

1/66
FIG. 1

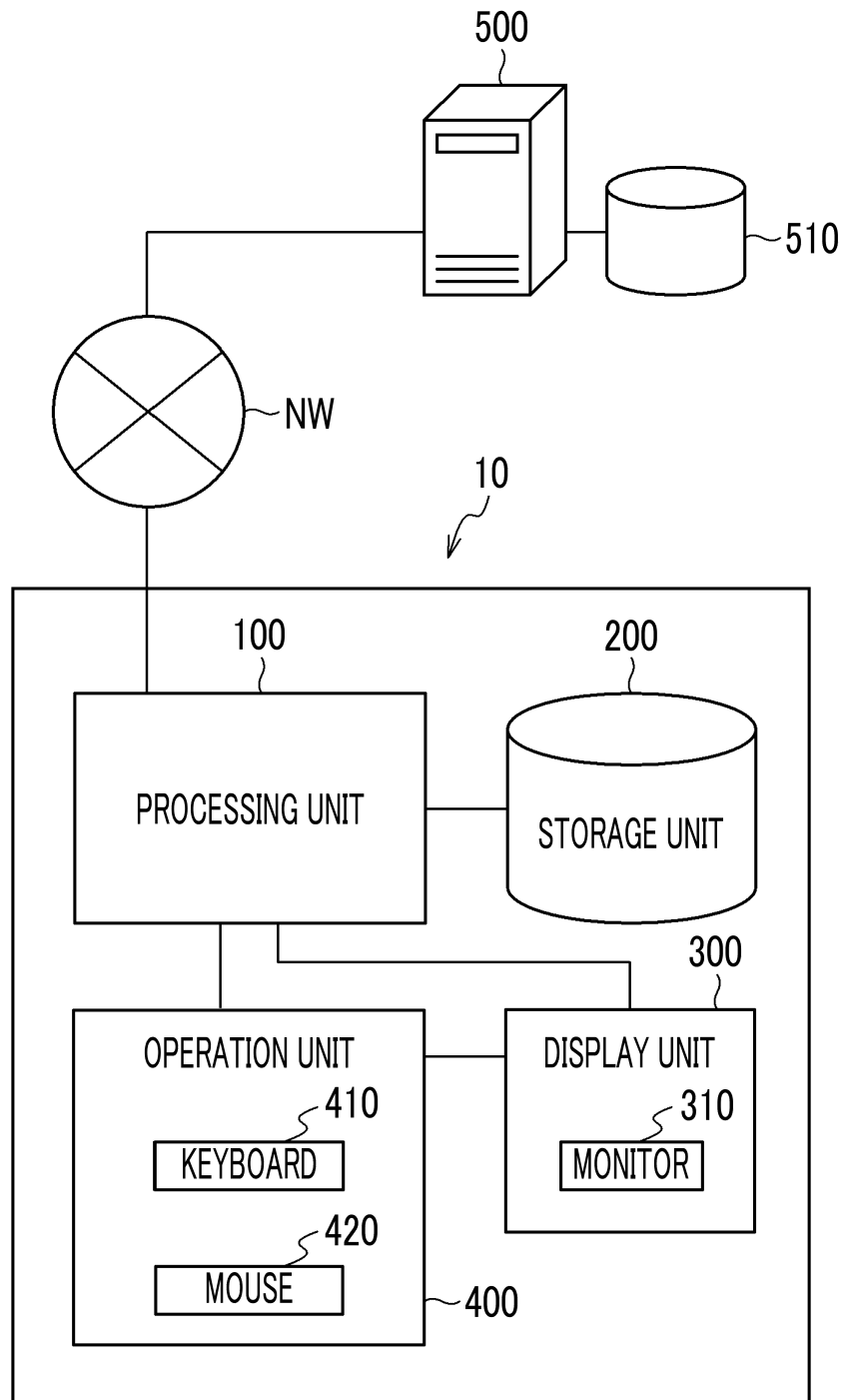


FIG. 2

100

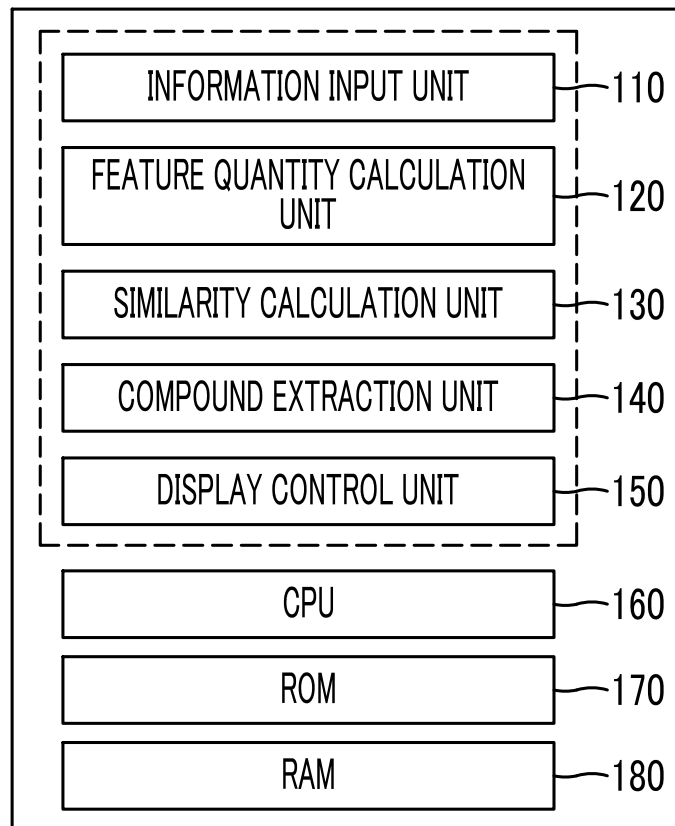
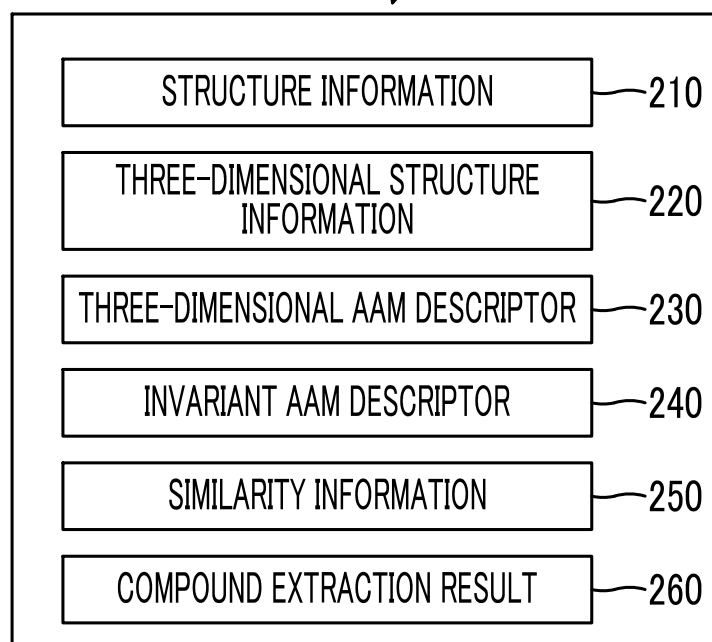


FIG. 3

200



3/66
FIG. 4

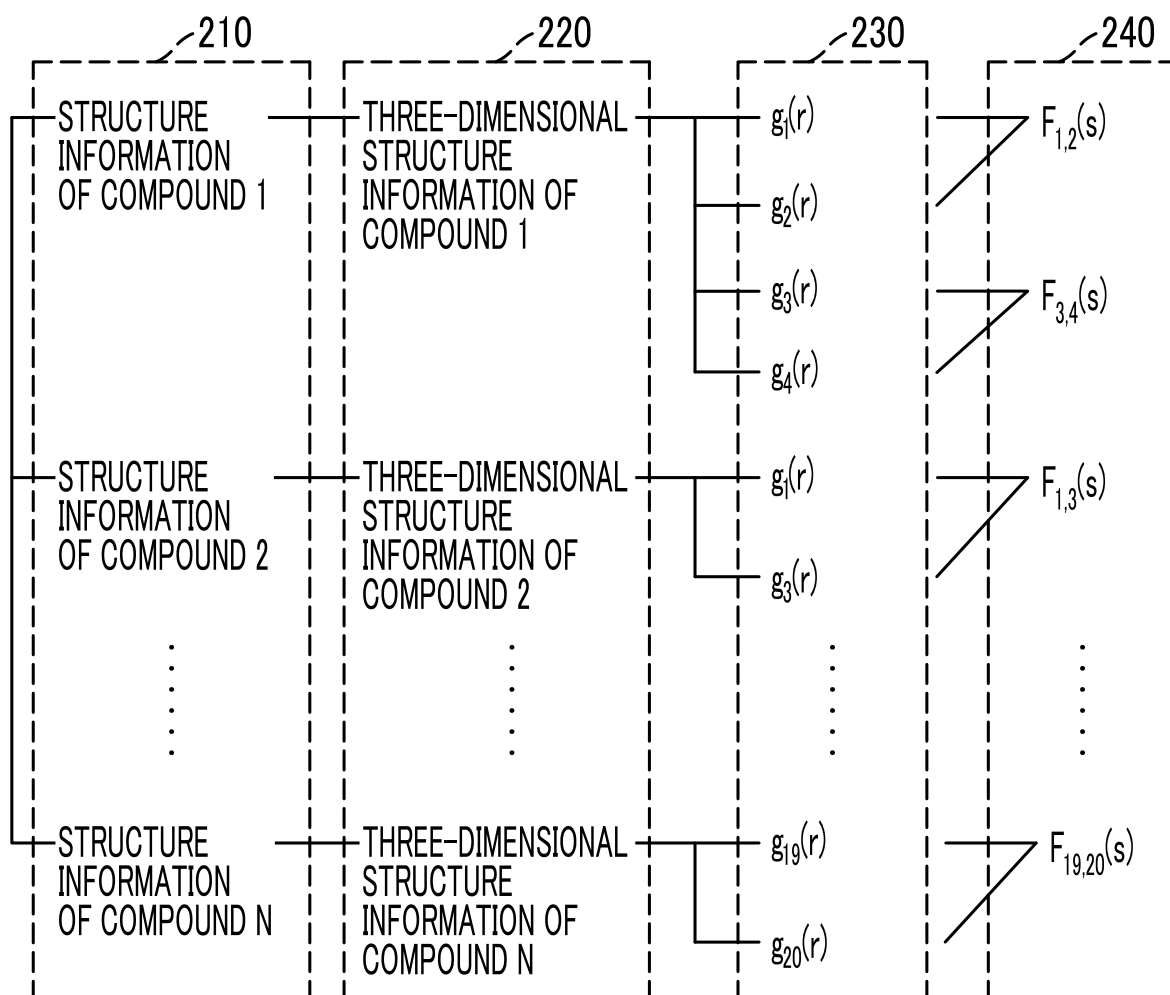


FIG. 5

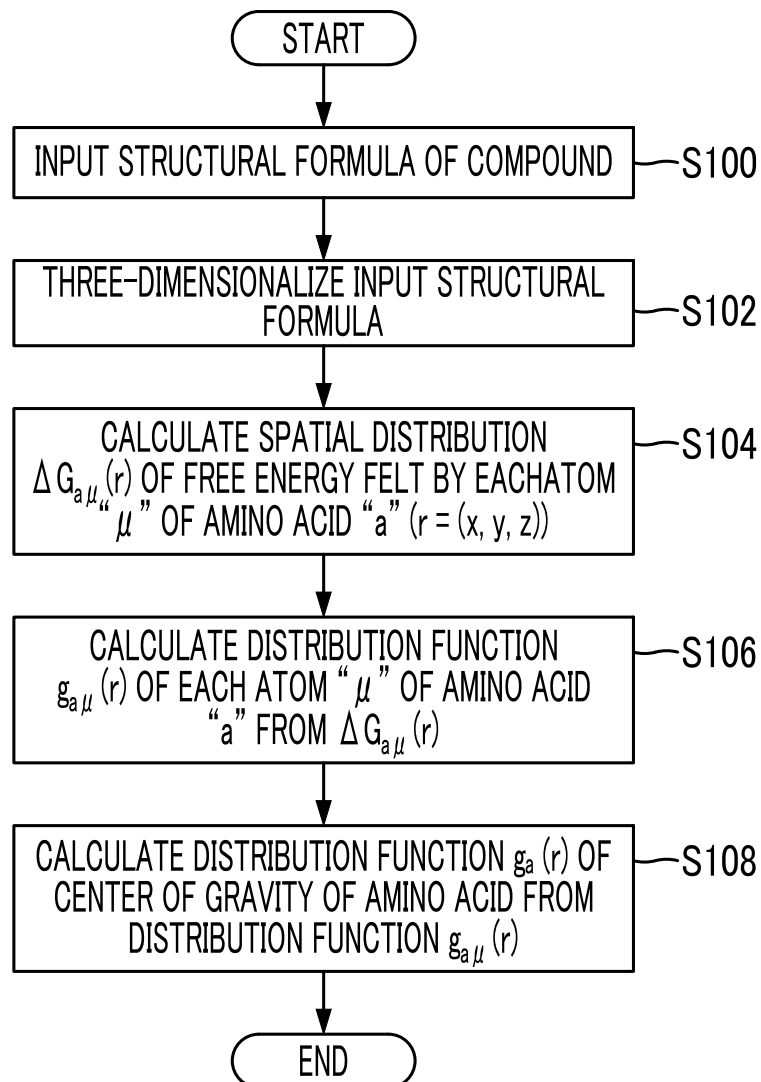


FIG. 6A

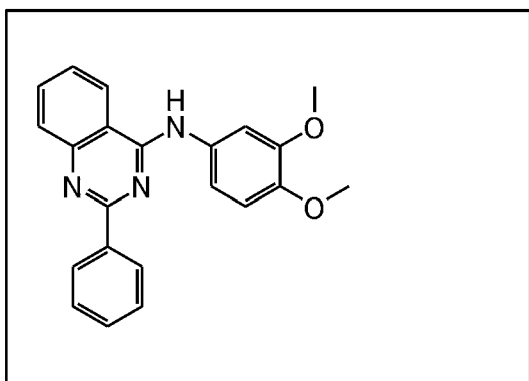


FIG. 6B

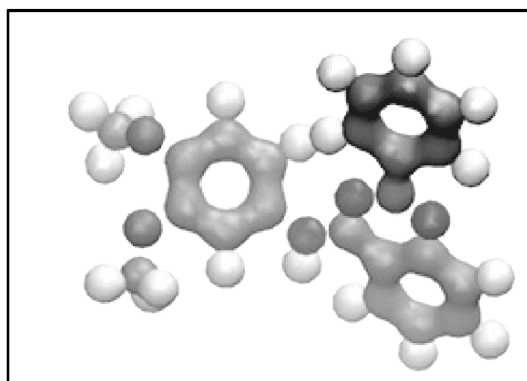


FIG. 7A

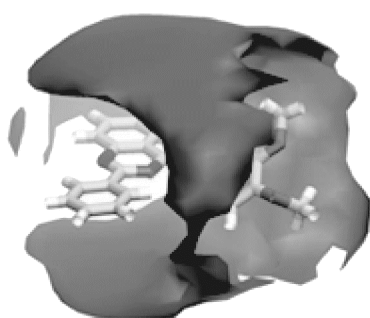
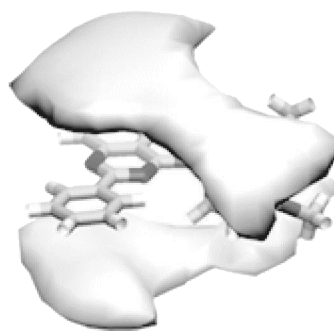


FIG. 7B



• • •

6/66
FIG. 8

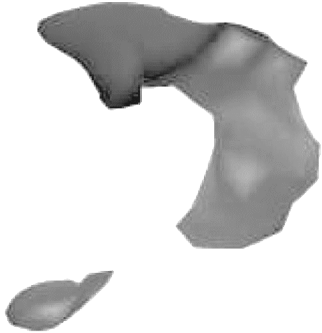
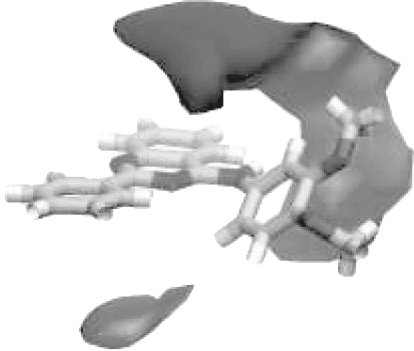
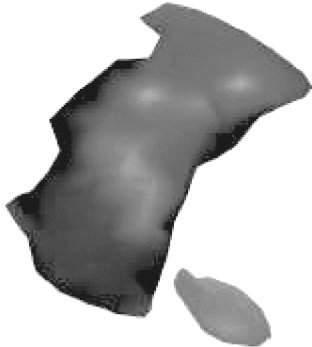
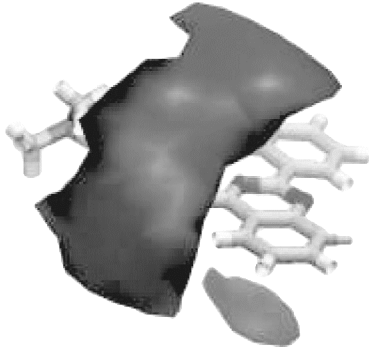
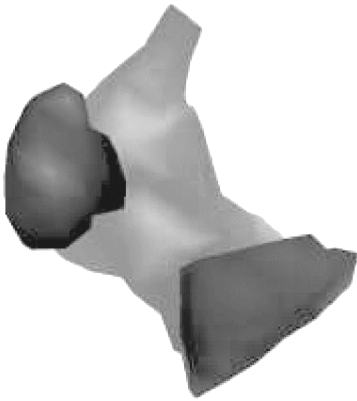
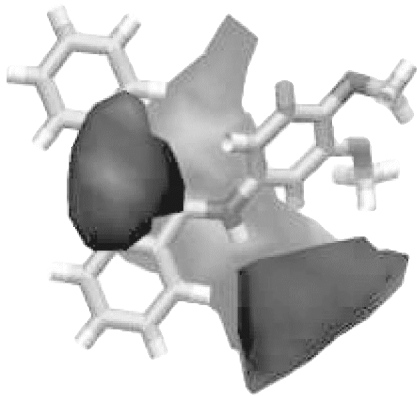
	THREE-DIMENSIONAL AAM DESCRIPTOR (LEVEL SURFACE WITH RESPECT TO THRESHOLD)	THREE-DIMENSIONAL AAM DESCRIPTOR (LEVEL SURFACE WITH RESPECT TO THRESHOLD) AND THREE-DIMENSIONAL STRUCTURE OF COMPOUND
DIRECTION 1	 A 3D surface plot showing a large, irregularly shaped volume with a smaller, separate lobe below it. The surface is smooth and shaded to show depth.	 The same 3D surface plot as in the previous cell, but with a white stick-model chemical structure overlaid. The structure consists of a central aromatic ring system with several substituents, including a long chain and a smaller ring.
DIRECTION 2	 A 3D surface plot showing a large, irregularly shaped volume with a smaller, separate lobe below it. The surface is smooth and shaded to show depth.	 The same 3D surface plot as in the previous cell, but with a white stick-model chemical structure overlaid. The structure is a different conformation or projection of the same molecule.
DIRECTION 3	 A 3D surface plot showing a large, irregularly shaped volume with a smaller, separate lobe below it. The surface is smooth and shaded to show depth.	 The same 3D surface plot as in the previous cell, but with a white stick-model chemical structure overlaid. The structure is a different conformation or projection of the same molecule.

FIG. 9

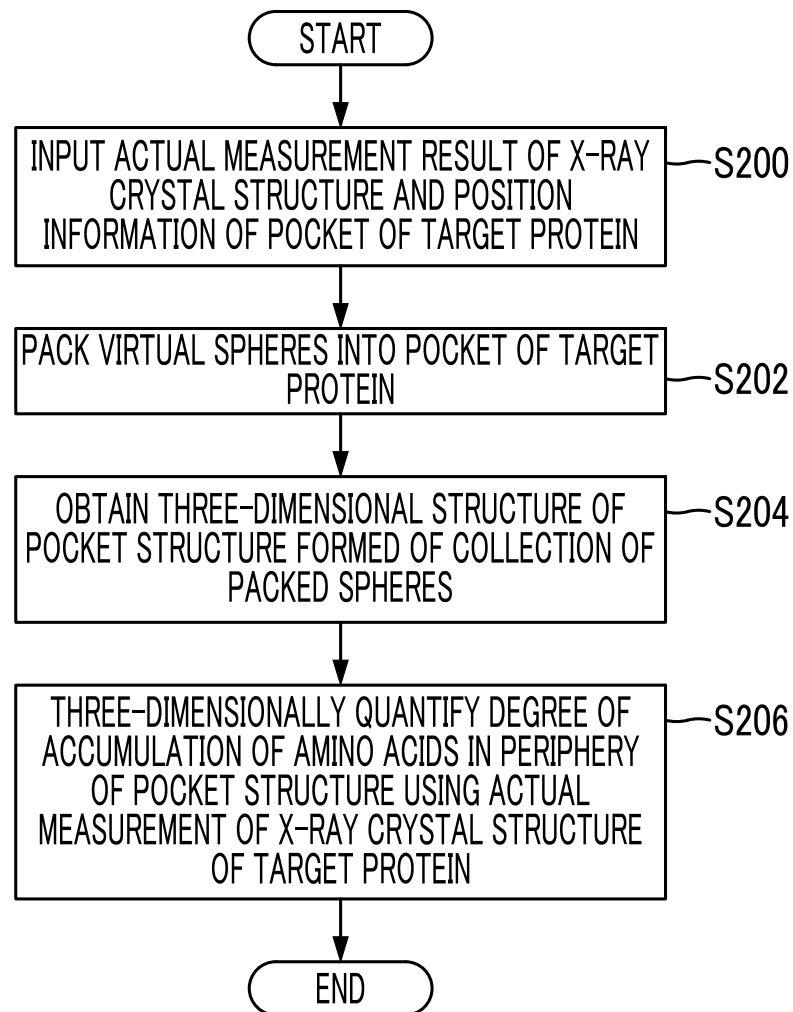


FIG. 10A

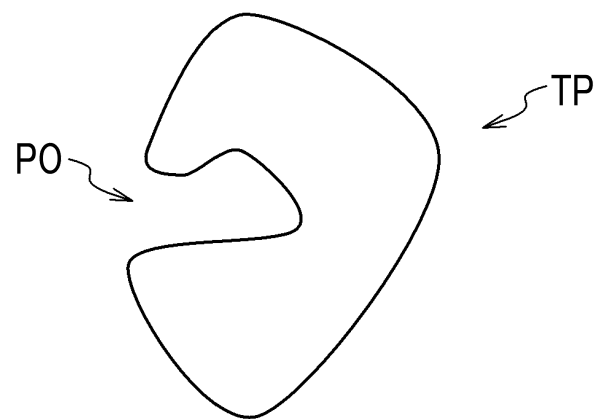


FIG. 10B

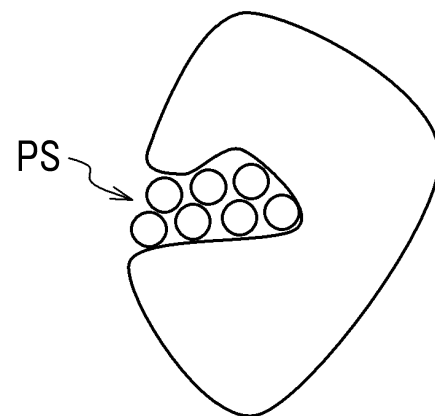
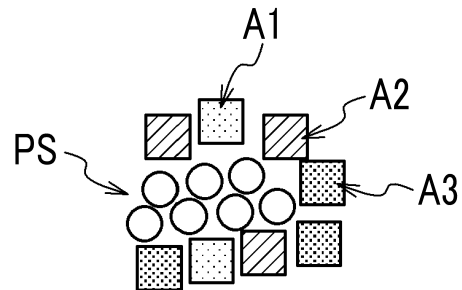


