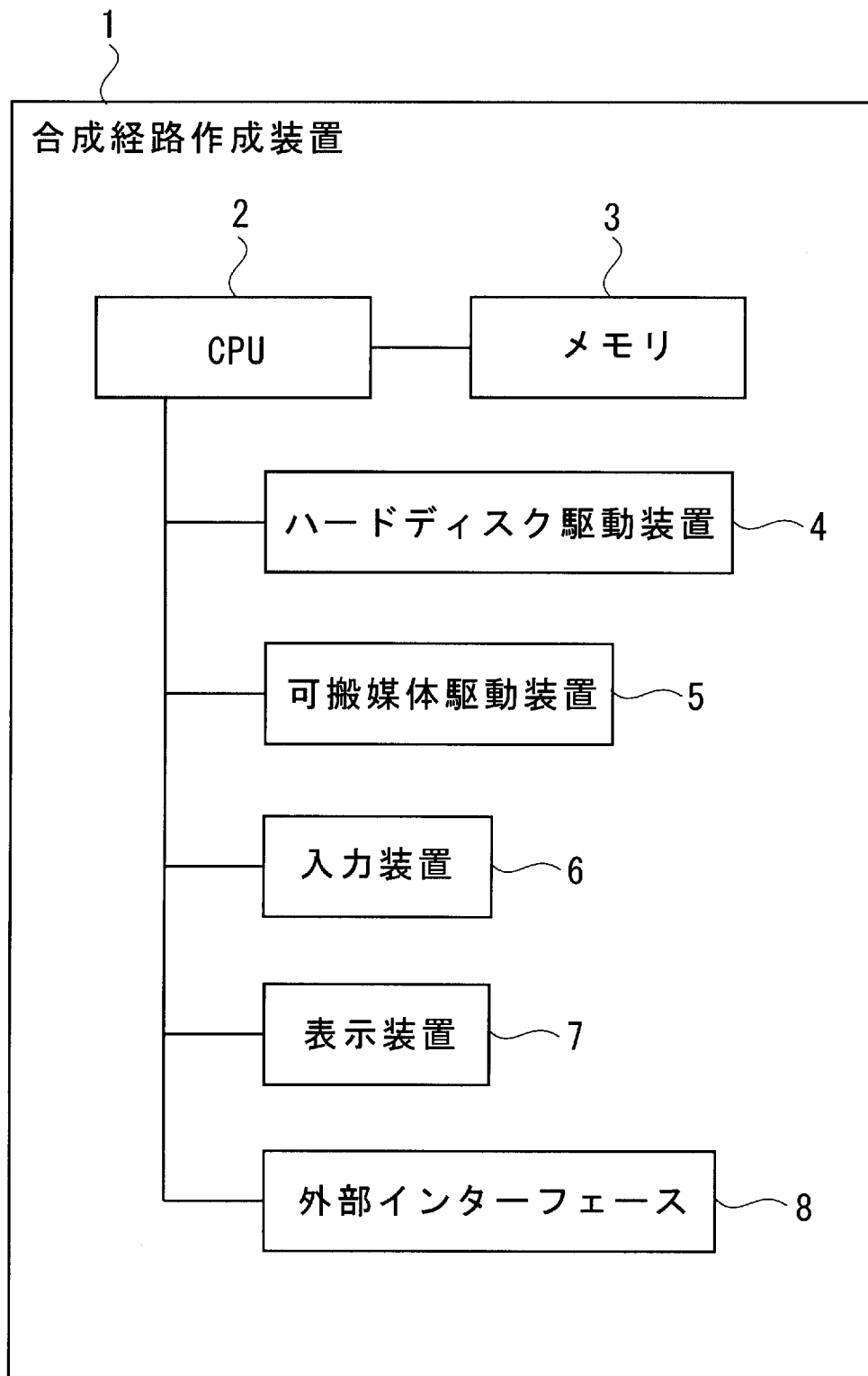
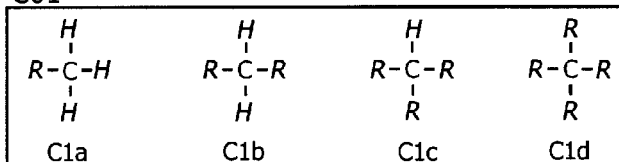


