Supplementary Information

Computer simulations to study the mechanisms of cold plasma-induced degradation of amoxicillin from pharmaceutical wastewater

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Simulation results

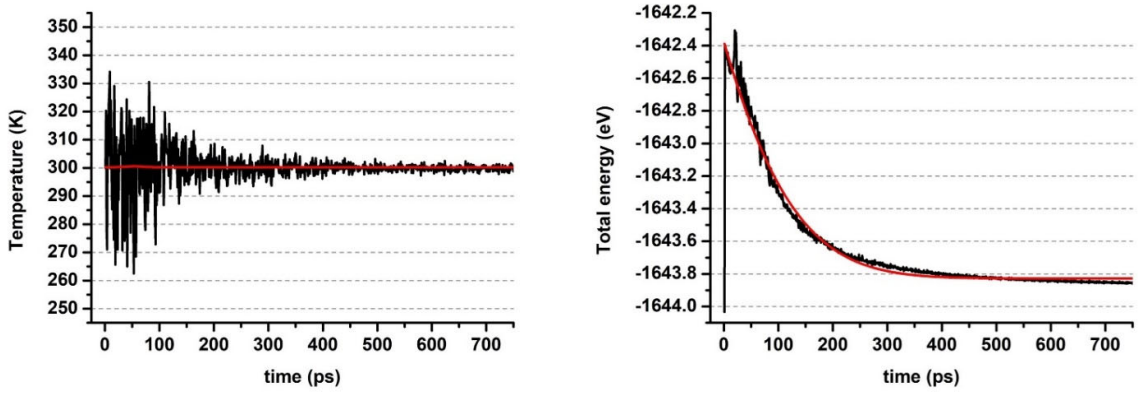


Figure S1. *Time evolution of the temperature and total energy of the amoxicillin model system. The red lines indicate the Gaussian curve fitting.*

