



Research Article

Putative Vegetal Inhibitors Against ns2 and vp4 Proteins of African Horse Sickness Virus: Molecular Modelling, Density Functional Theory Analysis, and Toxicokinetic Analyses

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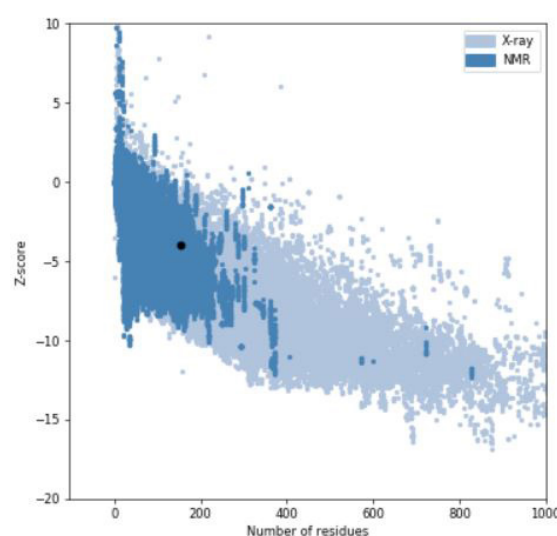
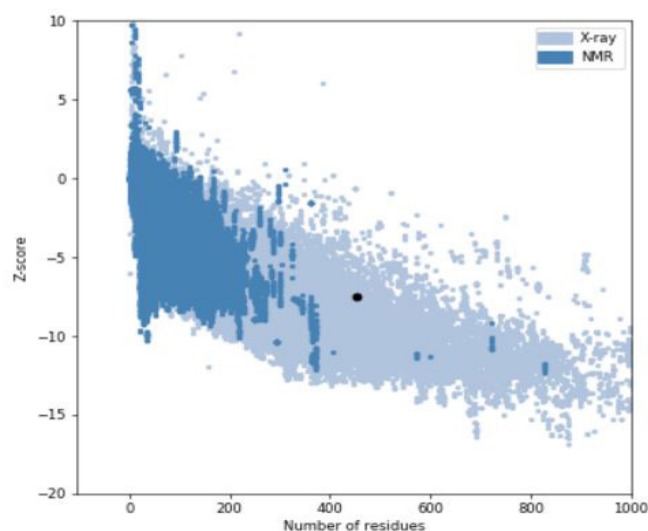
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Keywords | African horse sickness virus AHSV, ns2 vp4, Virtual screening, DFT, Epigallocatechin gallate, Plant biodiversity in Nigeria



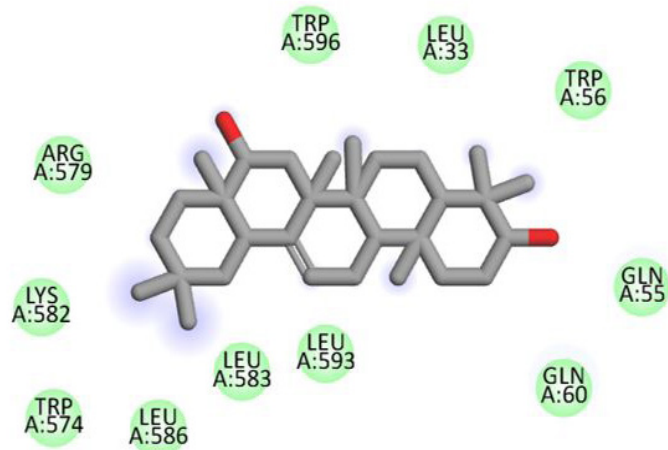
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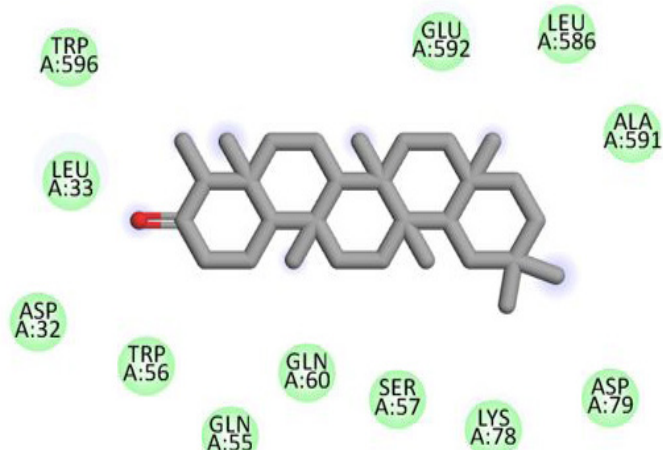


Supplementary Figure 1: The Z-score of homology modelled vp4 protein of AHSV. Z score value = -7.45, within the region of experimentally (x-ray) determined models.

Supplementary Figure 2: The Z-score of homology modelled ns2 protein of AHSV. Z score value = -3.96, within the region of experimentally (NMR) determined models.



Supplementary Figure 3: Maniladiol makes no strong molecular interaction with vp4 protein of African horse sickness virus.



Supplementary Figure 4: Friedelin makes no strong molecular interaction with vp4 protein of African horse sickness virus.

Supplementary Table 1: Molecular interactions of the top nine binding ligands to active site of ns2 protein of AHSV.

S. No	Ligand	Interacting residues involved in non van der waal interaction
1.	Warangalone	Thr 102, Arg 125, Ala 129, Pro 131, Val 130
2.	Uzarigenin	Ala 100, Ser 127
3.	Ursolic acid	Arg 160, Glu 94
4.	Maniladiol	-
5.	Luteolin	Thr 102, Ala 100, Thr 102, Phe 98, Glu 99
6.	Friedelin	-
7.	Epigallocatechin gallate	Asp 139, Lys 135, Asn 136, Arg 160, Pro 105, Met 138, Val 156
8.	Alpinumisoflavone	Ala 100, Glu 99, Ser 127
9.	Aurintricarboxylic acid	Met 143, Val 156, Arg 157, Arg 160, Met 138

Supplementary Table 2: Binding Affinity score (kCal/Mol) of ligands to ns2 and vp4 of AHSV.

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_92776_uff_E=205.59	-4.6	prepared_vp4_92776_uff_E=205.59	-6.2
Prepared_ns2_92776_uff_E=205.59	-4.5	prepared_vp4_92776_uff_E=205.59	-5.7
Prepared_ns2_92776_uff_E=205.59	-4.5	prepared_vp4_92776_uff_E=205.59	-5.7
Prepared_ns2_92776_uff_E=205.59	-4.4	prepared_vp4_92776_uff_E=205.59	-5.6
Prepared_ns2_92776_uff_E=205.59	-4.4	prepared_vp4_92776_uff_E=205.59	-5.5
Prepared_ns2_92776_uff_E=205.59	-4.1	prepared_vp4_92776_uff_E=205.59	-5.5
Prepared_ns2_92776_uff_E=205.59	-4	prepared_vp4_92776_uff_E=205.59	-5.5
Prepared_ns2_92776_uff_E=205.59	-3.9	prepared_vp4_92776_uff_E=205.59	-5.4
Prepared_ns2_92776_uff_E=205.59	-3.9	prepared_vp4_92776_uff_E=205.59	-5.1
Prepared_ns2_73207_uff_E=488.20	-6.4	prepared_vp4_73207_uff_E=488.20	-7.6
Prepared_ns2_73207_uff_E=488.20	-6.3	prepared_vp4_73207_uff_E=488.20	-7.6
Prepared_ns2_73207_uff_E=488.20	-6.3	prepared_vp4_73207_uff_E=488.20	-7.6
Prepared_ns2_73207_uff_E=488.20	-6.2	prepared_vp4_73207_uff_E=488.20	-7.1
Prepared_ns2_73207_uff_E=488.20	-6.2	prepared_vp4_73207_uff_E=488.20	-7
Prepared_ns2_73207_uff_E=488.20	-5.9	prepared_vp4_73207_uff_E=488.20	-7
Prepared_ns2_73207_uff_E=488.20	-5.7	prepared_vp4_73207_uff_E=488.20	-6.9
Prepared_ns2_73207_uff_E=488.20	-5.7	prepared_vp4_73207_uff_E=488.20	-6.8

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_73207_uff_E=488.20	-5.5	prepared_vp4_73207_uff_E=488.20	-6.6
Prepared_ns2_5379679_uff_E=474.91	-7.9	prepared_vp4_5379679_uff_E=474.91	-8.5
Prepared_ns2_5379679_uff_E=474.91	-7.6	prepared_vp4_5379679_uff_E=474.91	-8.2
Prepared_ns2_5379679_uff_E=474.91	-7.5	prepared_vp4_5379679_uff_E=474.91	-8.1
Prepared_ns2_5379679_uff_E=474.91	-7.4	prepared_vp4_5379679_uff_E=474.91	-7.8
Prepared_ns2_5379679_uff_E=474.91	-7.3	prepared_vp4_5379679_uff_E=474.91	-7.7
Prepared_ns2_5379679_uff_E=474.91	-7.1	prepared_vp4_5379679_uff_E=474.91	-7.6
Prepared_ns2_5379679_uff_E=474.91	-7	prepared_vp4_5379679_uff_E=474.91	-7.6
Prepared_ns2_5379679_uff_E=474.91	-6.8	prepared_vp4_5379679_uff_E=474.91	-7.4
Prepared_ns2_5379679_uff_E=474.91	-6.7	prepared_vp4_5379679_uff_E=474.91	-7.4
Prepared_ns2_5280441_uff_E=409.01	-6.8	prepared_vp4_5280441_uff_E=409.01	-8.1
Prepared_ns2_5280441_uff_E=409.01	-6.6	prepared_vp4_5280441_uff_E=409.01	-7.8
Prepared_ns2_5280441_uff_E=409.01	-6.6	prepared_vp4_5280441_uff_E=409.01	-7.7
Prepared_ns2_5280441_uff_E=409.01	-6.6	prepared_vp4_5280441_uff_E=409.01	-7.6
Prepared_ns2_5280441_uff_E=409.01	-6.5	prepared_vp4_5280441_uff_E=409.01	-7.5
Prepared_ns2_5280441_uff_E=409.01	-6.4	prepared_vp4_5280441_uff_E=409.01	-7.5
Prepared_ns2_5280441_uff_E=409.01	-6.3	prepared_vp4_5280441_uff_E=409.01	-7.4
Prepared_ns2_5280441_uff_E=409.01	-6.3	prepared_vp4_5280441_uff_E=409.01	-7.4
Prepared_ns2_5280441_uff_E=409.01	-6.3	prepared_vp4_5280441_uff_E=409.01	-7.4
Prepared_ns2_92760_uff_E=672.76	-8.2	prepared_vp4_92760_uff_E=672.76	-8.7
Prepared_ns2_92760_uff_E=672.76	-8.2	prepared_vp4_92760_uff_E=672.76	-8.4
Prepared_ns2_92760_uff_E=672.76	-7.9	prepared_vp4_92760_uff_E=672.76	-7.8
Prepared_ns2_92760_uff_E=672.76	-7.8	prepared_vp4_92760_uff_E=672.76	-7.7
Prepared_ns2_92760_uff_E=672.76	-7.4	prepared_vp4_92760_uff_E=672.76	-7.6
Prepared_ns2_92760_uff_E=672.76	-7.3	prepared_vp4_92760_uff_E=672.76	-7.5
Prepared_ns2_92760_uff_E=672.76	-7.1	prepared_vp4_92760_uff_E=672.76	-7.5
Prepared_ns2_92760_uff_E=672.76	-7	prepared_vp4_92760_uff_E=672.76	-7.2
Prepared_ns2_92760_uff_E=672.76	-7	prepared_vp4_92760_uff_E=672.76	-7.2
Prepared_ns2_64945_uff_E=805.65	-8	prepared_vp4_64945_uff_E=805.65	-9.1
Prepared_ns2_64945_uff_E=805.65	-7.7	prepared_vp4_64945_uff_E=805.65	-9.1
Prepared_ns2_64945_uff_E=805.65	-7.6	prepared_vp4_64945_uff_E=805.65	-8.8
Prepared_ns2_64945_uff_E=805.65	-7.4	prepared_vp4_64945_uff_E=805.65	-8.6
Prepared_ns2_64945_uff_E=805.65	-7.1	prepared_vp4_64945_uff_E=805.65	-8.5
Prepared_ns2_64945_uff_E=805.65	-7.1	prepared_vp4_64945_uff_E=805.65	-8.4
Prepared_ns2_64945_uff_E=805.65	-7	prepared_vp4_64945_uff_E=805.65	-8.2
Prepared_ns2_64945_uff_E=805.65	-7	prepared_vp4_64945_uff_E=805.65	-8.2
Prepared_ns2_64945_uff_E=805.65	-6.8	prepared_vp4_64945_uff_E=805.65	-8.2
Prepared_ns2_6029_uff_E=306.70	-6	prepared_vp4_6029_uff_E=306.70	-6.2
Prepared_ns2_6029_uff_E=306.70	-5.7	prepared_vp4_6029_uff_E=306.70	-6.2
Prepared_ns2_6029_uff_E=306.70	-5.6	prepared_vp4_6029_uff_E=306.70	-6.2
Prepared_ns2_6029_uff_E=306.70	-5.5	prepared_vp4_6029_uff_E=306.70	-6.1
Prepared_ns2_6029_uff_E=306.70	-5.5	prepared_vp4_6029_uff_E=306.70	-6.1
Prepared_ns2_6029_uff_E=306.70	-5.3	prepared_vp4_6029_uff_E=306.70	-6.1
Prepared_ns2_6029_uff_E=306.70	-5.3	prepared_vp4_6029_uff_E=306.70	-6.1
Prepared_ns2_6029_uff_E=306.70	-5.1	prepared_vp4_6029_uff_E=306.70	-6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_6029_uff_E=306.70	-5	prepared_vp4_6029_uff_E=306.70	-5.9
Prepared_ns2_73648_uff_E=595.02	-6.5	prepared_vp4_73648_uff_E=595.02	-7.1
Prepared_ns2_73648_uff_E=595.02	-6.5	prepared_vp4_73648_uff_E=595.02	-7.1
Prepared_ns2_73648_uff_E=595.02	-6.5	prepared_vp4_73648_uff_E=595.02	-7.1
Prepared_ns2_73648_uff_E=595.02	-6.5	prepared_vp4_73648_uff_E=595.02	-6.9
Prepared_ns2_73648_uff_E=595.02	-6.4	prepared_vp4_73648_uff_E=595.02	-6.8
Prepared_ns2_73648_uff_E=595.02	-6.3	prepared_vp4_73648_uff_E=595.02	-6.8
Prepared_ns2_73648_uff_E=595.02	-6.2	prepared_vp4_73648_uff_E=595.02	-6.8
Prepared_ns2_73648_uff_E=595.02	-6	prepared_vp4_73648_uff_E=595.02	-6.7
Prepared_ns2_73648_uff_E=595.02	-6	prepared_vp4_73648_uff_E=595.02	-6.7
Prepared_ns2_6305_uff_E=333.02	-6.2	prepared_vp4_6305_uff_E=333.02	-6.1
Prepared_ns2_6305_uff_E=333.02	-5.9	prepared_vp4_6305_uff_E=333.02	-6
Prepared_ns2_6305_uff_E=333.02	-5.9	prepared_vp4_6305_uff_E=333.02	-5.9
Prepared_ns2_6305_uff_E=333.02	-5.6	prepared_vp4_6305_uff_E=333.02	-5.9
Prepared_ns2_6305_uff_E=333.02	-5.6	prepared_vp4_6305_uff_E=333.02	-5.7
Prepared_ns2_6305_uff_E=333.02	-5.5	prepared_vp4_6305_uff_E=333.02	-5.7
Prepared_ns2_6305_uff_E=333.02	-5.3	prepared_vp4_6305_uff_E=333.02	-5.5
Prepared_ns2_6305_uff_E=333.02	-5.3	prepared_vp4_6305_uff_E=333.02	-5.3
Prepared_ns2_6305_uff_E=333.02	-5.2	prepared_vp4_6305_uff_E=333.02	-5.3
Prepared_ns2_451674_uff_E=1198.78	-7.8	prepared_vp4_451674_uff_E=1198.78	-9.1
Prepared_ns2_451674_uff_E=1198.78	-7.8	prepared_vp4_451674_uff_E=1198.78	-9
Prepared_ns2_451674_uff_E=1198.78	-7.6	prepared_vp4_451674_uff_E=1198.78	-8.9
Prepared_ns2_451674_uff_E=1198.78	-7.5	prepared_vp4_451674_uff_E=1198.78	-8.7
Prepared_ns2_451674_uff_E=1198.78	-7.3	prepared_vp4_451674_uff_E=1198.78	-8.6
Prepared_ns2_451674_uff_E=1198.78	-7.3	prepared_vp4_451674_uff_E=1198.78	-8.6
Prepared_ns2_451674_uff_E=1198.78	-7.2	prepared_vp4_451674_uff_E=1198.78	-8.5
Prepared_ns2_451674_uff_E=1198.78	-7.1	prepared_vp4_451674_uff_E=1198.78	-8.4
Prepared_ns2_451674_uff_E=1198.78	-6.9	prepared_vp4_451674_uff_E=1198.78	-8.3
Prepared_ns2_5541_uff_E=65.14	-4.6	prepared_vp4_5541_uff_E=65.14	-5.5
Prepared_ns2_5541_uff_E=65.14	-4.5	prepared_vp4_5541_uff_E=65.14	-5.2
Prepared_ns2_5541_uff_E=65.14	-4.4	prepared_vp4_5541_uff_E=65.14	-5.1
Prepared_ns2_5541_uff_E=65.14	-4.2	prepared_vp4_5541_uff_E=65.14	-5
Prepared_ns2_5541_uff_E=65.14	-4.1	prepared_vp4_5541_uff_E=65.14	-5
Prepared_ns2_5541_uff_E=65.14	-4.1	prepared_vp4_5541_uff_E=65.14	-5
Prepared_ns2_5541_uff_E=65.14	-4.1	prepared_vp4_5541_uff_E=65.14	-5
Prepared_ns2_5541_uff_E=65.14	-4.1	prepared_vp4_5541_uff_E=65.14	-4.9
Prepared_ns2_5541_uff_E=65.14	-4.1	prepared_vp4_5541_uff_E=65.14	-4.9
Prepared_ns2_68591_uff_E=413.79	-8.2	prepared_vp4_68591_uff_E=413.79	-8.5
Prepared_ns2_68591_uff_E=413.79	-7.3	prepared_vp4_68591_uff_E=413.79	-8.2
Prepared_ns2_68591_uff_E=413.79	-7.3	prepared_vp4_68591_uff_E=413.79	-8
Prepared_ns2_68591_uff_E=413.79	-7.3	prepared_vp4_68591_uff_E=413.79	-7.9
Prepared_ns2_68591_uff_E=413.79	-7.3	prepared_vp4_68591_uff_E=413.79	-7.9
Prepared_ns2_68591_uff_E=413.79	-7.2	prepared_vp4_68591_uff_E=413.79	-7.8
Prepared_ns2_68591_uff_E=413.79	-7.1	prepared_vp4_68591_uff_E=413.79	-7.6
Prepared_ns2_68591_uff_E=413.79	-7.1	prepared_vp4_68591_uff_E=413.79	-7.5

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_68591_uff_E=413.79	-7.1	prepared_vp4_68591_uff_E=413.79	-7.5
Prepared_ns2_9929901_uff_E=272.42	-6	prepared_vp4_9929901_uff_E=272.42	-7
Prepared_ns2_9929901_uff_E=272.42	-6	prepared_vp4_9929901_uff_E=272.42	-6.7
Prepared_ns2_9929901_uff_E=272.42	-5.9	prepared_vp4_9929901_uff_E=272.42	-6.6
Prepared_ns2_9929901_uff_E=272.42	-5.9	prepared_vp4_9929901_uff_E=272.42	-6.5
Prepared_ns2_9929901_uff_E=272.42	-5.9	prepared_vp4_9929901_uff_E=272.42	-6.5
Prepared_ns2_9929901_uff_E=272.42	-5.9	prepared_vp4_9929901_uff_E=272.42	-6.3
Prepared_ns2_9929901_uff_E=272.42	-5.9	prepared_vp4_9929901_uff_E=272.42	-6.3
Prepared_ns2_9929901_uff_E=272.42	-5.8	prepared_vp4_9929901_uff_E=272.42	-6.1
Prepared_ns2_9929901_uff_E=272.42	-5.8	prepared_vp4_9929901_uff_E=272.42	-6
Prepared_ns2_11463_uff_E=132.39	-4.5	prepared_vp4_11463_uff_E=132.39	-6.1
Prepared_ns2_11463_uff_E=132.39	-4.3	prepared_vp4_11463_uff_E=132.39	-5.6
Prepared_ns2_11463_uff_E=132.39	-4.3	prepared_vp4_11463_uff_E=132.39	-5.4
Prepared_ns2_11463_uff_E=132.39	-4.3	prepared_vp4_11463_uff_E=132.39	-5.4
Prepared_ns2_11463_uff_E=132.39	-4.2	prepared_vp4_11463_uff_E=132.39	-5.4
Prepared_ns2_11463_uff_E=132.39	-4.2	prepared_vp4_11463_uff_E=132.39	-5.4
Prepared_ns2_11463_uff_E=132.39	-4.2	prepared_vp4_11463_uff_E=132.39	-5.3
Prepared_ns2_11463_uff_E=132.39	-4.2	prepared_vp4_11463_uff_E=132.39	-5.3
Prepared_ns2_11463_uff_E=132.39	-4.2	prepared_vp4_11463_uff_E=132.39	-5.2
Prepared_ns2_17100_uff_E=147.80	-4.9	prepared_vp4_17100_uff_E=147.80	-5.8
Prepared_ns2_17100_uff_E=147.80	-4.7	prepared_vp4_17100_uff_E=147.80	-5.8
Prepared_ns2_17100_uff_E=147.80	-4.7	prepared_vp4_17100_uff_E=147.80	-5.7
Prepared_ns2_17100_uff_E=147.80	-4.5	prepared_vp4_17100_uff_E=147.80	-5.6
Prepared_ns2_17100_uff_E=147.80	-4.5	prepared_vp4_17100_uff_E=147.80	-5.5
Prepared_ns2_17100_uff_E=147.80	-4.5	prepared_vp4_17100_uff_E=147.80	-5.5
Prepared_ns2_17100_uff_E=147.80	-4.5	prepared_vp4_17100_uff_E=147.80	-5.5
Prepared_ns2_17100_uff_E=147.80	-4.5	prepared_vp4_17100_uff_E=147.80	-5.4
Prepared_ns2_17100_uff_E=147.80	-4.4	prepared_vp4_17100_uff_E=147.80	-5.3
Prepared_ns2_31408_uff_E=652.17	-5.1	prepared_vp4_31408_uff_E=652.17	-5.9
Prepared_ns2_31408_uff_E=652.17	-5	prepared_vp4_31408_uff_E=652.17	-5.7
Prepared_ns2_31408_uff_E=652.17	-4.8	prepared_vp4_31408_uff_E=652.17	-5.6
Prepared_ns2_31408_uff_E=652.17	-4.6	prepared_vp4_31408_uff_E=652.17	-5.2
Prepared_ns2_31408_uff_E=652.17	-4.5	prepared_vp4_31408_uff_E=652.17	-5.2
Prepared_ns2_31408_uff_E=652.17	-4.5	prepared_vp4_31408_uff_E=652.17	-5.1
Prepared_ns2_31408_uff_E=652.17	-4.4	prepared_vp4_31408_uff_E=652.17	-5.1
Prepared_ns2_31408_uff_E=652.17	-4.4	prepared_vp4_31408_uff_E=652.17	-4.9
Prepared_ns2_31408_uff_E=652.17	-4.4	prepared_vp4_31408_uff_E=652.17	-4.9
Prepared_ns2_592986_uff_E=117.06	-4.8	prepared_vp4_592986_uff_E=117.06	-5.5
Prepared_ns2_592986_uff_E=117.06	-4.5	prepared_vp4_592986_uff_E=117.06	-5.5
Prepared_ns2_592986_uff_E=117.06	-4.4	prepared_vp4_592986_uff_E=117.06	-5.3
Prepared_ns2_592986_uff_E=117.06	-4.4	prepared_vp4_592986_uff_E=117.06	-5.3
Prepared_ns2_592986_uff_E=117.06	-4.4	prepared_vp4_592986_uff_E=117.06	-5.2
Prepared_ns2_592986_uff_E=117.06	-4.3	prepared_vp4_592986_uff_E=117.06	-5.1
Prepared_ns2_592986_uff_E=117.06	-4.3	prepared_vp4_592986_uff_E=117.06	-5.1
Prepared_ns2_592986_uff_E=117.06	-4.2	prepared_vp4_592986_uff_E=117.06	-5.1