[図1]

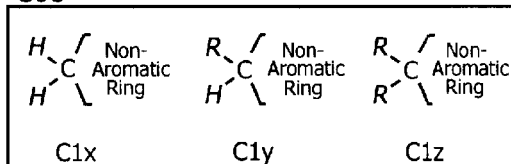


[図2]

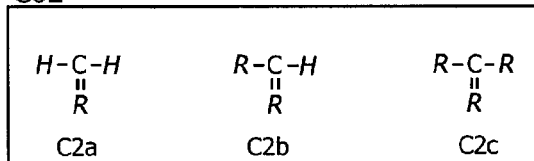
C01



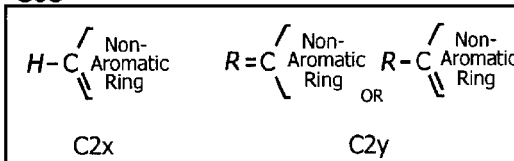
C08



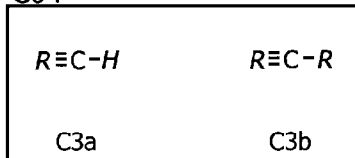
C02



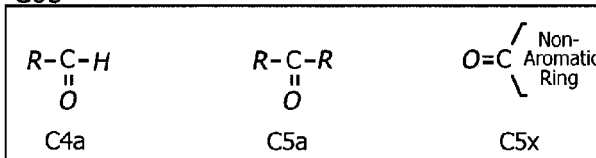
C03



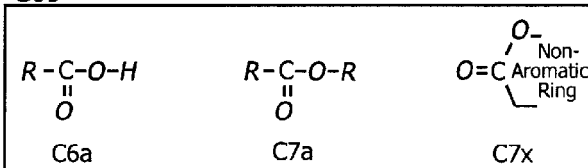
C04



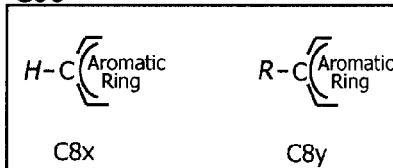
C05



C09



C06



[図3]

	識別番号A	識別番号B
1	C01	C1a
		C1b
		C1c
		C1d
2	C08	C1x
		C1y
		C1z
3	C02	C2a
		C2b
		C2c
4	C03	C2x
		C2y
5	C04	C3a
		C3b
6	C05	C4a
		C5a
		C5x
7	C09	C6a
		C7a
		C7x
8	C06	C8x
		C8y
9	C07	C0

