Untitled

url <- "https://github.com/dataprofessor/data/raw/master/acetylcholinesterase\_06\_bioactivity\_data\_3class\_pIC50\_pubchem\_fp.csv"  
download.file(url, destfile = "acetylcholinesterase\_06\_bioactivity\_data\_3class\_pIC50\_pubchem\_fp.csv")

df\_Ach <- read.csv("acetylcholinesterase\_06\_bioactivity\_data\_3class\_pIC50\_pubchem\_fp.csv")  
  
head(df\_Ach)

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## PubchemFP511 PubchemFP512 PubchemFP513 PubchemFP514 PubchemFP515 PubchemFP516  
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## 2 0 0 0 0 1 1  
## 3 0 0 0 0 1 1  
## 4 0 0 0 0 1 1  
## 5 0 0 0 0 1 1  
## 6 0 0 0 0 1 1  
## PubchemFP517 PubchemFP518 PubchemFP519 PubchemFP520 PubchemFP521 PubchemFP522  
## 1 1 1 1 1 0 0  
## 2 0 1 0 1 0 0  
## 3 1 1 1 1 0 0  
## 4 1 1 1 1 0 0  
## 5 1 1 1 1 0 0  
## 6 1 1 1 1 0 0  
## PubchemFP523 PubchemFP524 PubchemFP525 PubchemFP526 PubchemFP527 PubchemFP528  
## 1 1 1 0 0 0 0  
## 2 1 1 0 0 0 0  
## 3 1 1 0 0 0 0  
## 4 1 1 0 0 0 0  
## 5 1 1 0 0 0 0  
## 6 1 1 0 0 0 0  
## PubchemFP529 PubchemFP530 PubchemFP531 PubchemFP532 PubchemFP533 PubchemFP534  
## 1 0 1 0 0 0 0  
## 2 0 1 0 0 0 0  
## 3 0 1 0 0 0 0  
## 4 0 1 0 0 0 0  
## 5 0 1 0 0 0 0  
## 6 0 1 0 0 0 0  
## PubchemFP535 PubchemFP536 PubchemFP537 PubchemFP538 PubchemFP539 PubchemFP540  
## 1 0 0 0 1 0 1  
## 2 0 0 0 1 1 0  
## 3 0 0 0 1 0 1  
## 4 0 0 0 1 0 1  
## 5 0 0 0 1 0 1  
## 6 0 0 0 1 0 1  
## PubchemFP541 PubchemFP542 PubchemFP543 PubchemFP544 PubchemFP545 PubchemFP546  
## 1 0 0 0 0 1 0  
## 2 1 1 0 0 1 1  
## 3 0 0 0 0 1 0  
## 4 0 0 0 0 1 1  
## 5 1 1 0 0 1 0  
## 6 0 0 0 0 1 0  
## PubchemFP547 PubchemFP548 PubchemFP549 PubchemFP550 PubchemFP551 PubchemFP552  
## 1 0 0 1 1 0 1  
## 2 0 1 1 0 0 1  
## 3 0 0 1 1 0 1  
## 4 0 0 1 1 0 1  
## 5 0 1 1 0 0 1  
## 6 0 0 1 1 0 1  
## PubchemFP553 PubchemFP554 PubchemFP555 PubchemFP556 PubchemFP557 PubchemFP558  
## 1 0 0 1 1 0 0  
## 2 0 0 1 1 0 0  
## 3 0 0 1 1 0 0  
## 4 0 0 1 1 0 0  
## 5 0 0 1 1 0 0  
## 6 0 0 1 1 0 0  
## PubchemFP559 PubchemFP560 PubchemFP561 PubchemFP562 PubchemFP563 PubchemFP564  
## 1 0 1 0 0 0 1  
## 2 0 0 0 0 1 1  
## 3 0 1 0 0 0 1  
## 4 0 1 0 0 0 1  
## 5 0 1 0 0 0 1  
## 6 0 1 0 0 0 1  
## PubchemFP565 PubchemFP566 PubchemFP567 PubchemFP568 PubchemFP569 PubchemFP570  
## 1 0 0 0 0 0 1  
## 2 1 0 0 0 0 1  
## 3 0 0 0 0 0 1  
## 4 0 0 0 0 0 1  
## 5 1 0 0 0 0 1  
## 6 0 0 0 0 0 1  
## PubchemFP571 PubchemFP572 PubchemFP573 PubchemFP574 PubchemFP575 PubchemFP576  
## 1 0 1 0 0 0 1  
## 2 0 0 1 1 0 1  
## 3 0 1 0 0 0 1  
## 4 0 1 0 0 0 1  
## 5 0 1 1 1 0 1  
## 6 0 1 0 0 0 1  
## PubchemFP577 PubchemFP578 PubchemFP579 PubchemFP580 PubchemFP581 PubchemFP582  
## 1 0 1 0 0 0 1  
## 2 0 1 0 0 0 1  
## 3 0 1 0 0 0 1  
## 4 0 1 0 0 0 1  
## 5 0 1 0 0 0 1  
## 6 0 1 0 0 0 1  
## PubchemFP583 PubchemFP584 PubchemFP585 PubchemFP586 PubchemFP587 PubchemFP588  
## 1 0 1 1 1 0 0  
## 2 0 1 1 0 0 0  
## 3 0 1 1 0 0 0  
## 4 0 1 1 0 0 0  
## 5 0 1 1 0 0 0  
## 6 0 1 1 0 0 0  
## PubchemFP589 PubchemFP590 PubchemFP591 PubchemFP592 PubchemFP593 PubchemFP594  
## 1 0 0 1 1 0 0  
## 2 1 0 0 1 0 1  
## 3 0 0 1 1 0 0  
## 4 0 0 1 1 0 0  
## 5 1 0 0 1 0 1  
## 6 0 0 1 1 0 0  
## PubchemFP595 PubchemFP596 PubchemFP597 PubchemFP598 PubchemFP599 PubchemFP600  
## 1 1 1 0 1 1 1  
## 2 1 0 0 0 1 1  
## 3 1 1 0 1 1 1  
## 4 1 1 0 1 1 1  
## 5 1 1 0 0 1 1  
## 6 1 1 0 1 1 1  
## PubchemFP601 PubchemFP602 PubchemFP603 PubchemFP604 PubchemFP605 PubchemFP606  
## 1 0 0 1 0 0 0  
## 2 0 0 1 1 0 1  
## 3 0 0 1 0 0 0  
## 4 0 0 1 0 0 0  
## 5 0 0 1 1 0 1  
## 6 0 0 1 0 0 0  
## PubchemFP607 PubchemFP608 PubchemFP609 PubchemFP610 PubchemFP611 PubchemFP612  
## 1 1 1 0 0 0 0  
## 2 1 1 0 1 0 1  
## 3 1 1 0 0 0 0  
## 4 1 1 0 0 0 0  
## 5 1 1 0 0 0 0  
## 6 1 1 0 0 0 0  
## PubchemFP613 PubchemFP614 PubchemFP615 PubchemFP616 PubchemFP617 PubchemFP618  
## 1 1 0 0 1 0 1  
## 2 1 1 0 0 0 1  
## 3 1 0 0 1 0 1  
## 4 1 0 0 1 0 1  
## 5 1 0 0 1 0 1  
## 6 1 0 0 1 0 1  
## PubchemFP619 PubchemFP620 PubchemFP621 PubchemFP622 PubchemFP623 PubchemFP624  
## 1 0 0 0 0 0 0  
## 2 1 1 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 1 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP625 PubchemFP626 PubchemFP627 PubchemFP628 PubchemFP629 PubchemFP630  
## 1 0 0 0 1 0 0  
## 2 0 1 0 1 0 0  
## 3 0 0 0 1 0 0  
## 4 0 0 0 1 0 0  
## 5 0 1 0 1 0 0  
## 6 0 0 0 1 0 0  
## PubchemFP631 PubchemFP632 PubchemFP633 PubchemFP634 PubchemFP635 PubchemFP636  
## 1 0 0 1 1 0 1  
## 2 0 1 1 1 0 0  
## 3 0 0 1 1 0 1  
## 4 0 0 1 1 0 1  
## 5 0 0 1 1 0 1  
## 6 0 0 1 1 0 1  
## PubchemFP637 PubchemFP638 PubchemFP639 PubchemFP640 PubchemFP641 PubchemFP642  
## 1 0 0 0 1 0 0  
## 2 1 1 0 1 1 0  
## 3 0 0 0 1 0 0  
## 4 0 0 0 1 0 0  
## 5 1 0 0 1 1 0  
## 6 0 0 0 1 0 0  
## PubchemFP643 PubchemFP644 PubchemFP645 PubchemFP646 PubchemFP647 PubchemFP648  
## 1 0 1 1 1 1 0  
## 2 0 1 1 0 0 0  
## 3 0 1 1 1 1 0  
## 4 0 1 1 1 1 0  
## 5 0 1 0 1 1 0  
## 6 0 1 0 1 1 0  
## PubchemFP649 PubchemFP650 PubchemFP651 PubchemFP652 PubchemFP653 PubchemFP654  
## 1 0 0 0 0 0 1  
## 2 0 0 1 1 0 0  
## 3 0 0 0 0 0 1  
## 4 0 0 0 0 0 1  
## 5 0 0 1 0 0 1  
## 6 0 0 0 0 0 1  
## PubchemFP655 PubchemFP656 PubchemFP657 PubchemFP658 PubchemFP659 PubchemFP660  
## 1 0 1 1 0 0 1  
## 2 1 0 1 0 0 1  
## 3 0 1 1 0 0 1  
## 4 0 0 1 0 0 1  
## 5 1 0 1 0 0 1  
## 6 0 0 1 0 0 1  
## PubchemFP661 PubchemFP662 PubchemFP663 PubchemFP664 PubchemFP665 PubchemFP666  
## 1 0 0 0 1 1 0  
## 2 1 0 0 1 1 1  
## 3 0 0 0 1 1 0  
## 4 0 0 0 1 1 0  
## 5 0 0 0 1 1 1  
## 6 0 0 0 1 1 0  
## PubchemFP667 PubchemFP668 PubchemFP669 PubchemFP670 PubchemFP671 PubchemFP672  
## 1 0 1 0 0 0 0  
## 2 0 1 0 0 0 0  
## 3 0 1 0 0 0 0  
## 4 0 1 0 0 0 0  
## 5 0 1 0 0 0 0  
## 6 0 1 0 0 0 0  
## PubchemFP673 PubchemFP674 PubchemFP675 PubchemFP676 PubchemFP677 PubchemFP678  
## 1 0 1 0 0 1 1  
## 2 0 0 0 0 1 1  
## 3 0 1 0 0 1 1  
## 4 0 1 0 0 1 1  
## 5 0 1 0 0 1 1  
## 6 0 1 0 0 1 1  
## PubchemFP679 PubchemFP680 PubchemFP681 PubchemFP682 PubchemFP683 PubchemFP684  
## 1 1 0 0 0 1 0  
## 2 1 1 0 0 1 0  
## 3 1 0 0 0 1 0  
## 4 1 0 0 0 1 0  
## 5 1 1 0 0 1 0  
## 6 1 0 0 0 1 0  
## PubchemFP685 PubchemFP686 PubchemFP687 PubchemFP688 PubchemFP689 PubchemFP690  
## 1 0 0 0 1 0 0  
## 2 0 0 0 1 1 0  
## 3 0 0 0 1 0 0  
## 4 0 0 0 1 0 0  
## 5 0 0 0 1 1 0  
## 6 0 0 0 1 0 0  
## PubchemFP691 PubchemFP692 PubchemFP693 PubchemFP694 PubchemFP695 PubchemFP696  
## 1 0 0 0 0 0 0  
## 2 1 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 1 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP697 PubchemFP698 PubchemFP699 PubchemFP700 PubchemFP701 PubchemFP702  
## 1 0 0 0 0 0 0  
## 2 0 1 0 0 0 1  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 1  
## 6 0 0 0 0 0 0  
## PubchemFP703 PubchemFP704 PubchemFP705 PubchemFP706 PubchemFP707 PubchemFP708  
## 1 0 0 0 0 0 1  
## 2 1 0 0 0 0 1  
## 3 0 0 0 0 0 1  
## 4 0 0 0 0 0 1  
## 5 0 0 0 0 0 1  
## 6 0 0 0 0 0 1  
## PubchemFP709 PubchemFP710 PubchemFP711 PubchemFP712 PubchemFP713 PubchemFP714  
## 1 1 1 0 0 0 0  
## 2 1 1 0 0 0 0  
## 3 1 1 0 0 0 0  
## 4 1 1 0 0 0 0  
## 5 1 1 0 0 0 1  
## 6 1 1 0 0 0 0  
## PubchemFP715 PubchemFP716 PubchemFP717 PubchemFP718 PubchemFP719 PubchemFP720  
## 1 0 0 1 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 1 0 0 0  
## 4 0 0 1 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 1 0 0 0  
## PubchemFP721 PubchemFP722 PubchemFP723 PubchemFP724 PubchemFP725 PubchemFP726  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP727 PubchemFP728 PubchemFP729 PubchemFP730 PubchemFP731 PubchemFP732  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP733 PubchemFP734 PubchemFP735 PubchemFP736 PubchemFP737 PubchemFP738  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP739 PubchemFP740 PubchemFP741 PubchemFP742 PubchemFP743 PubchemFP744  
## 1 0 0 0 0 0 0  
## 2 0 0 0 1 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP745 PubchemFP746 PubchemFP747 PubchemFP748 PubchemFP749 PubchemFP750  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP751 PubchemFP752 PubchemFP753 PubchemFP754 PubchemFP755 PubchemFP756  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP757 PubchemFP758 PubchemFP759 PubchemFP760 PubchemFP761 PubchemFP762  
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## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP763 PubchemFP764 PubchemFP765 PubchemFP766 PubchemFP767 PubchemFP768  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP769 PubchemFP770 PubchemFP771 PubchemFP772 PubchemFP773 PubchemFP774  
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## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP775 PubchemFP776 PubchemFP777 PubchemFP778 PubchemFP779 PubchemFP780  
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## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 1  
## 4 0 0 0 0 0 1  
## 5 0 0 1 0 0 0  
## 6 0 0 0 0 0 1  
## PubchemFP781 PubchemFP782 PubchemFP783 PubchemFP784 PubchemFP785 PubchemFP786  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP787 PubchemFP788 PubchemFP789 PubchemFP790 PubchemFP791 PubchemFP792  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP793 PubchemFP794 PubchemFP795 PubchemFP796 PubchemFP797 PubchemFP798  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP799 PubchemFP800 PubchemFP801 PubchemFP802 PubchemFP803 PubchemFP804  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP805 PubchemFP806 PubchemFP807 PubchemFP808 PubchemFP809 PubchemFP810  
## 1 0 0 0 0 0 0  
## 2 1 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP811 PubchemFP812 PubchemFP813 PubchemFP814 PubchemFP815 PubchemFP816  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP817 PubchemFP818 PubchemFP819 PubchemFP820 PubchemFP821 PubchemFP822  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP823 PubchemFP824 PubchemFP825 PubchemFP826 PubchemFP827 PubchemFP828  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP829 PubchemFP830 PubchemFP831 PubchemFP832 PubchemFP833 PubchemFP834  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP835 PubchemFP836 PubchemFP837 PubchemFP838 PubchemFP839 PubchemFP840  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP841 PubchemFP842 PubchemFP843 PubchemFP844 PubchemFP845 PubchemFP846  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP847 PubchemFP848 PubchemFP849 PubchemFP850 PubchemFP851 PubchemFP852  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP853 PubchemFP854 PubchemFP855 PubchemFP856 PubchemFP857 PubchemFP858  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP859 PubchemFP860 PubchemFP861 PubchemFP862 PubchemFP863 PubchemFP864  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP865 PubchemFP866 PubchemFP867 PubchemFP868 PubchemFP869 PubchemFP870  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP871 PubchemFP872 PubchemFP873 PubchemFP874 PubchemFP875 PubchemFP876  
## 1 0 0 0 0 0 0  
## 2 0 0 0 0 0 0  
## 3 0 0 0 0 0 0  
## 4 0 0 0 0 0 0  
## 5 0 0 0 0 0 0  
## 6 0 0 0 0 0 0  
## PubchemFP877 PubchemFP878 PubchemFP879 PubchemFP880 pIC50  
## 1 0 0 0 0 6.124939  
## 2 0 0 0 0 7.000000  
## 3 0 0 0 0 4.301030  
## 4 0 0 0 0 6.522879  
## 5 0 0 0 0 6.096910  
## 6 0 0 0 0 5.619789

