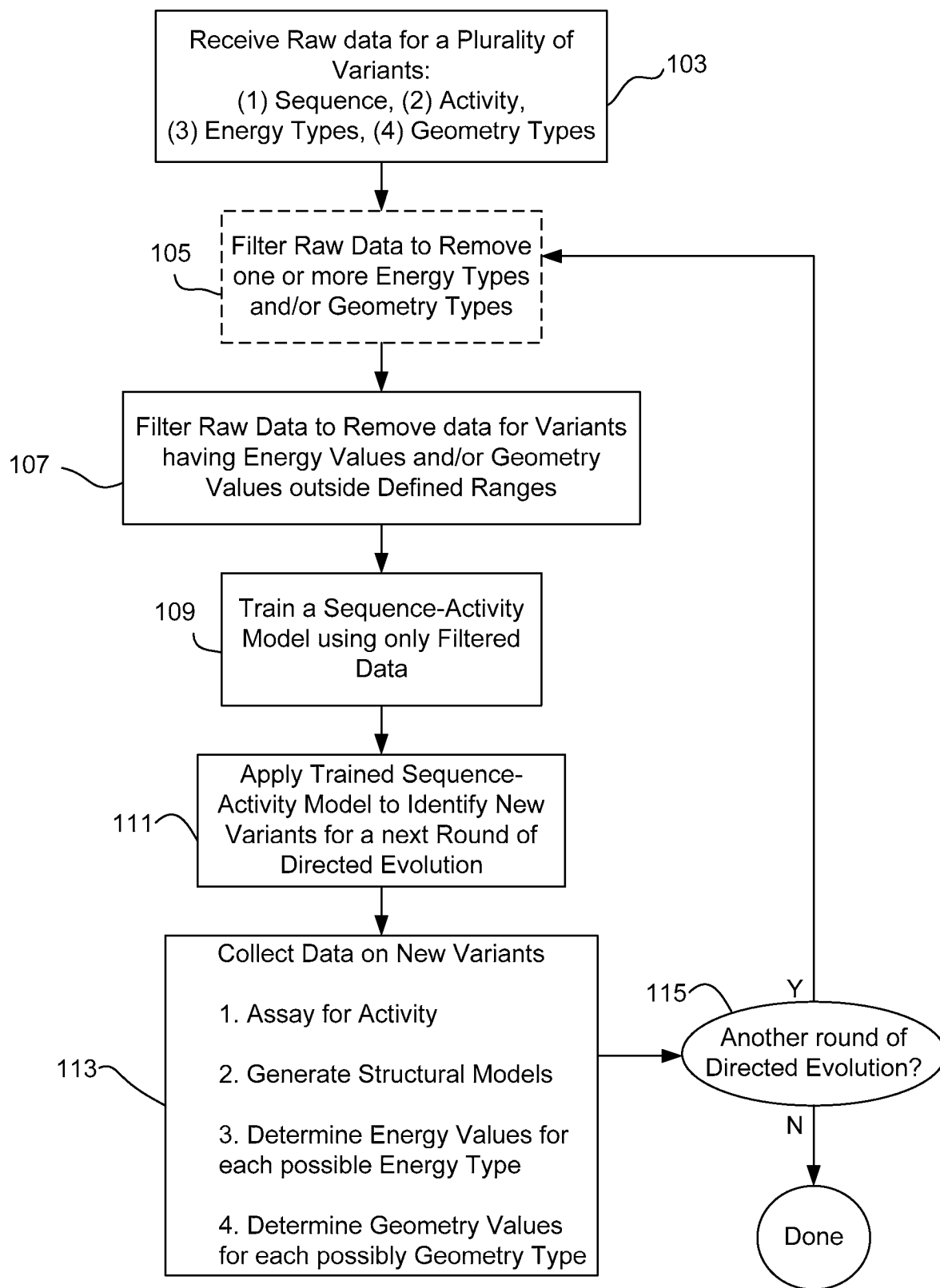
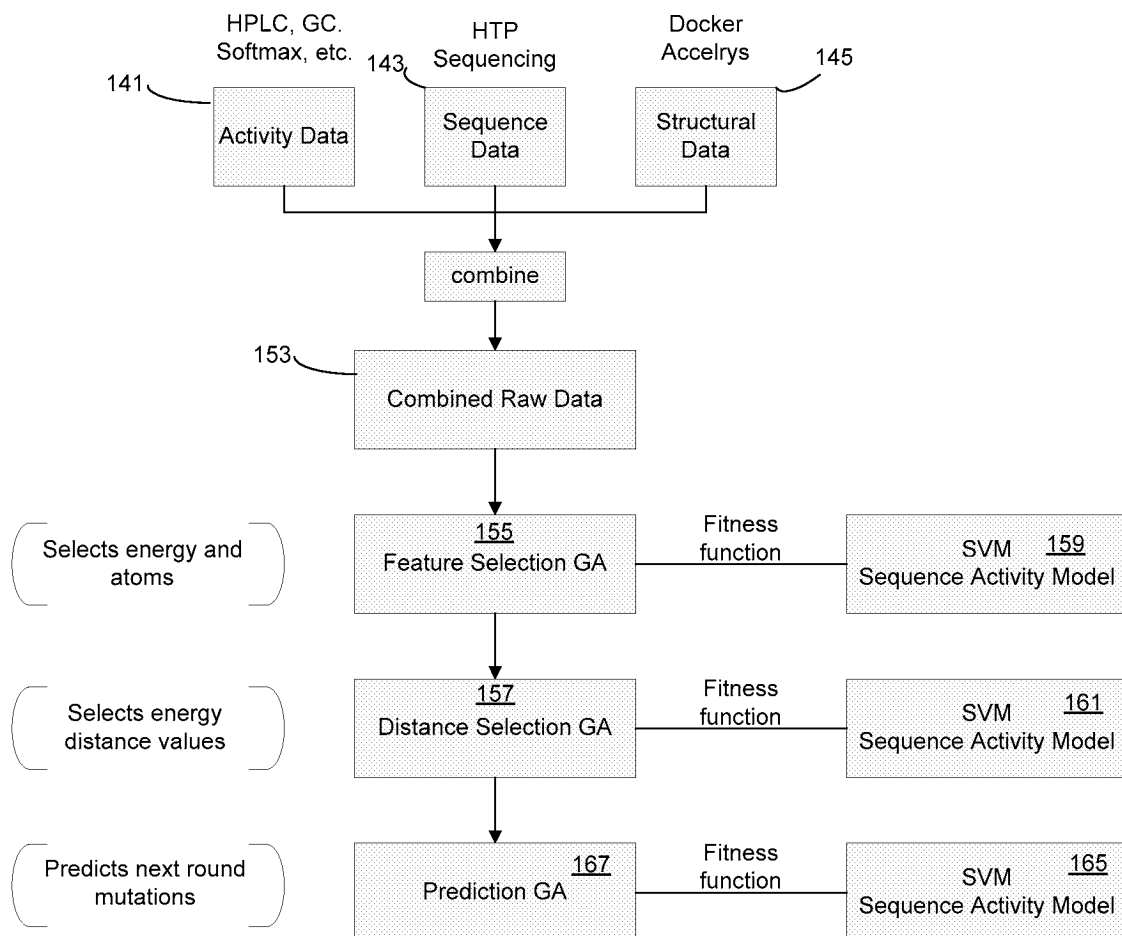
