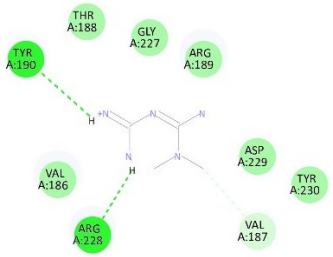
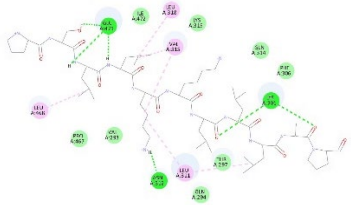
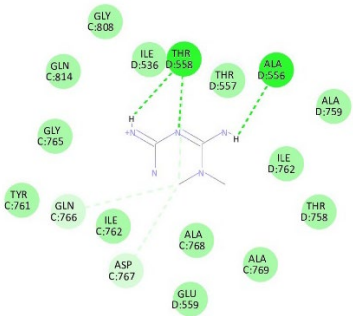
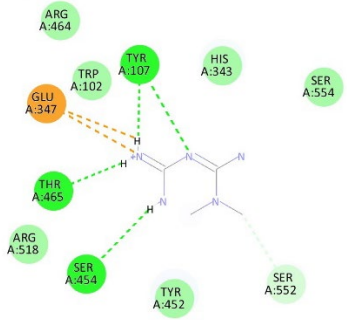
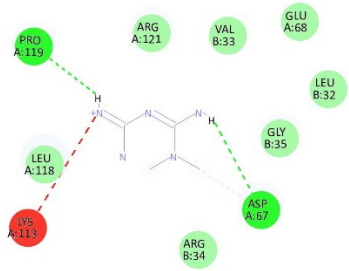
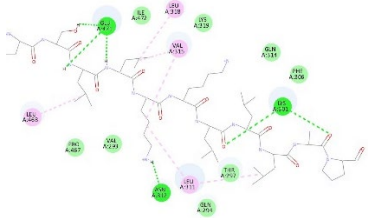
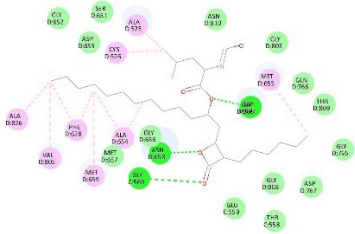
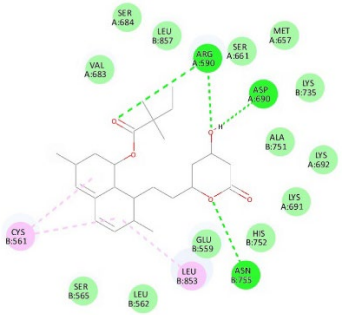
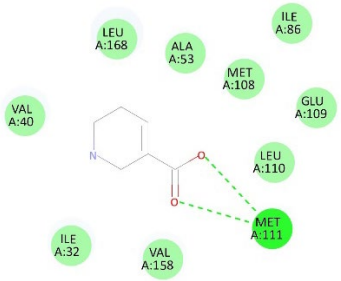
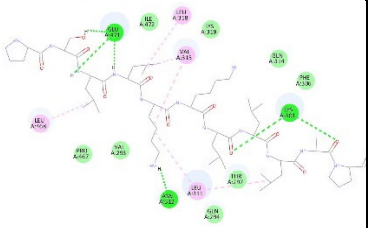
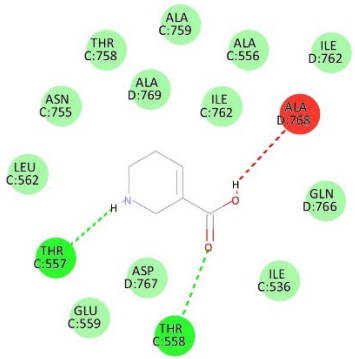
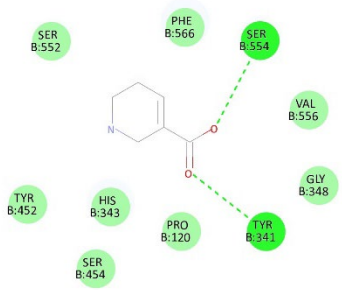
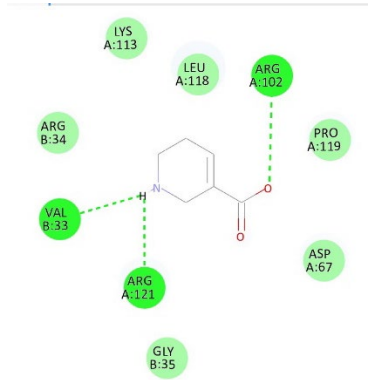
Tabel S1. Compounds and Peptides SMILE Canonical from FOE

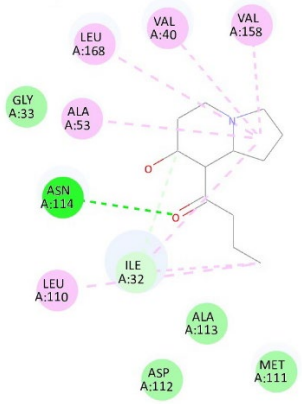
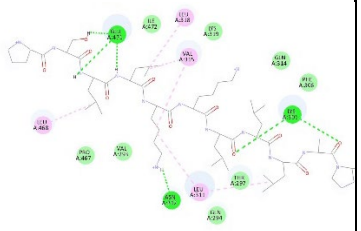
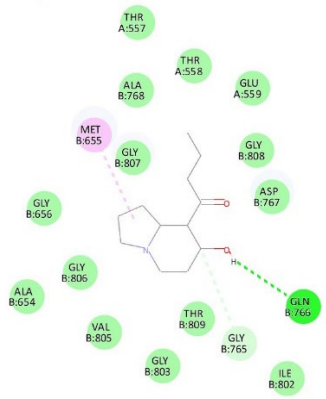
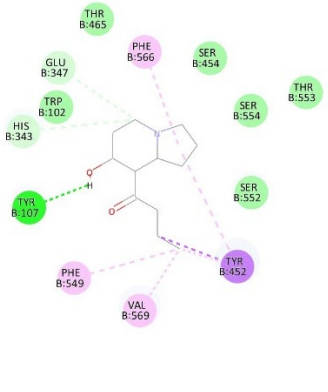
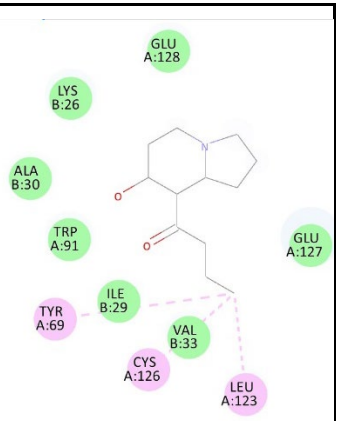
