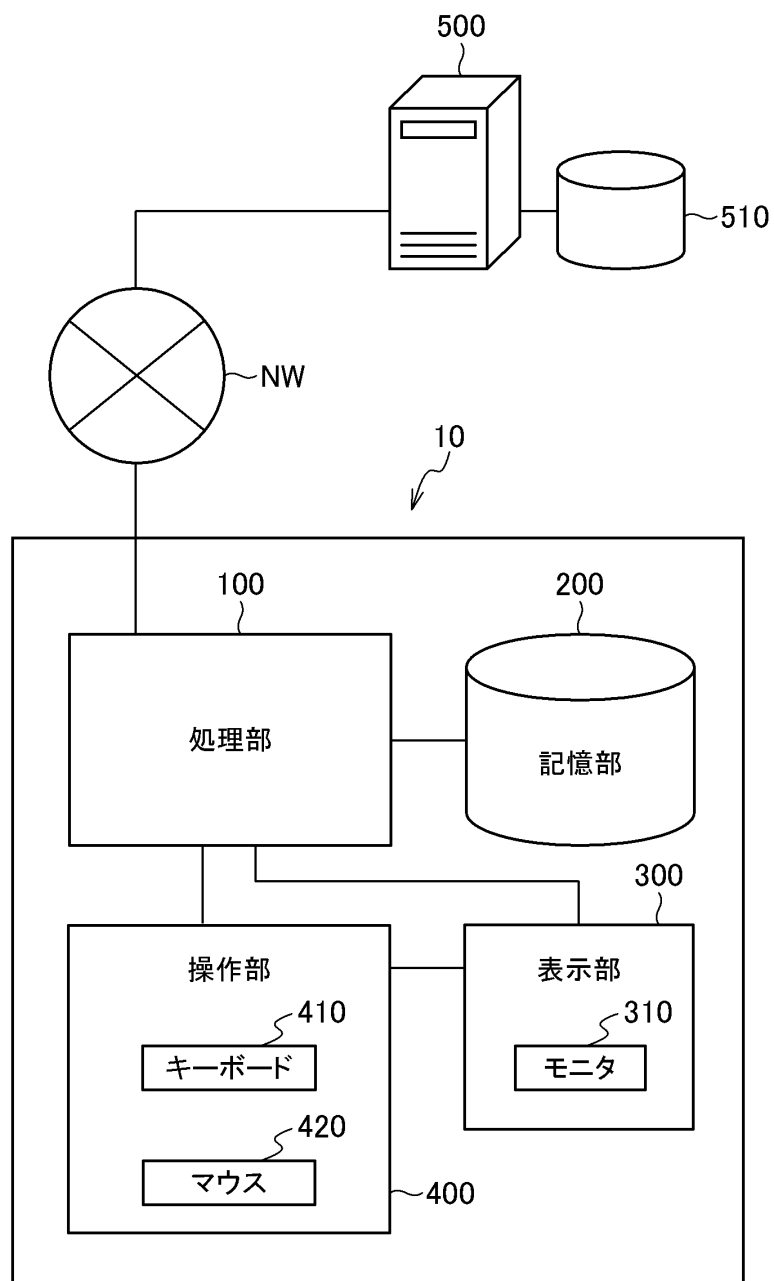
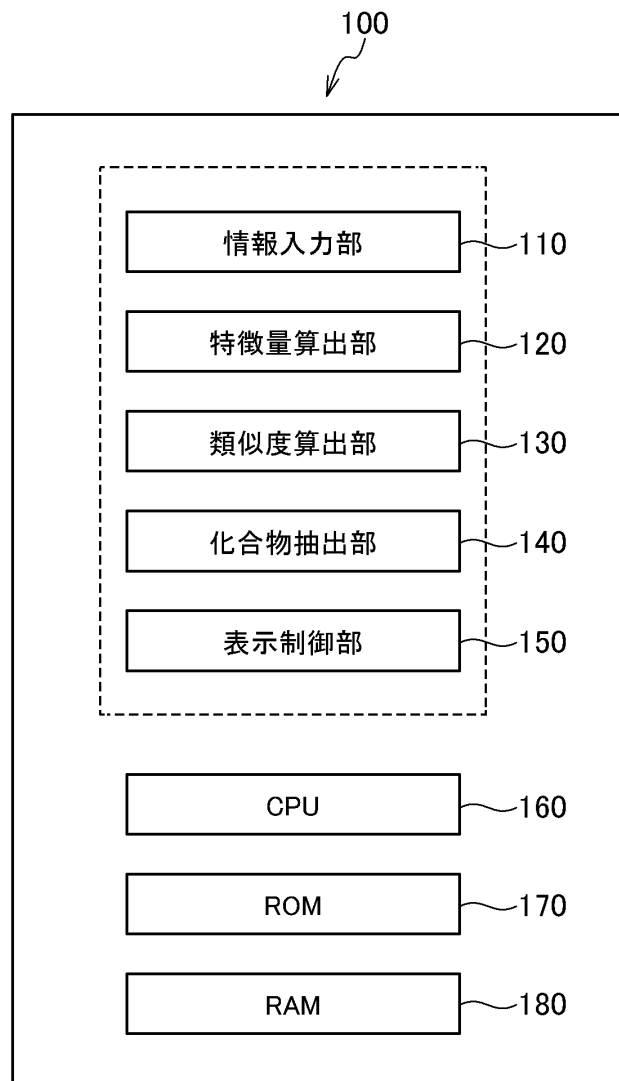


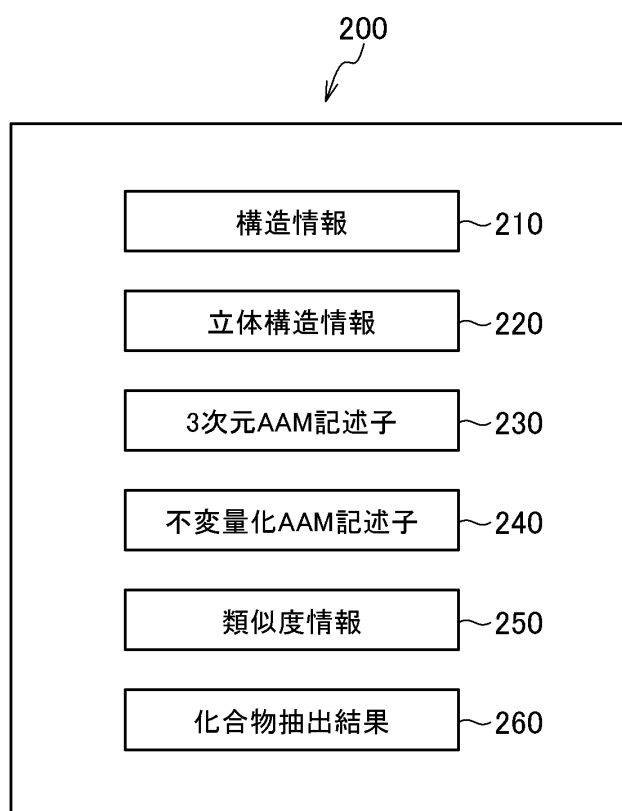
[図1]



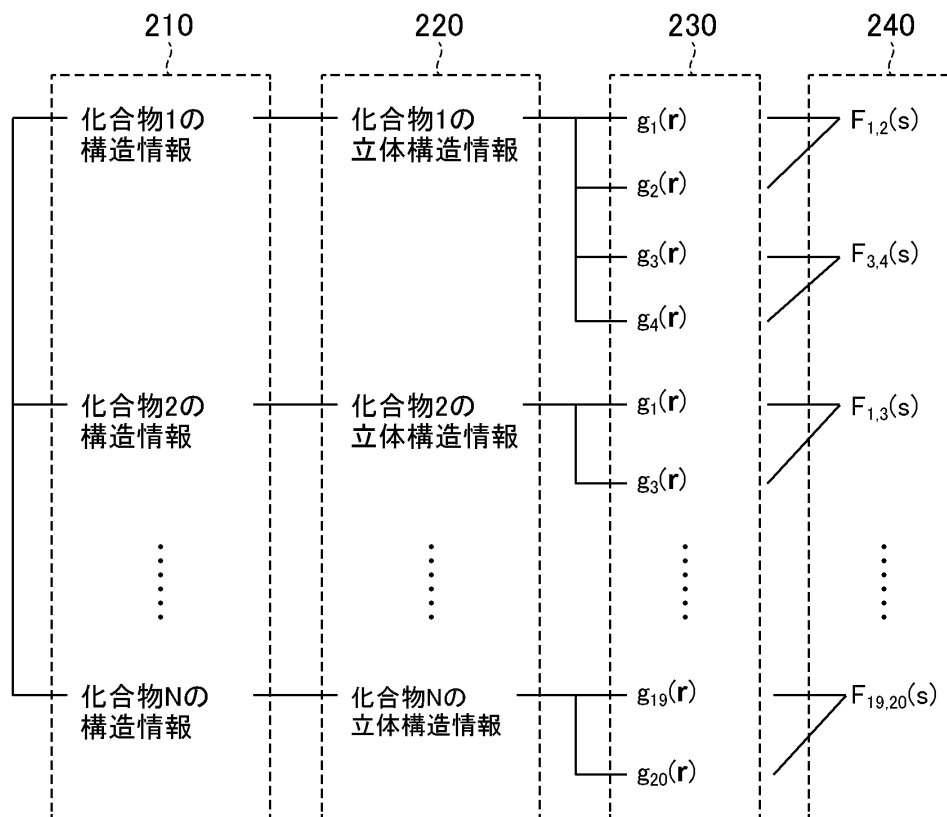
[図2]



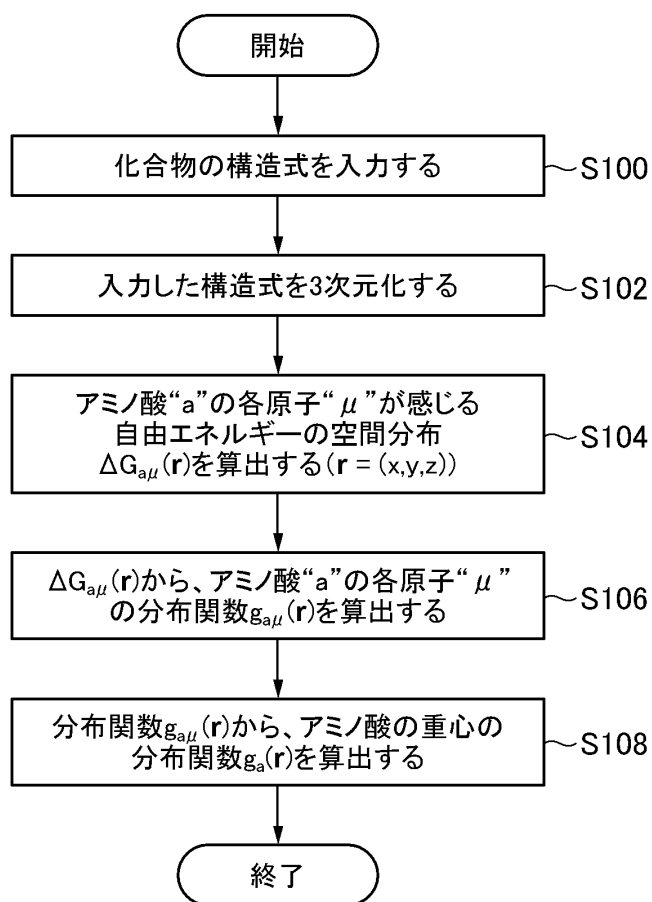
[図3]



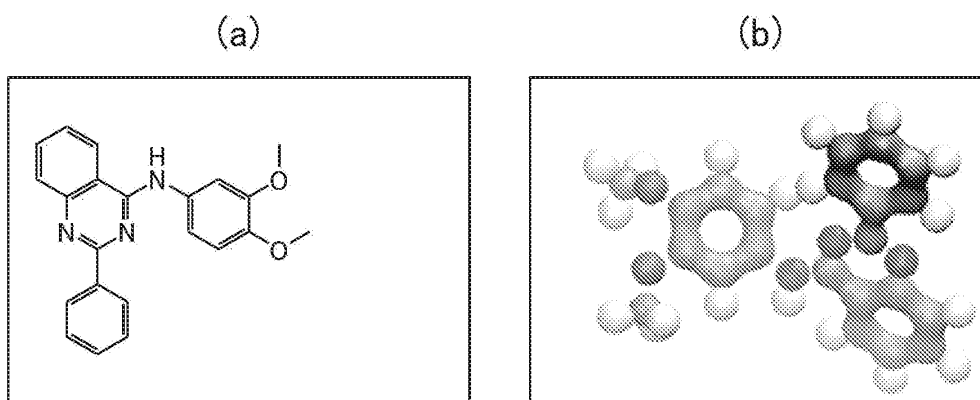
[図4]



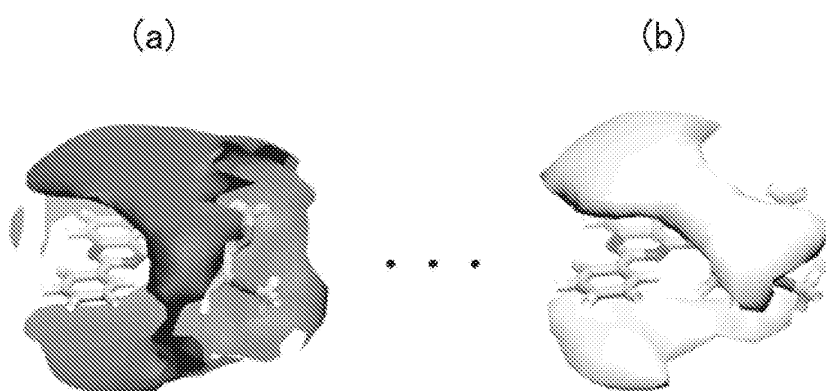
[図5]



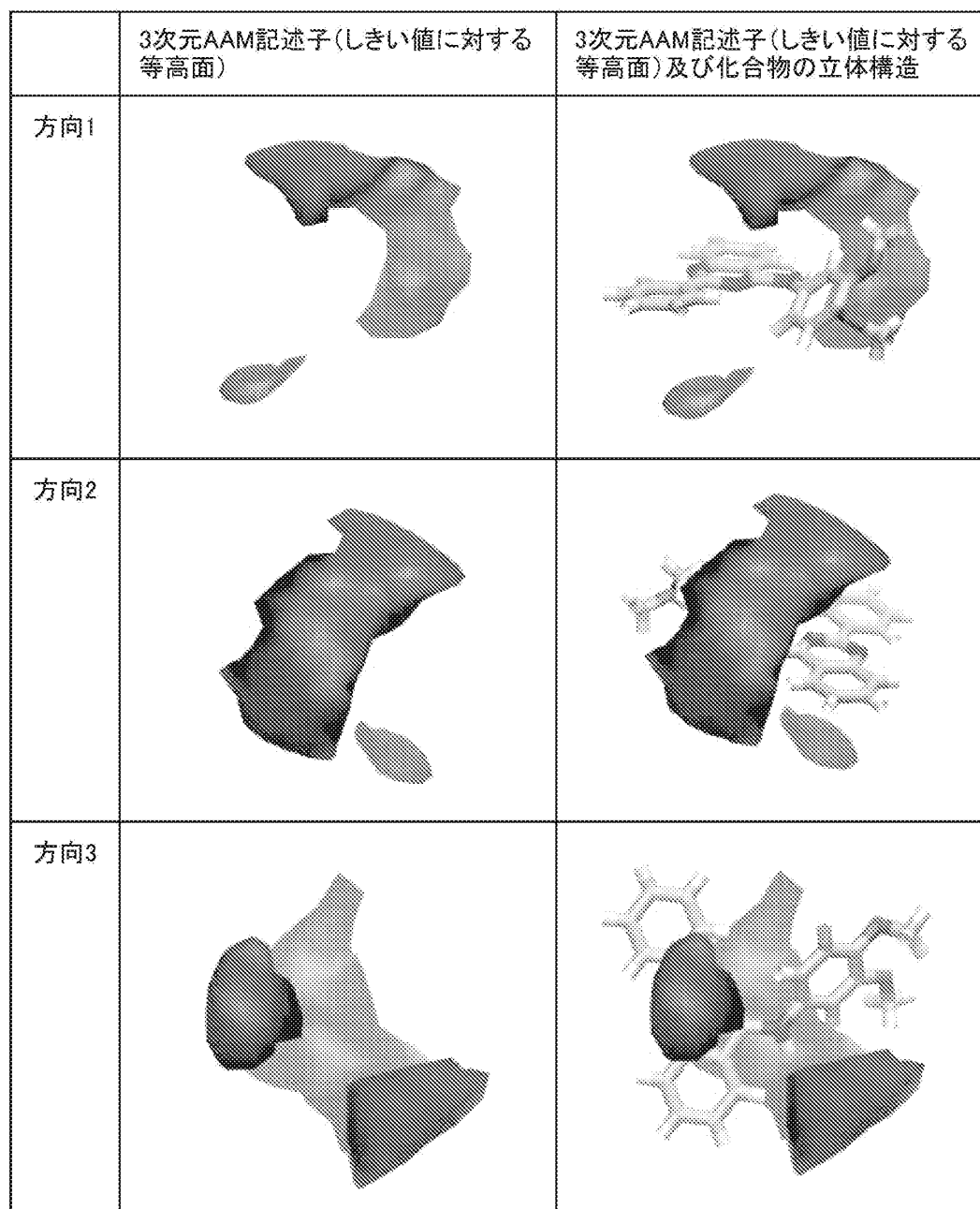
[図6]



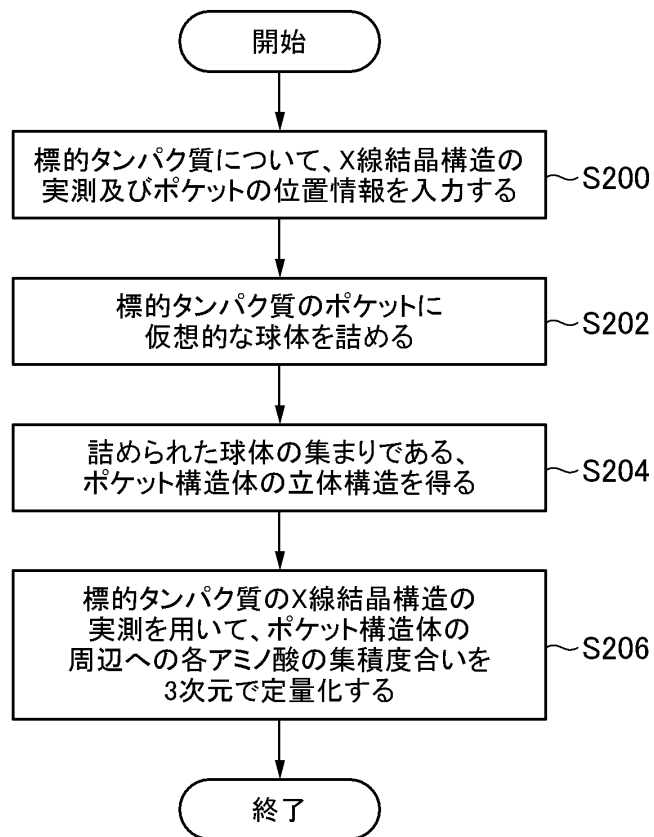
[図7]



