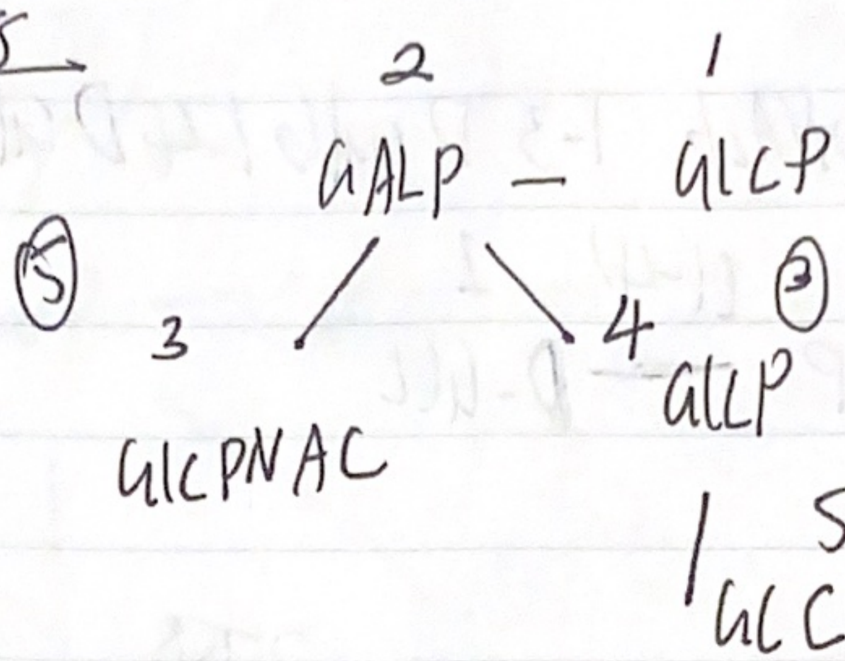
Processing doc. - non linear

circle ② → Res
non_circle 1 → PDB

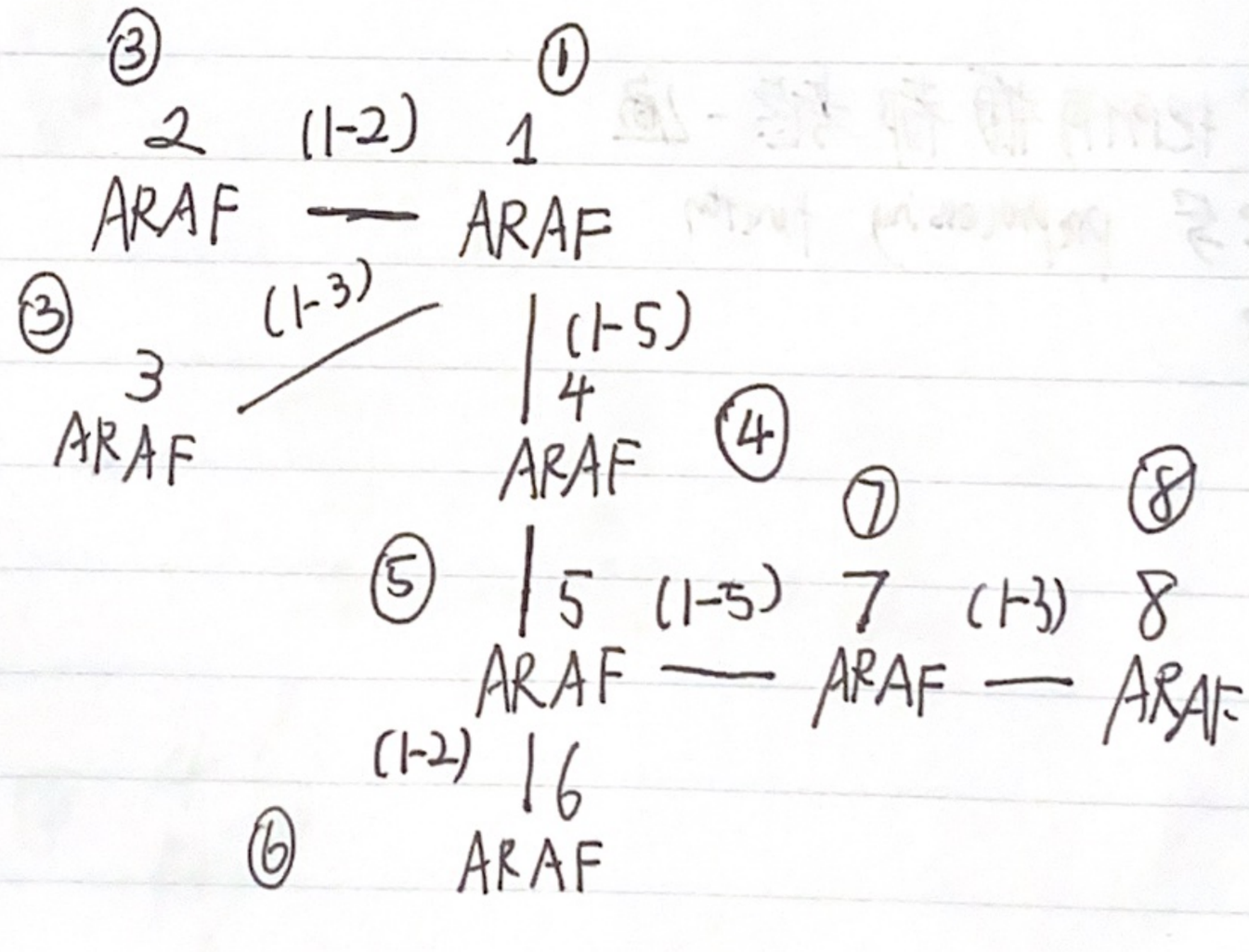
1

DB9948

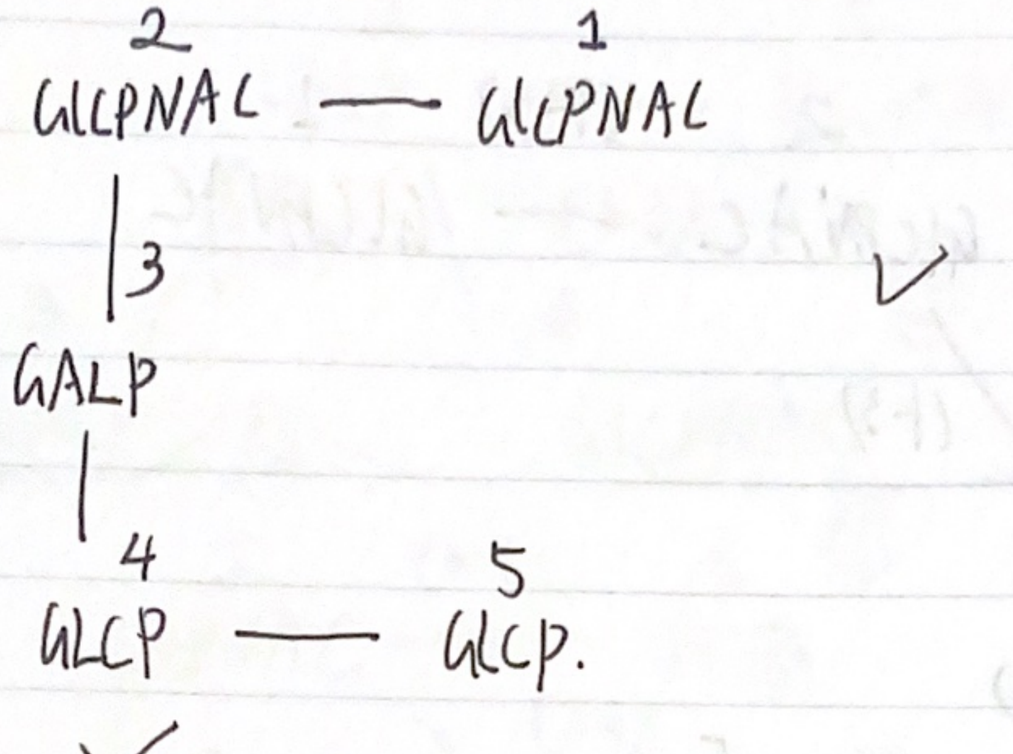


Res.	PDB
1	1
2	2
3	4
4	5
5	3

2. DB26476

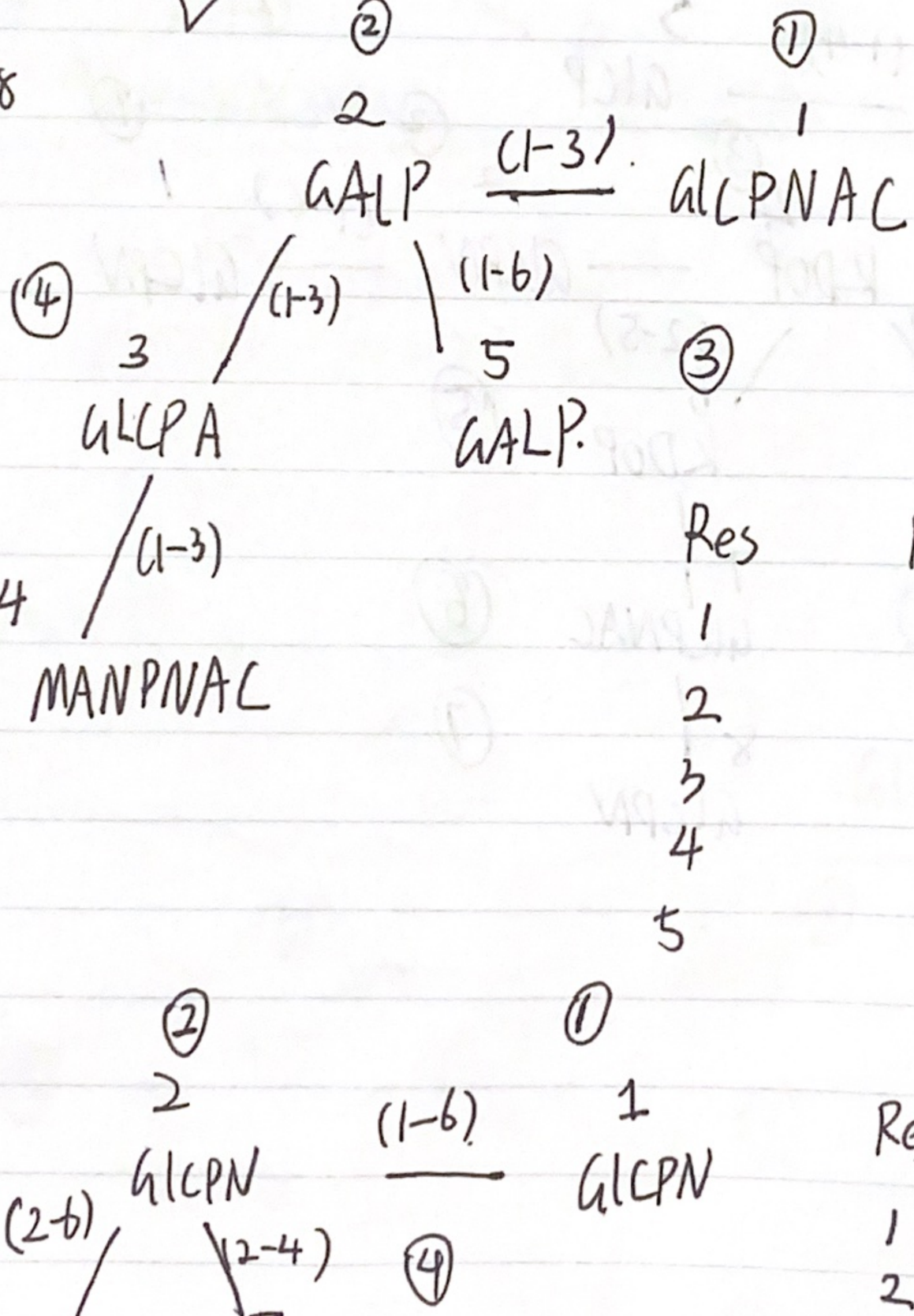


3. DB26405



4 PB 26521 ✓

5 DB 4858

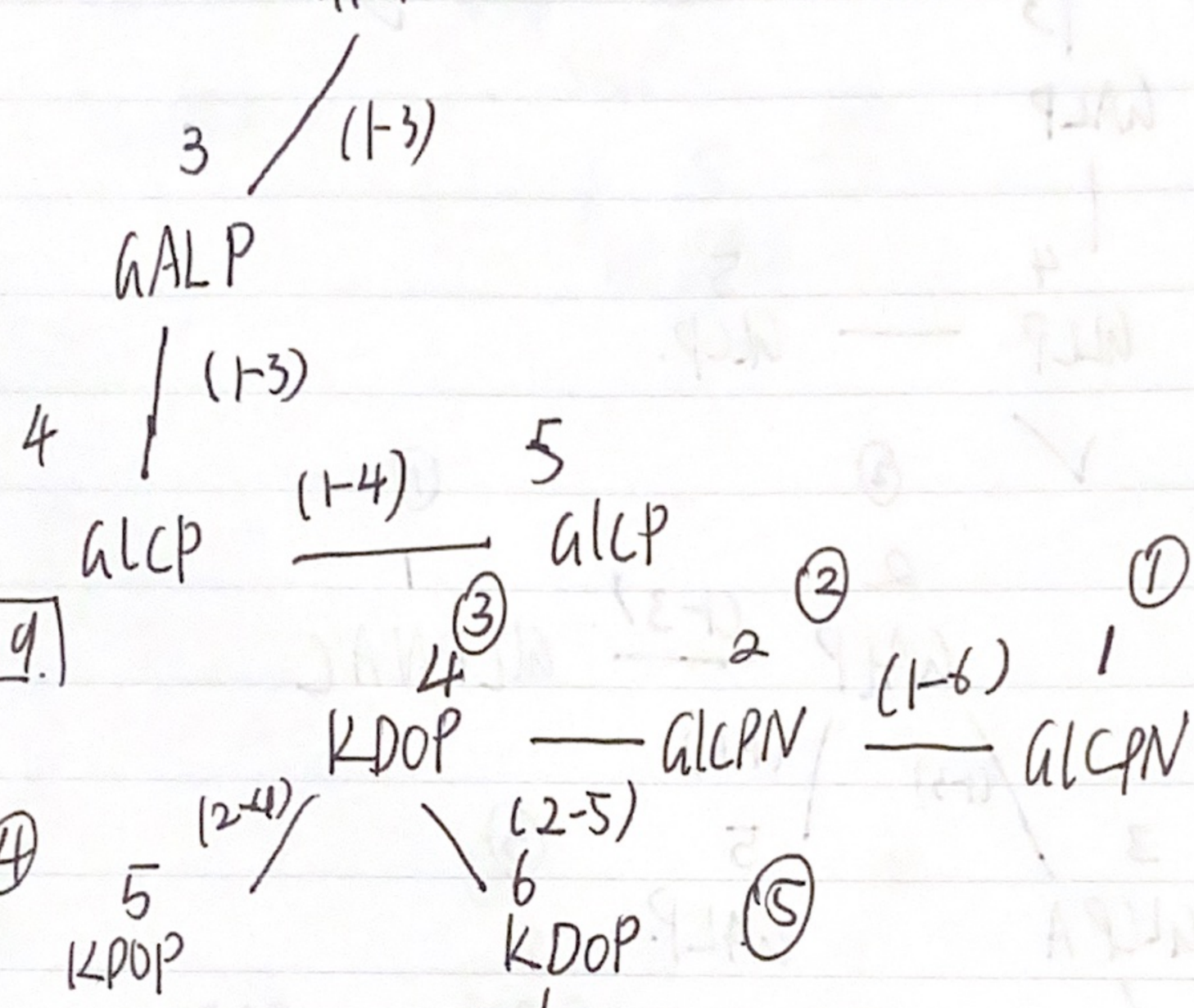


Res	PDB
1	1
2	2
3	5
4	3
5	4

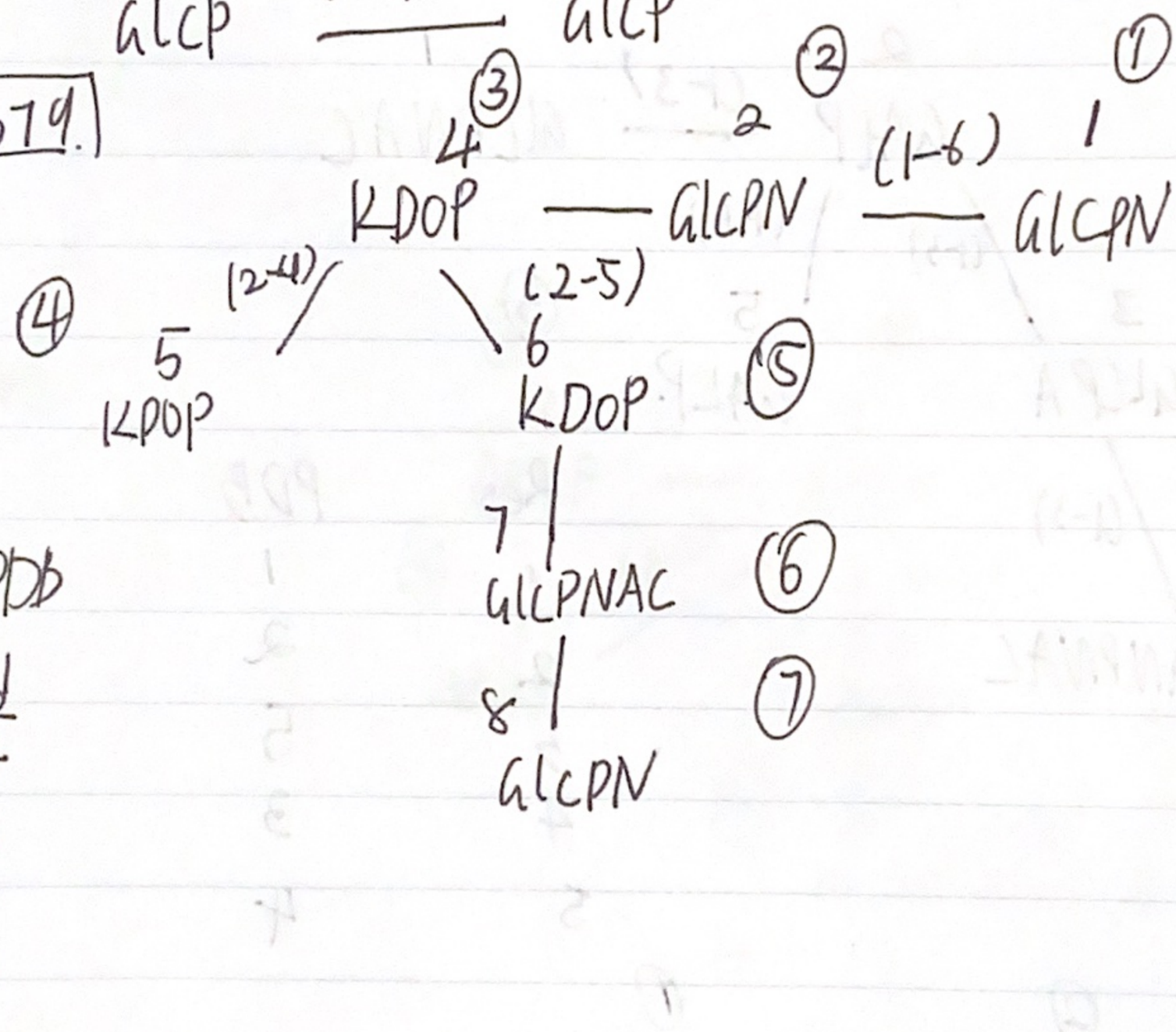
6 PB26370

Res	PDB
1	1
2	2
3	4
4	5

7. DB26404

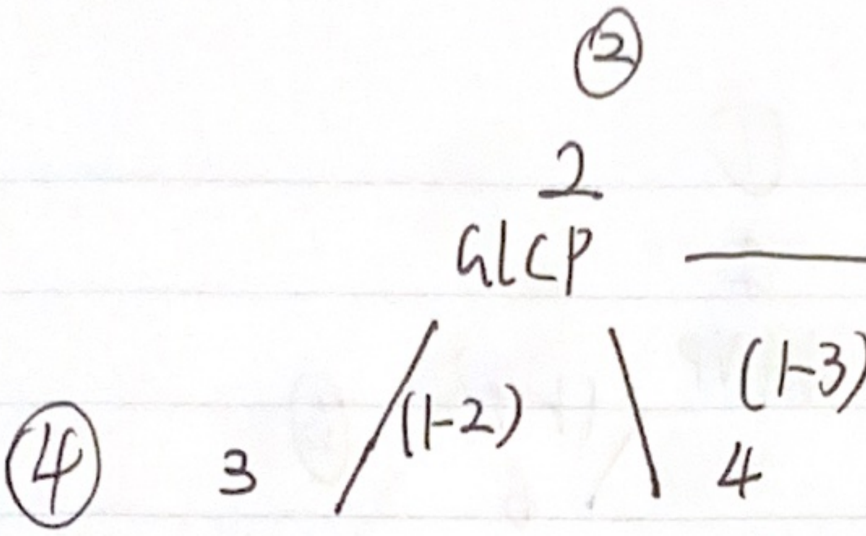


