Supplementary Materials to the paper entitled:

A naphthalene-based and hydroxyamide-functionalized hybrid Schiff base and its dimeric and dinuclear Zn(II) complex: synthesis, structural and theoretical characterization, optical, DPPH scavenging and *in silico* ADME properties

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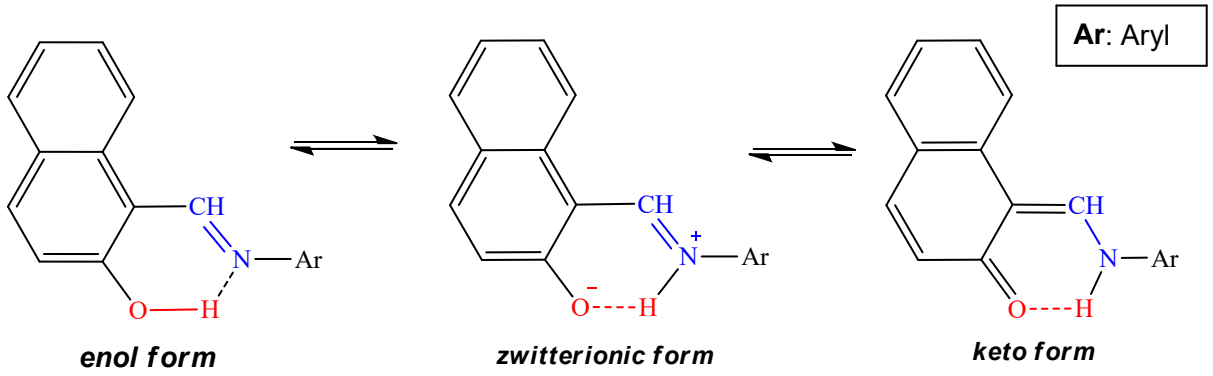
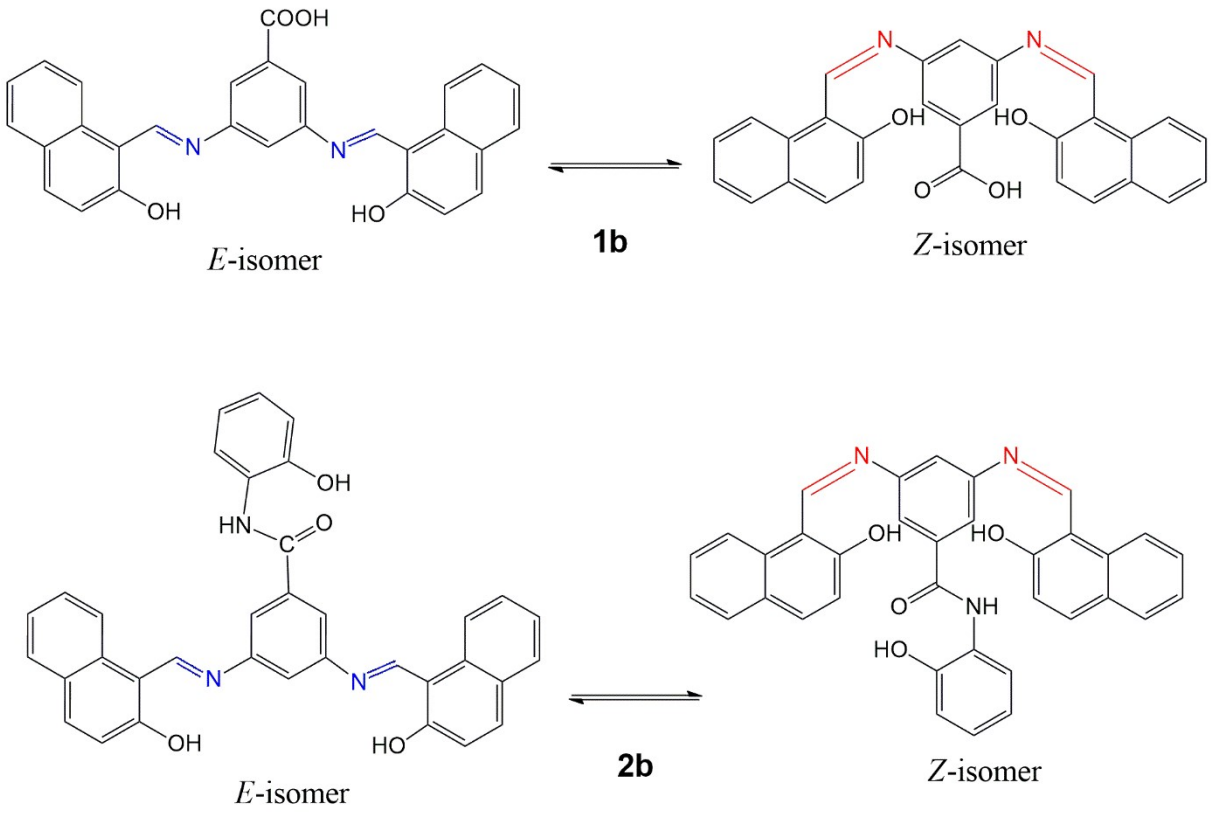
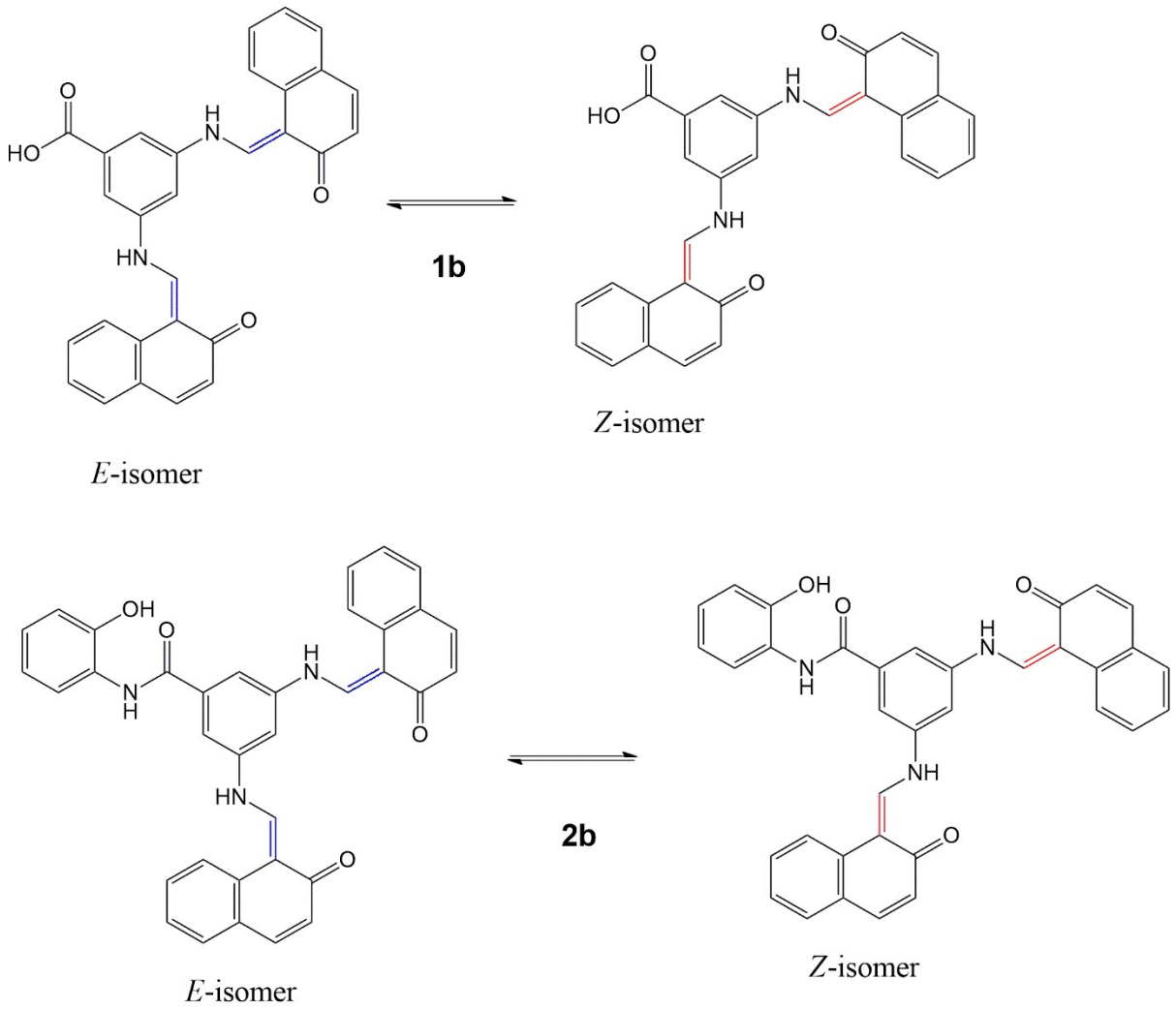
List of Content (Supplementary Materials)



Scheme S1. The enol-imine and keto-amine tautomeric equilibrium in ortho-hydroxy Schiff bases.



Scheme S2. Structural configurations of enol tautomer of **1b** and **2b**.



Scheme S3. Structural configurations of keto tautomer of **1b** and **2b**.

Table S1 Mass spectrum (HRMS) data of the compounds **1b**–**3b**.

Comp	Theor. Mol. Mass (*m/z*)	Detec.Mol. Mass (*m/z*)	RT (min)	Fragment ion		
				Mass (*m/z*)	Molecular formula	Assignment
1b	$[C_{29}H_{20}N_2O_4 + H]^+$ 461.1501 $[M + H]^+$	461.1489 $[M + H]^+$	8.2	921.2901 214.0861	$[C_{29}H_{20}N_2O_4]_2$ $[C_{13}H_{14}N_2O]^+$	*Dimeric Structure* $[M_2]^+$ 2-(((3-aminophenyl)amino)methyl)phenol
2b	$[C_{35}H_{25}N_3O_4 + H]^+$ 552.1923 $[M + H]^+$	552.1910 $[M + H]^+$	10.8	607.3902	$[C_{35}H_{25}N_3O_4 + C_3H_3O]^+$	
3b	$[Zn_2(C_{35}H_{23}N_3O_4)_2(H_2O)_2]\cdot 2H_2O$ 1334.2594 $[M]^+$	-	9.0	558.6808 214.2083	$[C_{35}H_{25}N_3O_4 + 7H]^+$ $[C_{13}H_{14}N_2O]^+$	 2-(((3-aminophenyl)amino)methyl)phenol
		-	9.9	513.5783	$[C_{35}H_{32}N_3O]^+$	3-(hydroxy(phenylamino)methyl)-*N*-(naphthalen-1-ylmethyl)-5-((naphthalen-1-ylmethyl)amino)benzenaminium
				452.5792	$[C_{31}H_{22}N_3O]^+$	2-((*E*)-((3-((*E*)-(naphthalen-1-ylmethylene)amino)-5-(phenylcarbamoyl)phenyl)imino)methyl)benzene-1-ylium
				321.3654	$[C_{20}H_{22}N_3O]^+$	3-(benzylamino)-5-(hydroxy(phenylamino)methyl)-benzenaminium
				214.2084	$[C_{13}H_{14}N_2O]^+$	2-(((3-aminophenyl)amino)methyl)phenol
		-	10.8	403.4622	$[C_{29}H_{27}N_2]^+$	3-methyl-*N*-(naphthalen-1-ylmethyl)-5-((naphthalen-1-ylmethyl)amino)benzenaminium
				214.2083	$[C_{13}H_{14}N_2O]^+$	2-(((3-aminophenyl)amino)methyl)phenol
		-	10.9	502.6026	$[C_{35}H_{24}N_3O]^+$	1-((*E*)-((3-((*E*)-(naphthalen-1-ylmethylene)amino)-5-(phenylcarbamoyl)phenyl)imino)methyl)naphthalen-2-ylium
				214.2085	$[C_{13}H_{14}N_2O]^+$	2-(((3-aminophenyl)amino)methyl)phenol
		-	11.0	507.5606	$[C_{35}H_{28}N_3O]^+$	1-(((3-((naphthalen-1-ylmethyl)amino)-5-(phenylcarbamoyl)phenyl)amino)methyl)naphthalen-2-ylium
				214.2086	$[C_{13}H_{14}N_2O]^+$	2-(((3-aminophenyl)amino)methyl)phenol
		1334.4077 $[M]^+$	12.0	214.2086	$[C_{13}H_{14}N_2O]^+$	*Dimeric Structure* 2-(((3-aminophenyl)amino)methyl)phenol

Table S2 Photophysical data of **1b**–**3b** at room temperature.

Comp.	Media	UV–Vis Absorption		FL Emission (λ_{ex} = 365 nm)		Stokes shift (nm)
		λ_{abs} (nm)	ε (L mol^{-1} cm^{-1})	λ_{em} (nm)	Intensity (a.u.)	
1b	DMSO (100 μM)	320	14,197	426	205.7	184
		391	11,074	504	431.9	
		444	11,593			
		467	11,291			
	DMSO (50 μM)	320	13,166	425	608.0	183
		394	10,118	503	663.4	
		444	11,248	728	29.5	
		467	10,950			
	DMF (100 μM)	320	22,697	426	211.5	179
		390	18,679	499	424.0	
		442	14,918			
		465	13,939			
	DMF (50 μM)	320	20,530	427	620.1	179
		390	18,242	499	716.3	
		443	15,522	726	34.8	
		465	14,644			
2b	DMSO (100 μM)	322	15,310	459	20.5	182
		394	14,869	504	406.8	
		443	12,923			
		468	12,583			
	DMSO (50 μM)	322	14,112	452	220.4	178
		393	14,432	500	513.2	
		443	12,604	730	26.4	
		467	12,282			
	DMF (100 μM)	320	18,830	457	56.7	180
		393	18,032	500	285.1	
		440	12,615			
		465	11,331			
	DMF (50 μM)	320	18,262	450	315.3	175
		390	18,574	495	377.4	
		441	13,664	727	147.5	
		465	12,600			
3b	DMSO (100 μM)	321	16,596	505	201.7	184
		395	16,118			
		444	13,998			
		468	13,616			
	DMSO (50 μM)	320	14,840	452	65.8	180
		396	14,836	500	457.6	
		443	13,462	727	11.8	
		467	13,066			
	DMF (100 μM)	322	22,738	453	46.9	179
		391	22,648	501	252.2	
		439	14,929			
		465	13,698			
	DMF (50 μM)	321	20,732	453	61.8	109
		390	21,574	499	331.4	
		440	14,694	730	33.4	
		465	13,486			

Table S3 The color purity parameters of the compounds **1b**–**3b**.