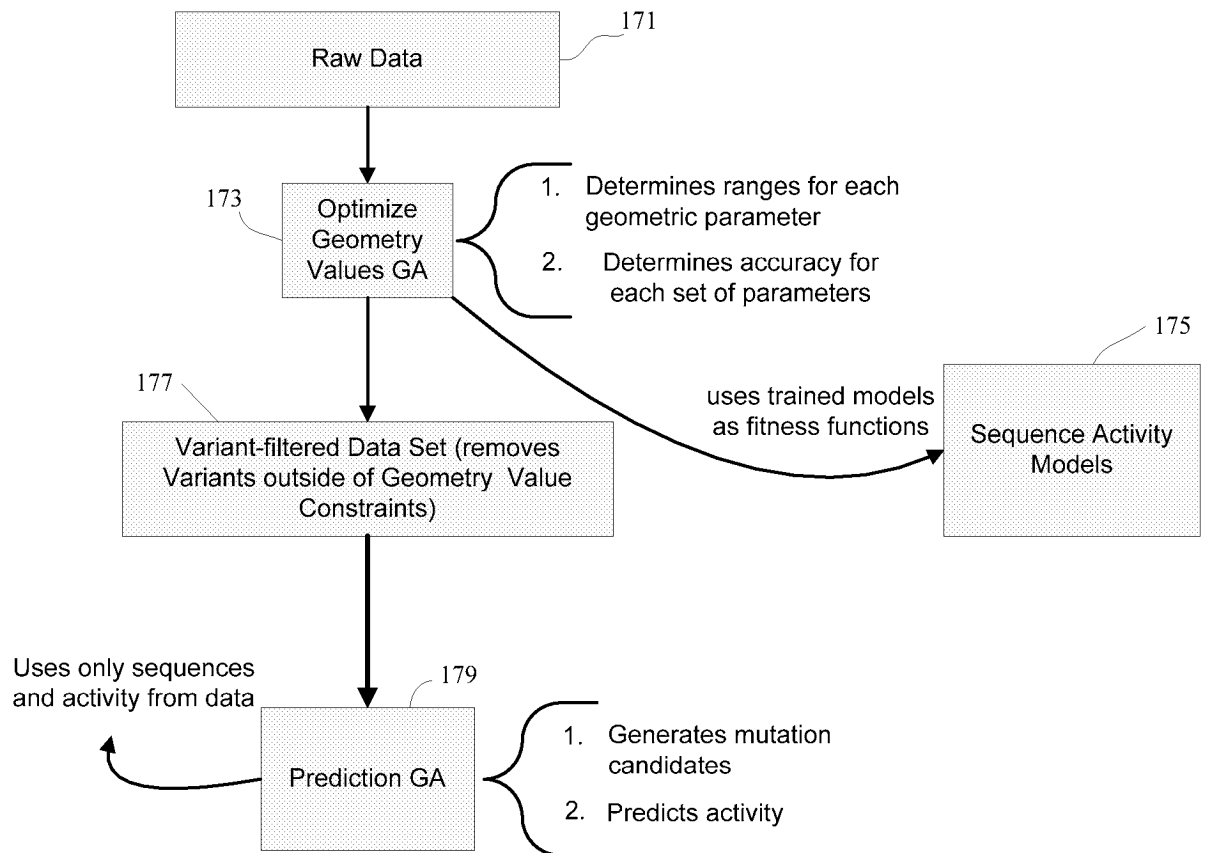


