

Supporting Information

Synthesis and experimental validation of new designed heterocyclic compounds with antiproliferative activity *versus* breast cancer cell line.

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Table of Contents:

Figure S1. PLS scores plot of Indole derivatives.

Figure S2. PLS scores plot of Benziloxindole derivatives.

Figure S3. PLS scores plot of Quinoline derivatives.

Figure S4. PLS scores plot of LCAPs derivatives.

Figure S5. PLS scores plot of Pyrimidinketone derivatives.

Table S1. Chemical structures of Pyrimidinketone derivatives.

Table S2. Chemical structures of Pyrrolopyrimidindione derivatives I.

Table S3. Chemical structures of Pyrrolopyrimidindione derivatives IIa.

Table S4. Chemical structures of Pyrrolopyrimidindione derivatives IIb.

Table S5. Chemical structures of Pyrrolopyrimidindione derivatives III.

Table S6. Chemical structures of Benziloxindole derivatives.

Table S7. Chemical structures of Indole derivatives.

Table S8. Chemical structures of LCAPs derivatives.

Table S9. Chemical structures of Quinoline derivatives.

Table S10. Chemical structures of Thiophene derivatives.

Table S11. Elemental analyses for compounds **2-19**.

PLS scores plot

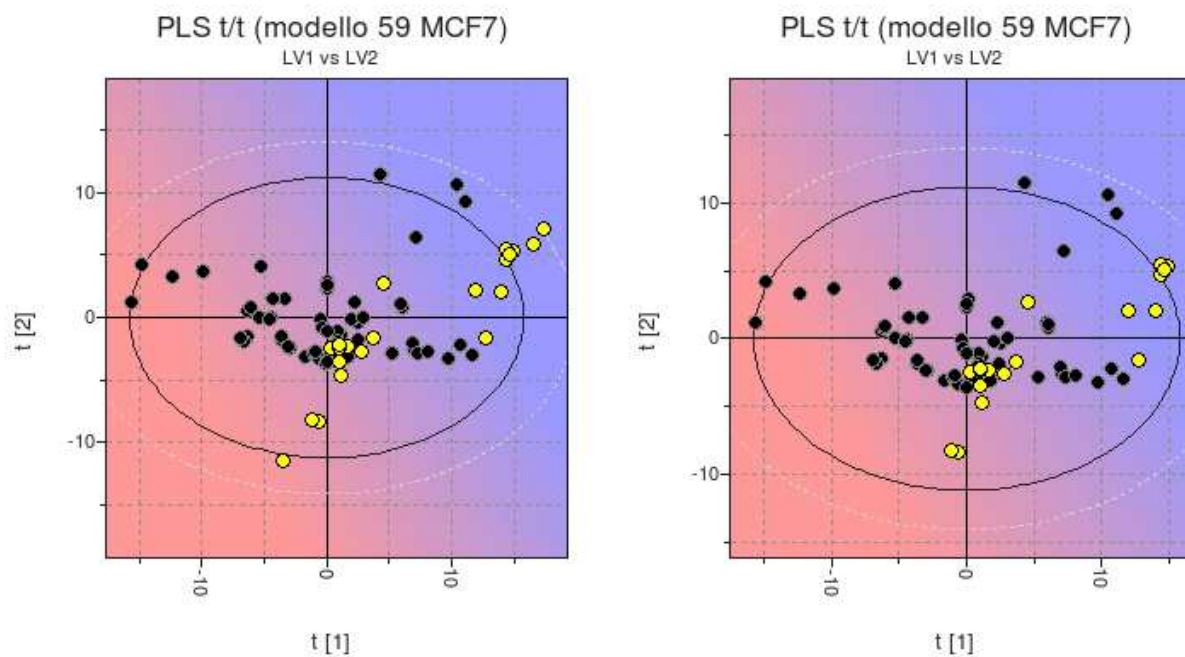


Figure S1. PLS scores plot of Indole derivatives: all compounds (left); after outlier or borderline elimination (right).

