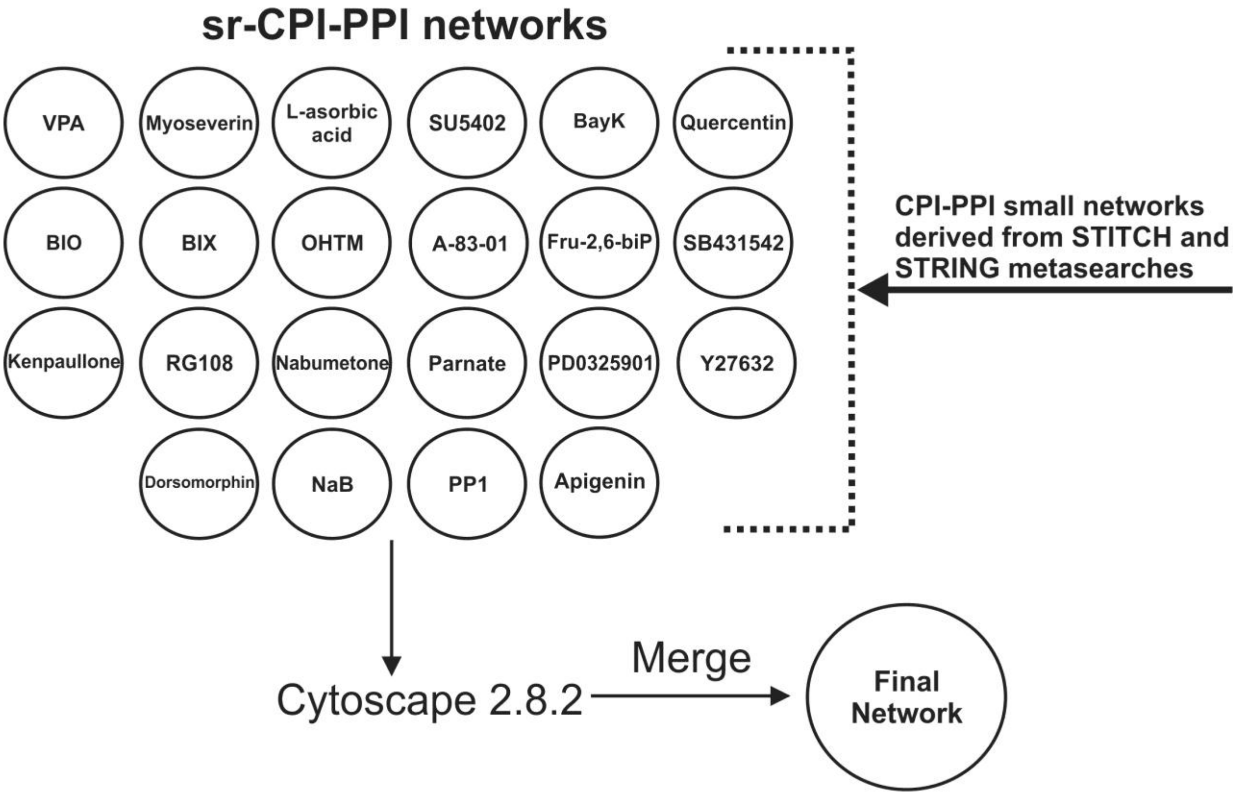
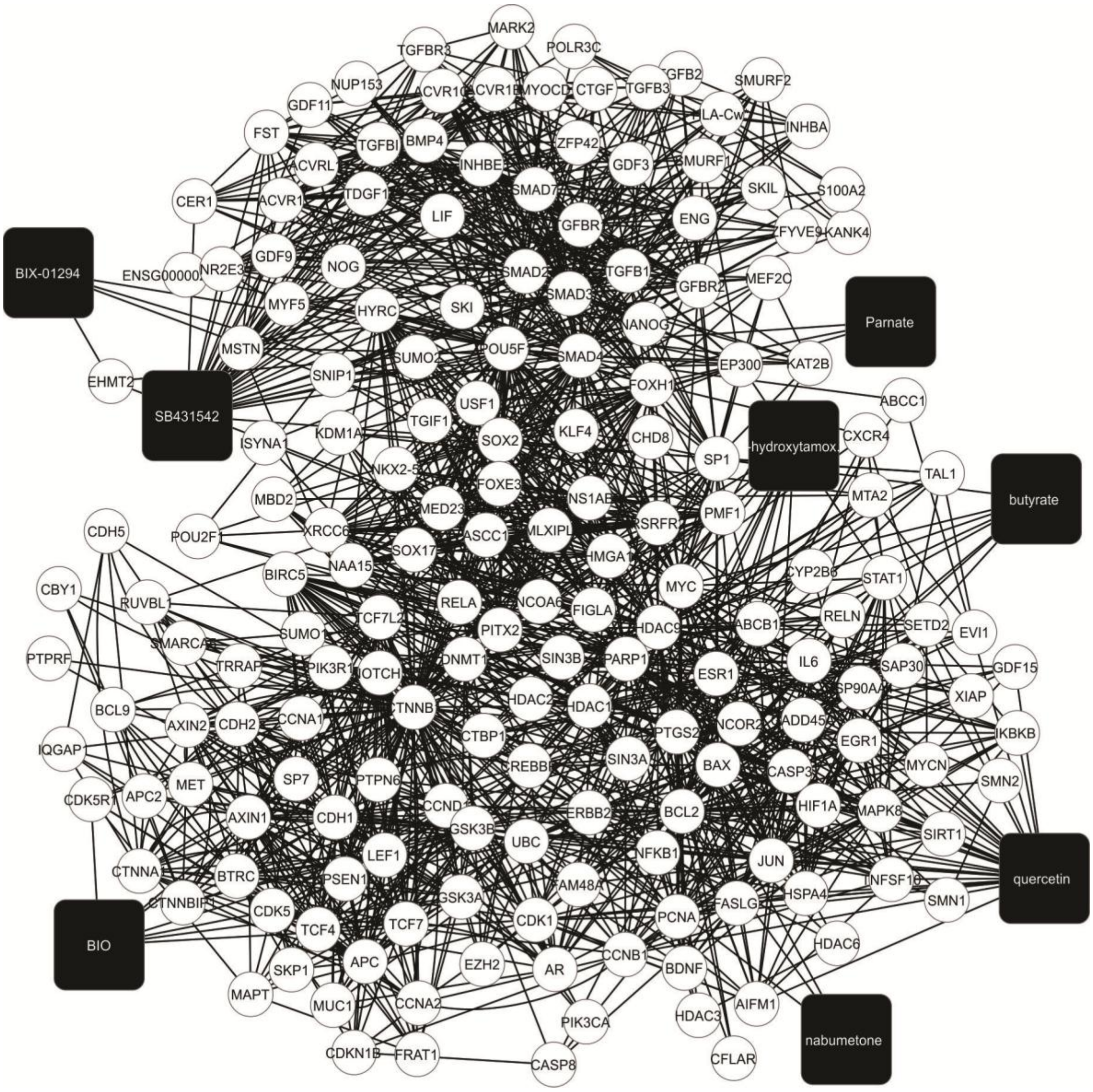
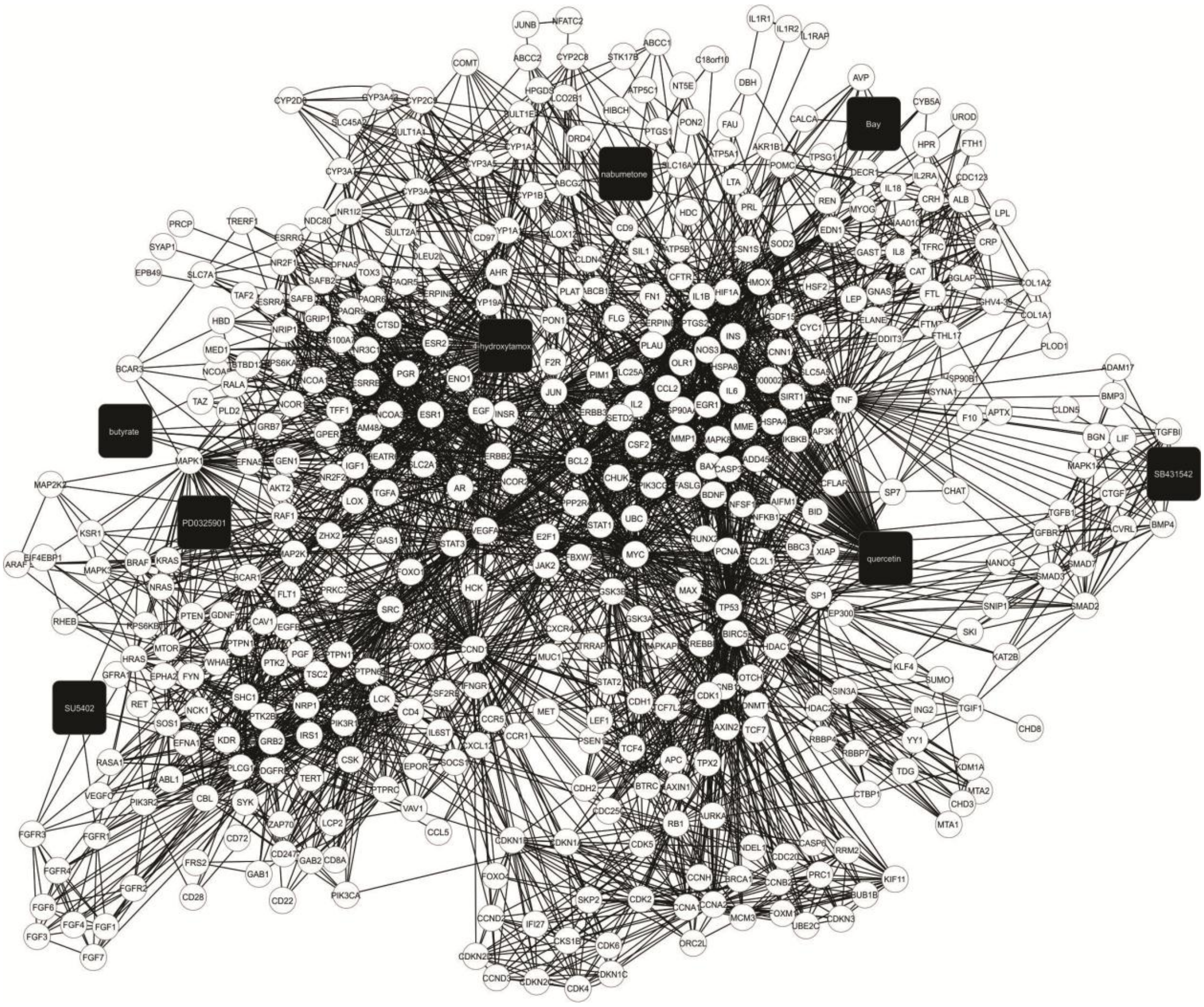