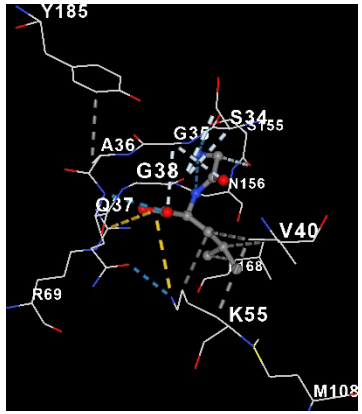
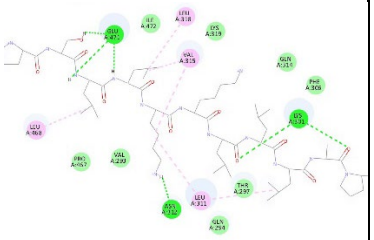
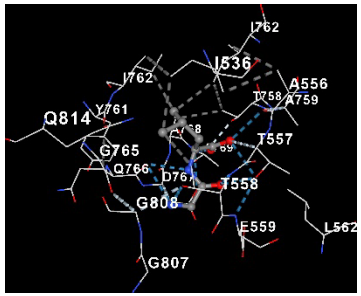
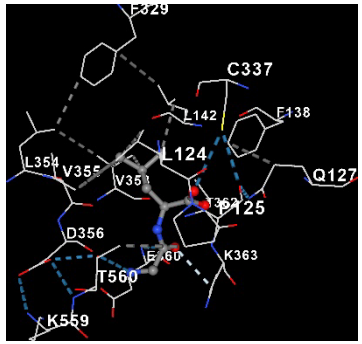
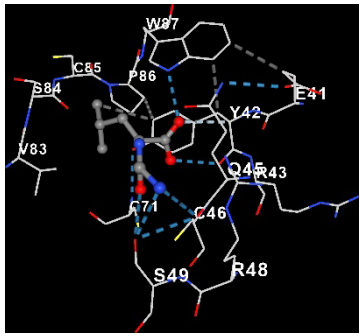
Compounds	**Compounds**	**SMILES Canonical**
C1	p-Cresol	CC1=CC=C(C=C1)O
C2	4-Fluorophenol	C1=CC(=CC=C1O)F
C3	Guvacine	C1CNCC(=C1)C(=O)O
C4	Furaneol	CC1C(=O)C(=C(O1)C)O
C5	p-cymene	CC1=CC=C(C=C1)C(C)C
C6	Elaeokanine C	CCCC(=O)C1C2CCCN2CCC1O
C7	Flavokawain A	COC1=CC=C(C=C1)C=CC(=O)C2=C(C=C(C=C2OC)OC)O
C8	3-hydroxy-3,4-bis[(4-hydroxy-3-methoxyphenyl)methyl]oxolan-2-one	COC1=C(C=CC(=C1)CC2COC(=O)C2(CC3=CC(=C(C=C3)O)OC)O)O
C9	Euparin	CC(=C)C1=CC2=CC(=C(C=C2O1)O)C(=O)C
C10	Eleutherol	CC1C2=C(C=C3C=CC=C(C3=C2O)OC)C(=O)O1

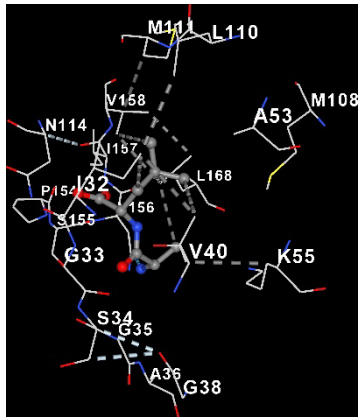
