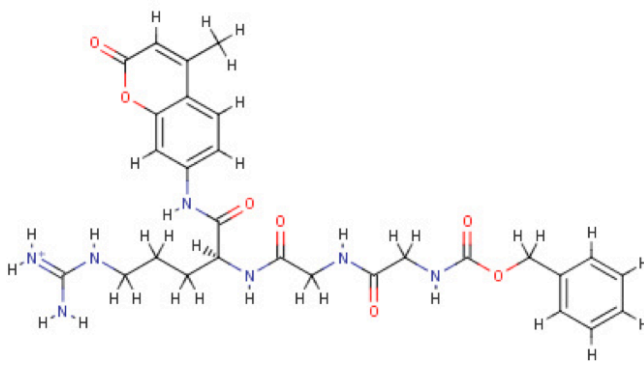
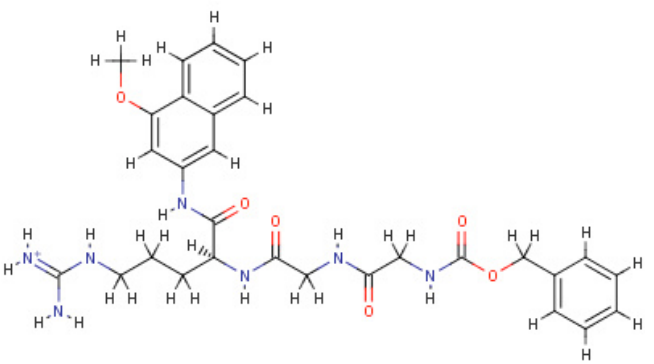
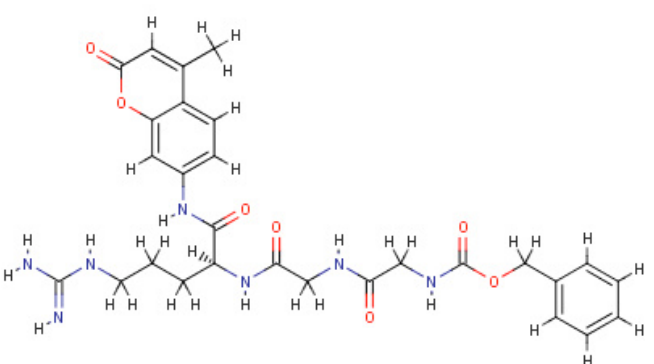
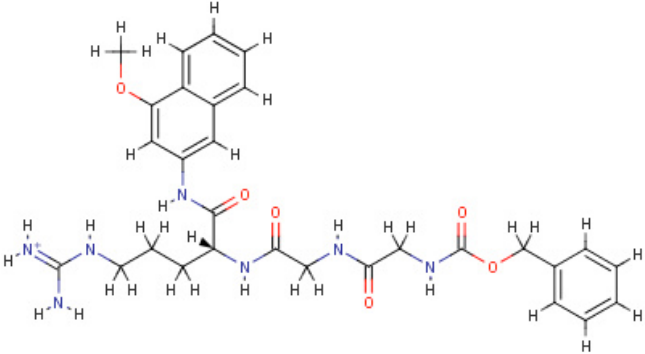
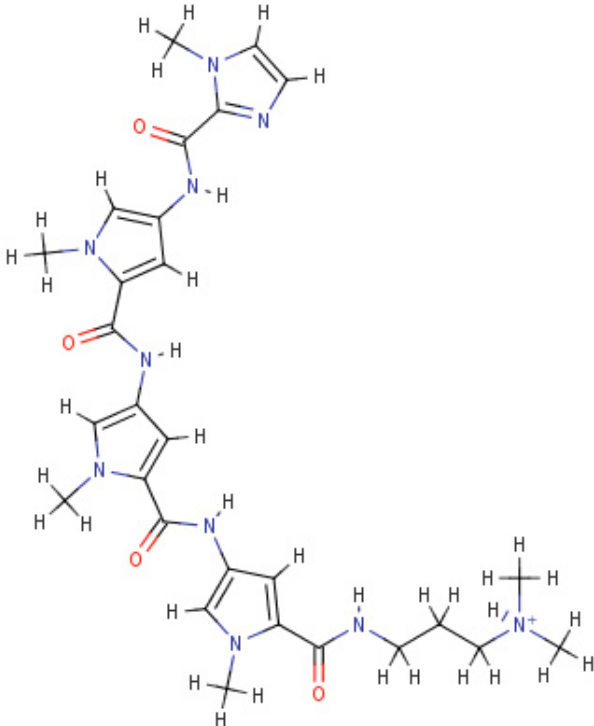
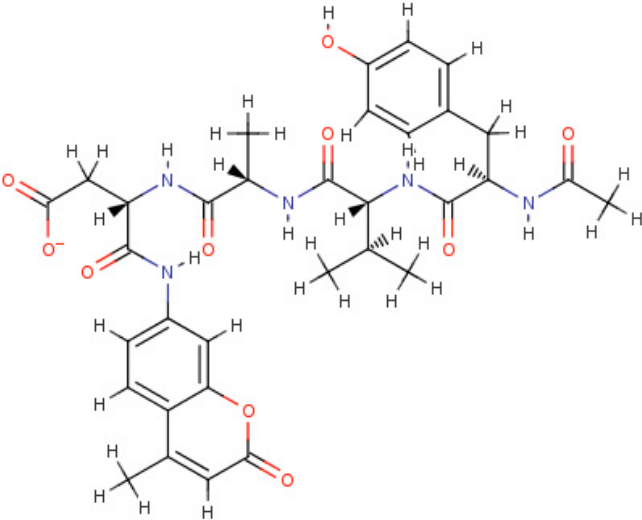
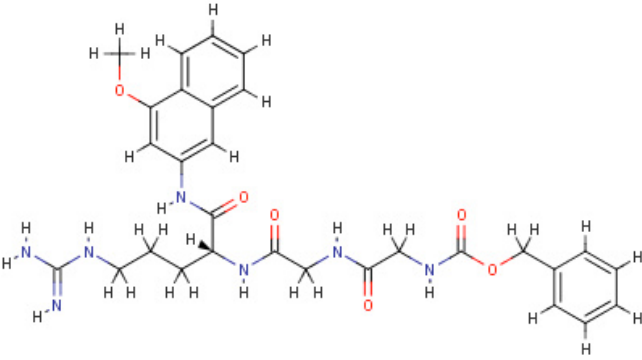
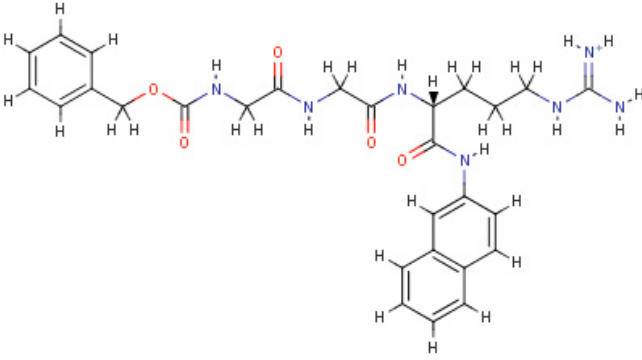
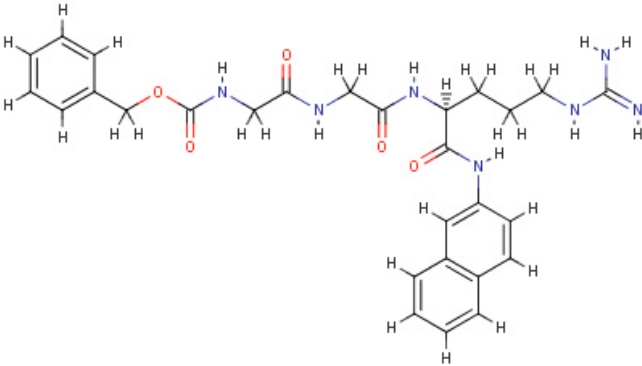
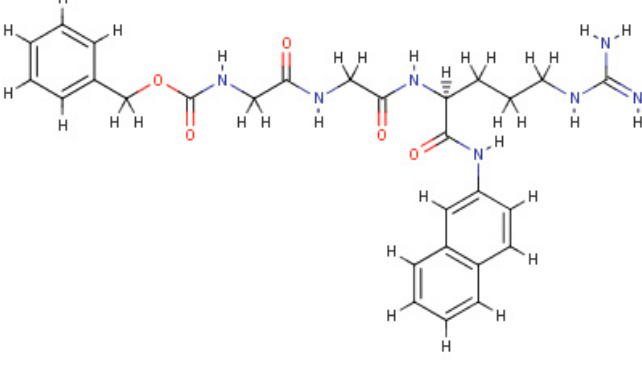
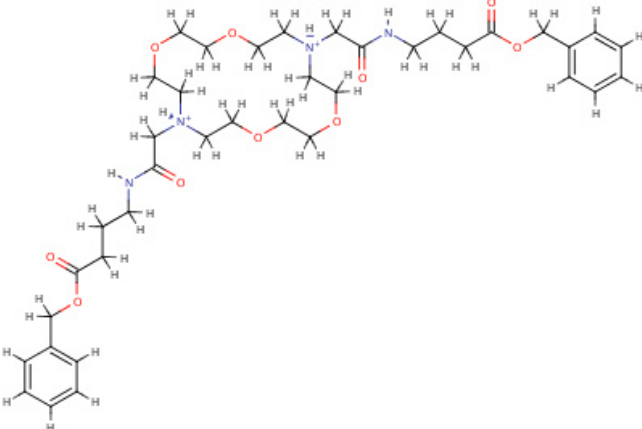