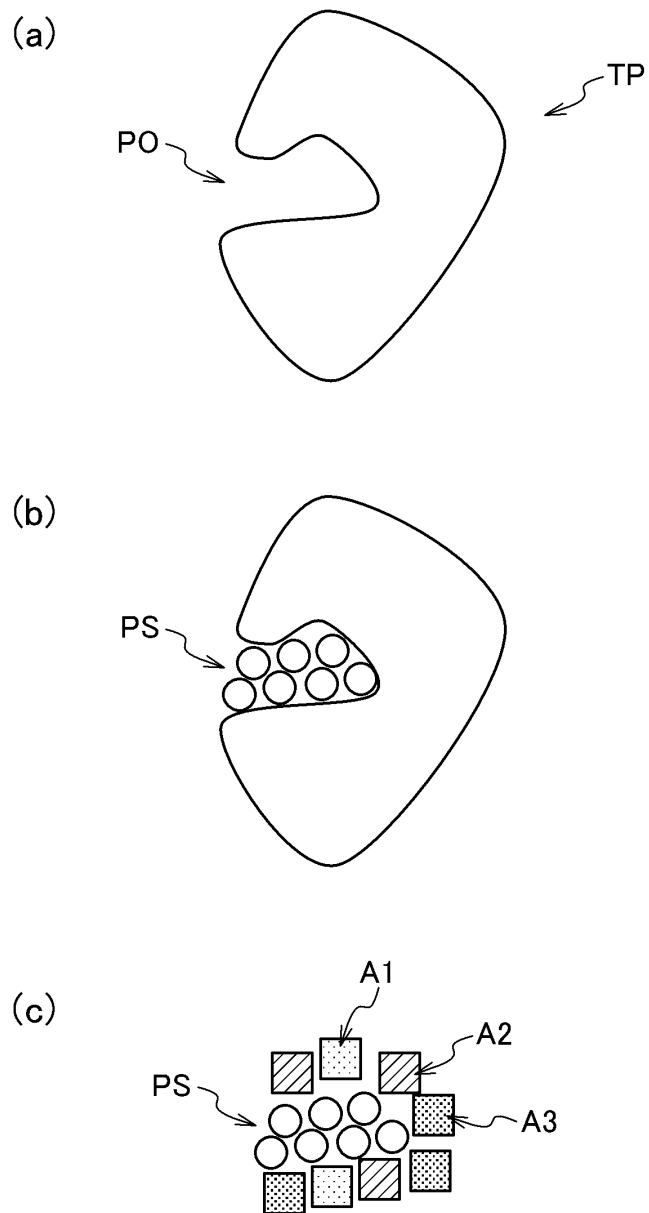
[図8]



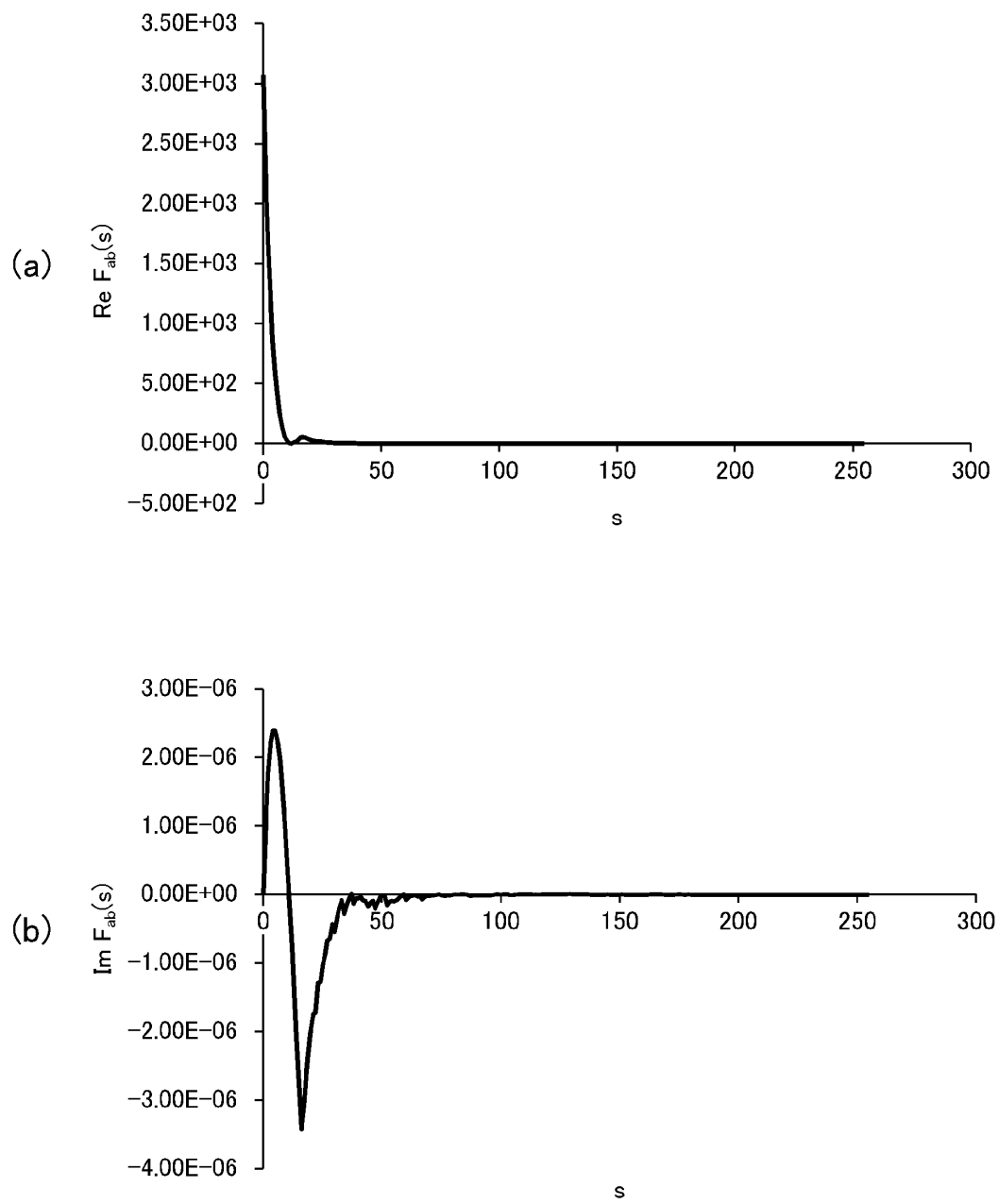
[図9]



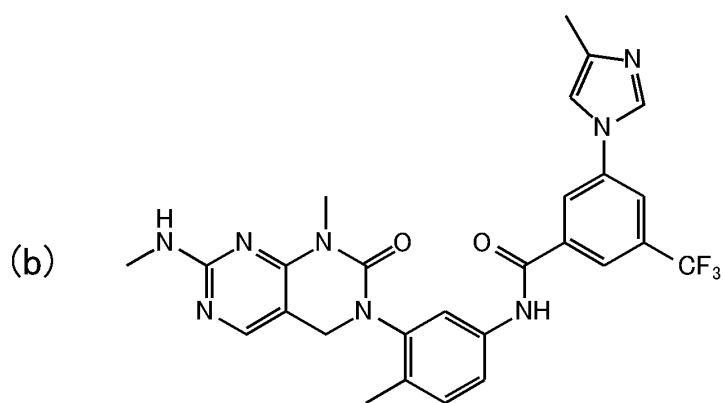
[図10]



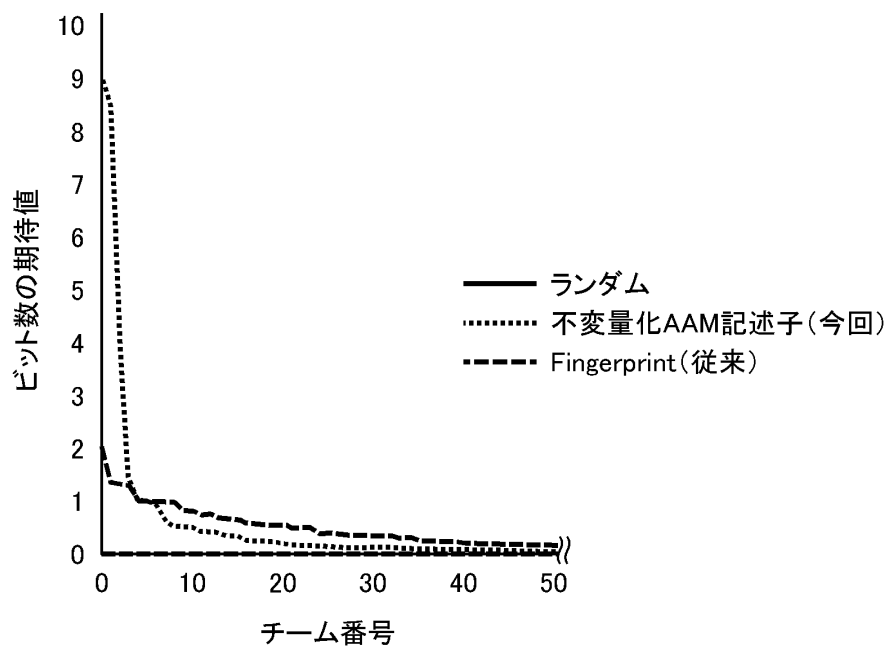
[図11]



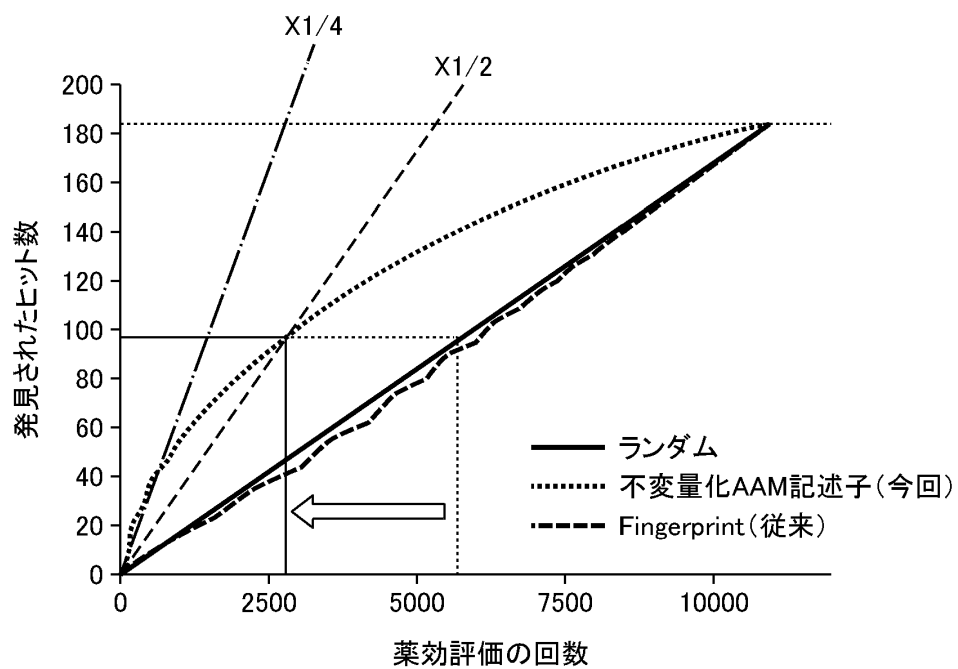
(a)

COc1ccc(Oc2ccc3c(c2)c(c[nH]3)C(=N4C=CC=C5C(=C4)N(C5)C6=CC=CC=C6O)cc2ccccc2

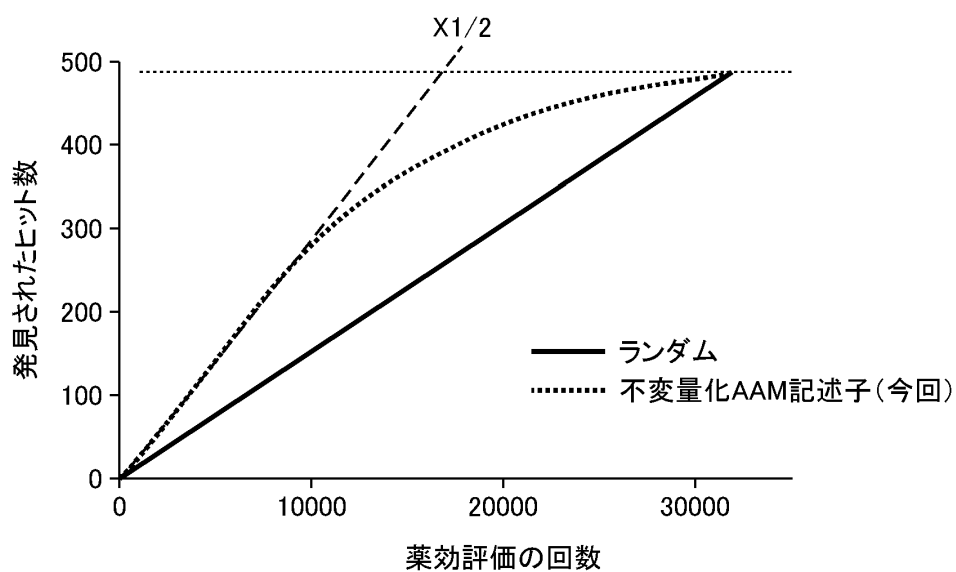
[図13]



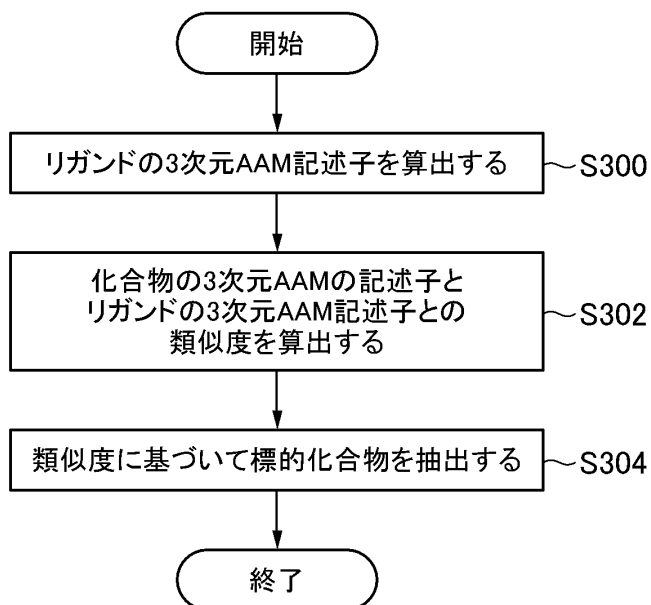
[図14]



[図15]



[図16]



[図17]

(a)

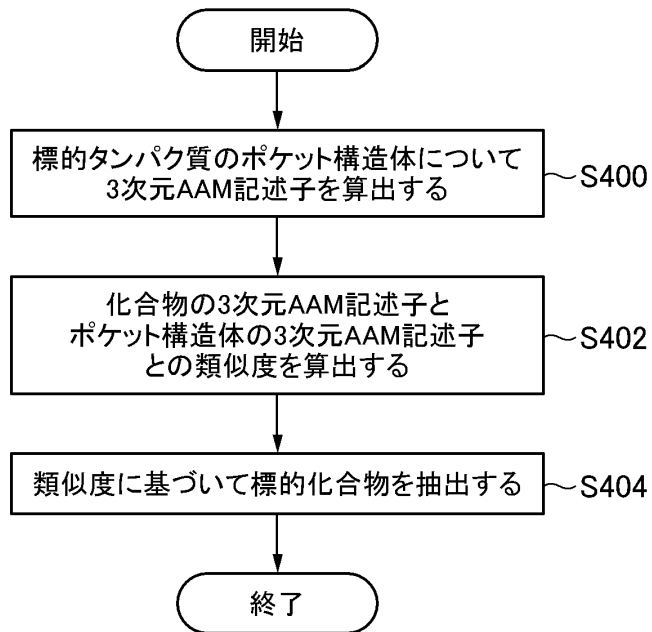
リガンド		化合物		類似度	抽出結果
識別情報	3次元 AAM記述子	識別情報	3次元 AAM記述子		
L00001	L00001_g1(r)	C00001	C00001_g1(r)	85%	抽出
		C00002	C00002_g1(r)	73%	抽出せず
		...	...	...	...
		C00100	C00100_g1(r)	91%	抽出
		...	...	...	...
		C01000	C01000_g1(r)	80%	抽出
		...	...	...	...

(b)

リガンド		化合物		類似度		抽出結果
識別情報	不変量化 AAM記述子	識別情報	不変量化 AAM記述子	数値	順位	
L00001	L00001_F ₁₂ (s)	C00100	C00100_F ₁₂ (s)	91%	1	抽出
		C00001	C00001_F ₁₂ (s)	85%	2	抽出
		...	...	...	...	...
		C01000	C01000_F ₁₂ (s)	80%	100	抽出
		...	...	...	...	...
		C00002	C00002_F ₁₂ (s)	73%	265	抽出せず
		...	...	...	...	...

抽出 ↑

[図18]



[図19]

(a)

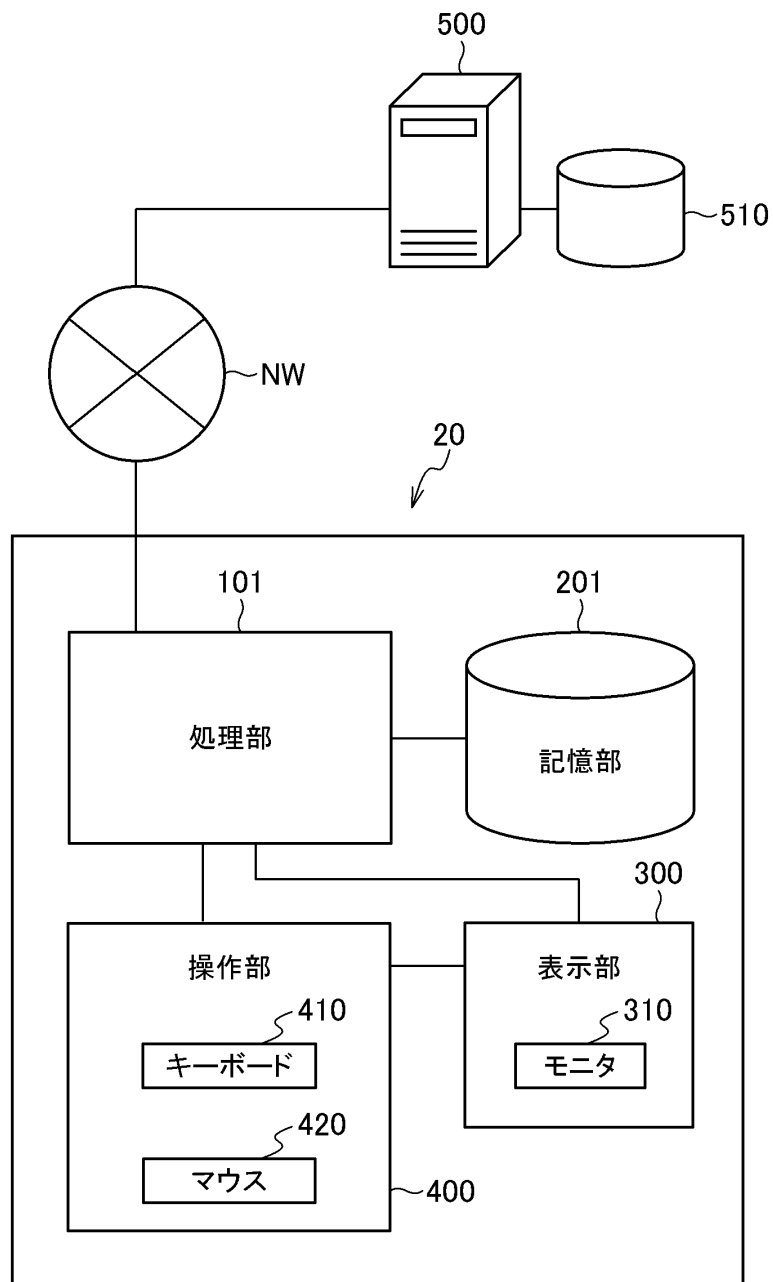
ポケット構造体		化合物		類似度	抽出結果
識別情報	3次元 AAM記述子	識別情報	3次元 AAM記述子		
P00001	P00001_g1(r)	C00001	C00001_g1(r)	85%	抽出
		C00002	C00002_g1(r)	73%	抽出せず
		...	...	...	...
		C00100	C00100_g1(r)	91%	抽出
		...	...	...	...
		C01000	C01000_g1(r)	80%	抽出
		...	...	...	...