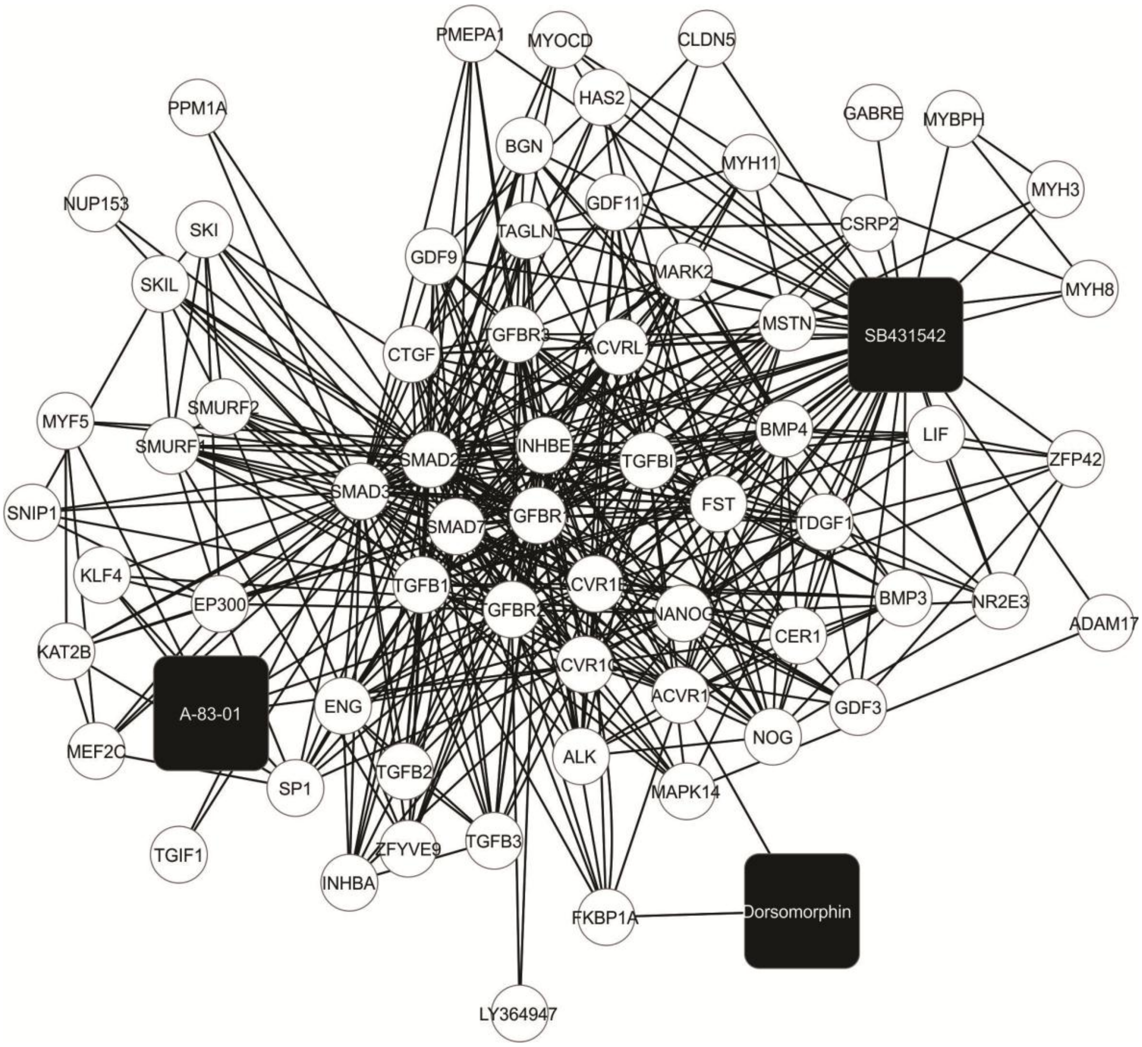
S-Figure 1: prospected small molecules, present in STITCH 3.1 database, related to in stem cell self-renewal, and plasticity maintenance. The 22 small networks were merged into one single network named sr-CPI-PPI network.



