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Supplementary data

Studies on racemic triglycerides as urease enzyme inhibitors

Hamdullah Khadim Sheikh[1], Tanzila Arshad[2], Haroon Khan[3], Uzma Habib[4], Cindy Juliet Cristancho Ortiz[5]

Table S1: Structure of reactant benzoic acid derivatives (9a-c)

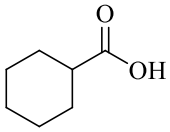
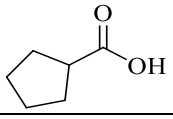
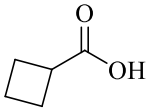
Code	Structure
9a	
9b	
9c	

Table S2: Molecular structure of mixed triglycerides (10a-c)

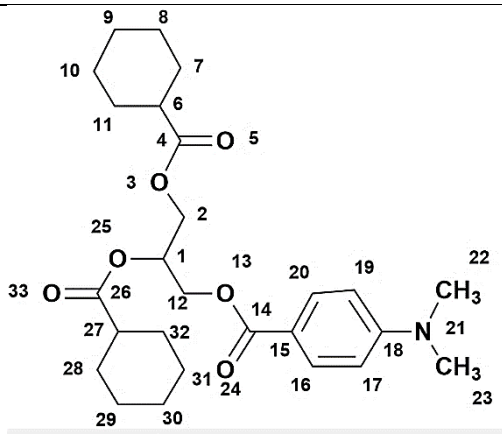
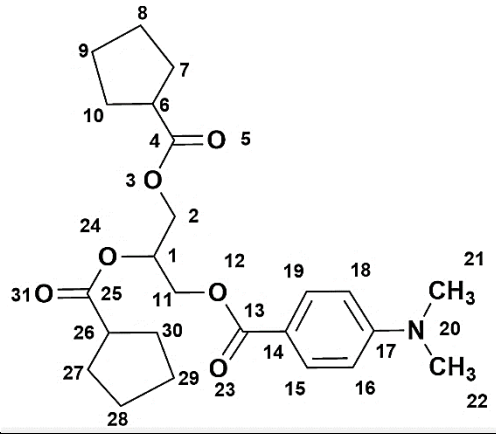
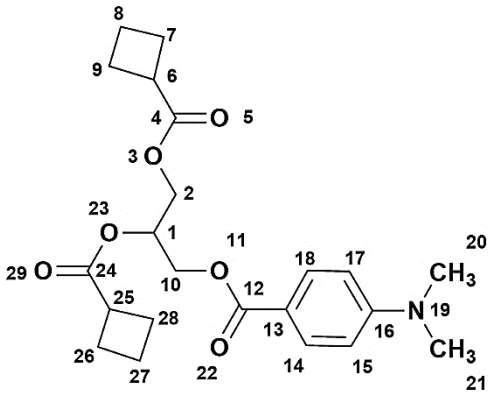
Code	Molecular Structure	Mol. Wt. g/mol
10a		**459.3**
10b		**431.3**
10c		**403.1**

Figure S1: Mass spectra of compound (10a)