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_592986_uff_E=117.06	-4.2	prepared_vp4_592986_uff_E=117.06	-5.1
Prepared_ns2_1110_uff_E=26.16	-4.1	prepared_vp4_1110_uff_E=26.16	-4.6
Prepared_ns2_1110_uff_E=26.16	-4	prepared_vp4_1110_uff_E=26.16	-4.6
Prepared_ns2_1110_uff_E=26.16	-3.9	prepared_vp4_1110_uff_E=26.16	-4.6
Prepared_ns2_1110_uff_E=26.16	-3.9	prepared_vp4_1110_uff_E=26.16	-4.3
Prepared_ns2_1110_uff_E=26.16	-3.9	prepared_vp4_1110_uff_E=26.16	-4.3
Prepared_ns2_1110_uff_E=26.16	-3.8	prepared_vp4_1110_uff_E=26.16	-4.3
Prepared_ns2_1110_uff_E=26.16	-3.7	prepared_vp4_1110_uff_E=26.16	-4.2
Prepared_ns2_1110_uff_E=26.16	-3.6	prepared_vp4_1110_uff_E=26.16	-4.2
Prepared_ns2_1110_uff_E=26.16	-3.6	prepared_vp4_1110_uff_E=26.16	-4.1
Prepared_ns2_5280794_uff_E=546.19	-7.6	prepared_vp4_5280794_uff_E=546.19	-8.6
Prepared_ns2_5280794_uff_E=546.19	-7.6	prepared_vp4_5280794_uff_E=546.19	-8.5
Prepared_ns2_5280794_uff_E=546.19	-7.5	prepared_vp4_5280794_uff_E=546.19	-8.4
Prepared_ns2_5280794_uff_E=546.19	-7.2	prepared_vp4_5280794_uff_E=546.19	-8.3
Prepared_ns2_5280794_uff_E=546.19	-7.1	prepared_vp4_5280794_uff_E=546.19	-7.9
Prepared_ns2_5280794_uff_E=546.19	-7	prepared_vp4_5280794_uff_E=546.19	-7.9
Prepared_ns2_5280794_uff_E=546.19	-6.8	prepared_vp4_5280794_uff_E=546.19	-7.7
Prepared_ns2_5280794_uff_E=546.19	-6.8	prepared_vp4_5280794_uff_E=546.19	-7.7
Prepared_ns2_5280794_uff_E=546.19	-6.8	prepared_vp4_5280794_uff_E=546.19	-7.6
Prepared_ns2_5281_uff_E=4383.69	-3.9	prepared_vp4_5281_uff_E=4383.69	-4.8
Prepared_ns2_5281_uff_E=4383.69	-3.8	prepared_vp4_5281_uff_E=4383.69	-4.3
Prepared_ns2_5281_uff_E=4383.69	-3.8	prepared_vp4_5281_uff_E=4383.69	-4.3
Prepared_ns2_5281_uff_E=4383.69	-3.7	prepared_vp4_5281_uff_E=4383.69	-4.1
Prepared_ns2_5281_uff_E=4383.69	-3.6	prepared_vp4_5281_uff_E=4383.69	-4.1
Prepared_ns2_5281_uff_E=4383.69	-3.5	prepared_vp4_5281_uff_E=4383.69	-4.1
Prepared_ns2_5281_uff_E=4383.69	-3.4	prepared_vp4_5281_uff_E=4383.69	-3.9
Prepared_ns2_5281_uff_E=4383.69	-3.4	prepared_vp4_5281_uff_E=4383.69	-3.9
Prepared_ns2_5281_uff_E=4383.69	-3.4	prepared_vp4_5281_uff_E=4383.69	-3.9
Prepared_ns2_638072_uff_E=248.91	-5.1	prepared_vp4_638072_uff_E=248.91	-5.6
Prepared_ns2_638072_uff_E=248.91	-5.1	prepared_vp4_638072_uff_E=248.91	-5.4
Prepared_ns2_638072_uff_E=248.91	-5.1	prepared_vp4_638072_uff_E=248.91	-5.4
Prepared_ns2_638072_uff_E=248.91	-5.1	prepared_vp4_638072_uff_E=248.91	-5.3
Prepared_ns2_638072_uff_E=248.91	-5	prepared_vp4_638072_uff_E=248.91	-5.3
Prepared_ns2_638072_uff_E=248.91	-5	prepared_vp4_638072_uff_E=248.91	-5
Prepared_ns2_638072_uff_E=248.91	-4.9	prepared_vp4_638072_uff_E=248.91	-5
Prepared_ns2_638072_uff_E=248.91	-4.9	prepared_vp4_638072_uff_E=248.91	-4.8
Prepared_ns2_638072_uff_E=248.91	-4.9	prepared_vp4_638072_uff_E=248.91	-4.8
Prepared_ns2_10168_uff_E=201.65	-7.2	prepared_vp4_10168_uff_E=201.65	-7.7
Prepared_ns2_10168_uff_E=201.65	-7.1	prepared_vp4_10168_uff_E=201.65	-7.4
Prepared_ns2_10168_uff_E=201.65	-6.8	prepared_vp4_10168_uff_E=201.65	-7.2
Prepared_ns2_10168_uff_E=201.65	-6.7	prepared_vp4_10168_uff_E=201.65	-7.2
Prepared_ns2_10168_uff_E=201.65	-6.7	prepared_vp4_10168_uff_E=201.65	-7
Prepared_ns2_10168_uff_E=201.65	-6.6	prepared_vp4_10168_uff_E=201.65	-6.9
Prepared_ns2_10168_uff_E=201.65	-6.5	prepared_vp4_10168_uff_E=201.65	-6.8
Prepared_ns2_10168_uff_E=201.65	-6.4	prepared_vp4_10168_uff_E=201.65	-6.8

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_10168_uff_E=201.65	-6.4	prepared_vp4_10168_uff_E=201.65	-6.7
Prepared_ns2_10446798_uff_E=298.22	-7.2	prepared_vp4_10446798_uff_E=298.22	-7.6
Prepared_ns2_10446798_uff_E=298.22	-6.8	prepared_vp4_10446798_uff_E=298.22	-7.3
Prepared_ns2_10446798_uff_E=298.22	-6.8	prepared_vp4_10446798_uff_E=298.22	-7.2
Prepared_ns2_10446798_uff_E=298.22	-6.8	prepared_vp4_10446798_uff_E=298.22	-7.1
Prepared_ns2_10446798_uff_E=298.22	-6.2	prepared_vp4_10446798_uff_E=298.22	-6.9
Prepared_ns2_10446798_uff_E=298.22	-6.2	prepared_vp4_10446798_uff_E=298.22	-6.9
Prepared_ns2_10446798_uff_E=298.22	-6.1	prepared_vp4_10446798_uff_E=298.22	-6.8
Prepared_ns2_10446798_uff_E=298.22	-6.1	prepared_vp4_10446798_uff_E=298.22	-6.7
Prepared_ns2_10446798_uff_E=298.22	-6.1	prepared_vp4_10446798_uff_E=298.22	-6.7
Prepared_ns2_637775_uff_E=206.17	-5.3	prepared_vp4_637775_uff_E=206.17	-5.9
Prepared_ns2_637775_uff_E=206.17	-5.3	prepared_vp4_637775_uff_E=206.17	-5.9
Prepared_ns2_637775_uff_E=206.17	-5.1	prepared_vp4_637775_uff_E=206.17	-5.8
Prepared_ns2_637775_uff_E=206.17	-5.1	prepared_vp4_637775_uff_E=206.17	-5.8
Prepared_ns2_637775_uff_E=206.17	-5.1	prepared_vp4_637775_uff_E=206.17	-5.7
Prepared_ns2_637775_uff_E=206.17	-5	prepared_vp4_637775_uff_E=206.17	-5.6
Prepared_ns2_637775_uff_E=206.17	-4.9	prepared_vp4_637775_uff_E=206.17	-5.4
Prepared_ns2_637775_uff_E=206.17	-4.9	prepared_vp4_637775_uff_E=206.17	-5.4
Prepared_ns2_637775_uff_E=206.17	-4.9	prepared_vp4_637775_uff_E=206.17	-5.4
Prepared_ns2_8742_uff_E=163.00	-5.4	prepared_vp4_8742_uff_E=163.00	-5.8
Prepared_ns2_8742_uff_E=163.00	-5.1	prepared_vp4_8742_uff_E=163.00	-5.8
Prepared_ns2_8742_uff_E=163.00	-5.1	prepared_vp4_8742_uff_E=163.00	-5.7
Prepared_ns2_8742_uff_E=163.00	-5	prepared_vp4_8742_uff_E=163.00	-5.6
Prepared_ns2_8742_uff_E=163.00	-4.9	prepared_vp4_8742_uff_E=163.00	-5.5
Prepared_ns2_8742_uff_E=163.00	-4.8	prepared_vp4_8742_uff_E=163.00	-5.5
Prepared_ns2_8742_uff_E=163.00	-4.7	prepared_vp4_8742_uff_E=163.00	-5.4
Prepared_ns2_8742_uff_E=163.00	-4.6	prepared_vp4_8742_uff_E=163.00	-5.4
Prepared_ns2_8742_uff_E=163.00	-4.6	prepared_vp4_8742_uff_E=163.00	-5.4
Prepared_ns2_338659_uff_E=528.05	-6.4	prepared_vp4_338659_uff_E=528.05	-7.7
Prepared_ns2_338659_uff_E=528.05	-6	prepared_vp4_338659_uff_E=528.05	-7.5
Prepared_ns2_338659_uff_E=528.05	-6	prepared_vp4_338659_uff_E=528.05	-7.5
Prepared_ns2_338659_uff_E=528.05	-5.9	prepared_vp4_338659_uff_E=528.05	-7.3
Prepared_ns2_338659_uff_E=528.05	-5.8	prepared_vp4_338659_uff_E=528.05	-7.3
Prepared_ns2_338659_uff_E=528.05	-5.8	prepared_vp4_338659_uff_E=528.05	-7.3
Prepared_ns2_338659_uff_E=528.05	-5.7	prepared_vp4_338659_uff_E=528.05	-7.1
Prepared_ns2_338659_uff_E=528.05	-5.7	prepared_vp4_338659_uff_E=528.05	-7
Prepared_ns2_338659_uff_E=528.05	-5.5	prepared_vp4_338659_uff_E=528.05	-6.9
Prepared_ns2_519764_uff_E=173.42	-4.6	prepared_vp4_519764_uff_E=173.42	-5.8
Prepared_ns2_519764_uff_E=173.42	-4.5	prepared_vp4_519764_uff_E=173.42	-5.8
Prepared_ns2_519764_uff_E=173.42	-4.5	prepared_vp4_519764_uff_E=173.42	-5.6
Prepared_ns2_519764_uff_E=173.42	-4.4	prepared_vp4_519764_uff_E=173.42	-5.6
Prepared_ns2_519764_uff_E=173.42	-4.3	prepared_vp4_519764_uff_E=173.42	-5.6
Prepared_ns2_519764_uff_E=173.42	-4.3	prepared_vp4_519764_uff_E=173.42	-5.6
Prepared_ns2_519764_uff_E=173.42	-4.3	prepared_vp4_519764_uff_E=173.42	-5.5
Prepared_ns2_519764_uff_E=173.42	-4.3	prepared_vp4_519764_uff_E=173.42	-5.3

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_519764_uff_E=173.42	-4.1	prepared_vp4_519764_uff_E=173.42	-5.3
Prepared_ns2_5202_uff_E=323.58	-5.2	prepared_vp4_5202_uff_E=323.58	-6.1
Prepared_ns2_5202_uff_E=323.58	-5.1	prepared_vp4_5202_uff_E=323.58	-5.8
Prepared_ns2_5202_uff_E=323.58	-5.1	prepared_vp4_5202_uff_E=323.58	-5.8
Prepared_ns2_5202_uff_E=323.58	-5.1	prepared_vp4_5202_uff_E=323.58	-5.7
Prepared_ns2_5202_uff_E=323.58	-5	prepared_vp4_5202_uff_E=323.58	-5.6
Prepared_ns2_5202_uff_E=323.58	-5	prepared_vp4_5202_uff_E=323.58	-5.5
Prepared_ns2_5202_uff_E=323.58	-5	prepared_vp4_5202_uff_E=323.58	-5.5
Prepared_ns2_5202_uff_E=323.58	-4.9	prepared_vp4_5202_uff_E=323.58	-5.3
Prepared_ns2_5202_uff_E=323.58	-4.8	prepared_vp4_5202_uff_E=323.58	-5.3
Prepared_ns2_124035_uff_E=383.91	-7.1	prepared_vp4_124035_uff_E=383.91	-8.8
Prepared_ns2_124035_uff_E=383.91	-6.9	prepared_vp4_124035_uff_E=383.91	-8.6
Prepared_ns2_124035_uff_E=383.91	-6.9	prepared_vp4_124035_uff_E=383.91	-7.9
Prepared_ns2_124035_uff_E=383.91	-6.8	prepared_vp4_124035_uff_E=383.91	-7.8
Prepared_ns2_124035_uff_E=383.91	-6.7	prepared_vp4_124035_uff_E=383.91	-7.7
Prepared_ns2_124035_uff_E=383.91	-6.6	prepared_vp4_124035_uff_E=383.91	-7.6
Prepared_ns2_124035_uff_E=383.91	-6.6	prepared_vp4_124035_uff_E=383.91	-7.6
Prepared_ns2_124035_uff_E=383.91	-6.5	prepared_vp4_124035_uff_E=383.91	-7.6
Prepared_ns2_124035_uff_E=383.91	-6.5	prepared_vp4_124035_uff_E=383.91	-7.5
Prepared_ns2_71815_uff_E=306.50	-4.5	prepared_vp4_71815_uff_E=306.50	-5.3
Prepared_ns2_71815_uff_E=306.50	-4.5	prepared_vp4_71815_uff_E=306.50	-5
Prepared_ns2_71815_uff_E=306.50	-4.2	prepared_vp4_71815_uff_E=306.50	-4.9
Prepared_ns2_71815_uff_E=306.50	-4.2	prepared_vp4_71815_uff_E=306.50	-4.8
Prepared_ns2_71815_uff_E=306.50	-4.2	prepared_vp4_71815_uff_E=306.50	-4.8
Prepared_ns2_71815_uff_E=306.50	-4.1	prepared_vp4_71815_uff_E=306.50	-4.7
Prepared_ns2_71815_uff_E=306.50	-4.1	prepared_vp4_71815_uff_E=306.50	-4.6
Prepared_ns2_71815_uff_E=306.50	-4	prepared_vp4_71815_uff_E=306.50	-4.6
Prepared_ns2_71815_uff_E=306.50	-4	prepared_vp4_71815_uff_E=306.50	-4.6
Prepared_ns2_5280460_uff_E=186.56	-5.6	prepared_vp4_5280460_uff_E=186.56	-6.9
Prepared_ns2_5280460_uff_E=186.56	-5.6	prepared_vp4_5280460_uff_E=186.56	-6.2
Prepared_ns2_5280460_uff_E=186.56	-5.6	prepared_vp4_5280460_uff_E=186.56	-6.1
Prepared_ns2_5280460_uff_E=186.56	-5.4	prepared_vp4_5280460_uff_E=186.56	-5.9
Prepared_ns2_5280460_uff_E=186.56	-5.4	prepared_vp4_5280460_uff_E=186.56	-5.9
Prepared_ns2_5280460_uff_E=186.56	-5.3	prepared_vp4_5280460_uff_E=186.56	-5.8
Prepared_ns2_5280460_uff_E=186.56	-5.3	prepared_vp4_5280460_uff_E=186.56	-5.8
Prepared_ns2_5280460_uff_E=186.56	-5.2	prepared_vp4_5280460_uff_E=186.56	-5.6
Prepared_ns2_5280460_uff_E=186.56	-5.1	prepared_vp4_5280460_uff_E=186.56	-5.6
Prepared_ns2_9793905_uff_E=85.21	-3.9	prepared_vp4_9793905_uff_E=85.21	-4.4
Prepared_ns2_9793905_uff_E=85.21	-3.9	prepared_vp4_9793905_uff_E=85.21	-4.1
Prepared_ns2_9793905_uff_E=85.21	-3.9	prepared_vp4_9793905_uff_E=85.21	-4.1
Prepared_ns2_9793905_uff_E=85.21	-3.9	prepared_vp4_9793905_uff_E=85.21	-4.1
Prepared_ns2_9793905_uff_E=85.21	-3.8	prepared_vp4_9793905_uff_E=85.21	-4.1
Prepared_ns2_9793905_uff_E=85.21	-3.7	prepared_vp4_9793905_uff_E=85.21	-4.1
Prepared_ns2_9793905_uff_E=85.21	-3.7	prepared_vp4_9793905_uff_E=85.21	-4
Prepared_ns2_9793905_uff_E=85.21	-3.7	prepared_vp4_9793905_uff_E=85.21	-4

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_9793905_uff_E=85.21	-3.6	prepared_vp4_9793905_uff_E=85.21	-4
Prepared_ns2_439503_uff_E=324.93	-5.7	prepared_vp4_439503_uff_E=324.93	-6.6
Prepared_ns2_439503_uff_E=324.93	-5.6	prepared_vp4_439503_uff_E=324.93	-6.3
Prepared_ns2_439503_uff_E=324.93	-5.6	prepared_vp4_439503_uff_E=324.93	-6.3
Prepared_ns2_439503_uff_E=324.93	-5.5	prepared_vp4_439503_uff_E=324.93	-6.2
Prepared_ns2_439503_uff_E=324.93	-5.5	prepared_vp4_439503_uff_E=324.93	-6.2
Prepared_ns2_439503_uff_E=324.93	-5.5	prepared_vp4_439503_uff_E=324.93	-6.2
Prepared_ns2_439503_uff_E=324.93	-5.4	prepared_vp4_439503_uff_E=324.93	-5.8
Prepared_ns2_439503_uff_E=324.93	-5.4	prepared_vp4_439503_uff_E=324.93	-5.5
Prepared_ns2_439503_uff_E=324.93	-5.3	prepared_vp4_439503_uff_E=324.93	-5.5
Prepared_ns2_72537_uff_E=237.73	-7.1	prepared_vp4_72537_uff_E=237.73	-7.3
Prepared_ns2_72537_uff_E=237.73	-6.5	prepared_vp4_72537_uff_E=237.73	-7
Prepared_ns2_72537_uff_E=237.73	-6.2	prepared_vp4_72537_uff_E=237.73	-6.8
Prepared_ns2_72537_uff_E=237.73	-6.2	prepared_vp4_72537_uff_E=237.73	-6.8
Prepared_ns2_72537_uff_E=237.73	-6.1	prepared_vp4_72537_uff_E=237.73	-6.6
Prepared_ns2_72537_uff_E=237.73	-6	prepared_vp4_72537_uff_E=237.73	-6.6
Prepared_ns2_72537_uff_E=237.73	-6	prepared_vp4_72537_uff_E=237.73	-6.5
Prepared_ns2_72537_uff_E=237.73	-5.9	prepared_vp4_72537_uff_E=237.73	-6.4
Prepared_ns2_72537_uff_E=237.73	-5.9	prepared_vp4_72537_uff_E=237.73	-6.4
Prepared_ns2_5281792_uff_E=209.67	-7.4	prepared_vp4_5281792_uff_E=209.67	-7.2
Prepared_ns2_5281792_uff_E=209.67	-7.3	prepared_vp4_5281792_uff_E=209.67	-6.9
Prepared_ns2_5281792_uff_E=209.67	-7.3	prepared_vp4_5281792_uff_E=209.67	-6.9
Prepared_ns2_5281792_uff_E=209.67	-7.3	prepared_vp4_5281792_uff_E=209.67	-6.8
Prepared_ns2_5281792_uff_E=209.67	-7.2	prepared_vp4_5281792_uff_E=209.67	-6.8
Prepared_ns2_5281792_uff_E=209.67	-7.1	prepared_vp4_5281792_uff_E=209.67	-6.7
Prepared_ns2_5281792_uff_E=209.67	-7.1	prepared_vp4_5281792_uff_E=209.67	-6.5
Prepared_ns2_5281792_uff_E=209.67	-7	prepared_vp4_5281792_uff_E=209.67	-6.5
Prepared_ns2_5281792_uff_E=209.67	-7	prepared_vp4_5281792_uff_E=209.67	-6.5
Prepared_ns2_643684_uff_E=131.80	-4.9	prepared_vp4_643684_uff_E=131.80	-5.7
Prepared_ns2_643684_uff_E=131.80	-4.7	prepared_vp4_643684_uff_E=131.80	-5.6
Prepared_ns2_643684_uff_E=131.80	-4.6	prepared_vp4_643684_uff_E=131.80	-5.5
Prepared_ns2_643684_uff_E=131.80	-4.5	prepared_vp4_643684_uff_E=131.80	-5.5
Prepared_ns2_643684_uff_E=131.80	-4.5	prepared_vp4_643684_uff_E=131.80	-5.4
Prepared_ns2_643684_uff_E=131.80	-4.5	prepared_vp4_643684_uff_E=131.80	-5.3
Prepared_ns2_643684_uff_E=131.80	-4.5	prepared_vp4_643684_uff_E=131.80	-5.3
Prepared_ns2_643684_uff_E=131.80	-4.4	prepared_vp4_643684_uff_E=131.80	-5.3
Prepared_ns2_643684_uff_E=131.80	-4.3	prepared_vp4_643684_uff_E=131.80	-5.3
Prepared_ns2_445154_uff_E=172.22	-6.5	prepared_vp4_445154_uff_E=172.22	-7.1
Prepared_ns2_445154_uff_E=172.22	-6.5	prepared_vp4_445154_uff_E=172.22	-7.1
Prepared_ns2_445154_uff_E=172.22	-6.2	prepared_vp4_445154_uff_E=172.22	-7.1
Prepared_ns2_445154_uff_E=172.22	-6.1	prepared_vp4_445154_uff_E=172.22	-6.9
Prepared_ns2_445154_uff_E=172.22	-6.1	prepared_vp4_445154_uff_E=172.22	-6.8
Prepared_ns2_445154_uff_E=172.22	-6.1	prepared_vp4_445154_uff_E=172.22	-6.8
Prepared_ns2_445154_uff_E=172.22	-5.9	prepared_vp4_445154_uff_E=172.22	-6.8
Prepared_ns2_445154_uff_E=172.22	-5.8	prepared_vp4_445154_uff_E=172.22	-6.7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_445154_uff_E=172.22	-5.8	prepared_vp4_445154_uff_E=172.22	-6.7
Prepared_ns2_3034034_uff_E=545.44	-6.6	prepared_vp4_3034034_uff_E=545.44	-7.4
Prepared_ns2_3034034_uff_E=545.44	-6.1	prepared_vp4_3034034_uff_E=545.44	-7.3
Prepared_ns2_3034034_uff_E=545.44	-6	prepared_vp4_3034034_uff_E=545.44	-7.1
Prepared_ns2_3034034_uff_E=545.44	-6	prepared_vp4_3034034_uff_E=545.44	-6.8
Prepared_ns2_3034034_uff_E=545.44	-5.9	prepared_vp4_3034034_uff_E=545.44	-6.7
Prepared_ns2_3034034_uff_E=545.44	-5.9	prepared_vp4_3034034_uff_E=545.44	-6.7
Prepared_ns2_3034034_uff_E=545.44	-5.9	prepared_vp4_3034034_uff_E=545.44	-6.4
Prepared_ns2_3034034_uff_E=545.44	-5.8	prepared_vp4_3034034_uff_E=545.44	-6.3
Prepared_ns2_3034034_uff_E=545.44	-5.7	prepared_vp4_3034034_uff_E=545.44	-6.2
Prepared_ns2_6508_uff_E=156.41	-5.6	prepared_vp4_6508_uff_E=156.41	-6
Prepared_ns2_6508_uff_E=156.41	-5.4	prepared_vp4_6508_uff_E=156.41	-6
Prepared_ns2_6508_uff_E=156.41	-5.1	prepared_vp4_6508_uff_E=156.41	-5.8
Prepared_ns2_6508_uff_E=156.41	-5	prepared_vp4_6508_uff_E=156.41	-5.8
Prepared_ns2_6508_uff_E=156.41	-4.9	prepared_vp4_6508_uff_E=156.41	-5.8
Prepared_ns2_6508_uff_E=156.41	-4.9	prepared_vp4_6508_uff_E=156.41	-5.6
Prepared_ns2_6508_uff_E=156.41	-4.9	prepared_vp4_6508_uff_E=156.41	-5.5
Prepared_ns2_6508_uff_E=156.41	-4.8	prepared_vp4_6508_uff_E=156.41	-5.5
Prepared_ns2_6508_uff_E=156.41	-4.7	prepared_vp4_6508_uff_E=156.41	-5.4
Prepared_ns2_5280459_uff_E=587.34	-7.5	prepared_vp4_5280459_uff_E=587.34	-8.1
Prepared_ns2_5280459_uff_E=587.34	-7.5	prepared_vp4_5280459_uff_E=587.34	-7.8
Prepared_ns2_5280459_uff_E=587.34	-7.2	prepared_vp4_5280459_uff_E=587.34	-7.8
Prepared_ns2_5280459_uff_E=587.34	-6.9	prepared_vp4_5280459_uff_E=587.34	-7.8
Prepared_ns2_5280459_uff_E=587.34	-6.8	prepared_vp4_5280459_uff_E=587.34	-7.7
Prepared_ns2_5280459_uff_E=587.34	-6.6	prepared_vp4_5280459_uff_E=587.34	-7.3
Prepared_ns2_5280459_uff_E=587.34	-6.4	prepared_vp4_5280459_uff_E=587.34	-7.2
Prepared_ns2_5280459_uff_E=587.34	-6.4	prepared_vp4_5280459_uff_E=587.34	-7.2
Prepared_ns2_5280459_uff_E=587.34	-6.4	prepared_vp4_5280459_uff_E=587.34	-7.2
Prepared_ns2_5280343_uff_E=380.43	-6.9	prepared_vp4_5280343_uff_E=380.43	-8.8
Prepared_ns2_5280343_uff_E=380.43	-6.7	prepared_vp4_5280343_uff_E=380.43	-7.9
Prepared_ns2_5280343_uff_E=380.43	-6.6	prepared_vp4_5280343_uff_E=380.43	-7.8
Prepared_ns2_5280343_uff_E=380.43	-6.6	prepared_vp4_5280343_uff_E=380.43	-7.5
Prepared_ns2_5280343_uff_E=380.43	-6.5	prepared_vp4_5280343_uff_E=380.43	-7.3
Prepared_ns2_5280343_uff_E=380.43	-6.4	prepared_vp4_5280343_uff_E=380.43	-7.3
Prepared_ns2_5280343_uff_E=380.43	-6.3	prepared_vp4_5280343_uff_E=380.43	-7.2
Prepared_ns2_5280343_uff_E=380.43	-6.1	prepared_vp4_5280343_uff_E=380.43	-7.2
Prepared_ns2_5280343_uff_E=380.43	-5.9	prepared_vp4_5280343_uff_E=380.43	-7
Prepared_ns2_8468_uff_E=150.75	-5.2	prepared_vp4_8468_uff_E=150.75	-5.9
Prepared_ns2_8468_uff_E=150.75	-4.8	prepared_vp4_8468_uff_E=150.75	-5.8
Prepared_ns2_8468_uff_E=150.75	-4.7	prepared_vp4_8468_uff_E=150.75	-5.6
Prepared_ns2_8468_uff_E=150.75	-4.7	prepared_vp4_8468_uff_E=150.75	-5.3
Prepared_ns2_8468_uff_E=150.75	-4.7	prepared_vp4_8468_uff_E=150.75	-5.3
Prepared_ns2_8468_uff_E=150.75	-4.5	prepared_vp4_8468_uff_E=150.75	-5.3
Prepared_ns2_8468_uff_E=150.75	-4.5	prepared_vp4_8468_uff_E=150.75	-5.2
Prepared_ns2_8468_uff_E=150.75	-4.5	prepared_vp4_8468_uff_E=150.75	-5.2