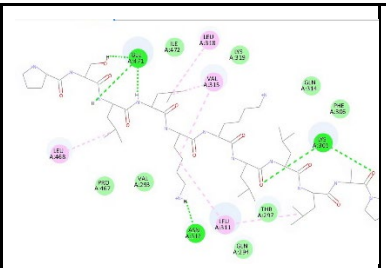
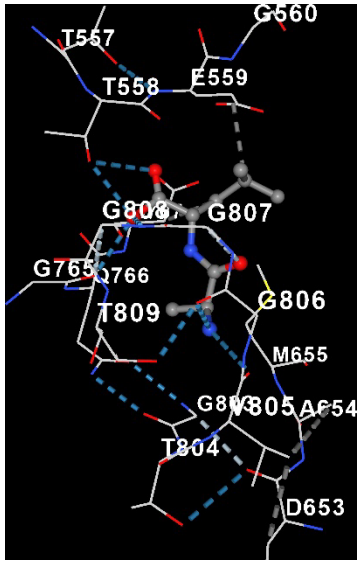
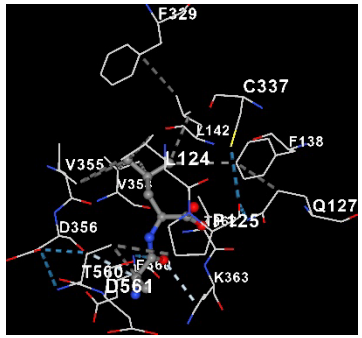
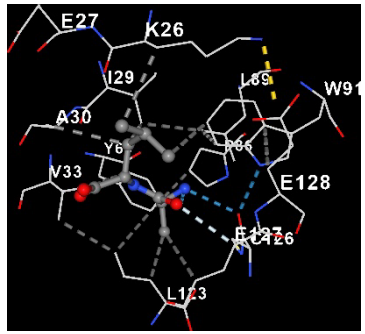
Peptides No	**Peptides**	**SMILES Canonical**
P1	Gly-Leu	CC(C)CC(C(=O)O)NC(=O)CN
P2	Ala-Leu	CC(C)CC(C(=O)O)NC(=O)C(C)N
P3	Val-Ser	CC(C)C(C(=O)NC(CO)C(=O)O)N
P4	Gly-Phe	C1=CC=C(C=C1)CC(C(=O)O)NC(=O)CN
P5	Ala-Phe	CC(C(=O)NC(CC1=CC=CC=C1)C(=O)O)N
P6	Asp-leu	CC(C)CC(C(=O)O)NC(=O)C(CC(=O)O)N
P7	Val-Met	CC(C)C(C(=O)NC(CCSC)C(=O)O)N
P8	Ala-Tyr	CC(C(=O)NC(CC1=CC=C(C=C1)O)C(=O)O)N
P9	Lys-Leu	CC(C)CC(C(=O)O)NC(=O)C(CCCCN)N
P10	Arg-Leu	CC(C)CC(C(=O)O)NC(=O)C(CCCN=C(N)N)N
P11	Arg-Glu	C(CC(C(=O)NC(CCC(=O)O)C(=O)O)N)CN=C(N)N

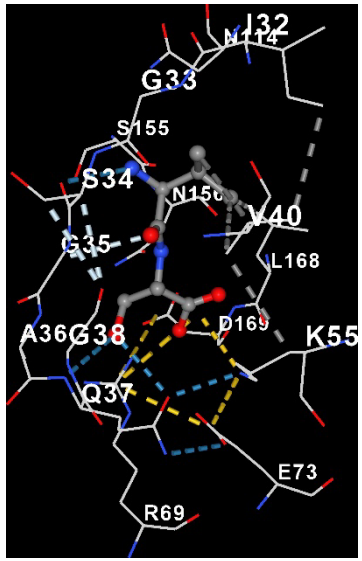
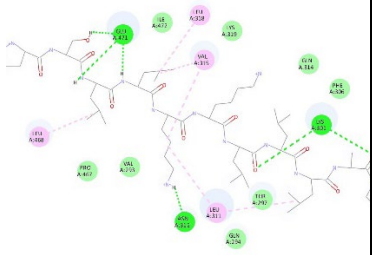
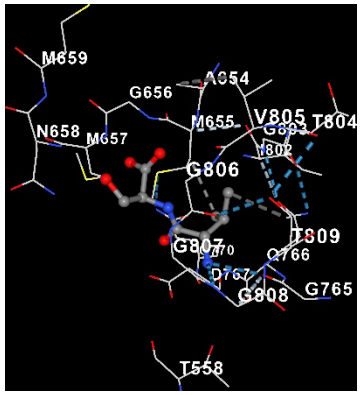