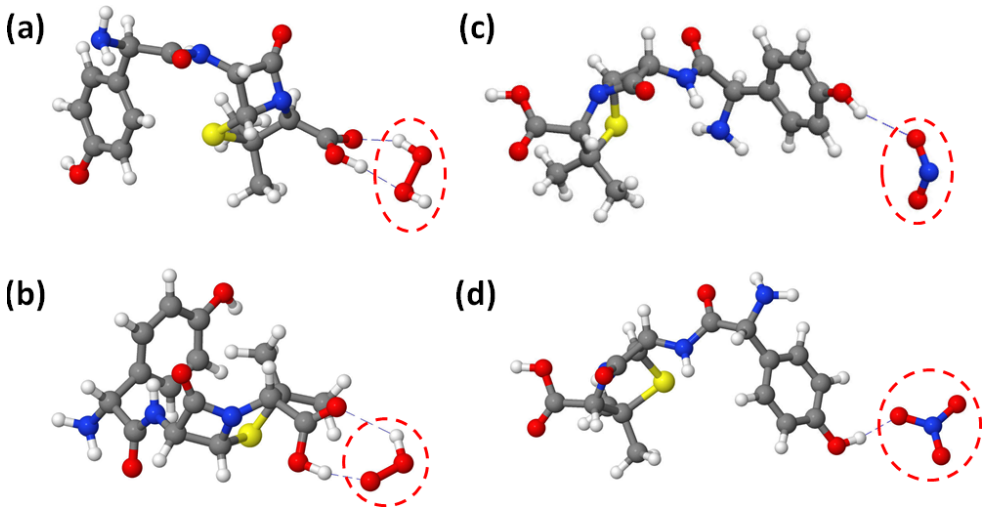
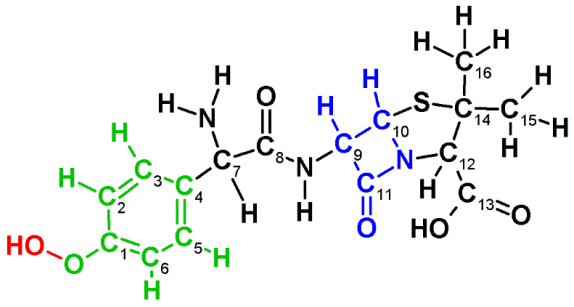
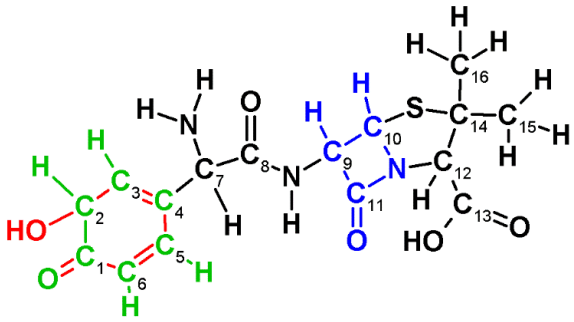
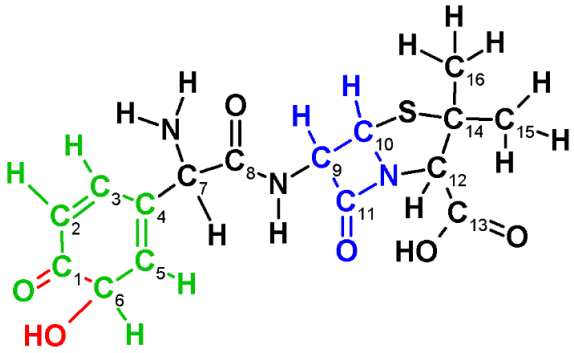
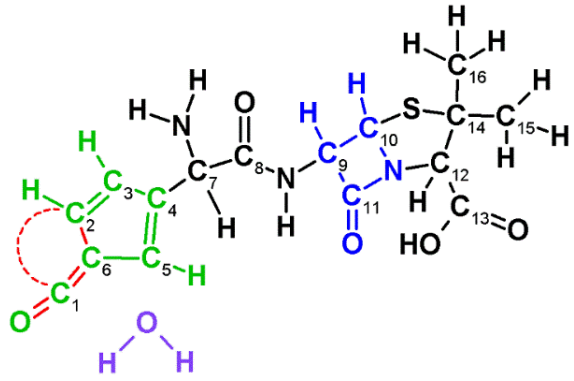
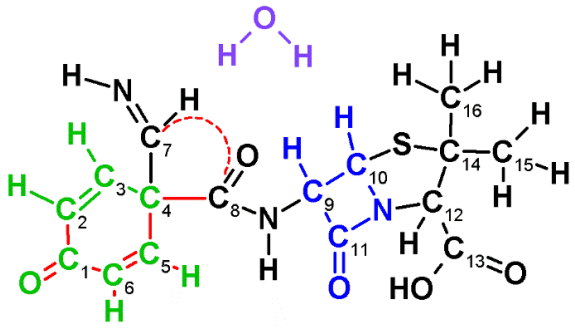
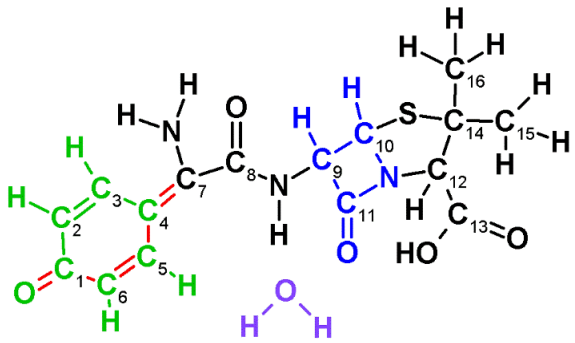
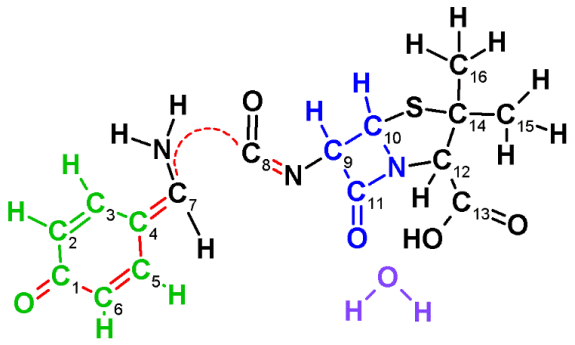
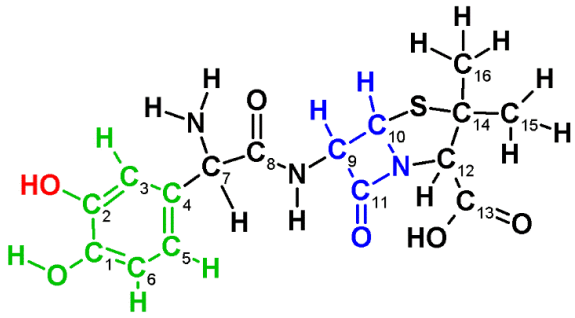
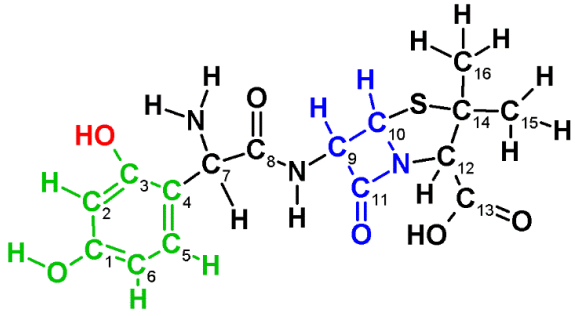
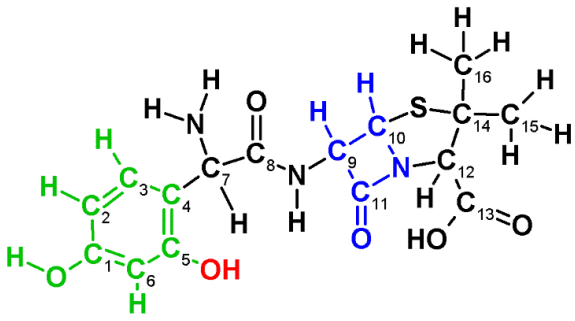
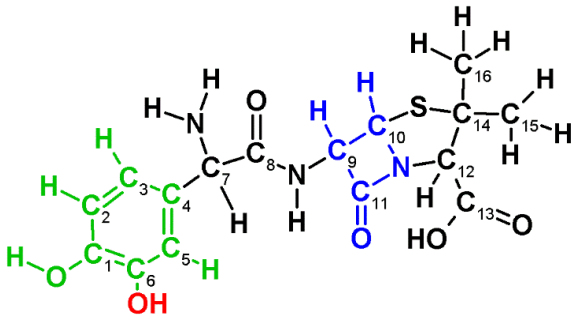
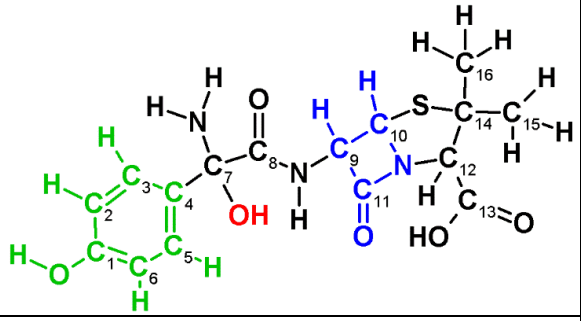
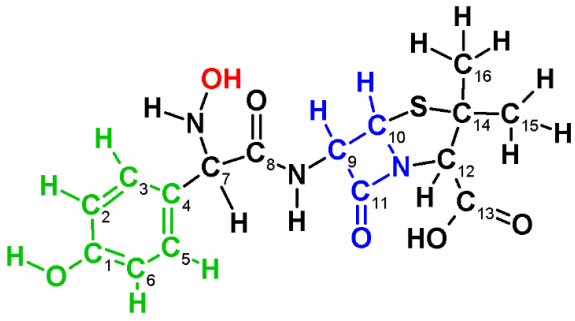
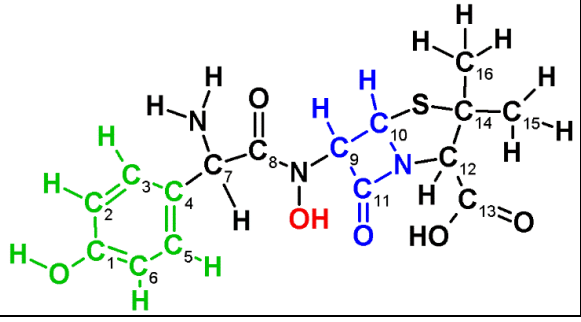


