

# LABORATORY NOTEBOOK

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DEPARTMENT BIOMOLECULAR CHEM.  
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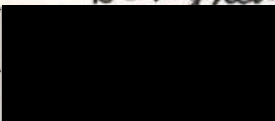
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## Genentech Laboratory Notebook Procedures

### Important steps for maintenance of your notebooks:

- 1) Use dark permanent ink to record all of your work in your notebook on a daily basis. Sign and date each day's entries.
- 2) Permanently affix all attachments without covering any other entries. Please attach copies of any computer data entered into your computer files. These data are considered part of your experimental record.
- 3) Make any changes in data in dark permanent ink and, if appropriate, initial and date in the margin. Ensure that the original entry remains visible. Leave no open areas. When the book is completed line out any unused portion of a page at the end of each experiment.
- 4) Have a witness who understands and is aware of your work, but who is not directly involved in your project, sign and date your notebook entries (not later than one month after you do the work).
- 5) Don't hold back data for later entry and don't keep a "rough draft" notebook.
- 6) Report the quantitative or qualitative results only. Avoid over broad and potentially inflammatory comments like "failed experiment", "doesn't work", or "toxic compound."
- 7) The source and character of starting materials should be described. Preferably, refer to the notebook pages describing the starting material and its method of preparation.
- 8) Be sure your notebook record is understandable. Omit abbreviations or slang that would not be understood by others working in your field. It is helpful to introduce each experiment with a statement of purpose, and make liberal use of cross-references to related experiments. While sufficient detail should be included to enable reproduction of experiments, it is acceptable to refer to conventional or published procedures. However, record any changes you may make to such procedures.
- 9) Record your ideas too, not just experimental data. This is important to demonstrate when an invention or thought occurred to you, and is an important part of establishing priority in inventorship contests. Don't hesitate to broaden the scope of your ideas; there is no reason to limit them to specific experiments planned for the next few days, although you should include as much detail as possible. Your notebook will not be published and there is no penalty for guessing wrong on notebook *idea* entries, so don't hesitate to let your imagination run.
- 10) Try to keep a different notebook for each product and/or project. Please complete the table of contents indicating which product and/or project this work concerns.

Genentech's success, and with it your own prosperity and research support, depends upon the quality and timing of your work. This may require that we prove what you did and when you did it in the face of a contrary challenge. Such challenges have and will continue to arise in judicial proceedings, in patent validity or infringement or challenge, inventorship priority contests and product liability actions. The key to winning in such cases is the ability to supply appropriate evidence.

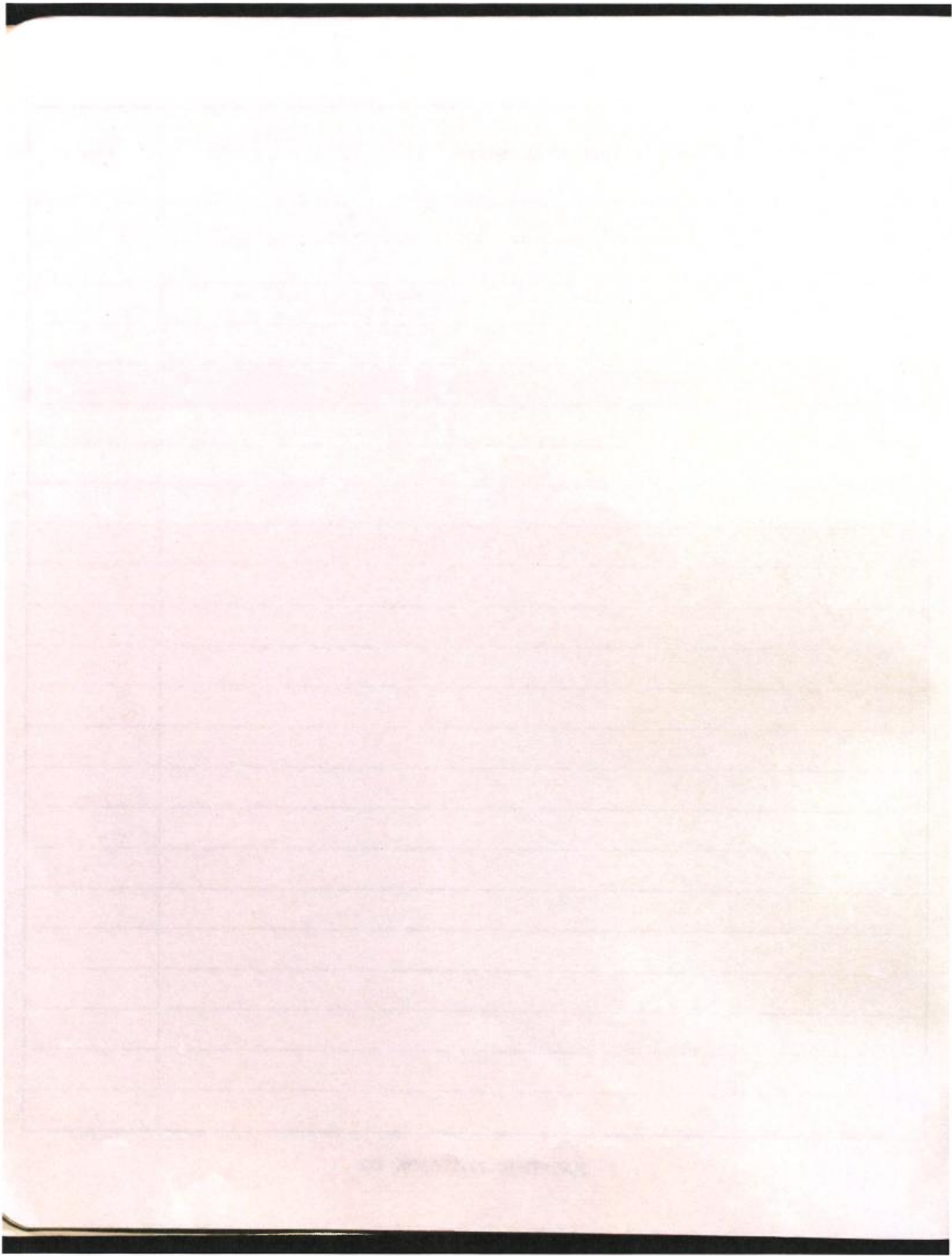
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[Faint, illegible handwritten text on lined paper, possibly bleed-through from the reverse side of the page.]

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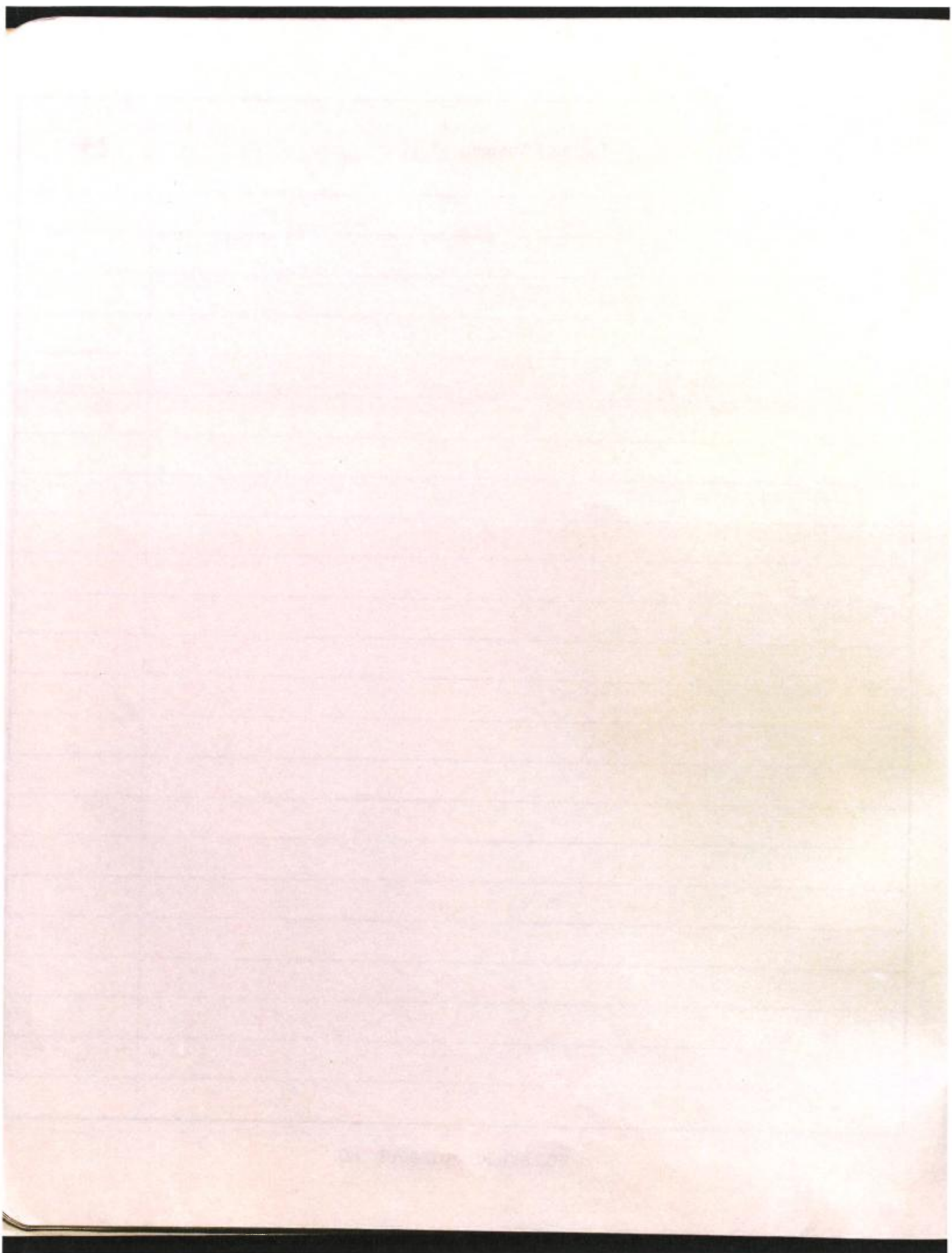
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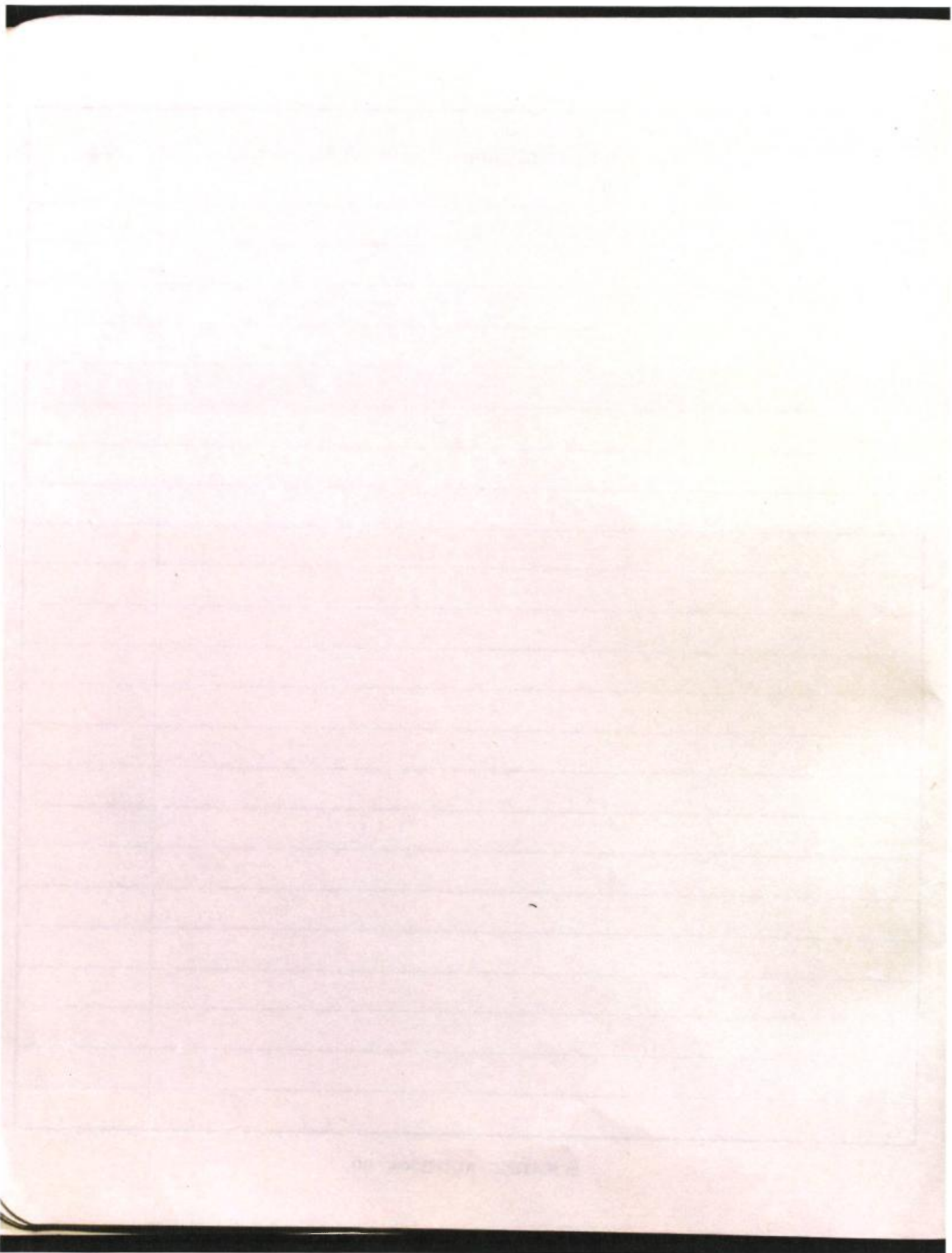












From Page No. \_\_\_\_\_ Based on Hydrogen Bonding & Backbone dihedral angle

1FB4 (V2) Q3-S7  
 (G9) G10-V12 (Q13)  
 (S17) L18-S25  
 A33-A40  
 (L45) E46-W47  
 A49-W52  
 D57-A61  
 F68-N73  
 T78-D84  
 (T91) G92-D99  
 Y107-G109  
 T112-S117

3FAB L4-S7 (G8)  
 L11-V12 (R13)  
 (T17) L18-S25  
 (Y32) Y33-Q39 (P40)  
 (L45) E46-F52  
 T56-T59  
 (V67) T68-V71  
 F78-L82 (S83)  
 (T90) A91-N98  
 (G110) S111-S116

2HFL (L4) Q5-S7  
 E10-M12 (K13)  
 (S17) V18-A24 (S25)  
 (W33) I34-Q39 (R40)  
 (L45) E46-L52  
 S57-H61  
 A68-D73  
 T78-N84  
 (S91) G92-H98  
 G105-S115

2MCP (V2) K3-S7  
 (G9) G10-V12 (Q13)  
 G16-S25  
 Y33-Q39 (P40)  
 (L45) I46-R52  
 T59-S63  
 F70-D75  
 I80-N86  
 (T93) A94-Y102 (Y103)  
 (W107) Y108-F109  
 T116-S121

1FBJ (L4) L5-S7  
 (G9) G10-G10 (L11)  
 L18-A23 (A24)  
 M34-Q39  
 (L45) E46-H52  
 T57-T61  
 F68-S71  
 (S78) L79-S84  
 (T91) A92-L99

(A106) Y107-G109  
 T112-T115

res in ( ) are outside h bond pattern, but have  $\beta$  strand's backbone dihedral angles

To Page No. \_\_\_\_\_

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Leonard Presta

11-20-89

From Page No. \_\_\_\_\_

All heavy variable domains superpositioned on 1FB4 HV using Insight (Biosym) program

Res	1FB4	1FBJ	2HFL	2MCP	3FAB
	18-25				
	34-39				
	46-52	Same	Same		
	57-61			59-63	56-60
	68-71			70-73	67-70
	78-84			80-86	77-83
	92-99			94-101	91-98

Superpositioning using N, Ca, C atoms (135 atoms)

1FB4 vs.	1FBJ	0.623 Å
	2MCP	0.425
	2HFL	0.913
	3FAB	0.854

Using 1FBJ as template

1FBJ vs	1FB4	0.623 Å
	2MCP	0.690
	2HFL	0.921
	3FAB	1.001

Using 2HFL as template

2HFL vs.	1FB4	0.913
	1FBJ	0.921
	2MCP	0.726
	3FAB	0.771

To Page No. \_\_\_\_\_

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11-20-89

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*Ca-Ca distances between analogous residues in the five crystal structures (superpositioned on IFB4) were used to define a set of residues to comprise the basic VH backbone. For a residue position to qualify, 4 of the 5 must have Ca-Ca distances  $\leq 1.0 \text{ \AA}$  (MATCH program). These residues were then used to calculate average coords. for N, Ca, C, O, Cs atoms using superpositioned coords. of the five crystal structures.*

```

*****
1FB4 and 3FAB are lambda-type 2MCP, 1FBJ AND 2HFL are kappa-type
() denotes beta-strand residues
Capital letters - Ca < 1.0A from 1FB4 HV
*****
1FB4 E(V Q L V Q S)G(G G V V Q)P G R(S L R L S C S S S)G F I F S
3FAB @ v (L E O S G) p g (l v r) p s q (S L T C T v s) G t s f d
1FBJ e v (L L E S G) G g l v q p g g (S L K L S C A A) S G f d f s
2HFL @ v (L L E S G) a (e l m k) p g A (S V K I S C K a s) g y t f s
2MCP e (V K L V E S G) G g L V q) P G (G S L R L S C A T S) g F T F S

1FB4 S Y (A M Y W V R Q A) P G K G (L E W) V (A I I) W) D D G S (D Q H Y A) D S V K
3FAB d (Y S) T W V R Q P P g r g (L E W I G Y V f) y h g - (t S D T) D T p l r
1FBJ k y (M S W V R Q) A P g k g (L E W I G E I H) p d s g (T I N G) E S l k
2HFL d Y (W I E W V K Q R) P G H G (L E W I G E I l) p g s g (s T N Y H) E r f k
2MCP d F (Y M E W V R Q P) P G K R (L E W I A A S) R N k g n k y (T E Y S) A S V K

1FB4 G R (F T I S R N) D S K N (T L F L Q M) D S L R P E D (T G V Y F C A
3FAB s R (T A) V N t s N Q (F S L R) S) s v t a a d (t A V Y Y C A
1FBJ d K (F I I S) R D n A K N (S L Y L Q M) s) k v r) s e d (t L Y Y C A
2HFL g (A T F T) d) t s S S (T A Y M Q L n) S l t s e d (s G V Y Y C L
2MCP G R (F I V S R) d) t s Q S (I L Y L Q M) N) A L R A E D (T A I Y Y C A

1FB4 R (D) G G H G F C S S A S C F G P L (Y W G) Q (T P V T V S) S A S
3FAB R n) l i a g c i d (W) Q (G S) v t v s) s a s
1FBJ R L) h y y g y n (a Y W G) Q (T L V t) v s a e s
2HFL (G) n y d f d (G W G O G T T L t v s) s a k
2MCP R N Y y) g s t (w y f) d V W G A G (T T V T V S) s e s
    
```

*2MCP A49 → B  
 IFB4 A49 → B  
 S92 → A  
 2HFL S92 → A  
 S105 → A*

*Circled residues were not used to calculate average coords.*

To Page No. 4

Witnessed & Understood by me,	Date	Invented by	Date
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From Page No. 3

```

IFB4.PDBASALA          62 residues and 306 atoms
GAP IN SEQUENCE:      0- 3 in file:IFB4.PDBASALA
GAP IN SEQUENCE:      8- 17 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     23- 33 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     41- 45 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     51- 58 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     62- 67 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     72- 76 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     83- 92 in file:IFB4.PDBASALA
GAP IN SEQUENCE:     98- 107 in file:IFB4.PDBASALA
IFBJ.PDBASALA          62 residues and 306 atoms
GAP IN SEQUENCE:      0- 3 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:      8- 17 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     23- 33 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     41- 45 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     51- 58 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     62- 67 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     72- 76 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     83- 92 in file:IFBJ.PDBASALA
GAP IN SEQUENCE:     98- 107 in file:IFBJ.PDBASALA
2HFL.PDBASALA          62 residues and 306 atoms
GAP IN SEQUENCE:      0- 3 in file:2HFL.PDBASALA
GAP IN SEQUENCE:      8- 17 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     23- 33 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     41- 45 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     51- 58 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     62- 67 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     72- 76 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     83- 92 in file:2HFL.PDBASALA
GAP IN SEQUENCE:     98- 105 in file:2HFL.PDBASALA
2MCP.PDBASALA          62 residues and 306 atoms
GAP IN SEQUENCE:      0- 3 in file:2MCP.PDBASALA
GAP IN SEQUENCE:      8- 17 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     23- 33 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     41- 45 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     51- 60 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     64- 69 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     74- 78 in file:2MCP.PDBASALA
GAP IN SEQUENCE:     85- 94 in file:2MCP.PDBASALA
GAP IN SEQUENCE:    100- 111 in file:2MCP.PDBASALA
3FAB.PDBASALA          62 residues and 306 atoms
GAP IN SEQUENCE:      0- 3 in file:3FAB.PDBASALA
GAP IN SEQUENCE:      8- 17 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     23- 33 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     41- 45 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     51- 57 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     61- 66 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     71- 75 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     82- 91 in file:3FAB.PDBASALA
GAP IN SEQUENCE:     97- 108 in file:3FAB.PDBASALA
GAP IN SEQUENCE:    108- 107 in file:3FAB.PDBASALA
MAXAT = 306 ; MAXRES = 62
B-factor range is: 2.00 to 33.72
B-factor BIN range is: 2 to 34
B-FACTOR STATS DO NOT INCLUDE 3FAB
Bin#   Range      Avg.Dst.  R.M.S.  #values  Dist range
  1  2.00 - 5.20   0.119   0.221   620   0.000 - 1.440
  2  5.20 - 8.40   0.364   0.423   145   0.037 - 1.306
  3  8.40 - 11.60  0.368   0.420   192   0.021 - 1.474
  4  11.60 - 14.80  0.372   0.417   235   0.035 - 1.016
  5  14.80 - 18.00  0.391   0.455   177   0.044 - 1.489
  6  18.00 - 21.20  0.434   0.490   104   0.065 - 1.505
  7  21.20 - 24.40  0.633   0.752    42   0.237 - 2.033
  8  24.40 - 27.60  0.616   0.828    9   0.265 - 1.866
  9  27.60 - 30.80  0.565   0.724    5   0.359 - 1.195
 10 30.80 - 34.00  0.268   0.268    1   0.268 - 0.268
    
```

Bond Lengths & Angles for HVONFB4HV

N-Ca	Ca-C	C-O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C-O	Ca-C-N	O-C-N	N-Ca-Cb	Cb-Ca-C
1.451	1.507	1.160	1.282	1.499	125.3	110.3	120.9	117.6	122.2	110.6	111.2
0.023	0.033	0.177	0.065	0.039	4.6	2.8	7.1	5.2	4.9	2.5	2.2
62	62	62	53	58	53	62	62	53	53	58	58

To Page No. \_\_\_\_\_

Witnessed & Understood by me,

Date

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Date

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*Leonard Prota*

11-26-89



From Page No. \_\_\_\_\_

Same treatment but using coords. superpositioned on 2HFL (instead of 1FB4)

\*\*\*\*\*  
 1FB4 and 3FAB are lambda-type 2MCP, 1FBJ AND 2HFL are kappa-type

( ) denotes beta-strand residues

capital letters = Ca < 1.0A from 2HFL HV

\*\*\*\*\*

```

2HFL @V Q(L Q Q) S) G A(E L M K) P G A(S V K I S C K) A S) G Y T F S
1FB4 e(v Q L Q) S) g(g g v v q) p g R(S L R L S C S) s s) g f i f s
3FAB @v Q(L E W) s) g(L v r) p s G(t) S L T C T V S) g t s f d
1FBJ e v K(L L E s) g(g G L) V Q P G G(S L K L S C A) a) s g f d f s
2MCP e(v K L V E s) g(g g l v q) p G G(S L R L S C A) T s) g F T F S
    
```

2MCP A49 → 8

1FB4 A49 → 8  
 592 → A

```

2HFL D Y W I E W V K Q R) P G H G L E W I G E I L) P G S G S(T N Y H) E R F K
1FB4 s Y A M Y W V R Q A) P G K G L E W V(A I I) W d d g s(d Q H Y A) D s v k
3FAB d(y Y S T W V R Q P) P g r g L E W I G Y V F) y - h g(t S D T) D T p l r
1FBJ k y W(M S W V R Q) A P G K G L E W I G E I h) p d s g(t I N Y T) S L K
2MCP d F Y M E W V R Q) P P g K R L E W I A A S r) n k g n k y(t T E Y S) A S V K
    
```

2HFL 592 → A  
 9105 → A

```

2HFL G K A T F T A D) T S S S(T A Y M Q L) N S L T S E D(S G V Y Y C L
1FB4 g r F T I S r n) d s K N(T L F L Q M d) S l r p e d(t G V Y F C A
3FAB s r V D M L V) n t s K N(Q F S L R L S) s v T A A D(T A V Y Y C A
1FBJ D k F I I S) r d n A K N(S L Y L Q M) s) K V R S E D(T A L Y Y C A
2MCP G r F I V S R D) T S Q S(I L Y L Q M) N) A l r a e d(t A I Y Y C A
    
```

```

2HFL H) G N Y D F D(G W G) G T F L T V S) S A K
1FB4 r d) g g h g f c s s a s c f g p d(Y W G) O G(T P V) t v s) s a s
3FAB R n) l i a g c i d v G H G S L V T V S) S a s
1FBJ r l) h y y g y n(a y W G) H G(T L V) T V S a e s
2MCP r n y y) g s t(w y f) d V W G A G(T T V) t v s) s e s
    
```

Bond Lengths & Angles for HVONHFLHV

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C-O	Ca-C-N	O-C-N	N-Ca-Cb	Cb-Ca-C
1.456	1.515	1.202	1.293	1.501	124.0	109.7	121.0	115.9	123.8	110.8	111.1
0.020	0.021	0.132	0.035	0.051	2.3	2.7	7.4	1.9	2.1	2.1	2.7
57	57	57	47	54	47	57	57	47	47	54	54

To compare the two average structures use N, Ca, C  
 of res: 3-6, 17-23, 33-41, 45-51, 58-62, 68-71, 76-83, 92-97,  
 108-109, 111-113

Avg HFL on Avg FB4 = 0.118 Å 165 atoms

Added res 16, 114 from HVONHFLHV. AV/SCRD to HVONFB4HV. AV/SCRD

To Page No. \_\_\_\_\_

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Date

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Leonard Presta

11-26-89

Project No. \_\_\_\_\_  
Book No. \_\_\_\_\_

TITLE *Seq. Alignments with  
Consensus Sequence*

From Page No. \_\_\_\_\_

\*\*\*\*\*  
1FB4 and 3FAB are lambda-type 2MCP, 1FBJ AND 2HFL are kappa-type

() denotes beta-strand residues

capital letters - Ca < 1.0A from 1FB4 HV

consensus sequence from Kabat et al., "Sequences of Proteins of Immunological Interest", 4th ed., 1987; numbering according to Kabat;

\* marks Kabat variance between 1 - 10, @ variance between 11 - 20

\*\*\*\*\*

```

1FB4 E(V Q L V Q S)G(G G V V Q)P G R(S L R L S C S S S)G F I F S
3FAB @ v q(L E Q S G)p g(l v r)p s q(t l S L T C T v s)G t s f d
1FBJ e v K(L L E S)G(G g l)v q p g g S(L K L S C A A)S G F d f s
2HFL @ v Q(L q q s)g a(e l m K)p g A(S V K I S C K a s)g y t f s
2MCP e(V K L V E S)G(G g L V q)P G(G S L R L S C A T S)g P T F S
con @ @ * @ * * @ @ @ Q * @ @ * @ @ * @ @ * @ * @ *
E V Q L V E S G G L V Q P G G S L K L S C A A S G F T F S
1 10 20 30

```

```

1FB4 S Y(A M Y W V R Q A)P G K G(L E W)V(A I I W)D D G S(D Q H Y A)D S V K
3FAB d(y y s T W V R Q P)p g r g(l E W I G Y V f)y h g -(t S D T)D T p l r
1FBJ k y W(M S W V R Q)A P g k g(L E W I G E I H)p d s g(T I N Y t)p s l k
2HFL d Y(W I E W V R Q R)P G H G(L E W I G E I l)p g s g(S T N Y H)E r f k
2MCP d F(Y M E W V R Q P)P G K R(L E W I A A S R)N k g n k y(T T E Y S)A S V K
con @ @ @ * * * * @ @ * * * * @ @ * *
S Y Y M H W V R Q A P G K G L E W I G Y I N P K A N S G S T N Y N E S F K
V
35a 40 50 abc 60

```

```

1FB4 G R(F T I S R N)D S K N(T L F L Q M D)S L R P E D(T G V Y F C A
3FAB s R(v T m l V)N t s k N Q(F S L R l S)s v t a a d(t A V Y Y C A
1FBJ d K(F Y I S)R D n A K N(S L Y L O M S)k v r)s e d(t a L Y Y C A
2HFL g k(A T F T a d)t s S S(T A Y M Q L N)S l t s e d(s G V Y Y C L
2MCP G R(F I V S R d)t s Q S(I L Y L Q M N)A L R A E D(T A I Y Y C A
con @ * @ @ @ * * * @ @ @ @ @ @ @ @ @ * * * * *
G R F T I S R D T S K S T A Y L Q M N S L T S E D T A V Y Y C A
70 80 abc 90

```

```

1FB4 R D)G G H G F C S S A S C F G P D(Y W G)Q G(T P V T V S)S A S
3FAB R n)l i a g c i d v W g Q(G S l v t v s)s a s
1FBJ R L)h y y g y n(a Y W G)Q G(T L v t)v s a e s
2HFL h)g n y d f d(G W G Q G T T L t v s)s a k
2MCP R N Y y) g s t (w y f)d V W G A G(T T V T V S)s e s
con @
R D Y Y Y G S S Y Y Y Y W Y F D Y W G Q G T T V T V S S
100 abcdefghi j k 110

```

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by <i>Leonard Presta</i>	<i>11-28-89</i>