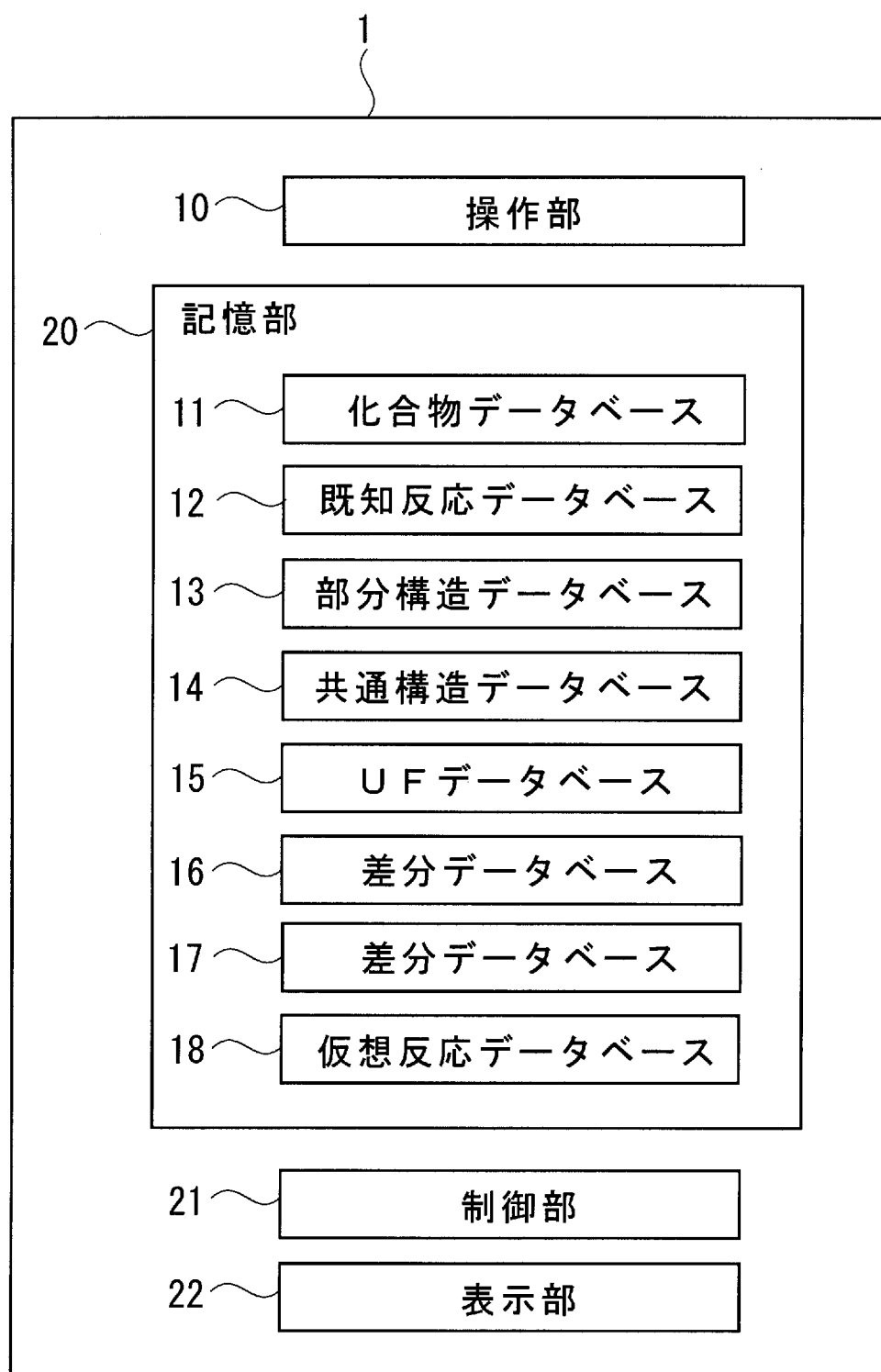
	識別番号A	識別番号B
10	S01	S1a
		S2a
		S2x
11	S04	S3a
		S3x
12	S02	S4a
13	S03	S0
14	P01	P1a
		P1b
15	X01	X
16	Z01	Z
17	R01	R
18	N01	N1a
		N1b
		N1c
		N1d
19	N06	N1x
		N1y
20	N02	N2a
		N2b
21	N07	N2x
		N2y

	識別番号A	識別番号B
22	N03	N3a
23	N04	N4x
		N4y
		N5x
		N5y
24	N05	N0
25	O01	O1a
		O1b
		O1c
		O1d
26	O05	O2a
		O2b
		O2c
		O2x
27	O02	O2a
		O2b
		O2c
		O2x
28	O03	O4a
		O5a
		O5x
29	O06	O6a
		O7a
		O7x
30	O04	O0