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_8468_uff_E=150.75	-4.5	prepared_vp4_8468_uff_E=150.75	-5.2
Prepared_ns2_440266_uff_E=99.61	-4.7	prepared_vp4_440266_uff_E=99.61	-5.7
Prepared_ns2_440266_uff_E=99.61	-4.7	prepared_vp4_440266_uff_E=99.61	-5.6
Prepared_ns2_440266_uff_E=99.61	-4.5	prepared_vp4_440266_uff_E=99.61	-5.3
Prepared_ns2_440266_uff_E=99.61	-4.5	prepared_vp4_440266_uff_E=99.61	-5.2
Prepared_ns2_440266_uff_E=99.61	-4.5	prepared_vp4_440266_uff_E=99.61	-5.2
Prepared_ns2_440266_uff_E=99.61	-4.5	prepared_vp4_440266_uff_E=99.61	-5.2
Prepared_ns2_440266_uff_E=99.61	-4.4	prepared_vp4_440266_uff_E=99.61	-5
Prepared_ns2_440266_uff_E=99.61	-4.4	prepared_vp4_440266_uff_E=99.61	-5
Prepared_ns2_440266_uff_E=99.61	-4.3	prepared_vp4_440266_uff_E=99.61	-4.8
Prepared_ns2_10205_uff_E=124.43	-5.6	prepared_vp4_10205_uff_E=124.43	-6.9
Prepared_ns2_10205_uff_E=124.43	-5.5	prepared_vp4_10205_uff_E=124.43	-6.9
Prepared_ns2_10205_uff_E=124.43	-5.5	prepared_vp4_10205_uff_E=124.43	-6.6
Prepared_ns2_10205_uff_E=124.43	-5.3	prepared_vp4_10205_uff_E=124.43	-6.6
Prepared_ns2_10205_uff_E=124.43	-5.2	prepared_vp4_10205_uff_E=124.43	-6.6
Prepared_ns2_10205_uff_E=124.43	-5.2	prepared_vp4_10205_uff_E=124.43	-6.4
Prepared_ns2_10205_uff_E=124.43	-5.2	prepared_vp4_10205_uff_E=124.43	-6.3
Prepared_ns2_10205_uff_E=124.43	-5.1	prepared_vp4_10205_uff_E=124.43	-6.3
Prepared_ns2_10205_uff_E=124.43	-5.1	prepared_vp4_10205_uff_E=124.43	-6.2
Prepared_ns2_638024_uff_E=357.43	-6.9	prepared_vp4_638024_uff_E=357.43	-7.6
Prepared_ns2_638024_uff_E=357.43	-6.7	prepared_vp4_638024_uff_E=357.43	-7.5
Prepared_ns2_638024_uff_E=357.43	-6.7	prepared_vp4_638024_uff_E=357.43	-7.5
Prepared_ns2_638024_uff_E=357.43	-6.6	prepared_vp4_638024_uff_E=357.43	-7.3
Prepared_ns2_638024_uff_E=357.43	-6.6	prepared_vp4_638024_uff_E=357.43	-7.2
Prepared_ns2_638024_uff_E=357.43	-6.6	prepared_vp4_638024_uff_E=357.43	-7.2
Prepared_ns2_638024_uff_E=357.43	-6.5	prepared_vp4_638024_uff_E=357.43	-7.1
Prepared_ns2_638024_uff_E=357.43	-6.5	prepared_vp4_638024_uff_E=357.43	-7
Prepared_ns2_638024_uff_E=357.43	-6.1	prepared_vp4_638024_uff_E=357.43	-7
Prepared_ns2_6654_uff_E=633.64	-4.5	prepared_vp4_6654_uff_E=633.64	-5.8
Prepared_ns2_6654_uff_E=633.64	-4.4	prepared_vp4_6654_uff_E=633.64	-5.7
Prepared_ns2_6654_uff_E=633.64	-4.3	prepared_vp4_6654_uff_E=633.64	-5.7
Prepared_ns2_6654_uff_E=633.64	-4.3	prepared_vp4_6654_uff_E=633.64	-5.5
Prepared_ns2_6654_uff_E=633.64	-4.2	prepared_vp4_6654_uff_E=633.64	-5.5
Prepared_ns2_6654_uff_E=633.64	-4	prepared_vp4_6654_uff_E=633.64	-5.5
Prepared_ns2_6654_uff_E=633.64	-4	prepared_vp4_6654_uff_E=633.64	-5.4
Prepared_ns2_6654_uff_E=633.64	-4	prepared_vp4_6654_uff_E=633.64	-5.4
Prepared_ns2_6654_uff_E=633.64	-4	prepared_vp4_6654_uff_E=633.64	-5.4
Prepared_ns2_667639_uff_E=172.66	-6.8	prepared_vp4_667639_uff_E=172.66	-7.5
Prepared_ns2_667639_uff_E=172.66	-6.7	prepared_vp4_667639_uff_E=172.66	-7.5
Prepared_ns2_667639_uff_E=172.66	-6.6	prepared_vp4_667639_uff_E=172.66	-7.3
Prepared_ns2_667639_uff_E=172.66	-5.9	prepared_vp4_667639_uff_E=172.66	-7.2
Prepared_ns2_667639_uff_E=172.66	-5.9	prepared_vp4_667639_uff_E=172.66	-7
Prepared_ns2_667639_uff_E=172.66	-5.9	prepared_vp4_667639_uff_E=172.66	-7
Prepared_ns2_667639_uff_E=172.66	-5.7	prepared_vp4_667639_uff_E=172.66	-6.7
Prepared_ns2_667639_uff_E=172.66	-5.7	prepared_vp4_667639_uff_E=172.66	-6.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_667639_uff_E=172.66	-5.7	prepared_vp4_667639_uff_E=172.66	-6.5
Prepared_ns2_12303662_uff_E=588.93	-7.1	prepared_vp4_12303662_uff_E=588.93	-8.1
Prepared_ns2_12303662_uff_E=588.93	-7	prepared_vp4_12303662_uff_E=588.93	-7.9
Prepared_ns2_12303662_uff_E=588.93	-7	prepared_vp4_12303662_uff_E=588.93	-7.9
Prepared_ns2_12303662_uff_E=588.93	-6.8	prepared_vp4_12303662_uff_E=588.93	-7.8
Prepared_ns2_12303662_uff_E=588.93	-6.6	prepared_vp4_12303662_uff_E=588.93	-7.7
Prepared_ns2_12303662_uff_E=588.93	-6.6	prepared_vp4_12303662_uff_E=588.93	-7.5
Prepared_ns2_12303662_uff_E=588.93	-6.5	prepared_vp4_12303662_uff_E=588.93	-7.5
Prepared_ns2_12303662_uff_E=588.93	-6.5	prepared_vp4_12303662_uff_E=588.93	-7.4
Prepared_ns2_12303662_uff_E=588.93	-6.5	prepared_vp4_12303662_uff_E=588.93	-7.3
Prepared_ns2_5280435_uff_E=165.89	-5.1	prepared_vp4_5280435_uff_E=165.89	-5.4
Prepared_ns2_5280435_uff_E=165.89	-5.1	prepared_vp4_5280435_uff_E=165.89	-5.3
Prepared_ns2_5280435_uff_E=165.89	-5	prepared_vp4_5280435_uff_E=165.89	-5.1
Prepared_ns2_5280435_uff_E=165.89	-5	prepared_vp4_5280435_uff_E=165.89	-5.1
Prepared_ns2_5280435_uff_E=165.89	-4.9	prepared_vp4_5280435_uff_E=165.89	-5
Prepared_ns2_5280435_uff_E=165.89	-4.9	prepared_vp4_5280435_uff_E=165.89	-4.9
Prepared_ns2_5280435_uff_E=165.89	-4.9	prepared_vp4_5280435_uff_E=165.89	-4.8
Prepared_ns2_5280435_uff_E=165.89	-4.8	prepared_vp4_5280435_uff_E=165.89	-4.6
Prepared_ns2_5280435_uff_E=165.89	-4.8	prepared_vp4_5280435_uff_E=165.89	-4.6
Prepared_ns2_10639_uff_E=212.65	-7.1	prepared_vp4_10639_uff_E=212.65	-7.4
Prepared_ns2_10639_uff_E=212.65	-6.7	prepared_vp4_10639_uff_E=212.65	-7.2
Prepared_ns2_10639_uff_E=212.65	-6.6	prepared_vp4_10639_uff_E=212.65	-7.1
Prepared_ns2_10639_uff_E=212.65	-6.5	prepared_vp4_10639_uff_E=212.65	-7
Prepared_ns2_10639_uff_E=212.65	-6.4	prepared_vp4_10639_uff_E=212.65	-7
Prepared_ns2_10639_uff_E=212.65	-6.3	prepared_vp4_10639_uff_E=212.65	-7
Prepared_ns2_10639_uff_E=212.65	-6.3	prepared_vp4_10639_uff_E=212.65	-6.9
Prepared_ns2_10639_uff_E=212.65	-6.2	prepared_vp4_10639_uff_E=212.65	-6.7
Prepared_ns2_10639_uff_E=212.65	-6.1	prepared_vp4_10639_uff_E=212.65	-6.6
Prepared_ns2_3314_uff_E=169.59	-4.6	prepared_vp4_3314_uff_E=169.59	-6
Prepared_ns2_3314_uff_E=169.59	-4.5	prepared_vp4_3314_uff_E=169.59	-5.9
Prepared_ns2_3314_uff_E=169.59	-4.5	prepared_vp4_3314_uff_E=169.59	-5.7
Prepared_ns2_3314_uff_E=169.59	-4.4	prepared_vp4_3314_uff_E=169.59	-5.6
Prepared_ns2_3314_uff_E=169.59	-4.3	prepared_vp4_3314_uff_E=169.59	-5.4
Prepared_ns2_3314_uff_E=169.59	-4.2	prepared_vp4_3314_uff_E=169.59	-5.4
Prepared_ns2_3314_uff_E=169.59	-4.2	prepared_vp4_3314_uff_E=169.59	-5.3
Prepared_ns2_3314_uff_E=169.59	-4.2	prepared_vp4_3314_uff_E=169.59	-5.3
Prepared_ns2_3314_uff_E=169.59	-4.1	prepared_vp4_3314_uff_E=169.59	-5.2
Prepared_ns2_323_uff_E=92.32	-5.3	prepared_vp4_323_uff_E=92.32	-6.6
Prepared_ns2_323_uff_E=92.32	-4.9	prepared_vp4_323_uff_E=92.32	-6.3
Prepared_ns2_323_uff_E=92.32	-4.9	prepared_vp4_323_uff_E=92.32	-6.1
Prepared_ns2_323_uff_E=92.32	-4.8	prepared_vp4_323_uff_E=92.32	-6.1
Prepared_ns2_323_uff_E=92.32	-4.7	prepared_vp4_323_uff_E=92.32	-6
Prepared_ns2_323_uff_E=92.32	-4.7	prepared_vp4_323_uff_E=92.32	-6
Prepared_ns2_323_uff_E=92.32	-4.7	prepared_vp4_323_uff_E=92.32	-5.9
Prepared_ns2_323_uff_E=92.32	-4.7	prepared_vp4_323_uff_E=92.32	-5.8

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_323_uff_E=92.32	-4.7	prepared_vp4_323_uff_E=92.32	-5.8
Prepared_ns2_441773_uff_E=426.67	-7	prepared_vp4_441773_uff_E=426.67	-8
Prepared_ns2_441773_uff_E=426.67	-6.6	prepared_vp4_441773_uff_E=426.67	-7.9
Prepared_ns2_441773_uff_E=426.67	-6.6	prepared_vp4_441773_uff_E=426.67	-7.6
Prepared_ns2_441773_uff_E=426.67	-6.5	prepared_vp4_441773_uff_E=426.67	-7.2
Prepared_ns2_441773_uff_E=426.67	-6.5	prepared_vp4_441773_uff_E=426.67	-7.2
Prepared_ns2_441773_uff_E=426.67	-6.3	prepared_vp4_441773_uff_E=426.67	-7.1
Prepared_ns2_441773_uff_E=426.67	-6.3	prepared_vp4_441773_uff_E=426.67	-7
Prepared_ns2_441773_uff_E=426.67	-6.1	prepared_vp4_441773_uff_E=426.67	-7
Prepared_ns2_441773_uff_E=426.67	-6.1	prepared_vp4_441773_uff_E=426.67	-7
Prepared_ns2_440832_uff_E=339.61	-7.1	prepared_vp4_440832_uff_E=339.61	-7.9
Prepared_ns2_440832_uff_E=339.61	-7	prepared_vp4_440832_uff_E=339.61	-7.8
Prepared_ns2_440832_uff_E=339.61	-6.8	prepared_vp4_440832_uff_E=339.61	-7.4
Prepared_ns2_440832_uff_E=339.61	-6.5	prepared_vp4_440832_uff_E=339.61	-7.2
Prepared_ns2_440832_uff_E=339.61	-6.3	prepared_vp4_440832_uff_E=339.61	-7.2
Prepared_ns2_440832_uff_E=339.61	-6.3	prepared_vp4_440832_uff_E=339.61	-7
Prepared_ns2_440832_uff_E=339.61	-6.3	prepared_vp4_440832_uff_E=339.61	-6.8
Prepared_ns2_440832_uff_E=339.61	-6.2	prepared_vp4_440832_uff_E=339.61	-6.6
Prepared_ns2_440832_uff_E=339.61	-6.1	prepared_vp4_440832_uff_E=339.61	-6.5
Prepared_ns2_854_uff_E=107.93	-4.5	prepared_vp4_854_uff_E=107.93	-4.9
Prepared_ns2_854_uff_E=107.93	-4.4	prepared_vp4_854_uff_E=107.93	-4.9
Prepared_ns2_854_uff_E=107.93	-4.3	prepared_vp4_854_uff_E=107.93	-4.8
Prepared_ns2_854_uff_E=107.93	-4.1	prepared_vp4_854_uff_E=107.93	-4.7
Prepared_ns2_854_uff_E=107.93	-4	prepared_vp4_854_uff_E=107.93	-4.7
Prepared_ns2_854_uff_E=107.93	-3.9	prepared_vp4_854_uff_E=107.93	-4.7
Prepared_ns2_854_uff_E=107.93	-3.9	prepared_vp4_854_uff_E=107.93	-4.6
Prepared_ns2_854_uff_E=107.93	-3.8	prepared_vp4_854_uff_E=107.93	-4.3
Prepared_ns2_854_uff_E=107.93	-3.8	prepared_vp4_854_uff_E=107.93	-4.3
Prepared_ns2_123409_uff_E=416.00	-4.4	prepared_vp4_123409_uff_E=416.00	-4.8
Prepared_ns2_123409_uff_E=416.00	-4.3	prepared_vp4_123409_uff_E=416.00	-4.6
Prepared_ns2_123409_uff_E=416.00	-4.3	prepared_vp4_123409_uff_E=416.00	-4.5
Prepared_ns2_123409_uff_E=416.00	-4.2	prepared_vp4_123409_uff_E=416.00	-4.5
Prepared_ns2_123409_uff_E=416.00	-4.2	prepared_vp4_123409_uff_E=416.00	-4.5
Prepared_ns2_123409_uff_E=416.00	-4.2	prepared_vp4_123409_uff_E=416.00	-4.5
Prepared_ns2_123409_uff_E=416.00	-4.2	prepared_vp4_123409_uff_E=416.00	-4.4
Prepared_ns2_123409_uff_E=416.00	-4.1	prepared_vp4_123409_uff_E=416.00	-4.4
Prepared_ns2_123409_uff_E=416.00	-4.1	prepared_vp4_123409_uff_E=416.00	-4.4
Prepared_ns2_985_uff_E=57.46	-4.3	prepared_vp4_985_uff_E=57.46	-4.8
Prepared_ns2_985_uff_E=57.46	-4.2	prepared_vp4_985_uff_E=57.46	-4.6
Prepared_ns2_985_uff_E=57.46	-4.1	prepared_vp4_985_uff_E=57.46	-4.6
Prepared_ns2_985_uff_E=57.46	-4	prepared_vp4_985_uff_E=57.46	-4.6
Prepared_ns2_985_uff_E=57.46	-4	prepared_vp4_985_uff_E=57.46	-4.5
Prepared_ns2_985_uff_E=57.46	-4	prepared_vp4_985_uff_E=57.46	-4.5
Prepared_ns2_985_uff_E=57.46	-3.8	prepared_vp4_985_uff_E=57.46	-4.5
Prepared_ns2_985_uff_E=57.46	-3.8	prepared_vp4_985_uff_E=57.46	-4.5

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_985_uff_E=57.46	-3.8	prepared_vp4_985_uff_E=57.46	-4.4
Prepared_ns2_445639_uff_E=80.35	-5	prepared_vp4_445639_uff_E=80.35	-4.8
Prepared_ns2_445639_uff_E=80.35	-4.8	prepared_vp4_445639_uff_E=80.35	-4.6
Prepared_ns2_445639_uff_E=80.35	-4.8	prepared_vp4_445639_uff_E=80.35	-4.6
Prepared_ns2_445639_uff_E=80.35	-4.8	prepared_vp4_445639_uff_E=80.35	-4.5
Prepared_ns2_445639_uff_E=80.35	-4.7	prepared_vp4_445639_uff_E=80.35	-4.3
Prepared_ns2_445639_uff_E=80.35	-4.7	prepared_vp4_445639_uff_E=80.35	-4.1
Prepared_ns2_445639_uff_E=80.35	-4.7	prepared_vp4_445639_uff_E=80.35	-4.1
Prepared_ns2_445639_uff_E=80.35	-4.7	prepared_vp4_445639_uff_E=80.35	-4
Prepared_ns2_445639_uff_E=80.35	-4.6	prepared_vp4_445639_uff_E=80.35	-3.9
Prepared_ns2_548230_uff_E=242.77	-5.7	prepared_vp4_548230_uff_E=242.77	-6.4
Prepared_ns2_548230_uff_E=242.77	-5.5	prepared_vp4_548230_uff_E=242.77	-6
Prepared_ns2_548230_uff_E=242.77	-5.4	prepared_vp4_548230_uff_E=242.77	-6
Prepared_ns2_548230_uff_E=242.77	-5.2	prepared_vp4_548230_uff_E=242.77	-5.9
Prepared_ns2_548230_uff_E=242.77	-5.1	prepared_vp4_548230_uff_E=242.77	-5.9
Prepared_ns2_548230_uff_E=242.77	-5.1	prepared_vp4_548230_uff_E=242.77	-5.8
Prepared_ns2_548230_uff_E=242.77	-5.1	prepared_vp4_548230_uff_E=242.77	-5.7
Prepared_ns2_548230_uff_E=242.77	-5	prepared_vp4_548230_uff_E=242.77	-5.6
Prepared_ns2_548230_uff_E=242.77	-5	prepared_vp4_548230_uff_E=242.77	-5.5
Prepared_ns2_5281553_uff_E=113.15	-4.3	prepared_vp4_5281553_uff_E=113.15	-5.5
Prepared_ns2_5281553_uff_E=113.15	-4.1	prepared_vp4_5281553_uff_E=113.15	-5.2
Prepared_ns2_5281553_uff_E=113.15	-4.1	prepared_vp4_5281553_uff_E=113.15	-4.9
Prepared_ns2_5281553_uff_E=113.15	-4	prepared_vp4_5281553_uff_E=113.15	-4.7
Prepared_ns2_5281553_uff_E=113.15	-4	prepared_vp4_5281553_uff_E=113.15	-4.7
Prepared_ns2_5281553_uff_E=113.15	-4	prepared_vp4_5281553_uff_E=113.15	-4.7
Prepared_ns2_5281553_uff_E=113.15	-3.9	prepared_vp4_5281553_uff_E=113.15	-4.6
Prepared_ns2_5281553_uff_E=113.15	-3.9	prepared_vp4_5281553_uff_E=113.15	-4.6
Prepared_ns2_5281553_uff_E=113.15	-3.9	prepared_vp4_5281553_uff_E=113.15	-4.5
Prepared_ns2_439260_uff_E=104.91	-5.1	prepared_vp4_439260_uff_E=104.91	-5.8
Prepared_ns2_439260_uff_E=104.91	-5.1	prepared_vp4_439260_uff_E=104.91	-5.7
Prepared_ns2_439260_uff_E=104.91	-5	prepared_vp4_439260_uff_E=104.91	-5.5
Prepared_ns2_439260_uff_E=104.91	-5	prepared_vp4_439260_uff_E=104.91	-5.5
Prepared_ns2_439260_uff_E=104.91	-5	prepared_vp4_439260_uff_E=104.91	-5.5
Prepared_ns2_439260_uff_E=104.91	-4.9	prepared_vp4_439260_uff_E=104.91	-5.4
Prepared_ns2_439260_uff_E=104.91	-4.9	prepared_vp4_439260_uff_E=104.91	-5.3
Prepared_ns2_439260_uff_E=104.91	-4.8	prepared_vp4_439260_uff_E=104.91	-5.3
Prepared_ns2_439260_uff_E=104.91	-4.8	prepared_vp4_439260_uff_E=104.91	-5.3
Prepared_ns2_72344_uff_E=703.11	-6.4	prepared_vp4_72344_uff_E=703.11	-7
Prepared_ns2_72344_uff_E=703.11	-6.4	prepared_vp4_72344_uff_E=703.11	-6.9
Prepared_ns2_72344_uff_E=703.11	-6.1	prepared_vp4_72344_uff_E=703.11	-6.9
Prepared_ns2_72344_uff_E=703.11	-6	prepared_vp4_72344_uff_E=703.11	-6.8
Prepared_ns2_72344_uff_E=703.11	-5.9	prepared_vp4_72344_uff_E=703.11	-6.7
Prepared_ns2_72344_uff_E=703.11	-5.8	prepared_vp4_72344_uff_E=703.11	-6.5
Prepared_ns2_72344_uff_E=703.11	-5.8	prepared_vp4_72344_uff_E=703.11	-6.2
Prepared_ns2_72344_uff_E=703.11	-5.7	prepared_vp4_72344_uff_E=703.11	-6.2