FIG. 10C



9/66
FIG. 11A

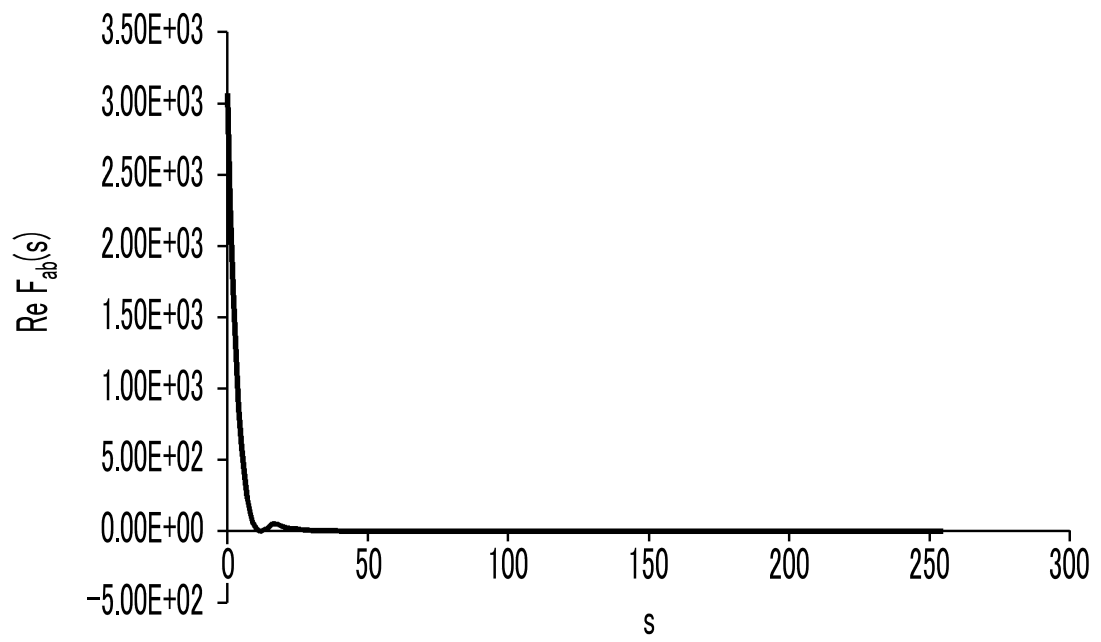
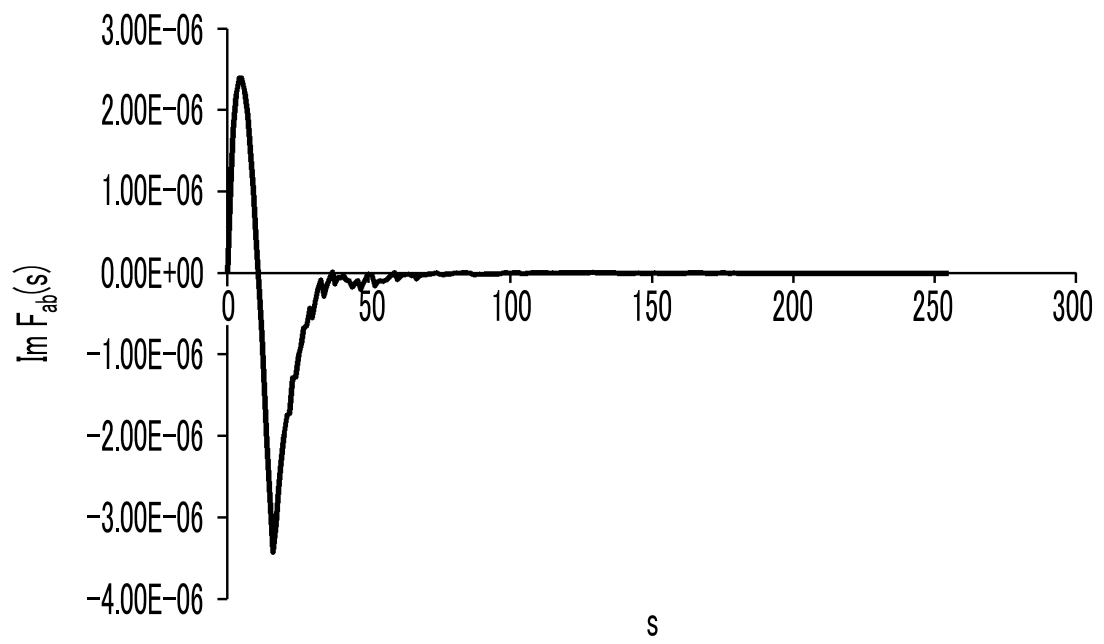


FIG. 11B



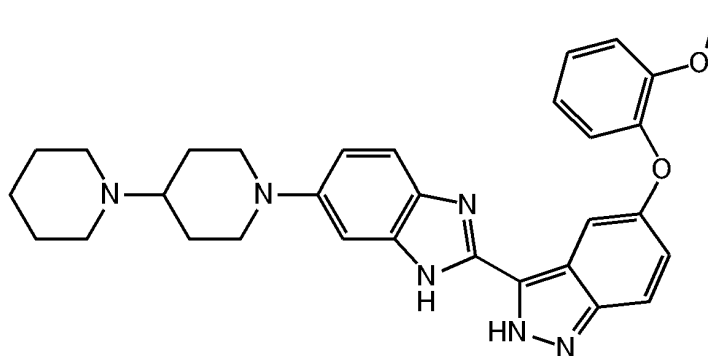


FIG. 12B

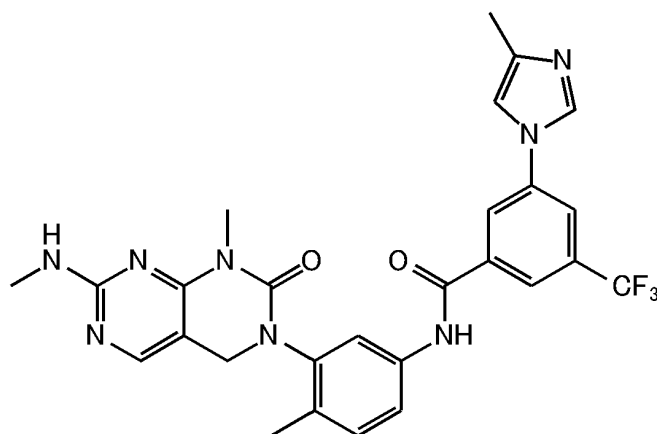
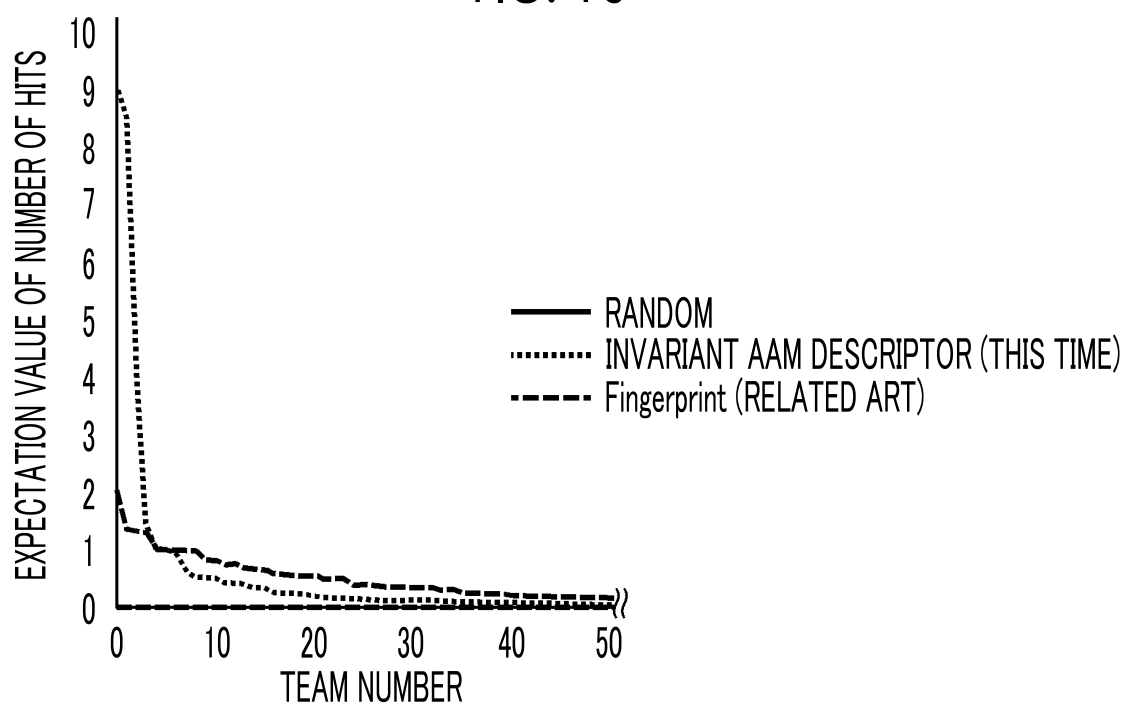


FIG. 13



11/66
FIG. 14

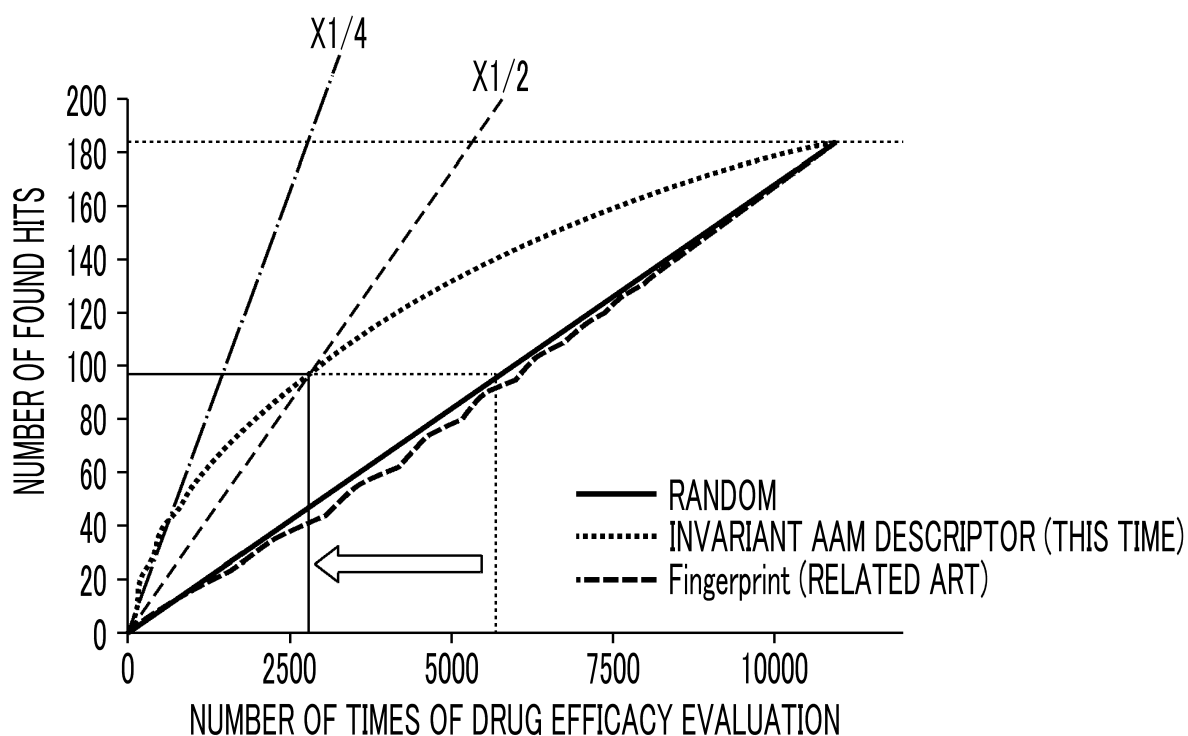


FIG. 15

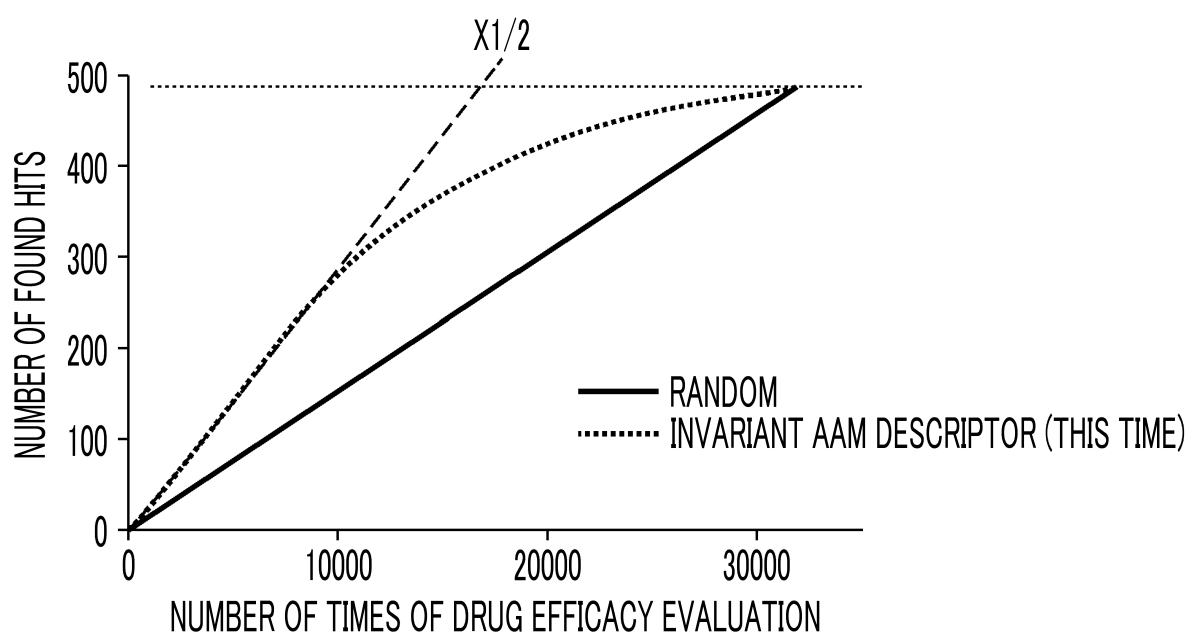


FIG. 16

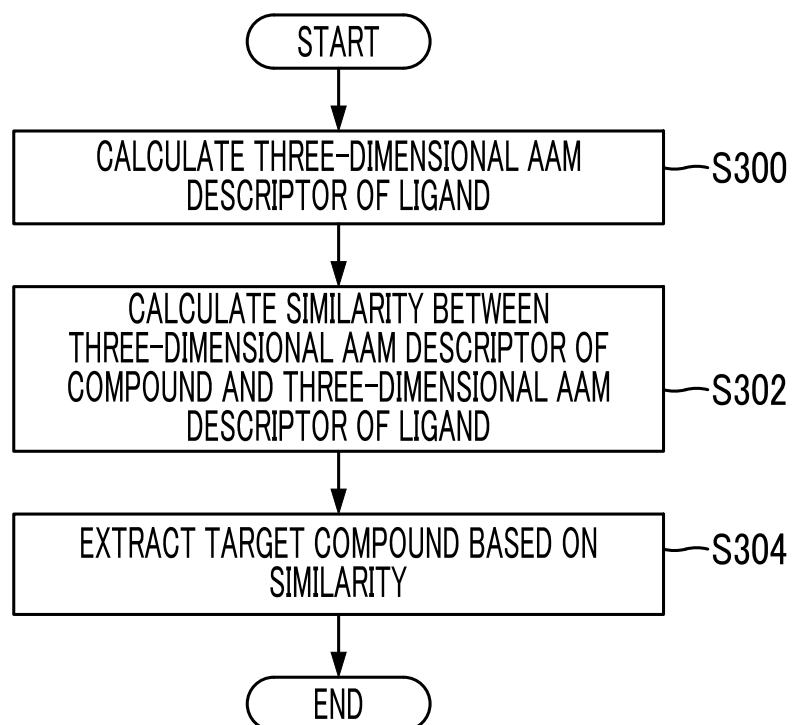


FIG. 17A

LIGAND	COMPOUND			SIMILARITY	EXTRACTION RESULT
	IDENTIFICATION INFORMATION	THREE-DIMENSIONAL AAM DESCRIPTOR	THREE-DIMENSIONAL AAM DESCRIPTOR		
L00001	L00001_g(r)	C00001	C00001_g1(r)	85%	EXTRACTED
		C00002	C00002_g1(r)	73%	NOT EXTRACTED
		...	...	...	...
		C00100	C00100_g1(r)	91%	EXTRACTED
		...	...	...	...
		C01000	C01000_g1(r)	80%	EXTRACTED
		...	...	...	...

FIG. 17B

LIGAND	COMPOUND			SIMILARITY		EXTRACTION RESULT
	IDENTIFICATION INFORMATION	INVARIANT AAM DESCRIPTOR	INVARIANT AAM DESCRIPTOR	VALUE	RANK	
L00001	L00001_F ₁₂ (s)	C00100	C00100_F ₁₂ (s)	91%	1	EXTRACTED
		C00001	C00001_F ₁₂ (s)	85%	2	EXTRACTED
		...	...	...	...	...
		C01000	C01000_F ₁₂ (s)	80%	100	EXTRACTED
		...	...	...	...	...
		C00002	C00002_F ₁₂ (s)	73%	265	NOT EXTRACTED
		...	...	...	...	...

EXTRACTED

FIG. 18

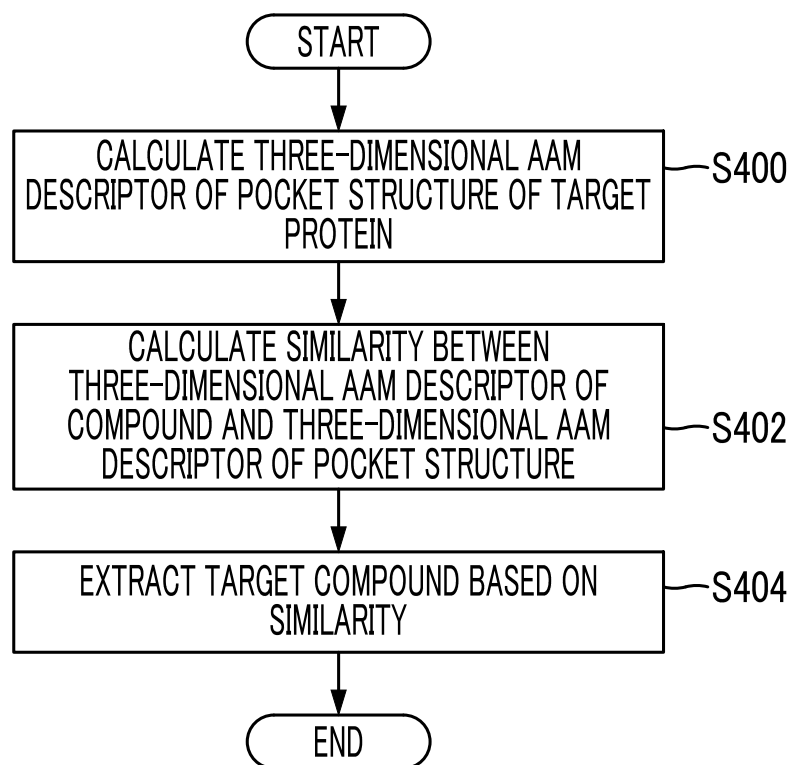


FIG. 19A

POCKET STRUCTURE		COMPOUND		SIMILARITY	EXTRACTION RESULT
IDENTIFICATION INFORMATION	THREE-DIMENSIONAL AAM DESCRIPTOR	IDENTIFICATION INFORMATION	THREE-DIMENSIONAL AAM DESCRIPTOR		
P00001	P00001_g(r)	C00001	C00001_g1(r)	85%	EXTRACTED
		C00002	C00002_g1(r)	73%	NOT EXTRACTED
		...	...	...	...
		C00100	C00100_g1(r)	91%	EXTRACTED
		...	...	...	...
		C01000	C01000_g1(r)	80%	EXTRACTED
		...	...	...	...

FIG. 19B

POCKET STRUCTURE		COMPOUND		SIMILARITY		EXTRACTION RESULT
IDENTIFICATION INFORMATION	INVARIANT AAM DESCRIPTOR	IDENTIFICATION INFORMATION	INVARIANT AAM DESCRIPTOR	VALUE	RANK	
P00001	P00001_F ₁₂ (s)	C00100	C00100_F ₁₂ (s)	91%	1	EXTRACTED
		C00001	C00001_F ₁₂ (s)	85%	2	EXTRACTED
		...	...	...	...	...
		C01000	C01000_F ₁₂ (s)	80%	100	EXTRACTED
		...	...	...	...	...
		C00001	C00001_F ₁₂ (s)	73%	265	NOT EXTRACTED
		...	...	...	...	...

