

Supporting Information

A Systematic Molecular Dynamics Approach to the Study of Peptide Keap1-Nrf2 Protein-Protein Interaction Inhibitors and Its Application to p62 Peptide

Meng-Chen Lu,^{a,b} Zhen-Wei Yuan,^{a,b} Yong-Lin Jiang,^{a,b} Zhi-Yun Chen,^{a,b} Qi-Dong You^{a,b,c*} and
Zheng-Yu Jiang^{a,b,c*}.

^aState Key Laboratory of Natural Medicines, China Pharmaceutical University, Nanjing 210009, China;

^bJiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, Nanjing;
210009, China

^cDepartment of Medicinal Chemistry, School of Pharmacy, China Pharmaceutical University, Nanjing
210009, China.

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1. The time-dependence of the RMSD of the backbone atoms;
2. Detailed results of Keap1-peptides binding energy calculation using different GB models;
3. The binding energy decomposition results of Keap1-p62 peptide;
4. The detailed procedures for the peptide synthesis

1. The time-dependence of the RMSD of the backbone atoms;

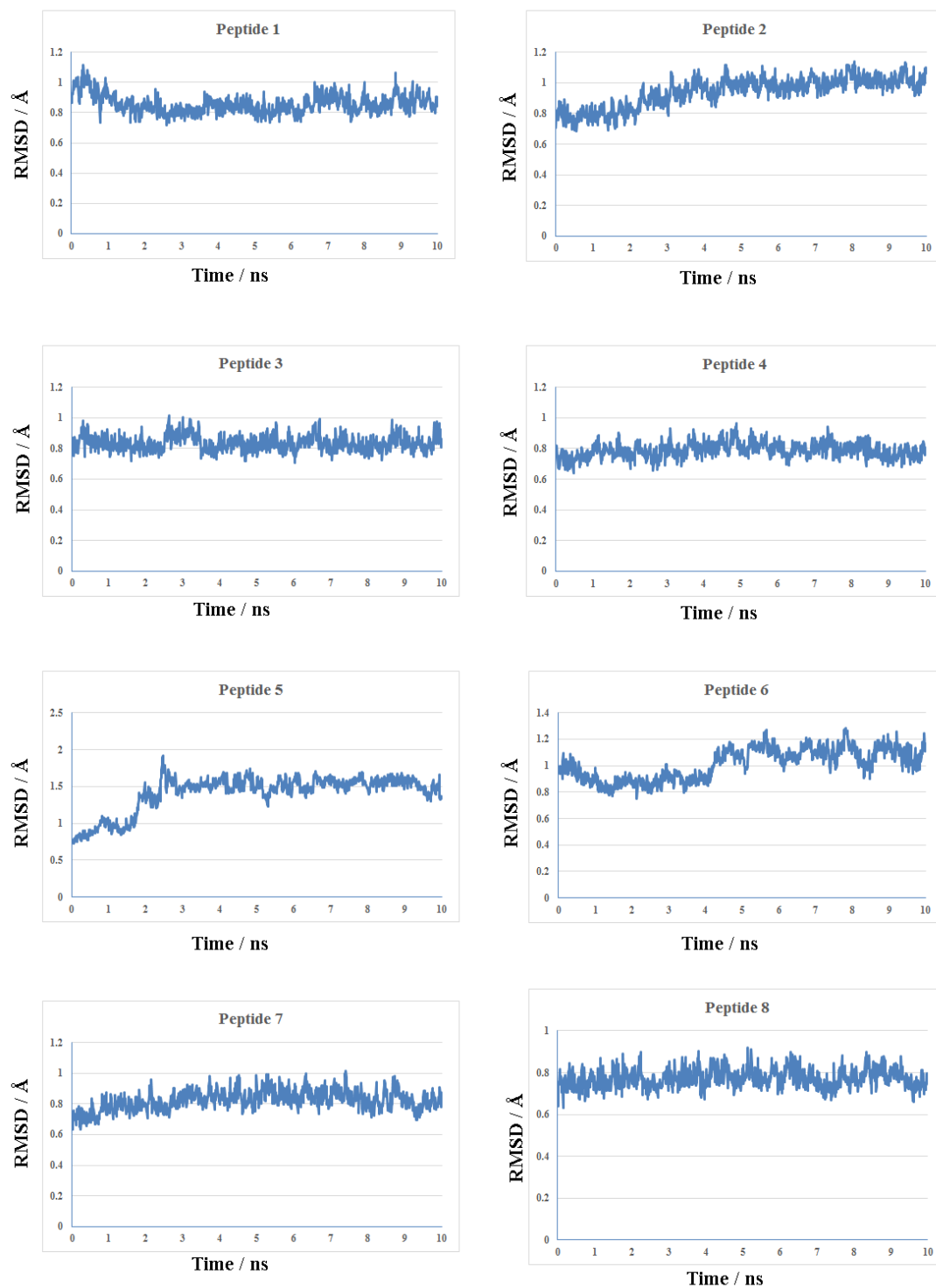


Figure S1. Stability examination for MD simulations. Time series of RMSD values of Keap1-peptide complexes are shown with respect to structures obtained at the end of the equilibration procedure