X <- df\_Ach[, !(names(df\_Ach) %in% c("pIC50"))]  
Y <- df\_Ach$pIC50

Data preprocessing

dim(X)

## [1] 4695 881

library(caret)

## Loading required package: ggplot2

## Loading required package: lattice

# Remove low variance features  
nzv <- nearZeroVar(X, saveMetrics = TRUE)  
X <- X[, !nzv$nzv]

dim(X)

## [1] 4695 323

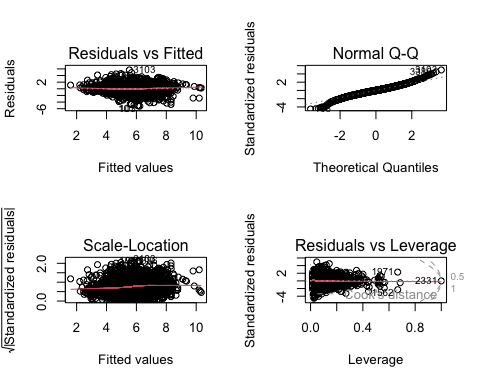
library(caret)  
  
# Set random seed for reproducibility  
set.seed(42)  
  
# Create data partitions  
trainIndex <- createDataPartition(Y, p = 0.8, list = FALSE)  
X\_train <- X[trainIndex, ]  
X\_test <- X[-trainIndex, ]  
Y\_train <- Y[trainIndex]  
Y\_test <- Y[-trainIndex]

Compare ML algorithms

# Fit a linear regression model using X\_train and Y\_train  
lm\_model <- lm(Y\_train ~ ., data = X\_train)  
  
# Create diagnostic plots  
par(mfrow = c(2,2))  
plot(lm\_model)

## Warning: not plotting observations with leverage one:  
## 13, 710, 874, 875, 1099, 1238, 1260, 2099, 2361

## Warning in sqrt(crit \* p \* (1 - hh)/hh): NaNs produced  
  
## Warning in sqrt(crit \* p \* (1 - hh)/hh): NaNs produced



summary(lm\_model)