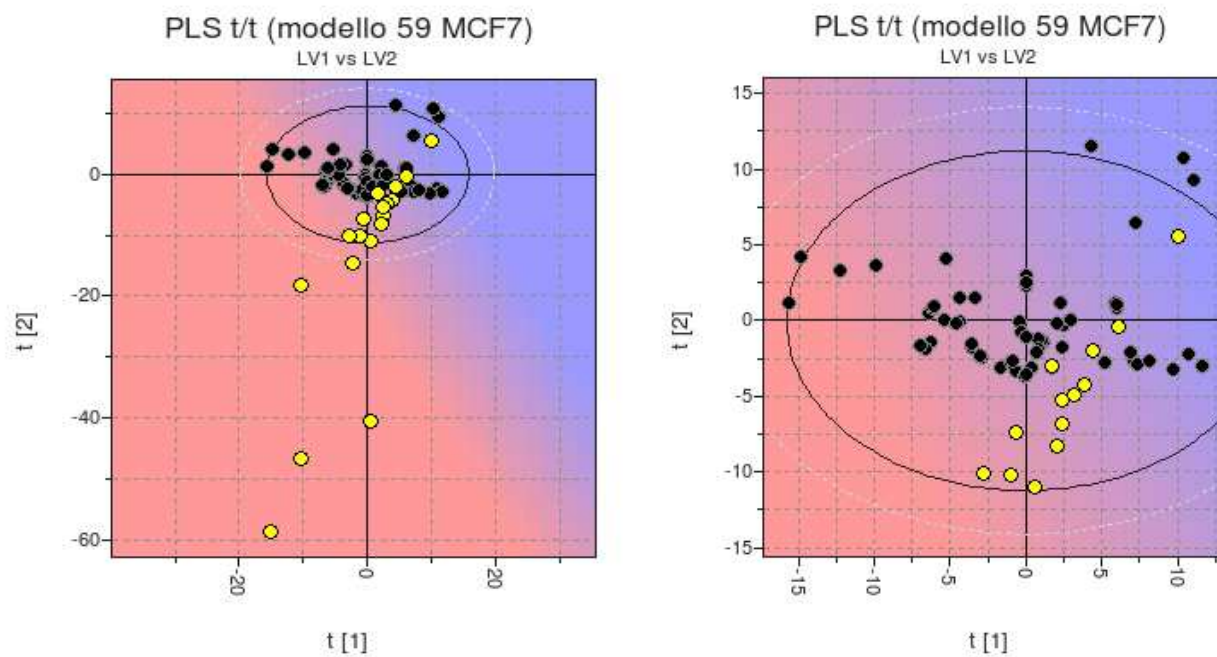


Figure S2. PLS scores plot of Benziloxindole derivatives: all compounds (left); after outlier or borderline elimination (right).