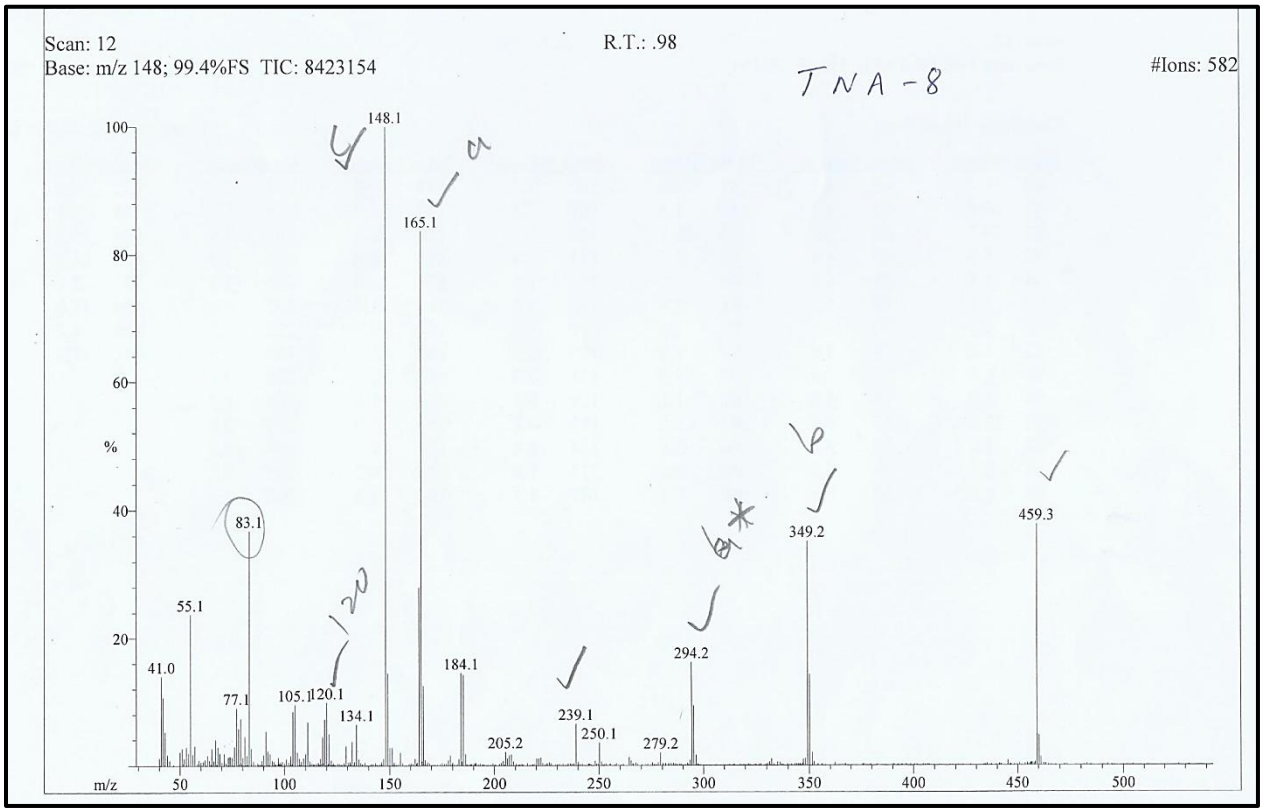


Figure S2: Mass spectra of compound 10b

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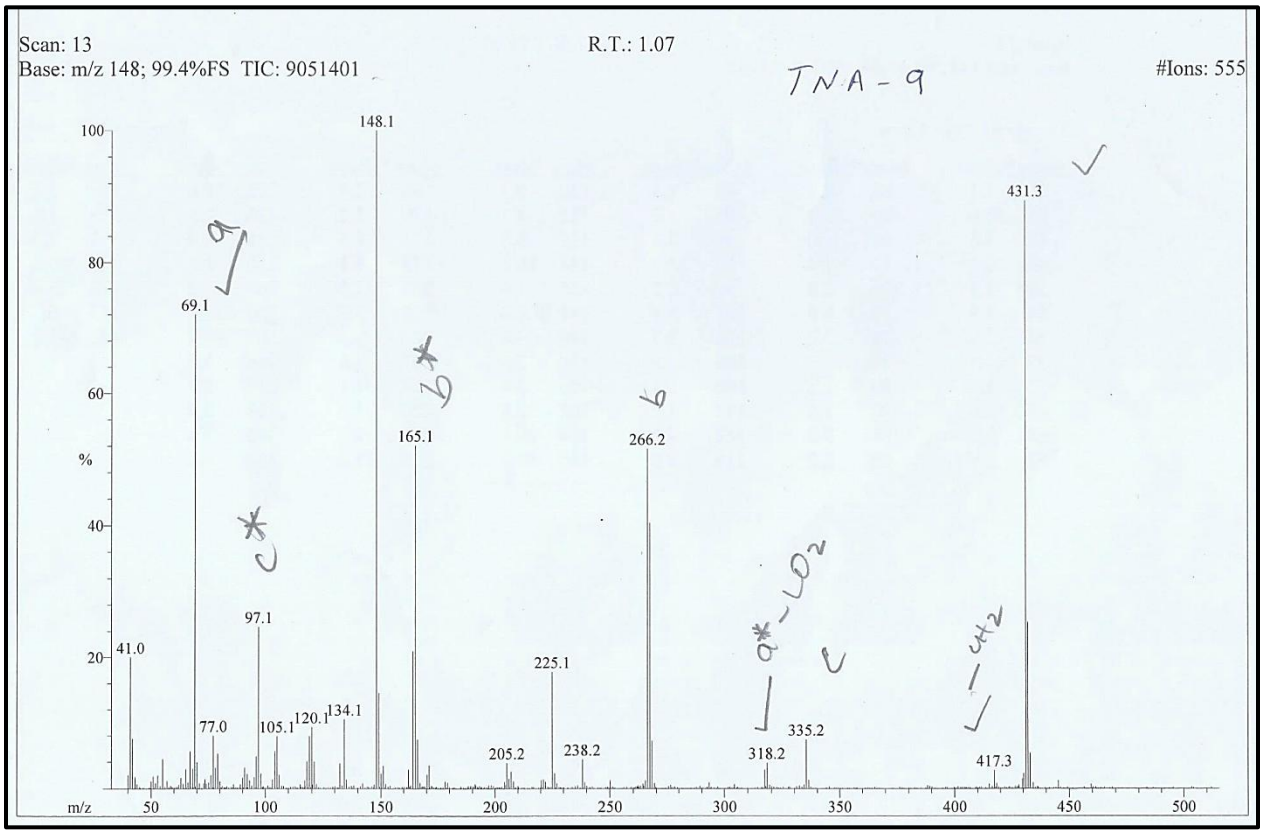


Figure S3: Mass spectra of compound 10c

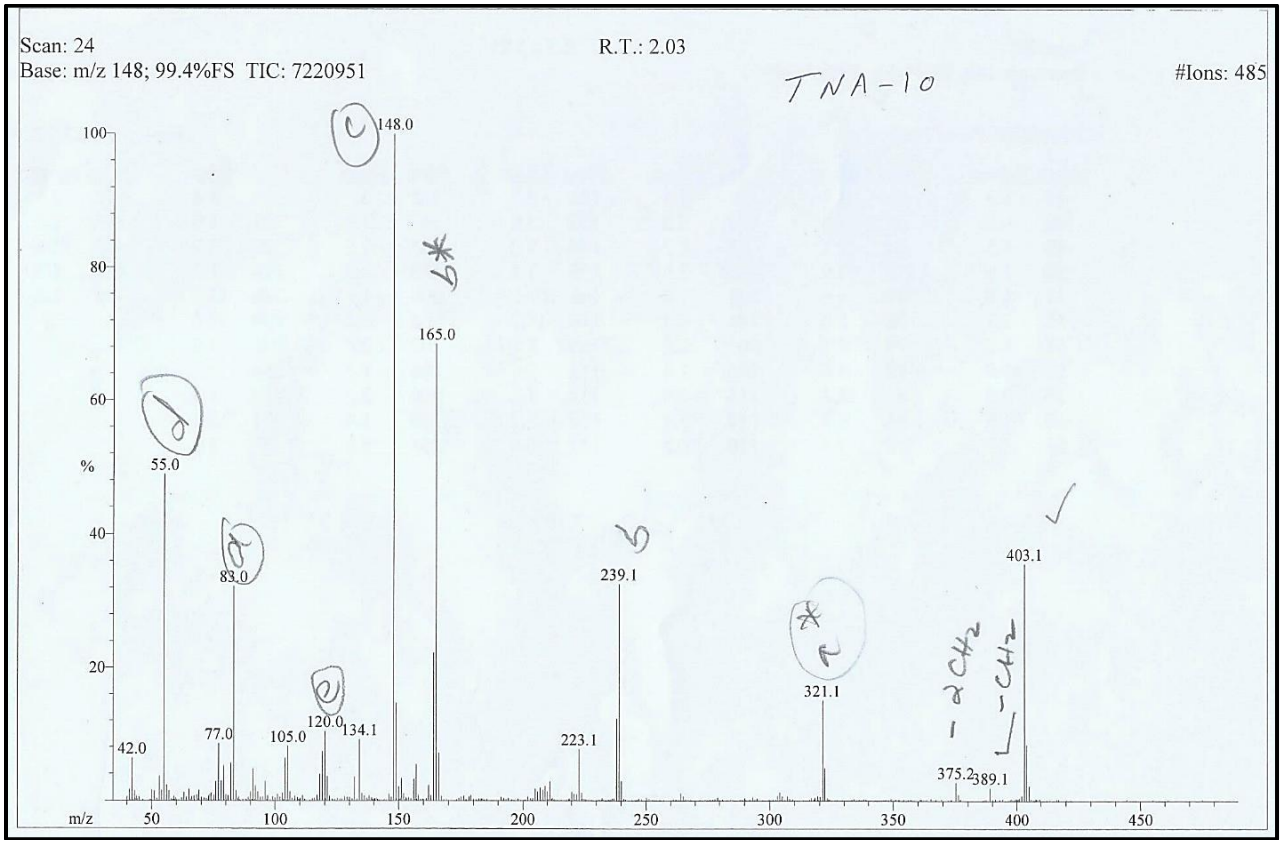


Figure S4: IR spectra of synthesized compounds (10a)