From Page No. \_\_\_\_\_

	1FB4	3FAB	1FBJ	2HFL	2MCP					
1	1000.0	129.9	1000.0	-131.5	1000.0	14.5				
2	-67.9	121.3	-145.2	-169.3	-77.8	134.3	129.9	-164.9	-86.1	109.7
3	-116.5	135.9	130.2	130.7	-158.2	149.2	81.0	-164.0	-124.2	140.5
4	-123.8	121.1	-107.0	143.4	-126.0	106.1	-122.8	123.3	-131.6	126.8
5	-120.5	110.1	-139.5	125.9	-98.4	110.5	-119.0	89.5	-134.7	116.0
6	-81.0	146.7	-109.3	157.1	-90.8	146.8	-95.7	151.0	-98.1	153.2
7	-152.4	152.6	-156.8	139.6	-140.3	168.6	-149.3	170.9	-151.2	170.1
8	115.4	-12.1	-178.6	-168.4	85.7	1.7	110.2	-98.5	80.0	96.7
9	-62.4	151.9	-82.1	163.4	-93.2	129.2	111.4	150.7	-174.6	145.7
10	-161.9	-171.0	-84.0	-69.2	-165.4	-147.9	-164.6	154.5	165.1	-143.5
11	-107.2	121.9	-93.3	142.3	-87.9	113.8	-109.0	134.5	-69.9	137.6
12	-134.7	163.7	-137.2	140.3	-116.3	-179.7	-155.6	141.1	-154.3	130.1
13	-96.8	159.9	-83.6	140.3	-130.8	139.2	-78.4	138.8	-79.5	144.1
14	-62.8	137.8	-65.1	135.3	-35.1	89.5	-52.8	133.9	-52.6	138.7
15	93.0	-10.3	104.0	-32.3	107.9	67.2	94.3	3.0	92.9	-20.8
16	-90.9	-179.2	-77.5	130.7	-157.7	158.3	-94.5	-149.9	-64.1	-175.2
17	-118.2	158.5	-61.7	146.7	-114.2	154.3	-151.0	169.1	-144.8	160.8
18	-140.8	164.7	-98.4	102.2	-147.6	172.8	-161.6	146.7	-151.0	160.1
19	-132.8	123.7	-90.1	140.3	-149.3	119.1	-124.4	109.7	-136.9	95.9
20	-97.4	148.6	-136.4	150.8	-100.4	139.1	-97.2	135.0	-82.5	148.8
21	-131.2	148.4	-137.5	143.5	-111.6	156.6	-101.6	163.7	-135.0	152.2
22	-131.9	104.9	-133.1	121.3	-147.5	106.3	-153.2	99.5	-126.6	107.5
23	-93.0	137.5	-109.6	120.2	-111.0	116.3	-86.8	124.2	-86.5	108.3
24	-125.0	164.5	-98.0	145.1	-127.2	125.5	-111.0	140.5	-98.4	116.6
25	-161.1	160.5	-159.6	153.2	-94.8	-150.8	-149.2	157.4	-135.1	158.8
26	87.5	13.2	84.2	-23.4	48.6	-12.0	85.8	0.2	85.8	21.3
27	-166.9	158.8	-89.3	141.5	-148.3	-172.9	-147.3	169.9	-169.3	166.6
28	-78.6	88.9	-79.3	107.7	-110.4	132.7	-76.1	94.2	-74.2	83.8
29	-49.0	-45.9	-74.5	47.4	-79.6	83.3	-73.7	-33.8	-48.9	-49.1
30	-65.7	-2.6	-116.7	-84.2	-157.5	-34.1	-64.2	11.8	-54.0	13.3
31	-91.7	-15.9	-43.9	-53.8	-79.3	35.3	-173.3	45.8	-166.0	38.6
32	-119.9	150.0	-60.5	167.9	-48.6	-132.6	-147.5	128.7	-136.8	140.9
33	-72.5	144.1	-159.4	100.2	65.9	91.8	-72.3	152.7	-71.1	131.5
34	-119.0	147.9	-82.0	121.9	-123.3	147.7	-126.8	141.6	-106.0	151.5
35	-110.7	163.3	-95.9	173.1	-153.7	171.0	-124.3	150.8	-138.4	147.0
36	-126.0	131.2	-127.4	80.6	-137.9	120.3	-119.0	120.1	-113.5	129.4
37	-133.5	141.1	-91.3	153.8	-95.2	162.0	-123.0	139.2	-133.6	142.3
38	-123.4	163.2	-131.7	163.5	-146.0	126.1	-113.4	137.9	-125.9	157.5
39	-143.9	108.8	-144.2	102.0	114.9	91.1	-129.3	111.0	-140.5	95.1
40	-75.1	138.9	-60.7	143.0	-55.9	155.5	-60.0	-179.1	-57.3	162.1
41	-54.9	122.4	-75.5	131.1	-57.1	125.2	-49.2	-71.6	-42.7	-57.5
42	85.6	-4.5	113.0	14.4	75.1	-29.7	-123.9	66.0	-127.7	59.5
43	-114.3	177.9	70.9	147.9	-77.8	-159.3	-146.0	157.9	-147.1	162.5
44	-82.5	179.7	128.5	118.9	-129.8	-170.3	-56.1	174.3	-61.5	169.6
45	-65.3	132.6	-100.7	136.5	-67.4	125.6	-77.7	162.5	-69.1	148.4
46	-129.6	112.3	-140.8	119.5	-127.0	117.5	-147.1	127.6	-134.3	123.6
47	-60.8	135.6	-68.3	143.0	-76.6	125.5	-88.0	134.4	-84.6	137.7
48	-102.6	-58.4	-105.0	-60.9	-90.5	-55.1	-107.3	-69.8	-119.0	-101.5
49	-154.9	164.0	178.2	-173.9	174.1	174.5	-135.9	-164.9	-80.0	176.7
50	-135.0	142.6	-151.1	173.2	-126.5	171.0	-172.5	162.9	-163.6	126.2
51	-128.1	134.1	-151.1	153.0	-153.2	149.6	-162.3	155.3	-104.0	166.4
52	-59.3	158.0	-115.7	153.0	-120.2	159.9	-109.3	98.2	-131.5	161.0
53	-41.2	-48.0	-52.6	-32.1	-83.1	-29.0	-51.8	-70.3	-69.6	149.2
54	-100.0	6.3	-64.8	-20.8	-45.0	-36.6	-30.5	-27.5	-68.7	65.5
55	70.8	15.0	83.5	45.1	-163.4	-22.6	-150.1	66.2	60.7	120.3
56	-70.6	-16.4	0.0	0.0	112.2	40.7	-33.4	67.6	-57.0	54.4
57	-156.6	155.5	-109.5	117.2	-85.9	146.6	-113.5	117.0	-65.5	155.8
58	-145.8	140.6	-126.9	169.9	-126.6	133.8	-102.9	167.4	-122.1	175.5
59	-130.2	145.3	-160.9	110.2	-118.3	153.7	-152.4	127.7	-157.4	141.0
60	-124.2	153.6	-87.1	154.4	-148.8	148.7	-132.3	135.9	-134.0	145.1
61	-65.1	141.0	-54.1	-101.9	-79.4	112.5	-78.6	131.8	-64.5	149.1
62	-46.4	-43.8	-177.2	-71.2	-36.7	-43.0	-9.9	-90.7	-56.1	-37.3
63	-58.9	-13.6	-46.9	-24.8	-65.7	-13.4	-34.9	-5.8	-60.9	-19.8
64	-126.3	-10.1	-84.7	-46.2	-120.0	3.0	-130.3	-49.3	-131.8	-11.3
65	-61.5	123.6	-18.8	107.2	-49.0	-50.0	-25.8	129.4	-52.8	118.6

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Book No. \_\_\_\_\_

TITLE *Crystal Struct. Backbone Coups*

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66	96.6	-27.1	140.8	-61.4	-74.1	30.1	92.1	-27.6	113.0	-34.7
67	-93.0	-28.5	-107.4	74.5	178.9	16.7	-91.1	-52.4	-103.0	-35.0
68	-106.9	140.6	-158.4	117.0	-145.1	128.8	-89.7	160.9	-94.3	149.5
69	-125.5	122.7	-130.1	131.1	-122.8	119.6	-155.3	116.9	-146.8	124.1
70	-91.5	132.6	-109.5	121.3	-89.0	135.9	-96.7	158.7	-98.5	129.5
71	-151.0	170.6	-104.4	149.5	-127.2	167.4	-156.8	175.8	-138.2	172.9
72	-146.5	159.2	-108.8	-159.8	-139.3	168.3	-157.9	144.5	-143.5	131.1
73	-130.5	86.7	-0.9	-139.3	-166.0	115.3	-121.7	91.9	-91.9	87.0
74	-61.8	-14.9	153.7	8.3	-52.6	1.3	-41.7	-49.7	-56.1	-34.5
75	-74.2	-40.1	118.0	-37.7	-135.7	-48.9	-51.9	-47.2	-65.6	-39.1
76	-105.9	13.1	-138.7	146.2	-73.0	-34.9	-99.6	6.3	-102.1	5.0
77	51.1	41.0	-3.5	120.0	77.3	44.5	45.8	47.0	57.9	45.6
78	-125.8	139.0	157.8	133.0	-127.2	123.7	-121.6	121.3	-119.8	140.9
79	-107.3	133.3	-142.1	149.9	-109.2	137.9	-111.1	136.9	-112.3	121.4
80	-110.7	155.9	-144.9	155.4	-112.8	169.8	-119.8	158.1	-102.4	154.8
81	-136.0	101.2	-116.7	137.0	-157.6	98.0	-125.0	112.6	-140.4	107.5
82	-86.3	115.3	-134.9	90.2	-74.7	147.4	-102.6	107.6	-89.7	114.8
83	-110.9	106.6	-87.2	109.2	-128.4	147.0	-110.2	123.0	-103.8	105.0
84	-105.3	157.9	-71.0	-176.1	-121.2	-144.5	-92.2	151.7	-103.8	143.3
85	41.4	52.4	77.2	-105.2	-46.5	84.1	31.9	76.5	46.1	70.0
86	-60.7	138.3	73.4	135.0	-77.8	121.6	-63.2	141.7	-73.8	154.4
87	-120.7	148.1	-152.9	173.8	-106.1	156.0	-122.9	-169.4	-133.0	171.4
88	-56.5	-25.6	-66.9	-34.0	-49.0	-21.9	-80.6	-38.5	-65.9	-30.9
89	-75.0	-0.4	-69.8	10.2	-91.6	24.3	-48.5	-19.8	-62.5	-17.7
90	-94.7	6.8	-124.5	17.5	-110.9	-1.4	-80.1	-7.7	-76.9	-10.2
91	-71.4	135.4	-91.0	112.6	-55.4	123.1	-70.6	152.3	-67.1	118.4
92	174.8	178.4	-168.4	-162.0	-176.4	-176.7	154.4	-178.4	-176.1	169.2
93	-95.7	129.2	-117.2	135.5	-114.2	126.7	-109.6	113.3	-82.0	128.2
94	-102.8	123.2	-109.2	122.0	-103.8	119.4	-92.2	130.1	-105.4	138.3
95	-105.4	137.8	-103.2	157.1	-106.0	145.5	-118.2	137.8	-126.5	144.7
96	-95.0	155.9	-129.8	85.5	-109.9	131.3	-107.3	128.3	-113.4	139.4
97	-144.0	153.7	-90.6	-167.8	-130.1	174.2	-131.2	-167.7	-135.3	159.6
98	-89.1	139.2	-134.5	107.5	-135.7	119.5	-135.9	138.8	-105.7	122.1
99	-81.3	129.4	-97.1	168.3	-71.1	179.6	-127.5	86.7	-100.0	90.4
100	-82.9	-5.5	-166.7	67.9	-160.0	-173.4	-126.5	79.3	-70.9	-46.8
106	-108.5	-54.2	145.7	76.3	-134.4	-166.8	-106.7	150.3	-127.6	129.0
107	-104.7	145.8	-75.0	-155.7	-174.4	133.0	-109.2	160.8	-111.5	156.4
108	-120.1	158.2	-170.8	176.7	-122.1	163.8	-84.7	179.2	-84.2	-176.1
109	-89.2	-167.2	-169.1	125.7	-101.0	166.2	-67.1	-41.8	-88.1	-24.6
110	-94.2	-19.5	-19.9	142.5	-79.8	-17.8	112.9	153.3	96.1	169.6
111	101.6	146.1	-112.1	160.4	77.4	168.7	-139.5	132.9	-154.0	126.5
112	-132.4	121.9	-101.5	139.4	-139.8	141.5	-91.9	142.1	-84.0	134.5
113	-76.0	136.7	-81.7	112.8	-84.0	147.1	-125.9	121.6	-129.3	114.9
114	-122.6	123.4	-115.3	117.5	-138.0	120.2	-117.4	99.7	-108.8	115.5
115	-120.4	115.2	-118.2	114.4	-119.0	108.5	-93.1	118.3	-100.6	104.1
116	-112.3	114.0	-95.4	122.9	-86.8	109.0	-165.7	145.9	-141.7	146.5
117	-142.4	148.9	-166.1	147.9	-173.3	150.1	-94.6	2.7	-69.0	-36.2
118	-69.9	-20.3	-66.8	-50.3	-101.4	10.5	-81.6	172.8	-59.3	-179.7
119	-65.0	155.7	-42.0	116.8	-78.3	142.9	-135.8	166.2	-137.6	144.9
120	-109.9	167.7	-65.2	148.1	-73.5	142.9	-43.0	122.7	-48.8	140.7
121	-59.0	123.2	-68.3	151.9	-71.0	138.2	-138.1	122.8	-148.9	113.9
122	-127.5	123.8	-153.9	130.9	-131.8	137.6	-74.6	164.7	-70.7	147.8
123	-67.0	155.3	-80.0	150.1	-99.9	146.8	-98.4	158.1	-62.2	1000.0

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*11-28-89*

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Due to averaging procedure, bond lengths & angles of the "average structure" are off from standard values. Therefore the "average structure" was subjected to energy minimization using the AMBER forcefield of the DISCOVER (Biosym) program. Ca atoms were constrained to remain in place with a force constant of 20.0

HVONFB4HV is the unminimized "average structure"

AMBER std.

mean  
Std.  
# values

Bond Lengths & Angles for HVONFB4HV

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.451	1.507	1.160	1.282	1.499	125.3	110.3	120.9	117.6	122.2	110.6	111.2
0.023	0.033	0.177	0.065	0.039	4.6	2.8	7.1	5.2	4.9	2.5	2.2
62	62	62	53	58	53	62	62	53	53	58	58

Bond Lengths & Angles for AVERAGE after 50 cycles minimization (.COR)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.450	1.522	1.230	1.334	1.528	123.6	109.4	120.1	116.6	123.3	109.8	111.1
0.005	0.006	0.002	0.005	0.003	1.2	1.9	0.9	1.3	0.6	1.2	1.1
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 100 cycles minimization (.COR2)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.452	1.524	1.231	1.335	1.530	124.0	109.5	120.1	116.6	123.3	109.8	111.1
0.004	0.005	0.003	0.004	0.002	1.1	1.6	0.7	1.0	0.5	0.9	0.8
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 200 cycles minimization (.COR3)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.526	1.230	1.337	1.530	124.2	109.7	120.2	116.6	123.3	109.8	111.1
0.003	0.003	0.002	0.002	0.001	0.9	1.4	0.6	0.8	0.4	0.6	0.6
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE (.COR4) after 300 cycles minimization (100 Ca released)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.528	1.231	1.338	1.531	124.2	109.9	120.4	116.5	123.1	109.5	111.2
0.002	0.002	0.001	0.001	0.001	0.6	0.9	0.4	0.4	0.2	0.3	0.5
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE (.COR5) after 600 cycles minimization (400 Ca released)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.454	1.528	1.230	1.338	1.531	124.1	110.0	120.5	116.5	123.1	109.6	111.3
0.002	0.002	0.001	0.001	0.001	0.6	0.8	0.4	0.4	0.2	0.4	0.6
64	64	64	55	60	55	64	64	55	55	60	60

Bond Lengths & Angles for AVERAGE after 200 cycles minimization with Ca at 20 (.COR3c)

N-Ca	Ca-C	C=O	C-N	Ca-Cb	C-N-Ca	N-Ca-C	Ca-C=O	Ca-C-N	O=C-N	N-Ca-Cb	Cb-Ca-C
1.455	1.528	1.231	1.338	1.531	124.2	110.0	120.4	116.5	123.1	109.5	111.2
0.002	0.002	0.001	0.001	0.001	0.6	0.8	0.4	0.4	0.2	0.3	0.4
64	64	64	55	60	55	64	64	55	55	60	60

- N-Ca 1.449
- Ca-C 1.522
- C=O 1.229
- C-N 1.335
- Ca-Cb 1.526
- C-N-Ca 121.9
- N-Ca-C 110.1
- Ca-C=O 120.4
- Ca-C-N 116.6
- O=C-N 122.9
- N-Ca-Cb 109.5
- Cb-Ca-C 111.1

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Dihedral Angles for AVERAGE after 200 cycles minimization

		PHI	PSI	OMEGA	
1.	ALA	3	1000.0	152.0	173.6
2.	ALA	4	-123.5	123.4	179.7
3.	ALA	5	-122.1	111.8	176.2
4.	ALA	6	-87.1	151.7	-179.6
5.	ALA	7	-150.5	160.8	177.9
6.	GLY	8	113.5	1000.0	1000.0
7.	ALA	16	1000.0	179.5	-175.3
8.	ALA	17	-128.2	161.6	171.8
9.	ALA	18	-147.0	164.7	174.4
10.	ALA	19	-134.2	112.6	174.1
11.	ALA	20	-90.7	143.4	176.6
12.	ALA	21	-118.2	155.8	179.7
13.	ALA	22	-140.9	104.1	-177.5
14.	ALA	23	-95.8	1000.0	1000.0
15.	ALA	33	1000.0	130.3	174.9
16.	ALA	34	-115.2	144.3	177.6
17.	ALA	35	-123.9	156.9	168.7
18.	ALA	36	-120.1	118.4	172.1
19.	ALA	37	-113.7	150.3	179.7
20.	ALA	38	-128.9	149.3	-178.7
21.	ALA	39	-134.7	100.5	172.5
22.	ALA	40	-58.8	163.1	-173.6
23.	ALA	41	-57.2	1000.0	1000.0
24.	ALA	45	1000.0	138.4	178.3
25.	ALA	46	-130.6	115.3	177.4
26.	ALA	47	-70.1	133.8	178.8
27.	ALA	48	-102.5	-64.9	-179.1
28.	GLY	49	-153.3	175.8	175.3
29.	ALA	50	-146.1	157.2	179.8
30.	ALA	51	-143.7	1000.0	1000.0
31.	ALA	58	1000.0	154.5	174.5
32.	ALA	59	-144.6	135.6	-177.8
33.	ALA	60	-124.0	149.8	173.5
34.	ALA	61	-69.1	155.6	-177.5
35.	ALA	62	-60.1	1000.0	1000.0
36.	ALA	67	1000.0	-19.2	167.7
37.	ALA	68	-99.4	143.1	174.0
38.	ALA	69	-137.6	117.2	177.2
39.	ALA	70	-87.9	139.8	177.3
40.	ALA	71	-140.4	171.1	-172.7
41.	ALA	72	-137.1	1000.0	1000.0
42.	ALA	76	1000.0	5.7	-173.8
43.	ALA	77	49.9	55.9	-174.2
44.	ALA	78	-134.2	129.2	175.4
45.	ALA	79	-112.1	135.8	-177.3
46.	ALA	80	-118.4	157.5	174.7
47.	ALA	81	-134.7	104.6	177.4
48.	ALA	82	-88.4	117.6	-173.7
49.	ALA	83	-109.7	1000.0	1000.0
50.	ALA	92	1000.0	172.2	170.3
51.	ALA	93	-95.6	126.0	-178.5
52.	ALA	94	-102.5	115.9	177.5
53.	ALA	95	-101.0	141.1	167.6
54.	ALA	96	-105.0	129.9	-178.1
55.	ALA	97	-128.6	165.3	-179.6
56.	ALA	98	-112.2	1000.0	1000.0
57.	ALA	107	1000.0	125.2	179.7
58.	ALA	108	-106.2	156.6	169.7
59.	GLY	109	-85.0	174.1	178.8
60.	ALA	110	-74.6	-25.5	-178.3
61.	GLY	111	91.3	154.5	173.9
62.	ALA	112	-133.2	136.4	-175.5
63.	ALA	113	-83.4	139.9	176.2
64.	ALA	114	-127.8	1000.0	1000.0

*.COR3*

Dihedral Angles for AVERAGE after 600 cycles minimization

		PHI	PSI	OMEGA	
1.	ALA	3	1000.0	161.6	173.1
2.	ALA	4	-118.1	88.1	-178.8
3.	ALA	5	-75.3	89.9	178.0
4.	ALA	6	-66.4	146.1	-177.3
5.	ALA	7	-160.4	174.0	-178.9
6.	GLY	8	68.0	1000.0	1000.0
7.	ALA	16	1000.0	163.8	175.6
8.	ALA	17	-117.6	167.3	178.2
9.	ALA	18	-146.4	162.0	179.6
10.	ALA	19	-134.8	91.8	178.0
11.	ALA	20	-77.9	154.5	-175.1
12.	ALA	21	-135.9	155.9	-179.5
13.	ALA	22	-150.1	93.8	-176.4
14.	ALA	23	-82.5	1000.0	1000.0
15.	ALA	33	1000.0	123.4	176.2
16.	ALA	34	-73.0	140.4	175.9
17.	ALA	35	-125.2	157.6	-179.5
18.	ALA	36	-147.0	136.1	-179.2
19.	ALA	37	-147.3	140.8	178.0
20.	ALA	38	-100.6	123.4	175.4
21.	ALA	39	-104.7	99.0	-178.2
22.	ALA	40	-70.3	156.3	177.8
23.	ALA	41	-67.5	1000.0	1000.0
24.	ALA	45	1000.0	163.3	179.3
25.	ALA	46	-135.6	121.6	179.8
26.	ALA	47	-62.8	126.1	179.3
27.	ALA	48	-88.6	-50.5	-179.6
28.	GLY	49	178.1	-172.6	-178.3
29.	ALA	50	-155.3	159.4	-178.1
30.	ALA	51	-160.9	1000.0	1000.0
31.	ALA	58	1000.0	172.5	-178.5
32.	ALA	59	-147.4	152.2	177.8
33.	ALA	60	-148.7	142.3	-178.8
34.	ALA	61	-72.6	158.4	-179.3
35.	ALA	62	-65.7	1000.0	1000.0
36.	ALA	67	1000.0	-49.5	-178.0
37.	ALA	68	-85.8	66.1	-179.8
38.	ALA	69	-74.4	100.7	174.6
39.	ALA	70	-64.8	145.8	-176.4
40.	ALA	71	-156.6	174.7	177.4
41.	ALA	72	-165.6	1000.0	1000.0
42.	ALA	76	1000.0	-43.4	-176.0
43.	ALA	77	57.5	64.5	177.8
44.	ALA	78	-146.2	126.9	172.1
45.	ALA	79	-85.2	166.2	-178.8
46.	ALA	80	-153.6	162.6	177.2
47.	ALA	81	-143.3	102.6	175.3
48.	ALA	82	-79.4	101.1	178.5
49.	ALA	83	-83.5	1000.0	1000.0
50.	ALA	92	1000.0	152.4	174.2
51.	ALA	93	-79.6	103.2	178.2
52.	ALA	94	-73.4	92.7	-175.8
53.	ALA	95	-95.6	110.0	170.8
54.	ALA	96	-79.7	160.3	-178.2
55.	ALA	97	-160.5	170.7	177.3
56.	ALA	98	-74.2	1000.0	1000.0
57.	ALA	107	1000.0	135.2	178.6
58.	ALA	108	-117.4	143.2	-179.5
59.	GLY	109	-82.0	169.7	174.7
60.	ALA	110	-62.7	-41.3	-179.8
61.	GLY	111	88.5	162.0	-178.0
62.	ALA	112	-123.8	129.1	177.6
63.	ALA	113	-66.3	120.0	-177.6
64.	ALA	114	-135.1	1000.0	1000.0

*.COR5*

RMS *.COR3* on *.COR3*      *.COR5* on *.COR3*  
 NcAcOcb      0.326      0.585  
 NcAcO      0.329      0.573  
 NcAc      0.259      0.493

To Page No. *11*

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by	

From Page No. *10*

Dihedral Angles for AVERAGE  
after 200 cycles minimization with Ca at 20.0  
50 cycles with Ca at 10.0  
100 cycles with Ca at 2.5  
100 cycles with Ca at 0.5

*.COR3C*

		PHI	PSI	OMEGA	
1.	ALA	3	1000.0	161.6	179.8
2.	ALA	4	-128.9	103.2	-177.6
3.	ALA	5	-96.6	101.0	174.3
4.	ALA	6	-73.2	146.1	-179.5
5.	ALA	7	-155.7	170.8	178.5
6.	GLY	8	69.6	1000.0	1000.0
7.	ALA	16	1000.0	168.8	178.3
8.	ALA	17	-118.7	164.8	177.2
9.	ALA	18	-150.6	157.8	-179.7
10.	ALA	19	-132.6	91.7	175.4
11.	ALA	20	-74.5	142.1	178.6
12.	ALA	21	-116.6	156.3	-179.9
13.	ALA	22	-146.0	97.6	-179.6
14.	ALA	23	-83.1	1000.0	1000.0
15.	ALA	33	1000.0	130.6	177.1
16.	ALA	34	-95.5	144.4	179.5
17.	ALA	35	-133.2	148.1	176.9
18.	ALA	36	-120.8	131.2	178.8
19.	ALA	37	-138.4	138.1	179.6
20.	ALA	38	-107.7	144.5	176.4
21.	ALA	39	-127.4	105.4	179.8
22.	ALA	40	-70.0	164.1	179.0
23.	ALA	41	-65.7	1000.0	1000.0
24.	ALA	45	1000.0	151.8	-179.3
25.	ALA	46	-140.5	112.5	177.8
26.	ALA	47	-62.7	123.9	-179.6
27.	ALA	48	-86.7	-51.8	-179.9
28.	GLY	49	-177.4	-172.0	-179.4
29.	ALA	50	-156.7	162.1	-179.3
30.	ALA	51	-157.5	1000.0	1000.0
31.	ALA	58	1000.0	170.4	178.3
32.	ALA	59	-142.9	153.6	-178.6
33.	ALA	60	-146.6	149.1	177.9
34.	ALA	61	-76.5	162.9	-178.4
35.	ALA	62	-66.1	1000.0	1000.0
36.	ALA	67	1000.0	-54.5	178.2
37.	ALA	68	-78.9	123.6	179.4
38.	ALA	69	-126.0	106.4	176.8
39.	ALA	70	-74.6	149.6	179.4
40.	ALA	71	-153.2	169.8	-179.3
41.	ALA	72	-140.7	1000.0	1000.0
42.	ALA	76	1000.0	-4.5	-176.9
43.	ALA	77	54.3	52.5	-175.1
44.	ALA	78	-134.6	114.8	169.5
45.	ALA	79	-82.3	157.2	-178.6
46.	ALA	80	-144.1	154.0	-178.8
47.	ALA	81	-138.2	96.8	178.3
48.	ALA	82	-80.8	102.0	177.6
49.	ALA	83	-85.8	1000.0	1000.0
50.	ALA	92	1000.0	155.1	175.3
51.	ALA	93	-85.2	105.3	178.8
52.	ALA	94	-83.1	106.5	179.8
53.	ALA	95	-107.4	124.0	169.6
54.	ALA	96	-84.2	152.2	179.5
55.	ALA	97	-151.5	158.9	178.6
56.	ALA	98	-83.8	1000.0	1000.0
57.	ALA	107	1000.0	133.1	178.1
58.	ALA	108	-119.9	141.3	179.9
59.	GLY	109	-81.2	174.7	177.8
60.	ALA	110	-64.6	-44.8	177.9

AVERAGE.PDB3					AVERAGE.PDB5						
Res#	Res#	Dist	D-A-AA	A-D-DD	A-D<	D-A<	Dist	D-A-AA	A-D-DD	A-D<	D-A<
6	4						2.98	98.0	132.8	32.3	-148.2
5	23	3.00	156.5	118.7	6.4	40.7	2.86	149.3	109.9	-18.2	55.3
23	5	2.98	142.8	119.5	-9.4	73.3	3.01	127.3	117.9	-14.8	72.5
7	21	2.90	147.3	128.1	10.0	-68.1	2.89	139.9	115.6	17.3	-83.6
21	7	2.90	154.0	122.8	-3.1	-61.4	2.94	131.3	113.1	4.9	-96.7
18	83	3.21	143.0	132.3	-5.1	-41.4	3.01	152.5	123.8	2.5	16.2
83	18	2.90	160.6	115.1	-2.5	-80.2	2.84	149.1	107.5	-28.5	-95.4
20	81	3.04	142.1	123.1	-11.6	61.3	2.98	139.9	113.2	-21.3	77.4
81	20	2.89	153.6	125.5	8.2	-49.3	2.94	134.3	124.7	2.9	-75.2
22	79	2.76	166.2	112.4	29.5	30.3	2.89	138.9	113.6	18.7	-89.3
79	22	3.00	143.1	122.9	-0.6	50.0	2.91	142.3	116.1	-22.6	70.9
34	51	2.97	164.4	125.2	-9.5	-42.9	2.84	152.8	110.8	-31.1	-92.8
51	34	2.95	166.3	126.7	7.5	-32.0	2.95	145.0	128.7	0.0	-57.8
35	97	2.89	147.7	120.6	2.4	-72.9	2.91	138.7	109.6	1.7	-92.6
97	35	2.95	143.6	126.7	-3.2	-63.6	2.92	136.0	116.7	17.7	-83.9
36	49	2.91	152.7	123.7	1.5	-75.9	2.93	158.2	108.3	25.4	-102.4
48	36	2.89	156.1	102.0	-0.3	-154.2	2.90	133.8	108.1	-14.3	-137.7
49	36	3.31	143.8	133.7	-10.8	-5.3	3.25	136.6	125.6	-3.2	-56.7
37	95	2.96	159.4	121.0	-15.8	-49.0	2.94	149.5	113.5	13.8	80.9
95	37	2.83	166.5	112.0	-15.6	-88.0	2.82	166.3	103.6	-17.8	101.3
38	46	2.87	150.9	117.6	6.1	68.3	2.87	155.1	120.9	-16.1	65.5
46	38	2.84	170.9	111.0	12.6	15.4	2.97	145.9	112.2	17.9	83.1
39	93	2.94	153.7	123.9	15.2	46.2	3.01	134.0	118.3	2.6	63.6
93	39	3.12	128.4	122.4	-5.4	77.8	2.93	130.3	117.5	-11.0	72.8
48	46						3.34	102.1	123.9	68.6	-159.8
61	48	2.72	170.0	112.7	13.2	-55.9	2.99	141.7	121.4	1.6	-103.9
50	59	2.95@	164.3	128.4	8.6	-23.5	2.97@	134.2	127.3	0.9	-68.7
59	50	3.13@	148.6	127.1	6.3	-60.3	2.91@	148.5	118.8	12.0	-69.7
69	67						3.05	88.1	140.3	11.6	-139.0
70	68						3.09	100.0	135.2	37.7	-150.2
69	82	2.90	154.4	126.1	13.2	20.6	2.92	145.9	108.3	-27.0	79.0
82	69	2.93	148.3	114.1	-7.8	63.7	2.92	143.0	109.6	-21.6	78.1
71	80	3.06	137.2	125.6	1.6	-65.8	2.92	136.1	111.6	13.8	-91.2
80	71	2.94	134.3	122.2	-6.4	-85.4	2.88	131.0	109.7	16.3	-104.2
78	76	3.42	74.1	114.2	90.1	130.4					
83	81						3.23	94.0	134.9	38.8	-143.5
92	114	3.13	153.2	131.7	38.6	-30.9	2.95	128.1	130.3	36.2	-100.1
114	92	2.94	161.8	114.1	12.0	88.7	2.92	150.6	105.9	7.9	94.0
94	92						3.27	94.1	135.2	40.0	-143.1
94	112	2.94	146.9	120.5	-2.6	66.2	2.85	141.6	109.1	-18.5	77.5
112	94	3.14	134.4	129.9	10.1	65.1	3.03	126.5	128.5	4.1	70.6
95	93						3.01	97.7	127.5	40.6	-146.7
109	96	2.80	159.7	107.6	25.9	94.3	2.87	150.8	105.5	0.7	-121.7
98	107	2.92	162.9	126.0	14.3	38.4	2.93	172.0	120.4	5.9	-54.4
114	112						3.29	101.1	123.8	64.0	-154.9

\* after dist denotes a possible alpha helix res  
@ after dist denotes a possible 3-10 helix res

61.	GLY	111	95.9	168.2	-177.5
62.	ALA	112	-135.3	130.7	179.0
63.	ALA	113	-71.5	138.8	178.5
64.	ALA	114	-141.1	1000.0	1000.0

*Hbonds*  
*.COR3(.PDB3) after 200 cycles*  
*.COR5(.PDB5) after 600 cycles*

To Page No. \_\_\_\_\_

Witnessed & Understood by me,

Date

Invented by

Date

Recorded by

*Leonard Presto*

*11-28-89*

From Page No. \_\_\_\_\_

Framework Model: to be used for generating model of a variable, heavy domain

Archetype model: special version of framework model to be used to generate model of a "consensus" human, variable heavy

Both based on HVONFB4HV after 200 cycles minimization (.COR3)

<u>B-sheet Framework Res.</u> (IFB4 numbering)	<u>Archetype Res.</u>	<u>Loop to insert</u>
4-7	4-7	1-7 (1-3 FB4, FBJ, MCP) 8-15
18-25	16-23	16-23 24-33
34-39	34-40	34-40 41-44
46-52	45-51	45-51 52-57
57-61	58-60	58-62 (61-62 FB4, HFL, MCP) 61-67 (framework) 63-65 (archetype)
68-71	68-72	66-83 (66-67 FB4, HFL, MCP) (73-76 FB4, FBJ, HFL, MCP) 73-76 (framework)
78-84	77-83	84-91
92-99	92-98	99-106
	107-108	109-111 (framework)
	112-114	115-123

For archetype model, inclusion of res 61, 62, 66, 67 assumes no Pro at 62 or 63 (as in 3FAB or 1FBT) and Gly at 66 (missing in 3FAB & 1FBT)

To Page No. \_\_\_\_\_

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Date \_\_\_\_\_

Recorded by

Leonard Presta

11-29-89



From Page No. \_\_\_\_\_

Remember Archetype & Consensus according to  
 Kabat et al Sequences of Proteins of Immunological  
 Interest 4th Ed 1987

Kabat	Archetype	Consensus	Kabat
57-61	58-62	58-60	57-59
65-82	66-83	68-72	67-71
88-94	92-98	77-83	76-82
102-109	107-114	92-98	88-94
		107-108	102-103
		112-114	107-109