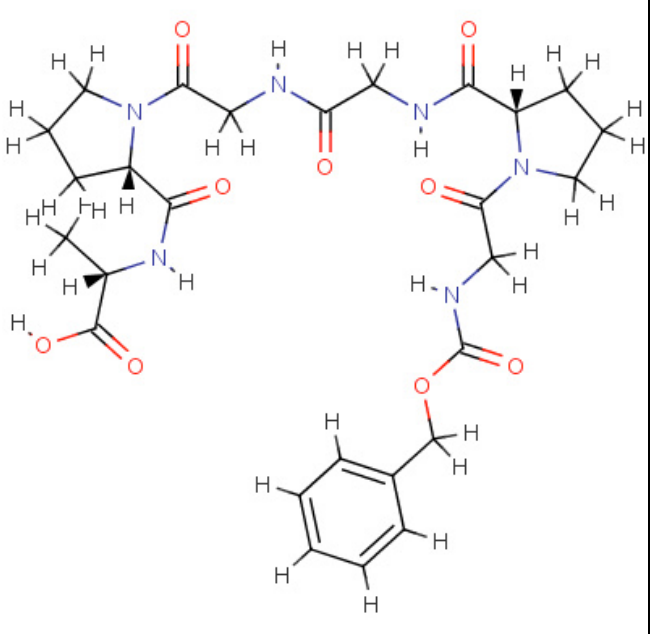
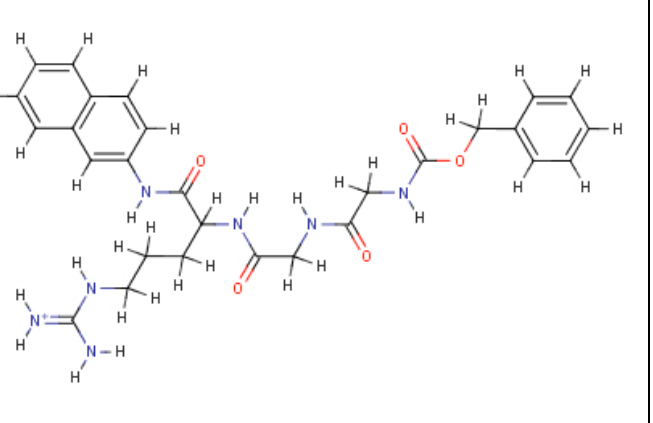
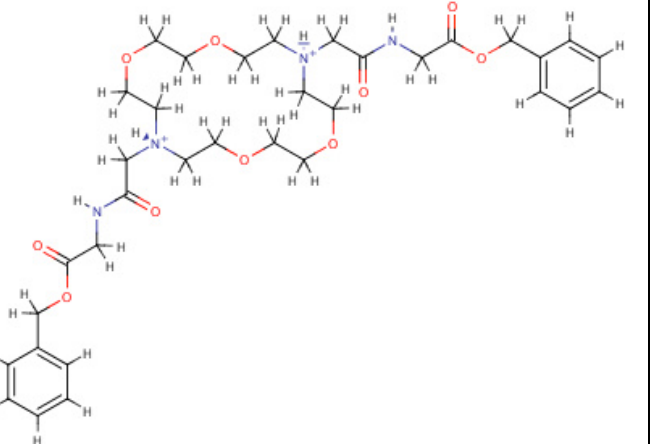
Table S1

