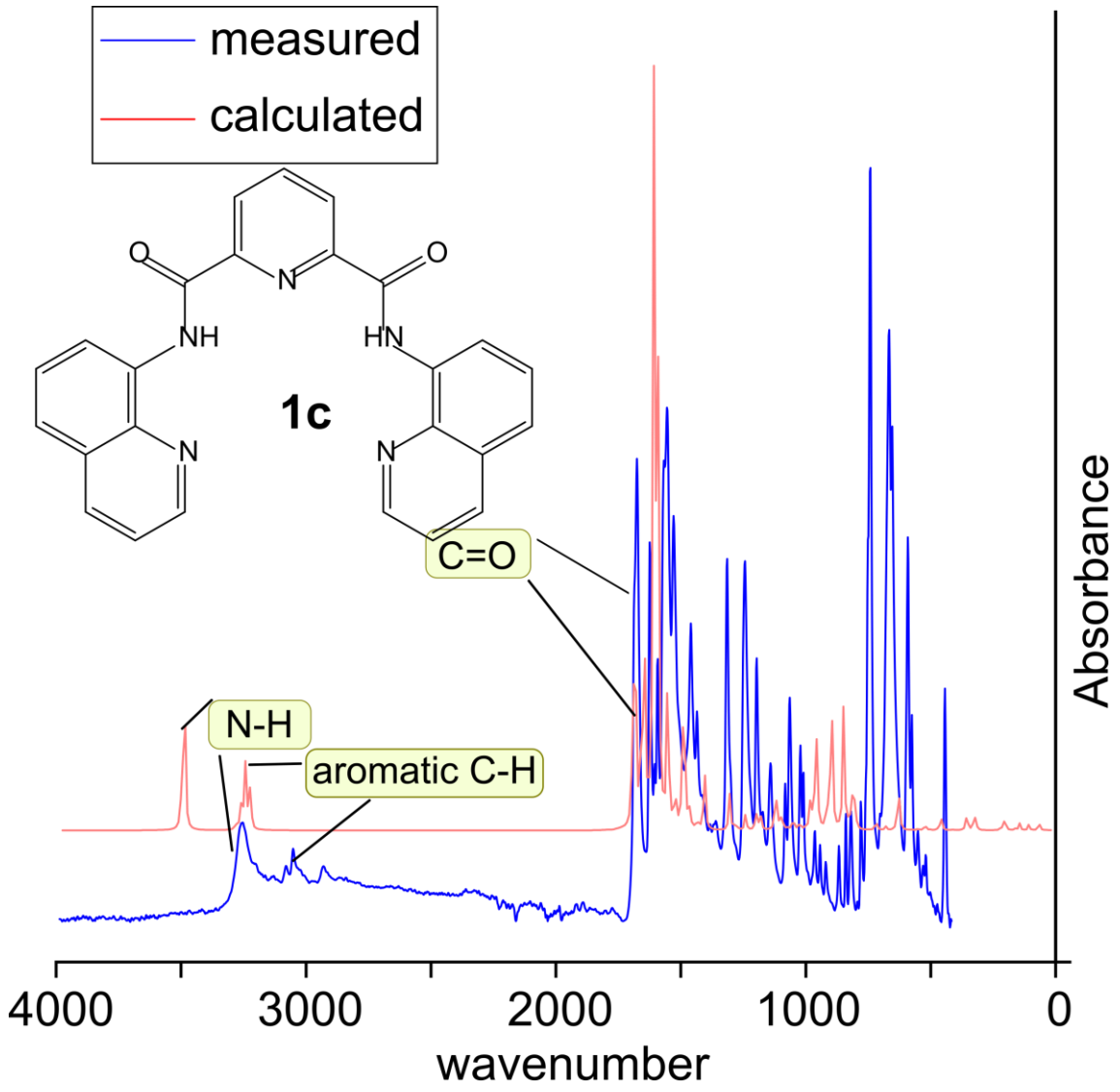


Figure S 3. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1c**.

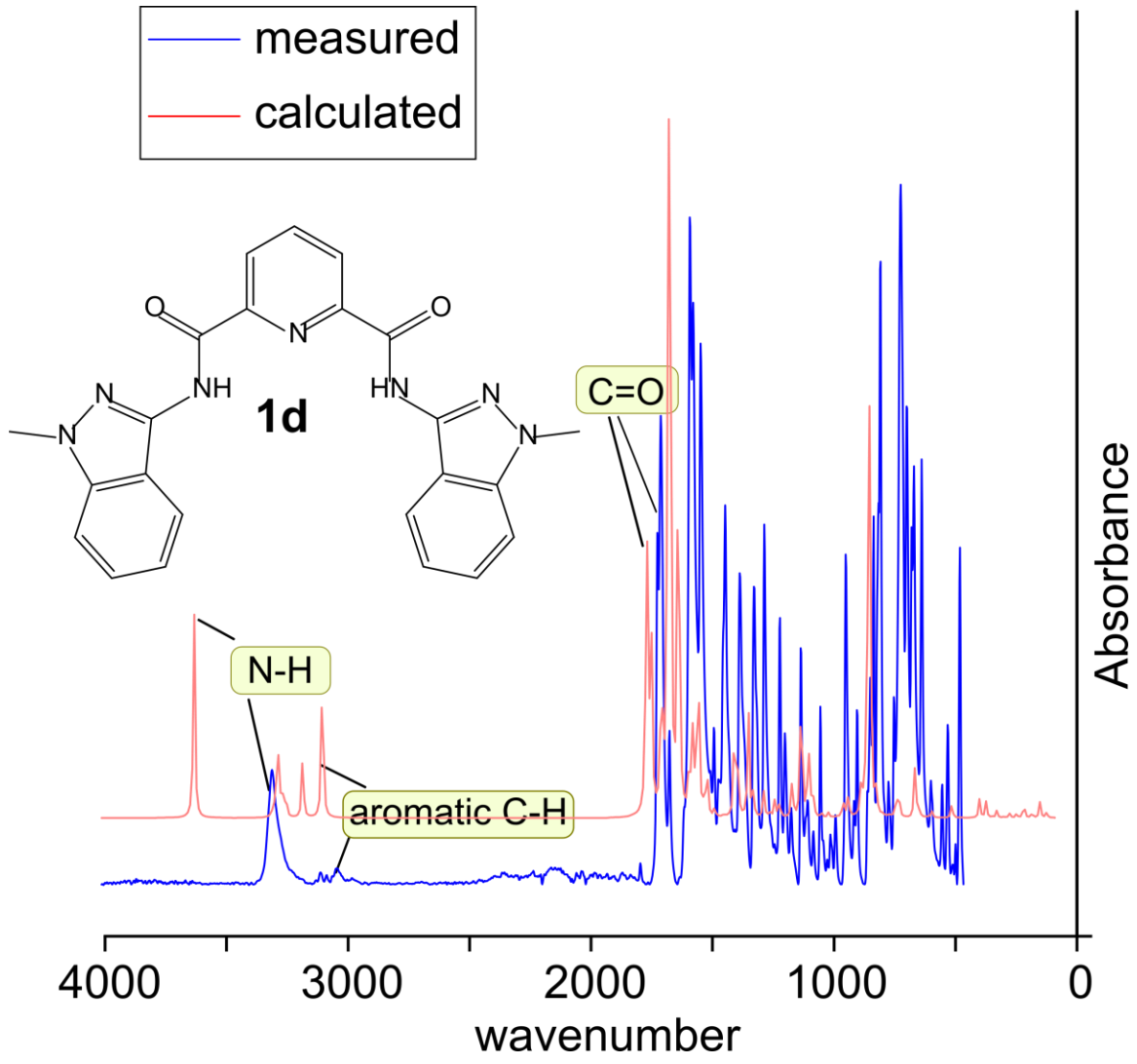


Figure S 4. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1d**.

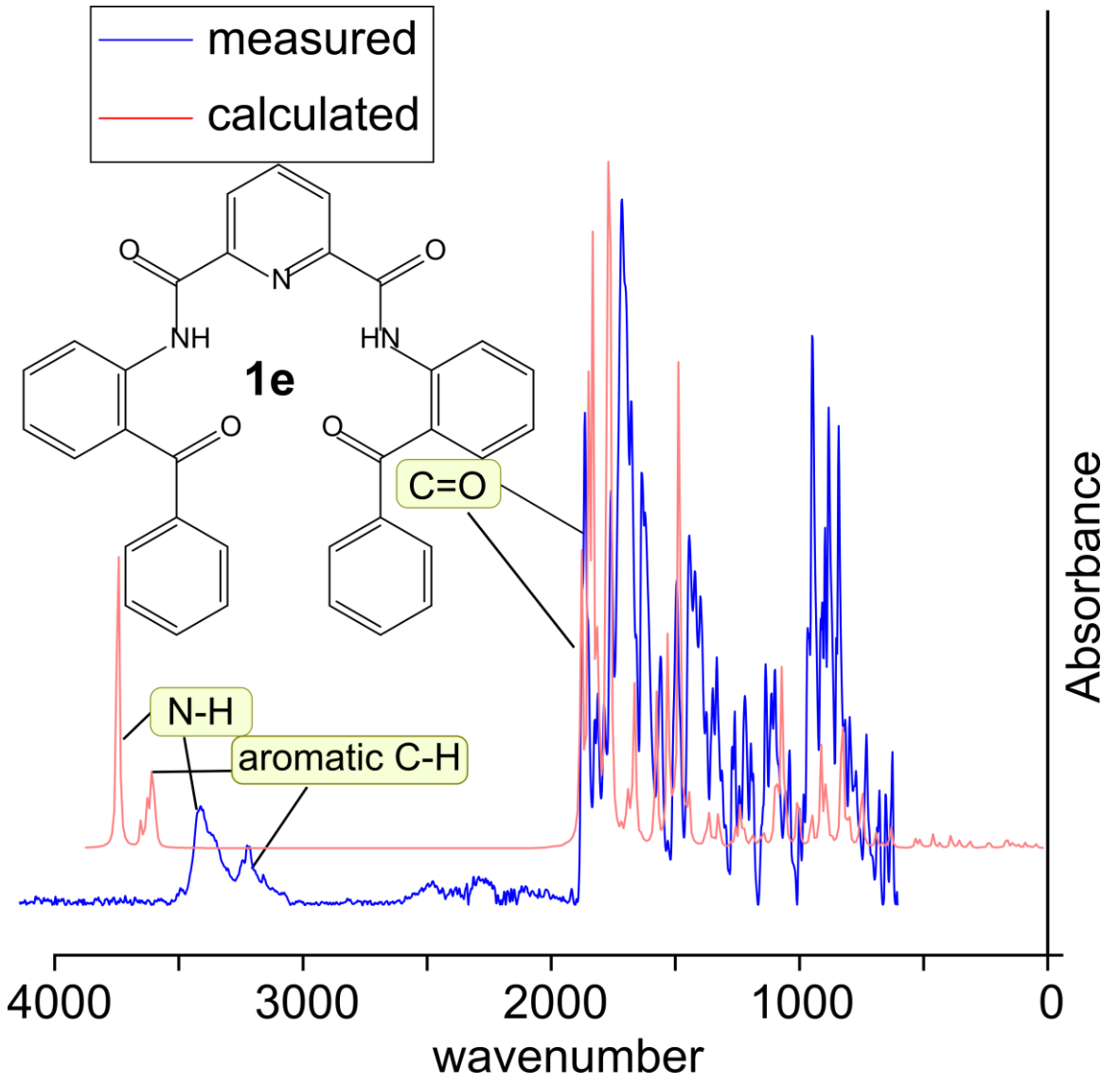


Figure S 5. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1e**.

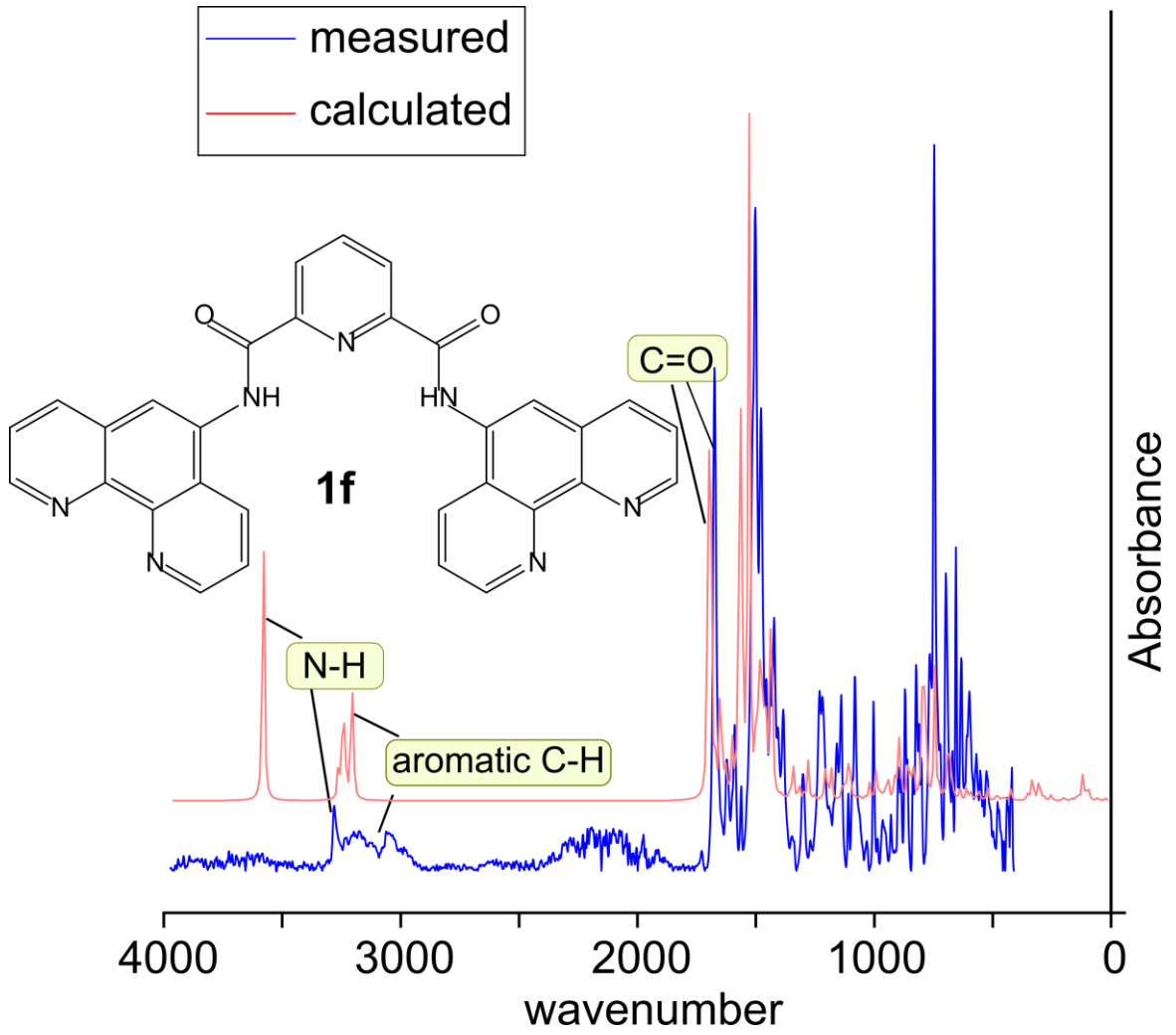


Figure S 6. IR spectra for a powder sample (blue) and from DFT calculated data in a vacuum (red) of **1f**.

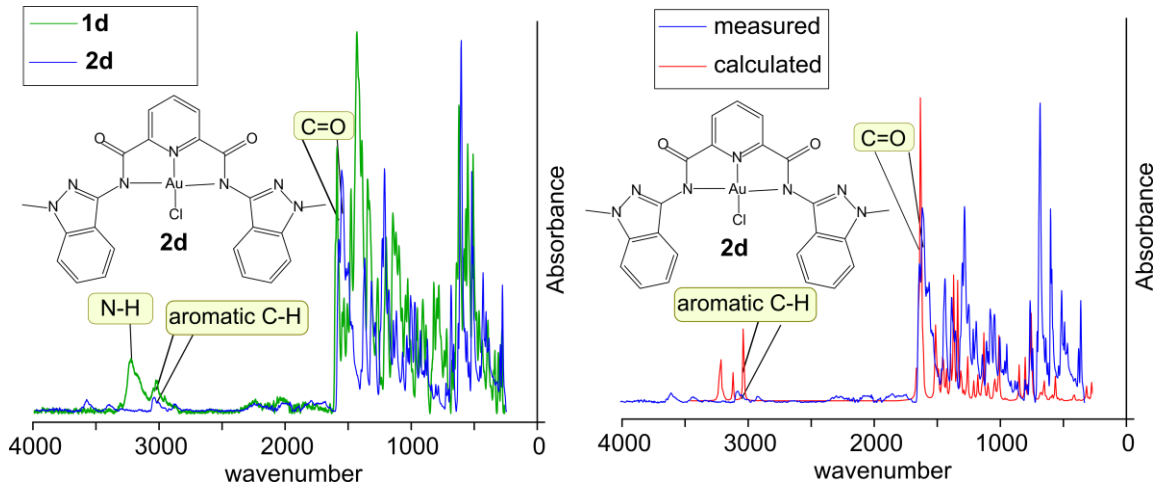


Figure S 7. Comparison of IR spectra for a powder sample of **1d** (green) and **2d** (blue) and from DFT calculated data in a vacuum (red) of **2d**.

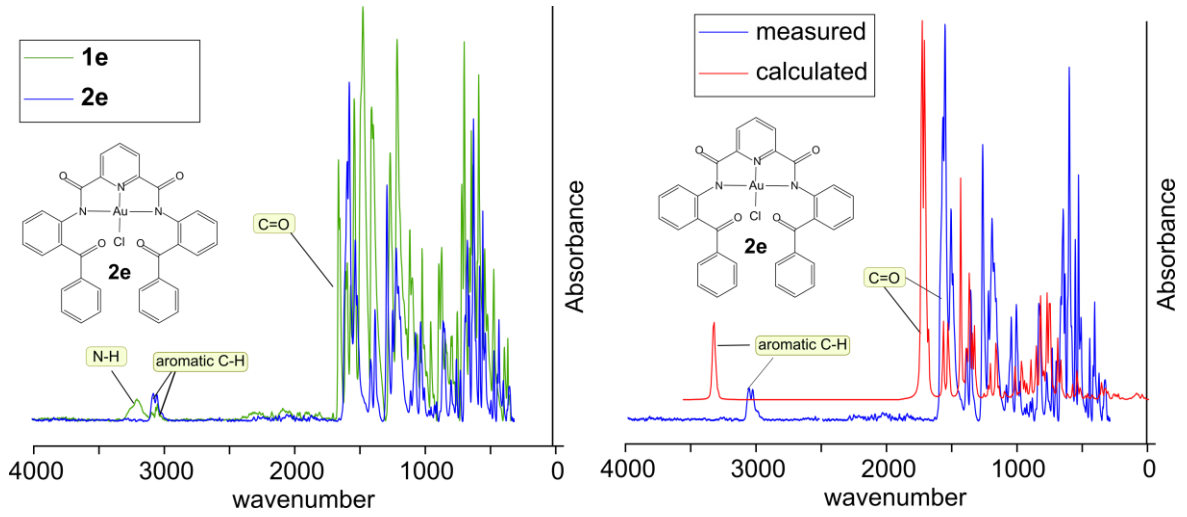


Figure S 8. Comparison of IR spectra for a powder sample of **1e** (green) and **2e** (blue) and from DFT calculated data in a vacuum (red) of **2e**

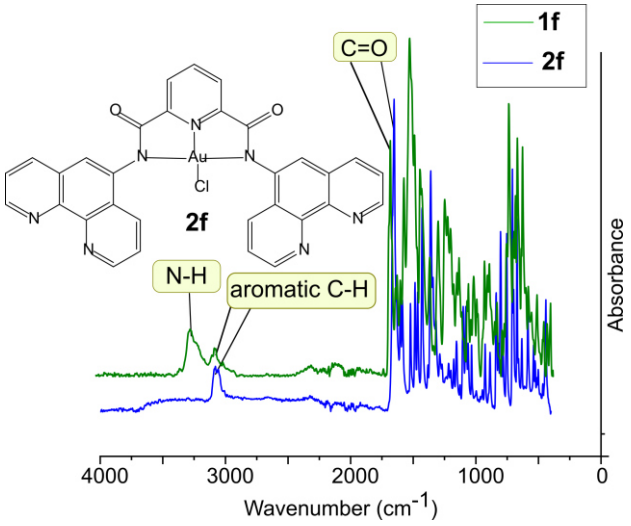


Figure S 9. Comparison of IR spectra for a powder sample of **1f** (green) and **2f** (blue).

S1.2. NMR spectroscopy

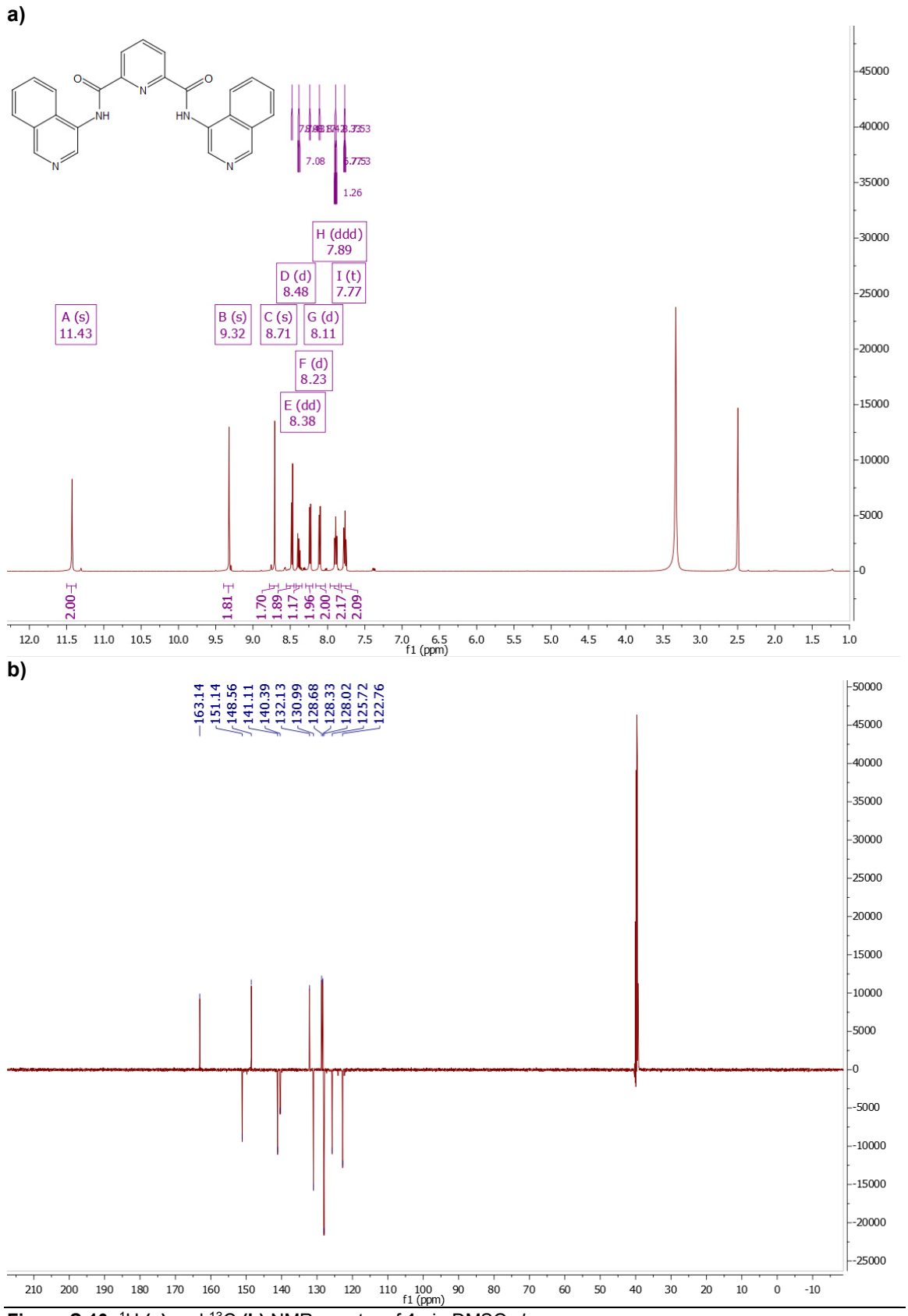
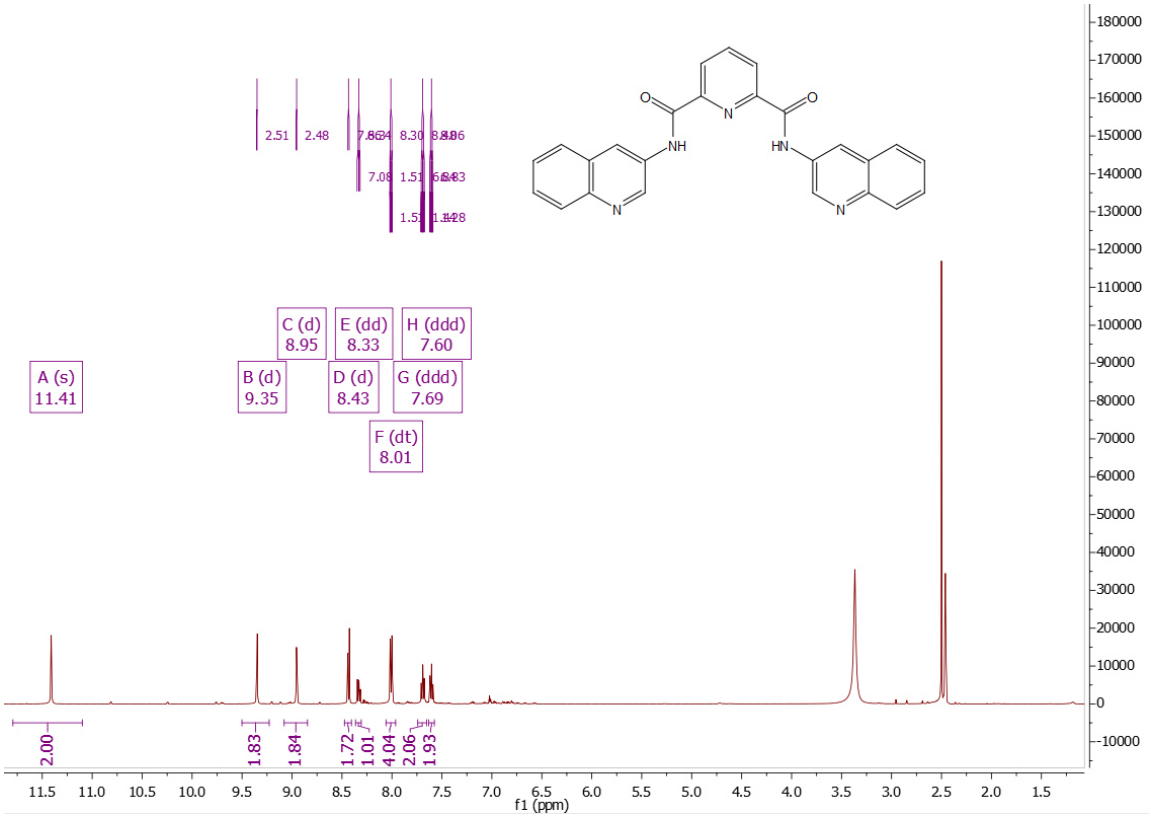


Figure S 10. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **1a** in DMSO-d_6.

a)



b)

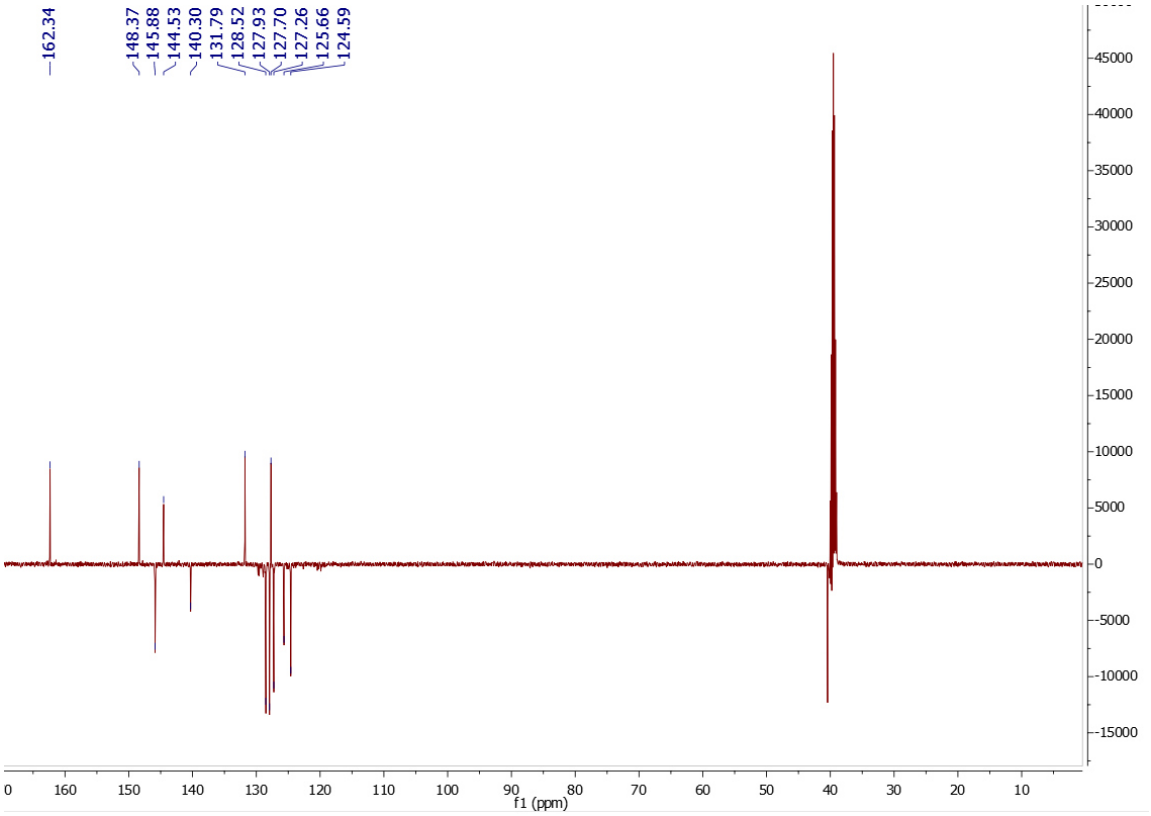


Figure S 11. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **1b** in DMSO-d_6.

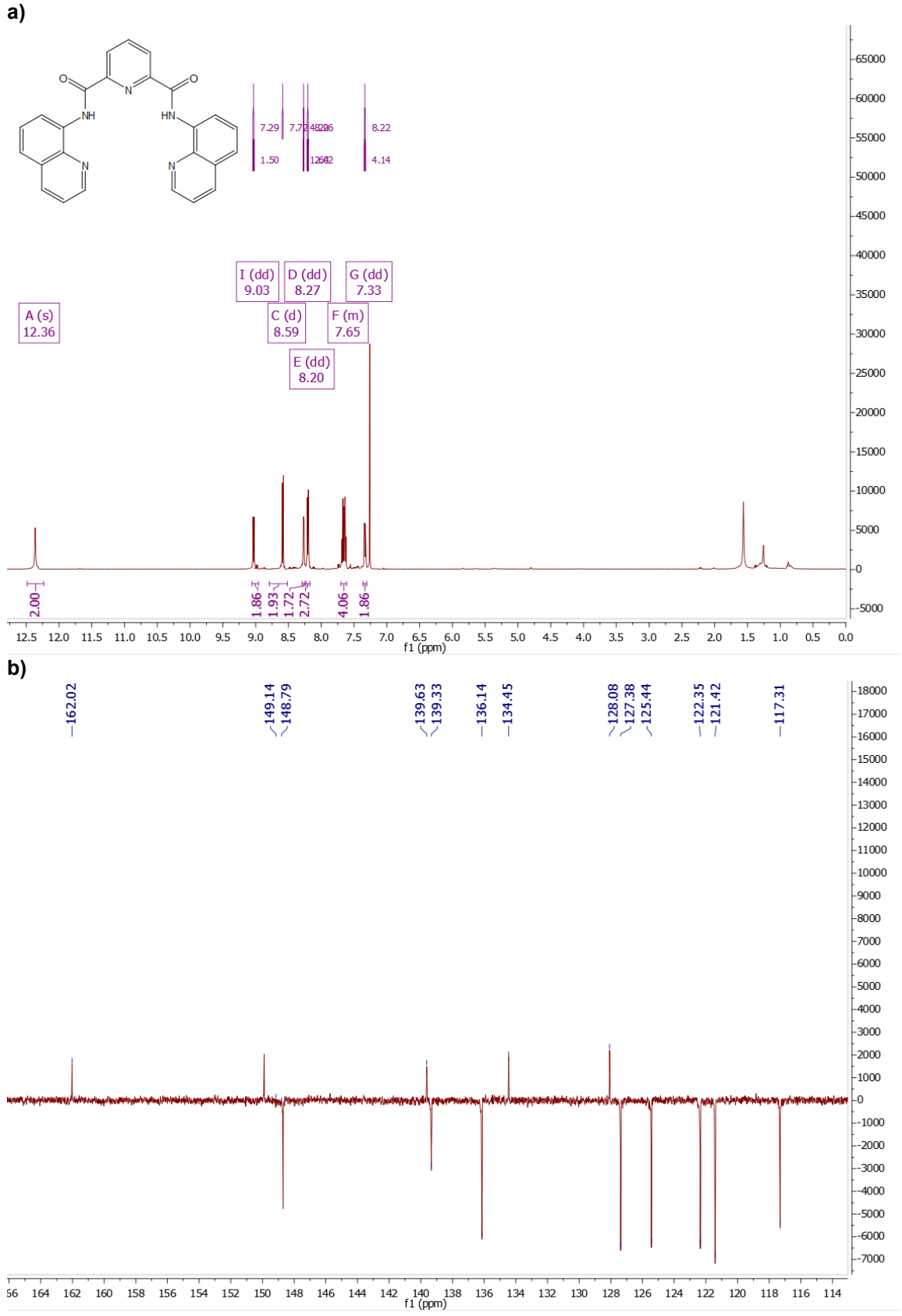


Figure S 12. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **1c** in DMSO-d_6.

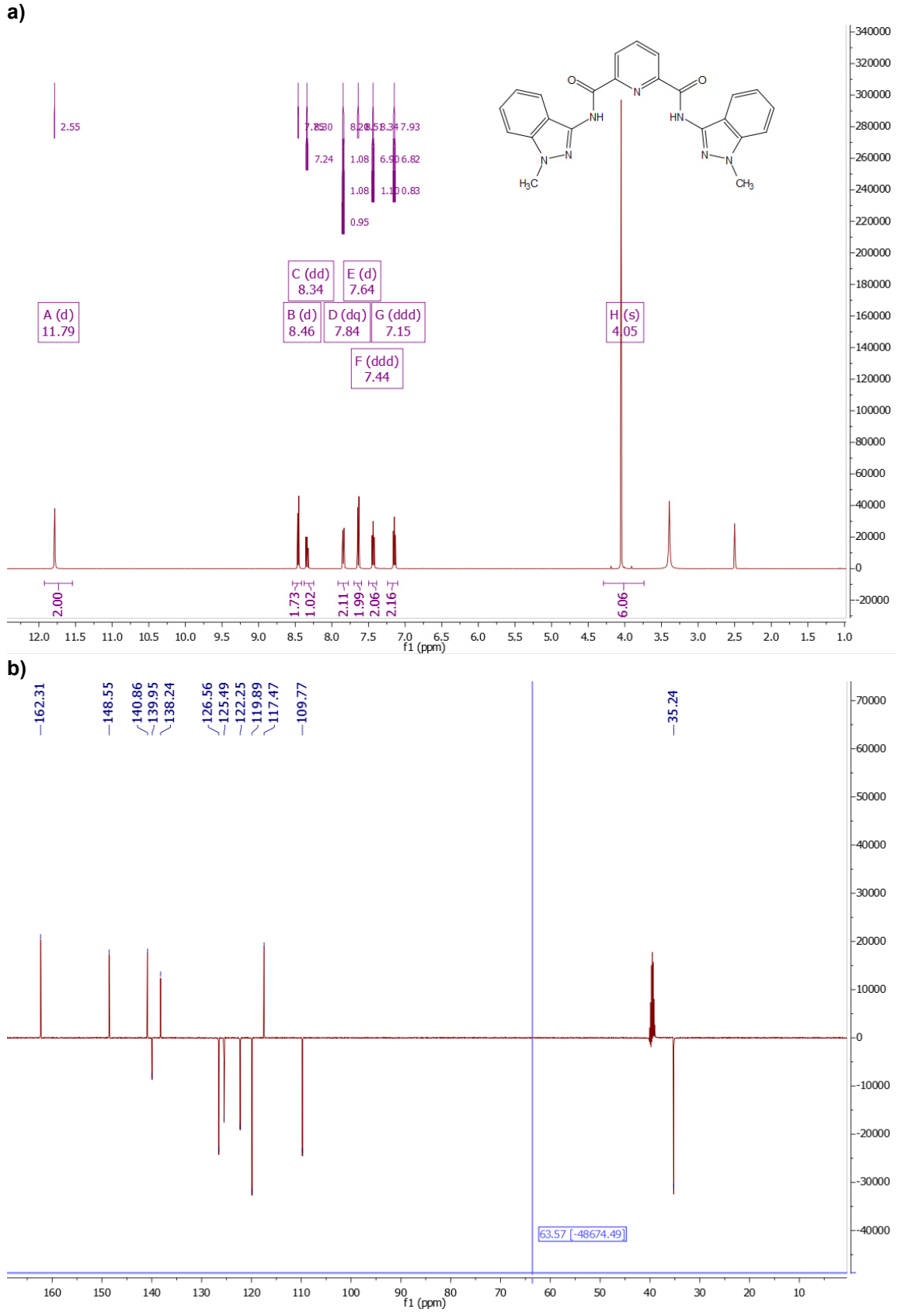


Figure S 13. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **1d** in DMSO-d_6.

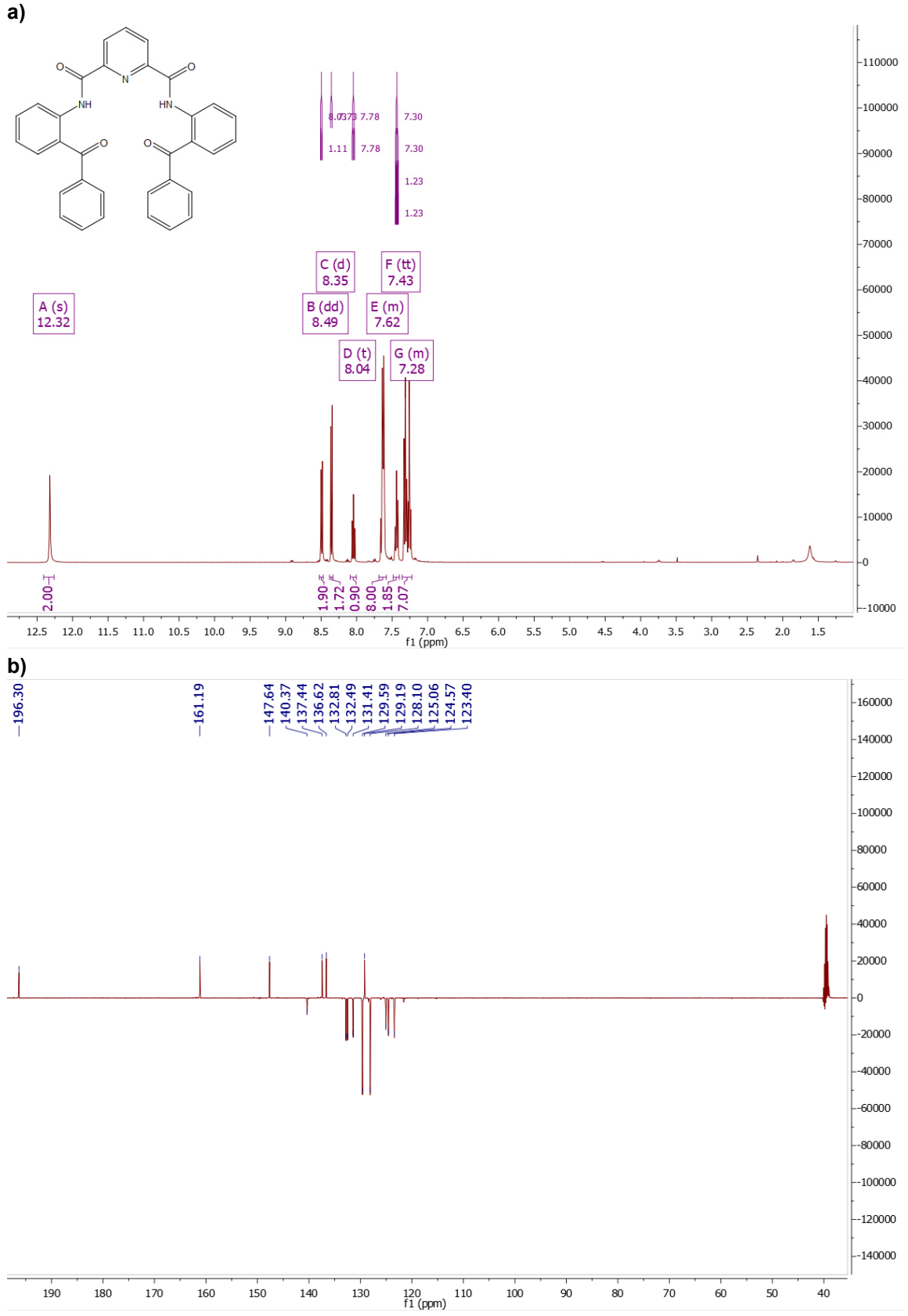


Figure S 14. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **2d** in MeCN-d_3.