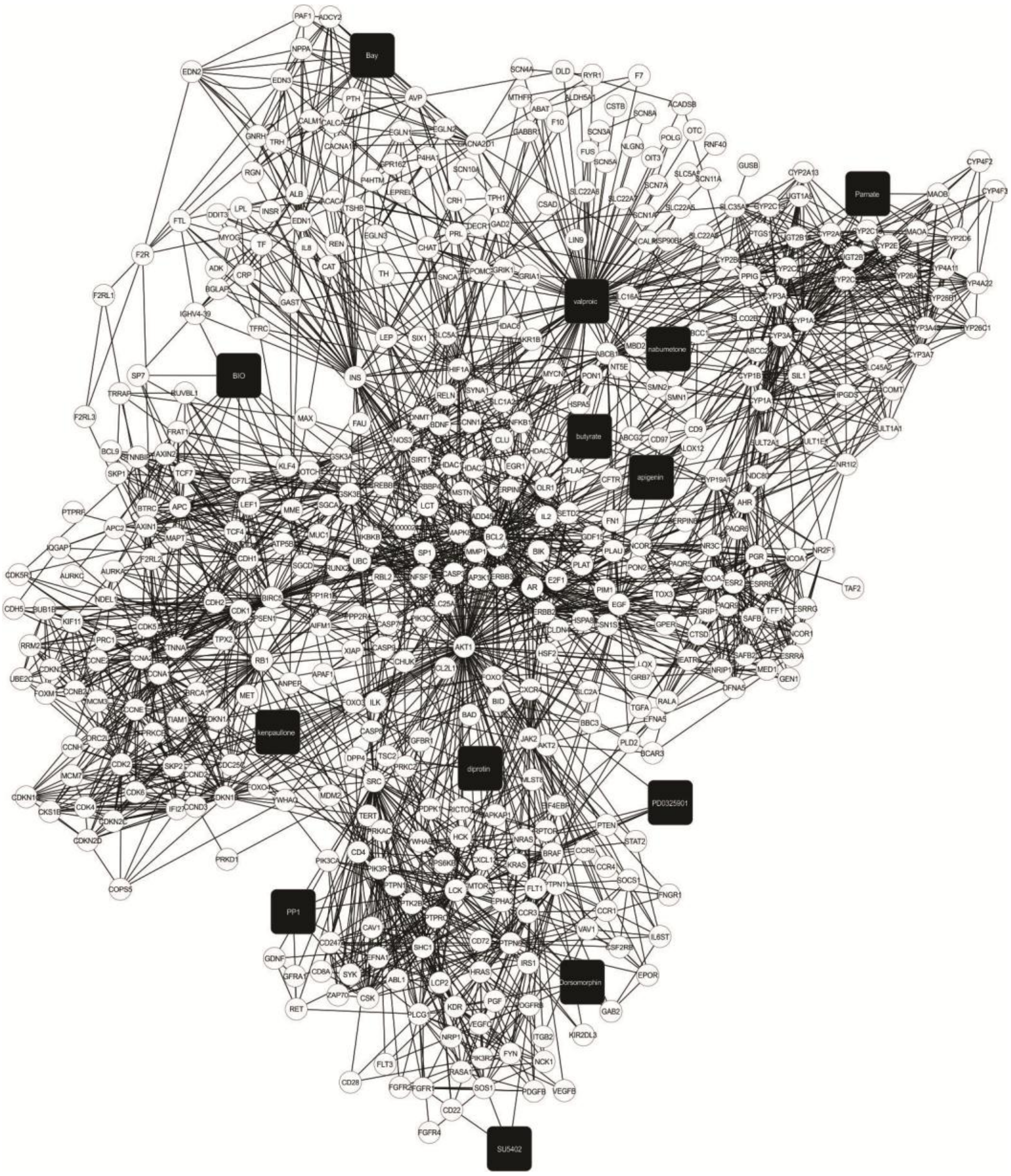
S-Figure 2: cluster 1, created by the program MCODE, with C*i* = 8,901. This cluster is composed of 191 nodes and 1700 edges. The 8 small molecules present in cluster 1 are: BIX-01294, SB431542, 4-hydroxytamoxifen, Parnate, sodium butyrate, quercetin. BIO and nabumentone.



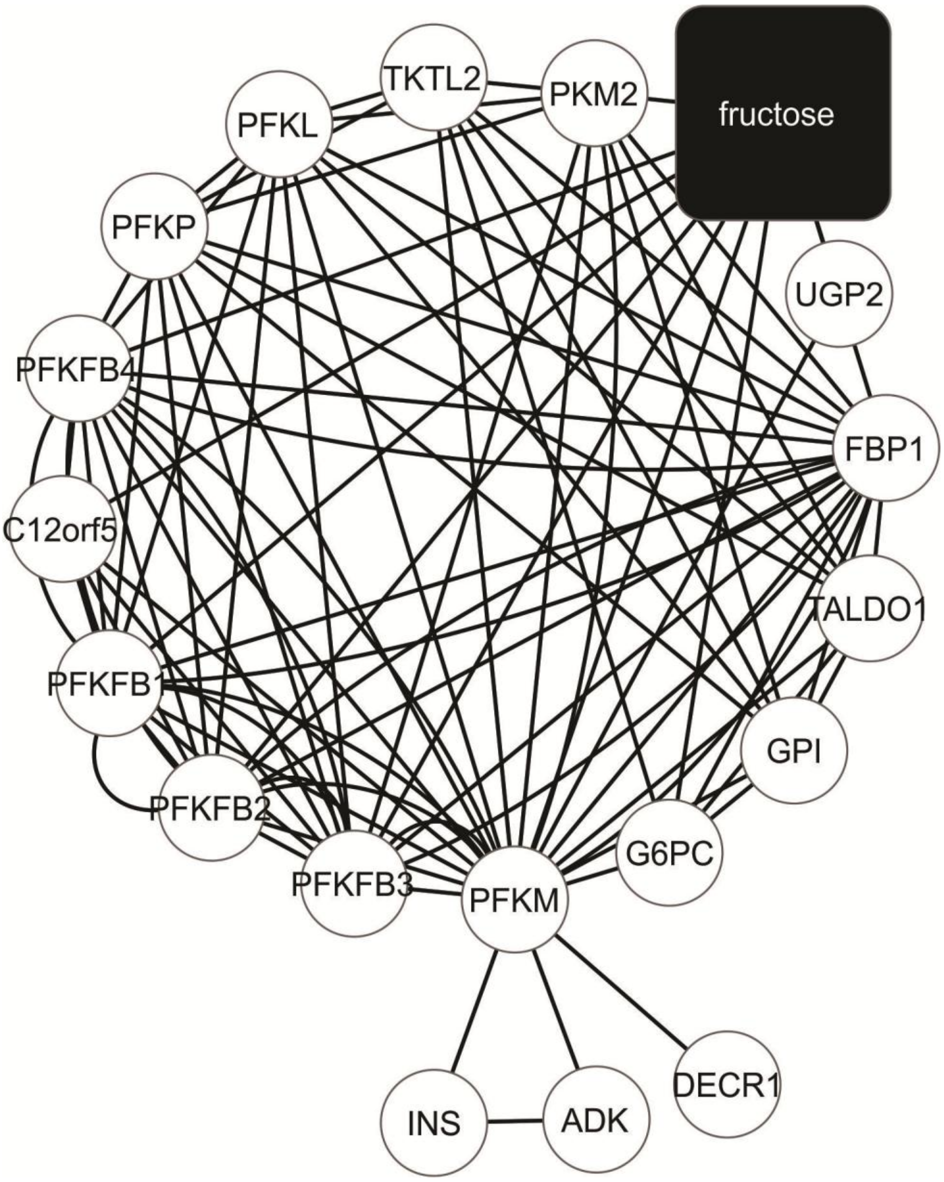
S-Figure 3: cluster 2, created by the program MCODE, with C*i* = 8,420. This cluster is composed of 424 nodes and 3570 edges. The 8 small molecules present in cluster 2 are: sodium butyrate, PD0325901, SU5402, 4-hydroxytamoxifen, nabumentone, Bayk8644, quercetin and SB431542.