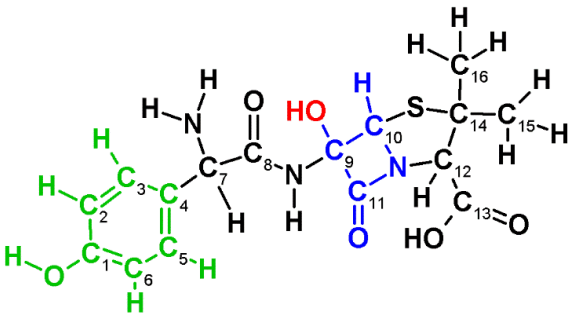
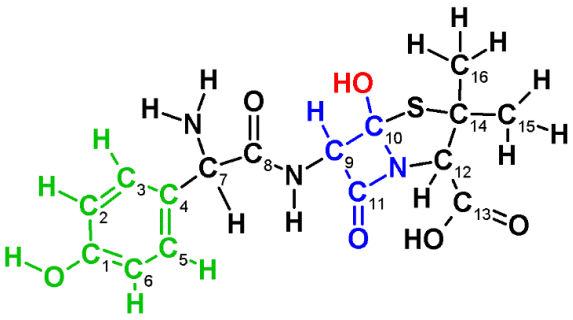
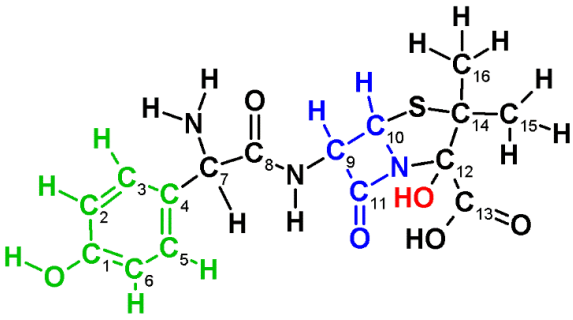
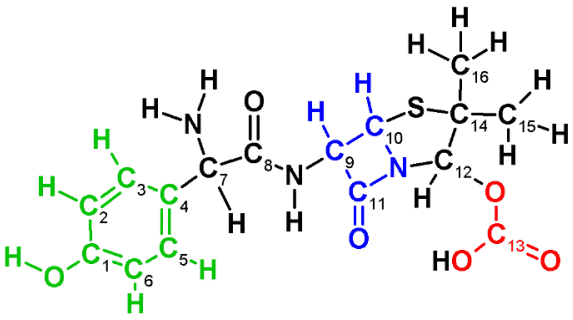
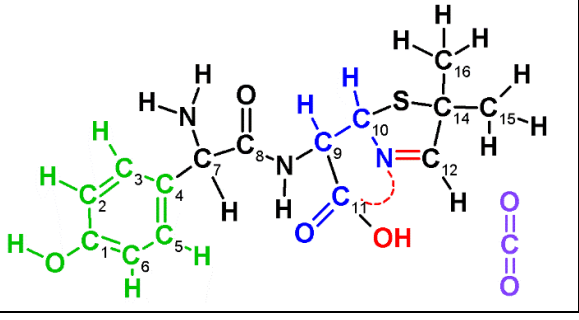
Figure S2. *Weak attractive interactions of H_2O_2 (a), HO_2 (b), NO_2^- (c) and NO_3^- (d), shown in red dashed circles, with amoxicillin.*