##   
## Call:  
## lm(formula = Y\_train ~ ., data = X\_train)  
##   
## Residuals:  
## Min 1Q Median 3Q Max   
## -5.2302 -0.6611 -0.0075 0.6538 5.6896   
##   
## Coefficients: (20 not defined because of singularities)  
## Estimate Std. Error t value Pr(>|t|)   
## (Intercept) 4.670753 0.255815 18.258 < 2e-16 \*\*\*  
## PubchemFP2 0.121498 0.095428 1.273 0.203038   
## PubchemFP3 0.159420 0.071234 2.238 0.025286 \*   
## PubchemFP12 -0.049918 0.099271 -0.503 0.615102   
## PubchemFP13 0.246140 0.099927 2.463 0.013819 \*   
## PubchemFP15 0.049728 0.097863 0.508 0.611388   
## PubchemFP16 0.253055 0.095313 2.655 0.007968 \*\*   
## PubchemFP18 0.174132 0.209579 0.831 0.406107   
## PubchemFP19 -0.059879 0.092733 -0.646 0.518505   
## PubchemFP20 -0.013046 0.084551 -0.154 0.877380   
## PubchemFP23 2.959695 1.214741 2.436 0.014881 \*   
## PubchemFP33 3.341833 0.480487 6.955 4.20e-12 \*\*\*  
## PubchemFP37 -0.388028 1.253381 -0.310 0.756895   
## PubchemFP143 0.068677 0.164820 0.417 0.676938   
## PubchemFP144 -0.200206 0.208018 -0.962 0.335894   
## PubchemFP145 0.002344 0.151072 0.016 0.987623   
## PubchemFP146 0.136105 0.197174 0.690 0.490064   
## PubchemFP150 0.198121 0.187052 1.059 0.289593   
## PubchemFP152 0.314081 0.204297 1.537 0.124293   
## PubchemFP153 -0.376376 0.222837 -1.689 0.091307 .   
## PubchemFP179 0.223989 0.192691 1.162 0.245142   
## PubchemFP180 0.163789 0.180486 0.907 0.364214   
## PubchemFP181 0.280311 0.195984 1.430 0.152728   
## PubchemFP182 0.636783 0.179441 3.549 0.000392 \*\*\*  
## PubchemFP184 -0.150574 0.204006 -0.738 0.460512   
## PubchemFP185 -0.165186 0.144454 -1.144 0.252900   
## PubchemFP186 0.333960 0.129062 2.588 0.009705 \*\*   
## PubchemFP187 -0.288205 0.182601 -1.578 0.114580   
## PubchemFP188 0.421623 0.189910 2.220 0.026475 \*   
## PubchemFP192 -0.099840 0.118308 -0.844 0.398785   
## PubchemFP193 0.010541 0.124721 0.085 0.932651   
## PubchemFP199 0.111576 0.110318 1.011 0.311894   
## PubchemFP200 -0.091035 0.137433 -0.662 0.507763   
## PubchemFP206 -0.179393 0.134492 -1.334 0.182337   
## PubchemFP256 0.081276 0.175336 0.464 0.643004   
## PubchemFP257 0.065790 0.125195 0.526 0.599268   
## PubchemFP258 0.414180 0.126691 3.269 0.001089 \*\*   
## PubchemFP259 -0.182393 0.098768 -1.847 0.064879 .   
## PubchemFP261 -0.185756 0.108197 -1.717 0.086100 .   
## PubchemFP286 0.029782 0.333834 0.089 0.928919   
## PubchemFP287 -3.076286 1.221934 -2.518 0.011862 \*   
## PubchemFP293 -3.242898 0.536868 -6.040 1.70e-09 \*\*\*  
## PubchemFP294 NA NA NA NA   
## PubchemFP299 -1.819914 0.912152 -1.995 0.046101 \*   
## PubchemFP300 -0.102316 0.510208 -0.201 0.841072   
## PubchemFP301 0.559154 1.220552 0.458 0.646898   
## PubchemFP308 -1.117482 0.302357 -3.696 0.000223 \*\*\*  
## PubchemFP333 -0.194007 0.309884 -0.626 0.531315   
## PubchemFP334 0.205300 0.436152 0.471 0.637879   
## PubchemFP335 0.181480 0.075132 2.415 0.015766 \*   
## PubchemFP338 -0.447514 0.116188 -3.852 0.000119 \*\*\*  
## PubchemFP339 -0.310215 0.157957 -1.964 0.049619 \*   
## PubchemFP340 0.174742 0.142604 1.225 0.220522   
## PubchemFP341 -0.053781 0.125347 -0.429 0.667907   
## PubchemFP342 1.299064 1.526396 0.851 0.394791   
## PubchemFP345 0.419607 0.176282 2.380 0.017351 \*   
## PubchemFP346 -0.122604 0.127124 -0.964 0.334890   
## PubchemFP349 0.303154 0.485596 0.624 0.532476   
## PubchemFP351 0.585111 0.398096 1.470 0.141714   
## PubchemFP352 -0.527483 0.275396 -1.915 0.055529 .   
## PubchemFP353 0.081130 0.315677 0.257 0.797192   
## PubchemFP355 -1.490754 1.070027 -1.393 0.163651   
## PubchemFP356 0.091415 0.360183 0.254 0.799663   
## PubchemFP357 0.818116 0.428269 1.910 0.056179 .   
## PubchemFP358 0.786302 0.648563 1.212 0.225452   
## PubchemFP359 0.430625 0.314571 1.369 0.171111   
## PubchemFP362 -1.092366 0.935960 -1.167 0.243248   
## PubchemFP364 0.329761 0.182878 1.803 0.071448 .   
## PubchemFP365 0.345918 0.382590 0.904 0.365981   
## PubchemFP366 0.176715 0.125264 1.411 0.158411   
## PubchemFP368 -0.559075 0.465852 -1.200 0.230178   
## PubchemFP370 0.930356 0.389298 2.390 0.016909 \*   
## PubchemFP371 -0.309557 0.502116 -0.617 0.537602   
## PubchemFP372 0.854166 1.525529 0.560 0.575574   
## PubchemFP373 0.563513 1.506153 0.374 0.708323   
## PubchemFP374 -0.016295 0.069117 -0.236 0.813637   
## PubchemFP375 -0.238504 1.047861 -0.228 0.819963   
## PubchemFP376 0.360494 0.464425 0.776 0.437675   
## PubchemFP377 0.049063 0.228136 0.215 0.829733   
## PubchemFP378 -0.173939 0.393896 -0.442 0.658817   
## PubchemFP379 -1.955396 1.138498 -1.718 0.085973 .   
## PubchemFP380 -0.570698 0.199487 -2.861 0.004251 \*\*   
## PubchemFP381 0.484369 0.354562 1.366 0.171995   
## PubchemFP382 -0.264645 0.242701 -1.090 0.275606   
## PubchemFP384 1.427743 1.685935 0.847 0.397134   
## PubchemFP385 -0.240344 0.107014 -2.246 0.024773 \*   
## PubchemFP386 -0.325277 0.238294 -1.365 0.172334   
## PubchemFP387 -0.460165 0.818858 -0.562 0.574180   
## PubchemFP389 0.521980 1.261451 0.414 0.679051   
## PubchemFP390 -0.943621 0.372168 -2.535 0.011273 \*   
## PubchemFP391 0.149895 0.093535 1.603 0.109127   
## PubchemFP392 0.418969 0.157827 2.655 0.007976 \*\*   
## PubchemFP393 1.576579 0.920852 1.712 0.086970 .   
## PubchemFP395 -1.036483 1.245265 -0.832 0.405275   
## PubchemFP396 -0.901427 0.378357 -2.382 0.017250 \*   
## PubchemFP397 0.078162 0.148253 0.527 0.598075   
## PubchemFP399 0.173007 0.736010 0.235 0.814176   
## PubchemFP400 -0.216907 0.448329 -0.484 0.628550   
## PubchemFP403 -0.232903 0.688753 -0.338 0.735270   
## PubchemFP405 -0.179629 0.180974 -0.993 0.320992   
## PubchemFP406 1.431479 0.406738 3.519 0.000438 \*\*\*  
## PubchemFP409 -0.501587 0.168155 -2.983 0.002875 \*\*   
## PubchemFP412 1.658366 0.522238 3.176 0.001509 \*\*   
## PubchemFP418 -1.454947 0.579553 -2.510 0.012103 \*   
## PubchemFP420 -0.200847 0.232950 -0.862 0.388644   
## PubchemFP423 -0.225085 1.280403 -0.176 0.860467   
## PubchemFP430 0.380542 0.320858 1.186 0.235699   
## PubchemFP431 -0.605275 0.385517 -1.570 0.116499   
## PubchemFP432 0.029156 0.150645 0.194 0.846545   
## PubchemFP434 -0.036326 0.358445 -0.101 0.919283   
## PubchemFP435 -2.323788 1.315965 -1.766 0.077511 .   
## PubchemFP437 -0.205124 0.284043 -0.722 0.470246   
## PubchemFP438 0.890932 0.373331 2.386 0.017066 \*   
## PubchemFP439 -0.213335 0.234998 -0.908 0.364039   
## PubchemFP440 0.171131 0.247704 0.691 0.489696   
## PubchemFP442 1.756770 0.632855 2.776 0.005534 \*\*   
## PubchemFP443 0.495771 0.252340 1.965 0.049530 \*   
## PubchemFP445 -0.627487 0.355727 -1.764 0.077827 .   
## PubchemFP447 1.450216 1.288697 1.125 0.260525   
## PubchemFP449 0.840789 0.356990 2.355 0.018567 \*   
## PubchemFP450 -0.019495 1.185062 -0.016 0.986875   
## PubchemFP451 0.433689 0.253738 1.709 0.087504 .   
## PubchemFP452 0.276432 0.305143 0.906 0.365048   
## PubchemFP453 1.099478 0.357374 3.077 0.002111 \*\*   
## PubchemFP454 1.107821 1.311085 0.845 0.398189   
## PubchemFP464 0.190471 0.299377 0.636 0.524672   
## PubchemFP470 6.941836 2.706832 2.565 0.010373 \*   
## PubchemFP472 -0.987535 0.835201 -1.182 0.237132   
## PubchemFP476 -1.181826 0.788789 -1.498 0.134152   
## PubchemFP482 1.110148 0.697738 1.591 0.111686   
## PubchemFP484 1.594195 1.004308 1.587 0.112523   
## PubchemFP485 0.817400 0.426686 1.916 0.055486 .   
## PubchemFP487 -0.154641 0.819656 -0.189 0.850366   
## PubchemFP491 0.210451 0.399767 0.526 0.598619   
## PubchemFP493 -0.629475 0.949708 -0.663 0.507498   
## PubchemFP495 -1.022975 1.047636 -0.976 0.328905   
## PubchemFP498 1.598118 0.502425 3.181 0.001482 \*\*   
## PubchemFP499 -2.184125 0.602811 -3.623 0.000295 \*\*\*  
## PubchemFP501 1.087522 1.022744 1.063 0.287703   
## PubchemFP502 -0.366322 0.361686 -1.013 0.311218   
## PubchemFP503 0.342696 0.393351 0.871 0.383694   
## PubchemFP504 -1.419284 1.234193 -1.150 0.250236   
## PubchemFP506 NA NA NA NA   
## PubchemFP507 -1.718201 0.535563 -3.208 0.001348 \*\*   
## PubchemFP514 -0.149413 0.345772 -0.432 0.665686   
## PubchemFP515 -0.313472 0.526051 -0.596 0.551283   
## PubchemFP516 0.045270 0.152568 0.297 0.766698   
## PubchemFP519 -0.479503 0.918422 -0.522 0.601638   
## PubchemFP520 NA NA NA NA   
## PubchemFP521 -0.365289 0.185249 -1.972 0.048703 \*   
## PubchemFP523 0.637262 1.163397 0.548 0.583892   
## PubchemFP527 -0.018045 0.667847 -0.027 0.978445   
## PubchemFP528 -0.396755 0.108862 -3.645 0.000272 \*\*\*  
## PubchemFP530 -0.348631 1.011888 -0.345 0.730465   
## PubchemFP535 0.216907 0.225195 0.963 0.335516   
## PubchemFP536 0.161606 0.517037 0.313 0.754632   
## PubchemFP538 -0.423971 0.353253 -1.200 0.230148   
## PubchemFP539 0.057016 0.208702 0.273 0.784721   
## PubchemFP540 -0.399324 0.345519 -1.156 0.247874   
## PubchemFP541 -1.491139 1.012811 -1.472 0.141037   
## PubchemFP542 0.421167 0.181306 2.323 0.020239 \*   
## PubchemFP544 2.894059 1.441161 2.008 0.044706 \*   
## PubchemFP545 -2.290849 0.660832 -3.467 0.000533 \*\*\*  
## PubchemFP546 0.444912 0.392286 1.134 0.256809   
## PubchemFP547 1.528852 0.501583 3.048 0.002321 \*\*   
## PubchemFP548 0.251627 1.030783 0.244 0.807158   
## PubchemFP549 -0.359910 0.730578 -0.493 0.622300   
## PubchemFP550 -1.173550 1.025860 -1.144 0.252716   
## PubchemFP552 NA NA NA NA   
## PubchemFP553 -0.426166 0.722800 -0.590 0.555495   
## PubchemFP555 -0.695190 0.422865 -1.644 0.100267   
## PubchemFP559 0.921408 0.163945 5.620 2.06e-08 \*\*\*  
## PubchemFP560 2.836204 1.600079 1.773 0.076393 .   
