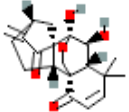
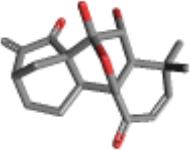
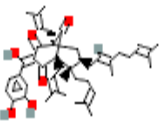
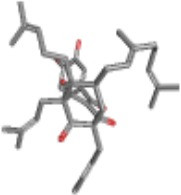
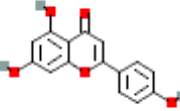
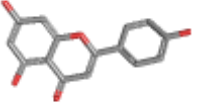

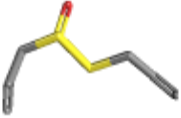
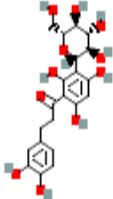
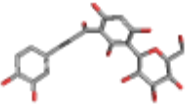
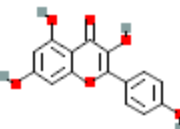
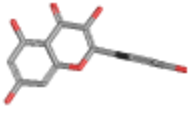
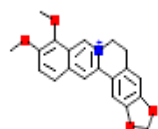
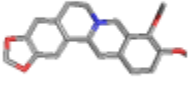
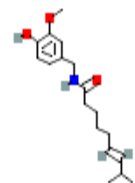

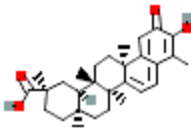
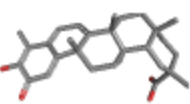


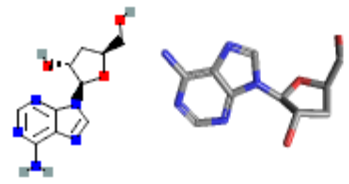
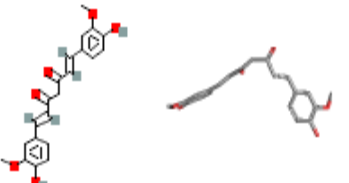
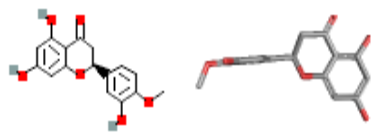
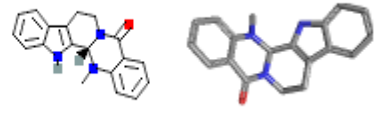
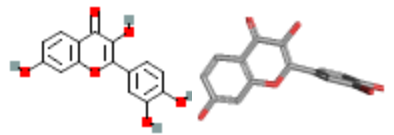
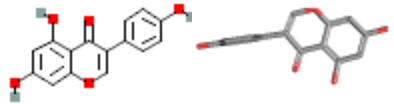
Majumder S, Panigrahi G K. Molecular docking and ADME evaluation of plant-based bioactive molecules targeting nonsense-mediated mRNA decay pathway factors to modulate tumorigenesis . Plant Science Today. 2024; 11(4): 1148-1155. <https://doi.org/10.14719/pst.3737>

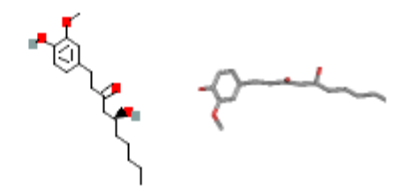
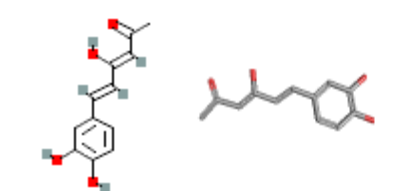
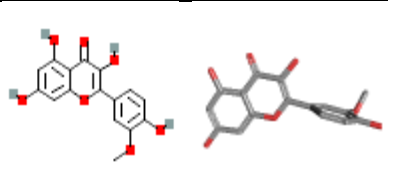
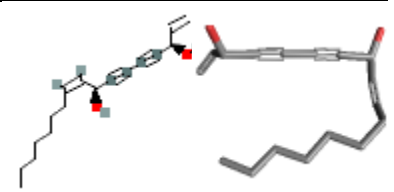
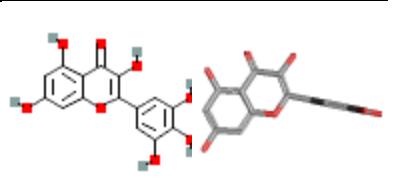
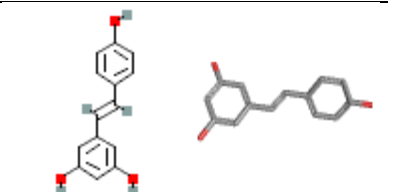
Supplementary table