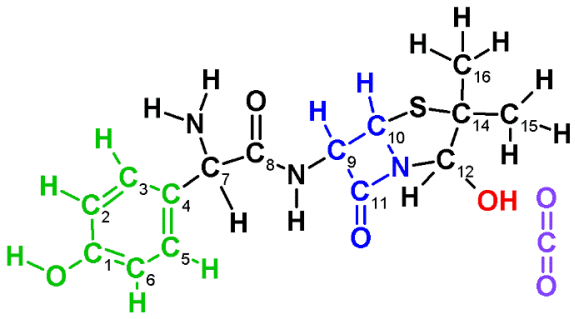
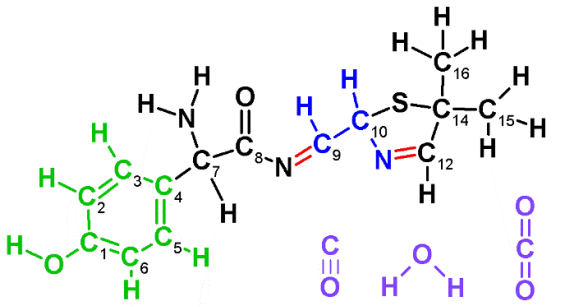
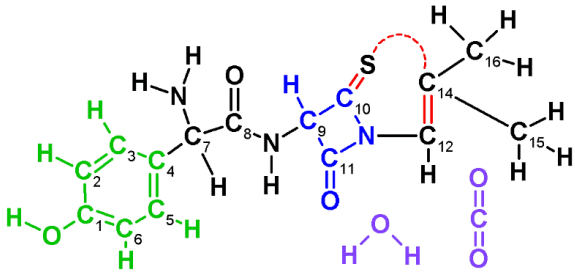
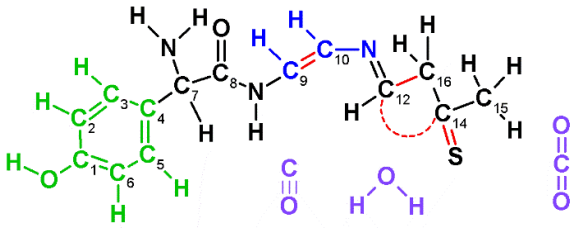
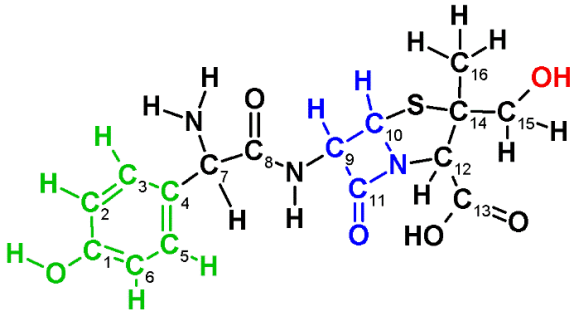
Table S1. *Overview of all the reaction events observed in the simulations following the interaction of O atoms with amoxicillin. Newly formed bonds and functional groups are shown in red, while dissociated bonds are indicated by red dashed lines. Detached species are illustrated in purple. The third column lists the number of times this reaction was observed (out of the 100 simulations). The last column summarizes the result of each reaction.*