8. DB26379.



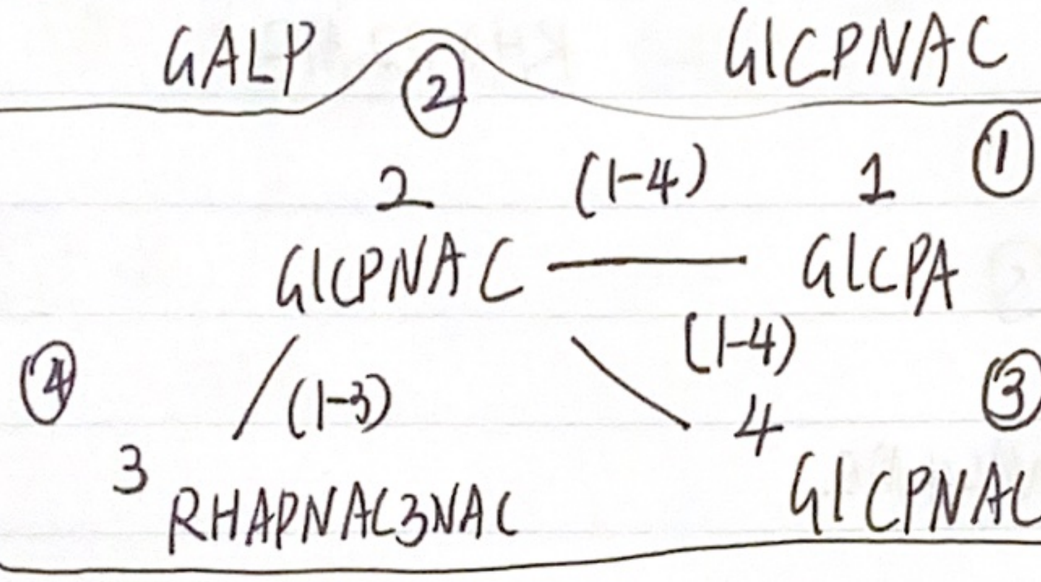
Res	PDB
1	2
2	4
3	5
4	6
5	7
6	8
7	

9. DB9023



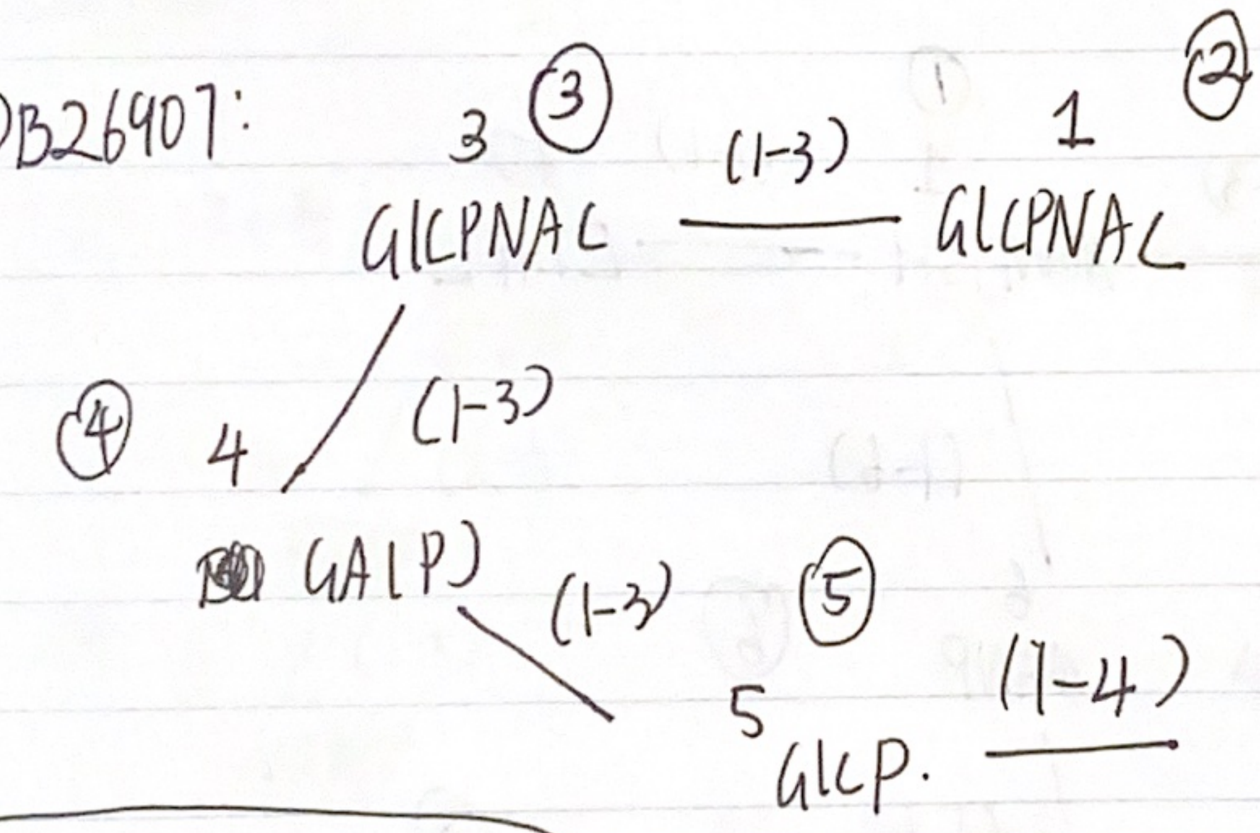
Res	Pdp
1	1
2	4
3	3
4	

10. PB9490



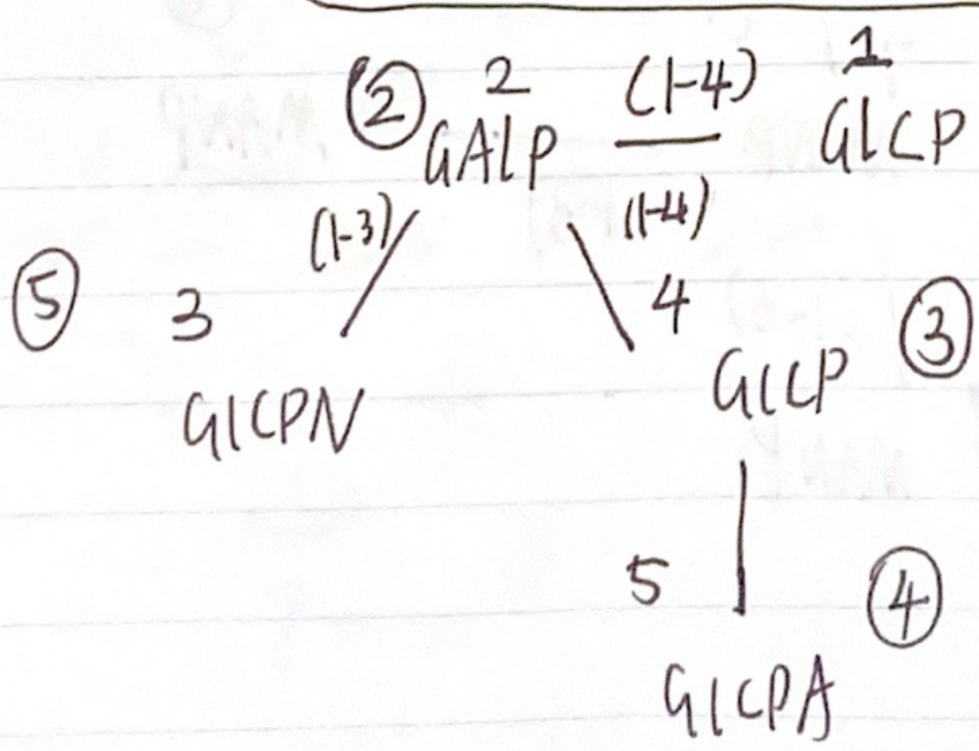
Res	pdP
1	1
2	2
3	4
4	3

11. PB26907:



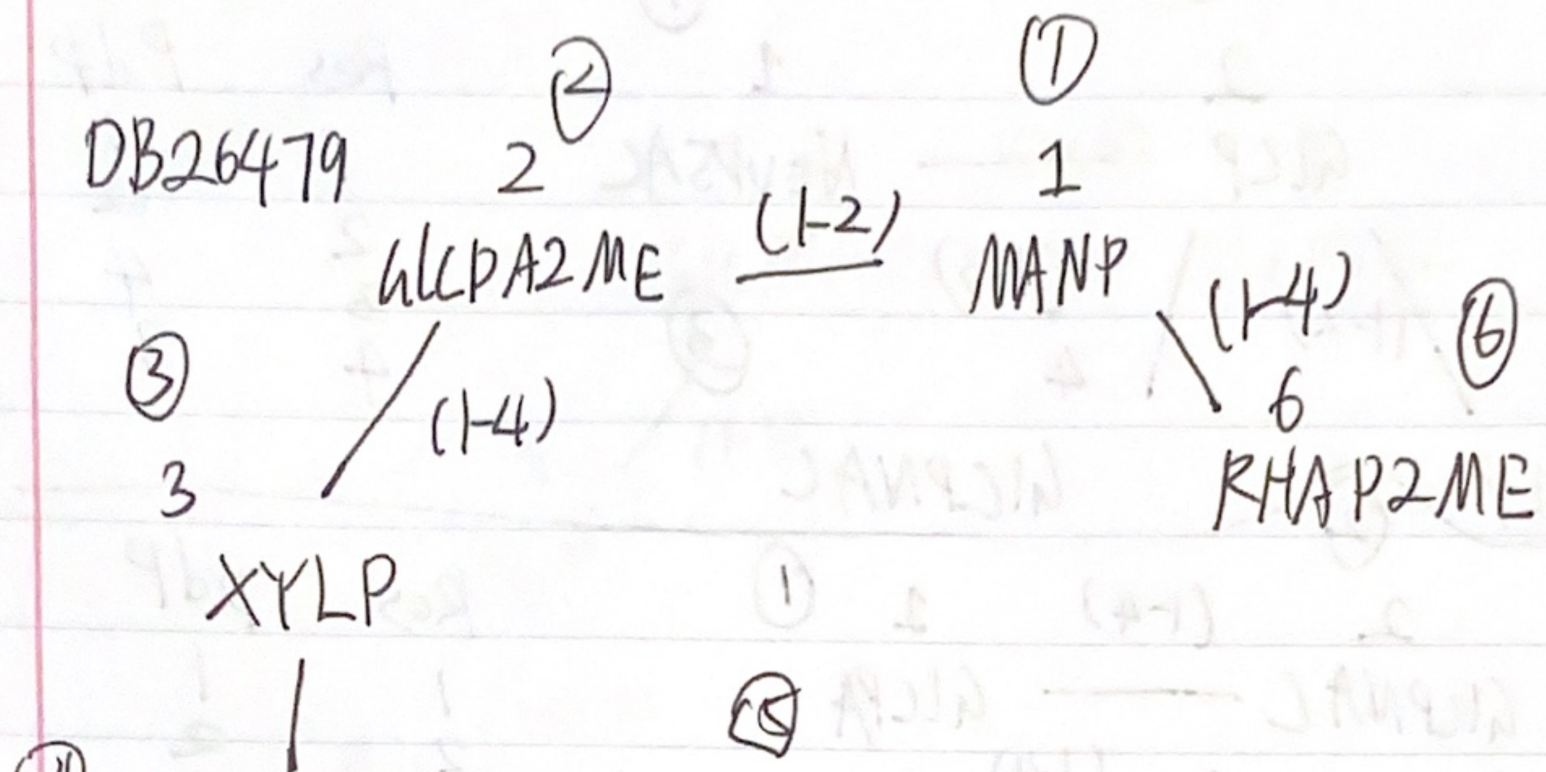
Res	Pdb 9991
1	1
2	3
3	4
4	5
5	6
6	6

12: DB9949

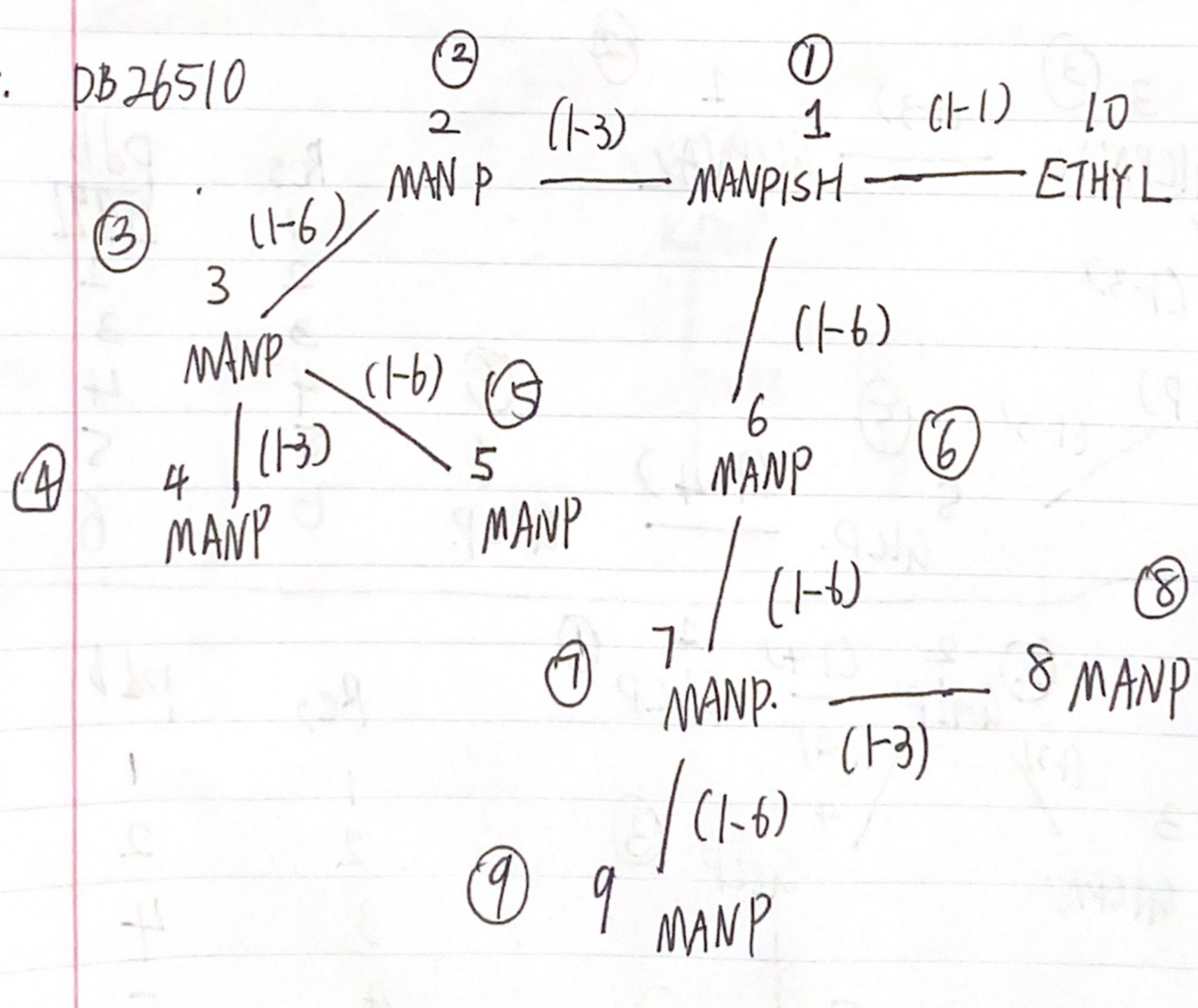


Res	pdb
1	1
2	2
3	4
4	5
5	3

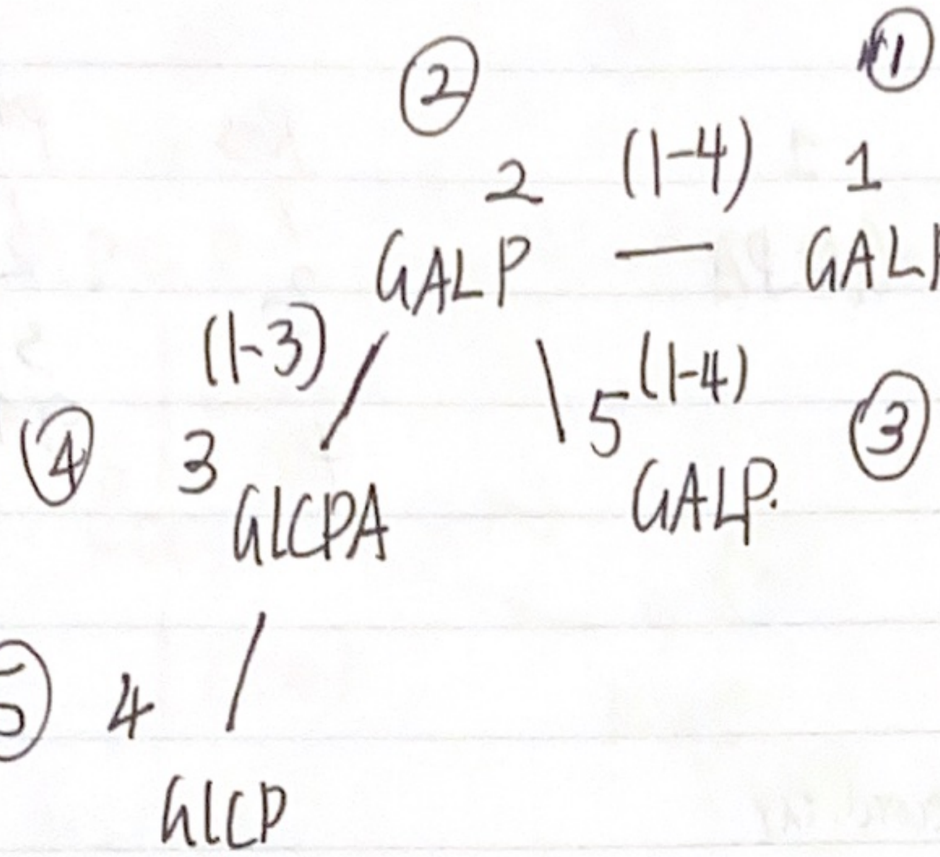
13. DB26479



14. DB26510