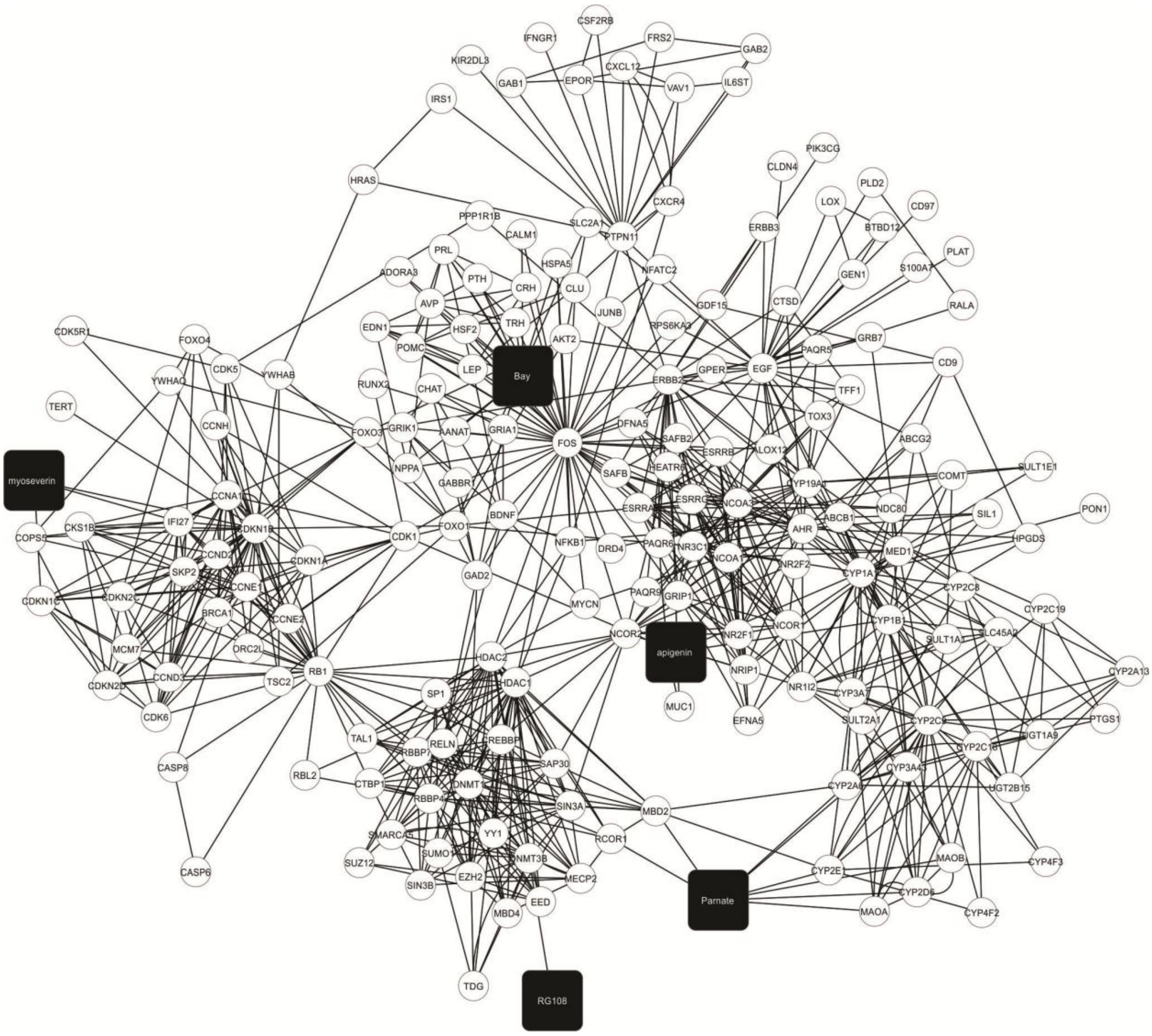
S-Figure 4: cluster 3, created by the program MCODE, with C*i* = 6,676. This cluster is composed of 68 nodes and 454 edges. The 3 small molecules present in cluster 3 are: A-83-01, dorsomorphin and SB431542.



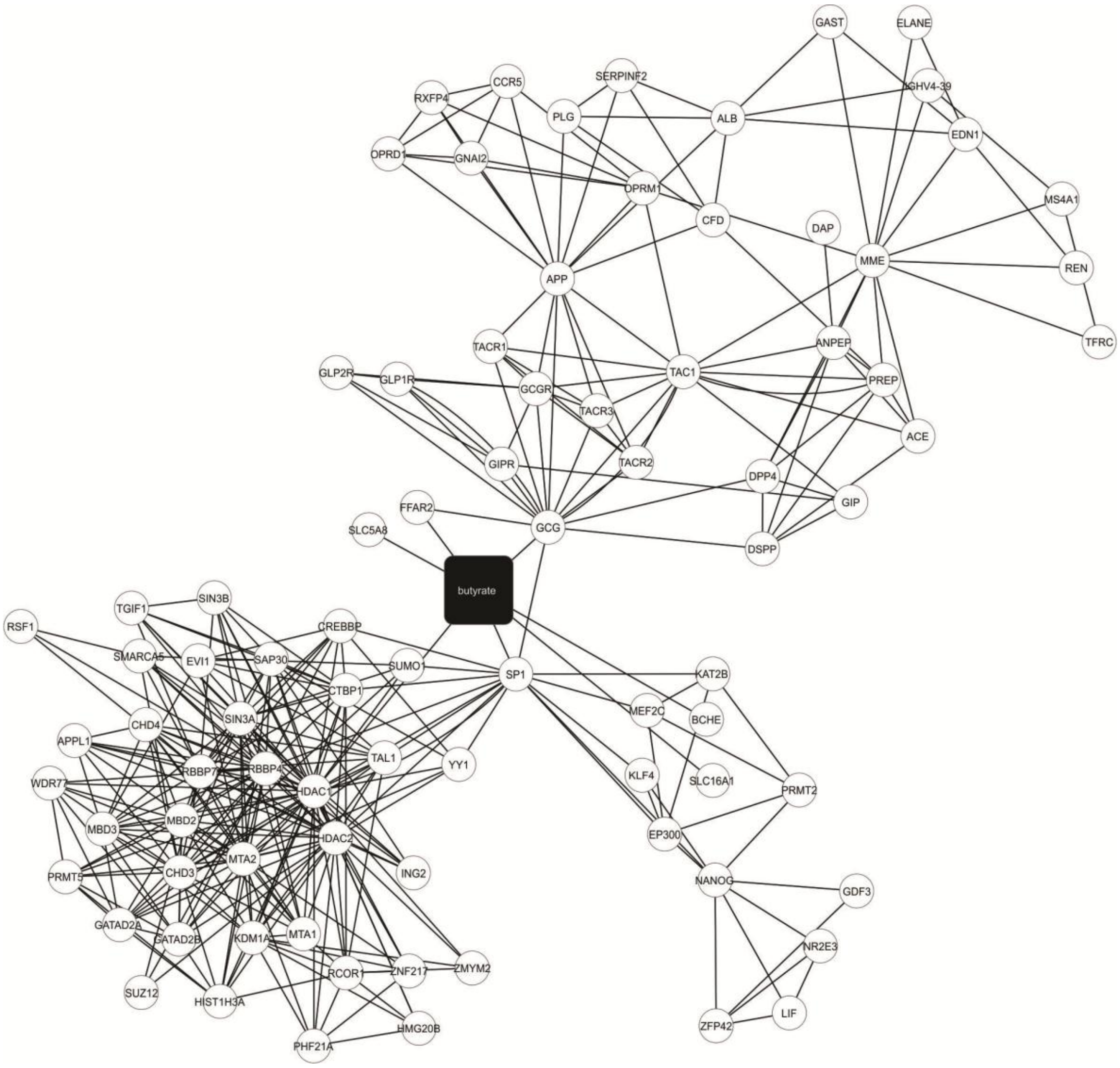
S-Figure 5: cluster 4, created by the program MCODE, with C*i* = 6,011. This cluster is composed of 445 nodes and 2675 edges. The 12 small molecules present in cluster are: kenpaullone, nabumetone, BIO, Parnate, PD032590, Bayk8644, SU5402, sodium butyrate, PP1, valproic acid, apigenin and dorsomorphin.