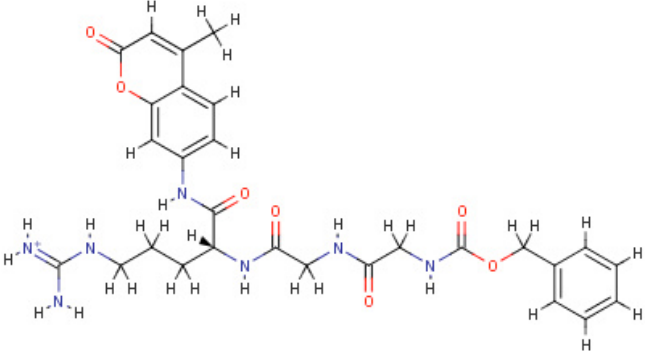
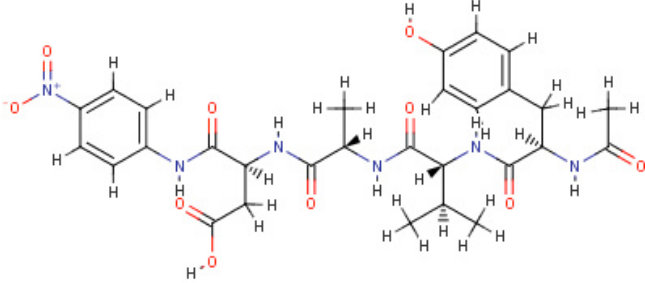
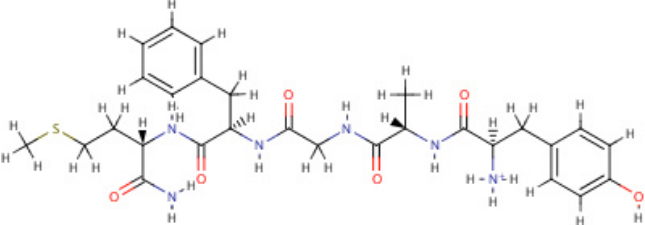
S. No.	pepMMsMIMIC Compound	Score	Mol. Wt.	Structure
1	MMs03919469	0.55	580.622	
2	MMs03919369	0.54	578.65	
3	MMs03919468	0.50	579.614	