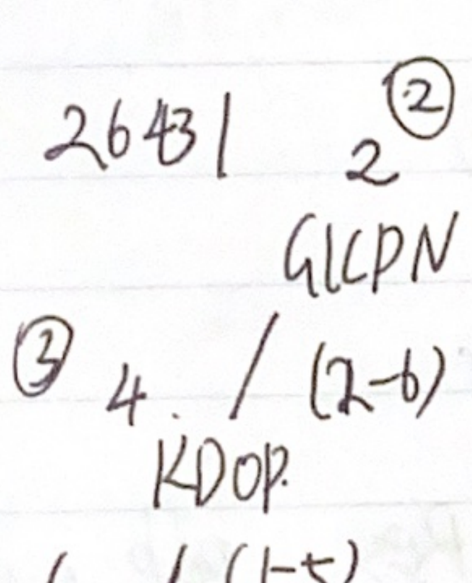
15. PB8939



Res	pdb
1	1
2	2
3	5
4	3
5	4

16. PB26122. ✓

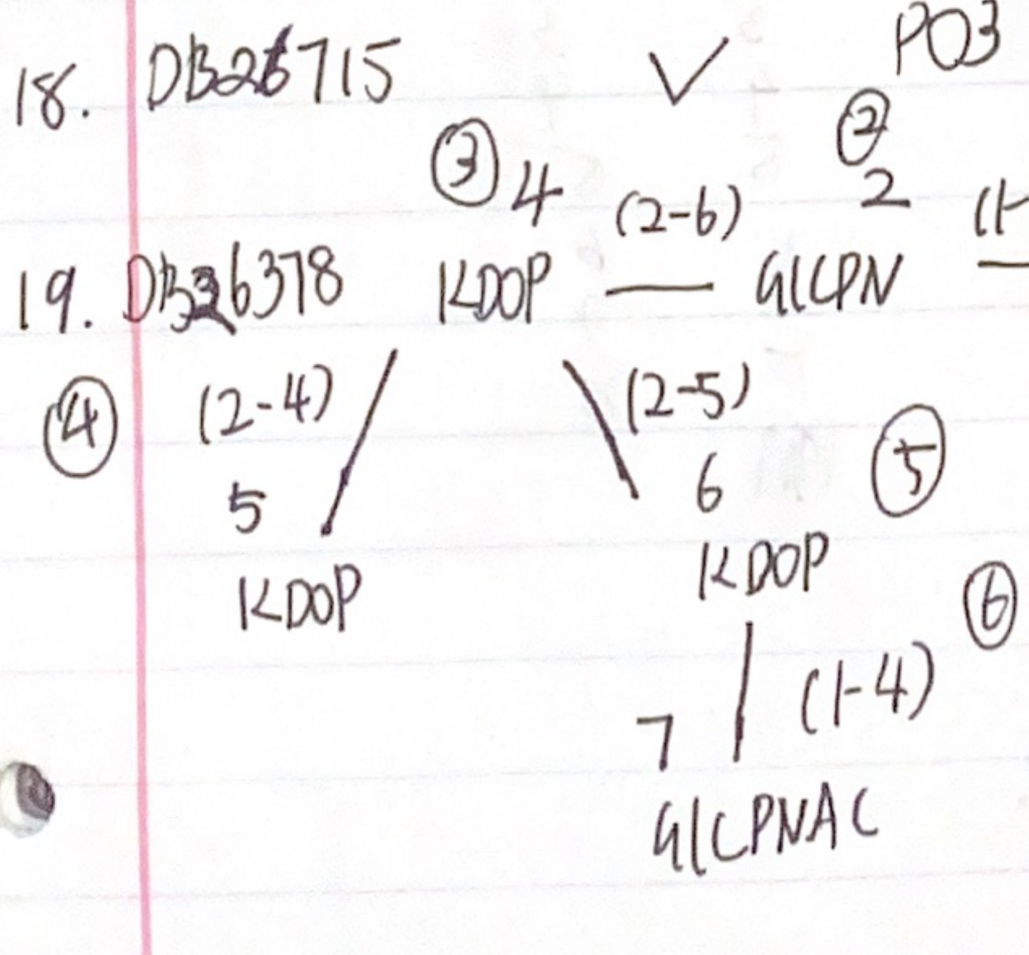
17 DB 26431



Res	pdb
1	1
2	2
3	4
4	6

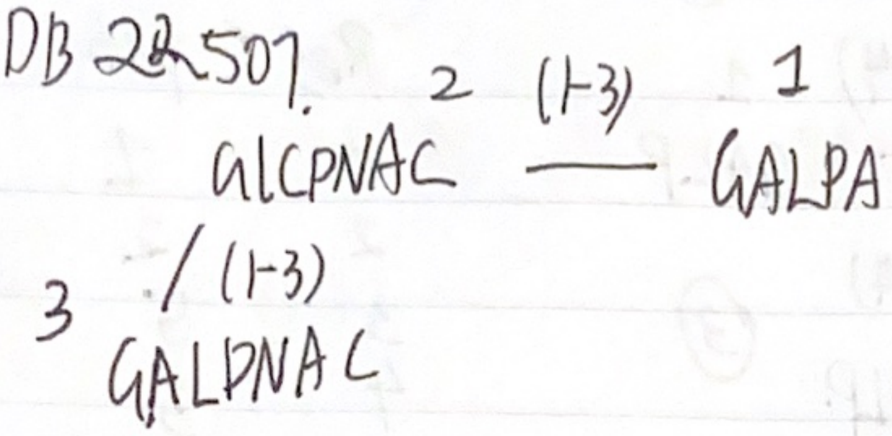
18. DB26715 ✓ PO3 in pdb

19. DB26378



Res	pdb
1	1
2	2
3	4
4	5
5	6
6	7

20 DB22507.



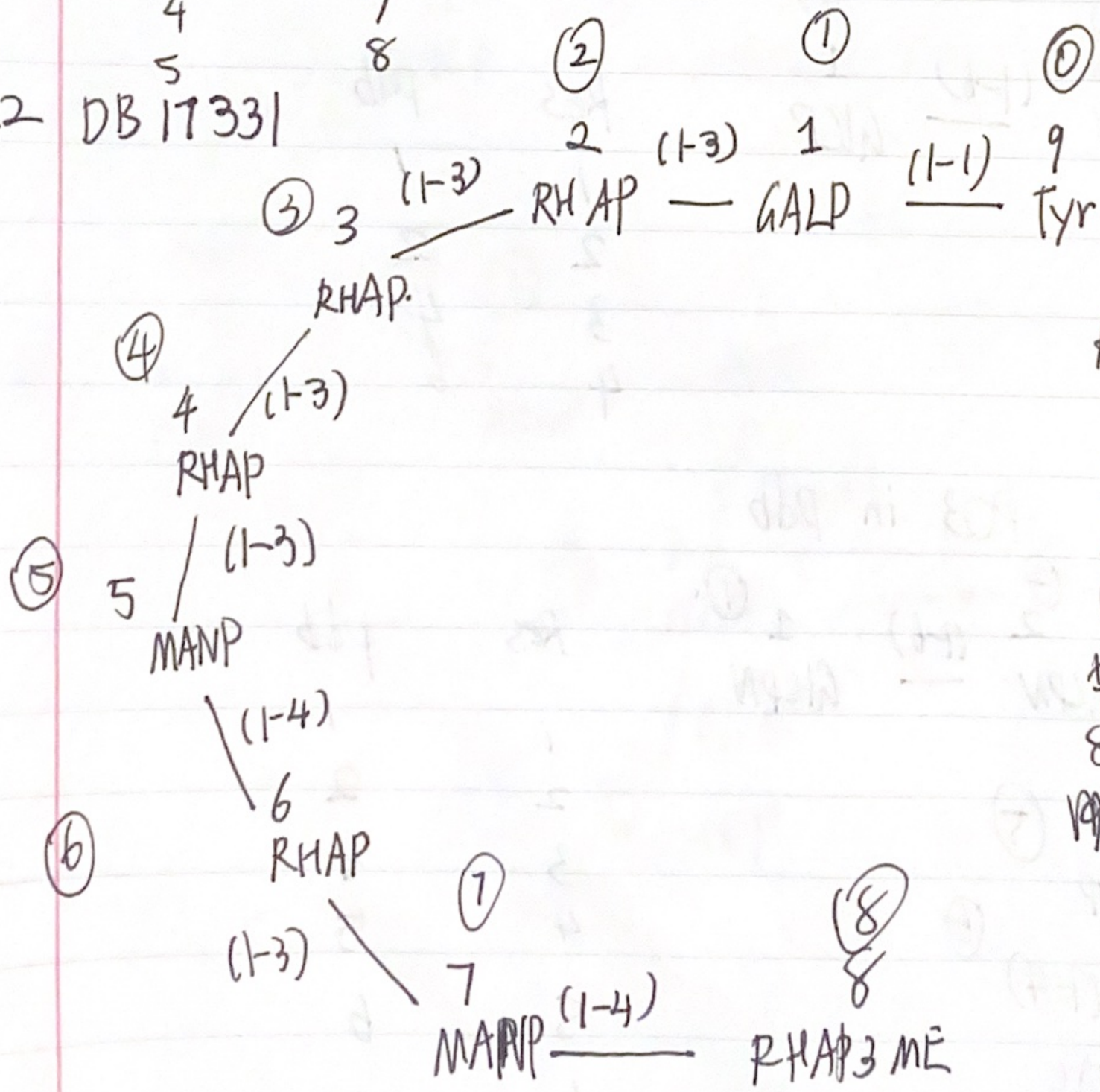
Res	pds
1	1
2	2
3	3
4	997

21. DB26682.

In nonlinear-preprocess_record.txt.

Res	pds
1	3
2	4
3	6
4	7
5	8

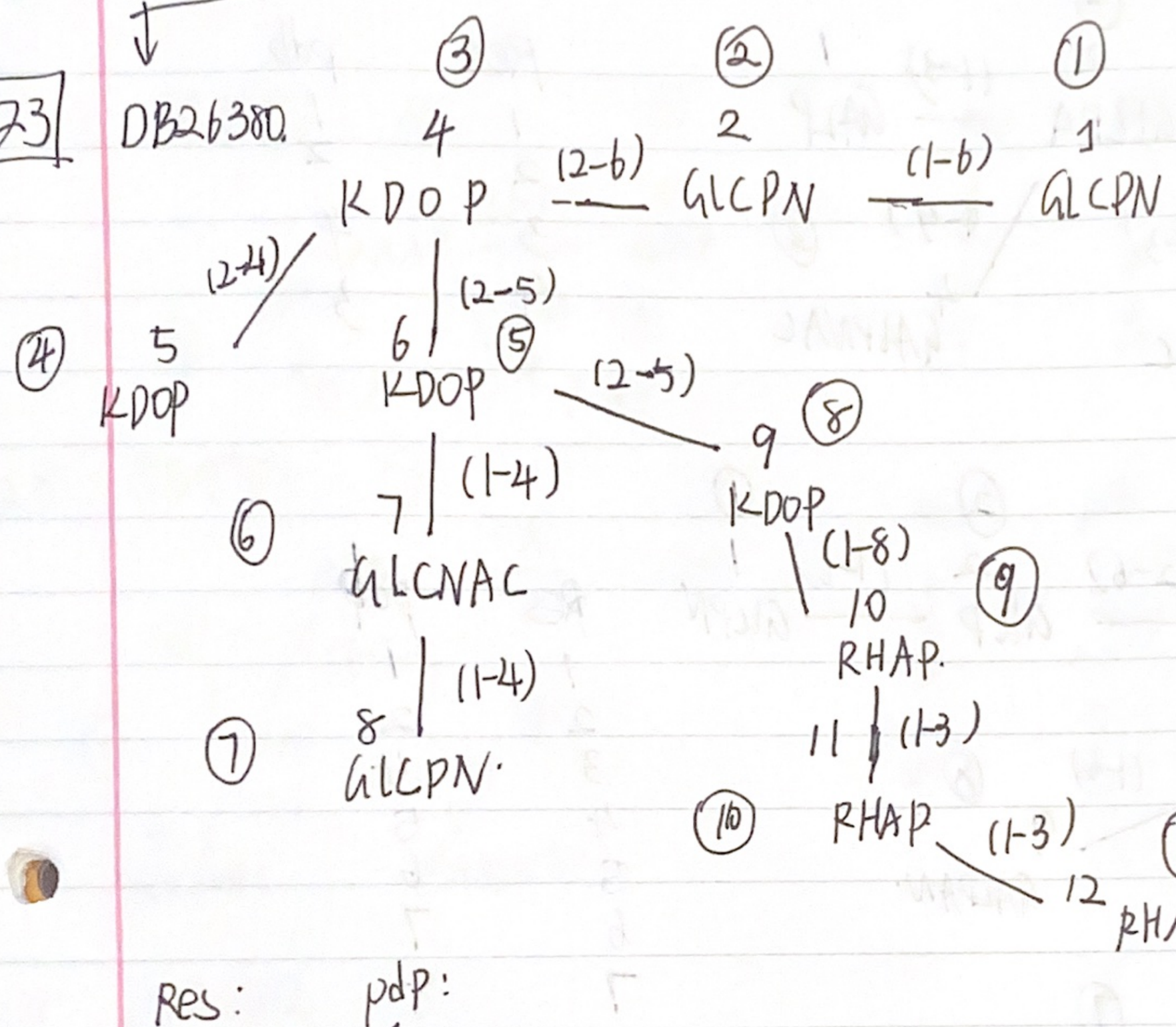