EXTRACTED

16/66
FIG. 20

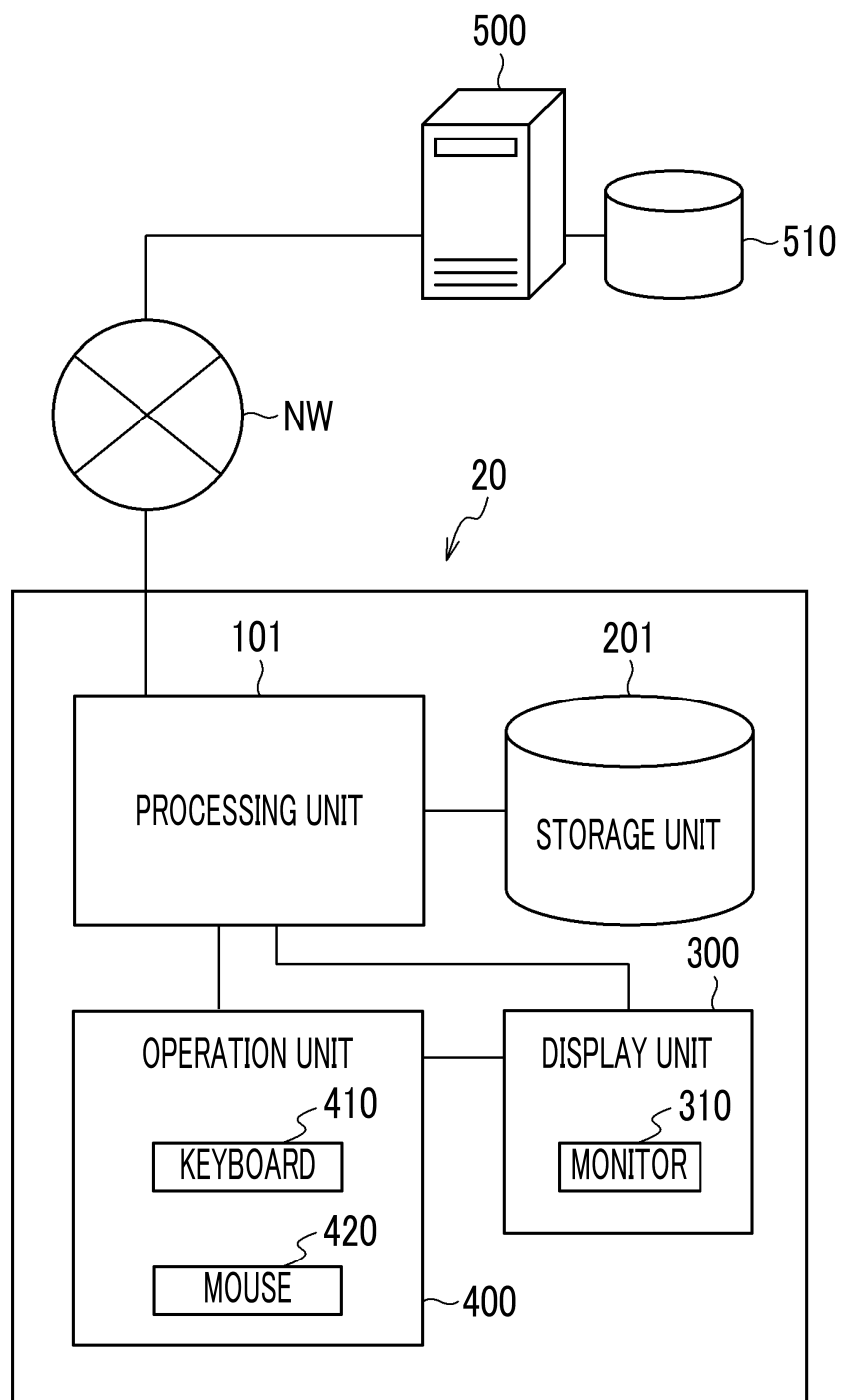


FIG. 21

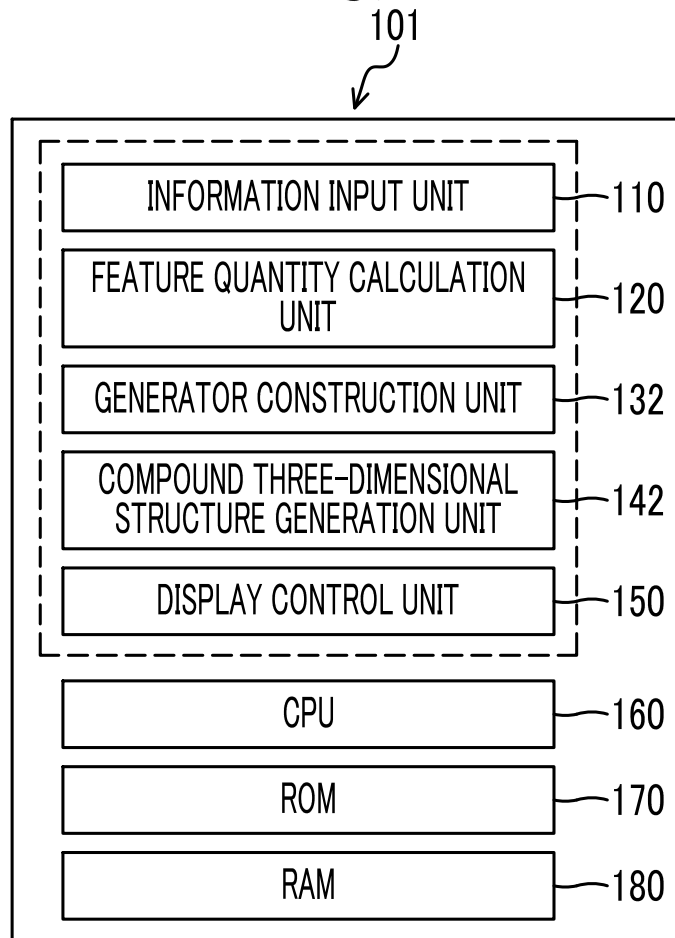


FIG. 22

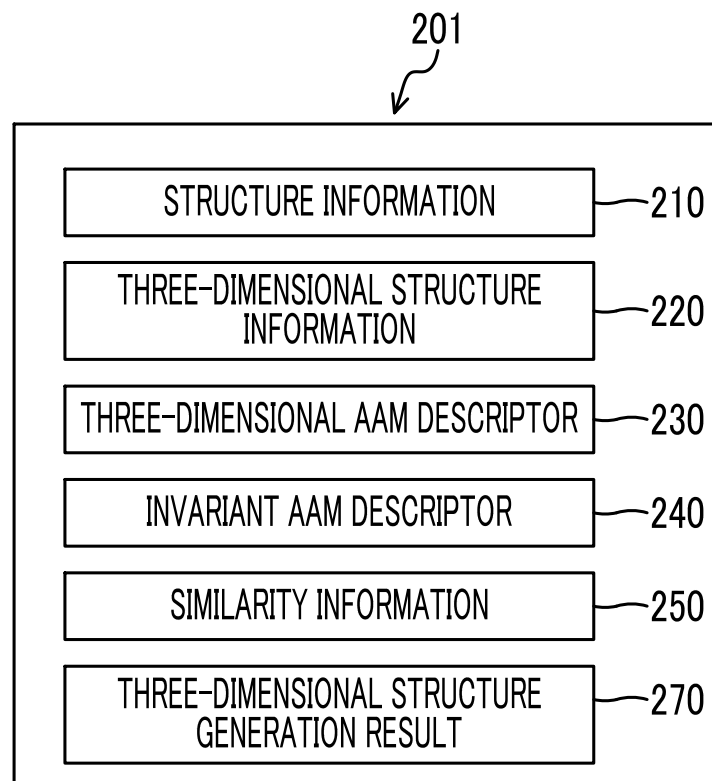
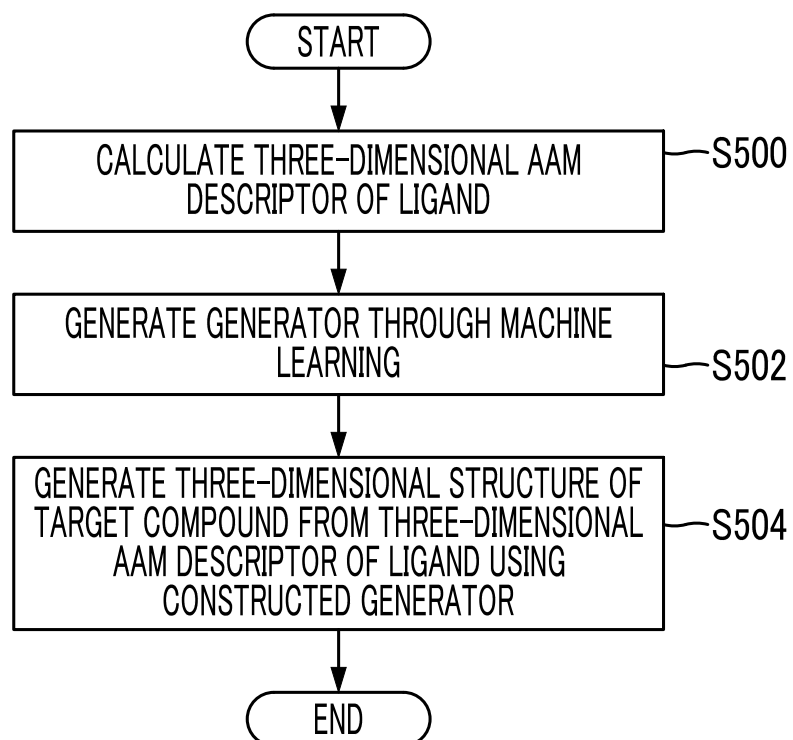
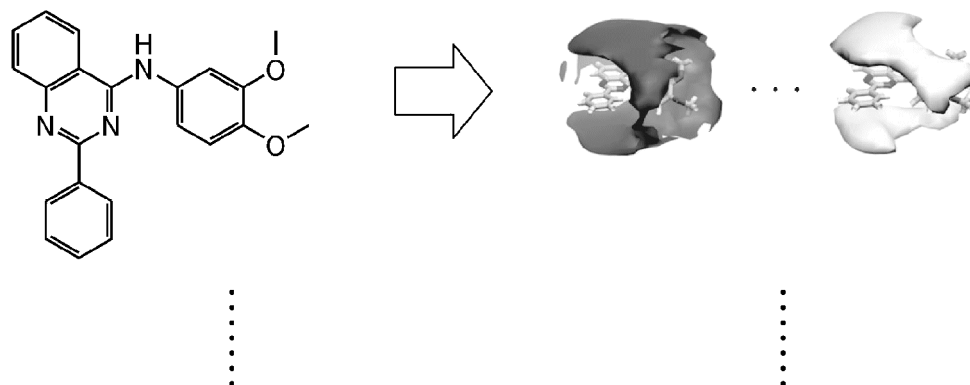


FIG. 23



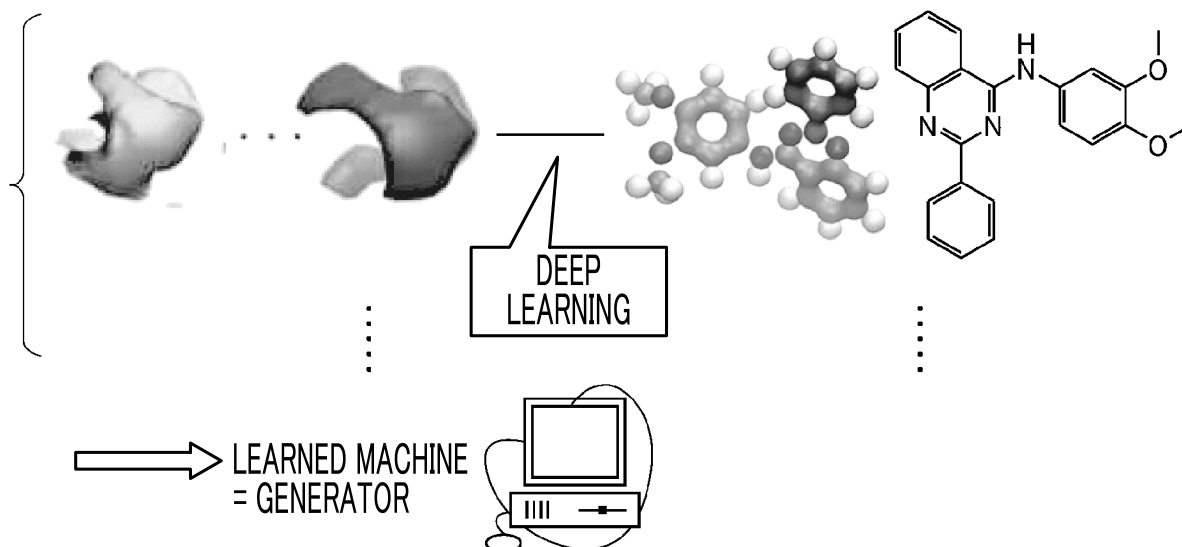
19/66
FIG. 24

Step1: CALCULATE THREE-DIMENSIONAL AAM DESCRIPTOR OF PLURALITY OF COMPOUNDS
AND CREATE PAIR OF STRUCTURAL FORMULA AND THREE-DIMENSIONAL AAM
DESCRIPTOR



Step2: THREE-DIMENSIONAL DESCRIPTOR
(EXPLANATORY VARIABLE)

THREE-DIMENSIONAL STRUCTURE
OF COMPOUND (TEACHER DATA)



20/66
FIG. 25

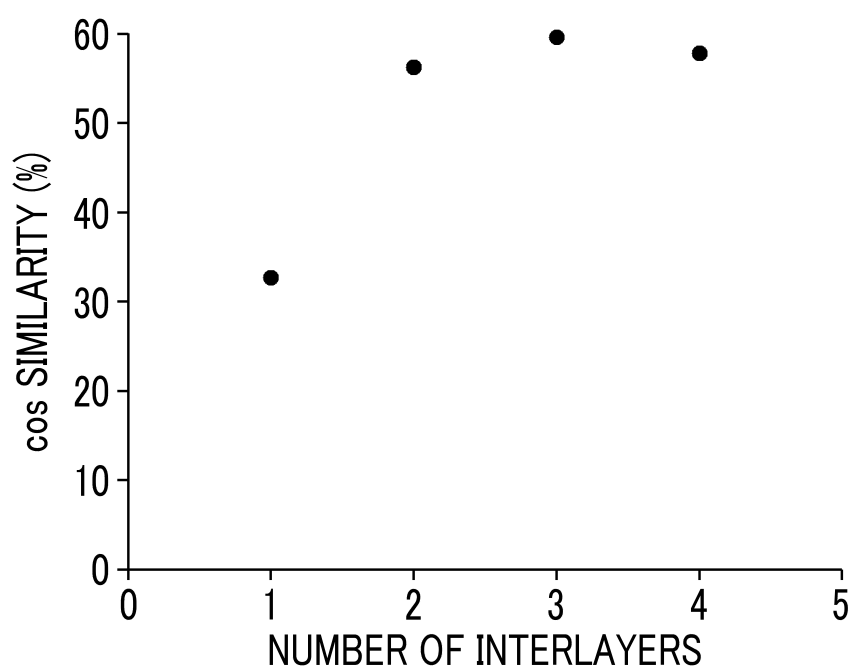
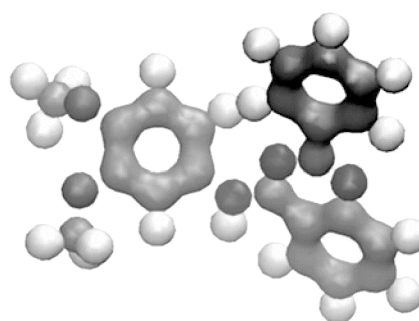


FIG. 26A



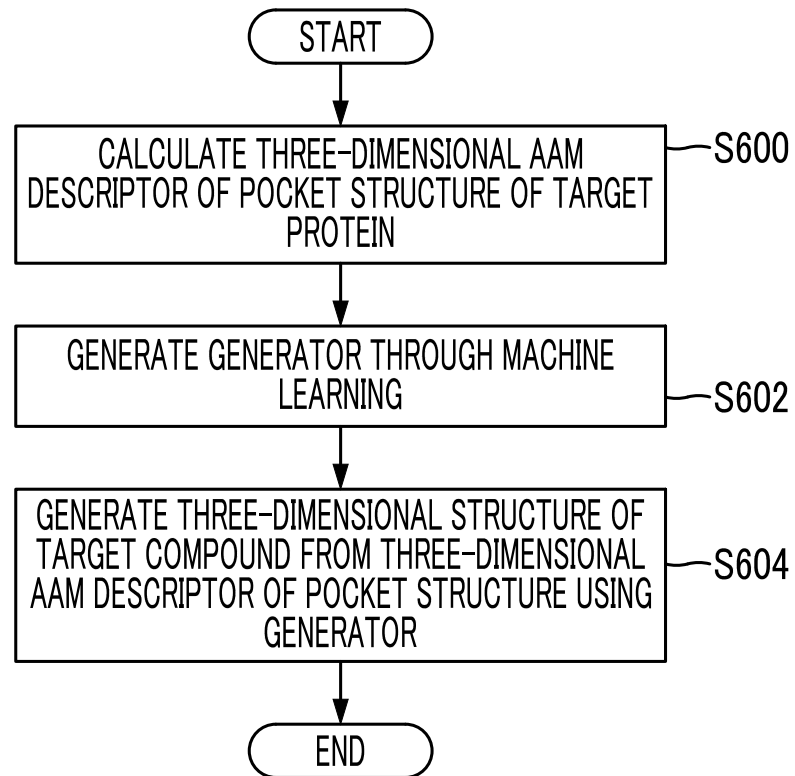
STRUCTURAL FORMULA
GENERATED FROM
THREE-DIMENSIONAL AAM
DESCRIPTOR

FIG. 26B



CORRECT STRUCTURAL
FORMULA

FIG. 27



22/66
FIG. 28

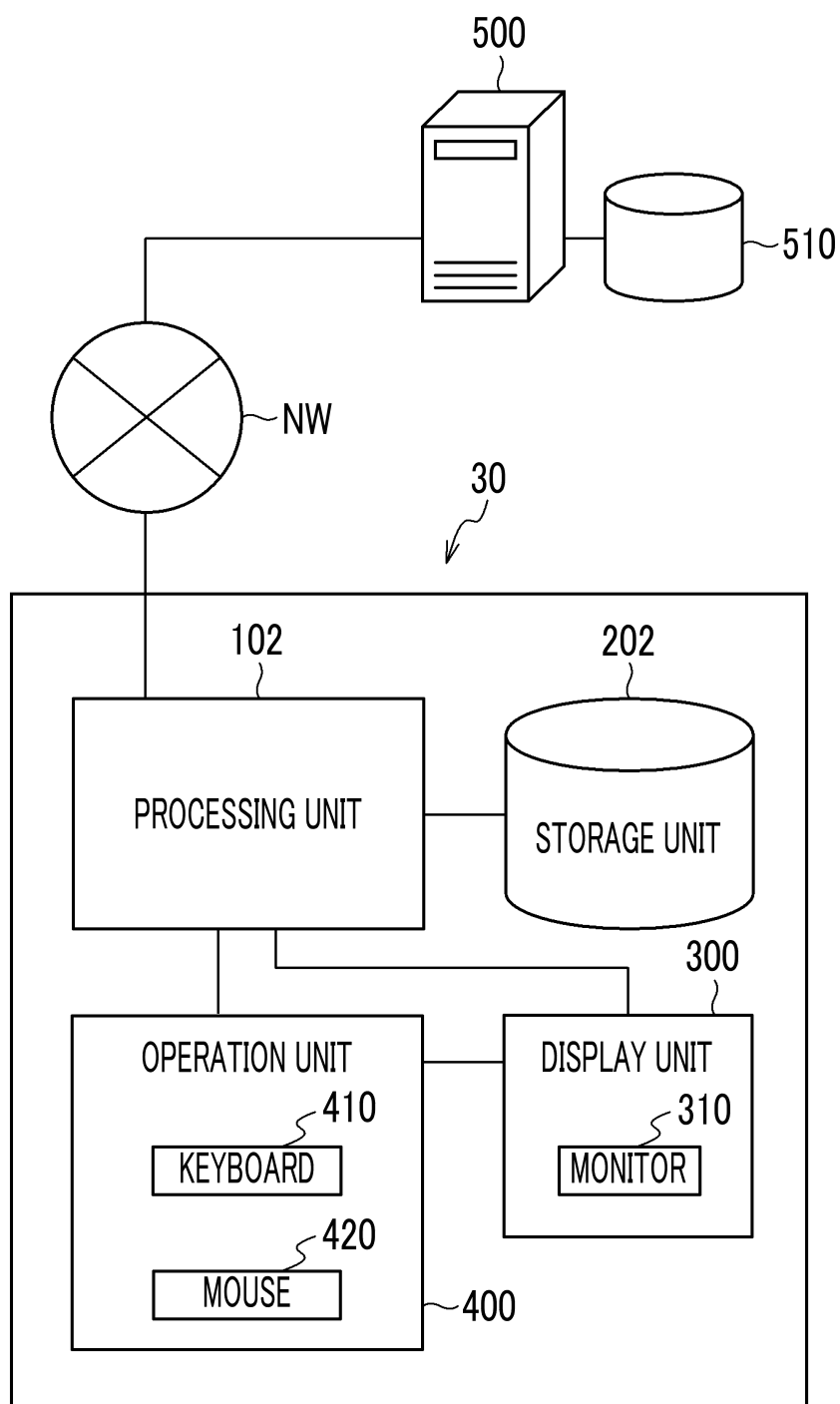


FIG. 29

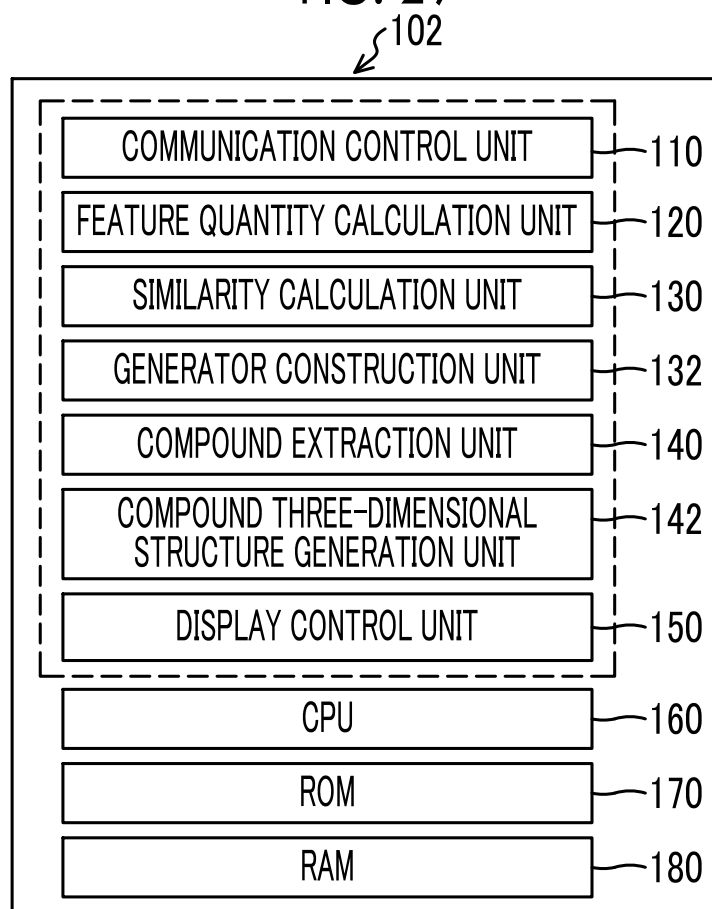


FIG. 30

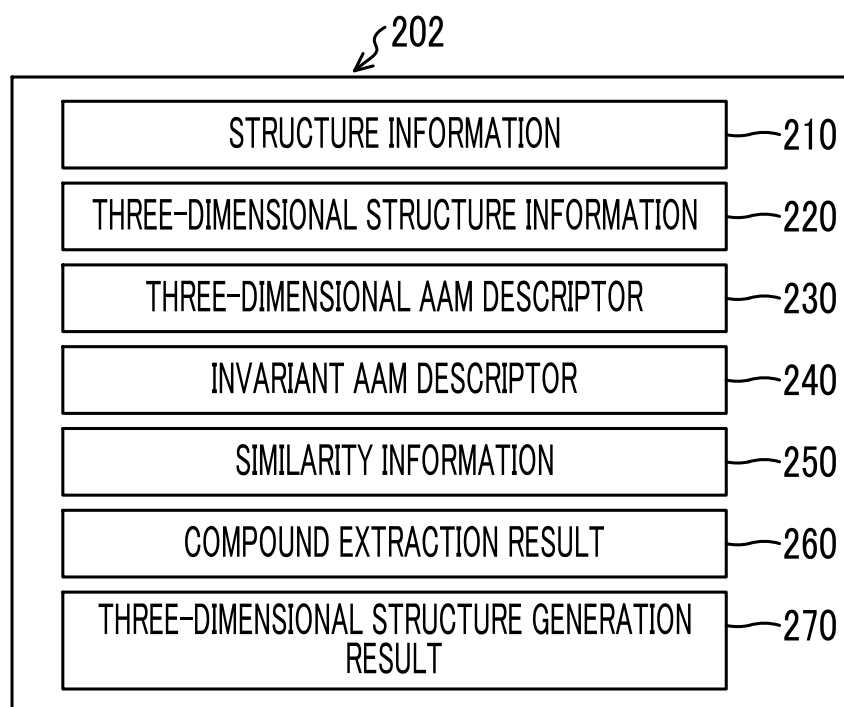
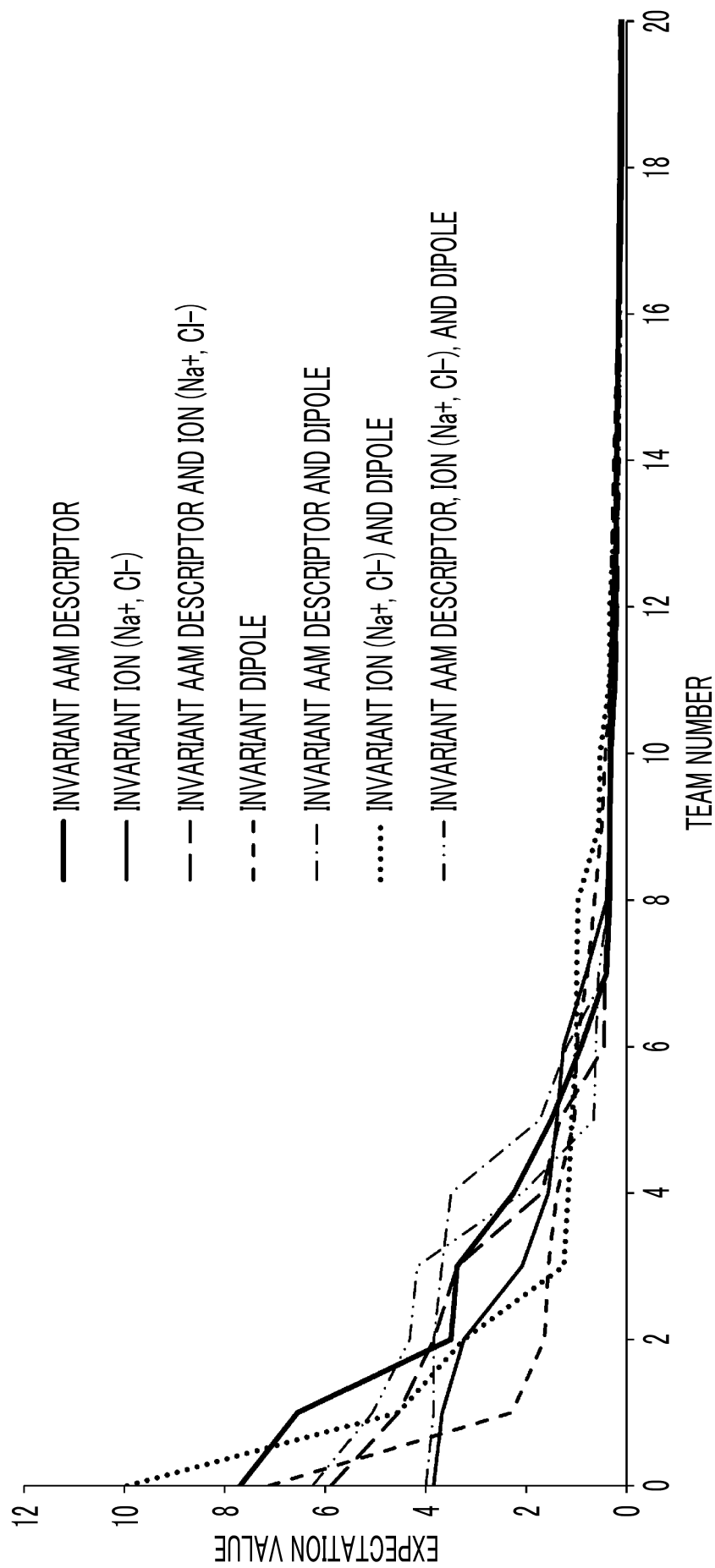