**FIG. 1A**

**FIG. 1B**

**FIG. 1C**

Variant	Activity	Sequence			Energy (kcal/mol)		Geometry (Å)				
		P1	P2	P3	Total	Interact	N ₁	P	C _(O)	C _(H3)	O _(H)
1	0.3	A	C	E	0.43	0.38	2.4	3.5	0.4	5.5	3.1
2	4.4	F	G	I	-2.1	-2.2	1.3	0.8	3.5	5.6	4.4
3	2.3	K	L	N	-3.1	-3.3	0.6	1.2	2.1	0.3	4.4
4	5.1	P	Q	S	-5.2	-5.6	0.3	0.7	1.1	3.1	2.1
5	1.3	T	V	Y	1.8	1.2	3.2	2.1	4.2	0.3	1.7
...	...	...	...	...	...	...	...	...	...	...	...
n	4.1	X	D	H	-4.1	-4.2	0.7	1.1	2.2	2.5	3.1

A. Raw Sequence Activity Data

							1	1	1	1	0	1	0
Variant	Activity	Sequence			Energy (kcal/mol)		Geometry (Å)						
		P1	P2	P3	Total	Interact	N ₁	P	C _(O)	C _(H3)	O _(H)		
1	0.3	A	C	E	0.43	0.38	2.4	3.5	0.4	5.5	3.1		
2	4.4	F	G	I	-2.1	-2.2	1.3	0.8	3.5	5.6	4.4		
3	2.3	K	L	N	-3.1	-3.3	0.6	1.2	2.1	0.3	4.4		
4	5.1	P	Q	S	-5.2	-5.6	0.3	0.7	1.1	3.1	2.1		
5	1.3	T	V	Y	1.8	1.2	3.2	2.1	4.2	0.3	1.7		
...	...	...	...	...	...	...	...	...	...	...	...		
n	4.1	X	D	H	-4.1	-4.2	0.7	1.1	2.2	2.5	3.1		

