

# Cheminformatics Assignment 2

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*December 2023*

Educts	Products	<i>k</i>	<i>c</i>	<i>n</i>	<i>t</i>
C=C, C=C	C1CCC1	0	4		
C=C, C=C	C1CCC1	1	4		
O, Cl, CC(=O)OCC	Cl, OCC, CC(=O)O	0	6		
O, Cl, CC(=O)OCC	Cl, OCC, CC(=O)O	1	6		
O, Cl, CC(=O)OCC	Cl, OCC, CC(=O)O	2	6		
C1C(O)CC(O)C(O)C1	C=CO, C=CO, C=CO	0	6		
C1C(O)CC(O)C(O)C1	C=CO, C=CO, C=CO	1	6		
CC=CC=CC, OC1C=CC=CC=1	C=CC=CC=C, OC(=C)C=CC=C	0	6		
CC=CC=CC, OC1C=CC=CC=1	C=CC=CC=C, OC(=C)C=CC=C	1	6		
CC=CC=CC, OC1C=CC=CC=1	C=CC=CC=C, OC(=C)C=CC=C	2	6		
CC, OC1C=CC=CC=1	C=C, OC(=C)C=CC=C	0	6		
CC, OC1C=CC=CC=1	C=C, OC(=C)C=CC=C	1	6		
CC, OC1C=CC=CC=1	C=C, OC(=C)C=CC=C	2	6		
OP(=O)(O)OP(=O)(O)O, O	O=P(O)(O)O, O=P(O)(O)O	0	4		
OP(=O)(O)OP(=O)(O)O, O	O=P(O)(O)O, O=P(O)(O)O	1	4		
OP(=O)(O)OP(=O)(O)O, O	O=P(O)(O)O, O=P(O)(O)O	0	6		
OP(=O)(O)OP(=O)(O)O, O	O=P(O)(O)O, O=P(O)(O)O	1	6		
C#N, C#N	N=CC#N	0	4		
C#N, C#N	N=CC#N	1	4		