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_72344_uff_E=703.11	-5.7	prepared_vp4_72344_uff_E=703.11	-6.1
Prepared_ns2_89594_uff_E=283.26	-4.7	prepared_vp4_89594_uff_E=283.26	-5.6
Prepared_ns2_89594_uff_E=283.26	-4.7	prepared_vp4_89594_uff_E=283.26	-5.5
Prepared_ns2_89594_uff_E=283.26	-4.6	prepared_vp4_89594_uff_E=283.26	-5.3
Prepared_ns2_89594_uff_E=283.26	-4.4	prepared_vp4_89594_uff_E=283.26	-5.3
Prepared_ns2_89594_uff_E=283.26	-4.3	prepared_vp4_89594_uff_E=283.26	-5.2
Prepared_ns2_89594_uff_E=283.26	-4.2	prepared_vp4_89594_uff_E=283.26	-5.2
Prepared_ns2_89594_uff_E=283.26	-4.2	prepared_vp4_89594_uff_E=283.26	-5.1
Prepared_ns2_89594_uff_E=283.26	-4.1	prepared_vp4_89594_uff_E=283.26	-5
Prepared_ns2_89594_uff_E=283.26	-4.1	prepared_vp4_89594_uff_E=283.26	-4.9
Prepared_ns2_160921_uff_E=423.55	-6.5	prepared_vp4_160921_uff_E=423.55	-7.5
Prepared_ns2_160921_uff_E=423.55	-6.4	prepared_vp4_160921_uff_E=423.55	-7.4
Prepared_ns2_160921_uff_E=423.55	-6.4	prepared_vp4_160921_uff_E=423.55	-7.1
Prepared_ns2_160921_uff_E=423.55	-6.3	prepared_vp4_160921_uff_E=423.55	-7
Prepared_ns2_160921_uff_E=423.55	-6.3	prepared_vp4_160921_uff_E=423.55	-7
Prepared_ns2_160921_uff_E=423.55	-6	prepared_vp4_160921_uff_E=423.55	-6.9
Prepared_ns2_160921_uff_E=423.55	-5.9	prepared_vp4_160921_uff_E=423.55	-6.7
Prepared_ns2_160921_uff_E=423.55	-5.9	prepared_vp4_160921_uff_E=423.55	-6.4
Prepared_ns2_160921_uff_E=423.55	-5.9	prepared_vp4_160921_uff_E=423.55	-6.4
Prepared_ns2_5316819_uff_E=299.28	-6.8	prepared_vp4_5316819_uff_E=299.28	-7.4
Prepared_ns2_5316819_uff_E=299.28	-6.5	prepared_vp4_5316819_uff_E=299.28	-7
Prepared_ns2_5316819_uff_E=299.28	-6.4	prepared_vp4_5316819_uff_E=299.28	-7
Prepared_ns2_5316819_uff_E=299.28	-6.4	prepared_vp4_5316819_uff_E=299.28	-6.6
Prepared_ns2_5316819_uff_E=299.28	-6.3	prepared_vp4_5316819_uff_E=299.28	-6.5
Prepared_ns2_5316819_uff_E=299.28	-6.3	prepared_vp4_5316819_uff_E=299.28	-6.4
Prepared_ns2_5316819_uff_E=299.28	-6	prepared_vp4_5316819_uff_E=299.28	-6.4
Prepared_ns2_5316819_uff_E=299.28	-6	prepared_vp4_5316819_uff_E=299.28	-6.4
Prepared_ns2_5316819_uff_E=299.28	-6	prepared_vp4_5316819_uff_E=299.28	-6.3
Prepared_ns2_5281119_uff_E=95.80	-4.9	prepared_vp4_5281119_uff_E=95.80	-5.5
Prepared_ns2_5281119_uff_E=95.80	-4.4	prepared_vp4_5281119_uff_E=95.80	-5.4
Prepared_ns2_5281119_uff_E=95.80	-4.3	prepared_vp4_5281119_uff_E=95.80	-5.3
Prepared_ns2_5281119_uff_E=95.80	-4.2	prepared_vp4_5281119_uff_E=95.80	-5.3
Prepared_ns2_5281119_uff_E=95.80	-4.2	prepared_vp4_5281119_uff_E=95.80	-5.3
Prepared_ns2_5281119_uff_E=95.80	-4.2	prepared_vp4_5281119_uff_E=95.80	-5.3
Prepared_ns2_5281119_uff_E=95.80	-4.1	prepared_vp4_5281119_uff_E=95.80	-5.2
Prepared_ns2_5281119_uff_E=95.80	-4.1	prepared_vp4_5281119_uff_E=95.80	-5.2
Prepared_ns2_5281119_uff_E=95.80	-4.1	prepared_vp4_5281119_uff_E=95.80	-5.1
Prepared_ns2_4276_uff_E=330.81	-5.1	prepared_vp4_4276_uff_E=330.81	-6
Prepared_ns2_4276_uff_E=330.81	-4.7	prepared_vp4_4276_uff_E=330.81	-5.9
Prepared_ns2_4276_uff_E=330.81	-4.6	prepared_vp4_4276_uff_E=330.81	-5.9
Prepared_ns2_4276_uff_E=330.81	-4.6	prepared_vp4_4276_uff_E=330.81	-5.6
Prepared_ns2_4276_uff_E=330.81	-4.6	prepared_vp4_4276_uff_E=330.81	-5.4
Prepared_ns2_4276_uff_E=330.81	-4.6	prepared_vp4_4276_uff_E=330.81	-5.4
Prepared_ns2_4276_uff_E=330.81	-4.4	prepared_vp4_4276_uff_E=330.81	-5.3
Prepared_ns2_4276_uff_E=330.81	-4.4	prepared_vp4_4276_uff_E=330.81	-5.2

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_4276_uff_E=330.81	-4.3	prepared_vp4_4276_uff_E=330.81	-5.1
Prepared_ns2_5281672_uff_E=388.01	-6.9	prepared_vp4_5281672_uff_E=388.01	-8.7
Prepared_ns2_5281672_uff_E=388.01	-6.8	prepared_vp4_5281672_uff_E=388.01	-8
Prepared_ns2_5281672_uff_E=388.01	-6.5	prepared_vp4_5281672_uff_E=388.01	-8
Prepared_ns2_5281672_uff_E=388.01	-6.5	prepared_vp4_5281672_uff_E=388.01	-7.8
Prepared_ns2_5281672_uff_E=388.01	-6.5	prepared_vp4_5281672_uff_E=388.01	-7.5
Prepared_ns2_5281672_uff_E=388.01	-6.4	prepared_vp4_5281672_uff_E=388.01	-7.4
Prepared_ns2_5281672_uff_E=388.01	-6.4	prepared_vp4_5281672_uff_E=388.01	-7.4
Prepared_ns2_5281672_uff_E=388.01	-6.3	prepared_vp4_5281672_uff_E=388.01	-7.1
Prepared_ns2_5281672_uff_E=388.01	-6.3	prepared_vp4_5281672_uff_E=388.01	-7.1
Prepared_ns2_31253_uff_E=90.99	-3.7	prepared_vp4_31253_uff_E=90.99	-4.5
Prepared_ns2_31253_uff_E=90.99	-3.6	prepared_vp4_31253_uff_E=90.99	-4.5
Prepared_ns2_31253_uff_E=90.99	-3.6	prepared_vp4_31253_uff_E=90.99	-4.4
Prepared_ns2_31253_uff_E=90.99	-3.6	prepared_vp4_31253_uff_E=90.99	-4.3
Prepared_ns2_31253_uff_E=90.99	-3.6	prepared_vp4_31253_uff_E=90.99	-4.2
Prepared_ns2_31253_uff_E=90.99	-3.5	prepared_vp4_31253_uff_E=90.99	-4.1
Prepared_ns2_31253_uff_E=90.99	-3.5	prepared_vp4_31253_uff_E=90.99	-4
Prepared_ns2_31253_uff_E=90.99	-3.4	prepared_vp4_31253_uff_E=90.99	-4
Prepared_ns2_31253_uff_E=90.99	-3.4	prepared_vp4_31253_uff_E=90.99	-3.9
Prepared_ns2_26447_uff_E=92.92	-4.4	prepared_vp4_26447_uff_E=92.92	-5.5
Prepared_ns2_26447_uff_E=92.92	-4.4	prepared_vp4_26447_uff_E=92.92	-5.5
Prepared_ns2_26447_uff_E=92.92	-4.3	prepared_vp4_26447_uff_E=92.92	-5.2
Prepared_ns2_26447_uff_E=92.92	-4.3	prepared_vp4_26447_uff_E=92.92	-5.2
Prepared_ns2_26447_uff_E=92.92	-4.2	prepared_vp4_26447_uff_E=92.92	-5.1
Prepared_ns2_26447_uff_E=92.92	-4.2	prepared_vp4_26447_uff_E=92.92	-4.9
Prepared_ns2_26447_uff_E=92.92	-4.1	prepared_vp4_26447_uff_E=92.92	-4.9
Prepared_ns2_26447_uff_E=92.92	-4.1	prepared_vp4_26447_uff_E=92.92	-4.9
Prepared_ns2_26447_uff_E=92.92	-4.1	prepared_vp4_26447_uff_E=92.92	-4.9
Prepared_ns2_397934_uff_E=827.74	-8.5	prepared_vp4_397934_uff_E=827.74	-9.6
Prepared_ns2_397934_uff_E=827.74	-8.5	prepared_vp4_397934_uff_E=827.74	-9.1
Prepared_ns2_397934_uff_E=827.74	-8.3	prepared_vp4_397934_uff_E=827.74	-8.8
Prepared_ns2_397934_uff_E=827.74	-7.8	prepared_vp4_397934_uff_E=827.74	-8.7
Prepared_ns2_397934_uff_E=827.74	-7.6	prepared_vp4_397934_uff_E=827.74	-8.6
Prepared_ns2_397934_uff_E=827.74	-7.6	prepared_vp4_397934_uff_E=827.74	-8.6
Prepared_ns2_397934_uff_E=827.74	-7.6	prepared_vp4_397934_uff_E=827.74	-8.5
Prepared_ns2_397934_uff_E=827.74	-7.5	prepared_vp4_397934_uff_E=827.74	-8.1
Prepared_ns2_397934_uff_E=827.74	-6.7	prepared_vp4_397934_uff_E=827.74	-8.1
Prepared_ns2_5281647_uff_E=412.79	-8	prepared_vp4_5281647_uff_E=412.79	-7.8
Prepared_ns2_5281647_uff_E=412.79	-7.7	prepared_vp4_5281647_uff_E=412.79	-7.7
Prepared_ns2_5281647_uff_E=412.79	-7.5	prepared_vp4_5281647_uff_E=412.79	-7.7
Prepared_ns2_5281647_uff_E=412.79	-7.4	prepared_vp4_5281647_uff_E=412.79	-7.6
Prepared_ns2_5281647_uff_E=412.79	-7.3	prepared_vp4_5281647_uff_E=412.79	-7.5
Prepared_ns2_5281647_uff_E=412.79	-7.2	prepared_vp4_5281647_uff_E=412.79	-7.5
Prepared_ns2_5281647_uff_E=412.79	-7	prepared_vp4_5281647_uff_E=412.79	-7.3
Prepared_ns2_5281647_uff_E=412.79	-7	prepared_vp4_5281647_uff_E=412.79	-7.2

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5281647_uff_E=412.79	-6.8	prepared_vp4_5281647_uff_E=412.79	-7.2
Prepared_ns2_5280445_uff_E=242.10	-7.9	prepared_vp4_5280445_uff_E=242.10	-8.8
Prepared_ns2_5280445_uff_E=242.10	-7.3	prepared_vp4_5280445_uff_E=242.10	-8
Prepared_ns2_5280445_uff_E=242.10	-7.1	prepared_vp4_5280445_uff_E=242.10	-8
Prepared_ns2_5280445_uff_E=242.10	-6.9	prepared_vp4_5280445_uff_E=242.10	-7.7
Prepared_ns2_5280445_uff_E=242.10	-6.9	prepared_vp4_5280445_uff_E=242.10	-7.6
Prepared_ns2_5280445_uff_E=242.10	-6.8	prepared_vp4_5280445_uff_E=242.10	-7.6
Prepared_ns2_5280445_uff_E=242.10	-6.6	prepared_vp4_5280445_uff_E=242.10	-7.6
Prepared_ns2_5280445_uff_E=242.10	-6.6	prepared_vp4_5280445_uff_E=242.10	-7.3
Prepared_ns2_5280445_uff_E=242.10	-6.5	prepared_vp4_5280445_uff_E=242.10	-7.3
Prepared_ns2_10250777_uff_E=317.22	-7.6	prepared_vp4_10250777_uff_E=317.22	-8.2
Prepared_ns2_10250777_uff_E=317.22	-7.2	prepared_vp4_10250777_uff_E=317.22	-8.2
Prepared_ns2_10250777_uff_E=317.22	-7	prepared_vp4_10250777_uff_E=317.22	-8.1
Prepared_ns2_10250777_uff_E=317.22	-7	prepared_vp4_10250777_uff_E=317.22	-8.1
Prepared_ns2_10250777_uff_E=317.22	-6.9	prepared_vp4_10250777_uff_E=317.22	-8
Prepared_ns2_10250777_uff_E=317.22	-6.9	prepared_vp4_10250777_uff_E=317.22	-8
Prepared_ns2_10250777_uff_E=317.22	-6.8	prepared_vp4_10250777_uff_E=317.22	-7.8
Prepared_ns2_10250777_uff_E=317.22	-6.8	prepared_vp4_10250777_uff_E=317.22	-7.7
Prepared_ns2_10250777_uff_E=317.22	-6.6	prepared_vp4_10250777_uff_E=317.22	-7.7
Prepared_ns2_259846_uff_E=928.19	-7.4	prepared_vp4_259846_uff_E=928.19	-8.9
Prepared_ns2_259846_uff_E=928.19	-7.3	prepared_vp4_259846_uff_E=928.19	-8.4
Prepared_ns2_259846_uff_E=928.19	-7.1	prepared_vp4_259846_uff_E=928.19	-8.4
Prepared_ns2_259846_uff_E=928.19	-7	prepared_vp4_259846_uff_E=928.19	-8.2
Prepared_ns2_259846_uff_E=928.19	-7	prepared_vp4_259846_uff_E=928.19	-8.1
Prepared_ns2_259846_uff_E=928.19	-7	prepared_vp4_259846_uff_E=928.19	-7.7
Prepared_ns2_259846_uff_E=928.19	-6.9	prepared_vp4_259846_uff_E=928.19	-7.6
Prepared_ns2_259846_uff_E=928.19	-6.8	prepared_vp4_259846_uff_E=928.19	-7.5
Prepared_ns2_259846_uff_E=928.19	-6.7	prepared_vp4_259846_uff_E=928.19	-7.4
Prepared_ns2_11128_uff_E=276.52	-5	prepared_vp4_11128_uff_E=276.52	-6.1
Prepared_ns2_11128_uff_E=276.52	-4.9	prepared_vp4_11128_uff_E=276.52	-5.8
Prepared_ns2_11128_uff_E=276.52	-4.8	prepared_vp4_11128_uff_E=276.52	-5.7
Prepared_ns2_11128_uff_E=276.52	-4.8	prepared_vp4_11128_uff_E=276.52	-5.6
Prepared_ns2_11128_uff_E=276.52	-4.8	prepared_vp4_11128_uff_E=276.52	-5.6
Prepared_ns2_11128_uff_E=276.52	-4.8	prepared_vp4_11128_uff_E=276.52	-5.3
Prepared_ns2_11128_uff_E=276.52	-4.7	prepared_vp4_11128_uff_E=276.52	-5.2
Prepared_ns2_11128_uff_E=276.52	-4.7	prepared_vp4_11128_uff_E=276.52	-5.1
Prepared_ns2_11128_uff_E=276.52	-4.4	prepared_vp4_11128_uff_E=276.52	-5
Prepared_ns2_6549_uff_E=118.54	-4.2	prepared_vp4_6549_uff_E=118.54	-5.2
Prepared_ns2_6549_uff_E=118.54	-4.2	prepared_vp4_6549_uff_E=118.54	-5.2
Prepared_ns2_6549_uff_E=118.54	-4.1	prepared_vp4_6549_uff_E=118.54	-5
Prepared_ns2_6549_uff_E=118.54	-4.1	prepared_vp4_6549_uff_E=118.54	-4.8
Prepared_ns2_6549_uff_E=118.54	-4	prepared_vp4_6549_uff_E=118.54	-4.8
Prepared_ns2_6549_uff_E=118.54	-3.9	prepared_vp4_6549_uff_E=118.54	-4.8
Prepared_ns2_6549_uff_E=118.54	-3.9	prepared_vp4_6549_uff_E=118.54	-4.7
Prepared_ns2_6549_uff_E=118.54	-3.9	prepared_vp4_6549_uff_E=118.54	-4.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_6549_uff_E=118.54	-3.8	prepared_vp4_6549_uff_E=118.54	-4.6
Prepared_ns2_22311_uff_E=102.50	-4.4	prepared_vp4_22311_uff_E=102.50	-5.7
Prepared_ns2_22311_uff_E=102.50	-4.4	prepared_vp4_22311_uff_E=102.50	-5.7
Prepared_ns2_22311_uff_E=102.50	-4.2	prepared_vp4_22311_uff_E=102.50	-5.5
Prepared_ns2_22311_uff_E=102.50	-4.2	prepared_vp4_22311_uff_E=102.50	-5.5
Prepared_ns2_22311_uff_E=102.50	-4.1	prepared_vp4_22311_uff_E=102.50	-5.4
Prepared_ns2_22311_uff_E=102.50	-4.1	prepared_vp4_22311_uff_E=102.50	-5.4
Prepared_ns2_22311_uff_E=102.50	-4.1	prepared_vp4_22311_uff_E=102.50	-5.3
Prepared_ns2_22311_uff_E=102.50	-4.1	prepared_vp4_22311_uff_E=102.50	-5.3
Prepared_ns2_22311_uff_E=102.50	-4	prepared_vp4_22311_uff_E=102.50	-5.3
Prepared_ns2_443013_uff_E=788.01	-7.1	prepared_vp4_443013_uff_E=788.01	-8.1
Prepared_ns2_443013_uff_E=788.01	-7	prepared_vp4_443013_uff_E=788.01	-8
Prepared_ns2_443013_uff_E=788.01	-7	prepared_vp4_443013_uff_E=788.01	-7.2
Prepared_ns2_443013_uff_E=788.01	-6.8	prepared_vp4_443013_uff_E=788.01	-7.2
Prepared_ns2_443013_uff_E=788.01	-6.7	prepared_vp4_443013_uff_E=788.01	-7.1
Prepared_ns2_443013_uff_E=788.01	-6.6	prepared_vp4_443013_uff_E=788.01	-7
Prepared_ns2_443013_uff_E=788.01	-6.6	prepared_vp4_443013_uff_E=788.01	-6.9
Prepared_ns2_443013_uff_E=788.01	-6.6	prepared_vp4_443013_uff_E=788.01	-6.7
Prepared_ns2_443013_uff_E=788.01	-6.4	prepared_vp4_443013_uff_E=788.01	-6.6
Prepared_ns2_261166_uff_E=511.48	-6.2	prepared_vp4_261166_uff_E=511.48	-6.6
Prepared_ns2_261166_uff_E=511.48	-6.2	prepared_vp4_261166_uff_E=511.48	-6.3
Prepared_ns2_261166_uff_E=511.48	-5.8	prepared_vp4_261166_uff_E=511.48	-6.1
Prepared_ns2_261166_uff_E=511.48	-5.8	prepared_vp4_261166_uff_E=511.48	-6.1
Prepared_ns2_261166_uff_E=511.48	-5.6	prepared_vp4_261166_uff_E=511.48	-5.9
Prepared_ns2_261166_uff_E=511.48	-5.5	prepared_vp4_261166_uff_E=511.48	-5.9
Prepared_ns2_261166_uff_E=511.48	-5.5	prepared_vp4_261166_uff_E=511.48	-5.9
Prepared_ns2_261166_uff_E=511.48	-5.5	prepared_vp4_261166_uff_E=511.48	-5.9
Prepared_ns2_261166_uff_E=511.48	-5.5	prepared_vp4_261166_uff_E=511.48	-5.9
Prepared_ns2_3893_uff_E=43.33	-4.4	prepared_vp4_3893_uff_E=43.33	-5
Prepared_ns2_3893_uff_E=43.33	-4.4	prepared_vp4_3893_uff_E=43.33	-4.8
Prepared_ns2_3893_uff_E=43.33	-4.2	prepared_vp4_3893_uff_E=43.33	-4.6
Prepared_ns2_3893_uff_E=43.33	-4	prepared_vp4_3893_uff_E=43.33	-4.6
Prepared_ns2_3893_uff_E=43.33	-4	prepared_vp4_3893_uff_E=43.33	-4.5
Prepared_ns2_3893_uff_E=43.33	-3.9	prepared_vp4_3893_uff_E=43.33	-4.5
Prepared_ns2_3893_uff_E=43.33	-3.9	prepared_vp4_3893_uff_E=43.33	-4.5
Prepared_ns2_3893_uff_E=43.33	-3.9	prepared_vp4_3893_uff_E=43.33	-4.4
Prepared_ns2_3893_uff_E=43.33	-3.9	prepared_vp4_3893_uff_E=43.33	-4.3
Prepared_ns2_73062_uff_E=480.62	-7.3	prepared_vp4_73062_uff_E=480.62	-8.3
Prepared_ns2_73062_uff_E=480.62	-7.2	prepared_vp4_73062_uff_E=480.62	-8.1
Prepared_ns2_73062_uff_E=480.62	-7	prepared_vp4_73062_uff_E=480.62	-8.1
Prepared_ns2_73062_uff_E=480.62	-6.7	prepared_vp4_73062_uff_E=480.62	-8
Prepared_ns2_73062_uff_E=480.62	-6.7	prepared_vp4_73062_uff_E=480.62	-7.9
Prepared_ns2_73062_uff_E=480.62	-6.6	prepared_vp4_73062_uff_E=480.62	-7.5
Prepared_ns2_73062_uff_E=480.62	-6.5	prepared_vp4_73062_uff_E=480.62	-7.4
Prepared_ns2_73062_uff_E=480.62	-6.5	prepared_vp4_73062_uff_E=480.62	-7.4

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_73062_uff_E=480.62	-6.3	prepared_vp4_73062_uff_E=480.62	-7.2
Prepared_ns2_5280863_uff_E=362.50	-7.4	prepared_vp4_5280863_uff_E=362.50	-8.4
Prepared_ns2_5280863_uff_E=362.50	-7.2	prepared_vp4_5280863_uff_E=362.50	-7.9
Prepared_ns2_5280863_uff_E=362.50	-6.7	prepared_vp4_5280863_uff_E=362.50	-7.8
Prepared_ns2_5280863_uff_E=362.50	-6.4	prepared_vp4_5280863_uff_E=362.50	-7.6
Prepared_ns2_5280863_uff_E=362.50	-6.3	prepared_vp4_5280863_uff_E=362.50	-7.6
Prepared_ns2_5280863_uff_E=362.50	-6.3	prepared_vp4_5280863_uff_E=362.50	-7.4
Prepared_ns2_5280863_uff_E=362.50	-6.2	prepared_vp4_5280863_uff_E=362.50	-7.3
Prepared_ns2_5280863_uff_E=362.50	-6.1	prepared_vp4_5280863_uff_E=362.50	-7.3
Prepared_ns2_5280863_uff_E=362.50	-6.1	prepared_vp4_5280863_uff_E=362.50	-7.2
Prepared_ns2_162350_uff_E=453.84	-7.3	prepared_vp4_162350_uff_E=453.84	-8.3
Prepared_ns2_162350_uff_E=453.84	-7.3	prepared_vp4_162350_uff_E=453.84	-8
Prepared_ns2_162350_uff_E=453.84	-7.2	prepared_vp4_162350_uff_E=453.84	-7.8
Prepared_ns2_162350_uff_E=453.84	-7.2	prepared_vp4_162350_uff_E=453.84	-7.7
Prepared_ns2_162350_uff_E=453.84	-7.1	prepared_vp4_162350_uff_E=453.84	-7.7
Prepared_ns2_162350_uff_E=453.84	-7.1	prepared_vp4_162350_uff_E=453.84	-7.7
Prepared_ns2_162350_uff_E=453.84	-7.1	prepared_vp4_162350_uff_E=453.84	-7.6
Prepared_ns2_162350_uff_E=453.84	-7.1	prepared_vp4_162350_uff_E=453.84	-7.5
Prepared_ns2_162350_uff_E=453.84	-6.8	prepared_vp4_162350_uff_E=453.84	-7.4
Prepared_ns2_853433_uff_E=170.74	-4.8	prepared_vp4_853433_uff_E=170.74	-6
Prepared_ns2_853433_uff_E=170.74	-4.7	prepared_vp4_853433_uff_E=170.74	-5.8
Prepared_ns2_853433_uff_E=170.74	-4.6	prepared_vp4_853433_uff_E=170.74	-5.5
Prepared_ns2_853433_uff_E=170.74	-4.6	prepared_vp4_853433_uff_E=170.74	-5.5
Prepared_ns2_853433_uff_E=170.74	-4.6	prepared_vp4_853433_uff_E=170.74	-5.4
Prepared_ns2_853433_uff_E=170.74	-4.6	prepared_vp4_853433_uff_E=170.74	-5.2
Prepared_ns2_853433_uff_E=170.74	-4.5	prepared_vp4_853433_uff_E=170.74	-5.2
Prepared_ns2_853433_uff_E=170.74	-4.5	prepared_vp4_853433_uff_E=170.74	-5.1
Prepared_ns2_853433_uff_E=170.74	-4.4	prepared_vp4_853433_uff_E=170.74	-5.1
Prepared_ns2_5318557_uff_E=272.58	-4.7	prepared_vp4_5318557_uff_E=272.58	-5.4
Prepared_ns2_5318557_uff_E=272.58	-4.7	prepared_vp4_5318557_uff_E=272.58	-5.3
Prepared_ns2_5318557_uff_E=272.58	-4.6	prepared_vp4_5318557_uff_E=272.58	-5.3
Prepared_ns2_5318557_uff_E=272.58	-4.6	prepared_vp4_5318557_uff_E=272.58	-5.2
Prepared_ns2_5318557_uff_E=272.58	-4.6	prepared_vp4_5318557_uff_E=272.58	-5.2
Prepared_ns2_5318557_uff_E=272.58	-4.5	prepared_vp4_5318557_uff_E=272.58	-5.1
Prepared_ns2_5318557_uff_E=272.58	-4.5	prepared_vp4_5318557_uff_E=272.58	-5
Prepared_ns2_5318557_uff_E=272.58	-4.4	prepared_vp4_5318557_uff_E=272.58	-4.9
Prepared_ns2_5318557_uff_E=272.58	-4.4	prepared_vp4_5318557_uff_E=272.58	-4.9
Prepared_ns2_68108_uff_E=100.81	-4.9	prepared_vp4_68108_uff_E=100.81	-6.4
Prepared_ns2_68108_uff_E=100.81	-4.8	prepared_vp4_68108_uff_E=100.81	-6.3
Prepared_ns2_68108_uff_E=100.81	-4.7	prepared_vp4_68108_uff_E=100.81	-5.9
Prepared_ns2_68108_uff_E=100.81	-4.7	prepared_vp4_68108_uff_E=100.81	-5.9
Prepared_ns2_68108_uff_E=100.81	-4.7	prepared_vp4_68108_uff_E=100.81	-5.6
Prepared_ns2_68108_uff_E=100.81	-4.7	prepared_vp4_68108_uff_E=100.81	-5.6
Prepared_ns2_68108_uff_E=100.81	-4.4	prepared_vp4_68108_uff_E=100.81	-5.5
Prepared_ns2_68108_uff_E=100.81	-4.4	prepared_vp4_68108_uff_E=100.81	-5.3