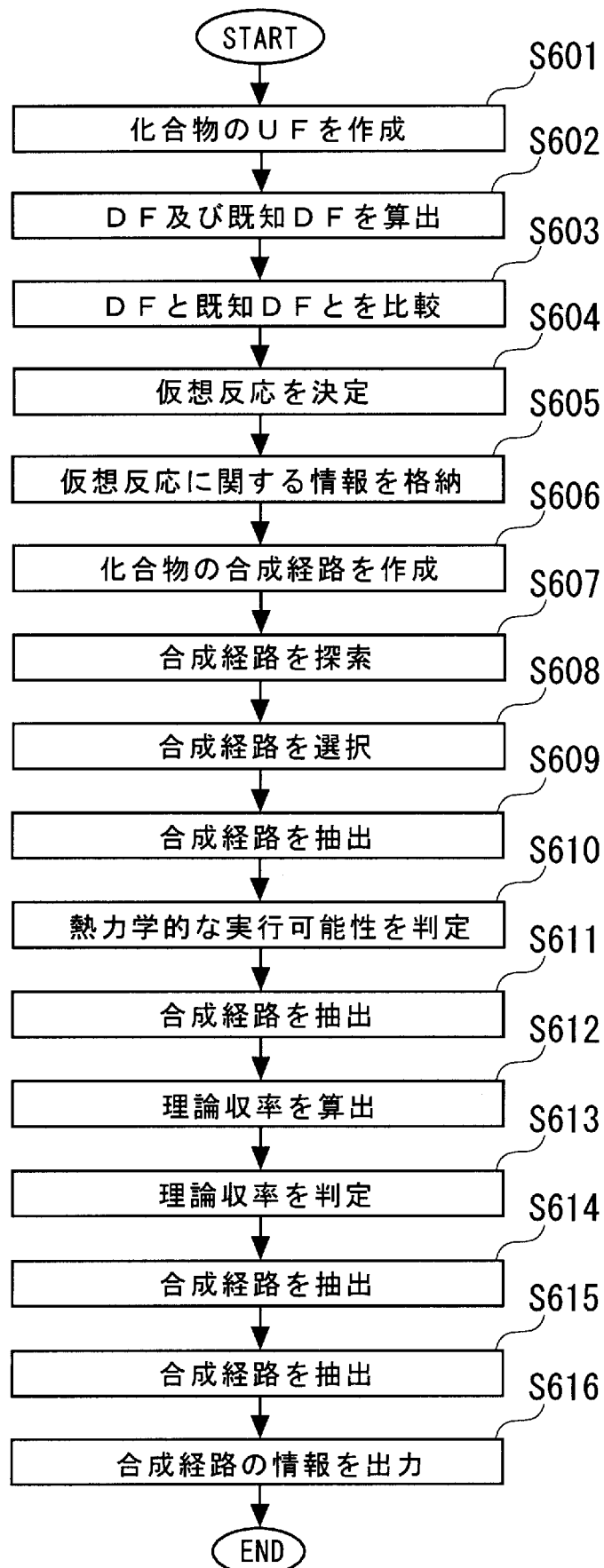
[図4]