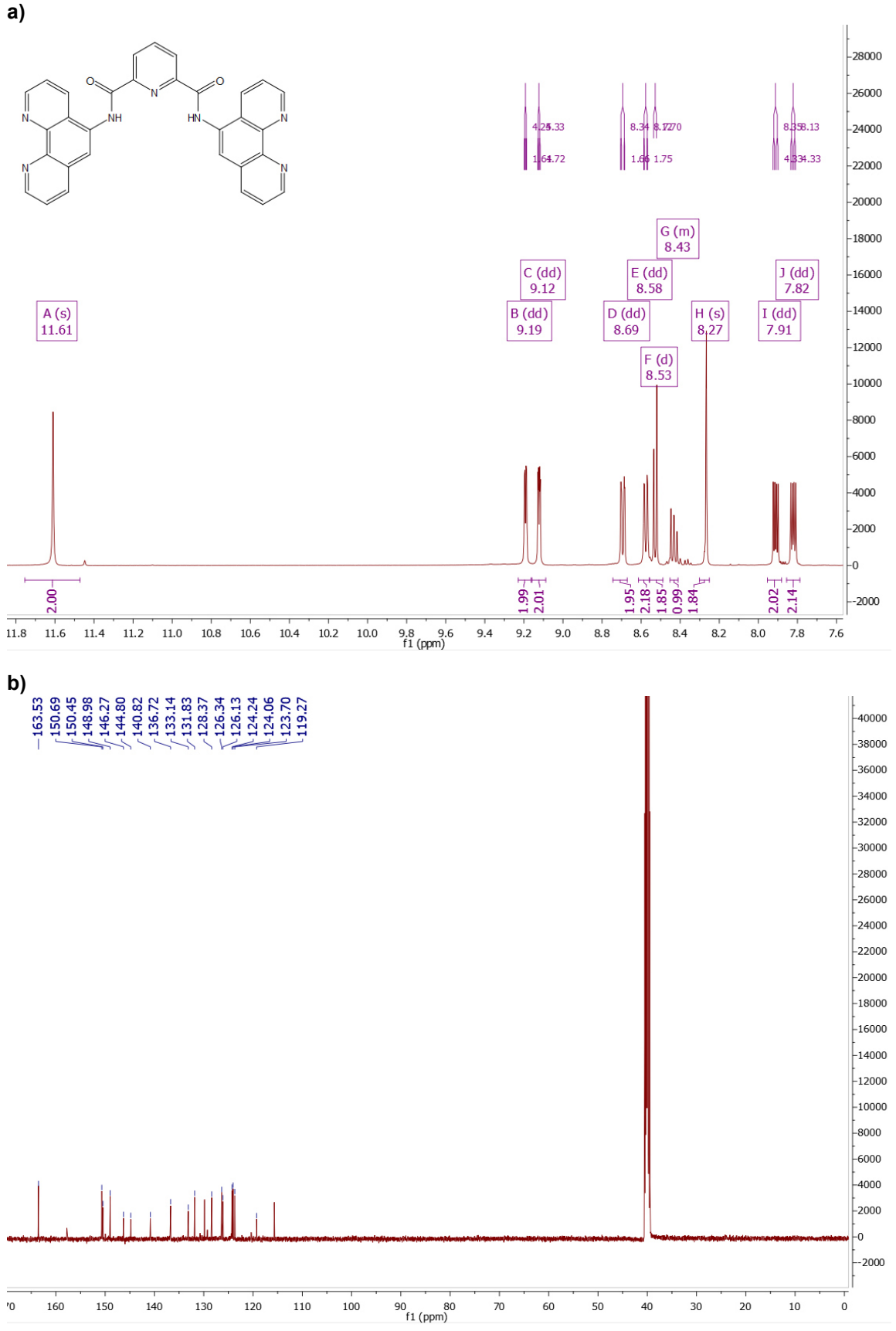


Figure S 15. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **1f** in DMSO-d_6.

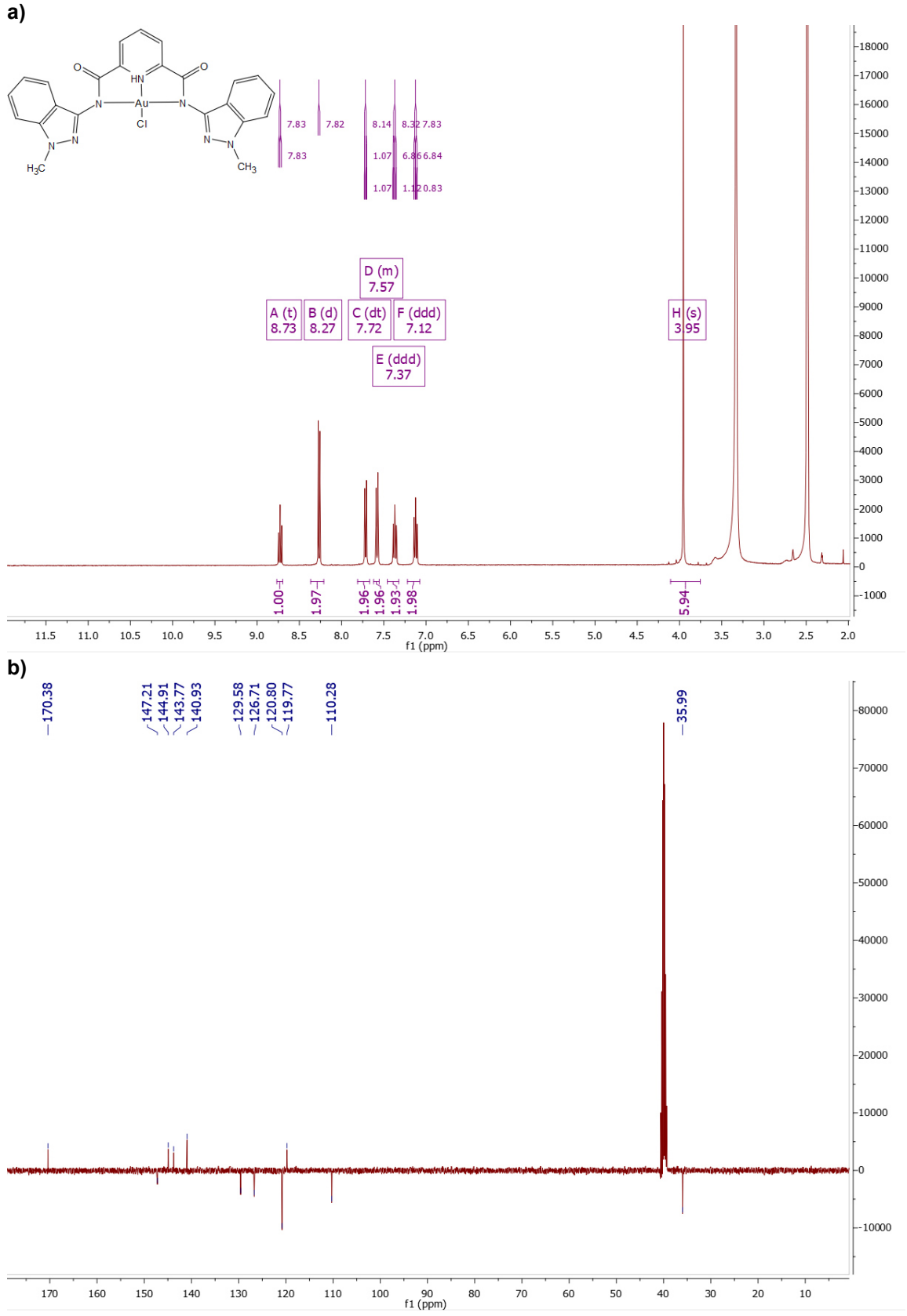
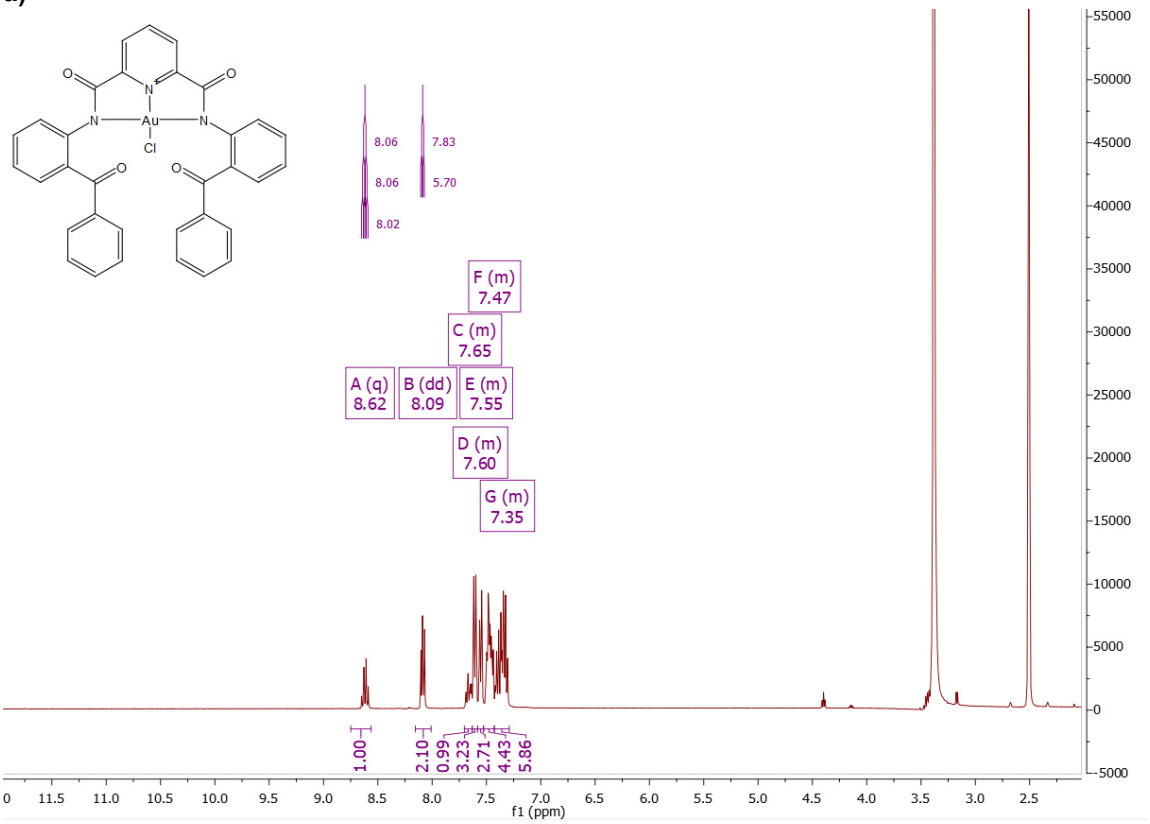


Figure S 16. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **2d** in DMSO-d_6.

a)



b)

Figure S 17. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **2e** in DMSO-d_6.

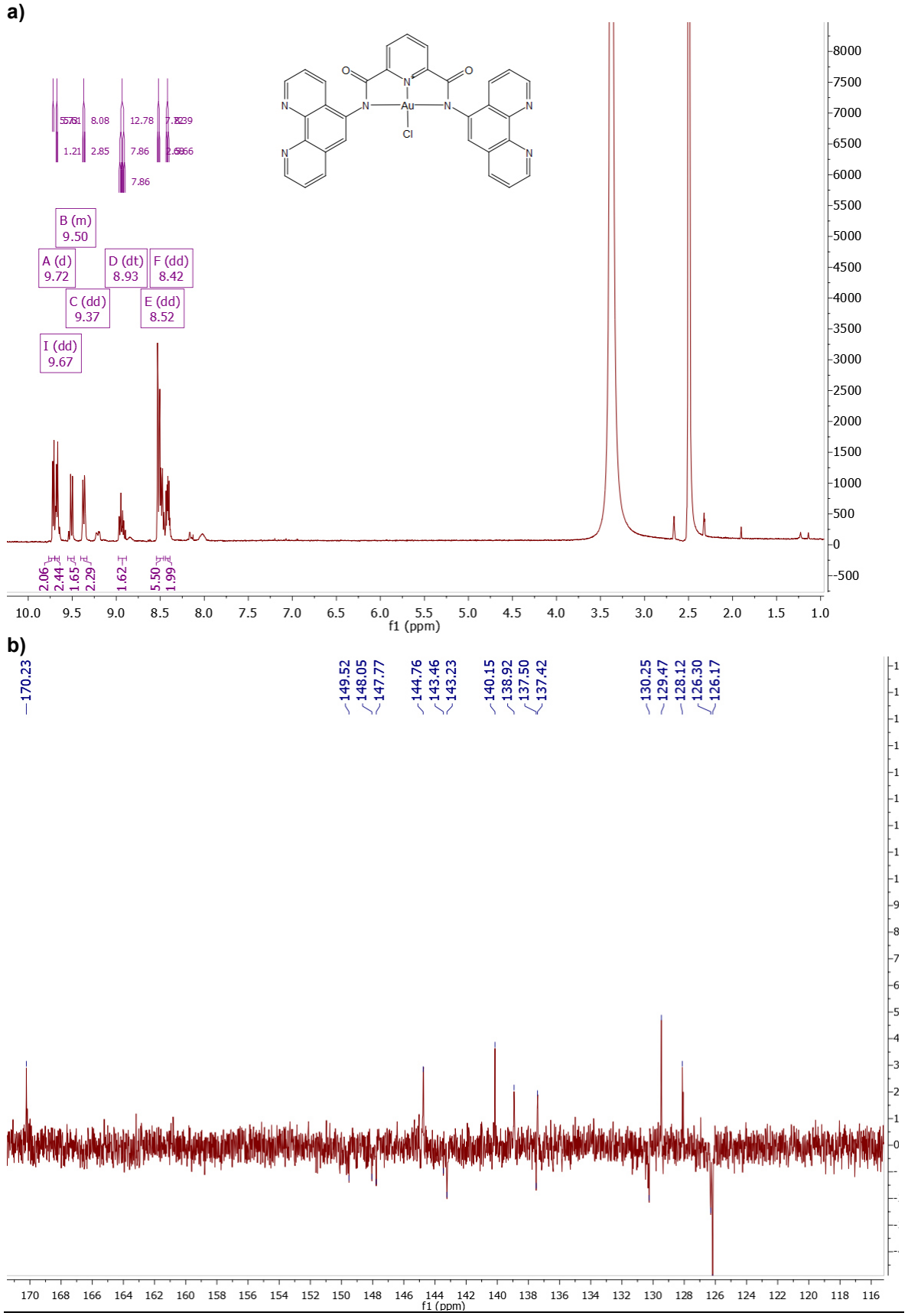


Figure S 18. ^{1}H **(a)** and ^{13}C **(b)** NMR spectra of **2f** in DMSO-d_6.

S1.3. UV-vis spectroscopy

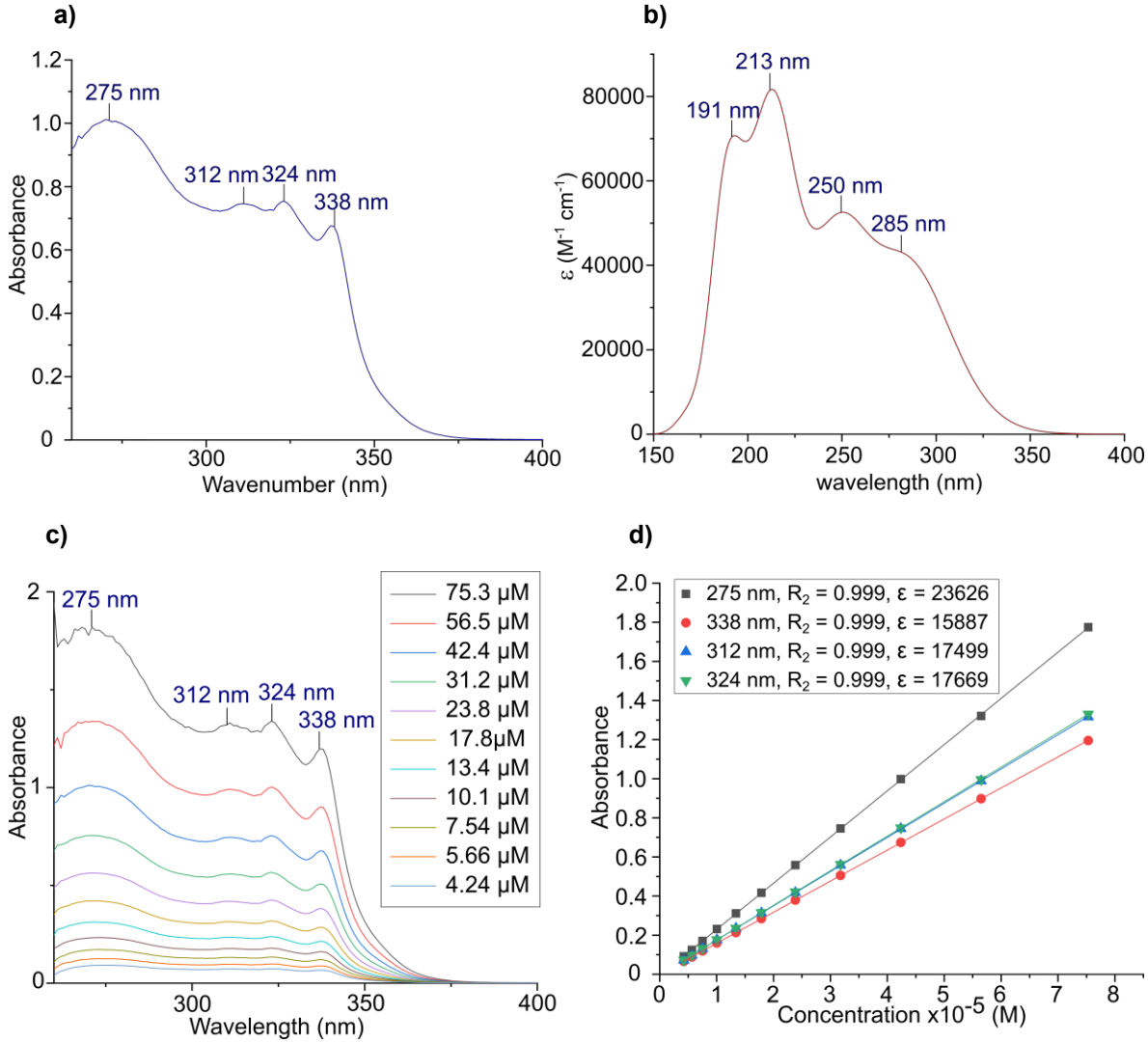


Figure S 19. **(a)** Experimental and **(b)** DFT-calculated electronic absorption spectra of **1b** in DMSO. The absorption maxima are indicated for the experimental spectrum at 275, 312, 324 and 338 nm. The absorption envelope for the DFT-calculated spectrum is plotted with a bandwidth of 2200 cm^{-1} (full width at half maximum intensity, FWHM). **(c)** Absorption spectra at a concentration range between 4 and 75 µM, to calculate the extinction coefficients at the λ_{max} in **(d)** (Beer-Lambert's Law).

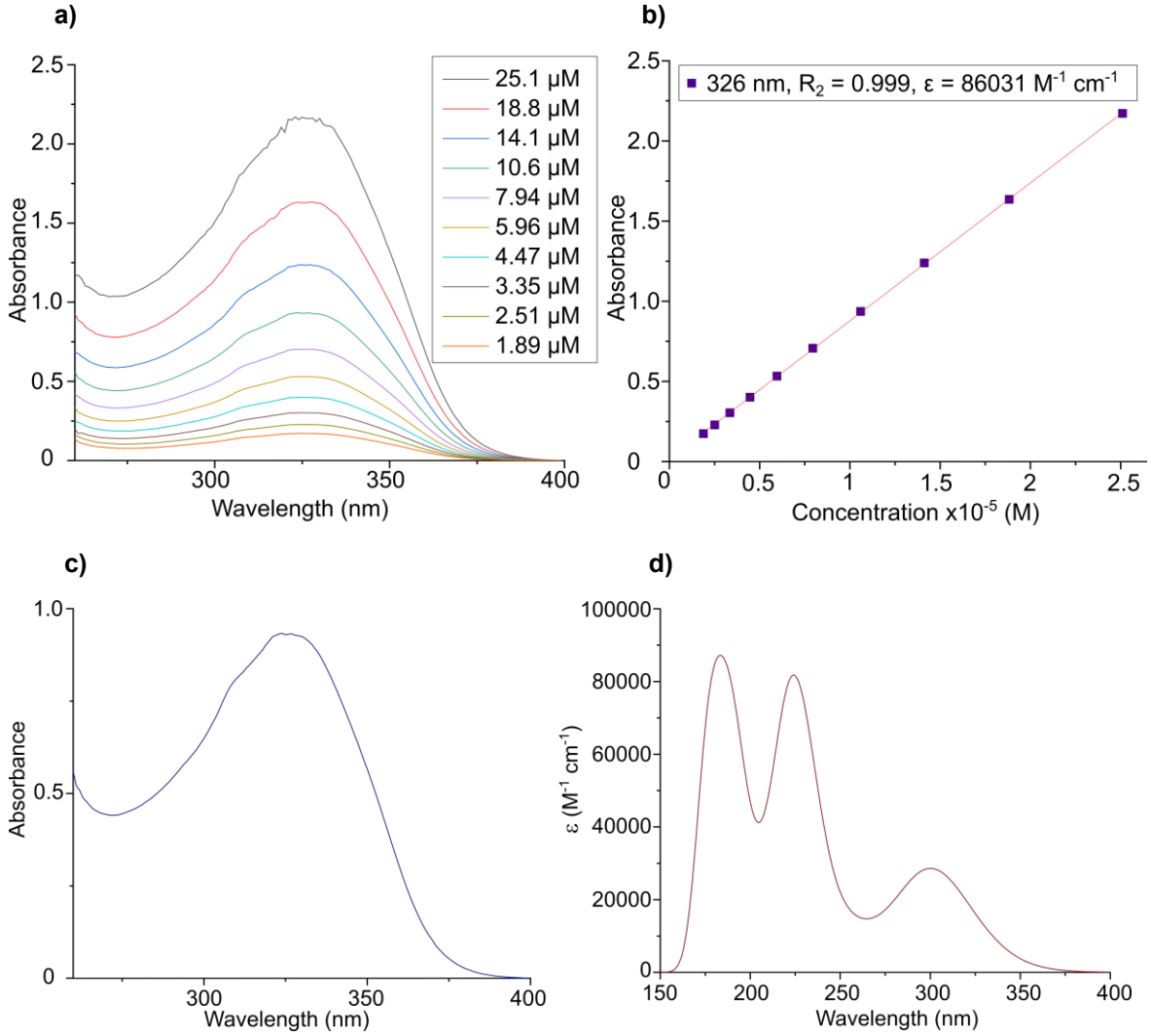


Figure S 20. (a) Experimental and **(b)** DFT-calculated electronic absorption spectra of **1c** in DMSO. The absorption maxima are indicated for the experimental spectrum at 326 nm. The absorption envelope for the DFT-calculated spectrum is plotted with a bandwidth of 2200 cm^{-1} (full width at half maximum intensity, FWHM). **(c)** Absorption spectra at a concentration range between 2 and 25 µM, to calculate the extinction coefficients at the λ_{max} in **(d)** (Beer-Lambert's Law).

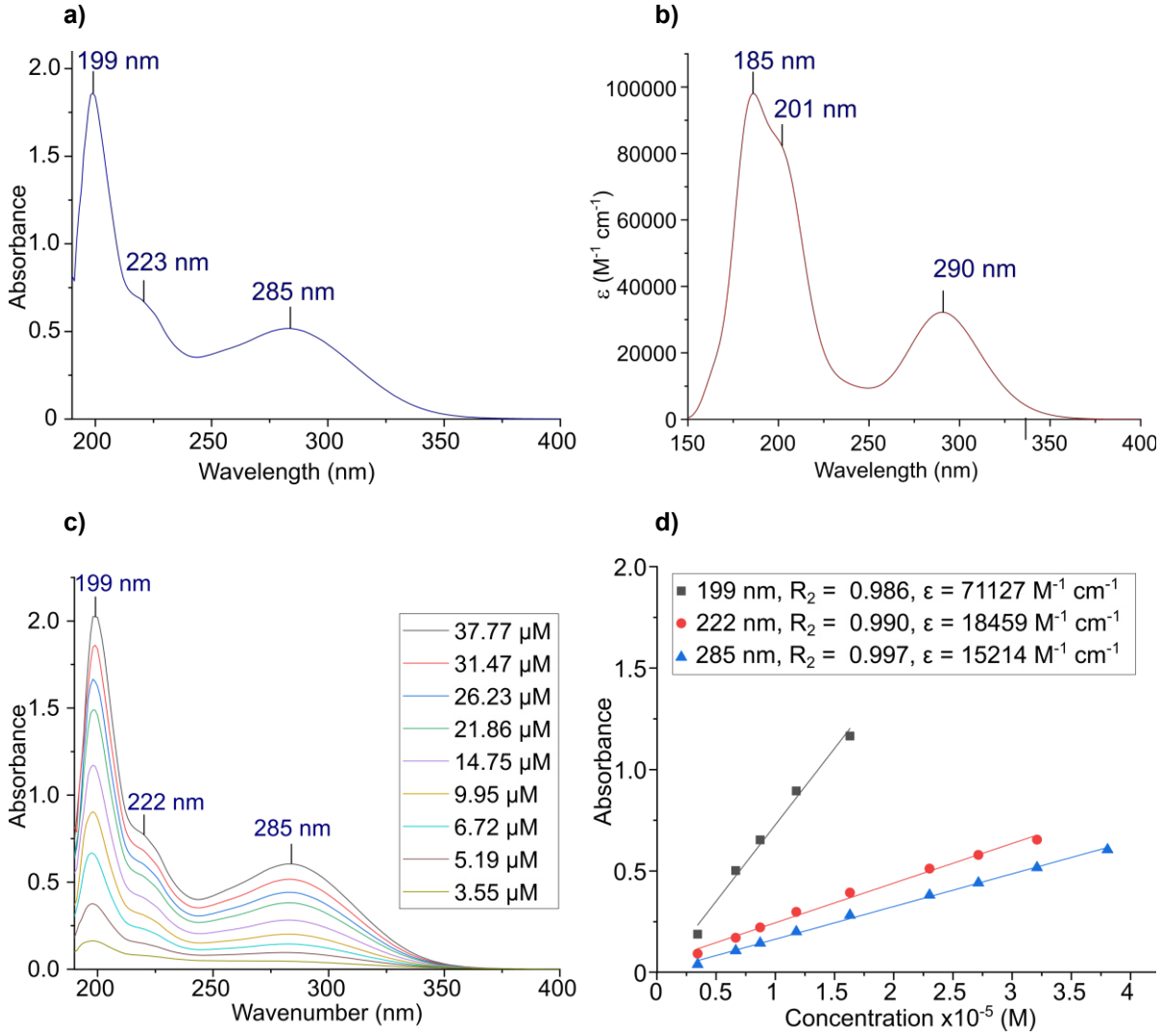


Figure S 21. (a) Experimental and **(b)** DFT-calculated electronic absorption spectra of **1d** in ACN. The absorption maxima are indicated for the experimental spectrum at 199, 223, 285 nm. The absorption envelope for the DFT-calculated spectrum is plotted with a bandwidth of 2200 cm^{-1} (full width at half maximum intensity, FWHM). **(c)** Absorption spectra at a concentration range between 4 and 38 μM, to calculate the extinction coefficients at the λ_{max} in **(d)** (Beer-Lambert's Law).

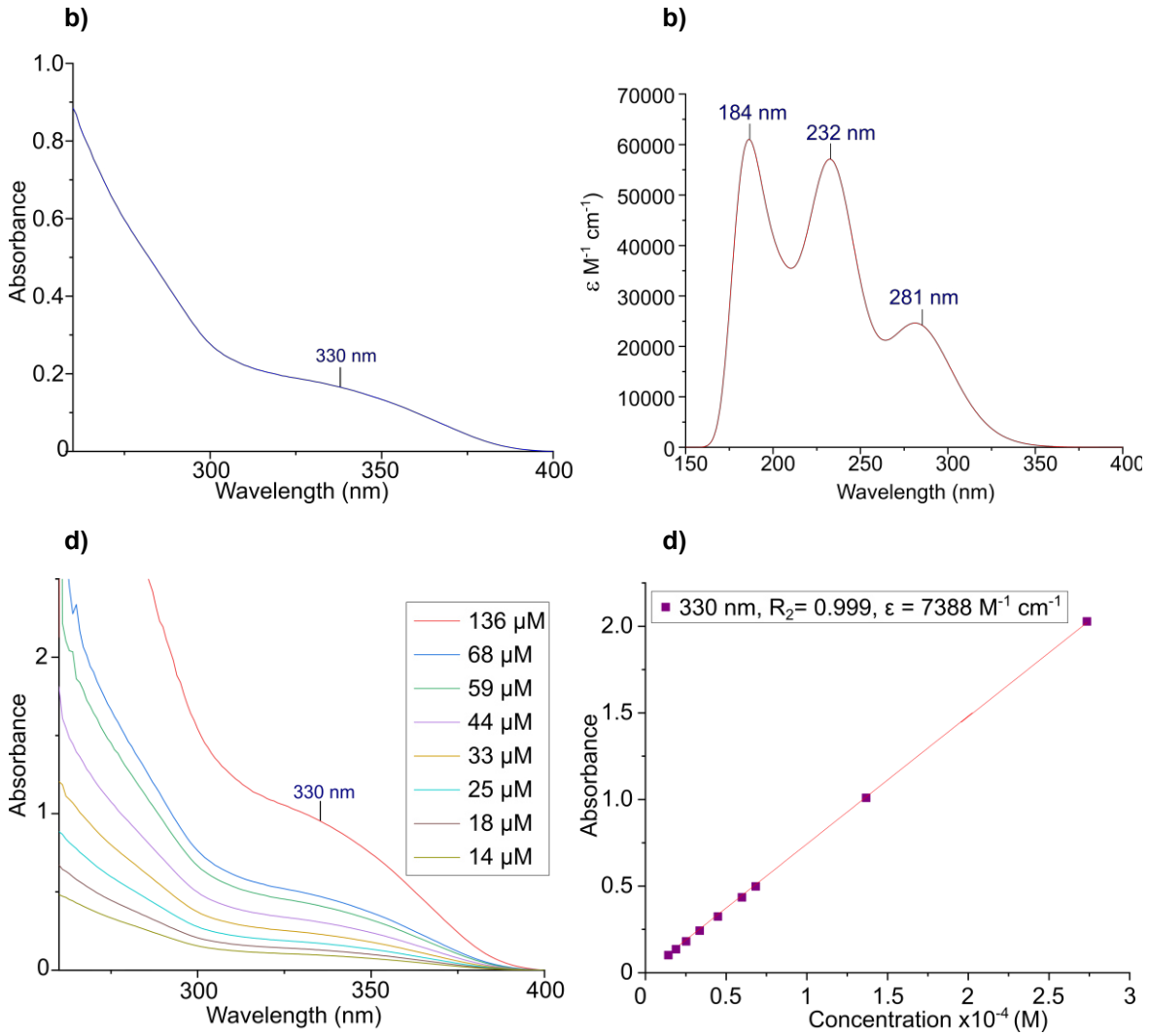


Figure S 22. (a) Experimental and **(b)** DFT-calculated electronic absorption spectra of **1e** in DMSO. The absorption maxima are indicated for the experimental spectrum at 330 nm. The absorption envelope for the DFT-calculated spectrum is plotted with a bandwidth of 2200 cm^{-1} (full width at half maximum intensity, FWHM). **(c)** Absorption spectra at a concentration range between 14 and 136 μM, to calculate the extinction coefficients at the λ_{max} in **(d)** (Beer-Lambert's Law).

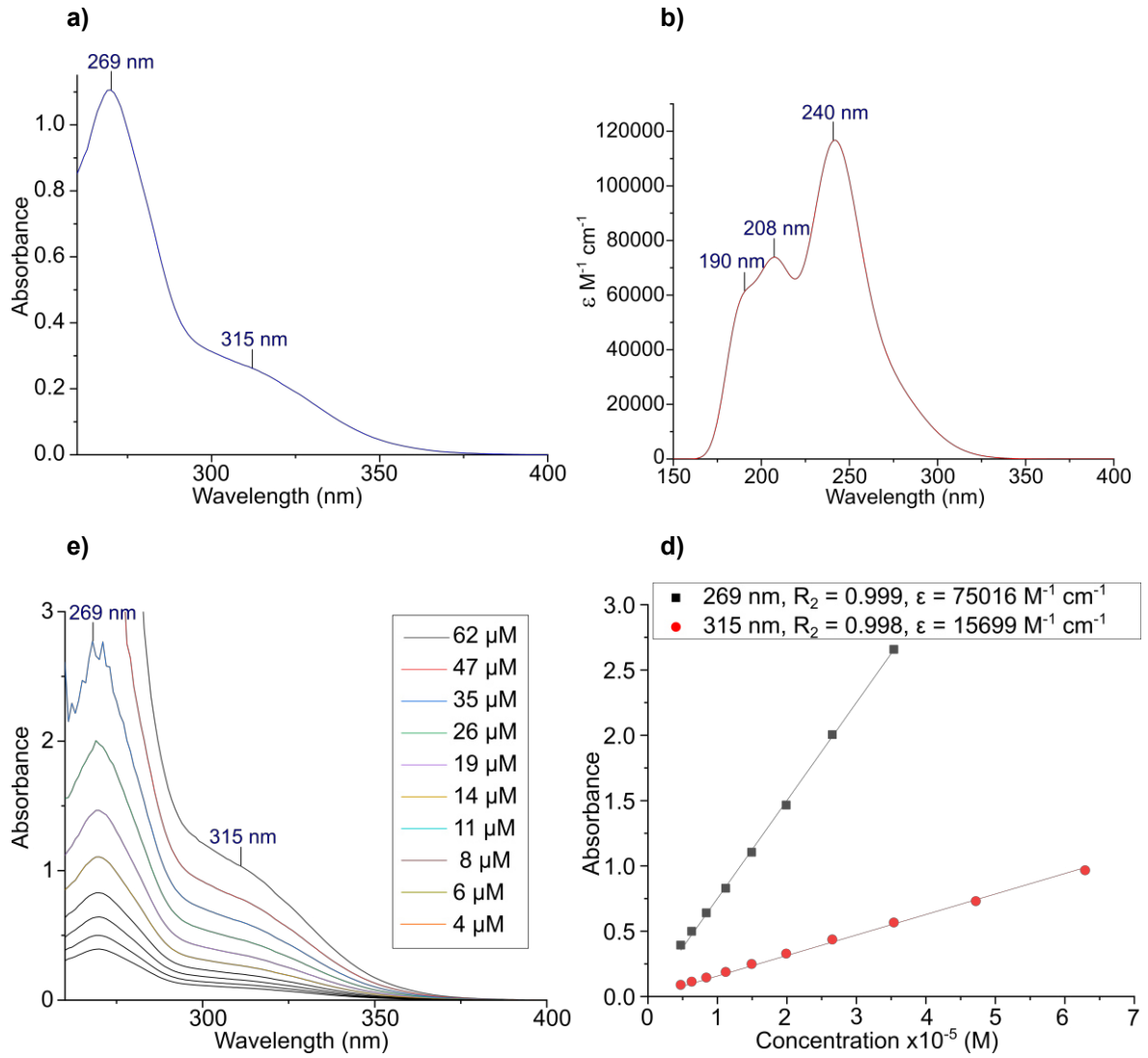


Figure S 23. (a) Experimental and **(b)** DFT-calculated electronic absorption spectra of **1f** in DMSO. The absorption maxima are indicated for the experimental spectrum at 269 and 315 nm. The absorption envelope for the DFT-calculated spectrum is plotted with a bandwidth of 2200 cm^{-1} (full width at half maximum intensity, FWHM). **(c)** Absorption spectra at a concentration range between 4 and 62 μM, to calculate the extinction coefficients at the λ_{max} in **(d)** (Beer-Lambert's Law).

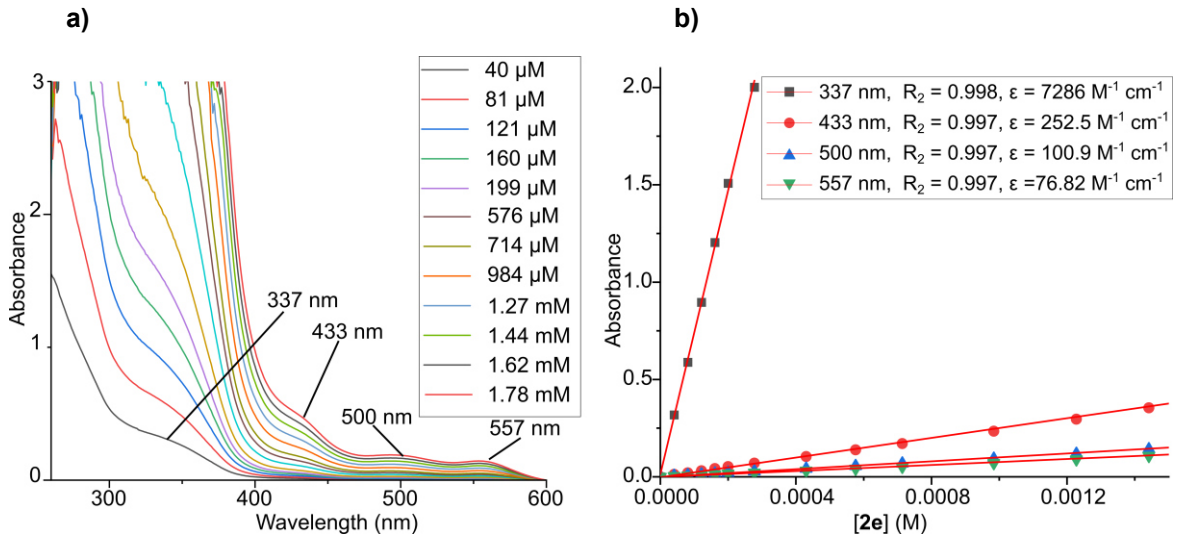


Figure S 24. (a) Experimental absorption spectra of **2e** in DMSO at a concentration range between 40 µM and 1.8 mM, to calculate the extinction coefficients at the λ_{max} (337 nm, 433 nm, 500 nm and 557 nm) in **(b)** (Beer-Lambert's Law)..

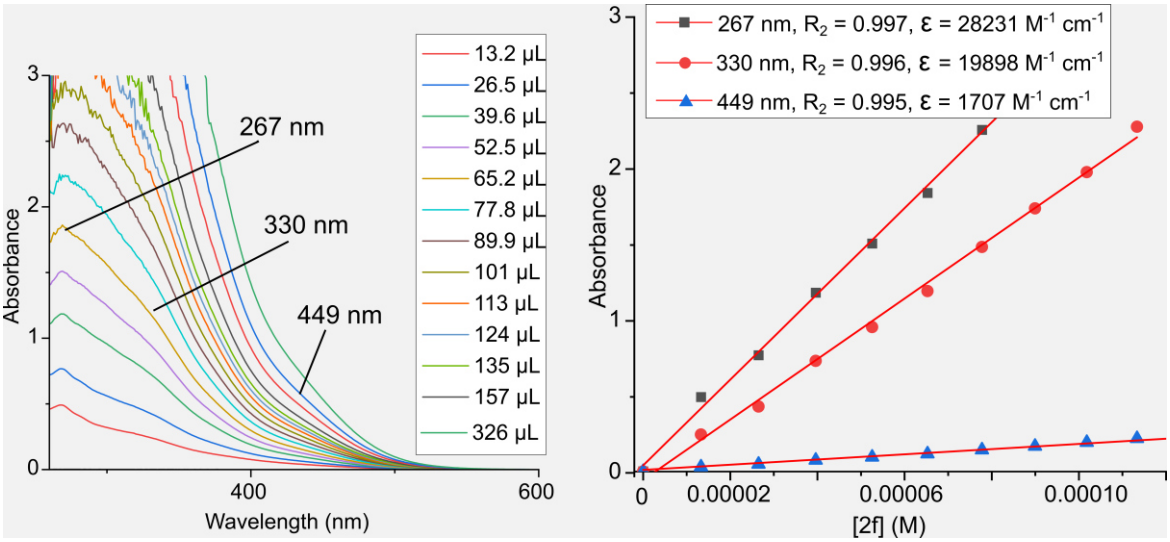


Figure S 25. (a) Experimental absorption spectra of **2f** in DMSO at a concentration range between 13 and 326 µM, to calculate the extinction coefficients at the λ_{max} (267 nm, 330 nm and 449 nm) in **(b)** (Beer-Lambert's

Table S1: Calculated energies for orbital levels involved in electron transition.