22 DB17331



Res	pdb	acty
0		
1	1	
2	2	
3	3	
4	4	
5	5	
6	6	
7	7	
8	8	
9		

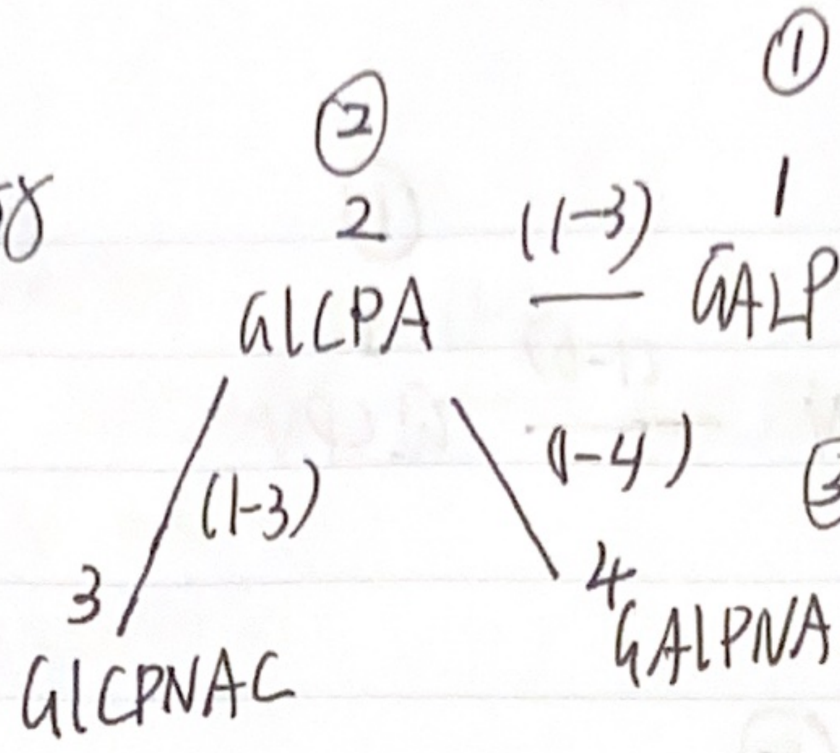
check this

23 DB26380.



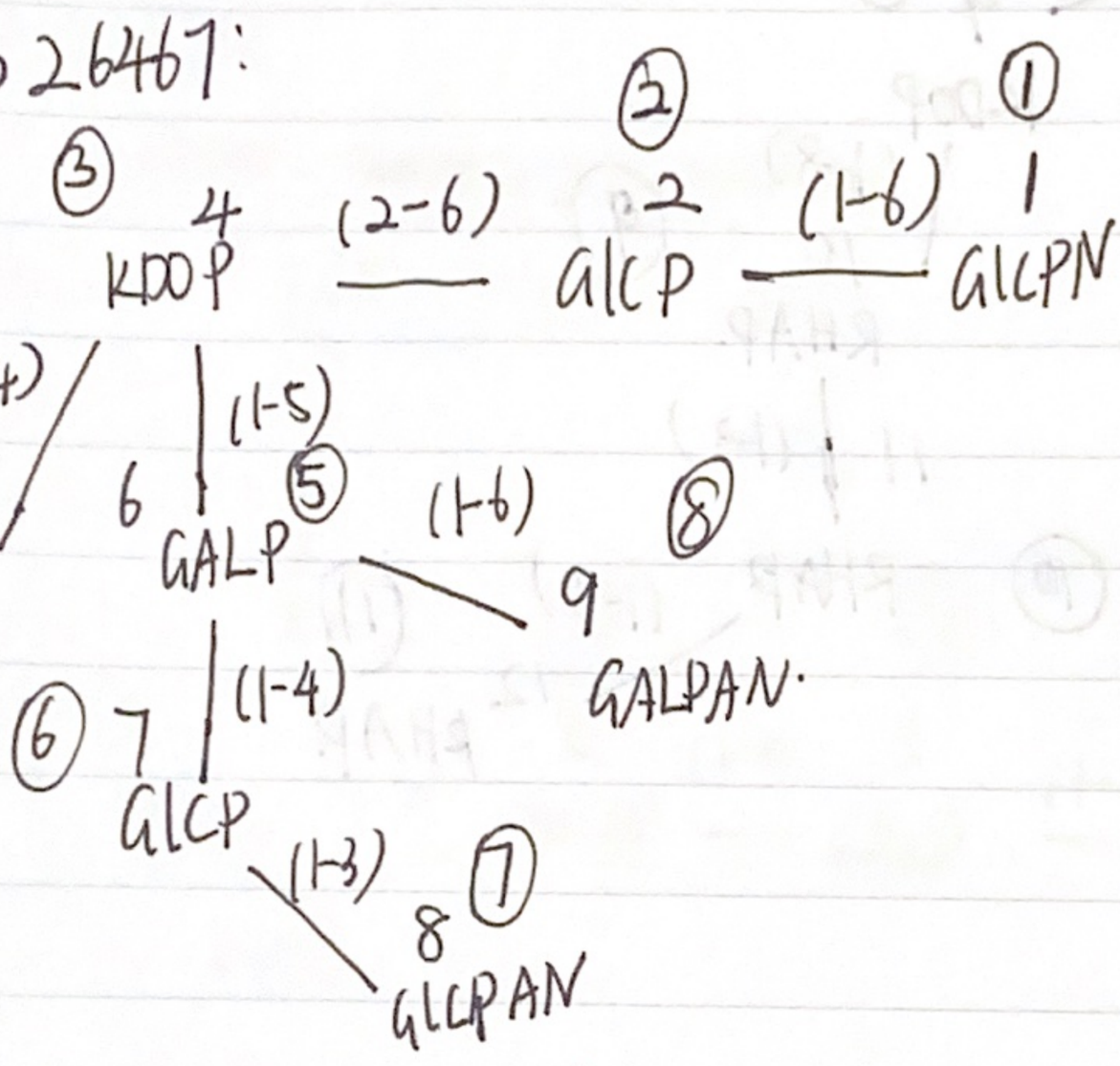
Res:	pdp:
1	1
2	2
3	4
4	5
5	6
6	7
7	8
8	9
9	10
10	11
11	12

24 DB9188



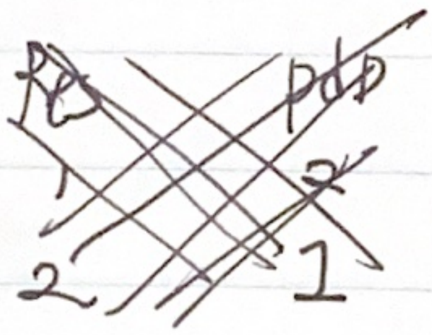
Res	pdb
1	1
2	2
3	4
4	3

25: DB 26467:

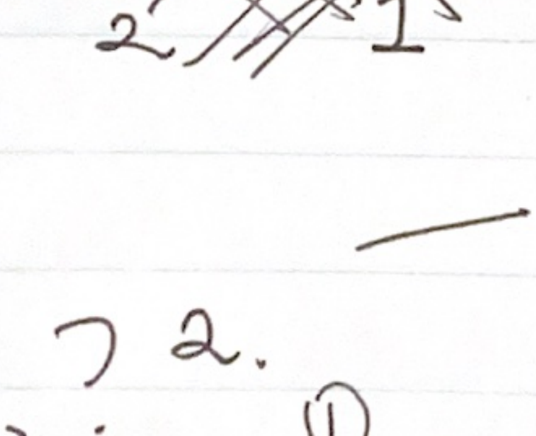


Res	pdb
1	1
2	2
3	4
4	5
5	6
6	7
7	8
8	9

26:



~~BD-GLCP~~
~~6~~

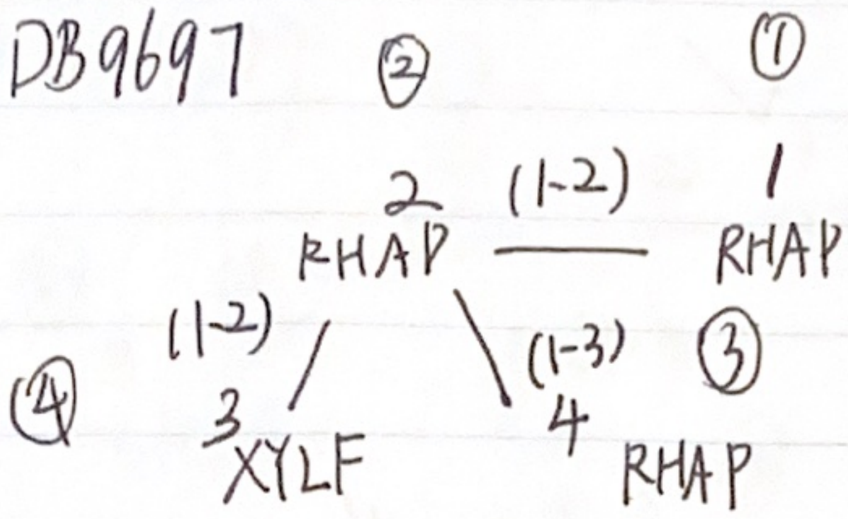


Res	pdb
1	999
2	1

7 2.