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_68108_uff_E=100.81	-4.4	prepared_vp4_68108_uff_E=100.81	-5.3
Prepared_ns2_798_uff_E=271.22	-4.4	prepared_vp4_798_uff_E=271.22	-5.9
Prepared_ns2_798_uff_E=271.22	-4.4	prepared_vp4_798_uff_E=271.22	-5.4
Prepared_ns2_798_uff_E=271.22	-4.3	prepared_vp4_798_uff_E=271.22	-4.9
Prepared_ns2_798_uff_E=271.22	-4.3	prepared_vp4_798_uff_E=271.22	-4.9
Prepared_ns2_798_uff_E=271.22	-4.2	prepared_vp4_798_uff_E=271.22	-4.9
Prepared_ns2_798_uff_E=271.22	-4.1	prepared_vp4_798_uff_E=271.22	-4.8
Prepared_ns2_798_uff_E=271.22	-4.1	prepared_vp4_798_uff_E=271.22	-4.7
Prepared_ns2_798_uff_E=271.22	-4	prepared_vp4_798_uff_E=271.22	-4.7
Prepared_ns2_798_uff_E=271.22	-4	prepared_vp4_798_uff_E=271.22	-4.6
Prepared_ns2_5281643_uff_E=608.46	-6.7	prepared_vp4_5281643_uff_E=608.46	-7.9
Prepared_ns2_5281643_uff_E=608.46	-6.7	prepared_vp4_5281643_uff_E=608.46	-7.9
Prepared_ns2_5281643_uff_E=608.46	-6.6	prepared_vp4_5281643_uff_E=608.46	-7.8
Prepared_ns2_5281643_uff_E=608.46	-6.6	prepared_vp4_5281643_uff_E=608.46	-7.7
Prepared_ns2_5281643_uff_E=608.46	-6.5	prepared_vp4_5281643_uff_E=608.46	-7.4
Prepared_ns2_5281643_uff_E=608.46	-6.3	prepared_vp4_5281643_uff_E=608.46	-7.3
Prepared_ns2_5281643_uff_E=608.46	-6	prepared_vp4_5281643_uff_E=608.46	-7
Prepared_ns2_5281643_uff_E=608.46	-6	prepared_vp4_5281643_uff_E=608.46	-7
Prepared_ns2_5281643_uff_E=608.46	-5.9	prepared_vp4_5281643_uff_E=608.46	-6.9
Prepared_ns2_82755_uff_E=106.56	-5.1	prepared_vp4_82755_uff_E=106.56	-5.9
Prepared_ns2_82755_uff_E=106.56	-4.9	prepared_vp4_82755_uff_E=106.56	-5.9
Prepared_ns2_82755_uff_E=106.56	-4.8	prepared_vp4_82755_uff_E=106.56	-5.7
Prepared_ns2_82755_uff_E=106.56	-4.7	prepared_vp4_82755_uff_E=106.56	-5.4
Prepared_ns2_82755_uff_E=106.56	-4.7	prepared_vp4_82755_uff_E=106.56	-5.3
Prepared_ns2_82755_uff_E=106.56	-4.7	prepared_vp4_82755_uff_E=106.56	-5.3
Prepared_ns2_82755_uff_E=106.56	-4.7	prepared_vp4_82755_uff_E=106.56	-5.2
Prepared_ns2_82755_uff_E=106.56	-4.6	prepared_vp4_82755_uff_E=106.56	-5.2
Prepared_ns2_82755_uff_E=106.56	-4.4	prepared_vp4_82755_uff_E=106.56	-5.2
Prepared_ns2_3652_uff_E=280.62	-6	prepared_vp4_3652_uff_E=280.62	-6.1
Prepared_ns2_3652_uff_E=280.62	-5.9	prepared_vp4_3652_uff_E=280.62	-6.1
Prepared_ns2_3652_uff_E=280.62	-5.9	prepared_vp4_3652_uff_E=280.62	-6
Prepared_ns2_3652_uff_E=280.62	-5.8	prepared_vp4_3652_uff_E=280.62	-6
Prepared_ns2_3652_uff_E=280.62	-5.7	prepared_vp4_3652_uff_E=280.62	-5.9
Prepared_ns2_3652_uff_E=280.62	-5.7	prepared_vp4_3652_uff_E=280.62	-5.9
Prepared_ns2_3652_uff_E=280.62	-5.6	prepared_vp4_3652_uff_E=280.62	-5.7
Prepared_ns2_3652_uff_E=280.62	-5.6	prepared_vp4_3652_uff_E=280.62	-5.7
Prepared_ns2_3652_uff_E=280.62	-5.6	prepared_vp4_3652_uff_E=280.62	-5.6
Prepared_ns2_441319624_uff_E=76.00	-5.5	prepared_vp4_441319624_uff_E=76.00	-6.1
Prepared_ns2_441319624_uff_E=76.00	-5.3	prepared_vp4_441319624_uff_E=76.00	-6
Prepared_ns2_441319624_uff_E=76.00	-5.3	prepared_vp4_441319624_uff_E=76.00	-6
Prepared_ns2_441319624_uff_E=76.00	-5.1	prepared_vp4_441319624_uff_E=76.00	-5.9
Prepared_ns2_441319624_uff_E=76.00	-4.9	prepared_vp4_441319624_uff_E=76.00	-5.8
Prepared_ns2_441319624_uff_E=76.00	-4.9	prepared_vp4_441319624_uff_E=76.00	-5.7
Prepared_ns2_441319624_uff_E=76.00	-4.9	prepared_vp4_441319624_uff_E=76.00	-5.7
Prepared_ns2_441319624_uff_E=76.00	-4.9	prepared_vp4_441319624_uff_E=76.00	-5.7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_441319624_uff_E=76.00	-4.9	prepared_vp4_441319624_uff_E=76.00	-5.6
Prepared_ns2_5281520_uff_E=195.77	-5.4	prepared_vp4_5281520_uff_E=195.77	-7
Prepared_ns2_5281520_uff_E=195.77	-5.3	prepared_vp4_5281520_uff_E=195.77	-6.9
Prepared_ns2_5281520_uff_E=195.77	-5.3	prepared_vp4_5281520_uff_E=195.77	-6.7
Prepared_ns2_5281520_uff_E=195.77	-5.2	prepared_vp4_5281520_uff_E=195.77	-6.6
Prepared_ns2_5281520_uff_E=195.77	-5	prepared_vp4_5281520_uff_E=195.77	-6.5
Prepared_ns2_5281520_uff_E=195.77	-5	prepared_vp4_5281520_uff_E=195.77	-6.4
Prepared_ns2_5281520_uff_E=195.77	-5	prepared_vp4_5281520_uff_E=195.77	-6.4
Prepared_ns2_5281520_uff_E=195.77	-4.9	prepared_vp4_5281520_uff_E=195.77	-6.4
Prepared_ns2_5281520_uff_E=195.77	-4.9	prepared_vp4_5281520_uff_E=195.77	-6.3
Prepared_ns2_135398633_uff_E=2044.77	-7	prepared_vp4_135398633_uff_E=1686.71	-8.5
Prepared_ns2_135398633_uff_E=2044.77	-6.8	prepared_vp4_135398633_uff_E=1686.71	-8.4
Prepared_ns2_135398633_uff_E=2044.77	-6.8	prepared_vp4_135398633_uff_E=1686.71	-7.9
Prepared_ns2_135398633_uff_E=2044.77	-6.6	prepared_vp4_135398633_uff_E=1686.71	-7.8
Prepared_ns2_135398633_uff_E=2044.77	-6.5	prepared_vp4_135398633_uff_E=1686.71	-7.7
Prepared_ns2_135398633_uff_E=2044.77	-6.5	prepared_vp4_135398633_uff_E=1686.71	-7.6
Prepared_ns2_135398633_uff_E=2044.77	-6.5	prepared_vp4_135398633_uff_E=1686.71	-7.5
Prepared_ns2_135398633_uff_E=2044.77	-6.5	prepared_vp4_135398633_uff_E=1686.71	-7.5
Prepared_ns2_135398633_uff_E=2044.77	-6.4	prepared_vp4_135398633_uff_E=1686.71	-7.5
Prepared_ns2_135398634_uff_E=306.57	-5.4	prepared_vp4_135398634_uff_E=306.57	-5.9
Prepared_ns2_135398634_uff_E=306.57	-5.4	prepared_vp4_135398634_uff_E=306.57	-5.9
Prepared_ns2_135398634_uff_E=306.57	-5.3	prepared_vp4_135398634_uff_E=306.57	-5.8
Prepared_ns2_135398634_uff_E=306.57	-5.2	prepared_vp4_135398634_uff_E=306.57	-5.6
Prepared_ns2_135398634_uff_E=306.57	-5.1	prepared_vp4_135398634_uff_E=306.57	-5.6
Prepared_ns2_135398634_uff_E=306.57	-4.9	prepared_vp4_135398634_uff_E=306.57	-5.5
Prepared_ns2_135398634_uff_E=306.57	-4.9	prepared_vp4_135398634_uff_E=306.57	-5.3
Prepared_ns2_135398634_uff_E=306.57	-4.8	prepared_vp4_135398634_uff_E=306.57	-5.3
Prepared_ns2_135398634_uff_E=306.57	-4.8	prepared_vp4_135398634_uff_E=306.57	-5.2
Prepared_ns2_5481224_uff_E=592.48	-7.2	prepared_vp4_5481224_uff_E=592.48	-9.3
Prepared_ns2_5481224_uff_E=592.48	-7.1	prepared_vp4_5481224_uff_E=592.48	-8.4
Prepared_ns2_5481224_uff_E=592.48	-6.8	prepared_vp4_5481224_uff_E=592.48	-8.3
Prepared_ns2_5481224_uff_E=592.48	-6.7	prepared_vp4_5481224_uff_E=592.48	-8.2
Prepared_ns2_5481224_uff_E=592.48	-6.6	prepared_vp4_5481224_uff_E=592.48	-8.2
Prepared_ns2_5481224_uff_E=592.48	-6.5	prepared_vp4_5481224_uff_E=592.48	-8
Prepared_ns2_5481224_uff_E=592.48	-6.5	prepared_vp4_5481224_uff_E=592.48	-7.8
Prepared_ns2_5481224_uff_E=592.48	-6.5	prepared_vp4_5481224_uff_E=592.48	-7.8
Prepared_ns2_5481224_uff_E=592.48	-6.5	prepared_vp4_5481224_uff_E=592.48	-7.7
Prepared_ns2_124886_uff_E=157.56	-5.5	prepared_vp4_124886_uff_E=157.56	-6
Prepared_ns2_124886_uff_E=157.56	-5.3	prepared_vp4_124886_uff_E=157.56	-5.9
Prepared_ns2_124886_uff_E=157.56	-5.3	prepared_vp4_124886_uff_E=157.56	-5.8
Prepared_ns2_124886_uff_E=157.56	-5.2	prepared_vp4_124886_uff_E=157.56	-5.7
Prepared_ns2_124886_uff_E=157.56	-5.2	prepared_vp4_124886_uff_E=157.56	-5.6
Prepared_ns2_124886_uff_E=157.56	-5.2	prepared_vp4_124886_uff_E=157.56	-5.4
Prepared_ns2_124886_uff_E=157.56	-5.1	prepared_vp4_124886_uff_E=157.56	-5.3
Prepared_ns2_124886_uff_E=157.56	-5.1	prepared_vp4_124886_uff_E=157.56	-5.2

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_124886_uff_E=157.56	-5	prepared_vp4_124886_uff_E=157.56	-5.2
Prepared_ns2_3086007_uff_E=797.18	-7.1	prepared_vp4_3086007_uff_E=797.18	-9
Prepared_ns2_3086007_uff_E=797.18	-7	prepared_vp4_3086007_uff_E=797.18	-8.3
Prepared_ns2_3086007_uff_E=797.18	-6.8	prepared_vp4_3086007_uff_E=797.18	-8.3
Prepared_ns2_3086007_uff_E=797.18	-6.7	prepared_vp4_3086007_uff_E=797.18	-8.1
Prepared_ns2_3086007_uff_E=797.18	-6.7	prepared_vp4_3086007_uff_E=797.18	-7.8
Prepared_ns2_3086007_uff_E=797.18	-6.6	prepared_vp4_3086007_uff_E=797.18	-7.8
Prepared_ns2_3086007_uff_E=797.18	-6.6	prepared_vp4_3086007_uff_E=797.18	-7.8
Prepared_ns2_3086007_uff_E=797.18	-6.5	prepared_vp4_3086007_uff_E=797.18	-7.8
Prepared_ns2_3086007_uff_E=797.18	-6.5	prepared_vp4_3086007_uff_E=797.18	-7.7
Prepared_ns2_5317570_uff_E=260.17	-5.5	prepared_vp4_5317570_uff_E=260.17	-6.8
Prepared_ns2_5317570_uff_E=260.17	-5.4	prepared_vp4_5317570_uff_E=260.17	-6.8
Prepared_ns2_5317570_uff_E=260.17	-5.4	prepared_vp4_5317570_uff_E=260.17	-6.7
Prepared_ns2_5317570_uff_E=260.17	-5.3	prepared_vp4_5317570_uff_E=260.17	-6.6
Prepared_ns2_5317570_uff_E=260.17	-5.1	prepared_vp4_5317570_uff_E=260.17	-6.5
Prepared_ns2_5317570_uff_E=260.17	-5	prepared_vp4_5317570_uff_E=260.17	-6.5
Prepared_ns2_5317570_uff_E=260.17	-4.9	prepared_vp4_5317570_uff_E=260.17	-6.4
Prepared_ns2_5317570_uff_E=260.17	-4.9	prepared_vp4_5317570_uff_E=260.17	-6.4
Prepared_ns2_5317570_uff_E=260.17	-4.9	prepared_vp4_5317570_uff_E=260.17	-6.4
Prepared_ns2_5281519_uff_E=318.41	-5.6	prepared_vp4_5281519_uff_E=318.41	-7
Prepared_ns2_5281519_uff_E=318.41	-5.3	prepared_vp4_5281519_uff_E=318.41	-7
Prepared_ns2_5281519_uff_E=318.41	-5.2	prepared_vp4_5281519_uff_E=318.41	-6.9
Prepared_ns2_5281519_uff_E=318.41	-5.2	prepared_vp4_5281519_uff_E=318.41	-6.9
Prepared_ns2_5281519_uff_E=318.41	-5.1	prepared_vp4_5281519_uff_E=318.41	-6.8
Prepared_ns2_5281519_uff_E=318.41	-5.1	prepared_vp4_5281519_uff_E=318.41	-6.8
Prepared_ns2_5281519_uff_E=318.41	-5	prepared_vp4_5281519_uff_E=318.41	-6.6
Prepared_ns2_5281519_uff_E=318.41	-4.9	prepared_vp4_5281519_uff_E=318.41	-6.6
Prepared_ns2_5281519_uff_E=318.41	-4.8	prepared_vp4_5281519_uff_E=318.41	-6.6
Prepared_ns2_1549026_uff_E=114.84	-4.5	prepared_vp4_1549026_uff_E=114.84	-5.4
Prepared_ns2_1549026_uff_E=114.84	-4.3	prepared_vp4_1549026_uff_E=114.84	-5.1
Prepared_ns2_1549026_uff_E=114.84	-4.3	prepared_vp4_1549026_uff_E=114.84	-5
Prepared_ns2_1549026_uff_E=114.84	-4.3	prepared_vp4_1549026_uff_E=114.84	-5
Prepared_ns2_1549026_uff_E=114.84	-4.2	prepared_vp4_1549026_uff_E=114.84	-5
Prepared_ns2_1549026_uff_E=114.84	-4.2	prepared_vp4_1549026_uff_E=114.84	-4.9
Prepared_ns2_1549026_uff_E=114.84	-4.1	prepared_vp4_1549026_uff_E=114.84	-4.9
Prepared_ns2_1549026_uff_E=114.84	-4	prepared_vp4_1549026_uff_E=114.84	-4.8
Prepared_ns2_1549026_uff_E=114.84	-4	prepared_vp4_1549026_uff_E=114.84	-4.8
Prepared_ns2_638011_uff_E=72.63	-4.6	prepared_vp4_638011_uff_E=72.63	-5.4
Prepared_ns2_638011_uff_E=72.63	-4.4	prepared_vp4_638011_uff_E=72.63	-5.4
Prepared_ns2_638011_uff_E=72.63	-4.4	prepared_vp4_638011_uff_E=72.63	-5.2
Prepared_ns2_638011_uff_E=72.63	-4.2	prepared_vp4_638011_uff_E=72.63	-5
Prepared_ns2_638011_uff_E=72.63	-4.2	prepared_vp4_638011_uff_E=72.63	-5
Prepared_ns2_638011_uff_E=72.63	-4.2	prepared_vp4_638011_uff_E=72.63	-5
Prepared_ns2_638011_uff_E=72.63	-4.1	prepared_vp4_638011_uff_E=72.63	-4.7
Prepared_ns2_638011_uff_E=72.63	-4.1	prepared_vp4_638011_uff_E=72.63	-4.4