Detailed results of Keap1-peptides binding energy calculation using different GB models

Peptide 1 igb-1

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2387.6512	19.1768	1.9177
EEL	-19412.2893	68.1303	6.8130
EGB	-3885.4421	49.6604	4.9660
ESURF	87.8151	1.4902	0.1490
G gas	-21799.9405	68.8024	6.8802
G solv	-3797.6269	48.9660	4.8966
TOTAL	-25597.5674	47.6222	4.7622

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2300.2622	19.2031	1.9203
EEL	-18876.5771	63.8142	6.3814
EGB	-3300.4302	45.0667	4.5067
ESURF	87.5260	1.4371	0.1437
G gas	-21176.8392	63.5484	6.3548
G solv	-3212.9042	44.4036	4.4404
TOTAL	-24389.7434	48.0280	4.8028

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.6613	3.3212	0.3321
EEL	-360.9128	15.5495	1.5550
EGB	-743.3165	14.0802	1.4080
ESURF	9.0695	0.2591	0.0259
G gas	-399.5741	15.1298	1.5130
G solv	-734.2470	14.1422	1.4142
TOTAL	-1133.8211	6.3364	0.6336

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-48.7277	5.2304	0.5230
EEL	-174.7994	30.3503	3.0350
EGB	158.3046	26.4195	2.6420
ESURF	-8.7804	0.4273	0.0427
DELTA G gas	-223.5272	28.9961	2.8996
DELTA G solv	149.5242	26.4105	2.6411
DELTA TOTAL	-74.0029	5.5892	0.5589

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2365.9254	25.7022	2.5702
EEL	-19343.7624	92.2672	9.2267
EGB	-3616.0456	62.0028	6.2003
ESURF	85.3028	1.7374	0.1737
G gas	-21709.6878	96.1110	9.6111
G solv	-3530.7428	61.0335	6.1033
TOTAL	-25240.4306	54.7529	5.4753

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2300.4518	25.6403	2.5640
EEL	-18833.4582	91.2983	9.1298
EGB	-3258.0474	61.0987	6.1099
ESURF	85.9586	1.7713	0.1771
G gas	-21133.9099	96.0209	9.6021
G solv	-3172.0888	60.1086	6.0109
TOTAL	-24305.9988	53.5086	5.3509

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-26.3472	2.2845	0.2284
EEL	-305.1784	10.2894	1.0289
EGB	-543.3516	7.8722	0.7872
ESURF	7.0085	0.1049	0.0105
G gas	-331.5257	10.0801	1.0080
G solv	-536.3431	7.8874	0.7887
TOTAL	-867.8688	5.9346	0.5935

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.1264	4.6093	0.4609
EEL	-205.1258	23.6197	2.3620
EGB	185.3535	21.6323	2.1632
ESURF	-7.6643	0.2381	0.0238
DELTA G gas	-244.2522	23.4830	2.3483
DELTA G solv	177.6892	21.5784	2.1578
DELTA TOTAL	-66.5630	4.6166	0.4617

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2372.7968	22.2382	2.2238
EEL	-19414.3537	71.2354	7.1235
EGB	-3621.9751	52.2753	5.2275
ESURF	86.1181	1.6700	0.1670
G gas	-21787.1505	76.3810	7.6381
G solv	-3535.8570	51.5356	5.1536
TOTAL	-25323.0074	57.4084	5.7408

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2306.1603	21.6142	2.1614
EEL	-18900.0650	74.0593	7.4059
EGB	-3263.5754	56.7433	5.6743
ESURF	86.9758	1.6523	0.1652
G gas	-21206.2253	79.0220	7.9022
G solv	-3176.5996	55.9666	5.5967
TOTAL	-24382.8249	57.0443	5.7044

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-26.7666	2.4583	0.2458
EEL	-316.0507	9.1415	0.9141
EGB	-535.6351	6.5910	0.6591
ESURF	6.9413	0.1029	0.0103
G gas	-342.8174	8.8522	0.8852
G solv	-528.6938	6.5883	0.6588
TOTAL	-871.5112	4.8431	0.4843

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.8698	4.5286	0.4529
EEL	-198.2380	24.0007	2.4001
EGB	177.2354	22.2016	2.2202
ESURF	-7.7990	0.2136	0.0214
DELTA G gas	-238.1078	23.9112	2.3911
DELTA G solv	169.4364	22.1819	2.2182
DELTA TOTAL	-68.6714	4.5578	0.4558

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2381.5894	21.5241	3.0440
EEL	-19390.8774	80.3311	11.3605
EGB	-3757.1154	48.7798	6.8985
ESURF	83.4579	1.3514	0.1911
G gas	-21772.4668	83.5272	11.8125
G solv	-3673.6575	48.4724	6.8550
TOTAL	-25446.1243	47.3785	6.7003

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2312.0231	21.7712	3.0789
EEL	-18971.5945	71.3050	10.0841
EGB	-3225.6353	43.8747	6.2048
ESURF	84.6543	1.2721	0.1799
G gas	-21283.6176	74.5703	10.5458
G solv	-3140.9811	43.4877	6.1501
TOTAL	-24424.5986	45.6611	6.4575