B. Sequence Activity Data Filtering Columns of Data

(GA individual: E Toal=1, E Interact=1, N₁=1, P=1, C_(O)=0, C_(H3)=1, O_(H)=0)

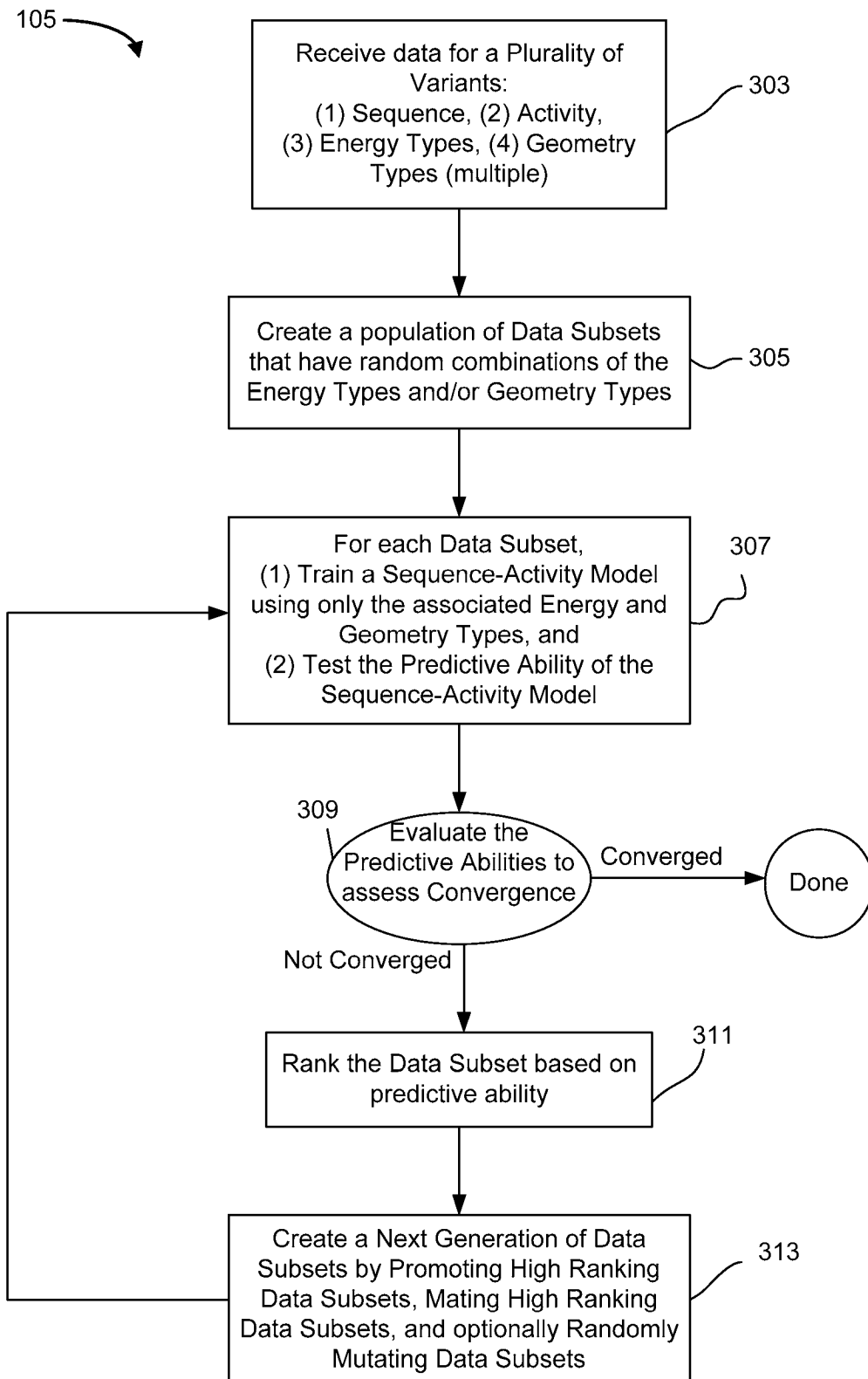
	Variant	Activity	Sequence			Energy (kcal/mol)		Geometry (Å)				
			P1	P2	P3	Total	Interact	N ₁	P	C _(O)	C _(H3)	O _(H)
P>2.8	1	0.3	A	C	E	0.43	0.38	2.4	3.5	0.4	5.5	3.1
	2	4.4	F	G	I	-2.1	-2.2	1.3	0.8	3.5	5.6	4.4
	3	2.3	K	L	N	-3.1	-3.3	0.6	1.2	2.1	0.3	4.4
	4	5.1	P	Q	S	-5.2	-5.6	0.3	0.7	1.1	3.1	2.1
E Total>1.5	5	1.3	T	V	Y	1.8	1.2	3.2	2.1	4.2	0.3	1.7
	...	...	...	...	...	...	...	...	...	...	...	...
	n	4.1	X	D	H	-4.1	-4.2	0.7	1.1	2.2	2.5	3.1