	1a	1b	1c	1d	1e	1f
HOMO-3	-0.26131	-0.25499	-0.26722	-0.25245	-0.25803	-0.25291
HOMO-2	-0.26052	-0.25494	-0.26520	-0.25198	-0.25551	-0.25287
HOMO-1	-0.22929	-0.23079	-0.22469	-0.21323	-0.23921	-0.24191
HOMO	-0.22759	-0.23079	-0.22379	-0.21190	-0.23754	-0.24092
LUMO	-0.09851	-0.09771	-0.09416	-0.09335	-0.09723	-0.09549
LUMO+1	-0.09815	-0.09720	-0.09242	-0.09136	-0.09199	-0.09421
LUMO+2	-0.07289	-0.07690	-0.07370	-0.05764	-0.07768	-0.08091
LUMO+3	-0.07080	-0.07457	-0.07275	-0.05730	-0.07368	-0.07950

Table S2: Difference in energy between different HOMO and LUMO energy levels in eV

Energy levels		Energy difference (eV)					
		1a	1b	1c	1d	1e	1f
HOMO	**LUMO**	-0.12908	-0.13308	-0.12963	-0.11855	-0.14031	-0.14543
	LUMO+1	-0.12944	-0.13359	-0.13137	-0.12054	-0.14555	-0.14671
	LUMO+2	-0.1547	-0.15389	-0.15009	-0.15426	-0.15986	-0.16001
	LUMO+3	-0.15679	-0.15622	-0.15104	-0.1546	-0.16386	-0.16142
HOMO-1	**LUMO**	-0.13078	-0.13308	-0.13053	-0.11988	-0.14198	-0.14642
	LUMO+1	-0.13114	-0.13359	-0.13227	-0.12187	-0.14722	-0.1477
	LUMO+2	-0.1564	-0.15389	-0.15099	-0.15559	-0.16153	-0.161
	LUMO+3	-0.15849	-0.15622	-0.15194	-0.15593	-0.16553	-0.16241
HOMO-2	**LUMO**	-0.16201	-0.15723	-0.17104	-0.15863	-0.15828	-0.15738
	LUMO+1	-0.16237	-0.15774	-0.17278	-0.16062	-0.16352	-0.15866
	LUMO+2	-0.18763	-0.17804	-0.1915	-0.19434	-0.17783	-0.17196
	LUMO+3	-0.18972	-0.18037	-0.19245	-0.19468	-0.18183	-0.17337
HOMO-3	**LUMO**	-0.1628	-0.15728	-0.17306	-0.1591	-0.1608	-0.15742
	LUMO+1	-0.16316	-0.15779	-0.1748	-0.16109	-0.16604	-0.1587
	LUMO+2	-0.18842	-0.17809	-0.19352	-0.19481	-0.18035	-0.172
	LUMO+3	-0.19051	-0.18042	-0.19447	-0.19515	-0.18435	-0.17341

S1.4. Mass spectroscopy

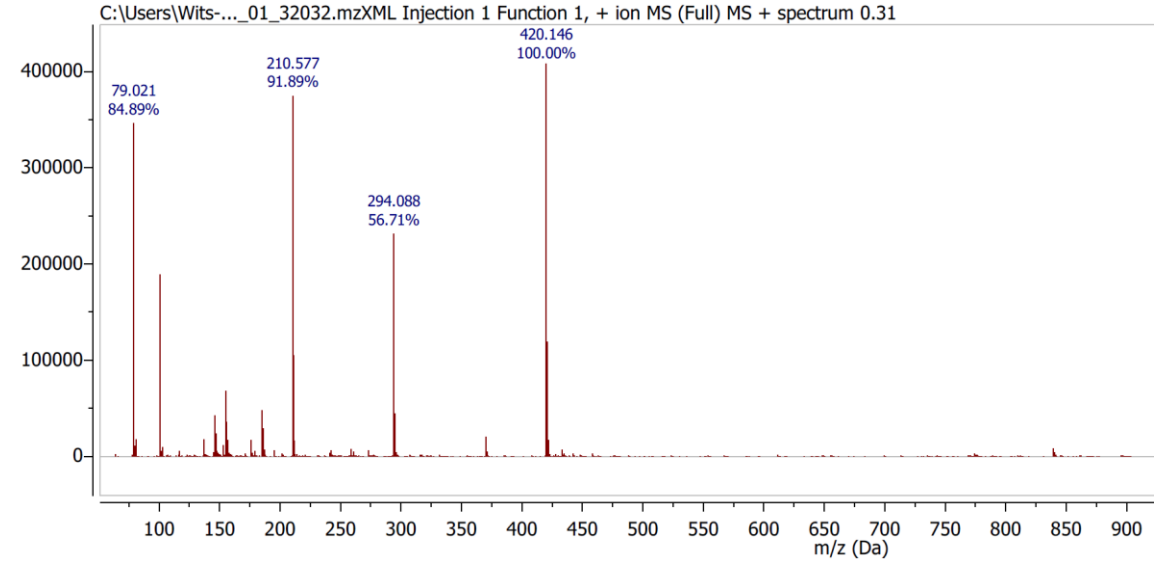


Figure S26. ESI-MS spectrum of **1a** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 420.416. The solid sample was dissolved in ACN (1 % DMSO) with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

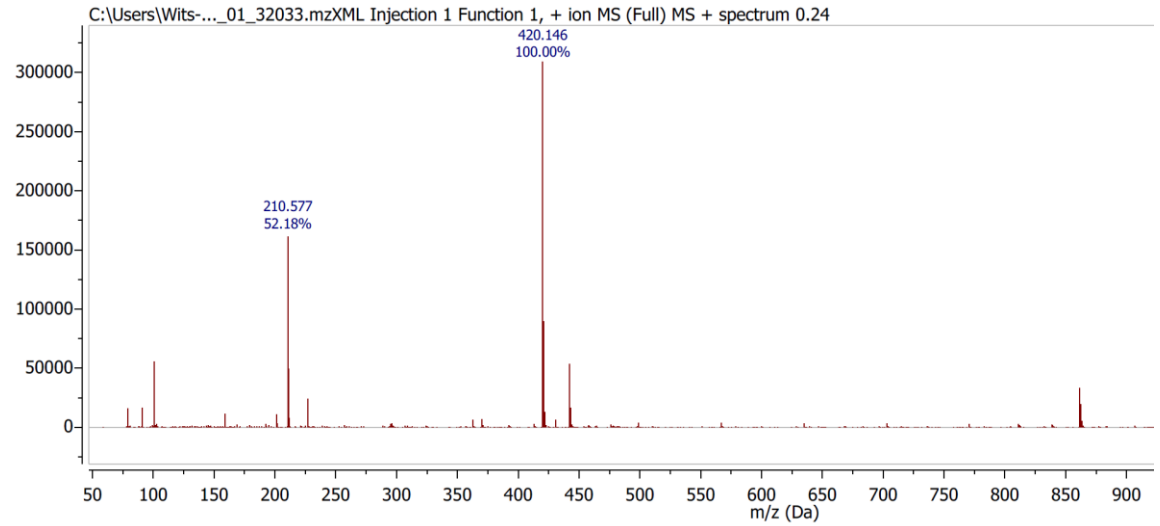


Figure S27. ESI-MS spectrum of **1b** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 420.146. The solid sample was dissolved in ACN (1 % DMSO) with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

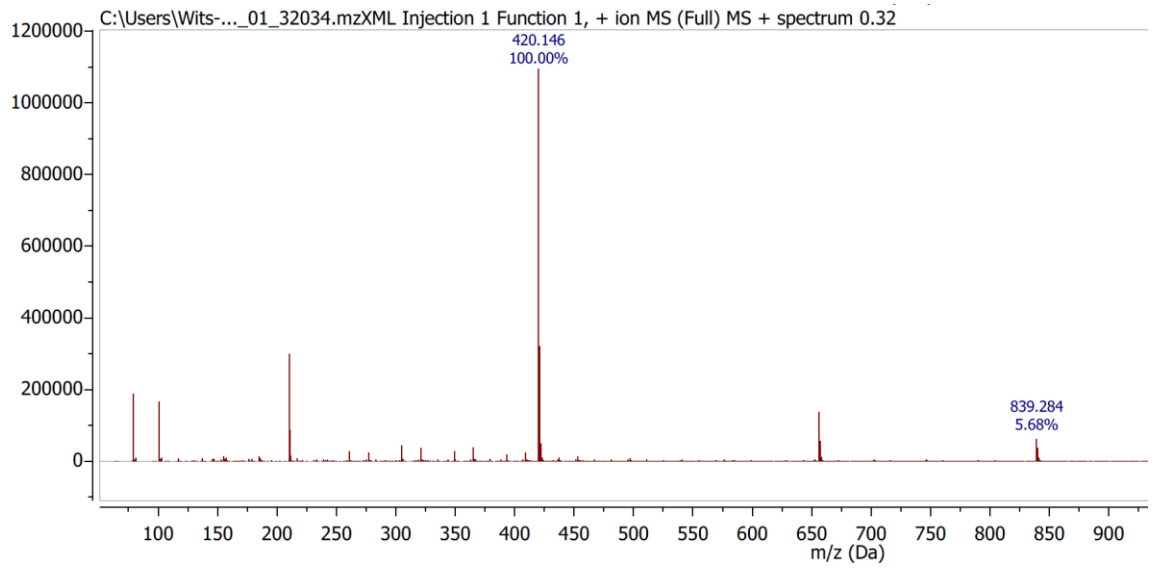


Figure S28. ESI-MS spectrum of **1c** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 420.146. The solid sample was dissolved in ACN (1 % DMSO) with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

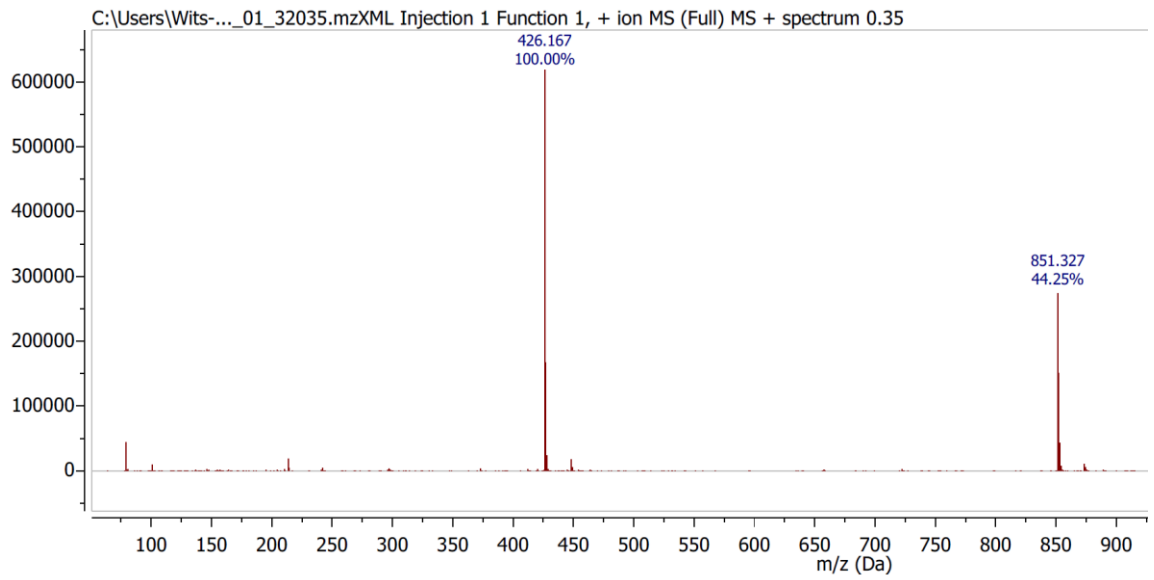


Figure S29. ESI-MS spectrum of **1d** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 420.146. The solid sample was dissolved in ACN with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

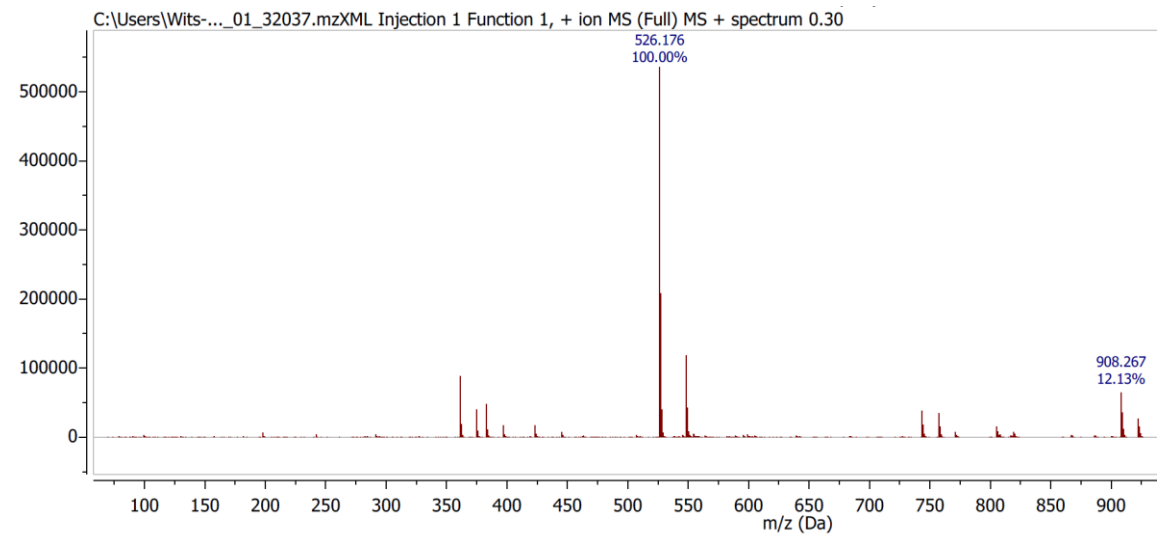


Figure S30. ESI-MS spectrum of **1e** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 426.167. The solid sample was dissolved in ACN (1 % DMSO) with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

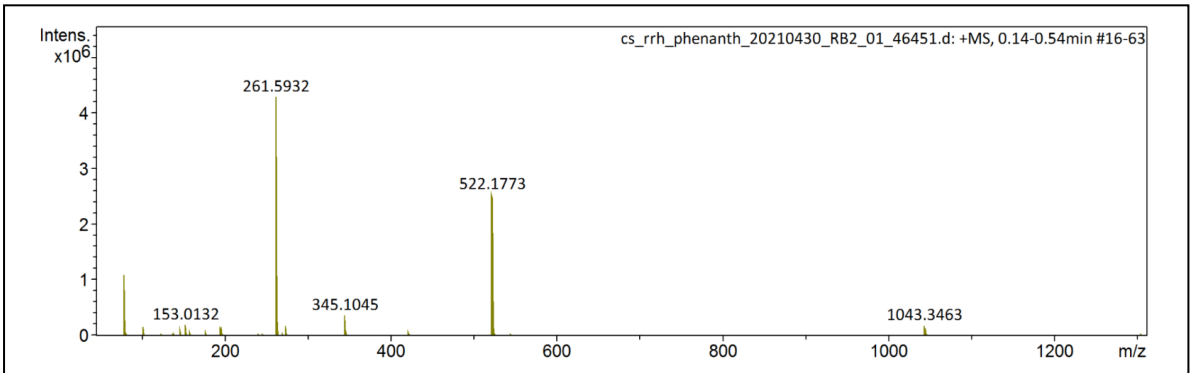


Figure S31. ESI-MS spectrum of **1f** for $C_{23}H_{18}N_5O_2$ $[M+H]^+$= 522.1773. The solid sample was dissolved in methanol with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

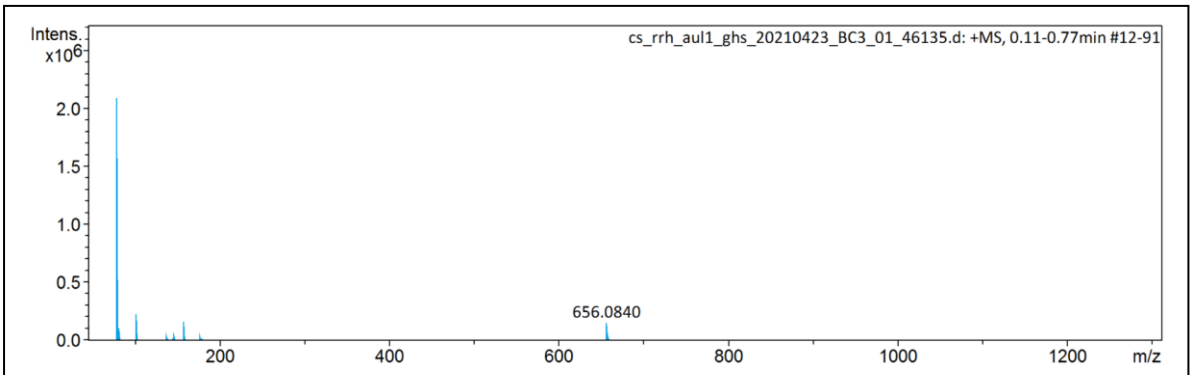


Figure S32. ESI-MS spectrum of **2d** for $C_{23}H_{18}N_7O_2$ $[M+H]^+$= 656.0840. The solid sample was dissolved in methanol with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

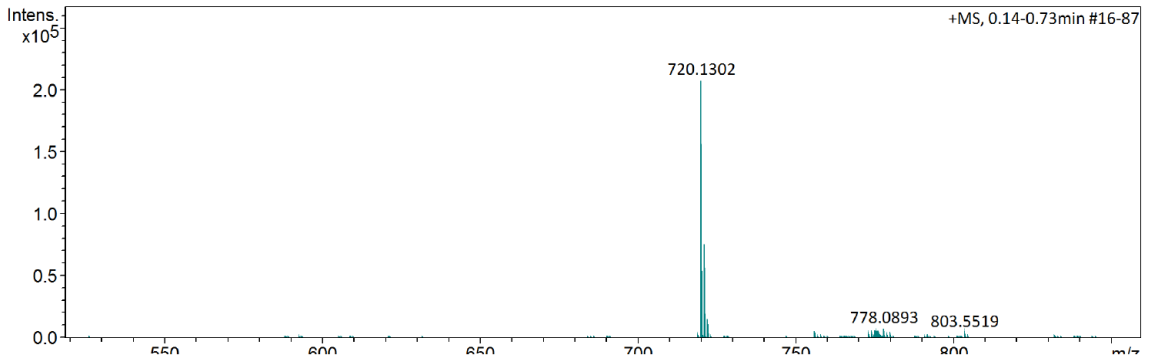


Figure S 33. ESI-MS spectrum of **2f** for $C_{33}H_{21}N_3O_4$ $[M\text{-}Cl]^+$. The solid sample was dissolved in methanol with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

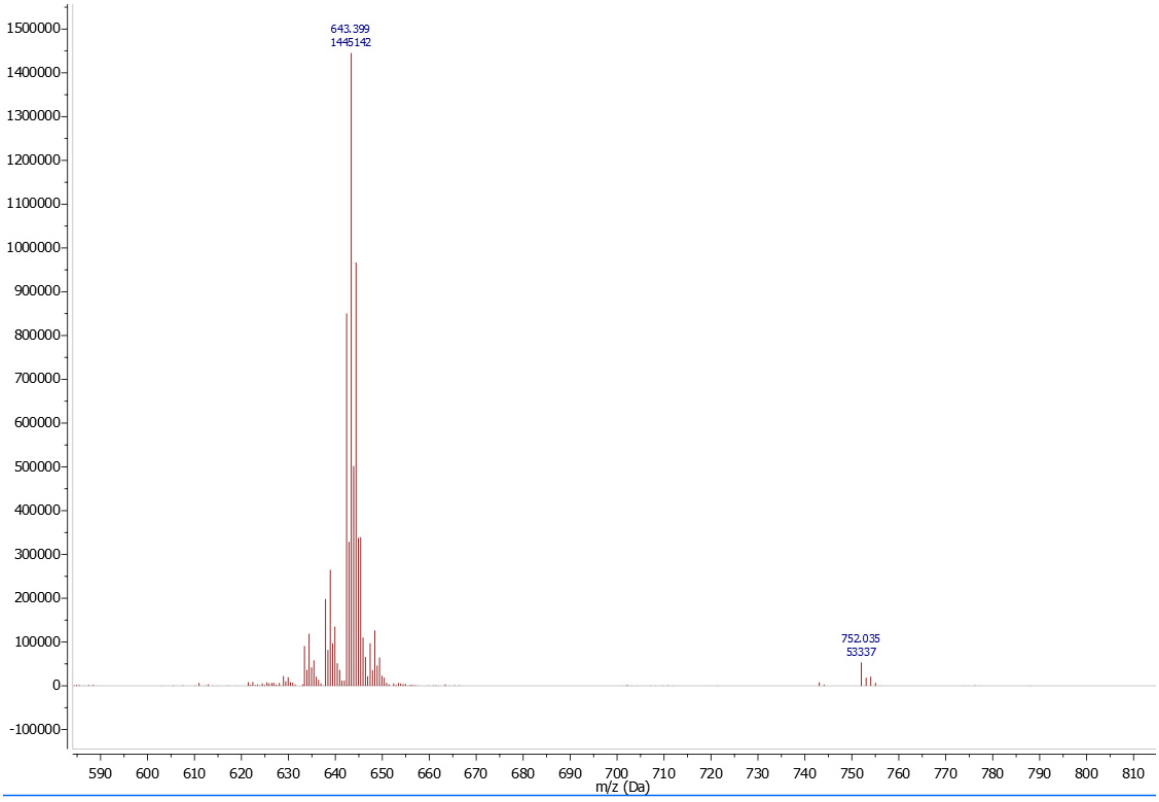


Figure S 34. ESI-MS spectrum of **2f** for $C_{31}H_{17}N_7O_2$ $[M\text{-}Cl]^+$. The solid sample was dissolved in methanol-DMSO with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode. The complex dissociated in solution.

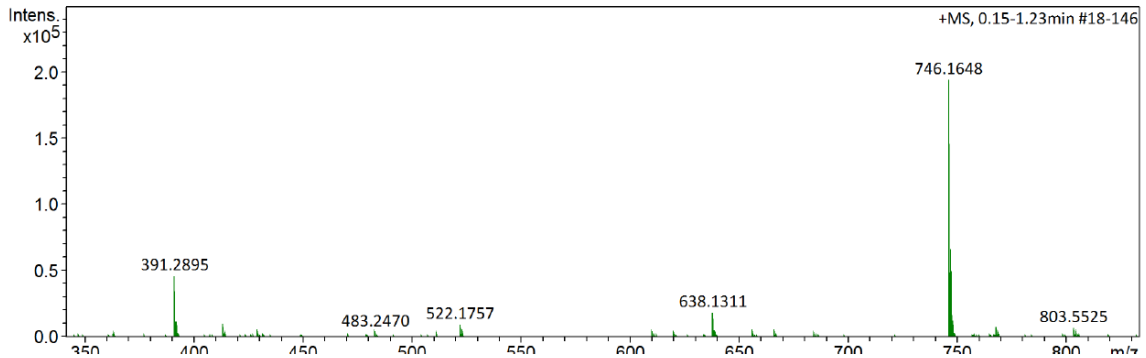


Figure S 35. ESI-MS spectrum of **2dT** for $C_{28}H_{14}N_9O_4$ $[M\text{-}Cl]^+$. The solid sample was dissolved in methanol with 0.1% formic acid (v/v) and the spectrum was recorded in positive ESI mode.

S2. Xray crystallographic data

S2.1. 1a

Crystal data and structure refinement for mo_18OV_RR_Sample_1_0m.

Identification code	mo_18OV_RR_Sample_1_0m
Empirical formula	$C_{25}H_{17}N_5O_2$
Formula weight	419.43
Temperature/K	173.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.7392(4)
b/Å	14.6766(8)
c/Å	15.2758(8)
α/°	90
β/°	102.656(2)
γ/°	90
Volume/Å^3	1911.70(17)
Z	4
ρ_{calc}g/cm^3	1.457
μ/mm^{-1}	0.096
F(000)	872.0
Crystal size/mm^3	0.4 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.526 to 66.466
Index ranges	-13 ≤ h ≤ 13, -22 ≤ k ≤ 22, -23 ≤ l ≤ 23
Reflections collected	38057
Independent reflections	7299 [R_{int} = 0.0277, R_{sigma} = 0.0189]
Data/restraints/parameters	7299/0/297
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1152
Final R indexes [all data]	R_1 = 0.0493, wR_2 = 0.1246
Largest diff. peak/hole / e Å^{-3}	0.45/-0.26

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for mo_18OV_RR_Sample_1_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor

Atom	*x*	*y*	*z*	U(eq)
O1	4583.2(7)	5203.8(5)	6499.7(4)	21.63(13)
O2	10872.7(8)	3485.8(5)	4888.9(4)	24.26(14)
N2	7638.8(7)	4567.1(4)	5463.4(4)	13.82(12)
N1	5900.0(8)	6089.3(4)	5670.6(4)	15.14(12)
N3	8881.3(8)	4275.0(5)	3970.2(4)	15.04(12)
N4	3320.9(10)	7902.2(6)	6244.8(5)	25.19(16)
N5	11133.9(10)	3581.5(5)	2293.8(5)	24.02(15)
C1	5662.7(9)	5319.0(5)	6113.8(5)	14.63(13)
C6	8690.7(9)	3898.2(5)	5485.9(5)	14.40(13)
C19	9028.5(9)	4982.4(5)	2531.0(5)	13.95(13)
C2	6845.0(9)	4575.4(5)	6121.3(5)	13.92(13)
C7	9593.5(9)	3867.7(5)	4754.3(5)	15.58(13)
C10	5050.0(9)	7531.4(5)	4917.2(5)	14.02(13)

C9	5015.9(9)	6900.4(5)	5625.7(5)	14.08(13)
C11	5885.7(9)	7392.4(5)	4232.1(5)	16.30(13)
C3	7045.8(10)	3928.7(5)	6805.9(5)	17.43(14)
C18	9473.1(9)	4277.3(5)	3180.7(5)	13.86(13)
C24	9725.7(9)	4959.4(6)	1773.9(5)	17.10(14)
C20	7959.3(9)	5694.2(5)	2590.5(5)	17.83(14)
C17	10470.1(10)	3598.9(5)	3018.0(5)	18.86(15)
C5	8998.2(10)	3231.0(5)	6153.0(5)	18.36(14)
C22	8304.8(11)	6315.8(6)	1173.8(6)	23.02(16)
C15	4204.5(10)	8358.0(6)	4920.9(5)	19.07(15)
C23	9357.2(11)	5643.2(6)	1105.6(6)	21.87(16)
C8	4154.2(10)	7116.5(6)	6254.9(5)	19.00(15)
C21	7601.0(11)	6336.9(6)	1920.3(6)	22.03(16)
C12	5899.1(11)	8054.8(6)	3599.5(6)	21.37(16)
C4	8151.9(10)	3246.7(6)	6822.3(5)	19.86(15)
C16	3364.3(12)	8492.7(6)	5602.1(7)	25.34(18)
C25	10783.1(11)	4246.4(6)	1707.1(6)	23.17(16)
C13	5067.3(12)	8882.1(6)	3609.3(6)	25.96(18)
C14	4229.3(12)	9026.5(6)	4254.9(6)	25.16(17)

Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_18OV_RR_Sample_1_0m. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	18.6(3)	25.1(3)	24.5(3)	5.0(2)	12.0(2)	1.0(2)
O2	17.3(3)	33.3(3)	23.0(3)	6.2(2)	6.2(2)	9.8(2)
N2	12.6(3)	15.8(3)	13.4(2)	1.7(2)	3.6(2)	0.0(2)
N1	13.9(3)	16.5(3)	16.5(3)	2.1(2)	6.4(2)	1.4(2)
N3	13.3(3)	17.6(3)	15.4(3)	2.6(2)	5.7(2)	3.1(2)
N4	28.0(4)	26.5(4)	24.9(3)	-4.2(3)	14.1(3)	5.0(3)
N5	27.7(4)	25.0(3)	22.4(3)	-1.6(3)	12.0(3)	8.1(3)
C1	13.9(3)	17.4(3)	12.9(3)	0.8(2)	3.6(2)	-0.4(2)
C6	13.4(3)	15.5(3)	14.3(3)	1.7(2)	3.1(2)	-0.2(2)
C19	13.2(3)	14.4(3)	14.6(3)	-0.3(2)	3.9(2)	-0.7(2)
C2	13.2(3)	15.6(3)	13.0(3)	1.4(2)	3.1(2)	-0.9(2)
C7	14.4(3)	16.8(3)	16.1(3)	2.0(2)	4.4(2)	1.1(2)
C10	12.8(3)	16.1(3)	13.3(3)	-0.8(2)	3.1(2)	0.2(2)
C9	12.7(3)	16.1(3)	13.8(3)	-1.6(2)	3.8(2)	0.3(2)
C11	15.0(3)	19.5(3)	15.2(3)	0.0(2)	5.1(2)	0.7(2)
C3	18.7(3)	20.0(3)	14.3(3)	3.9(2)	5.1(2)	-1.1(3)
C18	13.1(3)	14.7(3)	14.6(3)	-0.5(2)	5.1(2)	0.0(2)
C24	17.2(3)	19.8(3)	15.3(3)	-0.2(2)	5.8(2)	-0.4(3)
C20	17.2(3)	17.5(3)	19.8(3)	1.6(2)	6.2(3)	3.0(3)
C17	21.8(4)	16.7(3)	19.5(3)	-0.3(2)	7.6(3)	4.2(3)
C5	18.6(3)	17.2(3)	19.0(3)	4.6(3)	3.6(3)	2.2(3)
C22	25.6(4)	21.7(4)	20.7(4)	5.8(3)	2.9(3)	-0.6(3)
C15	19.2(4)	18.8(3)	19.5(3)	0.0(3)	4.7(3)	4.2(3)
C23	23.8(4)	26.1(4)	16.8(3)	3.2(3)	6.9(3)	-1.6(3)
C8	20.4(4)	22.0(3)	16.6(3)	-2.4(3)	8.5(3)	0.5(3)
C21	22.0(4)	19.3(3)	24.4(4)	3.6(3)	4.4(3)	4.4(3)
C12	22.8(4)	24.9(4)	17.7(3)	2.5(3)	7.3(3)	-0.8(3)

C4	22.0(4)	19.6(3)	18.0(3)	7.1(3)	4.4(3)	0.7(3)
C16	27.1(4)	23.6(4)	27.9(4)	-2.1(3)	11.7(3)	8.8(3)
C25	25.5(4)	27.0(4)	20.2(3)	-0.9(3)	11.9(3)	5.0(3)
C13	33.0(5)	23.0(4)	22.1(4)	6.4(3)	6.6(3)	1.6(3)
C14	29.2(4)	20.2(4)	25.7(4)	3.8(3)	5.4(3)	7.4(3)

Bond Lengths for mo_18OV_RR_Sample_1_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.2287(9)	C2	C3	1.3946(10)
O2	C7	1.2269(10)	C10	C9	1.4297(10)
N2	C6	1.3402(9)	C10	C11	1.4160(10)
N2	C2	1.3405(9)	C10	C15	1.4211(11)
N1	C1	1.3568(10)	C9	C8	1.3815(10)
N1	C9	1.4127(10)	C11	C12	1.3726(11)
N3	C7	1.3612(10)	C3	C4	1.3878(12)
N3	C18	1.4125(9)	C18	C17	1.3810(10)
N4	C8	1.3622(11)	C24	C23	1.4173(11)
N4	C16	1.3162(13)	C24	C25	1.4145(12)
N5	C17	1.3573(11)	C20	C21	1.3768(11)
N5	C25	1.3150(12)	C5	C4	1.3871(11)
C1	C2	1.5013(11)	C22	C23	1.3686(13)
C6	C7	1.5033(10)	C22	C21	1.4095(13)
C6	C5	1.3963(10)	C15	C16	1.4128(12)
C19	C18	1.4276(10)	C15	C14	1.4170(12)
C19	C24	1.4208(10)	C12	C13	1.4169(13)
C19	C20	1.4177(10)	C13	C14	1.3676(13)

Table 5 Bond Angles for mo_18OV_RR_Sample_1_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	N2	C2	116.88(6)	C8	C9	C10	118.88(7)
C1	N1	C9	125.77(6)	C12	C11	C10	120.24(7)
C7	N3	C18	124.75(6)	C4	C3	C2	118.49(7)
C16	N4	C8	117.59(7)	N3	C18	C19	120.03(6)
C25	N5	C17	117.65(7)	C17	C18	N3	121.02(7)
O1	C1	N1	124.85(7)	C17	C18	C19	118.94(7)
O1	C1	C2	119.72(7)	C23	C24	C19	119.94(7)
N1	C1	C2	115.43(6)	C25	C24	C19	118.67(7)
N2	C6	C7	118.14(6)	C25	C24	C23	121.39(7)
N2	C6	C5	123.62(7)	C21	C20	C19	120.19(7)
C5	C6	C7	118.25(7)	N5	C17	C18	124.01(7)
C24	C19	C18	116.66(7)	C4	C5	C6	118.54(7)
C20	C19	C18	124.91(7)	C23	C22	C21	119.80(8)
C20	C19	C24	118.42(7)	C16	C15	C10	118.50(7)
N2	C2	C1	117.98(6)	C16	C15	C14	121.61(8)
N2	C2	C3	123.73(7)	C14	C15	C10	119.90(8)
C3	C2	C1	118.28(7)	C22	C23	C24	120.42(8)
O2	C7	N3	124.91(7)	N4	C8	C9	123.92(8)
O2	C7	C6	119.76(7)	C20	C21	C22	121.20(8)
N3	C7	C6	115.33(6)	C11	C12	C13	121.06(8)
C11	C10	C9	124.46(7)	C5	C4	C3	118.72(7)
C11	C10	C15	118.61(7)	N4	C16	C15	124.18(8)
C15	C10	C9	116.92(7)	N5	C25	C24	123.94(8)
N1	C9	C10	118.73(6)	C14	C13	C12	119.84(8)
C8	C9	N1	122.37(7)	C13	C14	C15	120.35(8)

Table 6 Torsion Angles for mo_18OV_RR_Sample_1_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	N2	156.57(7)	C9	C10	C15	C14	177.99(8)
O1	C1	C2	C3	-22.86(11)	C11	C10	C9	N1	1.69(11)
N2	C6	C7	O2	156.02(8)	C11	C10	C9	C8	179.99(7)
N2	C6	C7	N3	-24.59(10)	C11	C10	C15	C16	179.63(8)
N2	C6	C5	C4	1.27(12)	C11	C10	C15	C14	-0.88(12)
N2	C2	C3	C4	1.42(12)	C11	C12	C13	C14	-0.28(14)
N1	C1	C2	N2	-23.96(10)	C18	N3	C7	O2	3.44(13)
N1	C1	C2	C3	156.60(7)	C18	N3	C7	C6	-175.92(7)
N1	C9	C8	N4	178.30(8)	C18	C19	C24	C23	-179.21(7)
N3	C18	C17	N5	-177.01(8)	C18	C19	C24	C25	0.72(11)
C1	N1	C9	C10	-159.70(7)	C18	C19	C20	C21	-179.42(8)
C1	N1	C9	C8	22.07(12)	C24	C19	C18	N3	177.36(7)
C1	C2	C3	C4	-179.18(7)	C24	C19	C18	C17	-3.34(11)
C6	N2	C2	C1	179.83(6)	C24	C19	C20	C21	0.78(12)
C6	N2	C2	C3	-0.77(11)	C20	C19	C18	N3	-2.44(11)
C6	C5	C4	C3	-0.56(12)	C20	C19	C18	C17	176.86(8)
C19	C18	C17	N5	3.70(13)	C20	C19	C24	C23	0.60(11)
C19	C24	C23	C22	-1.49(13)	C20	C19	C24	C25	-179.47(7)
C19	C24	C25	N5	2.00(14)	C17	N5	C25	C24	-1.89(14)
C19	C20	C21	C22	-1.32(13)	C5	C6	C7	O2	-23.71(11)
C2	N2	C6	C7	179.67(6)	C5	C6	C7	N3	155.68(7)
C2	N2	C6	C5	-0.61(11)	C15	C10	C9	N1	-177.11(7)
C2	C3	C4	C5	-0.68(12)	C15	C10	C9	C8	1.19(11)
C7	N3	C18	C19	-155.48(7)	C15	C10	C11	C12	1.39(11)
C7	N3	C18	C17	25.23(12)	C23	C24	C25	N5	-178.07(9)
C7	C6	C5	C4	-179.01(7)	C23	C22	C21	C20	0.43(14)
C10	C9	C8	N4	0.06(12)	C8	N4	C16	C15	0.67(15)
C10	C11	C12	C13	-0.83(13)	C21	C22	C23	C24	0.98(13)

C10 C15 C16 N4	0.60(14)	C12 C13 C14 C15	0.79(15)
C10 C15 C14 C13	-0.21(14)	C16 N4 C8 C9	-1.01(14)
C9 N1 C1 O1	4.19(13)	C16 C15 C14 C13	179.26(9)
C9 N1 C1 C2	-175.25(7)	C25 N5 C17 C18	-1.04(14)
C9 C10 C11 C12	-177.38(8)	C25 C24 C23 C22	178.58(9)
C9 C10 C15 C16	-1.50(11)	C14 C15 C16 N4	-78.88(10)

Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for mo_18OV_RR_Sample_1_0m.

Atom	x	y	z	U(eq)
H11	6439.03	6838.67	4210.18	20
H3A	6439.16	3954.34	7250.96	21
H20	7488.78	5727.76	3094.33	21
H17	10705.68	3114.7	3438.78	23
H5	9770.05	2776.26	6148.67	22
H22	8049.43	6767.1	719.44	28
H23	9843.74	5634.56	607.21	26
H8	4142.12	6691.68	6722.51	23
H21	6866.07	6803.09	1961.69	26
H12	6475.34	7957.06	3147.8	26
H4	8326.04	2799.39	7282.96	24
H16	2794.19	9044.64	5595.95	30
H25	11268.98	4247.95	1208.38	28
H13	5091.6	9335.26	3168.53	31
H14	3660.85	9577.97	4256.92	30
H3	7964(16)	4513(9)	3968(9)	26(3)
H1	6765(17)	6085(10)	5434(10)	31(3)

Experimental

Single crystals of $C_{25}H_{17}N_5O_2$ **[mo_18OV_RR_Sample_1_0m]** were **grown from XXX**. A suitable crystal was selected and **mounted in Paratone oil on a MiTeGen loop** on a **Bruker D8 Venture** diffractometer. The crystal was kept at 173.15 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [mo_18OV_RR_Sample_1_0m]

Crystal Data for $C_{25}H_{17}N_5O_2$ (M =419.43 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 8.7392(4) Å, b = 14.6766(8) Å, c = 15.2758(8) Å, β = 102.656(2)°, V = 1911.70(17) Å^3, Z = 4, T = 173.15 K, μ(MoKα) = 0.096 mm^{-1}, *Dcalc* = 1.457 g/cm^3, 38057 reflections measured (5.526° ≤ 2Θ ≤ 66.466°), 7299 unique (R_{int} = 0.0277, R_{sigma} = 0.0189) which were used in all calculations. The final R_1 was 0.0408 (I > 2σ(I)) and wR_2 was 0.1246 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C11(H11), C3(H3A), C20(H20), C17(H17), C5(H5), C22(H22), C23(H23), C8(H8),
 C21(H21), C12(H12), C4(H4), C16(H16), C25(H25), C13(H13), C14(H14)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.2. 1b
Crystal data and structure refinement for mo_21ov_RRH_3AmQuin_Pin_0m.

Identification code	mo_21ov_RRH_3AmQuin_Pin_0m
Empirical formula	$C_{27}H_{25}N_5O_4$
Formula weight	483.52
Temperature/K	153.000
Crystal system	triclinic
Space group	P-1
a/Å	7.2743(3)
b/Å	11.3528(5)
c/Å	14.9566(5)
α/°	76.6050(10)
β/°	78.8710(10)
γ/°	78.901(2)
Volume/Å3	1164.76(8)
Z	2
ρ_{calc}g/cm3	1.379
μ/mm-1	0.095
F(000)	508.000
Crystal size/mm3	0.368 × 0.237 × 0.096
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.778 to 66.428
Index ranges	-11 ≤ h ≤ 11, -17 ≤ k ≤ 17, -23 ≤ l ≤ 22
Reflections collected	85712
Independent reflections	8894 [R_{int} = 0.0459, R_{sigma} = 0.0265]
Data/restraints/parameters	8894/0/343
Goodness-of-fit on F2	1.067
Final R indexes [I>=2σ (I)]	R1 = 0.0487, wR2 = 0.1225
Final R indexes [all data]	R1 = 0.0663, wR2 = 0.1337
Largest diff. peak/hole / e Å-3	0.44/-0.34

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å$_2$×10^3) for mo_21ov_RRH_3AmQuin_Pin_0m. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

O2	7579.4(13)	11559.7(7)	4338.3(5)	24.64(17)
O1	3396.9(16)	8812.3(8)	8790.8(6)	32.7(2)
O2S	2682.3(13)	2974.2(8)	3809.4(6)	24.25(17)
O1S	2861.5(14)	5074.0(8)	4318.4(6)	29.91(19)
N3	7926.4(13)	9478.2(8)	4854.7(6)	16.48(15)
N2	5659.0(12)	9777.5(8)	6477.4(6)	15.77(15)
N1	4314.9(14)	7799.7(8)	7583.0(6)	19.23(17)
N5	10778.7(14)	7269.8(8)	3528.2(6)	20.83(17)
N4	2729.9(14)	4936.3(8)	7622.2(6)	20.72(17)
C16	12989.3(19)	8117.6(13)	1107.3(8)	29.8(3)
C17	12415(2)	9398.6(14)	929.0(8)	33.8(3)
C18	11328(2)	9965.0(12)	1612.2(8)	29.5(2)
C13	10743.2(15)	9272.8(10)	2507.0(7)	19.29(18)
C12	9623.5(15)	9826.8(9)	3231.8(7)	18.66(18)
C11	9075.2(14)	9089.8(9)	4073.6(7)	15.45(16)
C25	7249.7(14)	10656.1(9)	4940.5(7)	16.23(17)
C24	6043.1(14)	10794.4(9)	5862.2(7)	15.52(16)
C20	4644.5(14)	9916.8(9)	7305.5(7)	16.49(17)
C19	4077.4(15)	8787.6(9)	7980.3(7)	18.76(18)
C2	3701.8(14)	6670.2(9)	7990.2(7)	16.86(17)
C3	3403.6(15)	6189.7(10)	8929.7(7)	19.06(18)
C4	2741.7(15)	5046.8(9)	9233.4(7)	18.34(18)
C5	2372.0(15)	4462.2(9)	8559.5(7)	17.80(18)
C6	1569.1(16)	3367.5(10)	8851.6(8)	22.1(2)
C7	1212.5(19)	2851.2(11)	9779.9(8)	26.9(2)
C14	11299.6(15)	7984.9(10)	2677.0(7)	18.50(18)
C15	12443.6(17)	7420.8(11)	1965.5(8)	25.1(2)
C10	9710.1(15)	7808.4(9)	4181.0(7)	19.33(19)
C23	5383.0(15)	11970.0(9)	6030.1(7)	19.15(18)
C22	4355.7(16)	12100.6(10)	6897.2(8)	21.3(2)
C21	4006.0(16)	11052.4(9)	7554.4(7)	19.73(19)
C1	3374.6(16)	5985.9(9)	7364.5(7)	19.98(19)
C8	1650(2)	3405.2(11)	10450.5(8)	29.1(2)
C9	2383.0(18)	4481.4(11)	10188.1(8)	24.9(2)
C2S	1419(2)	3288.0(16)	3145.2(10)	39.1(3)
C1S	2447.1(19)	5102.3(11)	5285.8(8)	27.9(2)

Anisotropic Displacement Parameters (Å2×103) for mo_21ov_RRH_3AmQuin_Pin_0m. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Crystal	U11	U22	U33	U23	U13	U12
O2	35.1(4)	15.4(3)	19.7(3)	-0.6(3)	1.6(3)	-4.5(3)
O1	54.5(6)	22.7(4)	18.2(4)	-7.6(3)	8.9(4)	-9.8(4)
O2S	30.9(4)	20.6(4)	20.4(4)	-5.9(3)	0.2(3)	-4.1(3)
O1S	38.1(5)	21.5(4)	28.5(4)	-8.8(3)	-6.0(4)	4.4(4)
N3	19.5(4)	13.7(3)	14.6(3)	-2.0(3)	0.1(3)	-2.3(3)
N2	17.9(4)	13.8(3)	15.7(3)	-3.9(3)	-1.4(3)	-2.9(3)
N1	26.9(4)	15.7(4)	14.9(4)	-4.3(3)	2.5(3)	-7.1(3)
N5	24.1(4)	17.7(4)	19.5(4)	-4.8(3)	1.0(3)	-3.2(3)
N4	27.3(5)	17.6(4)	17.7(4)	-4.6(3)	-0.7(3)	-6.1(3)
C16	33.3(6)	38.3(7)	18.9(5)	-12.7(4)	2.6(4)	-6.5(5)
C17	41.8(7)	39.2(7)	15.7(5)	-3.2(4)	3.0(5)	-5.4(6)
C18	38.7(7)	27.5(6)	16.6(5)	0.6(4)	0.7(4)	-2.3(5)
C13	21.7(5)	20.8(4)	14.9(4)	-2.5(3)	-1.9(3)	-4.3(4)
C12	21.6(5)	16.9(4)	15.9(4)	-1.2(3)	-1.7(3)	-2.7(3)
C11	16.5(4)	14.9(4)	15.0(4)	-3.3(3)	-1.9(3)	-2.5(3)
C25	17.8(4)	14.4(4)	16.7(4)	-3.5(3)	-3.0(3)	-2.5(3)
C24	16.7(4)	13.9(4)	16.6(4)	-4.1(3)	-2.4(3)	-2.9(3)
C20	18.4(4)	14.8(4)	16.8(4)	-5.1(3)	-1.3(3)	-3.0(3)
C19	22.9(5)	15.1(4)	17.5(4)	-4.2(3)	0.0(3)	-3.1(3)
C2	19.4(4)	14.5(4)	16.2(4)	-3.1(3)	-0.5(3)	-3.7(3)
C3	22.7(5)	19.1(4)	15.9(4)	-3.2(3)	-1.9(3)	-6.1(4)
C4	19.6(4)	17.5(4)	17.1(4)	-1.8(3)	-2.3(3)	-3.4(3)
C5	19.1(4)	14.8(4)	18.4(4)	-3.4(3)	-0.6(3)	-2.3(3)
C6	24.6(5)	16.5(4)	24.5(5)	-4.8(4)	0.1(4)	-4.7(4)
C7	33.1(6)	18.2(5)	26.8(5)	0.7(4)	-0.1(4)	-8.3(4)
C14	19.6(4)	20.3(4)	16.3(4)	-5.1(3)	-1.8(3)	-4.1(3)
C15	27.9(5)	27.3(5)	21.6(5)	-11.3(4)	0.1(4)	-4.0(4)
C10	22.7(5)	15.0(4)	18.2(4)	-2.1(3)	0.4(3)	-2.9(3)
C23	22.3(5)	13.5(4)	21.6(4)	-4.1(3)	-1.6(4)	-3.8(3)
C22	25.4(5)	14.6(4)	24.3(5)	-8.1(3)	-0.8(4)	-2.4(4)
C21	23.4(5)	17.1(4)	19.6(4)	-8.2(3)	0.3(4)	-3.5(4)
C1	27.2(5)	17.3(4)	15.7(4)	-4.0(3)	-1.2(4)	-5.5(4)
C8	39.1(7)	24.9(5)	20.7(5)	4.3(4)	-3.3(4)	-10.5(5)
C9	31.9(6)	24.9(5)	17.7(4)	0.1(4)	-4.4(4)	-8.7(4)
C2S	32.3(7)	51.6(9)	34.3(7)	-13.6(6)	-7.1(5)	-0.7(6)
C1S	32.4(6)	23.1(5)	26.9(5)	-4.4(4)	-2.2(4)	-4.2(4)

Crystal data and structure refinement for mo_21ov_RRH_3AmQuin_Pin_0m.