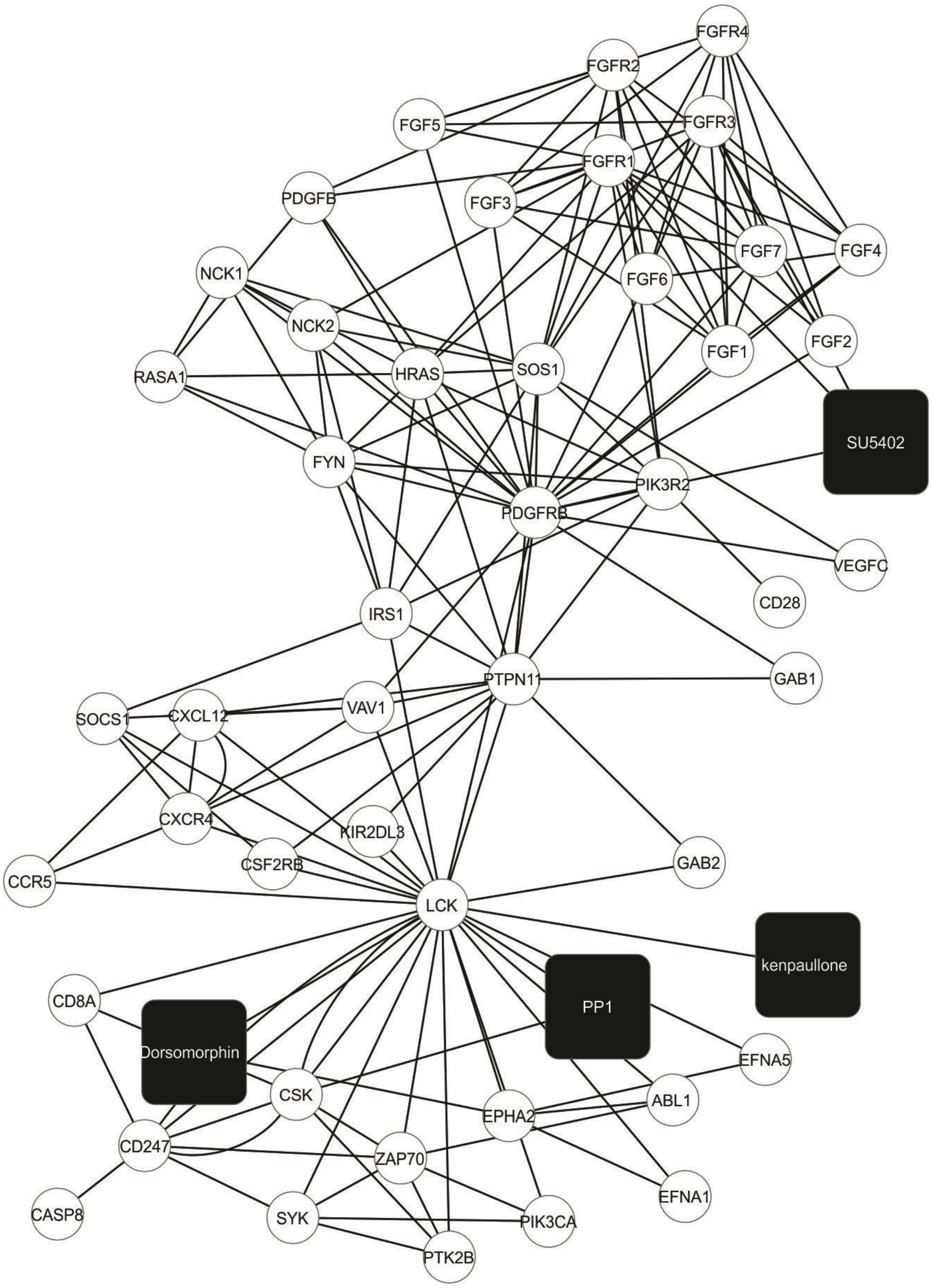
S-Figure 6: cluster 5, created by the program MCODE, with C*i* = 4,842. This cluster is composed of 19 nodes and 92 edges. The small molecules present in cluster 5 is fructose-2,6-biphosphate.



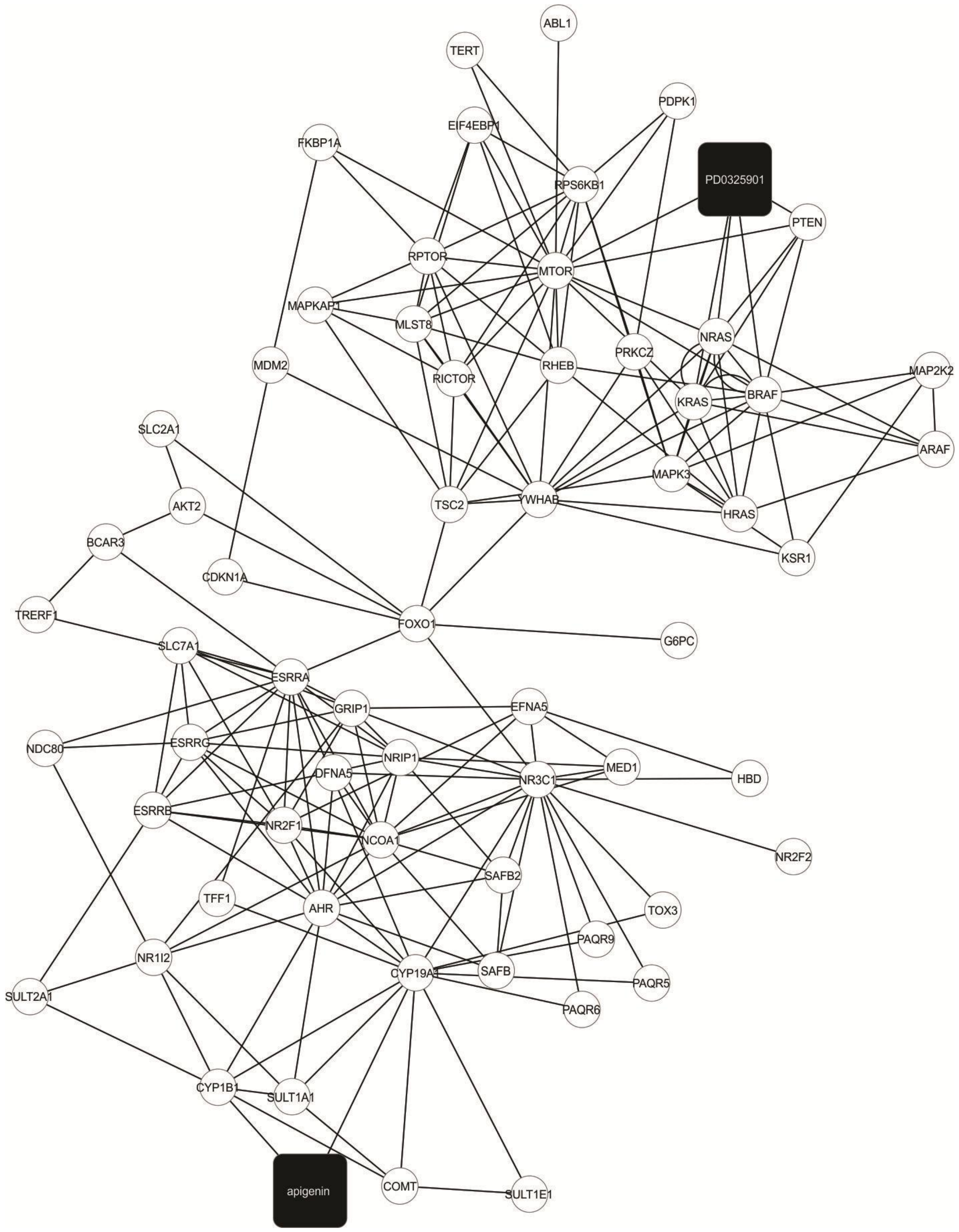
S-Figure 7: cluster 6, created by the program MCODE, with C*i* = 4,184. This cluster is composed of 185 nodes and 774 edges. The 5 small molecules present in cluster 6 are: Bayk8644, myoseverin, Parnate, apigenin and RG108.