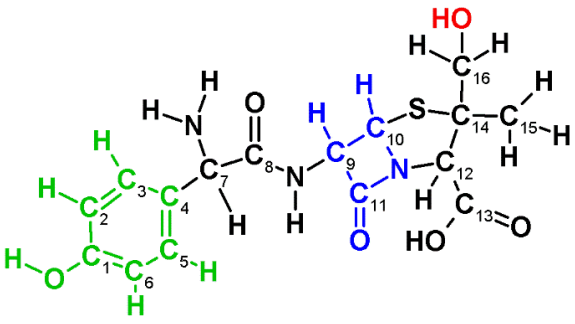
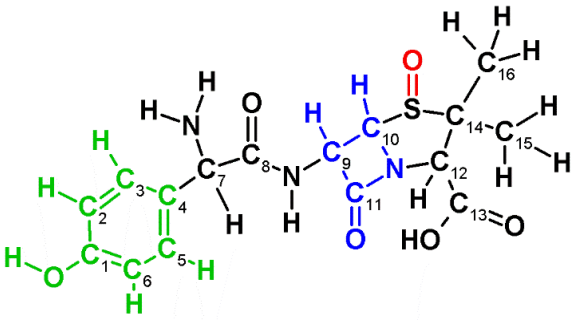
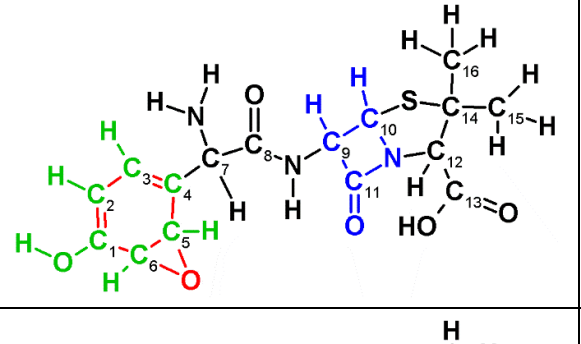
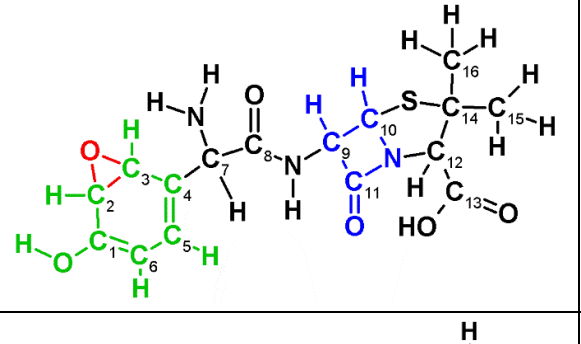
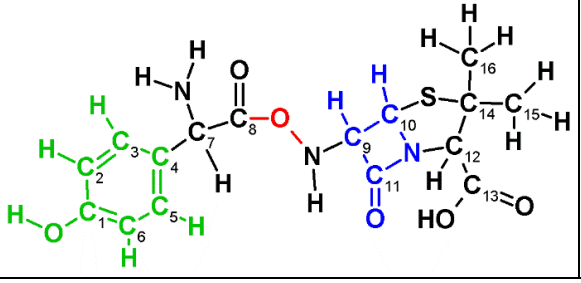
№	H-abstraction	Number of events	Structure	Consequence of reaction
1	C_1OH	8		C_1O-OH is formed (+16 Da)
2	C_1OH	1		Ketone is formed C_2-OH is formed (+16 Da)
3	C_1OH	1		Ketone is formed C_6-OH is formed (+16 Da)
4	C_1OH and C_6H	2		H_2O is formed C_1-C_2 is broken C_2-C_6, C_1=C_6 and C_1=O are formed (-2 Da)