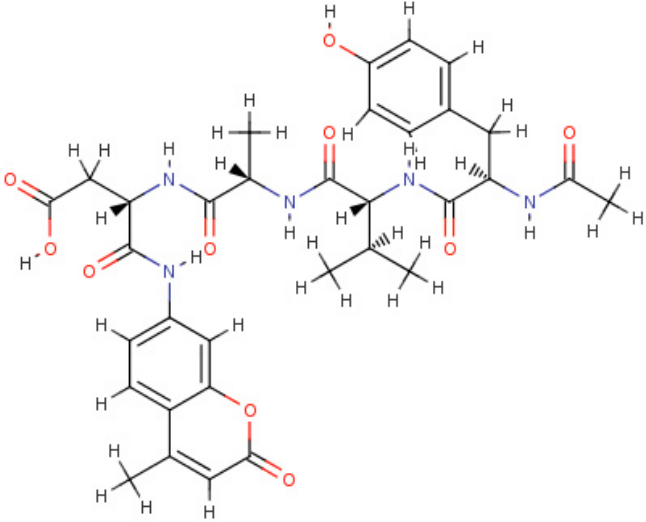
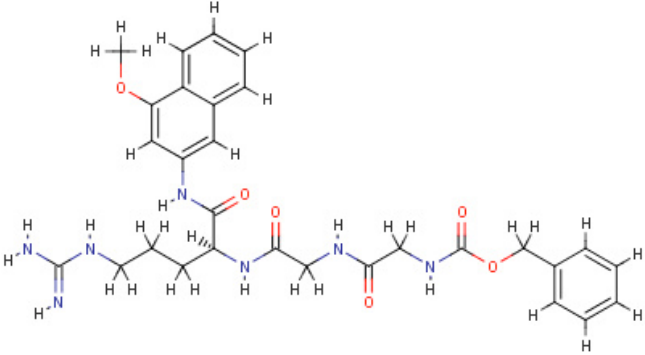
4	MMs03919367	0.49	578.65	 <p>The structure shows a benzene ring with a methoxy group (-OCH₃) at the top. An amide group (-NH-C(=O)-) is attached to the ring. This amide is linked to a guanidinium group, which is further connected to a carboxylate group (-COO-) via an amide linkage. The guanidinium group is shown with its characteristic three nitrogen atoms and a central carbon atom.</p>
5	MMs02548719	0.49	577.67	 <p>The structure consists of a chain of four pyrrole rings linked by amide bonds (-NH-C(=O)-). The chain starts with a pyrrole ring at the top, followed by three more pyrrole rings. The final pyrrole ring is linked to a guanidinium group (-N⁺(CH₃)₃), which is shown with its characteristic three nitrogen atoms and a central carbon atom. The guanidinium group is shown with its positive charge and three methyl groups.</p>