	101	102	101	102	101	102	101	102	101	102
C01	2	C03-N02	0	C06-O06	0	N02-N02	0	O04=O04	0	
C01-C01	1	C03-N03	0	C06-P01	0	N02-N06	0	O04=X01	0	
C01-C02	0	C03-N04	0	C06-R01	0	N02-O01	0	O04=Z01	0	
C01-C03	0	C03-N06	0	C06-S01	0	N02-O02	0	O05	0	
C01-C04	0	C03-N07	0	C06-S02	0	N02-O04	0	O05-O05	0	
C01-C05	0	C03-O01	0	C06-X01	0	N02-O05	0	O05-P01	0	
C01-C06	0	C03-O04	0	C06-Z01	0	N02-O06	0	O05-R01	0	
C01-C08	0	C03-O05	0	C06=C06	0	N02-R01	0	O05-S01	0	
C01-C09	1	C03-O06	0	C06=N02	0	N02-Z01	0	O05-S02	0	
C01-N01	0	C03-R01	0	C06=N04	0	N02=N02	0	O05-Z01	0	
C01-N02	0	C03-S01	0	C06=N07	0	N02=N05	0	O06	2	
C01-N03	0	C03-S02	0	C06=O03	0	N02=O02	0	O06-P01	0	
C01-N04	0	C03-S04	0	C06=O05	0	N02=P01	0	O06-R01	0	
C01-N06	0	C03-X01	0	C06=O06	0	N02=S02	0	O06-S01	0	
C01-N07	0	C03=C03	0	C06=S01	0	N03	0	O06-Z01	0	
C01-O01	1	C03=C07	0	C06=S03	0	N03=N03	0	P01	0	
C01-O04	0	C03=N02	0	C07	0	N03=N05	0	P01-S01	0	
C01-O05	0	C03=N05	0	C07=C07	0	N04	0	P01-X01	0	
C01-O06	0	C03=N06	0	C07-C08	0	N04-N04	0	P01-Z01	0	
C01-P01	0	C03=N07	0	C07=N02	0	N04-O01	0	P01=S03	0	
C01-R01	0	C03=S03	0	C07=O04	0	N04-O04	0	P01=Z01	0	
C01-S01	0	C04	0	C07=S03	0	N04-O05	0	R01	0	
C01-S02	0	C04=C04	0	C08	0	N04-O06	0	R01-S01	0	
C01-S03	0	C04=N03	0	C08-C08	0	N04-P01	0	R01-S02	0	
C01-S04	0	C04=O04	0	C08-C09	0	N04-R01	0	R01-S04	0	
C01-X01	0	C04-C04	0	C08-N01	0	N04-S01	0	R01-X01	0	
C01-Z01	0	C04-C05	0	C08-N02	0	N04-S02	0	R01-Z01	0	
C02	0	C04-C06	0	C08-N03	0	N04-Z01	0	S01	0	
C02-C02	0	C04-C08	0	C08-N04	0	N04=N04	0	S01-S01	0	
C02-C03	0	C04-C09	0	C08-N06	0	N05	0	S01-S02	0	
C02-C04	0	C04-N01	0	C08-N07	0	N05-S02	0	S01-S04	0	
C02-C05	0	C04-O01	0	C08-O01	0	N05=O02	0	S01-Z01	0	
C02-C06	0	C04-R01	0	C08-O04	0	N06	0	S02	0	
C02-C08	0	C04-S01	0	C08-O05	0	N06-N06	0	S02-S03	0	
C02-C09	0	C04-X01	0	C08-O06	0	N06-N07	0	S02-S04	0	
C02-N01	0	C04-Z01	0	C08-P01	0	N06-O01	0	S02-X01	0	
C02-N02	0	C05	0	C08-R01	0	N06-O05	0	S03	0	
C02-N04	0	C05-C05	0	C08-S01	0	N06-P01	0	S04	0	
C02-N06	0	C05-C06	0	C08-S02	0	N06-S01	0	S04-S04	0	
C02-O01	0	C05-C08	0	C08-S04	0	N06-S02	0	X01	0	
C02-O05	0	C05-C09	0	C08-X01	0	N06-Z01	0	X01-X01	0	
C02-O06	0	C05-N01	0	C08-Z01	0	N06=N07	0	X01-Z01	0	
C02-P01	0	C05-N02	0	C09	1	N07	0	Z01	0	
C02-R01	0	C05-N04	0	C09-C09	0	N07-N07	0	Z01-Z01	0	
C02-S01	0	C05-N05	0	C09-N01	0	N07-O04	0	Z01=Z01	0	
C02-S02	0	C05-N06	0	C09-N04	0	N07-O05	0			
C02-S03	0	C05-N07	0	C09-N06	0	N07-S01	0			
C02-S04	0	C05-O01	0	C09-O04	0	N07=N07	0			
C02-X01	0	C05-O05	0	C09-O06	1	N07=O02	0			
C02-Z01	0	C05-R01	0	C09-P01	0	O01	1			
C02=C02	0	C05-S01	0	C09-R01	0	O01-O01	0			
C02=C03	0	C05-S02	0	C09-S01	0	O01-O05	0			
C02=C06	0	C05-S04	0	C09-X01	0	O01-P01	0			
C02=C07	0	C05-X01	0	C09=O06	1	O01-R01	0			
C02=N02	0	C05-Z01	0	N01	0	O01-S02	0			
C02=N07	0	C05=O03	0	N01-N01	0	O01-X01	0			
C02=O04	0	C06	0	N01-N02	0	O01-Z01	0			
C02=R01	0	C06-C06	0	N01-N04	0	O02	0			
C02=S02	0	C06-C08	0	N01-N06	0	O02=P01	0			
C02=S03	0	C06-C09	0	N01-O01	0	O02=S01	0			
C03	0	C06-N01	0	N01-O04	0	O02=S02	0			
C03-C03	0	C06-N02	0	N01-O05	0	O02=S04	0			
C03-C04	0	C06-N03	0	N01-O06	0	O03	0			
C03-C05	0	C06-N04	0	N01-P01	0	O04	0			
C03-C06	0	C06-N06	0	N01-R01	0	O04-O05	0			
C03-C07	0	C06-N07	0	N01-S01	0	O04-P01	0			
C03-C08	0	C06-O01	0	N01-S02	0	O04-S02	0			
C03-C09	0	C06-O04	0	N01-Z01	0	O04-X01	0			
C03-N01	0	C06-O05	0	N02	0	O04-Z01	0			