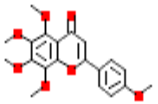
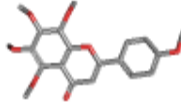
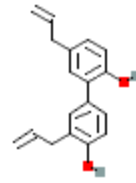
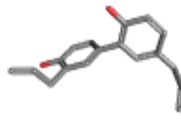
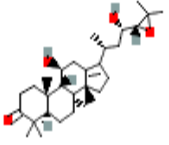
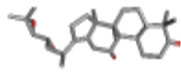
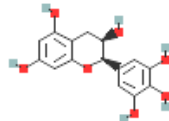
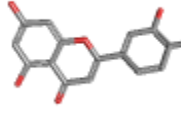
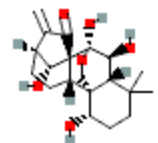
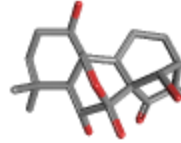
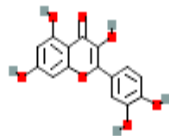
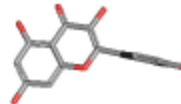
Table 1. List of phytochemicals used in preparing the ligand library.

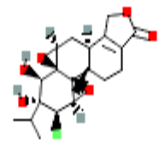
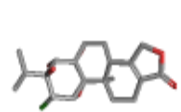
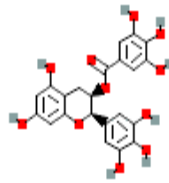
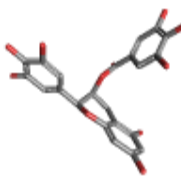
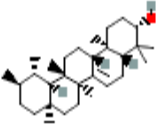
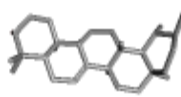
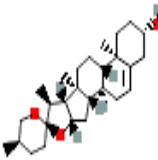
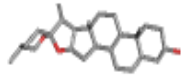
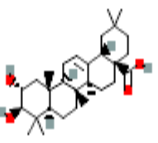
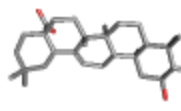
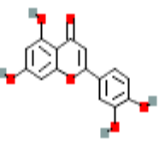
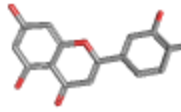
Sl. No.	Phytochemicals	PubChem CID	Molecular formula	Molecular weight (g/mol)	Chemical structure	
					2D	3D
1.	Eriocalyxin B	16202215	C ₂₀ H ₂₄ O ₅	344.4		
2.	Oblongifolin C	10100985	C ₄₃ H ₅₈ O ₆	670.9		
3.	Apigenin	5280443	C ₁₅ H ₁₀ O ₅	270.24		

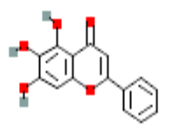
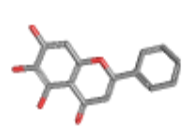
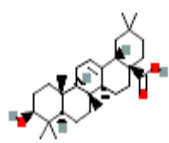
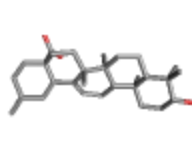
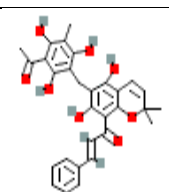
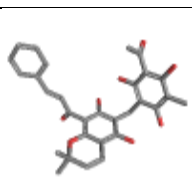
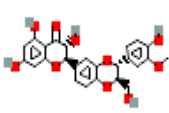
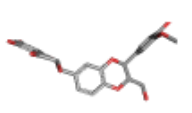
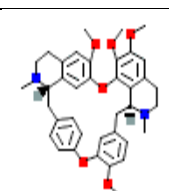
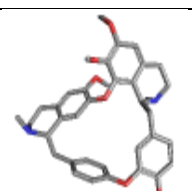
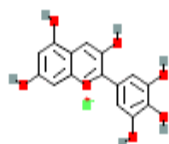
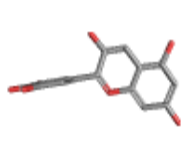
4.	Allicin	65036	$C_6H_{10}OS_2$	162.3		
5.	Aspalathin	11282394	$C_{21}H_{24}O_{11}$	452.4		
6.	Kaempferol	5280863	$C_{15}H_{10}O_6$	286.24		
7.	Berberine	2353	$C_{20}H_{18}NO_4^+$	336.4		
8.	Capsaicin	1548943	$C_{18}H_{27}NO_3$	305.4		
9.	Celastrol	122724	$C_{29}H_{38}O_4$	450.6g		