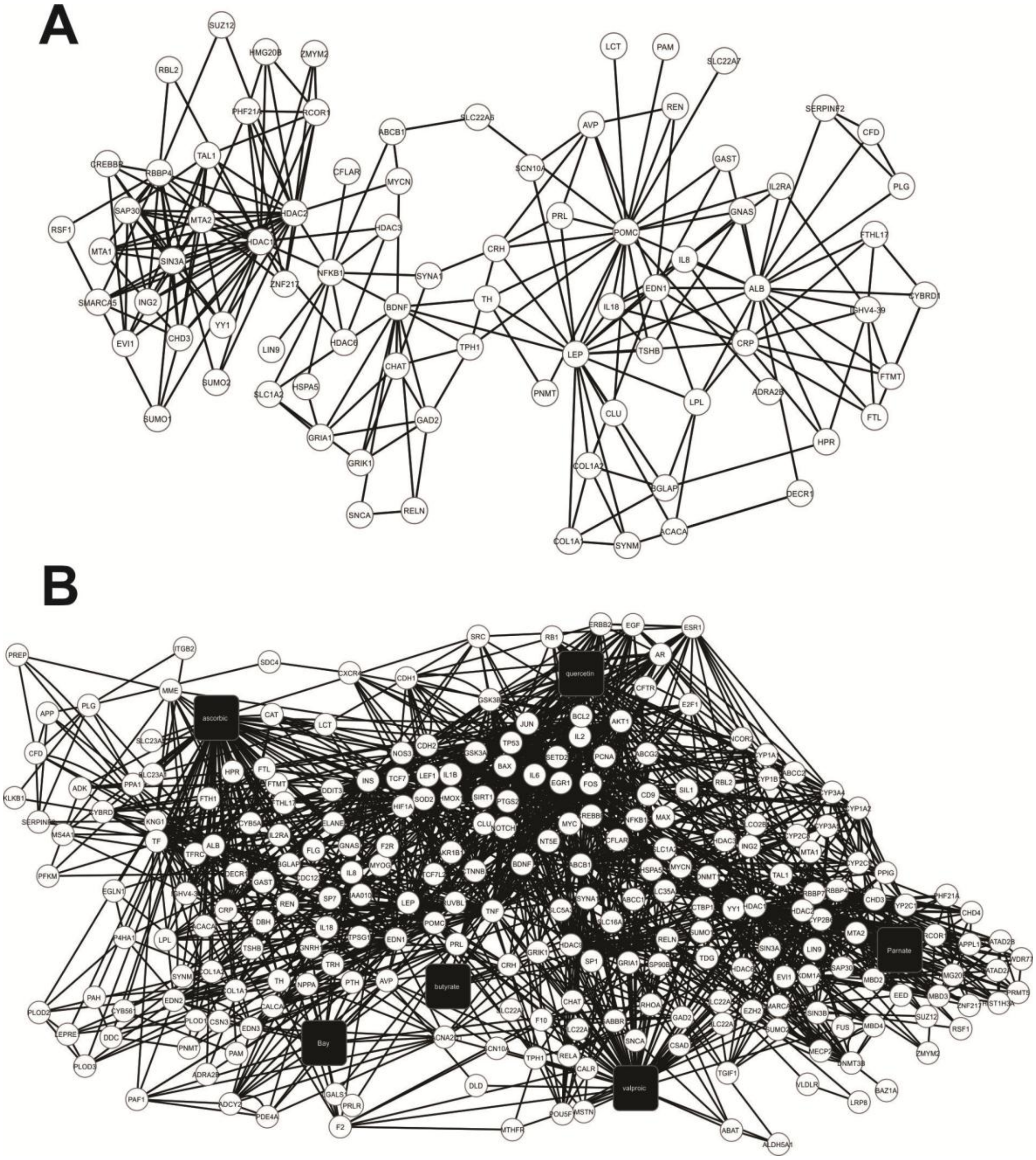
S-Figure 8: cluster 7, created by the program MCODE, with C*i* = 4,172. This cluster is composed of 87 nodes and 363 edges. The small molecule present in cluster 7 is sodium butyrate.



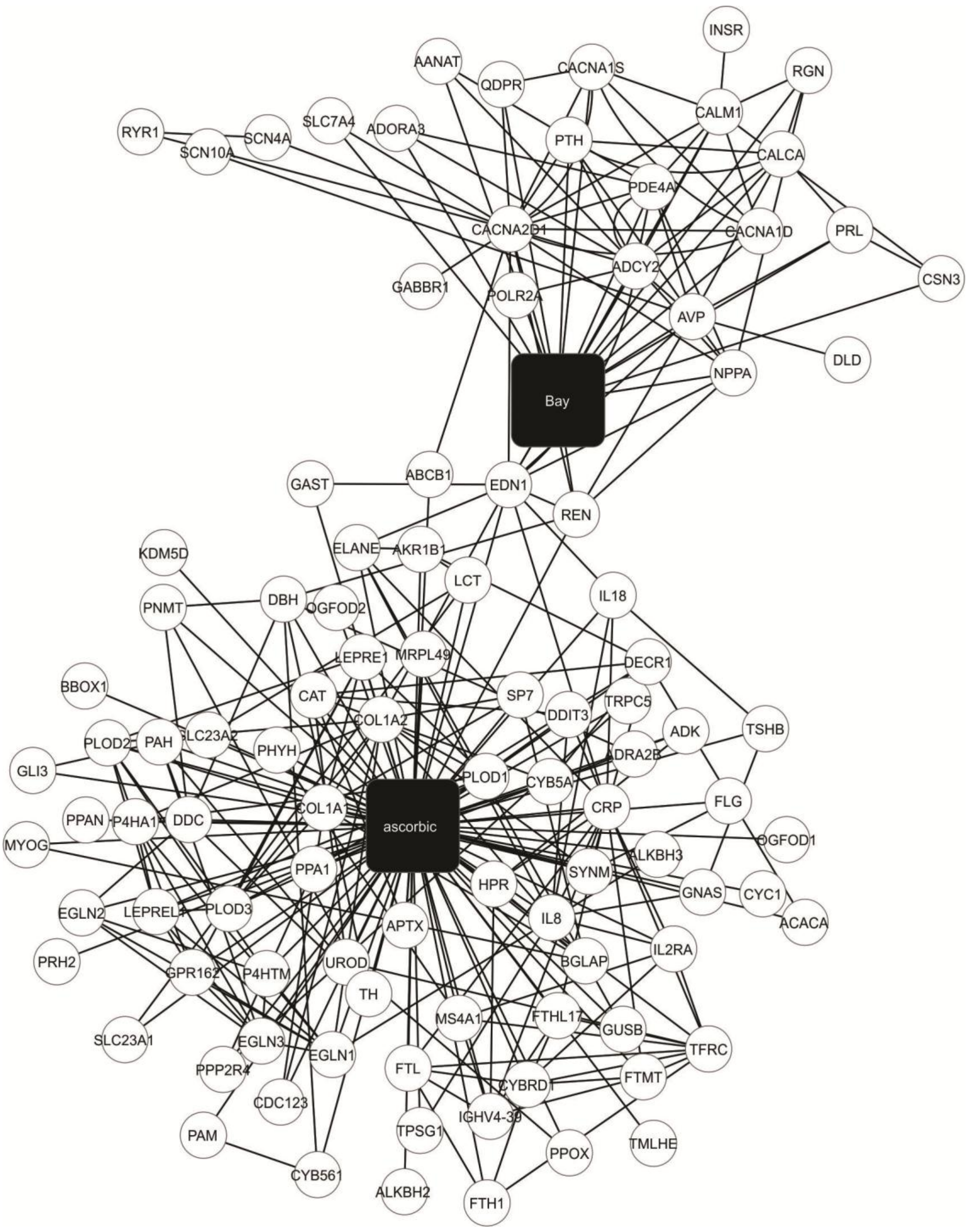
S-Figure 9: cluster 8, created by the program MCODE, with C*i* = 3,2. This cluster is composed of 50 nodes and 160 edges. The small molecules present in cluster 8 are: PP1, kenpaullone, dorsomorphin and SU5402.