To Page No. \_\_\_\_\_

Witnessed & Understood by me,

Date

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Date

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From Page No. \_\_\_\_\_

Dihedral Angles for ARCHETYPE

		PHI	PSI	OMEGA
1.	ALA	1	150.2	180.0
2.	ALA	2	-77.3	121.4
3.	ALA	3	-132.9	141.9
4.	ALA	4	-123.5	123.4
5.	ALA	5	-122.1	111.8
6.	ALA	6	-87.1	151.7
7.	ALA	7	-150.5	
8.	ALA	16		179.5
9.	ALA	17	-128.2	161.6
10.	ALA	18	-147.0	164.7
11.	ALA	19	-134.2	112.6
12.	ALA	20	-90.7	143.4
13.	ALA	21	-118.2	155.8
14.	ALA	22	-140.9	104.1
15.	ALA	23	-95.8	
16.	ALA	34		144.3
17.	ALA	35	-123.9	156.9
18.	ALA	36	-120.1	118.4
19.	ALA	37	-113.7	150.3
20.	ALA	38	-128.9	149.3
21.	ALA	39	-134.7	100.5
22.	ALA	40	-58.8	
23.	ALA	45		138.4
24.	ALA	46	-130.6	115.3
25.	ALA	47	-70.1	133.8
26.	ALA	48	-102.5	-64.9
27.	GLY	49	-153.3	175.8
28.	ALA	50	-146.1	157.2
29.	ALA	51	-143.7	
30.	ALA	57		154.5
31.	ALA	58	-144.6	135.6
32.	ALA	59	-124.0	149.8
33.	ALA	60	-74.1	145.6
34.	ALA	61	-37.9	
35.	GLY	65		-36.1
36.	ALA	66	-111.7	-19.2
37.	ALA	67	-99.4	145.5
38.	ALA	68	-137.6	117.2
39.	ALA	69	-87.9	139.8
40.	ALA	70	-140.4	171.1
41.	ALA	71	-137.1	116.2
42.	ALA	72	-82.7	89.6
43.	ALA	73	-52.9	-35.3
44.	ALA	74	-62.1	-25.5
45.	ALA	75	-111.1	5.6
46.	ALA	76	49.9	55.9
47.	ALA	77	-134.2	129.2
48.	ALA	78	-112.1	135.8
49.	ALA	79	-118.4	157.5
50.	ALA	80	-134.7	104.6
51.	ALA	81	-88.4	117.6
52.	ALA	82	-109.7	
53.	ALA	88		172.2
54.	ALA	89	-95.6	126.0
55.	ALA	90	-102.5	115.9
56.	ALA	91	-101.0	141.1
57.	ALA	92	-105.0	129.9
58.	ALA	93	-128.6	165.3
59.	ALA	94	-112.2	
60.	ALA	102		125.2
61.	ALA	103	-106.2	156.6
62.	GLY	104	-85.0	174.1
63.	ALA	105	-74.6	-25.5
64.	GLY	106	91.3	154.5
65.	ALA	107	-133.2	136.4
66.	ALA	108	-83.4	139.9
67.	ALA	109	-127.8	

FROM PDB FILE: ARCHETYPE.PDB

Doing residues: 1 to 67

Res	Res#	Atnm	Res	Res#	Atnm	Dist	D-A-AA	A-D-DD	A-D<	D-A<
ALA	5	N	ALA	23	O	3.00	156.5	118.7	6.4	40.7
ALA	23	N	ALA	5	O	2.98	142.8	119.5	-9.4	73.3
ALA	7	N	ALA	21	O	2.90	147.3	128.1	10.0	-68.1
ALA	21	N	ALA	7	O	2.90	154.0	122.8	-3.1	-61.4
ALA	18	N	ALA	82	O	3.21	143.0	132.3	-5.1	-41.4
ALA	82	N	ALA	18	O	2.90	160.6	115.1	-2.5	-80.2
ALA	20	N	ALA	80	O	3.04	142.1	123.1	-11.6	61.3
ALA	80	N	ALA	20	O	2.89	153.6	125.5	8.2	-49.3
ALA	22	N	ALA	78	O	2.76	166.2	112.4	29.5	30.3
ALA	78	N	ALA	22	O	3.00	143.1	122.9	-0.6	50.0
ALA	34	N	ALA	51	O	2.97	164.4	125.2	46.9	-42.9
ALA	51	N	ALA	34	O	2.95	166.3	126.7	7.5	-32.0
ALA	35	N	ALA	93	O	2.89	147.7	120.6	2.4	-72.9
ALA	93	N	ALA	35	O	2.95	143.6	126.7	-3.2	-63.6
ALA	36	N	GLY	49	O	2.91	152.7	123.7	1.5	-75.9
ALA	48	N	ALA	36	O	2.89	156.1	102.0	-0.3	-154.2
GLY	49	N	ALA	36	O	3.31	143.8	133.7	-10.8	-5.3
ALA	37	N	ALA	91	O	2.96	159.4	121.0	-15.8	-49.0
ALA	91	N	ALA	37	O	2.83	166.5	112.0	-15.6	-88.0
ALA	38	N	ALA	46	O	2.87*	150.9	117.6	6.1	68.3
ALA	46	N	ALA	38	O	2.84*	170.9	111.0	12.6	15.4
ALA	39	N	ALA	89	O	2.94	153.7	123.9	15.2	46.2
ALA	89	N	ALA	39	O	3.12	128.4	122.4	-5.4	77.8
ALA	60	N	ALA	48	O	2.72	170.0	111.7	15.9	-55.9
ALA	50	N	ALA	58	O	2.95@	164.3	128.4	8.6	-23.5
ALA	58	N	ALA	50	O	3.13@	148.6	127.1	6.3	-60.3
ALA	68	N	ALA	81	O	2.90	154.4	126.1	13.2	20.6
ALA	81	N	ALA	68	O	2.93	148.3	114.1	-7.8	63.7
ALA	70	N	ALA	79	O	3.06	137.2	125.6	1.6	-65.8
ALA	79	N	ALA	70	O	2.94	134.3	122.2	-6.4	-85.4
ALA	72	N	ALA	77	O	2.82	164.1	117.8	-32.2	-45.4
ALA	74	N	ALA	72	O	3.29	79.4	116.4	-75.1	-131.7
ALA	75	N	ALA	72	O	2.81@	127.9	108.6	-17.2	-101.5
ALA	76	N	ALA	72	O	3.00*	160.6	109.9	44.4	163.5
ALA	77	N	ALA	72	O	3.35	130.5	119.5	14.3	69.0
ALA	75	N	ALA	73	O	3.46	72.8	125.3	-64.7	-128.2
ALA	76	N	ALA	73	O	3.48@	100.3	107.6	-10.9	-90.2
ALA	77	N	ALA	75	O	3.42	74.1	114.2	90.1	130.4
ALA	88	N	ALA	109	O	3.13	153.2	131.7	38.6	-30.9
ALA	109	N	ALA	88	O	2.94	161.8	114.1	12.0	88.7
ALA	90	N	ALA	107	O	2.94	146.9	120.5	-2.6	66.2
ALA	107	N	ALA	90	O	3.14	134.4	129.9	10.1	65.1
GLY	104	N	ALA	92	O	2.80	159.7	107.6	25.9	94.3
ALA	94	N	ALA	102	O	2.92	162.9	126.0	14.3	38.4

\* after dist denotes a possible alpha helix res  
 @ after dist denotes a possible 3-10 helix res

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\* from 1FB4

Res	Conf	Res	Conf	Res	Conf
2 Val	175.8°	19 Arg	-174, 173, -85, 180	1 Glu	* 53, -66, -69
4 Leu	-73.9, 176.6	82 Met	-67, 179, 72	3 Ala	* -55, -82, -95
16 Gly		88 Ala		5 Val	* -166
17 Ser	-61.5	89 Val	168	6 Glu	* -60, 83, -16 <small>FB4 FBT</small>
20 Leu	-74, 177	90 Tyr	-68, 70	7 Ser	56 H <sub>2</sub> O
21 Ser	54	91 Tyr	-55, -79	18 Leu	* -68, 168
22 Cys	175	92 Cys	72	35 <del>His</del> Ser	-65, <del>100</del>
23 Ala		93 Ala		48 Val	* 176
34 Met	-66, -68, -59	103 Trp	-66, 68	50 <del>His</del> Val	<del>99, 75</del> 79
36 Trp	-73, 97	104 Gly		60 <del>Asn</del> Ala	-171, -28
37 Val	164	109 Val	173	61 <del>His</del> Asp	-65, <del>70, 90</del>
38 Arg	64, 169, 178, -174			66 Arg	* -45, -169, -74, 111
39 Glu	173, 176, 64			69 Ile	* -167, 168
40 Ala				71 Arg	* 60, -170, -60, 148
45 Leu	-65, 172			73 Asp	-73, -86
46 Glu	175, -153, 46			74 Ser	180
47 Trp	179, 78			76 Asn	-47, 171
49 Ala				94 Arg	* -166, 180, 73, 159
<del>50 His</del>	<del>79, -91</del>			102 Tyr	* -69, -88
51 Ile	-161, 178			105 Ala	* -57, 180, -118
57 Thr	45			107 Thr	180
58 <del>Asn</del> Trp	-71, <del>127</del> 90			108 Thr	* -60
59 Tyr	-62, -89				
65 Gly					
67 Phe	-64, <del>82</del> 17				
68 Thr	-40				
70 Ser	-52				
72 Asp	-178, 16				
75 Leu	-77, 180, 180, 180				
77 Thr	<del>78</del> -51				
78 Leu	176, 80				
80 Tyr	-59, -74				
81 Leu	179, 77				
82 Glu	178, 65, 56				

File: Archetype.PDBSC

@ Sidechain conf of res 69

X1 ~ 180 if 49 = Ala  
 ~ -40 if 49 = Gly

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Sg8 loops superimposed on Archetype

Prot res	RMS	NCaC	file
FB4 6,7,16,17	0.186		
FB4 7,16	0.159		LOOP1.FB4
FBJ 6,7,16,17	0.333		LOOP1.FBJ
HFL 5,6,16,17	0.263		#
6,7,16,17	0.559		LOOP1.HFL
FAB 6,7,16,17	0.525		LOOP1.FAB

file: Archetype.PDBLOOP1

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1FB4, 1FBJ have one conf and A40  
 2MCP, 2KFL have second conf and P40  
 model based on Human III - A40

Prot	res	RMS NCAC	file
1FB4	40, 45	0.126	LOOP3.FB4
1FBJ	40, 45	0.202	LOOP3.FBJ
2KFL	40, 45	0.195	LOOP3.KFL
2MCP	<del>40</del> , 40, 45	0.132	LOOP3.MCP

file: Archetype. PDBLPI-3

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Group 1: 1FB4, 2HFL, 2MCP

2: 3 tab ~~Pro~~ Pro @ 62

3: 1FB5 Pro @ 61

	Prot	res	RMS NC/C	Archetype
use	1FB4	62, 66	0.165	61, 65
	2MCP	64, 68	0.166	
	2HFL	62, 66	0.203	

File: Archetype.PDBLP1-4

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Prot	res	Archetype	RMS NC&C	
1FB4	82,83 92,93	81,82 88,89	0.157	Loop6.FB4
2mCP	84,85 94,95 on Loop6.FB4	"	0.206 0.203	.mCP
2KFL	82,83 92,93 on Loop6.FB4	"	0.191 0.486	.KFL .KFL2
1FBJ	82,83 92,93 on Loop6.FB4	81,82 88,89	0.311 0.449	.FBJ .FBJ2
3fab	81,82 91,92 on Loop6.FB4		0.327 0.588	.FAB .FAB2

file: Archetype.PDB1-6

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12-20-89

From Page No. \_\_\_\_\_ Heavy CDR1: Res 26-32 (Chothia/Lesk JMB 196:901 1987)  
Res 31-35 (Kabat 1987)

Prot	Res	Archetype Res	RMS NC&C	file
1FB4	22,23,34,35	22,23,34,35	0.178	LOOP.HI.FB4
2MCP	"	"	0.153	.MCP
1FBJ	"	"	0.294	.FBJ
2NFL	"	"	0.312	.NFL
3FAB	"	"	0.303	.FAB

Sidechains within 6 Å

Res	1FB4	1FBJ	2NFL	2MCP	3FAB	Hum III (Kabat)
F27	V2	V2		V2		V2
	L4			L4		L4
	S24	A24	A24	T24		A24
	F29	F29	F29	F29		F29
	Y32		Y32	F32		Y32
	M34	M34	I34	M34		M34
	R98	R98	H98	R100		R94
			F103			
F29	S24	A24		T24		A24
	F27	F27	F27	F27		F27
	M34	M34	I34	M34		M34
	R72		A72	R74		R71
	D74		T74	T76		D73
	N77	N77	S77	S79		N76
	L79	L79				L78
		Y32	P53			

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	1FB4	1FBJ	2NFL	2MCP	3FAB	Num III
M34	F27		F27	F27		F27
	F29	F29	F29	F29		F29
	Y32	Y32				Y32
	ISI	ISI		SSI		ISI
	R72			R74		R71
	L79	L79	A79	L81		L78
	R98	R98	H98			R94
	C22	C22	C22	C22		C22
	C96	C96	C96	C98		C92
				R100		
				T24		
				L4		

CDR1 Heavy Res 26-35b (26-32 Chathia/Leak; 31-35b Kabat)

Lengths Num I 10 Num II 10-12 (10=8; 11=1; 12=7) Num III 10 (Kabat 1987)

Res	I	II	III	#Aegs - #AA - # common
*26	J 10-2-9 E	J 12-1-12	J 58-3-56 VA	How other AAs
*27	Y 10-4-5 ADE	F 11-5-4 HLYS	F 56-2-55 I	
28	T 8-2-6 DE	S 11-3-9 TP	T 51-8-30 SNKI APL	
*29	F 8-2-7 A	L 10-4-5 IFV	F 53-4-47 IVL	
*30	S 8-5-3 NVIR	S 10-4-7 NTR	S 50-9-39 Gax BTPEAR	
31	D 8-7-2 RBSHTL	T 10-5-4 SHNR	DT 47-11-15/11 SARYKPEB	
32	Y 8-2-5 S	10-7 TSDERY	Y 50-10-21 SND FATHBV	
33	Y/A 8-6 TKDB	J 10-4-5 YTR	A 46-12-13 YAT SVWNLDEF	
*34	I 8-4-4 MNR	M 10-4-4 YVW	M 50-7-35 VIYLR	
35	H 8-5-3 SILD	10-8 CSRDAWTY	S 46-12-11 HDYNEFKVRT	
35a		V 8-3-6 SW		
35b		J 7-3-4 SA		

General: 26 GFTFSxYxMx

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Prot	Res	Archetype	RMS N/C
1FB4	50,51,58,59	50,51,57,58 <del>50,51,57,58</del>	0.120
2MCP	50,51,60,61	"	0.246
2HFL	50,51,58,59	"	0.232
1FBJ	50,51,58,59	"	0.275
3FAB	50,51,57,58	"	0.194

Heavy CDR2:  
Res 53-55 (Chothia / Lesk)  
50-65 (Kabat)

Human Subgroup I

Res	#Asps	#AA	#major	others
50	7	7	1(+)	GSIAWVE
	7	3	5(ILE)	PV
	7	6	2(ASN)	VAPHD
	6	3	4(PRO)	KL
53	7	6	2(SER)	MWRNY
	7	5	2(+)	PSTAD
	7	3	4(GLY)	DN
	7	5	2(+)	PGSRT
	7	4	4(THR)	PFE
	7	6	2(ASN)	QSVD
	7	3	5(TYR)	GK
60	6	4	3(ALA)	VNA
	6	3	3(PRO)	GY
	6	4	2(+)	KRIG
	6	3	3(PHE)	SK
	7	4	4(GLN)	WVK
65	7	5	3(GLY)	EVAS

Human Subgroup III

Res	34	12	6V	Sequence
50	34	12	6V	WAHYFYRTNIL
51	34	6	23I	RKVFM
52	33	11	6S	YSEWVTKLW Sex
52a	30	10	SE/SY	NBRKD SVW Sex
52b	8*	1		K
52c	8*	2		TS
53	33	12	10N	Asp YSKDTALERVQ
54	32	6	16Y	SANKV
55	31	8	10S	YAsp YNVKA
56	31	11		SDAsp TANLFIER Sex
57	33	8	15T	K Sex SQVI
58	32	11	10Y	HI STFALMVAsp
59	33	2	29Y	F
60	33	6	20A	GR TVI
61	33	5	19D	VAEN
62	34	20	32S	R
* related seqs (see Kabat)				
63	34	4	31V	ALF
64	33	4	21K	NQR
65	33	2	32B	A

Human Subgroup II

Res	#Asps	#AA	#major	others
50	10	7	3(ARG)	WFSYGE
	10	4	6(ILE)	VLD
	10	6	3(ASN) : 3(ASP)	YFIL
	2	2	1(+)	Y
53	9	5	4(TRP)	YHLAsp
	10	5	5(ASP) : 4(ASP)	NSHT
	10	2	6(ASP)	G
	10	4	5(ASP)	STK
	10	6	4(LYS)	TSIPN
	10	4	6(TYR)	RDN
	10	4	7(TYR)	WFD
60	10	5 : 6	3(+)	3(SER) NGTK
	10	3	5(THR)	PA
	10	2	9(SER)	P
	10	1	10(LEU)	
	10	3	4(ARG)	KE
65	10	3	5(SER)	TG

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CDR2 Heavy Res 50-65

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#Res 50-65

Hum I 17  
 II 17(1); 16(9)  
 III 17(21); 16(2); 19(8\*)

50 51 52 <sup>52a 53</sup> 54 55 56 57 58 59 60 61 62 63 64 65  
 I Y(A)(D) S V K G

CDR3 Heavy Res 95-102

Hum I 8(1); 10(1); 13(2); 16(1); 19(1)  
 II 9(2); 10(1); 11(1); 13(1); 15(2); 16(1); 18(2); 19(1)  
 III 5(1); 7(1); 9(2+8\*); 11(2); 12(2); 13(7); 17(2); 19(1)  
 10(5)

Heavy CDR3: Res 96-101 (Chothia/Lesk) Res 95-102 (Kabat)

3FAB = NEWM Human II

1FB4 = KOL Human III

2MCP = MCP 603 Mouse III(A)

1FBJ = J539 Mouse III(B)

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B-sheet h-bonds found in crystal structures and Archetype PDBEDR123 (consensus structure)

Res	FB1	FAB	FB5	MCP	HFL	Arch dist.	Res	FB1	FAB	FB5	MCP	HFL	Arch
3=25	✓	✓	-	✓	(1/2)	3.07 3.27*	52→56	✓	✓	(✓)	✓	✓	3.11*
5=23	✓	✓	✓	✓	✓	3.00 2.98	50=58	✓	(1/2)	✓	✓	✓	2.95 3.13*
7=21	✓	(✓)	✓	✓	-	2.90 2.90	48←60	✓	✓	(✓)	(✓)	(✓)	2.71
18=82	✓	✓	1/2	✓	✓	3.15* 2.90	15→82C	✓	-	✓	✓	✓	3.17*
20=80	✓	✓	✓	✓	✓	3.04 2.89	82C→16	✓	-	✓	✓	✓	3.28*
22=78	✓	(✓)	✓	✓	✓	3.76 3.00	12←112	✓	✓	-	✓	✓	2.94
24→76	✓	-	-	✓	✓	3.24*	→110	✓	(✓)	-	✓	✓	3.20
82A→66	✓	-	✓	✓	✓	2.91	10K	✓	(✓)	✓	✓	✓	3.14
81=68	✓	✓	✓	✓	✓	2.93 2.90	→108	(✓)	-	(✓)	✓	✓	-
79=70	✓	✓	1/2	✓	✓	2.66 3.06							
77←72	✓	(✓)	-	✓	✓	2.76							
88=109	✓	✓	✓	✓	✓	3.13* 2.94							
90=107	✓	✓	✓	✓	✓	2.94 3.14*							
92←104	✓	-	✓	✓	✓	2.80							
91→102	✓	-	✓	✓	✓	2.84							
↙ 101 ↘ 102	✓	-	-	✓	-	-							
39=89	✓	✓	1/2	✓	✓	2.94 3.12*							
37=91	✓	✓	✓	✓	✓	2.96 2.83							
35=93	✓	(1/2)	✓	✓	✓	2.89 2.95							
33←95	✓	✓	✓	✓	-	3.29*							
38=46	✓	✓	✓	✓	✓	2.87 2.84							
36←48	✓	✓	✓	✓	✓	2.89							
→49	✓	✓	✓	✓	✓	2.91							
34=51	✓	-	✓	✓	✓	2.97 2.95							

( ) = poor geometry  
\* = long distance in Archetype

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1-31-90

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		res #s ( ) long distance						
		HFM	HFL	MCP	F19	FBJ	FB4	FAB
S708	08 S21		7,21	7,21	7,21			
S1708	081 N82a	17,83					17,84	
W36NE1	0 F14 79	36,79		36,82		36,80	36,80	
R38 NE	0E E46	38,46				38,46	38,46	38,46
Nh1	0h Y90	38,93	(38,94)	(38,96)		38,94	38,94	
Nh1	0S D86			38,92			38,90	
Nh2	0E E46	38,46		38,46		38,46	38,46	38,46
W47 NE1	0 x49			47,49			47,49	
NE1	0E E35		47,35	47,35				
R66 Nh1	0S D86	66,89		69,92			67,90	66,89
Nh1	0 S82b	66,84					67,85	
Nh2	0S D86	66,89		69,92			67,90	66,89
Nh2	0 S62			69,65			67,63	
K66 NE2	0S D86		67,90		(67,90)			
x69 N	0h Y59	(59,69)	(70,60)	(72,62)		70,60	70,60	
Q81 NE2	0 L18			(84,18)		(82,18)	(82,18)	
NE2	0S D1N82a		(82,84)	84,86			(82,84)	
Y90 Oh	0 D86	<del>93,89</del>	94,90	96,92	94,90	94,90	94,90	93,89
R94 NE	0S D101			(100,110)	98,112		98,106	
Nh2	0S D101			100,110	98,112		98,106	
Q105 N	0E Q6			114,6		(110,6)	110,6	
Q106 N	0E Q6	106,6		115,6		111,6	111,6	

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2-6-90

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Archetype: PDBCDR123 → hvhumiii.pdb  
 human VH subgroup III

DS2aY Y102V T108L

Building 4DS VH from Archetype

(1) Conf. of residues 7-15 depends on identity of residues 9, 10; in human subgroup III Y9, Y10 in 4DS P9, E10; change conf. res 7-15 to (3HFM, 3FAB) conf.

(2) conf. of CDR2 (H2) dependent on position of Gly; in archetype, res 51-57 from 1FB4 -- replace with I51-T57 from 2HFL; conformation of H2 also dependent on res 71 -- when R, H2 folds "out", when A H2 folds "in"; since res 71 is A in 4DS and 2HFL, H2 taken from 2HFL

	49	50	51	52	53	54	55	56	71				
3FAB	D	Y	V	F	-	-	-	Y	H	S	T	} conf 1	
D1.3								D	D				
3HFM	D	Y	V	S	-	-	-	Y	S	D	S		R
2HFL	D	E	I	L	P	-	-	D	S	D	S	A	conf 2
2FB4	A	I	I	W	D	-	-	D	D	S	D	R	} conf 3
1FB3	D	E	I	H	P	-	-	D	S	D	T	R	
2MCP	A	A	S	R	N	K	D	N	K	Y	T	R	conf 4
4DS	D	R	I	Y	P	-	-	T	N	D	Y	A	

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From Page No. 27

(3) CDR1: use conf from 2HFL/2MCP

Seq	24	27	29	34	71	78	94
2FB4	S	F	F	M	R	L	R
1FBJ	A	F	F	M	R	L	R
2MCP	T	F	F	M	R	L	R
1F19	A	Y	F	V	V	A	R
2HFL	A	Y	F	I	A	A	R
3HFM	V	D	I	W	R	Y	N
3FAB	V	T	F	S	V	F	R
4DS	A	F	I	I	A	A	R
Hum III	A	F	F	M	R	L	R
mouse II	A	Y/F	F/I	M	A	A	R

conf1

conf2

(4) CDR3:

	94	100	101	105
2FB4	R D Y D H Y F C S S A S C F Y P		D Y W	
1F19	R S F Y Y S D L A V Y Y F		D S W	
3FAB	R N L I A D C I		D V W	
1FBJ	R L H Y Y D Y N		A Y W	
2HFL	H Y N Y D F		D Y W	
3HFM	N W D Y		D Y W	
2MCP	R N Y Y Y S T W Y F		D V W	
4DS	R W Y D D F Y A M		D Y W	

in one model; use H3 from 2MCP

Insight loop search gave one good one:

1PRC res C11-C19 PATTI-QT YFR YLSM-GEVLH To Page No. 29

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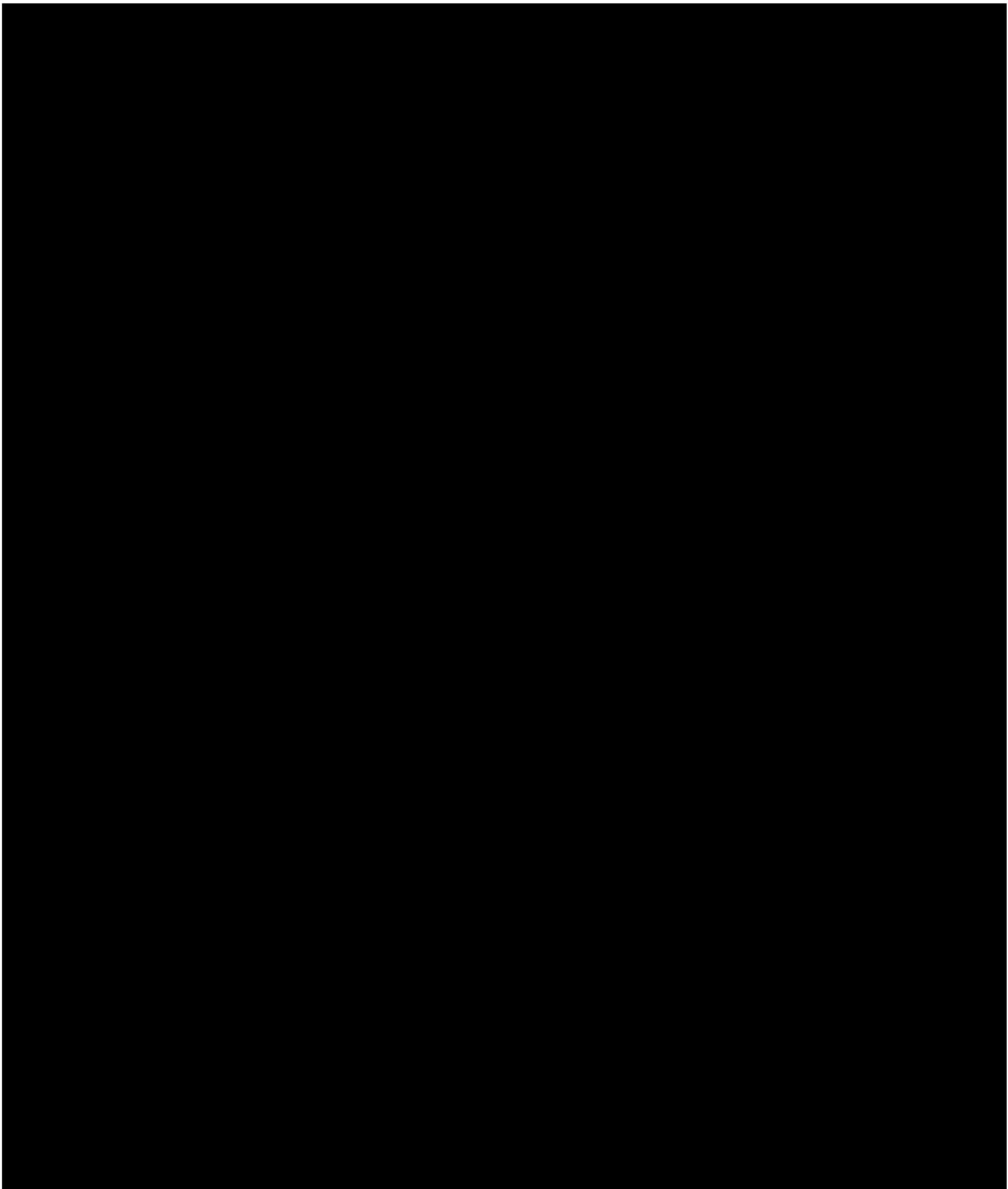
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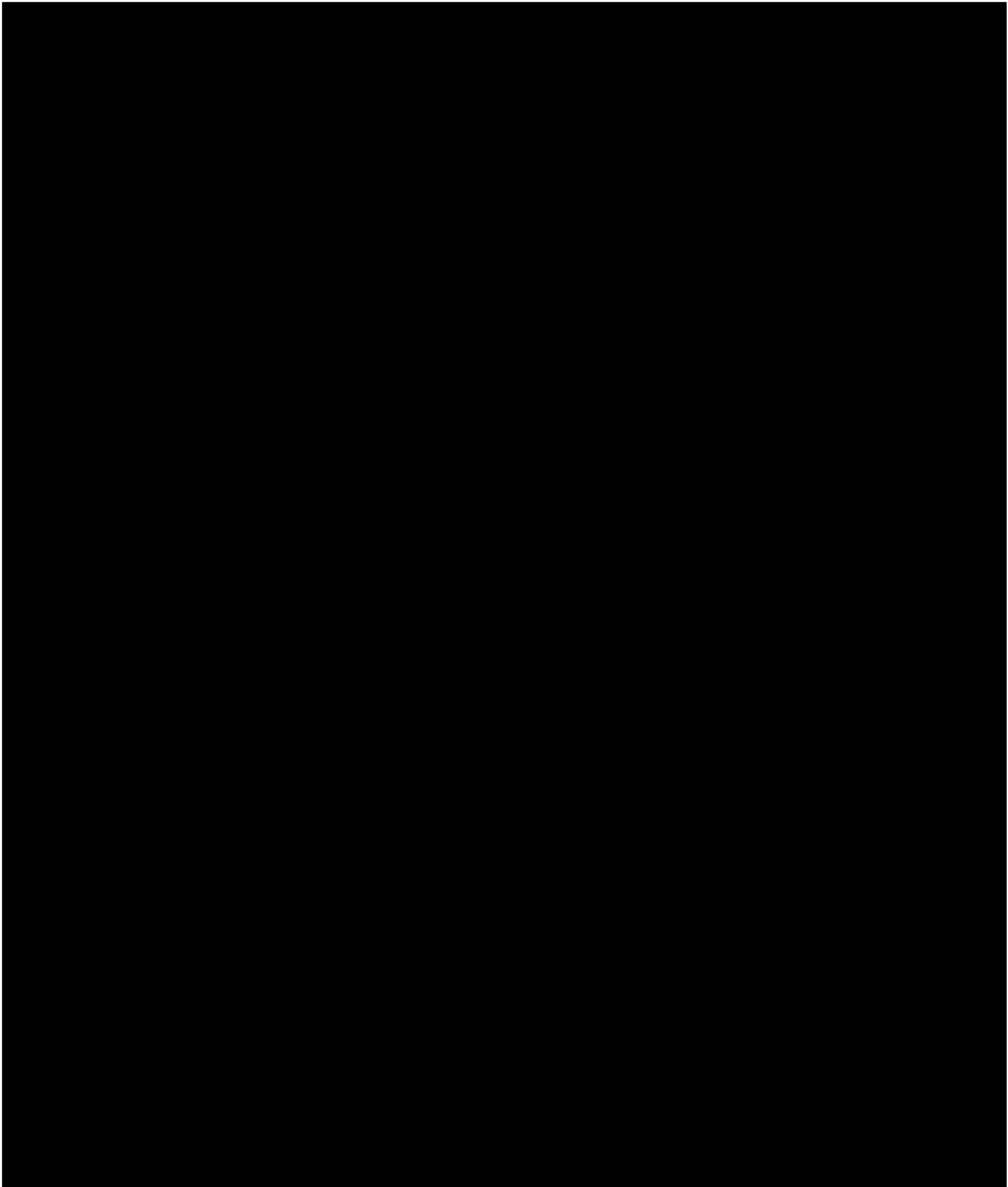
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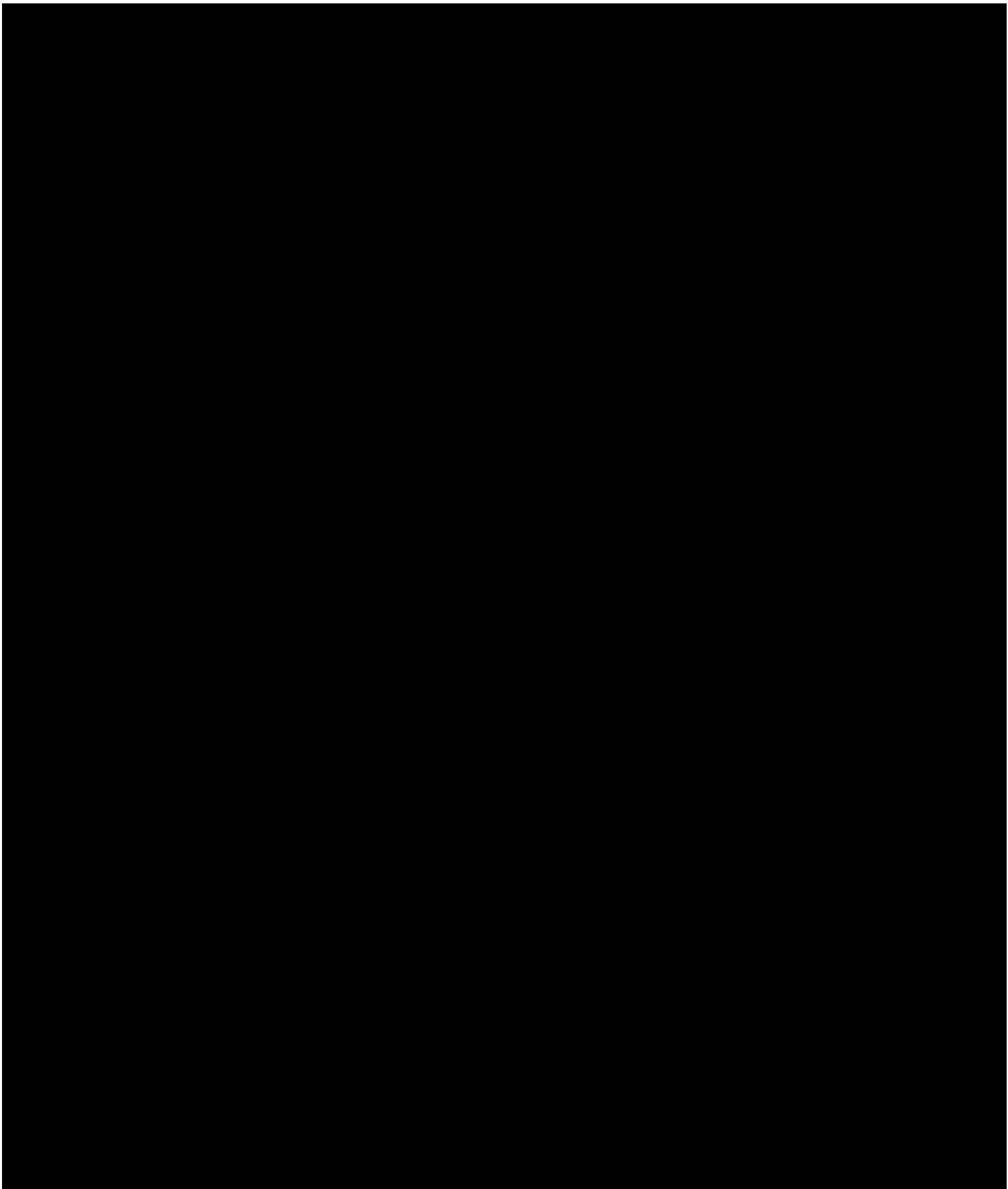