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_638011_uff_E=72.63	-4.1	prepared_vp4_638011_uff_E=72.63	-4.4
Prepared_ns2_3469_uff_E=78.01	-5.1	prepared_vp4_3469_uff_E=78.01	-5.9
Prepared_ns2_3469_uff_E=78.01	-4.9	prepared_vp4_3469_uff_E=78.01	-5.8
Prepared_ns2_3469_uff_E=78.01	-4.9	prepared_vp4_3469_uff_E=78.01	-5.8
Prepared_ns2_3469_uff_E=78.01	-4.9	prepared_vp4_3469_uff_E=78.01	-5.8
Prepared_ns2_3469_uff_E=78.01	-4.8	prepared_vp4_3469_uff_E=78.01	-5.7
Prepared_ns2_3469_uff_E=78.01	-4.7	prepared_vp4_3469_uff_E=78.01	-5.6
Prepared_ns2_3469_uff_E=78.01	-4.7	prepared_vp4_3469_uff_E=78.01	-5.6
Prepared_ns2_3469_uff_E=78.01	-4.7	prepared_vp4_3469_uff_E=78.01	-5.5
Prepared_ns2_3469_uff_E=78.01	-4.7	prepared_vp4_3469_uff_E=78.01	-5.4
Prepared_ns2_370_uff_E=77.82	-5.3	prepared_vp4_370_uff_E=77.82	-6.1
Prepared_ns2_370_uff_E=77.82	-5.3	prepared_vp4_370_uff_E=77.82	-5.9
Prepared_ns2_370_uff_E=77.82	-5.1	prepared_vp4_370_uff_E=77.82	-5.7
Prepared_ns2_370_uff_E=77.82	-5.1	prepared_vp4_370_uff_E=77.82	-5.7
Prepared_ns2_370_uff_E=77.82	-5	prepared_vp4_370_uff_E=77.82	-5.7
Prepared_ns2_370_uff_E=77.82	-5	prepared_vp4_370_uff_E=77.82	-5.6
Prepared_ns2_370_uff_E=77.82	-4.9	prepared_vp4_370_uff_E=77.82	-5.5
Prepared_ns2_370_uff_E=77.82	-4.9	prepared_vp4_370_uff_E=77.82	-5.4
Prepared_ns2_370_uff_E=77.82	-4.9	prepared_vp4_370_uff_E=77.82	-5.4
Prepared_ns2_91472_uff_E=973.63	-8	prepared_vp4_91472_uff_E=973.63	-8.6
Prepared_ns2_91472_uff_E=973.63	-8	prepared_vp4_91472_uff_E=973.63	-8.5
Prepared_ns2_91472_uff_E=973.63	-7.8	prepared_vp4_91472_uff_E=973.63	-8.3
Prepared_ns2_91472_uff_E=973.63	-7.7	prepared_vp4_91472_uff_E=973.63	-8.1
Prepared_ns2_91472_uff_E=973.63	-7.5	prepared_vp4_91472_uff_E=973.63	-8
Prepared_ns2_91472_uff_E=973.63	-7.5	prepared_vp4_91472_uff_E=973.63	-7.9
Prepared_ns2_91472_uff_E=973.63	-7.5	prepared_vp4_91472_uff_E=973.63	-7.7
Prepared_ns2_91472_uff_E=973.63	-7.5	prepared_vp4_91472_uff_E=973.63	-7.7
Prepared_ns2_91472_uff_E=973.63	-7.5	prepared_vp4_91472_uff_E=973.63	-7.6
Prepared_ns2_445858_uff_E=177.42	-5.3	prepared_vp4_445858_uff_E=177.42	-6
Prepared_ns2_445858_uff_E=177.42	-5.2	prepared_vp4_445858_uff_E=177.42	-6
Prepared_ns2_445858_uff_E=177.42	-5	prepared_vp4_445858_uff_E=177.42	-5.8
Prepared_ns2_445858_uff_E=177.42	-5	prepared_vp4_445858_uff_E=177.42	-5.8
Prepared_ns2_445858_uff_E=177.42	-4.9	prepared_vp4_445858_uff_E=177.42	-5.8
Prepared_ns2_445858_uff_E=177.42	-4.9	prepared_vp4_445858_uff_E=177.42	-5.7
Prepared_ns2_445858_uff_E=177.42	-4.8	prepared_vp4_445858_uff_E=177.42	-5.7
Prepared_ns2_445858_uff_E=177.42	-4.8	prepared_vp4_445858_uff_E=177.42	-5.6
Prepared_ns2_445858_uff_E=177.42	-4.8	prepared_vp4_445858_uff_E=177.42	-5.5
Prepared_ns2_3334_uff_E=383.33	-7	prepared_vp4_3334_uff_E=383.33	-7.3
Prepared_ns2_3334_uff_E=383.33	-6.9	prepared_vp4_3334_uff_E=383.33	-7.2
Prepared_ns2_3334_uff_E=383.33	-6.7	prepared_vp4_3334_uff_E=383.33	-7.1
Prepared_ns2_3334_uff_E=383.33	-6.7	prepared_vp4_3334_uff_E=383.33	-6.9
Prepared_ns2_3334_uff_E=383.33	-6.6	prepared_vp4_3334_uff_E=383.33	-6.9
Prepared_ns2_3334_uff_E=383.33	-6.6	prepared_vp4_3334_uff_E=383.33	-6.8
Prepared_ns2_3334_uff_E=383.33	-6.5	prepared_vp4_3334_uff_E=383.33	-6.7
Prepared_ns2_3334_uff_E=383.33	-6.5	prepared_vp4_3334_uff_E=383.33	-6.7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_3334_uff_E=383.33	-6.4	prepared_vp4_3334_uff_E=383.33	-6.7
Prepared_ns2_7136_uff_E=258.81	-4.8	prepared_vp4_7136_uff_E=258.81	-6.1
Prepared_ns2_7136_uff_E=258.81	-4.8	prepared_vp4_7136_uff_E=258.81	-6
Prepared_ns2_7136_uff_E=258.81	-4.7	prepared_vp4_7136_uff_E=258.81	-5.9
Prepared_ns2_7136_uff_E=258.81	-4.7	prepared_vp4_7136_uff_E=258.81	-5.8
Prepared_ns2_7136_uff_E=258.81	-4.7	prepared_vp4_7136_uff_E=258.81	-5.7
Prepared_ns2_7136_uff_E=258.81	-4.5	prepared_vp4_7136_uff_E=258.81	-5.6
Prepared_ns2_7136_uff_E=258.81	-4.4	prepared_vp4_7136_uff_E=258.81	-5.6
Prepared_ns2_7136_uff_E=258.81	-4.4	prepared_vp4_7136_uff_E=258.81	-5.4
Prepared_ns2_7136_uff_E=258.81	-4.4	prepared_vp4_7136_uff_E=258.81	-5.3
Prepared_ns2_5282184_uff_E=2055.50	-4.1	prepared_vp4_5282184_uff_E=2055.50	-4.9
Prepared_ns2_5282184_uff_E=2055.50	-4.1	prepared_vp4_5282184_uff_E=2055.50	-4.7
Prepared_ns2_5282184_uff_E=2055.50	-4.1	prepared_vp4_5282184_uff_E=2055.50	-4.7
Prepared_ns2_5282184_uff_E=2055.50	-4	prepared_vp4_5282184_uff_E=2055.50	-4.6
Prepared_ns2_5282184_uff_E=2055.50	-4	prepared_vp4_5282184_uff_E=2055.50	-4.5
Prepared_ns2_5282184_uff_E=2055.50	-3.9	prepared_vp4_5282184_uff_E=2055.50	-4.4
Prepared_ns2_5282184_uff_E=2055.50	-3.8	prepared_vp4_5282184_uff_E=2055.50	-4.3
Prepared_ns2_5282184_uff_E=2055.50	-3.8	prepared_vp4_5282184_uff_E=2055.50	-4.3
Prepared_ns2_5282184_uff_E=2055.50	-3.8	prepared_vp4_5282184_uff_E=2055.50	-4.3
Prepared_ns2_101761_uff_E=714.50	-8	prepared_vp4_101761_uff_E=714.50	-9.1
Prepared_ns2_101761_uff_E=714.50	-7.8	prepared_vp4_101761_uff_E=714.50	-8.8
Prepared_ns2_101761_uff_E=714.50	-7.6	prepared_vp4_101761_uff_E=714.50	-8.8
Prepared_ns2_101761_uff_E=714.50	-7.6	prepared_vp4_101761_uff_E=714.50	-8.4
Prepared_ns2_101761_uff_E=714.50	-7.6	prepared_vp4_101761_uff_E=714.50	-8.2
Prepared_ns2_101761_uff_E=714.50	-7.4	prepared_vp4_101761_uff_E=714.50	-8
Prepared_ns2_101761_uff_E=714.50	-7.2	prepared_vp4_101761_uff_E=714.50	-7.9
Prepared_ns2_101761_uff_E=714.50	-7.1	prepared_vp4_101761_uff_E=714.50	-7.8
Prepared_ns2_101761_uff_E=714.50	-7	prepared_vp4_101761_uff_E=714.50	-7.8
Prepared_ns2_169017_uff_E=519.91	-6.5	prepared_vp4_169017_uff_E=519.91	-7.8
Prepared_ns2_169017_uff_E=519.91	-6	prepared_vp4_169017_uff_E=519.91	-7.5
Prepared_ns2_169017_uff_E=519.91	-6	prepared_vp4_169017_uff_E=519.91	-7.3
Prepared_ns2_169017_uff_E=519.91	-5.9	prepared_vp4_169017_uff_E=519.91	-7.1
Prepared_ns2_169017_uff_E=519.91	-5.9	prepared_vp4_169017_uff_E=519.91	-6.9
Prepared_ns2_169017_uff_E=519.91	-5.8	prepared_vp4_169017_uff_E=519.91	-6.7
Prepared_ns2_169017_uff_E=519.91	-5.7	prepared_vp4_169017_uff_E=519.91	-6.6
Prepared_ns2_169017_uff_E=519.91	-5.7	prepared_vp4_169017_uff_E=519.91	-6.6
Prepared_ns2_169017_uff_E=519.91	-5.5	prepared_vp4_169017_uff_E=519.91	-6.5
Prepared_ns2_15478903_uff_E=536.07	-7.1	prepared_vp4_15478903_uff_E=536.07	-7.7
Prepared_ns2_15478903_uff_E=536.07	-7	prepared_vp4_15478903_uff_E=536.07	-7.4
Prepared_ns2_15478903_uff_E=536.07	-6.8	prepared_vp4_15478903_uff_E=536.07	-7.3
Prepared_ns2_15478903_uff_E=536.07	-6.8	prepared_vp4_15478903_uff_E=536.07	-7.3
Prepared_ns2_15478903_uff_E=536.07	-6.7	prepared_vp4_15478903_uff_E=536.07	-6.8
Prepared_ns2_15478903_uff_E=536.07	-6.6	prepared_vp4_15478903_uff_E=536.07	-6.6
Prepared_ns2_15478903_uff_E=536.07	-6.6	prepared_vp4_15478903_uff_E=536.07	-6.6
Prepared_ns2_15478903_uff_E=536.07	-6.6	prepared_vp4_15478903_uff_E=536.07	-6.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_15478903_uff_E=536.07	-6.5	prepared_vp4_15478903_uff_E=536.07	-6.6
Prepared_ns2_362562_uff_E=489.54	-6.9	prepared_vp4_362562_uff_E=489.54	-8.5
Prepared_ns2_362562_uff_E=489.54	-6.8	prepared_vp4_362562_uff_E=489.54	-8.2
Prepared_ns2_362562_uff_E=489.54	-6.8	prepared_vp4_362562_uff_E=489.54	-7.8
Prepared_ns2_362562_uff_E=489.54	-6.6	prepared_vp4_362562_uff_E=489.54	-7.6
Prepared_ns2_362562_uff_E=489.54	-6.4	prepared_vp4_362562_uff_E=489.54	-7.5
Prepared_ns2_362562_uff_E=489.54	-6.3	prepared_vp4_362562_uff_E=489.54	-7.4
Prepared_ns2_362562_uff_E=489.54	-6.3	prepared_vp4_362562_uff_E=489.54	-7.4
Prepared_ns2_362562_uff_E=489.54	-6.1	prepared_vp4_362562_uff_E=489.54	-7.4
Prepared_ns2_362562_uff_E=489.54	-6.1	prepared_vp4_362562_uff_E=489.54	-7.4
Prepared_ns2_65064_uff_E=325.39	-7.7	prepared_vp4_65064_uff_E=325.39	-8.8
Prepared_ns2_65064_uff_E=325.39	-7.7	prepared_vp4_65064_uff_E=325.39	-8.5
Prepared_ns2_65064_uff_E=325.39	-7.4	prepared_vp4_65064_uff_E=325.39	-8.5
Prepared_ns2_65064_uff_E=325.39	-7.4	prepared_vp4_65064_uff_E=325.39	-8.5
Prepared_ns2_65064_uff_E=325.39	-7.3	prepared_vp4_65064_uff_E=325.39	-8.3
Prepared_ns2_65064_uff_E=325.39	-7.3	prepared_vp4_65064_uff_E=325.39	-8.2
Prepared_ns2_65064_uff_E=325.39	-7.3	prepared_vp4_65064_uff_E=325.39	-8
Prepared_ns2_65064_uff_E=325.39	-7.2	prepared_vp4_65064_uff_E=325.39	-7.9
Prepared_ns2_65064_uff_E=325.39	-7.1	prepared_vp4_65064_uff_E=325.39	-7.7
Prepared_ns2_72276_uff_E=230.94	-7.5	prepared_vp4_72276_uff_E=230.94	-8
Prepared_ns2_72276_uff_E=230.94	-7.2	prepared_vp4_72276_uff_E=230.94	-7.6
Prepared_ns2_72276_uff_E=230.94	-7	prepared_vp4_72276_uff_E=230.94	-7.6
Prepared_ns2_72276_uff_E=230.94	-6.9	prepared_vp4_72276_uff_E=230.94	-7.4
Prepared_ns2_72276_uff_E=230.94	-6.7	prepared_vp4_72276_uff_E=230.94	-7.4
Prepared_ns2_72276_uff_E=230.94	-6.4	prepared_vp4_72276_uff_E=230.94	-7.4
Prepared_ns2_72276_uff_E=230.94	-6.4	prepared_vp4_72276_uff_E=230.94	-7.3
Prepared_ns2_72276_uff_E=230.94	-6.4	prepared_vp4_72276_uff_E=230.94	-7
Prepared_ns2_72276_uff_E=230.94	-6.3	prepared_vp4_72276_uff_E=230.94	-7
Prepared_ns2_3220_uff_E=196.51	-7	prepared_vp4_3220_uff_E=196.51	-7.3
Prepared_ns2_3220_uff_E=196.51	-6.7	prepared_vp4_3220_uff_E=196.51	-7.3
Prepared_ns2_3220_uff_E=196.51	-6.5	prepared_vp4_3220_uff_E=196.51	-7.2
Prepared_ns2_3220_uff_E=196.51	-6.5	prepared_vp4_3220_uff_E=196.51	-7.1
Prepared_ns2_3220_uff_E=196.51	-6.4	prepared_vp4_3220_uff_E=196.51	-7
Prepared_ns2_3220_uff_E=196.51	-6.4	prepared_vp4_3220_uff_E=196.51	-6.9
Prepared_ns2_3220_uff_E=196.51	-6.3	prepared_vp4_3220_uff_E=196.51	-6.9
Prepared_ns2_3220_uff_E=196.51	-6.2	prepared_vp4_3220_uff_E=196.51	-6.9
Prepared_ns2_3220_uff_E=196.51	-6.2	prepared_vp4_3220_uff_E=196.51	-6.9
Prepared_ns2_5281855_uff_E=227.58	-7	prepared_vp4_5281855_uff_E=227.58	-7.9
Prepared_ns2_5281855_uff_E=227.58	-6.9	prepared_vp4_5281855_uff_E=227.58	-7.9
Prepared_ns2_5281855_uff_E=227.58	-6.9	prepared_vp4_5281855_uff_E=227.58	-7.7
Prepared_ns2_5281855_uff_E=227.58	-6.8	prepared_vp4_5281855_uff_E=227.58	-7.7
Prepared_ns2_5281855_uff_E=227.58	-6.8	prepared_vp4_5281855_uff_E=227.58	-7.7
Prepared_ns2_5281855_uff_E=227.58	-6.8	prepared_vp4_5281855_uff_E=227.58	-7.6
Prepared_ns2_5281855_uff_E=227.58	-6.8	prepared_vp4_5281855_uff_E=227.58	-7.5
Prepared_ns2_5281855_uff_E=227.58	-6.8	prepared_vp4_5281855_uff_E=227.58	-7.5

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5281855_uff_E=227.58	-6.5	prepared_vp4_5281855_uff_E=227.58	-7.3
Prepared_ns2_439655_uff_E=76.10	-4.8	prepared_vp4_439655_uff_E=76.10	-4.8
Prepared_ns2_439655_uff_E=76.10	-4.8	prepared_vp4_439655_uff_E=76.10	-4.8
Prepared_ns2_439655_uff_E=76.10	-4.8	prepared_vp4_439655_uff_E=76.10	-4.7
Prepared_ns2_439655_uff_E=76.10	-4.8	prepared_vp4_439655_uff_E=76.10	-4.6
Prepared_ns2_439655_uff_E=76.10	-4.8	prepared_vp4_439655_uff_E=76.10	-4.6
Prepared_ns2_439655_uff_E=76.10	-4.6	prepared_vp4_439655_uff_E=76.10	-4.6
Prepared_ns2_439655_uff_E=76.10	-4.5	prepared_vp4_439655_uff_E=76.10	-4.6
Prepared_ns2_439655_uff_E=76.10	-4.5	prepared_vp4_439655_uff_E=76.10	-4.5
Prepared_ns2_439655_uff_E=76.10	-4.4	prepared_vp4_439655_uff_E=76.10	-4.4
Prepared_ns2_681_uff_E=104.20	-4.9	prepared_vp4_681_uff_E=104.20	-5.7
Prepared_ns2_681_uff_E=104.20	-4.9	prepared_vp4_681_uff_E=104.20	-5.6
Prepared_ns2_681_uff_E=104.20	-4.8	prepared_vp4_681_uff_E=104.20	-5.5
Prepared_ns2_681_uff_E=104.20	-4.7	prepared_vp4_681_uff_E=104.20	-5.4
Prepared_ns2_681_uff_E=104.20	-4.5	prepared_vp4_681_uff_E=104.20	-5.1
Prepared_ns2_681_uff_E=104.20	-4.5	prepared_vp4_681_uff_E=104.20	-5.1
Prepared_ns2_681_uff_E=104.20	-4.4	prepared_vp4_681_uff_E=104.20	-5
Prepared_ns2_681_uff_E=104.20	-4.4	prepared_vp4_681_uff_E=104.20	-5
Prepared_ns2_681_uff_E=104.20	-4.3	prepared_vp4_681_uff_E=104.20	-5
Prepared_ns2_10231_uff_E=304.43	-4.7	prepared_vp4_10231_uff_E=304.43	-6.2
Prepared_ns2_10231_uff_E=304.43	-4.6	prepared_vp4_10231_uff_E=304.43	-5.8
Prepared_ns2_10231_uff_E=304.43	-4.6	prepared_vp4_10231_uff_E=304.43	-5.6
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.5
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.4
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.3
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.3
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.2
Prepared_ns2_10231_uff_E=304.43	-4.5	prepared_vp4_10231_uff_E=304.43	-5.2
Prepared_ns2_11617_uff_E=59.19	-2.8	prepared_vp4_11617_uff_E=59.19	-3.5
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.4
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.4
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.4
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.3
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.3
Prepared_ns2_11617_uff_E=59.19	-2.7	prepared_vp4_11617_uff_E=59.19	-3.3
Prepared_ns2_11617_uff_E=59.19	-2.6	prepared_vp4_11617_uff_E=59.19	-3.3
Prepared_ns2_11617_uff_E=59.19	-2.6	prepared_vp4_11617_uff_E=59.19	-3.2
Prepared_ns2_5793_uff_E=184.96	-5.1	prepared_vp4_5793_uff_E=184.96	-6.1
Prepared_ns2_5793_uff_E=184.96	-5	prepared_vp4_5793_uff_E=184.96	-5.9
Prepared_ns2_5793_uff_E=184.96	-5	prepared_vp4_5793_uff_E=184.96	-5.9
Prepared_ns2_5793_uff_E=184.96	-4.9	prepared_vp4_5793_uff_E=184.96	-5.8
Prepared_ns2_5793_uff_E=184.96	-4.8	prepared_vp4_5793_uff_E=184.96	-5.7
Prepared_ns2_5793_uff_E=184.96	-4.8	prepared_vp4_5793_uff_E=184.96	-5.6
Prepared_ns2_5793_uff_E=184.96	-4.8	prepared_vp4_5793_uff_E=184.96	-5.6
Prepared_ns2_5793_uff_E=184.96	-4.7	prepared_vp4_5793_uff_E=184.96	-5.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5793_uff_E=184.96	-4.7	prepared_vp4_5793_uff_E=184.96	-5.5
Prepared_ns2_95478_uff_E=196.87	-5.5	prepared_vp4_95478_uff_E=196.87	-5.9
Prepared_ns2_95478_uff_E=196.87	-5.5	prepared_vp4_95478_uff_E=196.87	-5.5
Prepared_ns2_95478_uff_E=196.87	-5	prepared_vp4_95478_uff_E=196.87	-5.4
Prepared_ns2_95478_uff_E=196.87	-4.9	prepared_vp4_95478_uff_E=196.87	-5.4
Prepared_ns2_95478_uff_E=196.87	-4.9	prepared_vp4_95478_uff_E=196.87	-5.2
Prepared_ns2_95478_uff_E=196.87	-4.8	prepared_vp4_95478_uff_E=196.87	-5.2
Prepared_ns2_95478_uff_E=196.87	-4.8	prepared_vp4_95478_uff_E=196.87	-5
Prepared_ns2_95478_uff_E=196.87	-4.7	prepared_vp4_95478_uff_E=196.87	-4.9
Prepared_ns2_95478_uff_E=196.87	-4.6	prepared_vp4_95478_uff_E=196.87	-4.7
Prepared_ns2_14704457_uff_E=401.76	-7.3	prepared_vp4_14704457_uff_E=401.76	-8.6
Prepared_ns2_14704457_uff_E=401.76	-7.1	prepared_vp4_14704457_uff_E=401.76	-7.7
Prepared_ns2_14704457_uff_E=401.76	-7	prepared_vp4_14704457_uff_E=401.76	-7.4
Prepared_ns2_14704457_uff_E=401.76	-6.9	prepared_vp4_14704457_uff_E=401.76	-7.3
Prepared_ns2_14704457_uff_E=401.76	-6.8	prepared_vp4_14704457_uff_E=401.76	-7.2
Prepared_ns2_14704457_uff_E=401.76	-6.8	prepared_vp4_14704457_uff_E=401.76	-7
Prepared_ns2_14704457_uff_E=401.76	-6.8	prepared_vp4_14704457_uff_E=401.76	-7
Prepared_ns2_14704457_uff_E=401.76	-6.7	prepared_vp4_14704457_uff_E=401.76	-6.9
Prepared_ns2_14704457_uff_E=401.76	-6.6	prepared_vp4_14704457_uff_E=401.76	-6.6
Prepared_ns2_128853_uff_E=354.00	-6.8	prepared_vp4_128853_uff_E=354.00	-8.3
Prepared_ns2_128853_uff_E=354.00	-6.8	prepared_vp4_128853_uff_E=354.00	-8.1
Prepared_ns2_128853_uff_E=354.00	-6.4	prepared_vp4_128853_uff_E=354.00	-7.9
Prepared_ns2_128853_uff_E=354.00	-6.3	prepared_vp4_128853_uff_E=354.00	-7.5
Prepared_ns2_128853_uff_E=354.00	-6.3	prepared_vp4_128853_uff_E=354.00	-7.2
Prepared_ns2_128853_uff_E=354.00	-6.3	prepared_vp4_128853_uff_E=354.00	-7
Prepared_ns2_128853_uff_E=354.00	-6.1	prepared_vp4_128853_uff_E=354.00	-7
Prepared_ns2_128853_uff_E=354.00	-6.1	prepared_vp4_128853_uff_E=354.00	-6.9
Prepared_ns2_128853_uff_E=354.00	-6	prepared_vp4_128853_uff_E=354.00	-6.8
Prepared_ns2_8175_uff_E=34.10	-3.8	prepared_vp4_8175_uff_E=34.10	-4.5
Prepared_ns2_8175_uff_E=34.10	-3.6	prepared_vp4_8175_uff_E=34.10	-4.3
Prepared_ns2_8175_uff_E=34.10	-3.6	prepared_vp4_8175_uff_E=34.10	-4.2
Prepared_ns2_8175_uff_E=34.10	-3.5	prepared_vp4_8175_uff_E=34.10	-4.2
Prepared_ns2_8175_uff_E=34.10	-3.5	prepared_vp4_8175_uff_E=34.10	-4.2
Prepared_ns2_8175_uff_E=34.10	-3.5	prepared_vp4_8175_uff_E=34.10	-4.1
Prepared_ns2_8175_uff_E=34.10	-3.5	prepared_vp4_8175_uff_E=34.10	-4
Prepared_ns2_8175_uff_E=34.10	-3.5	prepared_vp4_8175_uff_E=34.10	-4
Prepared_ns2_8175_uff_E=34.10	-3.4	prepared_vp4_8175_uff_E=34.10	-3.9
Prepared_ns2_128861_uff_E=346.73	-6.8	prepared_vp4_128861_uff_E=346.73	-8.3
Prepared_ns2_128861_uff_E=346.73	-6.4	prepared_vp4_128861_uff_E=346.73	-7.9
Prepared_ns2_128861_uff_E=346.73	-6.3	prepared_vp4_128861_uff_E=346.73	-7.7
Prepared_ns2_128861_uff_E=346.73	-6.3	prepared_vp4_128861_uff_E=346.73	-7.2
Prepared_ns2_128861_uff_E=346.73	-6.2	prepared_vp4_128861_uff_E=346.73	-7.1
Prepared_ns2_128861_uff_E=346.73	-6.2	prepared_vp4_128861_uff_E=346.73	-7
Prepared_ns2_128861_uff_E=346.73	-6.1	prepared_vp4_128861_uff_E=346.73	-7
Prepared_ns2_128861_uff_E=346.73	-6	prepared_vp4_128861_uff_E=346.73	-7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_128861_uff_E=346.73	-6	prepared_vp4_128861_uff_E=346.73	-6.9
Prepared_ns2_637540_uff_E=98.26	-5.5	prepared_vp4_637540_uff_E=98.26	-6.1
Prepared_ns2_637540_uff_E=98.26	-5.3	prepared_vp4_637540_uff_E=98.26	-5.9
Prepared_ns2_637540_uff_E=98.26	-5.2	prepared_vp4_637540_uff_E=98.26	-5.8
Prepared_ns2_637540_uff_E=98.26	-5	prepared_vp4_637540_uff_E=98.26	-5.8
Prepared_ns2_637540_uff_E=98.26	-4.9	prepared_vp4_637540_uff_E=98.26	-5.8
Prepared_ns2_637540_uff_E=98.26	-4.9	prepared_vp4_637540_uff_E=98.26	-5.7
Prepared_ns2_637540_uff_E=98.26	-4.9	prepared_vp4_637540_uff_E=98.26	-5.7
Prepared_ns2_637540_uff_E=98.26	-4.9	prepared_vp4_637540_uff_E=98.26	-5.6
Prepared_ns2_637540_uff_E=98.26	-4.8	prepared_vp4_637540_uff_E=98.26	-5.5
Prepared_ns2_10970376_uff_E=505.33	-6.9	prepared_vp4_10970376_uff_E=505.33	-7.8
Prepared_ns2_10970376_uff_E=505.33	-6.8	prepared_vp4_10970376_uff_E=505.33	-7.8
Prepared_ns2_10970376_uff_E=505.33	-6.5	prepared_vp4_10970376_uff_E=505.33	-7.6
Prepared_ns2_10970376_uff_E=505.33	-6.5	prepared_vp4_10970376_uff_E=505.33	-7.5
Prepared_ns2_10970376_uff_E=505.33	-6.2	prepared_vp4_10970376_uff_E=505.33	-7.4
Prepared_ns2_10970376_uff_E=505.33	-6.2	prepared_vp4_10970376_uff_E=505.33	-7.2
Prepared_ns2_10970376_uff_E=505.33	-6.1	prepared_vp4_10970376_uff_E=505.33	-7
Prepared_ns2_10970376_uff_E=505.33	-6.1	prepared_vp4_10970376_uff_E=505.33	-7
Prepared_ns2_10970376_uff_E=505.33	-6.1	prepared_vp4_10970376_uff_E=505.33	-6.9
Prepared_ns2_7794_uff_E=88.05	-4.2	prepared_vp4_7794_uff_E=88.05	-5.4
Prepared_ns2_7794_uff_E=88.05	-4.2	prepared_vp4_7794_uff_E=88.05	-5.3
Prepared_ns2_7794_uff_E=88.05	-4.1	prepared_vp4_7794_uff_E=88.05	-5.2
Prepared_ns2_7794_uff_E=88.05	-4	prepared_vp4_7794_uff_E=88.05	-5.2
Prepared_ns2_7794_uff_E=88.05	-4	prepared_vp4_7794_uff_E=88.05	-5
Prepared_ns2_7794_uff_E=88.05	-4	prepared_vp4_7794_uff_E=88.05	-4.9
Prepared_ns2_7794_uff_E=88.05	-3.9	prepared_vp4_7794_uff_E=88.05	-4.7
Prepared_ns2_7794_uff_E=88.05	-3.9	prepared_vp4_7794_uff_E=88.05	-4.7
Prepared_ns2_7794_uff_E=88.05	-3.8	prepared_vp4_7794_uff_E=88.05	-4.7
Prepared_ns2_10208_uff_E=215.65	-7.2	prepared_vp4_10208_uff_E=215.65	-7.8
Prepared_ns2_10208_uff_E=215.65	-6.9	prepared_vp4_10208_uff_E=215.65	-7.5
Prepared_ns2_10208_uff_E=215.65	-6.7	prepared_vp4_10208_uff_E=215.65	-7.3
Prepared_ns2_10208_uff_E=215.65	-6.6	prepared_vp4_10208_uff_E=215.65	-7.2
Prepared_ns2_10208_uff_E=215.65	-6.6	prepared_vp4_10208_uff_E=215.65	-7.1
Prepared_ns2_10208_uff_E=215.65	-6.5	prepared_vp4_10208_uff_E=215.65	-7
Prepared_ns2_10208_uff_E=215.65	-6.4	prepared_vp4_10208_uff_E=215.65	-6.8
Prepared_ns2_10208_uff_E=215.65	-6.3	prepared_vp4_10208_uff_E=215.65	-6.8
Prepared_ns2_10208_uff_E=215.65	-6.2	prepared_vp4_10208_uff_E=215.65	-6.8
Prepared_ns2_5280666_uff_E=324.01	-7.1	prepared_vp4_5280666_uff_E=324.01	-8.5
Prepared_ns2_5280666_uff_E=324.01	-6.7	prepared_vp4_5280666_uff_E=324.01	-8
Prepared_ns2_5280666_uff_E=324.01	-6.7	prepared_vp4_5280666_uff_E=324.01	-7.8
Prepared_ns2_5280666_uff_E=324.01	-6.6	prepared_vp4_5280666_uff_E=324.01	-7.6
Prepared_ns2_5280666_uff_E=324.01	-6.4	prepared_vp4_5280666_uff_E=324.01	-7.5
Prepared_ns2_5280666_uff_E=324.01	-6.4	prepared_vp4_5280666_uff_E=324.01	-7.5
Prepared_ns2_5280666_uff_E=324.01	-6.3	prepared_vp4_5280666_uff_E=324.01	-7.4
Prepared_ns2_5280666_uff_E=324.01	-6.3	prepared_vp4_5280666_uff_E=324.01	-7.4