(b)

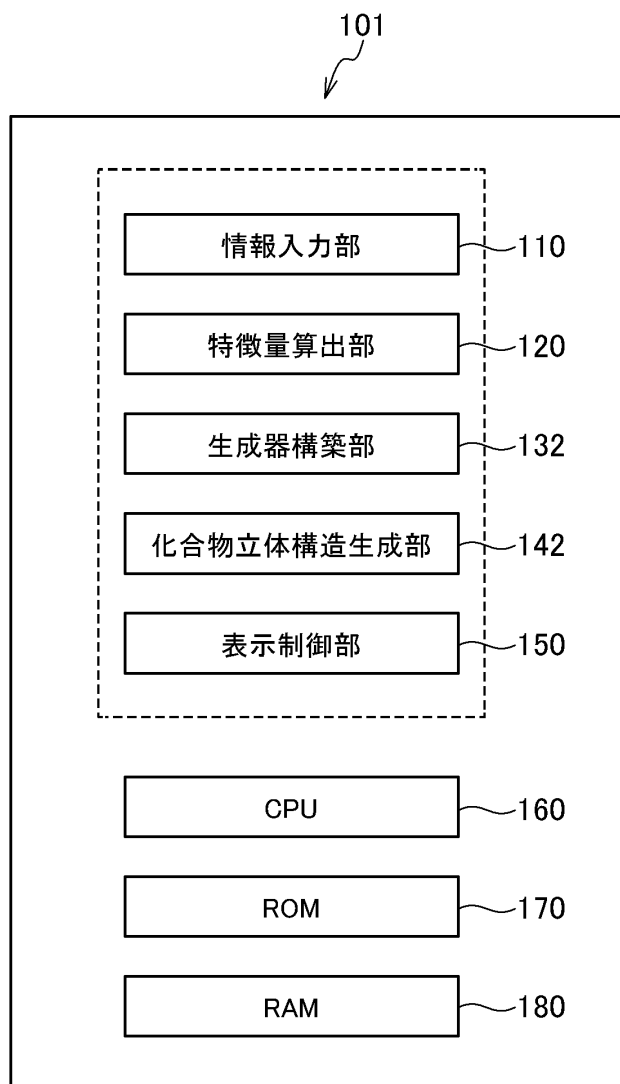
ポケット構造体		化合物		類似度		抽出結果
識別情報	不変量化 AAM記述子	識別情報	不変量化 AAM記述子	数値	順位	
P00001	P00001_F ₁₂ (s)	C00100	C00100_F ₁₂ (s)	91%	1	抽出
		C00001	C00001_F ₁₂ (s)	85%	2	抽出
		...	...	...	...	...
		C01000	C01000_F ₁₂ (s)	80%	100	抽出
		...	...	...	...	...
		C00001	C00001_F ₁₂ (s)	73%	265	抽出せず
		...	...	...	...	...

抽出 ↑

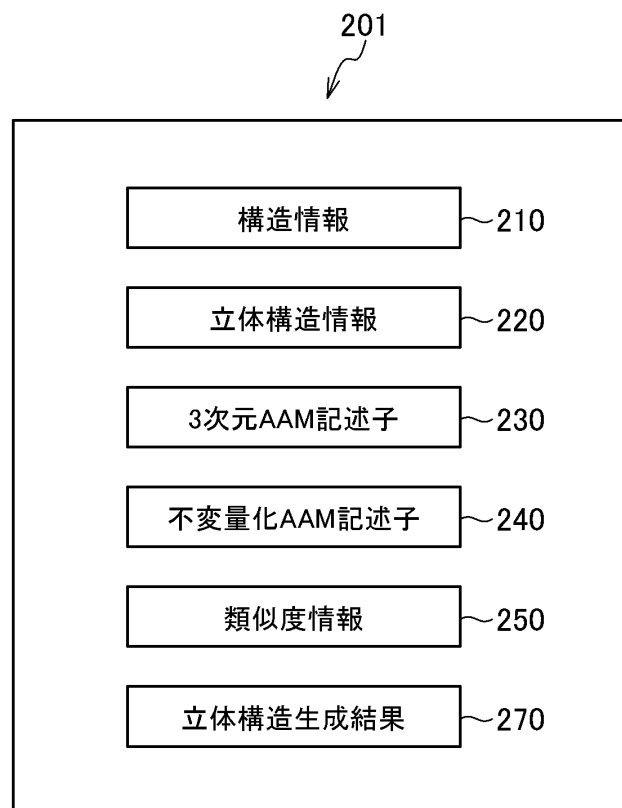
[図20]



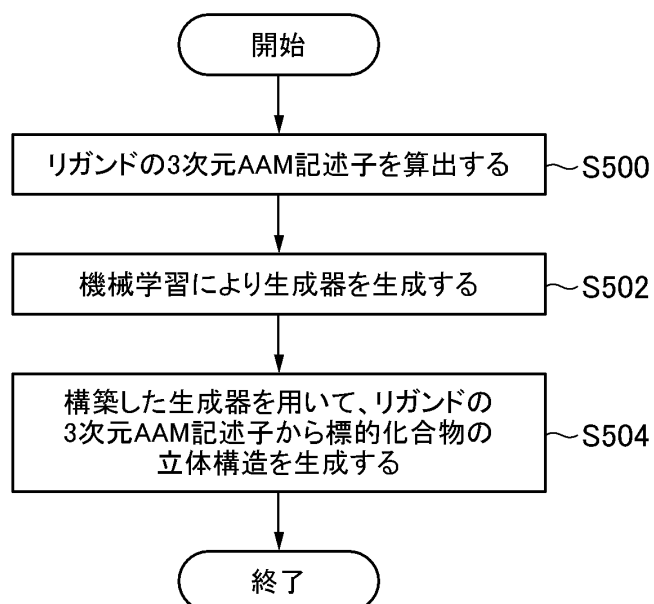
[図21]



[図22]

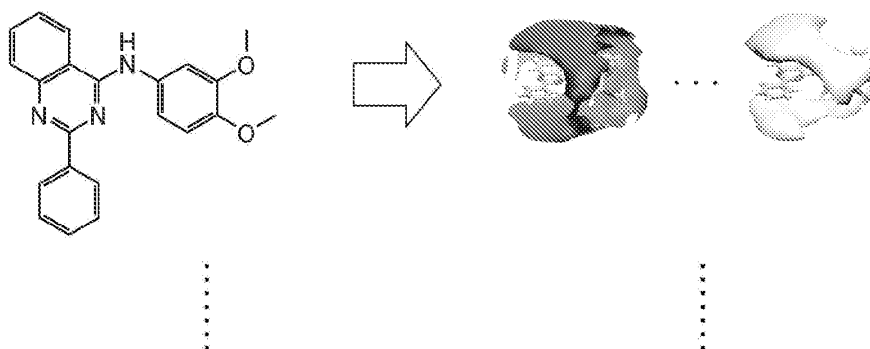


[図23]



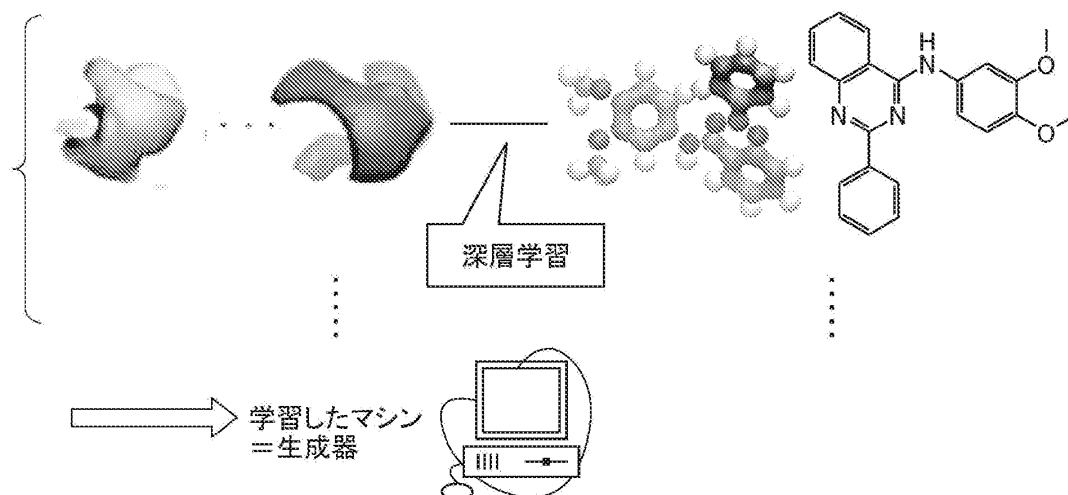
[図24]

Step1: 複数の化合物について3次元AAM記述子を算出し、構造式と3次元AAM記述子とのペアを作る

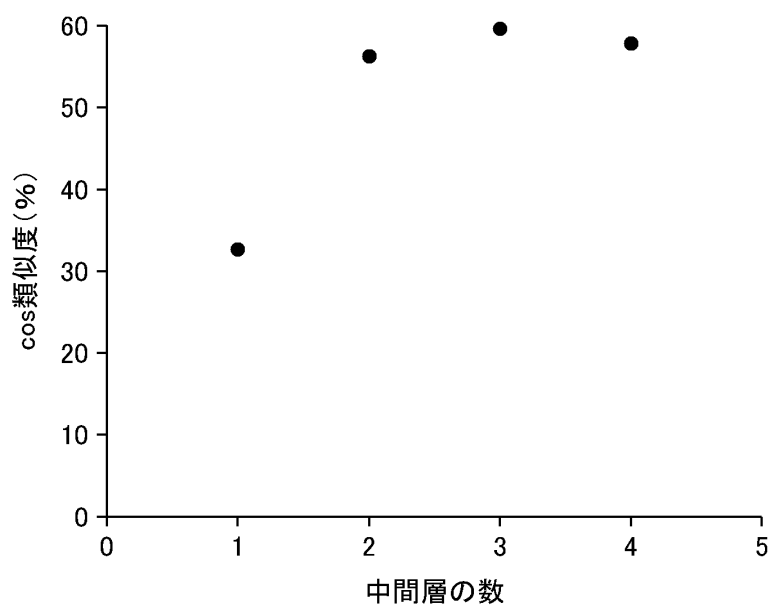


Step2: 3次元AAM記述子(説明変数)

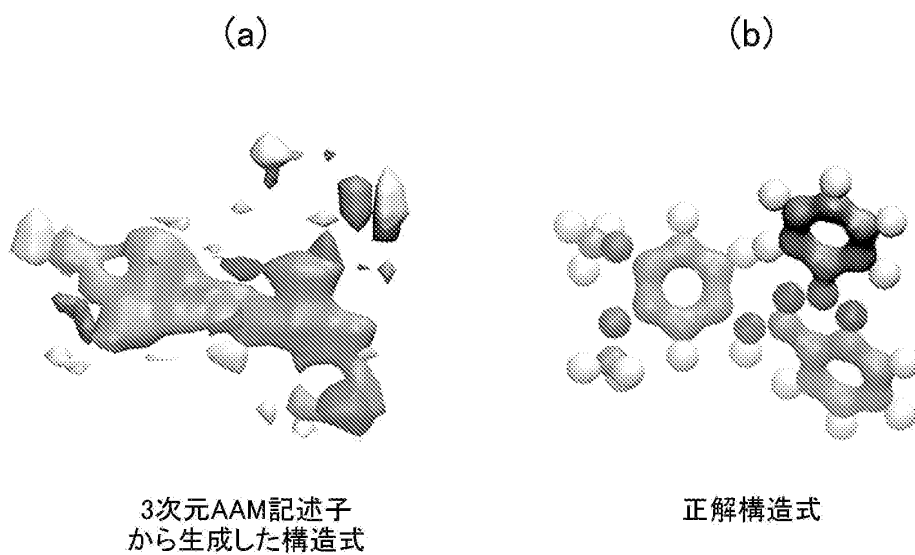
化合物の立体構造(教師データ)



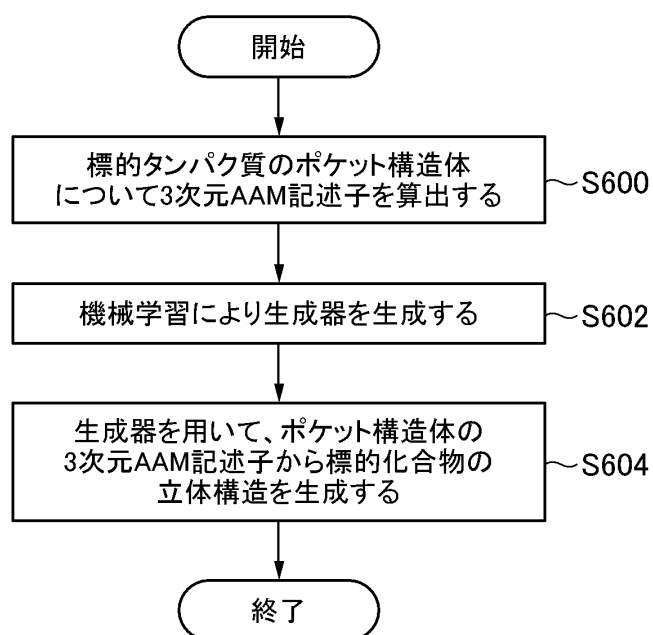
[図25]



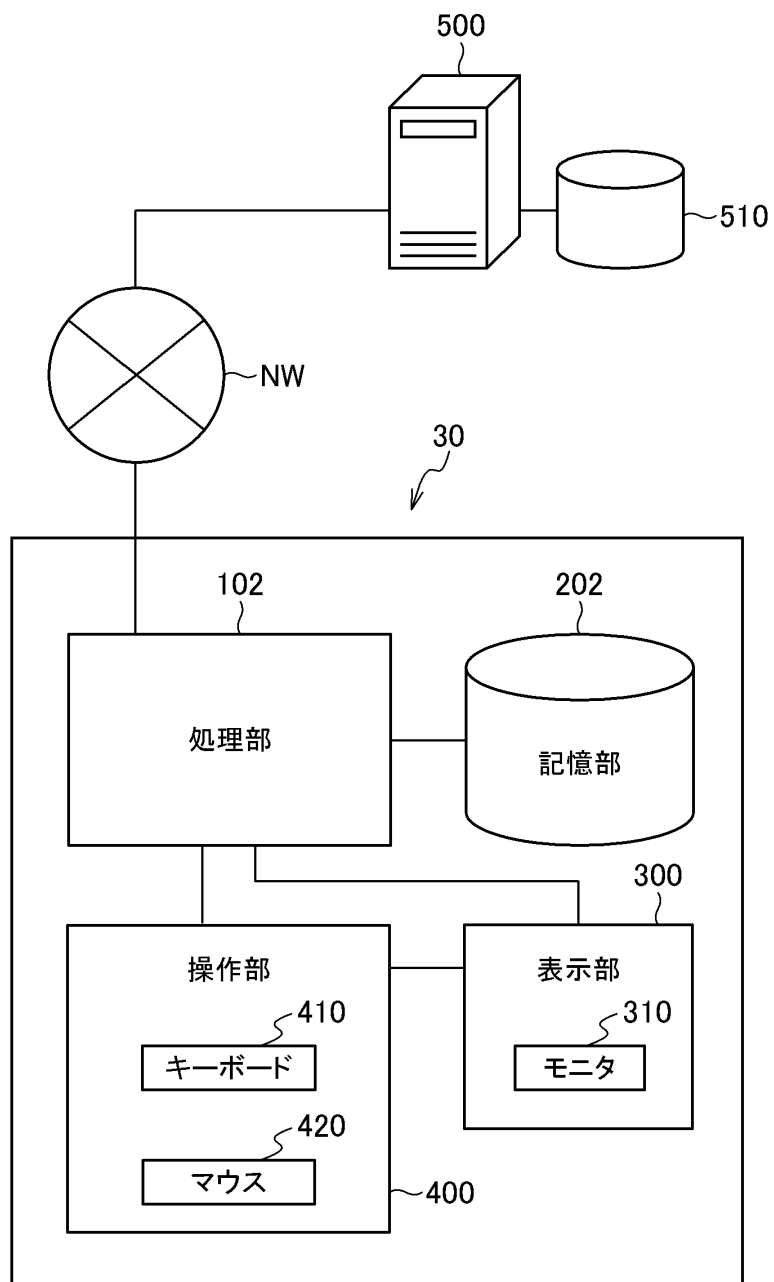
[図26]



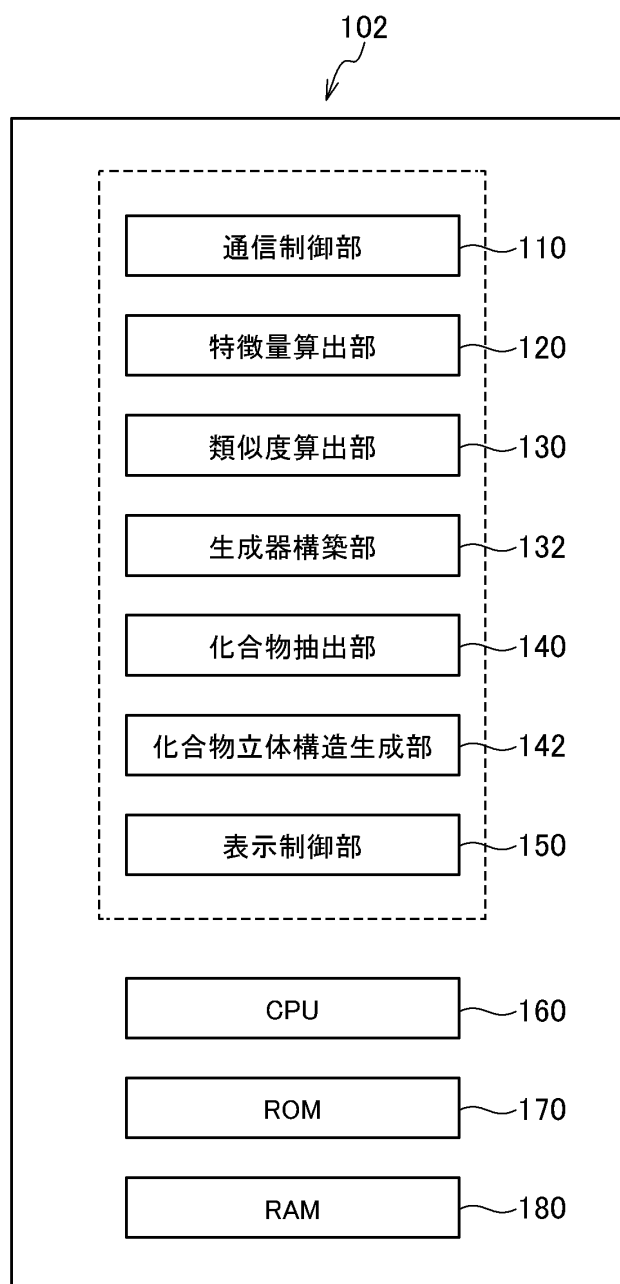
[図27]



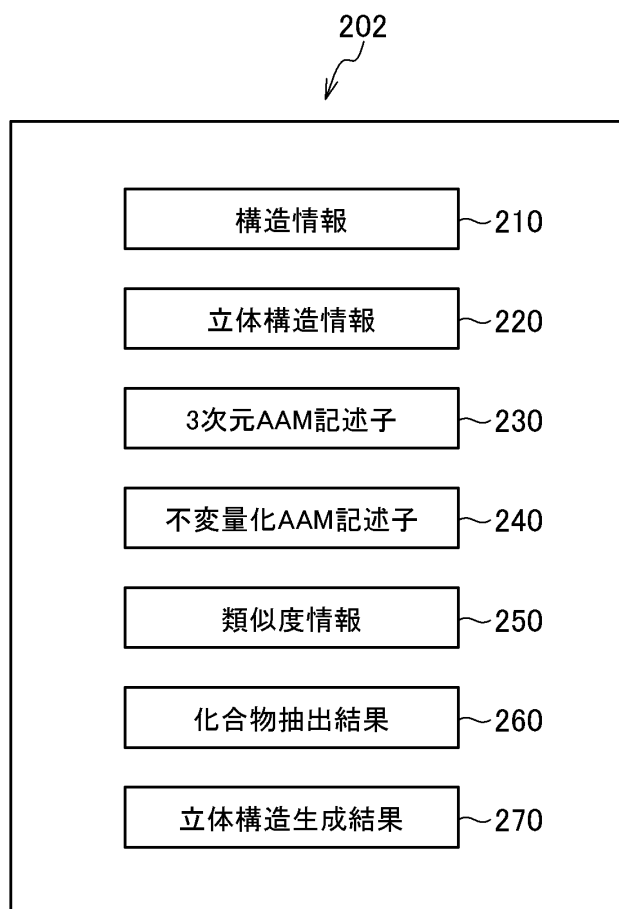
[図28]