## PubchemFP564 -2.866290 2.521186 -1.137 0.255667   
## PubchemFP565 1.622016 0.901756 1.799 0.072149 .   
## PubchemFP566 -0.698381 0.567486 -1.231 0.218534   
## PubchemFP567 0.010772 0.702977 0.015 0.987775   
## PubchemFP569 -1.437641 1.325342 -1.085 0.278116   
## PubchemFP570 -3.905121 2.058726 -1.897 0.057929 .   
## PubchemFP572 NA NA NA NA   
## PubchemFP573 -0.581837 0.847169 -0.687 0.492254   
## PubchemFP574 0.573392 1.096944 0.523 0.601204   
## PubchemFP575 -1.103506 0.400001 -2.759 0.005833 \*\*   
## PubchemFP576 0.305979 0.205585 1.488 0.136755   
## PubchemFP577 -0.264831 0.201515 -1.314 0.188866   
## PubchemFP578 0.468157 1.605170 0.292 0.770567   
## PubchemFP579 -0.451600 0.295050 -1.531 0.125963   
## PubchemFP580 -0.594477 0.155620 -3.820 0.000136 \*\*\*  
## PubchemFP581 0.181417 0.237568 0.764 0.445134   
## PubchemFP584 NA NA NA NA   
## PubchemFP585 1.366448 1.057057 1.293 0.196205   
## PubchemFP586 0.685555 0.291854 2.349 0.018882 \*   
## PubchemFP588 0.006833 0.160361 0.043 0.966013   
## PubchemFP589 NA NA NA NA   
## PubchemFP590 -0.738753 0.247752 -2.982 0.002885 \*\*   
## PubchemFP591 NA NA NA NA   
## PubchemFP592 -0.105460 0.349826 -0.301 0.763078   
## PubchemFP593 -0.723266 0.106945 -6.763 1.58e-11 \*\*\*  
## PubchemFP594 0.288212 0.405546 0.711 0.477333   
## PubchemFP595 NA NA NA NA   
## PubchemFP596 0.810089 0.375323 2.158 0.030967 \*   
## PubchemFP597 -0.636204 0.195844 -3.249 0.001171 \*\*   
## PubchemFP598 NA NA NA NA   
## PubchemFP599 -0.516422 0.222253 -2.324 0.020206 \*   
## PubchemFP600 -5.527824 1.904964 -2.902 0.003734 \*\*   
## PubchemFP601 0.612278 0.364388 1.680 0.092990 .   
## PubchemFP602 0.029081 0.522246 0.056 0.955596   
## PubchemFP603 NA NA NA NA   
## PubchemFP604 -1.050864 0.501367 -2.096 0.036155 \*   
## PubchemFP606 -0.680168 0.722593 -0.941 0.346623   
## PubchemFP607 0.048947 0.206012 0.238 0.812212   
## PubchemFP608 NA NA NA NA   
## PubchemFP611 0.906940 1.323767 0.685 0.493314   
## PubchemFP612 0.069849 0.173630 0.402 0.687500   
## PubchemFP613 -0.451712 0.236783 -1.908 0.056512 .   
## PubchemFP614 0.105449 0.158328 0.666 0.505444   
## PubchemFP615 -0.174708 0.199194 -0.877 0.380506   
## PubchemFP617 -0.209238 0.297883 -0.702 0.482467   
## PubchemFP618 -0.339097 0.416022 -0.815 0.415074   
## PubchemFP619 -0.047855 0.816700 -0.059 0.953277   
## PubchemFP620 0.706431 0.684871 1.031 0.302388   
## PubchemFP621 0.606647 0.375880 1.614 0.106632   
## PubchemFP622 0.240503 0.203854 1.180 0.238169   
## PubchemFP623 1.598493 0.965688 1.655 0.097957 .   
## PubchemFP624 0.925960 0.299242 3.094 0.001988 \*\*   
## PubchemFP625 -0.350705 0.278768 -1.258 0.208456   
## PubchemFP626 NA NA NA NA   
## PubchemFP628 0.222874 0.237822 0.937 0.348749   
## PubchemFP630 0.083059 0.731641 0.114 0.909622   
## PubchemFP632 -0.909192 0.692289 -1.313 0.189165   
## PubchemFP633 0.079723 0.606480 0.131 0.895425   
## PubchemFP634 -3.015411 2.487307 -1.212 0.225473   
## PubchemFP636 -0.096025 0.353400 -0.272 0.785856   
## PubchemFP637 0.596432 0.318849 1.871 0.061488 .   
## PubchemFP638 0.019579 0.093478 0.209 0.834109   
## PubchemFP639 0.598618 0.244360 2.450 0.014345 \*   
## PubchemFP641 -0.164737 0.314420 -0.524 0.600354   
## PubchemFP642 NA NA NA NA   
## PubchemFP643 0.301944 0.118673 2.544 0.010991 \*   
## PubchemFP645 -0.543999 0.120641 -4.509 6.72e-06 \*\*\*  
## PubchemFP646 0.582966 0.117813 4.948 7.85e-07 \*\*\*  
## PubchemFP651 NA NA NA NA   
## PubchemFP652 0.281865 0.165822 1.700 0.089258 .   
## PubchemFP653 0.998466 0.624416 1.599 0.109903   
## PubchemFP654 -2.013838 1.217460 -1.654 0.098192 .   
## PubchemFP655 0.061785 0.499173 0.124 0.901501   
## PubchemFP656 -0.000184 0.121516 -0.002 0.998792   
## PubchemFP657 NA NA NA NA   
## PubchemFP658 -0.267526 0.268100 -0.998 0.318418   
## PubchemFP659 0.653859 0.545663 1.198 0.230889   
## PubchemFP662 -0.293776 0.702218 -0.418 0.675714   
## PubchemFP664 2.463728 2.475727 0.995 0.319731   
## PubchemFP665 6.410387 1.917390 3.343 0.000837 \*\*\*  
## PubchemFP666 NA NA NA NA   
## PubchemFP667 0.140671 0.246695 0.570 0.568564   
## PubchemFP668 NA NA NA NA   
## PubchemFP671 -0.466870 0.705190 -0.662 0.507984   
## PubchemFP672 0.476801 0.170380 2.798 0.005163 \*\*   
## PubchemFP673 -0.268636 0.243273 -1.104 0.269558   
## PubchemFP674 -0.915269 0.258672 -3.538 0.000408 \*\*\*  
## PubchemFP677 NA NA NA NA   
## PubchemFP680 -0.166049 0.358493 -0.463 0.643260   
## PubchemFP681 0.106406 0.134330 0.792 0.428341   
## PubchemFP682 -0.209510 0.089948 -2.329 0.019905 \*   
## PubchemFP683 0.170897 0.297704 0.574 0.565972   
## PubchemFP684 -0.133421 0.306505 -0.435 0.663373   
## PubchemFP685 0.105830 0.121655 0.870 0.384403   
## PubchemFP686 0.135438 0.116395 1.164 0.244666   
## PubchemFP687 -0.051782 0.146687 -0.353 0.724104   
## PubchemFP688 0.583259 0.208416 2.799 0.005162 \*\*   
## PubchemFP689 0.031685 0.261092 0.121 0.903416   
## PubchemFP690 -0.062546 0.475760 -0.131 0.895415   
## PubchemFP691 -0.580947 0.216182 -2.687 0.007238 \*\*   
## PubchemFP692 0.065282 0.306059 0.213 0.831108   
## PubchemFP693 -0.383807 0.286367 -1.340 0.180247   
## PubchemFP694 -0.388526 0.258605 -1.502 0.133087   
## PubchemFP695 0.608759 0.121561 5.008 5.78e-07 \*\*\*  
## PubchemFP696 0.174608 0.101007 1.729 0.083956 .   
## PubchemFP697 0.277462 0.084799 3.272 0.001078 \*\*   
## PubchemFP698 -0.156755 0.114905 -1.364 0.172592   
## PubchemFP699 0.008339 0.129179 0.065 0.948532   
## PubchemFP700 0.021995 0.266619 0.082 0.934256   
## PubchemFP701 -0.233476 0.428061 -0.545 0.585495   
## PubchemFP702 0.367406 0.206210 1.782 0.074885 .   
## PubchemFP703 0.314279 0.123191 2.551 0.010780 \*   
## PubchemFP704 0.425524 0.215493 1.975 0.048387 \*   
## PubchemFP705 0.568292 0.301632 1.884 0.059641 .   
## PubchemFP706 0.158500 0.295715 0.536 0.592000   
## PubchemFP707 -0.461773 0.150285 -3.073 0.002138 \*\*   
## PubchemFP708 0.423502 0.401344 1.055 0.291403   
## PubchemFP709 -0.581820 0.309495 -1.880 0.060205 .   
## PubchemFP710 -0.303359 0.294119 -1.031 0.302419   
## PubchemFP711 -0.178413 0.451193 -0.395 0.692553   
## PubchemFP712 -0.101037 0.095517 -1.058 0.290223   
## PubchemFP713 0.343928 0.216070 1.592 0.111534   
## PubchemFP714 0.200085 0.346124 0.578 0.563253   
## PubchemFP716 -0.079360 0.234638 -0.338 0.735216   
## PubchemFP717 0.546960 1.075744 0.508 0.611171   
## PubchemFP721 -0.083430 0.663873 -0.126 0.900000   
## PubchemFP734 0.099444 0.208999 0.476 0.634240   
## PubchemFP735 0.290258 0.368822 0.787 0.431345   
## PubchemFP737 0.055742 0.211156 0.264 0.791809   
## PubchemFP740 -0.963252 0.674720 -1.428 0.153488   
## PubchemFP750 0.575152 0.151895 3.787 0.000155 \*\*\*  
## PubchemFP755 -0.037529 0.207785 -0.181 0.856680   
## PubchemFP756 -0.281209 0.368836 -0.762 0.445860   
## PubchemFP758 -0.020013 0.204306 -0.098 0.921972   
## PubchemFP761 -2.155333 1.352680 -1.593 0.111166   
## PubchemFP776 -0.375825 0.212318 -1.770 0.076798 .   
## PubchemFP777 -0.272159 0.330904 -0.822 0.410866   
## PubchemFP779 -0.009888 0.215566 -0.046 0.963415   
## PubchemFP780 -0.697827 1.065409 -0.655 0.512521   
## PubchemFP784 -0.169723 0.657199 -0.258 0.796227   
## PubchemFP797 -0.189588 0.200143 -0.947 0.343570   
## PubchemFP798 -0.120098 0.361476 -0.332 0.739725   
## PubchemFP800 0.251953 0.187753 1.342 0.179703   
## PubchemFP803 0.886323 0.426986 2.076 0.037989 \*   
## PubchemFP813 NA NA NA NA   
## PubchemFP818 0.072766 0.224719 0.324 0.746102   
## PubchemFP819 0.251399 0.360478 0.697 0.485596   
## PubchemFP821 0.115846 0.181438 0.638 0.523197   
## PubchemFP824 -0.584844 0.576846 -1.014 0.310719   
## PubchemFP839 -0.309139 0.169557 -1.823 0.068357 .   
## PubchemFP860 0.314372 0.218499 1.439 0.150303   
## ---  
## Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1  
##   
## Residual standard error: 1.175 on 3454 degrees of freedom  
## Multiple R-squared: 0.4766, Adjusted R-squared: 0.4307   
## F-statistic: 10.38 on 303 and 3454 DF, p-value: < 2.2e-16