Media	**1b**					**2b**					**3b**				
	[a] CP %	[b] CP %	dominant wavelength λ_{em} (nm)	x_d y_d	sample x_s y_s	[a] CP %	[b] CP %	dominant wavelength λ_{em} (nm)	x_d y_d	sample x_s y_s	[a] CP %	[b] CP %	dominant wavelength λ_{em} (nm)	x_d y_d	sample x_s y_s
DMSO (100 μM)	33.12	33.15	504	0.004 0.633	0.177 0.376	66.61	65.31	504	0.004 0.633	0.188 0.583	68.56	67.35	505	0.004 0.655	0.187 0.604
DMSO (50 μM)	36.19	38.54	503	0.004 0.610	0.166 0.263	58.20	56.78	500	0.008 0.538	0.177 0.489	39.18	39.62	500	0.008 0.538	0.169 0.357
DMF (100 μM)	39.79	40.51	499	0.010 0.513	0.170 0.344	51.11	49.62	500	0.008 0.538	0.192 0.467	52.50	51.18	501	0.006 0.563	0.182 0.477
DMF (50 μM)	43.25	45.91	499	0.010 0.513	0.165 0.261	49.38	52.11	495	0.023 0.413	0.171 0.261	54.41	53.04	499	0.010 0.513	0.178 0.460

[a] Standart illuminant C ($x_i = 0.31006$, $y_i = 0.31616$)

[b] Standart illuminant D65 ($x_i = 0.31271$, $y_i = 0.32902$)

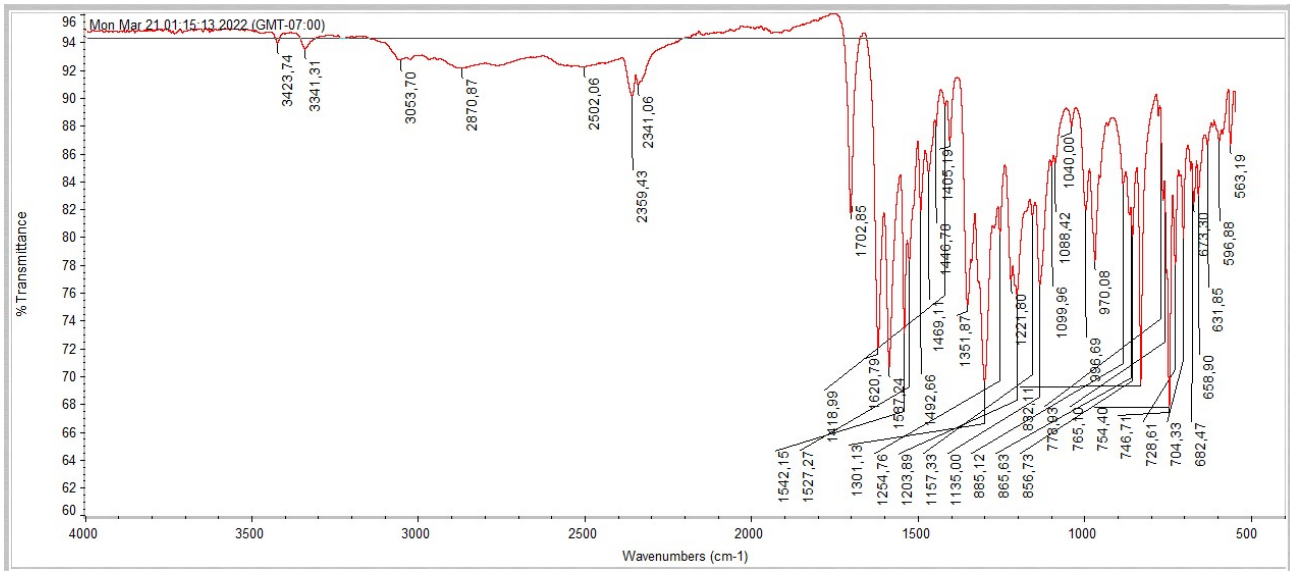
Table S4 Physicochemical properties of the compounds by *in silico* SwissADME technique.

Properties	**1b**	**2b**
Physicochemical properties	460.48 g/mol	551.59 g/mol
Mol. Wt.	$C_{29}H_{20}N_2O_4$	$C_{35}H_{25}N_3O_4$
No. of heavy atoms	35	42
No. of aromatic heavy atoms	26	32
Fraction Csp3	0.00	0.00
No. of rotatable bonds	5	7
No. of H-bond acceptors	6	6
No. of H-bond donors	3	4
Molar refractivity	139.85	169.13
TPSA	102.48 Å^2	114.51 Å^2
Lipophilicity		
Log $P_{o/w}$ (iLOGP)	3.47	4.32
Log $P_{o/w}$ (XLOGP3)	5.84	6.79
Log $P_{o/w}$ (WLOGP)	6.60	7.67
Log $P_{o/w}$ (MLOGP)	3.45	3.71
Log $P_{o/w}$ (SILICOS-IT)	6.37	7.16
Consensus Log $P_{o/w}$	5.15	5.93
Water solubility		
Log S (ESOL)	-6.59	-7.64
Solubility	[a] 1.17×10^{-4} mg/mL	[a] 1.27×10^{-5} mg/mL
Log S (Ali)	-7.76	-9.00
Solubility	[a] 7.94×10^{-6} mg/mL	[a] 5.49×10^{-7} mg/mL
Log S (SILICOS-IT)	-9.06	-11.52
Solubility	[a] 4.04×10^{-7} mg/mL	[b] 1.66×10^{-9} mg/mL

[a]poorly soluble, [b]insoluble

Table S5 Pharmacokinetic properties of the compounds by *in silico* SwissADME technique.

Properties	**1b**	**2b**
Pharmacokinetics		
GI absorption	Low	Low
BBB permeant	No	No
P-gp substrate	No	No
CYP1A2 inhibitor	No	No
CYP2C19 inhibitor	No	No
CYP2C9 inhibitor	No	No
CYP2D6 inhibitor	No	No
CYP3A4 inhibitor	No	No
Log K_p (skin permeation)	-4.96 cm/s	-4.84 cm/s
Drug-likeness		
Lipinski	Yes; 0 violation	Yes; 1 violation: MW>500
Ghose	No; 2 violations: WLOGP>5.6, MR>130	No; 3 violations: MW>480, WLOGP>5.6, MR>130
Veber	Yes	Yes
Egan	No; 1 violation: WLOGP>5.88	No; 1 violation: WLOGP>5.88
Muegge	No; 1 violation: XLOGP3>5	No; 1 violation: XLOGP3>5
Bioavailability score	0.56	0.55
Medicinal chemistry		
PAINS	0 alert	0 alert
Brenk	1 alert: imine_1	2 alerts: catechol, imine_1
Lead-likeness	No; 2 violations: MW>350, XLOGP3>3.5	No; 2 violations: MW>350, XLOGP3>3.5
Synthetic accessibility	3.31	3.69



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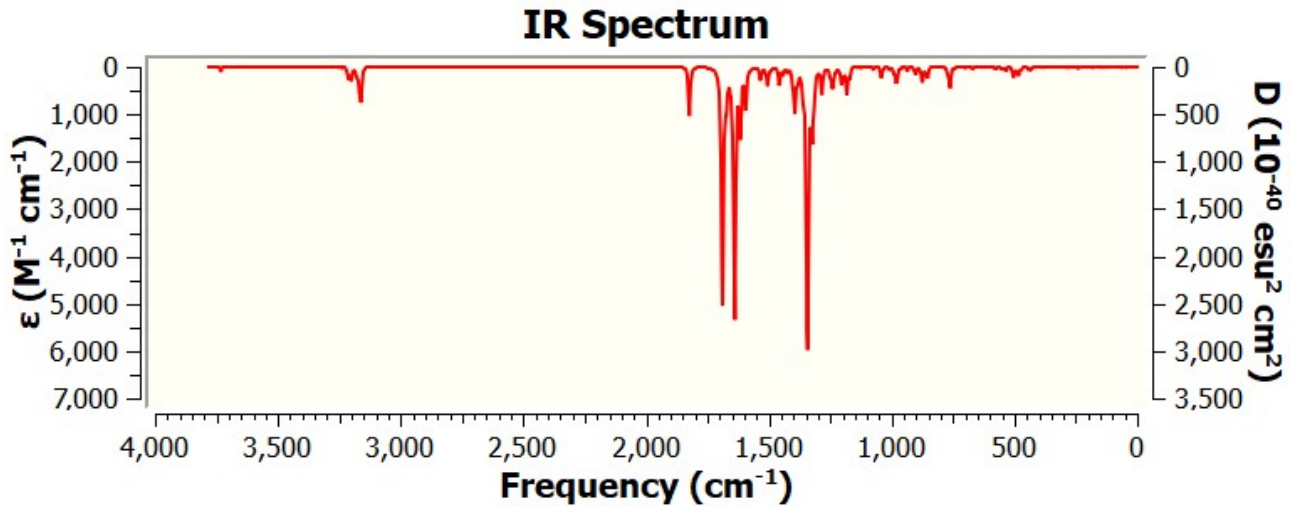
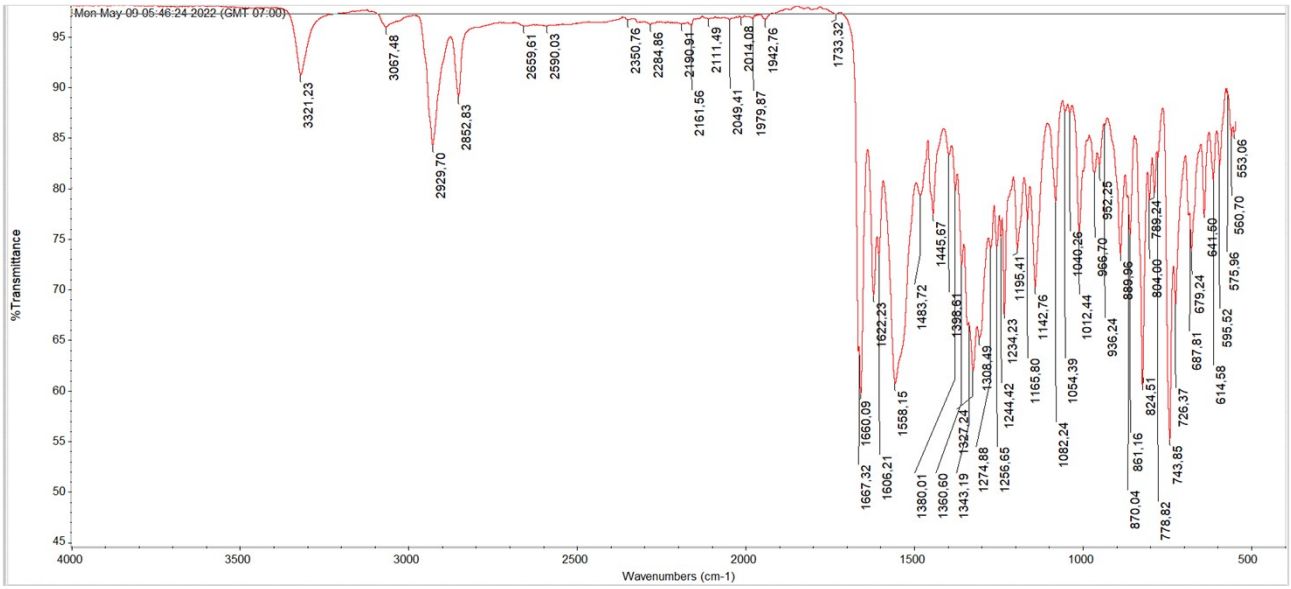
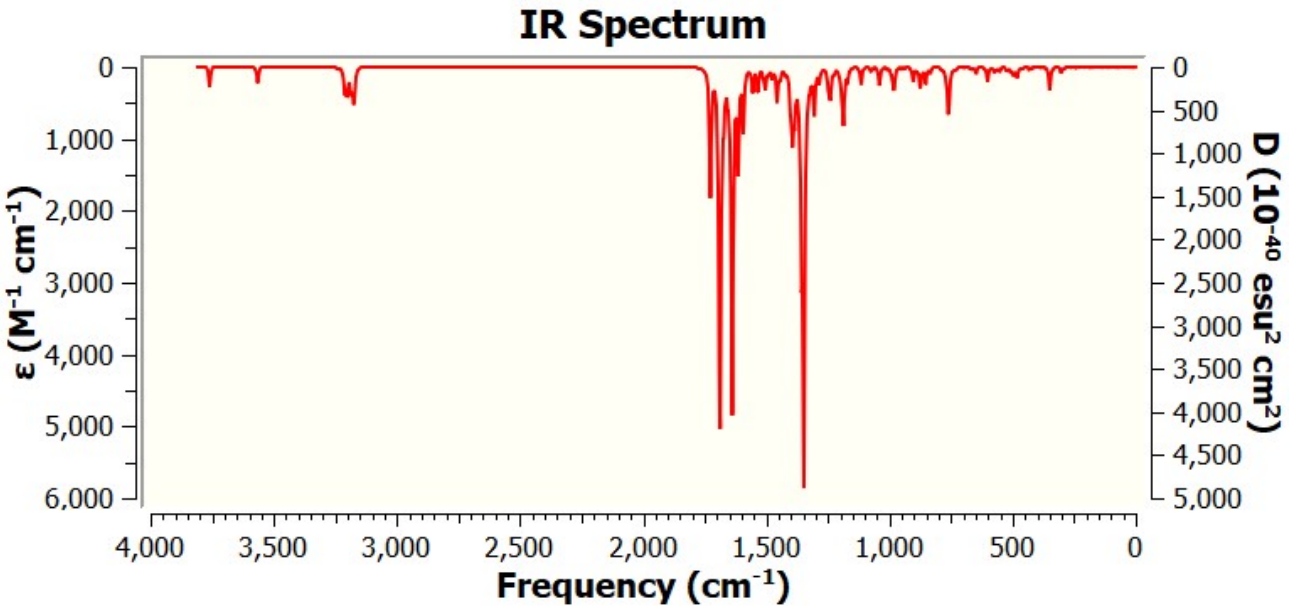


(b)

Fig. S1. Comparison between experimental IR spectrum of **1b (a)** in the solid state with the corresponding *(keto tautomer)* predicted in gas phase **(b)**.