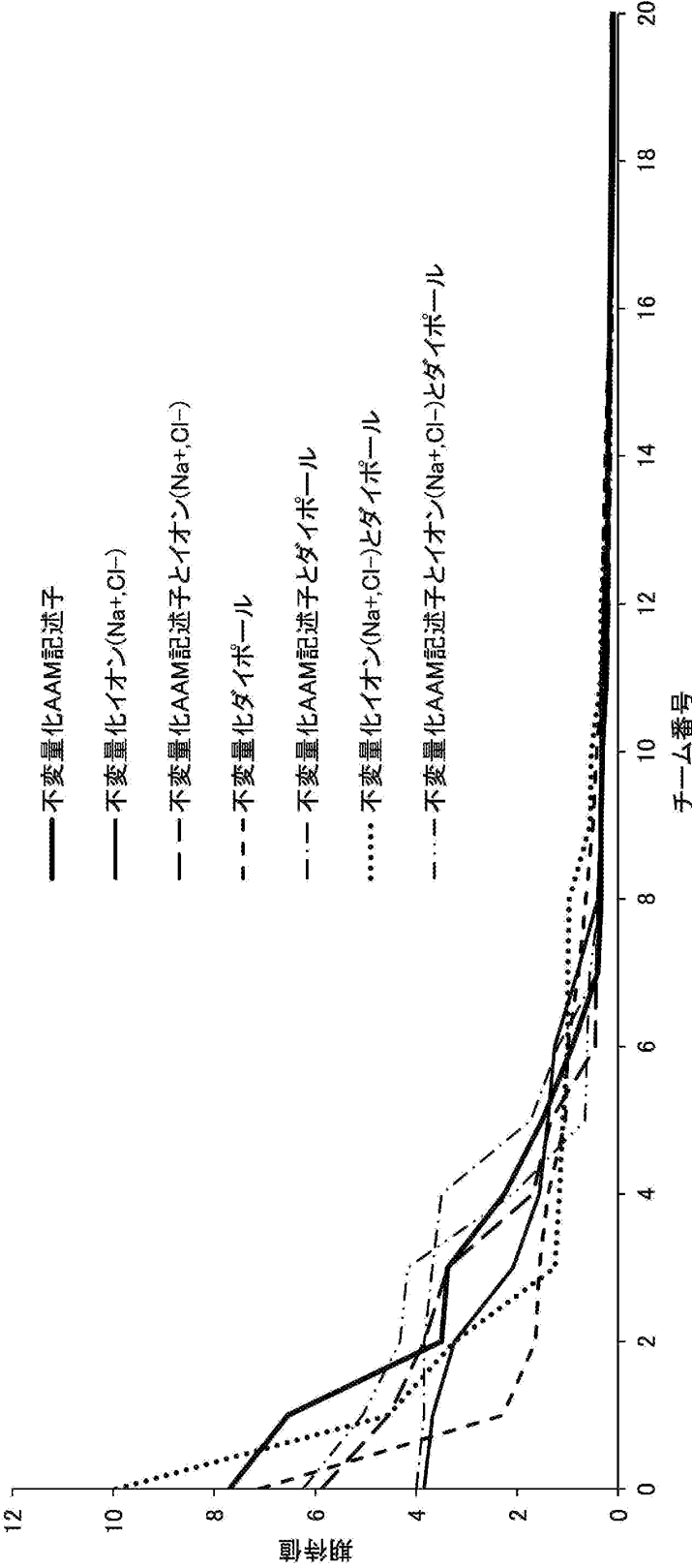
[図29]



[図30]

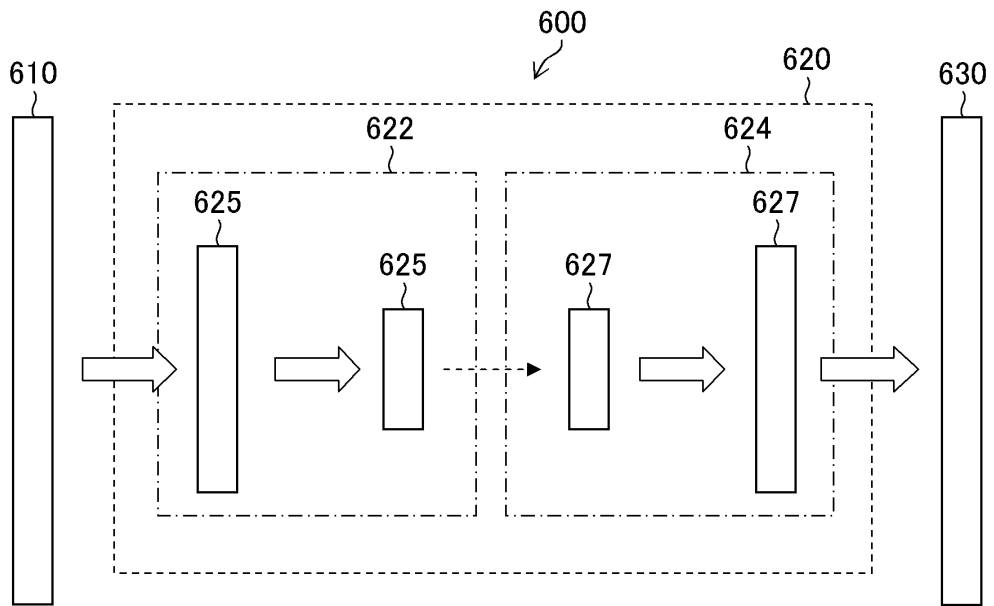


[図31]

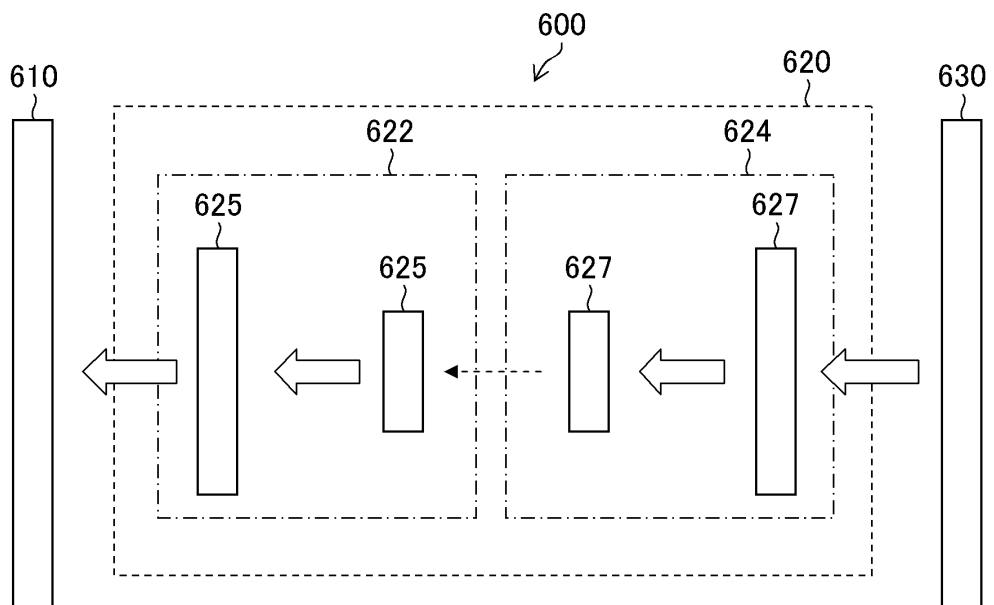


[図32]

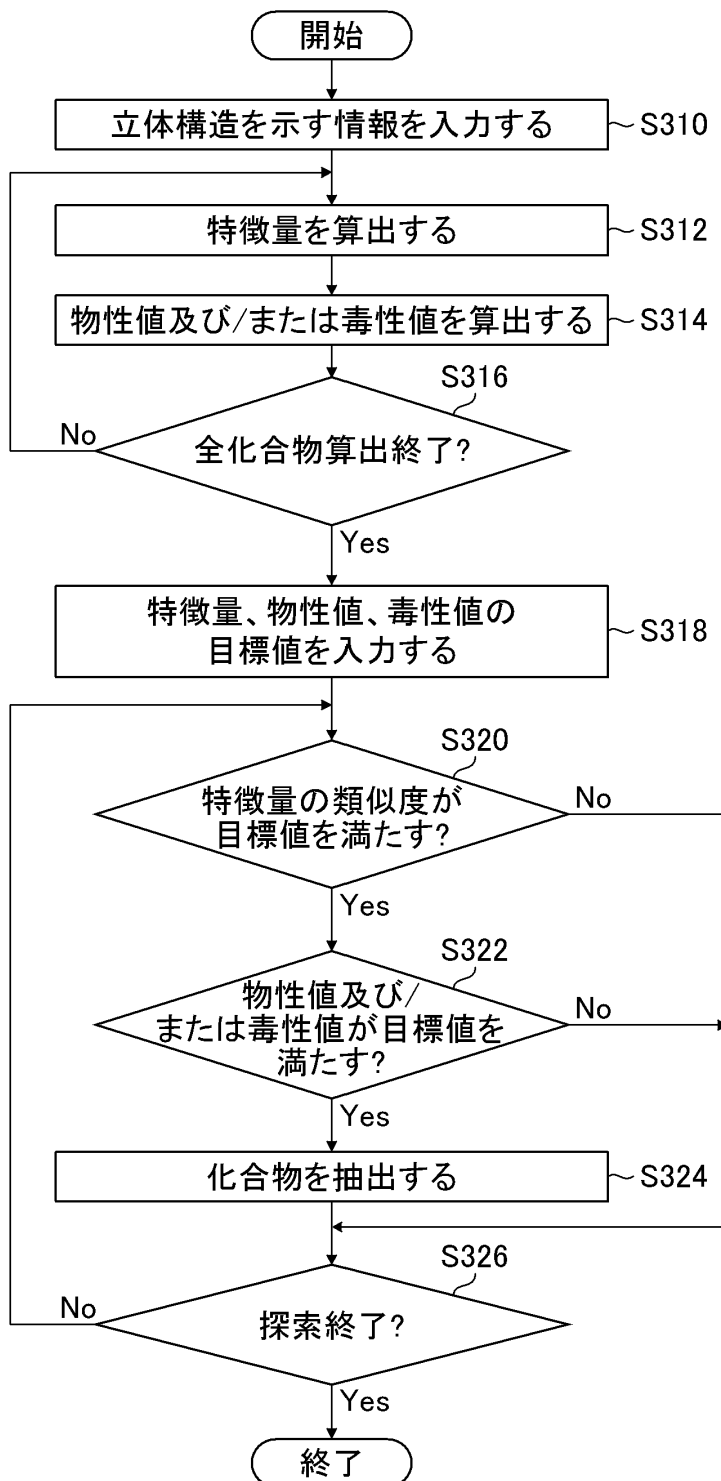
(a)



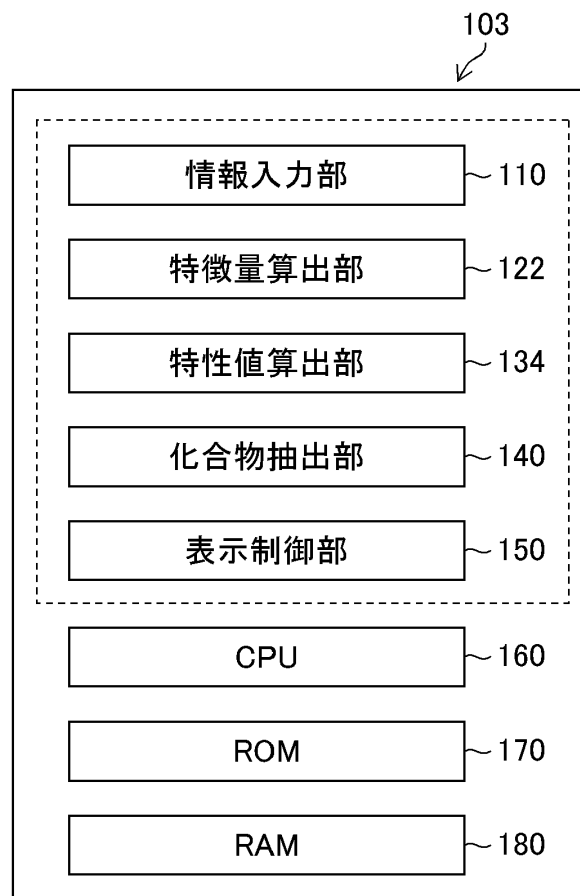
(b)



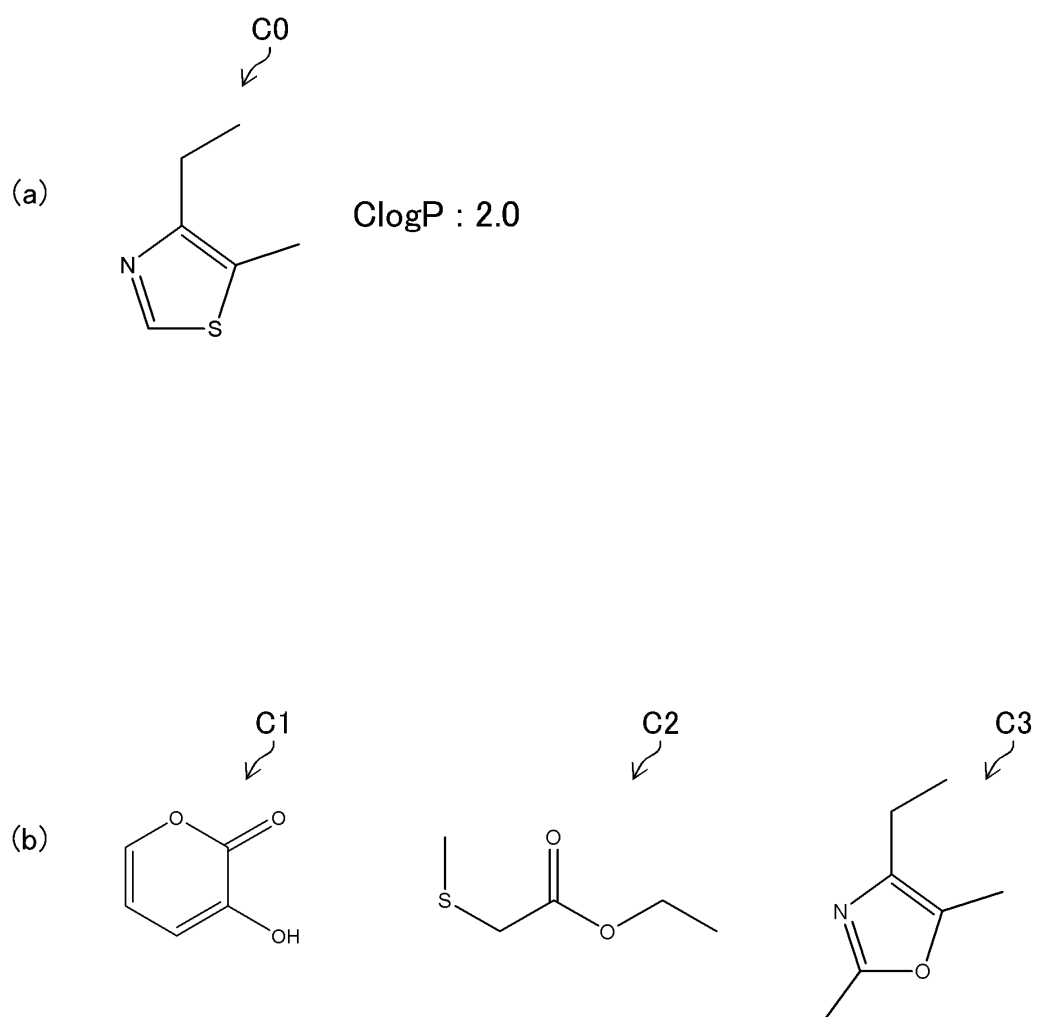
[図33]



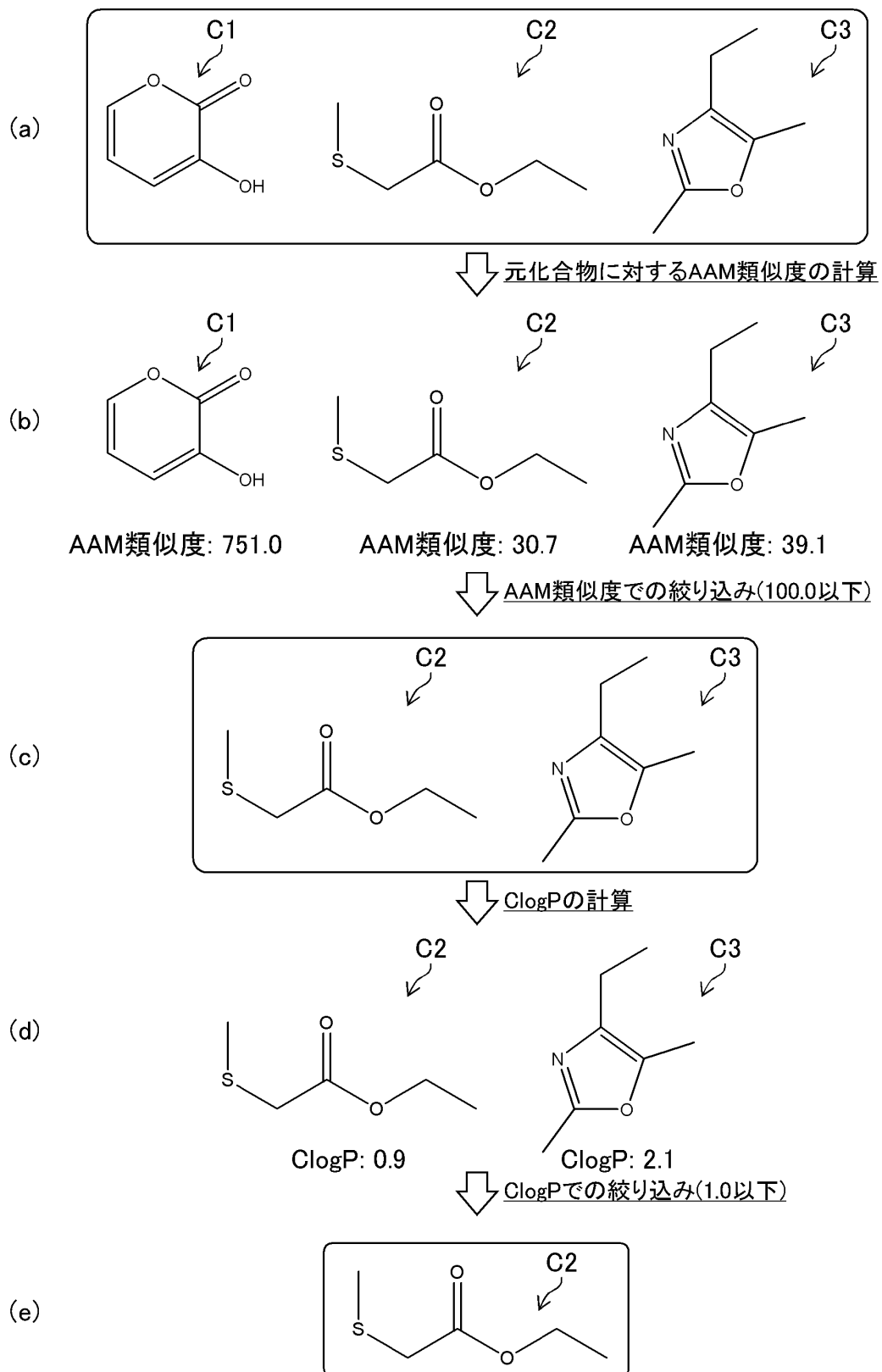
[図34]



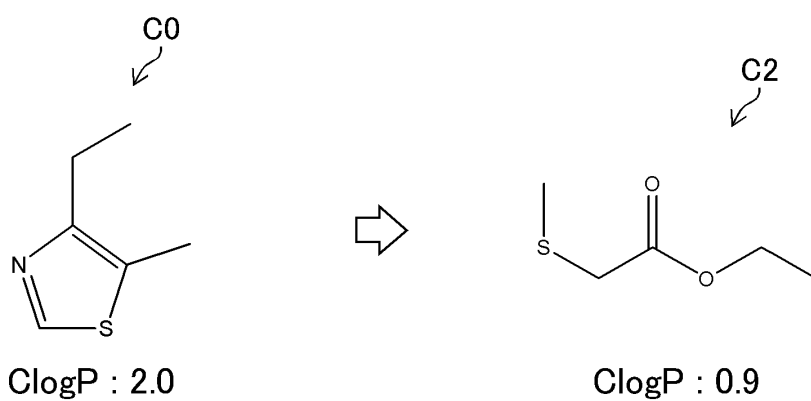
[図35]