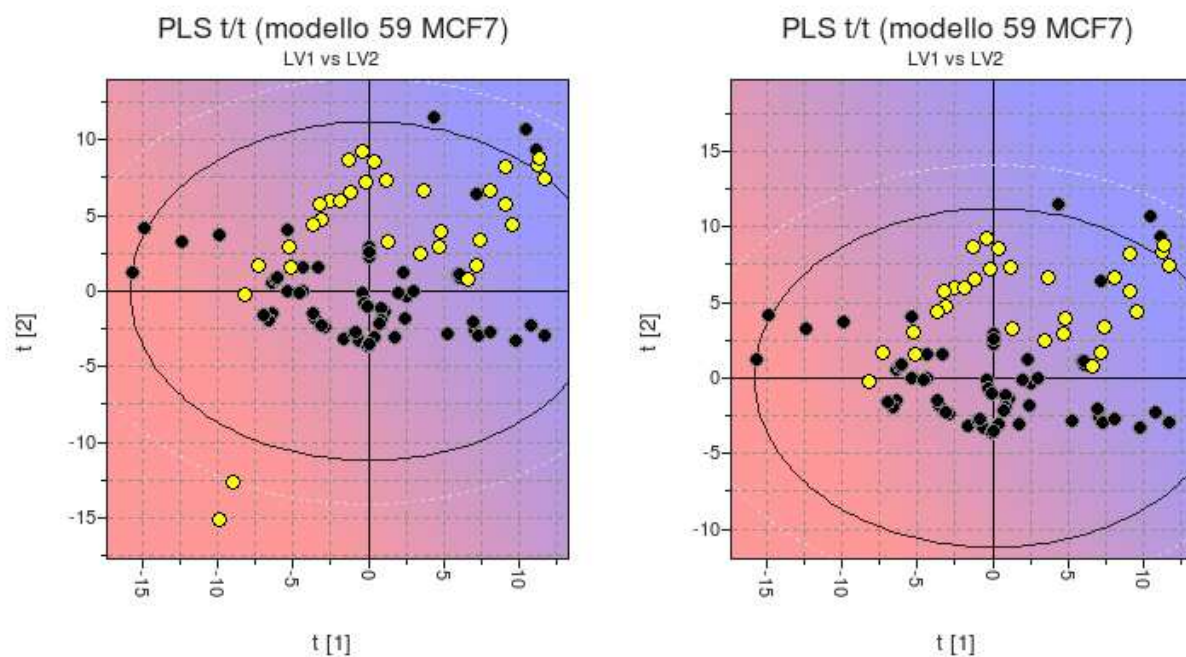


Figure S3. PLS scores plot of Quinoline derivatives: all compounds (left); after outlier or borderline elimination (right).

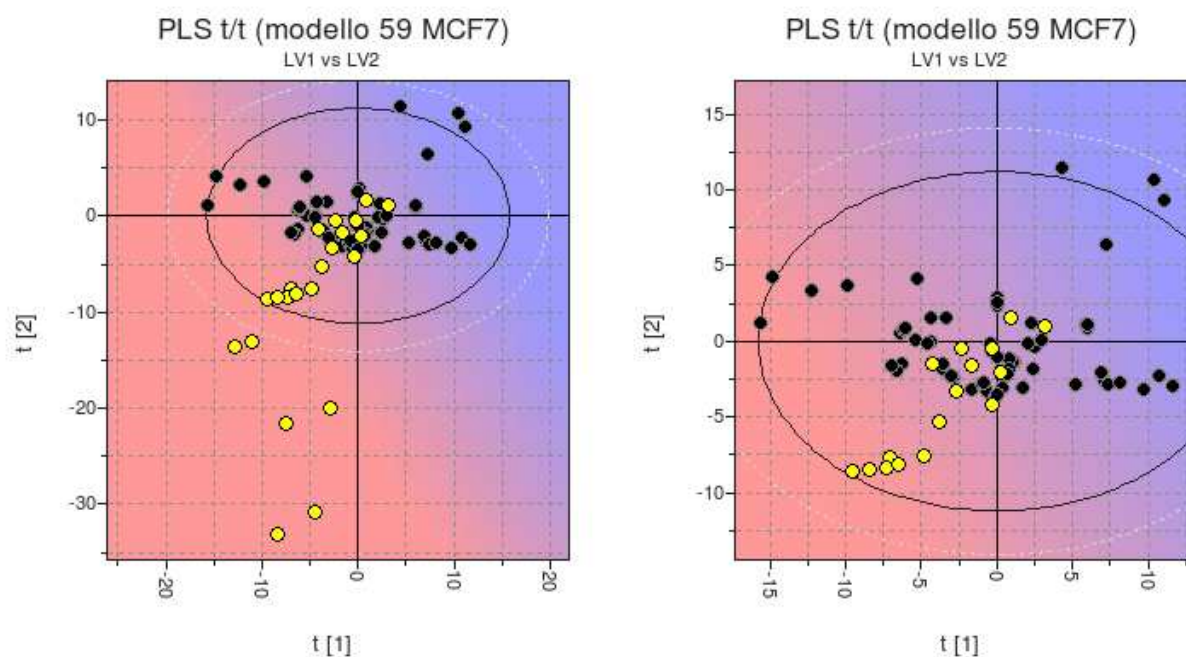


Figure S4. PLS scores plot of LCAPs derivatives: all compounds (left); after outlier or borderline elimination (right).