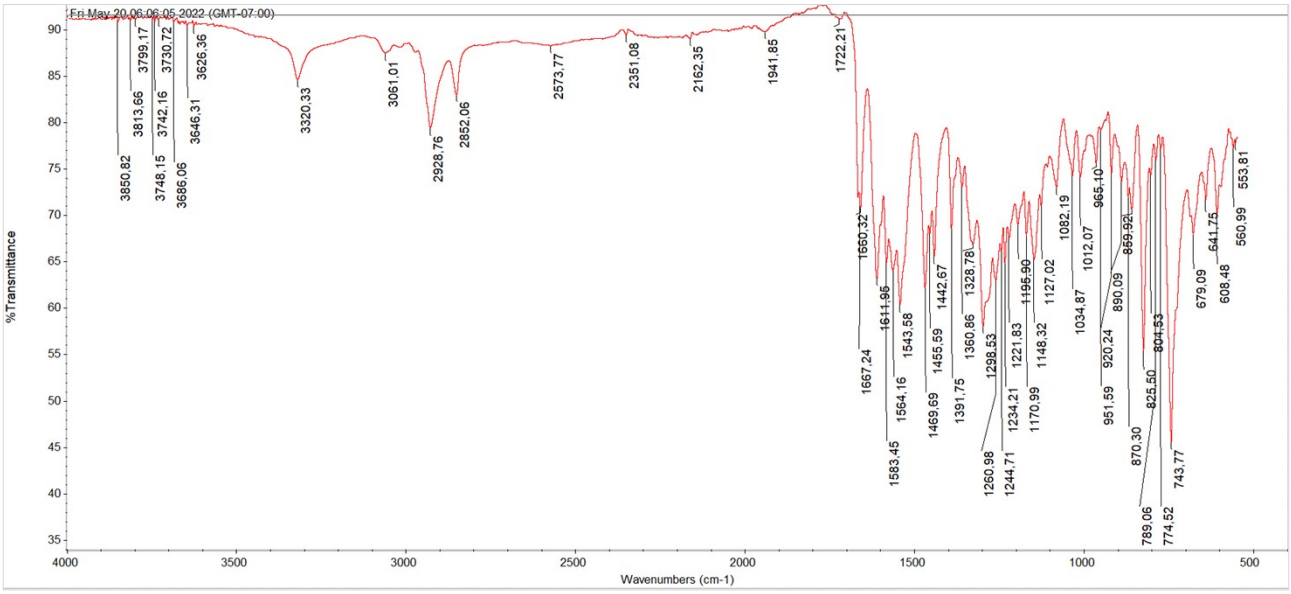


(a)



(b)

Fig. S2. Comparison between experimental IR spectrum of **2b (a)** in the solid state with the corresponding *(keto tautomer)* predicted in gas phase **(b)**.



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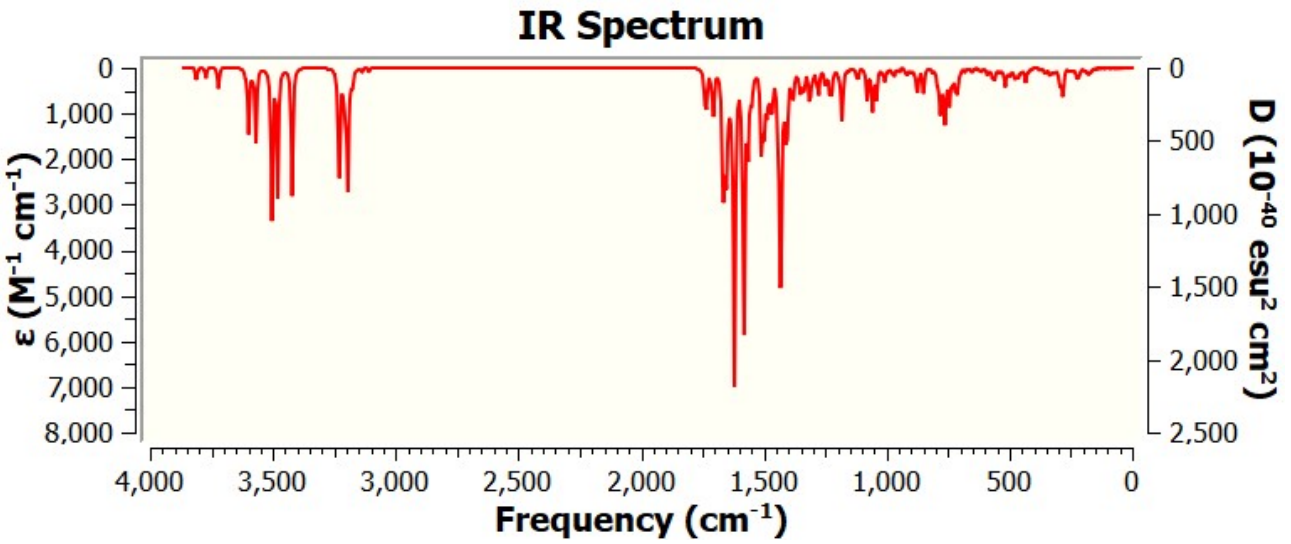


(b)

Fig. S3. Comparison between experimental IR spectrum of **3b (a)** in the solid state with the corresponding predicted in gas phase **(b)** *(ligand: enol tautomer)*.

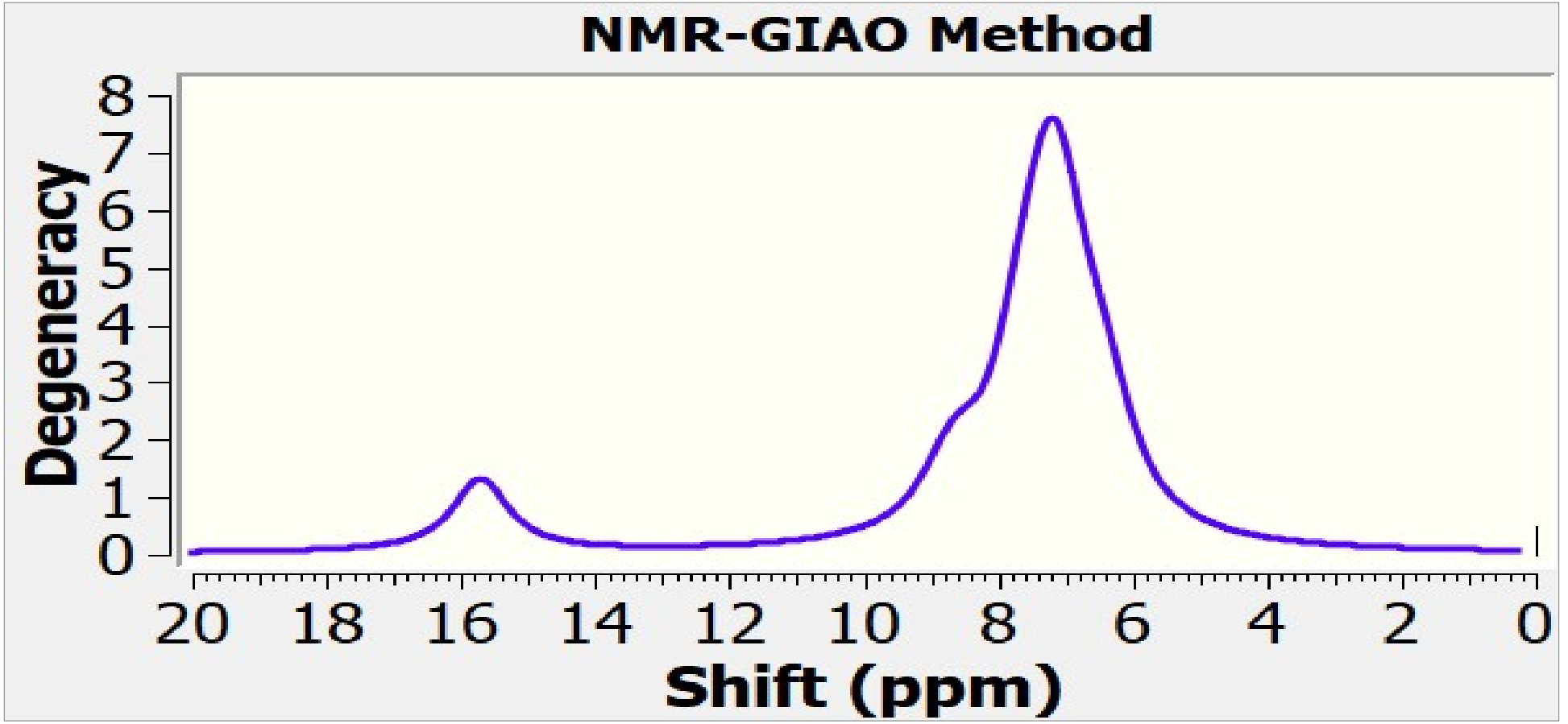


Fig. S4. Theoretical ^{1}H-NMR spectrum of **1b** *(keto tautomer)* in gas phase.

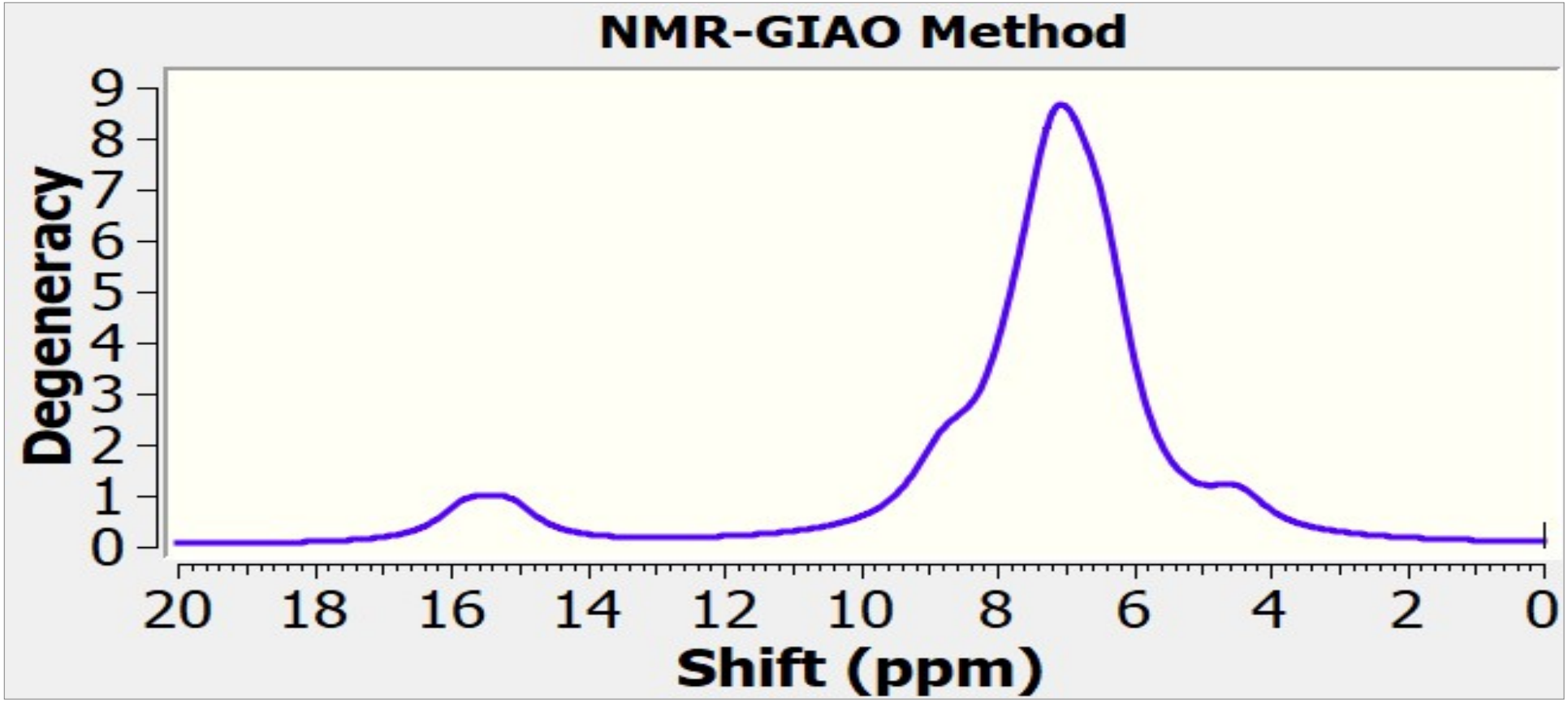


Fig. S5. Theoretical ^{1}H-NMR spectrum of **2b** *(keto tautomer)* in gas phase.

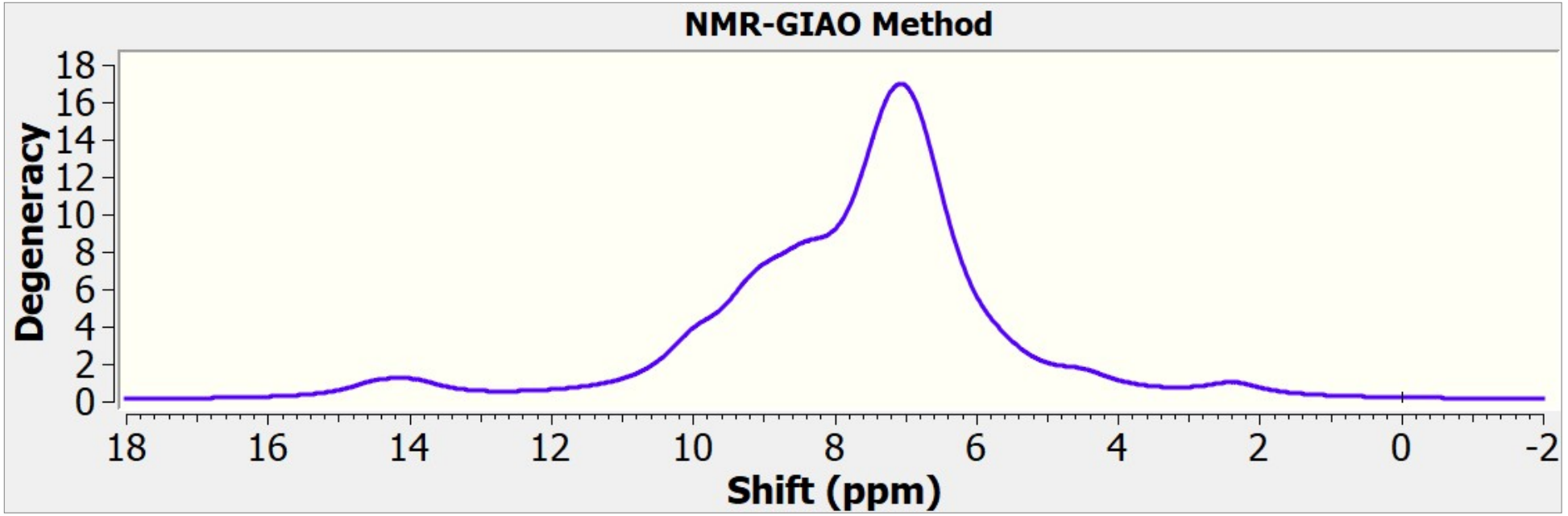


Fig. S6. Theoretical ^{1}H-NMR spectrum of homodinuclear dimeric structure of **3b** in gas phase *(ligand: keto tautomer)*.