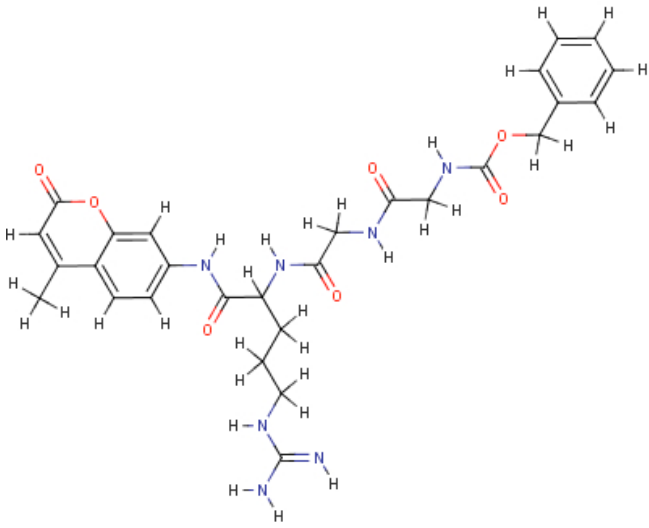
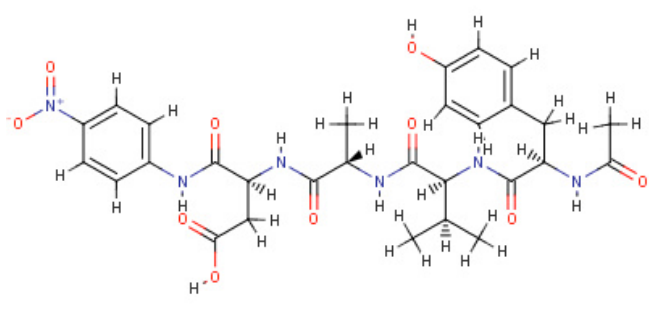
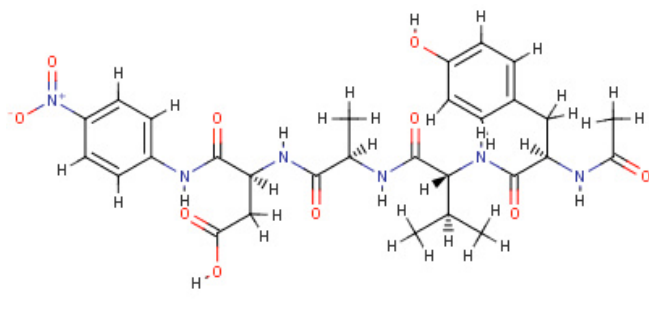
6	MMs03918861	0.49	664.692	
7	MMs03919366	0.45	577.642	
8	MMs03919425	0.45	548.624	

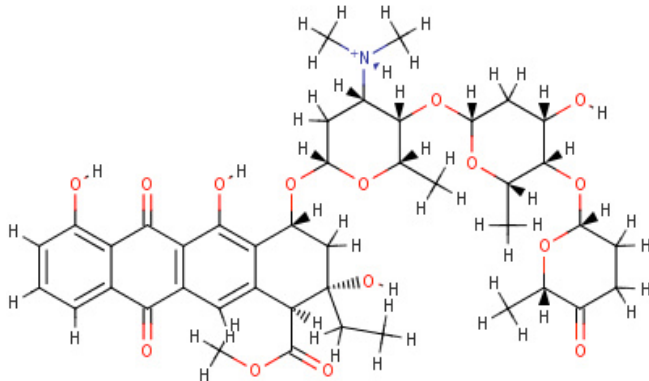
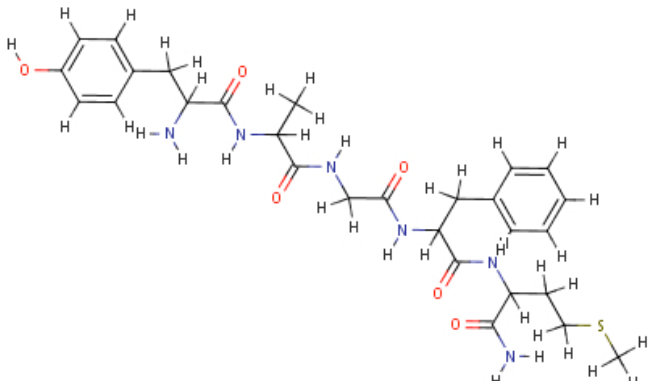
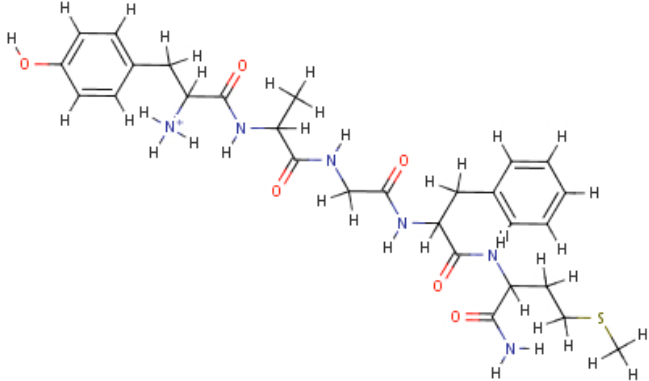
9	MMs03919422	0.45	547.616	 <p>The structure shows a peptide chain with a benzyl group at the N-terminus and a guanidino group at the C-terminus. The peptide backbone consists of several amino acid residues, including a proline ring. The guanidino group is attached to the side chain of the C-terminal residue.</p>
10	MMs03919424	0.44	547.616	 <p>This structure is identical to the one in row 9, showing a peptide chain with a benzyl group at the N-terminus and a guanidino group at the C-terminus.</p>
11	MMs03924092	0.43	730.9	 <p>The structure is a complex peptide derivative. It features a central peptide backbone with multiple modifications, including a benzyl group, a guanidino group, and a proline ring. The structure is highly branched and contains several amide bonds and side chains.</p>