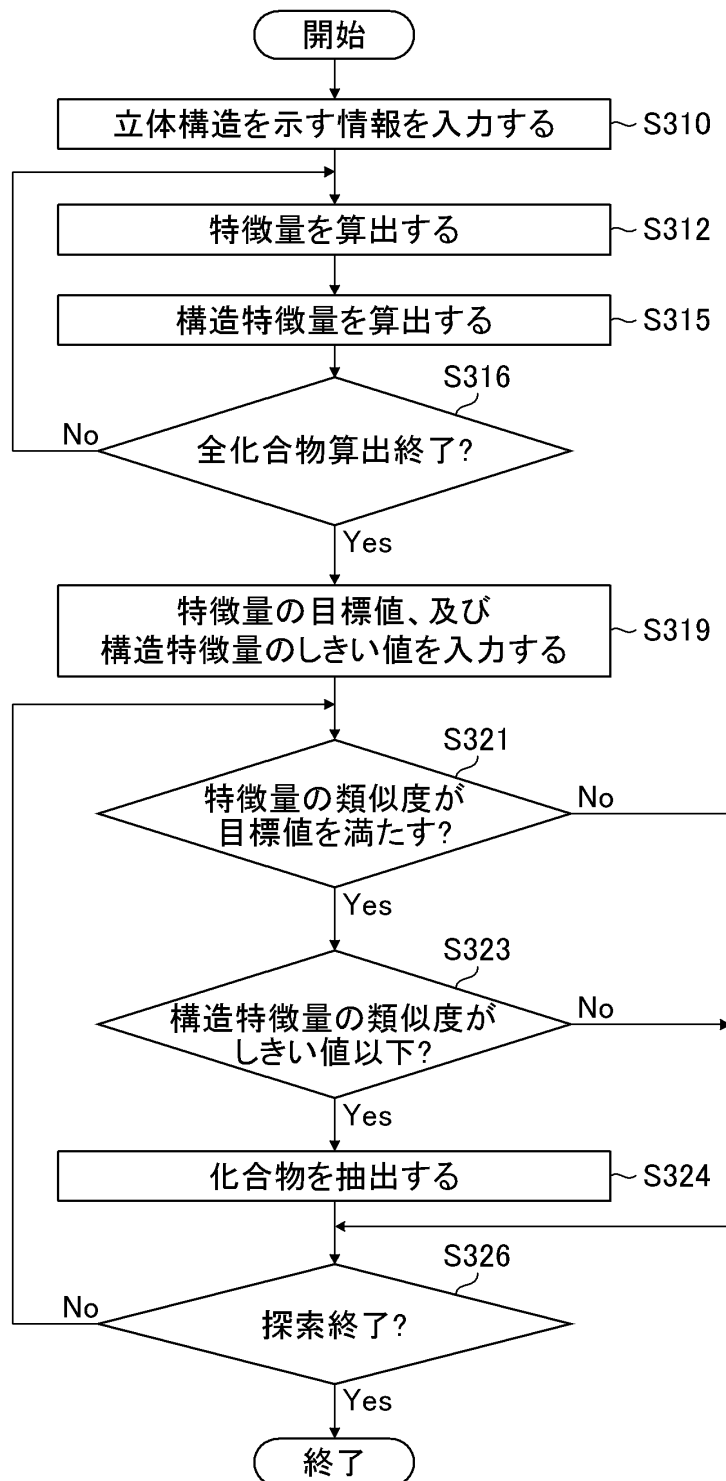
[図36]



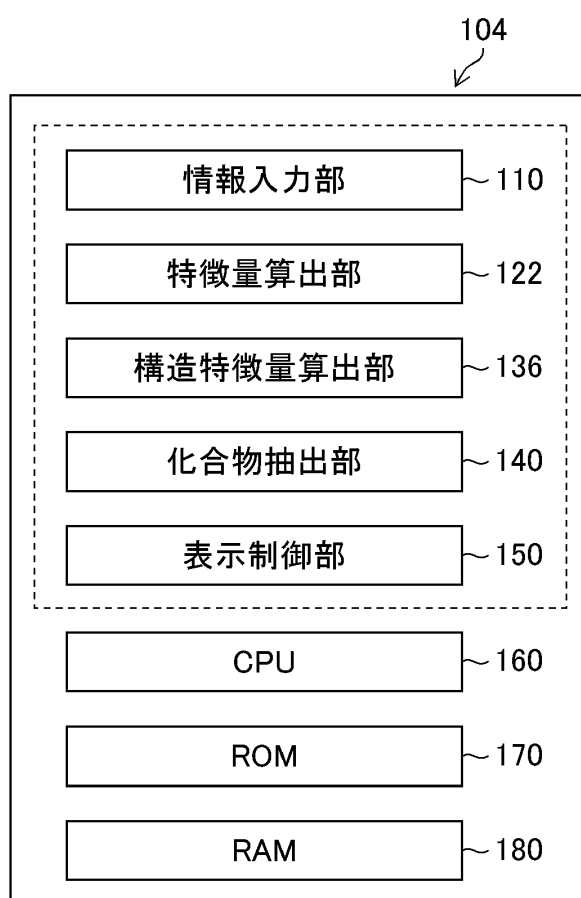
[図37]



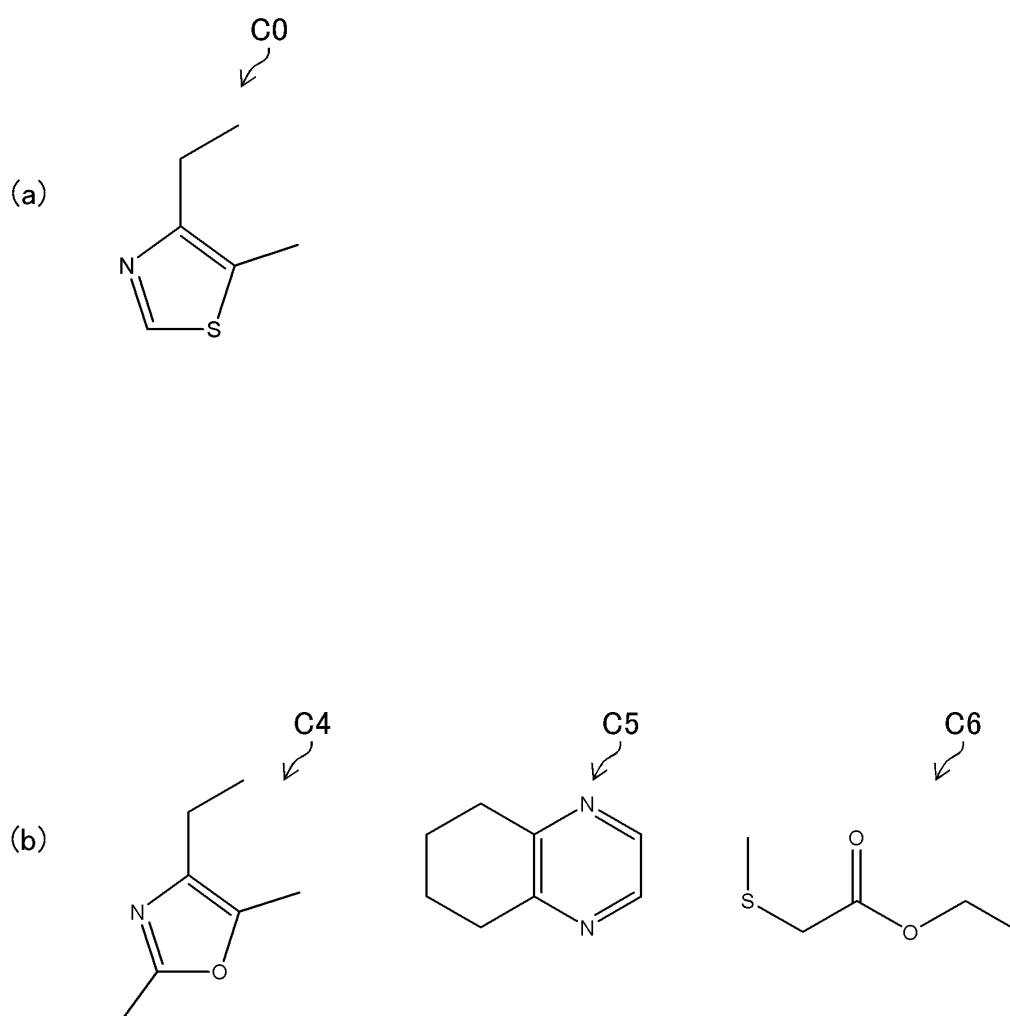
[図38]



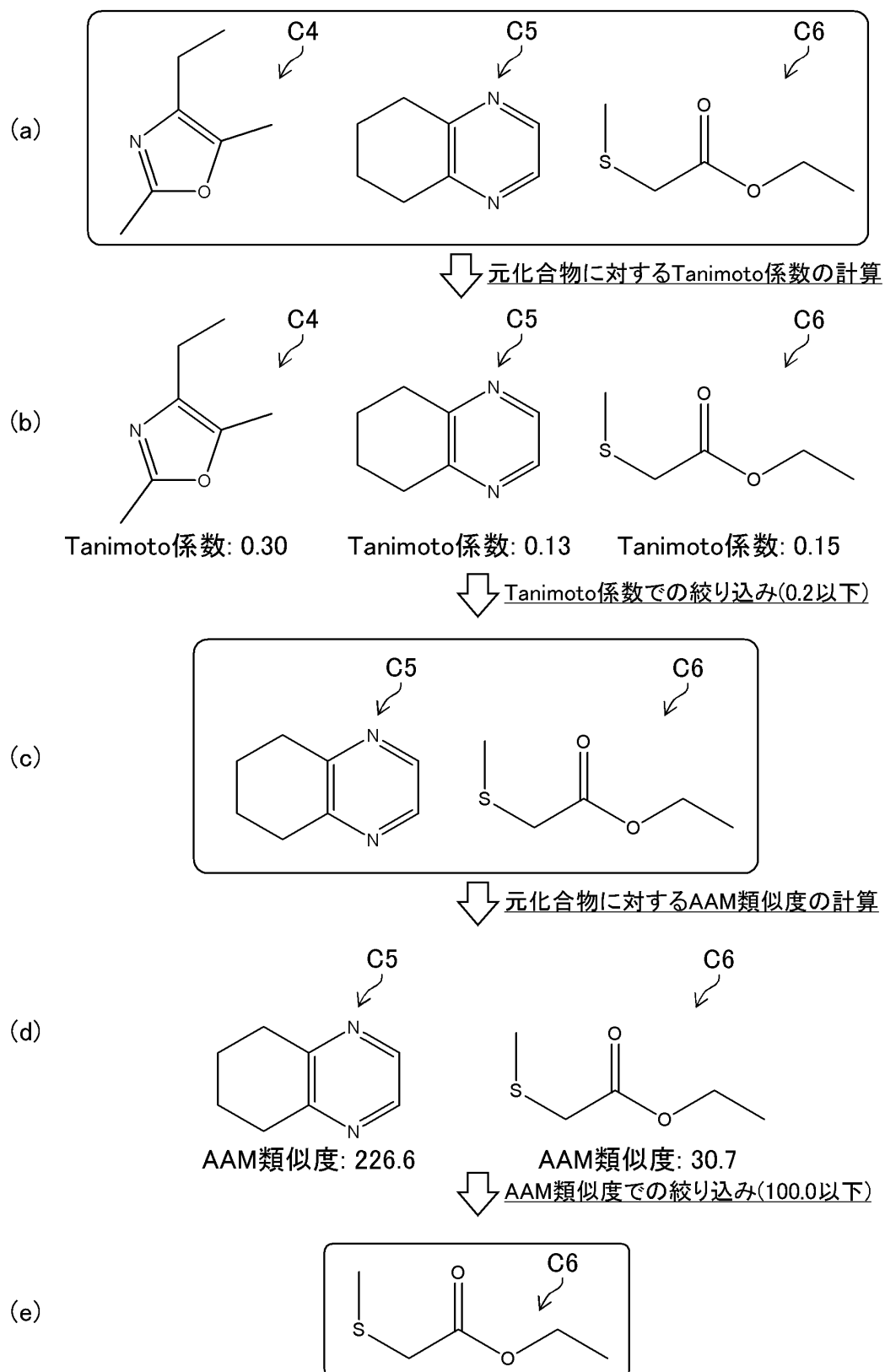
[図39]



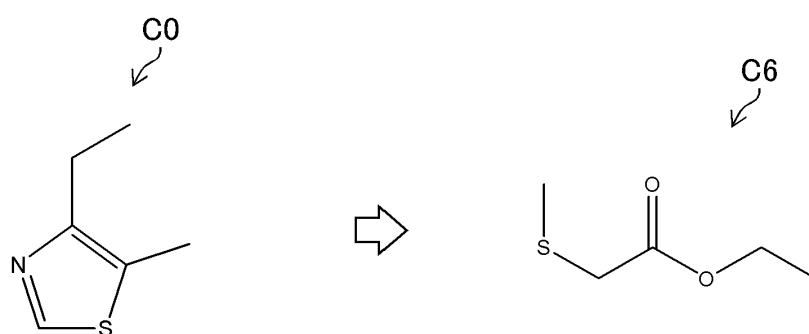
[図40]



[図41]



[図42]



[図43]

(a)

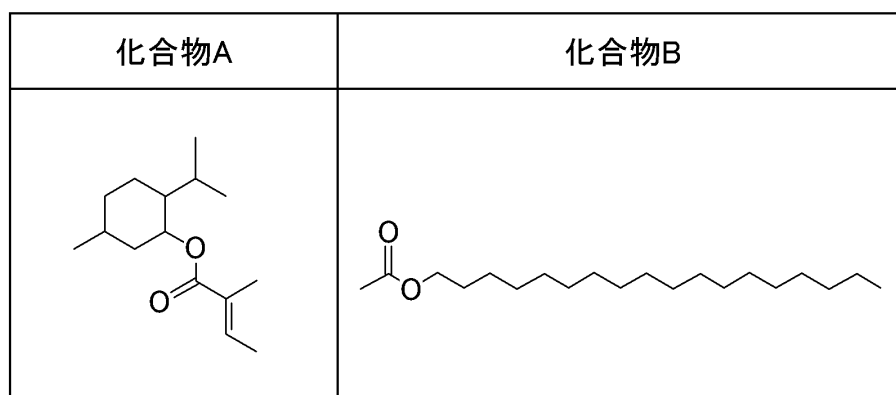
	化合物A	化合物B
ケース1		
ケース2		
ケース3		

(b)

	類似性距離 (AAM記述子)	化合物A ClogP	化合物B ClogP
ケース1	30.7	1.04	1.96
ケース2	44.7	1.64	3.40
ケース3	40.0	0.56	2.10

[図44]

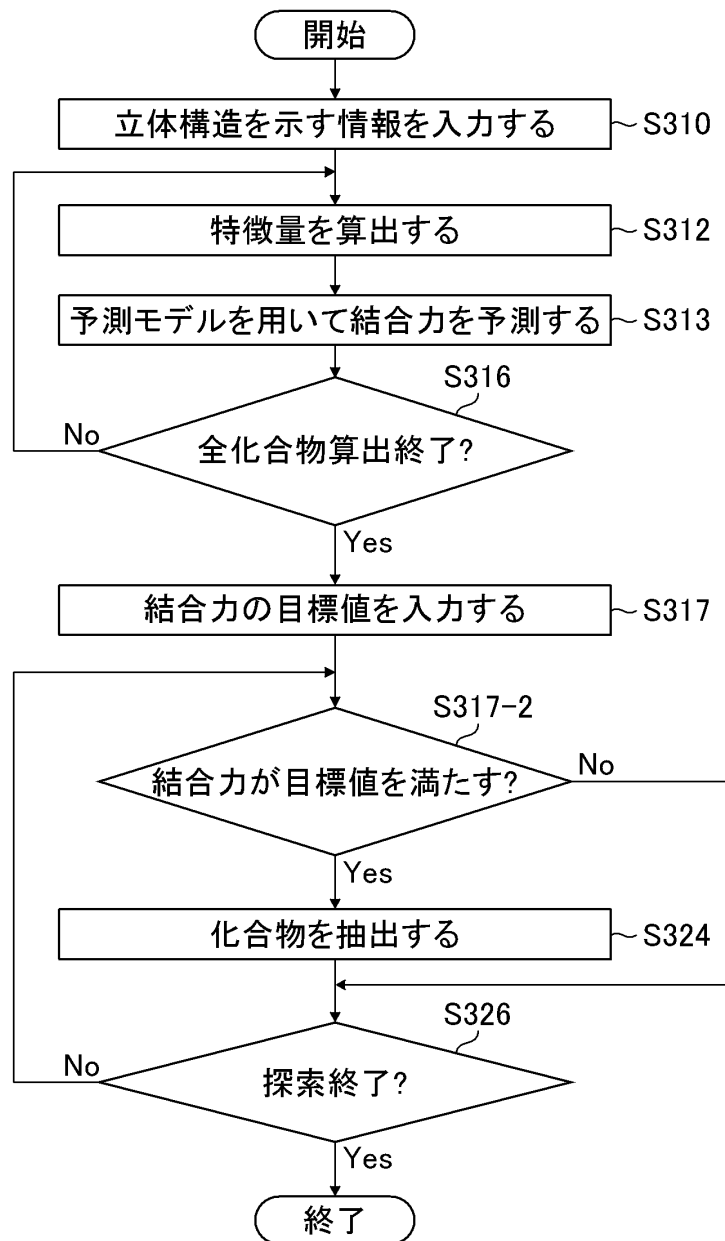
(a)



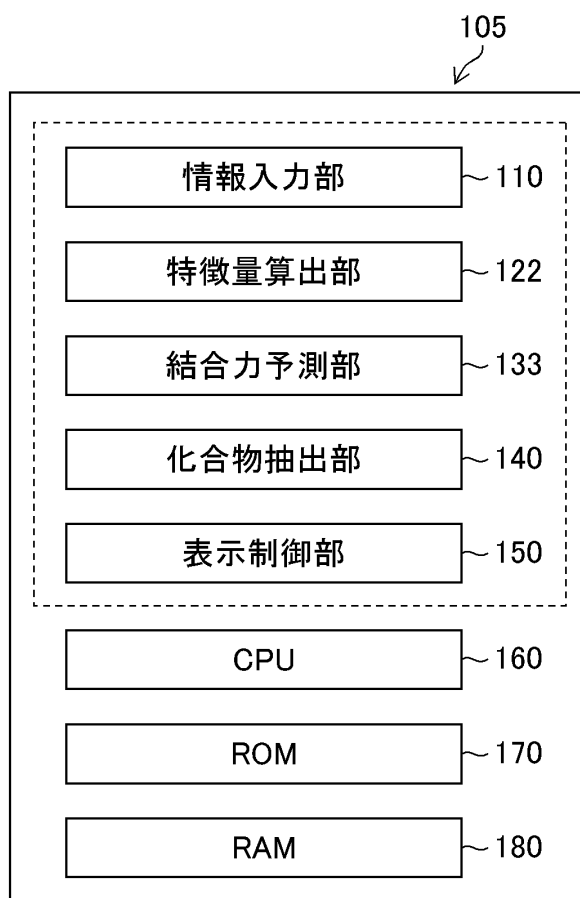
(b)