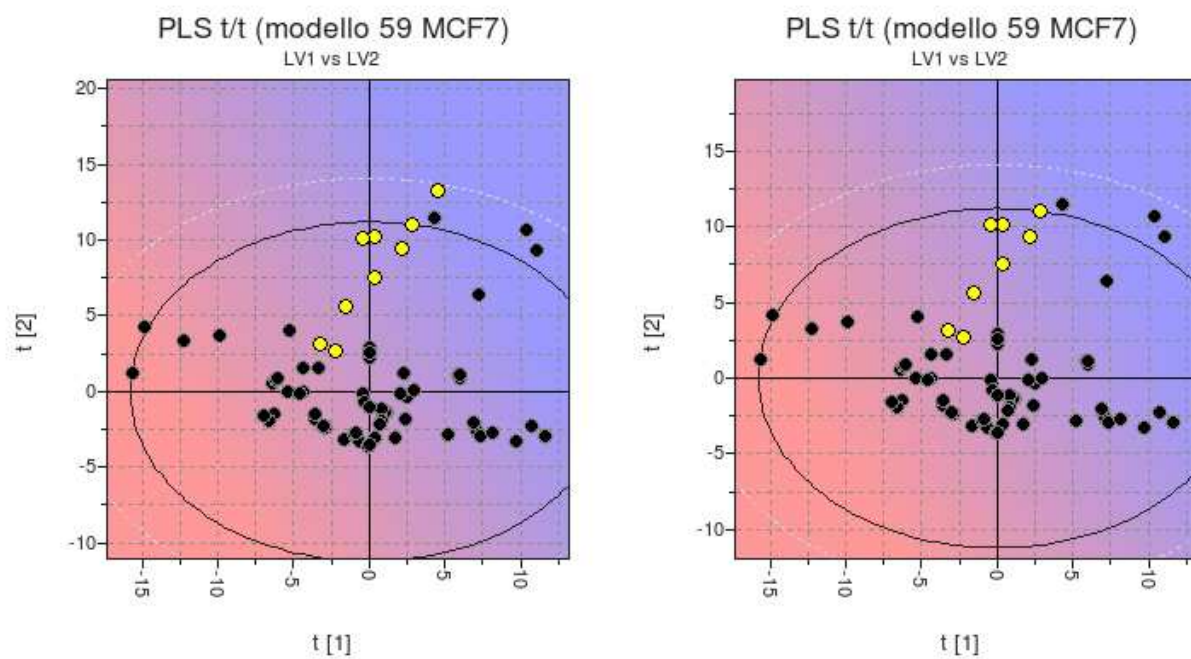


Figure S5. PLS scores plot of Pyrimidinketone derivatives: all compounds (left); after outlier or borderline elimination (right).

Chemical structures of 176 derivatives

Table S1. Chemical structures of Pyrimidinketone derivatives.

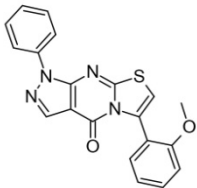
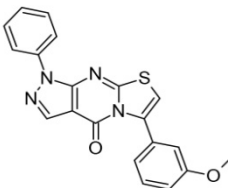
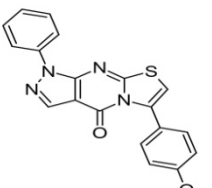
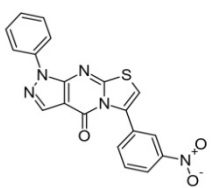
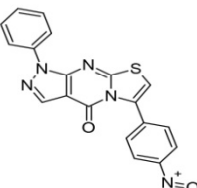
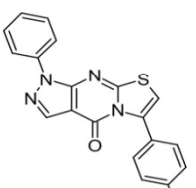
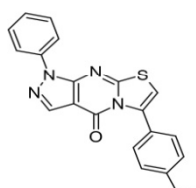
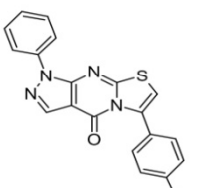
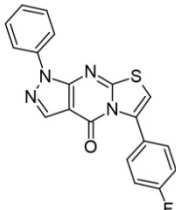
	PYRIMIDINKETONES DERIVATIVES			
	A	B	C	D
2				
3				
4				

Table S2. Chemical structures of Pyrrolopyrimidindione derivatives I.