# Load the necessary library  
library(tidyverse)

## ── Attaching core tidyverse packages ──────────────────────── tidyverse 2.0.0 ──  
## ✔ dplyr 1.1.1 ✔ readr 2.1.4  
## ✔ forcats 1.0.0 ✔ stringr 1.5.0  
## ✔ lubridate 1.9.2 ✔ tibble 3.2.1  
## ✔ purrr 1.0.1 ✔ tidyr 1.3.0  
## ── Conflicts ────────────────────────────────────────── tidyverse\_conflicts() ──  
## ✖ dplyr::filter() masks stats::filter()  
## ✖ dplyr::lag() masks stats::lag()  
## ✖ purrr::lift() masks caret::lift()  
## ℹ Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become errors

predictions1 <- predict(lm\_model, X\_test)

## Warning in predict.lm(lm\_model, X\_test): prediction from a rank-deficient fit  
## may be misleading

# Calculate R-squared  
SSE <- sum((Y\_train - predictions1)^2)

## Warning in Y\_train - predictions1: longer object length is not a multiple of  
## shorter object length

SST <- sum((Y\_train - mean(Y\_train))^2)  
R2 <- 1 - SSE/SST  
  
# Print the result  
print(paste0("R-squared: ", round(R2, 2)))

## [1] "R-squared: -0.47"

library (pls)

##   
## Attaching package: 'pls'

## The following object is masked from 'package:caret':  
##   
## R2

## The following object is masked from 'package:stats':  
##   
## loadings

set.seed(2)  
pcr.fit=pcr(Y\_train~., data=X\_train , scale=TRUE ,  
validation ="CV")

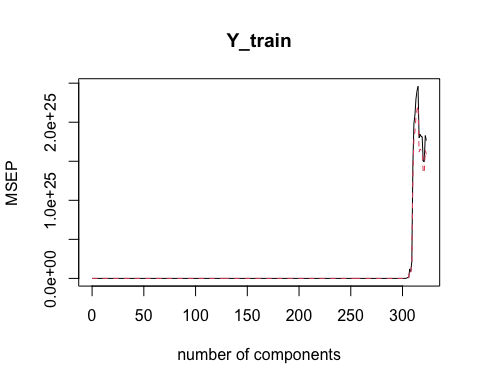
pcr.pred=predict (pcr.fit ,X\_test,ncomp =7)  
mean((pcr.pred -Y\_test)^2)

## [1] 2.056211

summary (pcr.fit)