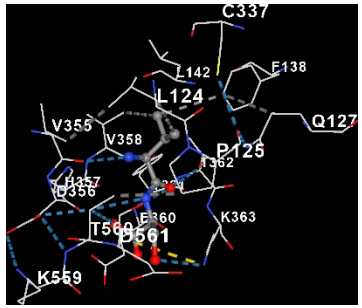
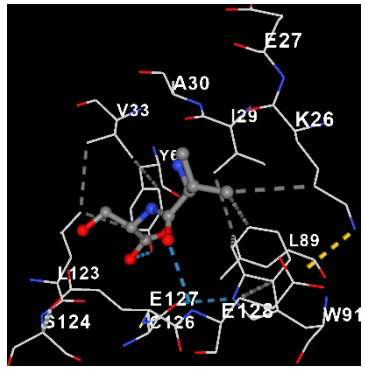
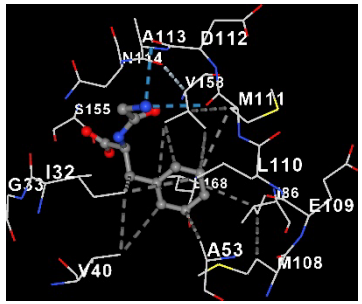
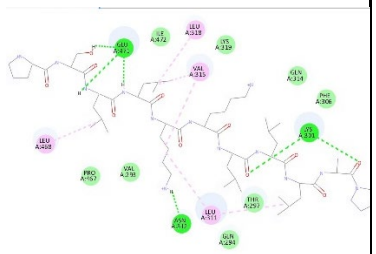
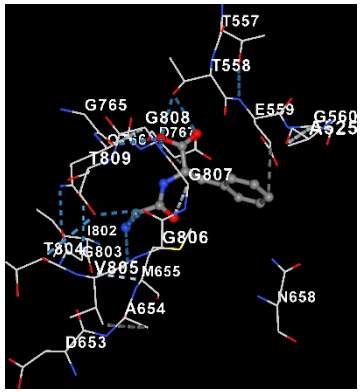
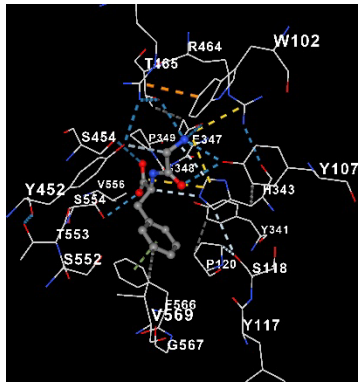
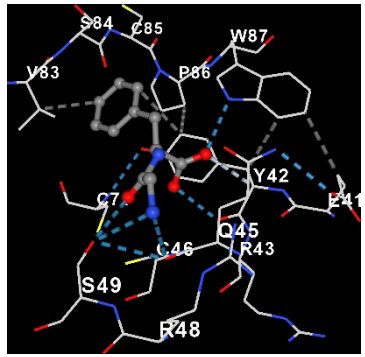
Table S2. Full Visualization of Amino Acid Interaction of FOE Properties against MAPK8, PPARG, HMGCR, CPT-1, and GLP-1

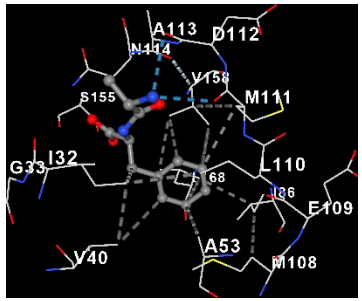
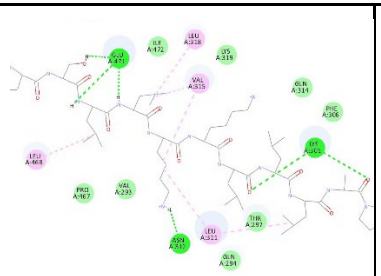
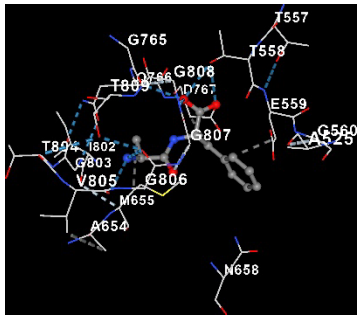
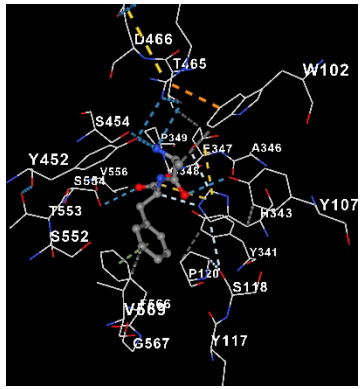
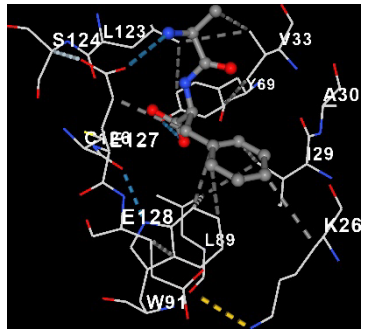
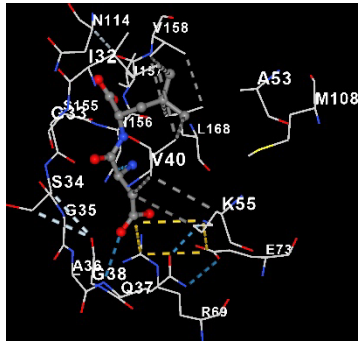
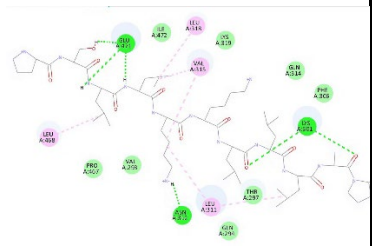
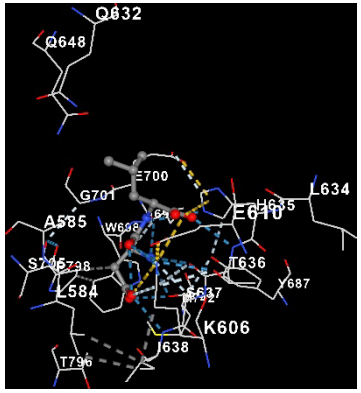
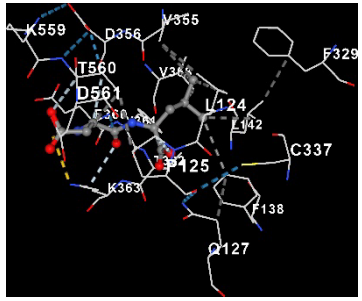