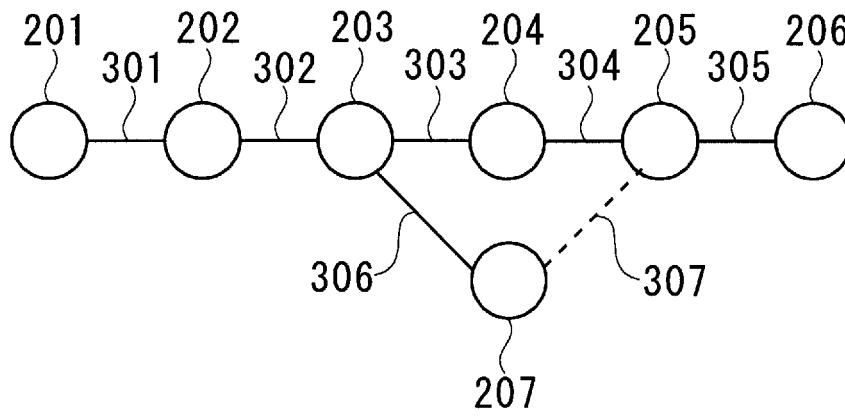
[図5]



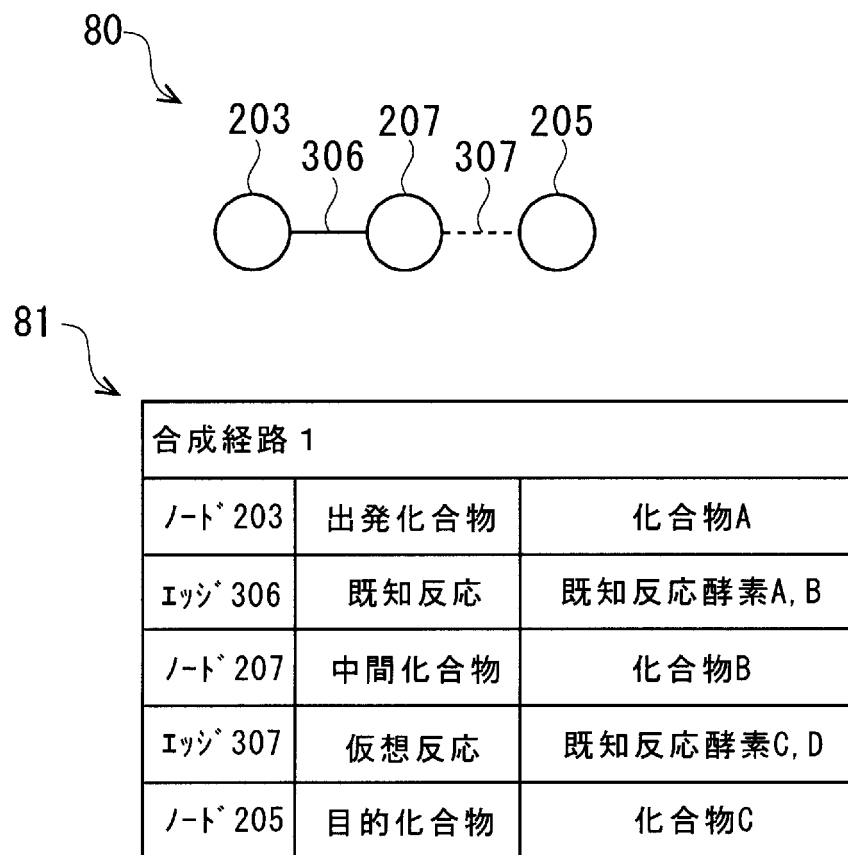
[図6]