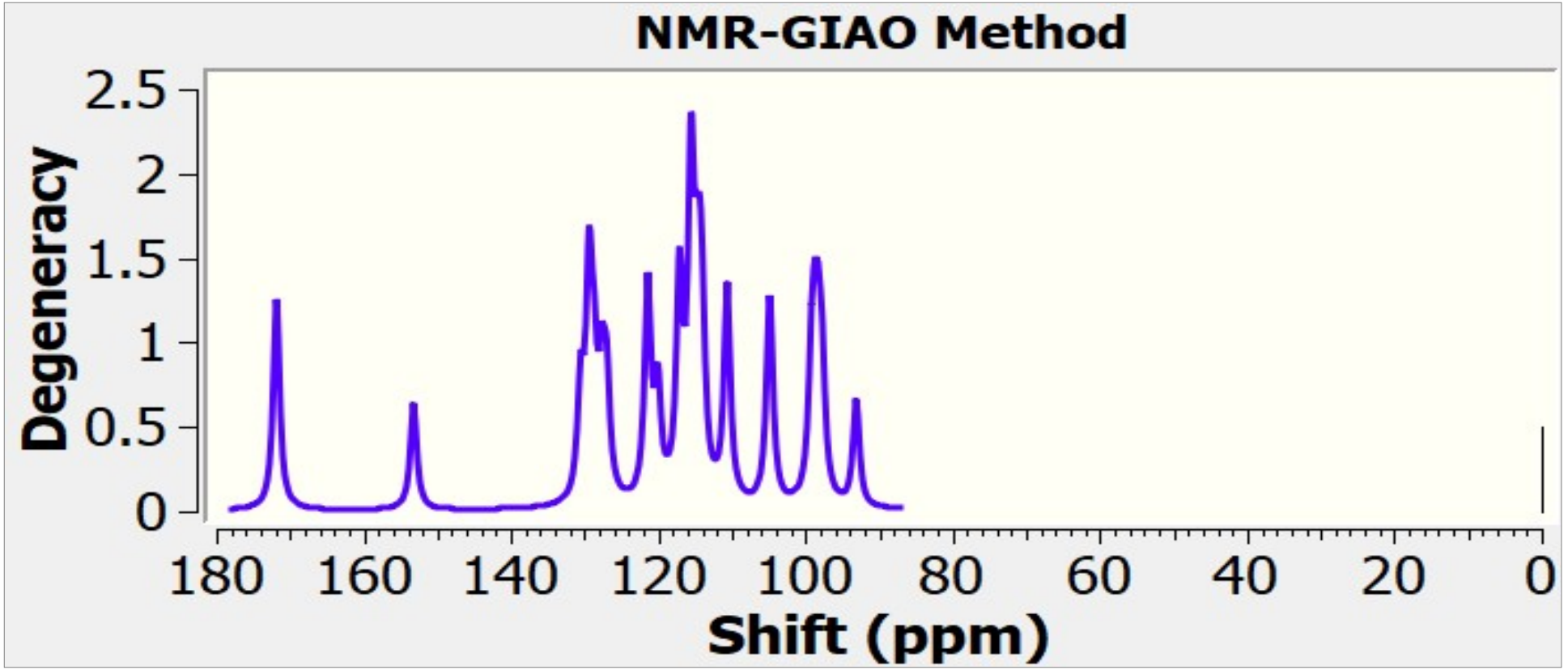


Fig. S7. Theoretical ^{13}C-NMR spectrum of **1b** *(keto tautomer)* in gas phase.

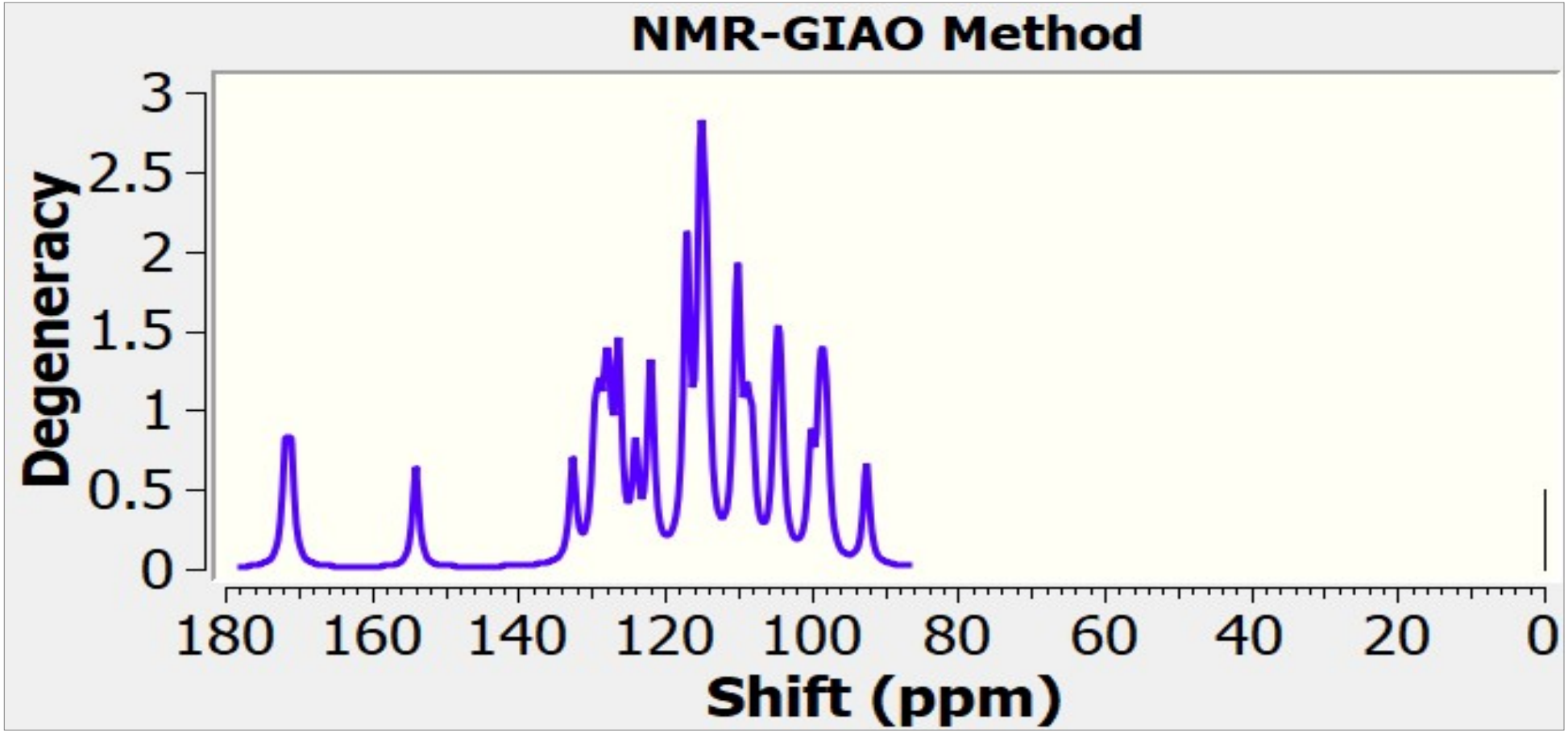


Fig. S8. Theoretical ^{13}C-NMR spectrum of **2b** *(keto tautomer)* in gas phase.

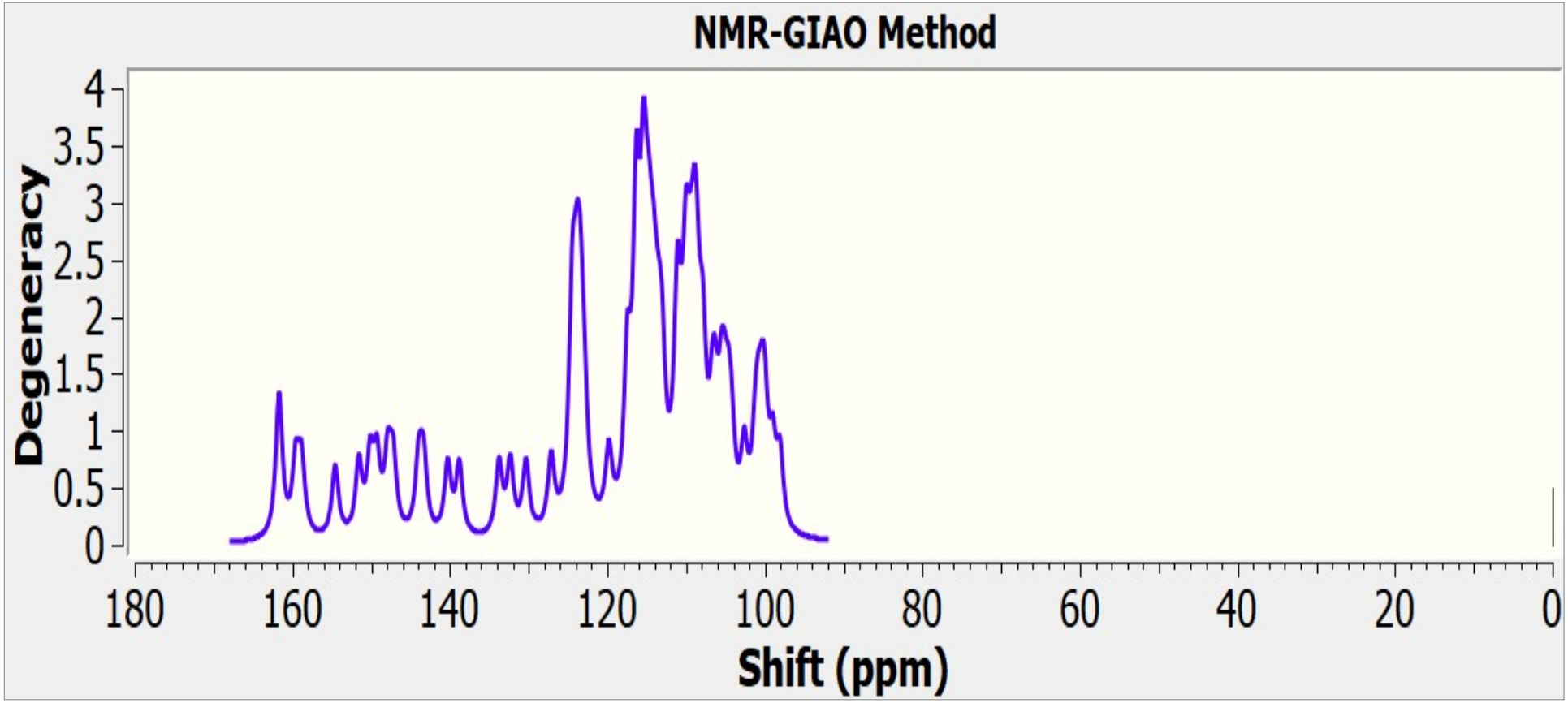


Fig. S9. Theoretical ^{13}C-NMR spectrum of homodinuclear dimeric structure of **3b** in gas phase *(ligand: keto tautomer)*.

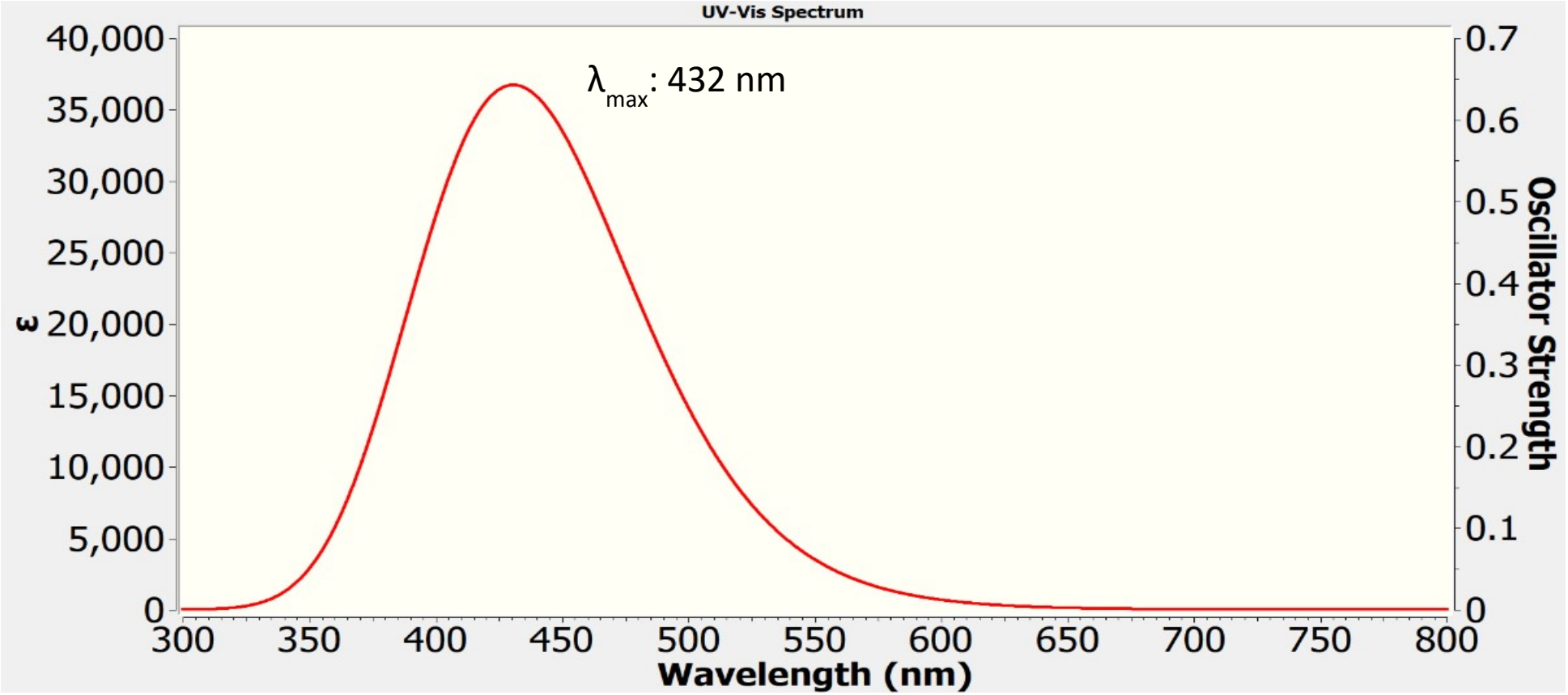


Fig. S10. Theoretical UV-Vis spectrum of **1b** (*keto tautomer)* in gas phase.