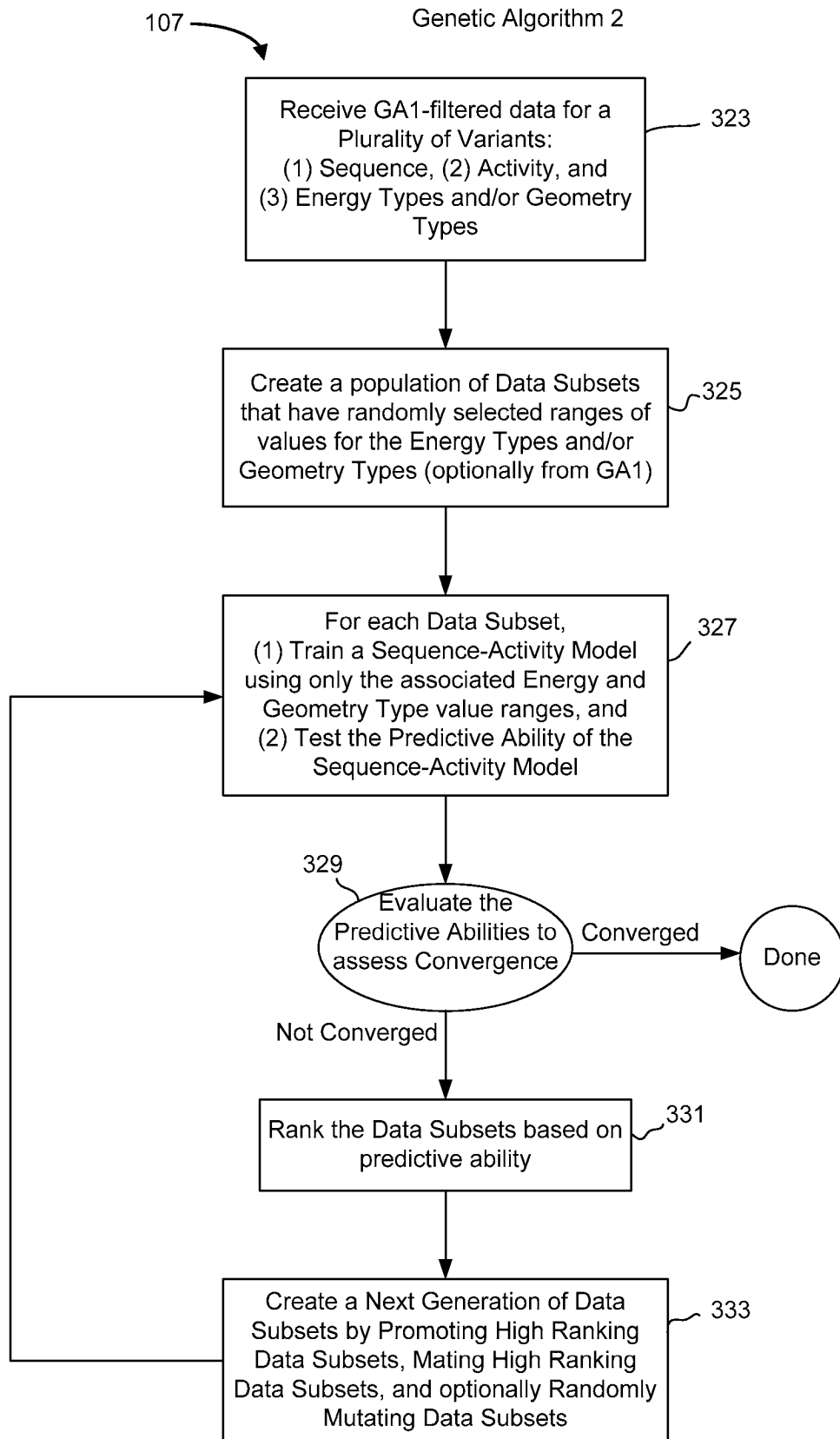
C. Sequence Activity Data Filtering Rows of Data