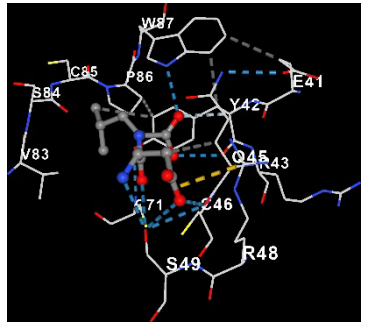
Compounds/Peptides and Control as Ligands	MAPK8 (3ELJ)	PPARG (8BF1)	HMGCR (2R4F)	CPT-1 (1NDB)	GLP-1 (4ZGM)
Control Metformin (4901)					
Control Orlistat (3034010)					

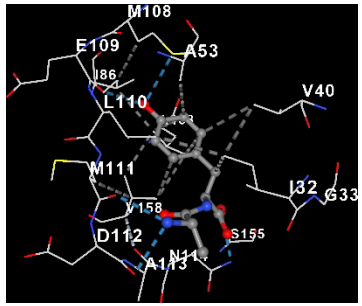
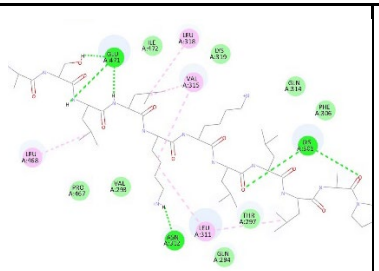
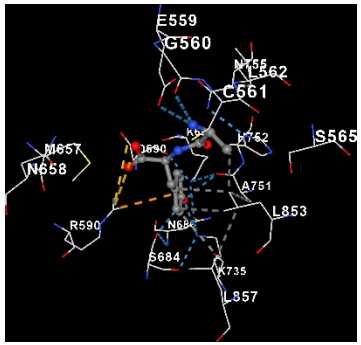
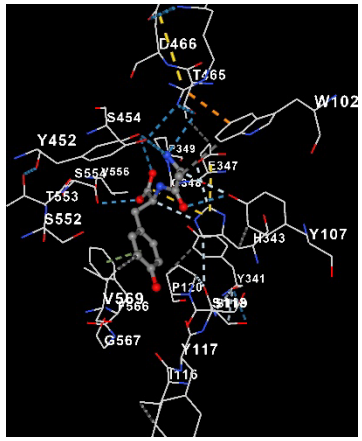
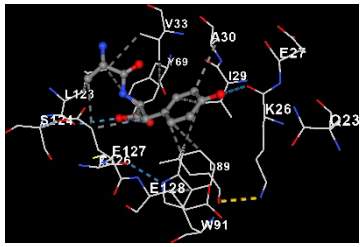
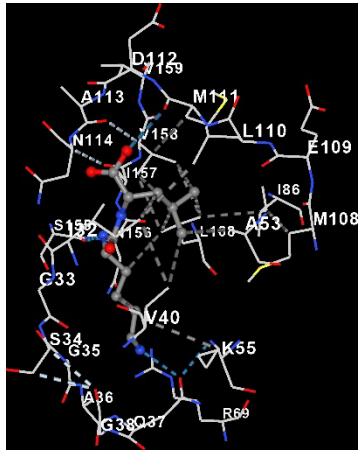
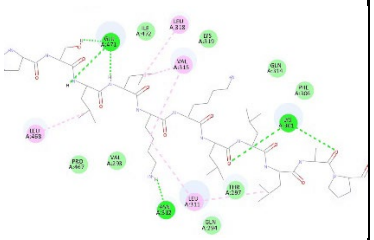
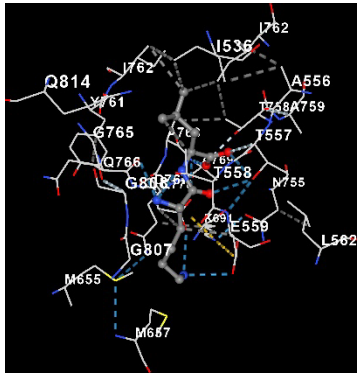
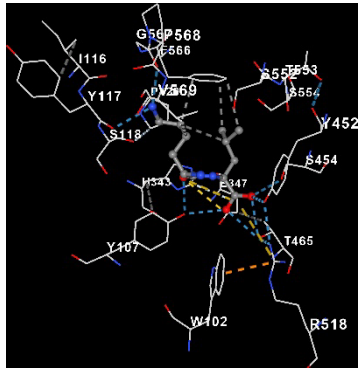
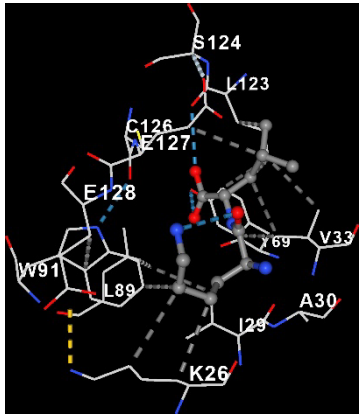
Control Simvastatin (54454)					
C3 (3532)					

C6 (442855)	 LEU A:168 VAL A:40 VAL A:158 GLY A:33 ALA A:53 ASN A:114 ILE A:32 LEU A:110 ALA A:113 ASP A:112 MET A:111		 