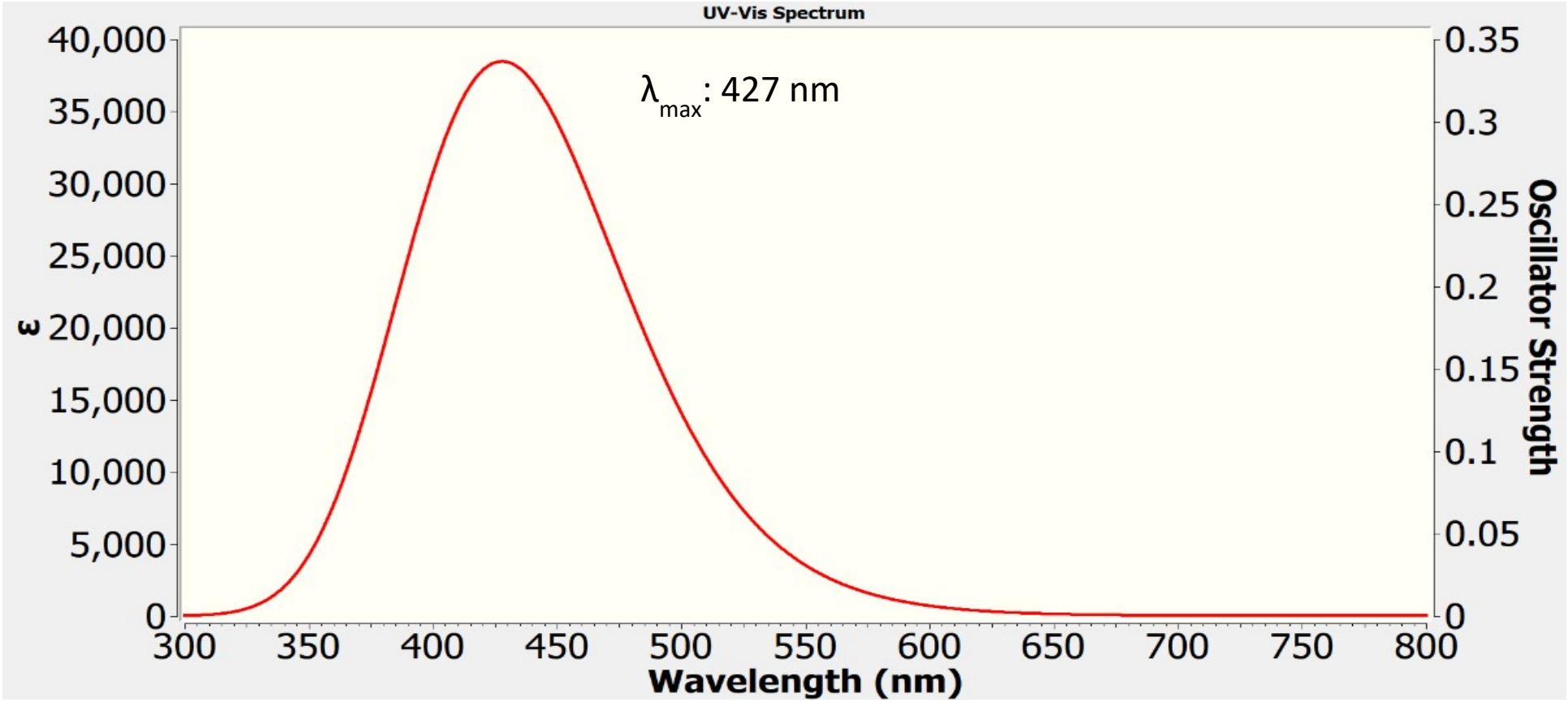


Fig. S11. Theoretical UV-Vis spectrum of **2b** *(keto tautomer)* in gas phase.

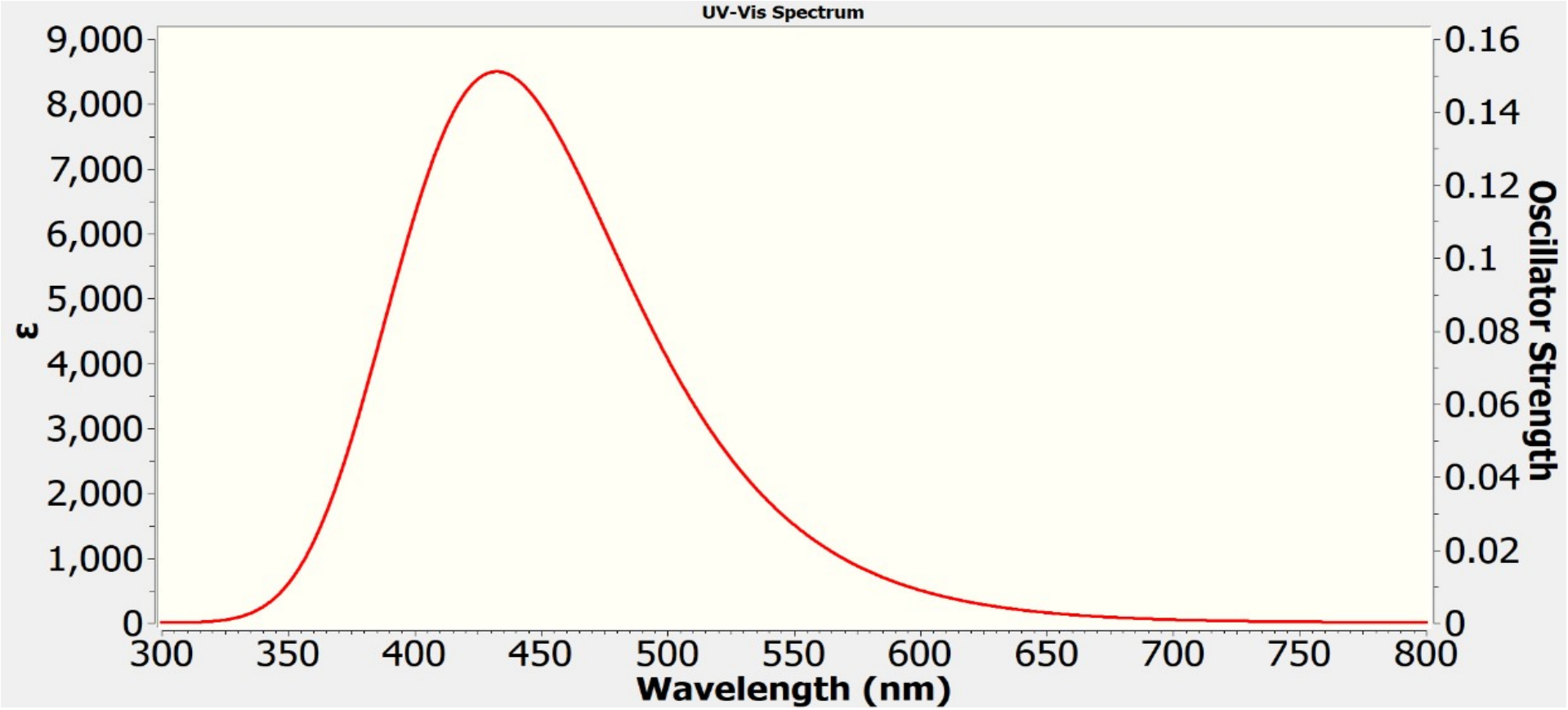


Fig. S12. Theoretical UV-Vis spectrum of homodinuclear dimeric structure of **3b** in gas phase *(ligand: keto tautomer)*.

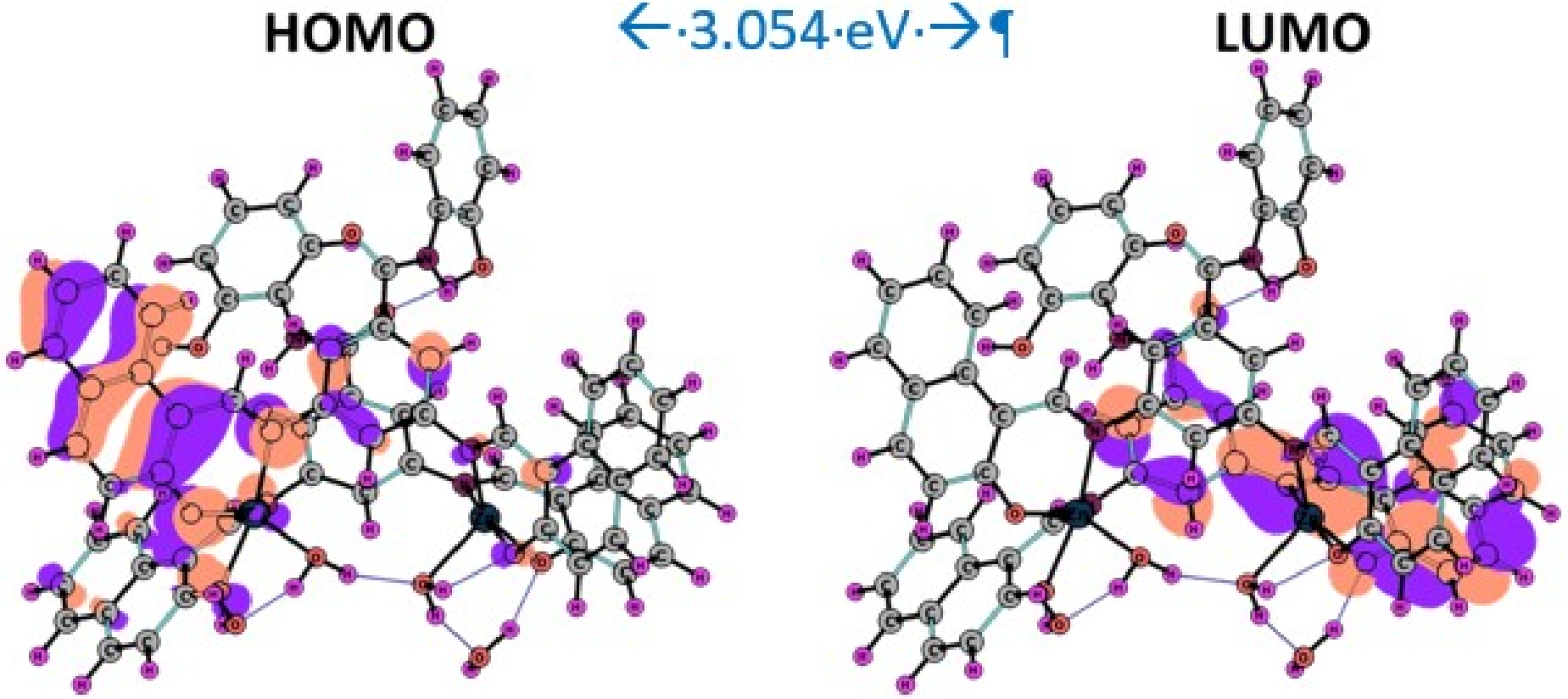


Fig. S13. Frontier MOs of homodinuclear dimeric structure of **3b** (*ligand: ketol tautomer*).

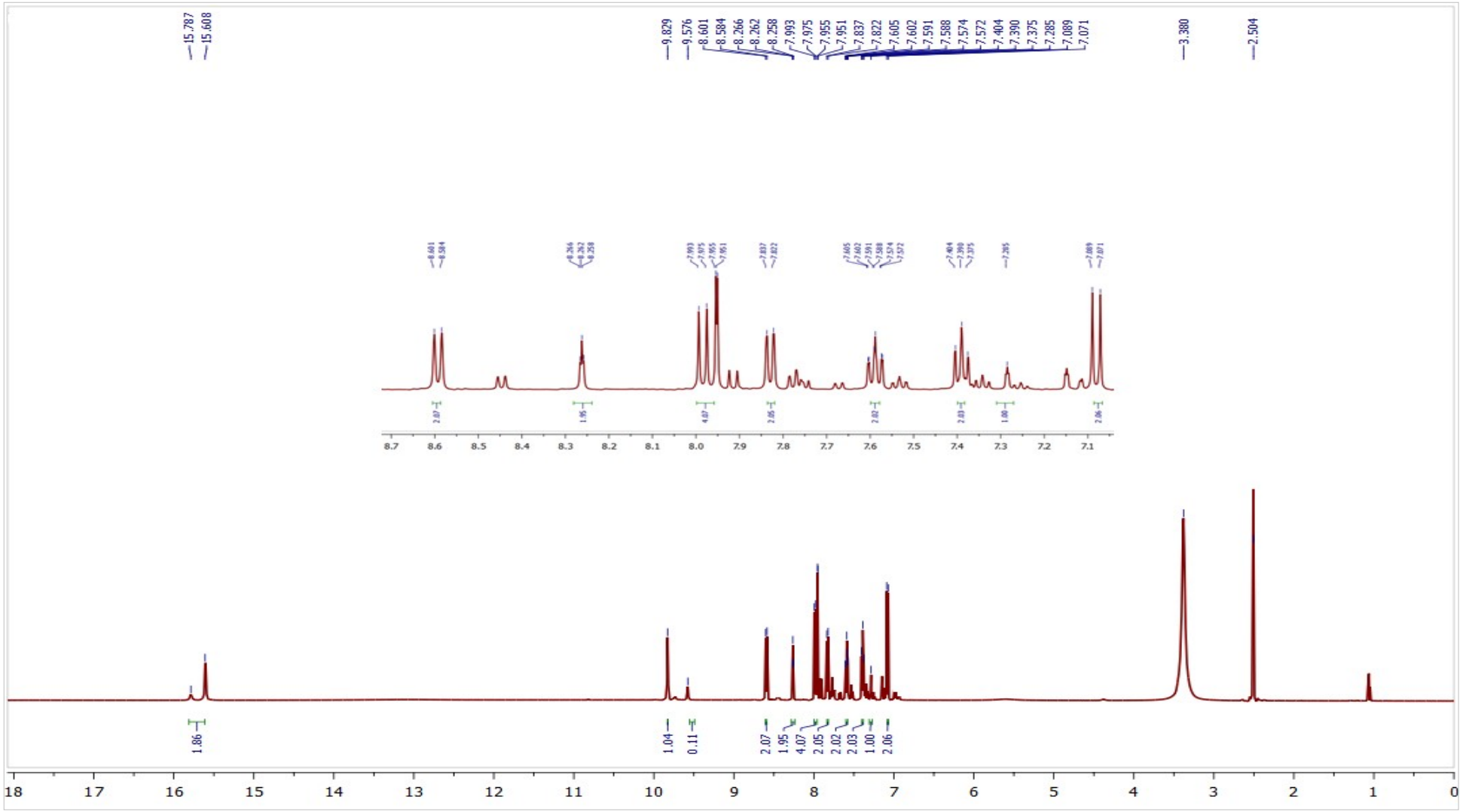


Fig. S14. ^{1}H-NMR spectrum of **1b** in DMSO-d_6.