FIG. 31



25/66
FIG. 32A

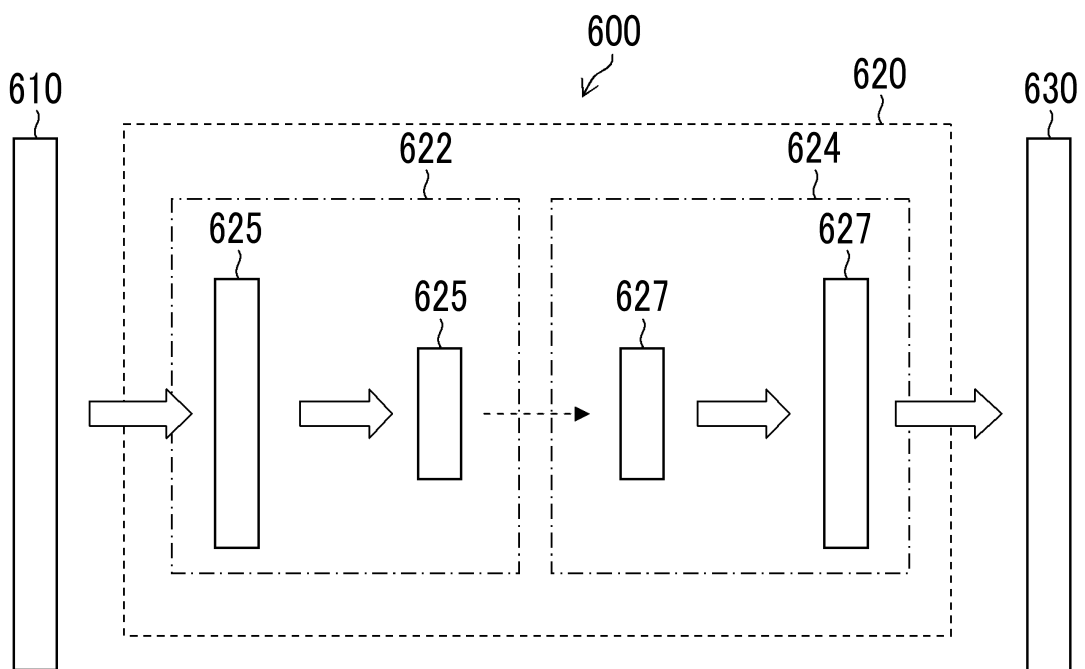


FIG. 32B

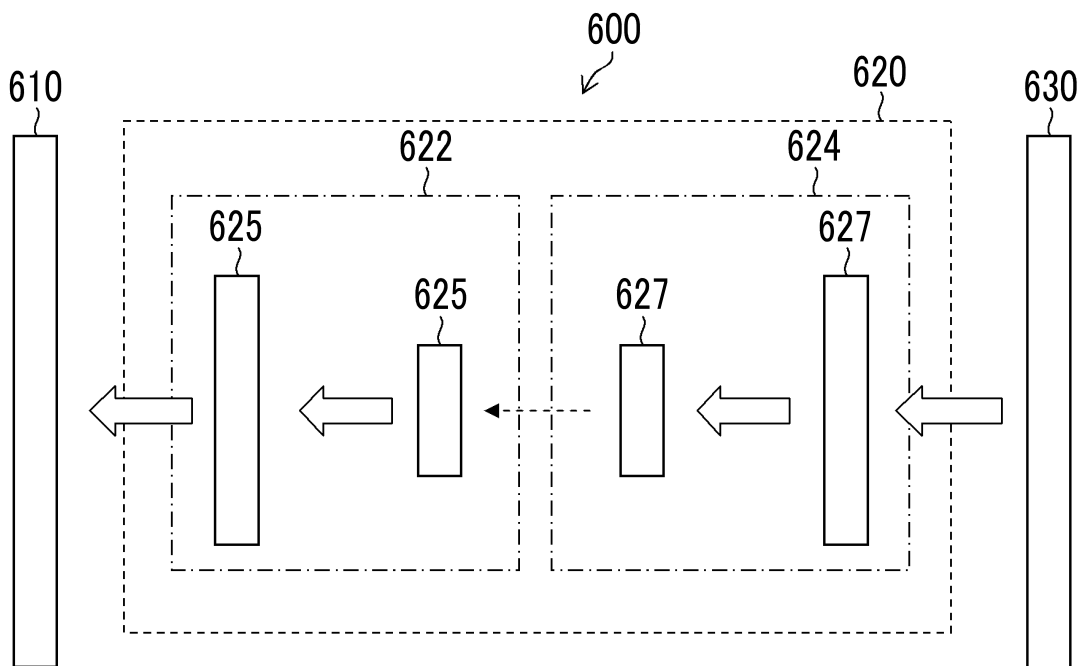


FIG. 33

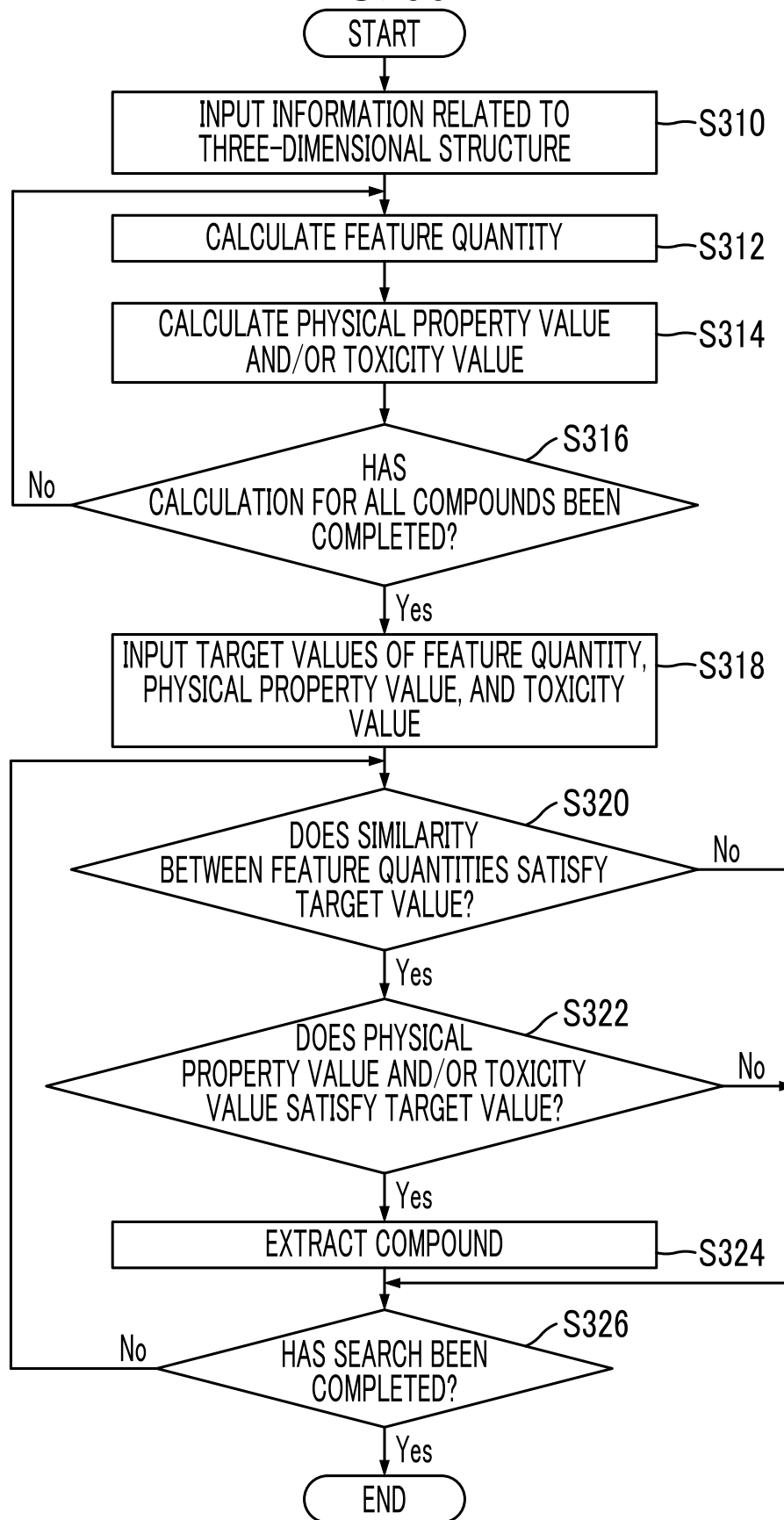


FIG. 34

103

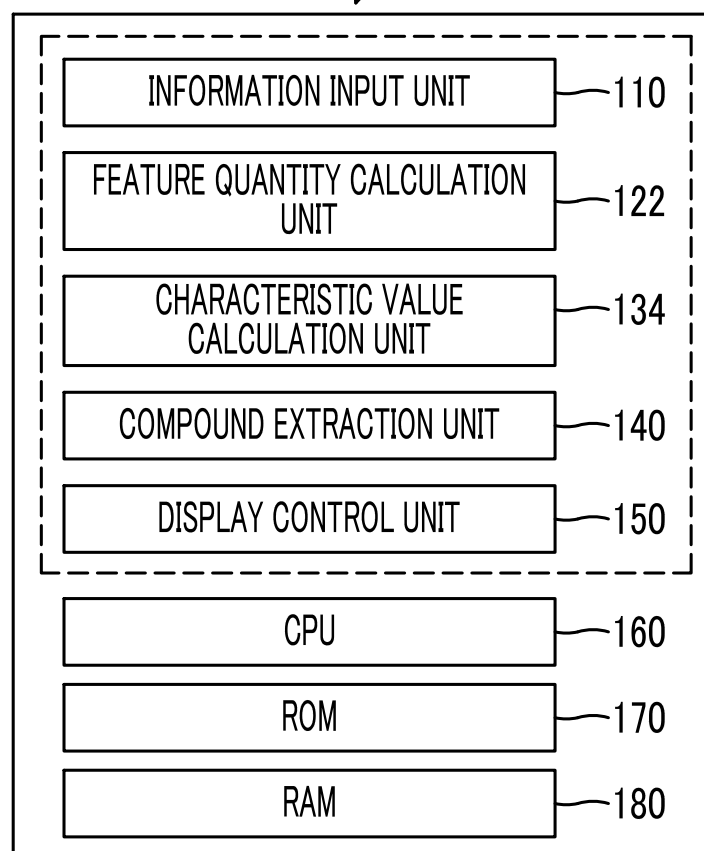
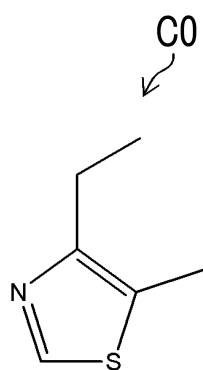
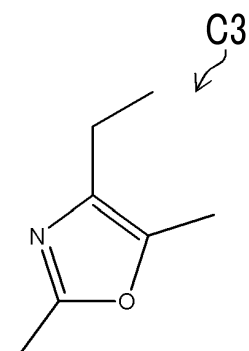
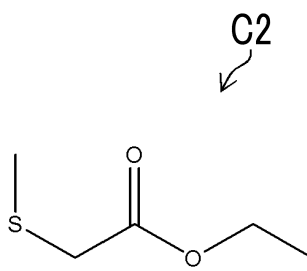
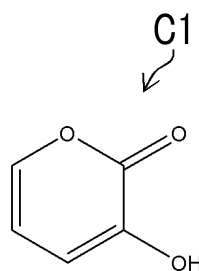


FIG. 35A

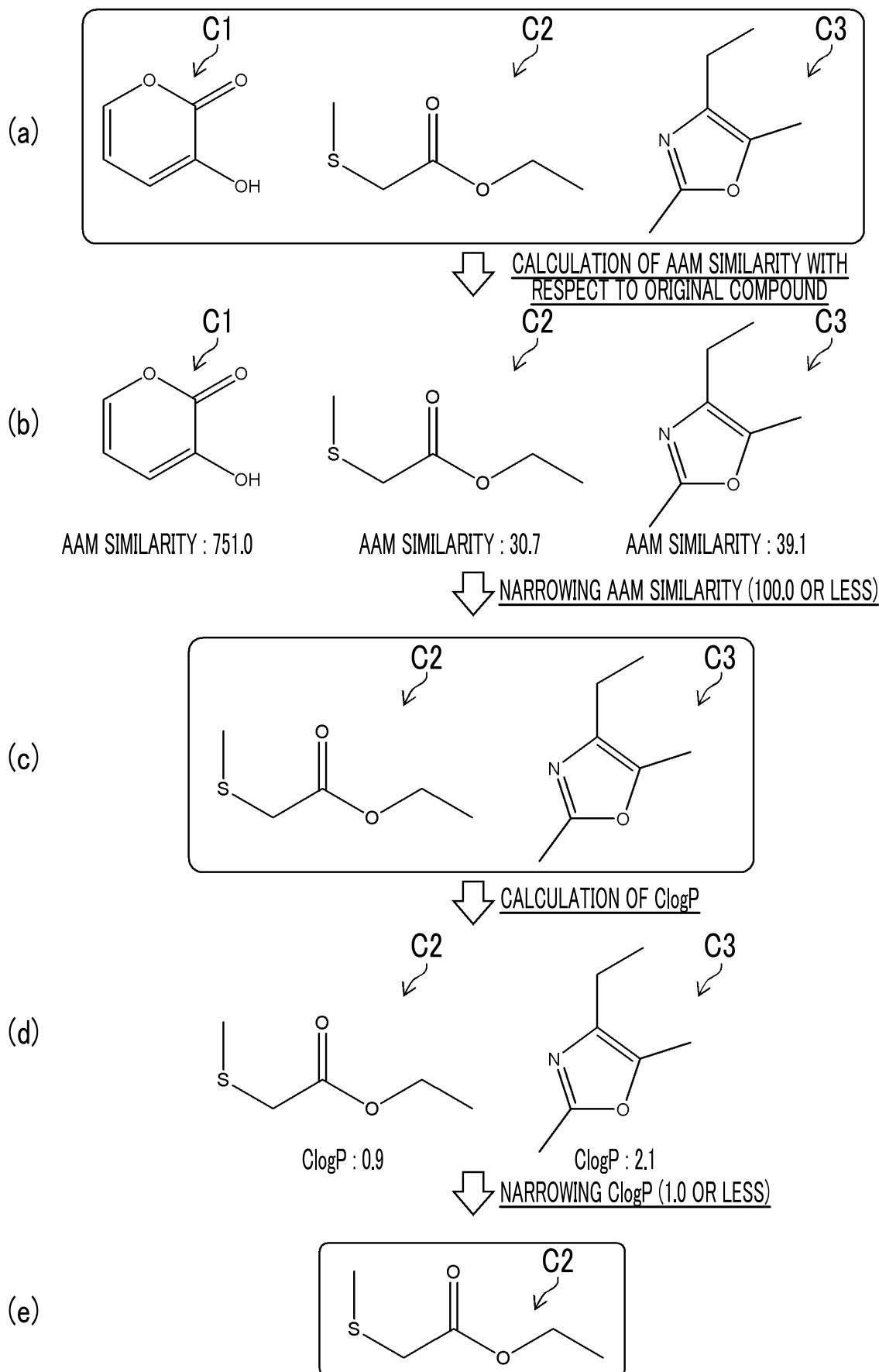


ClogP : 2.0

FIG. 35B



28/66
FIG. 36



29/66
FIG. 37

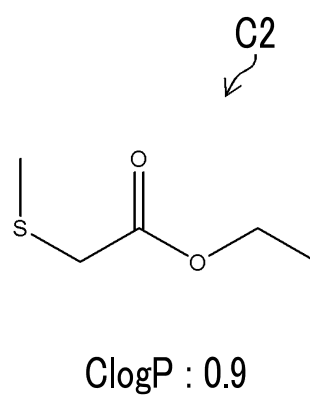
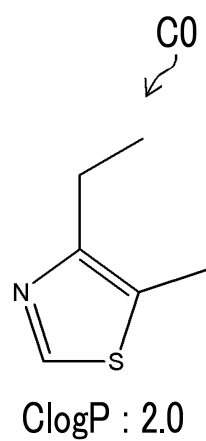
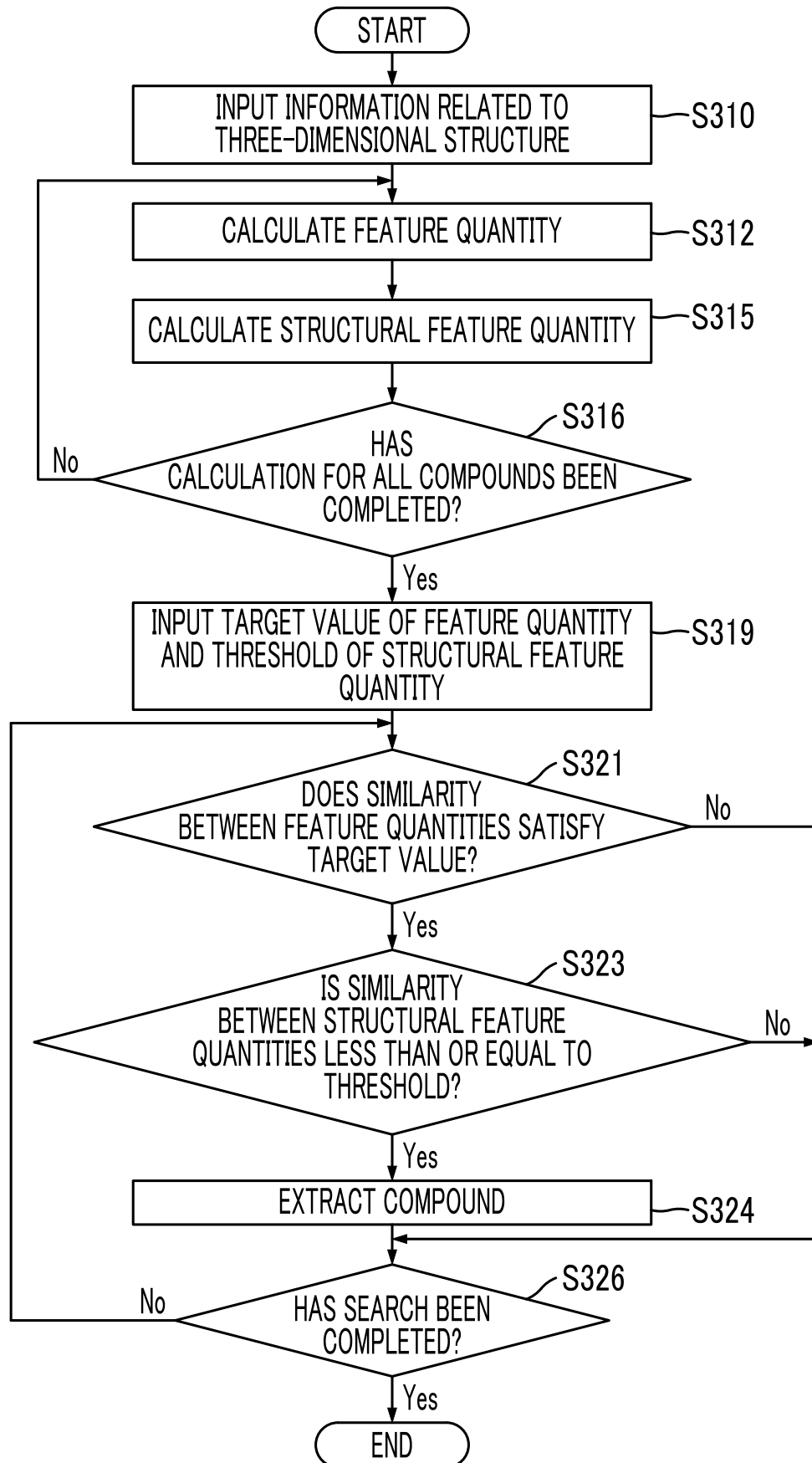


FIG. 38



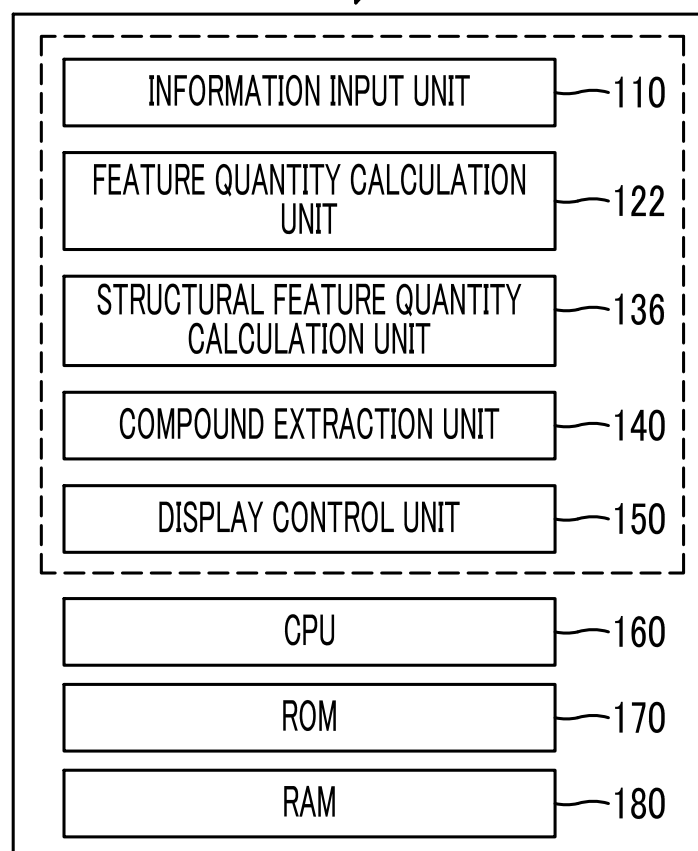


FIG. 40A

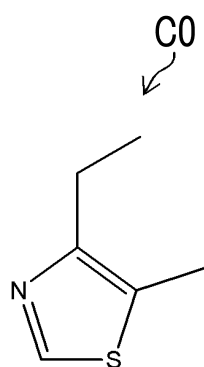
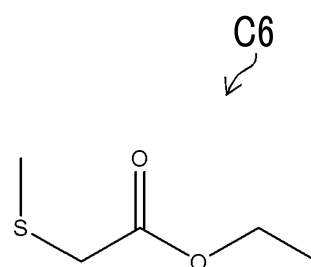
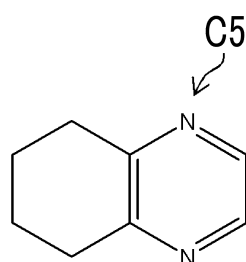
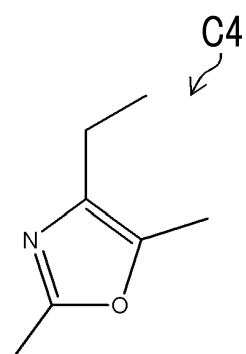
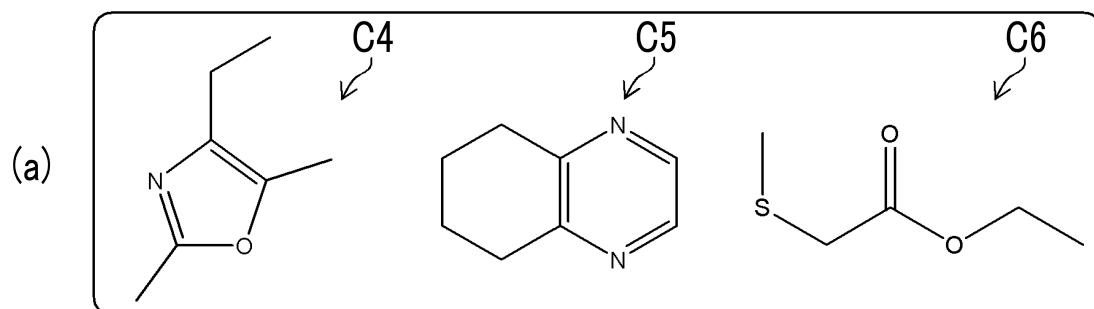