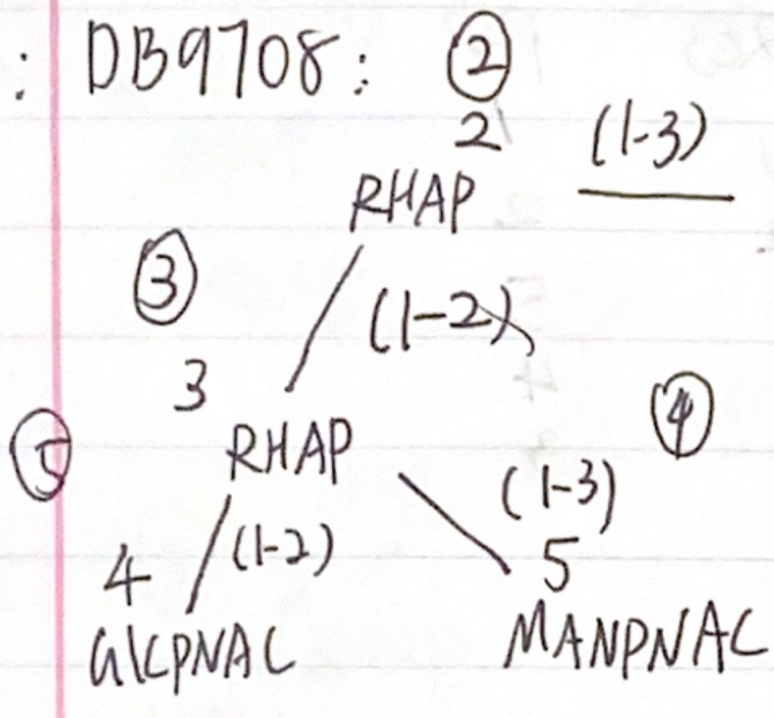
This is a non-monosaccharide component.

27: DB9697



Res	pdb
1	1
2	2
3	4
4	3

28: DB9708:



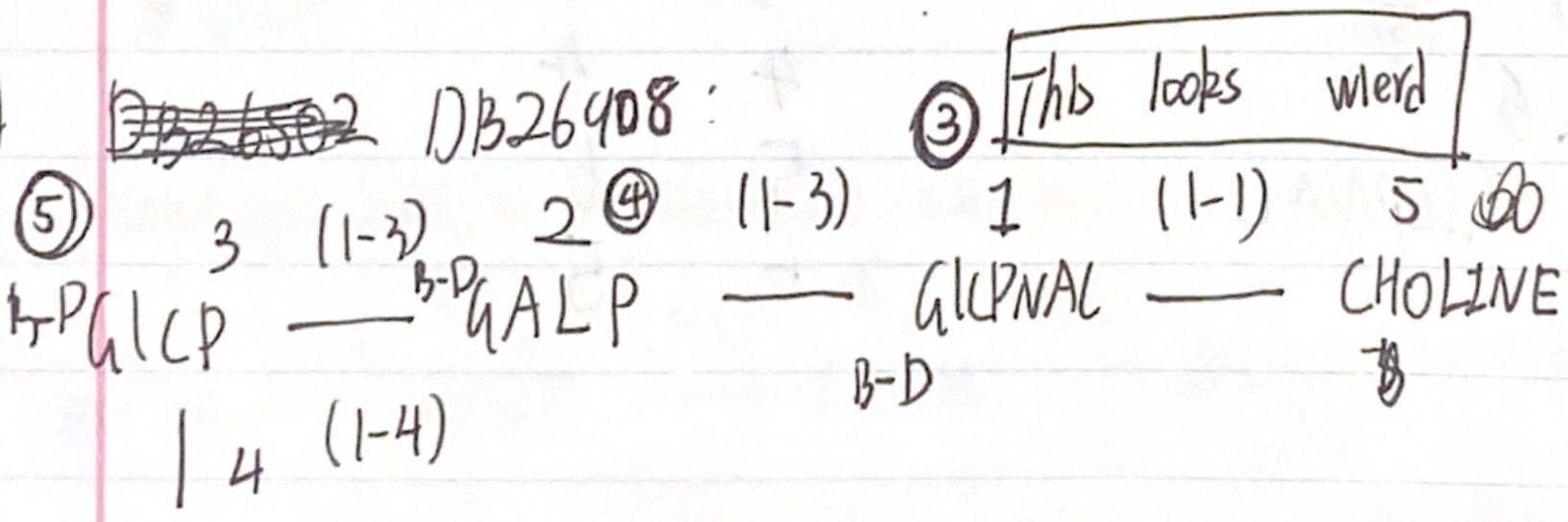
Res	pdb
1	1
2	2
3	3
4	5
5	4

29: DB26502

1-1, ... 9-9.

Include in nonlinear-preprocess-record.txt.

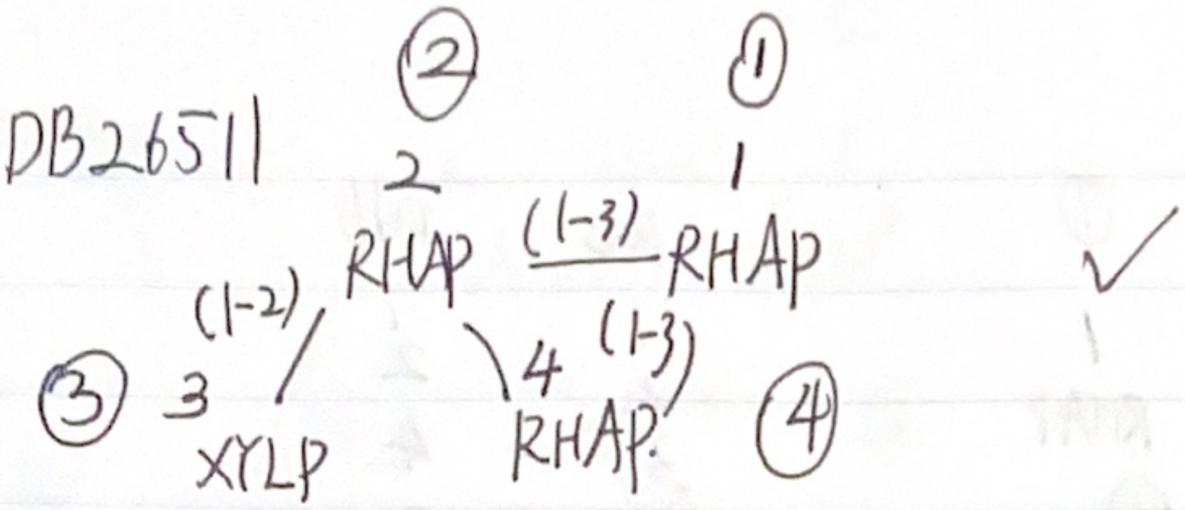
30 ~~DB26502~~ DB26408:



Res	pdb
1	999
2	999
3	1
4	2
5	3
6	4

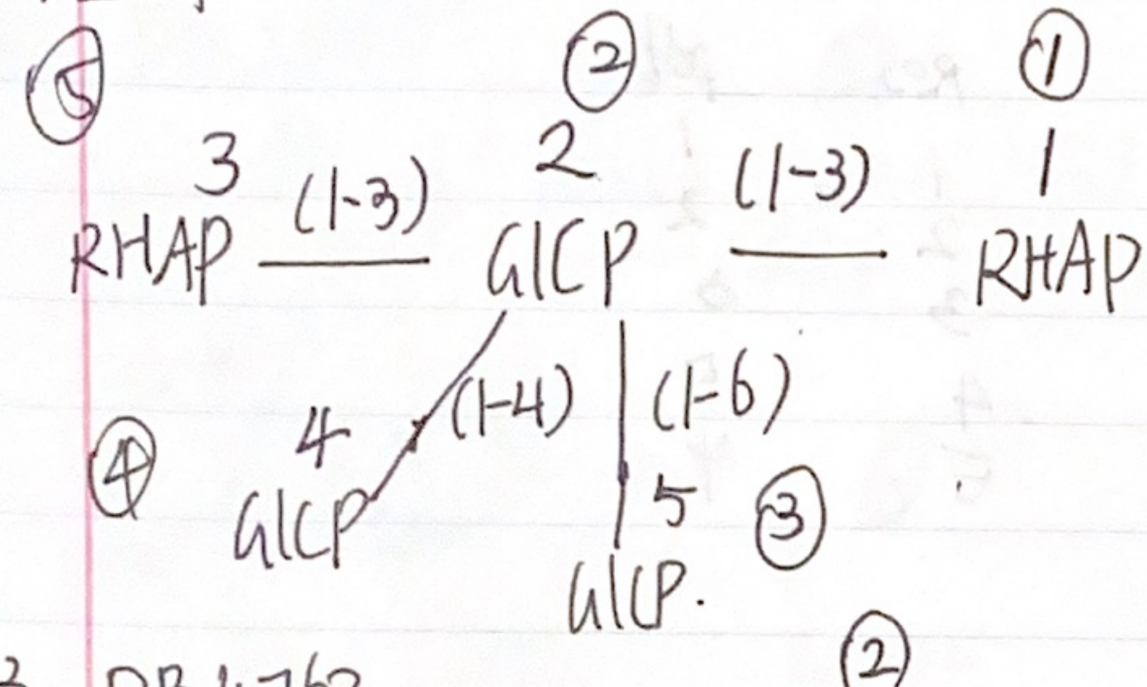
A-D GLCP ⑥

31 DB26511



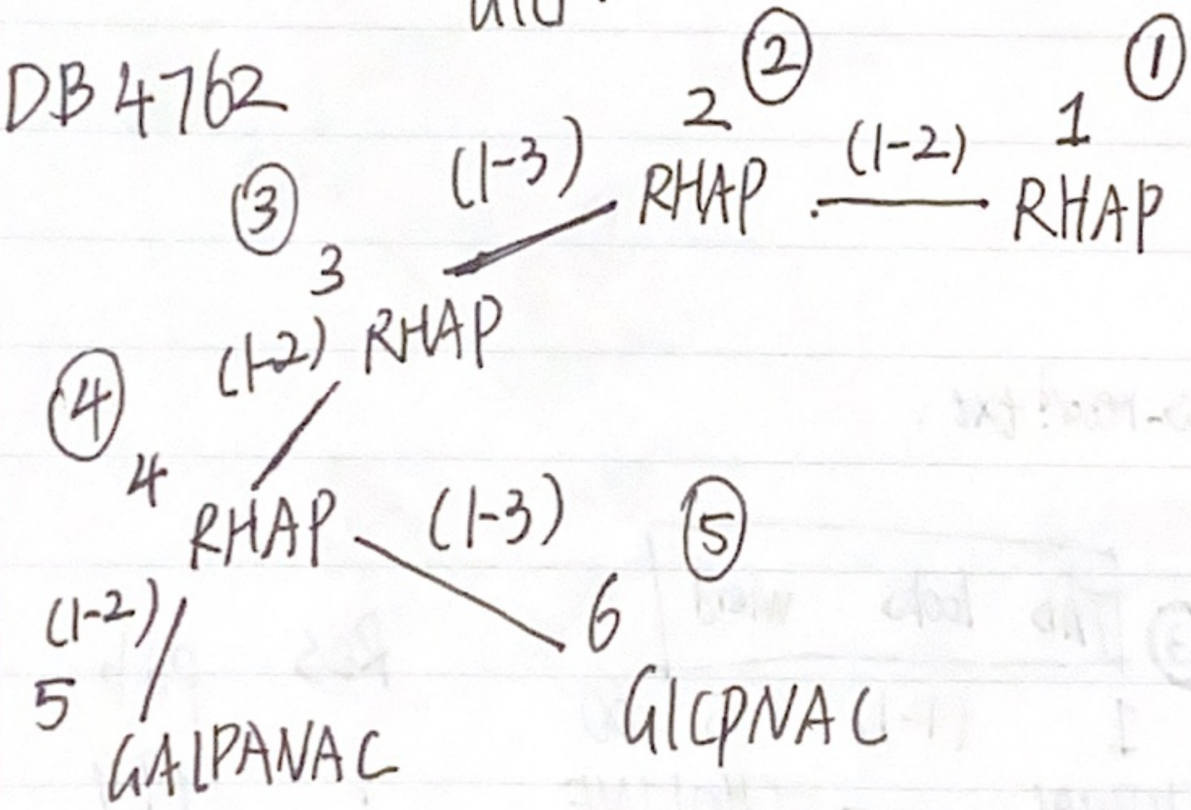
✓

32 DB9917



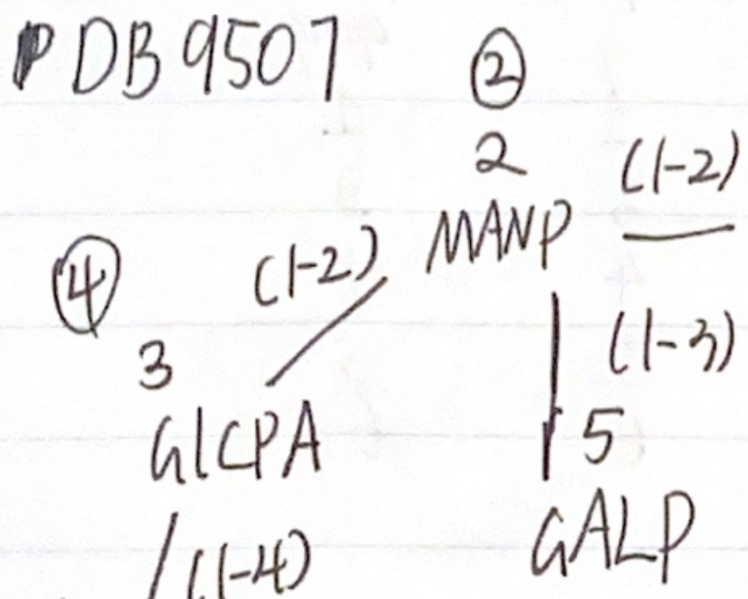
Res	pdb
1	1
2	2
3	5
4	4
5	3

33 DB4762



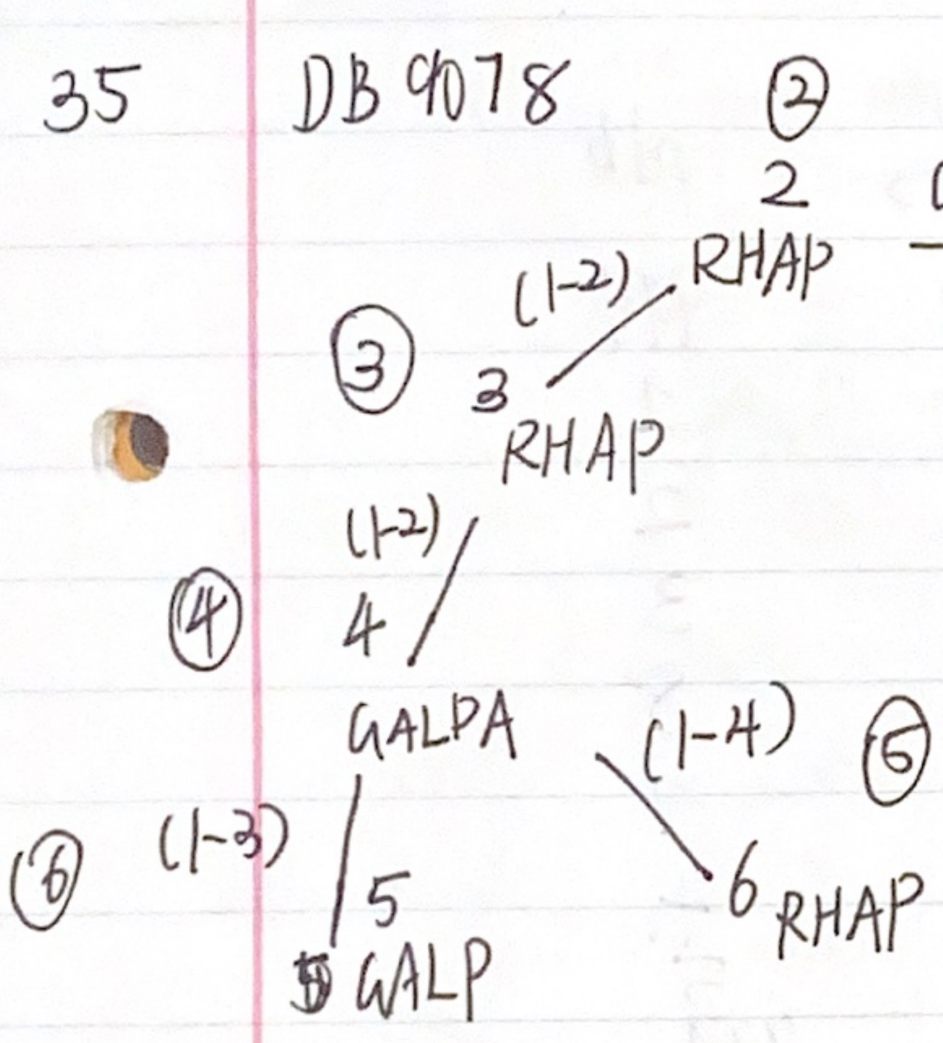
Res	pdb
1	1
2	2
3	3
4	4
5	6
6	5

34 PDB 9507



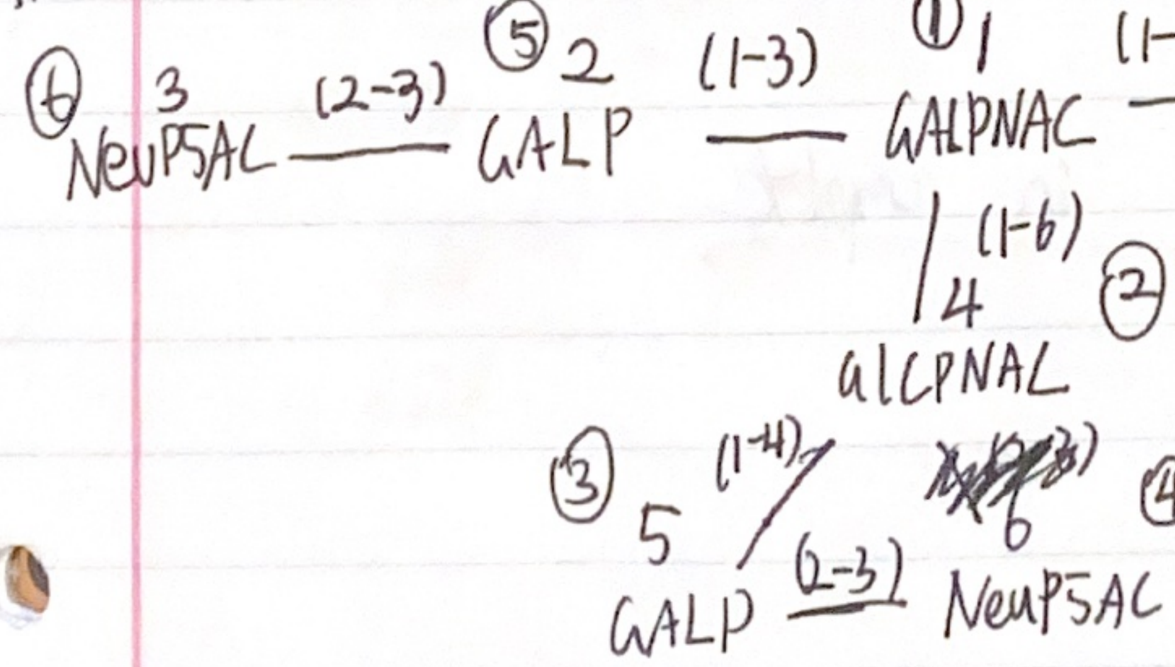
Res	pdb
1	1
2	2
3	5
4	3
5	4

35 DB 9078



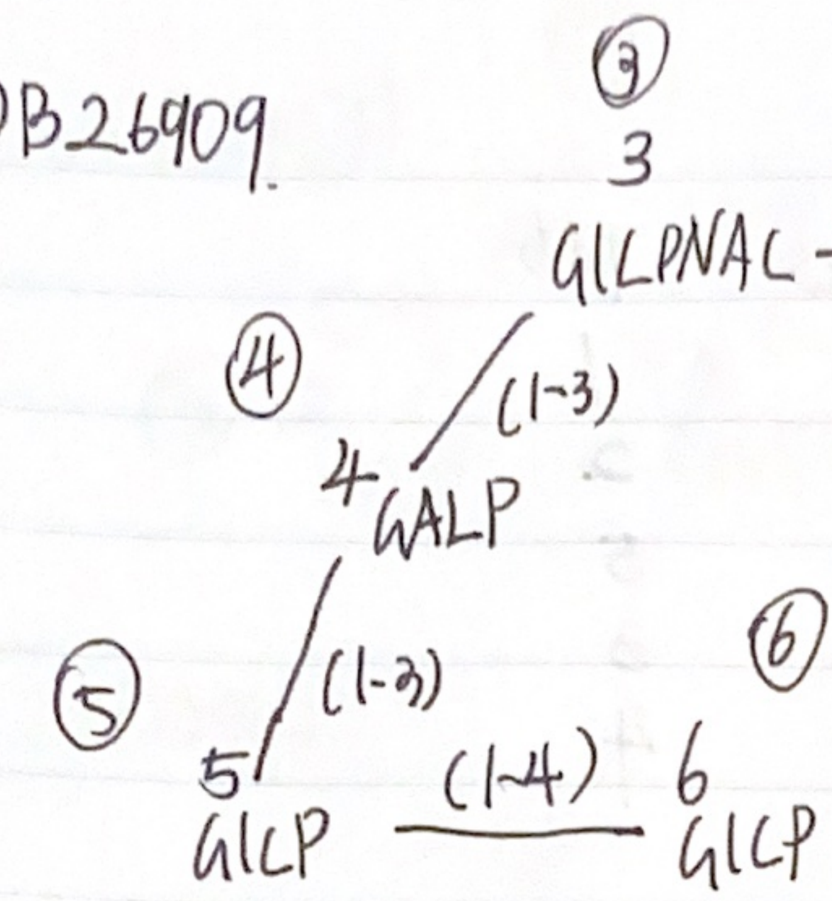
Res	pdb
1	1
2	2
3	3
4	4
5	6
6	5

36. NeuAcα2-3Galβ1-3(NeuAcα2-3Galβ1-4GlcNAcβ1-6)GAlNAc.



Res	pdb
1	1
2	4
3	5
4	6
5	2
6	3

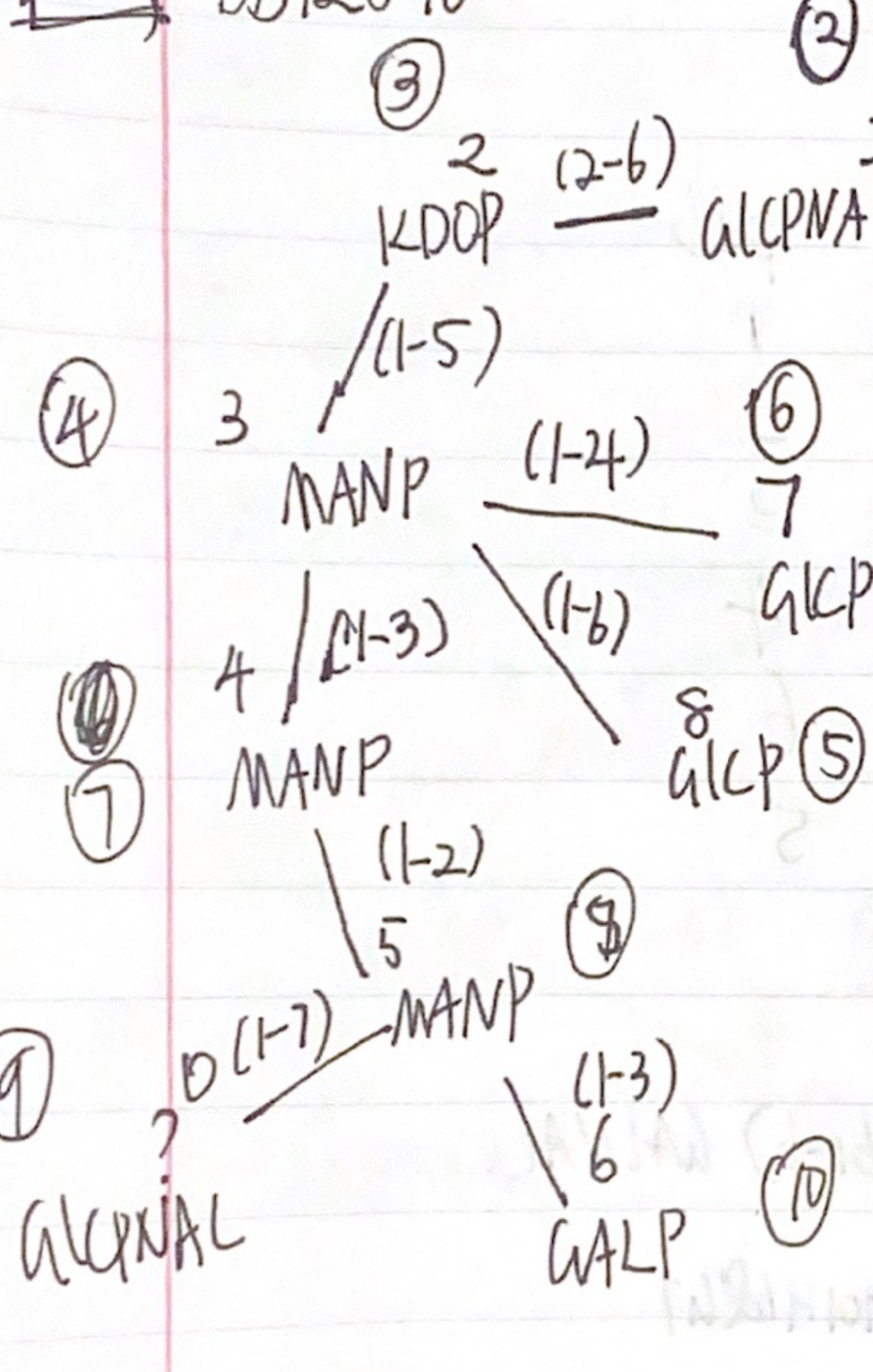
37 DB26909.



Res	pdb
1	999
2	1
3	3
4	4
5	5
6	6

B8 DB12870

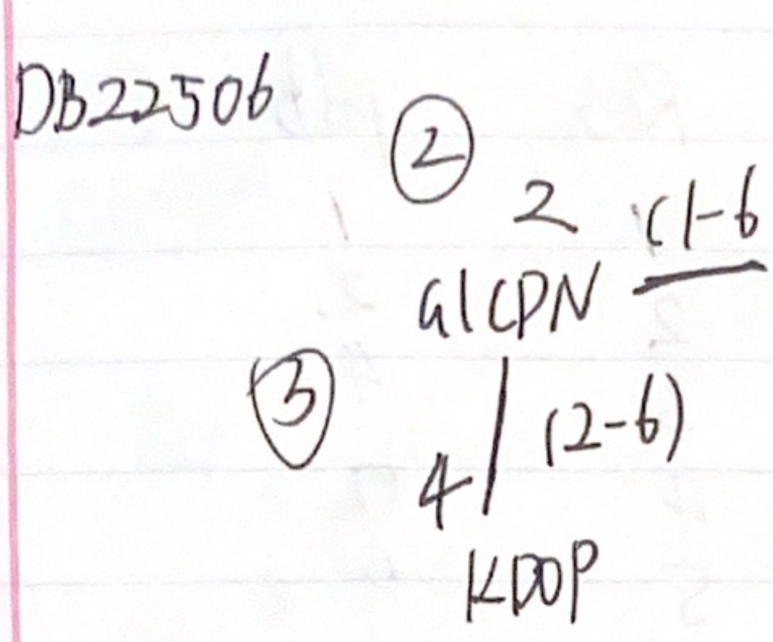
Are we include 1 or not?