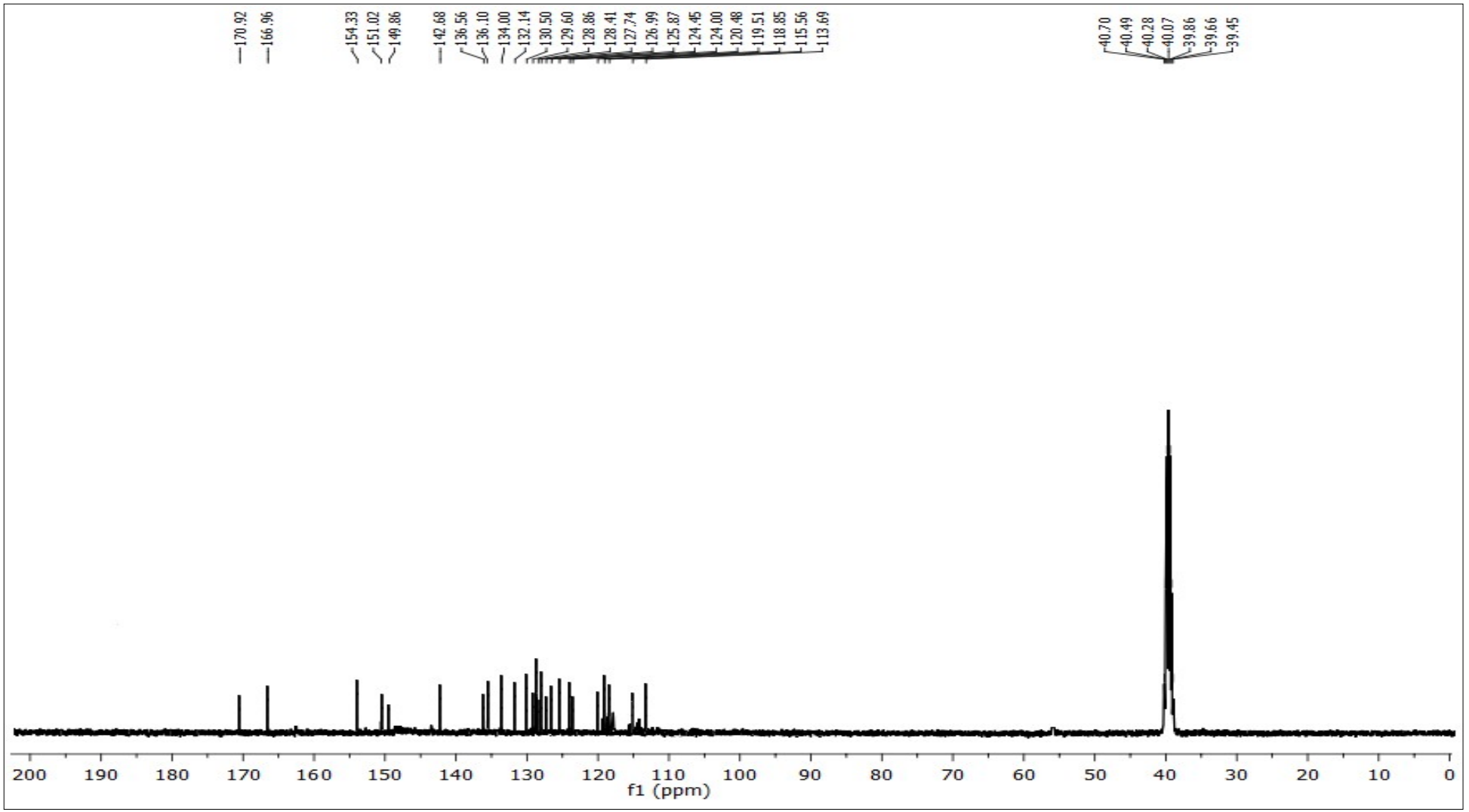


Fig. S15. ^{13}C-NMR spectrum of **1b** in DMSO-d_6.

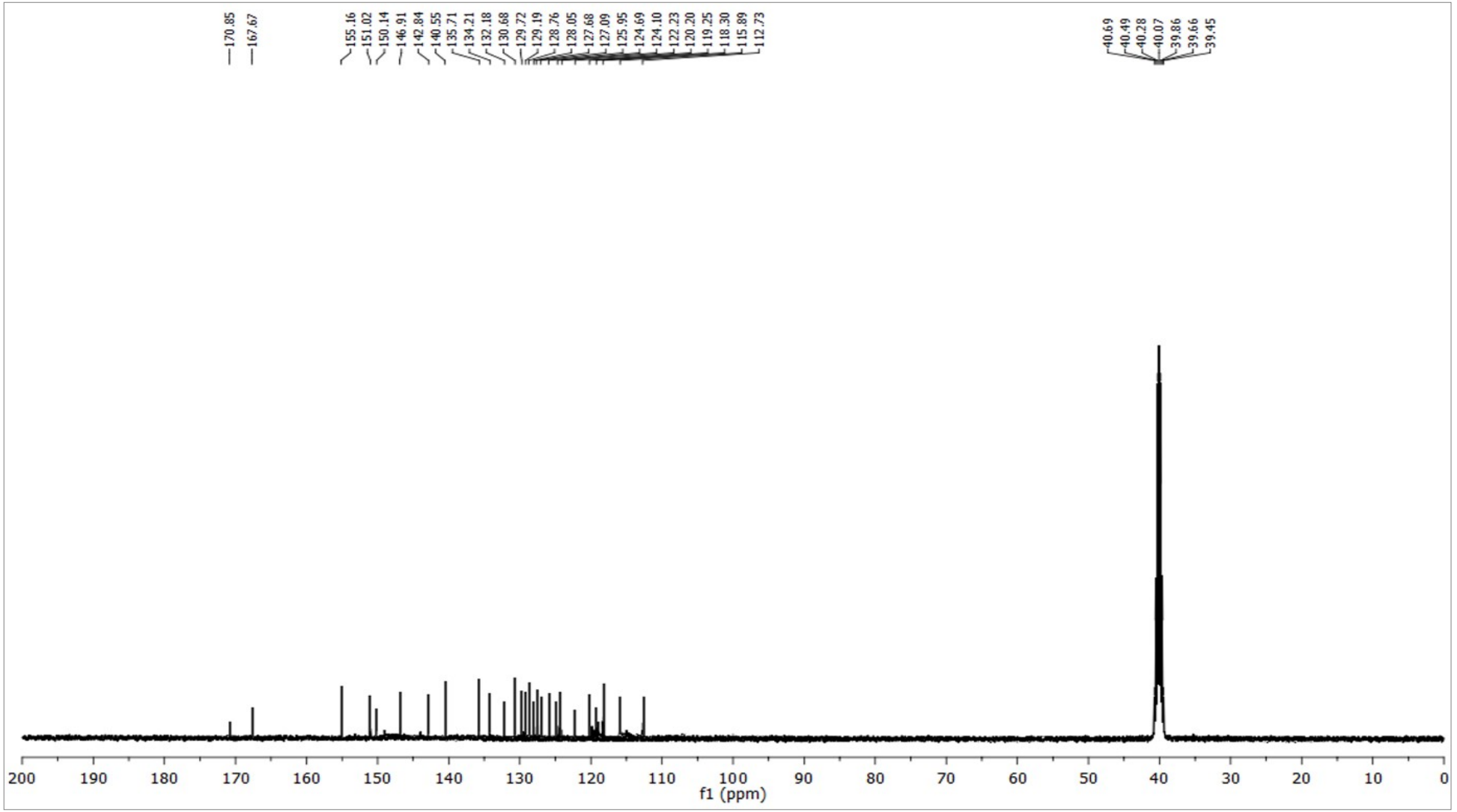
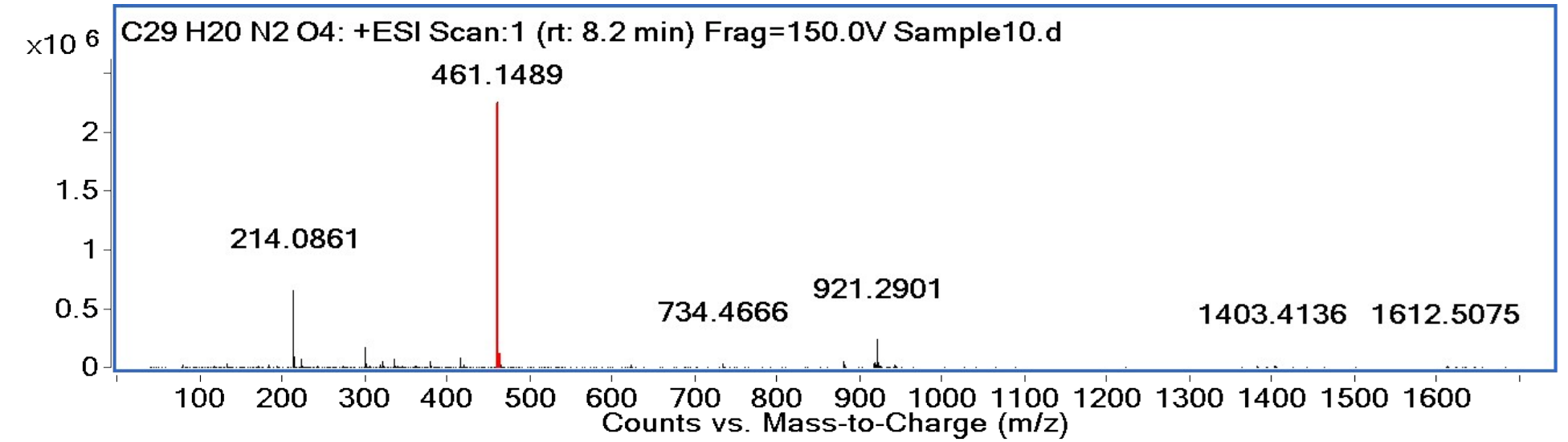


Fig. S16. ^{13}C-NMR spectrum of **2b** in DMSO-d_6.



Spectrum Identification Results: + Scan:1 (rt: 8.2 min) - Sample10.d

Automatically Show Columns

Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Score (MFG)
	MFG	C29 H20 N2 O4	(M+H)+	461.1489	98.91	1.38	98.91

Species	m/z	Score	Score (mass)	Score (MS)	Score (MFG)	Score (iso. spacing)	Height	Ion Formula
(M+H)+	461.1489	99.58	98.1	98.91	98.91	99.74	2255301	C29 H21 N2 O4

Height (Calc)	Height Su	Heigh	m/z (Calc)	Diff (mDa)	Height	Height %	Height Sum %	m/z	Diff (ppm)
2233599.7	71.8	100	461.1496	0.7	2255301	100	72.5	461.1489	1.52
725700.4	23.3	32.5	462.1528	0.4	719948.1	31.9	23.2	462.1524	0.95
132431.3	4.3	5.9	463.1557	0.7	118346.6	5.2	3.8	463.1551	1.41
17512.3	0.6	0.8	464.1585	0.3	15648.1	0.7	0.5	464.1583	0.58

Fig. S17. TOF-MS spectrum of **1b**.

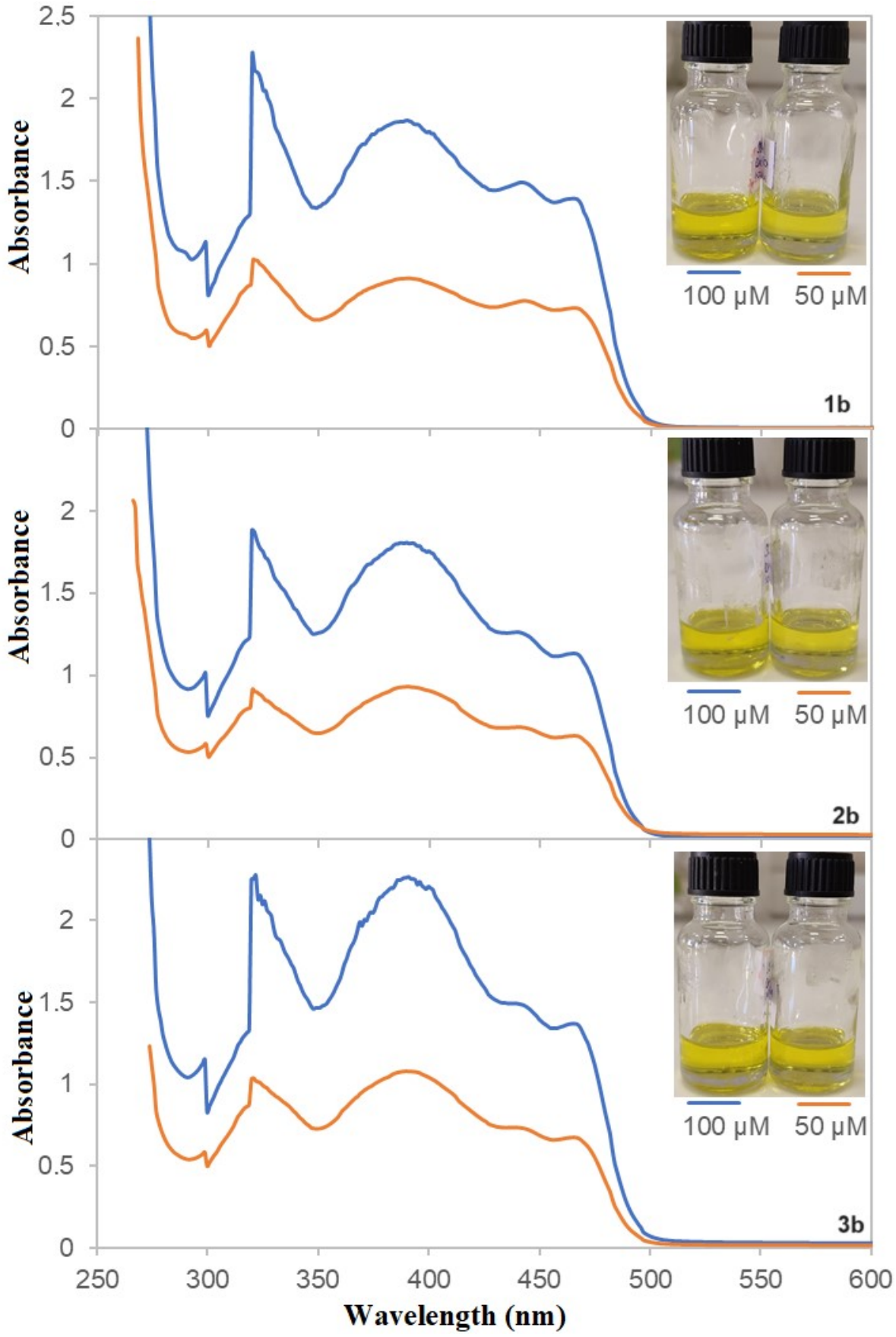


Fig. S18. UV–Vis spectra of the compounds **1b–3b** in DMSO at various concentrations.