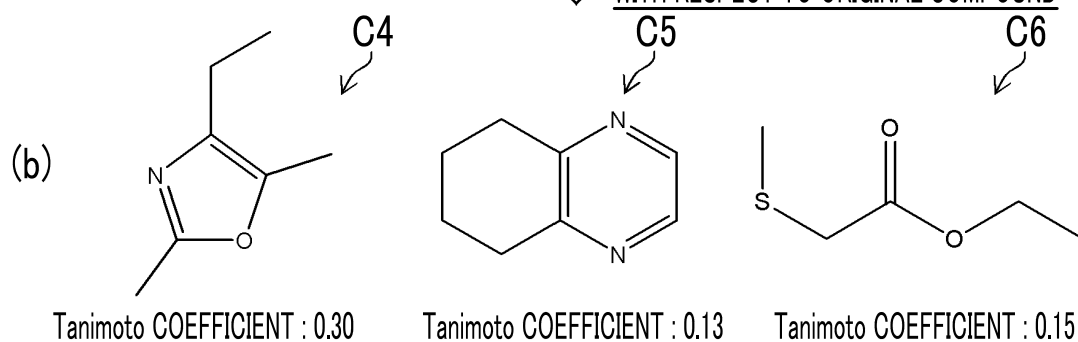
FIG. 40B



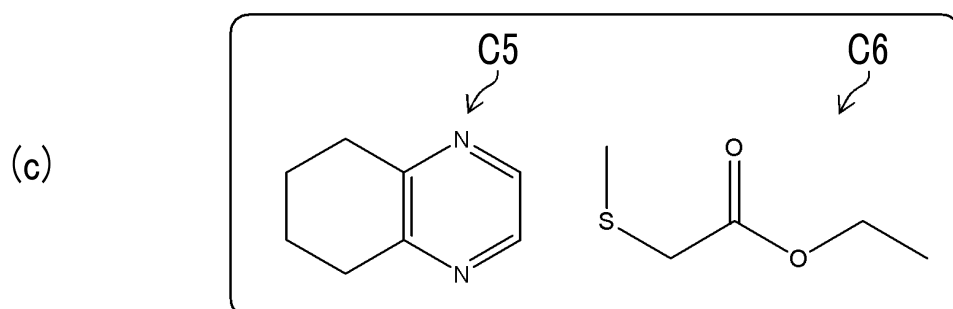
32/66
FIG. 41



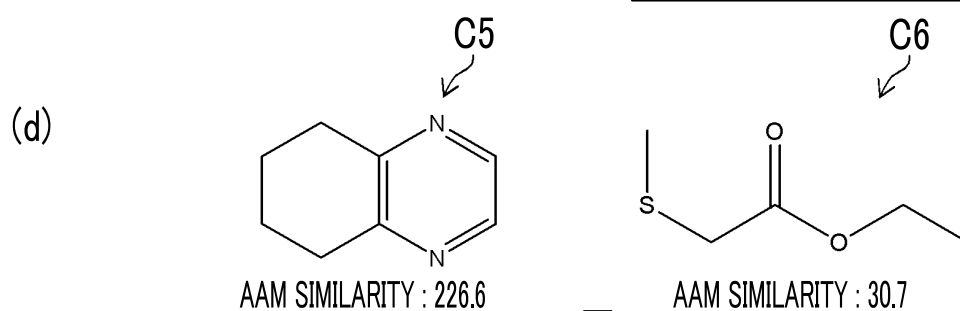
↓ CALCULATION OF Tanimoto COEFFICIENT
WITH RESPECT TO ORIGINAL COMPOUND



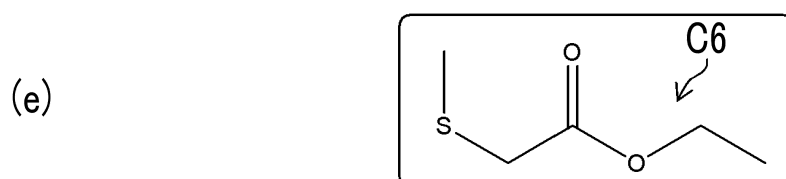
↓ NARROWING Tanimoto COEFFICIENT (0.2 OR LESS)



↓ CALCULATION OF AAM SIMILARITY WITH
RESPECT TO ORIGINAL COMPOUND



↓ NARROWING AAM SIMILARITY (100.0 OR LESS)



33/66
FIG. 42

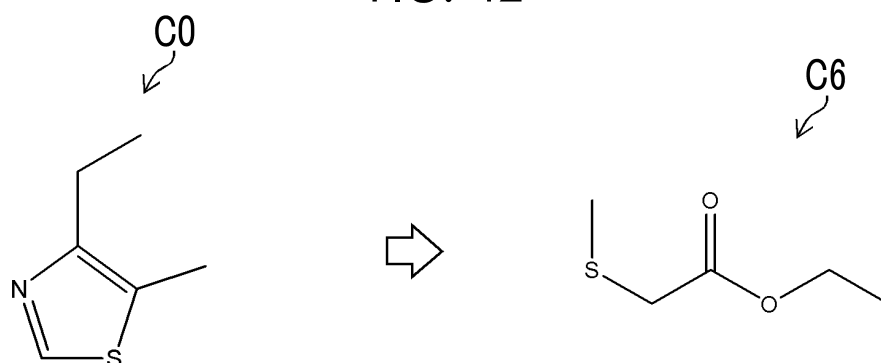


FIG. 43A

	COMPOUND A	COMPOUND B
CASE 1		
CASE 2		
CASE 3		

FIG. 43B

	SIMILARITY DISTANCE (AAM DESCRIPTOR)	COMPOUND A ClogP	COMPOUND B ClogP
CASE 1	30.7	1.04	1.96
CASE 2	44.7	1.64	3.40
CASE 3	40.0	0.56	2.10

34/66

FIG. 44A

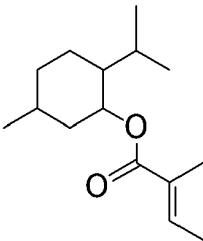
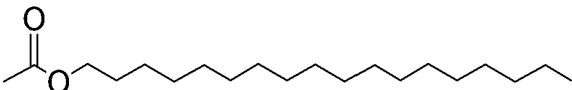
COMPOUND A	COMPOUND B
	