Res	pdb
1	999
2	1
3	2
4	3
5	8
6	7
7	4
8	5
9	999
10	6

PPB is in complete

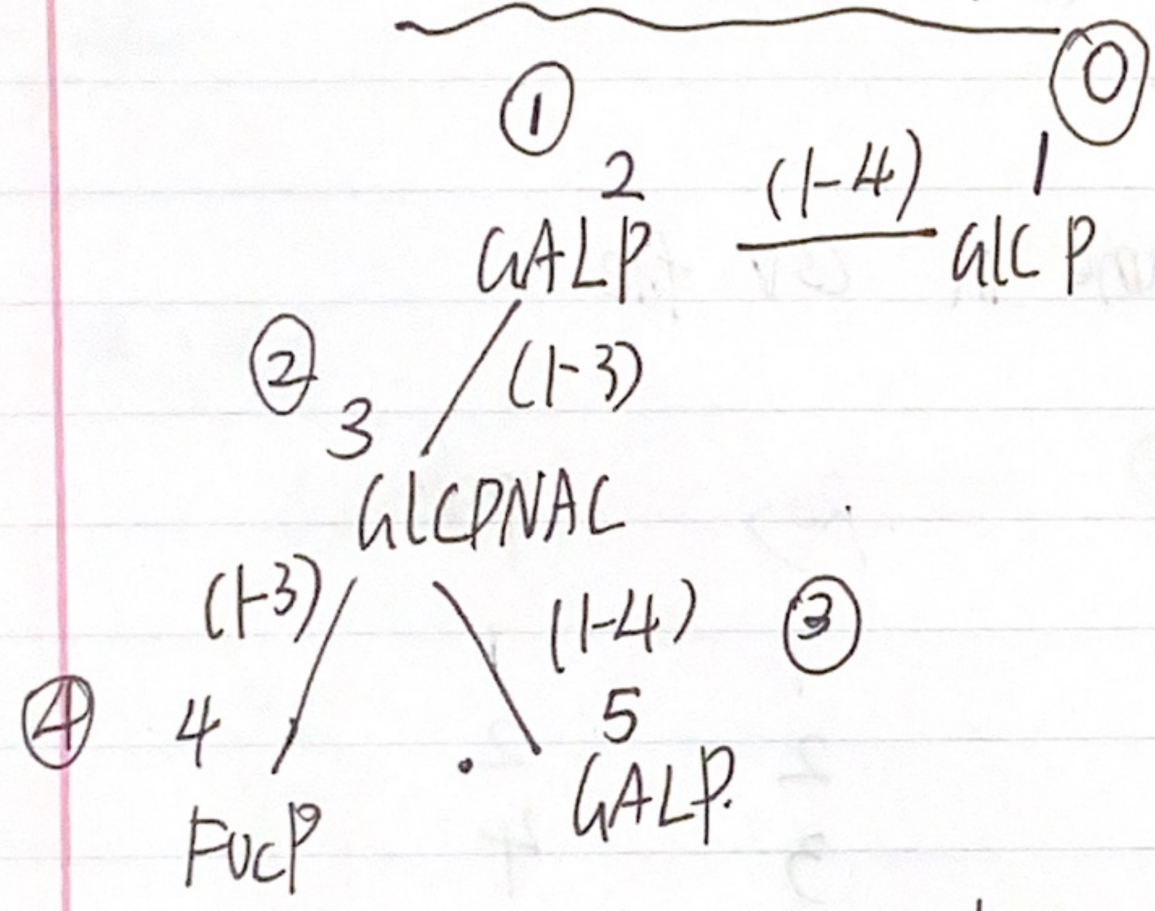
39 DB22506



Res	pdb
1	1
1	2
2	4
3	

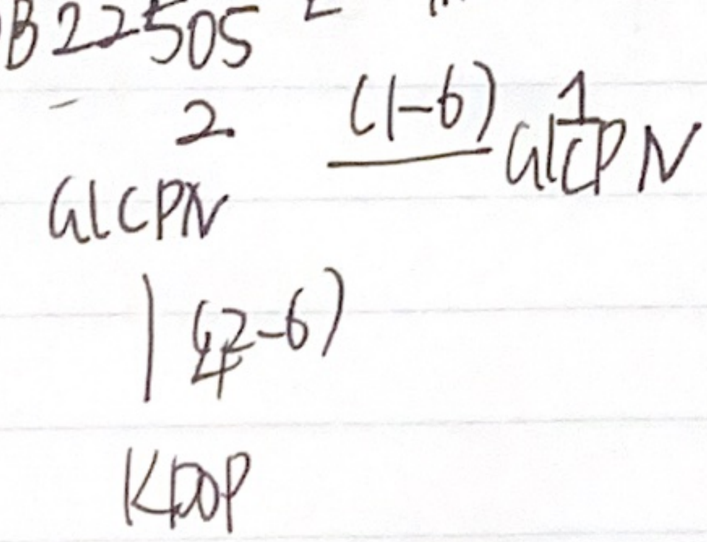
40 LFucpa 1-3 [DGalpb 1-4] DGlcpNAcb 1-3 DGalpb 1-4 DGlc.

↑ starts with HIA HIB. which to use?