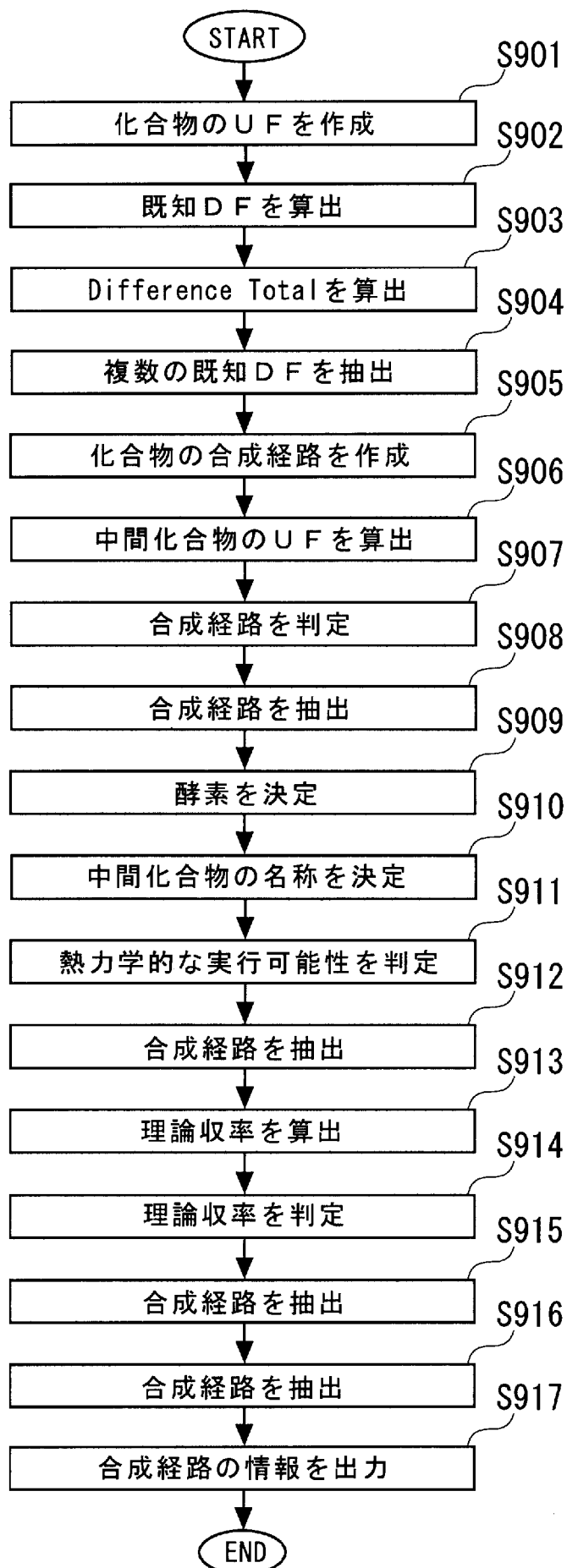
[図7]



[図8]



[図9]



[図10]