	類似性距離 (AAM記述子)	化合物A ClogP	化合物B ClogP
	12418.5	5.63	9.18

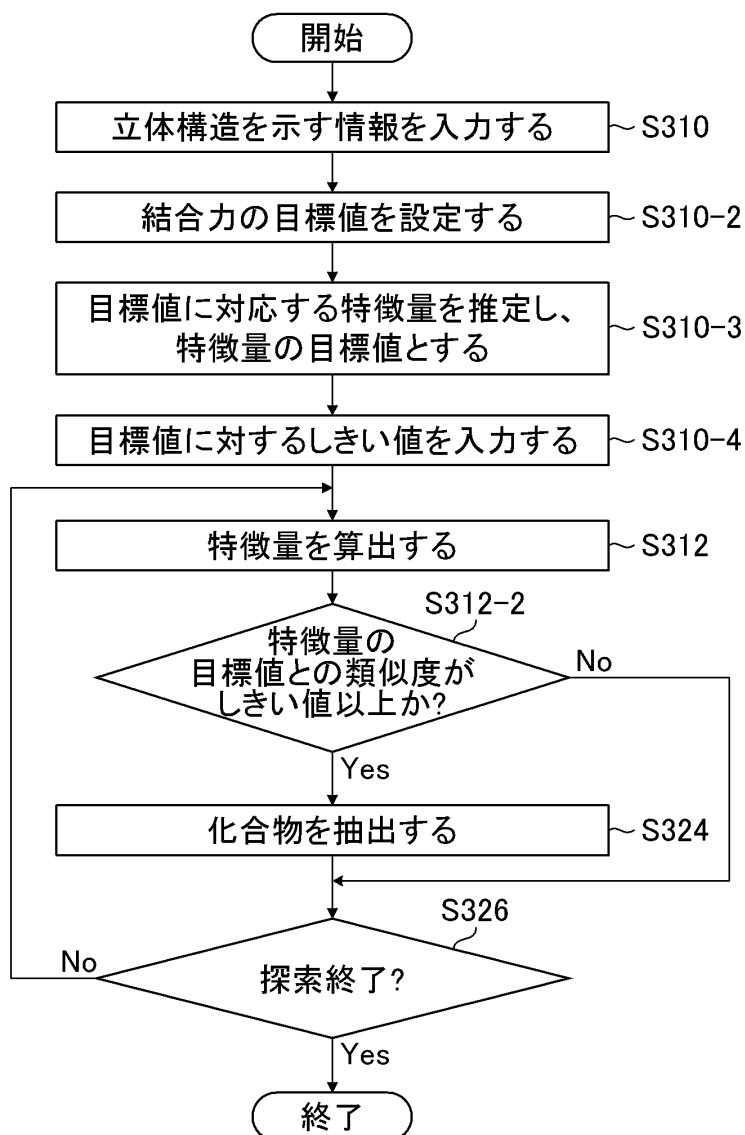
[図45]



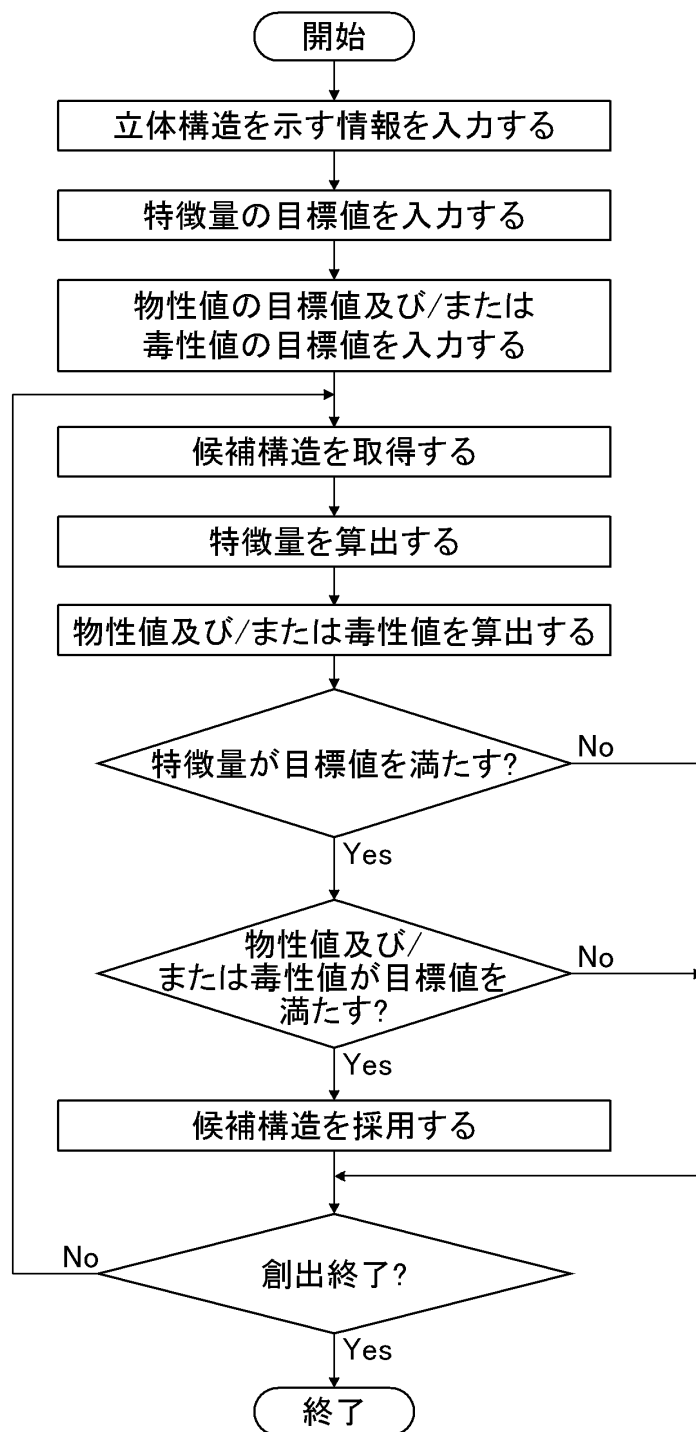
[図46]



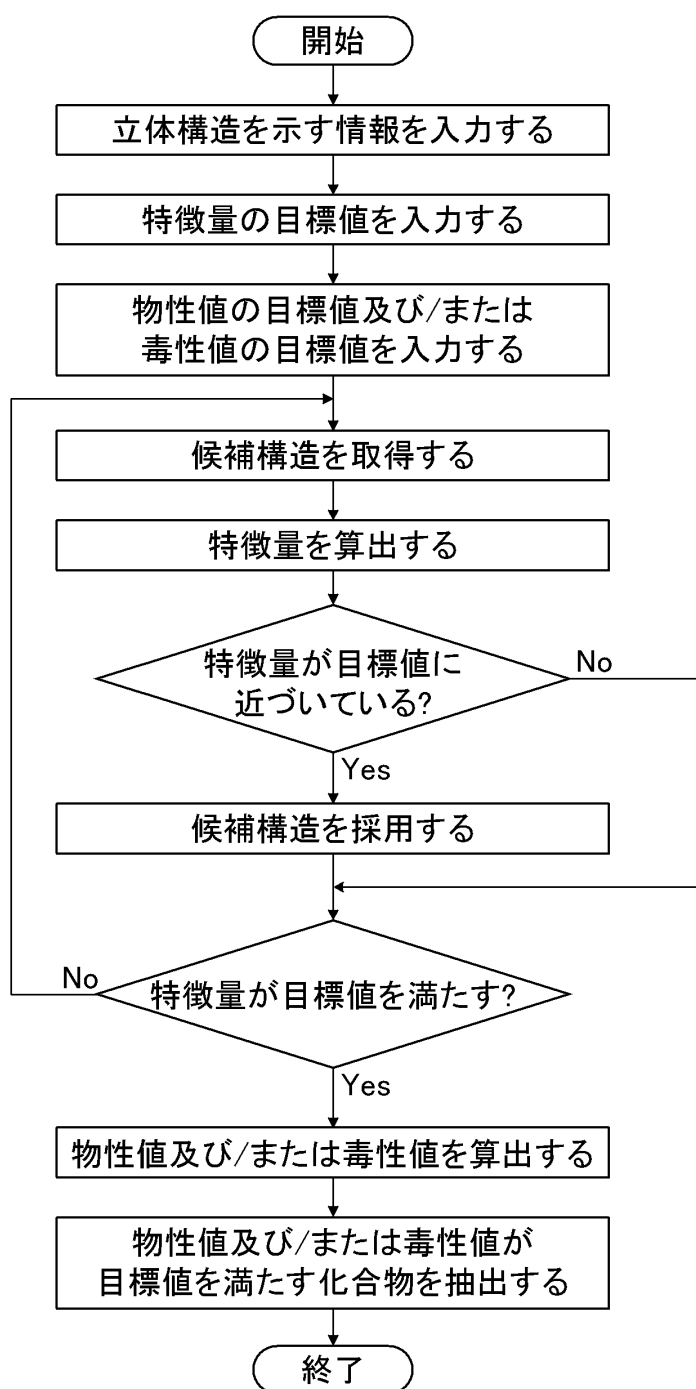
[図47]



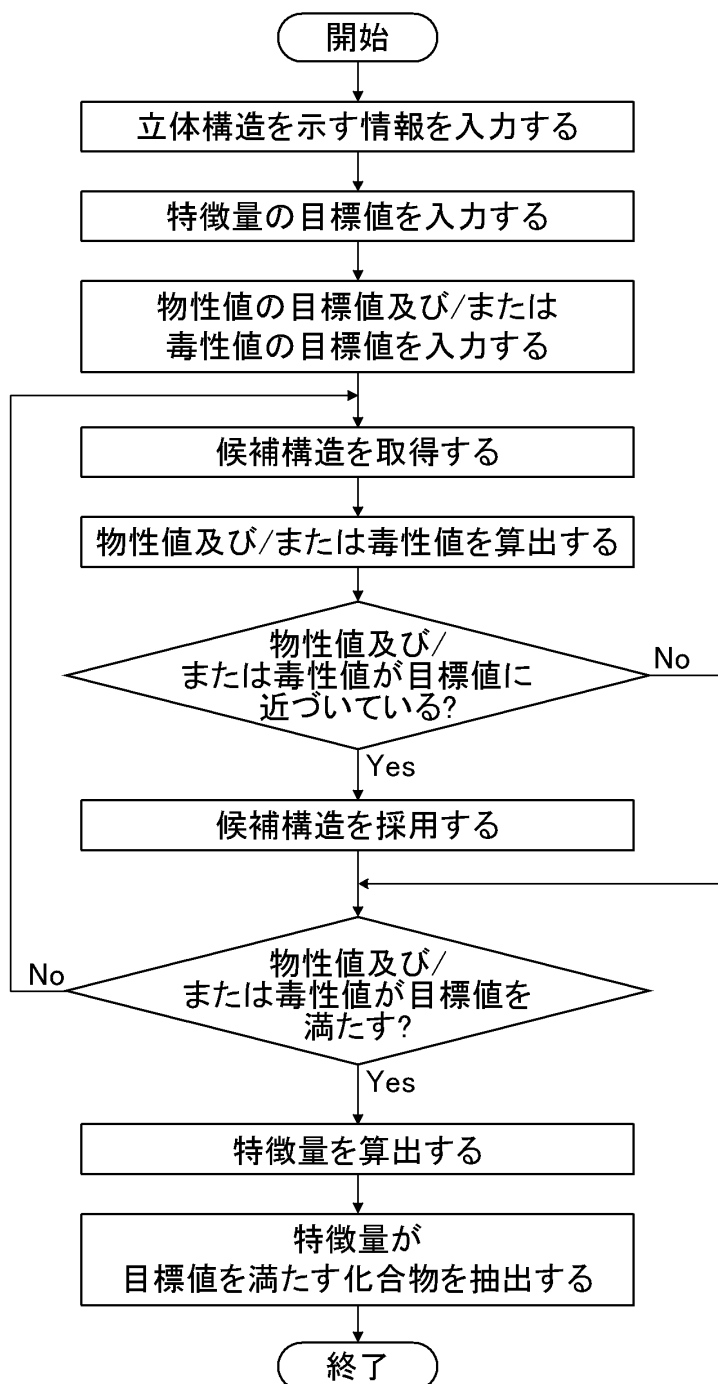
[図48]



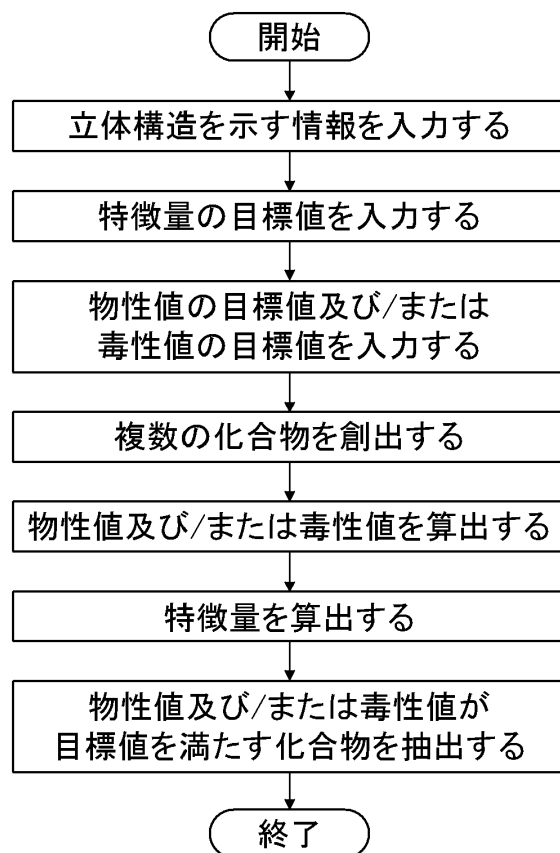
[図49]



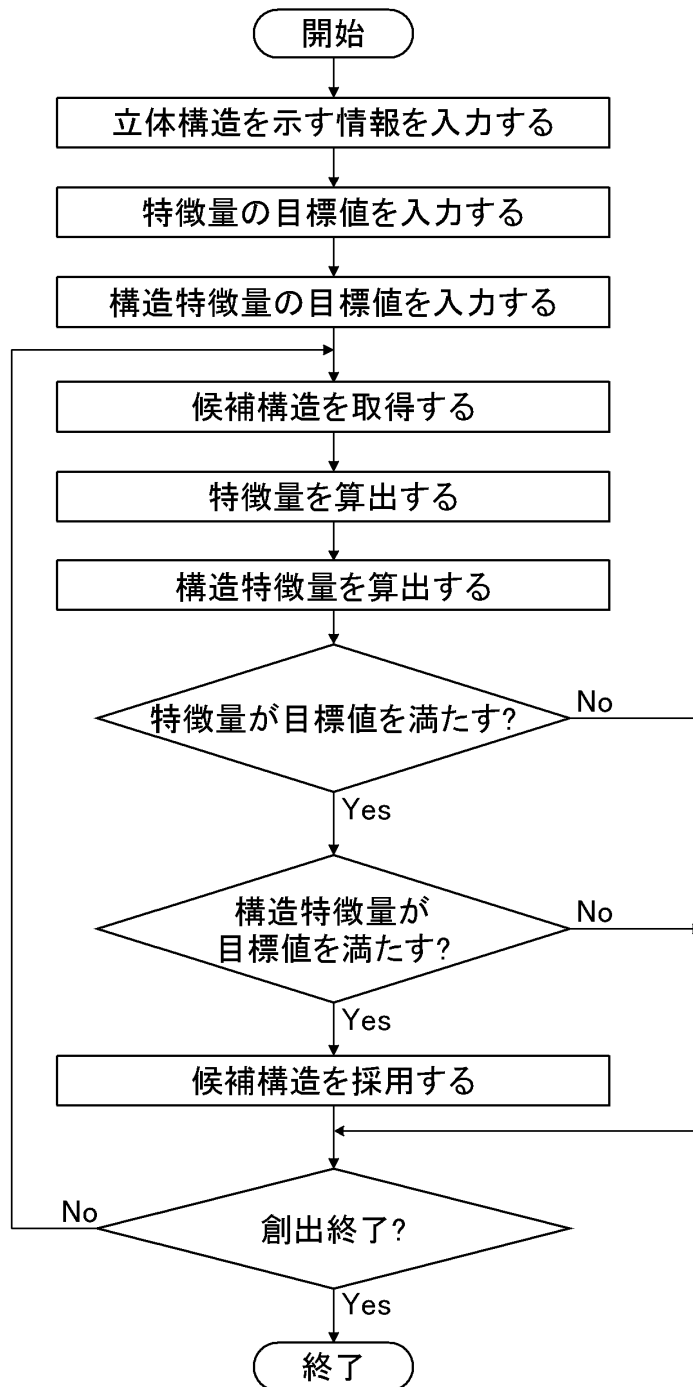
[図50]



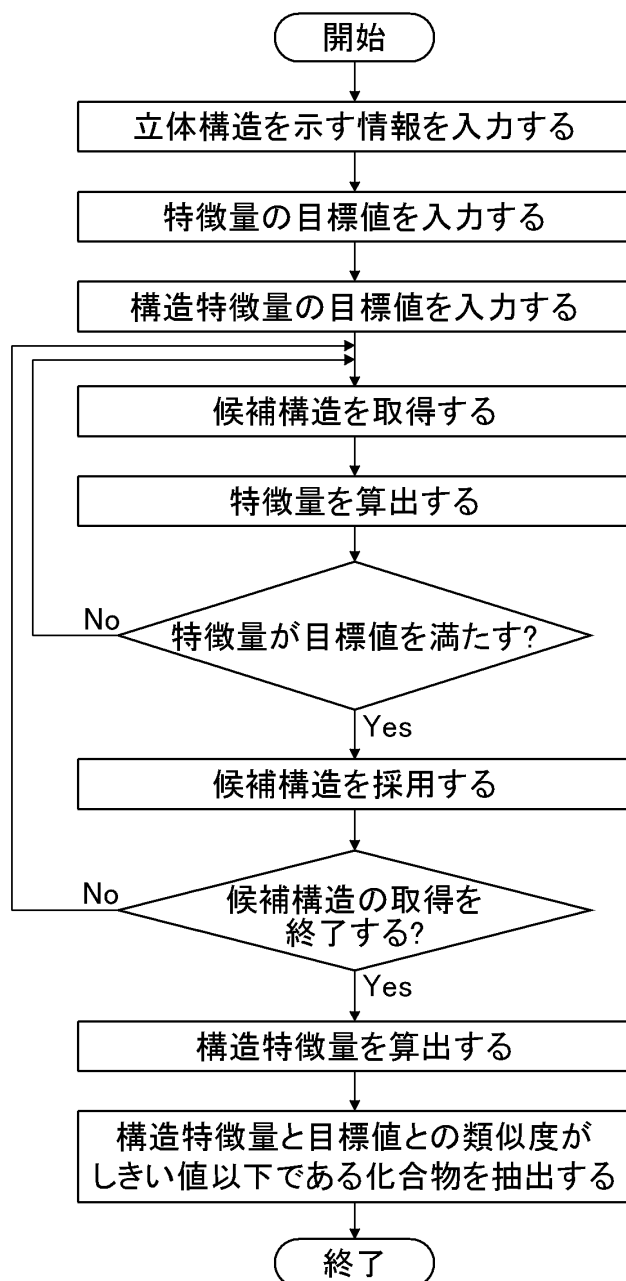
[図51]



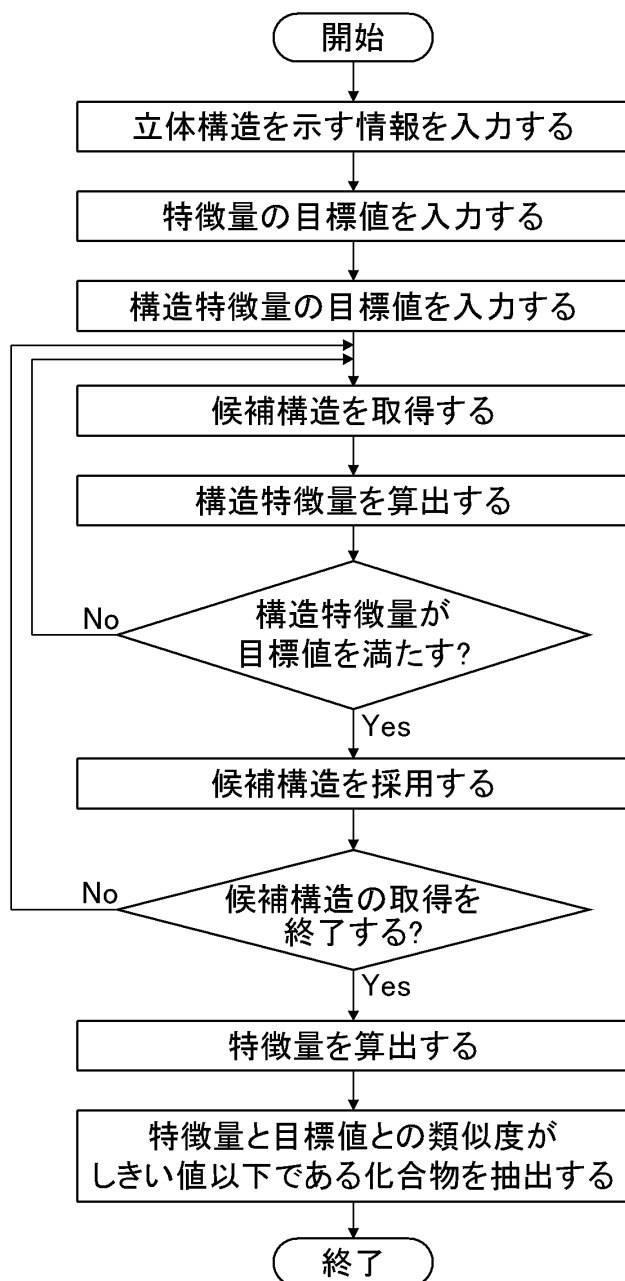
[図52]