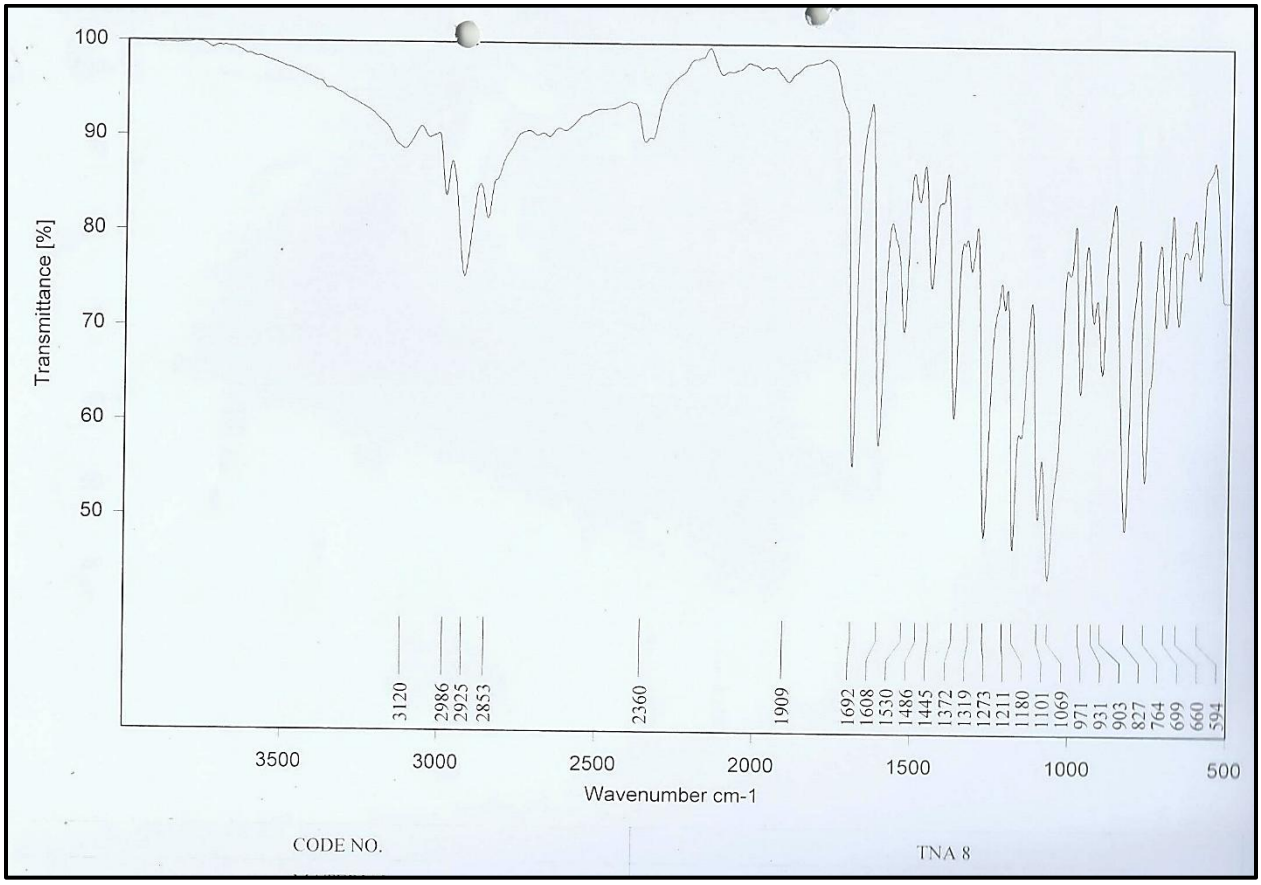


Figure S5: IR spectra of compound 10b

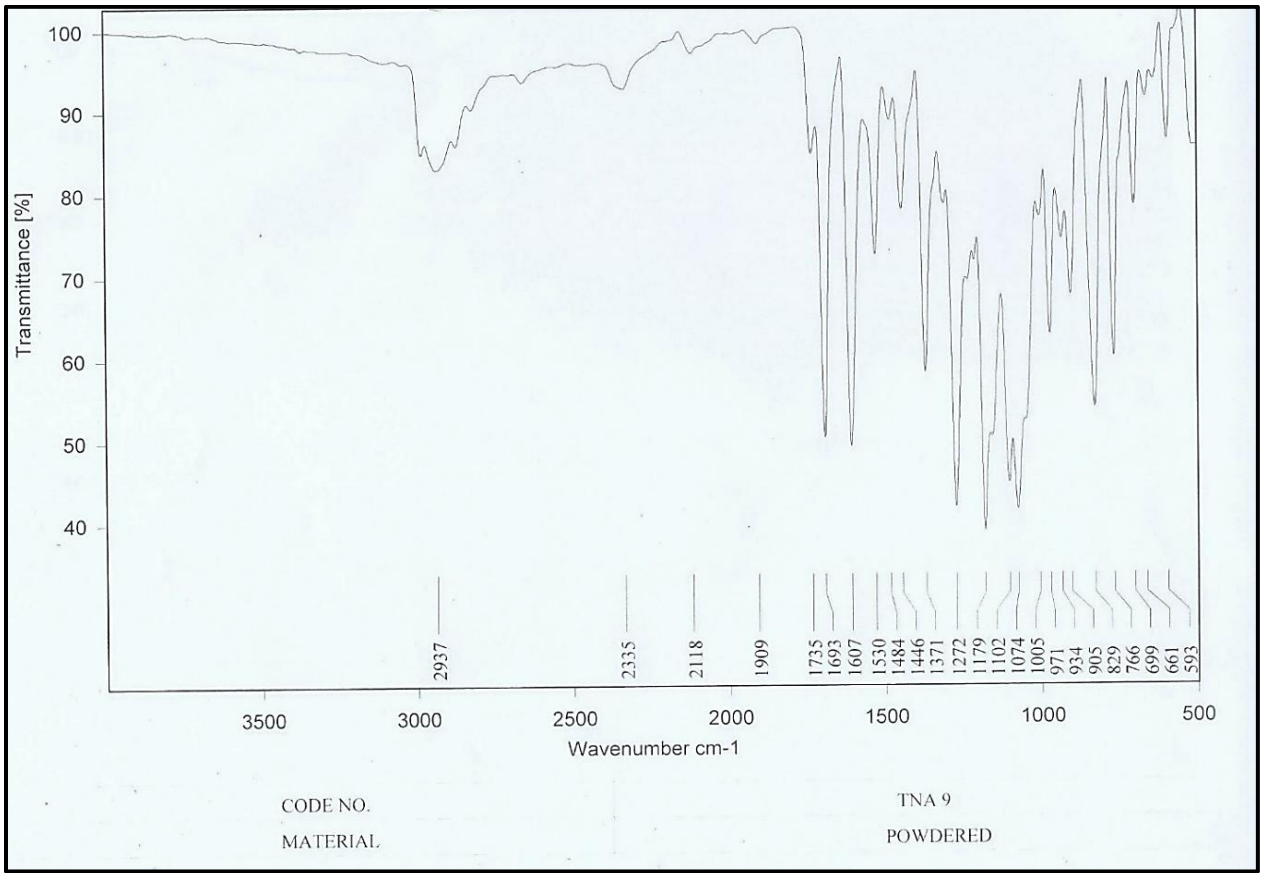


Figure S6: IR spectra of compound 10c

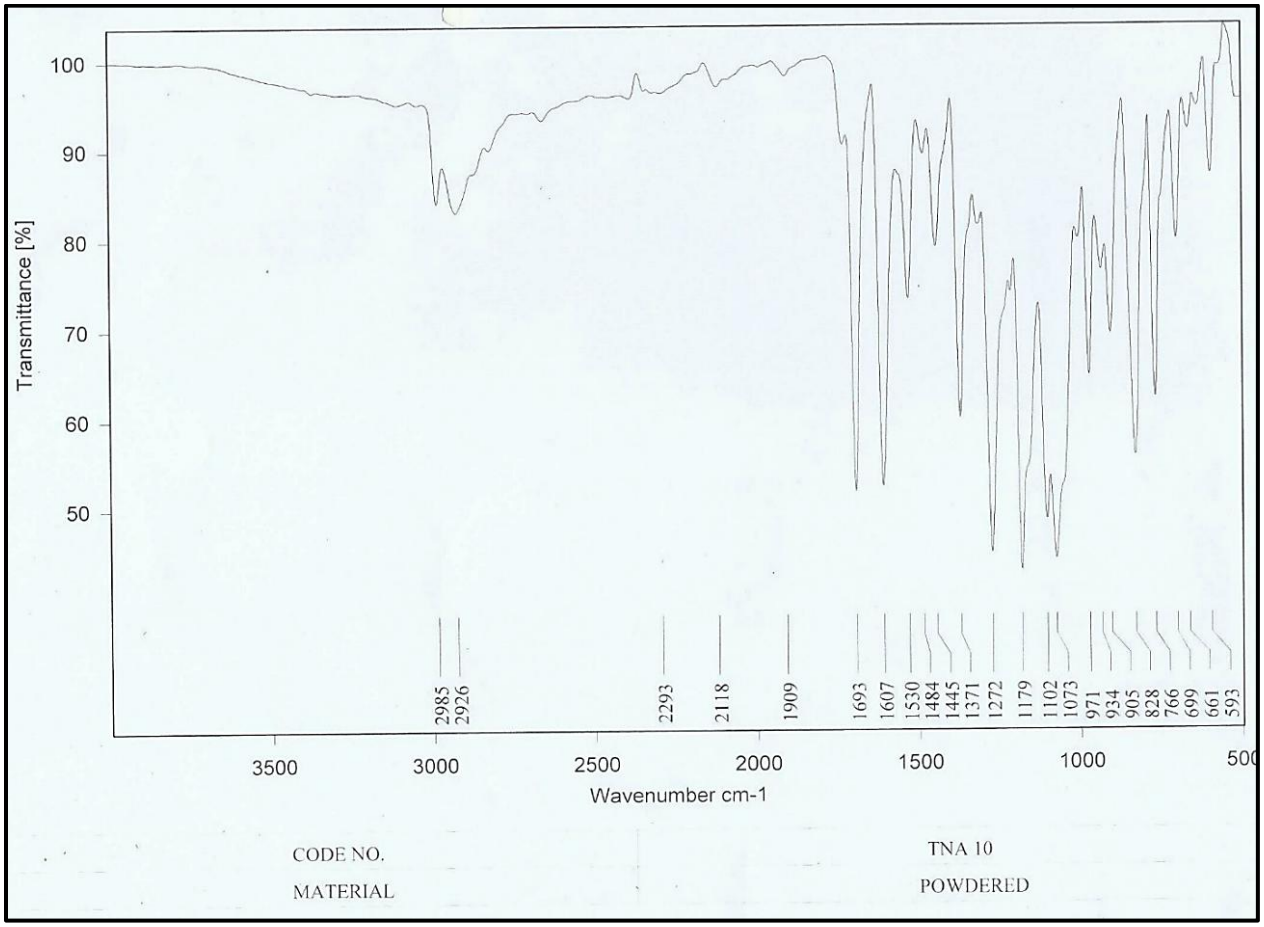


Figure S7: ^{13}C-NMR of compound 10a

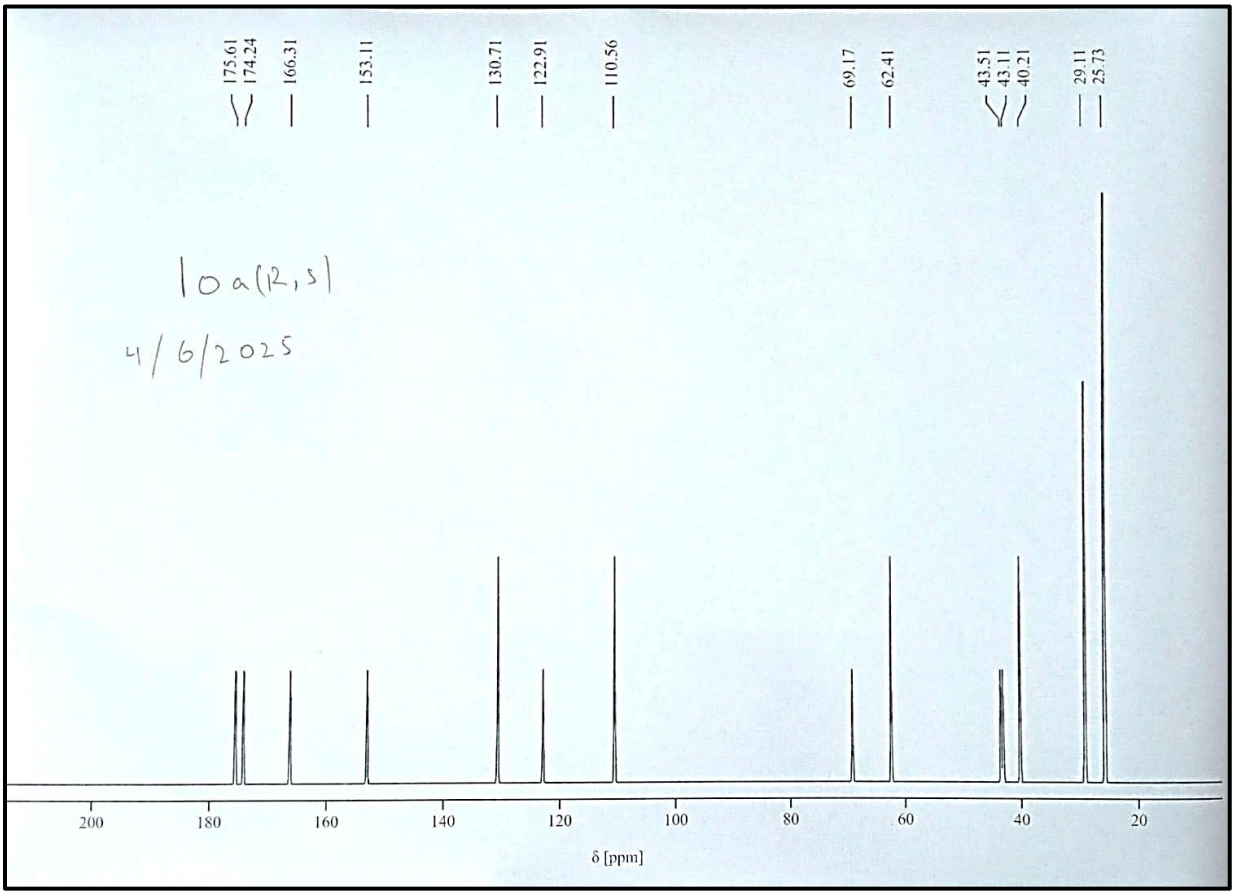


Figure S8: ^{13}C-NMR of compound 10b

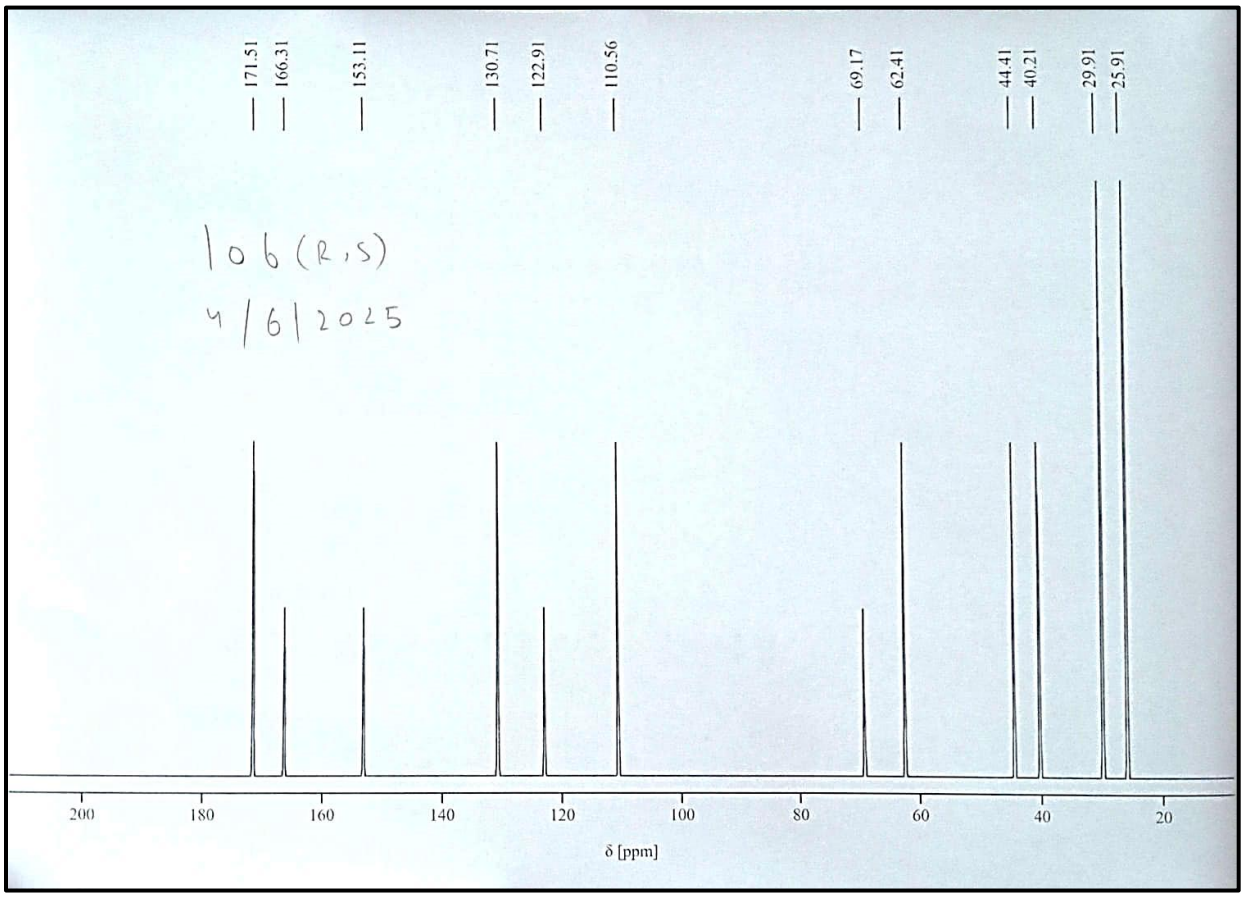
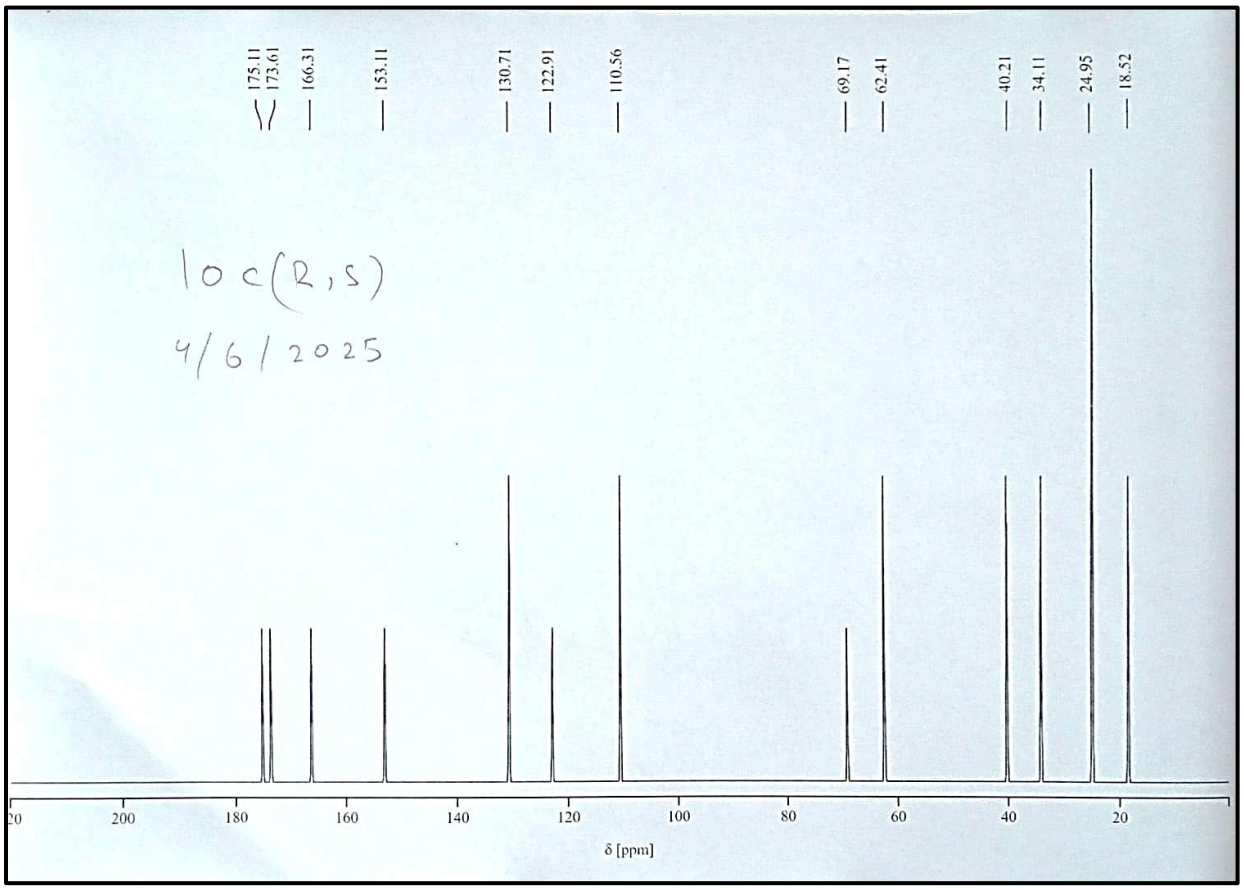


Figure S9: ^{13}C-NMR of compound 10c



Structural confirmation approach

The molecular structures of synthesized compounds (**10a–10c**) were confirmed by using IR, ^{13}C-NMR, mass spectrometry (EI-MS), and elemental analysis data.

- First, the molecular ion peak (M^+) in the EI-MS spectrum established the molecular weight and formulas. Fragmentation patterns in EI-MS supported the placement of substituents, as cleavage of the ester linkages gave characteristic acylium and aromatic fragments.
- The empirical formulas of the targeted compounds were validated by elemental analysis (CHN).
- The IR spectra identified key functional groups such as ester carbonyls (C=O), aromatic rings (C=C), dimethylamino groups (C–N), and aliphatic/alicyclic chains (C–H), present in compounds (**10a–10c**).
- The ^{13}C-NMR spectra provided details of C-skeleton; downfield peaks (δ 160–180 ppm) confirmed ester carbonyls (C=O); aromatic ring carbons (C=C) appeared at δ 110–155 ppm; the glycerol backbone carbons at δ 60–75 ppm; alicyclic and methyl carbons at δ 20–45 ppm.

Together, these data sets independently and also collectively confirmed the proposed molecular structures of **10a–10c**.

Figure S10: Visual summary of characterization of compounds (**10a**) using IR (blue) and ^{13}C-NMR (red) data. The IR identified functional groups are shaded (blue)