	Atom	Length/Å	Atom	Atom	Length/Å
O2	C25	1.2266(12)	C13	C14	1.4163(15)
O1	C19	1.2223(13)	C12	C11	1.3751(13)
O2S	C2S	1.4218(17)	C11	C10	1.4202(14)
O1S	C1S	1.4264(15)	C25	C24	1.5084(14)
N3	C11	1.4062(12)	C24	C23	1.3917(14)
N3	C25	1.3596(13)	C20	C19	1.5085(14)
N2	C24	1.3380(12)	C20	C21	1.3935(14)
N2	C20	1.3403(12)	C2	C3	1.3755(13)
N1	C19	1.3548(13)	C2	C1	1.4248(14)
N1	C2	1.4027(13)	C3	C4	1.4158(14)
N5	C14	1.3701(13)	C4	C5	1.4184(14)
N5	C10	1.3161(13)	C4	C9	1.4195(14)
N4	C5	1.3735(13)	C5	C6	1.4163(14)
N4	C1	1.3119(13)	C6	C7	1.3715(16)
C16	C17	1.411(2)	C7	C8	1.4125(18)
C16	C15	1.3728(17)	C14	C15	1.4155(15)
C17	C18	1.3708(18)	C23	C22	1.3910(15)
C18	C13	1.4182(15)	C22	C21	1.3874(15)
C13	C12	1.4185(14)	C8	C9	1.3708(16)

Bond Angles for mo_21ov_RRH_3AmQuin_Pin_0m.

C25	N3	C11	126.51(8)	O1	C19	C20	121.58(9)
C24	N2	C20	117.33(8)	N1	C19	C20	113.30(9)
C19	N1	C2	126.96(9)	N1	C2	C1	116.09(9)
C10	N5	C14	118.21(9)	C3	C2	N1	125.18(9)
C1	N4	C5	117.46(9)	C3	C2	C1	118.74(9)
C15	C16	C17	120.26(11)	C2	C3	C4	118.39(9)
C18	C17	C16	120.55(11)	C3	C4	C5	118.71(9)
C17	C18	C13	120.63(12)	C3	C4	C9	122.49(10)
C18	C13	C12	122.24(10)	C5	C4	C9	118.78(9)
C14	C13	C18	118.54(10)	N4	C5	C4	122.15(9)
C14	C13	C12	119.22(9)	N4	C5	C6	118.16(9)
C11	C12	C13	118.75(9)	C6	C5	C4	119.68(9)
N3	C11	C10	115.69(8)	C7	C6	C5	120.20(10)
C12	C11	N3	126.31(9)	C6	C7	C8	120.22(10)
C12	C11	C10	118.00(9)	N5	C14	C13	121.11(9)
O2	C25	N3	124.54(9)	N5	C14	C15	118.99(10)
O2	C25	C24	120.75(9)	C15	C14	C13	119.88(10)
N3	C25	C24	114.71(8)	C16	C15	C14	120.12(11)
N2	C24	C25	118.19(8)	N5	C10	C11	124.67(9)
N2	C24	C23	123.29(9)	C22	C23	C24	118.71(9)
C23	C24	C25	118.52(9)	C21	C22	C23	118.58(9)
N2	C20	C19	117.97(8)	C22	C21	C20	118.49(9)
N2	C20	C21	123.47(9)	N4	C1	C2	124.45(9)
C21	C20	C19	118.48(9)	C9	C8	C7	120.74(10)
O1	C19	N1	125.05(10)	C8	C9	C4	120.30(11)

Torsion Angles for mo_21ov_RRH_3AmQuin_Pin_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	C25	C24	N2	177.04(10)	C24	C23	C22	C21	-1.00(16)
O2	C25	C24	C23	-2.85(15)	C20	N2	C24	C25	177.57(9)
N3	C11	C10	N5	179.33(10)	C20	N2	C24	C23	-2.54(15)
N3	C25	C24	N2	-3.79(13)	C19	N1	C2	C3	-25.80(18)
N3	C25	C24	C23	176.32(9)	C19	N1	C2	C1	154.25(11)
N2	C24	C23	C22	3.51(16)	C19	C20	C21	C22	-173.26(10)
N2	C20	C19	O1	169.26(11)	C2	N1	C19	O1	5.53(19)
N2	C20	C19	N1	-13.78(14)	C2	N1	C19	C20	-171.31(10)
N2	C20	C21	C22	3.25(16)	C2	C3	C4	C5	-1.49(15)
N1	C2	C3	C4	178.62(10)	C2	C3	C4	C9	-179.65(10)
N1	C2	C1	N4	-177.25(11)	C3	C2	C1	N4	2.80(17)
N5	C14	C15	C16	-179.81(11)	C3	C4	C5	N4	3.51(16)
N4	C5	C6	C7	179.07(11)	C3	C4	C5	C6	-175.06(10)
C16	C17	C18	C13	-0.8(2)	C3	C4	C9	C8	176.60(12)
C17	C16	C15	C14	0.01(19)	C4	C5	C6	C7	-2.30(16)
C17	C18	C13	C12	179.83(12)	C5	N4	C1	C2	-0.88(17)
C17	C18	C13	C14	-0.24(19)	C5	C4	C9	C8	-1.55(17)
C18	C13	C12	C11	178.46(11)	C5	C6	C7	C8	-0.22(18)
C18	C13	C14	N5	179.89(11)	C6	C7	C8	C9	1.9(2)
C18	C13	C14	C15	1.12(16)	C7	C8	C9	C4	-1.0(2)
C13	C12	C11	N3	-178.08(10)	C14	N5	C10	C11	-1.08(16)
C13	C12	C11	C10	1.81(15)	C14	C13	C12	C11	-1.47(15)
C13	C14	C15	C16	-1.01(17)	C15	C16	C17	C18	0.9(2)
C12	C13	C14	N5	-0.17(16)	C10	N5	C14	C13	1.43(15)
C12	C13	C14	C15	-0.17(16)	C10	N5	C14	C15	-179.79(10)
C12	C11	C10	N5	-0.56(16)	C23	C22	C21	C20	-2.14(16)
C11	N3	C25	O2	-1.04(17)	C21	C20	C19	O1	-14.04(16)
C11	N3	C25	C24	-178.94(10)	C21	C20	C19	N1	162.92(10)
C25	N3	C11	C12	-4.50(17)	C1	N4	C5	C4	-2.30(16)
C25	N3	C11	C10	175.61(10)	C1	N4	C5	C6	176.29(10)
C25	C24	C23	C22	-176.60(9)	C1	C2	C3	C4	-1.43(15)
C24	N2	C20	C19	175.61(9)	C9	C4	C5	N4	-178.26(10)
C24	N2	C20	C21	-0.91(15)	C9	C4	C5	C6	3.17(15)

Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å ×10) for mo_21ov_RRH_3AmQuin_Pin_0m.

Atom	*x*	*y*	*z*	U(eq)
H16	13756.87	7735.54	631.58	36
H17	12783.57	9872.61	330.56	41
H18	10964.15	10829.53	1485.09	35
H12	9259.17	10690.83	3137.48	22
H3A	3636.12	6614.31	9364.28	23
H6	1276.56	2989.82	8403.17	27
H7	669.600	2118.41	9972.54	32
H15	12834.45	6558.54	2082.07	30
H10	9336.89	7304.19	4765.72	23
H23	5629.25	12669.64	5561.600	23
H22	3903.17	12890.54	7036.51	26
H21	3346.27	11107.69	8160.39	24
H1A	3641.57	6311.81	6716.58	24
H8	1432.99	3027.85	11090.51	35
H9	2652.36	4850.43	10647.26	30
H2SA	164.49	3635.65	3431.73	59
H2SB	1317.84	2551.75	2932.86	59
H2SC	1902.08	3892.96	2613.12	59
H1SA	3500.56	4619.82	5595.91	42
H1SB	1283.48	4754.67	5560.86	42
H1SC	2272.400	5951.81	5365.11	42
H3	7600(20)	8909(15)	5329(11)	24(4)
H1	4820(20)	7896(16)	6983(12)	34(4)
H2S	2800(30)	3617(18)	3976(13)	38(5)
H1S	2120(30)	5717(19)	4020(13)	46(5)

Experimental

Single crystals of C27H25N5O4 **[mo_21ov_RRH_3AmQuin_Pin_0m]** were **[]**. A suitable crystal was selected and **[]** on a diffractometer. The crystal was kept at 153.0 K during data collection. Using Olex2 [1], the structure was solved with the Unknown
[2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

2

3

Crystal structure determination of [mo_21ov_RRH_3AmQuin_Pin_0m]

Crystal Data for C27H25N5O4 (*M* =483.52 g/mol): triclinic, space group P-1 (no. 2), *a* = 7.2743(3) Å, *b* = 11.3528(5) Å, *c* = 14.9566(5) Å, *α* = 76.6050(10)°, *β* = 78.8710(10)°, *γ* = 78.901(2)°, *V* = 1164.76(8) Å3, *Z* = 2, *T* = 153.0 K, μ(MoKα) = 0.095 mm-1, *Dcalc* = 1.379 g/cm3, 85712 reflections measured (5.778° ≤ 2Θ ≤ 66.428°), 8894 unique (*R*int = 0.0459, Rsigma = 0.0265) which were used in all calculations. The final *R*1 was 0.0487 (I > 2σ(I)) and *wR*2 was 0.1337 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Aromatic/amide H refined with riding coordinates:

C16(H16), C17(H17), C18(H18), C12(H12), C3(H3A), C6(H6), C7(H7), C15(H15), C10(H10), C23(H23), C22(H22), C21(H21), C1(H1A), C8(H8), C9(H9)

2.b Idealised Me refined as rotating group:

Table 1 Crystal data and structure refinement for mo_21ov_RRH_3AmQuin_Pin_0m.
This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.3. 1c

Crystal data and structure refinement for mo_18OV_RRH8_Sample3_0m

Identification code	mo_18OV_RRH8_Sample3_0m
Empirical formula	$C_{25}H_{17}N_5O_2$
Formula weight	419.43
Temperature/K	173.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.4778(2)
b/Å	16.9420(7)
c/Å	25.8329(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1959.76(14)
Z	4
ρ_{calc}g/cm^3	1.4
μ/mm^{-1}	0.1
F(000)	872
Crystal size/mm^3	0.5 × 0.06 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.752 to 56.544
Index ranges	$-5 \le h \le 5$, $-22 \le k \le 22$, $-34 \le l \le 34$
Reflections collected	30705
Independent reflections	4830 [R_{int} = 0.0305, R_{sigma} = 0.0205]
Data/restraints/parameters	4830/0/357
Goodness-of-fit on F^2	1.0
Final R indexes [I>=2σ (I)]	R_1 = 0.0328, wR_2 = 0.0781
Final R indexes [all data]	R_1 = 0.0384, wR_2 = 0.0816
Largest diff. peak/hole / e Å^{-3}	0.20/-0.20
Flack parameter	-0.3(3)

Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for mo_18OV_RRH8_Sample3_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	11924(3)	7043.8(8)	7529.2(5)	30.6(3)
O2	7392(4)	6107.4(8)	4998.1(5)	34.8(3)
N4	4411(3)	4969.0(8)	7305.7(6)	22.0(3)
N5	6652(4)	3951.2(8)	6236.4(5)	22.8(3)
N1	8497(3)	6089.7(8)	7322.4(5)	20.0(3)
N3	6755(4)	5288.3(8)	5695.4(6)	24.8(3)
N2	9328(4)	6335.4(8)	6318.0(5)	20.2(3)
C17	4966(4)	3968.4(10)	5796.1(6)	18.4(3)
C18	5051(4)	4674.2(10)	5489.6(6)	20.8(3)
C1	10489(4)	6663.7(10)	7214.6(6)	20.7(3)
C8	5667(4)	5121.2(10)	7776.0(6)	19.2(3)
C13	4939(4)	4698.3(9)	8232.4(7)	20.9(3)
C23	3127(4)	2649.8(11)	5951.7(7)	25.7(4)
C9	7829(4)	5741.6(9)	7799.8(6)	18.7(3)
C2	10788(4)	6819.1(9)	6640.4(6)	20.5(3)
C10	9140(4)	5934.9(10)	8263.7(7)	21.8(3)
C16	2434(4)	4391.6(11)	7281.3(7)	26.0(4)
C7	7784(4)	5943.0(10)	5455.0(6)	24.0(4)
C20	1710(5)	4065.0(12)	4876.7(7)	28.6(4)
C24	4795(5)	2634.7(11)	6391.9(7)	27.5(4)
C22	3179(4)	3330.4(10)	5631.5(6)	21.3(3)
C21	1548(5)	3390.1(11)	5164.8(7)	27.0(4)
C19	3454(4)	4713.8(11)	5035.6(7)	25.8(4)
C11	8357(4)	5511.3(11)	8716.0(6)	24.8(4)
C12	6338(4)	4908.0(11)	8705.0(7)	24.7(4)
C25	6541(5)	3299.8(11)	6516.8(7)	25.6(4)
C3	12490(5)	7452.1(11)	6470.0(7)	26.7(4)
C15	1591(4)	3927.9(11)	7709.6(8)	27.5(4)
C14	2824(4)	4085.1(10)	8182.1(7)	24.3(4)
C6	9499(4)	6483.4(10)	5809.9(6)	22.3(4)
C4	12636(5)	7603.0(11)	5941.7(7)	30.3(4)
C5	11107(5)	7112.6(11)	5604.6(7)	28.1(4)

Anisotropic Displacement Parameters (Å2×103) for mo_18OV_RRH8_Sample3_0m. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U11	U22	U33	U23	U13	U12
O1	39.6(8)	27.6(6)	24.6(6)	2.3(5)	4.0(6)	10.3(6)
O2	51.9(9)	34.0(7)	18.6(6)	8.4(5)	3.9(6)	-7.3(7)
N4	21.2(7)	23.1(7)	21.8(7)	2.0(6)	1.1(6)	0.4(6)
N5	28.0(8)	22.4(7)	17.9(6)	0.2(5)	1.9(6)	-1.4(6)
N1	23.7(8)	21.1(7)	15.3(6)	0.7(5)	0.8(6)	-2.5(6)
N3	38.0(9)	21.4(7)	15.1(6)	2.7(5)	3.7(6)	-4.5(7)
N2	25.6(8)	17.0(6)	18.1(6)	1.8(5)	1.0(6)	0.1(6)
C17	20.2(8)	20.5(8)	14.6(7)	1.6(6)	2.4(6)	1.7(6)
C18	24.7(9)	21.7(8)	16.0(7)	2.0(6)	1.5(7)	0.3(7)
C1	23.5(9)	17.6(7)	20.8(7)	0.0(6)	1.3(7)	0.8(7)
C8	18.5(8)	18.7(7)	20.3(8)	0.6(6)	2.9(6)	4.5(6)
C13	21.1(9)	20.1(7)	21.3(8)	1.4(6)	5.2(7)	5.5(6)
C23	25.6(10)	22.3(8)	29.1(9)	2.0(7)	1.1(7)	-4.2(7)
C9	21.2(8)	17.4(7)	17.6(7)	0.5(6)	3.2(6)	4.1(6)
C2	24.6(9)	16.6(7)	20.5(8)	0.4(6)	1.5(7)	0.7(7)
C10	22.9(9)	22.6(8)	20.0(8)	2.7(6)	0.4(7)	2.0(7)
C16	24.9(9)	25.9(8)	27.1(8)	3.5(7)	0.9(7)	0.4(7)
C7	30.7(10)	22.1(8)	19.4(7)	3.5(6)	0.2(7)	0.1(7)
C20	28.2(10)	37.3(10)	20.2(8)	0.4(7)	6.2(7)	1.3(8)
C24	31.8(10)	22.3(8)	28.4(9)	4.7(7)	1.1(8)	0.0(8)
C22	19.9(8)	23.2(8)	20.7(7)	3.3(6)	1.7(6)	1.5(7)
C21	26.8(10)	29.2(9)	25.2(8)	5.4(7)	3.7(7)	-3.9(8)
C19	30.1(10)	28.2(9)	19.2(8)	2.3(7)	0.6(7)	3.5(7)
C11	29.6(10)	29.0(9)	16.0(7)	2.0(6)	0.2(7)	7.9(8)
C12	29.6(10)	27.1(9)	17.5(8)	2.6(6)	5.9(7)	7.7(8)
C25	28.3(10)	27.0(8)	21.5(8)	3.1(6)	3.2(7)	-1.0(8)
C3	30.7(10)	20.4(8)	28.9(8)	0.4(7)	3.1(8)	-4.5(8)
C15	23.9(9)	21.4(8)	37.1(10)	1.0(7)	5.0(8)	-2.4(8)
C14	24.4(9)	19.7(7)	28.9(8)	4.2(7)	7.6(7)	3.8(7)

Bond Lengths for mo_18OV_RRH8_Sample3_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.220(2)	C13	C12	1.417(3)
O2	C7	1.225(2)	C13	C14	1.412(3)
N4	C8	1.363(2)	C23	C24	1.361(3)
N4	C16	1.321(2)	C23	C22	1.419(2)
N5	C17	1.365(2)	C9	C10	1.374(2)
N5	C25	1.321(2)	C2	C3	1.387(2)
N1	C1	1.349(2)	C10	C11	1.415(2)
N1	C9	1.399(2)	C16	C15	1.409(3)
N3	C18	1.396(2)	C7	C6	1.506(2)
N3	C7	1.352(2)	C20	C21	1.366(3)
N2	C2	1.339(2)	C20	C19	1.410(3)
N2	C6	1.338(2)	C24	C25	1.409(3)
C17	C18	1.435(2)	C22	C21	1.413(2)
C17	C22	1.411(2)	C11	C12	1.365(3)
C18	C19	1.375(2)	C3	C4	1.390(3)
C1	C2	1.512(2)	C15	C14	1.366(3)
C8	C13	1.418(2)	C6	C5	1.391(2)
C8	C9	1.430(2)	C4	C5	1.385(3)

Bond Angles for mo_18OV_RRH8_Sample3_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C16	N4	C8	117.33(15)	N2	C2	C3	122.95(16)
C25	N5	C17	117.00(15)	C3	C2	C1	119.64(15)
C1	N1	C9	128.85(15)	C9	C10	C11	119.56(17)
C7	N3	C18	128.52(15)	N4	C16	C15	123.72(17)
C6	N2	C2	117.86(15)	O2	C7	N3	125.47(17)
N5	C17	C18	117.59(15)	O2	C7	C6	121.40(16)
N5	C17	C22	123.25(15)	N3	C7	C6	113.13(14)
C22	C17	C18	119.16(15)	C21	C20	C19	121.56(17)
N3	C18	C17	115.18(15)	C23	C24	C25	118.76(17)
C19	C18	N3	124.95(16)	C17	C22	C23	117.14(15)
C19	C18	C17	119.85(16)	C17	C22	C21	119.71(16)
O1	C1	N1	126.26(16)	C21	C22	C23	123.15(17)
O1	C1	C2	120.99(16)	C20	C21	C22	119.82(17)
N1	C1	C2	112.74(15)	C18	C19	C20	119.90(17)
N4	C8	C13	123.41(16)	C12	C11	C10	121.78(16)
N4	C8	C9	117.16(14)	C11	C12	C13	119.88(16)
C13	C8	C9	119.43(15)	N5	C25	C24	124.28(17)
C12	C13	C8	119.22(16)	C2	C3	C4	118.67(17)
C14	C13	C8	116.72(16)	C14	C15	C16	119.01(17)
C14	C13	C12	124.06(16)	C15	C14	C13	119.80(16)
C24	C23	C22	119.55(17)	N2	C6	C7	116.99(15)
N1	C9	C8	114.62(14)	N2	C6	C5	123.16(17)
C10	C9	N1	125.22(16)	C5	C6	C7	119.84(15)
C10	C9	C8	120.12(15)	C5	C4	C3	118.93(17)
N2	C2	C1	117.41(15)	C4	C5	C6	118.41(16)

Hydrogen Bonds for mo_18OV_RRH8_Sample3_0m.

D H A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N3H3N5	0.90(2)	2.21(2)	2.662(2)	110.4(18)
N3H3N2	0.90(2)	2.25(2)	2.657(2)	107.5(17)
N1H1N4	0.88(2)	2.16(2)	2.637(2)	113.1(17)
N1H1N2	0.88(2)	2.23(2)	2.6540(19)	109.5(18)

Torsion Angles for mo_18OV_RRH8_Sample3_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	N2	174.66(17)	C8	C9	C10	C11	0.6(2)
O1	C1	C2	C3	-6.4(3)	C13	C8	C9	N1	176.63(15)
O2	C7	C6	N2	167.49(18)	C13	C8	C9	C10	-1.3(2)
O2	C7	C6	C5	-11.1(3)	C23	C24	C25	N5	0.8(3)
N4	C8	C13	C12	-179.13(16)	C23	C22	C21	C20	180.00(19)
N4	C8	C13	C14	0.8(2)	C9	N1	C1	O1	-7.2(3)
N4	C8	C9	N1	-3.3(2)	C9	N1	C1	C2	173.86(16)
N4	C8	C9	C10	178.82(16)	C9	C8	C13	C12	1.0(2)
N4	C16	C15	C14	1.2(3)	C9	C8	C13	C14	−179.07(15)
N5	C17	C18	N3	-3.3(2)	C9	C10	C11	C12	0.5(3)
N5	C17	C18	C19	178.31(16)	C2	N2	C6	C7	−178.66(16)
N5	C17	C22	C23	1.2(3)	C2	N2	C6	C5	-0.1(3)
N5	C17	C22	C21	178.70(17)	C2	C3	C4	C5	-0.7(3)
N1	C1	C2	N2	-6.3(2)	C10	C11	C12	C13	-0.8(3)
N1	C1	C2	C3	172.67(17)	C16	N4	C8	C13	-0.5(2)
N1	C9	C10	C11	-177.10(17)	C16	N4	C8	C9	179.40(16)
N3	C18	C19	C20	-177.36(18)	C16	C15	C14	C13	-0.8(3)
N3	C7	C6	N2	-11.9(2)	C7	N3	C18	C17	164.20(18)
N3	C7	C6	C5	169.52(18)	C7	N3	C18	C19	-17.5(3)
N2	C2	C3	C4	1.5(3)	C7	C6	C5	C4	179.37(18)
N2	C6	C5	C4	0.9(3)	C24	C23	C22	C17	-0.8(3)
C17	N5	C25	C24	-0.5(3)	C24	C2	C22	C21	179.09(19)
C17	C18	C19	C20	0.9(3)	C22	C17	C18	N3	176.87(15)
C17	C22	C21	C20	-0.1(3)	C22	C17	C18	C19	-1.5(2)
C18	N3	C7	O2	-0.6(3)	C22	C23	C24	C25	-0.1(3)
C18	N3	C7	C6	178.72(17)	C21	C20	C19	C18	0.2(3)
C18	C17	C22	C23	-178.96(16)	C19	C20	C21	C22	-0.6(3)
C18	C17	C22	C21	1.1(2)	C12	C13	C14	C15	179.85(17)
C1	N1	C9	C8	-177.56(16)	C25	N5	C17	C18	179.61(16)
C1	N1	C9	C10	0.2(3)	C25	N5	C17	C22	-0.6(3)
C1	C2	C3	C4	-177.43(17)	C3	C4	C5	C6	-0.4(3)
C8	N4	C16	C15	-0.6(3)	C14	C13	C12	C11	-79.92(17)
C8	C13	C12	C11	0.0(3)	C6	N2	C2	C1	177.87(15)
C8	C13	C14	C15	-0.1(2)	C6	N2	C2	C3	-1.1(3)

Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for mo_18OV_RRH8_Sample3_0m.

Atom	*x*	*y*	*z*	U(eq)
H10	10570(50)	6339(12)	8269(8)	22(5)
H11	9380(50)	5661(13)	9042(8)	31(6)
H3	7410(60)	5199(13)	6018(9)	33(6)
H19	3470(50)	5193(13)	4823(9)	33(6)
H3A	13560(50)	7784(13)	6720(8)	31(6)
H16	1570(50)	4312(13)	6933(8)	33(6)
H4	13760(60)	8038(13)	5807(9)	36(6)
H25	7840(50)	3275(12)	6829(8)	25(5)
H21	340(50)	2958(13)	5062(9)	33(6)
H12	5790(60)	4620(13)	9010(9)	34(6)
H23	1980(60)	2217(14)	5853(8)	32(6)
H24	4770(60)	2193(15)	6626(9)	41(7)
H1	7580(60)	5858(13)	7061(8)	29(6)
H5	11180(50)	7187(13)	5236(9)	33(6)
H15	130(60)	3514(13)	7655(8)	34(6)
H14	2340(50)	3795(12)	8493(8)	23(5)
H20	620(60)	4109(14)	4558(9)	40(7)

Experimental
Single crystals of C25H17N5O2 **[mo_18OV_RRH8_Sample3_0m]** were **[]**. A suitable crystal was selected and **[]** on a **Bruker D8 Venture** diffractometer. The crystal was kept at 173.15 K during data collection. Using Olex2 [1], the structure was
solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package
using Unknown minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

2

3

Crystal structure determination of [mo_18OV_RRH8_Sample3_0m]
Crystal Data for C25H17N5O2 (*M* =419.43 g/mol): orthorhombic, space group P212121 (no. 19), *a* = 4.4778(2) Å, *b* = 16.9420(7) Å, *c* = 25.8329(10) Å, *V* = 1959.76(14) Å3, *Z* = 4, *T* = 173.15 K, μ(MoKα) = 0.094 mm-1, *Dcalc* = 1.422 g/cm3, 30705
reflections measured (5.752° ≤ 2Θ ≤ 56.544°), 4830 unique (*R*int = 0.0305, Rsigma = 0.0205) which were used in all calculations.

The final *R*1 was 0.0328 (I > 2σ(I)) and *wR*2 was 0.0816 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

S2.4. 1d

Table 1 Crystal data and structure refinement for RRH84.

Identification code	RRH84
Empirical formula	$C_{23}H_{19}N_7O_2$
Formula weight	425.45
Temperature/K	153.15
Crystal system	monoclinic
Space group	P2/c
a/Å	10.4220(2)
b/Å	11.8014(3)
c/Å	8.6298(2)
α/°	90
β/°	112.0760(10)
γ/°	90
Volume/Å^3	983.60(4)
Z	2
ρ_{calc}g/cm^3	1.437
μ/mm^{-1}	0.097
F(000)	444.0
Crystal size/mm^3	0.495 × 0.296 × 0.126
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.218 to 63.288
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -12 ≤ l ≤ 10
Reflections collected	23433
Independent reflections	3319 [R_{int} = 0.0293, R_{sigma} = 0.0173]
Data/restraints/parameters	3319/0/151
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0429, wR_2 = 0.1150
Final R indexes [all data]	R_1 = 0.0517, wR_2 = 0.1230
Largest diff. peak/hole / e Å^{-3}	0.52/-0.25

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for RRH84. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6806.7(8)	3781.7(6)	6818.3(8)	23.54(17)
N1	5000	4123.7(9)	2500	15.1(2)
N4	8925.5(9)	6769.4(7)	8658.1(10)	19.53(17)
N2	6901.2(8)	5247.7(7)	5110.9(9)	17.07(16)
N3	8443.7(8)	5767.0(7)	7862.7(10)	17.92(16)
C3	5721.9(9)	3536.0(8)	3879.5(10)	15.21(17)
C5	7628.2(9)	6044.2(8)	6315.5(11)	15.53(17)
C11	8410.8(10)	7675.2(8)	7637.4(12)	18.51(18)
C6	7565.4(9)	7240.1(8)	6061.7(11)	16.65(17)
C4	6529.5(9)	4199.8(8)	5423.2(11)	16.07(17)
C2	5737.7(10)	2355.6(8)	3944.9(12)	19.29(18)
C7	6892.4(11)	7975.3(9)	4732.3(13)	22.4(2)
C1	5000	1760.3(12)	2500	21.7(3)
C10	8584.9(12)	8842.7(9)	7949.9(14)	26.0(2)
C12	9743.8(11)	6771.8(10)	10435.6(12)	24.9(2)
C8	7075.5(13)	9129.1(10)	5035.7(15)	29.3(2)
C9	7905.5(13)	9550.5(9)	6629.0(16)	31.0(2)

Anisotropic Displacement Parameters ($Å^2×10^3$) for RRH84. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	33.1(4)	23.1(3)	12.3(3)	3.2(3)	6.1(3)	-0.5(3)
N1	16.6(5)	17.9(5)	10.6(4)	0	4.9(4)	0
N4	20.5(4)	22.4(4)	12.6(3)	-1.8(3)	2.7(3)	-2.3(3)
N2	22.4(4)	18.6(4)	8.9(3)	-0.5(3)	4.4(3)	-1.0(3)
N3	19.1(3)	20.3(4)	12.7(3)	-0.7(3)	4.1(3)	-0.6(3)
C3	16.0(4)	17.6(4)	12.1(3)	0.2(3)	5.3(3)	0.6(3)
C5	17.0(4)	18.4(4)	11.4(4)	-0.3(3)	5.5(3)	0.7(3)
C11	19.2(4)	21.2(4)	16.1(4)	-1.8(3)	7.7(3)	-1.6(3)
C6	18.2(4)	18.3(4)	14.2(4)	0.7(3)	6.9(3)	1.4(3)
C4	17.3(4)	18.8(4)	11.5(4)	0.1(3)	4.7(3)	2.0(3)
C2	19.6(4)	18.0(4)	19.4(4)	2.5(3)	6.3(3)	2.1(3)
C7	26.0(4)	23.2(4)	18.0(4)	3.4(3)	8.3(4)	5.1(4)
C1	22.7(6)	15.5(6)	24.7(6)	0	6.6(5)	0
C10	30.5(5)	21.8(5)	26.7(5)	-6.3(4)	11.8(4)	-5.0(4)
C12	22.8(4)	34.9(5)	12.1(4)	-2.7(4)	1.1(3)	-4.4(4)
C8	37.4(6)	22.6(5)	29.8(5)	7.7(4)	14.7(5)	6.8(4)
C9	41.3(6)	17.8(4)	37.5(6)	-0.1(4)	19.0(5)	0.3(4)

Bond Lengths for RRH84.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C4	1.2309(11)	C3	C2	1.3941(13)
N1	C3	1.3383(10)	C5	C6	1.4259(13)
N1	C3[1]	1.3383(10)	C11	C6	1.4101(13)
N4	N3	1.3652(11)	C11	C10	1.4025(14)
N4	C11	1.3606(13)	C6	C7	1.3986(13)
N4	C12	1.4481(12)	C2	C1	1.3852(12)
N2	C5	1.3951(11)	C7	C8	1.3861(15)
N2	C4	1.3530(12)	C10	C9	1.3755(16)
N3	C5	1.3263(11)	C8	C9	1.4114(17)
C3	C4	1.5013(12)			

[1]1-X,+Y,1/2-Z

Bond Angles for RRH84.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3[1]	N1	C3	117.57(11)	C10	C11	C6	122.14(9)
N3	N4	C12	119.55(8)	C11	C6	C5	103.67(8)
C11	N4	N3	111.98(8)	C7	C6	C5	136.05(9)
C11	N4	C12	128.04(9)	C7	C6	C11	120.27(9)
C4	N2	C5	125.69(8)	O1	C4	N2	125.58(9)
C5	N3	N4	105.54(8)	O1	C4	C3	120.39(8)
N1	C3	C4	117.33(8)	N2	C4	C3	114.03(7)
N1	C3	C2	123.23(9)	C1	C2	C3	118.44(9)
C2	C3	C4	119.43(8)	C8	C7	C6	117.61(10)
N2	C5	C6	124.87(8)	C2	C1	C2[1]	119.06(12)
N3	C5	N2	123.16(8)	C9	C10	C11	116.62(10)
N3	C5	C6	111.95(8)	C7	C8	C9	121.37(10)
N4	C11	C6	106.84(8)	C10	C9	C8	121.97(10)
N4	C11	C10	131.01(9)				

[1]1-X,+Y,1/2-Z

Torsion Angles for RRH84.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C3	C4	O1	154.63(8)	C5	N2	C4	C3	178.57(8)
N1	C3	C4	N2	-25.79(10)	C5	C6	C7	C8	177.54(10)
N1	C3	C2	C1	1.77(12)	C11	N4	N3	C5	0.73(10)
N4	N3	C5	N2	-178.20(8)	C11	C6	C7	C8	-0.88(14)
N4	N3	C5	C6	0.35(10)	C11	C10	C9	C8	-0.10(17)
N4	C11	C6	C5	1.59(10)	C6	C11	C10	C9	-1.07(15)
N4	C11	C6	C7	-179.54(8)	C6	C7	C8	C9	-0.27(16)
N4	C11	C10	C9	−179.62(10)	C4	N2	C5	N3	23.82(14)
N2	C5	C6	C11	177.30(8)	C4	N2	C5	C6	-154.55(9)
N2	C5	C6	C7	-1.29(17)	C4	C3	C2	C1	-179.16(7)
N3	N4	C11	C6	-1.51(11)	C2	C3	C4	O1	-24.49(13)
N3	N4	C11	C10	177.20(10)	C2	C3	C4	N2	155.08(8)
N3	C5	C6	C11	-1.23(10)	C7	C8	C9	C10	0.79(18)
N3	C5	C6	C7	−179.82(10)	C10	C11	C6	C5	-177.27(9)
C3[1]	N1	C3	C4	-179.99(8)	C10	C11	C6	C7	1.60(14)
C3[1]	N1	C3	C2	-0.90(6)	C12	N4	N3	C5	173.80(8)
C3	C2	C1	C2[1]	-0.82(6)	C12	N4	C11	C6	-173.85(9)
C5	N2	C4	O1	-1.88(15)	C12	N4	C11	C10	4.86(17)

[1]1-X,+Y,1/2-Z

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for RRH84.

Atom	*x*	*y*	*z*	U(eq)
H2A	6242.62	1968.47	4956.57	23
H7	6329.98	7694.07	3659.93	27
H1	4999.99	955.34	2500.02	26
H10	9143.77	9130.01	9019.82	31
H12A	9137.51	6901.31	11053.64	37
H12B	10437.3	7376.63	10694.7	37
H12C	10210.32	6039.1	10761.35	37
H8	6633.09	9646.97	4152.83	35
H9	7997.74	10346.84	6793.99	37
H2	6704(16)	5443(14)	4060(20)	38(4)

Experimental

Single crystals of $C_{23}H_{19}N_7O_2$ [RRH84] were [by slow evaporation of the solvent]. A clear pale-yellow shard-like specimen of C23H19N7O2, approximate dimensions 0.126 mm x 0.296 mm x 0.495 mm, was used for the X-ray crystallographic analysis by mounting the crystal in Paratone oil on a MiTeGeN microgripper cryoloop. The X-ray intensity data were measured on a Bruker APEX-II CCD diffractometer. The crystal was kept at 153.15 K during data collection. A total of 3031 frames were collected. The total exposure time was 8.42 hours. The integration of the data using a monoclinic unit cell yielded a total of 23461 reflections to a maximum θ angle of 31.64° (0.68 Å resolution), of which 3323 were independent (average redundancy 7.060, completeness = 99.9%, R_{int} = 2.94%, $R\sigma$ = 1.80%) and 2791 (83.99%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.4220(2) Å, b = 11.8014(3) Å, c = 8.6298(2) Å, β = 112.0760(10)°, volume = 983.60(4) Å^3, are based upon the refinement of the XYZ-centroids of 107 reflections above 20 $\sigma(I)$ with 8.598° < 2θ < 55.29°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.941. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9520 and 0.9880. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation. The final anisotropic full-matrix least-squares refinement on F^2 with 151 variables converged at R_1 = 4.29%, for the observed data and wR_2 = 12.30% for all data. The goodness-of-fit was 1.052. The largest peak in the final difference electron density synthesis was 0.52 e$^-$/Å^3 and the largest hole was -0.25 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.437 g/cm^3 and F(000), 444 e$^-$.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [RRH84]

Crystal Data for $C_{23}H_{19}N_7O_2$ (M =425.45 g/mol): monoclinic, space group P2/c (no. 13), a = 10.4220(2) Å, b = 11.8014(3) Å, c = 8.6298(2) Å, β = 112.0760(10)°, V = 983.60(4) Å^3, Z = 2, T = 153.15 K, μ(MoKα) = 0.097 mm^{-1}, *Dcalc* = 1.437 g/cm^3, 23433 reflections measured (4.218° ≤ 2Θ ≤ 63.288°), 3319 unique (R_{int} = 0.0293, R_{sigma} = 0.0173) which were used in all calculations. The final R_1 was 0.0429 (I > 2σ(I)) and wR_2 was 0.1230 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C2(H2A), C7(H7), C1(H1), C10(H10), C8(H8), C9(H9)
2.b Idealised Me refined as rotating group:
 C12(H12A,H12B,H12C)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.5. 1e

Crystal data and structure refinement for 19oa_rr_bzkpin_0m.