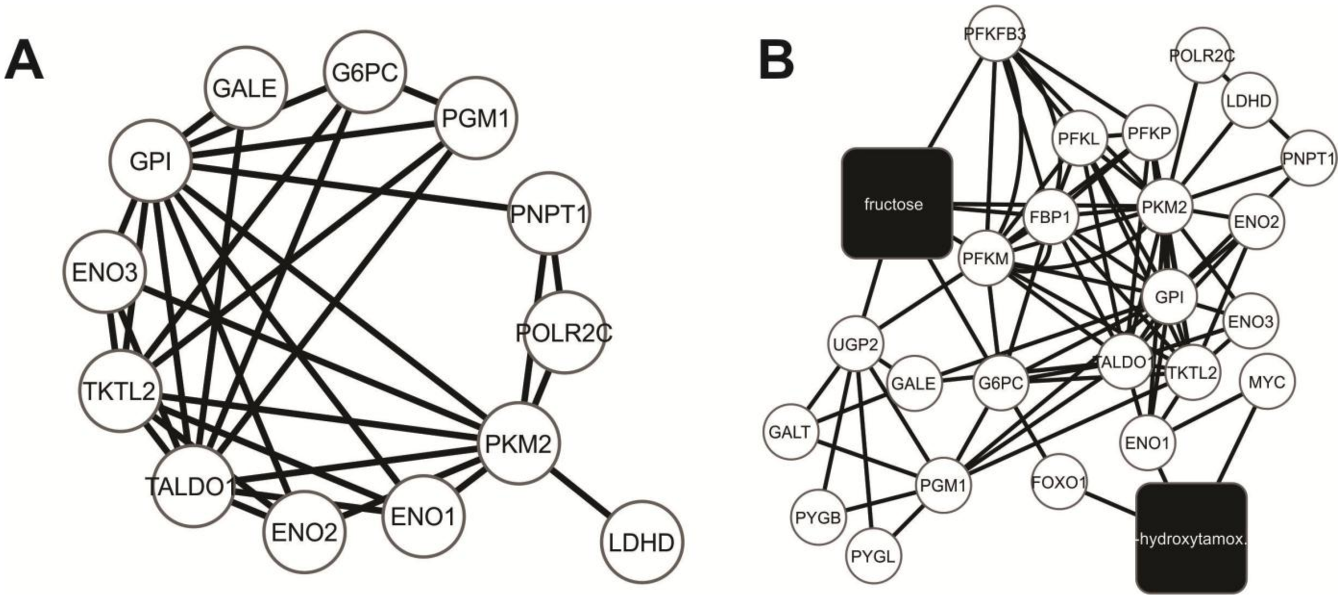
S-Figure 10: cluster 9, created by the program MCODE, with C*i* = 3,109. This cluster is composed of 64 nodes and 199 edges. The 2 small molecules present in cluster 9 are: apigenin and PD0325901.



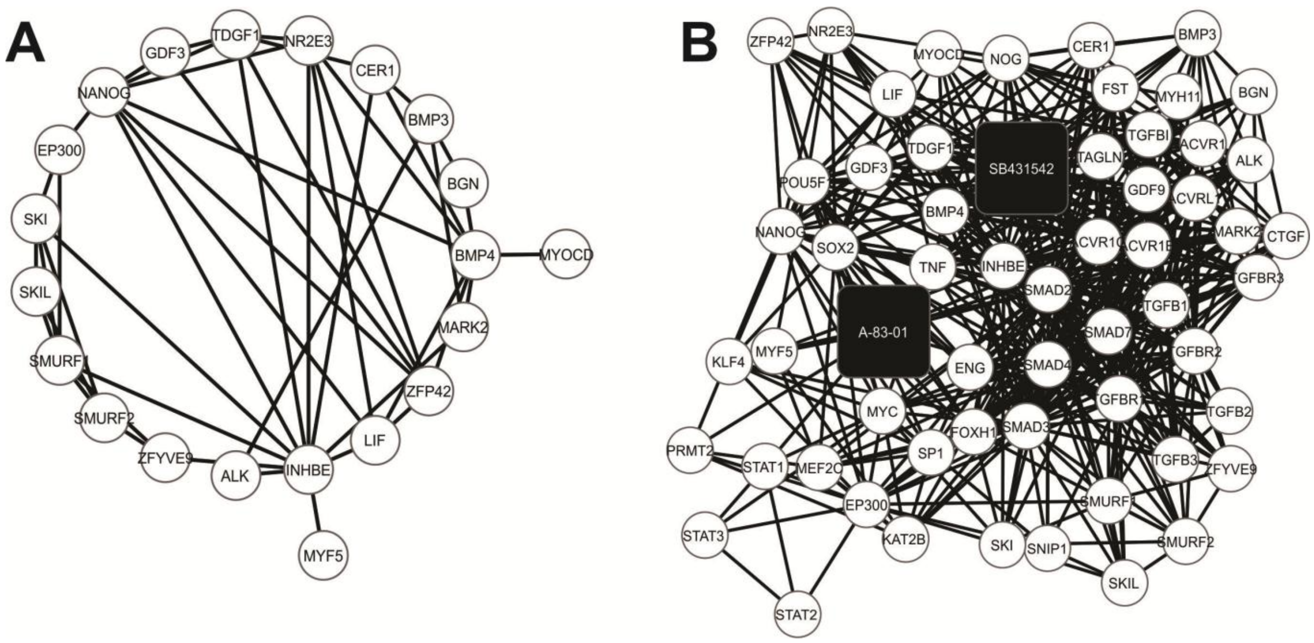
S-Figure 11: A) cluster 10, created by the program MCODE, with C*i* = 2,817, composed by 82 nodes and 231 edges. It however did not presented any small molecules. Therefore, we expanded the network for the adjacent nodes for each node and obtained the network in B. The cluster 10B contains 246 nodes and 1707 edges. The 6 small molecules present in cluster 10 are: Bayk8644, sodium butyrate, valproic acid, Parnate, quercetin and ascorbic acid.