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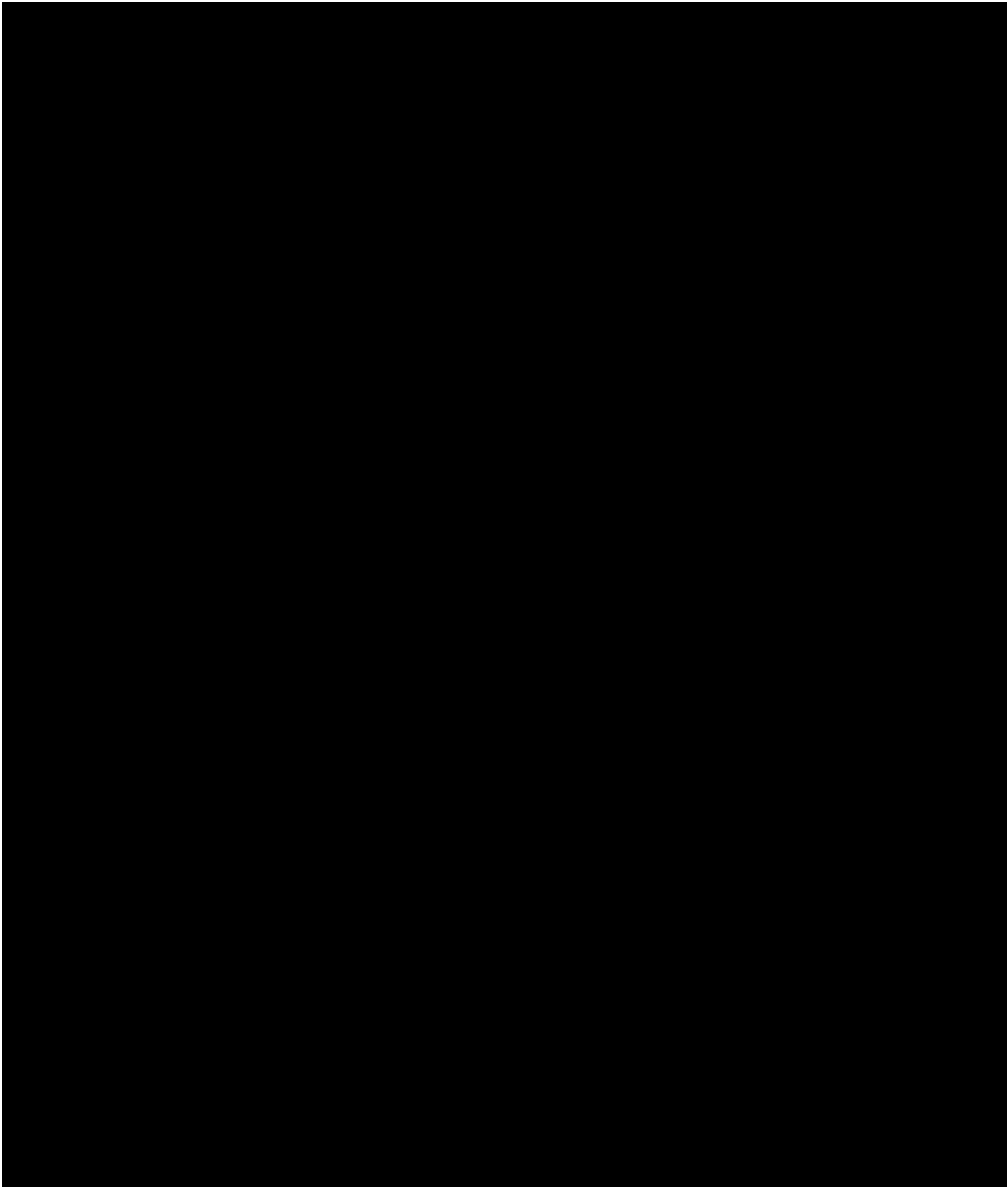
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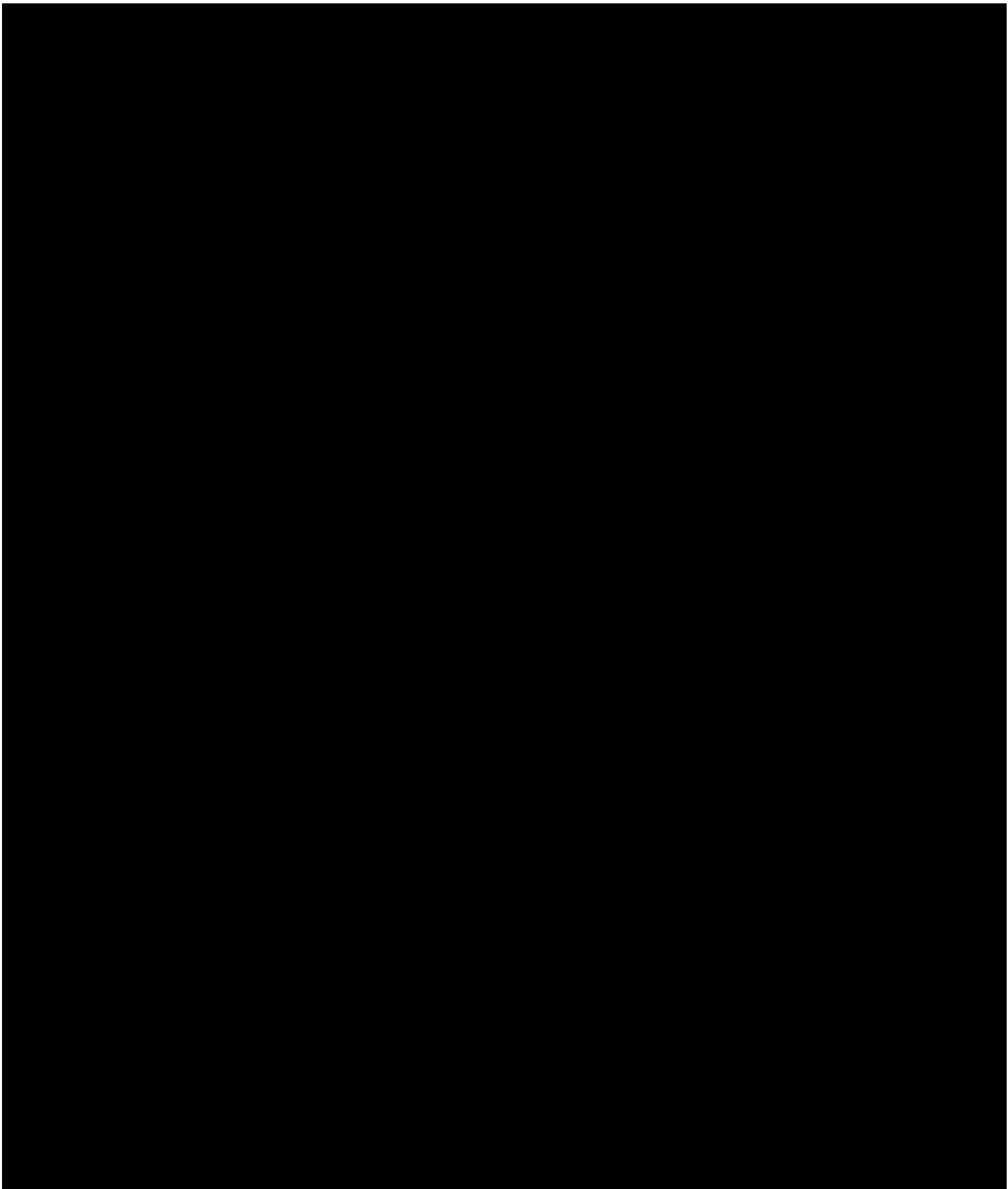
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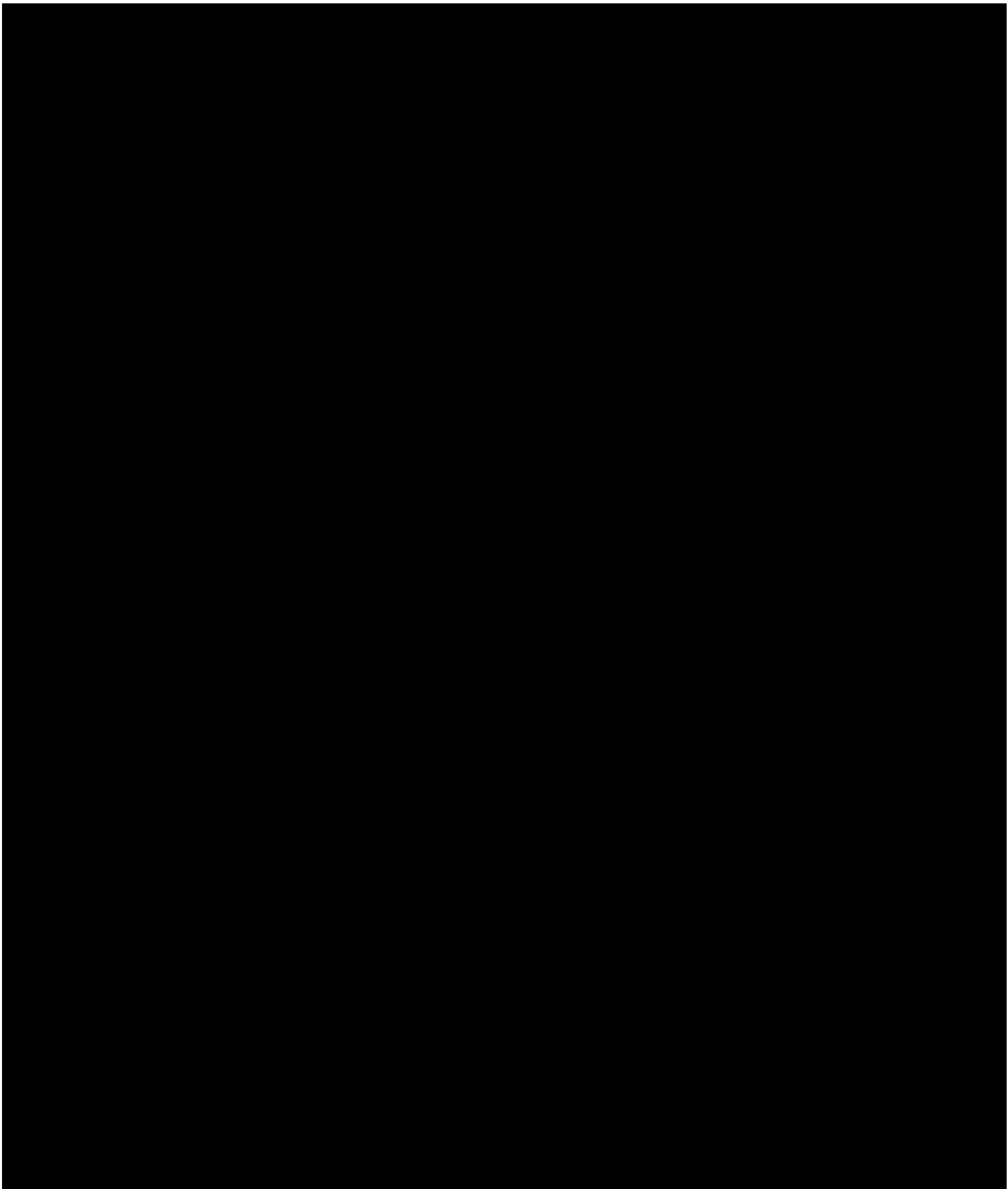
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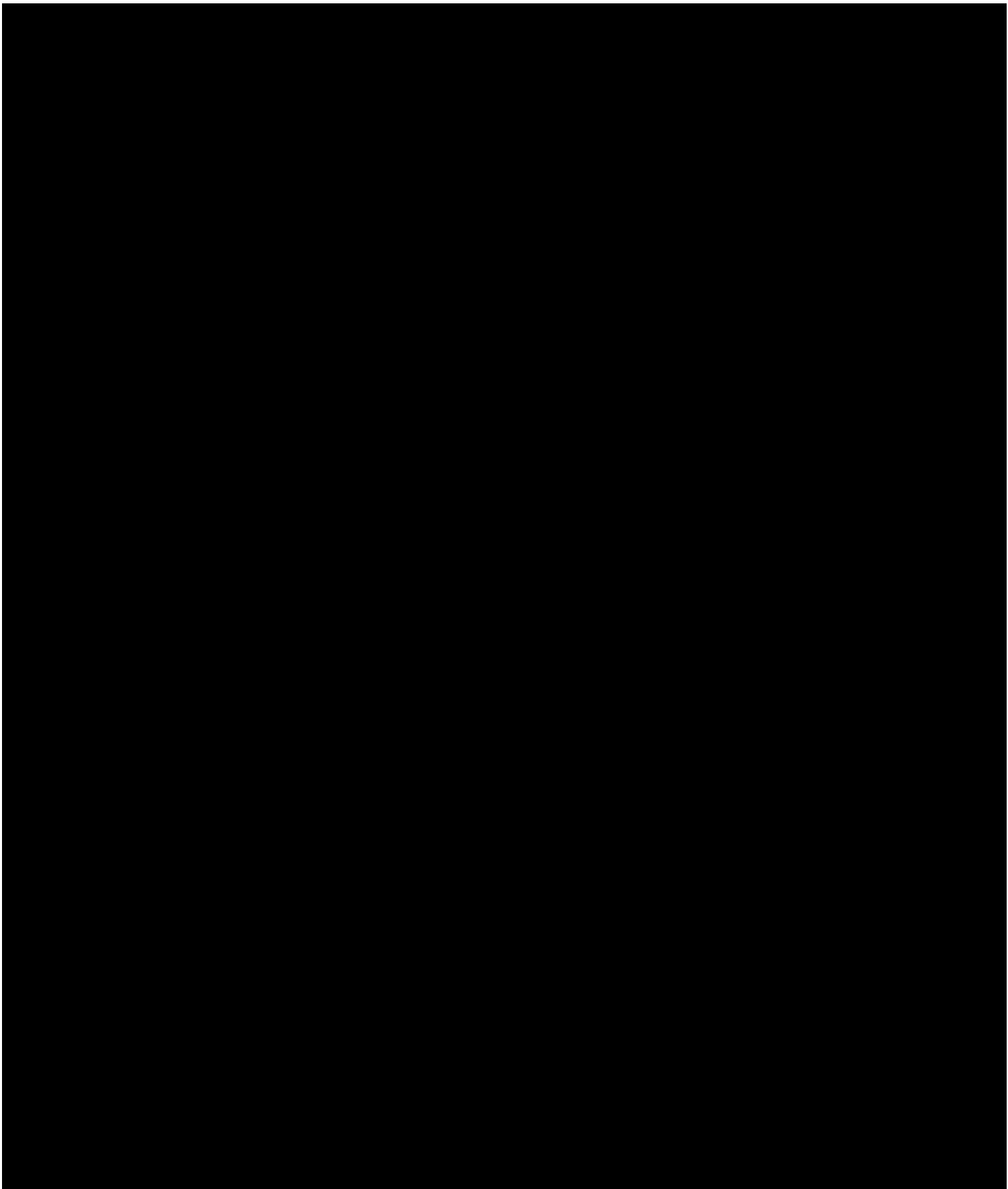
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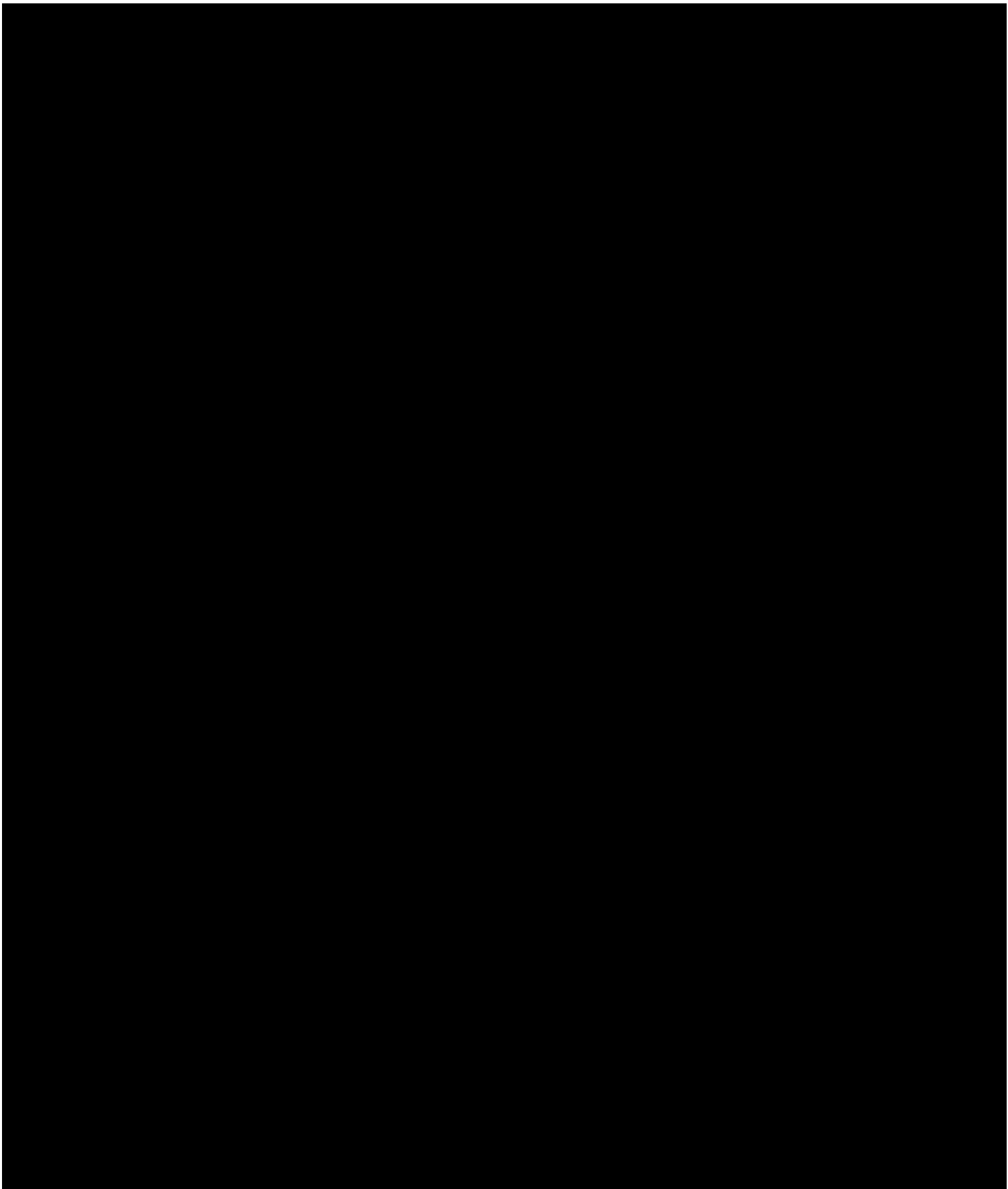