Identification code	19oa_rr_bzkpin_0m
Empirical formula	$C_{33}H_{23}N_3O_4$
Formula weight	525.54
Temperature/K	153.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.4952(2)
b/Å	18.3345(4)
c/Å	16.2123(3)
α/°	90
β/°	90.6890(10)
γ/°	90
Volume/Å^3	2524.97(9)
Z	4
ρ_{calc}g/cm^3	1.382
μ/mm^{-1}	0.092
F(000)	1096.0
Crystal size/mm^3	0.22 × 0.16 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.354 to 56.762
Index ranges	-11 ≤ h ≤ 11, -24 ≤ k ≤ 24, -21 ≤ l ≤ 20
Reflections collected	38759
Independent reflections	6322 [R_{int} = 0.0562, R_{sigma} = 0.0479]
Data/restraints/parameters	6322/0/361
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0800, wR_2 = 0.1098
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 19oa_rr_bzkpin_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	9710.7(19)	3879.6(8)	2243.4(9)	25.5(3)
C2	9271(2)	3181.5(8)	2016.3(10)	27.2(4)
C3	7889(2)	3068.6(9)	1575.1(10)	28.6(4)
C4	6973(2)	3657.5(9)	1337.3(10)	28.6(4)
C5	7444.3(19)	4363.3(8)	1529.9(10)	25.5(3)
C6	8812.1(18)	4473.8(8)	1990.9(9)	21.8(3)
C7	9292.1(18)	5217.4(8)	2293.5(9)	23.1(3)
C8	9644.3(17)	5814.3(8)	1698.1(9)	20.4(3)
C9	9565.5(18)	5676.4(8)	848.7(9)	23.2(3)
C10	9983.0(19)	6196.7(8)	278.0(9)	24.9(3)
C11	10523.1(19)	6869.1(9)	550.5(10)	26.7(4)
C12	10620.2(19)	7027.8(8)	1380.1(9)	25.0(3)
C13	10175.2(18)	6509.8(8)	1959.8(9)	21.2(3)
C14	11087.2(18)	7170.3(8)	3213.4(9)	23.8(3)
C15	10757.2(18)	7177.0(8)	4122.1(9)	21.7(3)
C16	11769(2)	7531.5(9)	4667.8(10)	27.9(4)
C17	11422(2)	7518.6(9)	5499.6(10)	32.1(4)
C18	10087(2)	7158.9(9)	5756.6(10)	28.6(4)
C19	9131.2(18)	6822.8(8)	5168.8(9)	21.4(3)
C20	7638.0(19)	6449.4(8)	5420.6(9)	22.7(3)
C21	5126.2(18)	6012.0(8)	4778.0(9)	22.3(3)
C22	4303(2)	5929.8(8)	5513.7(10)	28.5(4)
C23	2772(2)	5669.3(9)	5502.6(11)	33.5(4)
C24	2031(2)	5497.3(9)	4764.1(11)	32.7(4)
C25	2828.2(19)	5579.9(8)	4033.3(11)	27.7(4)
C26	4383.4(18)	5827.7(8)	4016.6(10)	22.9(3)
C27	5162.6(19)	5920.3(8)	3208.2(10)	23.9(3)
C28	4482.2(18)	5578.8(9)	2441.9(9)	24.4(3)
C29	3906.8(19)	4866.4(9)	2411.3(10)	27.3(4)
C30	3416(2)	4567.5(10)	1668.4(11)	34.8(4)
C31	3464(2)	4978.4(11)	954.6(11)	39.2(4)
C32	4013(2)	5689.5(11)	982.7(11)	40.4(5)
C33	4539(2)	5982.8(9)	1718.0(10)	32.3(4)
N1	10203.4(16)	6672.3(7)	2801.8(7)	23.4(3)
N2	9459.0(15)	6827.7(6)	4363.8(7)	20.0(3)
N3	6666.7(15)	6288.4(7)	4774.0(8)	22.5(3)
O1	9445.4(15)	5294.7(6)	3042.7(7)	34.2(3)
O2	12056.3(15)	7577.9(7)	2912.7(7)	40.6(3)
O3	7367.9(14)	6335.8(6)	6149.5(6)	31.4(3)
O4	6364.1(14)	6288.8(6)	3134.8(7)	34.3(3)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 19oa_rr_bzkpin_0m. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	23.2(8)	30.3(8)	22.9(8)	2.0(6)	-2.4(6)	-2.7(7)
C2	30.4(9)	23.6(8)	27.7(9)	3.9(7)	-2.7(7)	2.0(7)
C3	34.0(10)	22.4(8)	29.5(9)	-2.3(6)	0.1(7)	-4.6(7)
C4	24.2(9)	29.9(8)	31.5(9)	-1.5(7)	-4.7(7)	-5.5(7)
C5	23.2(9)	24.9(8)	28.5(9)	1.7(6)	-2.5(7)	-0.8(7)
C6	23.0(8)	22.5(7)	19.9(8)	1.6(6)	1.5(6)	-2.8(6)
C7	20.9(8)	25.8(8)	22.6(8)	-0.1(6)	0.7(6)	-3.4(6)
C8	19.0(8)	20.5(7)	21.5(8)	-0.8(6)	0.7(6)	-1.6(6)
C9	24.9(9)	21.9(7)	22.8(8)	-1.1(6)	-1.1(6)	0.2(6)
C10	27.5(9)	28.5(8)	18.6(8)	0.9(6)	-0.3(6)	1.1(7)
C11	28.9(9)	25.9(8)	25.2(8)	6.4(6)	2.4(7)	-1.4(7)
C12	26.3(9)	20.8(7)	27.8(8)	0.4(6)	0.0(7)	-3.3(6)
C13	18.9(8)	23.1(7)	21.4(8)	-1.3(6)	0.9(6)	-0.5(6)
C14	21.1(8)	24.2(8)	26.2(8)	-1.0(6)	-2.0(6)	-3.0(7)
C15	20.3(8)	18.8(7)	25.8(8)	-1.8(6)	-2.8(6)	2.0(6)
C16	25.3(9)	27.1(8)	31.0(9)	-4.0(7)	-3.8(7)	-4.0(7)
C17	33.5(10)	32.1(9)	30.5(9)	-8.2(7)	-8.1(8)	-3.7(8)
C18	33.8(10)	28.6(8)	23.2(8)	-4.3(7)	-3.0(7)	1.1(7)
C19	24.5(8)	16.7(7)	23.0(8)	-0.5(6)	-1.7(6)	5.1(6)
C20	28.4(9)	16.6(7)	23.2(8)	-1.1(6)	0.5(7)	5.8(6)
C21	23.0(8)	16.1(7)	27.9(8)	3.8(6)	4.5(7)	2.1(6)
C22	31.1(10)	24.6(8)	29.9(9)	5.4(7)	6.2(7)	4.6(7)
C23	34.2(10)	26.3(8)	40.3(10)	8.2(7)	16.1(8)	5.0(7)
C24	22.3(9)	24.7(8)	51.4(11)	6.2(8)	10.8(8)	0.2(7)
C25	23.2(9)	20.8(7)	39.0(10)	1.8(7)	1.8(7)	2.0(7)
C26	21.5(8)	16.9(7)	30.4(9)	3.6(6)	4.1(7)	2.5(6)
C27	22.0(8)	19.4(7)	30.2(9)	4.4(6)	-0.6(7)	0.0(6)
C28	17.9(8)	28.3(8)	27.1(8)	2.9(6)	-0.6(6)	0.8(6)
C29	21.3(9)	28.0(8)	32.8(9)	2.1(7)	-0.4(7)	-1.2(7)
C30	21.4(9)	38.9(10)	44.0(11)	-9.2(8)	0.5(8)	-4.4(7)
C31	26.3(10)	59.4(12)	31.8(10)	-7.8(9)	-7.3(8)	-0.5(9)

C32	36.9(11)	55.1(12)	28.9(10)	10.5(8)	-5.4(8)	6.1(9)
C33	33.7(10)	32.0(9)	31.3(9)	7.5(7)	-2.2(8)	1.2(8)
N1	27.8(7)	22.6(6)	20.0(6)	-1.6(5)	3.2(5)	-7.4(6)
N2	21.1(7)	17.0(6)	21.9(7)	-1.1(5)	-1.8(5)	2.0(5)
N3	23.8(7)	23.1(6)	20.7(7)	0.8(5)	2.9(5)	-0.7(5)
O1	50.3(8)	30.5(6)	21.7(6)	0.2(5)	-0.9(5)	-11.9(6)
O2	40.3(8)	50.0(8)	31.7(7)	-0.3(6)	0.2(6)	-24.8(6)
O3	39.4(7)	33.1(6)	21.7(6)	0.4(5)	2.1(5)	0.1(5)
O4	32.5(7)	40.2(7)	30.2(6)	1.2(5)	2.2(5)	-15.2(6)

Bond Lengths for 19oa_rr_bzkpin_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.382(2)	C17	C18	1.380(2)
C1	C6	1.389(2)	C18	C19	1.389(2)
C2	C3	1.383(2)	C19	C20	1.502(2)
C3	C4	1.383(2)	C19	N2	1.3378(19)
C4	C5	1.389(2)	C20	N3	1.3588(19)
C5	C6	1.389(2)	C20	O3	1.2244(18)
C6	C7	1.504(2)	C21	C22	1.398(2)
C7	C8	1.492(2)	C21	C26	1.420(2)
C7	O1	1.2283(18)	C21	N3	1.4035(19)
C8	C9	1.401(2)	C22	C23	1.386(2)
C8	C13	1.416(2)	C23	C24	1.382(3)
C9	C10	1.378(2)	C24	C25	1.380(2)
C10	C11	1.386(2)	C25	C26	1.398(2)
C11	C12	1.378(2)	C26	C27	1.485(2)
C12	C13	1.392(2)	C27	C28	1.501(2)
C13	N1	1.3972(18)	C27	O4	1.2310(18)
C14	C15	1.503(2)	C28	C29	1.395(2)
C14	N1	1.3528(19)	C28	C33	1.389(2)
C14	O2	1.2181(18)	C29	C30	1.383(2)
C15	C16	1.388(2)	C30	C31	1.382(3)
C15	N2	1.3381(19)	C31	C32	1.385(3)
C16	C17	1.384(2)	C32	C33	1.377(2)

Bond Angles for 19oa_rr_bzkpin_0m.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C6	120.14(15)	C18	C19	C20	120.30(14)
C1	C2	C3	120.10(15)	N2	C19	C18	122.65(15)
C2	C3	C4	119.91(14)	N2	C19	C20	117.03(13)
C3	C4	C5	120.31(15)	N3	C20	C19	113.35(13)
C6	C5	C4	119.60(15)	O3	C20	C19	120.56(14)
C1	C6	C7	117.98(14)	O3	C20	N3	126.06(15)
C5	C6	C1	119.83(14)	C22	C21	C26	119.63(15)
C5	C6	C7	121.98(14)	C22	C21	N3	121.25(15)
C8	C7	C6	120.65(13)	N3	C21	C26	119.10(13)
O1	C7	C6	116.89(13)	C23	C22	C21	120.34(16)
O1	C7	C8	122.38(14)	C24	C23	C22	120.50(16)
C9	C8	C7	119.73(13)	C25	C24	C23	119.71(16)
C9	C8	C13	117.93(13)	C24	C25	C26	121.73(16)
C13	C8	C7	122.17(13)	C21	C26	C27	122.80(14)
C10	C9	C8	121.69(14)	C25	C26	C21	118.08(14)
C9	C10	C11	119.25(14)	C25	C26	C27	119.06(15)
C12	C11	C10	120.98(14)	C26	C27	C28	120.76(14)
C11	C12	C13	120.11(14)	O4	C27	C26	121.80(14)
C12	C13	C8	120.02(14)	O4	C27	C28	117.42(14)
C12	C13	N1	120.84(13)	C29	C28	C27	123.46(14)
N1	C13	C8	119.11(13)	C33	C28	C27	117.37(14)
N1	C14	C15	112.34(13)	C33	C28	C29	119.00(15)
O2	C14	C15	121.48(14)	C30	C29	C28	120.25(16)
O2	C14	N1	126.18(14)	C31	C30	C29	120.11(17)
C16	C15	C14	120.48(14)	C30	C31	C32	119.92(17)
N2	C15	C14	116.57(13)	C33	C32	C31	120.10(17)
N2	C15	C16	122.95(14)	C32	C33	C28	120.58(17)
C17	C16	C15	118.37(16)	C14	N1	C13	128.96(13)
C18	C17	C16	119.20(15)	C19	N2	C15	118.09(13)
C17	C18	C19	118.72(15)	C20	N3	C21	129.23(13)

Hydrogen Bonds for 19oa_rr_bzkpin_0m.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C22	H22	O3	0.95	2.25	2.886(2)	123.4
N1	H1A	O1	0.88	2.06	2.6368(16)	122.3
N3	H3A	O4	0.88	1.95	2.6669(16)	137.5

Torsion Angles for 19oa_rr_bzkpin_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	2.1(2)	C21	C22	C23	C24	-0.9(2)
C1	C6	C7	C8	122.93(16)	C21	C26	C27	C28	167.17(14)
C1	C6	C7	O1	-53.9(2)	C21	C26	C27	O4	-14.3(2)
C2	C1	C6	C5	1.9(2)	C22	C21	C26	C25	1.1(2)
C2	C1	C6	C7	176.71(14)	C22	C21	C26	C27	178.15(13)
C2	C3	C4	C5	0.9(2)	C22	C21	N3	C20	6.6(2)
C3	C4	C5	C6	-2.5(2)	C22	C23	C24	C25	0.5(2)
C4	C5	C6	C1	1.1(2)	C23	C24	C25	C26	0.7(2)
C4	C5	C6	C7	-173.48(14)	C24	C25	C26	C21	-1.5(2)
C5	C6	C7	C8	-62.4(2)	C24	C25	C26	C27	-178.65(14)
C5	C6	C7	O1	120.82(17)	C25	C26	C27	C28	-15.8(2)
C6	C1	C2	C3	-3.5(2)	C25	C26	C27	O4	162.72(15)
C6	C7	C8	C9	-1.6(2)	C26	C21	C22	C23	0.1(2)
C6	C7	C8	C13	-176.77(14)	C26	C21	N3	C20	-174.73(14)
C7	C8	C9	C10	-175.58(15)	C26	C27	C28	C29	-43.8(2)
C7	C8	C13	C12	174.35(14)	C26	C27	C28	C33	140.86(15)
C7	C8	C13	N1	-7.4(2)	C27	C28	C29	C30	-174.65(15)
C8	C9	C10	C11	1.2(2)	C27	C28	C33	C32	176.57(15)
C8	C13	N1	C14	156.38(15)	C28	C29	C30	C31	-1.3(3)
C9	C8	C13	C12	-0.9(2)	C29	C28	C33	C32	1.0(3)
C9	C8	C13	N1	177.37(14)	C29	C30	C31	C32	0.4(3)
C9	C10	C11	C12	-1.2(2)	C30	C31	C32	C33	1.2(3)
C10	C11	C12	C13	0.1(2)	C31	C32	C33	C28	-1.9(3)
C11	C12	C13	C8	1.0(2)	C33	C28	C29	C30	0.6(2)
C11	C12	C13	N1	-177.28(14)	N1	C14	C15	C16	166.02(14)
C12	C13	N1	C14	-25.3(2)	N1	C14	C15	N2	-13.94(19)

C13	C8	C9	C10	-0.2(2)	N2	C15	C16	C17	0.4(2)
C14	C15	C16	C17	-179.57(14)	N2	C19	C20	N3	-12.07(18)
C14	C15	N2	C19	179.96(13)	N2	C19	C20	O3	169.97(13)
C15	C14	N1	C13	179.76(14)	N3	C21	C22	C23	178.72(14)
C15	C16	C17	C18	-0.2(2)	N3	C21	C26	C25	-177.59(13)
C16	C15	N2	C19	0.0(2)	N3	C21	C26	C27	-0.5(2)
C16	C17	C18	C19	-0.2(2)	O1	C7	C8	C9	175.02(15)
C17	C18	C19	C20	-177.76(14)	O1	C7	C8	C13	-0.2(2)
C17	C18	C19	N2	0.6(2)	O2	C14	C15	C16	-13.8(2)
C18	C19	C20	N3	166.42(13)	O2	C14	C15	N2	166.20(15)
C18	C19	C20	O3	-11.5(2)	O2	C14	N1	C13	-0.4(3)
C18	C19	N2	C15	-0.5(2)	O3	C20	N3	C21	5.0(2)
C19	C20	N3	C21	-172.85(13)	O4	C27	C28	C29	137.62(16)
C20	C19	N2	C15	177.93(12)	O4	C27	C28	C33	-37.7(2)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 19oa_rr_bzkpin_0m.

Atom	*x*	*y*	*z*	U(eq)
H1	10629.3	3953.26	2572.91	31
H2	9919.25	2778.65	2163.43	33
H3	7569.98	2587.15	1435.4	34
H4	6016.27	3578.86	1040.97	34
H5	6834.89	4768.02	1347.35	31
H9	9215.24	5212.38	661.27	28
H10	9901.43	6095.48	-295.58	30
H11	10830.96	7225.91	159.3	32
H12	10991.65	7491.56	1556.79	30
H16	12678.54	7777.06	4475.18	33
H17	12093.52	7754.51	5888.96	39
H18	9827.76	7141.53	6324.6	34
H22	4796.61	6053.14	6023.86	34
H23	2227.24	5608.58	6006.24	40
H24	978.01	5322.96	4759.67	39
H25	2306.06	5465.28	3528.32	33
H29	3851.64	4585.68	2902.6	33
H30	3045.94	4078.81	1648.75	42
H31	3120.34	4773.47	445.27	47
H32	4027.11	5975.28	494.05	48
H33	4945.05	6465.61	1730.14	39
H1A	9556.96	6415.28	3106.58	28
H3A	7059.57	6368.97	4282.54	27

Experimental

Single crystals of $C_{33}H_{23}N_3O_4$ [19oa_rr_bzkpin_0m] were [ROOM TEMPERATURE]. A suitable crystal was selected and [] on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 153.15 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2.

Crystal structure determination of [19oa_rr_bzkpin_0m]

Crystal Data for $C_{33}H_{23}N_3O_4$ (M =525.54 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 8.4952(2) Å, b = 18.3345(4) Å, c = 16.2123(3) Å, β = 90.6890(10)°, V = 2524.97(9) Å^3, Z = 4, T = 153.15 K, μ(MoKα) = 0.092 mm^{-1}, *Dcalc* = 1.382 g/cm^3, 38759 reflections measured (3.354° ≤ 2Θ ≤ 56.762°), 6322 unique (R_{int} = 0.0562, R_{sigma} = 0.0479) which were used in all calculations. The final R_1 was 0.0452 (I > 2σ(I)) and wR_2 was 0.1098 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All N(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C1(H1), C2(H2), C3(H3), C4(H4), C5(H5), C9(H9), C10(H10), C11(H11), C12(H12),
 C16(H16), C17(H17), C18(H18), C22(H22), C23(H23), C24(H24), C25(H25), C29(H29),
  C30(H30), C31(H31), C32(H32), C33(H33), N1(H1A), N3(H3A)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.6. 2d

Crystal data and structure refinement for 19OA_RRH114_P-1.

Identification code	19OA_RRH114_P-1
Empirical formula	$C_{23}H_{17}AuClN_7O_2$
Formula weight	1311.70
Temperature/K	153.15
Crystal system	triclinic
Space group	P-1
a/Å	8.8115(3)
b/Å	10.4987(3)
c/Å	12.0821(4)
α/°	82.449(2)
β/°	74.233(2)
γ/°	81.344(2)
Volume/Å^3	1058.58(6)
Z	2
ρ_{calc}g/cm^3	2.058
μ/mm^{-1}	7.114
F(000)	632.0
Crystal size/mm^3	0.161 × 0.094 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.518 to 66.494
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -18 ≤ l ≤ 18
Reflections collected	59569
Independent reflections	8133 [R_{int} = 0.0387, R_{sigma} = 0.0240]
Data/restraints/parameters	8133/0/309
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0194, wR_2 = 0.0423
Final R indexes [all data]	R_1 = 0.0241, wR_2 = 0.0437
Largest diff. peak/hole / e Å^{-3}	2.51/-1.09

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 19OA_RRH114_P-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au1	7316.2(2)	4918.9(2)	5197.8(2)	16.16(2)
Cl1	7173.2(7)	3149.5(5)	6497.0(4)	27.64(10)
O2	10785(2)	4991.5(16)	2176.1(15)	32.7(4)
O1	4226(2)	8197.9(16)	5883.5(14)	29.4(3)
N3	9260(2)	4257.7(16)	3955.0(14)	20.6(3)
N1	5423(2)	6090.6(16)	6076.1(14)	19.3(3)
N4	3303(2)	5038.1(16)	8851.5(14)	19.9(3)
N7	10692(2)	2289.8(17)	4554.8(15)	22.4(3)
N5	3818(2)	4947.7(17)	7691.2(14)	20.9(3)
N2	7434(2)	6456.1(16)	4077.5(13)	17.7(3)
N6	11228(2)	1112.9(17)	4133.8(15)	22.3(3)
C22	10026(2)	2262.8(19)	2864.6(16)	18.8(3)
C1	5196(2)	7300(2)	5504.0(17)	21.2(4)
C2	6334(2)	7458(2)	4329.0(16)	20.6(4)
C14	4696(2)	6694.4(19)	8142.0(16)	18.9(3)
C9	3791(2)	6087.8(19)	9159.5(16)	18.8(3)
C17	10888(2)	1067.4(19)	3102.5(17)	20.2(3)
C15	4662(2)	5925.6(19)	7262.9(16)	18.7(3)
C7	9688(2)	5156(2)	3035.7(17)	22.5(4)
C10	3506(2)	6564(2)	10241.4(17)	23.3(4)
C23	9965(2)	2971.7(19)	3807.4(17)	19.5(3)
C5	8789(3)	7501(2)	2346.4(18)	27.8(4)
C6	8642(2)	6420(2)	3136.4(17)	21.5(4)
C21	9483(3)	2498(2)	1860.7(18)	23.0(4)
C11	4148(3)	7673(2)	10247.5(19)	28.5(4)
C8	2316(3)	4119(2)	9584.4(19)	27.7(4)
C20	9864(3)	1539(2)	1117.3(19)	29.0(4)

C13	5347(3)	7826(2)	8180.2(18)	26.6(4)
C12	5054(3)	8305(2)	9237(2)	31.6(5)
C19	10774(3)	366(2)	1353(2)	29.7(5)
C18	11273(3)	94(2)	2349.3(19)	25.8(4)
C4	7644(3)	8564(2)	2554.2(19)	29.9(5)
C3	6400(3)	8550(2)	3544.2(18)	26.7(4)
C16	12127(3)	124(2)	4721(2)	28.1(4)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 19OA_RRH114_P-1. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	19.58(3)	16.66(3)	10.94(3)	-2.58(2)	-0.77(2)	-2.87(2)
Cl1	36.7(3)	21.0(2)	18.5(2)	1.69(17)	0.47(19)	0.23(19)
O2	34.8(9)	26.9(8)	27.1(8)	-7.8(6)	12.9(7)	-8.6(7)
O1	31.6(8)	27.2(8)	21.1(7)	0.0(6)	-0.6(6)	8.5(6)
N3	22.7(8)	19.8(8)	16.4(7)	-4.8(6)	1.0(6)	-1.7(6)
N1	21.8(8)	19.6(7)	12.5(6)	-1.6(6)	0.6(6)	0.6(6)
N4	21.5(8)	21.6(8)	13.0(7)	-0.6(6)	1.9(6)	-3.9(6)
N7	22.1(8)	25.5(8)	19.6(8)	-6.6(6)	-3.7(6)	-2.6(6)
N5	22.8(8)	23.0(8)	14.5(7)	-1.5(6)	-0.8(6)	-2.9(6)
N2	21.8(7)	18.0(7)	12.6(6)	-1.4(5)	-2.4(5)	-4.4(6)
N6	22.7(8)	23.9(8)	20.0(8)	-4.4(6)	-5.9(6)	0.8(6)
C22	18.0(8)	20.4(8)	17.5(8)	-3.9(7)	-2.2(6)	-3.1(7)
C1	22.6(9)	24.9(9)	14.1(8)	-1.5(7)	-2.4(7)	-1.0(7)
C2	22.7(9)	23.4(9)	15.1(8)	-1.1(7)	-3.7(7)	-3.8(7)
C14	18.1(8)	21.6(9)	15.0(8)	-1.4(6)	-1.4(6)	-1.7(7)
C9	17.2(8)	21.3(9)	15.4(8)	0.2(6)	-2.1(6)	0.4(7)
C17	19.3(8)	21.4(9)	19.2(8)	-5.1(7)	-2.0(7)	-2.2(7)
C15	18.7(8)	20.8(8)	13.1(7)	-0.9(6)	0.3(6)	-0.4(7)
C7	24.9(9)	21.0(9)	19.0(8)	-5.4(7)	2.9(7)	-7.0(7)
C10	22.2(9)	30.1(10)	14.2(8)	-3.4(7)	0.1(7)	-0.3(8)
C23	19.1(8)	20.5(9)	17.2(8)	-5.6(7)	-0.4(6)	-2.0(7)
C5	34.3(11)	27.3(10)	18.2(9)	-0.4(8)	2.7(8)	-11.3(9)
C6	24.7(9)	21.9(9)	16.6(8)	-4.5(7)	0.9(7)	-8.2(7)
C21	25.7(10)	22.2(9)	22.8(9)	-3.5(7)	-7.8(7)	-3.7(7)
C11	30.8(11)	34.5(12)	19.5(9)	-9.2(8)	-2.6(8)	-3.2(9)
C8	30.6(11)	28.0(10)	20.2(9)	1.4(8)	1.8(8)	-8.8(8)
C20	40.5(12)	28.7(11)	21.5(9)	-3.7(8)	-10.9(9)	-9.3(9)

C13	29.3(10)	29.2(11)	19.9(9)	-2.1(8)	-1.1(8)	-9.1(8)
C12	37.2(12)	31.6(11)	27.8(11)	-8.3(9)	-5.0(9)	-11.3(9)
C19	40.6(12)	24.1(10)	25.3(10)	-9.8(8)	-5.2(9)	-6.4(9)
C18	30.2(10)	20.0(9)	26.3(10)	-6.1(8)	-4.9(8)	-1.2(8)
C4	39.9(12)	25.2(10)	20.7(9)	4.6(8)	-2.4(9)	-7.7(9)
C3	31.6(11)	23.9(10)	20.5(9)	3.3(7)	-3.8(8)	-0.6(8)
C16	29.0(10)	28.8(11)	26.4(10)	0.1(8)	-9.8(8)	-0.4(8)

Bond Lengths for 19OA_RRH114_P-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Cl1	2.2644(5)	C22	C17	1.404(3)
Au1	N3	2.0464(16)	C22	C23	1.426(3)
Au1	N1	2.0458(16)	C22	C21	1.401(3)
Au1	N2	1.9615(16)	C1	C2	1.504(3)
O2	C7	1.222(2)	C2	C3	1.386(3)
O1	C1	1.219(3)	C14	C9	1.403(3)
N3	C7	1.367(3)	C14	C15	1.425(3)
N3	C23	1.411(3)	C14	C13	1.406(3)
N1	C1	1.378(3)	C9	C10	1.406(3)
N1	C15	1.408(2)	C17	C18	1.400(3)
N4	N5	1.363(2)	C7	C6	1.497(3)
N4	C9	1.369(3)	C10	C11	1.371(3)
N4	C8	1.443(3)	C5	C6	1.381(3)
N7	N6	1.367(2)	C5	C4	1.387(3)
N7	C23	1.321(3)	C21	C20	1.380(3)
N5	C15	1.325(3)	C11	C12	1.409(3)
N2	C2	1.325(3)	C20	C19	1.405(3)
N2	C6	1.330(2)	C13	C12	1.378(3)
N6	C17	1.367(3)	C19	C18	1.372(3)
N6	C16	1.440(3)	C4	C3	1.386(3)

Bond Angles for 19OA_RRH114_P-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	Au1	Cl1	99.24(5)	C9	C14	C15	104.18(17)
N1	Au1	Cl1	98.93(5)	C9	C14	C13	119.98(18)
N1	Au1	N3	161.83(7)	C13	C14	C15	135.81(18)
N2	Au1	Cl1	179.75(5)	N4	C9	C14	106.66(16)
N2	Au1	N3	81.00(7)	N4	C9	C10	130.91(18)
N2	Au1	N1	80.83(7)	C14	C9	C10	122.42(19)
C7	N3	Au1	113.33(14)	N6	C17	C22	106.71(17)
C7	N3	C23	116.46(16)	N6	C17	C18	131.08(19)
C23	N3	Au1	128.62(13)	C18	C17	C22	122.21(19)
C1	N1	Au1	113.58(12)	N1	C15	C14	127.71(18)
C1	N1	C15	117.53(16)	N5	C15	N1	120.68(18)
C15	N1	Au1	126.43(13)	N5	C15	C14	111.59(16)
N5	N4	C9	111.63(15)	O2	C7	N3	126.0(2)
N5	N4	C8	120.25(17)	O2	C7	C6	120.21(19)
C9	N4	C8	128.07(17)	N3	C7	C6	113.78(17)
C23	N7	N6	105.65(16)	C11	C10	C9	116.13(19)
C15	N5	N4	105.92(16)	N3	C23	C22	126.10(18)
C2	N2	Au1	117.73(13)	N7	C23	N3	121.88(18)
C2	N2	C6	125.13(17)	N7	C23	C22	112.00(17)
C6	N2	Au1	117.12(14)	C6	C5	C4	118.5(2)
N7	N6	C17	111.69(17)	N2	C6	C7	114.65(17)
N7	N6	C16	120.91(17)	N2	C6	C5	118.6(2)
C17	N6	C16	127.27(18)	C5	C6	C7	126.67(18)
C17	C22	C23	103.90(17)	C20	C21	C22	117.8(2)
C21	C22	C17	119.96(18)	C10	C11	C12	122.5(2)
C21	C22	C23	136.13(19)	C21	C20	C19	121.3(2)
O1	C1	N1	125.94(18)	C12	C13	C14	117.8(2)
O1	C1	C2	120.87(19)	C13	C12	C11	121.1(2)

N1	C1	C2	113.16(17)	C18	C19	C20	122.0(2)
N2	C2	C1	114.50(17)	C19	C18	C17	116.7(2)
N2	C2	C3	118.38(18)	C3	C4	C5	120.7(2)
C3	C2	C1	126.98(19)	C4	C3	C2	118.7(2)

Torsion Angles for 19OA_RRH114_P-1.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Au1	N3	C7	O2	-78.60(19)	C9	C14	C15	N5	0.3(2)
Au1	N3	C7	C6	-0.2(2)	C9	C14	C13	C12	-0.4(3)
Au1	N3	C23	N7	-67.5(3)	C9	C10	C11	C12	-0.4(3)
Au1	N3	C23	C22	113.9(2)	C17	C22	C23	N3	178.07(18)
Au1	N1	C1	O1	-74.28(18)	C17	C22	C23	N7	-0.6(2)
Au1	N1	C1	C2	3.4(2)	C17	C22	C21	C20	-1.8(3)
Au1	N1	C15	N5	-68.6(2)	C15	N1	C1	O1	-10.9(3)
Au1	N1	C15	C14	109.7(2)	C15	N1	C1	C2	166.82(17)
Au1	N2	C2	C1	4.2(2)	C15	C14	C9	N4	0.5(2)
Au1	N2	C2	C3	179.85(16)	C15	C14	C9	C10	-178.98(18)
Au1	N2	C6	C7	3.9(2)	C15	C14	C13	C12	177.6(2)
Au1	N2	C6	C5	178.06(16)	C7	N3	C23	N7	128.0(2)
O2	C7	C6	N2	176.2(2)	C7	N3	C23	C22	-50.6(3)
O2	C7	C6	C5	-1.7(3)	C10	C11	C12	C13	-0.4(4)
O1	C1	C2	N2	172.9(2)	C23	N3	C7	O2	-11.7(3)
O1	C1	C2	C3	-2.7(3)	C23	N3	C7	C6	166.65(17)
N3	C7	C6	N2	-2.3(3)	C23	N7	N6	C17	2.1(2)
N3	C7	C6	C5	179.8(2)	C23	N7	N6	C16	178.26(19)
N1	C1	C2	N2	-5.0(3)	C23	C22	C17	N6	1.8(2)
N1	C1	C2	C3	179.5(2)	C23	C22	C17	C18	177.38(19)
N4	N5	C15	N1	177.71(17)	C23	C22	C21	C20	177.1(2)
N4	N5	C15	C14	-0.9(2)	C5	C4	C3	C2	0.7(4)
N4	C9	C10	C11	-178.5(2)	C6	N2	C2	C1	-73.93(18)
7	N6	C17	C22	-2.5(2)	C6	N2	C2	C3	2.0(3)
N7	N6	C17	C18	176.6(2)	C6	C5	C4	C3	1.3(4)
N5	N4	C9	C14	-1.1(2)	C21	C22	C17	N6	-79.00(18)
N5	N4	C9	C10	178.3(2)	C21	C22	C17	C18	1.8(3)

N2	C2	C3	C4	-2.4(3)	C21	C22	C23	N3	-0.9(4)
N6	N7	C23	N3	-79.58(17)	C21	C22	C23	N7	-179.6(2)
N6	N7	C23	C22	-0.8(2)	C21	C20	C19	C18	2.7(4)
N6	C17	C18	C19	-178.6(2)	C8	N4	N5	C15	178.98(18)
C22	C17	C18	C19	0.4(3)	C8	N4	C9	C14	-178.6(2)
C22	C21	C20	C19	-0.4(3)	C8	N4	C9	C10	0.8(4)
C1	N1	C15	N5	130.4(2)	C20	C19	C18	C17	-2.6(3)
C1	N1	C15	C14	-51.3(3)	C13	C14	C9	N4	179.07(19)
C1	C2	C3	C4	173.0(2)	C13	C14	C9	C10	-0.4(3)
C2	N2	C6	C7	-77.95(18)	C13	C14	C15	N1	3.5(4)
C2	N2	C6	C5	0.1(3)	C13	C14	C15	N5	-178.0(2)
C14	C9	C10	C11	0.8(3)	C4	C5	C6	N2	-1.8(3)
C14	C13	C12	C11	0.8(4)	C4	C5	C6	C7	176.0(2)
C9	N4	N5	C15	1.3(2)	C16	N6	C17	C22	-178.4(2)
C9	C14	C15	N1	-78.26(19)	C16	N6	C17	C18	0.7(4)

Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 19OA_RRH114_P-1.

Atom	*x*	*y*	*z*	U(eq)
H10	2902.53	6141.18	10928.4	28
H5	9654.28	7516.16	1675.96	33
H21	8872.4	3292.21	1696.77	28
H11	3976.46	8029.11	10960.9	34
H8A	1226.58	4334.6	9504.75	42
H8B	2320.31	4151.55	10390.31	42
H8C	2729.15	3245.78	9355.74	42
H20	9504.25	1674.36	432.94	35
H13	5968.04	8246.42	7500.33	32
H12	5469.62	9074.06	9284.27	38
H19	11052.62	-257	806.46	36
H18	11850.54	-714.04	2519.27	31
H4	7712.54	9309.53	2012.28	36
H3	5608.51	9274.28	3682.3	32
H16A	13237.69	293.4	4518.08	42
H16B	12069.41	-723.12	4488.14	42
H16C	11684.63	129.05	5558.12	42

Experimental

Single crystals of $C_{23}H_{17}AuClN_7O_2$ **[19OA_RRH114_P-1]** were **[grown from DMSO/tBuOH by vapour diffusion]**. A suitable crystal was selected and **[mounted in Paratone oil on a 100 um MiTeGeN cryoloop.]** on a **'Bruker APEX-II CCD'** diffractometer. The crystal was kept at 153.15 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [19OA_RRH114_P-1]

Crystal Data for $C_{23}H_{17}AuClN_7O_2$ (M =1311.70 g/mol): triclinic, space group P-1 (no. 2), a = 8.8115(3) Å, b = 10.4987(3) Å, c = 12.0821(4) Å, α = 82.449(2)°, β = 74.233(2)°, γ = 81.344(2)°, V = 1058.58(6) Å^3, Z = 2, T = 153.15 K, μ(MoKα) = 7.114 mm^{-1}, *Dcalc* = 2.058 g/cm^3, 59569 reflections measured (3.518° ≤ 2Θ ≤ 66.494°), 8133 unique (R_{int} = 0.0387, R_{sigma} = 0.0240) which were used in all calculations. The final R_1 was 0.0194 (I > 2σ(I)) and wR_2 was 0.0437 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C10(H10), C5(H5), C21(H21), C11(H11), C20(H20), C13(H13), C12(H12), C19(H19),
 C18(H18), C4(H4), C3(H3)
2.b Idealised Me refined as rotating group:
 C8(H8a,H8b,H8c), C16(H16a,H16b,H16c)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.7. 2e

Crystal data and structure refinement for 19oa_rr_bzkpin_0m.

Identification code	19oa_rr_bzkpin_0m
Empirical formula	$C_{33}H_{23}N_3O_4$
Formula weight	525.54
Temperature/K	153.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.4952(2)
b/Å	18.3345(4)
c/Å	16.2123(3)
α/°	90
β/°	90.6890(10)
γ/°	90
Volume/Å^3	2524.97(9)
Z	4
ρ_{calc}g/cm^3	1.382
μ/mm^{-1}	0.092
F(000)	1096.0
Crystal size/mm^3	0.22 × 0.16 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.354 to 56.762
Index ranges	$-11 \leq h \leq 11$, $-24 \leq k \leq 24$, $-21 \leq l \leq 20$
Reflections collected	38759
Independent reflections	6322 [R_{int} = 0.0562, R_{sigma} = 0.0479]
Data/restraints/parameters	6322/0/361
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0800, wR_2 = 0.1098
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25

Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 19oa_rr_bzkpin_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	9710.7(19)	3879.6(8)	2243.4(9)	25.5(3)
C2	9271(2)	3181.5(8)	2016.3(10)	27.2(4)
C3	7889(2)	3068.6(9)	1575.1(10)	28.6(4)
C4	6973(2)	3657.5(9)	1337.3(10)	28.6(4)
C5	7444.3(19)	4363.3(8)	1529.9(10)	25.5(3)
C6	8812.1(18)	4473.8(8)	1990.9(9)	21.8(3)
C7	9292.1(18)	5217.4(8)	2293.5(9)	23.1(3)
C8	9644.3(17)	5814.3(8)	1698.1(9)	20.4(3)
C9	9565.5(18)	5676.4(8)	848.7(9)	23.2(3)
C10	9983.0(19)	6196.7(8)	278.0(9)	24.9(3)
C11	10523.1(19)	6869.1(9)	550.5(10)	26.7(4)
C12	10620.2(19)	7027.8(8)	1380.1(9)	25.0(3)
C13	10175.2(18)	6509.8(8)	1959.8(9)	21.2(3)
C14	11087.2(18)	7170.3(8)	3213.4(9)	23.8(3)
C15	10757.2(18)	7177.0(8)	4122.1(9)	21.7(3)
C16	11769(2)	7531.5(9)	4667.8(10)	27.9(4)
C17	11422(2)	7518.6(9)	5499.6(10)	32.1(4)
C18	10087(2)	7158.9(9)	5756.6(10)	28.6(4)
C19	9131.2(18)	6822.8(8)	5168.8(9)	21.4(3)
C20	7638.0(19)	6449.4(8)	5420.6(9)	22.7(3)
C21	5126.2(18)	6012.0(8)	4778.0(9)	22.3(3)
C22	4303(2)	5929.8(8)	5513.7(10)	28.5(4)
C23	2772(2)	5669.3(9)	5502.6(11)	33.5(4)
C24	2031(2)	5497.3(9)	4764.1(11)	32.7(4)
C25	2828.2(19)	5579.9(8)	4033.3(11)	27.7(4)
C26	4383.4(18)	5827.7(8)	4016.6(10)	22.9(3)
C27	5162.6(19)	5920.3(8)	3208.2(10)	23.9(3)

C28	4482.2(18)	5578.8(9)	2441.9(9)	24.4(3)
C29	3906.8(19)	4866.4(9)	2411.3(10)	27.3(4)
C30	3416(2)	4567.5(10)	1668.4(11)	34.8(4)
C31	3464(2)	4978.4(11)	954.6(11)	39.2(4)
C32	4013(2)	5689.5(11)	982.7(11)	40.4(5)
C33	4539(2)	5982.8(9)	1718.0(10)	32.3(4)
N1	10203.4(16)	6672.3(7)	2801.8(7)	23.4(3)
N2	9459.0(15)	6827.7(6)	4363.8(7)	20.0(3)
N3	6666.7(15)	6288.4(7)	4774.0(8)	22.5(3)
O1	9445.4(15)	5294.7(6)	3042.7(7)	34.2(3)
O2	12056.3(15)	7577.9(7)	2912.7(7)	40.6(3)
O3	7367.9(14)	6335.8(6)	6149.5(6)	31.4(3)
O4	6364.1(14)	6288.8(6)	3134.8(7)	34.3(3)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 19oa_rr_bzkpin_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	23.2(8)	30.3(8)	22.9(8)	2.0(6)	-2.4(6)	-2.7(7)
C2	30.4(9)	23.6(8)	27.7(9)	3.9(7)	-2.7(7)	2.0(7)
C3	34.0(10)	22.4(8)	29.5(9)	-2.3(6)	0.1(7)	-4.6(7)
C4	24.2(9)	29.9(8)	31.5(9)	-1.5(7)	-4.7(7)	-5.5(7)
C5	23.2(9)	24.9(8)	28.5(9)	1.7(6)	-2.5(7)	-0.8(7)
C6	23.0(8)	22.5(7)	19.9(8)	1.6(6)	1.5(6)	-2.8(6)
C7	20.9(8)	25.8(8)	22.6(8)	-0.1(6)	0.7(6)	-3.4(6)
C8	19.0(8)	20.5(7)	21.5(8)	-0.8(6)	0.7(6)	-1.6(6)
C9	24.9(9)	21.9(7)	22.8(8)	-1.1(6)	-1.1(6)	0.2(6)
C10	27.5(9)	28.5(8)	18.6(8)	0.9(6)	-0.3(6)	1.1(7)
C11	28.9(9)	25.9(8)	25.2(8)	6.4(6)	2.4(7)	-1.4(7)
C12	26.3(9)	20.8(7)	27.8(8)	0.4(6)	0.0(7)	-3.3(6)
C13	18.9(8)	23.1(7)	21.4(8)	-1.3(6)	0.9(6)	-0.5(6)
C14	21.1(8)	24.2(8)	26.2(8)	-1.0(6)	-2.0(6)	-3.0(7)
C15	20.3(8)	18.8(7)	25.8(8)	-1.8(6)	-2.8(6)	2.0(6)
C16	25.3(9)	27.1(8)	31.0(9)	-4.0(7)	-3.8(7)	-4.0(7)
C17	33.5(10)	32.1(9)	30.5(9)	-8.2(7)	-8.1(8)	-3.7(8)
C18	33.8(10)	28.6(8)	23.2(8)	-4.3(7)	-3.0(7)	1.1(7)
C19	24.5(8)	16.7(7)	23.0(8)	-0.5(6)	-1.7(6)	5.1(6)
C20	28.4(9)	16.6(7)	23.2(8)	-1.1(6)	0.5(7)	5.8(6)
C21	23.0(8)	16.1(7)	27.9(8)	3.8(6)	4.5(7)	2.1(6)
C22	31.1(10)	24.6(8)	29.9(9)	5.4(7)	6.2(7)	4.6(7)
C23	34.2(10)	26.3(8)	40.3(10)	8.2(7)	16.1(8)	5.0(7)
C24	22.3(9)	24.7(8)	51.4(11)	6.2(8)	10.8(8)	0.2(7)
C25	23.2(9)	20.8(7)	39.0(10)	1.8(7)	1.8(7)	2.0(7)
C26	21.5(8)	16.9(7)	30.4(9)	3.6(6)	4.1(7)	2.5(6)
C27	22.0(8)	19.4(7)	30.2(9)	4.4(6)	-0.6(7)	0.0(6)

C28	17.9(8)	28.3(8)	27.1(8)	2.9(6)	-0.6(6)	0.8(6)
C29	21.3(9)	28.0(8)	32.8(9)	2.1(7)	-0.4(7)	-1.2(7)
C30	21.4(9)	38.9(10)	44.0(11)	-9.2(8)	0.5(8)	-4.4(7)
C31	26.3(10)	59.4(12)	31.8(10)	-7.8(9)	-7.3(8)	-0.5(9)
C32	36.9(11)	55.1(12)	28.9(10)	10.5(8)	-5.4(8)	6.1(9)
C33	33.7(10)	32.0(9)	31.3(9)	7.5(7)	-2.2(8)	1.2(8)
N1	27.8(7)	22.6(6)	20.0(6)	-1.6(5)	3.2(5)	-7.4(6)
N2	21.1(7)	17.0(6)	21.9(7)	-1.1(5)	-1.8(5)	2.0(5)
N3	23.8(7)	23.1(6)	20.7(7)	0.8(5)	2.9(5)	-0.7(5)
O1	50.3(8)	30.5(6)	21.7(6)	0.2(5)	-0.9(5)	-11.9(6)
O2	40.3(8)	50.0(8)	31.7(7)	-0.3(6)	0.2(6)	-24.8(6)
O3	39.4(7)	33.1(6)	21.7(6)	0.4(5)	2.1(5)	0.1(5)
O4	32.5(7)	40.2(7)	30.2(6)	1.2(5)	2.2(5)	-15.2(6)

Bond Lengths for 19oa_rr_bzkpin_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.382(2)	C17	C18	1.380(2)
C1	C6	1.389(2)	C18	C19	1.389(2)
C2	C3	1.383(2)	C19	C20	1.502(2)
C3	C4	1.383(2)	C19	N2	1.3378(19)
C4	C5	1.389(2)	C20	N3	1.3588(19)
C5	C6	1.389(2)	C20	O3	1.2244(18)
C6	C7	1.504(2)	C21	C22	1.398(2)
C7	C8	1.492(2)	C21	C26	1.420(2)
C7	O1	1.2283(18)	C21	N3	1.4035(19)
C8	C9	1.401(2)	C22	C23	1.386(2)
C8	C13	1.416(2)	C23	C24	1.382(3)
C9	C10	1.378(2)	C24	C25	1.380(2)
C10	C11	1.386(2)	C25	C26	1.398(2)
C11	C12	1.378(2)	C26	C27	1.485(2)
C12	C13	1.392(2)	C27	C28	1.501(2)
C13	N1	1.3972(18)	C27	O4	1.2310(18)
C14	C15	1.503(2)	C28	C29	1.395(2)
C14	N1	1.3528(19)	C28	C33	1.389(2)
C14	O2	1.2181(18)	C29	C30	1.383(2)
C15	C16	1.388(2)	C30	C31	1.382(3)
C15	N2	1.3381(19)	C31	C32	1.385(3)
C16	C17	1.384(2)	C32	C33	1.377(2)

Bond Angles for 19oa_rr_bzkpin_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	120.14(15)	C18	C19	C20	120.30(14)
C1	C2	C3	120.10(15)	N2	C19	C18	122.65(15)
C2	C3	C4	119.91(14)	N2	C19	C20	117.03(13)
C3	C4	C5	120.31(15)	N3	C20	C19	113.35(13)
C6	C5	C4	119.60(15)	O3	C20	C19	120.56(14)
C1	C6	C7	117.98(14)	O3	C20	N3	126.06(15)
C5	C6	C1	119.83(14)	C22	C21	C26	119.63(15)
C5	C6	C7	121.98(14)	C22	C21	N3	121.25(15)
C8	C7	C6	120.65(13)	N3	C21	C26	119.10(13)
O1	C7	C6	116.89(13)	C23	C22	C21	120.34(16)
O1	C7	C8	122.38(14)	C24	C23	C22	120.50(16)
C9	C8	C7	119.73(13)	C25	C24	C23	119.71(16)
C9	C8	C13	117.93(13)	C24	C25	C26	121.73(16)
C13	C8	C7	122.17(13)	C21	C26	C27	122.80(14)
C10	C9	C8	121.69(14)	C25	C26	C21	118.08(14)
C9	C10	C11	119.25(14)	C25	C26	C27	119.06(15)
C12	C11	C10	120.98(14)	C26	C27	C28	120.76(14)
C11	C12	C13	120.11(14)	O4	C27	C26	121.80(14)
C12	C13	C8	120.02(14)	O4	C27	C28	117.42(14)
C12	C13	N1	120.84(13)	C29	C28	C27	123.46(14)
N1	C13	C8	119.11(13)	C33	C28	C27	117.37(14)
N1	C14	C15	112.34(13)	C33	C28	C29	119.00(15)
O2	C14	C15	121.48(14)	C30	C29	C28	120.25(16)
O2	C14	N1	126.18(14)	C31	C30	C29	120.11(17)
C16	C15	C14	120.48(14)	C30	C31	C32	119.92(17)
N2	C15	C14	116.57(13)	C33	C32	C31	120.10(17)
N2	C15	C16	122.95(14)	C32	C33	C28	120.58(17)
C17	C16	C15	118.37(16)	C14	N1	C13	128.96(13)
C18	C17	C16	119.20(15)	C19	N2	C15	118.09(13)
C17	C18	C19	118.72(15)	C20	N3	C21	129.23(13)

Hydrogen Bonds for 19oa_rr_bzkpin_0m.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C22	H22	O3	0.95	2.25	2.886(2)	123.4
N1	H1A	O1	0.88	2.06	2.6368(16)	122.3
N3	H3A	O4	0.88	1.95	2.6669(16)	137.5

Torsion Angles for 19oa_rr_bzkpin_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	2.1(2)	C21	C22	C23	C24	-0.9(2)
C1	C6	C7	C8	122.93(16)	C21	C26	C27	C28	167.17(14)
C1	C6	C7	O1	-53.9(2)	C21	C26	C27	O4	-14.3(2)
C2	C1	C6	C5	1.9(2)	C22	C21	C26	C25	1.1(2)
C2	C1	C6	C7	176.71(14)	C22	C21	C26	C27	178.15(13)
C2	C3	C4	C5	0.9(2)	C22	C21	N3	C20	6.6(2)
C3	C4	C5	C6	-2.5(2)	C22	C23	C24	C25	0.5(2)
C4	C5	C6	C1	1.1(2)	C23	C24	C25	C26	0.7(2)
C4	C5	C6	C7	-173.48(14)	C24	C25	C26	C21	-1.5(2)
C5	C6	C7	C8	-62.4(2)	C24	C25	C26	C27	-178.65(14)
C5	C6	C7	O1	120.82(17)	C25	C26	C27	C28	-15.8(2)
C6	C1	C2	C3	-3.5(2)	C25	C26	C27	O4	162.72(15)
C6	C7	C8	C9	-1.6(2)	C26	C21	C22	C23	0.1(2)
C6	C7	C8	C13	-176.77(14)	C26	C21	N3	C20	-174.73(14)
C7	C8	C9	C10	-175.58(15)	C26	C27	C28	C29	-43.8(2)
C7	C8	C13	C12	174.35(14)	C26	C27	C28	C33	140.86(15)
C7	C8	C13	N1	-7.4(2)	C27	C28	C29	C30	-174.65(15)
C8	C9	C10	C11	1.2(2)	C27	C28	C33	C32	176.57(15)
C8	C13	N1	C14	156.38(15)	C28	C29	C30	C31	-1.3(3)
C9	C8	C13	C12	-0.9(2)	C29	C28	C33	C32	1.0(3)
C9	C8	C13	N1	177.37(14)	C29	C30	C31	C32	0.4(3)
C9	C10	C11	C12	-1.2(2)	C30	C31	C32	C33	1.2(3)
C10	C11	C12	C13	0.1(2)	C31	C32	C33	C28	-1.9(3)
C11	C12	C13	C8	1.0(2)	C33	C28	C29	C30	0.6(2)
C11	C12	C13	N1	-177.28(14)	N1	C14	C15	C16	166.02(14)
C12	C13	N1	C14	-25.3(2)	N1	C14	C15	N2	-13.94(19)
C13	C8	C9	C10	-0.2(2)	N2	C15	C16	C17	0.4(2)
C14	C15	C16	C17	-179.57(14)	N2	C19	C20	N3	-12.07(18)

C14	C15	N2	C19	179.96(13)	N2	C19	C20	O3	169.97(13)
C15	C14	N1	C13	179.76(14)	N3	C21	C22	C23	178.72(14)
C15	C16	C17	C18	-0.2(2)	N3	C21	C26	C25	-177.59(13)
C16	C15	N2	C19	0.0(2)	N3	C21	C26	C27	-0.5(2)
C16	C17	C18	C19	-0.2(2)	O1	C7	C8	C9	175.02(15)
C17	C18	C19	C20	-177.76(14)	O1	C7	C8	C13	-0.2(2)
C17	C18	C19	N2	0.6(2)	O2	C14	C15	C16	-13.8(2)
C18	C19	C20	N3	166.42(13)	O2	C14	C15	N2	166.20(15)
C18	C19	C20	O3	-11.5(2)	O2	C14	N1	C13	-0.4(3)
C18	C19	N2	C15	-0.5(2)	O3	C20	N3	C21	5.0(2)
C19	C20	N3	C21	-172.85(13)	O4	C27	C28	C29	137.62(16)
C20	C19	N2	C15	177.93(12)	O4	C27	C28	C33	-37.7(2)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 19oa_rr_bzkpin_0m.