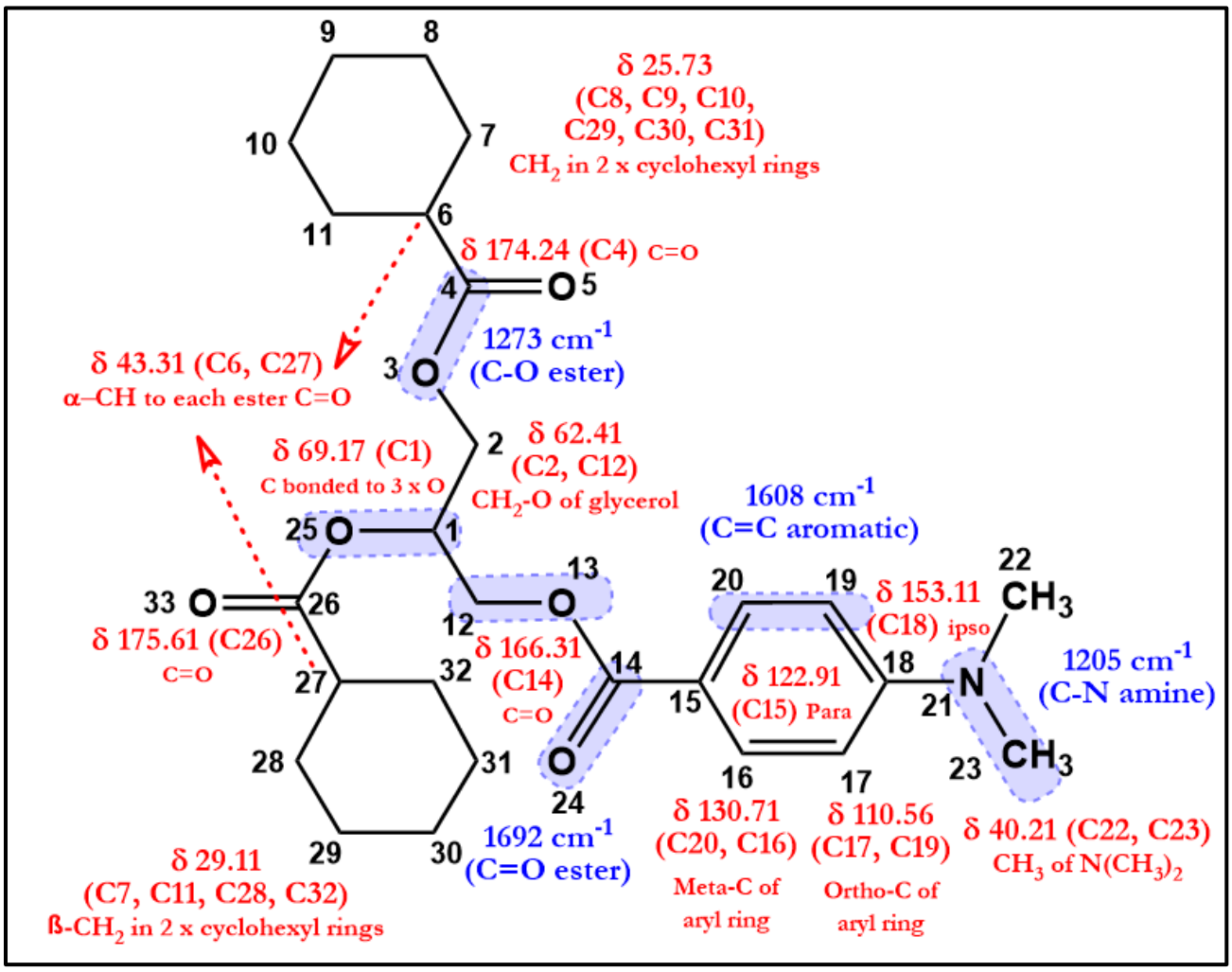


Figure S11: Strongest binding (highest absolute binding energy) docked conformations of 10a(R), 10a(S) and thiourea ligands within the same binding pocket

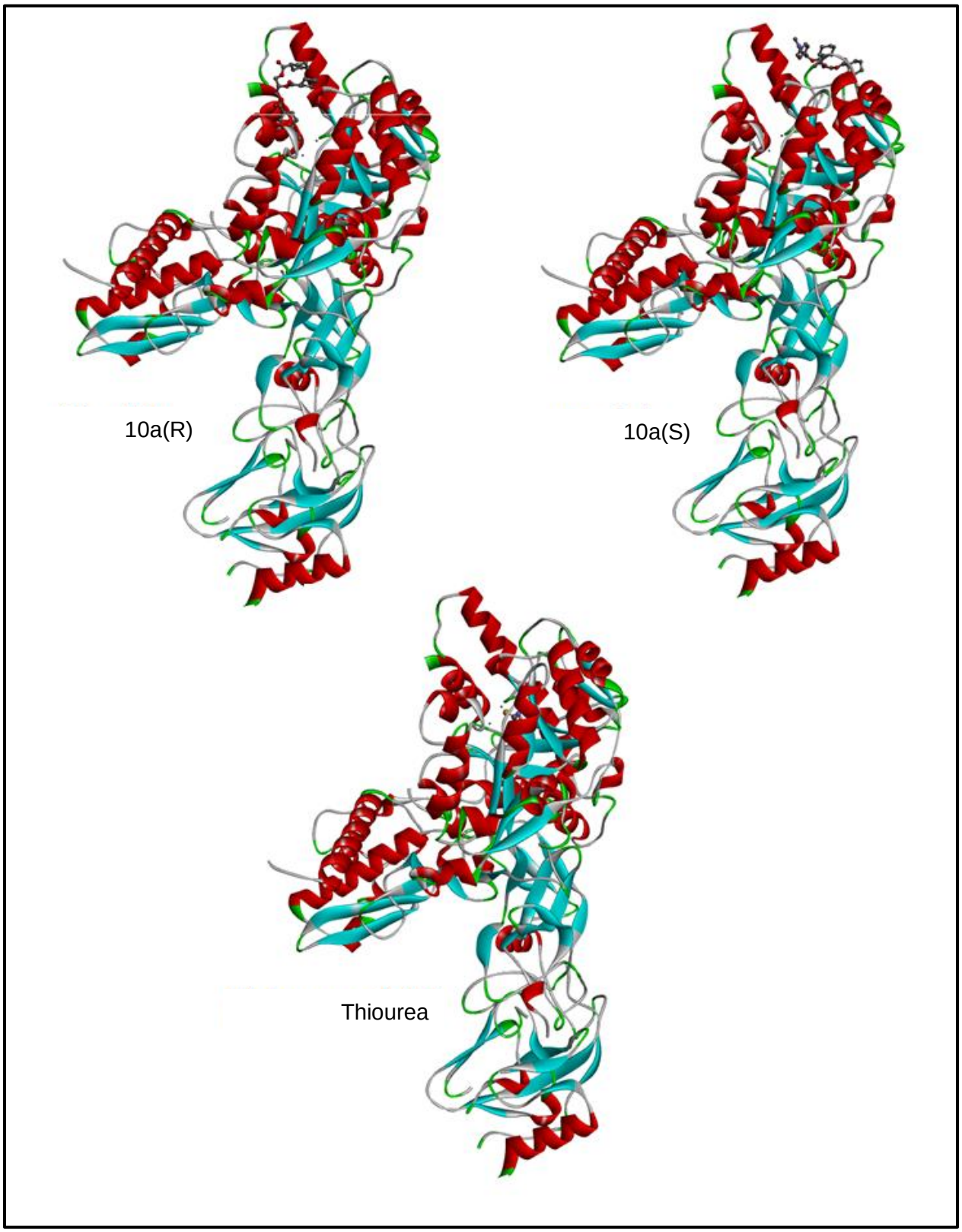


Figure S12: Principle component analysis: Variances of PC_1-PC_3 for scoring function 1