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5280666_uff_E=324.01	-6.2	prepared_vp4_5280666_uff_E=324.01	-7.2
Prepared_ns2_305_uff_E=103.14	-3.2	prepared_vp4_305_uff_E=103.14	-3.6
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.6
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.4
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_305_uff_E=103.14	-3	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_305_uff_E=103.14	-2.9	prepared_vp4_305_uff_E=103.14	-3.3
Prepared_ns2_2719_uff_E=262.55	-5.7	prepared_vp4_2719_uff_E=262.55	-5.6
Prepared_ns2_2719_uff_E=262.55	-5.5	prepared_vp4_2719_uff_E=262.55	-5.1
Prepared_ns2_2719_uff_E=262.55	-5.5	prepared_vp4_2719_uff_E=262.55	-4.9
Prepared_ns2_2719_uff_E=262.55	-5.4	prepared_vp4_2719_uff_E=262.55	-4.9
Prepared_ns2_2719_uff_E=262.55	-5.4	prepared_vp4_2719_uff_E=262.55	-4.7
Prepared_ns2_2719_uff_E=262.55	-5.3	prepared_vp4_2719_uff_E=262.55	-4.6
Prepared_ns2_2719_uff_E=262.55	-5.2	prepared_vp4_2719_uff_E=262.55	-4.6
Prepared_ns2_2719_uff_E=262.55	-5.1	prepared_vp4_2719_uff_E=262.55	-4.4
Prepared_ns2_2719_uff_E=262.55	-5.1	prepared_vp4_2719_uff_E=262.55	-4.1
Prepared_ns2_1794427_uff_E=254.42	-6.9	prepared_vp4_1794427_uff_E=254.42	-8.2
Prepared_ns2_1794427_uff_E=254.42	-6.6	prepared_vp4_1794427_uff_E=254.42	-7.9
Prepared_ns2_1794427_uff_E=254.42	-6.5	prepared_vp4_1794427_uff_E=254.42	-7.2
Prepared_ns2_1794427_uff_E=254.42	-6.4	prepared_vp4_1794427_uff_E=254.42	-7.1
Prepared_ns2_1794427_uff_E=254.42	-6.3	prepared_vp4_1794427_uff_E=254.42	-7.1
Prepared_ns2_1794427_uff_E=254.42	-6.3	prepared_vp4_1794427_uff_E=254.42	-7
Prepared_ns2_1794427_uff_E=254.42	-6.3	prepared_vp4_1794427_uff_E=254.42	-6.9
Prepared_ns2_1794427_uff_E=254.42	-6.3	prepared_vp4_1794427_uff_E=254.42	-6.9
Prepared_ns2_1794427_uff_E=254.42	-6.2	prepared_vp4_1794427_uff_E=254.42	-6.8
Prepared_ns2_9064_uff_E=204.84	-7.7	prepared_vp4_9064_uff_E=204.84	-8.4
Prepared_ns2_9064_uff_E=204.84	-7.3	prepared_vp4_9064_uff_E=204.84	-7.7
Prepared_ns2_9064_uff_E=204.84	-7.1	prepared_vp4_9064_uff_E=204.84	-7
Prepared_ns2_9064_uff_E=204.84	-6.7	prepared_vp4_9064_uff_E=204.84	-7
Prepared_ns2_9064_uff_E=204.84	-6.6	prepared_vp4_9064_uff_E=204.84	-6.9
Prepared_ns2_9064_uff_E=204.84	-6.5	prepared_vp4_9064_uff_E=204.84	-6.9
Prepared_ns2_9064_uff_E=204.84	-6.4	prepared_vp4_9064_uff_E=204.84	-6.8
Prepared_ns2_9064_uff_E=204.84	-6.4	prepared_vp4_9064_uff_E=204.84	-6.8
Prepared_ns2_9064_uff_E=204.84	-6.2	prepared_vp4_9064_uff_E=204.84	-6.7
Prepared_ns2_5377796_uff_E=422.89	-6.5	prepared_vp4_5377796_uff_E=422.89	-7.4
Prepared_ns2_5377796_uff_E=422.89	-6.4	prepared_vp4_5377796_uff_E=422.89	-7.4
Prepared_ns2_5377796_uff_E=422.89	-6.4	prepared_vp4_5377796_uff_E=422.89	-7.3
Prepared_ns2_5377796_uff_E=422.89	-6.3	prepared_vp4_5377796_uff_E=422.89	-7.2
Prepared_ns2_5377796_uff_E=422.89	-6.1	prepared_vp4_5377796_uff_E=422.89	-7.2
Prepared_ns2_5377796_uff_E=422.89	-5.9	prepared_vp4_5377796_uff_E=422.89	-7.1
Prepared_ns2_5377796_uff_E=422.89	-5.9	prepared_vp4_5377796_uff_E=422.89	-7
Prepared_ns2_5377796_uff_E=422.89	-5.9	prepared_vp4_5377796_uff_E=422.89	-6.9

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5377796_uff_E=422.89	-5.8	prepared_vp4_5377796_uff_E=422.89	-6.8
Prepared_ns2_5354499_uff_E=737.77	-5.7	prepared_vp4_5354499_uff_E=737.77	-6.8
Prepared_ns2_5354499_uff_E=737.77	-5.6	prepared_vp4_5354499_uff_E=737.77	-6.8
Prepared_ns2_5354499_uff_E=737.77	-5.5	prepared_vp4_5354499_uff_E=737.77	-6.7
Prepared_ns2_5354499_uff_E=737.77	-5.4	prepared_vp4_5354499_uff_E=737.77	-6.6
Prepared_ns2_5354499_uff_E=737.77	-5.4	prepared_vp4_5354499_uff_E=737.77	-6.6
Prepared_ns2_5354499_uff_E=737.77	-5.1	prepared_vp4_5354499_uff_E=737.77	-6.5
Prepared_ns2_5354499_uff_E=737.77	-5.1	prepared_vp4_5354499_uff_E=737.77	-6.4
Prepared_ns2_5354499_uff_E=737.77	-5.1	prepared_vp4_5354499_uff_E=737.77	-6.4
Prepared_ns2_5354499_uff_E=737.77	-5.1	prepared_vp4_5354499_uff_E=737.77	-6.3
Prepared_ns2_10449654_uff_E=264.49	-7.5	prepared_vp4_10449654_uff_E=264.49	-8.4
Prepared_ns2_10449654_uff_E=264.49	-7.4	prepared_vp4_10449654_uff_E=264.49	-8.2
Prepared_ns2_10449654_uff_E=264.49	-7.3	prepared_vp4_10449654_uff_E=264.49	-8
Prepared_ns2_10449654_uff_E=264.49	-7.1	prepared_vp4_10449654_uff_E=264.49	-8
Prepared_ns2_10449654_uff_E=264.49	-7.1	prepared_vp4_10449654_uff_E=264.49	-7.8
Prepared_ns2_10449654_uff_E=264.49	-7.1	prepared_vp4_10449654_uff_E=264.49	-7.7
Prepared_ns2_10449654_uff_E=264.49	-7.1	prepared_vp4_10449654_uff_E=264.49	-7.6
Prepared_ns2_10449654_uff_E=264.49	-6.9	prepared_vp4_10449654_uff_E=264.49	-7.6
Prepared_ns2_10449654_uff_E=264.49	-6.9	prepared_vp4_10449654_uff_E=264.49	-7.4
Prepared_ns2_1548943_uff_E=156.51	-6.1	prepared_vp4_1548943_uff_E=156.51	-6.1
Prepared_ns2_1548943_uff_E=156.51	-5.7	prepared_vp4_1548943_uff_E=156.51	-5.6
Prepared_ns2_1548943_uff_E=156.51	-5.7	prepared_vp4_1548943_uff_E=156.51	-5.6
Prepared_ns2_1548943_uff_E=156.51	-5.7	prepared_vp4_1548943_uff_E=156.51	-5.6
Prepared_ns2_1548943_uff_E=156.51	-5.7	prepared_vp4_1548943_uff_E=156.51	-5.3
Prepared_ns2_1548943_uff_E=156.51	-5.7	prepared_vp4_1548943_uff_E=156.51	-5.3
Prepared_ns2_1548943_uff_E=156.51	-5.6	prepared_vp4_1548943_uff_E=156.51	-5.3
Prepared_ns2_1548943_uff_E=156.51	-5.6	prepared_vp4_1548943_uff_E=156.51	-5.3
Prepared_ns2_1548943_uff_E=156.51	-5.6	prepared_vp4_1548943_uff_E=156.51	-5.2
Prepared_ns2_6557_uff_E=22.27	-2.9	prepared_vp4_6557_uff_E=22.27	-3.9
Prepared_ns2_6557_uff_E=22.27	-2.9	prepared_vp4_6557_uff_E=22.27	-3.8
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.7
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.7
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.6
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.5
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.5
Prepared_ns2_6557_uff_E=22.27	-2.8	prepared_vp4_6557_uff_E=22.27	-3.5
Prepared_ns2_6557_uff_E=22.27	-2.7	prepared_vp4_6557_uff_E=22.27	-3.4
Prepared_ns2_173183_uff_E=573.30	-6.9	prepared_vp4_173183_uff_E=573.30	-8.2
Prepared_ns2_173183_uff_E=573.30	-6.8	prepared_vp4_173183_uff_E=573.30	-8.1
Prepared_ns2_173183_uff_E=573.30	-6.8	prepared_vp4_173183_uff_E=573.30	-8
Prepared_ns2_173183_uff_E=573.30	-6.7	prepared_vp4_173183_uff_E=573.30	-8
Prepared_ns2_173183_uff_E=573.30	-6.7	prepared_vp4_173183_uff_E=573.30	-7.9
Prepared_ns2_173183_uff_E=573.30	-6.5	prepared_vp4_173183_uff_E=573.30	-7.8
Prepared_ns2_173183_uff_E=573.30	-6.5	prepared_vp4_173183_uff_E=573.30	-7.8
Prepared_ns2_173183_uff_E=573.30	-6.4	prepared_vp4_173183_uff_E=573.30	-7.7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_173183_uff_E=573.30	-6.4	prepared_vp4_173183_uff_E=573.30	-7.6
Prepared_ns2_689043_uff_E=98.60	-5.5	prepared_vp4_689043_uff_E=98.60	-6.2
Prepared_ns2_689043_uff_E=98.60	-5.3	prepared_vp4_689043_uff_E=98.60	-6.2
Prepared_ns2_689043_uff_E=98.60	-5.2	prepared_vp4_689043_uff_E=98.60	-6.2
Prepared_ns2_689043_uff_E=98.60	-5.2	prepared_vp4_689043_uff_E=98.60	-6
Prepared_ns2_689043_uff_E=98.60	-5.2	prepared_vp4_689043_uff_E=98.60	-5.9
Prepared_ns2_689043_uff_E=98.60	-5.1	prepared_vp4_689043_uff_E=98.60	-5.8
Prepared_ns2_689043_uff_E=98.60	-5.1	prepared_vp4_689043_uff_E=98.60	-5.8
Prepared_ns2_689043_uff_E=98.60	-5	prepared_vp4_689043_uff_E=98.60	-5.7
Prepared_ns2_689043_uff_E=98.60	-5	prepared_vp4_689043_uff_E=98.60	-5.7
Prepared_ns2_3931_uff_E=81.58	-5.2	prepared_vp4_3931_uff_E=81.58	-5.8
Prepared_ns2_3931_uff_E=81.58	-5	prepared_vp4_3931_uff_E=81.58	-5.7
Prepared_ns2_3931_uff_E=81.58	-5	prepared_vp4_3931_uff_E=81.58	-5.4
Prepared_ns2_3931_uff_E=81.58	-4.8	prepared_vp4_3931_uff_E=81.58	-5.4
Prepared_ns2_3931_uff_E=81.58	-4.8	prepared_vp4_3931_uff_E=81.58	-5.3
Prepared_ns2_3931_uff_E=81.58	-4.8	prepared_vp4_3931_uff_E=81.58	-5.2
Prepared_ns2_3931_uff_E=81.58	-4.7	prepared_vp4_3931_uff_E=81.58	-5.1
Prepared_ns2_3931_uff_E=81.58	-4.7	prepared_vp4_3931_uff_E=81.58	-5.1
Prepared_ns2_3931_uff_E=81.58	-4.7	prepared_vp4_3931_uff_E=81.58	-5
Prepared_ns2_37034_uff_E=267.32	-5.8	prepared_vp4_37034_uff_E=267.32	-7.1
Prepared_ns2_37034_uff_E=267.32	-5.8	prepared_vp4_37034_uff_E=267.32	-6.9
Prepared_ns2_37034_uff_E=267.32	-5.7	prepared_vp4_37034_uff_E=267.32	-6.9
Prepared_ns2_37034_uff_E=267.32	-5.6	prepared_vp4_37034_uff_E=267.32	-6.8
Prepared_ns2_37034_uff_E=267.32	-5.5	prepared_vp4_37034_uff_E=267.32	-6.8
Prepared_ns2_37034_uff_E=267.32	-5.5	prepared_vp4_37034_uff_E=267.32	-6.5
Prepared_ns2_37034_uff_E=267.32	-5.4	prepared_vp4_37034_uff_E=267.32	-6.2
Prepared_ns2_37034_uff_E=267.32	-5.3	prepared_vp4_37034_uff_E=267.32	-6.1
Prepared_ns2_37034_uff_E=267.32	-5.3	prepared_vp4_37034_uff_E=267.32	-6
Prepared_ns2_14896_uff_E=713.31	-4.4	prepared_vp4_14896_uff_E=713.31	-5.9
Prepared_ns2_14896_uff_E=713.31	-4.4	prepared_vp4_14896_uff_E=713.31	-5.6
Prepared_ns2_14896_uff_E=713.31	-4.3	prepared_vp4_14896_uff_E=713.31	-5.6
Prepared_ns2_14896_uff_E=713.31	-4.3	prepared_vp4_14896_uff_E=713.31	-5.6
Prepared_ns2_14896_uff_E=713.31	-4.2	prepared_vp4_14896_uff_E=713.31	-5.6
Prepared_ns2_14896_uff_E=713.31	-4.2	prepared_vp4_14896_uff_E=713.31	-5.5
Prepared_ns2_14896_uff_E=713.31	-4.2	prepared_vp4_14896_uff_E=713.31	-5.5
Prepared_ns2_14896_uff_E=713.31	-4.2	prepared_vp4_14896_uff_E=713.31	-5.5
Prepared_ns2_14896_uff_E=713.31	-4.2	prepared_vp4_14896_uff_E=713.31	-5.5
Prepared_ns2_14896_uff_E=713.31	-4.1	prepared_vp4_14896_uff_E=713.31	-5.4
Prepared_ns2_11142_uff_E=124.80	-4.3	prepared_vp4_11142_uff_E=124.80	-6
Prepared_ns2_11142_uff_E=124.80	-4.3	prepared_vp4_11142_uff_E=124.80	-5.6
Prepared_ns2_11142_uff_E=124.80	-4.3	prepared_vp4_11142_uff_E=124.80	-5.6
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.5
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.4
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.3
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.3
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.3

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_11142_uff_E=124.80	-4.2	prepared_vp4_11142_uff_E=124.80	-5.3
Prepared_ns2_247_uff_E=88.22	-3.5	prepared_vp4_247_uff_E=88.22	-4
Prepared_ns2_247_uff_E=88.22	-3.3	prepared_vp4_247_uff_E=88.22	-3.7
Prepared_ns2_247_uff_E=88.22	-3.2	prepared_vp4_247_uff_E=88.22	-3.7
Prepared_ns2_247_uff_E=88.22	-3.2	prepared_vp4_247_uff_E=88.22	-3.6
Prepared_ns2_247_uff_E=88.22	-3.1	prepared_vp4_247_uff_E=88.22	-3.6
Prepared_ns2_247_uff_E=88.22	-3.1	prepared_vp4_247_uff_E=88.22	-3.5
Prepared_ns2_247_uff_E=88.22	-3.1	prepared_vp4_247_uff_E=88.22	-3.4
Prepared_ns2_247_uff_E=88.22	-3	prepared_vp4_247_uff_E=88.22	-3.4
Prepared_ns2_247_uff_E=88.22	-3	prepared_vp4_247_uff_E=88.22	-3.3
Prepared_ns2_57339298_uff_E=852.99	-5.6	prepared_vp4_57339298_uff_E=856.62	-7
Prepared_ns2_57339298_uff_E=852.99	-5.5	prepared_vp4_57339298_uff_E=856.62	-7
Prepared_ns2_57339298_uff_E=852.99	-5.4	prepared_vp4_57339298_uff_E=856.62	-7
Prepared_ns2_57339298_uff_E=852.99	-5.4	prepared_vp4_57339298_uff_E=856.62	-7
Prepared_ns2_57339298_uff_E=852.99	-5.3	prepared_vp4_57339298_uff_E=856.62	-6.9
Prepared_ns2_57339298_uff_E=852.99	-5.2	prepared_vp4_57339298_uff_E=856.62	-6.8
Prepared_ns2_57339298_uff_E=852.99	-5.2	prepared_vp4_57339298_uff_E=856.62	-6.8
Prepared_ns2_57339298_uff_E=852.99	-5.1	prepared_vp4_57339298_uff_E=856.62	-6.7
Prepared_ns2_57339298_uff_E=852.99	-5	prepared_vp4_57339298_uff_E=856.62	-6.4
Prepared_ns2_5281515_uff_E=740.89	-5.5	prepared_vp4_5281515_uff_E=740.89	-7.1
Prepared_ns2_5281515_uff_E=740.89	-5.3	prepared_vp4_5281515_uff_E=740.89	-6.7
Prepared_ns2_5281515_uff_E=740.89	-5.2	prepared_vp4_5281515_uff_E=740.89	-6.7
Prepared_ns2_5281515_uff_E=740.89	-5.2	prepared_vp4_5281515_uff_E=740.89	-6.5
Prepared_ns2_5281515_uff_E=740.89	-5.1	prepared_vp4_5281515_uff_E=740.89	-6.5
Prepared_ns2_5281515_uff_E=740.89	-5.1	prepared_vp4_5281515_uff_E=740.89	-6.4
Prepared_ns2_5281515_uff_E=740.89	-5.1	prepared_vp4_5281515_uff_E=740.89	-6.3
Prepared_ns2_5281515_uff_E=740.89	-5.1	prepared_vp4_5281515_uff_E=740.89	-6.3
Prepared_ns2_5281515_uff_E=740.89	-5.1	prepared_vp4_5281515_uff_E=740.89	-6.2
Prepared_ns2_10104370_uff_E=146.78	-4.9	prepared_vp4_10104370_uff_E=146.78	-6.6
Prepared_ns2_10104370_uff_E=146.78	-4.8	prepared_vp4_10104370_uff_E=146.78	-6.4
Prepared_ns2_10104370_uff_E=146.78	-4.7	prepared_vp4_10104370_uff_E=146.78	-6.4
Prepared_ns2_10104370_uff_E=146.78	-4.6	prepared_vp4_10104370_uff_E=146.78	-6.4
Prepared_ns2_10104370_uff_E=146.78	-4.6	prepared_vp4_10104370_uff_E=146.78	-6.3
Prepared_ns2_10104370_uff_E=146.78	-4.6	prepared_vp4_10104370_uff_E=146.78	-6
Prepared_ns2_10104370_uff_E=146.78	-4.6	prepared_vp4_10104370_uff_E=146.78	-6
Prepared_ns2_10104370_uff_E=146.78	-4.5	prepared_vp4_10104370_uff_E=146.78	-6
Prepared_ns2_10104370_uff_E=146.78	-4.4	prepared_vp4_10104370_uff_E=146.78	-5.9
Prepared_ns2_5490064_uff_E=670.36	-7.2	prepared_vp4_5490064_uff_E=670.36	-7.5
Prepared_ns2_5490064_uff_E=670.36	-7.1	prepared_vp4_5490064_uff_E=670.36	-7.1
Prepared_ns2_5490064_uff_E=670.36	-6.7	prepared_vp4_5490064_uff_E=670.36	-6.9
Prepared_ns2_5490064_uff_E=670.36	-6.6	prepared_vp4_5490064_uff_E=670.36	-6.9
Prepared_ns2_5490064_uff_E=670.36	-6.6	prepared_vp4_5490064_uff_E=670.36	-6.8
Prepared_ns2_5490064_uff_E=670.36	-6.5	prepared_vp4_5490064_uff_E=670.36	-6.8
Prepared_ns2_5490064_uff_E=670.36	-6.4	prepared_vp4_5490064_uff_E=670.36	-6.7
Prepared_ns2_5490064_uff_E=670.36	-6.3	prepared_vp4_5490064_uff_E=670.36	-6.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5490064_uff_E=670.36	-6.2	prepared_vp4_5490064_uff_E=670.36	-6.5
Prepared_ns2_2259_uff_E=545.05	-7.4	prepared_vp4_2259_uff_E=545.05	-8.5
Prepared_ns2_2259_uff_E=545.05	-7.3	prepared_vp4_2259_uff_E=545.05	-8.1
Prepared_ns2_2259_uff_E=545.05	-7.3	prepared_vp4_2259_uff_E=545.05	-7.9
Prepared_ns2_2259_uff_E=545.05	-6.9	prepared_vp4_2259_uff_E=545.05	-7.8
Prepared_ns2_2259_uff_E=545.05	-6.9	prepared_vp4_2259_uff_E=545.05	-7.8
Prepared_ns2_2259_uff_E=545.05	-6.9	prepared_vp4_2259_uff_E=545.05	-7.8
Prepared_ns2_2259_uff_E=545.05	-6.8	prepared_vp4_2259_uff_E=545.05	-7.6
Prepared_ns2_2259_uff_E=545.05	-6.6	prepared_vp4_2259_uff_E=545.05	-7.5
Prepared_ns2_2259_uff_E=545.05	-6.6	prepared_vp4_2259_uff_E=545.05	-7.5
Prepared_ns2_2259_uff_E=559.39	-7.6	prepared_vp4_2259_uff_E=559.39	-8.4
Prepared_ns2_2259_uff_E=559.39	-7.3	prepared_vp4_2259_uff_E=559.39	-8.3
Prepared_ns2_2259_uff_E=559.39	-6.8	prepared_vp4_2259_uff_E=559.39	-7.8
Prepared_ns2_2259_uff_E=559.39	-6.7	prepared_vp4_2259_uff_E=559.39	-7.7
Prepared_ns2_2259_uff_E=559.39	-6.7	prepared_vp4_2259_uff_E=559.39	-7.6
Prepared_ns2_2259_uff_E=559.39	-6.6	prepared_vp4_2259_uff_E=559.39	-7.6
Prepared_ns2_2259_uff_E=559.39	-6.6	prepared_vp4_2259_uff_E=559.39	-7.3
Prepared_ns2_2259_uff_E=559.39	-6.6	prepared_vp4_2259_uff_E=559.39	-6.9
Prepared_ns2_2259_uff_E=559.39	-6.5	prepared_vp4_2259_uff_E=559.39	-6.8
Prepared_ns2_2259_uff_E=547.22	-7.6	prepared_vp4_2259_uff_E=547.22	-9.2
Prepared_ns2_2259_uff_E=547.22	-7.5	prepared_vp4_2259_uff_E=547.22	-7.8
Prepared_ns2_2259_uff_E=547.22	-7.2	prepared_vp4_2259_uff_E=547.22	-7.7
Prepared_ns2_2259_uff_E=547.22	-7	prepared_vp4_2259_uff_E=547.22	-7.3
Prepared_ns2_2259_uff_E=547.22	-6.9	prepared_vp4_2259_uff_E=547.22	-7.3
Prepared_ns2_2259_uff_E=547.22	-6.9	prepared_vp4_2259_uff_E=547.22	-7
Prepared_ns2_2259_uff_E=547.22	-6.9	prepared_vp4_2259_uff_E=547.22	-6.9
Prepared_ns2_2259_uff_E=547.22	-6.8	prepared_vp4_2259_uff_E=547.22	-6.9
Prepared_ns2_2259_uff_E=547.22	-6.7	prepared_vp4_2259_uff_E=547.22	-6.9
Prepared_ns2_2259_uff_E=544.22	-7.1	prepared_vp4_2259_uff_E=544.22	-7.5
Prepared_ns2_2259_uff_E=544.22	-7	prepared_vp4_2259_uff_E=544.22	-6.8
Prepared_ns2_2259_uff_E=544.22	-6.8	prepared_vp4_2259_uff_E=544.22	-6.7
Prepared_ns2_2259_uff_E=544.22	-6.8	prepared_vp4_2259_uff_E=544.22	-6.7
Prepared_ns2_2259_uff_E=544.22	-6.6	prepared_vp4_2259_uff_E=544.22	-6.5
Prepared_ns2_2259_uff_E=544.22	-6.6	prepared_vp4_2259_uff_E=544.22	-6.5
Prepared_ns2_2259_uff_E=544.22	-6.5	prepared_vp4_2259_uff_E=544.22	-6.5
Prepared_ns2_2259_uff_E=544.22	-6.5	prepared_vp4_2259_uff_E=544.22	-6.4
Prepared_ns2_2259_uff_E=544.22	-6.4	prepared_vp4_2259_uff_E=544.22	-6.4
Prepared_ns2_54670067_uff_E=200.65	-5.2	prepared_vp4_54670067_uff_E=200.65	-5.4
Prepared_ns2_54670067_uff_E=200.65	-4.9	prepared_vp4_54670067_uff_E=200.65	-5.4
Prepared_ns2_54670067_uff_E=200.65	-4.8	prepared_vp4_54670067_uff_E=200.65	-5.3
Prepared_ns2_54670067_uff_E=200.65	-4.8	prepared_vp4_54670067_uff_E=200.65	-5.2
Prepared_ns2_54670067_uff_E=200.65	-4.6	prepared_vp4_54670067_uff_E=200.65	-5.2
Prepared_ns2_54670067_uff_E=200.65	-4.6	prepared_vp4_54670067_uff_E=200.65	-5.2
Prepared_ns2_54670067_uff_E=200.65	-4.5	prepared_vp4_54670067_uff_E=200.65	-5.1
Prepared_ns2_54670067_uff_E=200.65	-4.5	prepared_vp4_54670067_uff_E=200.65	-5.1