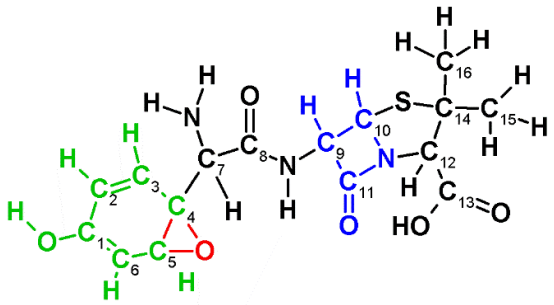
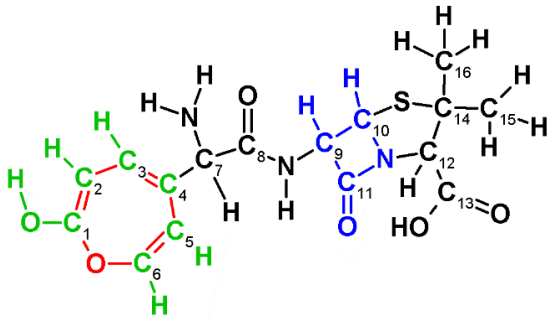
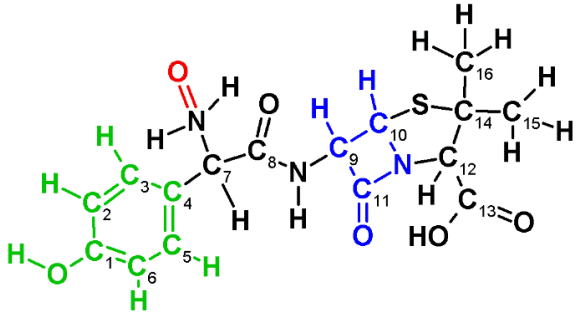
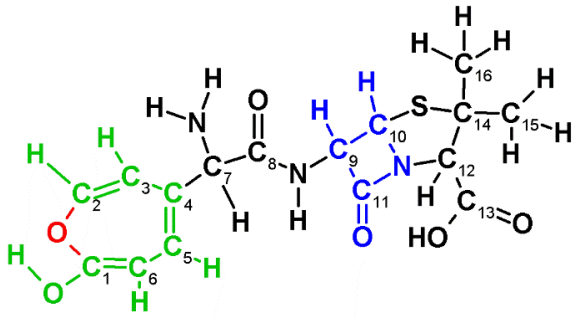
5	C_1OH and C_7NH	1		Ketone is formed H_2O is formed C_7-C_8 is broken C_4-C_8 is formed (-2 Da)
6	C_1OH and C_7H	1		Ketone is formed H_2O is formed C_5=C_6 and C_4=C_7 are formed (-2 Da)
7	C_1OH and C_8NH	2		Ketone is formed H_2O is formed C_7-C_8 is broken C_5=C_6, C_4=C_7 and C_8=N are formed (fragmentation of amoxicillin) (-2 Da)
8	C_2H	5		C_2-OH is formed (+16 Da)
9	C_3H	3		C_3-OH is formed (+16 Da)