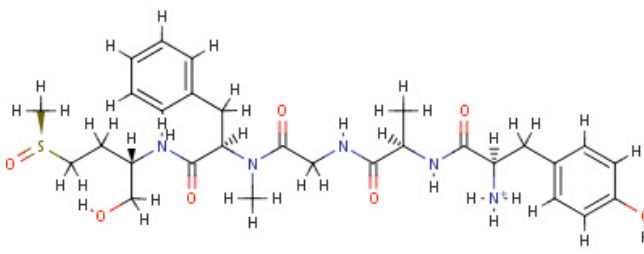
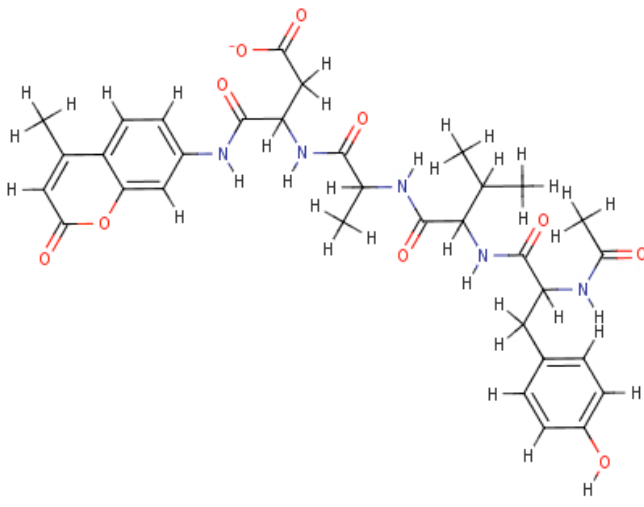
12	MMs03919433	0.42	588.618	
13	MMs03919423	0.41	548.624	
14	MMs03924085	0.40	674.792	

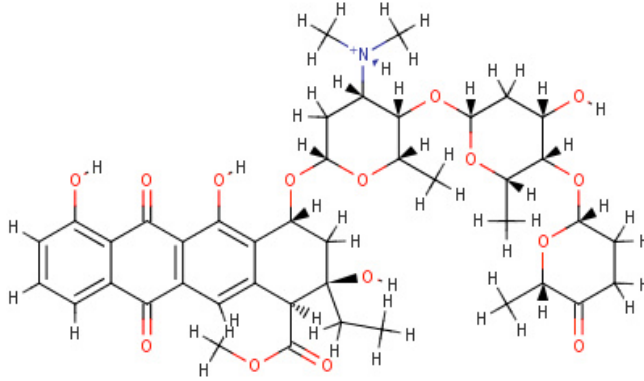
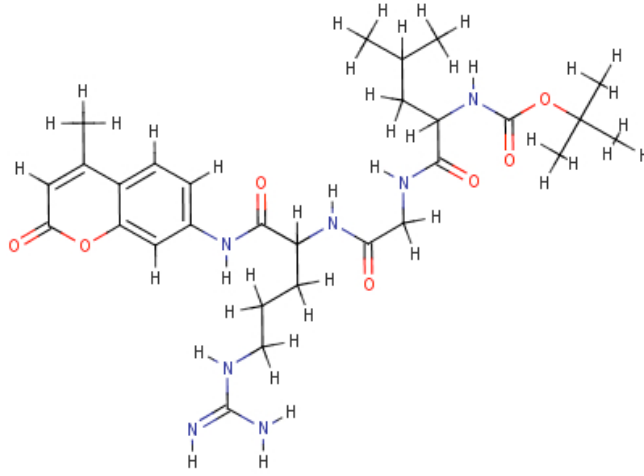
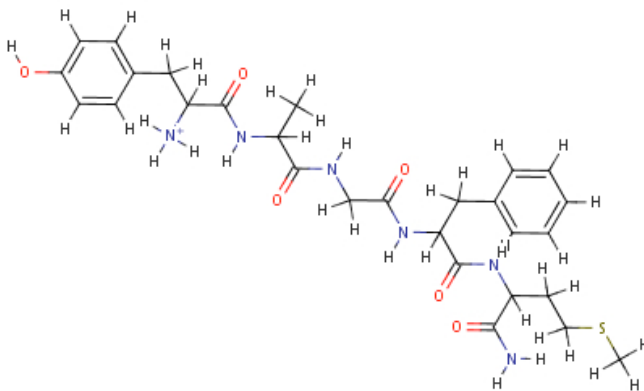
15	MMs03919467	0.39	580.622	
16	MMs03918885	0.37	628.639	
17	MMs02467784	0.36	587.722	