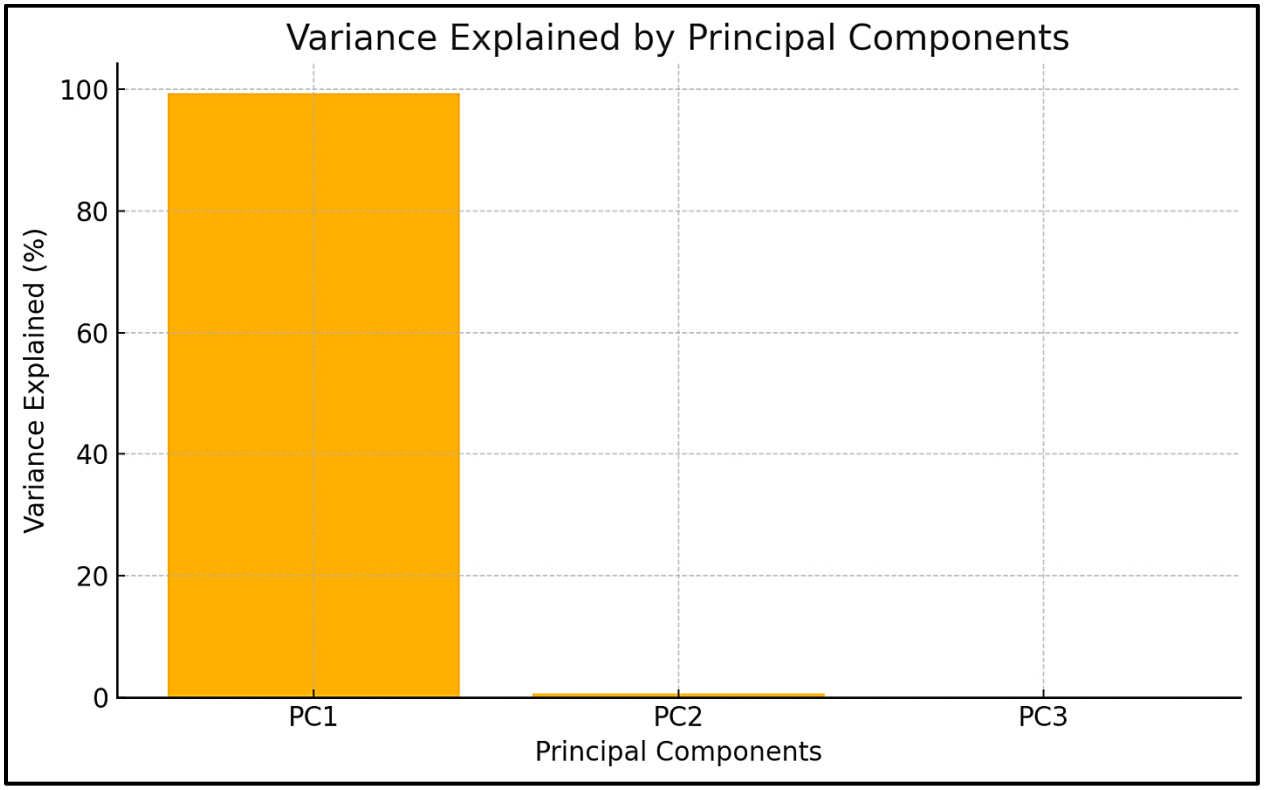


Figure S13: Principle component analysis: PC_1-PC_3 loadings for scoring function 1

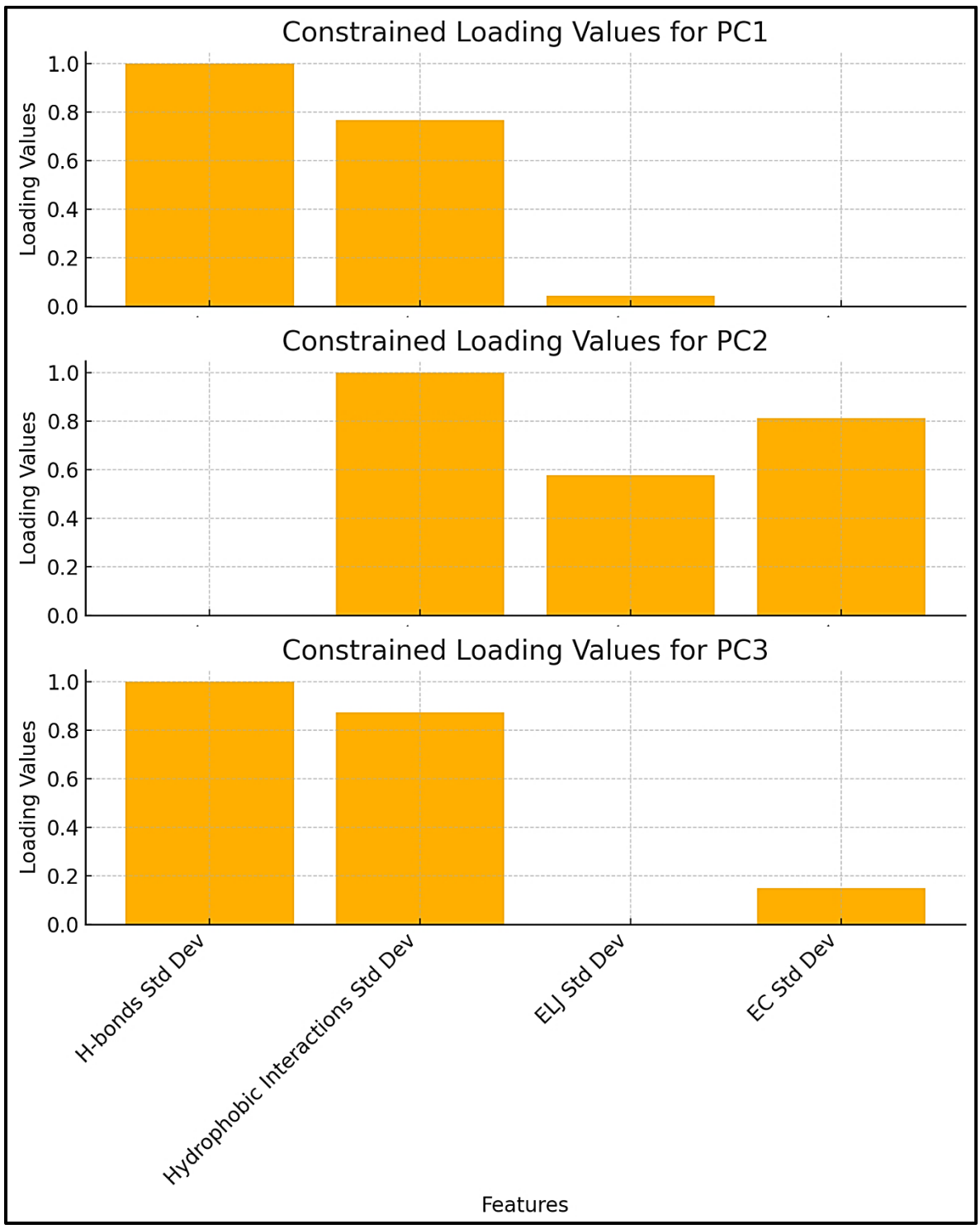


Figure S14: Principle component analysis: Variances of PC_1-PC_3 for scoring functions 2

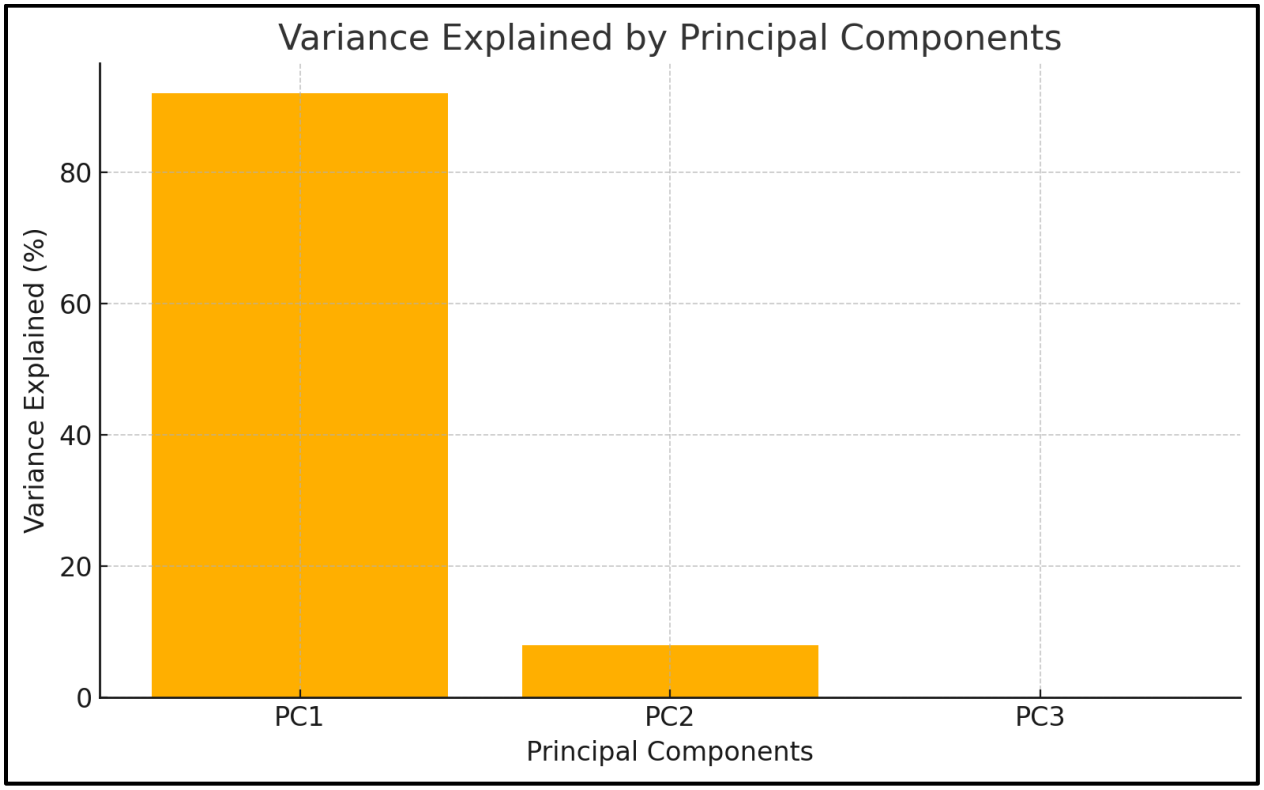


Figure S15: Principle component analysis: PC_1-PC_3 loadings for scoring functions 2