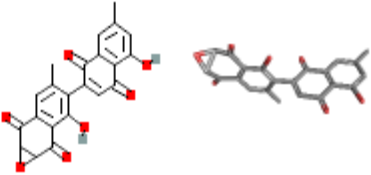

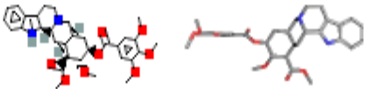

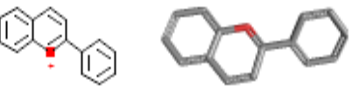
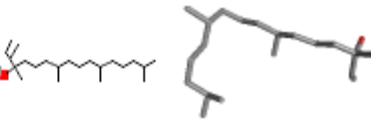
10.	Cordycepin	6303	$C_{10}H_{13}N_5O_3$	251.24	
11.	Curcumin	969516	$C_{21}H_{20}O_6$	368.4	
12.	Hesperetin	72281	$C_{16}H_{14}O_6$	302.28	
13.	Evodiamine	442088	$C_{19}H_{17}N_3O$	303.4	
14.	Fisetin	5281614	$C_{15}H_{10}O_6$	286.24	
15.	Genistein	5280961	$C_{15}H_{10}O_5$	270.24	

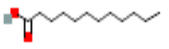

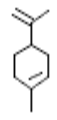
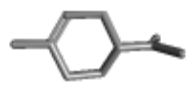
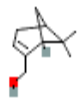
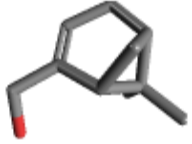
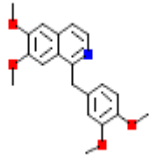
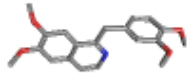
16.	Gingerol	442793	$C_{17}H_{26}O_4$	294.4	
17.	Hispolon	10082188	$C_{12}H_{12}O_4$	220.22	
18.	Isorhamnetin	5281654	$C_{16}H_{12}O_7$	316.26	
19.	Falcarindiol	5281148	$C_{17}H_{24}O_2$	260.399	
20.	Myricetin	5281672	$C_{15}H_{10}O_8$	318.23g	
21.	Resveratrol	445154	$C_{14}H_{12}O_3$	228.24	

22.	Tangeritin	68077	$C_{20}H_{20}O_7$	372.4		
23.	Honokiol	72303	$C_{18}H_{18}O_2$	266.3		
24.	Alisol B	15558620	$C_{30}H_{48}O_4$	472.7		
25.	Epigallocatechin	72277	$C_{15}H_{14}O_7$	306.27		
26.	Oridonin	5321010	$C_{20}H_{28}O_6$	364.4		
27.	Quercetin	5280343	$C_{15}H_{10}O_7$	302.23		

28.	Tripchlorolide	159588	$C_{20}H_{25}ClO_6$	396.9		
29.	Epigallocatechin gallate	65064	$C_{22}H_{18}O_{11}$	458.4		
30.	Baurenol	111220	$C_{30}H_{50}O$	426.7		
31.	Diosgenin	99474	$C_{27}H_{42}O_3$	414.6		
32.	Maslinic acid	73659	$C_{30}H_{48}O_4$	472.7		
33.	Luteolin	5280445	$C_{15}H_{10}O_6$	286.24		

34.	Baicalein	5281605	$C_{15}H_{10}O_5$	270.24g		
35.	Oleanolic acid	10494	$C_{30}H_{48}O_3$	456.7		
36.	Rottlerin	5281847	$C_{30}H_{28}O_8$	516.5		
37.	Silibinin	31553	$C_{25}H_{22}O_{10}$	482.4		
38.	Tetrandrine	73078	$C_{38}H_{42}N_2O_6$	622.7		
39.	Delphinidin	68245	$C_{15}H_{11}ClO_7$	338.69		

40.	Diosquinone	122720	$C_{22}H_{14}O_7$	390.3	
41.	Alpha-pinene	6654	$C_{10}H_{16}$	136.23g	
42.	Deserpidine	8550	$C_{32}H_{38}N_2O_8$	578.7	
43.	Eugenol	3314	$C_{10}H_{12}O_2$	164.2	
44.	Flavylium	145858	$C_{15}H_{11}O^+$	207.25	
45.	Isophytol	10453	$C_{20}H_{40}O$	296.5	

46.	Lauric acid	3893	$C_{12}H_{24}O_2$	200.32		
47.	Limonene	22311	$C_{10}H_{16}$	136.23		
48.	Myrtenol	10582	$C_{10}H_{16}O$	152.23		
49.	Papaverine	4680	$C_{20}H_{21}NO_4$	339.4		
50.	Trihydroxyisoflavone	5284648	$C_{15}H_{10}O_5$	270.24	