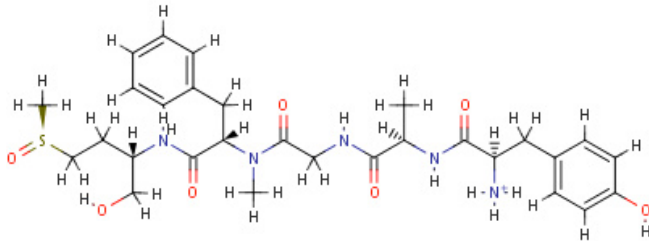
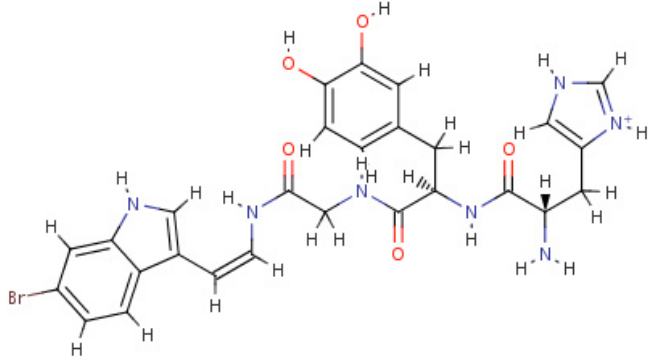
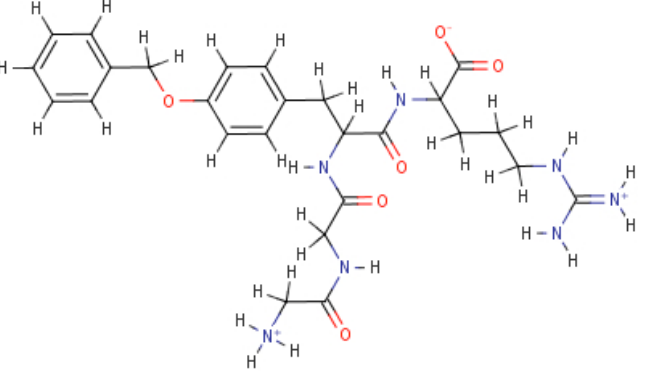
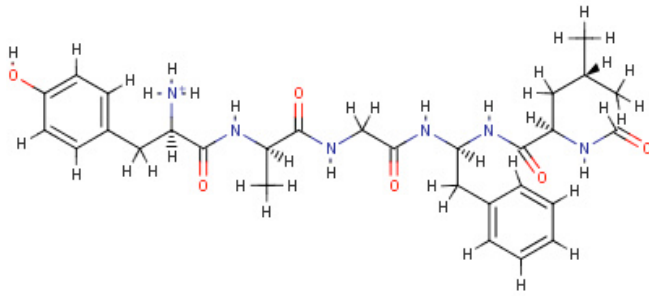
18	MMs03918860	0.36	665.7	 <p>The structure shows a central chain of amide and ester linkages. On the left, a benzene ring is attached to a nitrogen atom, which is part of an amide group. On the right, another benzene ring is attached to a carbon atom, which is part of an ester group. The molecule contains several chiral centers indicated by wedged and dashed bonds.</p>
19	MMs03919368	0.36	577.642	 <p>The structure shows a central chain of amide and ester linkages. On the left, a benzene ring is attached to a nitrogen atom, which is part of an amide group. On the right, another benzene ring is attached to a carbon atom, which is part of an ester group. The molecule contains several chiral centers indicated by wedged and dashed bonds.</p>

20	MMs03919466	0.36	579.614	
21	MMs03918883	0.32	628.639	
22	MMs03918889	0.30	628.639	

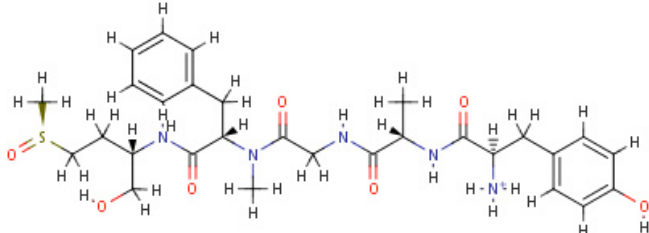
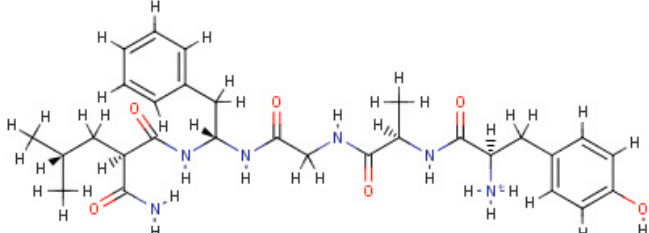
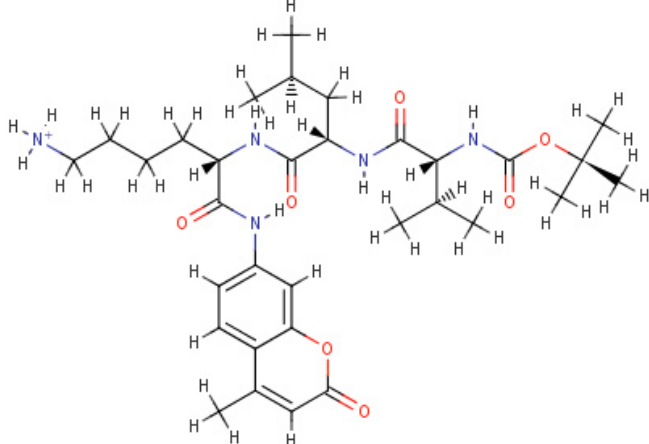
23	MMs01727547	0.29	812.886	
24	MMs02467779	0.29	586.714	
25	MMs02467780	0.28	587.722	