FIG. 44B

	SIMILARITY DISTANCE (AAM DESCRIPTOR)	COMPOUND A ClogP	COMPOUND B ClogP
	12418.5	5.63	9.18

FIG. 45

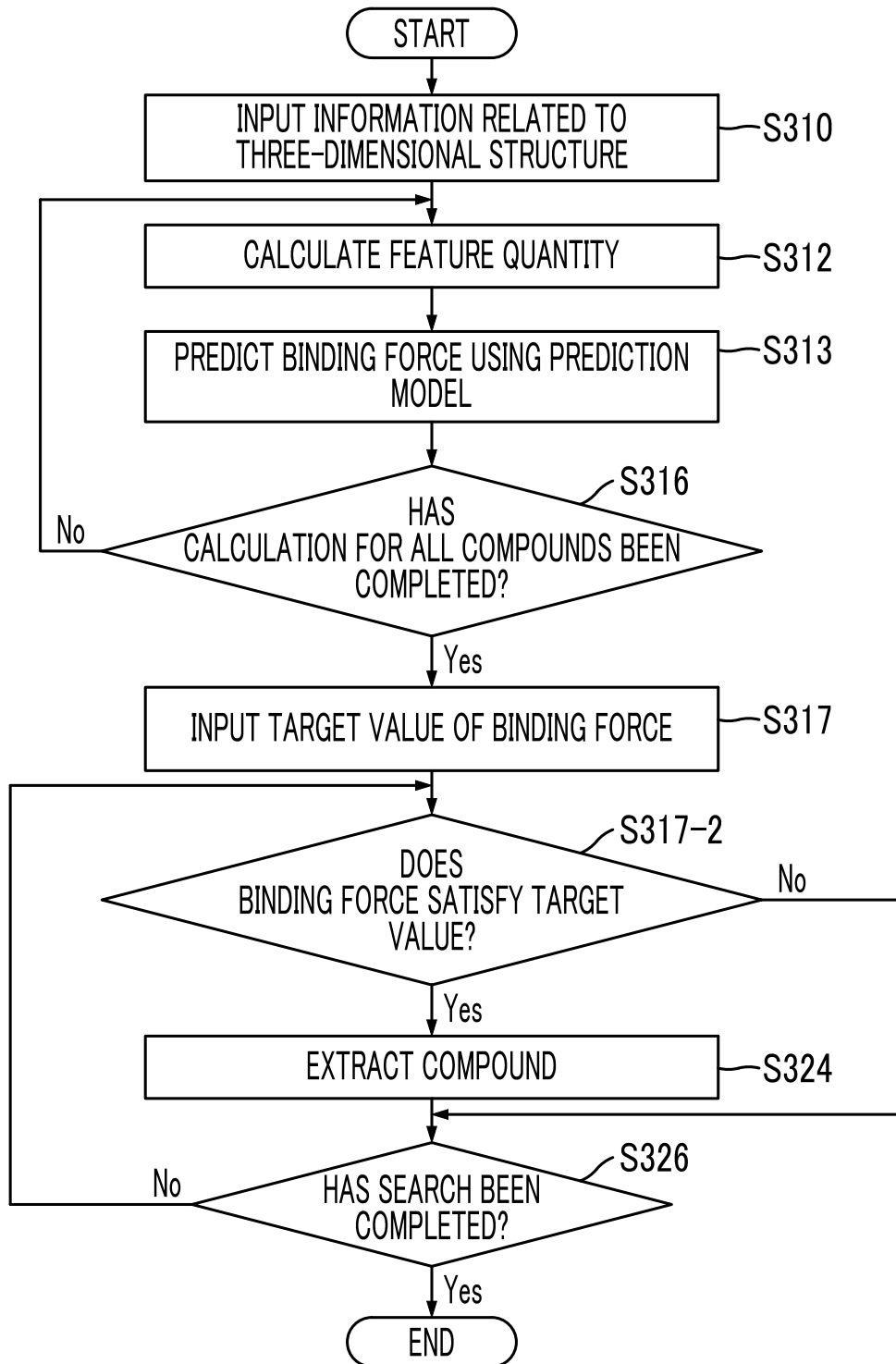


FIG. 46

105
↙

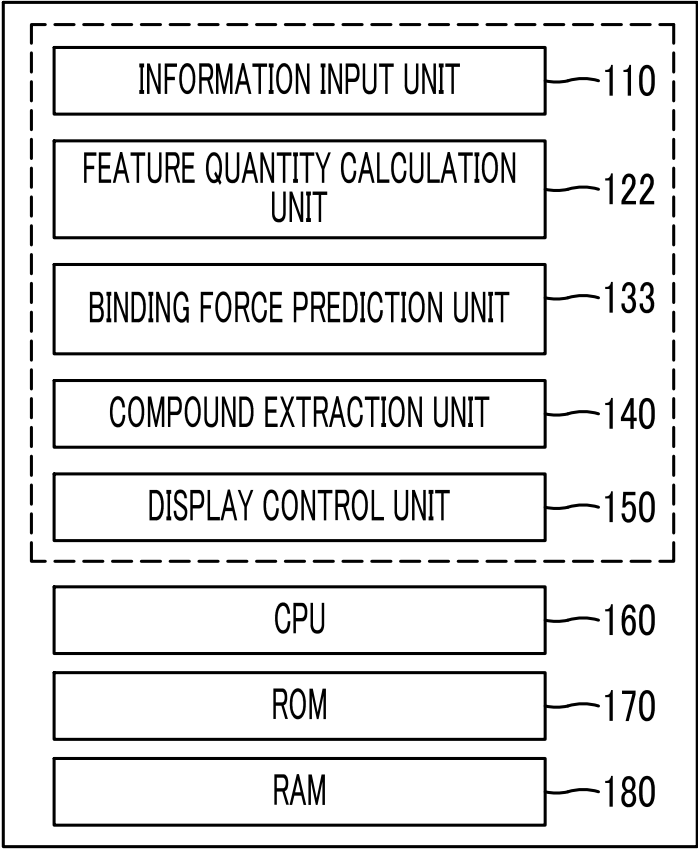


FIG. 47

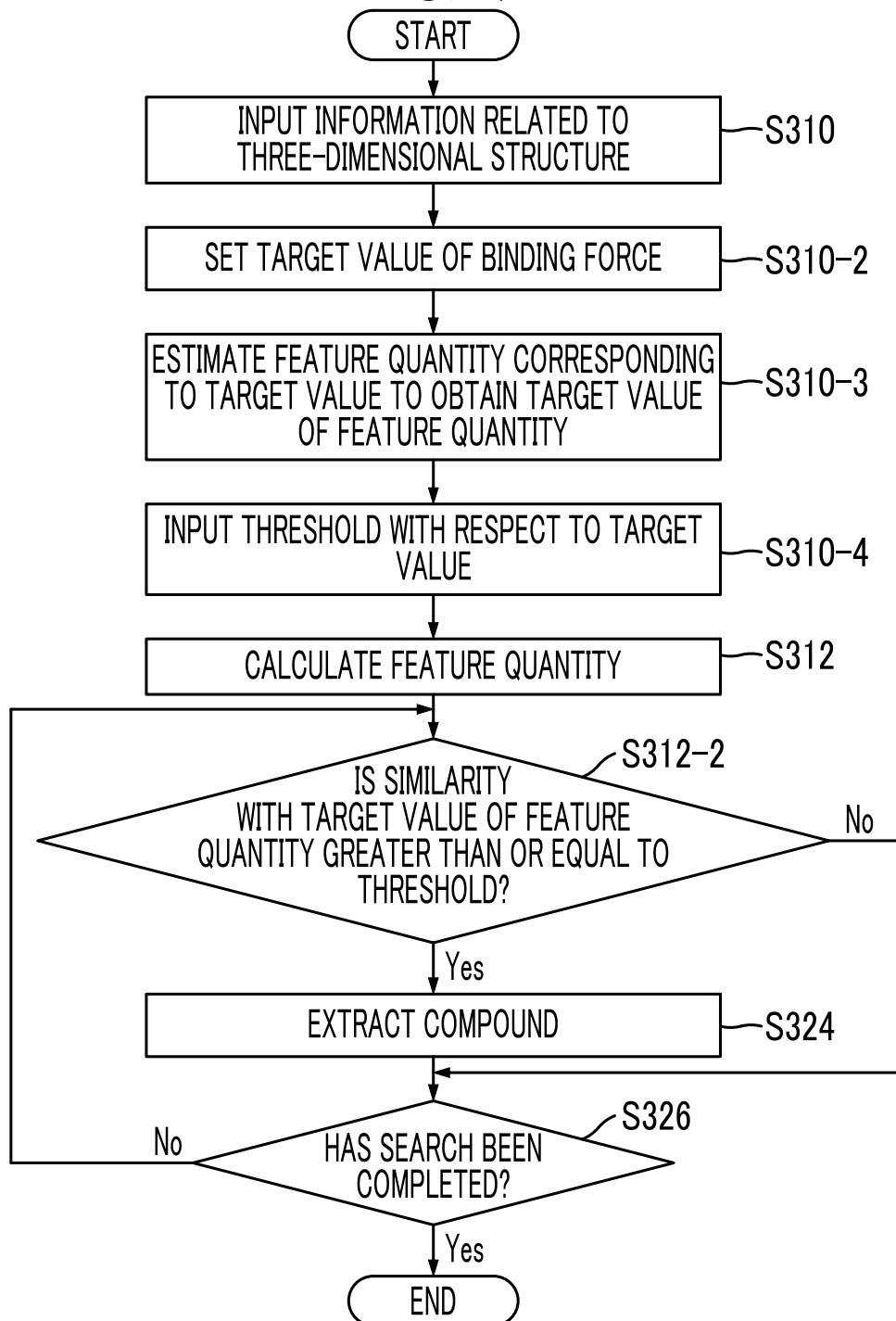


FIG. 48

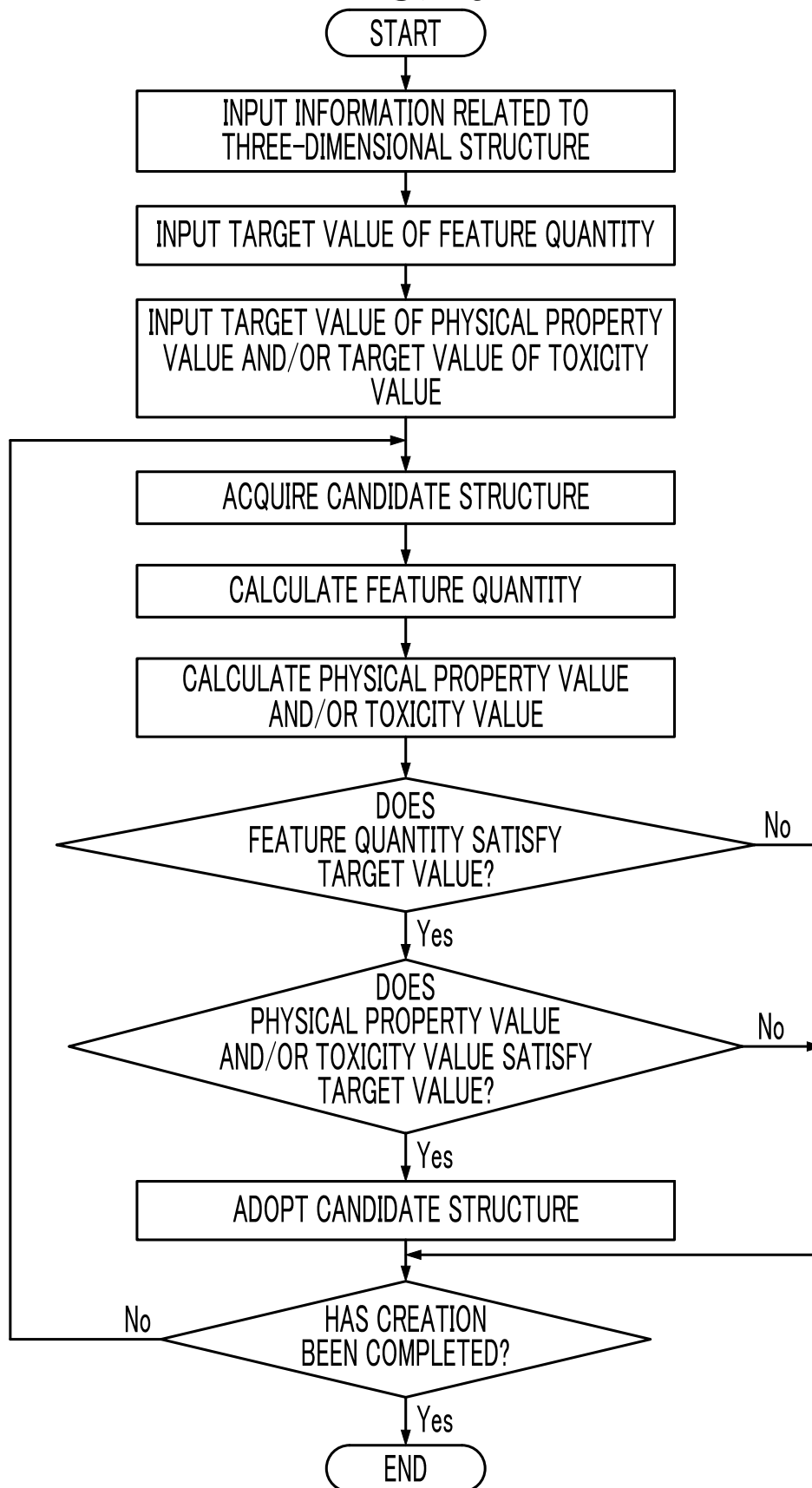


FIG. 49

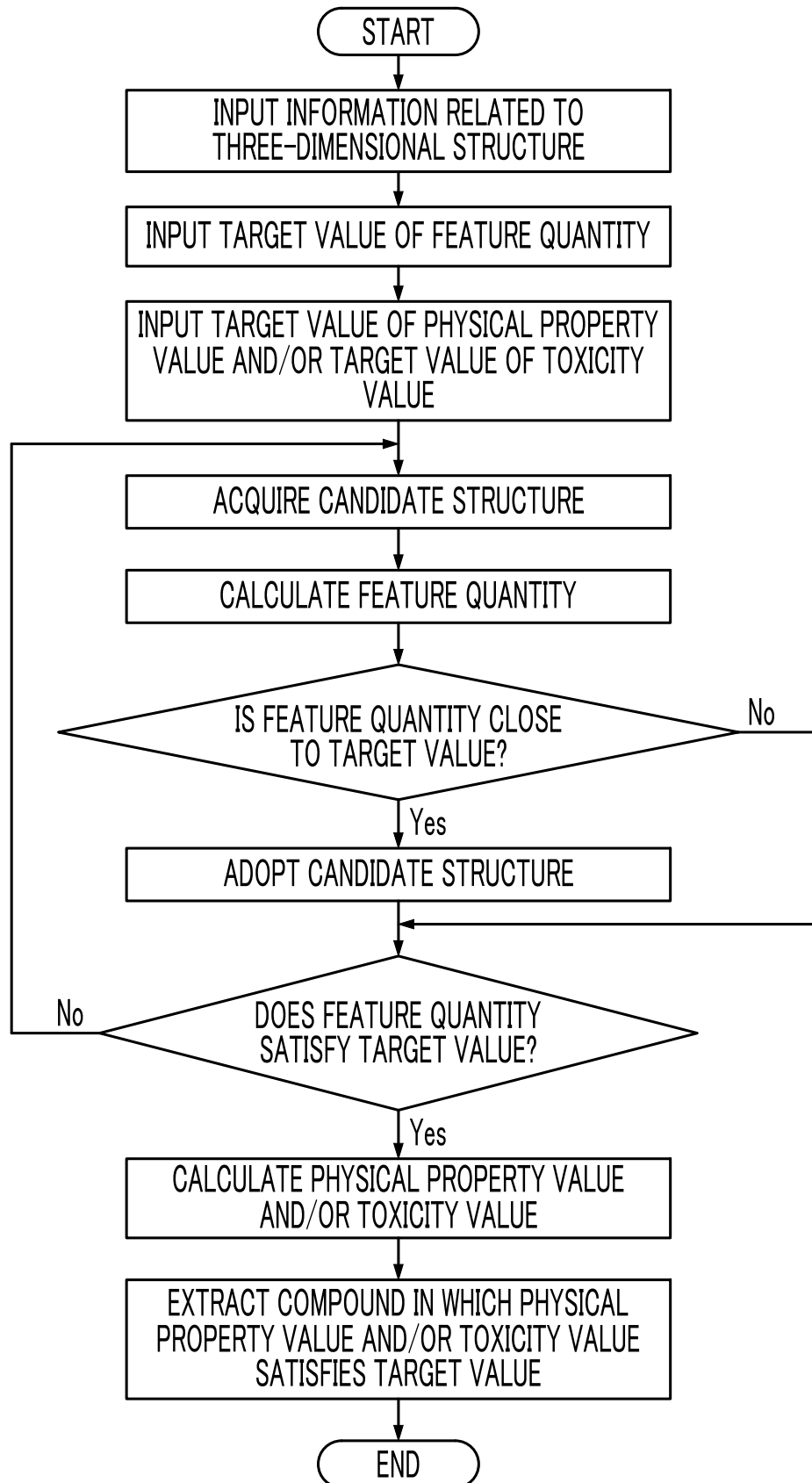


FIG. 50

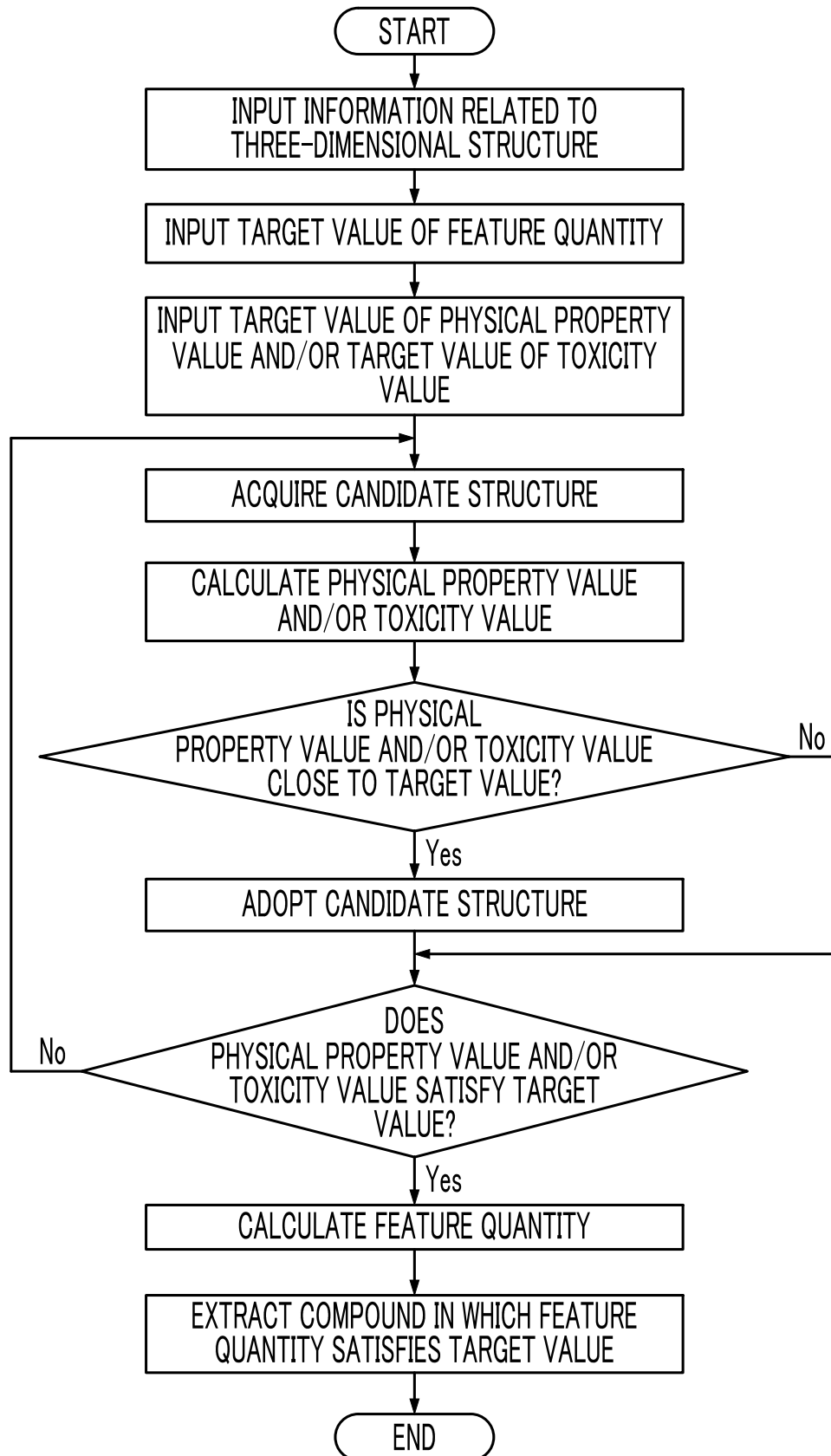


FIG. 51

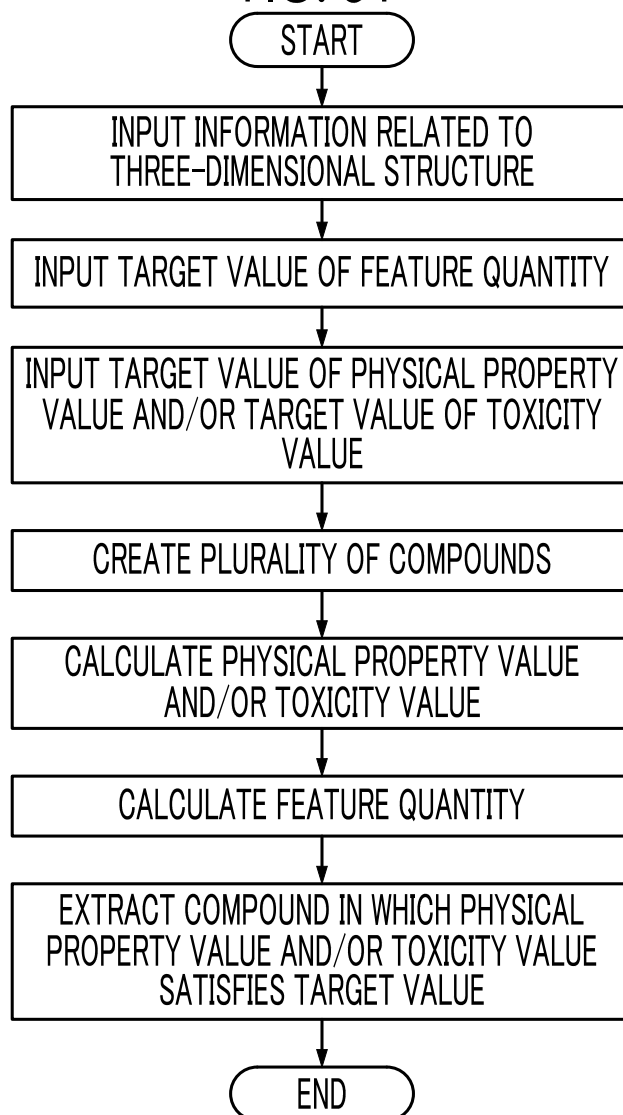


FIG. 52

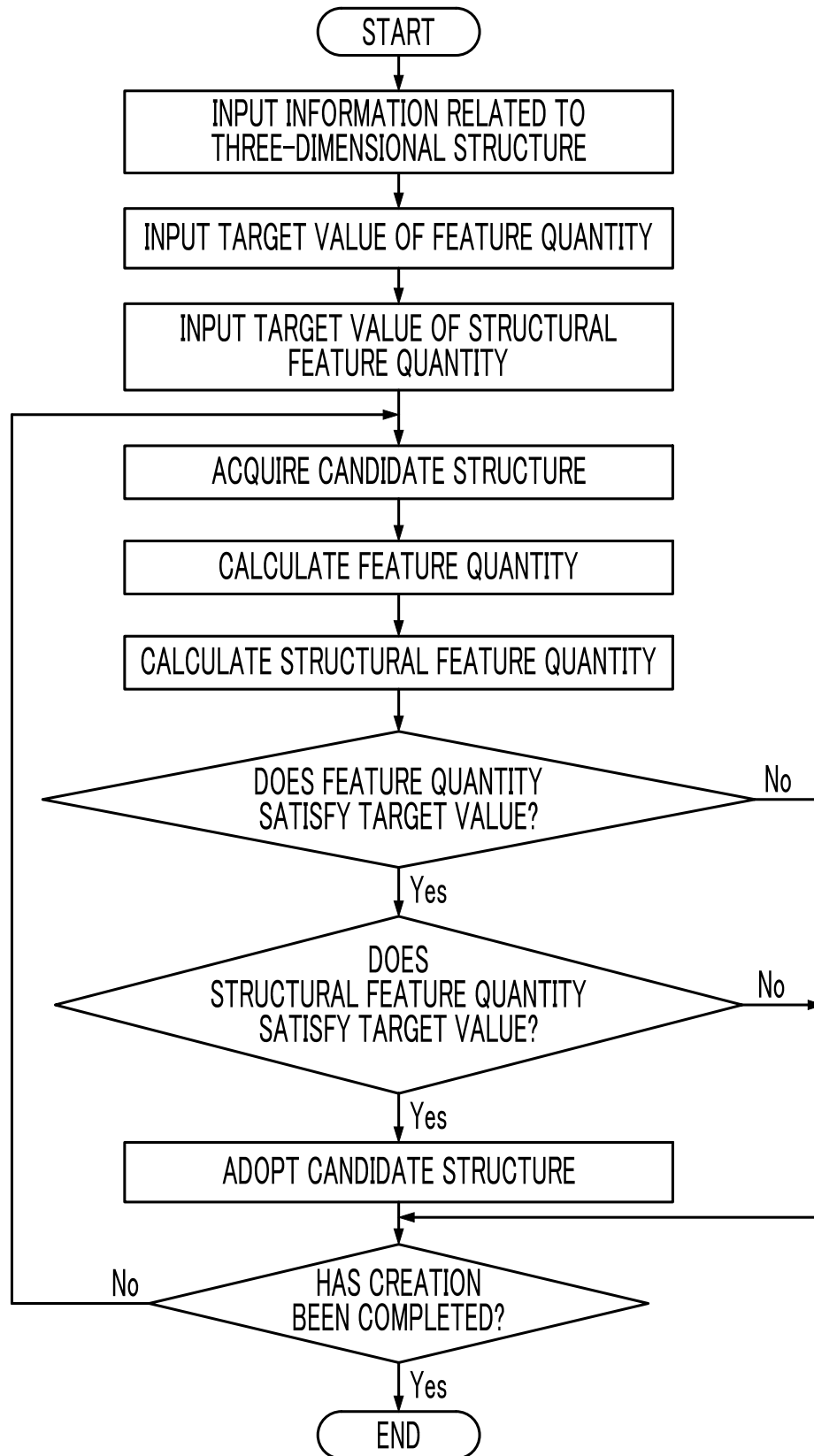


FIG. 53

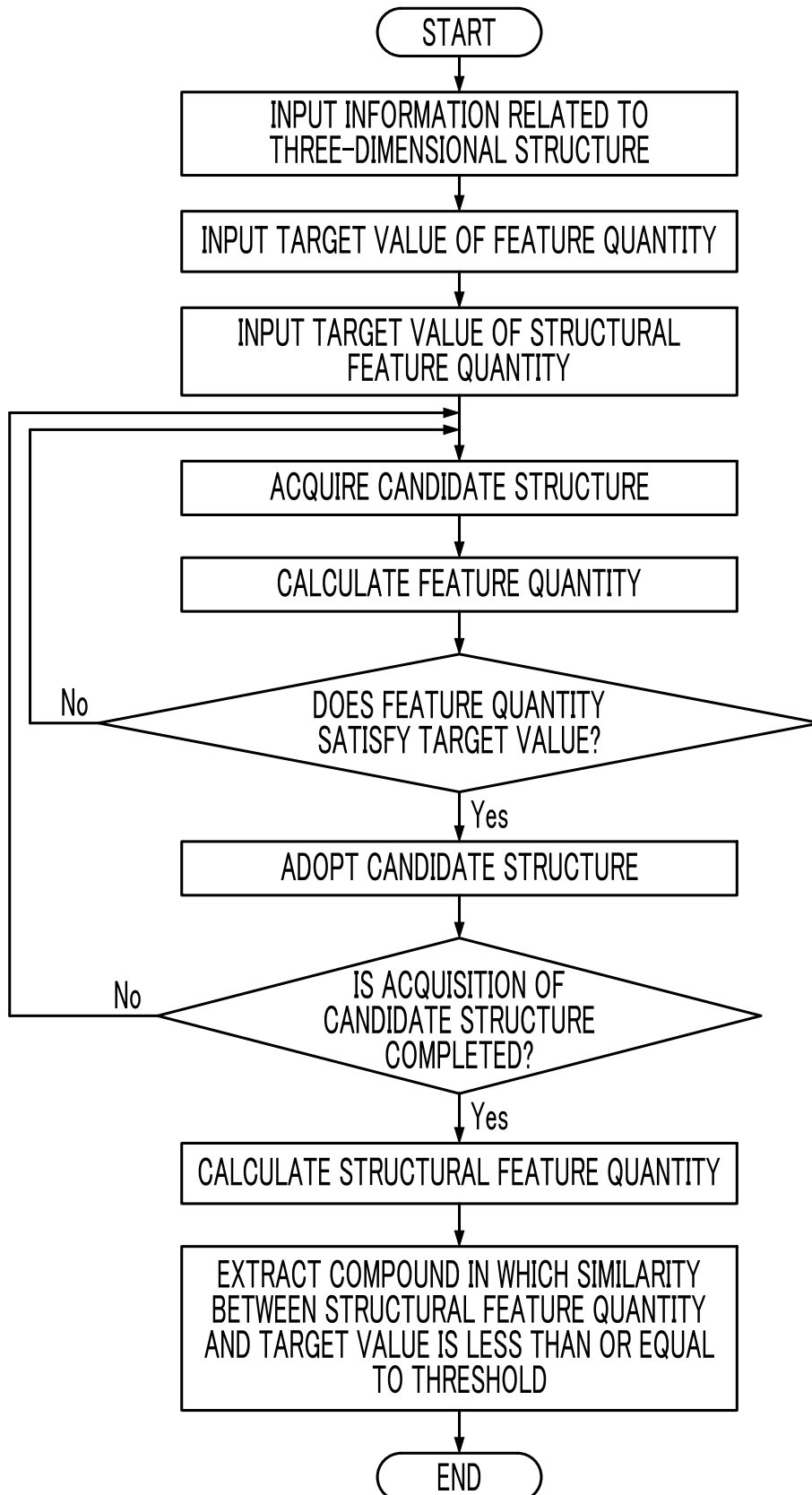


FIG. 54

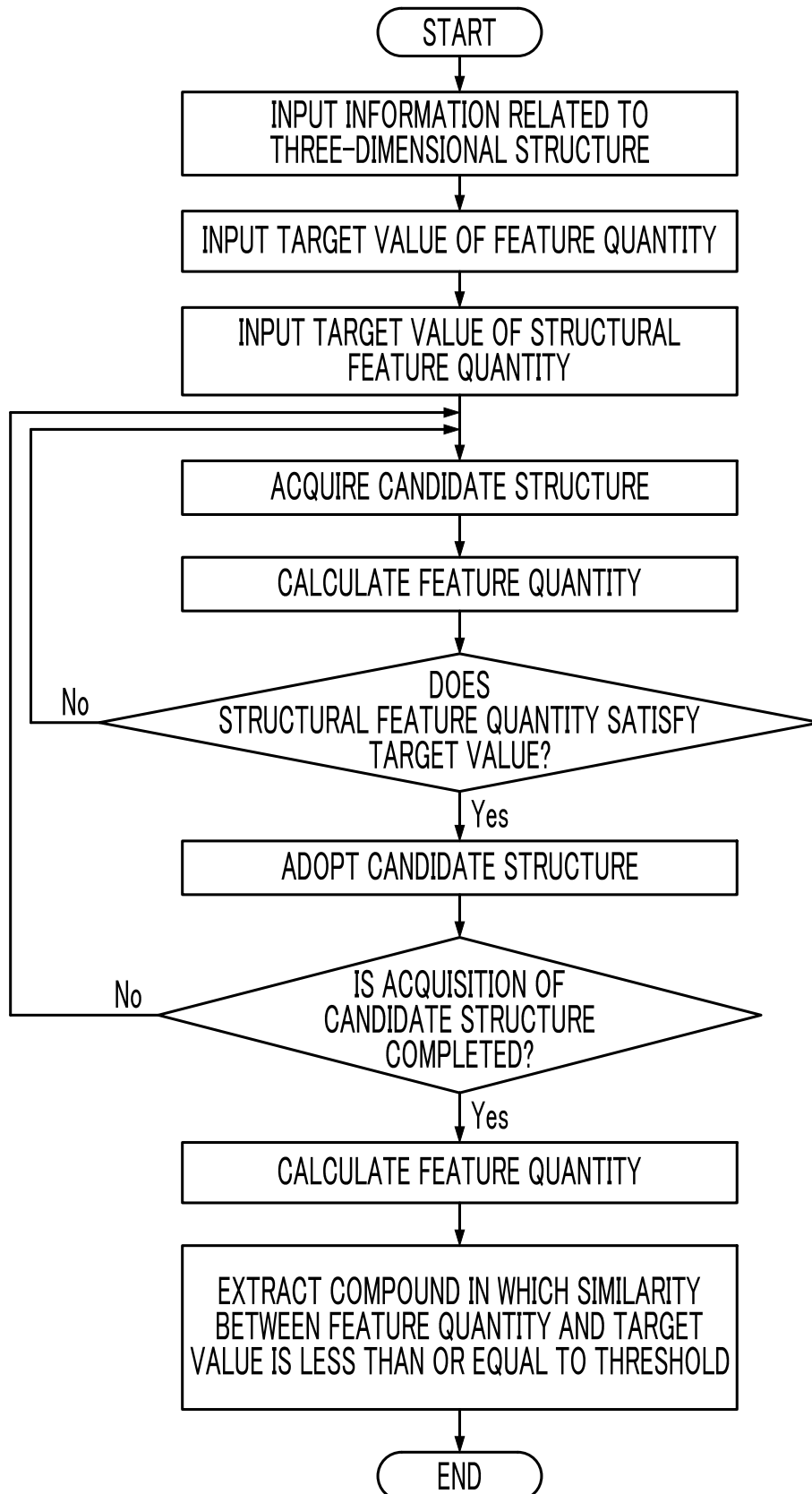


FIG. 55

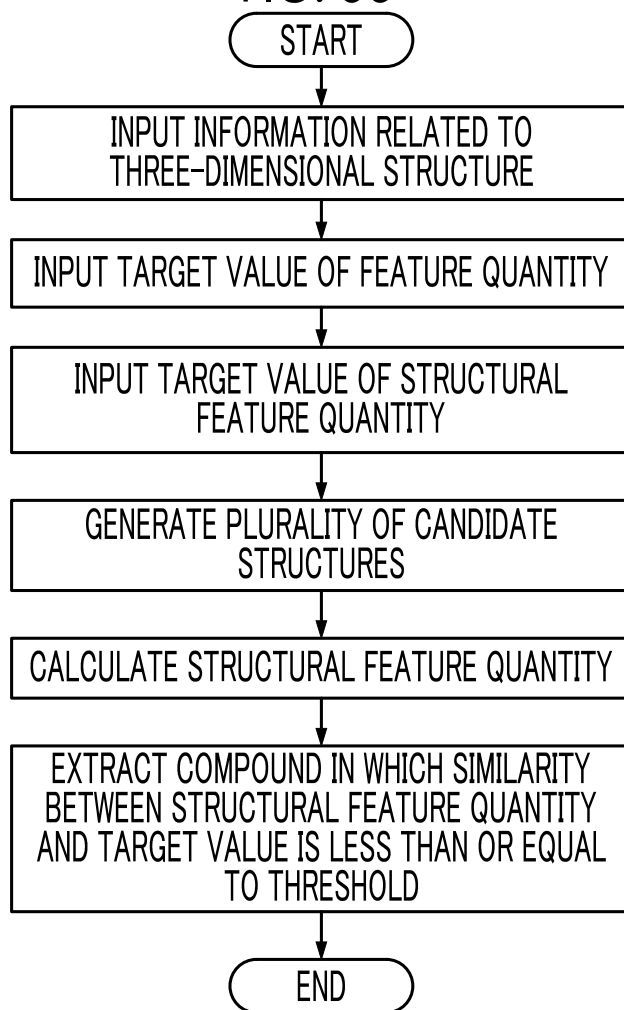


FIG. 56

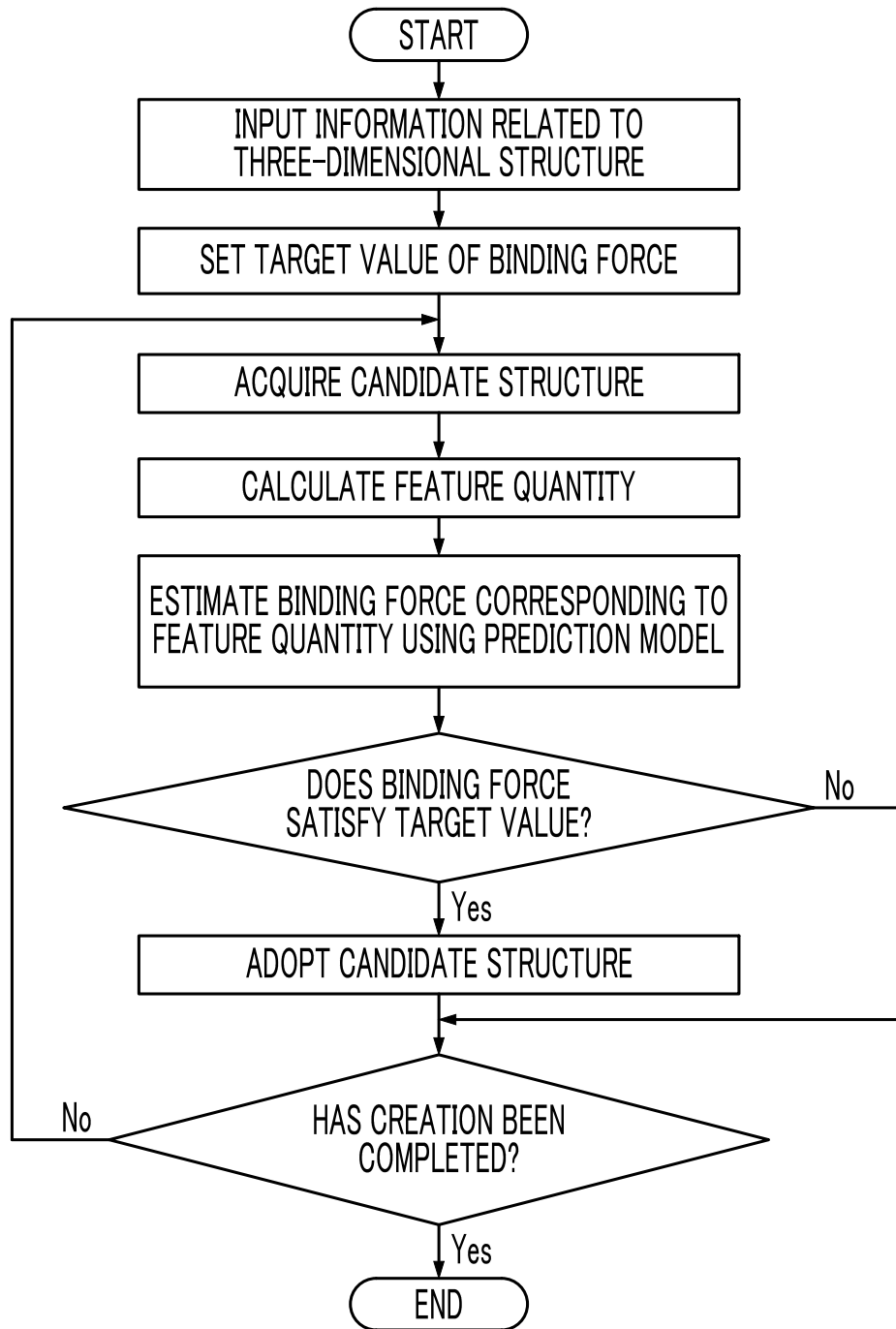


FIG. 57

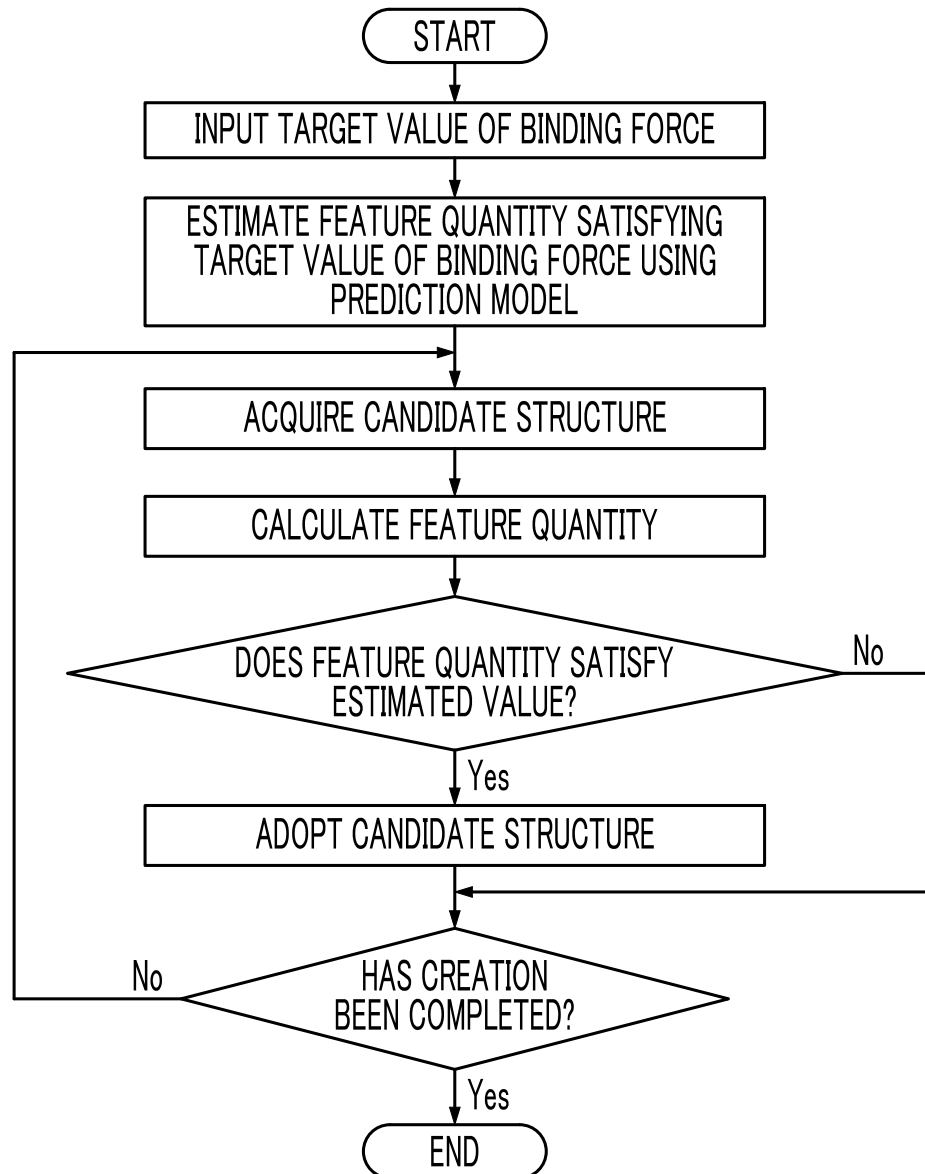


FIG. 58

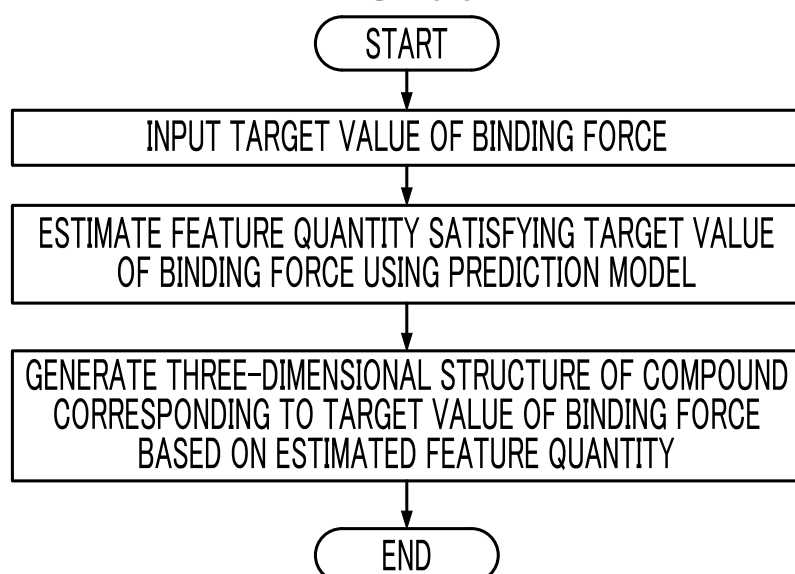