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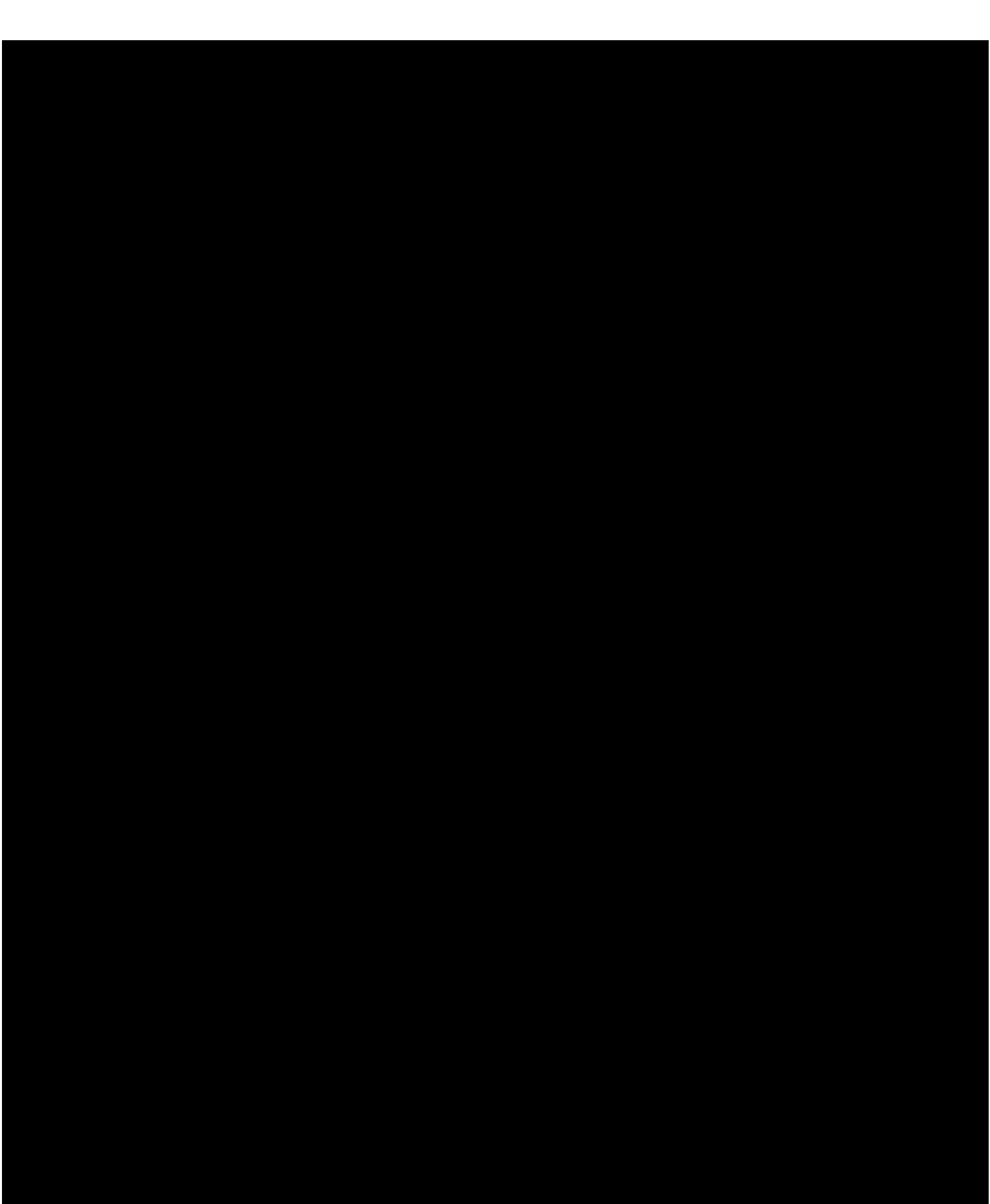
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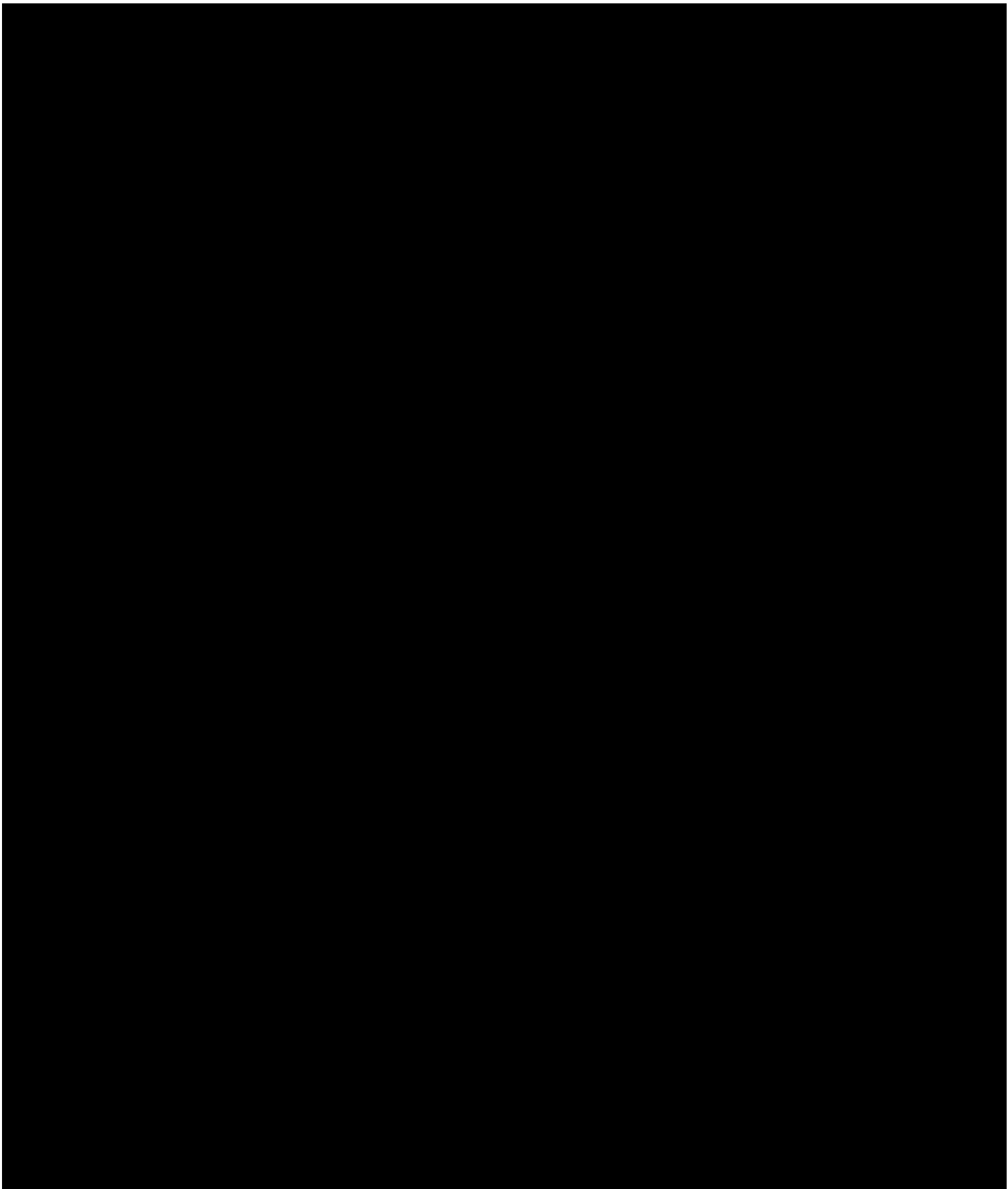
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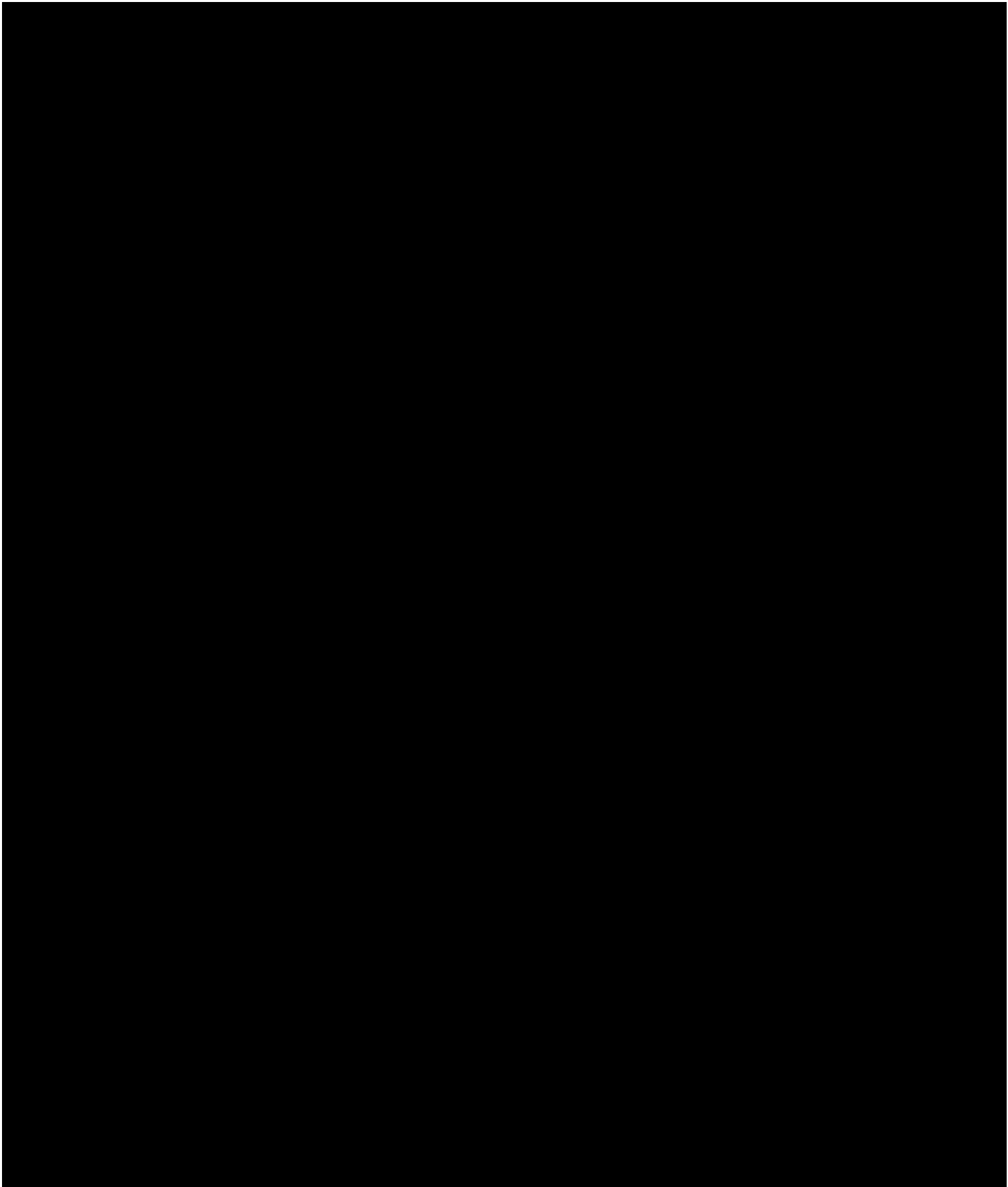
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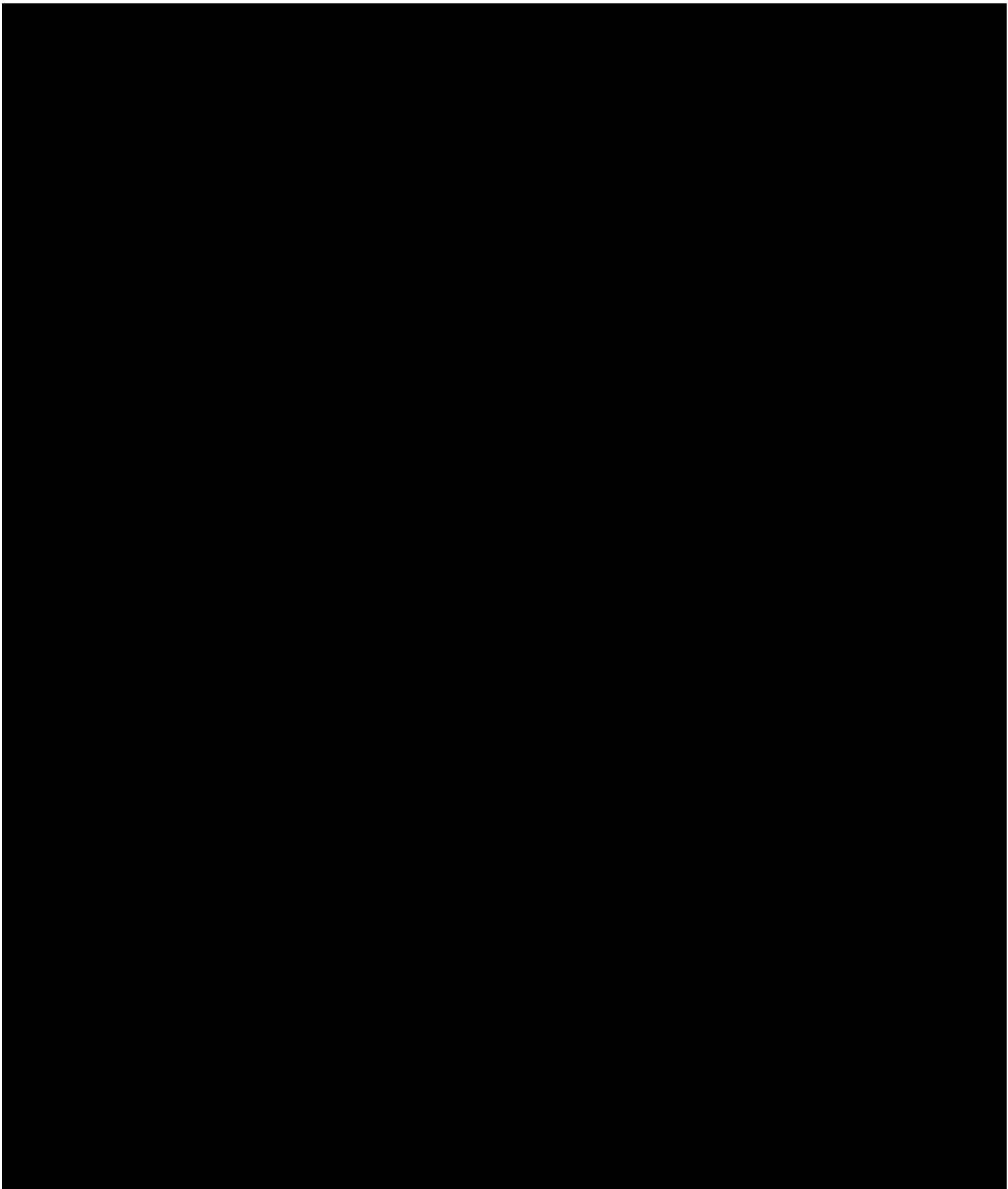
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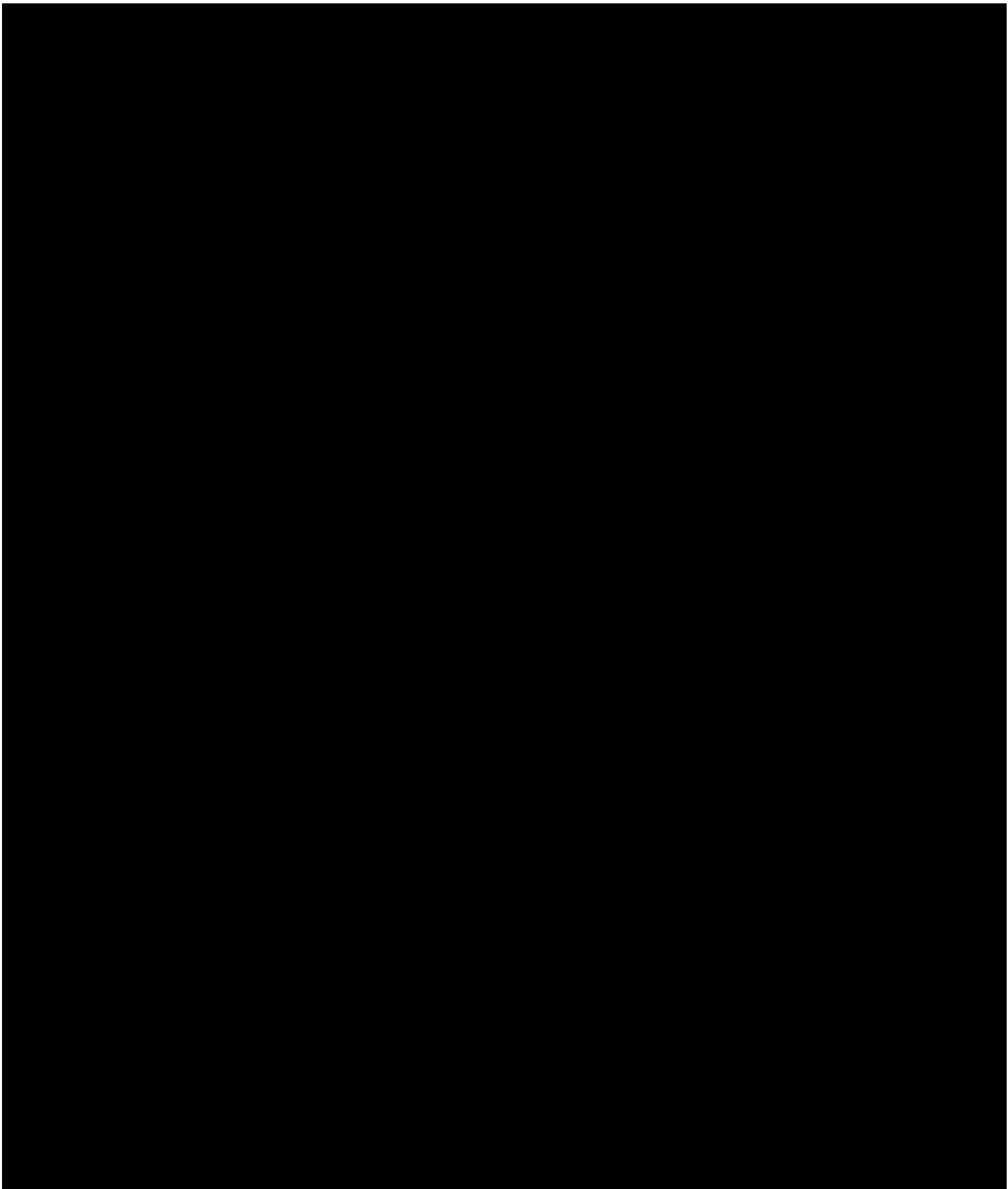
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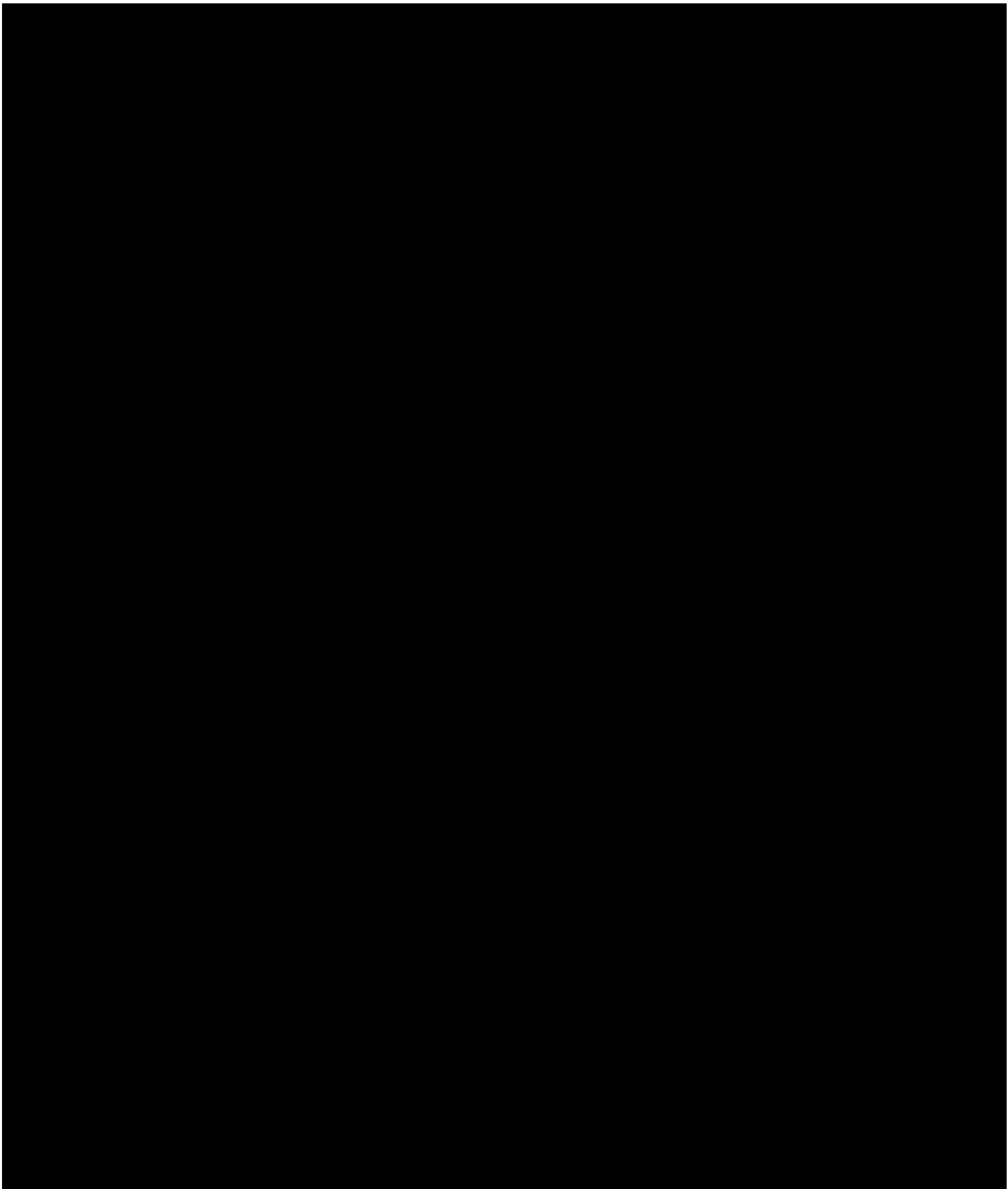
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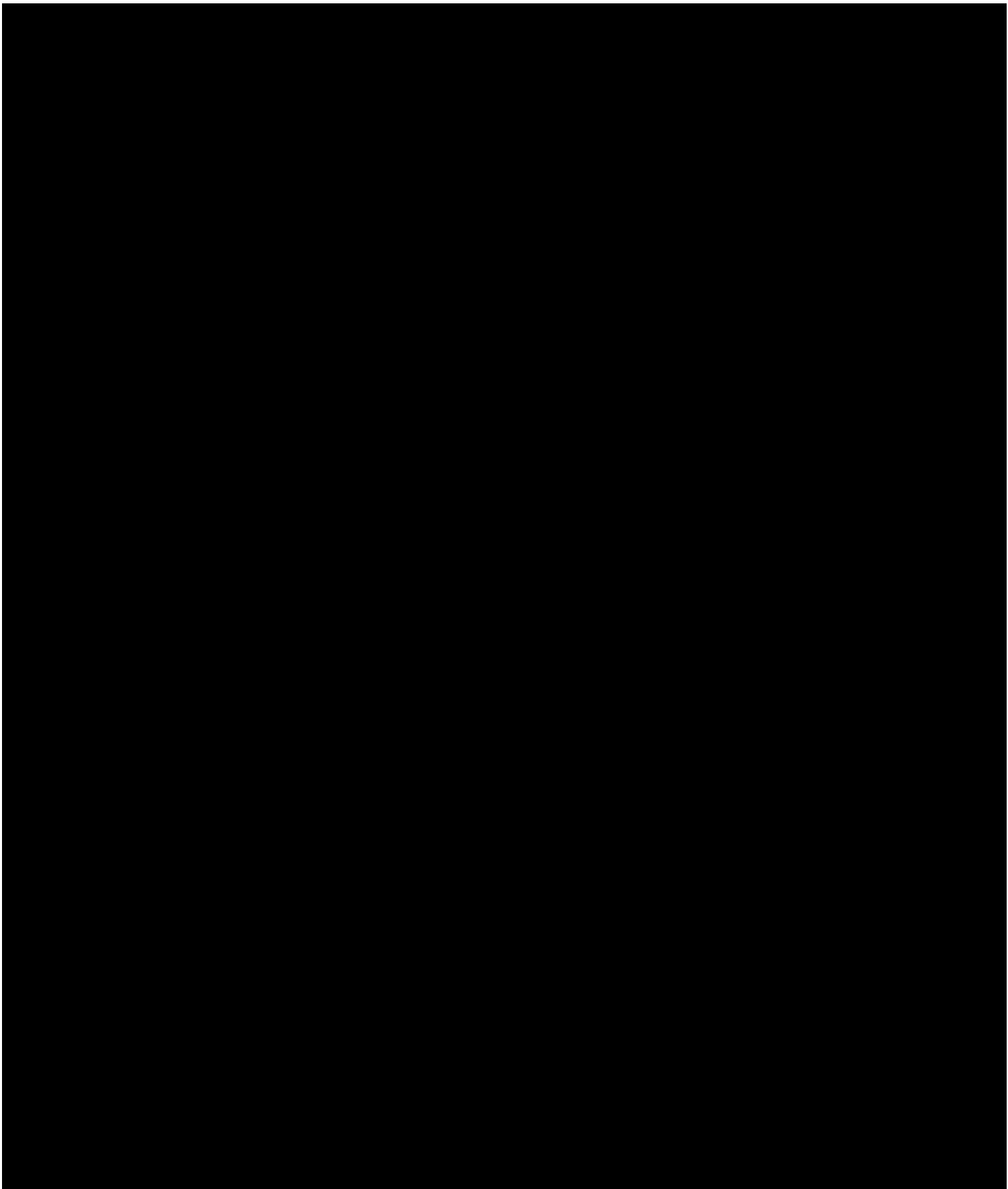
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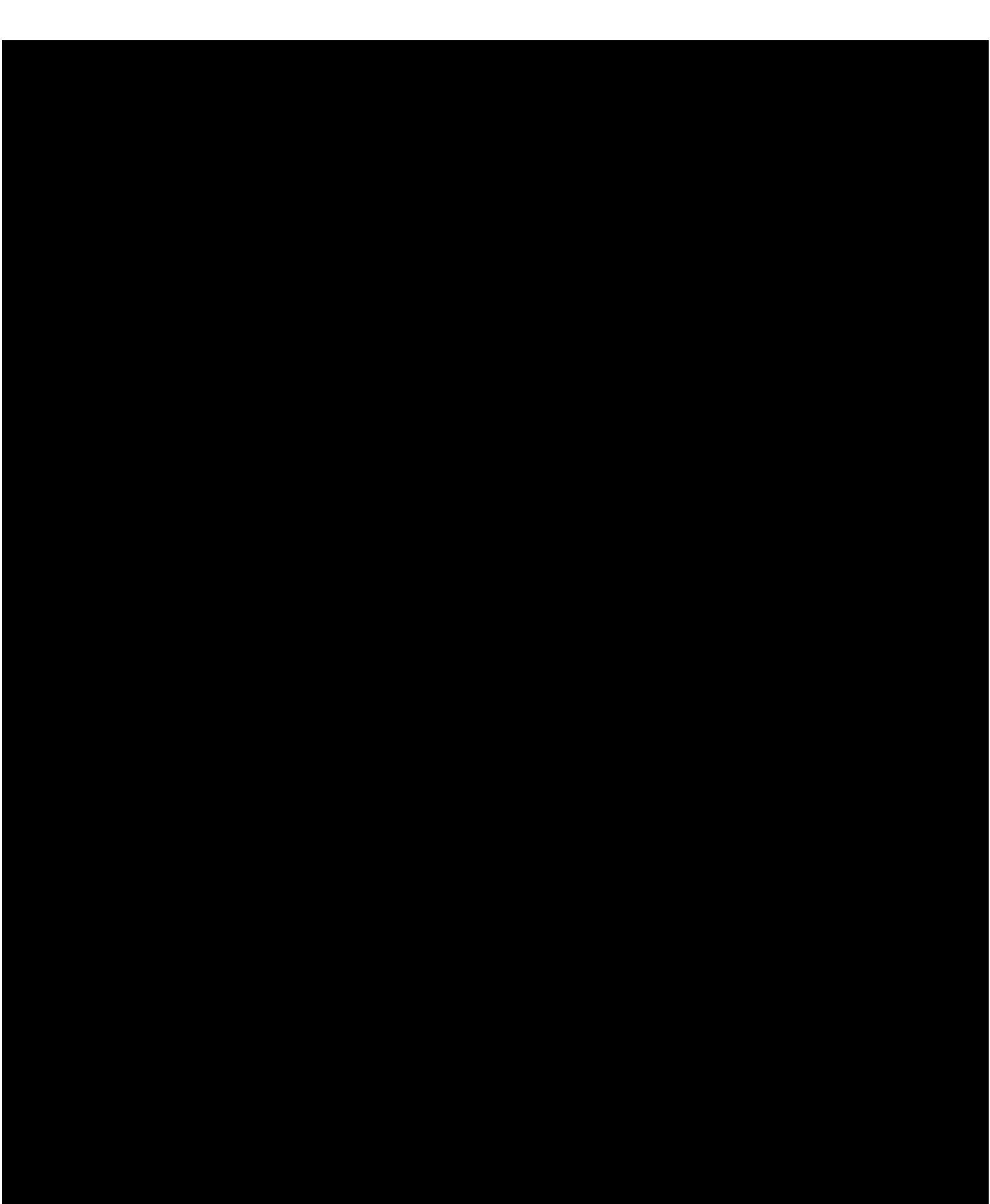
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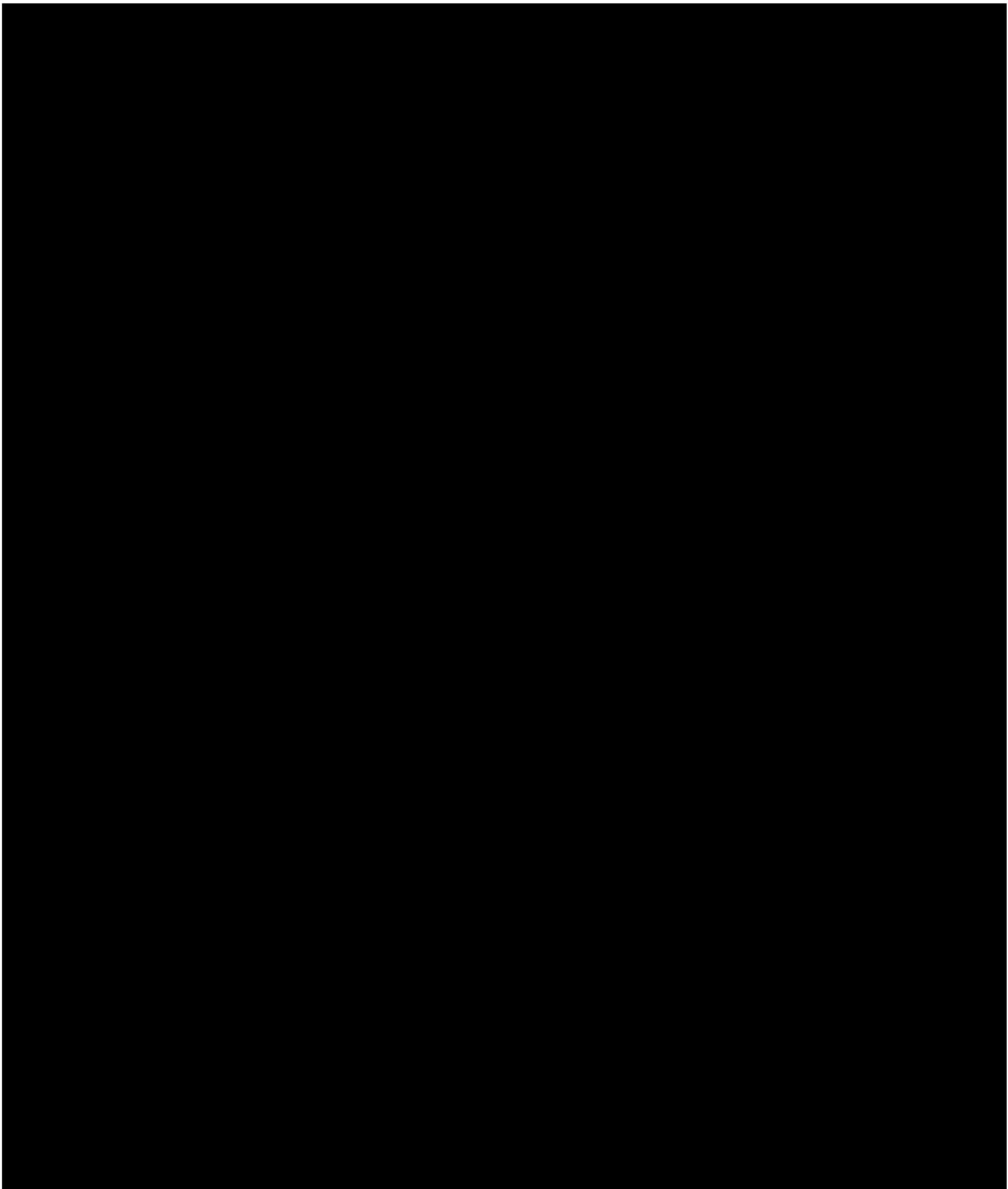
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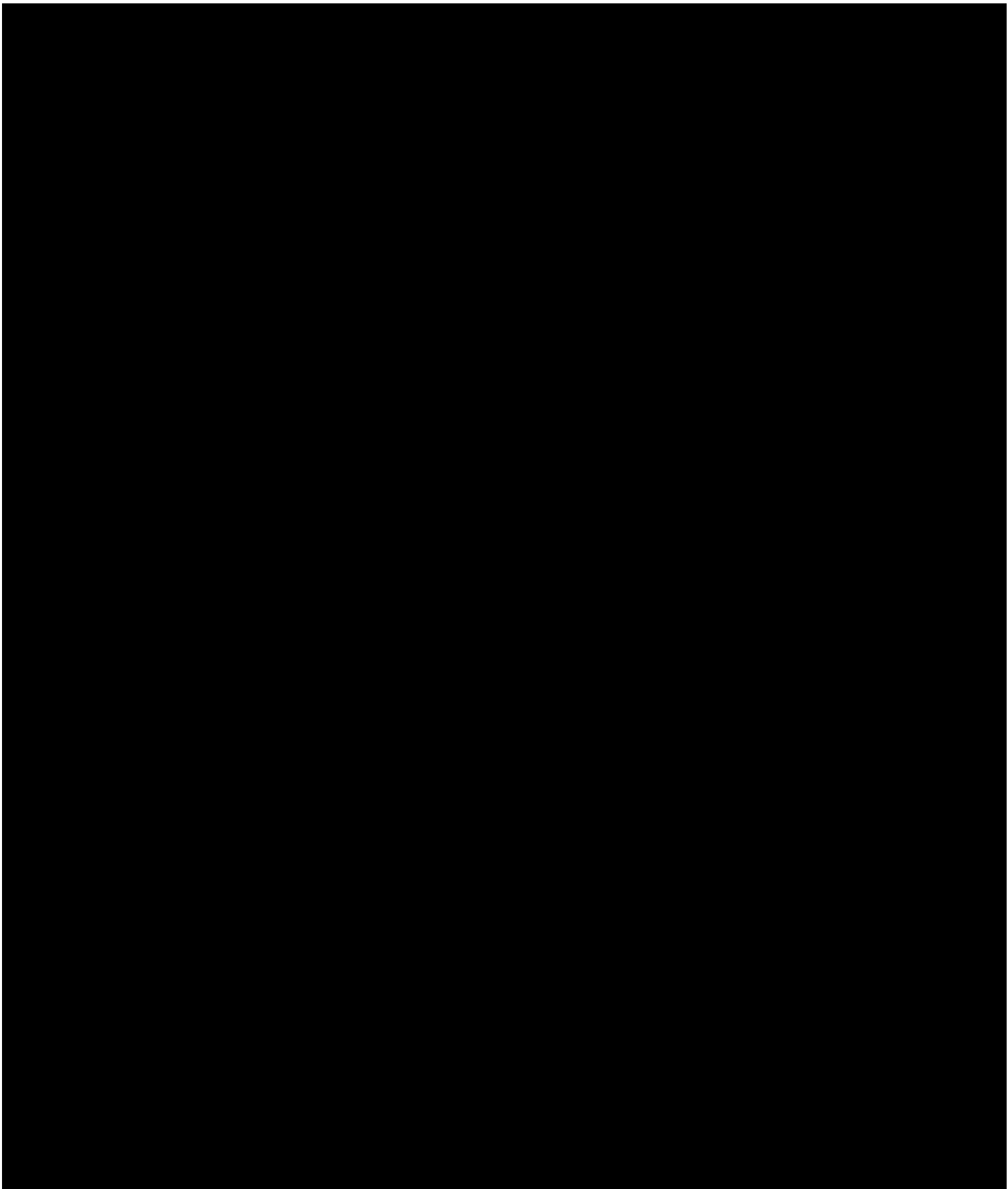