1	出発化合物, 既知DF1, 既知DF2, 既知DF3, 目的化合物
2	出発化合物, 既知DF1, 既知DF3, 既知DF2, 目的化合物
3	出発化合物, 既知DF2, 既知DF1, 既知DF3, 目的化合物
4	出発化合物, 既知DF2, 既知DF3, 既知DF1, 目的化合物
5	出発化合物, 既知DF3, 既知DF1, 既知DF2, 目的化合物
6	出発化合物, 既知DF3, 既知DF2, 既知DF1, 目的化合物

DF組合せ群

既知DF1 + 既知DF2 + 既知DF3 = Difference Total = 目的化合物DF - 出発化合物DF

[図11]

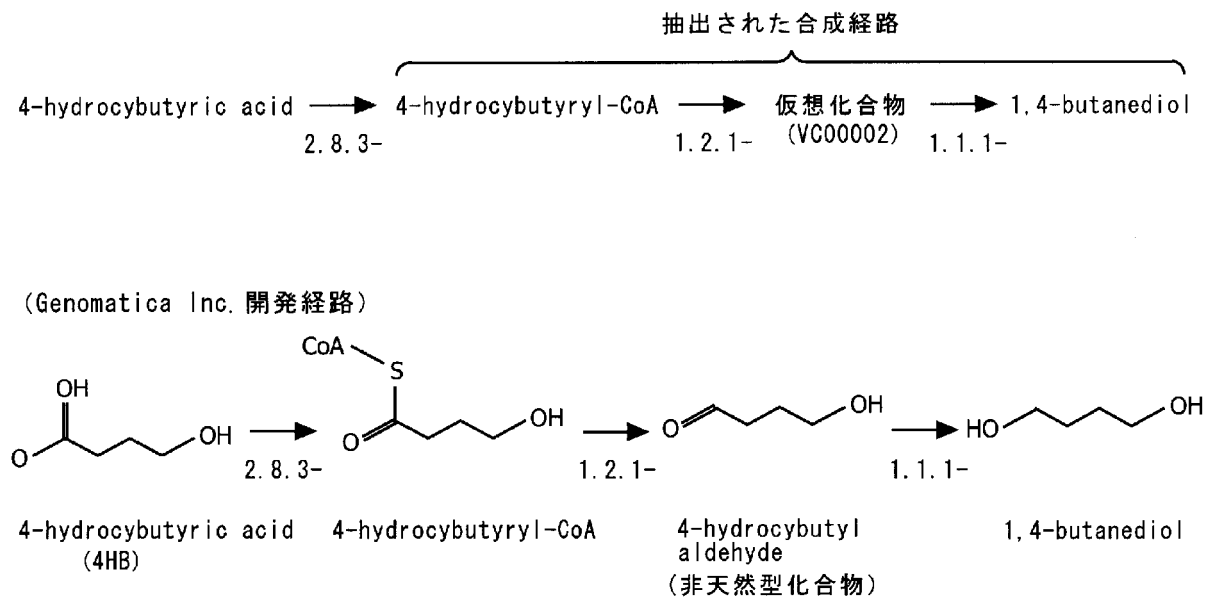
121

出発化合物	化合物a	UF1		
	既知反応	既知DF1	UF3-UF4	既知反応酵素A, B
			UF5-UF6	既知反応酵素C, D
中間化合物A	化合物b	UF14		
	既知反応	既知DF2	UF7-UF8	既知反応酵素E, F
中間化合物B	化合物c	UF13		
	仮想反応	既知DF3	UF9-UF10	既知反応酵素G, H
			UF11-UF12	既知反応酵素I, J
目的化合物	化合物d	UF2		

122

出発化合物	化合物a	UF1		
	既知反応	既知DF1	UF3-UF4	既知反応酵素A, B
			UF5-UF6	既知反応酵素C, D
中間化合物A	化合物b	UF14		
	仮想反応	既知DF4	UF15-UF16	既知反応酵素K, L
中間化合物C	VC0001	UF21		
	仮想反応	既知DF5	UF17-UF18	既知反応酵素M, N
			UF19-UF20	既知反応酵素O, P
目的化合物	化合物D	UF2		

[図12]



[図13]