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_54670067_uff_E=200.65	-4.4	prepared_vp4_54670067_uff_E=200.65	-5.1
Prepared_ns2_5280443_uff_E=233.26	-7.4	prepared_vp4_5280443_uff_E=233.26	-8.5
Prepared_ns2_5280443_uff_E=233.26	-7	prepared_vp4_5280443_uff_E=233.26	-7.9
Prepared_ns2_5280443_uff_E=233.26	-6.8	prepared_vp4_5280443_uff_E=233.26	-7.9
Prepared_ns2_5280443_uff_E=233.26	-6.8	prepared_vp4_5280443_uff_E=233.26	-7.7
Prepared_ns2_5280443_uff_E=233.26	-6.7	prepared_vp4_5280443_uff_E=233.26	-7.5
Prepared_ns2_5280443_uff_E=233.26	-6.7	prepared_vp4_5280443_uff_E=233.26	-7.5
Prepared_ns2_5280443_uff_E=233.26	-6.4	prepared_vp4_5280443_uff_E=233.26	-7.5
Prepared_ns2_5280443_uff_E=233.26	-6.3	prepared_vp4_5280443_uff_E=233.26	-7.5
Prepared_ns2_5280443_uff_E=233.26	-6.3	prepared_vp4_5280443_uff_E=233.26	-7.3
Prepared_ns2_6780_uff_E=133.80	-6.2	prepared_vp4_6780_uff_E=133.80	-7.3
Prepared_ns2_6780_uff_E=133.80	-5.8	prepared_vp4_6780_uff_E=133.80	-7.3
Prepared_ns2_6780_uff_E=133.80	-5.7	prepared_vp4_6780_uff_E=133.80	-7.2
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-7.1
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-7
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-7
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-6.8
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-6.7
Prepared_ns2_6780_uff_E=133.80	-5.6	prepared_vp4_6780_uff_E=133.80	-6.6
Prepared_ns2_145858_uff_E=178.56	-6.4	prepared_vp4_145858_uff_E=178.56	-8.1
Prepared_ns2_145858_uff_E=178.56	-6.3	prepared_vp4_145858_uff_E=178.56	-7.8
Prepared_ns2_145858_uff_E=178.56	-6.3	prepared_vp4_145858_uff_E=178.56	-7.5
Prepared_ns2_145858_uff_E=178.56	-6.3	prepared_vp4_145858_uff_E=178.56	-7.4
Prepared_ns2_145858_uff_E=178.56	-6.1	prepared_vp4_145858_uff_E=178.56	-7.4
Prepared_ns2_145858_uff_E=178.56	-5.9	prepared_vp4_145858_uff_E=178.56	-7.3
Prepared_ns2_145858_uff_E=178.56	-5.8	prepared_vp4_145858_uff_E=178.56	-7.2
Prepared_ns2_145858_uff_E=178.56	-5.8	prepared_vp4_145858_uff_E=178.56	-7
Prepared_ns2_145858_uff_E=178.56	-5.8	prepared_vp4_145858_uff_E=178.56	-6.9
Prepared_ns2_656516_uff_E=524.62	-7	prepared_vp4_656516_uff_E=524.62	-8.5
Prepared_ns2_656516_uff_E=524.62	-6.9	prepared_vp4_656516_uff_E=524.62	-8.5
Prepared_ns2_656516_uff_E=524.62	-6.7	prepared_vp4_656516_uff_E=524.62	-8.3
Prepared_ns2_656516_uff_E=524.62	-6.6	prepared_vp4_656516_uff_E=524.62	-8.1
Prepared_ns2_656516_uff_E=524.62	-6.6	prepared_vp4_656516_uff_E=524.62	-8
Prepared_ns2_656516_uff_E=524.62	-6.5	prepared_vp4_656516_uff_E=524.62	-7.9
Prepared_ns2_656516_uff_E=524.62	-6.5	prepared_vp4_656516_uff_E=524.62	-7.8
Prepared_ns2_656516_uff_E=524.62	-6.4	prepared_vp4_656516_uff_E=524.62	-7.7
Prepared_ns2_656516_uff_E=524.62	-6.3	prepared_vp4_656516_uff_E=524.62	-7.7
Prepared_ns2_5490139_uff_E=404.13	-8.3	prepared_vp4_5490139_uff_E=404.13	-8.8
Prepared_ns2_5490139_uff_E=404.13	-8	prepared_vp4_5490139_uff_E=404.13	-8.5
Prepared_ns2_5490139_uff_E=404.13	-7.8	prepared_vp4_5490139_uff_E=404.13	-8.3
Prepared_ns2_5490139_uff_E=404.13	-7.4	prepared_vp4_5490139_uff_E=404.13	-7.8
Prepared_ns2_5490139_uff_E=404.13	-7.3	prepared_vp4_5490139_uff_E=404.13	-7.8
Prepared_ns2_5490139_uff_E=404.13	-6.9	prepared_vp4_5490139_uff_E=404.13	-7.8
Prepared_ns2_5490139_uff_E=404.13	-6.9	prepared_vp4_5490139_uff_E=404.13	-7.7
Prepared_ns2_5490139_uff_E=404.13	-6.9	prepared_vp4_5490139_uff_E=404.13	-7.7

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_5490139_uff_E=404.13	-6.9	prepared_vp4_5490139_uff_E=404.13	-7.7
Prepared_ns2_10398656_uff_E=220.84	-5.3	prepared_vp4_10398656_uff_E=220.84	-6.8
Prepared_ns2_10398656_uff_E=220.84	-5.3	prepared_vp4_10398656_uff_E=220.84	-6.7
Prepared_ns2_10398656_uff_E=220.84	-5.2	prepared_vp4_10398656_uff_E=220.84	-6.6
Prepared_ns2_10398656_uff_E=220.84	-5.2	prepared_vp4_10398656_uff_E=220.84	-6.3
Prepared_ns2_10398656_uff_E=220.84	-5.2	prepared_vp4_10398656_uff_E=220.84	-6.3
Prepared_ns2_10398656_uff_E=220.84	-5.1	prepared_vp4_10398656_uff_E=220.84	-6.2
Prepared_ns2_10398656_uff_E=220.84	-5	prepared_vp4_10398656_uff_E=220.84	-6.2
Prepared_ns2_10398656_uff_E=220.84	-5	prepared_vp4_10398656_uff_E=220.84	-6.2
Prepared_ns2_10398656_uff_E=220.84	-5	prepared_vp4_10398656_uff_E=220.84	-6.2
Prepared_ns2_12305761_uff_E=413.77	-6.4	prepared_vp4_12305761_uff_E=413.77	-8.2
Prepared_ns2_12305761_uff_E=413.77	-6.4	prepared_vp4_12305761_uff_E=413.77	-7.8
Prepared_ns2_12305761_uff_E=413.77	-6.4	prepared_vp4_12305761_uff_E=413.77	-7.5
Prepared_ns2_12305761_uff_E=413.77	-6.3	prepared_vp4_12305761_uff_E=413.77	-7.2
Prepared_ns2_12305761_uff_E=413.77	-6.2	prepared_vp4_12305761_uff_E=413.77	-7.2
Prepared_ns2_12305761_uff_E=413.77	-6.2	prepared_vp4_12305761_uff_E=413.77	-7.2
Prepared_ns2_12305761_uff_E=413.77	-6.2	prepared_vp4_12305761_uff_E=413.77	-7
Prepared_ns2_12305761_uff_E=413.77	-6.2	prepared_vp4_12305761_uff_E=413.77	-7
Prepared_ns2_12305761_uff_E=413.77	-6.1	prepared_vp4_12305761_uff_E=413.77	-6.9
Prepared_ns2_160190_uff_E=380.73	-6.9	prepared_vp4_160190_uff_E=380.73	-7.7
Prepared_ns2_160190_uff_E=380.73	-6.4	prepared_vp4_160190_uff_E=380.73	-7.3
Prepared_ns2_160190_uff_E=380.73	-6.3	prepared_vp4_160190_uff_E=380.73	-6.9
Prepared_ns2_160190_uff_E=380.73	-6.2	prepared_vp4_160190_uff_E=380.73	-6.9
Prepared_ns2_160190_uff_E=380.73	-6.1	prepared_vp4_160190_uff_E=380.73	-6.8
Prepared_ns2_160190_uff_E=380.73	-6	prepared_vp4_160190_uff_E=380.73	-6.8
Prepared_ns2_160190_uff_E=380.73	-6	prepared_vp4_160190_uff_E=380.73	-6.6
Prepared_ns2_160190_uff_E=380.73	-6	prepared_vp4_160190_uff_E=380.73	-6.5
Prepared_ns2_160190_uff_E=380.73	-5.9	prepared_vp4_160190_uff_E=380.73	-6.5
Prepared_ns2_10207_uff_E=212.95	-6.9	prepared_vp4_10207_uff_E=212.95	-7.5
Prepared_ns2_10207_uff_E=212.95	-6.6	prepared_vp4_10207_uff_E=212.95	-7.4
Prepared_ns2_10207_uff_E=212.95	-6.5	prepared_vp4_10207_uff_E=212.95	-7
Prepared_ns2_10207_uff_E=212.95	-6.3	prepared_vp4_10207_uff_E=212.95	-7
Prepared_ns2_10207_uff_E=212.95	-6.3	prepared_vp4_10207_uff_E=212.95	-7
Prepared_ns2_10207_uff_E=212.95	-6.2	prepared_vp4_10207_uff_E=212.95	-6.9
Prepared_ns2_10207_uff_E=212.95	-6.2	prepared_vp4_10207_uff_E=212.95	-6.7
Prepared_ns2_10207_uff_E=212.95	-6.1	prepared_vp4_10207_uff_E=212.95	-6.6
Prepared_ns2_10207_uff_E=212.95	-6	prepared_vp4_10207_uff_E=212.95	-6.5
Prepared_ns2_87310_uff_E=139.89	-4.1	prepared_vp4_87310_uff_E=139.89	-4.5
Prepared_ns2_87310_uff_E=139.89	-4.1	prepared_vp4_87310_uff_E=139.89	-4.5
Prepared_ns2_87310_uff_E=139.89	-4	prepared_vp4_87310_uff_E=139.89	-4.5
Prepared_ns2_87310_uff_E=139.89	-4	prepared_vp4_87310_uff_E=139.89	-4.4
Prepared_ns2_87310_uff_E=139.89	-4	prepared_vp4_87310_uff_E=139.89	-4.4
Prepared_ns2_87310_uff_E=139.89	-3.9	prepared_vp4_87310_uff_E=139.89	-4.4
Prepared_ns2_87310_uff_E=139.89	-3.9	prepared_vp4_87310_uff_E=139.89	-4.4
Prepared_ns2_87310_uff_E=139.89	-3.9	prepared_vp4_87310_uff_E=139.89	-4.3

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ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_87310_uff_E=139.89	-3.8	prepared_vp4_87310_uff_E=139.89	-4.3
Prepared_ns2_65036_uff_E=111.54	-3.3	prepared_vp4_65036_uff_E=111.54	-3.9
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.8
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.6
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.6
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.6
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.5
Prepared_ns2_65036_uff_E=111.54	-3.2	prepared_vp4_65036_uff_E=111.54	-3.5
Prepared_ns2_65036_uff_E=111.54	-3.1	prepared_vp4_65036_uff_E=111.54	-3.5
Prepared_ns2_65036_uff_E=111.54	-3	prepared_vp4_65036_uff_E=111.54	-3.4
Prepared_ns2_6442612_uff_E=131.21	-5.2	prepared_vp4_6442612_uff_E=131.21	-5.6
Prepared_ns2_6442612_uff_E=131.21	-5.2	prepared_vp4_6442612_uff_E=131.21	-5.4
Prepared_ns2_6442612_uff_E=131.21	-5	prepared_vp4_6442612_uff_E=131.21	-5.4
Prepared_ns2_6442612_uff_E=131.21	-5	prepared_vp4_6442612_uff_E=131.21	-5.1
Prepared_ns2_6442612_uff_E=131.21	-5	prepared_vp4_6442612_uff_E=131.21	-5.1
Prepared_ns2_6442612_uff_E=131.21	-4.9	prepared_vp4_6442612_uff_E=131.21	-5
Prepared_ns2_6442612_uff_E=131.21	-4.8	prepared_vp4_6442612_uff_E=131.21	-5
Prepared_ns2_6442612_uff_E=131.21	-4.8	prepared_vp4_6442612_uff_E=131.21	-4.9
Prepared_ns2_6442612_uff_E=131.21	-4.7	prepared_vp4_6442612_uff_E=131.21	-4.8
Prepared_ns2_6429274_uff_E=813.38	-5.9	prepared_vp4_6429274_uff_E=813.38	-7.5
Prepared_ns2_6429274_uff_E=813.38	-5.6	prepared_vp4_6429274_uff_E=813.38	-7
Prepared_ns2_6429274_uff_E=813.38	-5.4	prepared_vp4_6429274_uff_E=813.38	-6.9
Prepared_ns2_6429274_uff_E=813.38	-5.3	prepared_vp4_6429274_uff_E=813.38	-6.8
Prepared_ns2_6429274_uff_E=813.38	-5.3	prepared_vp4_6429274_uff_E=813.38	-6.6
Prepared_ns2_6429274_uff_E=813.38	-5.3	prepared_vp4_6429274_uff_E=813.38	-6.4
Prepared_ns2_6429274_uff_E=813.38	-5.2	prepared_vp4_6429274_uff_E=813.38	-6.4
Prepared_ns2_6429274_uff_E=813.38	-5.2	prepared_vp4_6429274_uff_E=813.38	-6.3
Prepared_ns2_6429274_uff_E=813.38	-5.2	prepared_vp4_6429274_uff_E=813.38	-6.2
Prepared_ns2_168114_uff_E=235.63	-4.9	prepared_vp4_168114_uff_E=235.63	-6
Prepared_ns2_168114_uff_E=235.63	-4.6	prepared_vp4_168114_uff_E=235.63	-5.9
Prepared_ns2_168114_uff_E=235.63	-4.6	prepared_vp4_168114_uff_E=235.63	-5.8
Prepared_ns2_168114_uff_E=235.63	-4.6	prepared_vp4_168114_uff_E=235.63	-5.6
Prepared_ns2_168114_uff_E=235.63	-4.5	prepared_vp4_168114_uff_E=235.63	-5.5
Prepared_ns2_168114_uff_E=235.63	-4.4	prepared_vp4_168114_uff_E=235.63	-5.5
Prepared_ns2_168114_uff_E=235.63	-4.4	prepared_vp4_168114_uff_E=235.63	-5.5
Prepared_ns2_168114_uff_E=235.63	-4.4	prepared_vp4_168114_uff_E=235.63	-5.4
Prepared_ns2_168114_uff_E=235.63	-4.4	prepared_vp4_168114_uff_E=235.63	-5.4
Prepared_ns2_123387_uff_E=43.12	-3.5	prepared_vp4_123387_uff_E=43.12	-5
Prepared_ns2_123387_uff_E=43.12	-3.5	prepared_vp4_123387_uff_E=43.12	-4.9
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.8
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.7
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.7
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.6
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.6
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_123387_uff_E=43.12	-3.3	prepared_vp4_123387_uff_E=43.12	-4.6
Prepared_ns2_5281794_uff_E=155.38	-4.9	prepared_vp4_5281794_uff_E=155.38	-6
Prepared_ns2_5281794_uff_E=155.38	-4.8	prepared_vp4_5281794_uff_E=155.38	-5.9
Prepared_ns2_5281794_uff_E=155.38	-4.8	prepared_vp4_5281794_uff_E=155.38	-5.6
Prepared_ns2_5281794_uff_E=155.38	-4.7	prepared_vp4_5281794_uff_E=155.38	-5.6
Prepared_ns2_5281794_uff_E=155.38	-4.6	prepared_vp4_5281794_uff_E=155.38	-5.5
Prepared_ns2_5281794_uff_E=155.38	-4.6	prepared_vp4_5281794_uff_E=155.38	-5.5
Prepared_ns2_5281794_uff_E=155.38	-4.6	prepared_vp4_5281794_uff_E=155.38	-5.4
Prepared_ns2_5281794_uff_E=155.38	-4.6	prepared_vp4_5281794_uff_E=155.38	-5.4
Prepared_ns2_5281794_uff_E=155.38	-4.5	prepared_vp4_5281794_uff_E=155.38	-5.3
Prepared_ns2_152430_uff_E=568.19	-6.8	prepared_vp4_152430_uff_E=568.19	-7.3
Prepared_ns2_152430_uff_E=568.19	-6.5	prepared_vp4_152430_uff_E=568.19	-7.1
Prepared_ns2_152430_uff_E=568.19	-6.4	prepared_vp4_152430_uff_E=568.19	-6.9
Prepared_ns2_152430_uff_E=568.19	-6.4	prepared_vp4_152430_uff_E=568.19	-6.6
Prepared_ns2_152430_uff_E=568.19	-6.3	prepared_vp4_152430_uff_E=568.19	-6.5
Prepared_ns2_152430_uff_E=568.19	-6.1	prepared_vp4_152430_uff_E=568.19	-6.5
Prepared_ns2_152430_uff_E=568.19	-6	prepared_vp4_152430_uff_E=568.19	-6.4
Prepared_ns2_152430_uff_E=568.19	-6	prepared_vp4_152430_uff_E=568.19	-6.4
Prepared_ns2_152430_uff_E=568.19	-5.9	prepared_vp4_152430_uff_E=568.19	-6.2
Prepared_ns2_9958_uff_E=84.92	-4.7	prepared_vp4_9958_uff_E=84.92	-5.5
Prepared_ns2_9958_uff_E=84.92	-4.6	prepared_vp4_9958_uff_E=84.92	-5.5
Prepared_ns2_9958_uff_E=84.92	-4.6	prepared_vp4_9958_uff_E=84.92	-5.3
Prepared_ns2_9958_uff_E=84.92	-4.5	prepared_vp4_9958_uff_E=84.92	-5.2
Prepared_ns2_9958_uff_E=84.92	-4.4	prepared_vp4_9958_uff_E=84.92	-5.2
Prepared_ns2_9958_uff_E=84.92	-4.4	prepared_vp4_9958_uff_E=84.92	-5.2
Prepared_ns2_9958_uff_E=84.92	-4.2	prepared_vp4_9958_uff_E=84.92	-5.2
Prepared_ns2_9958_uff_E=84.92	-4.2	prepared_vp4_9958_uff_E=84.92	-5.1
Prepared_ns2_9958_uff_E=84.92	-4.2	prepared_vp4_9958_uff_E=84.92	-5.1
Prepared_ns2_12040_uff_E=60.22	-3.6	prepared_vp4_12040_uff_E=60.22	-4.5
Prepared_ns2_12040_uff_E=60.22	-3.5	prepared_vp4_12040_uff_E=60.22	-4.4
Prepared_ns2_12040_uff_E=60.22	-3.5	prepared_vp4_12040_uff_E=60.22	-4.4
Prepared_ns2_12040_uff_E=60.22	-3.5	prepared_vp4_12040_uff_E=60.22	-4.3
Prepared_ns2_12040_uff_E=60.22	-3.4	prepared_vp4_12040_uff_E=60.22	-4.2
Prepared_ns2_12040_uff_E=60.22	-3.4	prepared_vp4_12040_uff_E=60.22	-4.1
Prepared_ns2_12040_uff_E=60.22	-3.4	prepared_vp4_12040_uff_E=60.22	-4.1
Prepared_ns2_12040_uff_E=60.22	-3.4	prepared_vp4_12040_uff_E=60.22	-4
Prepared_ns2_12040_uff_E=60.22	-3.4	prepared_vp4_12040_uff_E=60.22	-4
Prepared_ns2_11747_uff_E=21.80	-3.5	prepared_vp4_11747_uff_E=21.80	-4.1
Prepared_ns2_11747_uff_E=21.80	-3.4	prepared_vp4_11747_uff_E=21.80	-3.8
Prepared_ns2_11747_uff_E=21.80	-3.2	prepared_vp4_11747_uff_E=21.80	-3.8
Prepared_ns2_11747_uff_E=21.80	-3.2	prepared_vp4_11747_uff_E=21.80	-3.8
Prepared_ns2_11747_uff_E=21.80	-3.1	prepared_vp4_11747_uff_E=21.80	-3.7
Prepared_ns2_11747_uff_E=21.80	-3.1	prepared_vp4_11747_uff_E=21.80	-3.7
Prepared_ns2_11747_uff_E=21.80	-3.1	prepared_vp4_11747_uff_E=21.80	-3.6
Prepared_ns2_11747_uff_E=21.80	-3.1	prepared_vp4_11747_uff_E=21.80	-3.6

Table continues on next page.....

ns2		vp4	
Ligand	Affinity	Ligands	Affinity
Prepared_ns2_11747_uff_E=21.80	-3	prepared_vp4_11747_uff_E=21.80	-3.6
Prepared_ns2_19707_uff_E=25.13	-3.5	prepared_vp4_19707_uff_E=25.13	-4.4
Prepared_ns2_19707_uff_E=25.13	-3.4	prepared_vp4_19707_uff_E=25.13	-4.1
Prepared_ns2_19707_uff_E=25.13	-3.4	prepared_vp4_19707_uff_E=25.13	-4
Prepared_ns2_19707_uff_E=25.13	-3.4	prepared_vp4_19707_uff_E=25.13	-4
Prepared_ns2_19707_uff_E=25.13	-3.4	prepared_vp4_19707_uff_E=25.13	-3.9
Prepared_ns2_19707_uff_E=25.13	-3.3	prepared_vp4_19707_uff_E=25.13	-3.9
Prepared_ns2_19707_uff_E=25.13	-3.3	prepared_vp4_19707_uff_E=25.13	-3.9
Prepared_ns2_19707_uff_E=25.13	-3.3	prepared_vp4_19707_uff_E=25.13	-3.8
Prepared_ns2_19707_uff_E=25.13	-3.2	prepared_vp4_19707_uff_E=25.13	-3.7
Prepared_ns2_2758_uff_E=344.57	-4.6	prepared_vp4_2758_uff_E=344.57	-6
Prepared_ns2_2758_uff_E=344.57	-4.5	prepared_vp4_2758_uff_E=344.57	-5.7
Prepared_ns2_2758_uff_E=344.57	-4.5	prepared_vp4_2758_uff_E=344.57	-5.5
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.5
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.5
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.4
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.4
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.4
Prepared_ns2_2758_uff_E=344.57	-4.4	prepared_vp4_2758_uff_E=344.57	-5.4
Prepared_ns2_27867_uff_E=106.82	-4.9	prepared_vp4_27867_uff_E=106.82	-5.9
Prepared_ns2_27867_uff_E=106.82	-4.7	prepared_vp4_27867_uff_E=106.82	-5.9
Prepared_ns2_27867_uff_E=106.82	-4.7	prepared_vp4_27867_uff_E=106.82	-5.7
Prepared_ns2_27867_uff_E=106.82	-4.6	prepared_vp4_27867_uff_E=106.82	-5.6
Prepared_ns2_27867_uff_E=106.82	-4.6	prepared_vp4_27867_uff_E=106.82	-5.6
Prepared_ns2_27867_uff_E=106.82	-4.6	prepared_vp4_27867_uff_E=106.82	-5.5
Prepared_ns2_27867_uff_E=106.82	-4.6	prepared_vp4_27867_uff_E=106.82	-5.4
Prepared_ns2_27867_uff_E=106.82	-4.5	prepared_vp4_27867_uff_E=106.82	-5.3
Prepared_ns2_27867_uff_E=106.82	-4.5	prepared_vp4_27867_uff_E=106.82	-5.3