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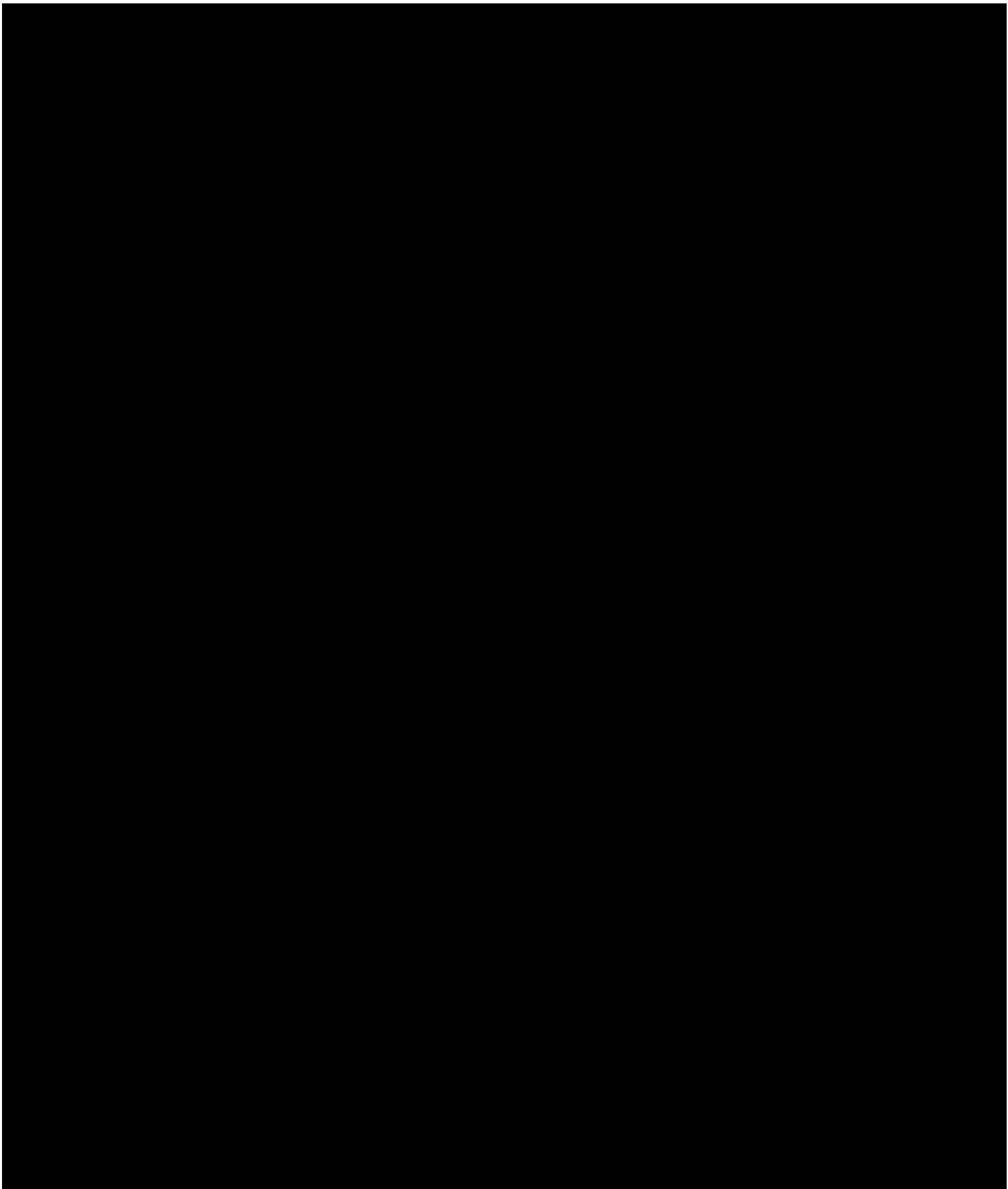
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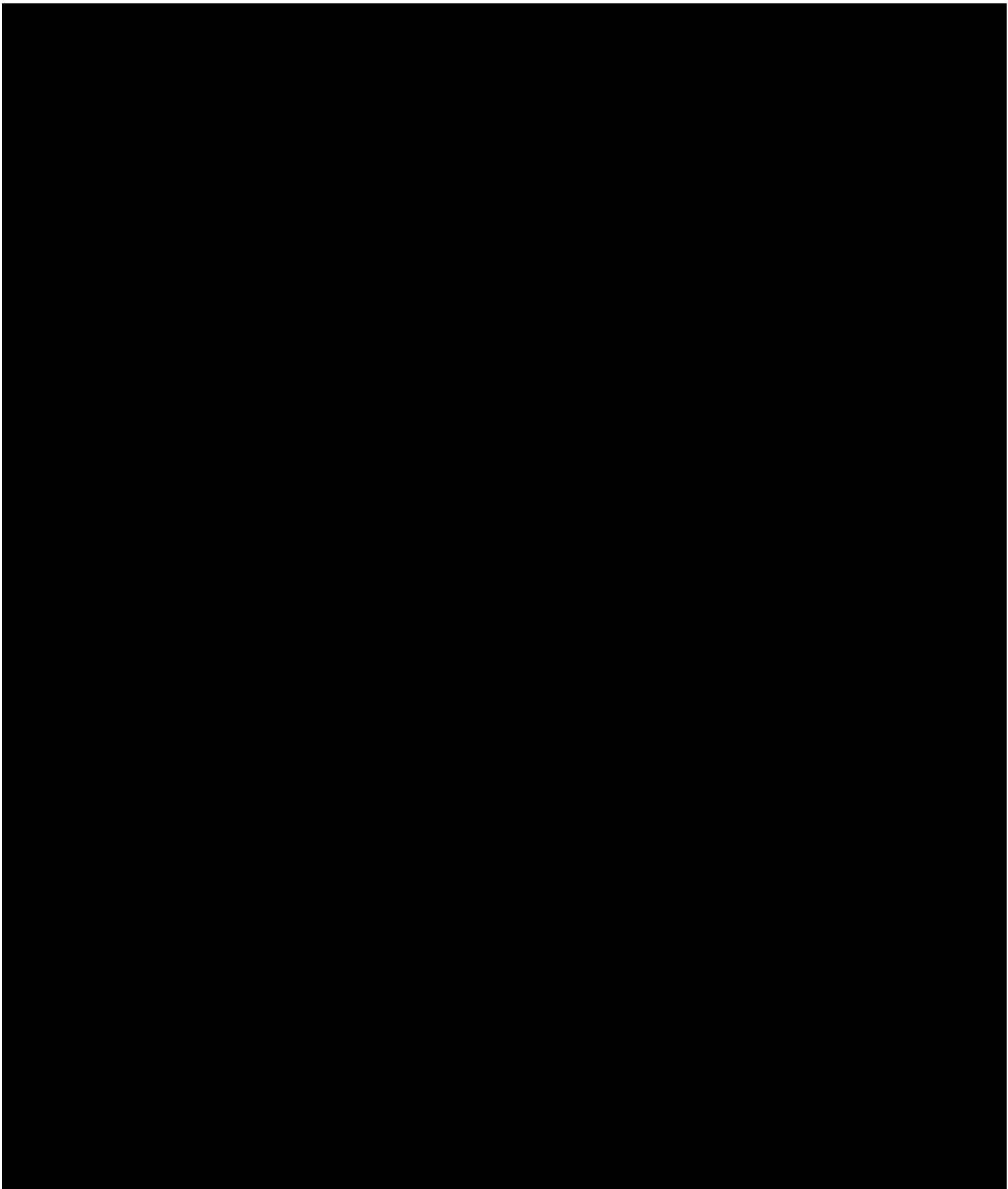
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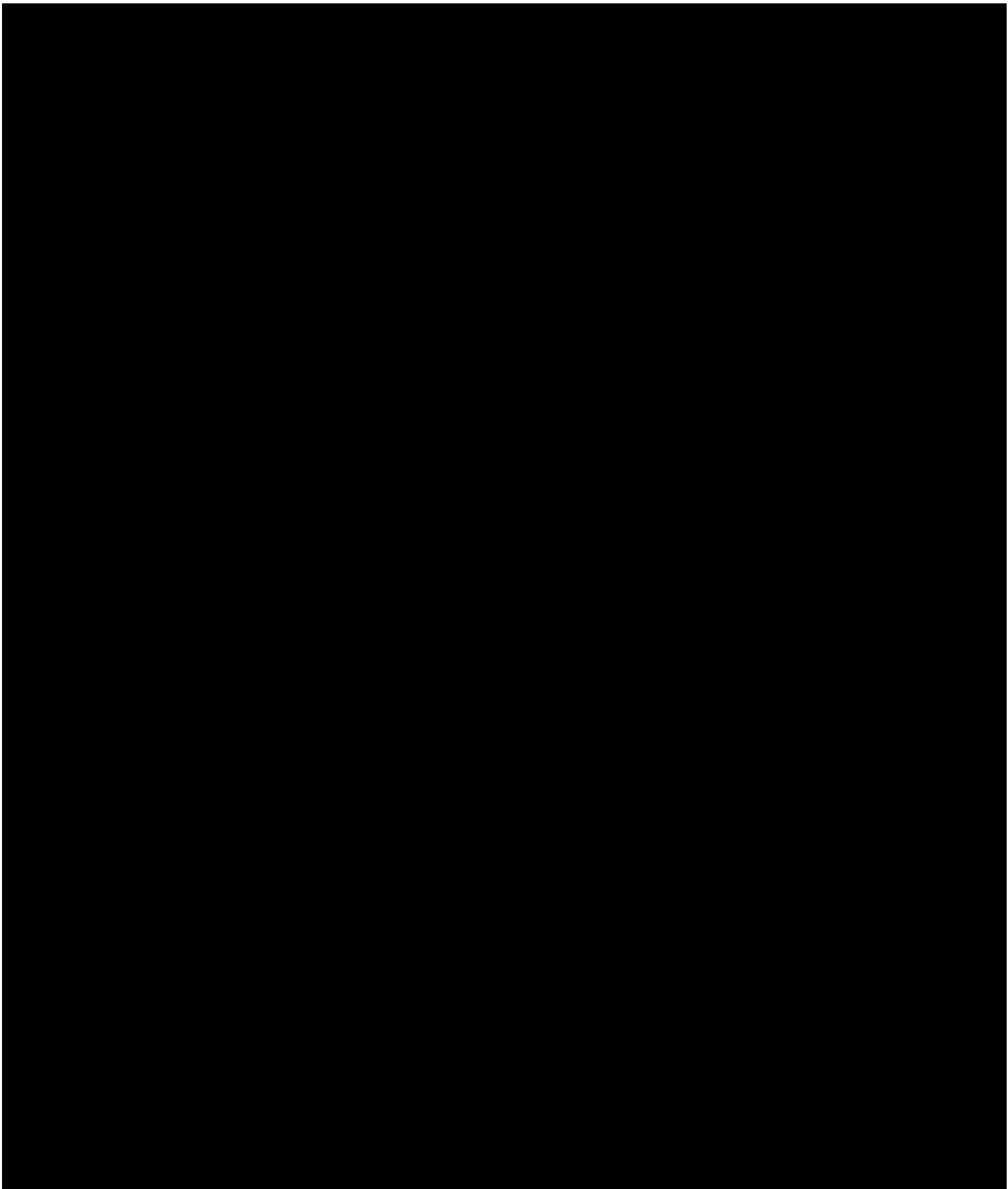
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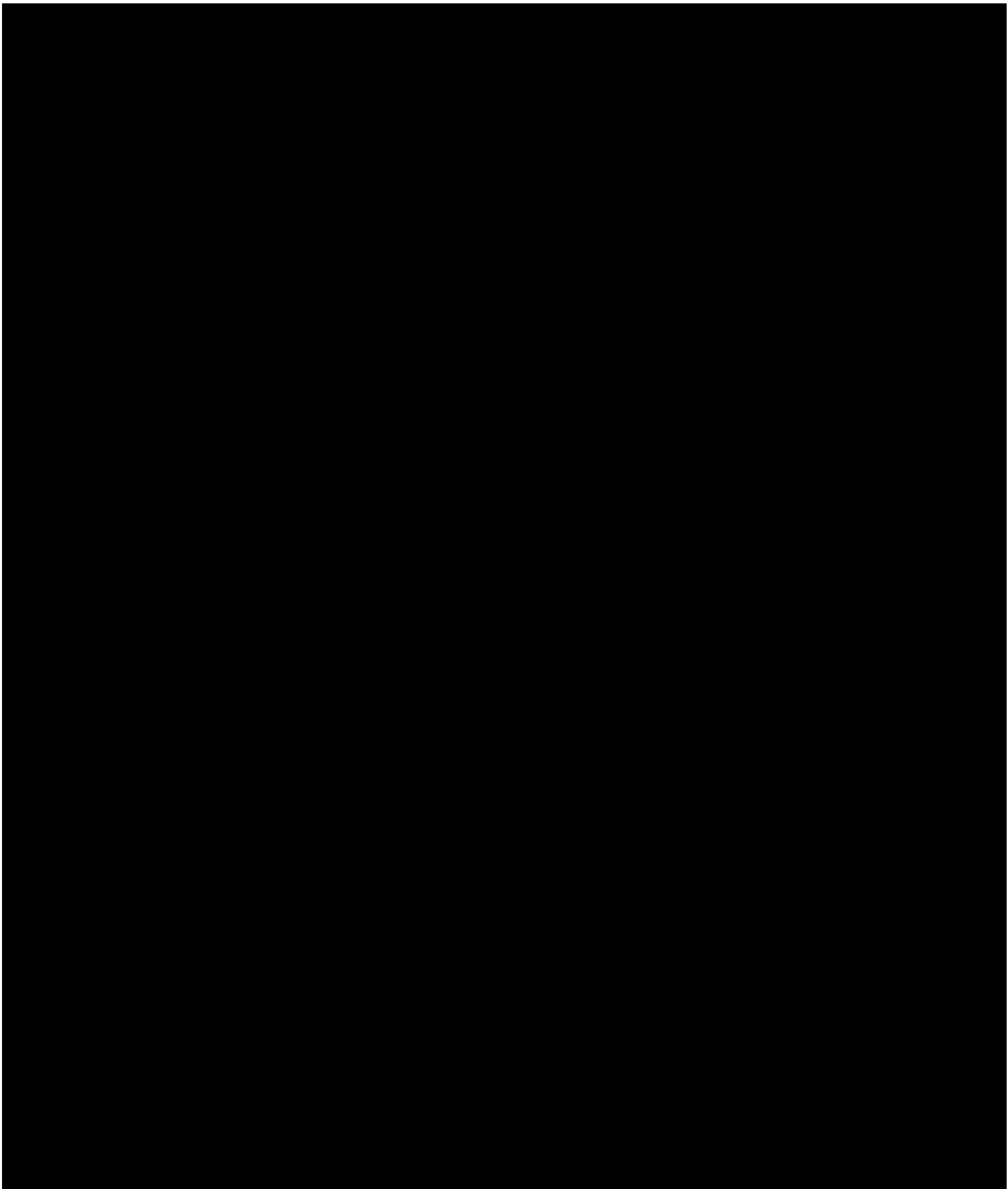
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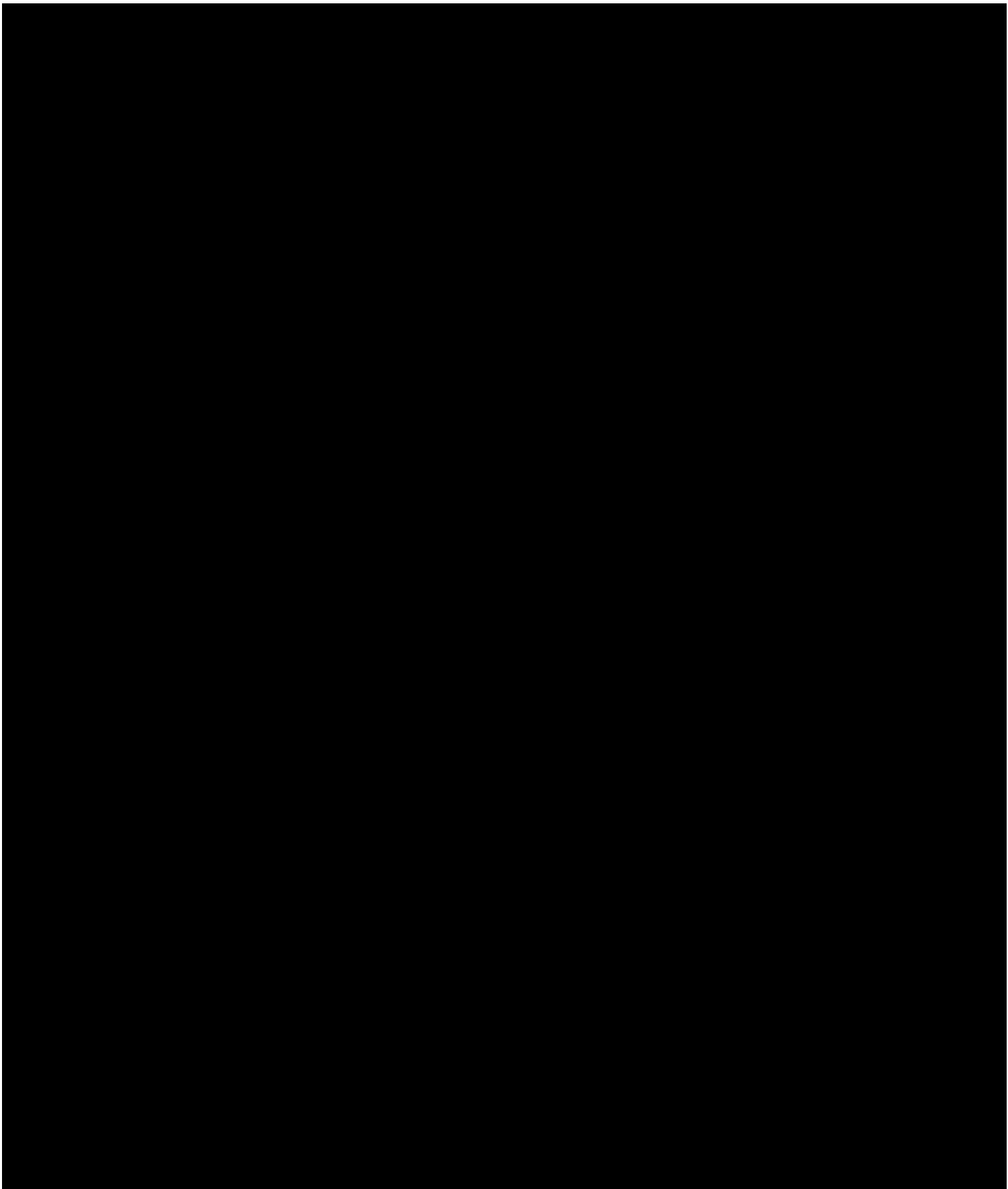
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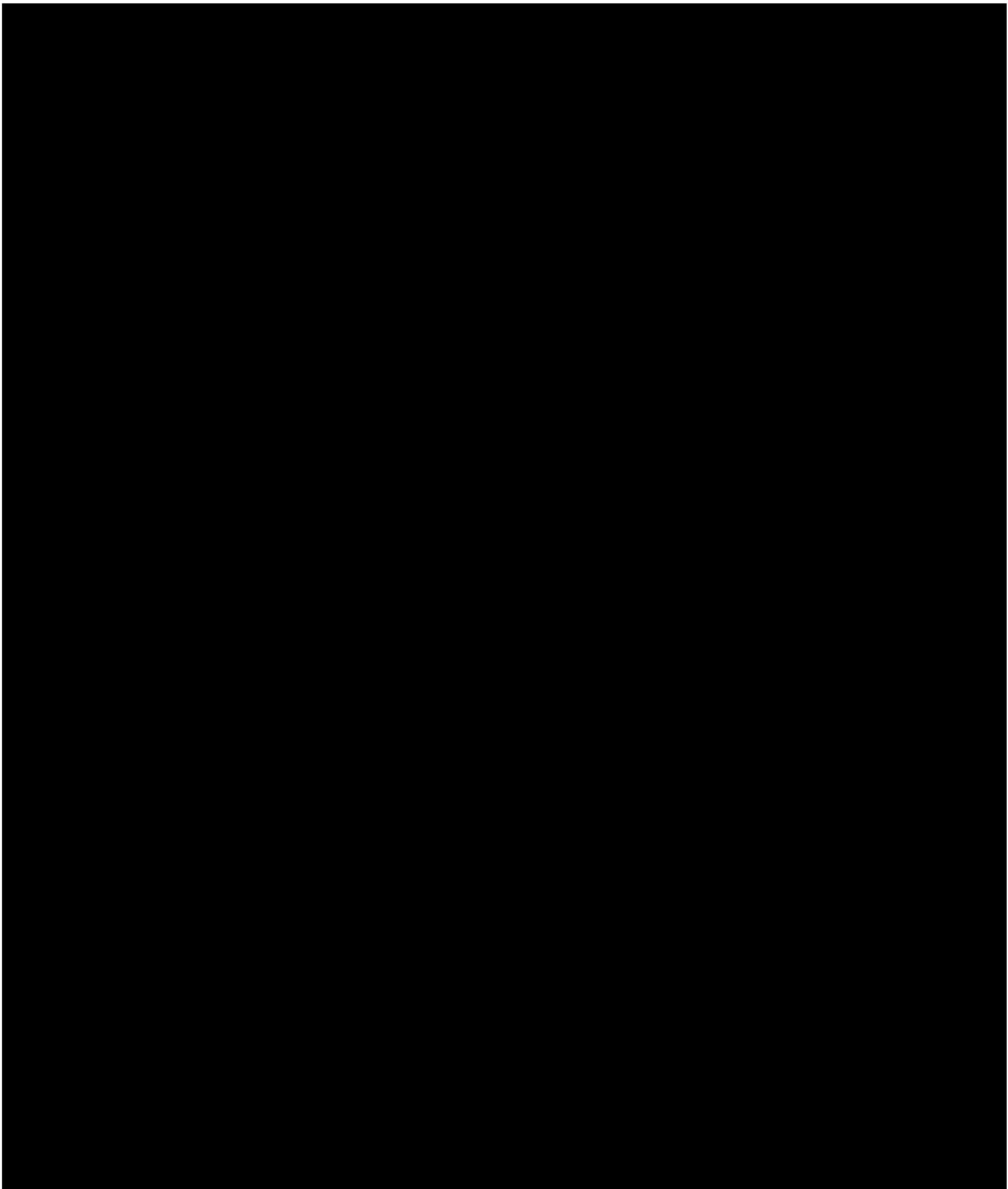
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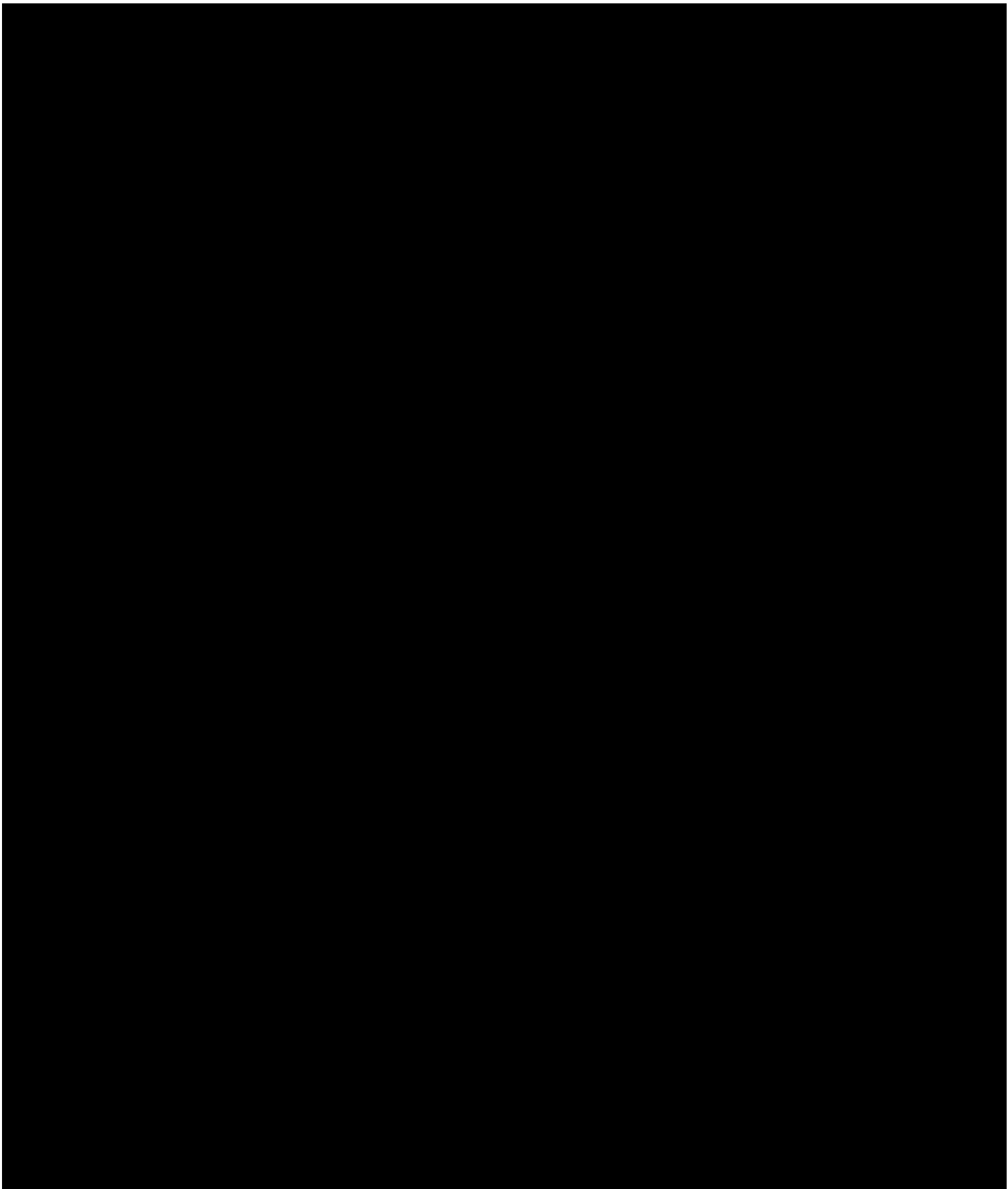
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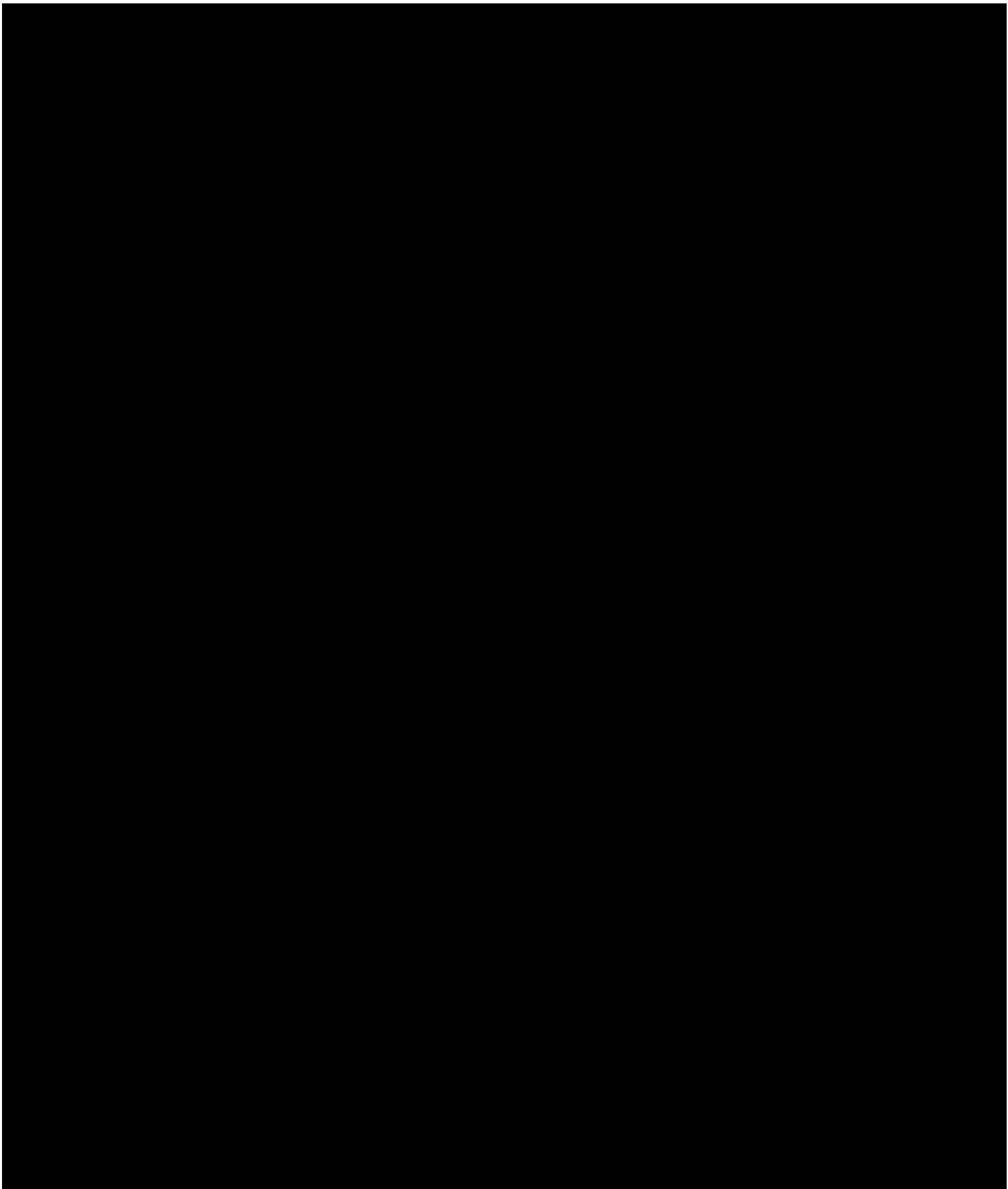
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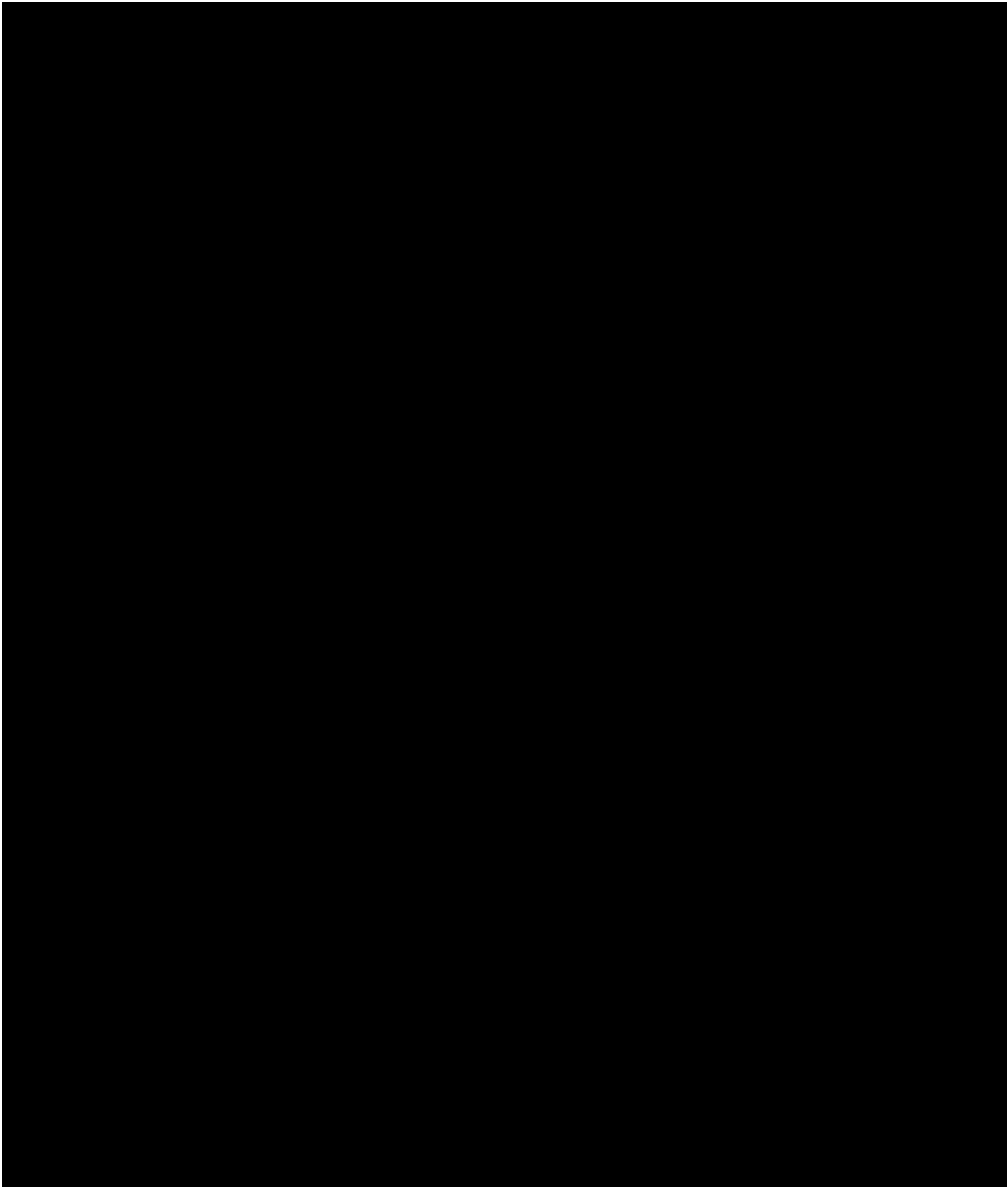
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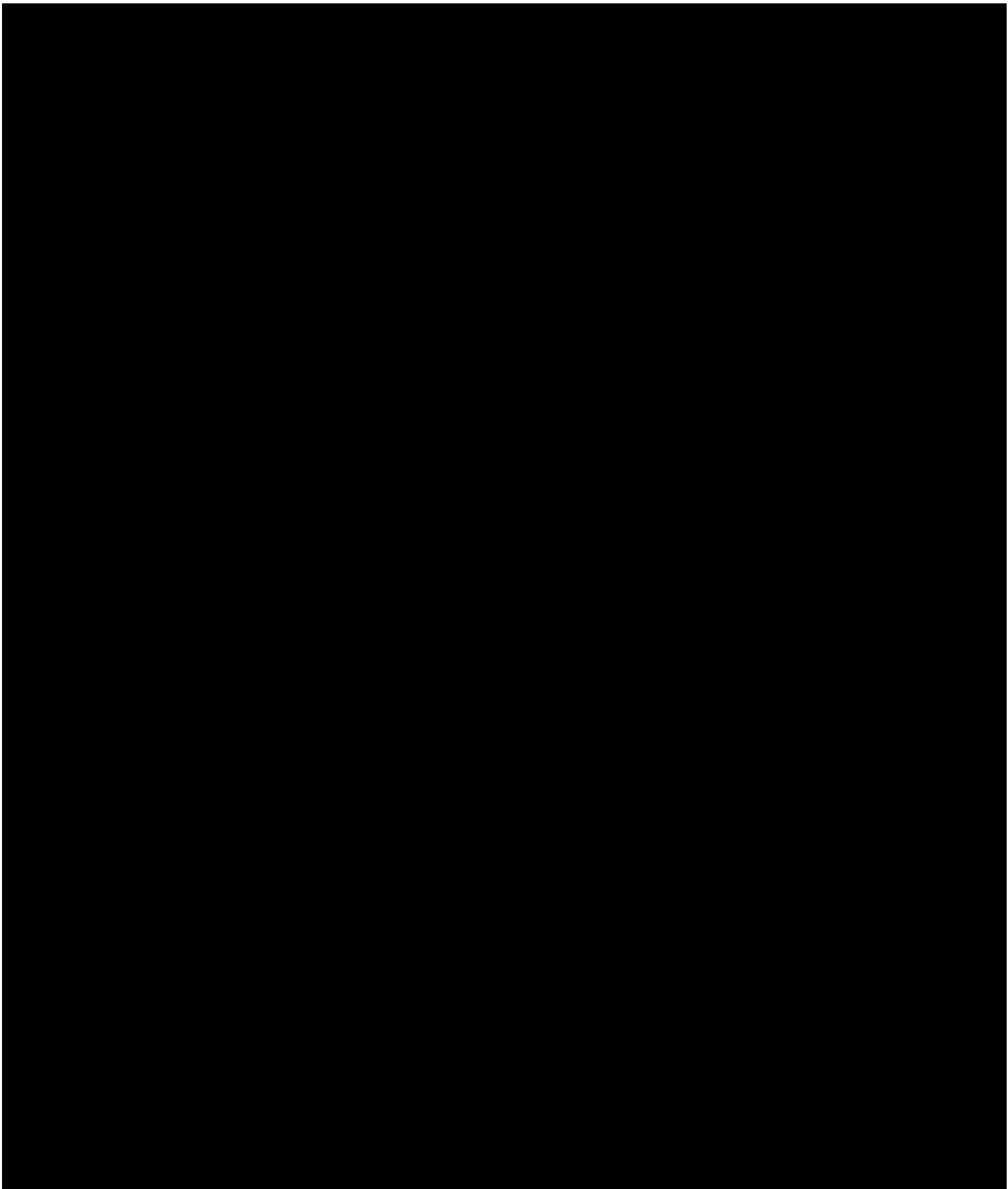