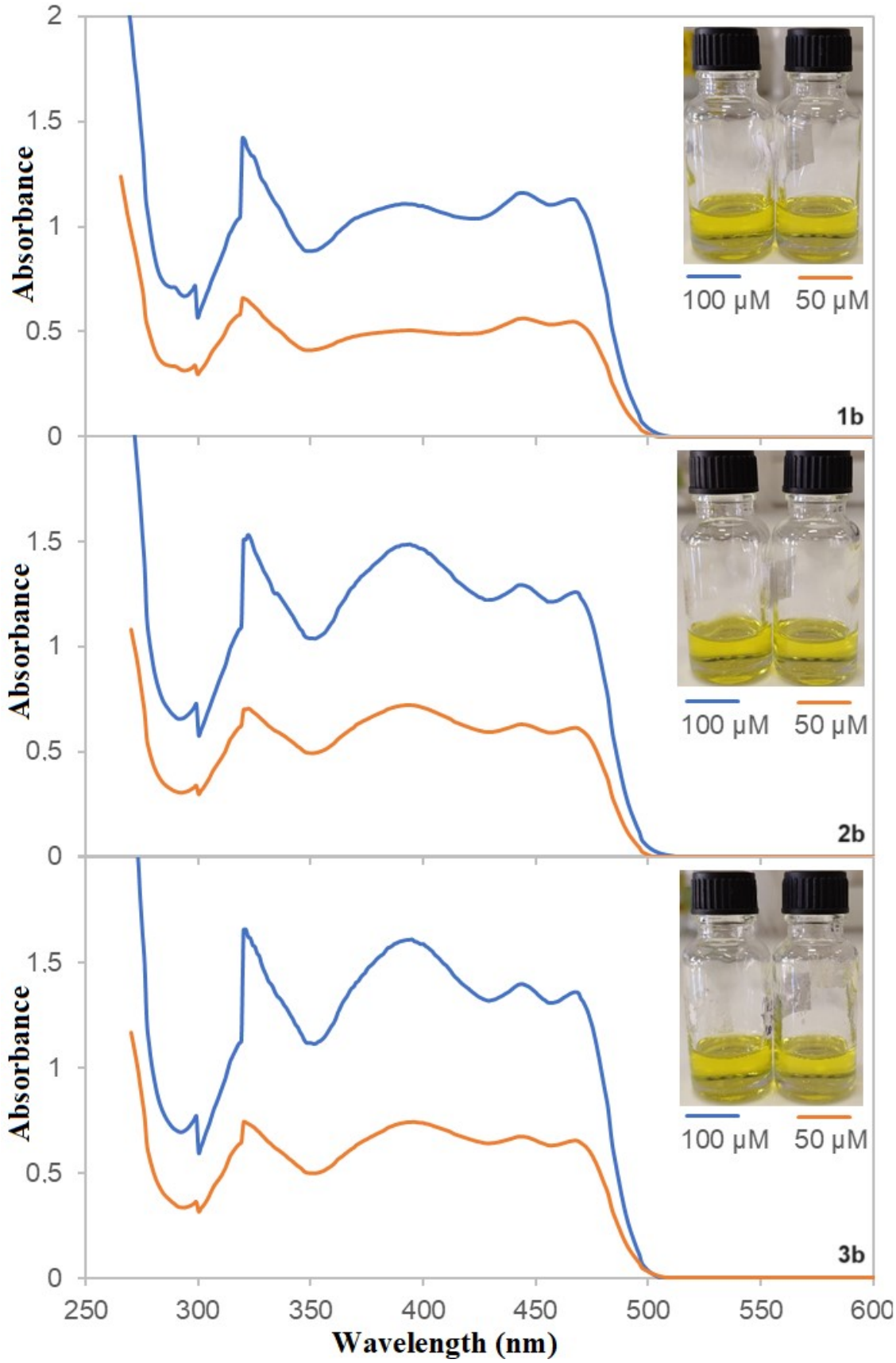


Fig. S19. UV–Vis spectra of the compounds **1b–3b** in DMF at various concentrations.

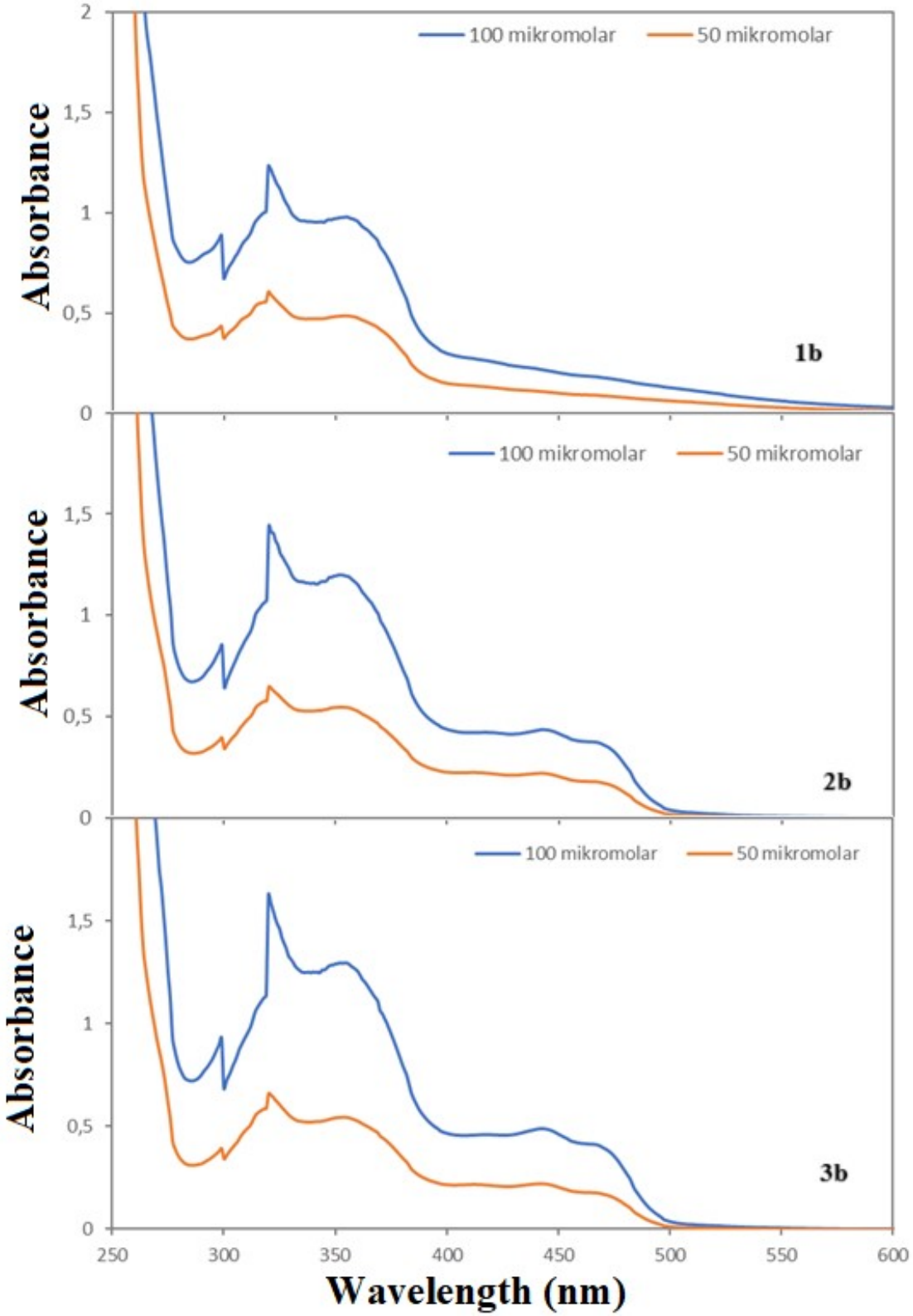


Fig. S20. UV–Vis spectra of the compounds **1b–3b** in DMSO at various concentrations recorded a few months later

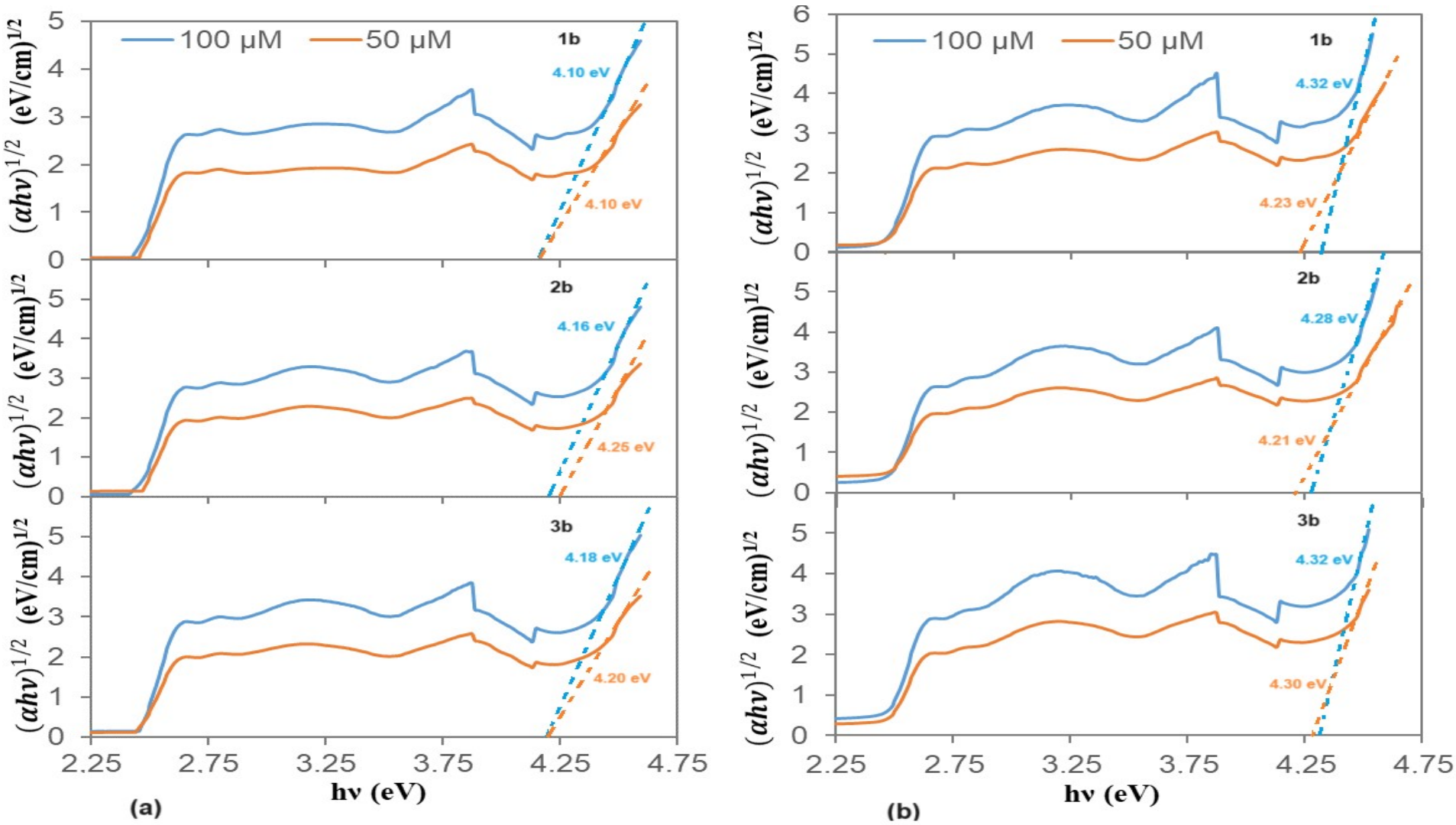


Fig. S21. Tauc's plots for the indirect allowed transition of the compounds **1b–3b** in DMSO **(a)** and DMF **(b)**.