## Data: X dimension: 3758 323   
## Y dimension: 3758 1  
## Fit method: svdpc  
## Number of components considered: 323  
##   
## VALIDATION: RMSEP  
## Cross-validated using 10 random segments.  
## (Intercept) 1 comps 2 comps 3 comps 4 comps 5 comps 6 comps  
## CV 1.557 1.554 1.513 1.482 1.472 1.469 1.464  
## adjCV 1.557 1.554 1.513 1.482 1.471 1.469 1.464  
## 7 comps 8 comps 9 comps 10 comps 11 comps 12 comps 13 comps  
## CV 1.464 1.465 1.464 1.464 1.457 1.452 1.448  
## adjCV 1.464 1.465 1.464 1.464 1.456 1.451 1.448  
## 14 comps 15 comps 16 comps 17 comps 18 comps 19 comps 20 comps  
## CV 1.444 1.444 1.443 1.444 1.425 1.418 1.417  
## adjCV 1.444 1.444 1.443 1.444 1.425 1.417 1.417  
## 21 comps 22 comps 23 comps 24 comps 25 comps 26 comps 27 comps  
## CV 1.411 1.411 1.411 1.406 1.407 1.405 1.404  
## adjCV 1.410 1.410 1.411 1.406 1.406 1.404 1.403  
## 28 comps 29 comps 30 comps 31 comps 32 comps 33 comps 34 comps  
## CV 1.404 1.404 1.404 1.402 1.395 1.395 1.378  
## adjCV 1.404 1.404 1.404 1.400 1.395 1.394 1.377  
## 35 comps 36 comps 37 comps 38 comps 39 comps 40 comps 41 comps  
## CV 1.377 1.376 1.376 1.376 1.376 1.375 1.372  
## adjCV 1.376 1.375 1.375 1.376 1.376 1.374 1.371  
## 42 comps 43 comps 44 comps 45 comps 46 comps 47 comps 48 comps  
## CV 1.368 1.367 1.364 1.364 1.357 1.355 1.354  
## adjCV 1.367 1.366 1.363 1.363 1.355 1.352 1.352  
## 49 comps 50 comps 51 comps 52 comps 53 comps 54 comps 55 comps  
## CV 1.354 1.354 1.354 1.355 1.354 1.355 1.355  
## adjCV 1.353 1.353 1.353 1.354 1.353 1.354 1.354  
## 56 comps 57 comps 58 comps 59 comps 60 comps 61 comps 62 comps  
## CV 1.351 1.349 1.348 1.348 1.347 1.346 1.343  
## adjCV 1.349 1.347 1.348 1.347 1.346 1.346 1.342  
## 63 comps 64 comps 65 comps 66 comps 67 comps 68 comps 69 comps  
## CV 1.338 1.335 1.335 1.330 1.330 1.329 1.329  
## adjCV 1.336 1.334 1.334 1.328 1.328 1.327 1.328  
## 70 comps 71 comps 72 comps 73 comps 74 comps 75 comps 76 comps  
## CV 1.328 1.328 1.328 1.323 1.323 1.321 1.321  
## adjCV 1.328 1.327 1.327 1.321 1.321 1.321 1.319  
## 77 comps 78 comps 79 comps 80 comps 81 comps 82 comps 83 comps  
## CV 1.320 1.320 1.319 1.319 1.315 1.315 1.310  
## adjCV 1.318 1.318 1.318 1.318 1.315 1.314 1.308  
## 84 comps 85 comps 86 comps 87 comps 88 comps 89 comps 90 comps  
## CV 1.308 1.305 1.305 1.305 1.304 1.305 1.305  
## adjCV 1.307 1.303 1.303 1.303 1.303 1.303 1.303  
## 91 comps 92 comps 93 comps 94 comps 95 comps 96 comps 97 comps  
## CV 1.305 1.303 1.302 1.302 1.302 1.302 1.301  
## adjCV 1.304 1.302 1.300 1.301 1.301 1.300 1.300  
## 98 comps 99 comps 100 comps 101 comps 102 comps 103 comps  
## CV 1.302 1.301 1.299 1.295 1.293 1.292  
## adjCV 1.300 1.300 1.298 1.292 1.291 1.290  
## 104 comps 105 comps 106 comps 107 comps 108 comps 109 comps  
## CV 1.292 1.294 1.293 1.293 1.293 1.292  
## adjCV 1.291 1.291 1.291 1.291 1.290 1.290  
## 110 comps 111 comps 112 comps 113 comps 114 comps 115 comps  
## CV 1.293 1.294 1.294 1.295 1.294 1.295  
## adjCV 1.290 1.292 1.292 1.293 1.292 1.294  
## 116 comps 117 comps 118 comps 119 comps 120 comps 121 comps  
## CV 1.294 1.292 1.288 1.288 1.288 1.286  
## adjCV 1.292 1.287 1.286 1.286 1.285 1.284  
## 122 comps 123 comps 124 comps 125 comps 126 comps 127 comps  
## CV 1.286 1.287 1.287 1.287 1.288 1.289  
## adjCV 1.284 1.284 1.285 1.285 1.286 1.286  
## 128 comps 129 comps 130 comps 131 comps 132 comps 133 comps  
## CV 1.288 1.288 1.288 1.287 1.285 1.275  
## adjCV 1.286 1.286 1.285 1.285 1.284 1.272  
## 134 comps 135 comps 136 comps 137 comps 138 comps 139 comps  
## CV 1.269 1.269 1.269 1.270 1.271 1.270  
## adjCV 1.265 1.266 1.267 1.268 1.268 1.268  
## 140 comps 141 comps 142 comps 143 comps 144 comps 145 comps  
## CV 1.269 1.268 1.266 1.267 1.268 1.266  
## adjCV 1.266 1.265 1.264 1.264 1.265 1.265  
## 146 comps 147 comps 148 comps 149 comps 150 comps 151 comps  
## CV 1.264 1.264 1.264 1.264 1.264 1.263  
## adjCV 1.261 1.261 1.261 1.261 1.261 1.260  
## 152 comps 153 comps 154 comps 155 comps 156 comps 157 comps  
## CV 1.263 1.262 1.261 1.261 1.259 1.259  
## adjCV 1.260 1.260 1.258 1.258 1.255 1.256  
## 158 comps 159 comps 160 comps 161 comps 162 comps 163 comps  
## CV 1.259 1.258 1.256 1.255 1.252 1.251  
## adjCV 1.256 1.255 1.253 1.252 1.248 1.248  
## 164 comps 165 comps 166 comps 167 comps 168 comps 169 comps  
## CV 1.252 1.252 1.252 1.251 1.249 1.247  
## adjCV 1.248 1.248 1.249 1.248 1.246 1.244  
## 170 comps 171 comps 172 comps 173 comps 174 comps 175 comps  
## CV 1.247 1.247 1.246 1.246 1.246 1.245  
## adjCV 1.244 1.244 1.243 1.243 1.243 1.241  
## 176 comps 177 comps 178 comps 179 comps 180 comps 181 comps  
## CV 1.246 1.247 1.246 1.245 1.244 1.244  
## adjCV 1.243 1.243 1.243 1.242 1.240 1.240  
## 182 comps 183 comps 184 comps 185 comps 186 comps 187 comps  
## CV 1.244 1.245 1.245 1.246 1.246 1.246  
## adjCV 1.241 1.241 1.241 1.242 1.243 1.243  
## 188 comps 189 comps 190 comps 191 comps 192 comps 193 comps  
## CV 1.246 1.246 1.244 1.243 1.242 1.243  
## adjCV 1.242 1.243 1.242 1.239 1.238 1.239  
## 194 comps 195 comps 196 comps 197 comps 198 comps 199 comps  
## CV 1.243 1.242 1.242 1.243 1.243 1.242  
## adjCV 1.239 1.239 1.239 1.239 1.239 1.238  
## 200 comps 201 comps 202 comps 203 comps 204 comps 205 comps  
## CV 1.243 1.243 1.241 1.241 1.242 1.242  
## adjCV 1.239 1.239 1.238 1.237 1.238 1.238  
## 206 comps 207 comps 208 comps 209 comps 210 comps 211 comps  
## CV 1.242 1.242 1.241 1.241 1.241 1.239  
## adjCV 1.238 1.239 1.237 1.237 1.235 1.235  
## 212 comps 213 comps 214 comps 215 comps 216 comps 217 comps  
## CV 1.239 1.238 1.238 1.237 1.238 1.238  
## adjCV 1.234 1.234 1.233 1.233 1.233 1.234  
## 218 comps 219 comps 220 comps 221 comps 222 comps 223 comps  
## CV 1.238 1.238 1.238 1.239 1.239 1.239  
## adjCV 1.234 1.234 1.234 1.235 1.235 1.235  
## 224 comps 225 comps 226 comps 227 comps 228 comps 229 comps  
## CV 1.238 1.239 1.239 1.239 1.239 1.239  
## adjCV 1.234 1.235 1.234 1.234 1.235 1.235  
## 230 comps 231 comps 232 comps 233 comps 234 comps 235 comps  
## CV 1.238 1.239 1.238 1.239 1.239 1.239  
## adjCV 1.234 1.234 1.234 1.234 1.234 1.234  
## 236 comps 237 comps 238 comps 239 comps 240 comps 241 comps  
## CV 1.239 1.238 1.237 1.238 1.239 1.240  
## adjCV 1.234 1.234 1.233 1.233 1.235 1.236  
## 242 comps 243 comps 244 comps 245 comps 246 comps 247 comps  
## CV 1.241 1.240 1.240 1.240 1.239 1.237  
## adjCV 1.236 1.235 1.235 1.236 1.234 1.233  
## 248 comps 249 comps 250 comps 251 comps 252 comps 253 comps  
## CV 1.238 1.238 1.237 1.237 1.237 1.236  
## adjCV 1.234 1.233 1.232 1.232 1.232 1.232  
## 254 comps 255 comps 256 comps 257 comps 258 comps 259 comps  
## CV 1.237 1.236 1.235 1.234 1.233 1.233  
## adjCV 1.233 1.231 1.230 1.229 1.228 1.227  
## 260 comps 261 comps 262 comps 263 comps 264 comps 265 comps  
## CV 1.233 1.233 1.233 1.234 1.236 1.236  
## adjCV 1.227 1.227 1.228 1.229 1.231 1.230  
## 266 comps 267 comps 268 comps 269 comps 270 comps 271 comps  
## CV 1.236 1.236 1.237 1.237 1.237 1.236  
## adjCV 1.230 1.231 1.232 1.232 1.232 1.231  
## 272 comps 273 comps 274 comps 275 comps 276 comps 277 comps  
## CV 1.236 1.237 1.238 1.238 1.238 1.239  
## adjCV 1.231 1.231 1.232 1.232 1.233 1.233  
## 278 comps 279 comps 280 comps 281 comps 282 comps 283 comps  
## CV 1.239 1.239 1.239 1.240 1.240 1.240  
## adjCV 1.233 1.234 1.233 1.234 1.235 1.234  
## 284 comps 285 comps 286 comps 287 comps 288 comps 289 comps  
## CV 1.240 1.241 1.242 1.243 1.241 1.240  
## adjCV 1.235 1.235 1.236 1.237 1.235 1.234  
## 290 comps 291 comps 292 comps 293 comps 294 comps 295 comps  
## CV 1.240 1.238 1.239 1.239 1.238 1.239  
## adjCV 1.234 1.232 1.233 1.233 1.232 1.233  
## 296 comps 297 comps 298 comps 299 comps 300 comps 301 comps  
## CV 1.239 1.239 1.240 1.242 1.242 1.248  
## adjCV 1.233 1.233 1.234 1.236 1.236 1.241  
## 302 comps 303 comps 304 comps 305 comps 306 comps 307 comps  
## CV 6.390e+09 9.959e+10 1.912e+11 3.236e+11 3.371e+11 1.102e+12  
## adjCV 6.062e+09 9.448e+10 1.814e+11 3.070e+11 3.198e+11 1.045e+12  
## 308 comps 309 comps 310 comps 311 comps 312 comps 313 comps  
## CV 9.435e+11 1.477e+12 3.803e+12 4.450e+12 4.573e+12 4.795e+12  
## adjCV 8.950e+11 1.401e+12 3.608e+12 4.222e+12 4.338e+12 4.548e+12  
## 314 comps 315 comps 316 comps 317 comps 318 comps 319 comps  
## CV 4.899e+12 4.959e+12 4.240e+12 4.293e+12 4.265e+12 4.255e+12  
## adjCV 4.648e+12 4.704e+12 4.022e+12 4.073e+12 4.046e+12 