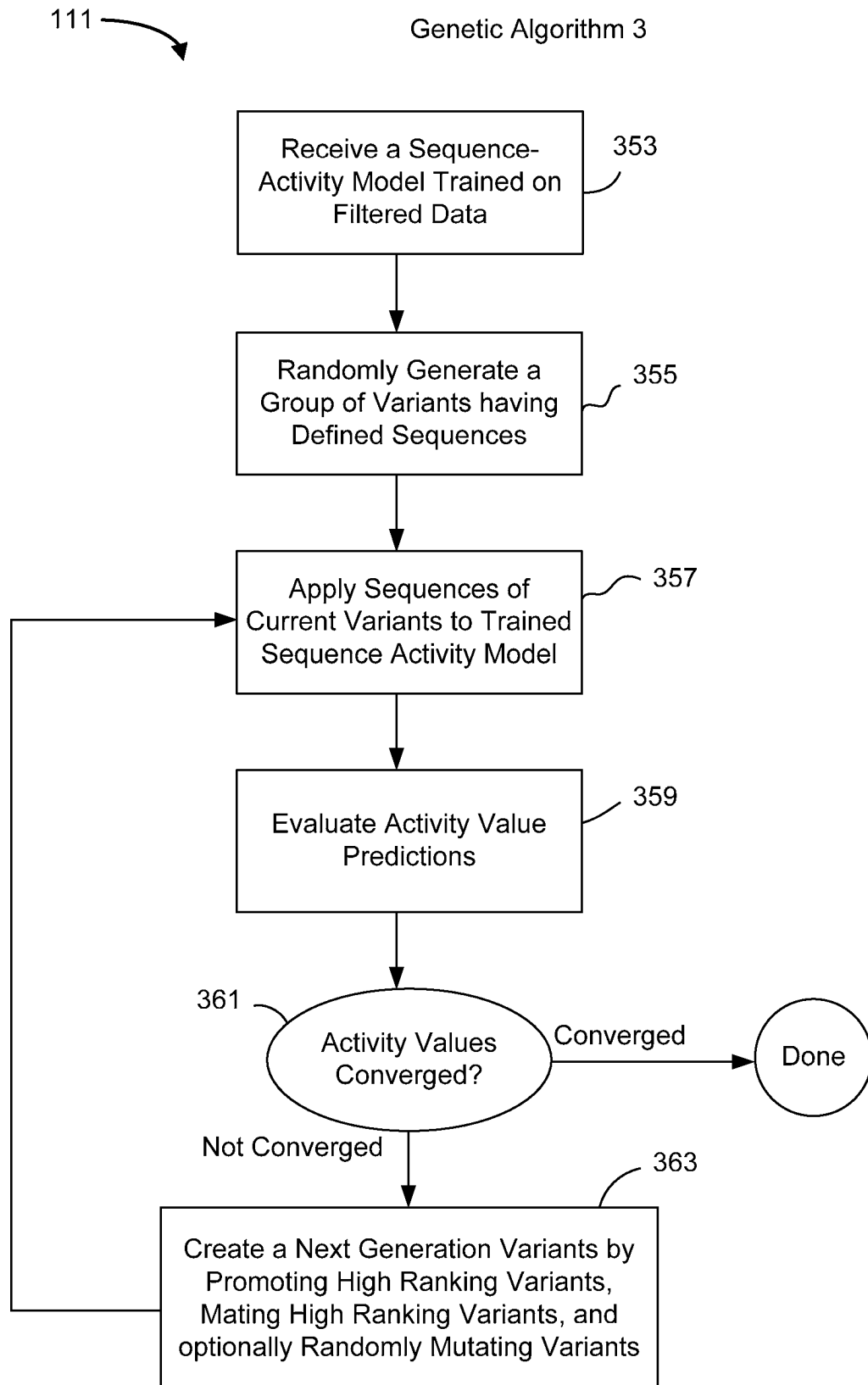
(GA individual: E Toal>1.5, E Interact>1.5, N₁>3.3, P>2.8, C_(O)>3.6, C_(H3)>6, O_(H)>6)