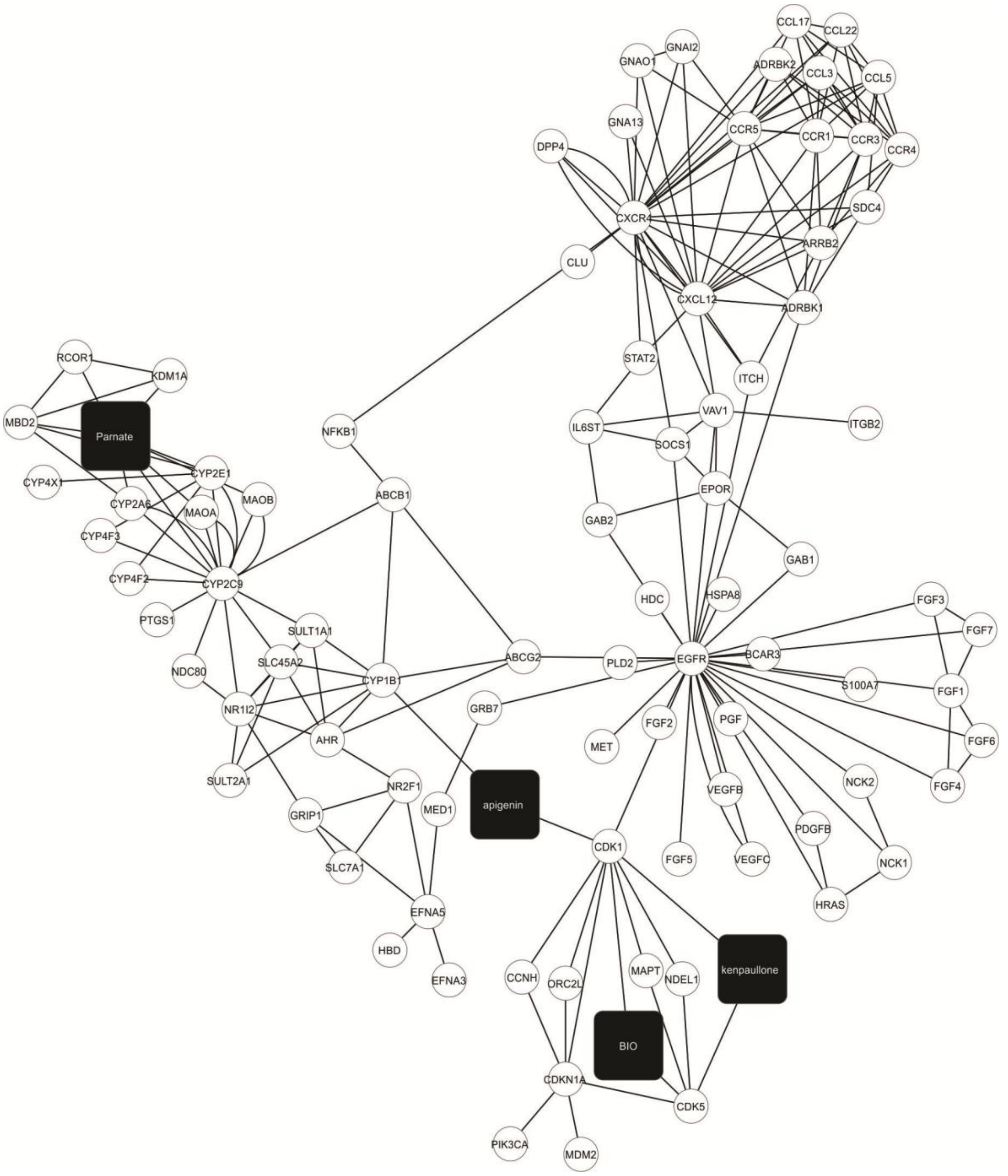
S-Figure 12: cluster 11, created by the program MCODE, with C*i* = 2,769, composed by 104 nodes and 288 edges. The 2 small molecules present in cluster 11 are: Bayk8644 and ascorbic acid.



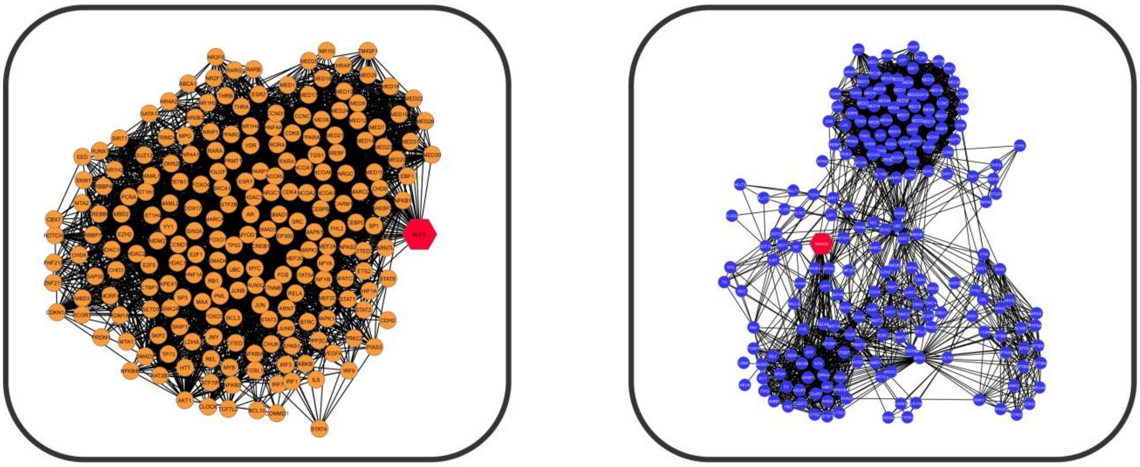
S-Figure 13: A) cluster 12, created by the program MCODE, with C*i* = 2,462, composed by 13 nodes and 32 edges. It however did not presented any small molecules. Therefore, we expanded the network for the adjacent nodes for each node and obtained the network in B. The cluster 13B contains 26 nodes and 86 edges. The 2 small molecules present in cluster 12 are: 4-hydroxytamoxifen and fructose-2,6-biphosphate.



S-Figure 14: A) cluster 13, created by the program MCODE, with C*i* = 2,238, composed by 21 nodes and 47 edges. It however did not presented any small molecules. Therefore, we expanded the network for the adjacent nodes for each node and obtained the network in B. The cluster 14B contains 59 nodes and 500 edges. The 2 small molecules present in cluster 13 are: SB431542 and A-83-01.

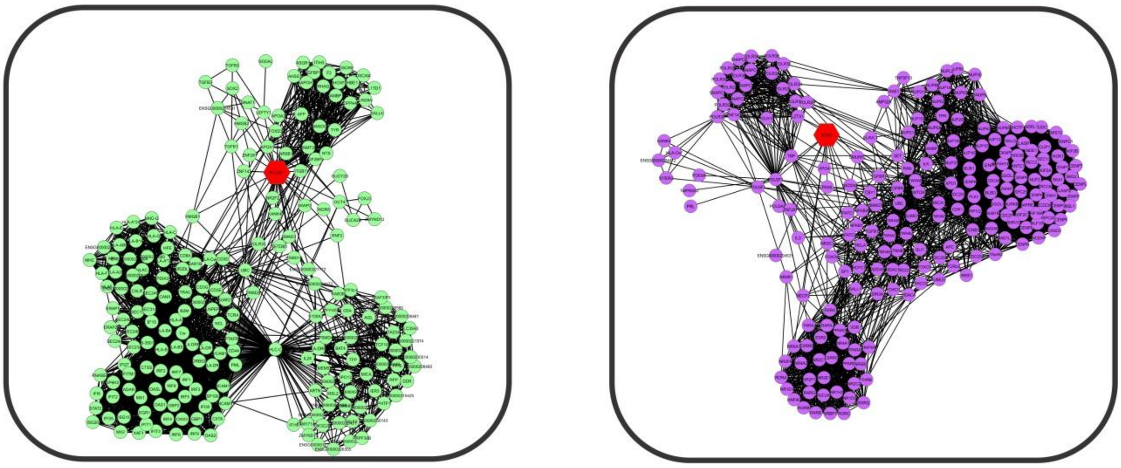


S-Figure 15: cluster 14, created by the program MCODE, with C*i* = 2,234. This cluster is composed of 94 nodes and 210 edges. The 5 small molecules present in cluster 14 are: Parnate, apigenin, BIO, and kenpaullone.



KLF4 network

NANOG network



OCT4 network

SOX2 network

S-Figure 16: networks designed for each classical pluripotency-associated factor. The main proteins (KLF4, NANOG, OCT4 and SOX2) are colored in red. Each network was used in the analysis performed by the program Interference 1.0.