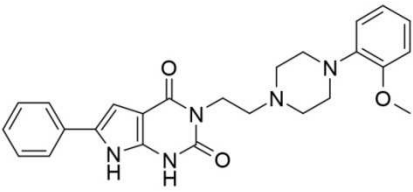
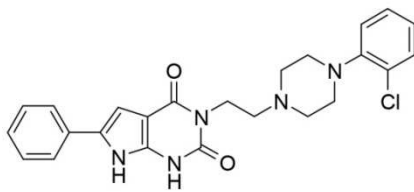
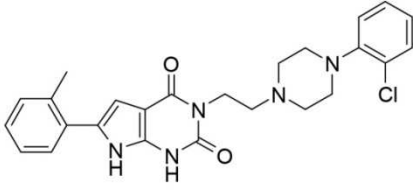
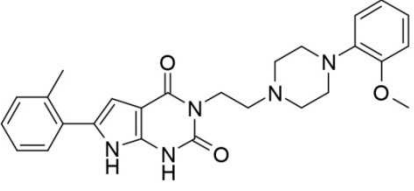
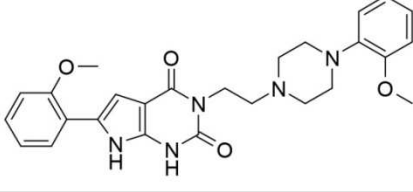
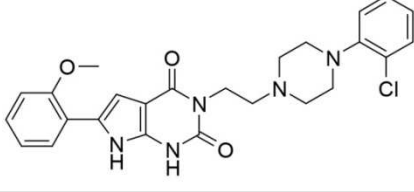
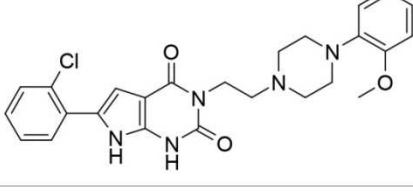
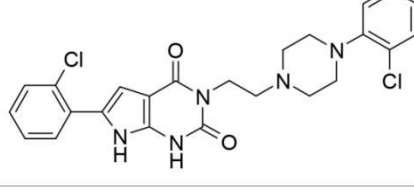
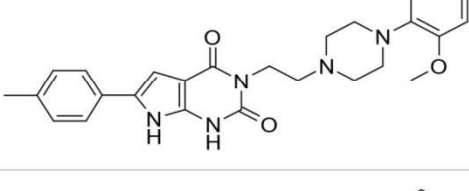
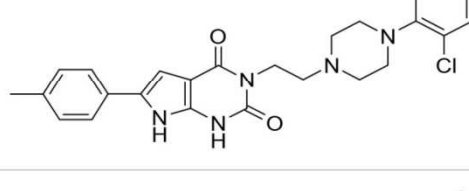
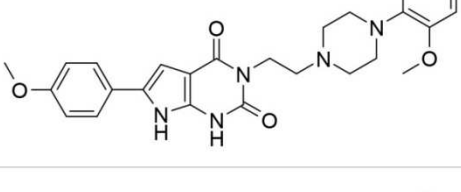
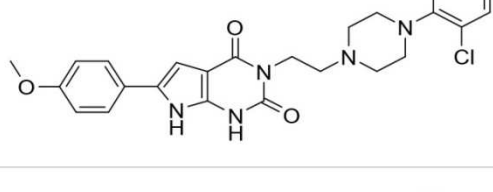
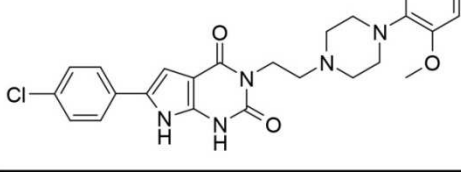
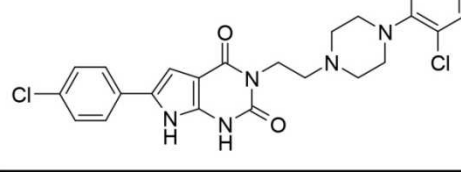
	PYRROLOPYRIMIDINDIONE DERIVATIVES I	
	A	B
2		
3		
4		
5		
6		
7		
8		

Table S3. Chemical structures of Pyrrolopyrimidindione derivatives IIa.