10	C_5H	7		C_5-OH is formed (+16 Da)
11	C_6H	7		C_6-OH is formed (+16 Da)
12	C_7H	1		C_7-OH is formed (+16 Da)
13	C_7NH	13		C_7N-OH is formed (+16 Da)
14	C_8NH	1		C_8N-OH is formed (+16 Da)

15	C_9H	1		C_9-OH is formed (+16 Da)
16	$C_{10}H$	1		C_{10}-OH is formed (+16 Da)
17	$C_{12}H$	4		C_{12}-OH is formed (+16 Da)
18	$C_{13}OH$	2		C_{12}-C_{13} is broken $C_{13}O$-C_{12} is formed (+16 Da)
19	$C_{13}OH$	1		C_{12}-C_{13} is broken CO_2 and C_{11}-OH are formed C_{11}-N is broken C_{12}=N is formed (β-lactam ring is opened) (-28 Da)

20	$C_{13}OH$	1		C_{12}-C_{13} is broken CO_2 and C_{12}-OH are formed (-28 Da)
21	$C_{13}OH$ and C_8NH	3		C_{12}-C_{13} is broken CO_2 and C_{12}=N are formed C_{11}-N and C_9-C_{11} are broken CO, H_2O and C_9=N are formed (β-lactam ring is opened) (-74 Da)
22	$C_{13}OH$ and $C_{10}H$	1		C_{12}-C_{13} is broken CO_2 is formed C_{14}-S is broken H_2O, C_{10}=S and C_{12}=C_{14} are formed (-46 Da)
23	$C_{13}OH$ and $C_{16}H$	1		C_{12}-C_{13} is broken CO_2 and C_{12}=N are formed C_{11}-N and C_9-C_{11} are broken CO, H_2O and C_9=C_{10} are formed C_{10}-S and C_{12}-C_{14} are broken C_{12}-C_{16} and C_{14}=S are formed (β-lactam ring is opened) (-74 Da)
24	$C_{15}H$	9		C_{15}-OH is formed (+16 Da)

25	$C_{16}H$	7		C_{16}-OH is formed (+16 Da)
26	–	4		S=O is formed (+16 Da)
27	–	4		C_5-O-C_6 is formed (+16 Da)
28	–	1		C_2-O-C_3 is formed (+16 Da)
29	–	1		C_8-N is broken C_8-O-N is formed (+16 Da)

30	–	2		C_5-O-C_4 is formed (+16 Da)
31	–	1		C_1-C_6 is broken C_1-O-C_6 is formed (+16 Da)
32	–	2		C_7N-O is formed (+16 Da) (not stable N=O bond)
33	–	1		C_1-C_2 is broken C_1-O-C_2 is formed (+16 Da)
TOTAL		**100**		