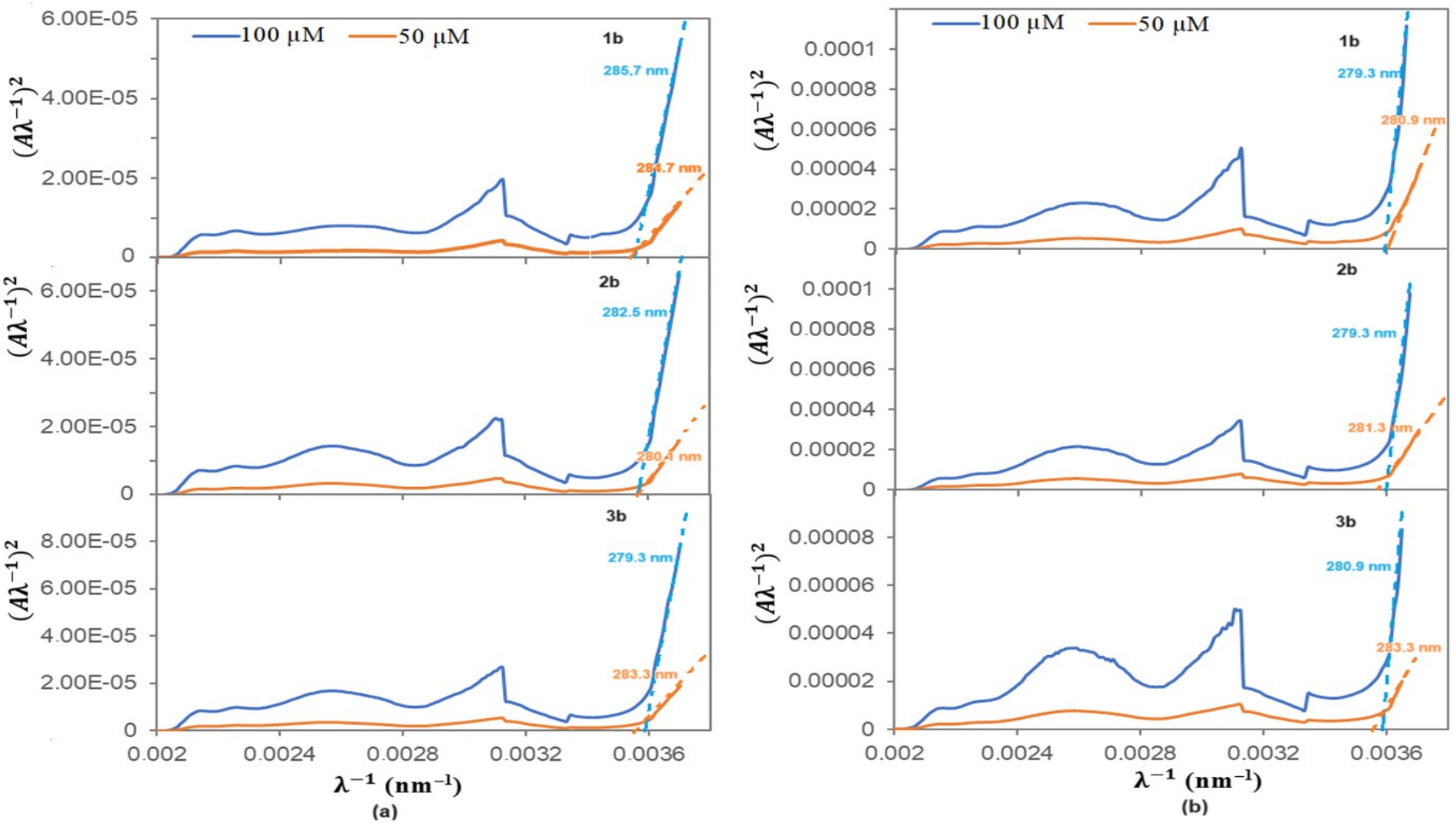


Fig. S22. ASF plots for the direct allowed transition of **1b–3b** in **(a)** DMSO and **(b)** DMF.

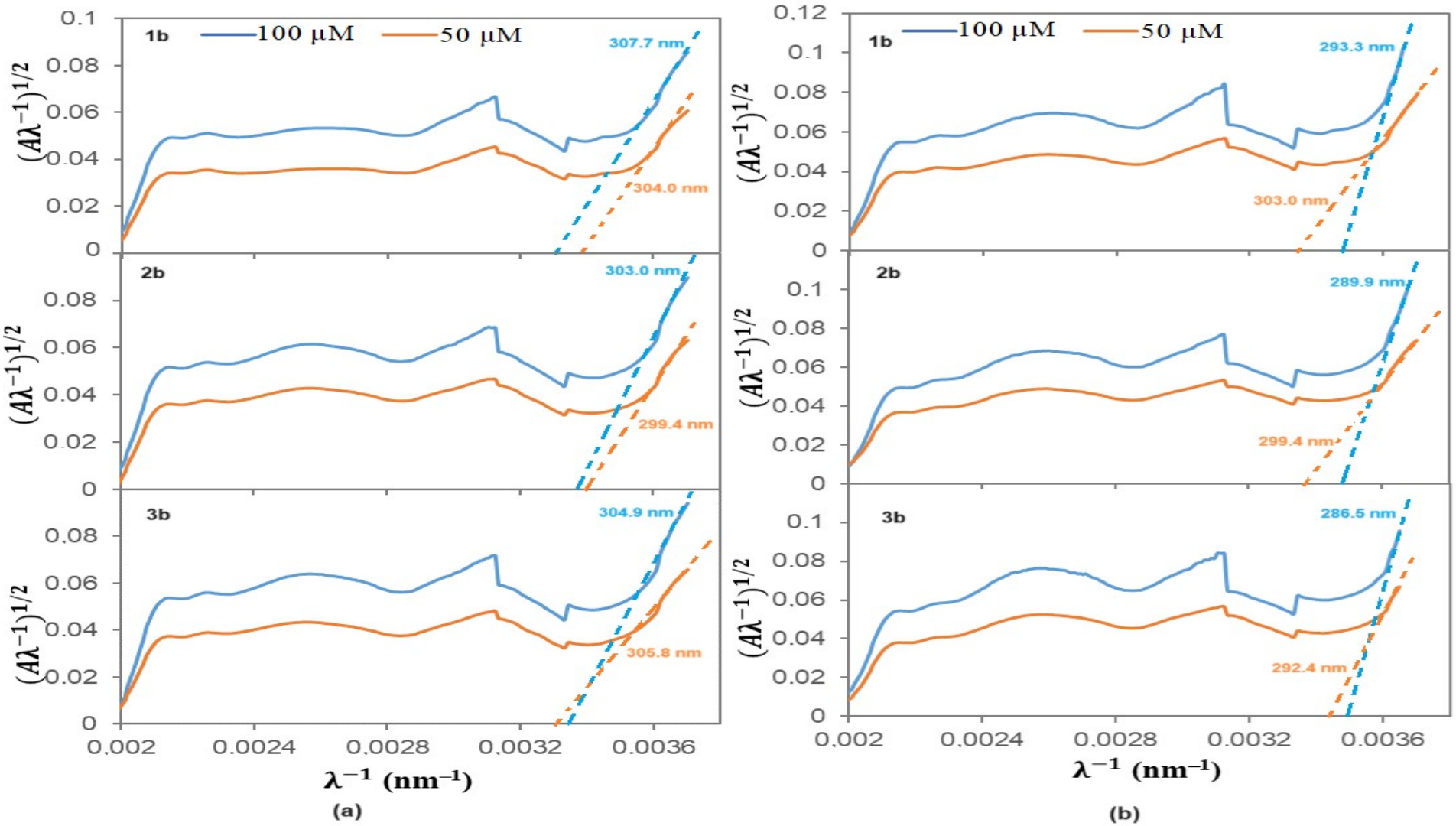


Fig. S23. ASF plots for the indirect allowed transition of the compounds **1b–3b** in DMSO **(a)** and DMF **(b)**.

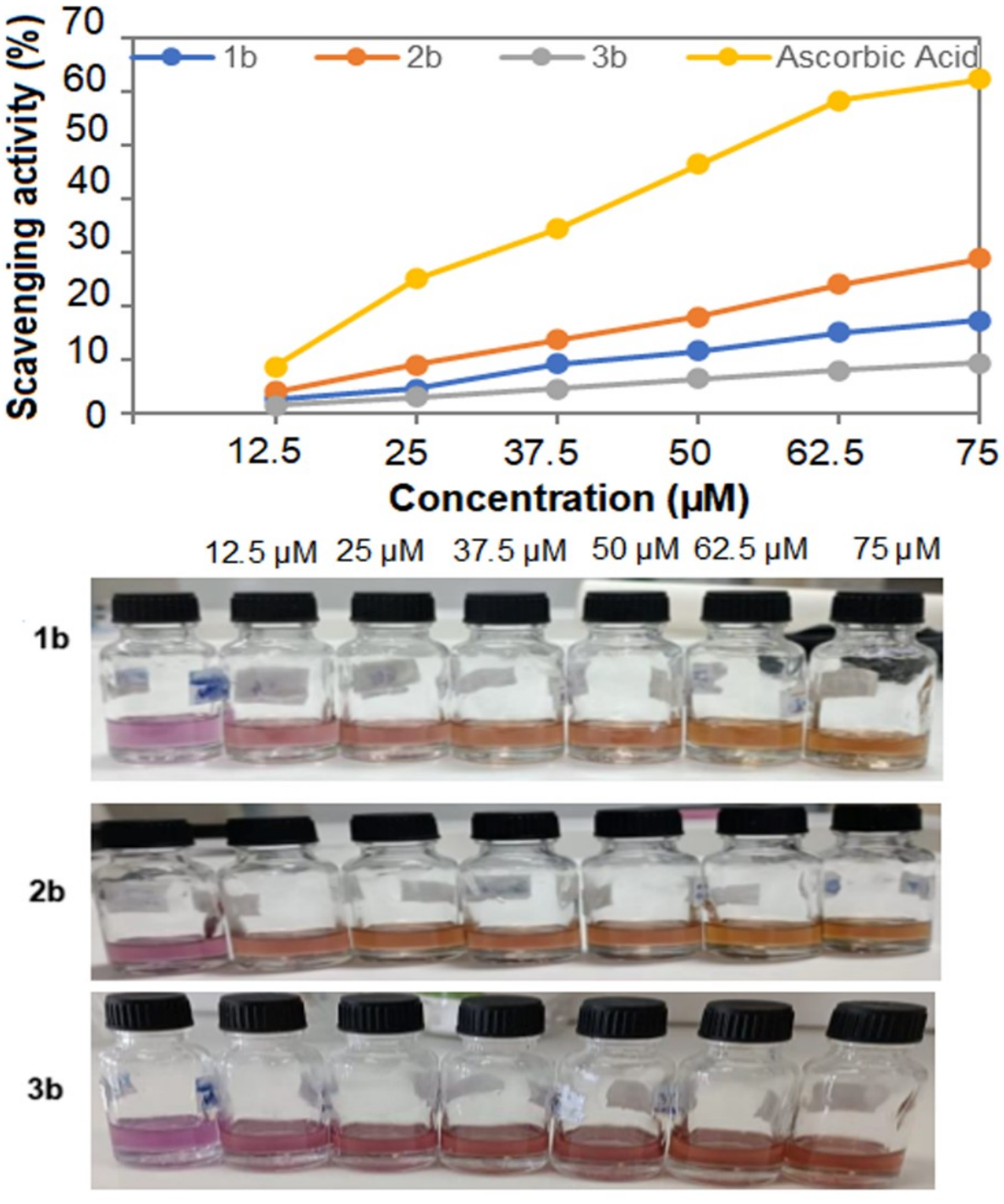


Fig. S24. Comparable chart for the percentage of scavenging activity of **1b–3b** at various concentrations. The data given is average ± SD of three experiments.

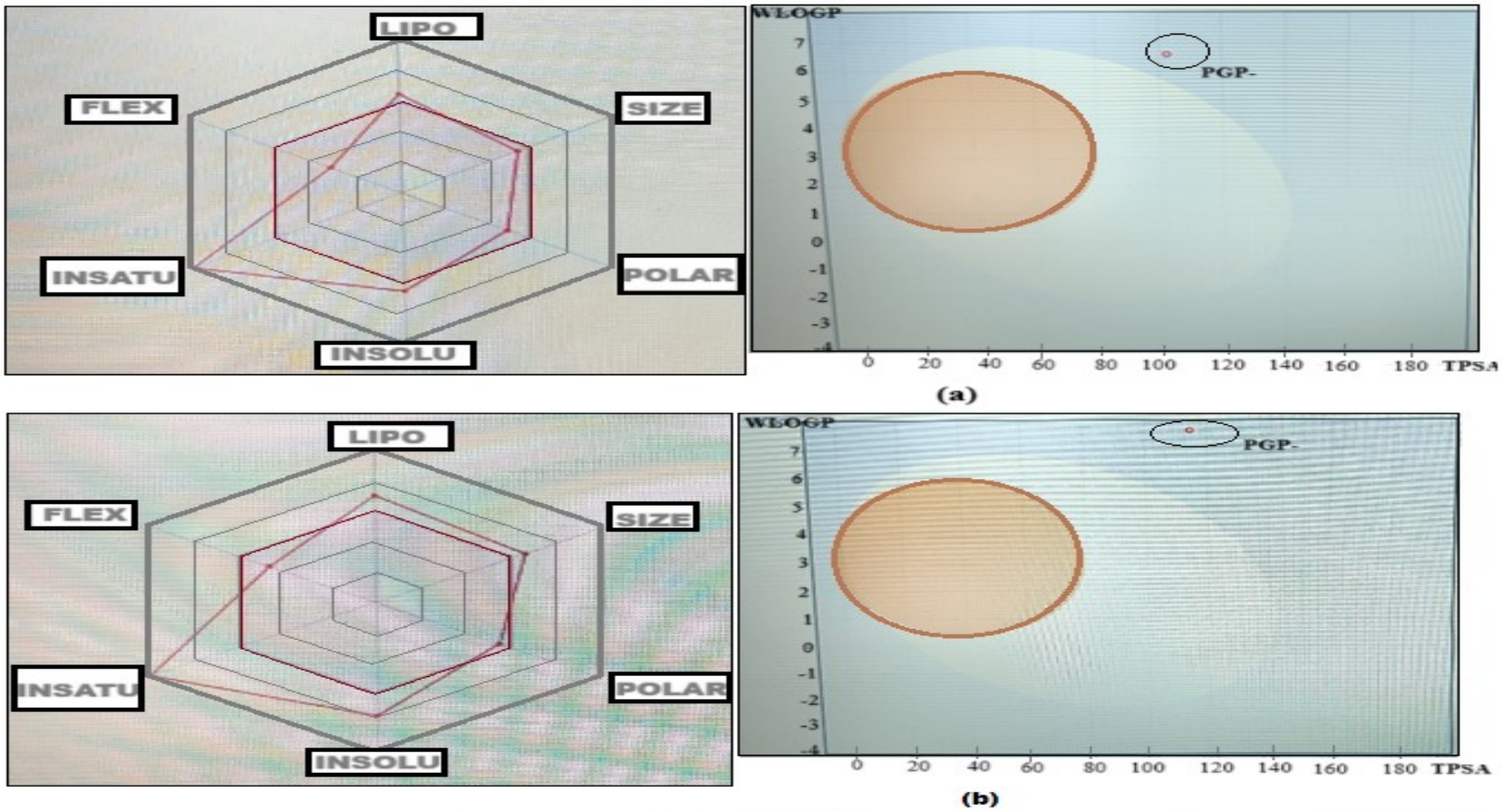


Fig. S25. Bioavailability radar plots and Boiled-Egg graphs of the molecules **(a) 1b** and **(b) 2b** obtained by SwissADME web tool.