Atom	*x*	*y*	*z*	U(eq)
H1	10629.3	3953.26	2572.91	31
H2	9919.25	2778.65	2163.43	33
H3	7569.98	2587.15	1435.4	34
H4	6016.27	3578.86	1040.97	34
H5	6834.89	4768.02	1347.35	31
H9	9215.24	5212.38	661.27	28
H10	9901.43	6095.48	-295.58	30
H11	10830.96	7225.91	159.3	32
H12	10991.65	7491.56	1556.79	30
H16	12678.54	7777.06	4475.18	33
H17	12093.52	7754.51	5888.96	39
H18	9827.76	7141.53	6324.6	34
H22	4796.61	6053.14	6023.86	34
H23	2227.24	5608.58	6006.24	40
H24	978.01	5322.96	4759.67	39
H25	2306.06	5465.28	3528.32	33
H29	3851.64	4585.68	2902.6	33
H30	3045.94	4078.81	1648.75	42
H31	3120.34	4773.47	445.27	47
H32	4027.11	5975.28	494.05	48
H33	4945.05	6465.61	1730.14	39
H1A	9556.96	6415.28	3106.58	28
H3A	7059.57	6368.97	4282.54	27

Experimental

Single crystals of $C_{33}H_{23}N_3O_4$ [19oa_rr_bzkpin_0m] were [ROOM TEMPERATURE]. A suitable crystal was selected and [] on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 153.15 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

2.

Crystal structure determination of [19oa_rr_bzkpin_0m]

Crystal Data for $C_{33}H_{23}N_3O_4$ (M =525.54 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 8.4952(2) Å, b = 18.3345(4) Å, c = 16.2123(3) Å, β = 90.6890(10)°, V = 2524.97(9) Å^3, Z = 4, T = 153.15 K, μ(MoKα) = 0.092 mm^{-1}, *Dcalc* = 1.382 g/cm^3, 38759 reflections measured (3.354° ≤ 2Θ ≤ 56.762°), 6322 unique (R_{int} = 0.0562, R_{sigma} = 0.0479) which were used in all calculations. The final R_1 was 0.0452 (I > 2σ(I)) and wR_2 was 0.1098 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All N(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C1(H1), C2(H2), C3(H3), C4(H4), C5(H5), C9(H9), C10(H10), C11(H11), C12(H12),
 C16(H16), C17(H17), C18(H18), C22(H22), C23(H23), C24(H24), C25(H25), C29(H29),
  C30(H30), C31(H31), C32(H32), C33(H33), N1(H1A), N3(H3A)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.8. 2di

Crystal data and structure refinement for 19oa_RR_H91_AuInDZ_0a.

Identification code	19oa_RR_H91_AuInDZ_0a
Empirical formula	$C_{23}H_{17}AgAuClFN_7O_2$
Formula weight	782.72
Temperature/K	173.15
Crystal system	triclinic
Space group	P-1
a/Å	8.670(3)
b/Å	11.448(4)
c/Å	13.101(5)
α/°	105.909(19)
β/°	97.97(2)
γ/°	97.98(2)
Volume/Å^3	1216.9(8)
Z	2
ρ_{calc}g/cm^3	2.136
μ/mm^{-1}	6.979
F(000)	744.0
Crystal size/mm^3	0.18 × 0.05 × 0.044
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.29 to 56.89
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 15, -17 ≤ l ≤ 17
Reflections collected	33090
Independent reflections	6077 [R_{int} = 0.0829, R_{sigma} = 0.0654]
Data/restraints/parameters	6077/0/327
Goodness-of-fit on F^2	1.112
Final R indexes [I>=2σ (I)]	R_1 = 0.0532, wR_2 = 0.1244
Final R indexes [all data]	R_1 = 0.0811, wR_2 = 0.1381
Largest diff. peak/hole / e Å^{-3}	3.55/-2.86

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 19oa_RR_H91_AuInDZ_0a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au1	4583.8(4)	6709.3(3)	5609.0(3)	21.42(12)
Ag1	3629.4(9)	9677.9(6)	6876.4(6)	26.17(18)
Cl1	2088(3)	6084(2)	5852(2)	36.6(6)
F1	3316(9)	10441(5)	5508(5)	42.4(17)
O1	5656(10)	5864(7)	2600(6)	38.0(18)
O2	8027(10)	8861(7)	8142(6)	39.2(18)
N1	4240(11)	5926(7)	3975(6)	28.7(18)
N2	6771(10)	7171(7)	5405(6)	22.8(16)
N3	5611(10)	7703(7)	7162(6)	28.1(18)
N4	2075(11)	4436(7)	2828(7)	30.9(19)
N5	762(11)	4458(8)	2120(7)	35(2)
N6	3919(10)	8901(7)	8044(7)	28.3(18)
N7	3344(10)	9108(7)	8985(7)	27.9(18)
C1	5614(12)	6143(8)	3558(8)	27(2)
C2	7059(12)	6800(8)	4402(8)	26(2)
C3	8563(13)	7123(10)	4219(8)	33(2)
C4	9735(14)	7854(10)	5108(9)	40(3)
C5	9377(13)	8193(10)	6131(8)	34(2)
C6	7843(12)	7842(8)	6268(8)	27(2)
C7	7173(13)	8169(8)	7289(8)	29(2)
C8	2777(12)	5610(8)	3252(8)	24.8(19)
C9	1943(12)	6417(8)	2861(8)	25.4(19)
C10	2141(15)	7707(10)	3031(10)	38(3)
C11	1021(17)	8120(11)	2428(12)	49(3)
C12	-252(16)	7334(13)	1708(11)	51(3)
C13	-477(15)	6059(11)	1517(10)	42(3)
C14	635(13)	5620(9)	2106(8)	29(2)
C15	-362(16)	3324(10)	1541(10)	49(3)
C16	4829(12)	8042(8)	8026(8)	26(2)
C17	4854(12)	7674(8)	8970(7)	24.6(19)
C18	5564(14)	6806(9)	9352(8)	32(2)
C19	5306(15)	6696(10)	10336(9)	40(3)
C20	4361(14)	7449(10)	10944(9)	36(2)
C21	3664(13)	8273(9)	10583(8)	31(2)
C22	3900(12)	8384(8)	9576(8)	25(2)
C23	2257(12)	9957(9)	9224(9)	32(2)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 19oa_RR_H91_AuInDZ_0a. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	24.3(2)	20.13(17)	16.37(17)	2.33(12)	1.45(13)	1.43(12)
Ag1	30.4(4)	21.5(3)	22.9(4)	5.0(3)	-0.6(3)	1.5(3)
Cl1	31.5(14)	39.1(13)	34.4(14)	5.3(11)	9.3(11)	-1.0(10)
F1	66(5)	17(3)	39(4)	12(2)	-7(3)	0(3)
O1	44(5)	43(4)	19(4)	2(3)	3(3)	-1(3)
O2	41(5)	42(4)	21(4)	-3(3)	1(3)	-9(3)
N1	40(5)	26(4)	13(4)	1(3)	-3(4)	1(3)
N2	26(4)	26(4)	17(4)	5(3)	10(3)	6(3)
N3	31(5)	29(4)	17(4)	-1(3)	4(3)	-4(3)
N4	34(5)	23(4)	30(5)	4(3)	-2(4)	2(3)
N5	35(5)	34(4)	26(5)	-1(4)	-3(4)	-1(4)
N6	34(5)	23(4)	20(4)	-2(3)	2(4)	-3(3)
N7	28(5)	26(4)	24(4)	2(3)	3(4)	1(3)
C1	34(6)	25(4)	16(5)	3(3)	0(4)	-1(4)
C2	27(5)	26(4)	24(5)	7(4)	3(4)	2(4)
C3	39(6)	39(5)	18(5)	2(4)	9(4)	2(4)
C4	32(6)	46(6)	33(6)	3(5)	7(5)	-9(5)
C5	31(6)	42(6)	22(5)	3(4)	-1(4)	-3(4)
C6	33(6)	24(4)	20(5)	4(3)	5(4)	1(4)
C7	33(6)	24(4)	25(5)	5(4)	5(4)	-1(4)
C8	25(5)	25(4)	20(5)	3(3)	2(4)	-3(4)
C9	28(5)	26(4)	21(5)	7(4)	6(4)	3(4)
C10	48(7)	31(5)	39(6)	12(5)	21(6)	7(5)
C11	63(9)	36(6)	69(9)	29(6)	38(8)	24(6)
C12	45(8)	70(9)	49(8)	28(7)	12(6)	23(7)
C13	43(7)	45(6)	36(6)	10(5)	3(5)	16(5)
C14	35(6)	35(5)	22(5)	11(4)	12(4)	11(4)
C15	52(8)	37(6)	40(7)	3(5)	-16(6)	-8(5)
C16	28(5)	25(4)	18(5)	1(3)	1(4)	-6(4)
C17	26(5)	26(4)	17(4)	0(3)	5(4)	-1(4)
C18	42(6)	30(5)	19(5)	1(4)	6(4)	4(4)
C19	55(8)	33(5)	28(6)	7(4)	-1(5)	7(5)
C20	47(7)	37(5)	21(5)	8(4)	5(5)	-3(5)
C21	31(6)	32(5)	22(5)	0(4)	7(4)	-1(4)
C22	29(5)	22(4)	19(5)	1(3)	3(4)	-3(4)
C23	29(6)	28(5)	31(6)	-1(4)	1(4)	0(4)

Bond Lengths for 19oa_RR_H91_AuInDZ_0a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Cl1	2.277(3)	N7	C23	1.450(13)
Au1	N1	2.042(8)	C1	C2	1.502(14)
Au1	N2	1.971(8)	C2	C3	1.377(15)
Au1	N3	2.043(8)	C3	C4	1.411(15)
Ag1	F1	2.200(6)	C4	C5	1.380(15)
Ag1	N6	1.973(8)	C5	C6	1.386(15)
O1	C1	1.214(12)	C6	C7	1.507(14)
O2	C7	1.243(12)	C8	C9	1.408(13)
N1	C1	1.397(14)	C9	C10	1.414(13)
N1	C8	1.411(13)	C9	C14	1.415(14)
N2	C2	1.336(12)	C10	C11	1.383(18)
N2	C6	1.329(12)	C11	C12	1.37(2)
N3	C7	1.355(13)	C12	C13	1.393(18)
N3	C16	1.392(13)	C13	C14	1.385(15)
N4	N5	1.372(12)	C16	C17	1.410(13)
N4	C8	1.325(12)	C17	C18	1.405(14)
N5	C14	1.355(13)	C17	C22	1.410(13)
N5	C15	1.454(13)	C18	C19	1.374(15)
N6	N7	1.367(12)	C19	C20	1.432(17)
N6	C16	1.341(13)	C20	C21	1.343(15)
N7	C22	1.371(12)	C21	C22	1.400(14)

Bond Angles for 19oa_RR_H91_AuInDZ_0a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
N1	Au1	Cl1	98.2(3)	C4	C5	C6	119.2(10)
N1	Au1	N3	161.9(3)	N2	C6	C5	118.5(9)
N2	Au1	Cl1	177.1(2)	N2	C6	C7	113.4(9)
N2	Au1	N1	81.6(3)	C5	C6	C7	128.1(9)
N2	Au1	N3	80.5(3)	O2	C7	N3	125.6(10)
N3	Au1	Cl1	99.8(3)	O2	C7	C6	119.9(9)
N6	Ag1	F1	176.7(3)	N3	C7	C6	114.4(8)
C1	N1	Au1	112.5(6)	N4	C8	N1	120.1(8)
C1	N1	C8	117.5(8)	N4	C8	C9	112.7(9)
C8	N1	Au1	126.1(7)	C9	C8	N1	127.2(8)
C2	N2	Au1	117.3(7)	C8	C9	C10	136.2(10)
C6	N2	Au1	117.9(6)	C8	C9	C14	103.9(8)
C6	N2	C2	124.7(9)	C10	C9	C14	119.8(9)
C7	N3	Au1	113.9(7)	C11	C10	C9	116.8(11)
C7	N3	C16	119.4(8)	C12	C11	C10	122.6(11)
C16	N3	Au1	126.3(7)	C11	C12	C13	122.0(12)
C8	N4	N5	104.7(8)	C14	C13	C12	116.6(12)
N4	N5	C15	120.3(9)	N5	C14	C9	106.3(8)
C14	N5	N4	112.4(8)	N5	C14	C13	131.5(10)
C14	N5	C15	127.2(10)	C13	C14	C9	122.2(9)
N7	N6	Ag1	130.3(6)	N3	C16	C17	131.2(9)
C16	N6	Ag1	122.2(7)	N6	C16	N3	118.7(8)
C16	N6	N7	107.5(8)	N6	C16	C17	110.1(9)
N6	N7	C22	110.2(8)	C16	C17	C22	105.3(9)
N6	N7	C23	120.9(8)	C18	C17	C16	134.1(9)
C22	N7	C23	128.9(9)	C18	C17	C22	120.6(9)
O1	C1	N1	124.0(9)	C19	C18	C17	117.4(10)
O1	C1	C2	121.8(10)	C18	C19	C20	120.8(10)
N1	C1	C2	114.1(8)	C21	C20	C19	122.4(10)
N2	C2	C1	114.1(9)	C20	C21	C22	117.4(10)
N2	C2	C3	119.3(9)	N7	C22	C17	107.0(8)
C3	C2	C1	126.4(9)	N7	C22	C21	131.5(9)
C2	C3	C4	117.9(10)	C21	C22	C17	121.5(9)
C5	C4	C3	120.3(10)				

Torsion Angles for 19oa_RR_H91_AuInDZ_0a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Au1	N1	C1	O1	-173.0(8)	C2	C3	C4	C5	2.1(17)
Au1	N1	C1	C2	5.0(10)	C3	C4	C5	C6	-2.1(17)
Au1	N1	C8	N4	-105.9(10)	C4	C5	C6	N2	1.0(15)
Au1	N1	C8	C9	77.3(12)	C4	C5	C6	C7	-176.1(10)
Au1	N2	C2	C1	3.7(10)	C5	C6	C7	O2	1.9(16)
Au1	N2	C2	C3	178.7(7)	C5	C6	C7	N3	178.7(10)
Au1	N2	C6	C5	-178.7(7)	C6	N2	C2	C1	-175.2(8)
Au1	N2	C6	C7	-1.2(10)	C6	N2	C2	C3	-0.2(14)
Au1	N3	C7	O2	175.5(8)	C7	N3	C16	N6	101.3(11)
Au1	N3	C7	C6	-1.1(10)	C7	N3	C16	C17	-75.6(13)
Au1	N3	C16	N6	-70.4(10)	C8	N1	C1	O1	-13.9(14)
Au1	N3	C16	C17	112.7(11)	C8	N1	C1	C2	164.1(8)
Ag1	N6	N7	C22	-177.7(6)	C8	N4	N5	C14	-0.5(12)
Ag1	N6	N7	C23	4.5(12)	C8	N4	N5	C15	-176.4(10)
Ag1	N6	C16	N3	0.9(12)	C8	C9	C10	C11	177.8(12)
Ag1	N6	C16	C17	178.5(6)	C8	C9	C14	N5	1.2(11)
O1	C1	C2	N2	172.3(9)	C8	C9	C14	C13	-178.7(10)
O1	C1	C2	C3	-2.3(15)	C9	C10	C11	C12	1.3(18)
N1	C1	C2	N2	-5.8(12)	C10	C9	C14	N5	180.0(9)
N1	C1	C2	C3	179.7(9)	C10	C9	C14	C13	0.1(15)
N1	C8	C9	C10	-3.1(19)	C10	C11	C12	C13	-2(2)
N1	C8	C9	C14	175.5(10)	C11	C12	C13	C14	1.2(19)
N2	C2	C3	C4	-0.9(15)	C12	C13	C14	N5	179.7(11)
N2	C6	C7	O2	-175.3(9)	C12	C13	C14	C9	-0.4(17)
N2	C6	C7	N3	1.5(12)	C14	C9	C10	C11	-0.5(15)
N3	C16	C17	C18	-4.7(18)	C15	N5	C14	C9	175.1(11)
N3	C16	C17	C22	176.5(9)	C15	N5	C14	C13	-5(2)
N4	N5	C14	C9	-0.5(12)	C16	N3	C7	O2	2.8(15)
N4	N5	C14	C13	179.4(11)	C16	N3	C7	C6	-173.8(8)
N4	C8	C9	C10	179.9(11)	C16	N6	N7	C22	0.4(10)
N4	C8	C9	C14	-1.6(11)	C16	N6	N7	C23	-177.4(8)
N5	N4	C8	N1	-176.0(9)	C16	C17	C18	C19	-179.5(11)
N5	N4	C8	C9	1.3(12)	C16	C17	C22	N7	0.8(10)
N6	N7	C22	C17	-0.8(10)	C16	C17	C22	C21	-179.3(9)
N6	N7	C22	C21	179.3(10)	C17	C18	C19	C20	-0.6(16)
N6	C16	C17	C18	178.2(10)	C18	C17	C22	N7	-178.1(9)
N6	C16	C17	C22	-0.6(10)	C18	C17	C22	C21	1.7(14)
N7	N6	C16	N3	-177.4(8)	C18	C19	C20	C21	1.3(18)
N7	N6	C16	C17	0.1(10)	C19	C20	C21	C22	-0.4(16)
C1	N1	C8	N4	98.1(11)	C20	C21	C22	N7	178.8(10)
C1	N1	C8	C9	-78.7(13)	C20	C21	C22	C17	-1.0(14)
C1	C2	C3	C4	173.4(10)	C22	C17	C18	C19	-0.9(15)
C2	N2	C6	C5	0.2(14)	C23	N7	C22	C17	176.8(9)
C2	N2	C6	C7	177.7(8)	C23	N7	C22	C21	-3.1(17)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 19oa_RR_H91_AuInDZ_0a.

Atom	*x*	*y*	*z*	U(eq)
H3	8805.07	6861.86	3515.28	40
H4	10774.21	8114.64	5002.97	48
H5	10173.82	8661.67	6734.16	41
H10	3003.23	8263.96	3536.95	45
H11	1136.3	8980.83	2514.02	59
H12	-1001.1	7671.2	1328.32	61
H13	-1348.02	5517.33	1008.43	50
H15A	31.87	2621.54	1705.57	73
H15B	-487.58	3207.01	762.75	73
H15C	-1388.67	3378.92	1765.66	73
H18	6197.09	6315.15	8946.83	39
H19	5759.63	6112.3	10615.62	48
H20	4222.39	7362.58	11628.54	44
H21	3034.66	8762.02	10995.03	37
H23A	2644.6	10719.76	9061.22	48
H23B	2184.79	10151.31	9990.41	48
H23C	1206.63	9575.62	8781.72	48

Experimental

Single crystals of $C_{23}H_{17}AgAuClFN_7O_2$ [**19oa_RR_H91_AuInDZ_0a**] were crystallized by vapor diffusion of methanol into a DMSO solution of the compound. A suitable crystal was selected and mounted in NVH oil on a MiTeGen 100-micron cryoloop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173.15 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [19oa_RR_H91_AuInDZ_0a]

Crystal Data for $C_{23}H_{17}AgAuClFN_7O_2$ (*M* =782.72 g/mol): triclinic, space group P-1 (no. 2), *a* = 8.670(3) Å, *b* = 11.448(4) Å, *c* = 13.101(5) Å, *α* = 105.909(19)°, *β* = 97.97(2)°, *γ* = 97.98(2)°, *V* = 1216.9(8) Å^3, *Z* = 2, *T* = 173.15 K, μ(MoKα) = 6.979 mm^{-1}, *Dcalc* = 2.136 g/cm^3, 33090 reflections measured (3.29° ≤ 2Θ ≤ 56.89°), 6077 unique (R_{int} = 0.0829, R_{sigma} = 0.0654) which were used in all calculations. The final R_1 was 0.0532 (I > 2σ(I)) and wR_2 was 0.1381 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C3(H3), C4(H4), C5(H5), C10(H10), C11(H11), C12(H12), C13(H13), C18(H18),
 C19(H19), C20(H20), C21(H21)
2.b Idealised Me refined as rotating group:
 C15(H15A,H15B,H15C), C23(H23A,H23B,H23C)

S2.9. 2dii

Crystal data and structure refinement for 19oa_rr_rrh113_0m

Identification code	19oa_rr_rrh113_0m
Empirical formula	$C_{46}H_{32}Au_{2.71}Cl_{2.71}N_{14}O_4$
Formula weight	1474.70
Temperature/K	153.2
Crystal system	triclinic
Space group	P-1
a/Å	8.5381(4)
b/Å	11.3000(5)
c/Å	13.1055(6)
α/°	104.735(2)
β/°	97.970(3)
γ/°	98.032(3)
Volume/Å^3	1190.64(10)
Z	1
ρ_{calc}g/cm^3	2.057
μ/mm^{-1}	8.542
F(000)	698.0
Crystal size/mm^3	0.05 × 0.035 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.268 to 58.068
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 15, -17 ≤ l ≤ 17
Reflections collected	32923
Independent reflections	6309 [R_{int} = 0.0476, R_{sigma} = 0.0405]
Data/restraints/parameters	6309/0/328
Goodness-of-fit on F^2	1.336
Final R indexes [I>=2σ (I)]	R_1 = 0.0569, wR_2 = 0.1326
Final R indexes [all data]	R_1 = 0.0728, wR_2 = 0.1390
Largest diff. peak/hole / e Å^{-3}	3.96/-3.72

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 19oa_rr_rrh113_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au1	5389.1(5)	3248.4(4)	4417.9(3)	23.52(11)
Au2	6261.9(12)	301.9(9)	3209.8(8)	19.6(3)
Cl1	7906(3)	3912(3)	4180(2)	37.1(6)
Cl2	6384(13)	-383(8)	4674(7)	48(2)
O1	1970(10)	1032(8)	1918(6)	41(2)
O2	4278(11)	4050(8)	7405(6)	43(2)
N1	4388(12)	2222(9)	2890(7)	37(2)
N2	3214(11)	2753(9)	4637(7)	30.0(19)
N3	5683(11)	4050(8)	6021(7)	30.0(19)
N4	6117(12)	1015(9)	1998(7)	36(2)
N5	6677(11)	823(8)	1064(7)	33(2)
N6	7882(11)	5590(8)	7109(7)	30.9(19)
N7	9210(11)	5611(9)	7807(8)	35(2)
C1	2809(13)	1714(10)	2750(8)	31(2)
C2	2136(13)	2039(10)	3781(8)	31(2)
C3	590(14)	1615(12)	3901(9)	40(3)
C4	226(14)	1964(13)	4919(10)	43(3)
C5	1360(14)	2690(12)	5778(9)	41(3)
C6	2894(14)	3082(11)	5610(8)	32(2)
C7	4347(13)	3784(11)	6447(8)	31(2)
C8	5203(13)	1878(10)	2025(8)	31(2)
C9	5153(12)	2308(10)	1109(8)	30(2)
C10	4464(14)	3189(11)	746(10)	38(3)
C11	4724(16)	3312(11)	-259(10)	43(3)
C12	5680(15)	2610(11)	-840(10)	40(3)
C13	6376(14)	1720(11)	-503(9)	36(3)
C14	6126(12)	1587(9)	498(8)	27(2)

C15	7742(15)	-48(11)	788(10)	41(3)
C16	7191(12)	4413(9)	6742(8)	25(2)
C17	8056(13)	3627(10)	7193(8)	28(2)
C18	7895(15)	2356(11)	7087(10)	37(3)
C19	9041(16)	1960(13)	7734(12)	46(3)
C20	10349(17)	2825(14)	8425(11)	50(3)
C21	10536(14)	4056(12)	8532(10)	39(3)
C22	9367(13)	4454(10)	7898(8)	31(2)
C23	10337(16)	6760(12)	8343(11)	50(3)

Anisotropic Displacement Parameters ($Å^2×10^3$) for 19oa_rr_rrh113_0m. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	24.17(19)	25.84(19)	17.43(16)	4.29(12)	3.16(12)	-1.87(13)
Au2	23.6(6)	12.0(5)	22.4(5)	6.8(3)	-1.0(4)	2.4(3)
Cl1	29.2(13)	44.3(15)	32.2(13)	6.0(11)	8.5(11)	-5.7(11)
Cl2	74(6)	30(4)	37(4)	23(3)	-16(4)	-3(4)
O1	39(5)	48(5)	25(4)	2(3)	4(3)	-10(4)
O2	44(5)	57(5)	24(4)	5(4)	13(4)	0(4)
N1	38(5)	40(5)	23(4)	-1(4)	7(4)	-13(4)
N2	29(5)	36(5)	22(4)	7(4)	-1(3)	4(4)
N3	30(5)	32(5)	25(4)	7(3)	3(4)	-2(4)
N4	41(5)	29(5)	28(5)	0(4)	4(4)	-13(4)
N5	33(5)	30(5)	29(5)	1(4)	5(4)	-1(4)
N6	27(5)	31(5)	33(5)	9(4)	3(4)	0(4)
N7	31(5)	30(5)	36(5)	5(4)	-2(4)	-3(4)
C1	32(6)	32(5)	25(5)	3(4)	6(4)	-3(4)
C2	30(5)	37(6)	22(5)	7(4)	4(4)	0(4)
C3	28(6)	60(8)	27(5)	5(5)	3(4)	-1(5)
C4	26(6)	61(8)	36(6)	10(6)	7(5)	0(5)
C5	26(6)	61(8)	30(6)	4(5)	8(5)	-2(5)
C6	35(6)	39(6)	21(5)	8(4)	7(4)	5(5)
C7	25(5)	40(6)	22(5)	5(4)	1(4)	1(4)
C8	29(5)	29(5)	23(5)	-3(4)	4(4)	-10(4)
C9	23(5)	32(5)	27(5)	4(4)	4(4)	-10(4)
C10	35(6)	31(6)	41(6)	-1(5)	8(5)	1(5)
C11	54(8)	33(6)	42(7)	16(5)	1(6)	3(5)
C12	41(7)	36(6)	42(6)	14(5)	8(5)	-3(5)
C13	32(6)	44(6)	26(5)	4(5)	8(4)	-4(5)
C14	21(5)	25(5)	27(5)	0(4)	4(4)	-6(4)

C15	35(6)	33(6)	45(7)	4(5)	-4(5)	0(5)
C16	25(5)	26(5)	21(4)	4(4)	6(4)	-4(4)
C17	27(5)	32(5)	23(5)	5(4)	9(4)	1(4)
C18	36(6)	35(6)	45(7)	12(5)	18(5)	6(5)
C19	43(7)	45(7)	66(9)	30(7)	22(7)	16(6)
C20	42(7)	65(9)	47(7)	16(7)	10(6)	22(7)
C21	31(6)	53(7)	37(6)	17(5)	5(5)	13(5)
C22	30(5)	33(6)	29(5)	9(4)	8(4)	4(4)
C23	35(7)	46(7)	51(8)	-9(6)	4(6)	-7(6)

Bond Lengths for 19oa_rr_rrh113_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Cl1	2.265(3)	N7	C23	1.451(14)
Au1	N1	2.037(9)	C1	C2	1.520(14)
Au1	N2	1.945(9)	C2	C3	1.385(15)
Au1	N3	2.030(9)	C3	C4	1.383(16)
Au2	Cl2	2.240(7)	C4	C5	1.372(16)
Au2	N4	1.953(10)	C5	C6	1.389(15)
O1	C1	1.224(12)	C6	C7	1.508(15)
O2	C7	1.226(12)	C8	C9	1.402(15)
N1	C1	1.358(14)	C9	C10	1.375(17)
N1	C8	1.412(13)	C9	C14	1.427(15)
N2	C2	1.342(13)	C10	C11	1.404(17)
N2	C6	1.313(13)	C11	C12	1.386(18)
N3	C7	1.367(13)	C12	C13	1.372(18)
N3	C16	1.427(13)	C13	C14	1.400(14)
N4	N5	1.353(13)	C16	C17	1.418(15)
N4	C8	1.327(16)	C17	C18	1.393(15)
N5	C14	1.362(14)	C17	C22	1.401(14)
N5	C15	1.445(15)	C18	C19	1.400(18)
N6	N7	1.349(13)	C19	C20	1.41(2)
N6	C16	1.314(13)	C20	C21	1.346(19)
N7	C22	1.365(14)	C21	C22	1.405(16)

Bond Angles for 19oa_rr_rrh113_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Au1	Cl1	99.9(3)	C4	C5	C6	118.8(11)
N2	Au1	Cl1	177.5(3)	N2	C6	C5	119.1(10)
N2	Au1	N1	81.1(4)	N2	C6	C7	113.3(9)
N2	Au1	N3	80.5(4)	C5	C6	C7	127.4(10)
N3	Au1	Cl1	98.5(3)	O2	C7	N3	125.7(10)
N3	Au1	N1	161.5(3)	O2	C7	C6	121.0(10)
N4	Au2	Cl2	175.6(4)	N3	C7	C6	113.2(9)
C1	N1	Au1	114.7(7)	N4	C8	N1	120.1(10)
C1	N1	C8	118.1(9)	N4	C8	C9	111.7(10)
C8	N1	Au1	126.7(7)	C9	C8	N1	128.2(11)
C2	N2	Au1	117.5(7)	C8	C9	C14	103.0(10)
C6	N2	Au1	118.9(7)	C10	C9	C8	136.0(11)
C6	N2	C2	123.6(10)	C10	C9	C14	121.0(10)
C7	N3	Au1	113.7(7)	C9	C10	C11	116.9(11)
C7	N3	C16	116.9(8)	C12	C11	C10	121.5(12)
C16	N3	Au1	124.9(7)	C13	C12	C11	123.0(11)
N5	N4	Au2	136.0(8)	C12	C13	C14	116.1(11)
C8	N4	Au2	116.2(7)	N5	C14	C9	108.0(9)
C8	N4	N5	107.7(9)	N5	C14	C13	130.5(10)
N4	N5	C14	109.7(9)	C13	C14	C9	121.6(11)
N4	N5	C15	122.0(10)	N6	C16	N3	120.5(10)
C14	N5	C15	128.3(10)	N6	C16	C17	112.6(9)
C16	N6	N7	105.1(9)	C17	C16	N3	126.8(9)
N6	N7	C22	112.5(9)	C18	C17	C16	136.5(10)
N6	N7	C23	121.3(10)	C18	C17	C22	119.9(11)
C22	N7	C23	126.1(11)	C22	C17	C16	103.6(9)
O1	C1	N1	126.5(10)	C17	C18	C19	117.7(12)
O1	C1	C2	121.0(10)	C18	C19	C20	120.3(12)

N1	C1	C2	112.5(9)	C21	C20	C19	122.9(13)
N2	C2	C1	114.2(9)	C20	C21	C22	116.7(12)
N2	C2	C3	119.8(10)	N7	C22	C17	106.1(10)
C3	C2	C1	125.9(10)	N7	C22	C21	131.4(11)
C4	C3	C2	117.4(11)	C17	C22	C21	122.4(11)
C5	C4	C3	121.2(11)				

Torsion Angles for 19oa_rr_rrh113_0m.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Au1	N1	C1	O1	-177.4(10)	C2	C3	C4	C5	-1(2)
Au1	N1	C1	C2	0.3(13)	C3	C4	C5	C6	0(2)
Au1	N1	C8	N4	72.5(12)	C4	C5	C6	N2	0.2(19)
Au1	N1	C8	C9	-109.8(12)	C4	C5	C6	C7	-174.3(12)
Au1	N2	C2	C1	0.5(13)	C5	C6	C7	O2	2(2)
Au1	N2	C2	C3	177.2(9)	C5	C6	C7	N3	-179.2(12)
Au1	N2	C6	C5	-177.5(9)	C6	N2	C2	C1	-176.5(10)
Au1	N2	C6	C7	-2.2(13)	C6	N2	C2	C3	0.3(18)
Au1	N3	C7	O2	172.0(10)	C7	N3	C16	N6	-101.6(12)
Au1	N3	C7	C6	-6.9(12)	C7	N3	C16	C17	74.3(14)
Au1	N3	C16	N6	104.0(10)	C8	N1	C1	O1	-4.7(19)
Au1	N3	C16	C17	-80.2(12)	C8	N1	C1	C2	173.0(10)
Au2	N4	N5	C14	177.6(7)	C8	N4	N5	C14	0.8(11)
Au2	N4	N5	C15	-4.4(15)	C8	N4	N5	C15	178.8(9)
Au2	N4	C8	N1	-0.7(12)	C8	C9	C10	C11	-179.7(11)
Au2	N4	C8	C9	-178.7(6)	C8	C9	C14	N5	-0.6(10)
O1	C1	C2	N2	177.3(11)	C8	C9	C14	C13	179.2(9)
O1	C1	C2	C3	0.8(19)	C9	C10	C11	C12	-2.3(17)
N1	C1	C2	N2	-0.5(15)	C10	C9	C14	N5	178.3(9)
N1	C1	C2	C3	-177.0(12)	C10	C9	C14	C13	-2.0(15)
N1	C8	C9	C10	4.7(19)	C10	C11	C12	C13	2.8(19)
N1	C8	C9	C14	-176.7(9)	C11	C12	C13	C14	-2.6(17)
N2	C2	C3	C4	0.4(19)	C12	C13	C14	N5	-178.2(10)
N2	C6	C7	O2	-172.9(11)	C12	C13	C14	C9	2.2(15)
N2	C6	C7	N3	6.0(14)	C14	C9	C10	C11	1.9(15)
N3	C16	C17	C18	4.9(19)	C15	N5	C14	C9	-177.9(10)
N3	C16	C17	C22	-175.5(9)	C15	N5	C14	C13	2.4(18)
N4	N5	C14	C9	-0.1(11)	C16	N3	C7	O2	14.7(17)

N4	N5	C14	C13	-179.8(10)	C16	N3	C7	C6	-164.1(9)
N4	C8	C9	C10	-177.5(11)	C16	N6	N7	C22	-0.6(12)
N4	C8	C9	C14	1.1(11)	C16	N6	N7	C23	177.0(10)
N5	N4	C8	N1	176.8(8)	C16	C17	C18	C19	-178.0(12)
N5	N4	C8	C9	-1.2(11)	C16	C17	C22	N7	-1.0(11)
N6	N7	C22	C17	1.0(12)	C16	C17	C22	C21	179.1(10)
N6	N7	C22	C21	-179.0(11)	C17	C18	C19	C20	-3.1(18)
N6	C16	C17	C18	-178.9(12)	C18	C17	C22	N7	178.7(10)
N6	C16	C17	C22	0.7(11)	C18	C17	C22	C21	-1.2(16)
N7	N6	C16	N3	176.3(9)	C18	C19	C20	C21	3(2)
N7	N6	C16	C17	-0.1(12)	C19	C20	C21	C22	-1.2(19)
C1	N1	C8	N4	-99.1(13)	C20	C21	C22	N7	-179.4(12)
C1	N1	C8	C9	78.5(14)	C20	C21	C22	C17	0.6(17)
C1	C2	C3	C4	176.8(12)	C22	C17	C18	C19	2.4(16)
C2	N2	C6	C5	-0.6(18)	C23	N7	C22	C17	-176.5(11)
C2	N2	C6	C7	174.6(10)	C23	N7	C22	C21	3(2)

Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 19oa_rr_rrh113_0m.

Atom	*x*	*y*	*z*	U(eq)
H3	-190.52	1103.81	3307.8	49
H4	-829.39	1696.89	5025.64	51
H5	1100.03	2919.74	6474.66	49
H10	3840.66	3690.67	1157.02	46
H11	4234.01	3890.02	-547.77	51
H12	5860.34	2751.73	-1502.03	48
H13	6992.49	1222.4	-924.08	43
H15A	8803.64	282.84	1243.63	61
H15B	7841.51	-172.66	33.27	61
H15C	7302.26	-844.79	898.86	61
H18	7037.29	1777.01	6593.19	45
H19	8935.8	1103.88	7706.48	56
H20	11132.29	2526.76	8832.51	60
H23A	10997.2	6980.92	7840.97	75
H23B	11033.58	6647.06	8958.76	75
H23C	9743.04	7426.87	8592.36	75

Atomic Occupancy for 19oa_rr_rrh113_0m.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Au2	0.353(2)	Cl2	0.353(2)		

Experimental

Single crystals of $C_{46}H_{32}Au_{2.71}Cl_{2.71}N_{14}O_4$ **[19oa_rr_rrh113_0m]** were **[grown from a DMSO solution of the complex into which was diffused deionised water as the non-solvent]**. A suitable crystal was selected and **[mounted in Paratone(R) oil on a MiTeGeN microgripper cryoloop]** on a **'Bruker APEX-II CCD'** diffractometer. The crystal was kept at 153.2 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [19oa_rr_rrh113_0m]

Crystal Data for $C_{46}H_{32}Au_{2.71}Cl_{2.71}N_{14}O_4$ (M =1474.70 g/mol): triclinic, space group P-1 (no. 2), a = 8.5381(4) Å, b = 11.3000(5) Å, c = 13.1055(6) Å, α = 104.735(2)°, β = 97.970(3)°, γ = 98.032(3)°, V = 1190.64(10) Å^3, Z = 1, T = 153.2 K, μ(MoKα) = 8.542 mm^{-1}, *Dcalc* = 2.057 g/cm^3, 32923 reflections measured (3.268° ≤ 2Θ ≤ 58.068°), 6309 unique (R_{int} = 0.0476, R_{sigma} = 0.0405) which were used in all calculations. The final R_1 was 0.0569 (I > 2σ(I)) and wR_2 was 0.1390 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Others
 Sof(Au2)=Sof(Cl2)=FVAR(1)
3.a Aromatic/amide H refined with riding coordinates:
 C3(H3), C4(H4), C5(H5), C10(H10), C11(H11), C12(H12), C13(H13), C18(H18),
 C19(H19), C20(H20)
3.b Idealised Me refined as rotating group:
 C15(H15A,H15B,H15C), C23(H23A,H23B,H23C)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.10. 3d

Crystal data and structure refinement for 19OV_RR_PdIndz_0m.