THR A:557 THR A:558 ALA B:768 GLU A:559 MET B:655 GLY B:807 GLY B:808 ASP B:767 GLY B:656 GLY B:806 ALA B:654 VAL B:805 THR B:809 GLN B:766 GLY B:765 GLY B:803 ILE B:802	 THR B:465 PHE B:566 SER B:454 GLU B:347 THR B:553 TRP B:102 SER B:554 HIS B:343 SER B:552 TYR B:107 TYR B:452 PHE B:549 VAL B:569	 GLU A:128 LYS B:26 ALA B:30 TRP A:91 GLU A:127 ILE B:29 TYR A:69 VAL B:33 CYS A:126 LEU A:123
P1	 Y185 S34 G35 A36 G38 N156 Q37 V40 R69 K55 M108		 I762 I536 A556 Q814 T557 G765 T558 G808 E559 G807	 C337 L142 F138 L124 Q127 L354 V355 P125 D356 K363 T560 K559	 W97 C85 S84 P86 E41 Y42 V83 Q45 R43 C71 C46 S49 R48

P2	 M111 L110 V158 A53 M108 N114 I157 L168 P154 I32 156 S155 G33 V40 K55 S34 G35 A36 G38		 T557 G560 T558 E559 G807 G765 Q766 T809 G806 M655 T804 D653	 F329 C337 L142 F138 L124 V355 Q127 D356 T560 D561 K363	 E27 K26 I29 W91 A30 V33 E128 L123