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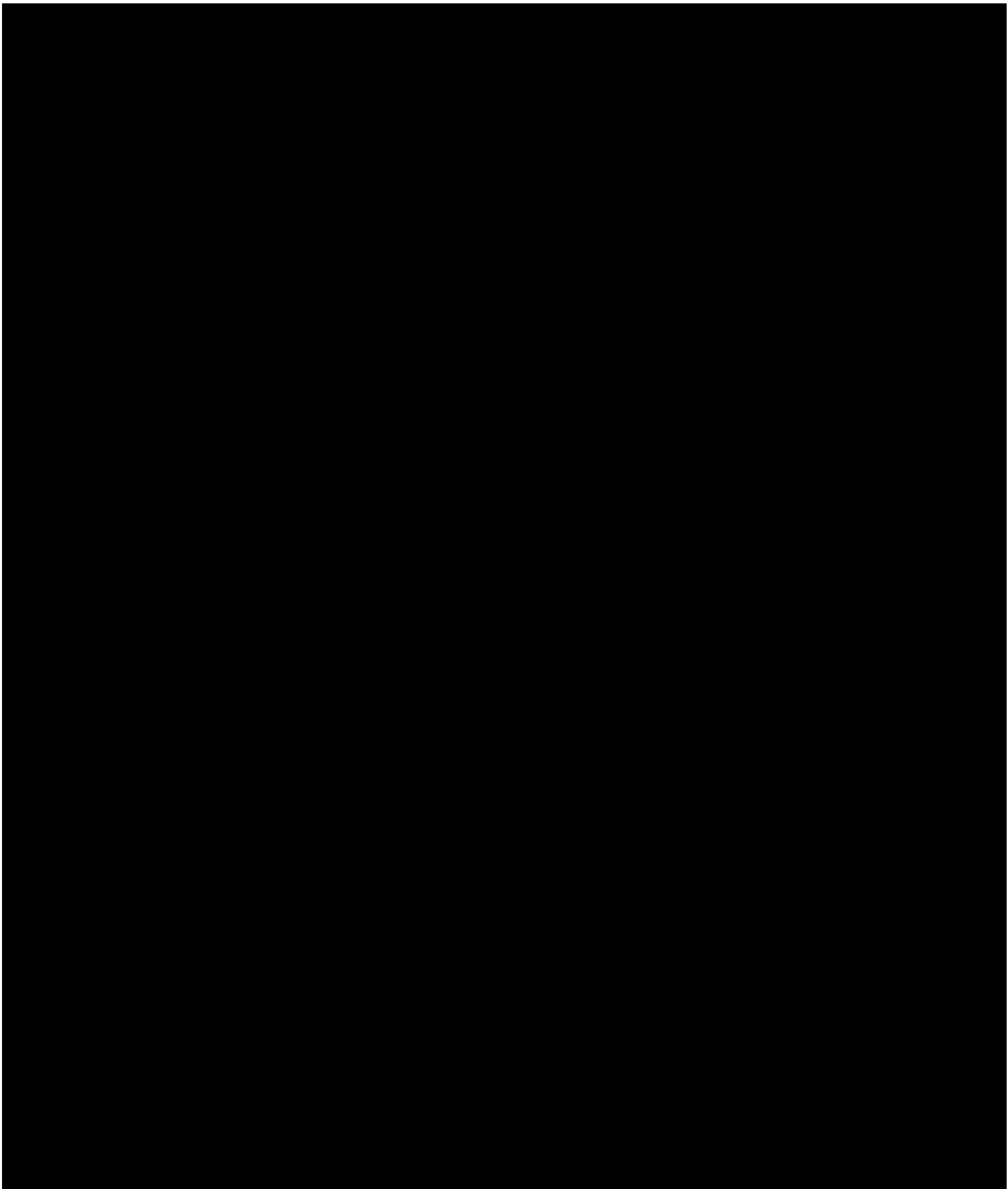
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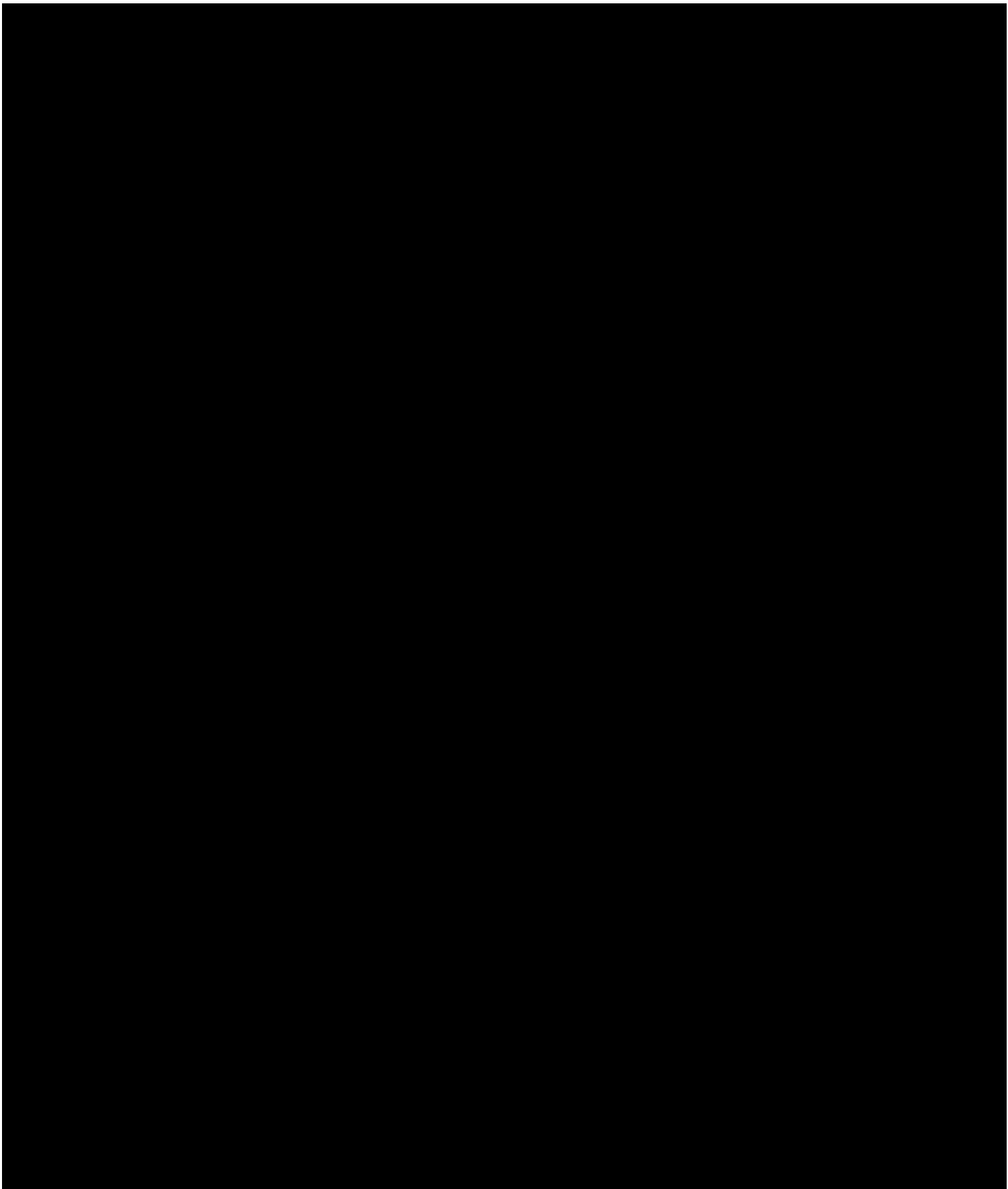
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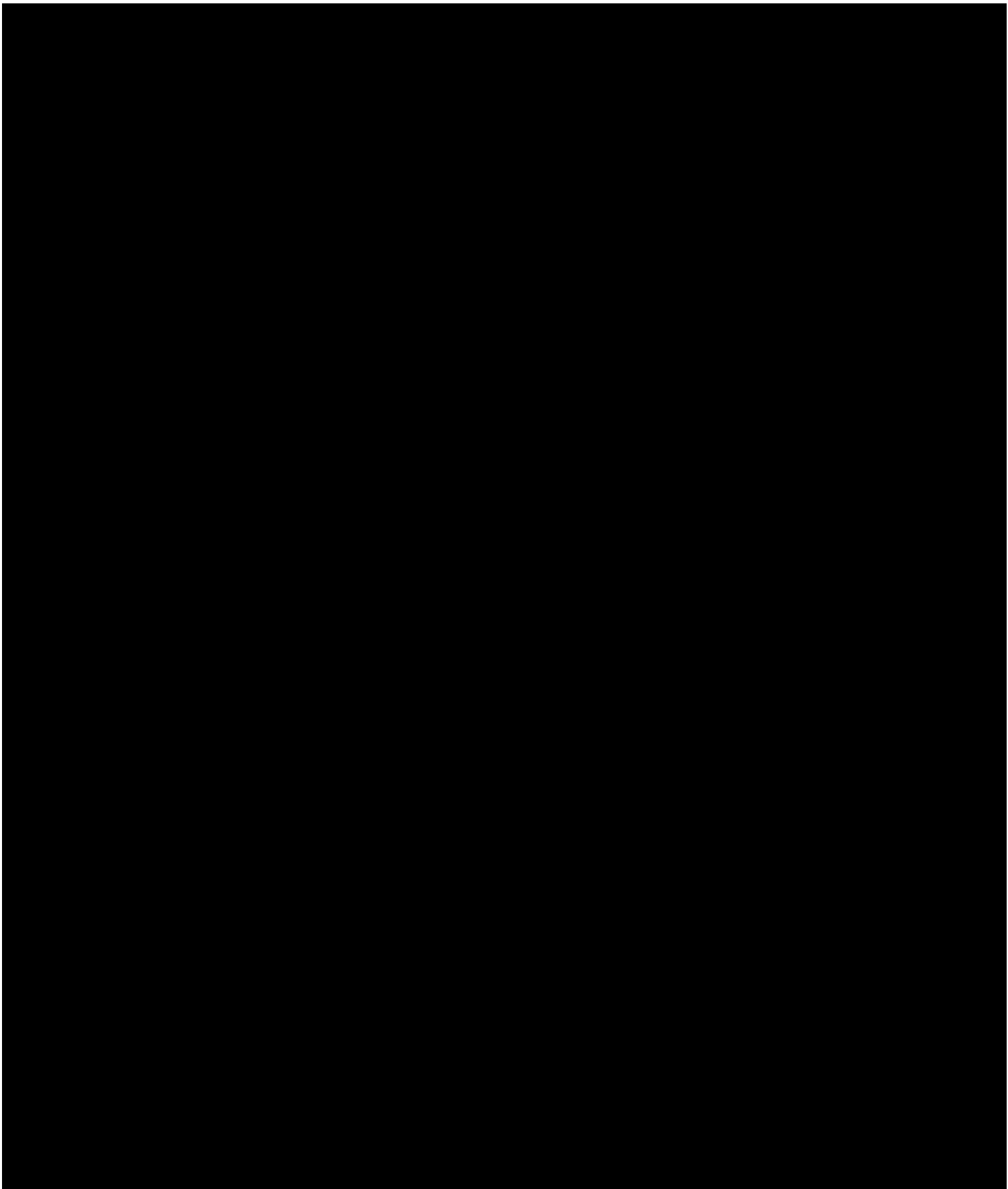
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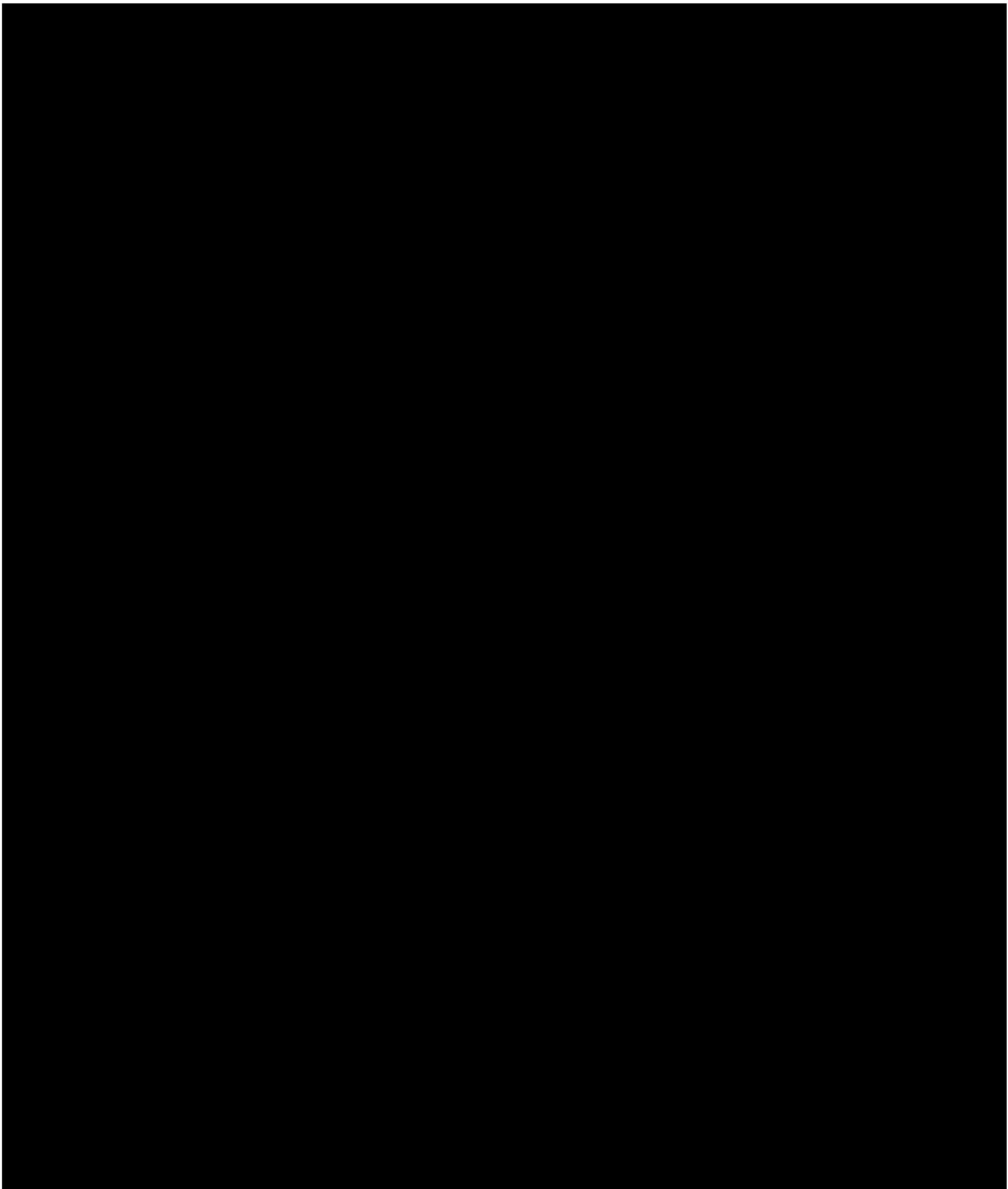
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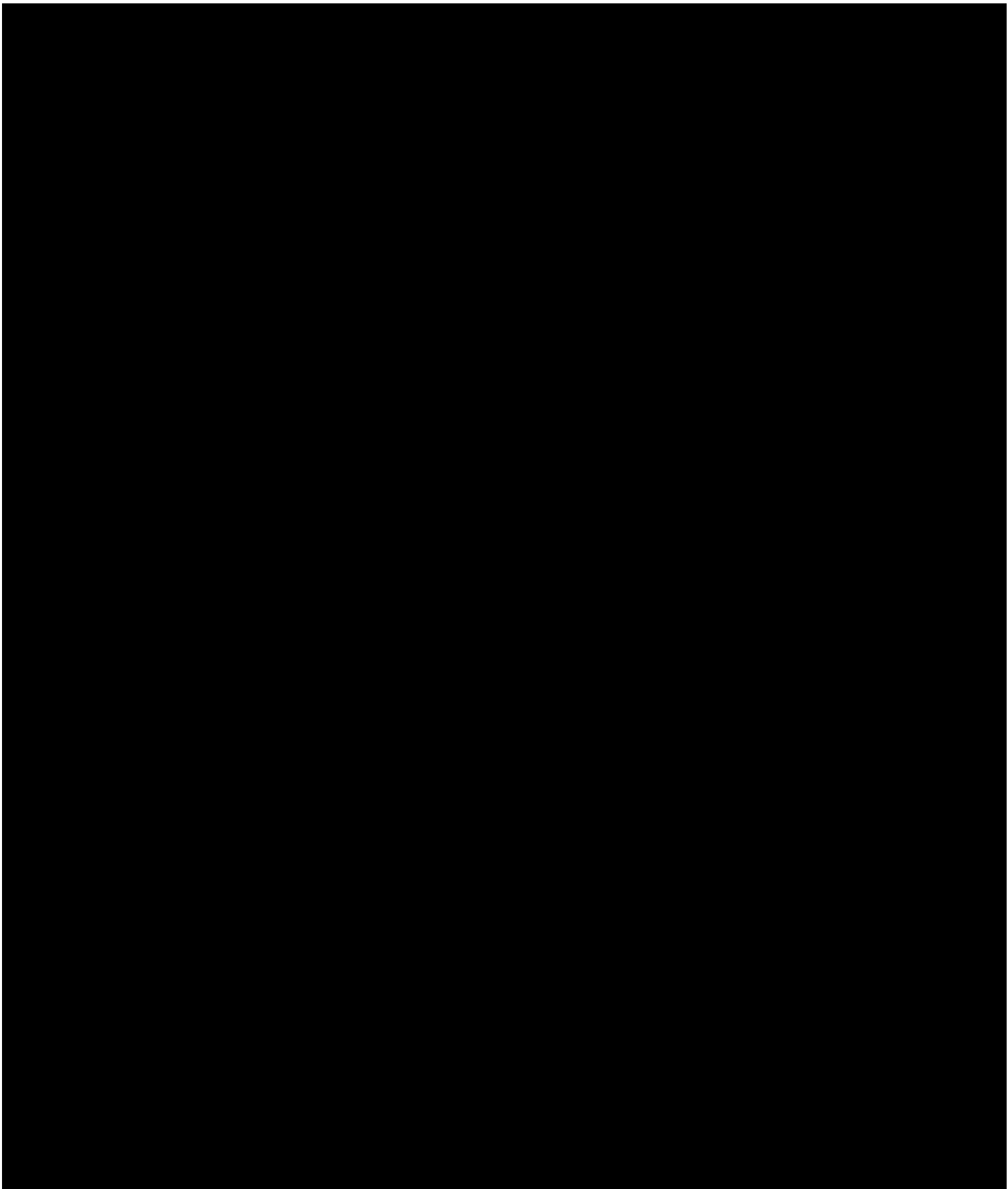
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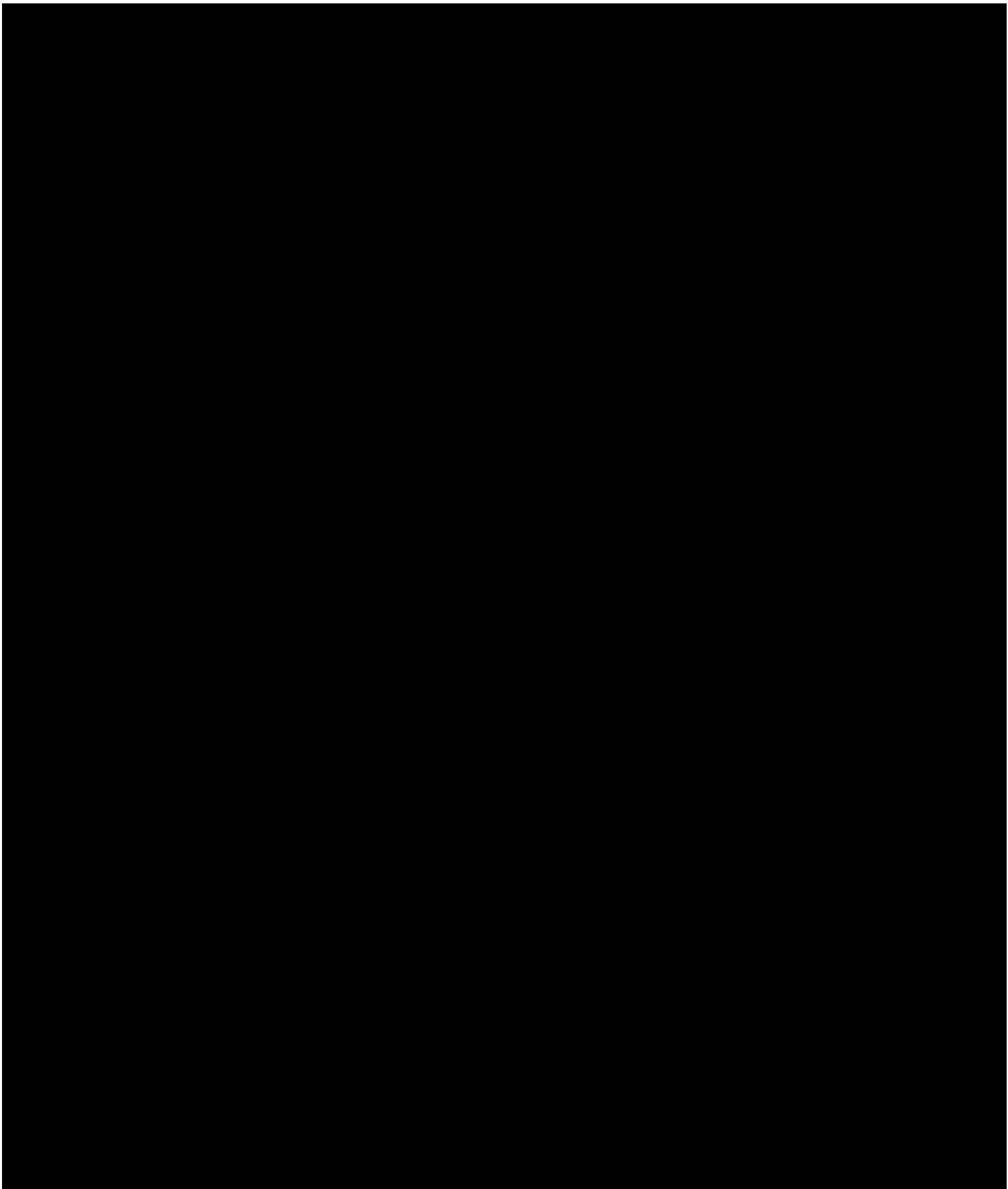
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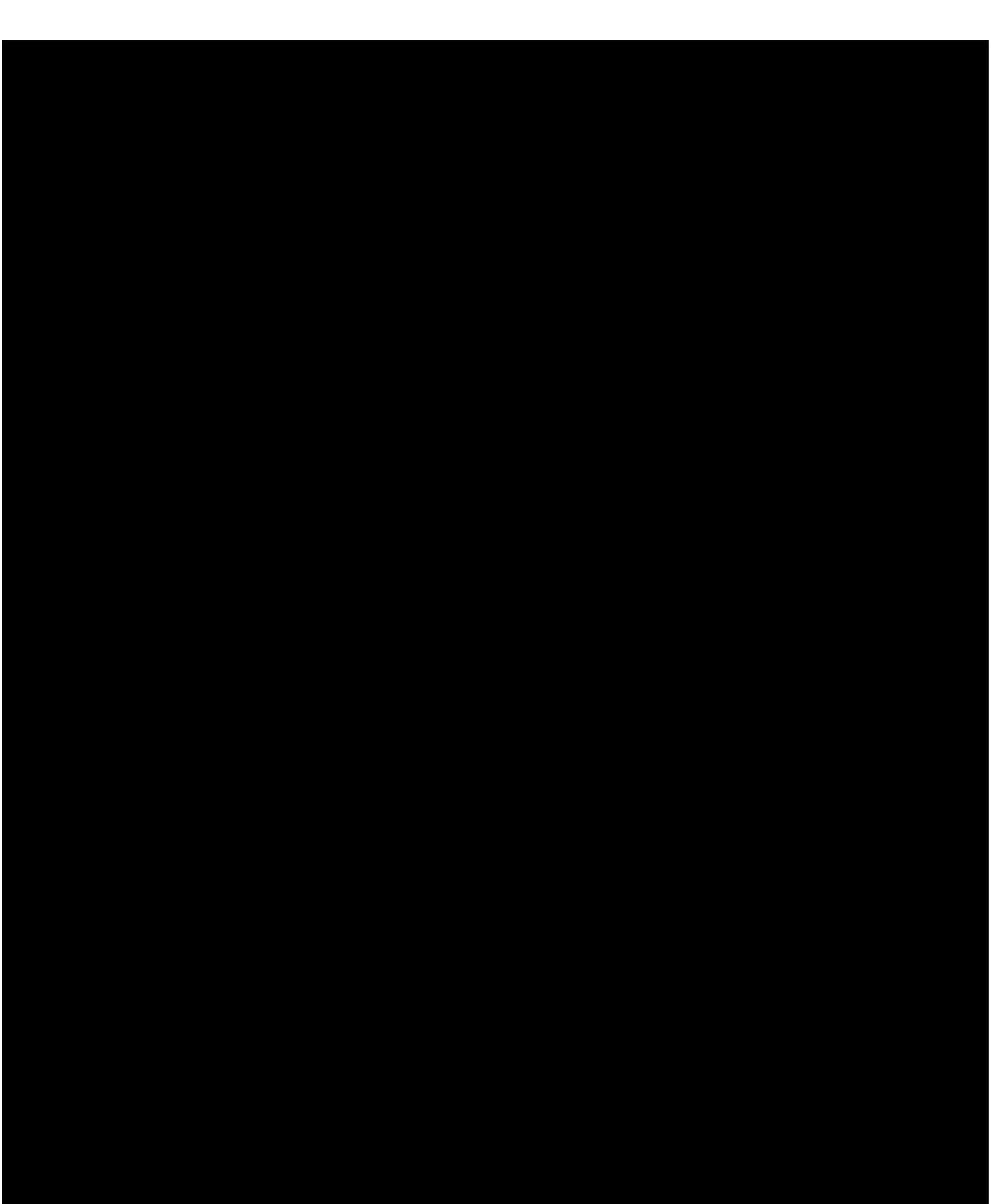
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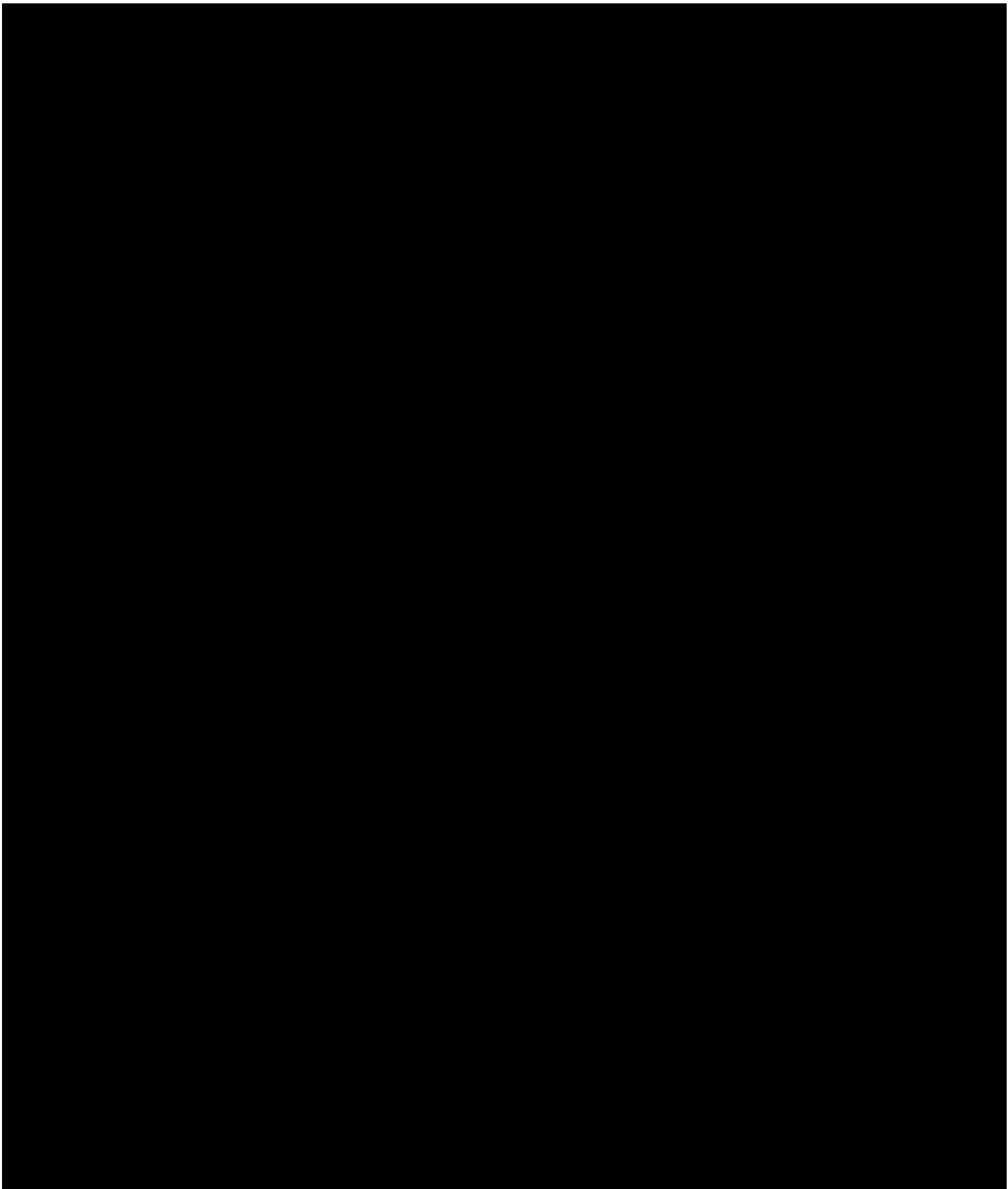
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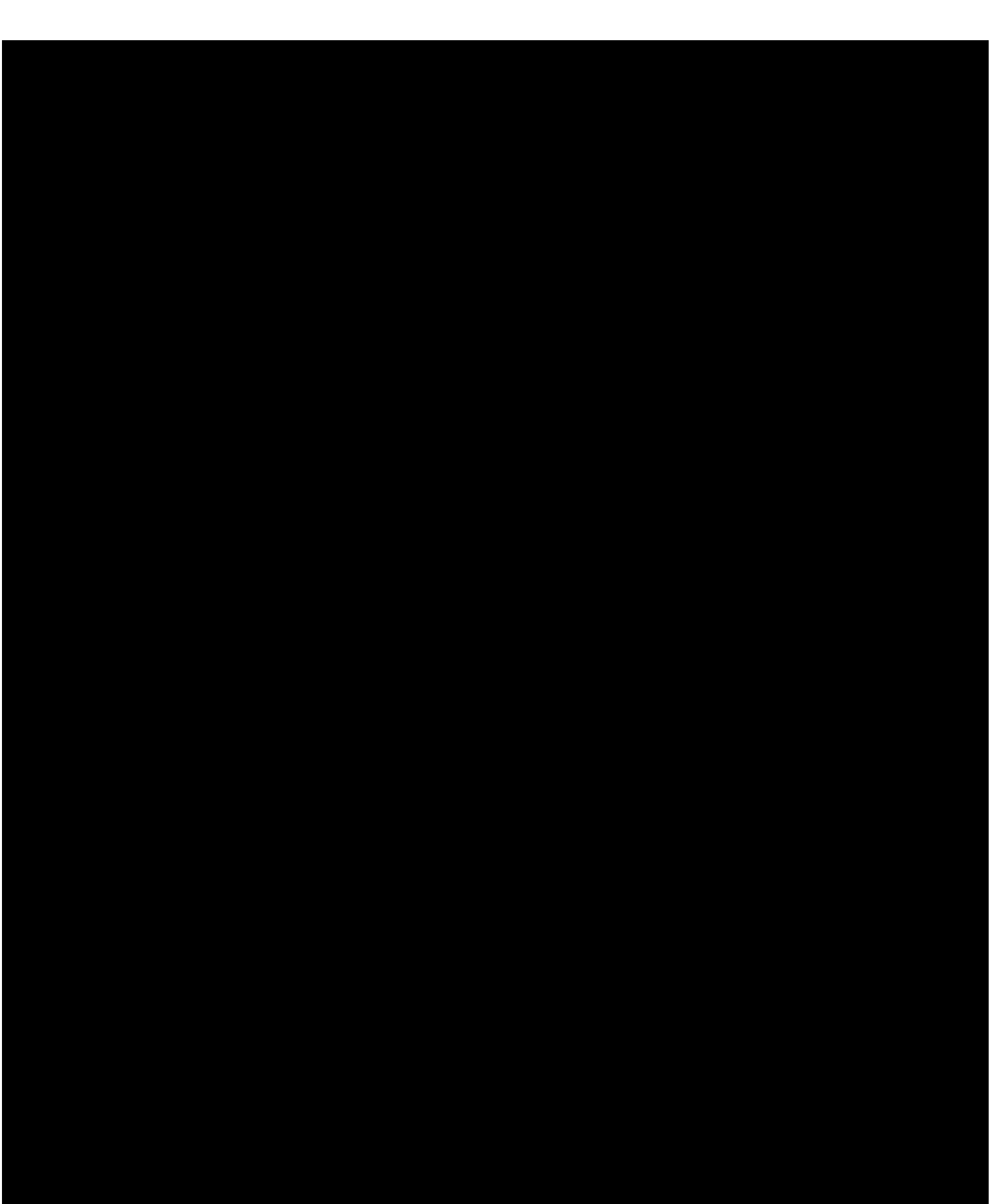
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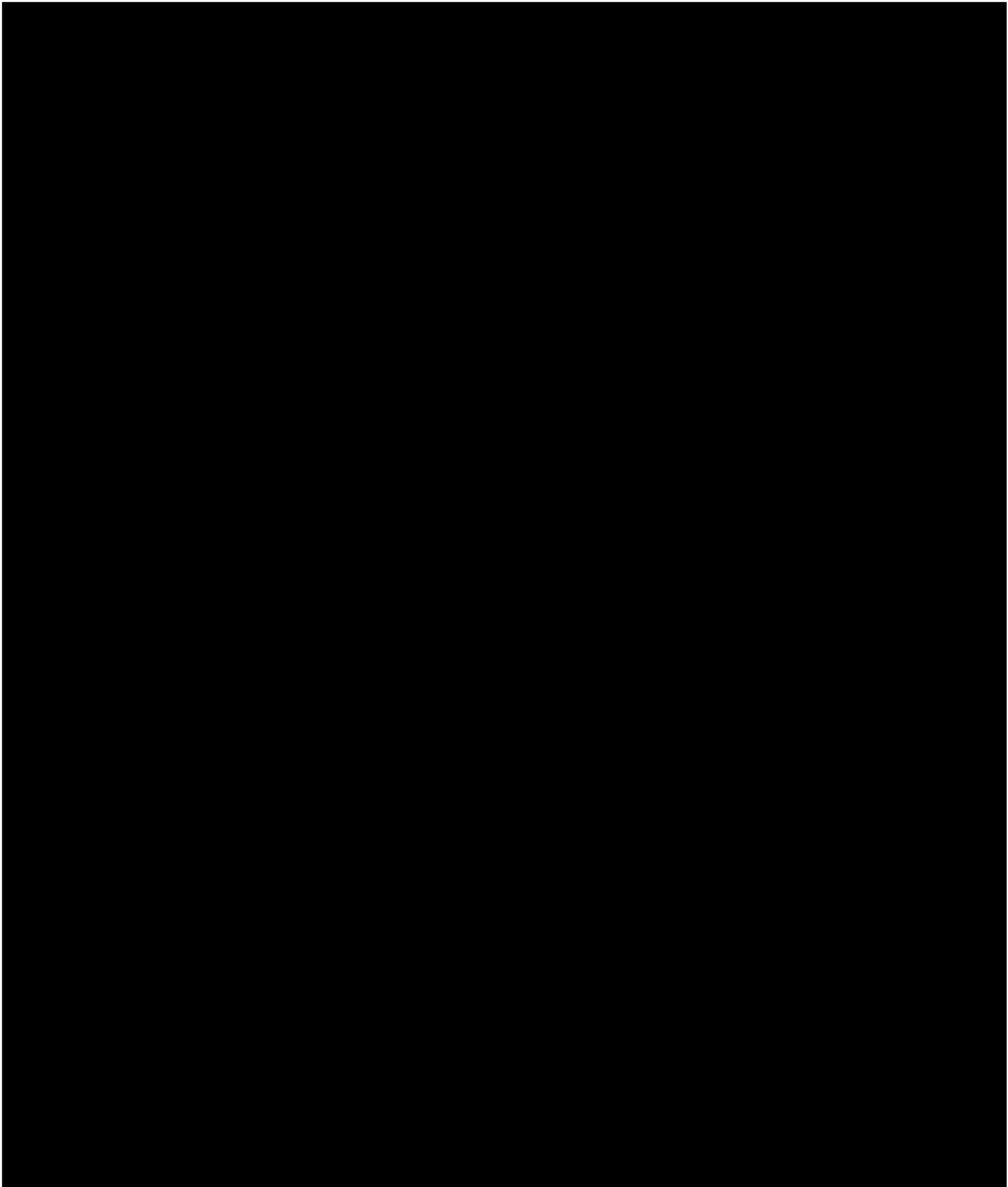