Identification code	19OV_RR_PdIndz_0m
Empirical formula	$C_{23}H_{19}Cl_2N_7O_2Pd$
Formula weight	602.75
Temperature/K	152.95
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.4125(4)
b/Å	14.3306(7)
c/Å	18.7046(9)
α/°	90
β/°	95.258(2)
γ/°	90
Volume/Å^3	2245.47(19)
Z	4
ρ_{calc}g/cm^3	1.783
μ/mm^{-1}	1.103
F(000)	1208.0
Crystal size/mm^3	0.334 × 0.204 × 0.154
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.632 to 59.296
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -26 ≤ l ≤ 25
Reflections collected	43715
Independent reflections	6314 [R_{int} = 0.0344, R_{sigma} = 0.0236]
Data/restraints/parameters	6314/2/326
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0292, wR_2 = 0.0639
Final R indexes [all data]	R_1 = 0.0406, wR_2 = 0.0685
Largest diff. peak/hole / e Å^{-3}	0.52/-0.52

Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 19OV_RR_PdIndz_0m. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Pd1	3126.7(2)	8146.6(2)	5336.7(2)	17.75(5)
Cl1	1029.5(6)	7854.3(4)	6000.5(3)	25.37(11)
Cl2	5232.8(6)	8464.0(4)	4683.2(3)	25.98(11)
O1	5464.9(19)	4827.5(11)	6369.3(9)	26.4(3)
O2	-222(2)	5787.7(12)	3480.6(9)	32.3(4)
N1	5638(2)	8410.4(12)	6572.7(10)	23.4(4)
N2	4680(2)	7792.8(12)	6181.8(9)	19.1(3)
N3	4285(2)	6220.8(13)	6029.6(11)	24.4(4)
N4	2471(2)	5472.8(12)	5021.4(9)	20.0(4)
N5	1042(2)	6790.3(13)	4305.1(10)	25.4(4)
N6	1552(2)	8352.7(12)	4470.6(10)	19.8(4)
N7	1076(2)	9199.6(13)	4195.5(10)	22.8(4)
C1	5192(3)	9378.8(16)	6611.0(14)	34.4(6)
C2	6689(2)	7934.4(14)	7028.7(11)	19.1(4)
C3	7852(3)	8280.3(15)	7544.2(12)	24.2(5)
C4	8769(3)	7633.8(16)	7931.0(12)	25.7(5)
C5	8554(3)	6670.8(16)	7815.1(12)	25.2(5)
C6	7405(3)	6327.7(15)	7316.1(12)	22.4(4)
C7	6439(2)	6973.0(14)	6913.2(11)	17.2(4)
C8	5141(2)	6937.1(14)	6376.0(11)	17.2(4)
C9	4490(3)	5279.3(14)	6006.0(11)	19.9(4)

C10	3320(2)	4859.2(15)	5430.8(11)	20.5(4)
C11	3195(3)	3902.1(15)	5314.0(12)	24.0(4)
C12	2130(3)	3592.9(16)	4754.8(13)	25.1(5)
C13	1265(3)	4233.3(16)	4319.2(12)	23.6(4)
C14	1480(2)	5176.1(15)	4470.4(11)	20.3(4)
C15	652(3)	5939.3(15)	4018.6(11)	21.2(4)
C16	716(2)	7697.0(15)	4097.7(11)	20.4(4)
C17	-358(2)	8107.2(16)	3564.8(11)	20.7(4)
C18	-1518(3)	7783.9(18)	3032.4(12)	26.2(5)
C19	-2322(3)	8436.8(19)	2600.2(12)	29.9(5)
C20	-2000(3)	9394.6(19)	2679.4(13)	31.5(5)
C21	-893(3)	9735.3(18)	3197.2(13)	29.3(5)
C22	-78(2)	9073.4(16)	3647.1(11)	22.1(4)
C23	1729(3)	10052.4(16)	4522.8(14)	30.6(5)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 19OV_RR_PdIndz_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	19.65(8)	15.45(7)	16.35(8)	-1.02(6)	-8.00(5)	-0.12(6)
Cl1	23.8(2)	27.3(3)	23.9(3)	2.8(2)	-3.8(2)	-2.7(2)
Cl2	23.5(2)	30.7(3)	22.7(3)	0.1(2)	-3.3(2)	-0.5(2)
O1	31.0(8)	18.9(7)	26.9(8)	0.0(6)	-9.8(7)	1.2(6)
O2	35.4(9)	31.4(9)	26.6(9)	-7.3(7)	-15.2(7)	-1.3(7)
N1	28.6(9)	14.7(8)	23.7(9)	-4.0(7)	-14.4(8)	0.0(7)
N2	21.6(8)	16.1(8)	17.7(8)	-2.8(7)	-8.9(7)	-0.8(7)
N3	27.2(9)	15.4(8)	27.2(10)	-0.6(7)	-15.4(8)	-1.5(7)
N4	23.1(9)	17.7(8)	18.6(8)	-1.8(7)	-1.8(7)	-4.3(7)
N5	30.9(10)	21.9(9)	20.3(9)	-0.4(7)	-13.6(8)	-4.7(8)
N6	21.0(8)	19.3(9)	17.7(8)	0.2(6)	-5.8(7)	0.8(7)
N7	24.5(9)	20.4(9)	21.3(9)	0.6(7)	-9.6(7)	3.2(7)
C1	46.5(15)	16.7(10)	36.0(13)	-7.3(9)	-17.5(11)	6.5(10)
C2	20.8(10)	18.9(10)	16.4(9)	-1.5(7)	-5.3(8)	0.0(7)
C3	26.0(11)	21.2(11)	23.2(11)	-4.7(8)	-8.9(9)	-2.8(8)
C4	24.6(11)	27.6(12)	22.3(11)	-2.4(9)	-11.0(9)	-2.5(9)
C5	26.3(11)	24.2(11)	22.9(11)	1.2(8)	-9.8(9)	3.9(8)
C6	24.1(10)	18.2(10)	23.2(11)	-0.8(8)	-7.0(8)	0.9(8)
C7	18.0(9)	18.1(10)	14.6(9)	-2.2(7)	-3.2(7)	-1.0(7)
C8	19.3(9)	15.7(9)	15.7(9)	-0.4(7)	-3.3(7)	-0.7(7)
C9	22.4(10)	17.4(9)	19.4(10)	-1.6(8)	-1.1(8)	-3.3(8)

C10	21.5(10)	17.9(10)	21.6(10)	-1.5(8)	-1.2(8)	-2.9(8)
C11	25.9(10)	18.6(10)	26.9(11)	-2.2(9)	-1.4(9)	-2.5(8)
C12	25.4(11)	18.8(10)	30.6(12)	-6.3(9)	-0.7(9)	-6.1(8)
C13	23.2(10)	24.7(11)	22.4(11)	-6.9(8)	-1.0(8)	-6.3(8)
C14	20.2(9)	21.9(10)	18.2(10)	-3.4(8)	-1.1(8)	-3.9(8)
C15	20.8(10)	24.1(10)	18.0(10)	-2.5(8)	-2.0(8)	-4.2(8)
C16	19.8(10)	23.4(11)	16.9(10)	0.4(8)	-3.5(8)	-2.5(8)
C17	18.1(9)	27.9(11)	15.3(9)	-0.5(8)	-2.9(7)	1.7(8)
C18	21.5(10)	34.9(12)	21.0(11)	-5.2(9)	-4.2(8)	-1.0(9)
C19	20.6(10)	48.8(15)	18.7(11)	-4.8(10)	-7.3(8)	7.1(10)
C20	27.9(11)	44.5(15)	20.4(11)	1.0(10)	-6.7(9)	14.1(11)
C21	28.8(12)	31.7(12)	26.1(12)	0.4(9)	-4.8(9)	8.6(10)
C22	19.7(10)	28.6(11)	16.7(10)	-1.1(8)	-5.4(8)	2.8(8)
C23	32.4(12)	19.3(11)	37.2(14)	-2.2(9)	-11.7(10)	0.9(9)

Bond Lengths for 19OV_RR_PdIndz_0m.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	Cl1	2.2873(6)	C2	C3	1.400(3)
Pd1	Cl2	2.2884(6)	C2	C7	1.407(3)
Pd1	N2	2.0207(17)	C3	C4	1.369(3)
Pd1	N6	2.0183(17)	C4	C5	1.406(3)
O1	C9	1.205(3)	C5	C6	1.372(3)
O2	C15	1.210(3)	C6	C7	1.404(3)
N1	N2	1.364(2)	C7	C8	1.416(3)
N1	C1	1.441(3)	C9	C10	1.515(3)
N1	C2	1.355(3)	C10	C11	1.391(3)
N2	C8	1.327(3)	C11	C12	1.386(3)
N3	C8	1.380(3)	C12	C13	1.388(3)
N3	C9	1.361(3)	C13	C14	1.389(3)
N4	C10	1.330(3)	C14	C15	1.513(3)
N4	C14	1.334(3)	C16	C17	1.411(3)
N5	C15	1.360(3)	C17	C18	1.407(3)
N5	C16	1.376(3)	C17	C22	1.411(3)
N6	N7	1.364(2)	C18	C19	1.373(3)
N6	C16	1.332(3)	C19	C20	1.404(4)
N7	C22	1.358(3)	C20	C21	1.371(3)
N7	C23	1.452(3)	C21	C22	1.404(3)

Bond Angles for 19OV_RR_PdIndz_0m.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	Pd1	Cl2	178.97(2)	N2	C8	N3	115.59(18)
N2	Pd1	Cl1	90.28(5)	N2	C8	C7	110.36(17)
N2	Pd1	Cl2	89.49(6)	N3	C8	C7	134.04(18)
N6	Pd1	Cl1	88.86(5)	O1	C9	N3	126.6(2)
N6	Pd1	Cl2	91.47(5)	O1	C9	C10	123.47(19)
N6	Pd1	N2	173.87(7)	N3	C9	C10	109.93(18)
N2	N1	C1	120.51(18)	N4	C10	C9	115.19(18)
C2	N1	N2	109.29(17)	N4	C10	C11	122.2(2)
C2	N1	C1	127.69(18)	C11	C10	C9	122.56(19)
N1	N2	Pd1	124.38(14)	C12	C11	C10	117.9(2)
C8	N2	Pd1	126.72(14)	C11	C12	C13	120.0(2)
C8	N2	N1	108.01(16)	C12	C13	C14	118.2(2)
C9	N3	C8	133.63(19)	N4	C14	C13	121.9(2)
C10	N4	C14	119.89(19)	N4	C14	C15	115.11(18)
C15	N5	C16	134.50(19)	C13	C14	C15	123.02(19)
N7	N6	Pd1	125.54(13)	O2	C15	N5	126.5(2)
C16	N6	Pd1	126.39(15)	O2	C15	C14	123.3(2)
C16	N6	N7	107.93(17)	N5	C15	C14	110.24(18)
N6	N7	C23	120.23(17)	N5	C16	C17	133.7(2)
C22	N7	N6	109.34(18)	N6	C16	N5	115.90(18)
C22	N7	C23	130.31(19)	N6	C16	C17	110.43(19)
N1	C2	C3	129.03(19)	C18	C17	C16	136.1(2)

N1	C2	C7	108.45(17)	C18	C17	C22	119.9(2)
C3	C2	C7	122.52(19)	C22	C17	C16	104.02(18)
C4	C3	C2	116.6(2)	C19	C18	C17	117.7(2)
C3	C4	C5	121.6(2)	C18	C19	C20	121.6(2)
C6	C5	C4	122.0(2)	C21	C20	C19	122.3(2)
C5	C6	C7	117.8(2)	C20	C21	C22	116.5(2)
C2	C7	C8	103.84(17)	N7	C22	C17	108.28(18)
C6	C7	C2	119.43(18)	N7	C22	C21	129.7(2)
C6	C7	C8	136.72(19)	C21	C22	C17	122.0(2)

Torsion Angles for 19OV_RR_PdIndz_0m.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pd1	N2	C8	N3	-10.6(3)	C4	C5	C6	C7	0.5(4)
Pd1	N2	C8	C7	169.71(14)	C5	C6	C7	C2	0.6(3)
Pd1	N6	N7	C22	-175.48(15)	C5	C6	C7	C8	-178.3(2)
Pd1	N6	N7	C23	0.9(3)	C6	C7	C8	N2	179.9(2)
Pd1	N6	C16	N5	-4.0(3)	C6	C7	C8	N3	0.3(4)
Pd1	N6	C16	C17	175.21(14)	C7	C2	C3	C4	0.9(3)
O1	C9	C10	N4	-171.7(2)	C8	N3	C9	O1	8.4(4)
O1	C9	C10	C11	5.2(4)	C8	N3	C9	C10	-170.2(2)
N1	N2	C8	N3	179.89(19)	C9	N3	C8	N2	170.4(2)
N1	N2	C8	C7	0.2(2)	C9	N3	C8	C7	-10.0(4)
N1	C2	C3	C4	-179.5(2)	C9	C10	C11	C12	-177.4(2)
N1	C2	C7	C6	179.0(2)	C10	N4	C14	C13	1.9(3)
N1	C2	C7	C8	-1.8(2)	C10	N4	C14	C15	-176.67(19)
N2	N1	C2	C3	-177.6(2)	C10	C11	C12	C13	1.9(3)
N2	N1	C2	C7	2.0(3)	C11	C12	C13	C14	-1.2(3)
N3	C9	C10	N4	6.9(3)	C12	C13	C14	N4	-0.7(3)
N3	C9	C10	C11	-176.2(2)	C12	C13	C14	C15	177.7(2)
N4	C10	C11	C12	-0.8(3)	C13	C14	C15	O2	-2.3(3)
N4	C14	C15	O2	176.3(2)	C13	C14	C15	N5	178.0(2)
N4	C14	C15	N5	-3.5(3)	C14	N4	C10	C9	175.77(19)
N5	C16	C17	C18	-0.2(5)	C14	N4	C10	C11	-1.1(3)
N5	C16	C17	C22	179.6(2)	C15	N5	C16	N6	-168.9(2)

N6	N7	C22	C17	0.0(2)	C15	N5	C16	C17	12.1(5)
N6	N7	C22	C21	-178.4(2)	C16	N5	C15	O2	-4.3(4)
N6	C16	C17	C18	-179.2(2)	C16	N5	C15	C14	175.4(2)
N6	C16	C17	C22	0.6(2)	C16	N6	N7	C22	0.4(2)
N7	N6	C16	N5	-179.86(19)	C16	N6	N7	C23	176.8(2)
N7	N6	C16	C17	-0.6(2)	C16	C17	C18	C19	-179.1(2)
C1	N1	N2	Pd1	25.5(3)	C16	C17	C22	N7	-0.3(2)
C1	N1	N2	C8	-164.7(2)	C16	C17	C22	C21	178.2(2)
C1	N1	C2	C3	-15.8(4)	C17	C18	C19	C20	0.4(4)
C1	N1	C2	C7	163.8(2)	C18	C17	C22	N7	179.5(2)
C2	N1	N2	Pd1	-171.18(15)	C18	C17	C22	C21	-1.9(3)
C2	N1	N2	C8	-1.4(2)	C18	C19	C20	C21	-1.2(4)
C2	C3	C4	C5	0.1(4)	C19	C20	C21	C22	0.4(4)
C2	C7	C8	N2	1.0(2)	C20	C21	C22	N7	179.4(2)
C2	C7	C8	N3	-178.6(2)	C20	C21	C22	C17	1.2(3)
C3	C2	C7	C6	-1.3(3)	C22	C17	C18	C19	1.1(3)
C3	C2	C7	C8	177.9(2)	C23	N7	C22	C17	-175.9(2)
C3	C4	C5	C6	-0.8(4)	C23	N7	C22	C21	5.7(4)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 19OV_RR_PdIndz_0m.

Atom	*x*	*y*	*z*	U(eq)
H3	3520(30)	6420(20)	5755(14)	34(8)
H5	1660(30)	6750(20)	4674(11)	36(8)
H1A	4709.9	9584.49	6140.62	52
H1B	6143.2	9755.2	6750.01	52
H1C	4420.42	9455.13	6968.56	52
H3A	7998.28	8931.08	7621.73	29
H4	9569.71	7840.96	8286.63	31
H5A	9224.77	6245.13	8090.44	30
H6	7267.18	5675.15	7245.55	27
H11	3819.26	3474.07	5608.24	29
H12	1992.28	2943.14	4669.74	30
H13	546.3	4032.18	3928.34	28
H18	-1737.2	7136.66	2973.94	31
H19	-3114.65	8235.59	2238.82	36
H20	-2570.06	9821.51	2362.97	38
H21	-687.23	10384.84	3248.86	35
H23A	1467.04	10085.48	5022.08	46
H23B	1268.39	10591.9	4256.55	46
H23C	2890.72	10055.3	4510.73	46

Experimental

Single crystals of $C_{23}H_{19}Cl_2N_7O_2Pd$ [19OV_RR_PdIndz_0m] were [grown from DMSO-water solution]. A suitable crystal was selected and [mounted in Paratone oil on a MiTeGeN microgripper cryoloop] on a diffractometer. The crystal was kept at 152.95 K during data collection. Using Olex2 [1], the structure was solved with the Unknown [2] structure solution program using Unknown and refined with the Unknown [3] refinement package using Unknown minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2.

Crystal structure determination of [19OV_RR_PdIndz_0m]

Crystal Data for $C_{23}H_{19}Cl_2N_7O_2Pd$ (M =602.75 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 8.4125(4) Å, b = 14.3306(7) Å, c = 18.7046(9) Å, β = 95.258(2)°, V = 2245.47(19) Å^3, Z = 4, T = 152.95 K, μ(MoKα) = 1.103 mm^{-1}, $Dcalc$ = 1.783 g/cm^3, 43715 reflections measured (5.632° ≤ 2Θ ≤ 59.296°), 6314 unique (R_{int} = 0.0344, R_{sigma} = 0.0236) which were used in all calculations. The final R_1 was 0.0292 (I > 2σ(I)) and wR_2 was 0.0685 (all data).

Refinement model description

Number of restraints - 2, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Restrained distances
 N5-H5
 0.85 with sigma of 0.02
 N3-H3
 0.85 with sigma of 0.02
3.a Aromatic/amide H refined with riding coordinates:
 C3(H3A), C4(H4), C5(H5A), C6(H6), C11(H11), C12(H12), C13(H13), C18(H18),
 C19(H19), C20(H20), C21(H21)
3.b Idealised Me refined as rotating group:
 C1(H1A,H1B,H1C), C23(H23A,H23B,H23C)
```

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S2.11. 2dT

Crystal data and structure refinement for AuIndz_Thy_MS.

Identification code	AuIndz_Thy_MS
Empirical formula	$C_{28}H_{25}AuN_9O_{5.5}$
Formula weight	772.54
Temperature/K	173.0
Crystal system	triclinic
Space group	P-1
a/Å	10.3116(7)
b/Å	11.8798(7)
c/Å	13.2653(8)
α/°	69.269(2)
β/°	68.398(2)
γ/°	86.901(2)
Volume/Å^3	1407.59(15)
Z	2
ρ_{calc}g/cm^3	1.823
μ/mm^{-1}	5.285
F(000)	758.0
Crystal size/mm^3	0.18 × 0.15 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.874 to 61.17
Index ranges	-14 ≤ h ≤ 14, -16 ≤ k ≤ 16, -18 ≤ l ≤ 18
Reflections collected	86078
Independent reflections	8624 [R_{int} = 0.0366, R_{sigma} = 0.0188]
Data/restraints/parameters	8624/2/420
Goodness-of-fit on F^2	1.103
Final R indexes [I>=2σ (I)]	R_1 = 0.0196, wR_2 = 0.0382
Final R indexes [all data]	R_1 = 0.0257, wR_2 = 0.0410
Largest diff. peak/hole / e Å^{-3}	1.94/-1.21

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AuIndz_Thy_MS. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au1	7504.1(2)	3409.4(2)	5102.7(2)	19.21(2)
O1	6541.4(19)	3200.1(15)	8429.5(13)	30.1(4)
O2	9593.3(19)	6476.2(15)	2436.2(14)	31.7(4)
O3	9079(2)	1298.1(17)	4654.8(17)	37.4(4)
O4	4975(2)	2884.4(18)	4649.9(18)	39.0(4)
N1	6702(2)	2691.4(17)	6865.9(15)	23.5(4)
N2	8001.2(18)	4778.0(15)	5421.2(15)	18.7(3)
N3	8522(2)	4533.1(17)	3453.9(15)	22.6(4)
N4	6687(2)	634.6(17)	7993.0(16)	24.6(4)
N5	5710(2)	-316.2(17)	8707.6(16)	24.1(4)
N6	9856(2)	3690.4(18)	2052.0(17)	27.6(4)
N7	9708(2)	3489.8(18)	1150.5(16)	26.1(4)
N8	7012(2)	2079.8(16)	4660.9(16)	23.9(4)
N9	7883(2)	667(2)	3785(2)	34.7(5)
C1	6910(2)	3439(2)	7384.1(18)	22.0(4)
C2	7653(2)	4651.5(19)	6532.9(18)	20.0(4)
C3	8003(2)	5604(2)	6780(2)	25.8(4)
C4	8677(2)	6662(2)	5854(2)	27.5(5)
C5	8994(2)	6760(2)	4708(2)	25.6(4)
C6	8650(2)	5773.3(18)	4509.4(18)	20.1(4)
C7	8969(2)	5649.1(19)	3342.0(18)	22.1(4)
C8	5996(2)	1543(2)	7584.1(18)	22.5(4)
C9	4540(2)	1197.4(19)	8008.5(18)	21.6(4)
C10	3351(3)	1763(2)	7865(2)	28.4(5)
C11	2079(3)	1094(2)	8478(2)	34.7(5)
C12	1962(3)	-120(2)	9231(2)	34.0(5)
C13	3103(2)	-699(2)	9384(2)	27.9(5)

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AuIndz_Thy_MS. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C14	4404(2)	-20.0(19)	8749.4(18)	21.9(4)
C15	6148(3)	-1478(2)	9257(2)	31.5(5)
C16	8749(2)	4247.7(19)	2464.2(18)	22.1(4)
C17	7839(2)	4398(2)	1853.9(18)	22.9(4)
C18	6555(3)	4881(3)	1940(2)	34.3(6)
C19	5982(3)	4838(3)	1167(3)	46.9(8)
C20	6670(3)	4327(3)	315(2)	43.0(7)
C21	7938(3)	3859(2)	202(2)	30.0(5)
C22	8509(2)	3892.7(19)	1000.6(18)	21.8(4)
C23	10722(3)	2843(3)	525(2)	38.8(6)
C24	5830(3)	2169(2)	4390(2)	27.6(5)
C25	5682(3)	1394(2)	3791(2)	31.3(5)
C26	6720(3)	701(2)	3509(2)	35.6(6)
C27	8060(3)	1342(2)	4386(2)	27.4(5)
C28	4414(3)	1462(3)	3485(3)	45.7(7)
O1S	10369(2)	-488(2)	3256(2)	45.5(5)
O2S	5353(5)	5346(5)	4423(4)	54.2(12)

Anisotropic Displacement Parameters ($Å^2×10^3$) for AuIndz_Thy_MS. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	22.60(4)	21.22(4)	16.25(4)	-7.95(3)	-8.59(3)	0.59(3)
O1	38.5(10)	33.1(9)	17.4(7)	-11.2(7)	-6.6(7)	-0.2(7)
O2	40.1(10)	26.5(8)	22.1(8)	-3.3(6)	-9.1(7)	-1.8(7)
O3	35.9(10)	34.8(9)	46.7(11)	-15.7(8)	-20.6(9)	6.8(8)
O4	35.9(10)	42.9(10)	52.6(12)	-27.1(9)	-23.2(9)	8.2(8)
N1	28.8(10)	25.4(9)	15.3(8)	-7.7(7)	-5.9(7)	-4.3(7)
N2	18.8(8)	21.7(8)	19.0(8)	-9.4(7)	-8.8(7)	2.2(6)
N3	28.4(10)	25.2(9)	13.6(8)	-4.7(7)	-8.7(7)	-2.8(7)
N4	23.0(9)	28.8(9)	20.3(9)	-7.9(7)	-6.9(7)	0.1(7)
N5	23.6(9)	23.5(9)	22.2(9)	-5.5(7)	-8.0(7)	3.4(7)
N6	29.2(10)	32.9(10)	24.3(9)	-10.6(8)	-14.3(8)	6.1(8)
N7	27.2(10)	32.4(10)	22.8(9)	-13.9(8)	-10.7(8)	7.8(8)
N8	28.9(10)	22.9(9)	21.4(9)	-9.2(7)	-9.2(8)	-2.5(7)
N9	36.8(12)	31.2(11)	39.8(12)	-21.0(10)	-10.8(10)	4.9(9)
C1	21.8(10)	26.3(10)	19.2(9)	-10.1(8)	-7.3(8)	1.8(8)
C2	17.6(9)	25.7(10)	19.1(9)	-11.0(8)	-6.7(8)	2.6(8)
C3	24.5(11)	33.9(12)	25.7(11)	-17.3(9)	-10.4(9)	2.1(9)
C4	25.9(11)	29.8(11)	34.0(12)	-18.1(10)	-12.5(10)	1.3(9)
C5	24.4(11)	23.3(10)	30.6(11)	-10.5(9)	-11.0(9)	0.4(8)
C6	19.4(10)	21.1(9)	21.2(9)	-7.1(8)	-9.4(8)	2.2(7)
C7	23.5(10)	25.1(10)	19.7(9)	-7.4(8)	-11.2(8)	3.9(8)
C8	25.3(11)	25.1(10)	17.7(9)	-9.6(8)	-6.5(8)	-0.5(8)
C9	25.1(10)	21.6(9)	18.2(9)	-8.3(8)	-7.1(8)	2.3(8)
C10	31.5(12)	24.9(11)	29.9(12)	-10.4(9)	-12.8(10)	8.0(9)
C11	25.1(12)	36.5(13)	41.7(14)	-14.5(11)	-12.3(11)	10.7(10)
C12	22.2(11)	35.1(13)	37.6(13)	-11.4(11)	-4.8(10)	0.0(9)
C13	27.2(12)	23.1(10)	28.2(11)	-7.1(9)	-6.4(9)	-0.4(9)

Anisotropic Displacement Parameters ($Å^2×10^3$) for AuIndz_Thy_MS. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C14	24.0(10)	21.8(10)	20.1(10)	-8.7(8)	-7.7(8)	3.5(8)
C15	32.4(13)	27.8(11)	28.9(12)	-4.8(9)	-11.7(10)	9.6(10)
C16	25.2(11)	25.7(10)	16.2(9)	-6.3(8)	-9.5(8)	0.8(8)
C17	25.9(11)	28.5(11)	16.0(9)	-9.4(8)	-8.3(8)	2.6(8)
C18	32.7(13)	52.2(16)	28.0(12)	-23.0(11)	-15.8(10)	18.0(11)
C19	36.6(15)	82(2)	43.2(16)	-35.9(16)	-27.5(13)	27.4(15)
C20	40.7(15)	72(2)	34.3(14)	-28.3(14)	-25.5(12)	14.8(14)
C21	33.9(13)	41.2(13)	20.0(10)	-15.8(10)	-11.1(9)	3.8(10)
C22	23.9(10)	25.2(10)	16.9(9)	-8.2(8)	-7.4(8)	1.7(8)
C23	37.1(14)	45.5(15)	40.8(15)	-25.4(13)	-14.8(12)	18.8(12)
C24	31.5(12)	27.6(11)	25.5(11)	-11.1(9)	-10.9(9)	-1.0(9)
C25	37.9(14)	34.5(12)	26.8(11)	-13.3(10)	-15.0(10)	-2.8(10)
C26	45.7(16)	32.4(13)	33.1(13)	-18.0(11)	-12.9(12)	-2.4(11)
C27	32.0(12)	20.0(10)	25.9(11)	-8.1(8)	-5.8(9)	-1.1(9)
C28	52.2(18)	50.2(17)	50.3(17)	-24.0(14)	-30.1(15)	-0.2(14)
O1S	32.4(11)	53.6(13)	49.5(12)	-26.9(11)	-6.8(9)	7.0(9)
O2S	73(3)	43(2)	43(2)	-26(2)	-9(2)	17(2)

Bond Lengths for AuIndz_Thy_MS.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	N1	2.0302(17)	N9	C27	1.373(3)
Au1	N2	1.9547(17)	C1	C2	1.506(3)
Au1	N3	2.0153(17)	C2	C3	1.382(3)
Au1	N8	2.0141(18)	C3	C4	1.395(3)
O1	C1	1.222(3)	C4	C5	1.395(3)
O2	C7	1.219(3)	C5	C6	1.379(3)
O3	C27	1.222(3)	C6	C7	1.520(3)
O4	C24	1.233(3)	C8	C9	1.421(3)
N1	C1	1.367(3)	C9	C10	1.408(3)
N1	C8	1.406(3)	C9	C14	1.411(3)
N2	C2	1.336(3)	C10	C11	1.373(4)
N2	C6	1.336(3)	C11	C12	1.415(4)
N3	C7	1.367(3)	C12	C13	1.374(3)
N3	C16	1.405(3)	C13	C14	1.402(3)
N4	N5	1.361(3)	C16	C17	1.417(3)
N4	C8	1.325(3)	C17	C18	1.395(3)
N5	C14	1.360(3)	C17	C22	1.407(3)
N5	C15	1.450(3)	C18	C19	1.374(4)
N6	N7	1.360(3)	C19	C20	1.414(4)
N6	C16	1.325(3)	C20	C21	1.371(4)
N7	C22	1.359(3)	C21	C22	1.400(3)
N7	C23	1.448(3)	C24	C25	1.458(3)
N8	C24	1.381(3)	C25	C26	1.338(4)
N8	C27	1.380(3)	C25	C28	1.496(4)
N9	C26	1.372(4)	O2S	O2S[1]	1.378(10)

[1]1-X,1-Y,1-Z

Bond Angles for AuIndz_Thy_MS.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Au1	N1	81.13(7)	O2	C7	N3	126.6(2)
N2	Au1	N3	81.17(7)	O2	C7	C6	120.9(2)
N2	Au1	N8	175.98(7)	N3	C7	C6	112.48(18)
N3	Au1	N1	162.18(7)	N1	C8	C9	127.9(2)
N8	Au1	N1	102.69(7)	N4	C8	N1	120.3(2)
N8	Au1	N3	95.05(7)	N4	C8	C9	111.73(19)
C1	N1	Au1	113.95(14)	C10	C9	C8	136.1(2)
C1	N1	C8	118.10(17)	C10	C9	C14	120.2(2)
C8	N1	Au1	127.94(14)	C14	C9	C8	103.68(19)
C2	N2	Au1	117.54(14)	C11	C10	C9	117.6(2)
C2	N2	C6	125.04(18)	C10	C11	C12	121.3(2)
C6	N2	Au1	117.41(14)	C13	C12	C11	122.4(2)
C7	N3	Au1	114.94(14)	C12	C13	C14	116.3(2)
C7	N3	C16	120.42(18)	N5	C14	C9	106.95(19)
C16	N3	Au1	124.62(14)	N5	C14	C13	130.9(2)
C8	N4	N5	106.04(18)	C13	C14	C9	122.1(2)
N4	N5	C15	119.65(19)	N3	C16	C17	127.1(2)
C14	N5	N4	111.58(18)	N6	C16	N3	120.85(19)
C14	N5	C15	128.7(2)	N6	C16	C17	111.84(19)
C16	N6	N7	105.53(18)	C18	C17	C16	135.4(2)
N6	N7	C23	120.2(2)	C18	C17	C22	120.5(2)
C22	N7	N6	112.05(18)	C22	C17	C16	104.02(19)
C22	N7	C23	127.6(2)	C19	C18	C17	117.5(2)
C24	N8	Au1	117.20(15)	C18	C19	C20	121.2(2)
C27	N8	Au1	115.66(15)	C21	C20	C19	122.5(2)
C27	N8	C24	125.12(19)	C20	C21	C22	116.0(2)
C26	N9	C27	122.0(2)	N7	C22	C17	106.54(18)
O1	C1	N1	125.9(2)	N7	C22	C21	131.3(2)

Bond Angles for AuIndz_Thy_MS.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C2	120.59(19)	C21	C22	C17	122.2(2)
N1	C1	C2	113.52(18)	O4	C24	N8	119.8(2)
N2	C2	C1	113.84(18)	O4	C24	C25	123.7(2)
N2	C2	C3	118.6(2)	N8	C24	C25	116.5(2)
C3	C2	C1	127.56(19)	C24	C25	C28	118.1(2)
C2	C3	C4	118.3(2)	C26	C25	C24	117.7(2)
C5	C4	C3	121.0(2)	C26	C25	C28	124.1(2)
C6	C5	C4	118.3(2)	C25	C26	N9	123.1(2)
N2	C6	C5	118.7(2)	O3	C27	N8	122.1(2)
N2	C6	C7	113.85(18)	O3	C27	N9	122.4(2)
C5	C6	C7	127.4(2)	N9	C27	N8	115.5(2)

Torsion Angles for AuIndz_Thy_MS.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au1	N1	C1	O1	-78.87(19)	C4	C5	C6	C7	-176.1(2)
Au1	N1	C1	C2	1.8(2)	C5	C6	C7	O2	-0.1(4)
Au1	N1	C8	N4	95.4(2)	C5	C6	C7	N3	177.9(2)
Au1	N1	C8	C9	-87.8(3)	C6	N2	C2	C1	179.14(19)
Au1	N2	C2	C1	-0.1(2)	C6	N2	C2	C3	-1.3(3)
Au1	N2	C2	C3	179.50(16)	C7	N3	C16	N6	94.8(3)
Au1	N2	C6	C5	178.97(16)	C7	N3	C16	C17	-91.0(3)
Au1	N2	C6	C7	-3.0(2)	C8	N1	C1	O1	0.4(3)
Au1	N3	C7	O2	-79.39(19)	C8	N1	C1	C2	-78.99(19)
Au1	N3	C7	C6	2.7(2)	C8	N4	N5	C14	0.4(2)
Au1	N3	C16	N6	-87.0(2)	C8	N4	N5	C15	177.2(2)
Au1	N3	C16	C17	87.2(3)	C8	C9	C10	C11	-178.3(2)
Au1	N8	C24	O4	-14.9(3)	C8	C9	C14	N5	-1.1(2)
Au1	N8	C24	C25	164.65(16)	C8	C9	C14	C13	177.8(2)

Torsion Angles for AuIndz_Thy_MS.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au1	N8	C27	O3	17.0(3)	C9	C10	C11	C12	0.3(4)
Au1	N8	C27	N9	-162.60(16)	C10	C9	C14	N5	179.62(19)
O1	C1	C2	N2	179.5(2)	C10	C9	C14	C13	-1.5(3)
O1	C1	C2	C3	-0.1(4)	C10	C11	C12	C13	-0.7(4)
O4	C24	C25	C26	176.8(3)	C11	C12	C13	C14	0.0(4)
O4	C24	C25	C28	-0.6(4)	C12	C13	C14	N5	179.7(2)
N1	C1	C2	N2	-1.1(3)	C12	C13	C14	C9	1.1(3)
N1	C1	C2	C3	179.3(2)	C14	C9	C10	C11	0.7(3)
N1	C8	C9	C10	3.5(4)	C15	N5	C14	C9	-175.9(2)
N1	C8	C9	C14	-175.6(2)	C15	N5	C14	C13	5.3(4)
N2	C2	C3	C4	1.4(3)	C16	N3	C7	O2	-1.0(4)
N2	C6	C7	O2	-177.9(2)	C16	N3	C7	C6	-178.93(18)
N2	C6	C7	N3	0.1(3)	C16	N6	N7	C22	-1.1(3)
N3	C16	C17	C18	3.5(4)	C16	N6	N7	C23	-177.5(2)
N3	C16	C17	C22	-175.7(2)	C16	C17	C18	C19	-178.9(3)
N4	N5	C14	C9	0.5(2)	C16	C17	C22	N7	0.3(2)
N4	N5	C14	C13	-178.3(2)	C16	C17	C22	C21	179.9(2)
N4	C8	C9	C10	-179.5(2)	C17	C18	C19	C20	-0.1(5)
N4	C8	C9	C14	1.4(2)	C18	C17	C22	N7	-179.1(2)
N5	N4	C8	N1	176.14(18)	C18	C17	C22	C21	0.5(4)
N5	N4	C8	C9	-1.1(2)	C18	C19	C20	C21	-0.6(5)
N6	N7	C22	C17	0.5(3)	C19	C20	C21	C22	1.3(4)
N6	N7	C22	C21	-179.1(2)	C20	C21	C22	N7	178.3(3)
N6	C16	C17	C18	178.2(3)	C20	C21	C22	C17	-1.2(4)
N6	C16	C17	C22	-1.0(3)	C22	C17	C18	C19	0.2(4)
N7	N6	C16	N3	176.36(19)	C23	N7	C22	C17	176.5(2)
N7	N6	C16	C17	1.3(3)	C23	N7	C22	C21	-3.1(4)
N8	C24	C25	C26	-2.8(3)	C24	N8	C27	O3	-179.7(2)

Torsion Angles for AuIndz_Thy_MS.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N8	C24	C25	C28	179.8(2)	C24	N8	C27	N9	0.7(3)
C1	N1	C8	N4	-83.7(3)	C24	C25	C26	N9	1.8(4)
C1	N1	C8	C9	93.1(3)	C26	N9	C27	O3	178.5(2)
C1	C2	C3	C4	-179.1(2)	C26	N9	C27	N8	-1.9(3)
C2	N2	C6	C5	-0.3(3)	C27	N8	C24	O4	-178.0(2)
C2	N2	C6	C7	177.74(19)	C27	N8	C24	C25	1.6(3)
C2	C3	C4	C5	-0.1(3)	C27	N9	C26	C25	0.6(4)
C3	C4	C5	C6	-1.4(3)	C28	C25	C26	N9	179.0(3)
C4	C5	C6	N2	1.6(3)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for AuIndz_Thy_MS.

Atom	*x*	*y*	*z*	U(eq)
H3	7790.58	5538.43	7559.46	31
H4	8924.54	7327.1	6006.65	33
H5	9434.63	7488.33	4079.94	31
H10	3426.87	2579.03	7362.66	34
H11	1260.74	1452.39	8393.74	42
H12	1061.05	-549.9	9646.89	41
H13	3014.09	-1513.81	9891.57	33
H15A	6607.35	-1847.08	8674.44	47
H15B	5326.54	-2007.23	9867.84	47
H15C	6804.15	-1366.07	9598.3	47
H18	6094.5	5226.31	2510.99	41
H19	5108.13	5158.58	1205.79	56
H20	6235.74	4306.4	-198.72	52
H21	8402.51	3530.58	-382.09	36
H23A	10604	1986.14	1014.14	58

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for AuIndz_Thy_MS.

Atom	*x*	*y*	*z*	U(eq)
H23B	11669.82	3178.21	324.13	58
H23C	10577.63	2927.88	-188.04	58
H28A	4350.39	791.18	3233.2	68
H28B	4485.71	2230.41	2853.99	68
H28C	3574.62	1407.86	4167.16	68
H9	8600(40)	140(30)	3540(30)	59(10)
H26	6710(30)	150(30)	3110(30)	41(8)
H1SA	10690(110)	-110(90)	3670(80)	310(50)
H1SB	11180(40)	-580(50)	2650(40)	130(20)
H2S	5100(40)	5540(30)	5020(40)	56(11)

Atomic Occupancy for AuIndz_Thy_MS.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O2S	0.5				

Experimental

Single crystals of $C_{28}H_{25}AuN_9O_{5.5}$ **[AuIndz_Thy_MS]** were **[grown from THF-water]**. A suitable crystal was selected and **[mounted in Paratone oil on a Hampton nylon cryoloop]** on a **Bruker D8 Venture** diffractometer. The crystal was kept at 173.0 K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [AuIndz_Thy_MS]

Crystal Data for $C_{28}H_{25}AuN_9O_{5.5}$ (M =772.54 g/mol): triclinic, space group P-1 (no. 2), a = 10.3116(7) Å, b = 11.8798(7) Å, c = 13.2653(8) Å, α = 69.269(2)°, β = 68.398(2)°, γ = 86.901(2)°, V = 1407.59(15) Å^3, Z = 2, T = 173.0 K, μ(MoKα) = 5.285 mm^{-1}, *Dcalc* = 1.823 g/cm^3, 86078 reflections measured (5.874° ≤ 2Θ ≤ 61.17°), 8624 unique (R_{int} = 0.0366, R_{sigma} = 0.0188) which were used in all calculations. The final R_1 was 0.0196 (I > 2σ(I)) and wR_2 was 0.0410 (all data).

Refinement model description

Number of restraints - 2, number of constraints - unknown.

Details:

```
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
```

```
  All C(H,H,H) groups
2. Restrained distances
 H1SA-O1S
 0.96 with sigma of 0.02
 O1S-H1SB
 0.96 with sigma of 0.02
3. Others
 Fixed Sof: O2S(0.5)
4.a Aromatic/amide H refined with riding coordinates:
 C3(H3), C4(H4), C5(H5), C10(H10), C11(H11), C12(H12), C13(H13), C18(H18),
 C19(H19), C20(H20), C21(H21)
4.b Idealised Me refined as rotating group:
 C15(H15A,H15B,H15C), C23(H23A,H23B,H23C), C28(H28A,H28B,H28C)
```

This report has been created with Olex2, compiled on 2020.11.12 svn.r5f609507 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

S3. CD spectrometry

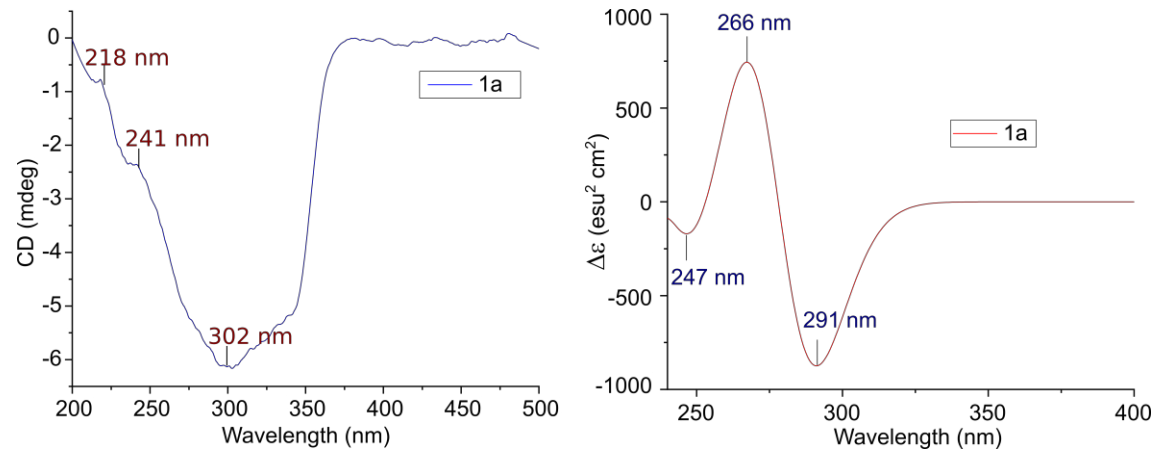


Figure S 36. Experimental **a)** and DFT-calculated **(b)** CD spectra of C_2 symmetry **1a** in 2-methoxyethanol. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

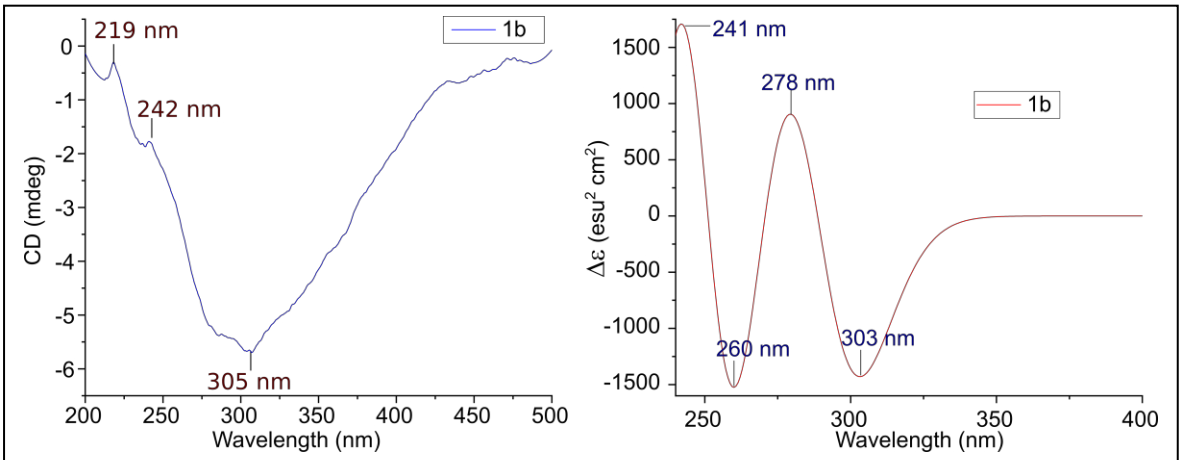


Figure S 37. Experimental **a)** and DFT-calculated **(b)** CD spectra of C_2 symmetry **1b** in 2-methoxyethanol. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

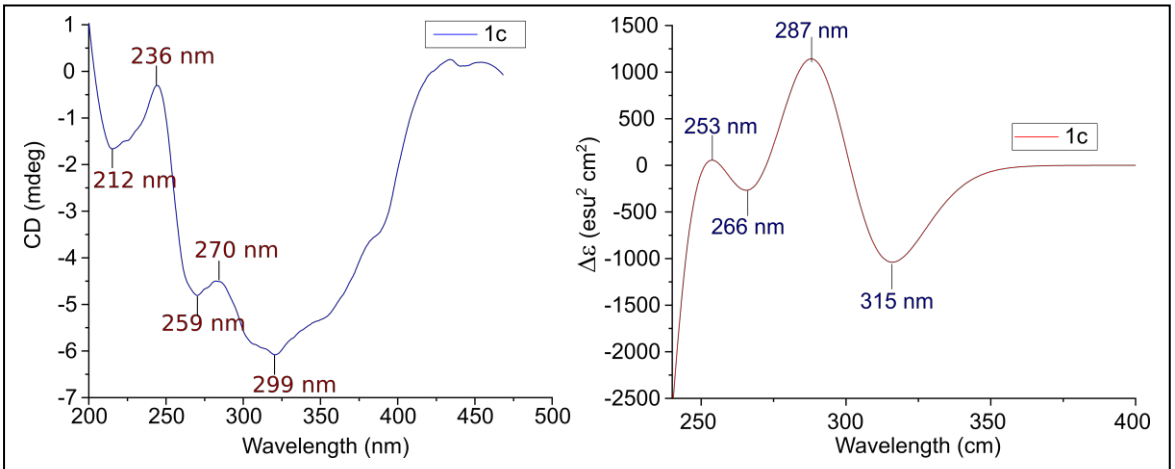


Figure S 38. Experimental **a)** and DFT-calculated **(b)** CD spectra of C_2 symmetry **1c** in chloroform. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

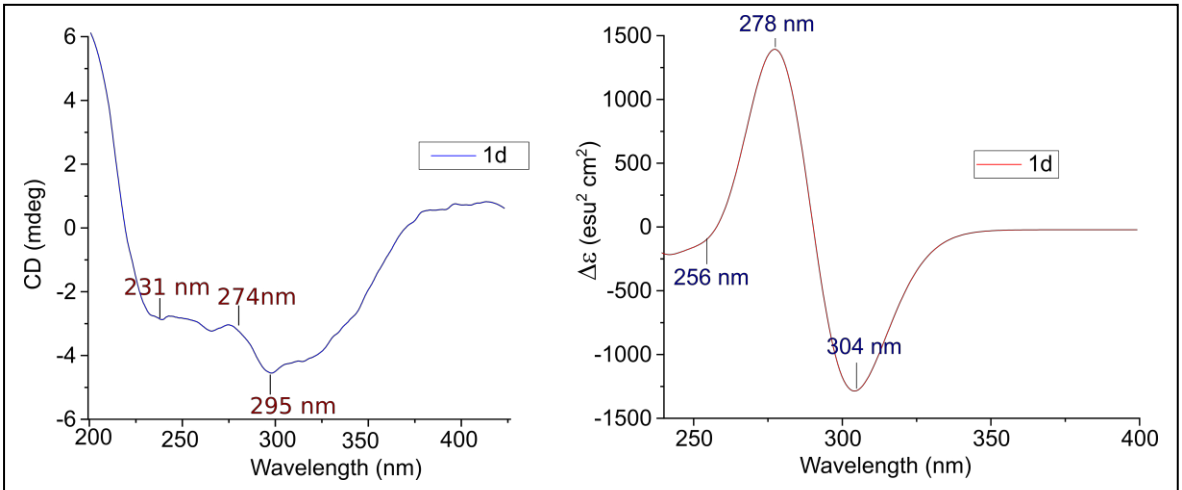


Figure S 39. Experimental **a)** and DFT-calculated **(b)** CD spectra of C_2 symmetry **1d** in DMSO. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

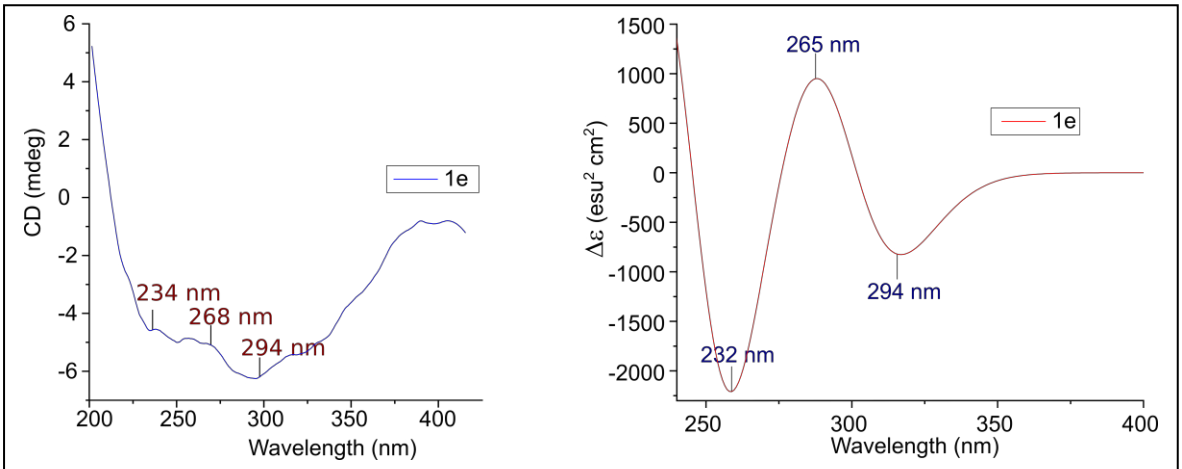


Figure S 40. Experimental **a)** and DFT-calculated **(b)** CD spectra of C_2 symmetry **1a** in DMSO. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

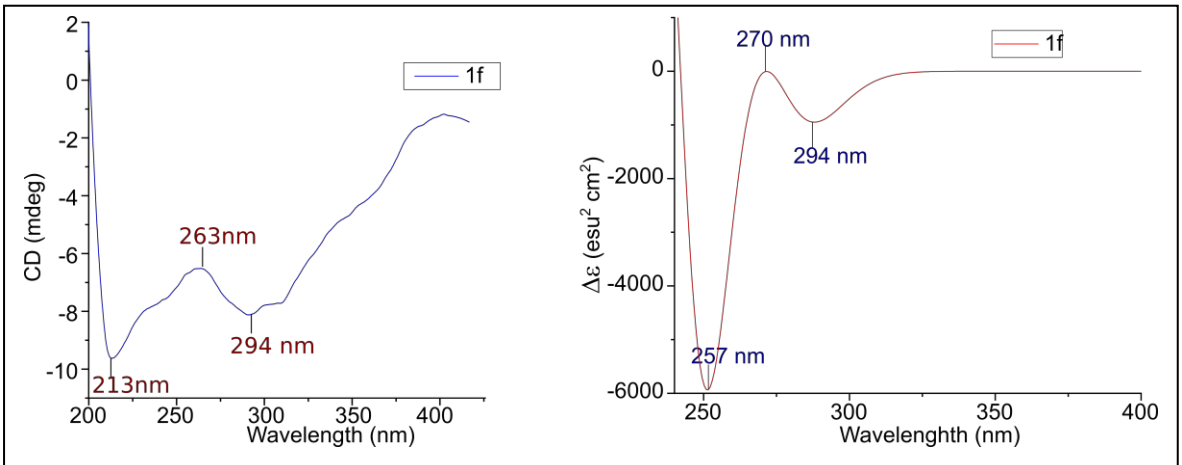


Figure S 41. Experimental a) and DFT-calculated **(b)** CD spectra of C_2 symmetry **1f** in 2-methoxyethanol. The CD for the DFT-calculated spectrum is plotted with full width at half maximum intensity (FWHM) of 3000 cm^{-1}.

S4. Binding studies

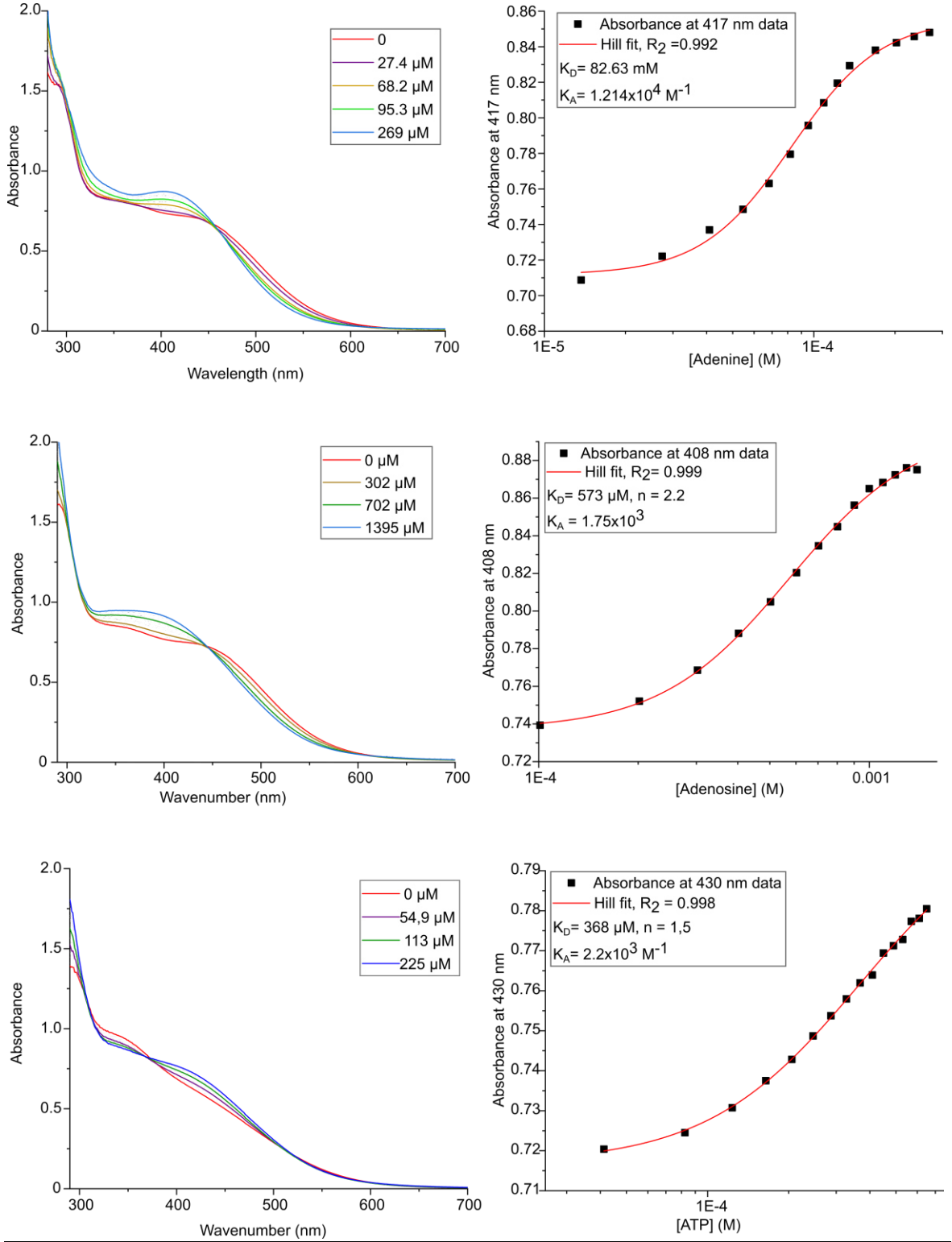


Figure S 42. A representative of the triplicates for the UV-vis absorption spectra of 117 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO (red spectrum) after sequential additions of DNA components (adenine, adenosine and ATP) and final concentration before precipitation (blue spectrum). The graphs on the right are an illustration of the Uv-vis titration spectra at specified wavelengths with a change in ratio of **2d** to the DNA components.

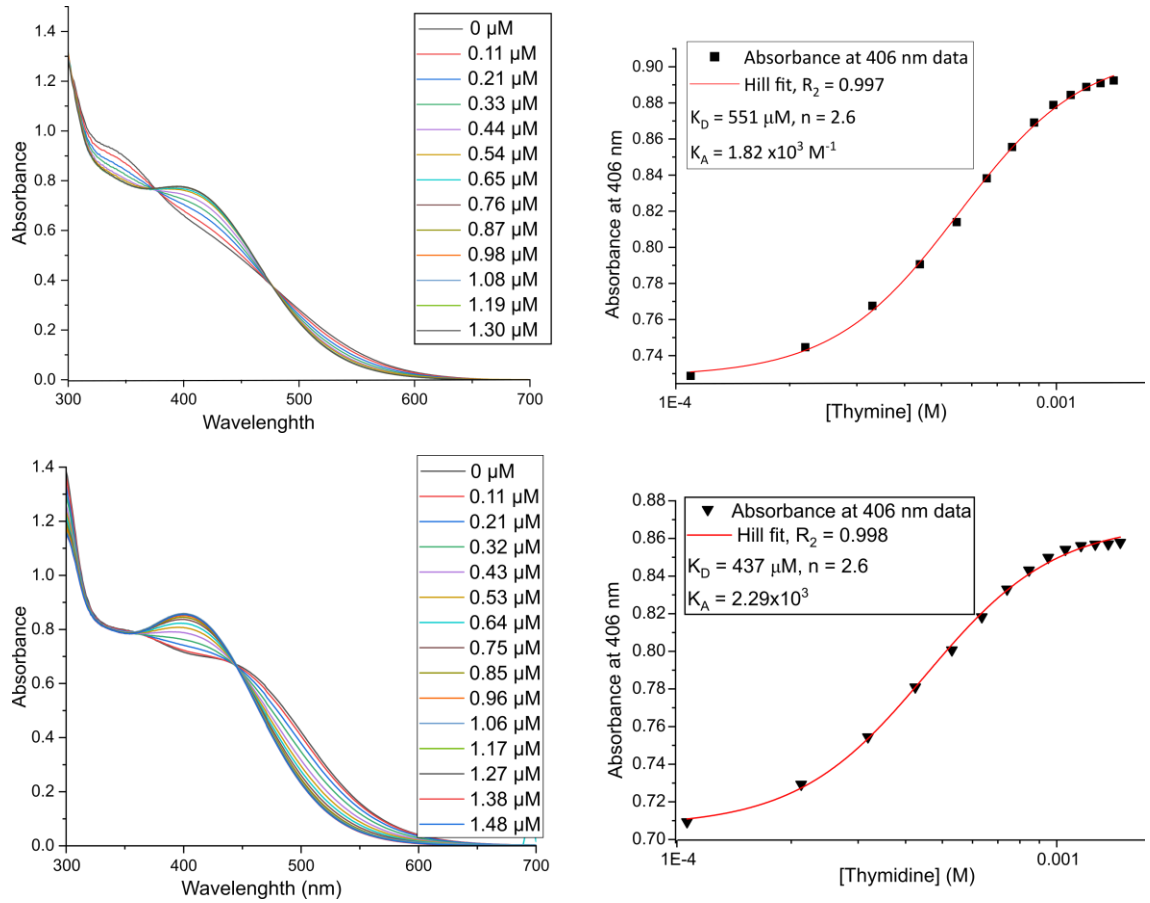


Figure S 43. A representative of the triplicates for the UV-vis absorption spectra of 117 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO after sequential additions of DNA components (thymine and thymidine) and final concentration before precipitation. The graphs on the right are an illustration of the Uv-vis titration spectra at specified wavelengths with a change in ratio of **2d** to the DNA components.

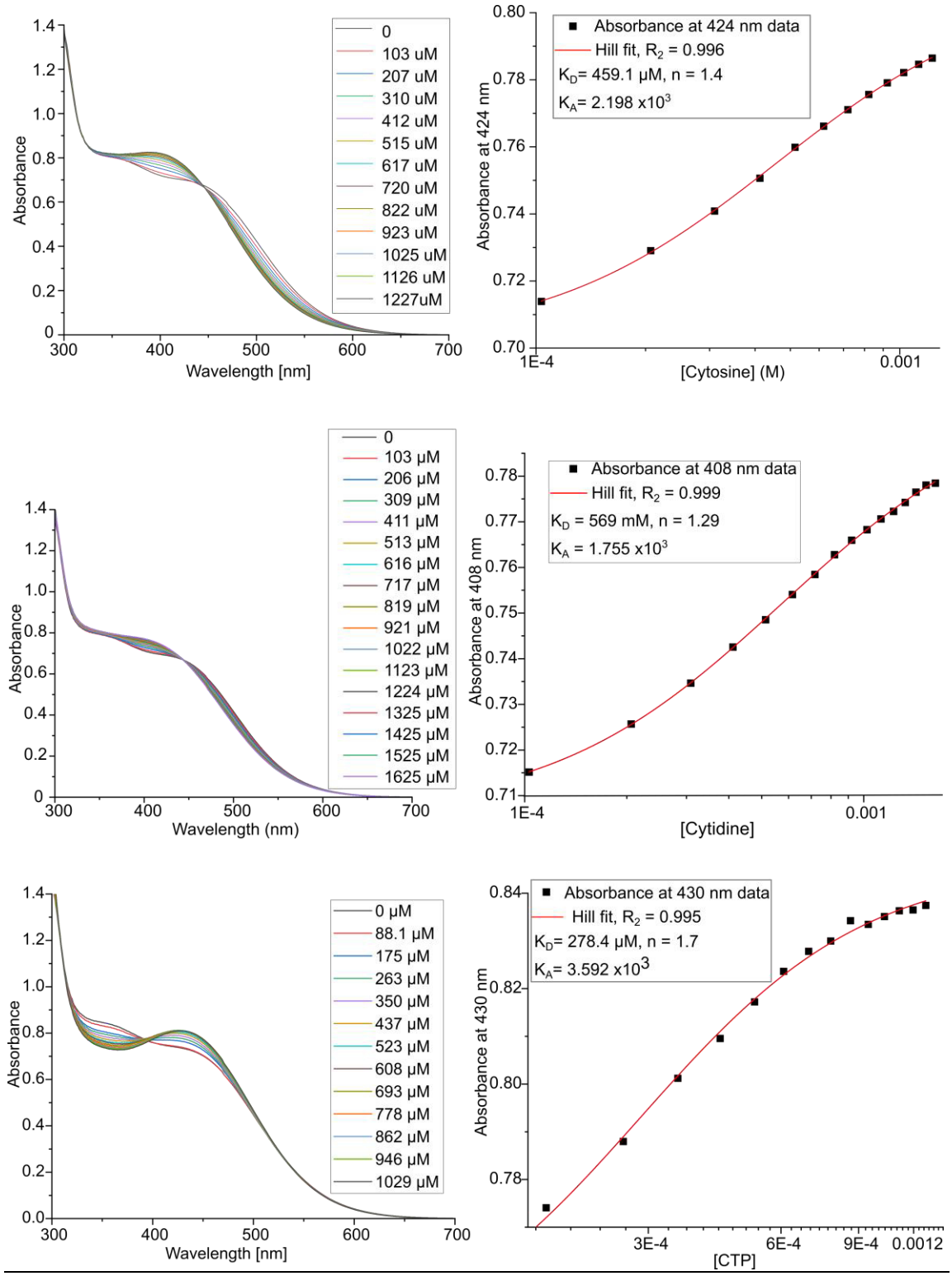


Figure S 44. A representative of the triplicates for the UV-vis absorption spectra of 117 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO after sequential additions of DNA components (cytosine, cytidine and CTP) and final concentration before precipitation. The graphs on the right are an illustration of the Uv-vis titration spectra at specified wavelengths with a change in ratio of **2d** to the DNA components.

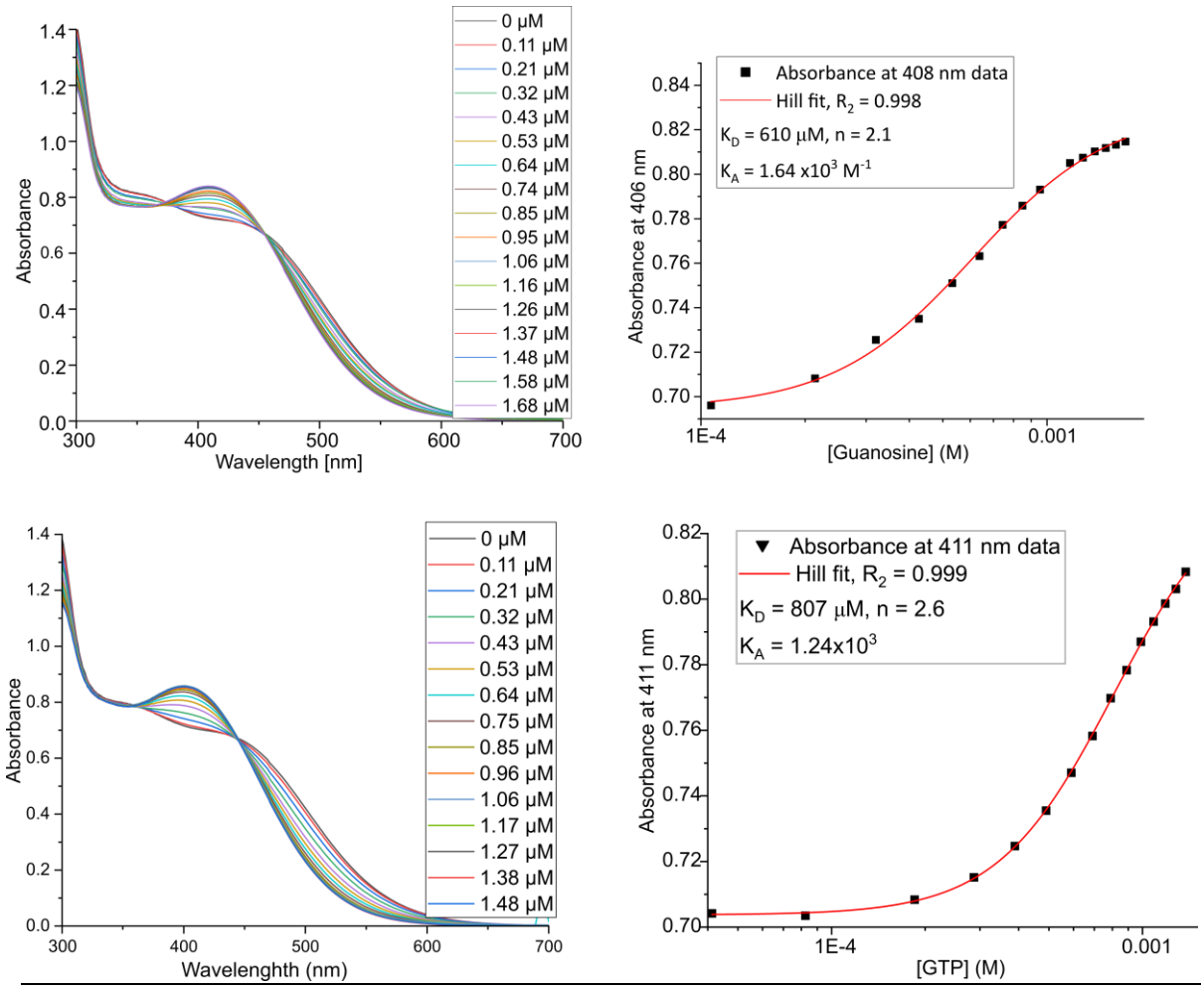


Figure S 45. A representative of the triplicates for the UV-vis absorption spectra of 117 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO after sequential additions of DNA components (guanosine and GTP) and final concentration before precipitation. The graphs on the right are an illustration of the Uv-vis titration spectra at specified wavelengths with a change in ratio of **2d** to the DNA components.

S5. Kinetics studies

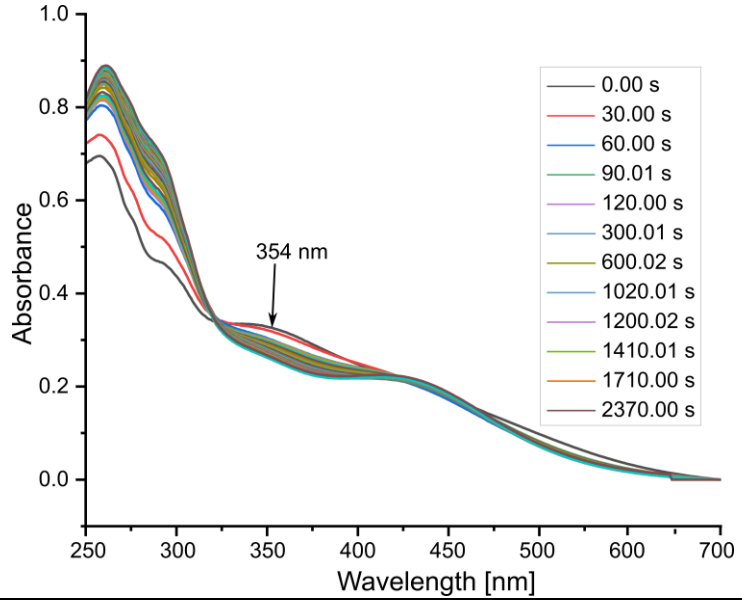


Figure S 46. An illustration of the absobance of a solution of **2d** and GSH in 0.10 M TRIS-HCl buffer 10% DMSO as a function of time, the spectra was scanned in 30s intervalsfor 2000s. The wavelength 324 nm was selected for the kinetics studies.

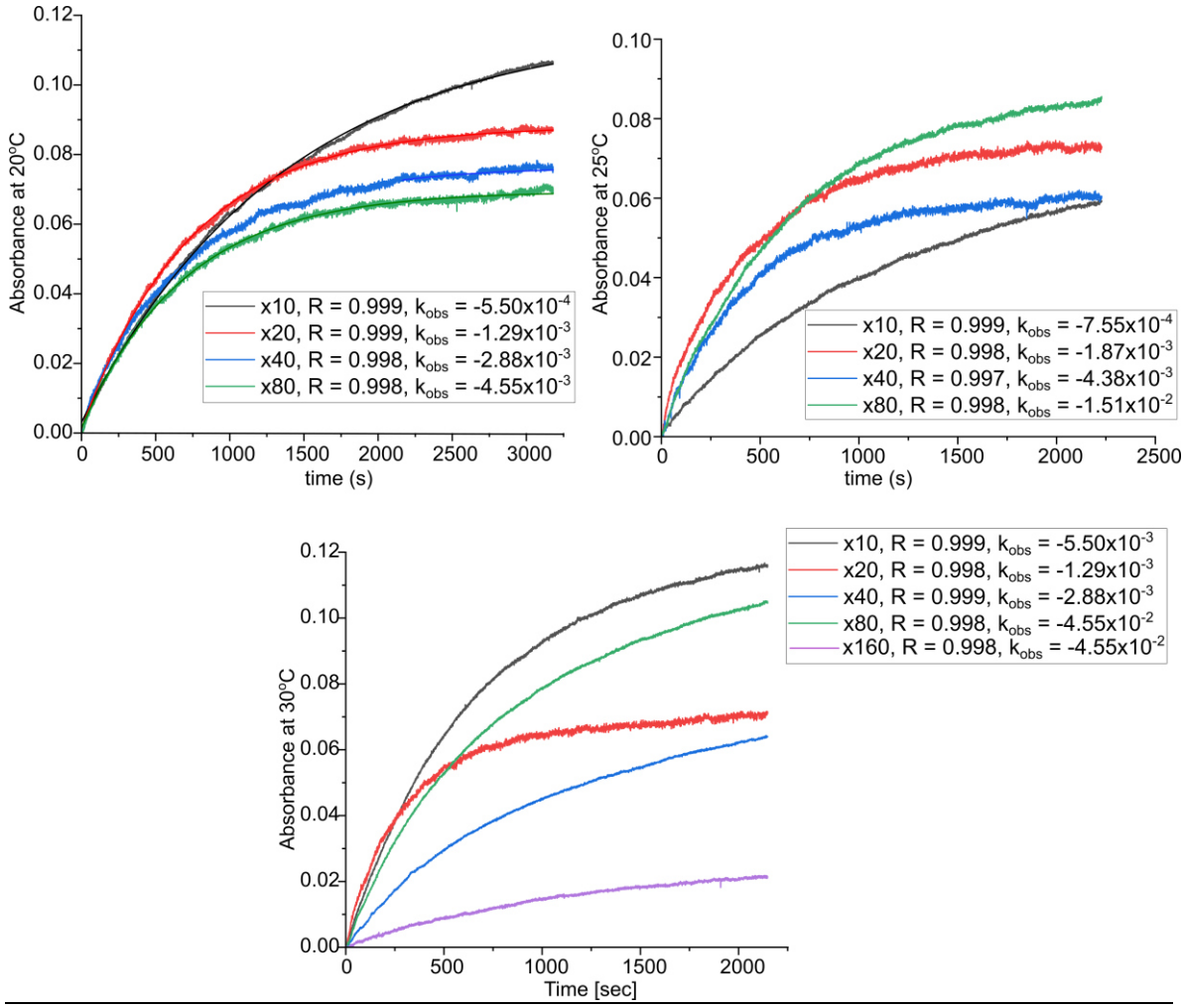


Figure S 47. Time dependence of the binding of GSH to **2d** with ratios of [2d]:[GSH] between 10 and 160 at 20, 25 and 30 °C

S6. HSA Binding

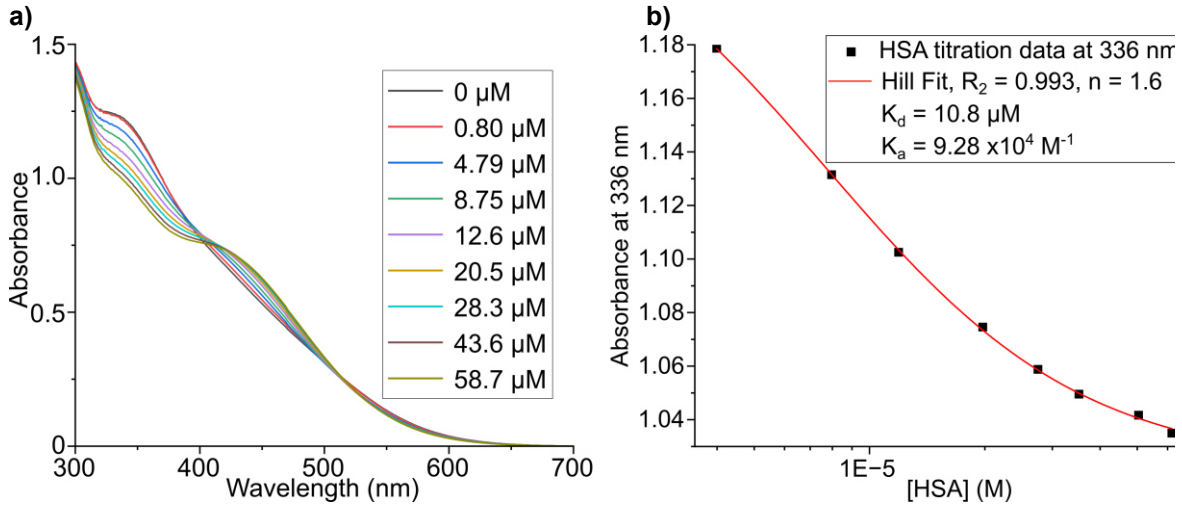


Figure S 48. a) A representation of the triplicates for the UV-vis absorption spectra of 150 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO after sequential additions of HSA from (0 µM to 58.7 µM) before precipitation at 15 °C **b)** An illustration of the Uv-vis titration spectra at 336 nm with a change in concentration of the ratio of **2d**:HSA at 15 °C**.**

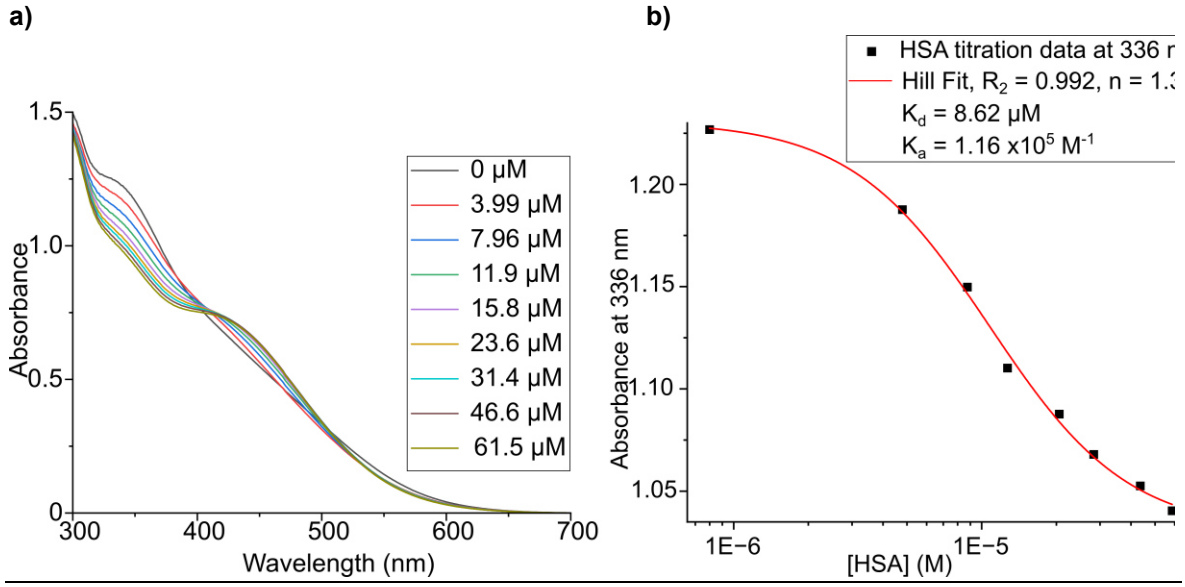


Figure S 49. a) A representation of the triplicates for the UV-vis absorption spectra of 150 µM **2d** in 0.10 M TRIS-HCl buffer 10% DMSO after sequential additions of HSA from (0 µM to 61.5 µM) before precipitation at 25 °C **b)** An illustration of the Uv-vis titration spectra at 336 nm with a change in concentration of the ratio of **2d**:HSA at 25 °C.

S7. Equations and derivations

S7.1. Hill equations

$y = y_{max} * x^n / (K_D + x^n)$

$y_{max}=(y_0+(y-y_0)$

thus

$y = (y_0+(y-y_0) * x^n / (K_D + x^n)$

$[DNA] = 1/(1+(K_D/[L])^n)$

$K_D = ([DNA][L])/[DNA-L]$

$K_A = K_D^{-1}$ (M^{-1})

S7.2. PKa equation

For the proposed speciation equation

[**2d**H_2]$^{2+}$ ⇌ [**2d**H]$^+$ ⇌ [**2d**] ⇌ [**2d**H_2O]$^+$ ⇌ [**2d**OH]

where the equilibrium constants for the forward reactions are k_1, k_2, k_3 and k_4 from left to right, and A, B, C, D, and E are the molar concentrations of [**2d**H_2]$^{2+}$, [**2d**H]$^+$, [**2d**], [**2d**H_2O]$^+$ and [**2d**OH] respectively.

k_1: A ⇌ B+H^+; k_2: B ⇌ C+H^+; k_3: C ⇌ D+Cl^- and k_4: D ⇌ E+H^+

Total concentration is

[T] = [A] + [B] + [C] + [D] + [E],

Therefore

$k_1 = \frac{[B][H^+]}{[A]}$, $k_2 = \frac{[B][H^+]}{[A]}$, $k_3 = \frac{[B][Cl^-]}{[A]}$, $k_4 = \frac{[B][H^+]}{[A]}$

[T] In terms of A,

$[B] = \frac{k_1[A]}{[H^+]}$; $[C] = \frac{k_2[B]}{[H^+]} = \frac{k_1k_2[A]}{[H^+]^2}$; $[D] = \frac{k_3[C]}{[Cl^-]} = \frac{k_1k_2k_3[A]}{[H^+]^2[Cl^-]}$ and $[E] = \frac{k_4[D]}{[H^+]} = \frac{k_1k_2k_3k_4[A]}{[H^+]^3[Cl^-]}$

Thus,

$[T] = [A] + \frac{k_1[A]}{[H^+]} + \frac{k_1k_2[A]}{[H^+]^2} + \frac{k_1k_2k_3[A]}{[H^+]^2[Cl^-]} + \frac{k_1k_2k_3k_4[A]}{[H^+]^3[Cl^-]}$

And,

$[T] = \frac{[A][H^+]^3[Cl^-]+k_1[A][H^+]^2[Cl^-]+k_1k_2[A][H^+][Cl^-]+k_1k_2k_3[A][H^+]+k_1k_2k_3k_4[A]}{[H^+]^3[Cl^-]}$,

$= [A]\frac{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}{[H^+]^3[Cl^-]}$

thus

$[A] = \frac{[H^+]^3[Cl^-][T]}{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}$

Following the same principles,

$[T] = [B]\frac{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}{k_1[H^+]^2[Cl^-]}$

$[B] = \frac{k_1[H^+]^2[Cl^-][T]}{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}$

and

$[T] = [C]\frac{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}{k_1k_2[H^+][Cl^-]}$

$[C] = \frac{k_1k_2[H^+][Cl^-][T]}{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}$

and

$[T] = [D]\frac{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}{[H^+]}$

$[D] = \frac{k_1k_2k_3[H^+][T]}{[H^+]^3[Cl^-]+k_1[H^+]^2[Cl^-]+k_1k_2[H^+][Cl^-]+k_1k_2k_3[H^+]+k_1k_2k_3k_4}$

and

$[T]= [E]\frac{[\mathrm{H}^+]^3[\mathrm{Cl}^-]+k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-]+k_1k_2[\mathrm{H}^+][\mathrm{Cl}^-]+k_1k_2k_3[\mathrm{H}^+]+ k_1k_2k_3k_4}{k_1k_2k_3k_4}$

$[E] =\frac{k_1k_2k_3k_4}{[\mathrm{H}^+]^3[\mathrm{Cl}^-]+k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-]+k_1k_2[\mathrm{H}^+][\mathrm{Cl}^-]+k_1k_2k_3[\mathrm{H}^+]+ k_1k_2k_3k_4}$

If,

$z = [\mathrm{H}^+]^3[\mathrm{Cl}^-] + k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-] + k_1k_2[\mathrm{H}^+][\mathrm{Cl}^-] + k_1k_2k_3[\mathrm{H}^+] + \ k_1k_2k_3k_4,$

and total absorbance of solution A_T if A_A, A_B, A_C, A_D and A_E represent the fractional contributions of each species to the total absorbance is

$[T]\cdot A_T = f([A]\cdot A_A) + f([B]\cdot A_B) + f([C]\cdot A_C) + f([D]\cdot A_D) + f([E]\cdot A_E)$

Then

$[A] =\frac{[\mathrm{H}^+]^3[\mathrm{Cl}^-][\mathrm{T}]}{z}$,$[B] =\frac{k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-][\mathrm{T}]}{z}$, $[C] =\frac{k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-][\mathrm{T}]}{z}$, $[D] =\frac{k_1k_2k_3[\mathrm{H}^+][\mathrm{T}]}{z}$ and $[E] =\frac{k_1k_2k_3k_4}{z}$

and

$A_T = \frac{[\mathrm{H}^+]^3[\mathrm{Cl}^-]A_A+k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-]A_B+k_1[\mathrm{H}^+]^2[\mathrm{Cl}^-]A_C+k_1k_2k_3[\mathrm{H}^+]A_D+k_1k_2k_3k_4A_E}{z}$,

Assuming that

$[\mathrm{H}^+] = \ [\mathrm{Cl}^-],$

$A_T = \frac{[\mathrm{H}^+]^4A_A+k_1[\mathrm{H}^+]^3A_B+k_1[\mathrm{H}^+]^2A_C+k_1k_2k_3[\mathrm{H}^+]A_D+k_1k_2k_3k_4A_E}{z}$.

$pH = \ -\log[H^+],$

then $[H^+] = 10^{-pH}$,

and

$A_T = (A_A\times10^{-4pH} + k_1A_B\times10^{-3pH} + k_1k_2\ A_C\times10^{-2pH}+ k_1k_2k_3\ A_D\times10^{-pH} + k_1k_2k_3k_4A_E)/(\ 10^{-4pH} + k_1\times10^{-3pH} + k_1k_2\times10^{-2pH} + k_1k_2k_3\times10^{-pH} + k_1k_2k_3k_4)$.