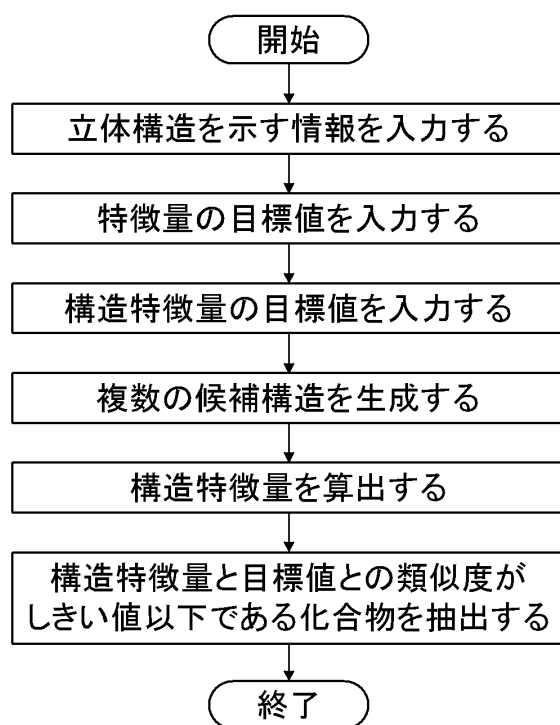
[図53]



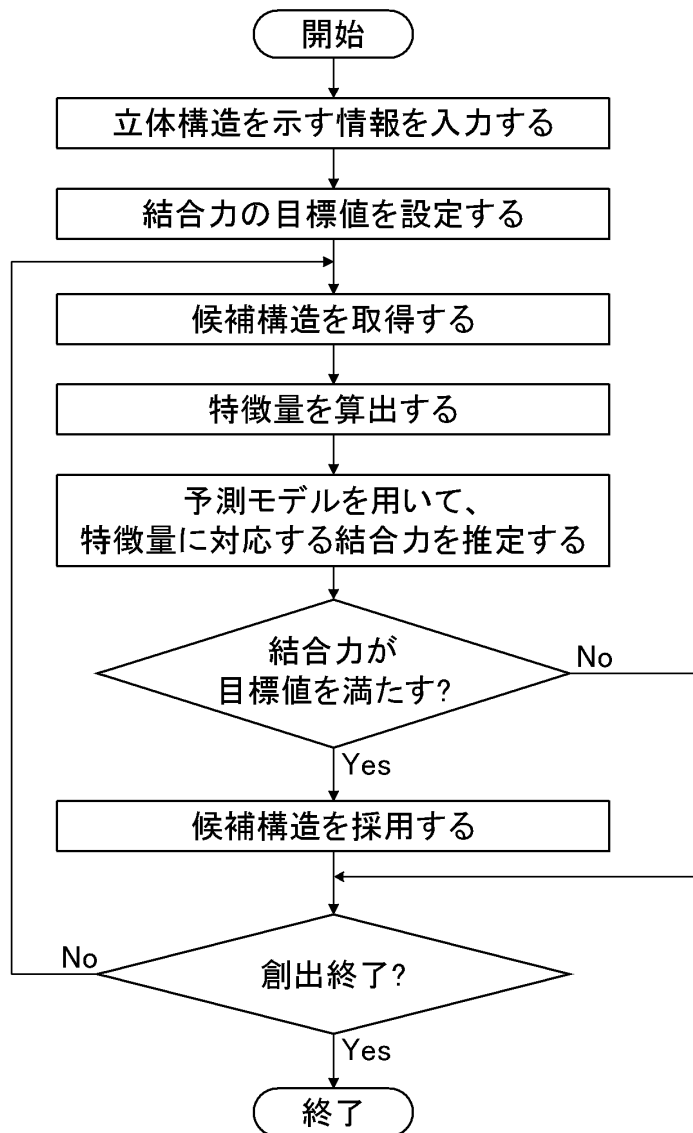
[図54]



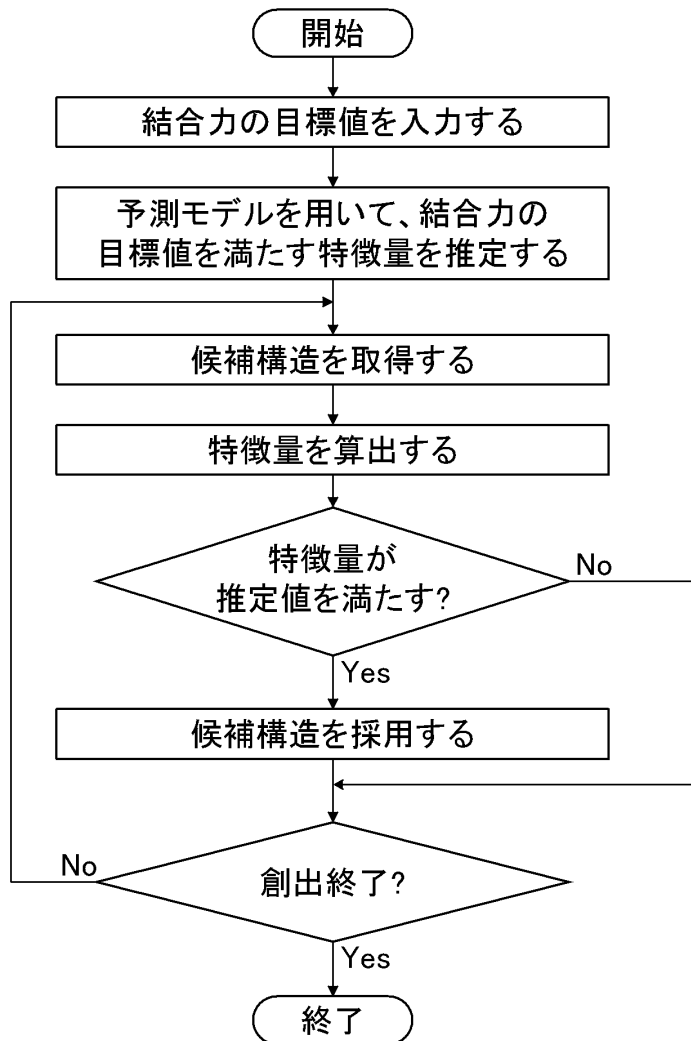
[図55]



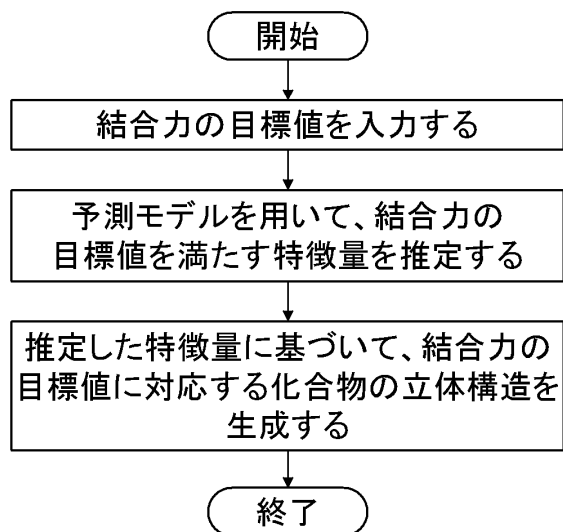
[図56]



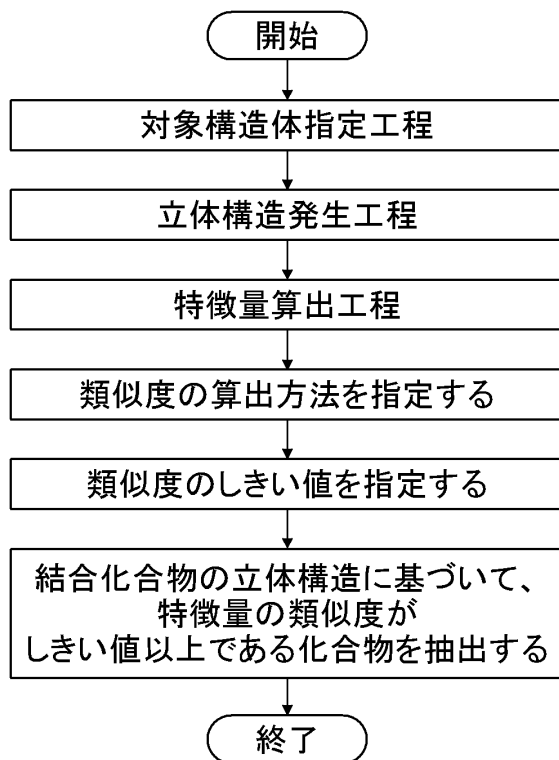
[図57]



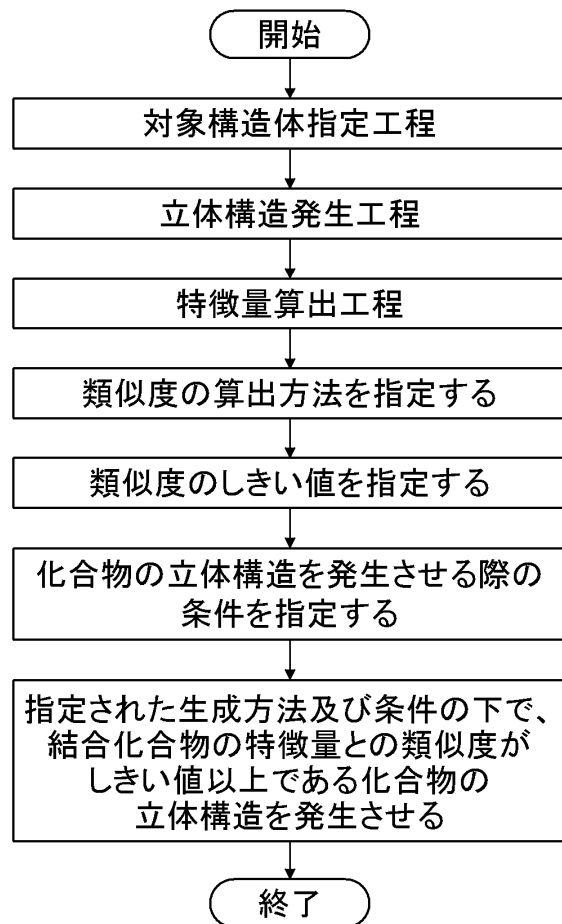
[図58]



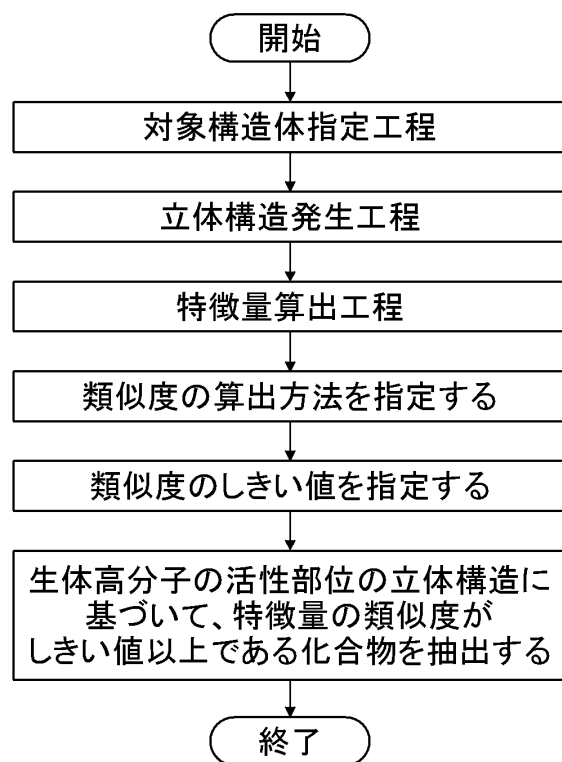
[図59]



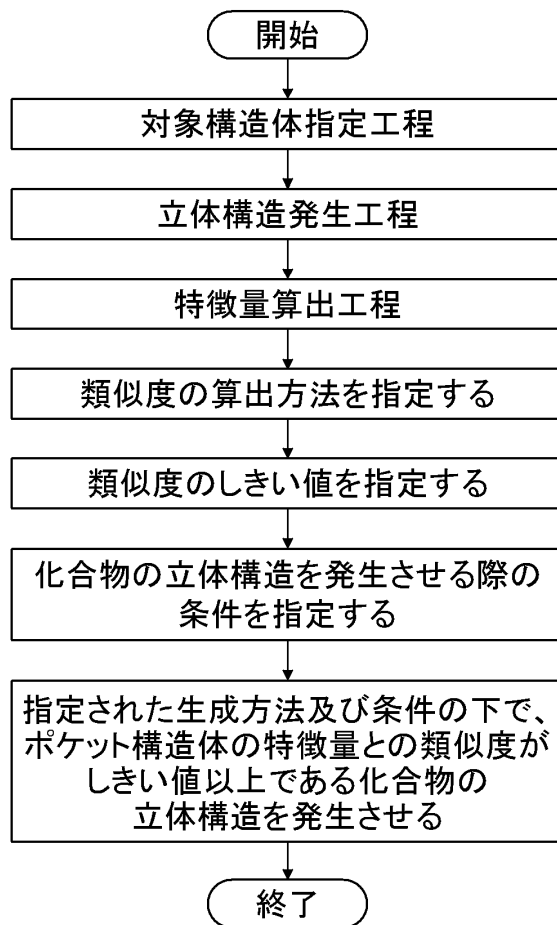
[図60]



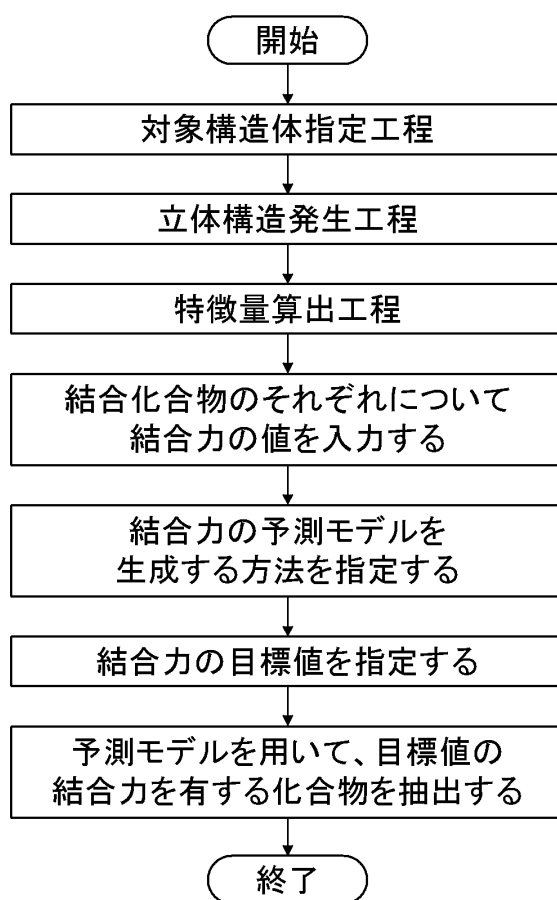
[図61]



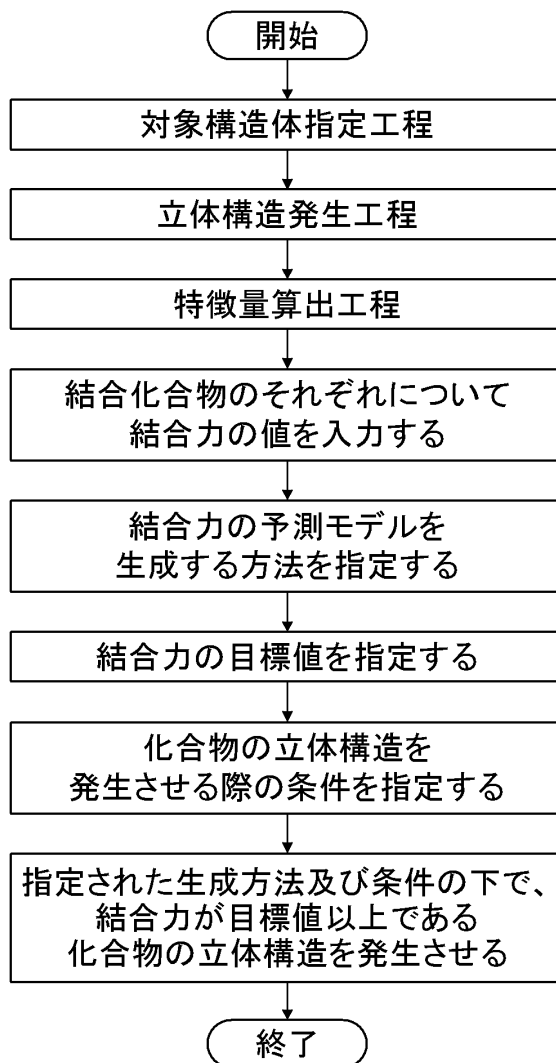
[図62]



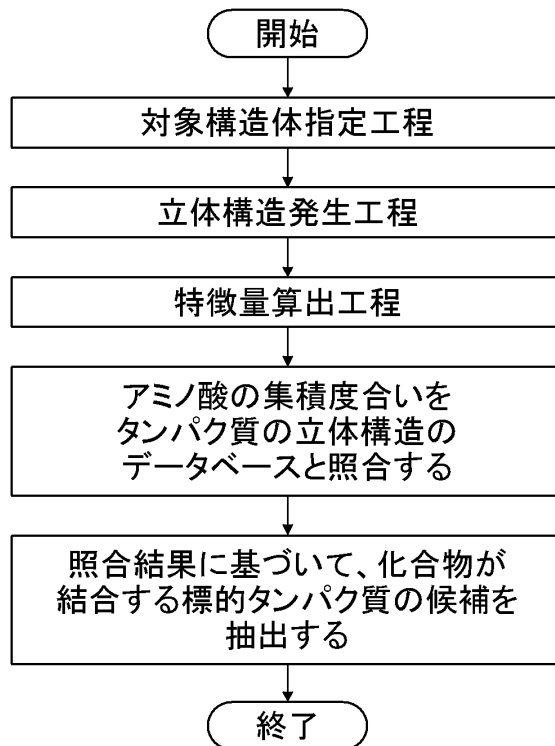
[図63]



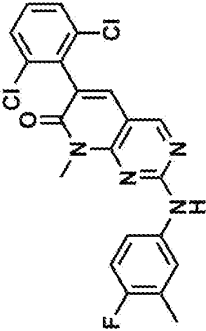
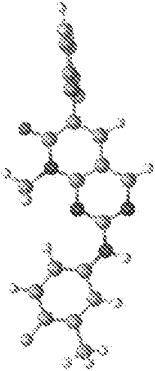
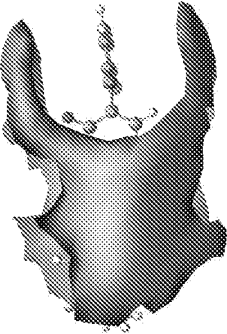
[図64]



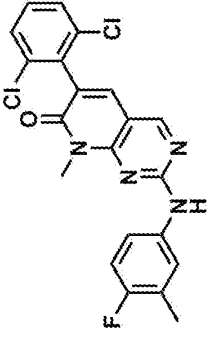
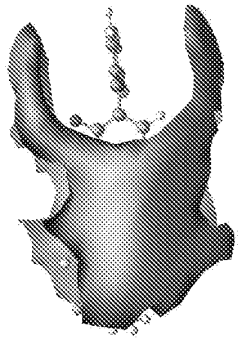
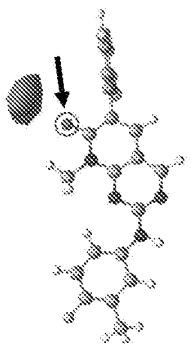
[図65]



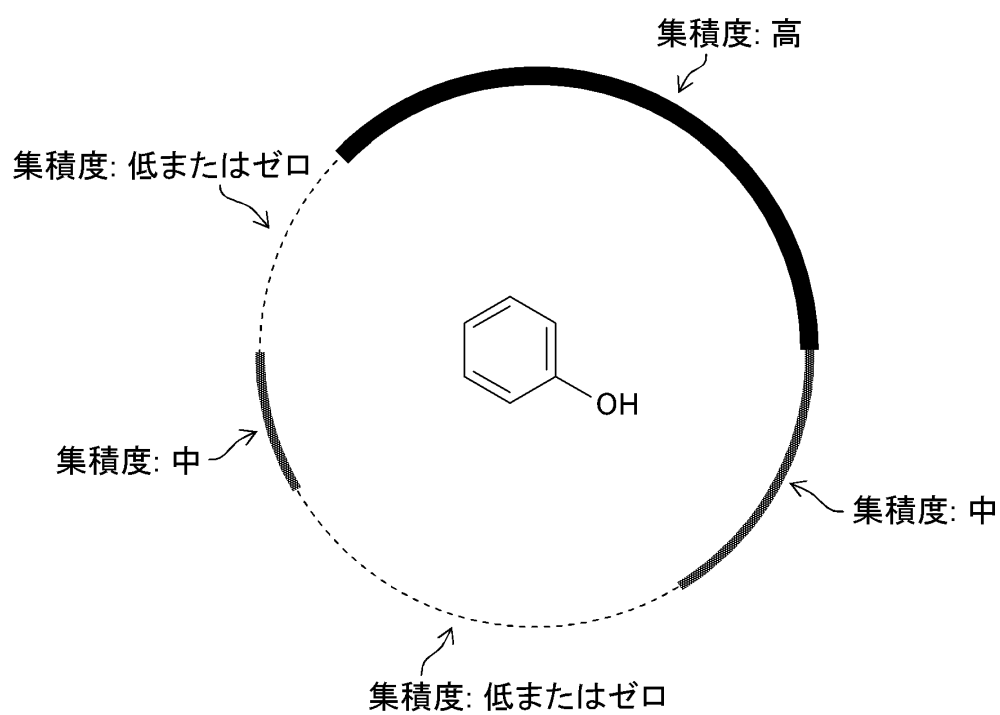
[図66]

化合物				特徴量(各アミノ酸の集積度合い)	
名前	構造式	立体構造	アラニン	...	...
lig001				...	...
lig002	...	...	...	...	...