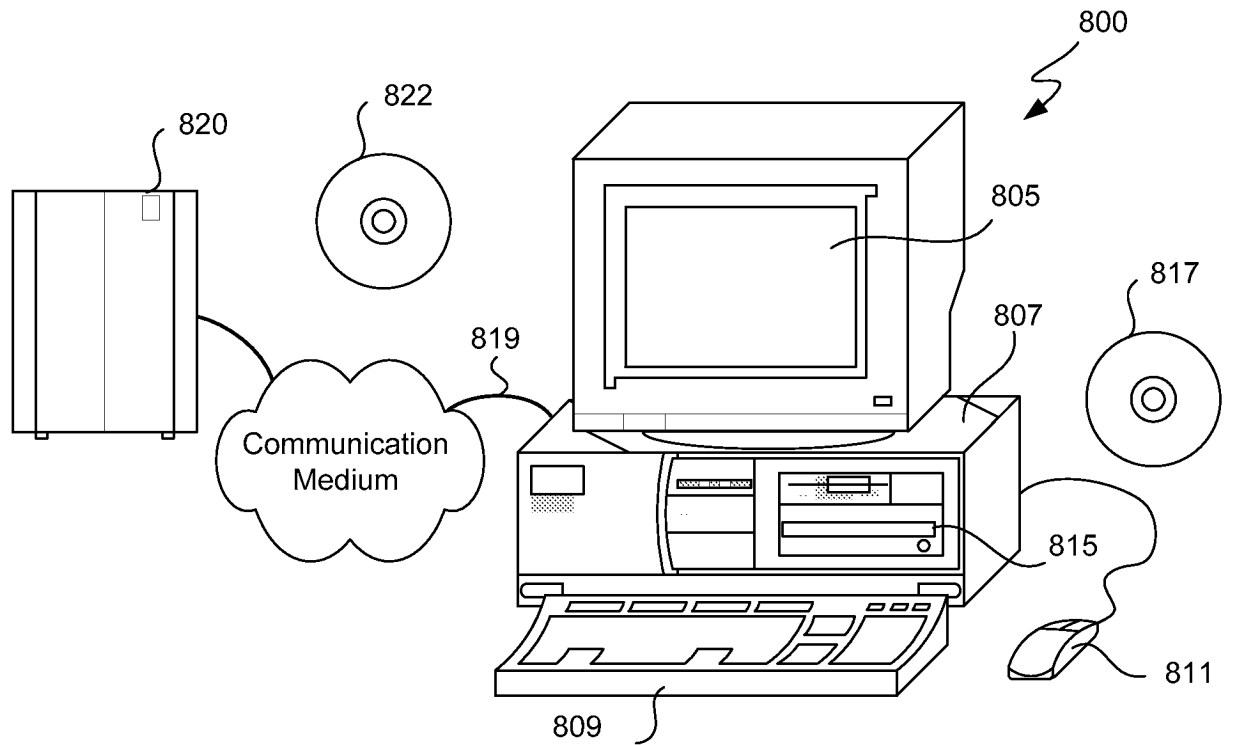
FIG. 2

Genetic Algorithm 1

**FIG. 3A**

**FIG. 3B**

**FIG. 3C**

**FIG. 4**