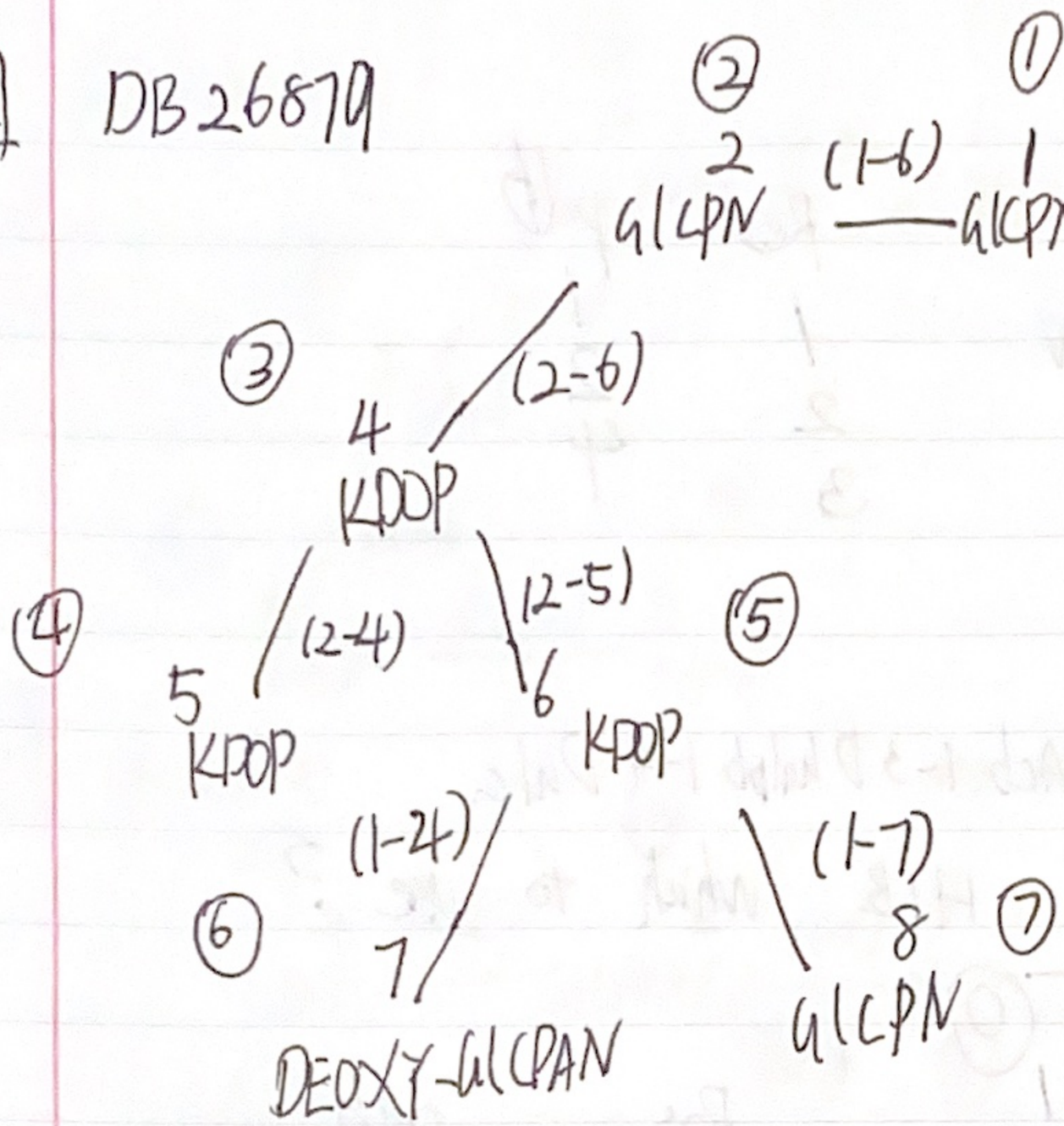
Res	pdb
0	999
1	2 3
2	5
3	4
4	

41 DB22505 ← this is exactly same as 22506



Res	pdb
1	1
2	2
3	4

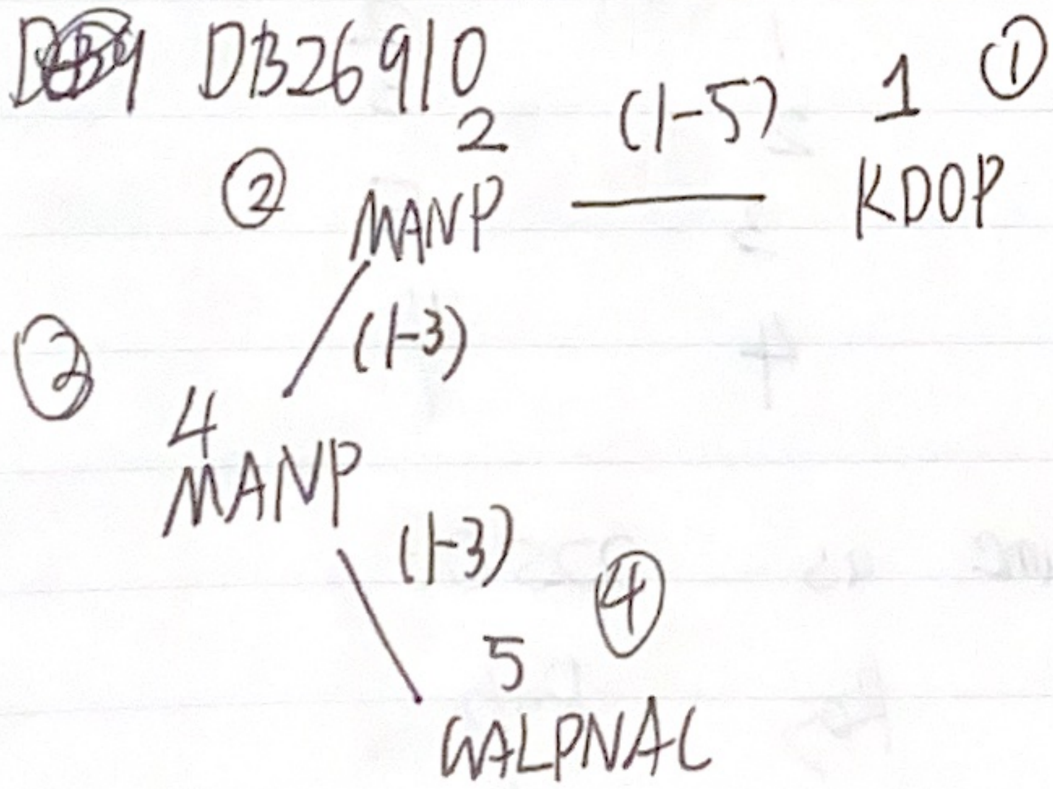
42 DB26879



Res	pdb
1	1
2	2
3	4
4	5
5	6
6	7
7	8

Needs correct monosaccharidename in csv file

43 ~~DB26910~~ DB26910

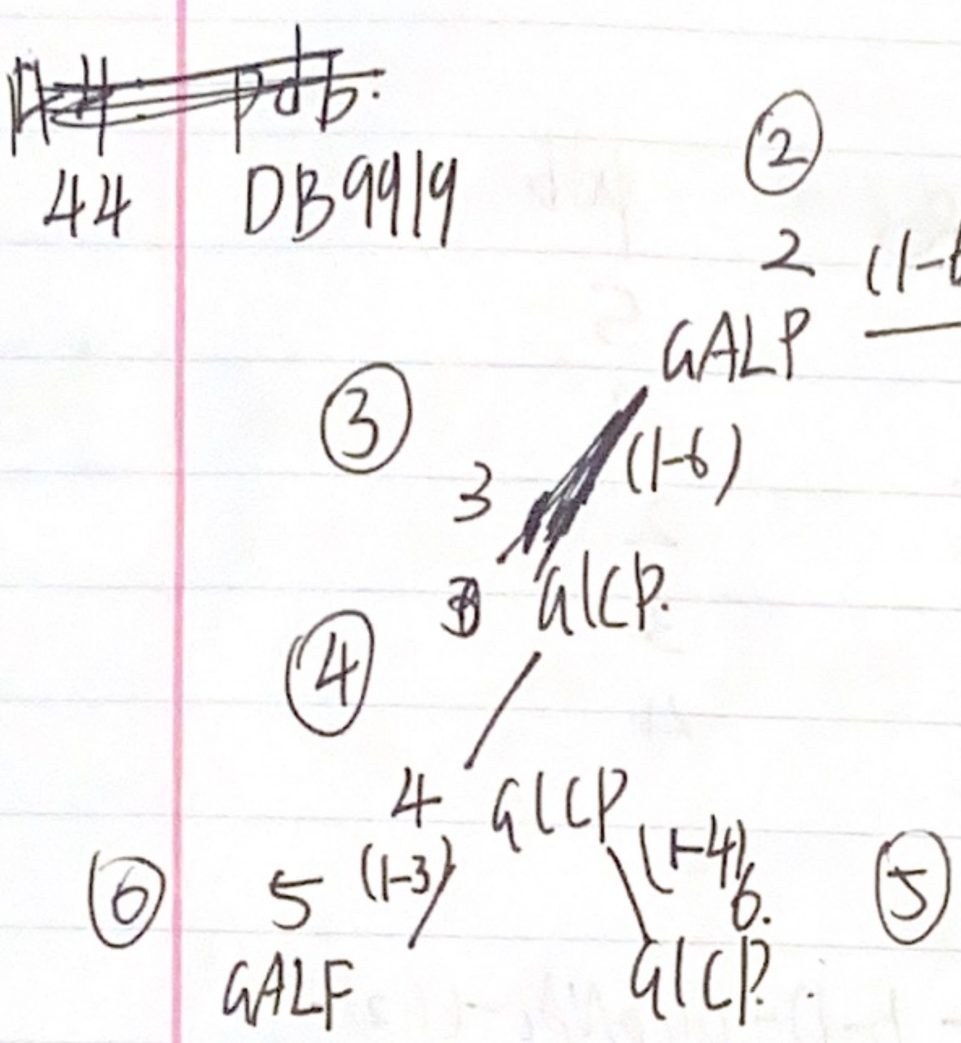


Res	pdb
1	1
2	2
3	4
4	5

HEPP change to MANP

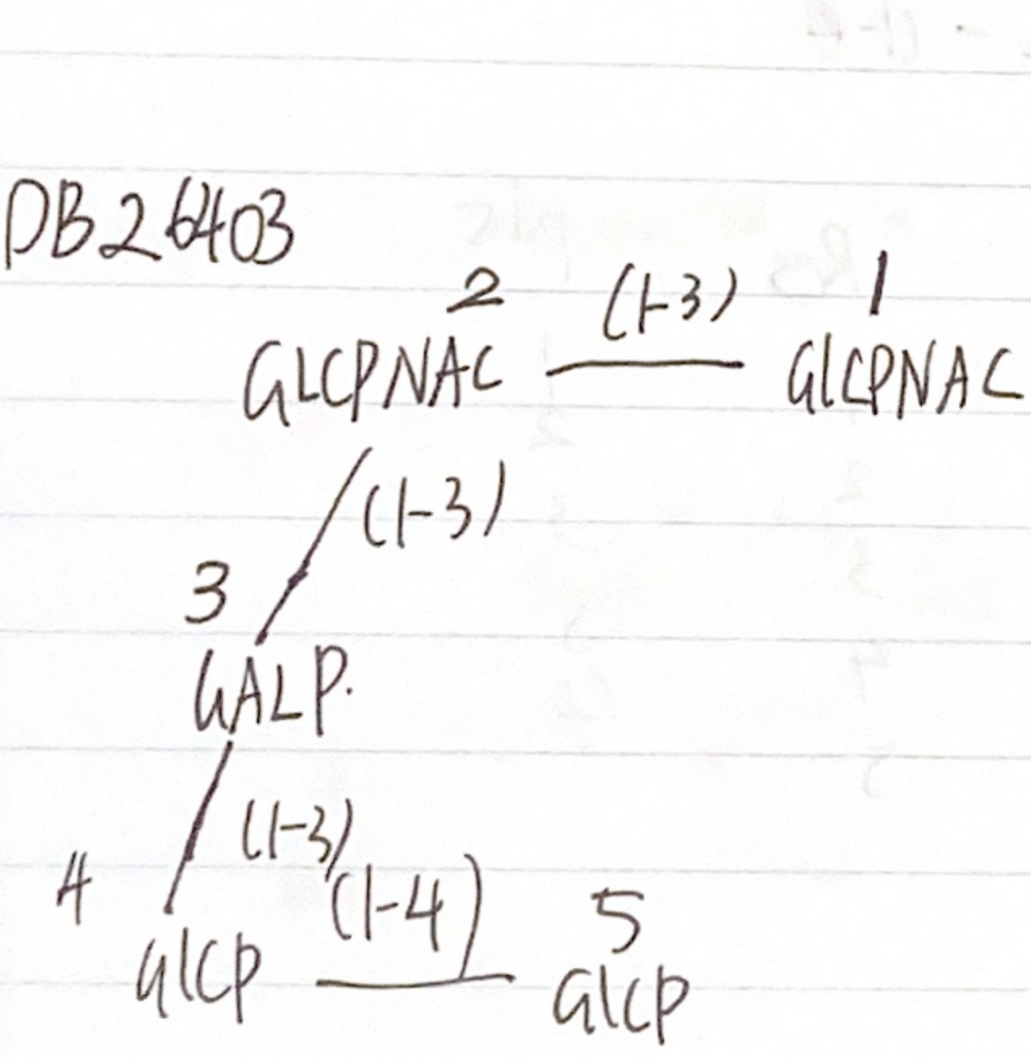
~~Red pdb.~~

44 DB9919



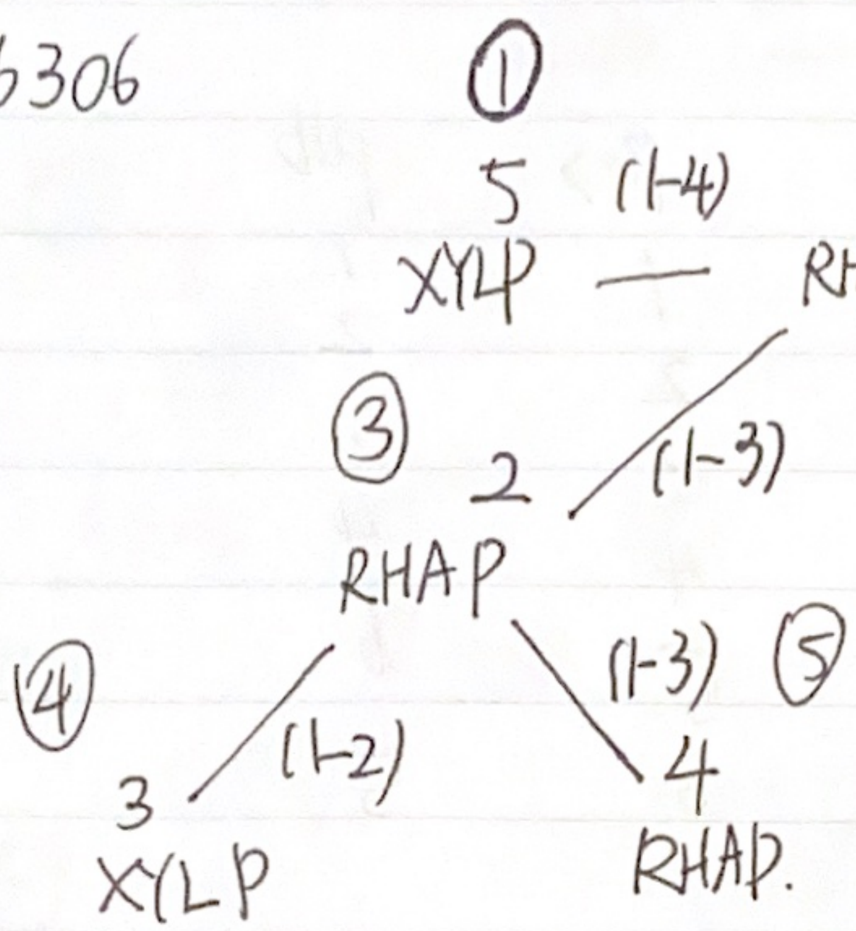
Res	pdb
1	1
2	2
3	3
4	4
5	6
6	5

45 DB26403



✓

46 DB26306

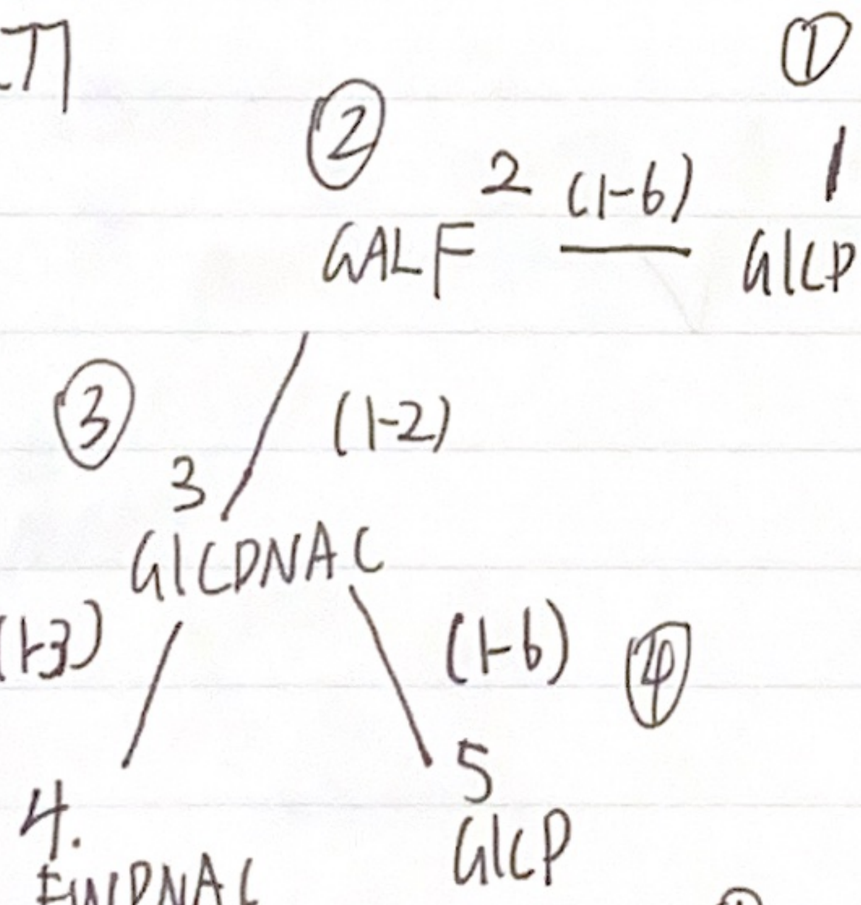


Res	pdb
1	5
2	1
3	2
4	3
5	4

47 Repeat-4)-a-D-Manp-(1-4)-a-D-GulpA-(1-3)-b-D-GlcpNAc-(1-2)-a-D-Gulp-(1-3)-a-L-Rhap2NAc-(1-

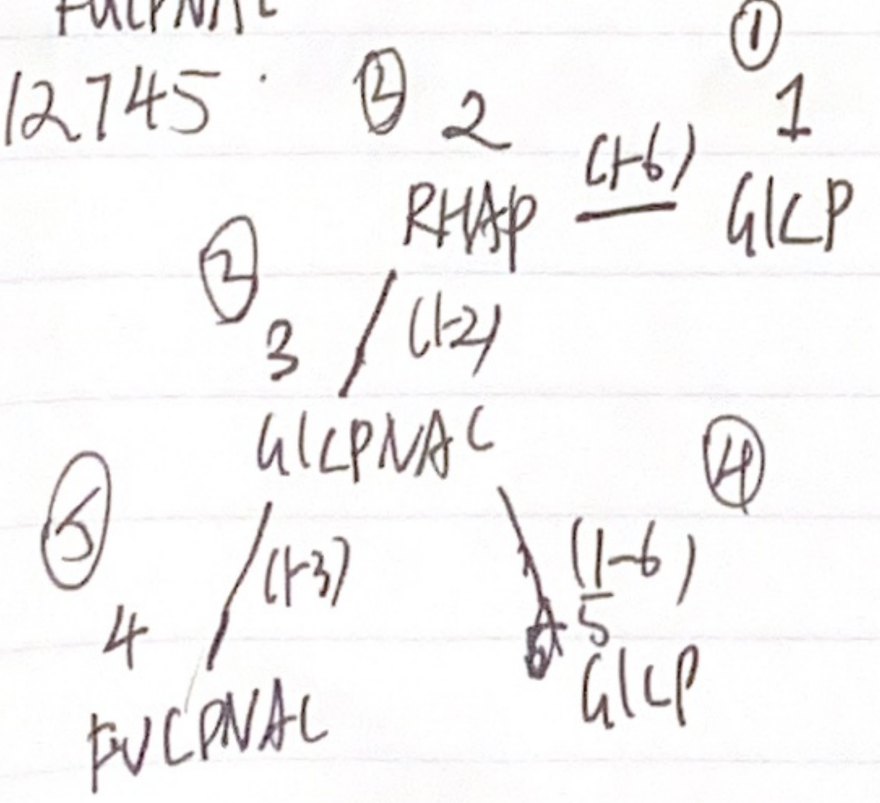
✓

48 DB RT7



Res	pdb
1	1
2	2
3	3
4	5
5	4

44 DB12745



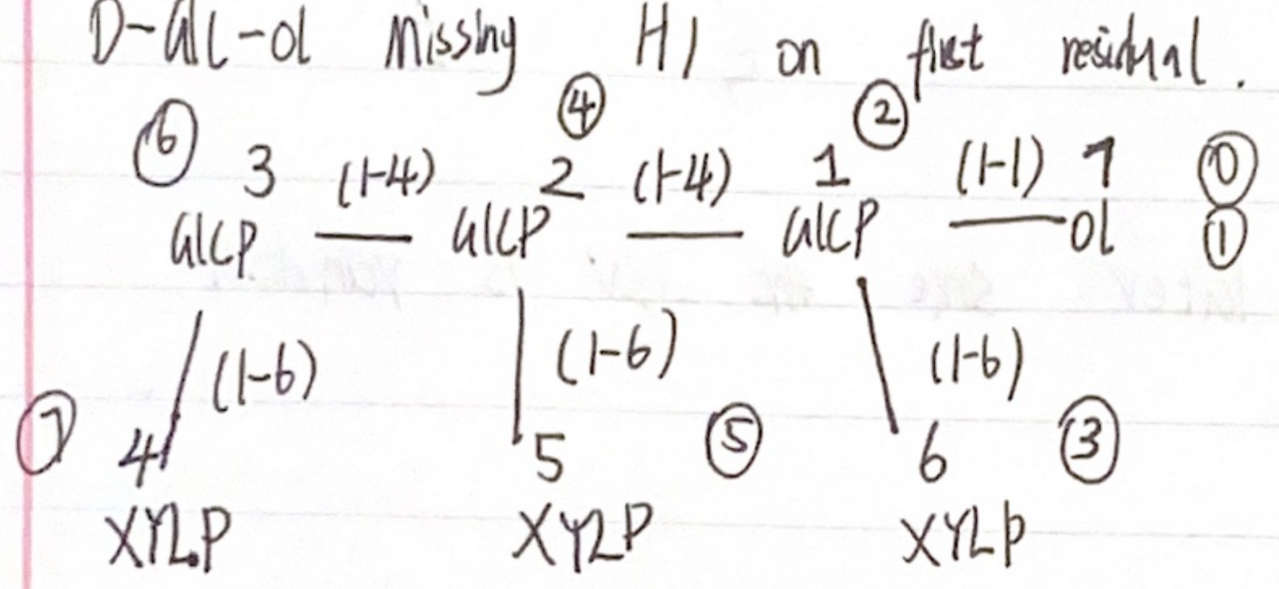
Res	pdb
1	1
2	2
3	3
4	5
5	4

50 DB26810

Rare a-L-6-deoxy-Talp. ✓

51 DB 3758

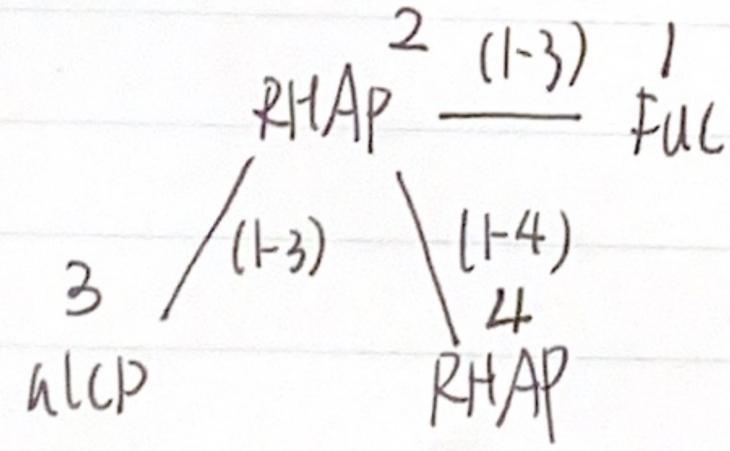
D-GlcNAc-ol Missing H1 on first residual.



Res	pdb
0	qqq
1	qqq
2	1
3	6
4	2
5	5
6	3
7	4

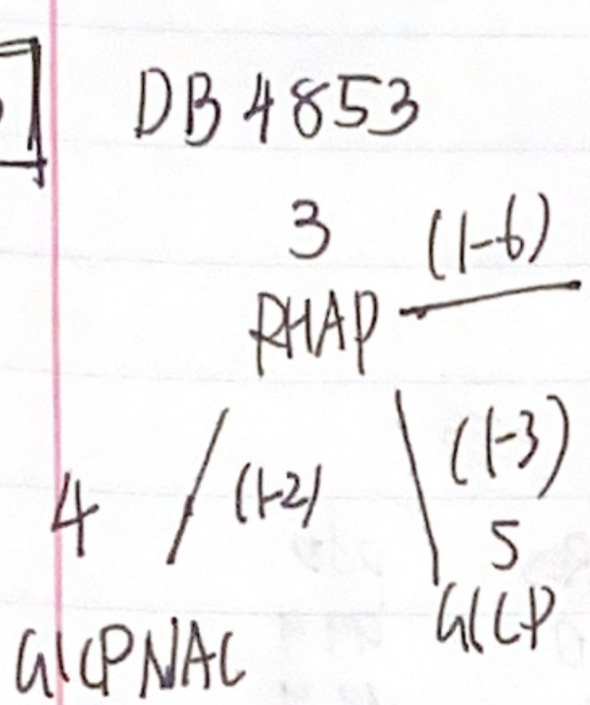
Assigned by connections in .csv

52 DB 4717



Res	pdb
1	1
2	2
3	4
4	3

53 DB4853



Res	pdb
1	3
2	5
3	4
4	1
5	2

? We may exclude this later. since the .csv is random and contain 2 Glcp.