26	MMs02391032	0.27	604.749	
27	MMs03918857	0.27	664.692	

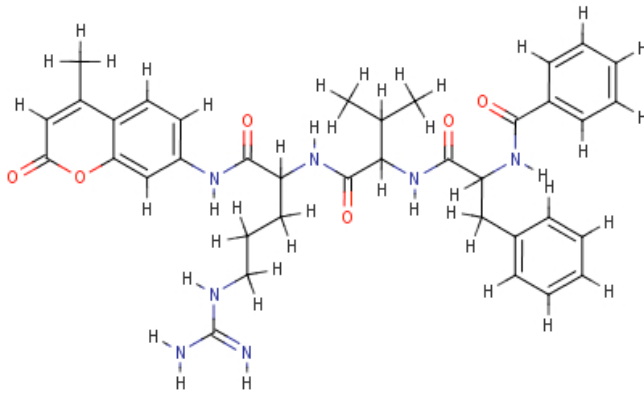
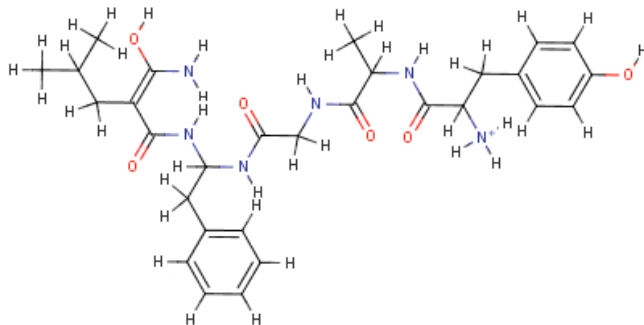
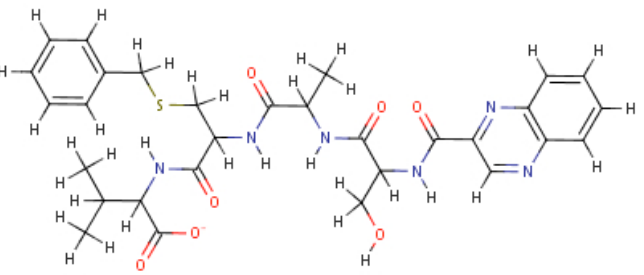
31	MMs01727549	0.25	812.886	
32	MMs03919145	0.25	601.705	
33	MMs02467786	0.25	587.722	

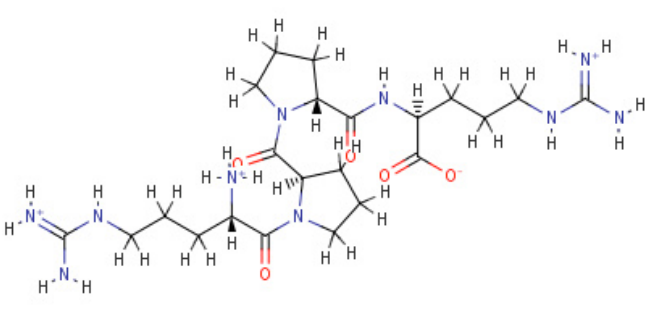
34	MMs02391028	0.25	604.749	
35	MMs02489379	0.25	611.477	
36	MMs02481161	0.24	542.617	
37	MMs02514534	0.24	569.683	

38	MMs02467782	0.24	587.722	
39	MMs03919122	0.23	573.675	
40	MMs02514549	0.23	569.683	

41	MMs02391026	0.23	604.749	
42	MMs02514564	0.23	569.683	
43	MMs03919120	0.23	616.78	

44	MMs03919124	0.22	573.675	
45	MMs03919146	0.22	602.713	
46	MMs02514537	0.22	569.683	

47	MMs03919198	0.22	681.794	
48	MMs02514563	0.22	569.683	
49	MMs02421858	0.21	623.711	
50	MMs02487107	0.21	526.643	

				
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