	PYRROLOPYRIMIDINDIONE DERIVATIVES II	
	A	B
2		
3		
4		
5		
6		
7		
8		
9		
10		

Table S4. Chemical structures of Pyrrolopyrimidindione derivatives IIb.

PYRROLOPYRIMIDINDIONE DERIVATIVES II		
	A	B
11		
12		
13		

Table S5. Chemical structures of Pyrrolopyrimidindione derivatives III.

PYRROLOPYRIMIDINDIONE DERIVATIVES III			
	A	B	C
2			
3			
4			
5			
6			
7			
8			
9			

Table S6. Chemical structures of Benziloxindole derivatives.

	BENZILOXYINDOLE DERIVATIVES		
	A	B	C
2			
3			
4			
5			
6			
7			

Table S7. Chemical structures of Indole derivatives.

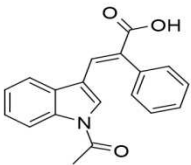
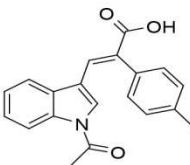
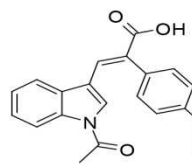
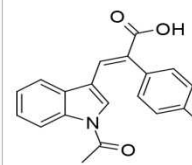
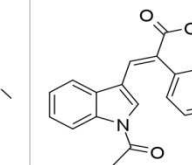
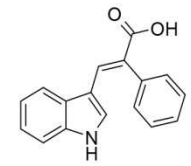
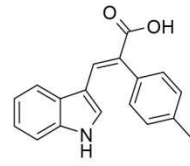
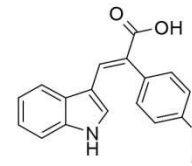

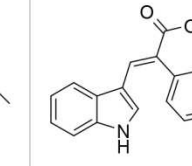
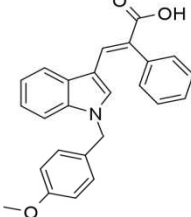
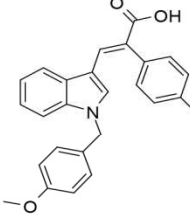
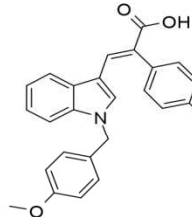
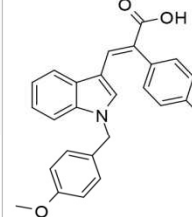
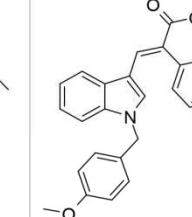
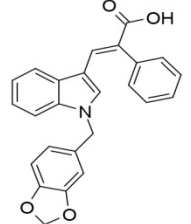
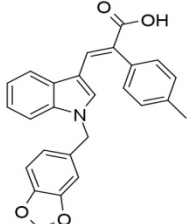
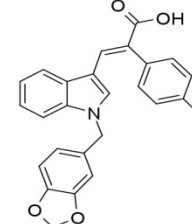
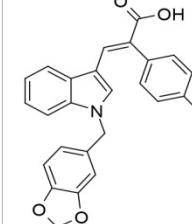
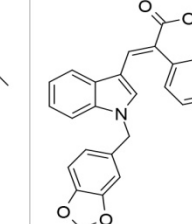
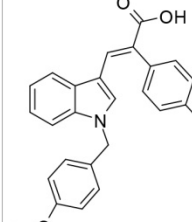
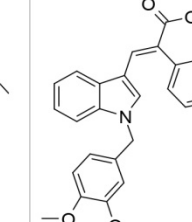
	INDOLE DERIVATIVES				
	A	B	C	D	E
2					
3					
4					
5					
6					

Table S8. Chemical structures of LCAPs derivatives.