FIG. 59

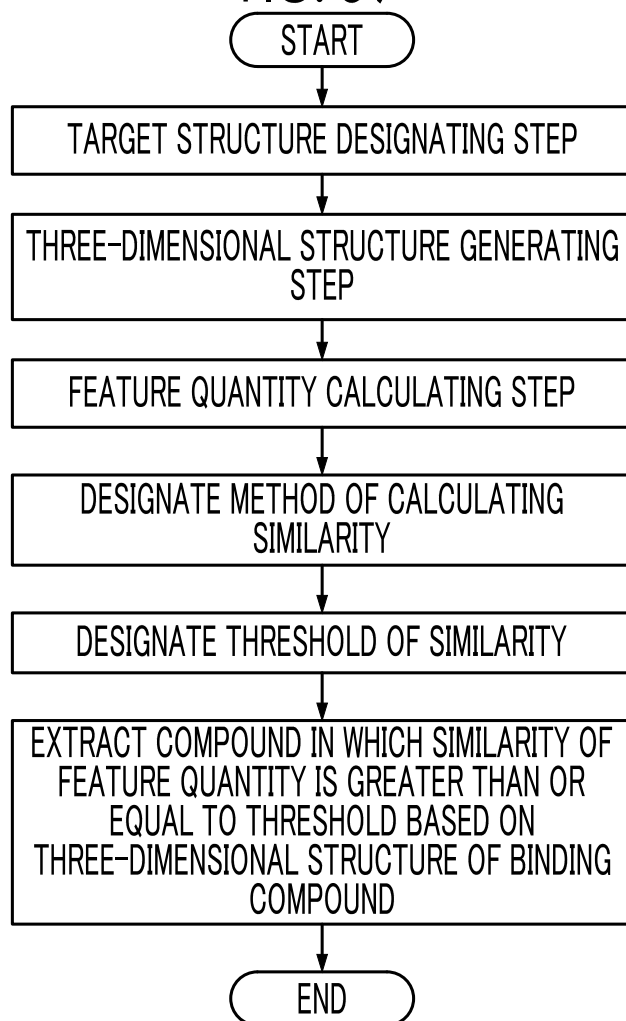


FIG. 60

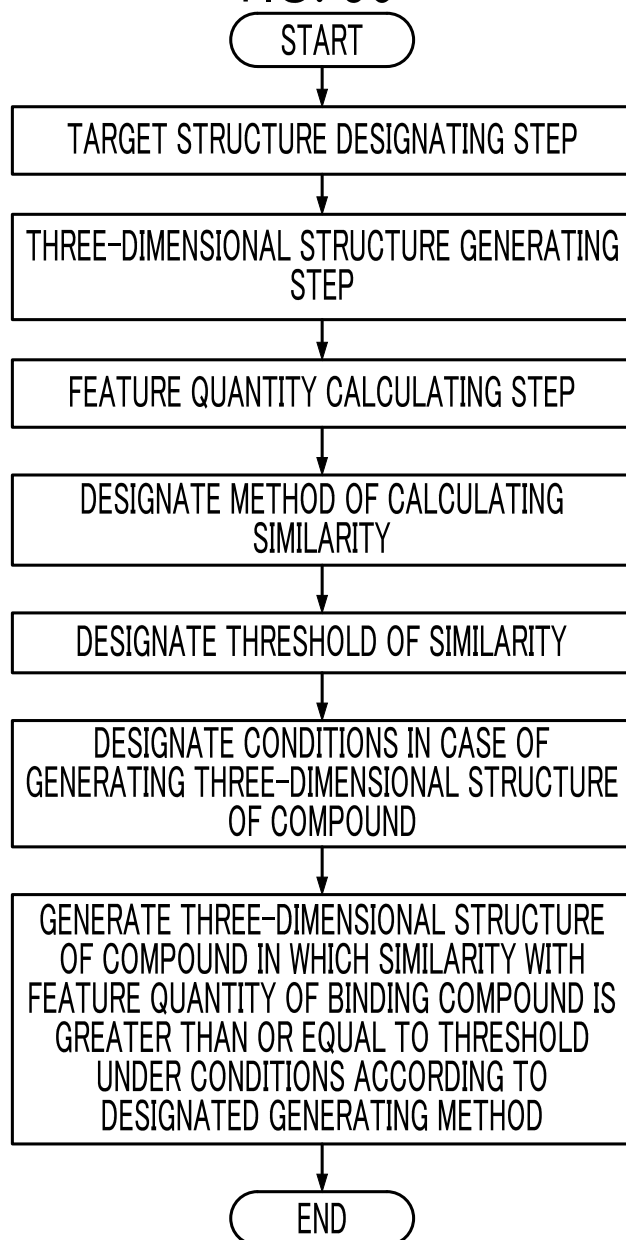


FIG. 61

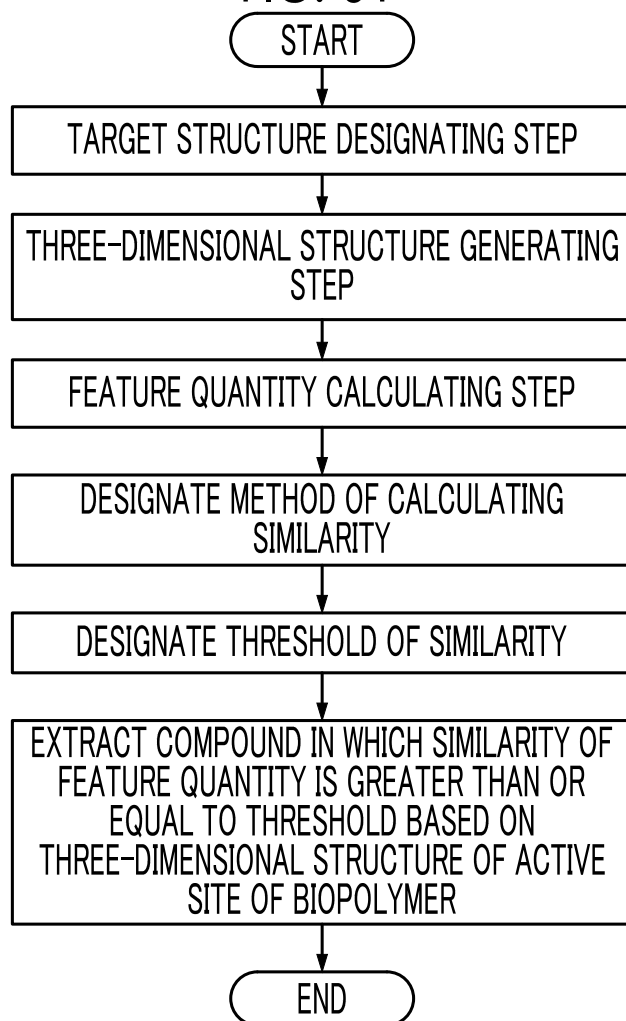


FIG. 62

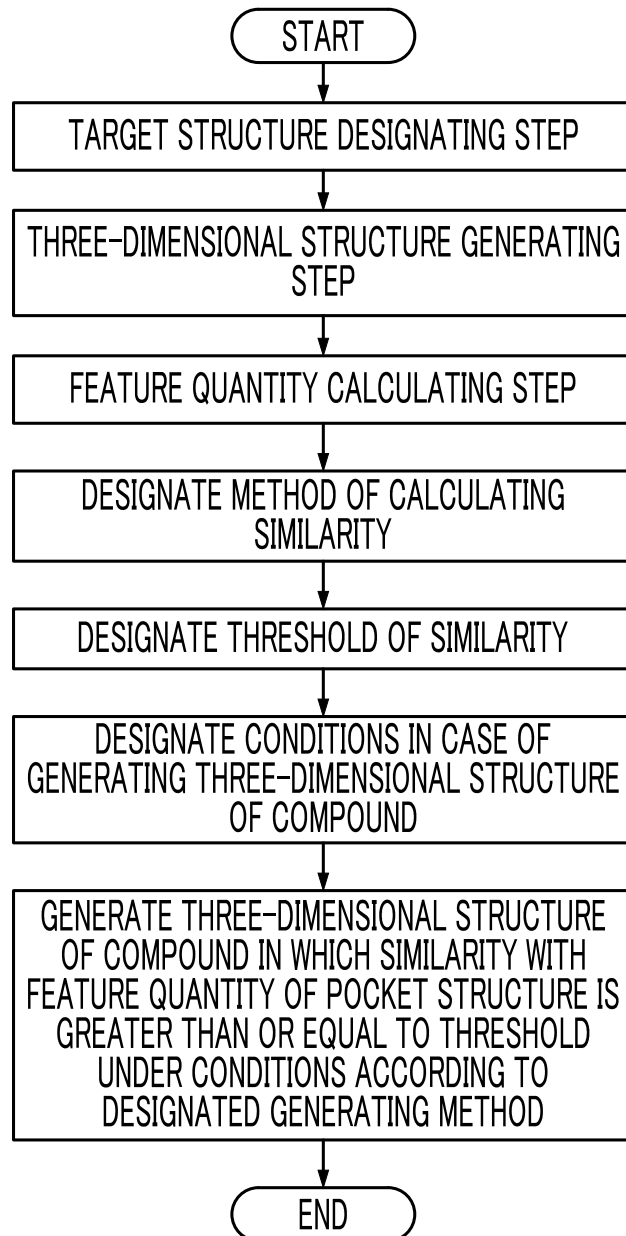


FIG. 63

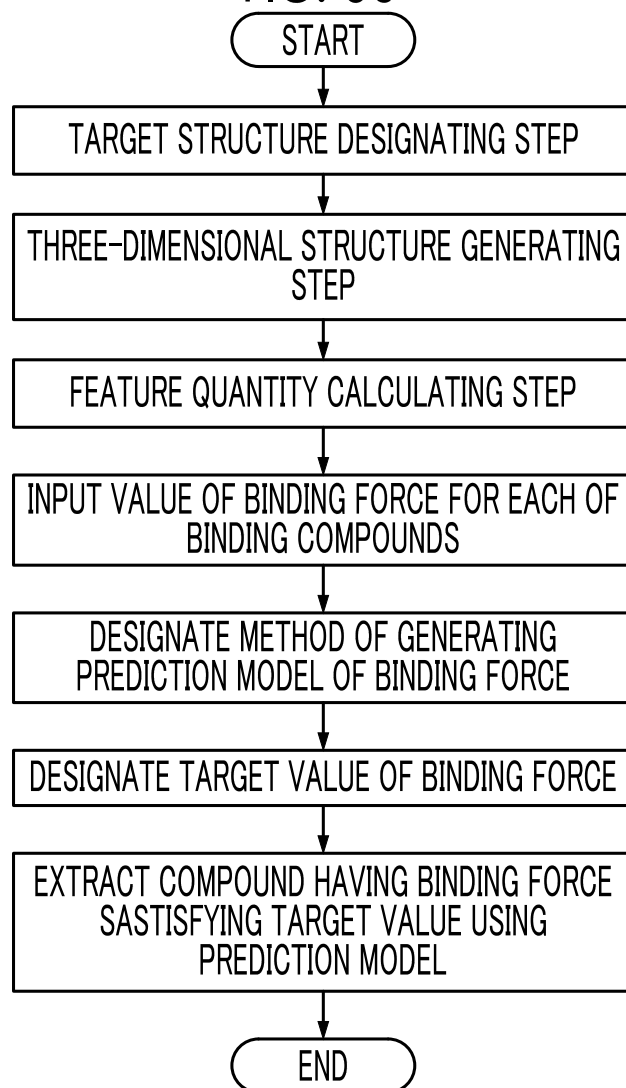


FIG. 64

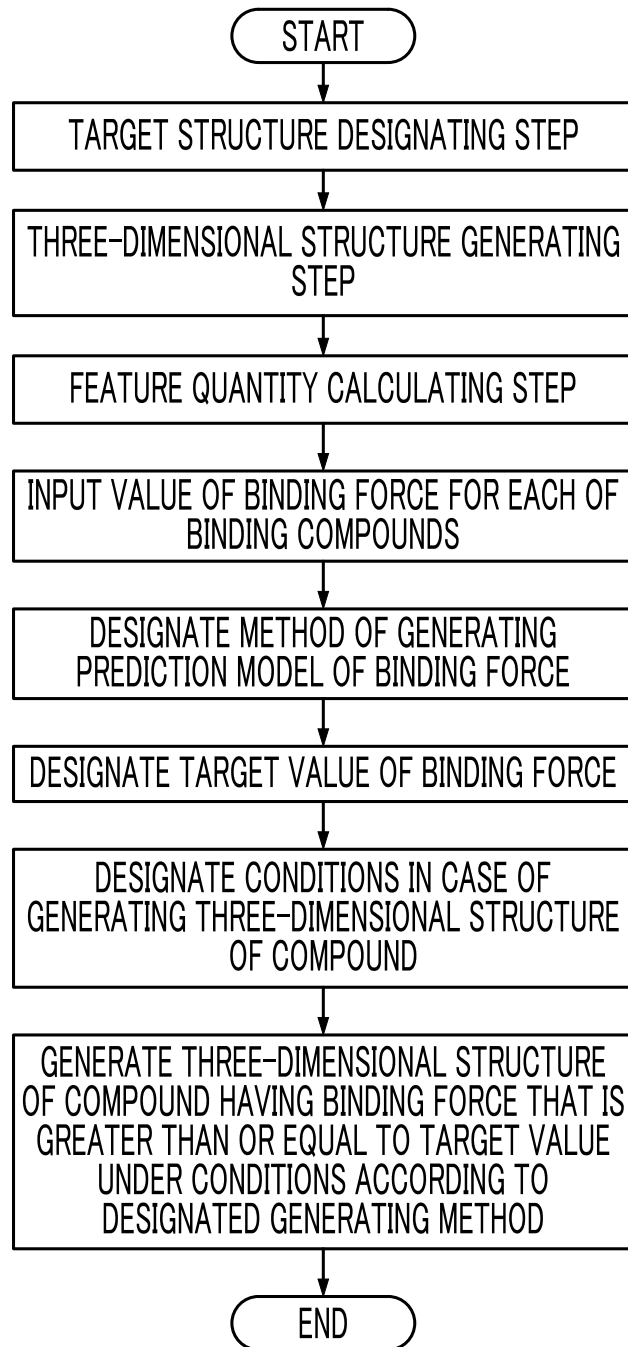


FIG. 65

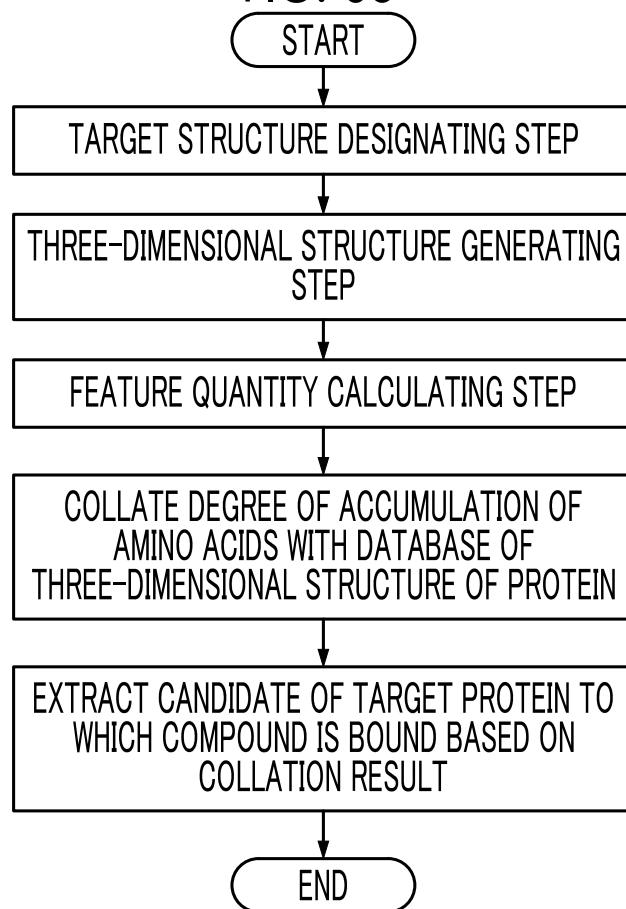


FIG. 66

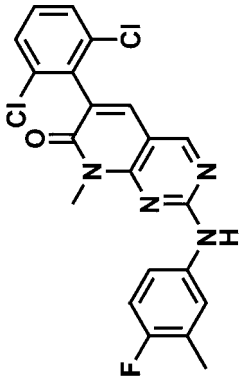
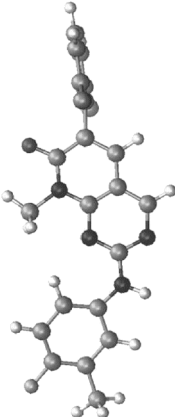
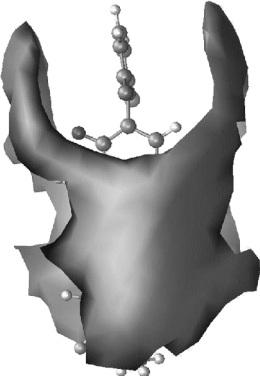
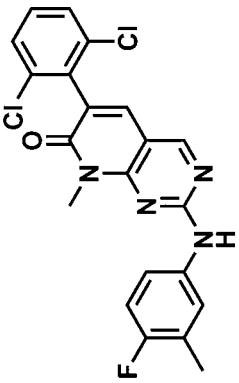
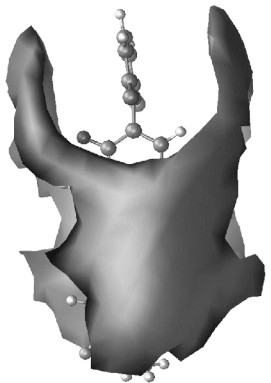
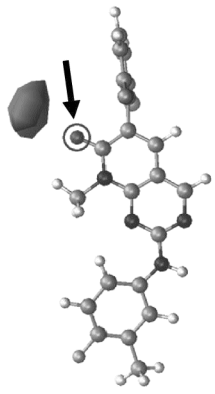
COMPOUND				FEATURE QUANTITY (DEGREE OF ACCUMULATION OF EACH AMINO ACID)	
NAME	STRUCTURAL FORMULA	THREE-DIMENSIONAL STRUCTURE	ALANINE		
lig001				...	
lig002	...	...	...	...	