4.036e+12  
## 320 comps 321 comps 322 comps 323 comps  
## CV 3.877e+12 3.867e+12 4.276e+12 4.203e+12  
## adjCV 3.678e+12 3.669e+12 4.057e+12 3.988e+12  
##   
## TRAINING: % variance explained  
## 1 comps 2 comps 3 comps 4 comps 5 comps 6 comps 7 comps 8 comps  
## X 14.2499 25.738 31.487 36.58 40.56 44.28 47.45 50.46  
## Y\_train 0.4135 5.679 9.573 10.83 11.18 11.86 11.86 11.87  
## 9 comps 10 comps 11 comps 12 comps 13 comps 14 comps 15 comps  
## X 53.23 55.65 57.76 59.68 61.49 63.13 64.62  
## Y\_train 12.13 12.15 13.12 13.70 14.17 14.63 14.73  
## 16 comps 17 comps 18 comps 19 comps 20 comps 21 comps 22 comps  
## X 65.99 67.34 68.57 69.69 70.78 71.78 72.72  
## Y\_train 14.85 14.88 17.20 18.04 18.12 18.88 18.96  
## 23 comps 24 comps 25 comps 26 comps 27 comps 28 comps 29 comps  
## X 73.62 74.48 75.27 75.99 76.67 77.35 78.01  
## Y\_train 18.99 19.52 19.52 19.78 20.05 20.05 20.06  
## 30 comps 31 comps 32 comps 33 comps 34 comps 35 comps 36 comps  
## X 78.63 79.22 79.81 80.34 80.87 81.37 81.86  
## Y\_train 20.18 20.78 21.20 21.36 23.17 23.43 23.45  
## 37 comps 38 comps 39 comps 40 comps 41 comps 42 comps 43 comps  
## X 82.32 82.78 83.22 83.64 84.06 84.46 84.85  
## Y\_train 23.47 23.49 23.52 23.62 24.09 24.50 24.64  
## 44 comps 45 comps 46 comps 47 comps 48 comps 49 comps 50 comps  
## X 85.24 85.61 85.95 86.29 86.62 86.94 87.25  
## Y\_train 25.18 25.20 26.20 26.32 26.39 26.45 26.48  
## 51 comps 52 comps 53 comps 54 comps 55 comps 56 comps 57 comps  
## X 87.56 87.86 88.15 88.43 88.70 88.96 89.22  
## Y\_train 26.57 26.58 26.67 26.70 26.75 27.24 27.49  
## 58 comps 59 comps 60 comps 61 comps 62 comps 63 comps 64 comps  
## X 89.48 89.73 89.98 90.21 90.44 90.67 90.88  
## Y\_train 27.50 27.63 27.80 27.88 28.19 28.77 29.03  
## 65 comps 66 comps 67 comps 68 comps 69 comps 70 comps 71 comps  
## X 91.08 91.28 91.48 91.66 91.85 92.03 92.21  
## Y\_train 29.04 29.61 29.61 29.83 29.86 29.90 30.06  
## 72 comps 73 comps 74 comps 75 comps 76 comps 77 comps 78 comps  
## X 92.39 92.56 92.73 92.89 93.05 93.20 93.35  
## Y\_train 30.12 30.62 30.66 30.66 30.89 31.05 31.10  
## 79 comps 80 comps 81 comps 82 comps 83 comps 84 comps 85 comps  
## X 93.50 93.64 93.78 93.92 94.06 94.18 94.30  
## Y\_train 31.21 31.35 31.64 31.74 32.31 32.56 32.86  
## 86 comps 87 comps 88 comps 89 comps 90 comps 91 comps 92 comps  
## X 94.43 94.55 94.67 94.78 94.90 95.01 95.12  
## Y\_train 32.98 33.00 33.04 33.04 33.04 33.05 33.16  
## 93 comps 94 comps 95 comps 96 comps 97 comps 98 comps 99 comps  
## X 95.23 95.33 95.43 95.53 95.63 95.72 95.82  
## Y\_train 33.54 33.56 33.60 33.78 33.81 33.94 33.94  
## 100 comps 101 comps 102 comps 103 comps 104 comps 105 comps  
## X 95.91 96.00 96.09 96.17 96.26 96.34  
## Y\_train 34.11 34.68 34.82 34.95 34.95 35.08  
## 106 comps 107 comps 108 comps 109 comps 110 comps 111 comps  
## X 96.42 96.51 96.58 96.66 96.73 96.81  
## Y\_train 35.17 35.22 35.22 35.26 35.27 35.28  
## 112 comps 113 comps 114 comps 115 comps 116 comps 117 comps  
## X 96.88 96.95 97.02 97.09 97.15 97.22  
## Y\_train 35.38 35.38 35.43 35.49 35.70 36.22  
## 118 comps 119 comps 120 comps 121 comps 122 comps 123 comps  
## X 97.28 97.34 97.40 97.46 97.52 97.58  
## Y\_train 36.23 36.23 36.53 36.66 36.67 36.68  
## 124 comps 125 comps 126 comps 127 comps 128 comps 129 comps  
## X 97.63 97.68 97.74 97.79 97.84 97.89  
## Y\_train 36.74 36.74 36.75 36.78 36.83 36.83  
## 130 comps 131 comps 132 comps 133 comps 134 comps 135 comps  
## X 97.93 97.98 98.03 98.07 98.11 98.16  
## Y\_train 37.00 37.02 37.19 38.00 38.55 38.65  
## 136 comps 137 comps 138 comps 139 comps 140 comps 141 comps  
## X 98.20 98.24 98.28 98.32 98.36 98.39  
## Y\_train 38.66 38.66 38.76 38.84 39.01 39.02  
## 142 comps 143 comps 144 comps 145 comps 146 comps 147 comps  
## X 98.43 98.46 98.50 98.53 98.57 98.60  
## Y\_train 39.29 39.29 39.29 39.37 39.78 39.84  
## 148 comps 149 comps 150 comps 151 comps 152 comps 153 comps  
## X 98.63 98.66 98.69 98.72 98.75 98.78  
## Y\_train 39.86 39.90 40.00 40.12 40.12 40.13  
## 154 comps 155 comps 156 comps 157 comps 158 comps 159 comps  
## X 98.81 98.84 98.86 98.89 98.92 98.94  
## Y\_train 40.26 40.48 40.63 40.63 40.74 40.74  
## 160 comps 161 comps 162 comps 163 comps 164 comps 165 comps  
## X 98.97 98.99 99.01 99.04 99.06 99.08  
## Y\_train 41.02 41.03 41.34 41.41 41.42 41.44  
## 166 comps 167 comps 168 comps 169 comps 170 comps 171 comps  
## X 99.11 99.13 99.15 99.17 99.19 99.21  
## Y\_train 41.52 41.61 41.77 41.98 42.05 42.07  
## 172 comps 173 comps 174 comps 175 comps 176 comps 177 comps  
## X 99.23 99.25 99.27 99.28 99.30 99.32  
## Y\_train 42.09 42.11 42.25 42.41 42.41 42.48  
## 178 comps 179 comps 180 comps 181 comps 182 comps 183 comps  
## X 99.34 99.35 99.37 99.39 99.40 99.42  
## Y\_train 42.51 42.62 42.70 42.72 42.72 42.85  
## 184 comps 185 comps 186 comps 187 comps 188 comps 189 comps  
## X 99.43 99.45 99.46 99.48 99.49 99.50  
## Y\_train 42.88 42.88 42.89 42.89 42.98 43.02  
## 190 comps 191 comps 192 comps 193 comps 194 comps 195 comps  
## X 99.52 99.53 99.54 99.56 99.57 99.58  
## Y\_train 43.02 43.39 43.43 43.46 43.46 43.50  
## 196 comps 197 comps 198 comps 199 comps 200 comps 201 comps  
## X 99.59 99.60 99.62 99.63 99.64 99.65  
## Y\_train 43.51 43.52 43.54 43.70 43.72 43.77  
## 202 comps 203 comps 204 comps 205 comps 206 comps 207 comps  
## X 99.66 99.67 99.68 99.69 99.70 99.71  
## Y\_train 43.81 43.97 43.99 43.99 44.02 44.11  
## 208 comps 209 comps 210 comps 211 comps 212 comps 213 comps  
## X 99.71 99.72 99.73 99.74 99.75 99.76  
## Y\_train 44.23 44.29 44.51 44.52 44.60 44.65  
## 214 comps 215 comps 216 comps 217 comps 218 comps 219 comps  
## X 99.76 99.77 99.78 99.79 99.79 99.80  
## Y\_train 44.65 44.71 44.73 44.74 44.75 44.76  
## 220 comps 221 comps 222 comps 223 comps 224 comps 225 comps  
## X 99.81 99.81 99.82 99.82 99.83 99.84  
## Y\_train 44.76 44.77 44.77 44.82 44.92 44.93  
## 226 comps 227 comps 228 comps 229 comps 230 comps 231 comps  
## X 99.84 99.85 99.85 99.86 99.86 99.87  
## Y\_train 44.98 44.99 44.99 44.99 45.10 45.13  
## 232 comps 233 comps 234 comps 235 comps 236 comps 237 comps  
## X 99.87 99.88 99.88 99.89 99.89 99.90  
## Y\_train 45.14 45.27 45.27 45.29 45.29 45.31  
## 238 comps 239 comps 240 comps 241 comps 242 comps 243 comps  
## X 99.9 99.91 99.91 99.91 99.92 99.92  
## Y\_train 45.4 45.41 45.42 45.42 45.42 45.47  
## 244 comps 245 comps 246 comps 247 comps 248 comps 249 comps  
## X 99.92 99.93 99.93 99.93 99.94 99.94  
## Y\_train 45.51 45.52 45.67 45.67 45.67 45.82  
## 250 comps 251 comps 252 comps 253 comps 254 comps 255 comps  
## X 99.94 99.95 99.95 99.95 99.95 99.96  
## Y\_train 45.87 45.93 45.94 45.98 46.01 46.27  
## 256 comps 257 comps 258 comps 259 comps 260 comps 261 comps  
## X 99.96 99.96 99.96 99.96 99.97 99.97  
## Y\_train 46.33 46.40 46.52 46.52 46.52 46.54  
## 262 comps 263 comps 264 comps 265 comps 266 comps 267 comps  
## X 99.97 99.97 99.97 99.98 99.98 99.98  
## Y\_train 46.54 46.55 46.60 46.61 46.63 46.63  
## 268 comps 269 comps 270 comps 271 comps 272 comps 273 comps  
## X 99.98 99.98 99.98 99.98 99.99 99.99  
## Y\_train 46.64 46.64 46.71 46.76 46.77 46.77  
## 274 comps 275 comps 276 comps 277 comps 278 comps 279 comps  
## X 99.99 99.99 99.99 99.99 99.99 99.99  
## Y\_train 46.78 46.79 46.79 46.81 46.82 46.86  
## 280 comps 281 comps 282 comps 283 comps 284 comps 285 comps  
## X 99.99 99.99 99.99 99.99 100.00 100.00  
## Y\_train 46.92 46.93 46.94 46.97 46.97 47.05  
## 286 comps 287 comps 288 comps 289 comps 290 comps 291 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.06 47.06 47.17 47.23 47.33 47.37  
## 292 comps 293 comps 294 comps 295 comps 296 comps 297 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.39 47.39 47.42 47.42 47.45 47.47  
## 298 comps 299 comps 300 comps 301 comps 302 comps 303 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.47 47.48 47.48 47.52 47.52 47.66  
## 304 comps 305 comps 306 comps 307 comps 308 comps 309 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.66 47.76 47.76 47.76 47.76 47.77  
## 310 comps 311 comps 312 comps 313 comps 314 comps 315 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.77 47.77 47.79 47.79 47.79 47.81  
## 316 comps 317 comps 318 comps 319 comps 320 comps 321 comps  
## X 100.00 100.00 100.00 100.00 100.00 100.00  
## Y\_train 47.81 47.82 47.83 47.84 47.85 47.88  
## 322 comps 323 comps  
## X 100.0 100.0  
## Y\_train 47.9 47.9