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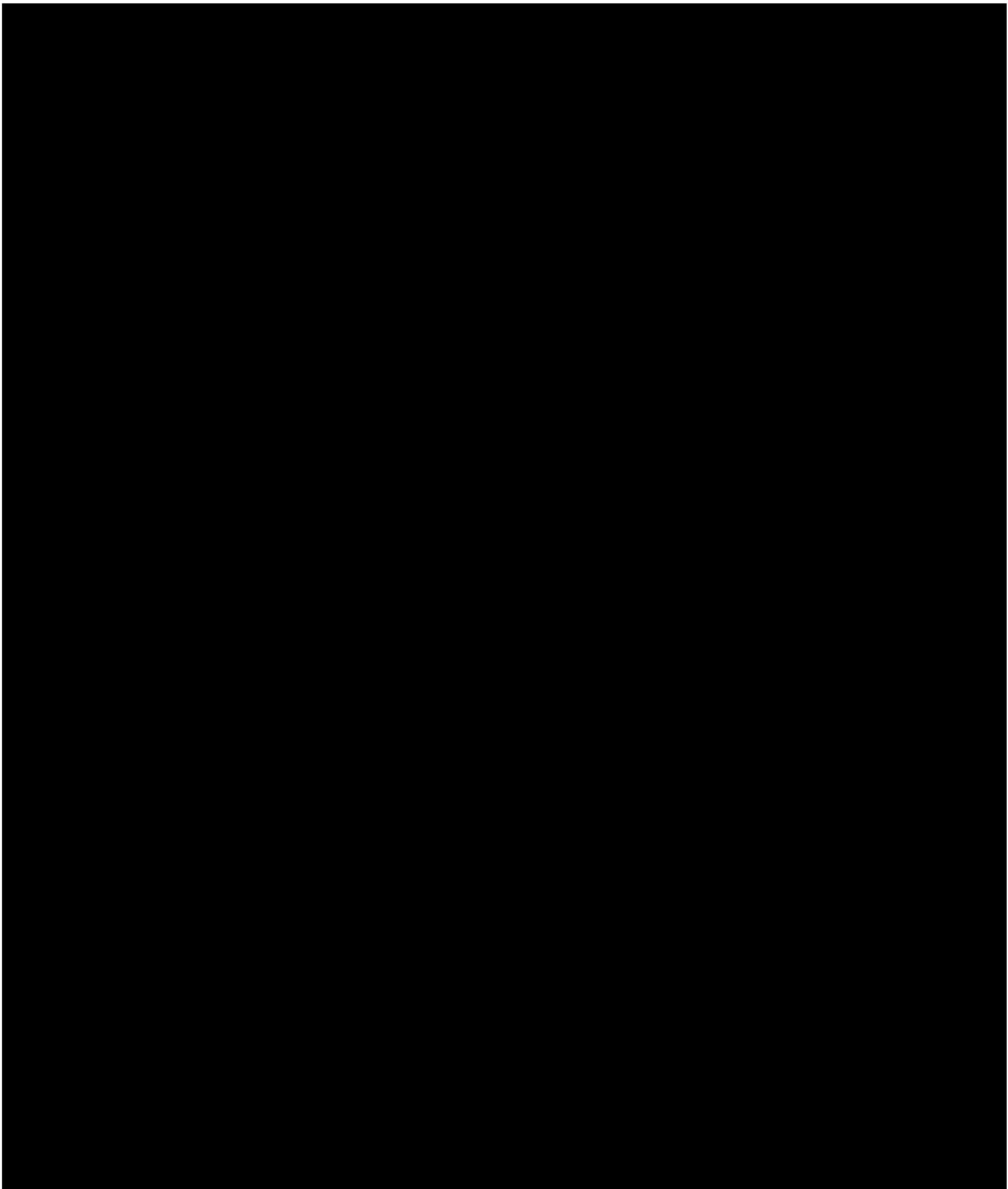
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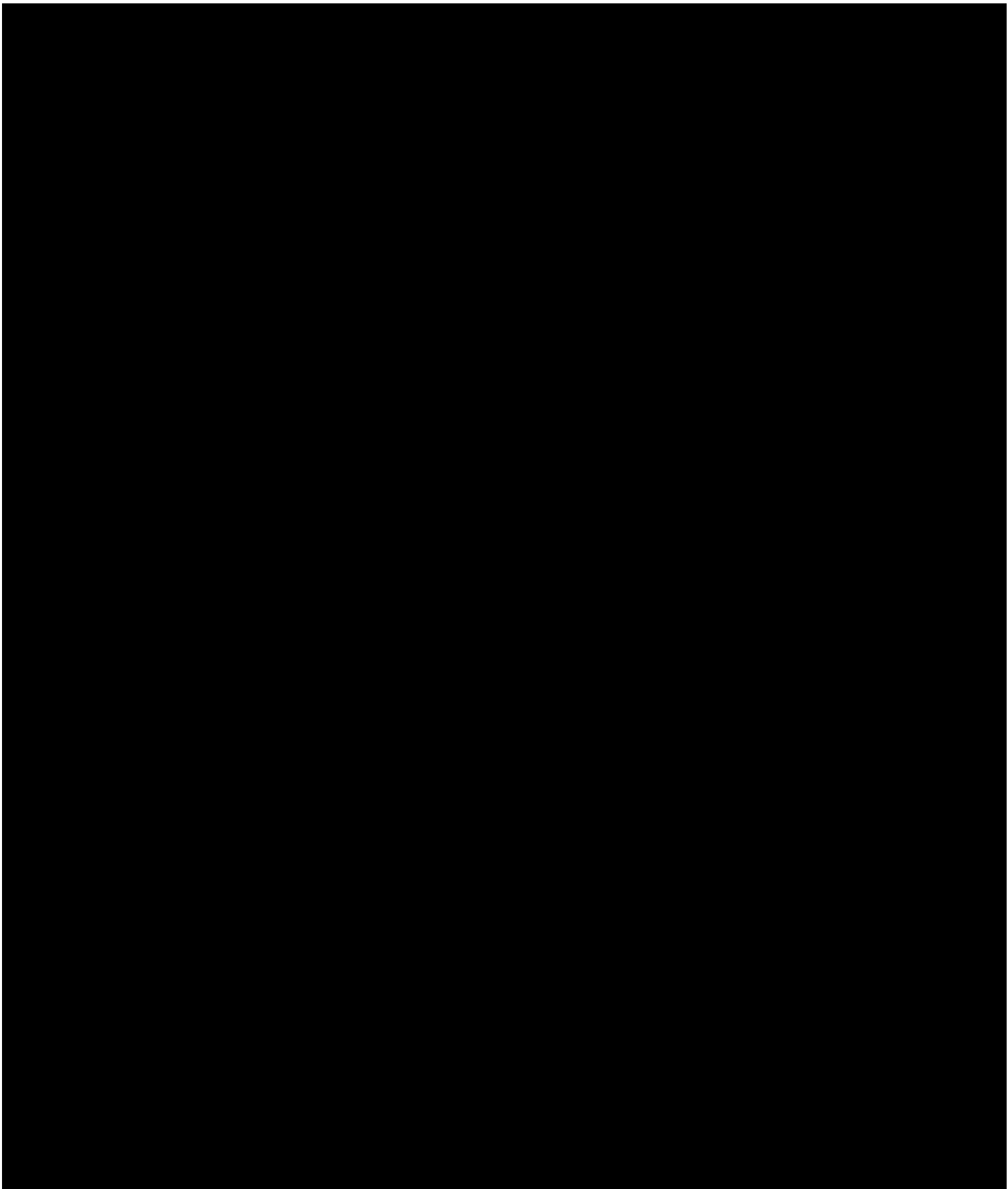
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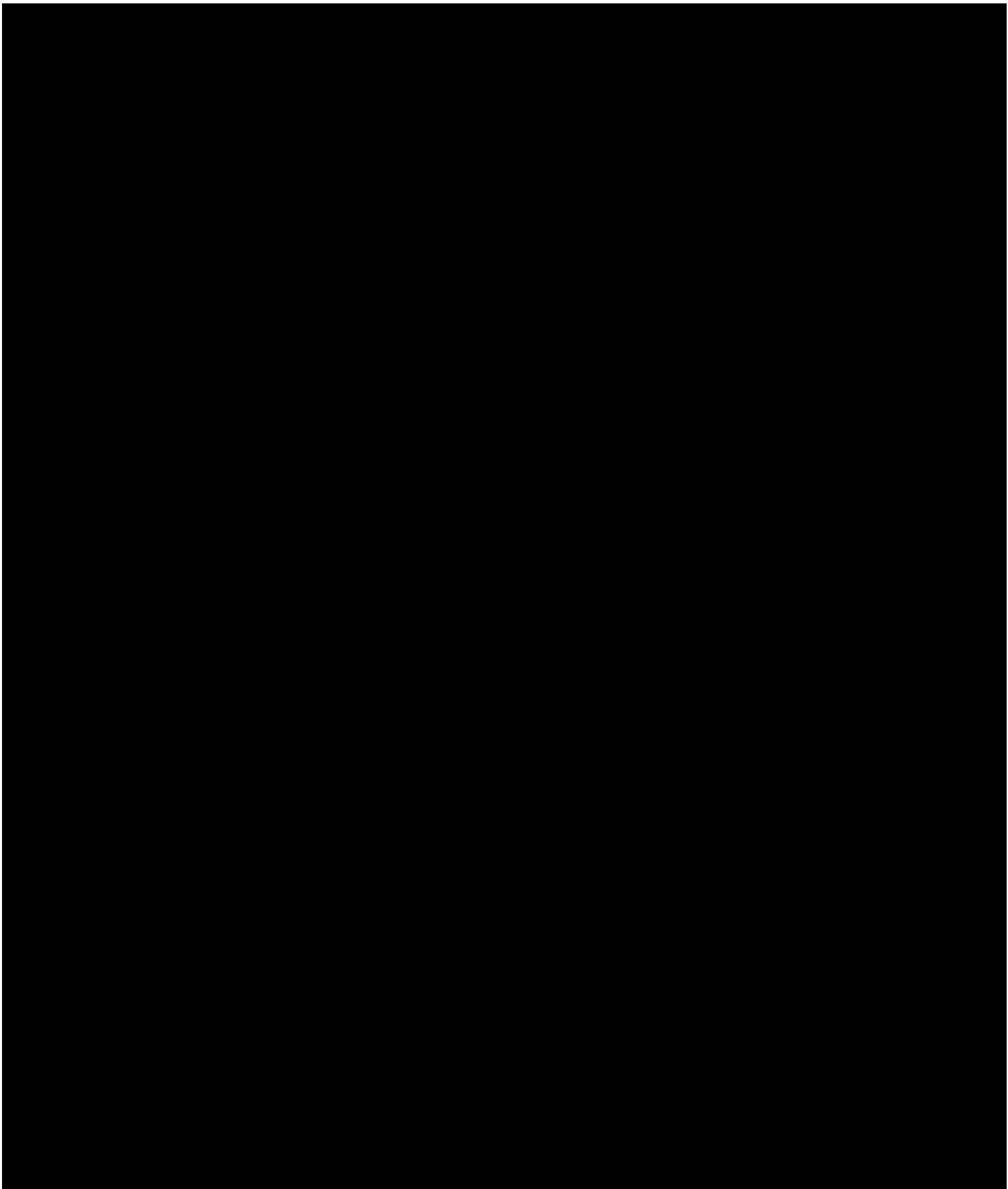
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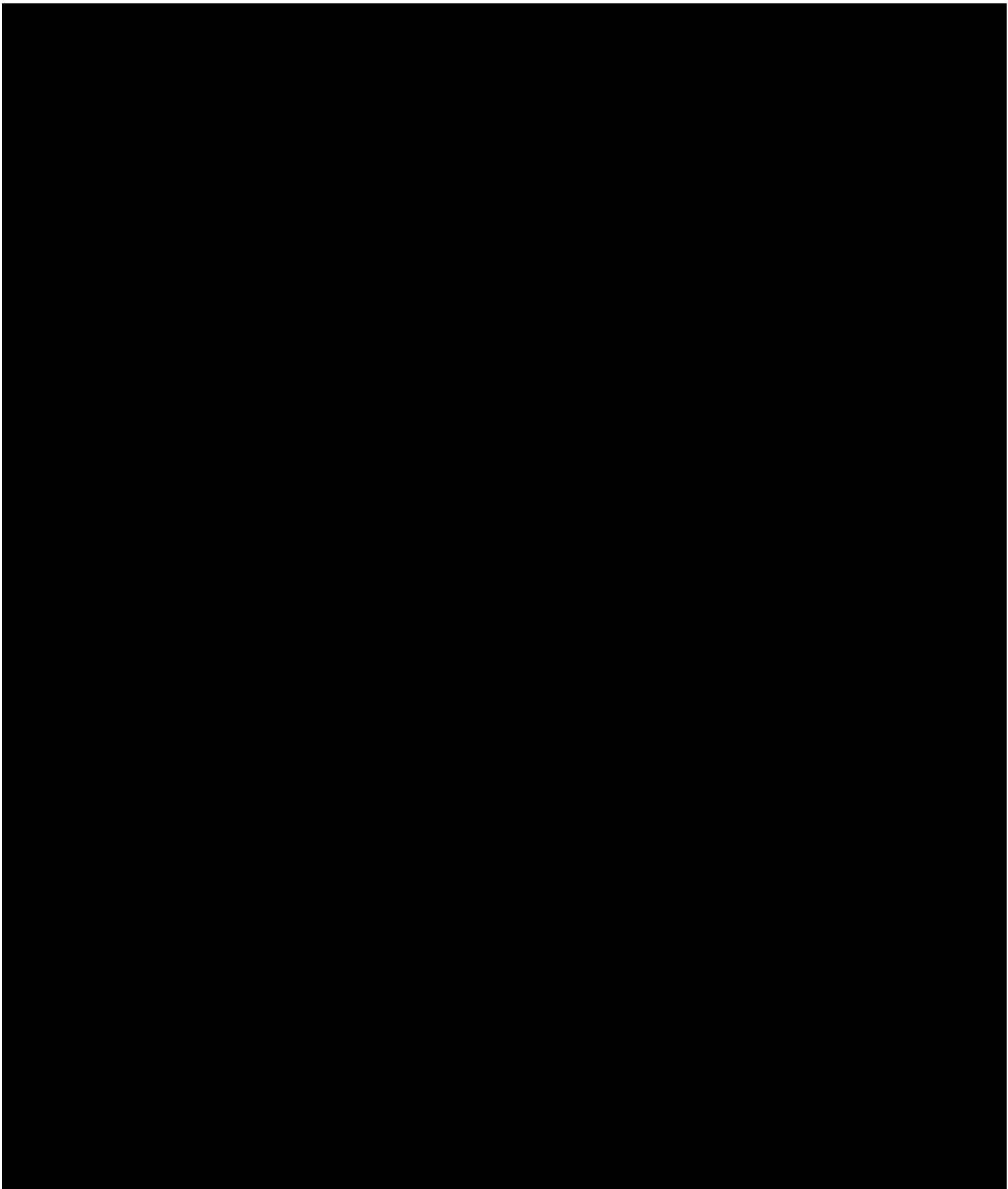
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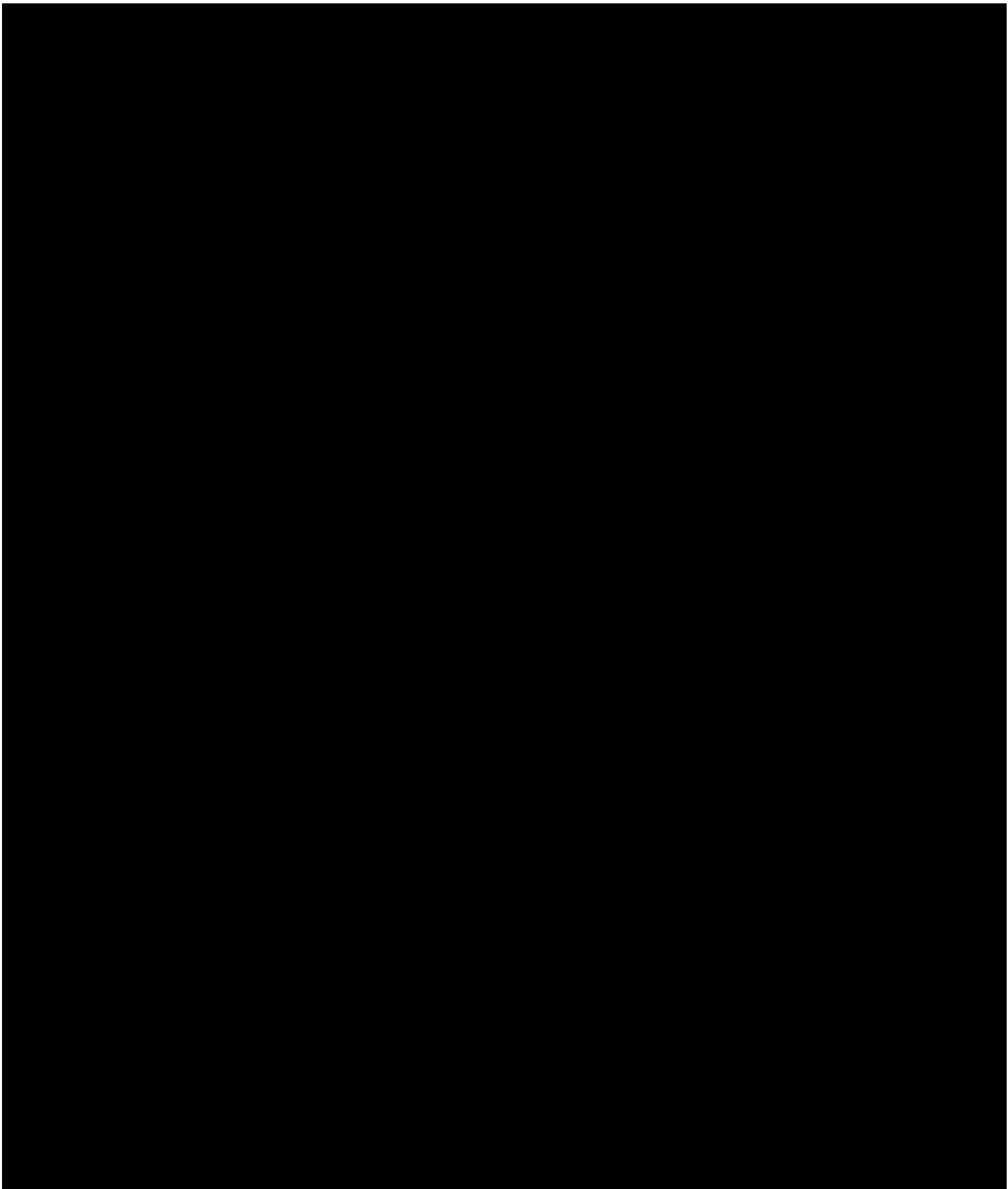
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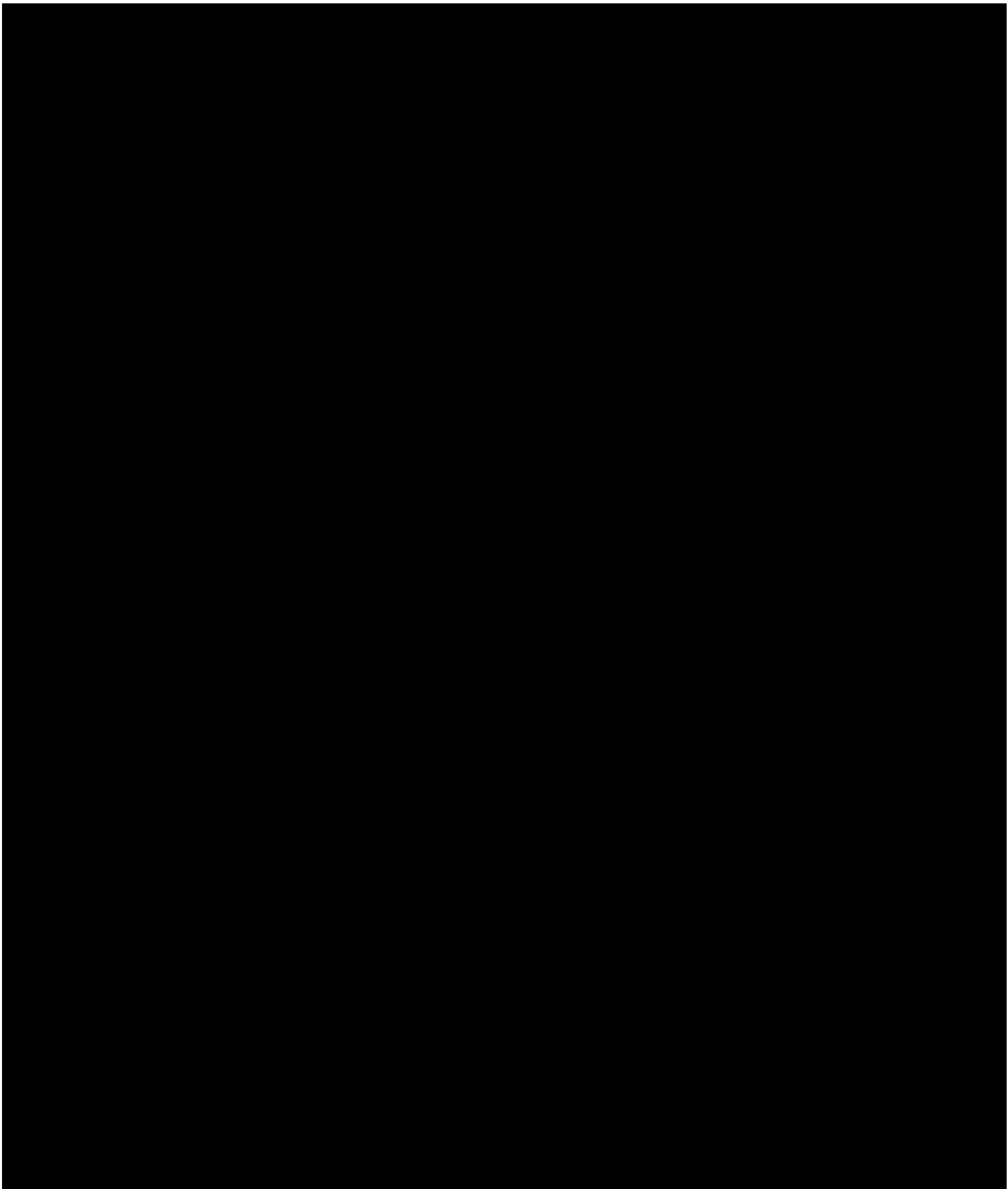
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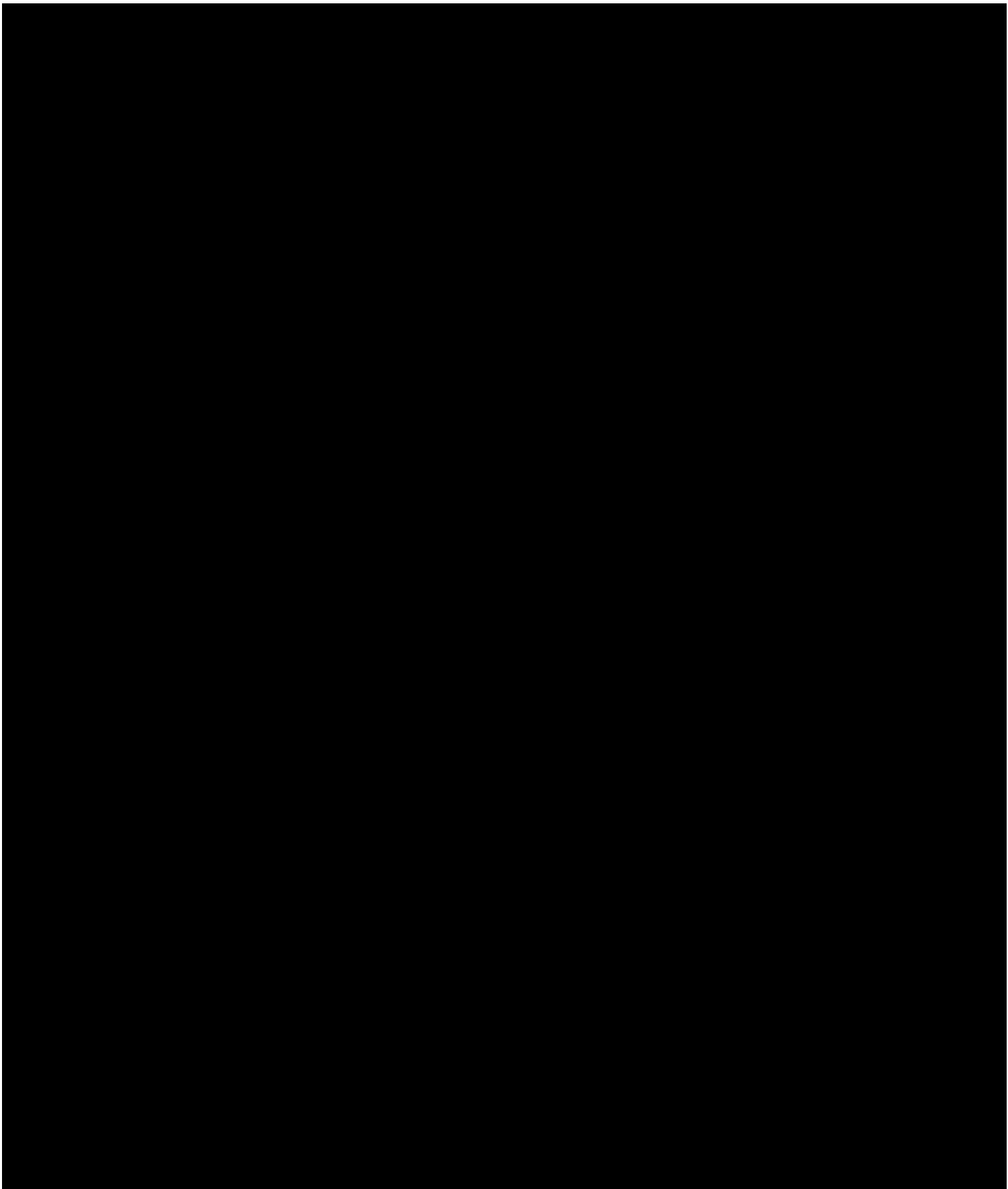
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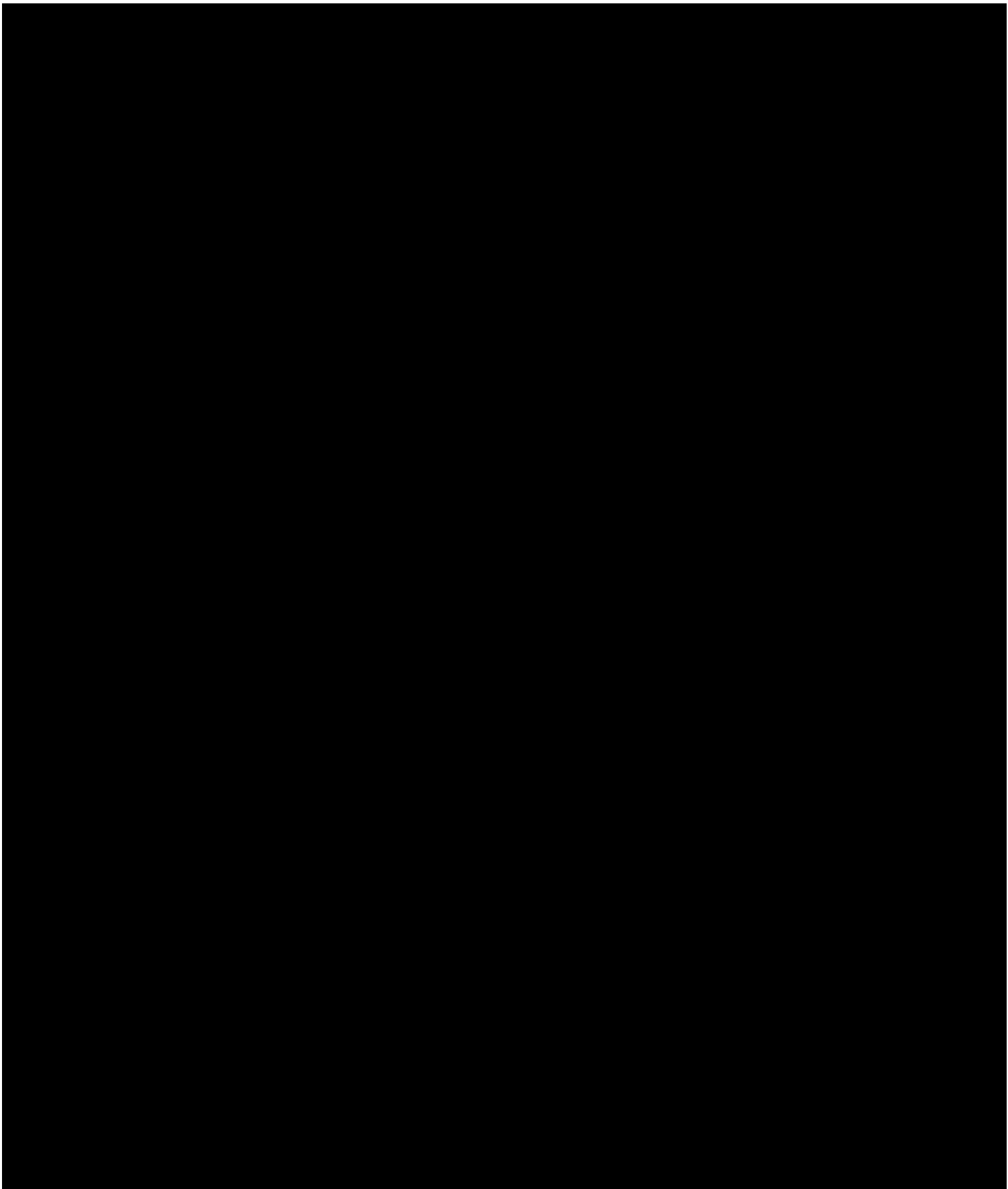
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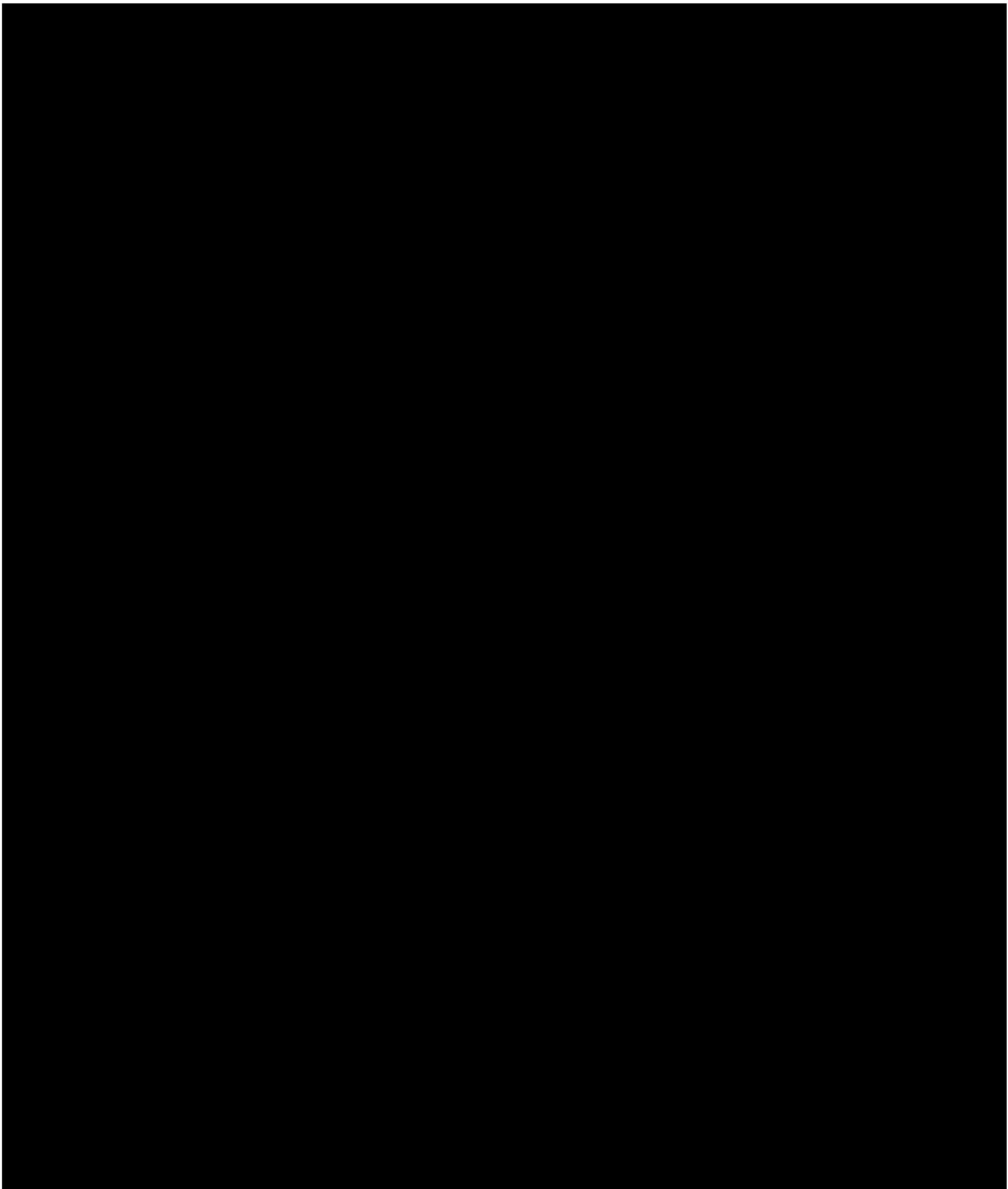
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