FIG. 67

NAME	STRUCTURAL FORMULA	DEGREE OF ACCUMULATION OF AMINO ACIDS	SHARE OF SELECTED ATOM GROUP IN DEGREE OF ACCUMULATION OF AMINO ACIDS
lig001			

57/66
FIG. 68

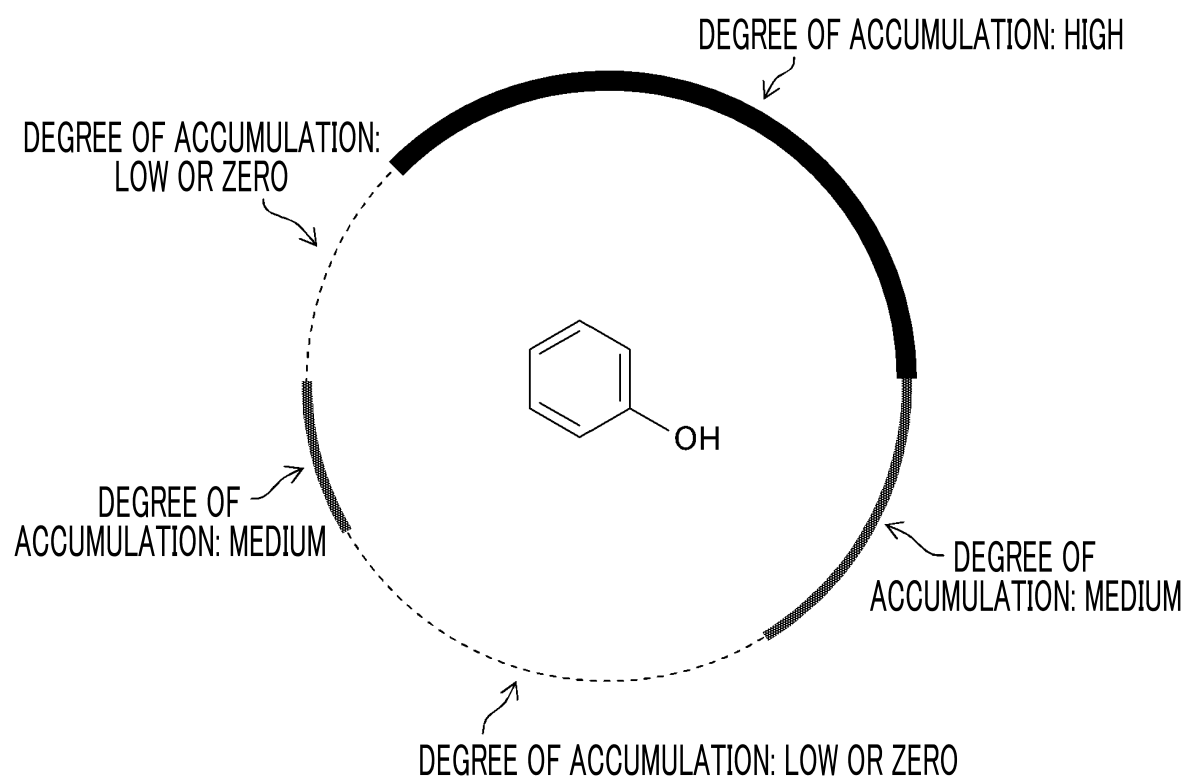


FIG. 69B

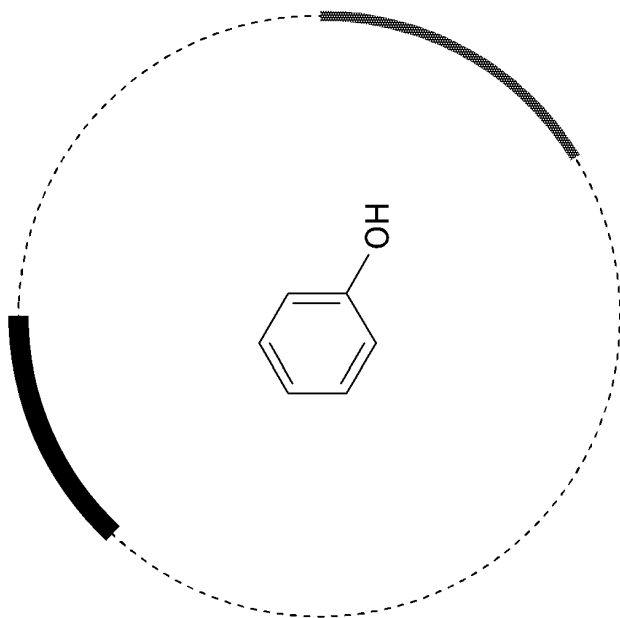
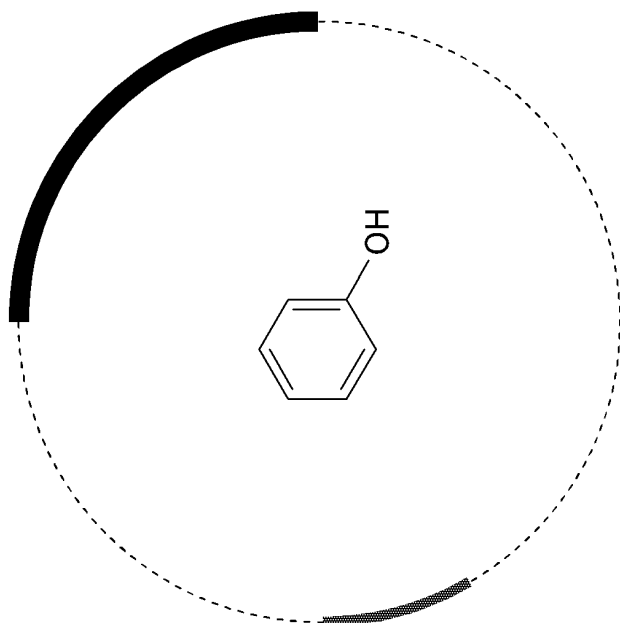


FIG. 69A



59/66
FIG. 70

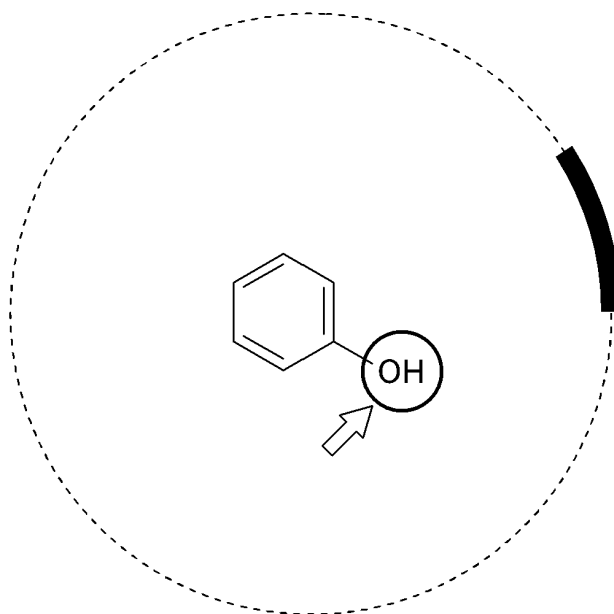
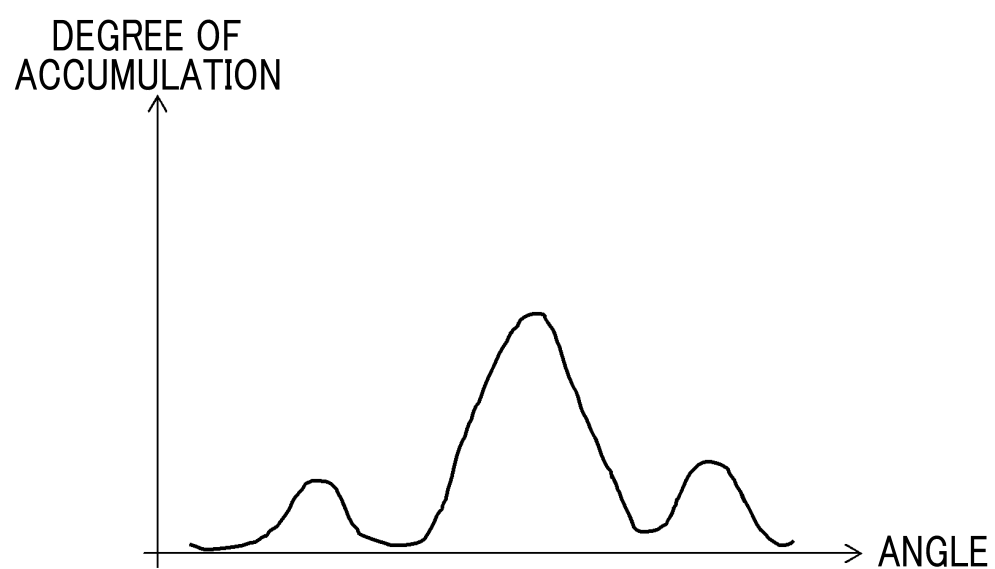
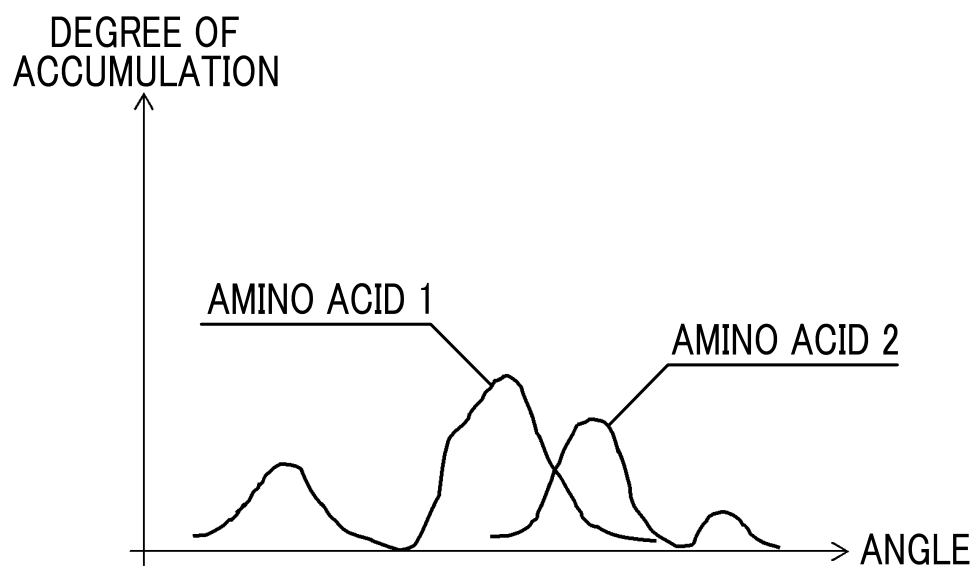


FIG. 71



60/66
FIG. 72



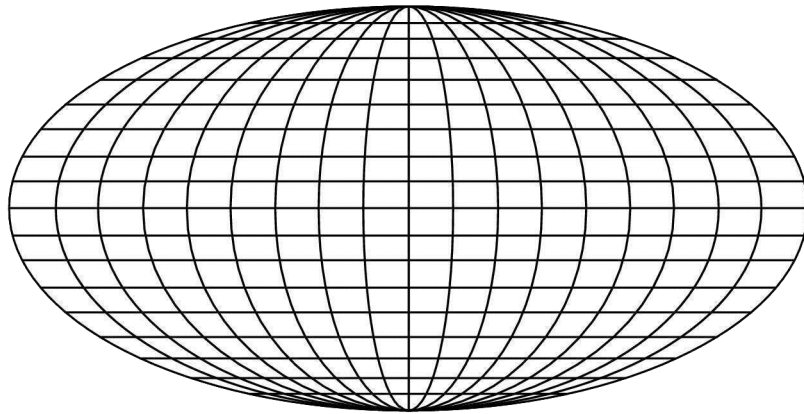
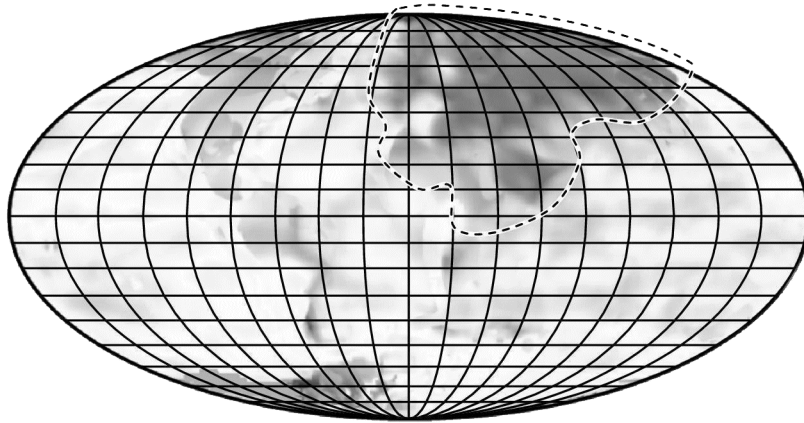


FIG. 73B

DEGREE OF ACCUMULATION: HIGH

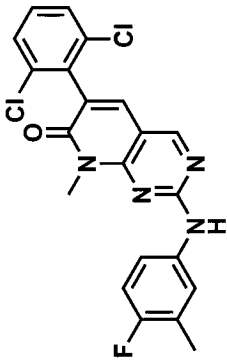
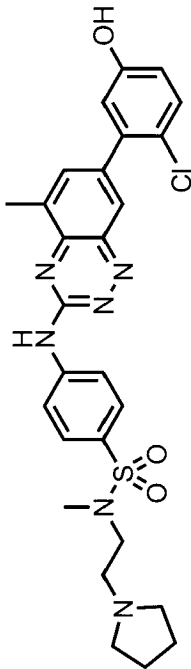


DEGREE OF
ACCUMULATION: LOW

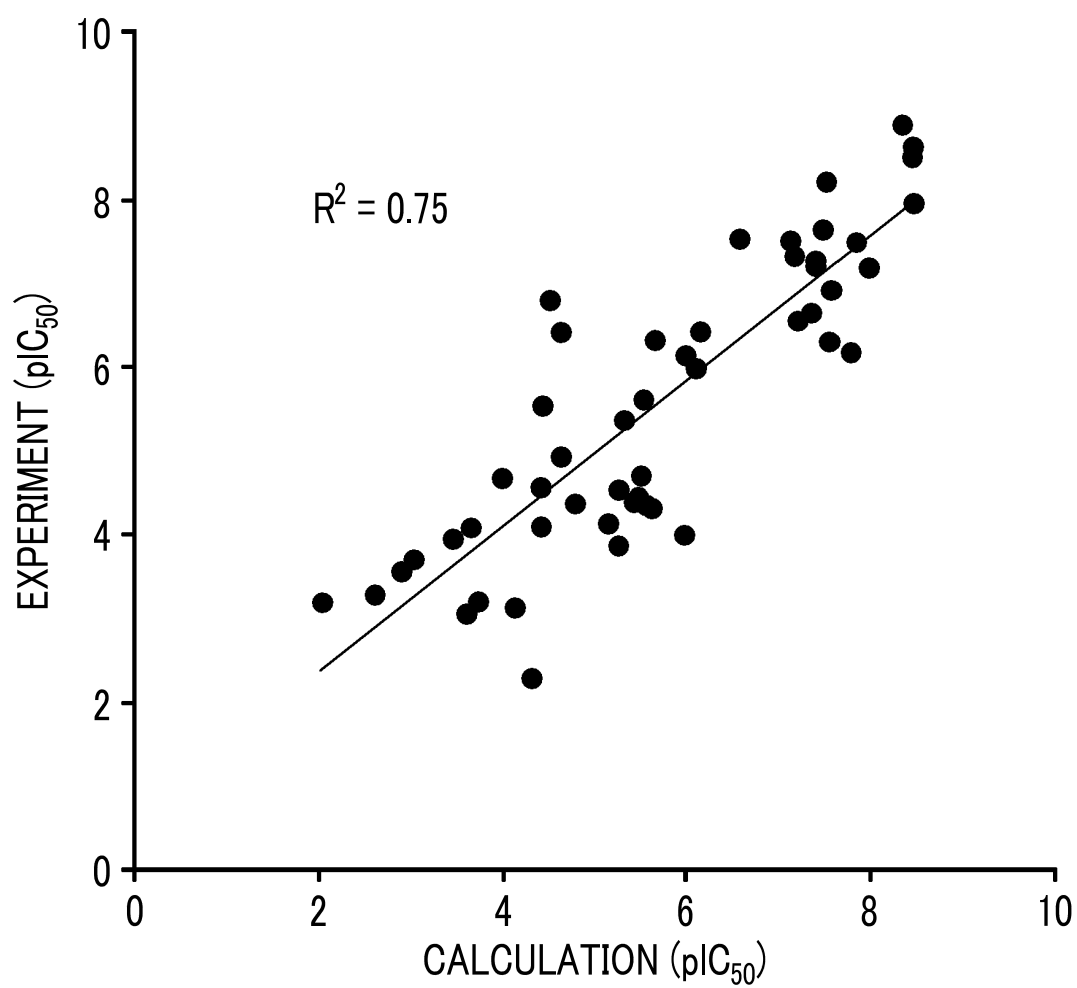
DEGREE OF
ACCUMULATION: HIGH



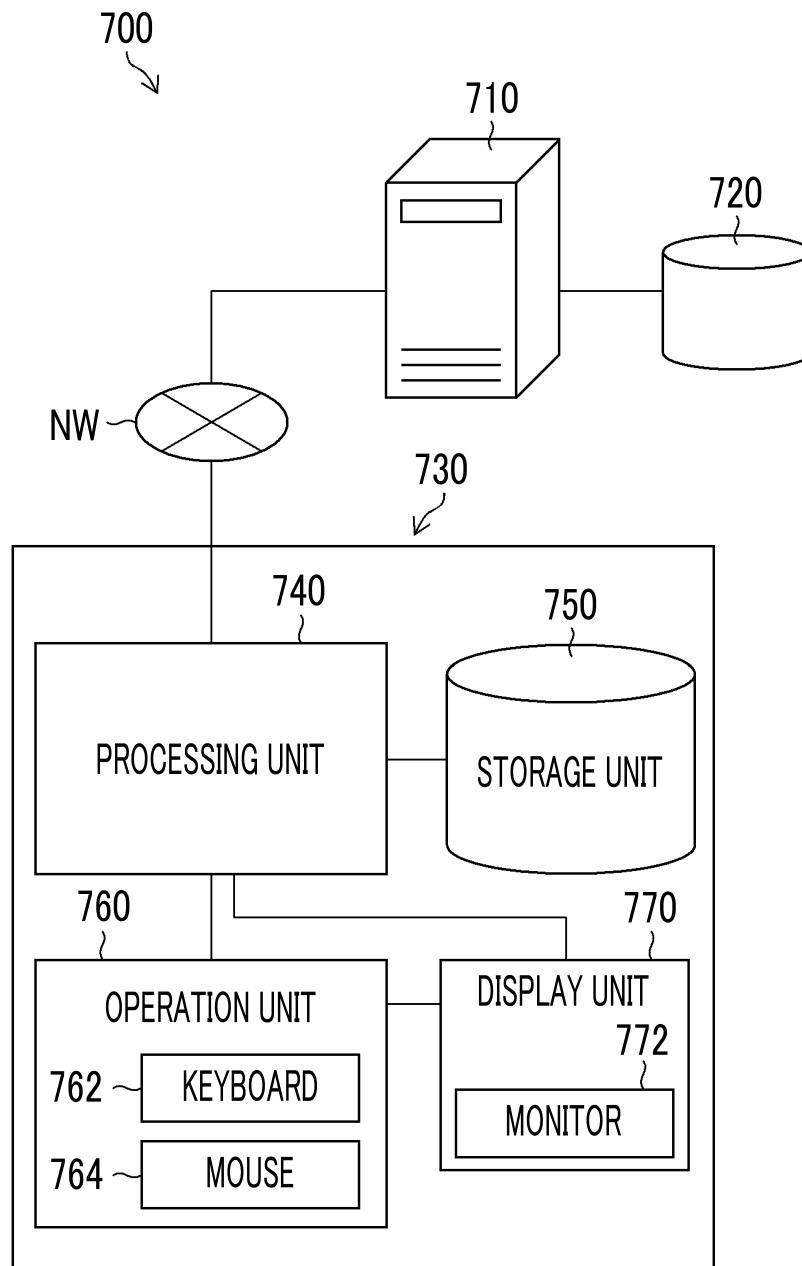
FIG. 74

NAME	STRUCTURAL FORMULA	SIMILARITY WITH TARGET COMPOUND
TARGET COMPOUND		-
COMPOUND TO BE SCREENED		0.1
	...	...
	...	...

63/66
FIG. 75



64/66
FIG. 76



65/66
FIG. 77

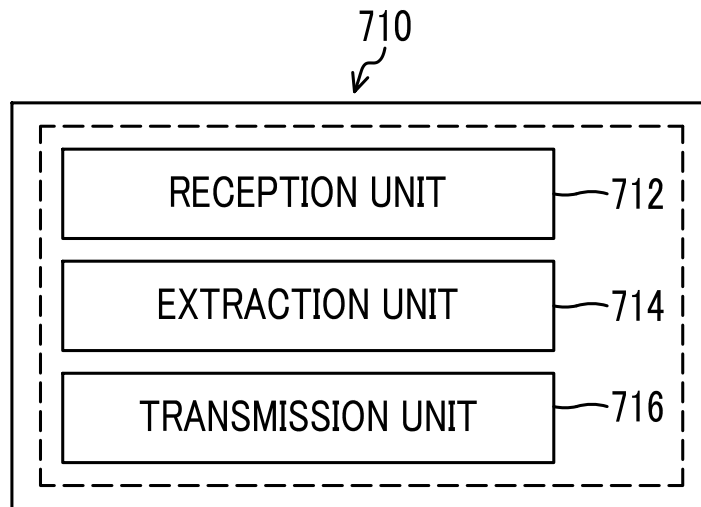
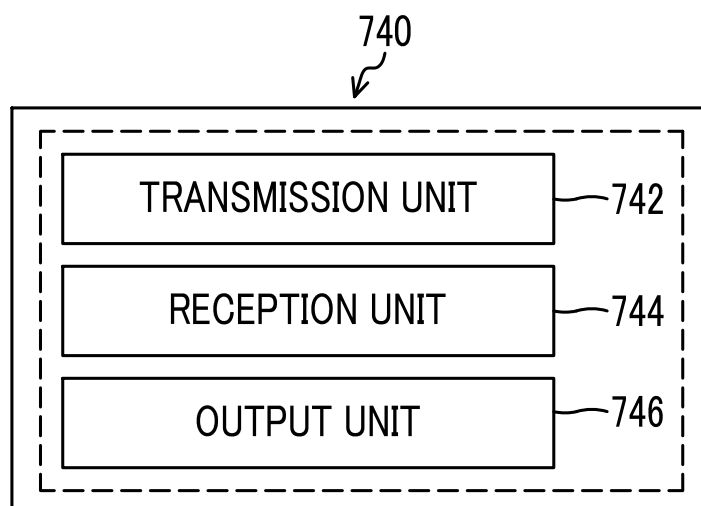


FIG. 78



66/66
FIG. 79

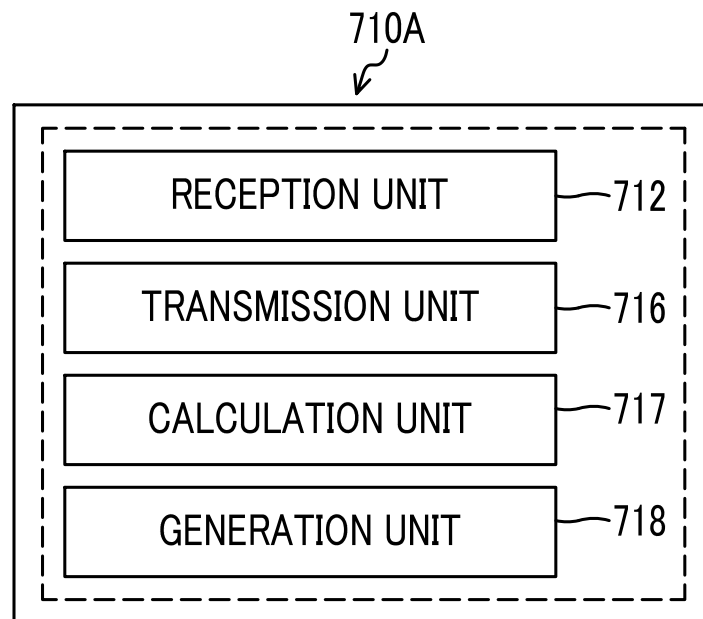


FIG. 80