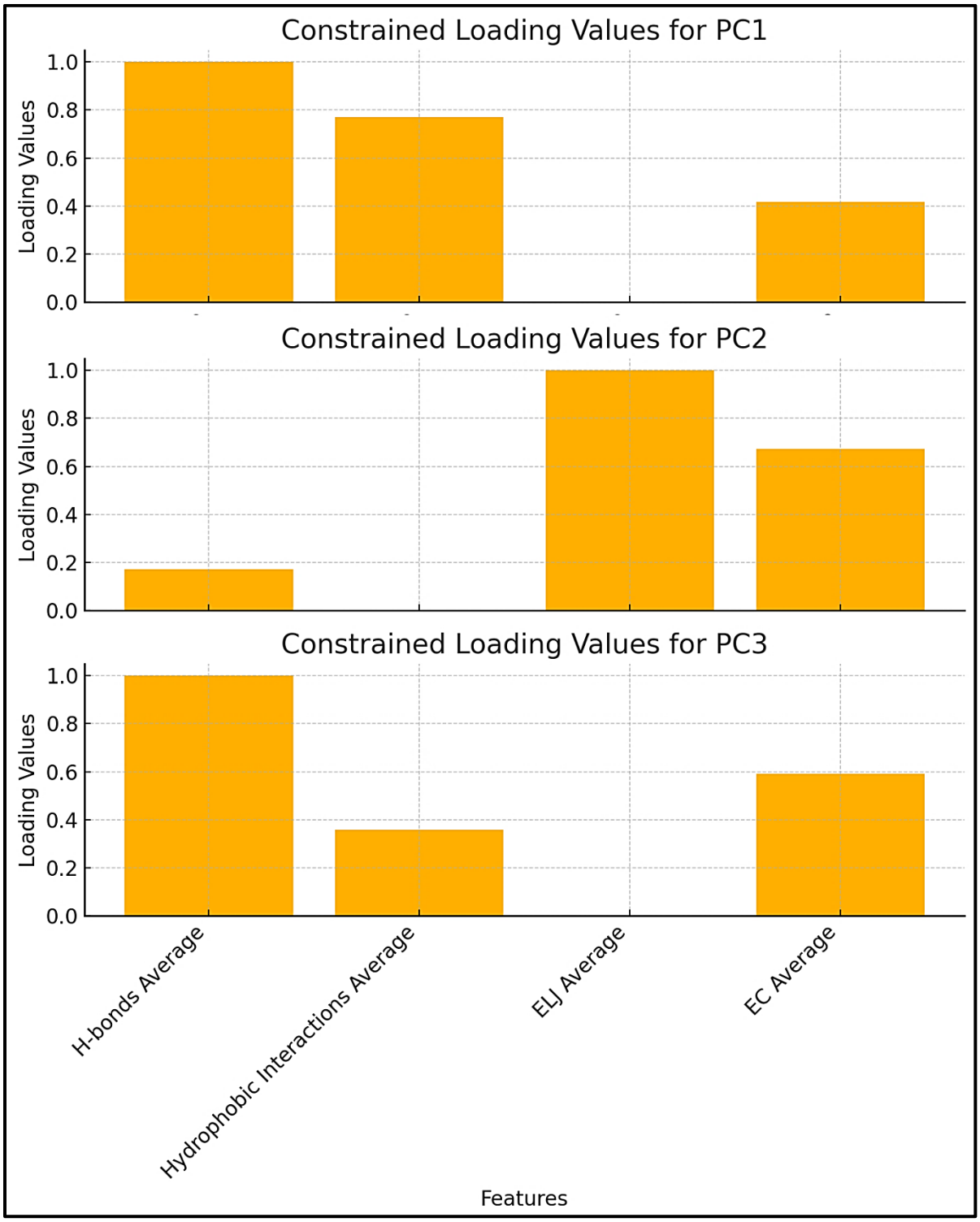


Table S3: Static factors (and their normalized values) derived from MD simulations of ligands **10a**(R), **10a**(S), and thiourea

Scoring function 1: Fluctuation of interaction				
Ligand	**H-bonds standard deviation**	**Hydrophobic Interactions standard deviation**	**E_{LJ} standard deviation**	**E_C standard deviation**
10a(R)	0.4406 (1.000)	0.0112 (1.000)	16.0230 (0.149)	18.8534 (0.845)
10a(S)	0.4495 (0.989)	0.0134 (0.962)	17.3344 (0.000)	14.3857 (1.000)
TU	1.2745 (0.000)	0.0690 (0.000)	8.5319 (1.000)	43.2982 (0.000)
Scoring function 2: Strength of interaction				
Ligand	**H-bonds Average**	**Hydrophobic Interactions Average**	**E_{LJ} Average**	**E_C Average**
10a(R)	0.2605 (0.043)	0.2104 (1.000)	-142.9213 (1.000)	-31.2136 (0.250)
10a(S)	0.1859 (0.000)	0.2163 (0.830)	-90.2286 (0.456)	-9.5395 (0.000)
TU	1.9400 (1.000)	0.2451 (0.000)	-46.1404 (0.000)	-96.2209 (1.000)

Table S4. Principal components loadings (PC_1-PC_3) of normalized static factors of the MD properties of ligands **10a**(R), **10a**(S), thiourea) along with their %variances, and calculated weights to indicate the relative importance of each static factor of MD properties

Scoring function 1: Fluctuation of interaction					
	PC (Variance)	**H-bonds standard deviation**	**Hydrophobic interactions standard deviation**	**E_{LJ} standard deviation**	**E_C standard deviation**
Pre-normalization	PC_1 (99.33)	0.518	0.510	0.486	0.485
	PC_2 (0.66)	0.411	0.555	0.494	0.528
	PC_3 (0.00)	0.743	0.654	0.034	0.140
Post-normalization	PC_1 (99.33)	1.000	0.769	0.042	0.000
	PC_2 (0.66)	0.000	1.000	0.577	0.814
	PC_3 (0.00)	1.000	0.874	0.000	0.150
Scoring function 2: Strength of interaction					
	PC (Variance)	**H-bonds average**	**Hydrophobic interactions average**	**E_{LJ} average**	**E_C average**
Pre-normalization	PC_1 (92.03)	0.551	0.524	0.435	0.483
	PC_2 (7.96)	0.239	0.126	0.779	0.565
	PC_3 (0.00)	0.800	0.328	0.063	0.498
Post-normalization	PC_1 (92.03)	1.000	0.771	0.000	0.417
	PC_2 (7.96)	0.173	0.000	1.000	0.673
	PC_3 (0.00)	1.000	0.360	0.000	0.591

Table S5: Calculation of combined weights from *PCA* analysis

Scoring function 1: Fluctuation of interaction	
MD property	**Combined weights**
H-bonds standard deviation	0.3212
Hydrophobic Interactions standard deviation	0.4244
E_{LJ} standard deviation	0.0994
E_C standard deviation	0.1547
Scoring function 2: Strength of interaction	
MD property	**Combined weights**
H-bonds average	0.3631
Hydrophobic interactions average	0.1889
E_{LJ} average	0.1670
E_C average	0.2808

Figure S16: Variances and PC_1-PC_3 component loadings of scoring functions 1 and 2