	LCAPs		
	A	B	C
2			
3			
4			
5			
6			
7			
8			
9			

Table S9. Chemical structures of Quinoline derivatives.

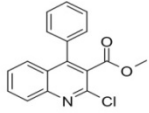
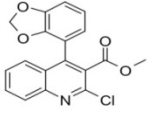
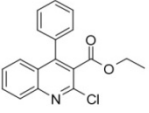
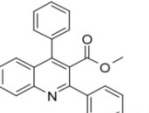
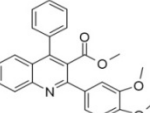
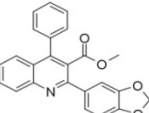
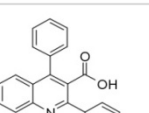
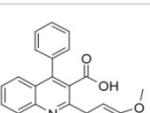
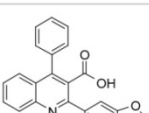
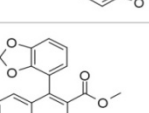
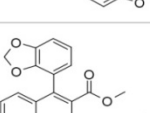
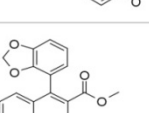
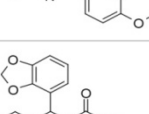
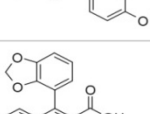
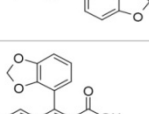
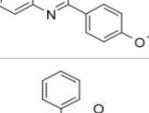
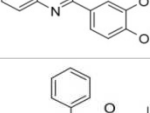
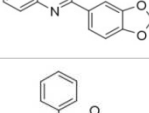
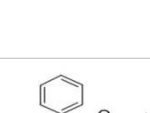
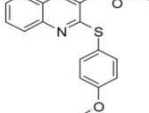
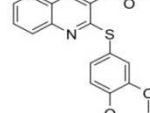
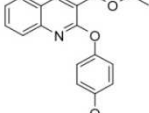
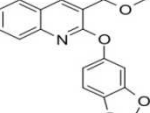
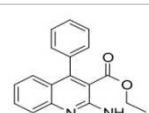
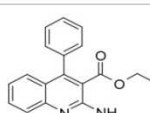
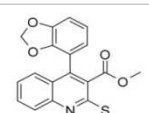
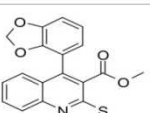
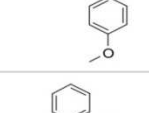
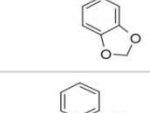
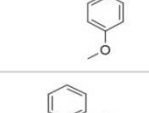
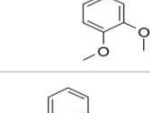
	QUINOLINE DERIVATIVES			
	A	B	C	D
2				
3				
4				
5				
6				
7				
8				
9				
10				

Table S10. Chemical structures of Thiophene derivatives.

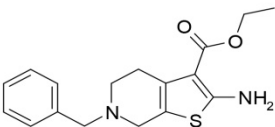
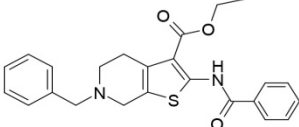
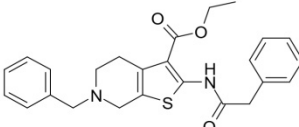
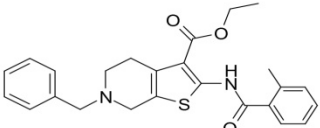
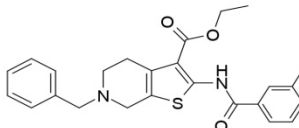
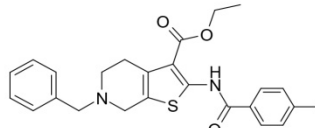
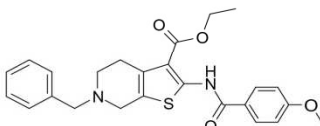
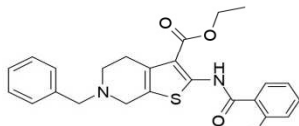
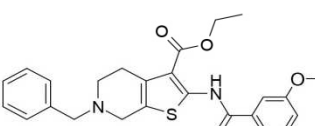
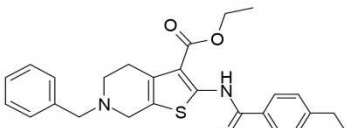
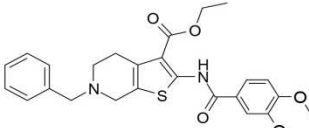
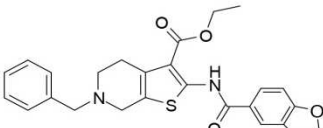
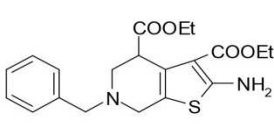
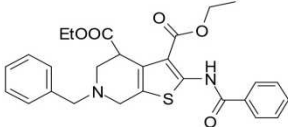
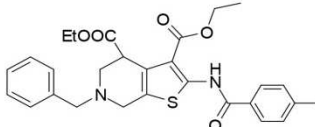
	Thiophene derivatives		
	A	B	C
2			
3			
4			
5			
6			