P3	 I32 N114 G33 S155 S34 N150 V40 G35 L168 A36 G38 D169 K55 Q37 E73 R69		 M659 G656 A654 N658 M657 M655 V805 T804 G806 T809 G807 Q766 D767 G808 G765 T558	 C337 F138 L124 Q127 V355 V358 P125 K363 K559	 E27 A30 V33 I29 K26 L89 L123 E127 S124 E126 E128 W91
P4	 A113 D112 N114 V158 S155 M111 I32 G33 L110 E168 I86 E109 A53 V40 M108		 T557 T558 G765 G808 E559 T809 G807 I802 G806 T804 G803 V805 M655 A654 N658 D653	 R464 W102 T465 S454 E347 Y107 Y452 S554 T343 T553 Y341 S552 P120 S118 Y117 G567	 S84 C85 W87 V83 P86 Y42 C7 Q45 C46 R43 S49 R48

P5	 A113 D112 N114 V158 S155 M111 G33 I32 L110 E109 V40 A53 M108		 T557 G765 T558 G808 D767 E559 G807 G806 V805 M655 A654 N658	 D466 T465 W102 S454 Y452 E347 A346 Y107 H343 S552 Y341 P120 S178 Y117 G567	 S124 L123 Y33 Y69 A30 E127 29 E128 L89 K26 W91
P6	 N114 V158 I32 A53 M108 L168 V40 S34 G35 K55 E73 A36 G38 Q37		 Q632 Q648 G701 L634 A585 E610 L584 T636 K606 J638 T796	 K559 D356 V355 F329 T560 D561 L124 C337 P125 F138 Q127	 W87 C85 P86 E41 S84 Y42 V83 Q45 R43 Y71 E46 S49 R48

P8	 M108 E109 A53 I86 L110 V40 M111 I32 G33 V158 D112 S155 A113		 E559 G560 C561 S565 M657 N658 R590 A751 L853 S684 L857	 D466 T465 W102 S454 Y452 T553 S552 E347 H343 Y107 Y341 V569 G567 Y117	 V33 A30 E27 I29 K26 Q23 L123 S124 E127 E128 W91
P9	 D112 A113 M111 L110 E109 N114 I86 M108 A53 G33 V40 S34 G35 K55 A36 R69		 I762 I536 Q814 A556 G765 T557 T558 N755 E559 L562 G807 M655 M657	 I116 Y117 S118 Y452 S454 T465 Y107 W102 R518	 S124 L123 C126 E127 E128 V33 Y69 W91 L89 A30 I29 K26