validationplot(pcr.fit ,val.type="MSEP")



lm.pred=predict (lm\_model ,newdata = X\_test)

## Warning in predict.lm(lm\_model, newdata = X\_test): prediction from a  
## rank-deficient fit may be misleading

mean((lm.pred -Y\_test)^2)

## [1] 1.338069

# Calculate R-squared  
pcr.pred1=predict (pcr.fit ,newdata = X\_test)  
SSE.pcr <- sum((Y\_train - pcr.pred1)^2)

## Warning in Y\_train - pcr.pred1: longer object length is not a multiple of  
## shorter object length

SST.pcr <- sum((Y\_train - mean(Y\_train))^2)  
R2.pcr <- 1 - SSE.pcr/SST.pcr  
  
# Print the result  
print(paste0("R-squared: ", round(R2.pcr, 2)))

## [1] "R-squared: -6.66907539917111e+24"

# Perform PCA on X\_train  
pca <- prcomp(X\_train, center = TRUE, scale. = TRUE)  
  
# Get the loadings for the first principal component  
loadings <- pca$rotation[, 1]  
  
# Sort the compounds in descending order of contribution to the first PC  
contributions <- sort(loadings, decreasing = TRUE)  
  
# Get the indices of the compounds that contribute the most to the first PC  
top\_indices <- order(loadings, decreasing = TRUE)[1:10]  
  
# Print the top contributing compounds  
colnames(X\_train[, top\_indices])

## [1] "PubchemFP418" "PubchemFP442" "PubchemFP453" "PubchemFP358" "PubchemFP387"  
## [6] "PubchemFP530" "PubchemFP523" "PubchemFP396" "PubchemFP472" "PubchemFP506"

# Calculate correlation matrix between descriptors and pIC50  
cor\_mat <- cor(df\_Ach[,3:ncol(df\_Ach)])

## Warning in cor(df\_Ach[, 3:ncol(df\_Ach)]): the standard deviation is zero

# Get correlation values with pIC50  
cor\_values <- cor\_mat[,1]  
  
# Sort correlation values in descending order  
sorted\_cor <- sort(cor\_values, decreasing = TRUE)  
  
# Print sorted correlation values  
print(sorted\_cor)

## PubchemFP2 PubchemFP12 PubchemFP540 PubchemFP345 PubchemFP365   
## 1.0000000000 0.4878138879 0.3429885136 0.3282573840 0.3230548010   
## PubchemFP11 PubchemFP391 PubchemFP679 PubchemFP688 PubchemFP710   
## 0.2516377916 0.2434415724 0.2298335778 0.2270028577 0.2267094214   
## PubchemFP709 PubchemFP683 PubchemFP186 PubchemFP3 PubchemFP390   
## 0.2256520196 0.2179630036 0.2160080195 0.2142971256 0.2110697349   
## PubchemFP696 PubchemFP351 PubchemFP192 PubchemFP14 PubchemFP285   
## 0.2087805398 0.2036945697 0.2034030444 0.2016834549 0.2016834549   
## PubchemFP185 PubchemFP392 PubchemFP592 PubchemFP613 PubchemFP656   
## 0.1987214400 0.1971411567 0.1953244106 0.1924996146 0.1891133572   
## PubchemFP199 PubchemFP528 PubchemFP708 PubchemFP179 PubchemFP582   
## 0.1885298109 0.1862152463 0.1785083401 0.1768759691 0.1737681064   
## PubchemFP374 PubchemFP698 PubchemFP689 PubchemFP680 PubchemFP643   
## 0.1727484390 0.1657098855 0.1642949628 0.1641287781 0.1640259847   
## PubchemFP193 PubchemFP646 PubchemFP19 PubchemFP405 PubchemFP637   
## 0.1607315419 0.1574422755 0.1562742720 0.1515565288 0.1456960369   
## PubchemFP699 PubchemFP335 PubchemFP333 PubchemFP607 PubchemFP434   
## 0.1445286305 0.1444995677 0.1443025461 0.1424692708 0.1414881760   
## PubchemFP420 PubchemFP257 PubchemFP13 PubchemFP604 PubchemFP178   
## 0.1412615158 0.1402117473 0.1380079789 0.1379988157 0.1374567217   
## PubchemFP594 PubchemFP666 PubchemFP476 PubchemFP565 PubchemFP589   
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