Table S11. Elemental analyses for compounds **2-19**.

Comp.	MW Molecular Formula	C% Calc. Found	H%	N%	S%
2	392.43 C ₂₀ H ₁₆ N ₄ O ₃ S	61.21 61.03	4.11 4.26	14.28 14.29	8.17 8.22
3	392.43 C ₂₀ H ₁₆ N ₄ O ₃ S	61.21 60.92	4.11 4.14	14.28 14.32	8.17 8.28
4	392.43 C ₂₀ H ₁₆ N ₄ O ₃ S	61.21 60.97	4.11 4.14	14.28 14.40	8.17 8.06
5	C ₂₀ H ₁₆ N ₄ O ₂ S 376.43	63.81 63.48	4.28 4.25	14.88 14.72	8.52 8.66
6	C ₁₉ H ₁₃ N ₅ O ₄ S 407.40	56.01 55.87	3.22 3.48	17.19 17.32	7.87 7.70
7	C ₁₉ H ₁₃ N ₅ O ₄ S 407.40	56.01 56.08	3.22 3.40	17.19 17.03	7.87 7.91
8	C ₁₉ H ₁₃ ClN ₄ O ₂ S 396.85	57.50 57.26	3.30 3.38	14.12 14.56	8.08 7.98
9	C ₁₉ H ₁₃ BrN ₄ O ₂ S 441.30	51.71 52.08	2.97 2.93	12.70 12.55	7.27 7.00
10	C ₁₉ H ₁₃ FN ₄ O ₂ S 380.39	59.99 60.22	3.44 3.36	14.73 14.62	8.43 8.28
11	C ₂₀ H ₁₄ N ₄ O ₂ S 374.41	64.16 64.28	3.77 3.90	14.96 15.15	8.56 8.60
12	C ₂₀ H ₁₄ N ₄ O ₂ S 374.41	64.16 64.35	3.77 3.79	14.96 15.02	8.56 8.31
13	C ₂₀ H ₁₄ N ₄ O ₂ S 374.41	64.16 63.99	3.77 4.02	14.96 15.01	8.56 8.89
14	C ₂₀ H ₁₄ N ₄ OS 358.41	67.02 66.74	3.94 3.88	15.63 15.54	8.95 8.89
15	C ₁₉ H ₁₁ N ₅ O ₃ S 389.38	58.61 58.47	2.85 2.83	17.99 18.03	8.23 8.15
16	C ₁₉ H ₁₁ N ₅ O ₃ S 389.38	58.61 58.45	2.85 2.82	17.99 17.99	8.23 8.09
17	C ₁₉ H ₁₁ ClN ₄ OS · ½H ₂ O 387.83	58.83 58.81	2.83 2.85	14.43 14.30	8.26 8.12
18	C ₁₉ H ₁₁ BrN ₄ OS 423.28	53.91 53.69	2.62 2.59	13.24 13.36	7.58 7.30
19	C ₁₉ H ₁₁ FN ₄ OS 362.38	62.97 62.46	3.06 3.09	15.46 15.19	8.85 8.81