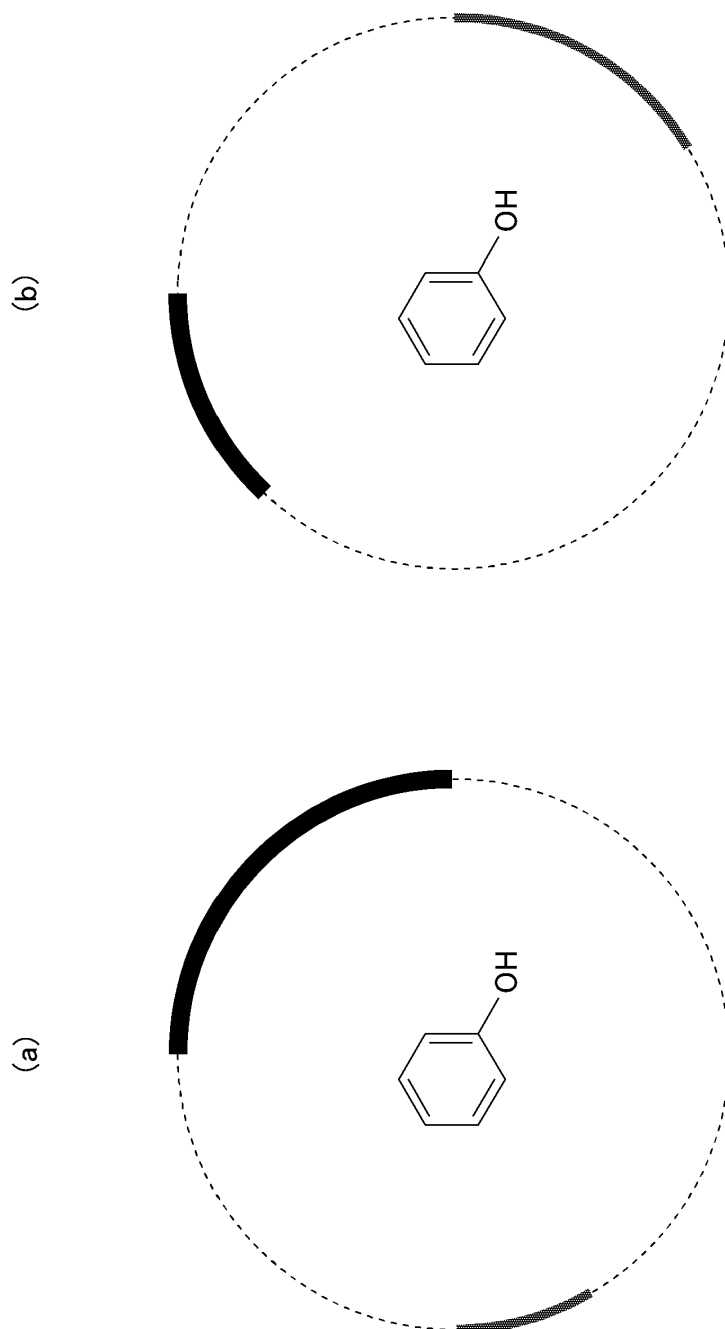
[図67]

名前	構造式	アミノ酸の集積度合い	アミノ酸の集積度合いにおける 選択原子群の持ち分
lig001			

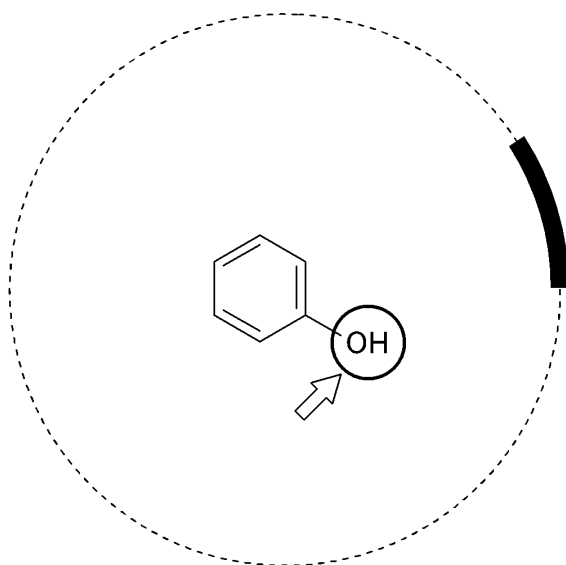
[図68]



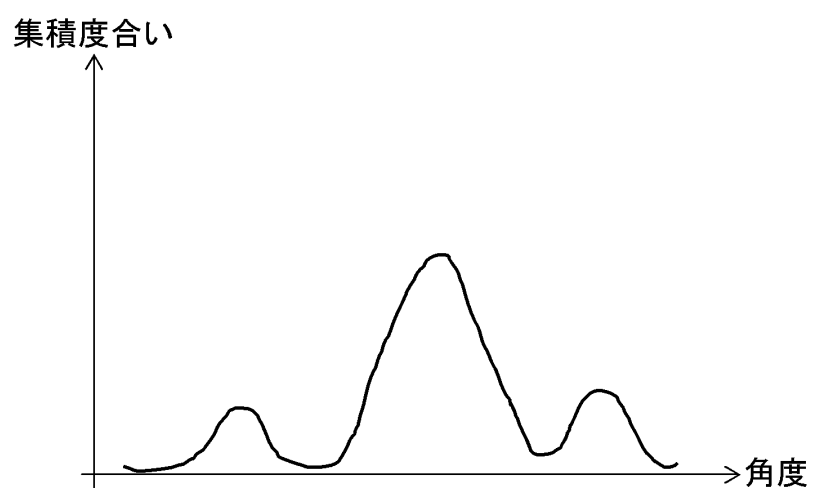
[図69]



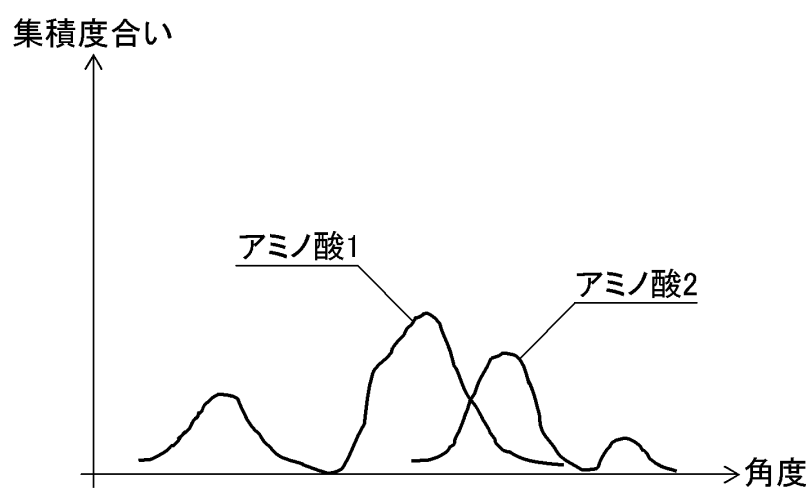
[図70]



[図71]

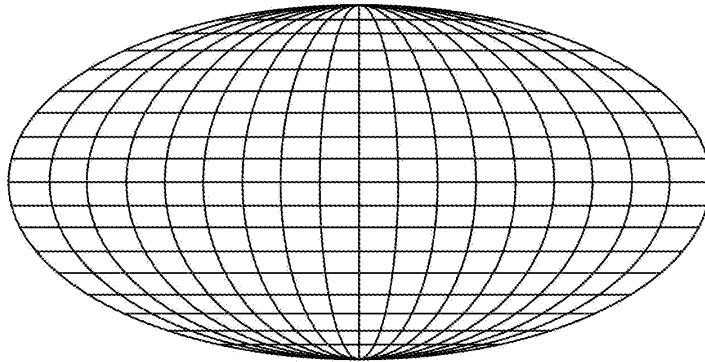


[図72]

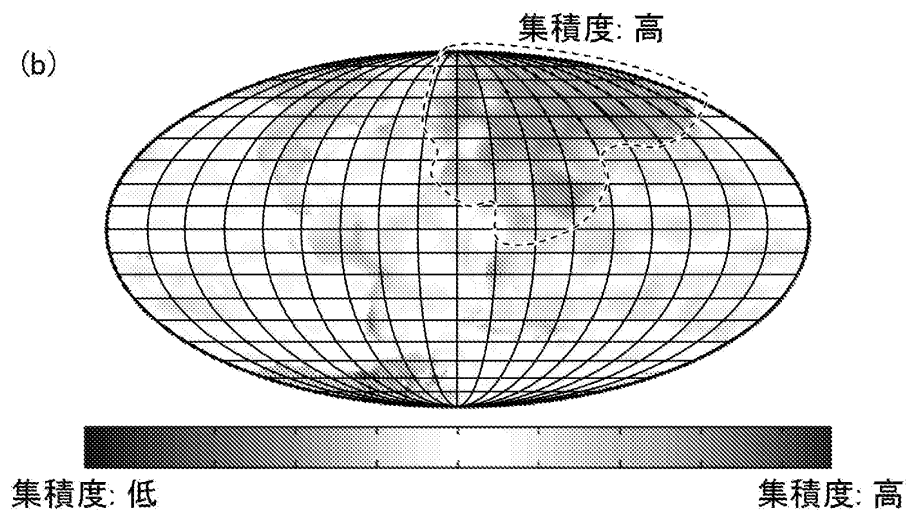


[図73]

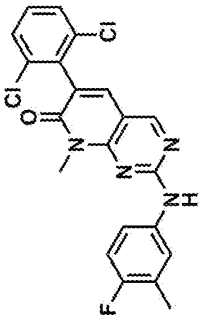
(a)



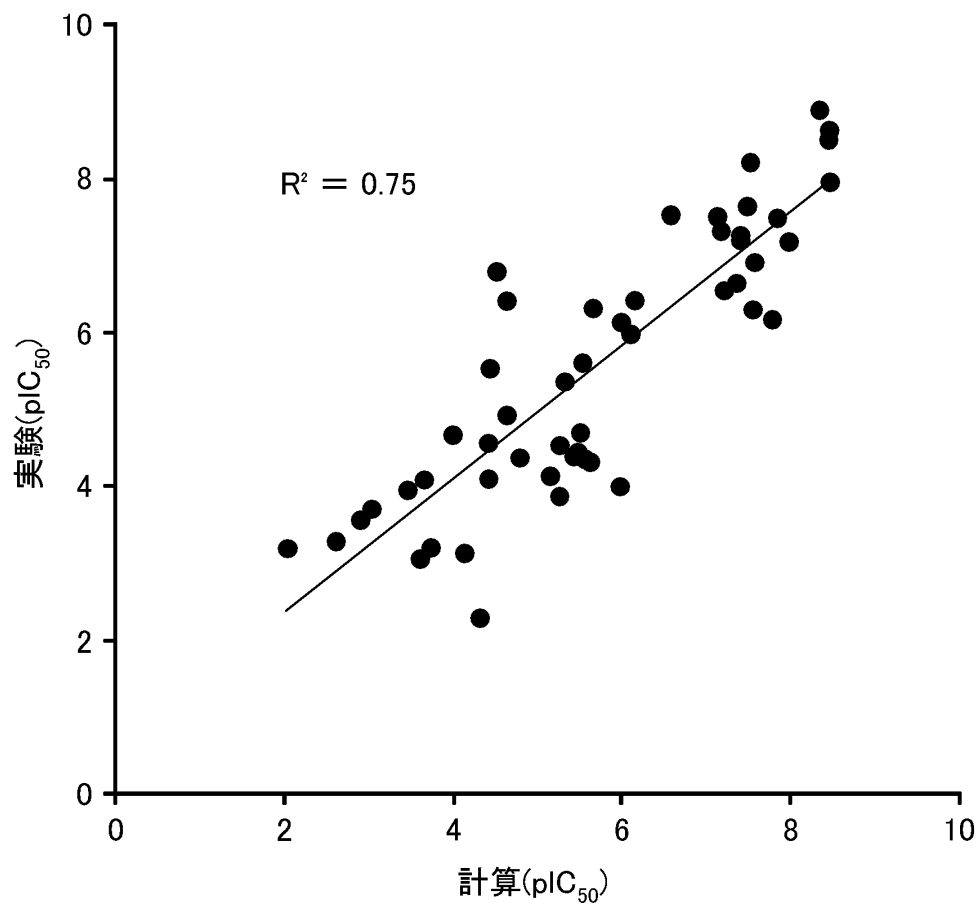
(b)



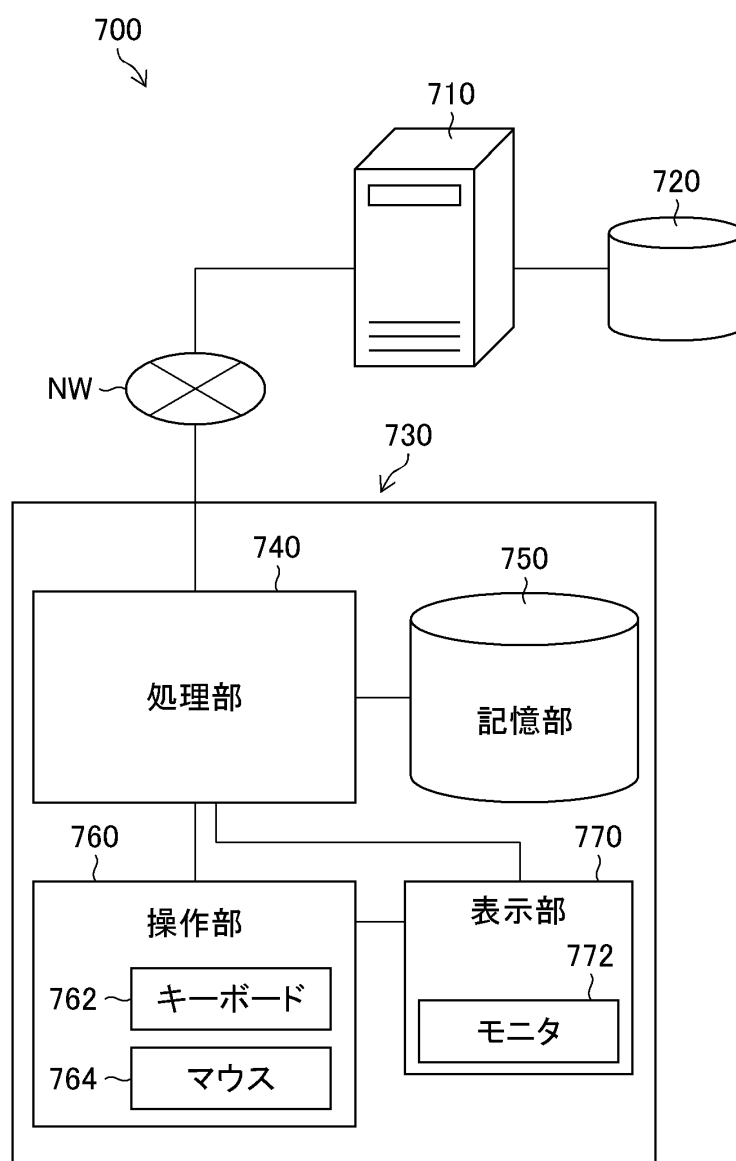
[図74]

名前	構造式	目標化合物との類似度
目標化合物		-
スクリーニング対象化合物		0.1
	...	...
	...	...

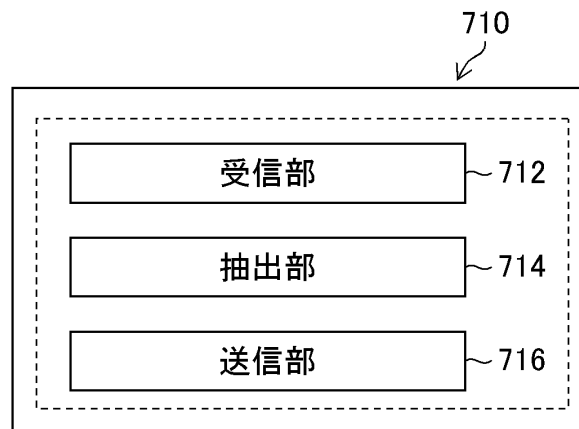
[図75]



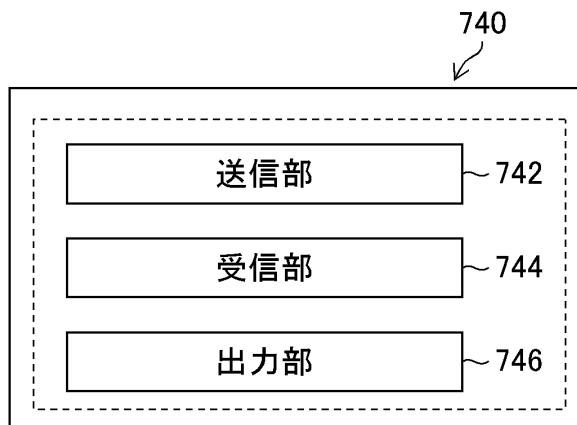
[図76]



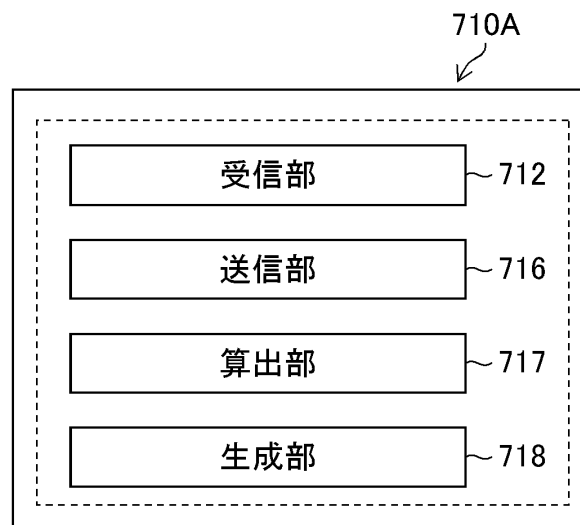
[図77]



[図78]



[図79]



[図80]