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-23.5725	1.8489	0.2615
EEL	-150.3608	11.6977	1.6543
EGB	-770.7494	8.6775	1.2272
ESURF	7.6679	0.1336	0.0189
G gas	-173.9334	11.5724	1.6366
G solv	-763.0815	8.7051	1.2311
TOTAL	-937.0149	5.4309	0.7680

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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VDWAALS	-45.9938	5.1660	0.7306
EEL	-268.9221	30.8589	4.3641
EGB	239.2694	26.1957	3.7046
ESURF	-8.8643	0.3868	0.0547
DELTA G gas	-314.9159	29.9961	4.2421
DELTA G solv	230.4051	26.0692	3.6867
DELTA TOTAL	-84.5108	6.4974	0.9189

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2410.7302	22.5309	2.2531
EEL	-19976.5849	69.9237	6.9924
EGB	-3425.2152	49.7798	4.9780
ESURF	91.1540	1.7170	0.1717
G gas	-22387.3151	70.2434	7.0243
G solv	-3334.0612	49.3053	4.9305
TOTAL	-25721.3763	47.6990	4.7699

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2319.8026	21.9843	2.1984
EEL	-19402.3346	66.7774	6.6777
EGB	-3257.9934	49.0804	4.9080
ESURF	91.8210	1.7732	0.1773
G gas	-21722.1372	67.2576	6.7258
G solv	-3166.1724	48.4628	4.8463
TOTAL	-24888.3096	46.4667	4.6467

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-37.5985	3.5105	0.3510
EEL	-432.5804	31.9942	3.1994
EGB	-313.2388	26.7248	2.6725
ESURF	7.8249	0.2990	0.0299
G gas	-470.1789	30.9907	3.0991
G solv	-305.4139	26.5926	2.6593
TOTAL	-775.5928	7.6828	0.7683

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-53.3292	4.2783	0.4278
EEL	-141.6698	31.7486	3.1749
EGB	146.0170	27.7487	2.7749
ESURF	-8.4920	0.4119	0.0412
DELTA G gas	-194.9990	31.7190	3.1719
DELTA G solv	137.5251	27.5909	2.7591
DELTA TOTAL	-57.4740	6.6157	0.6616

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2428.5611	21.8551	2.1855
EEL	-20010.2669	96.1764	9.6176
EGB	-3520.7227	58.4202	5.8420
ESURF	89.0645	1.5383	0.1538
G gas	-22438.8280	92.3950	9.2395
G solv	-3431.6582	57.9599	5.7960
TOTAL	-25870.4862	57.0984	5.7098

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2342.0129	22.2165	2.2216
EEL	-19398.0455	90.5244	9.0524
EGB	-3296.0690	62.7198	6.2720
ESURF	90.4213	1.6801	0.1680
G gas	-21740.0584	88.4823	8.8482
G solv	-3205.6477	61.9630	6.1963
TOTAL	-24945.7060	57.1052	5.7105

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-32.6770	2.4083	0.2408
EEL	-445.3235	9.9760	0.9976
EGB	-394.1839	7.7668	0.7767
ESURF	7.4127	0.1429	0.0143
G gas	-478.0005	10.2636	1.0264
G solv	-386.7712	7.7588	0.7759
TOTAL	-864.7717	5.0326	0.5033

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-53.8713	4.9699	0.4970
EEL	-166.8979	33.1336	3.3134
EGB	169.5301	29.2110	2.9211
ESURF	-8.7695	0.3383	0.0338
DELTA G gas	-220.7692	33.3965	3.3396
DELTA G solv	160.7607	29.1283	2.9128
DELTA TOTAL	-60.0085	6.1963	0.6196

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2373.3748	19.5314	1.9531
EEL	-19513.0766	85.5949	8.5595
EGB	-3420.2210	59.3700	5.9370
ESURF	84.3971	1.7785	0.1778
G gas	-21886.4514	88.3930	8.8393
G solv	-3335.8239	58.4079	5.8408
TOTAL	-25222.2752	52.8180	5.2818

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2306.6445	19.6232	1.9623
EEL	-18863.9705	82.0675	8.2067
EGB	-3248.3713	59.0588	5.9059
ESURF	85.5950	1.8224	0.1822
G gas	-21170.6151	83.9460	8.3946
G solv	-3162.7762	58.1407	5.8141
TOTAL	-24333.3913	50.7157	5.0716

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-28.5069	2.5135	0.2514
EEL	-432.0760	9.5044	0.9504
EGB	-364.7793	6.1559	0.6156
ESURF	6.6085	0.1257	0.0126
G gas	-460.5828	8.9930	0.8993
G solv	-358.1707	6.1892	0.6189
TOTAL	-818.7536	6.1020	0.6102

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.2234	4.1597	0.4160
EEL	-217.0301	22.7958	2.2796
EGB	192.9295	18.8847	1.8885
ESURF	-7.8064	0.2085	0.0208
DELTA G gas	-255.2534	22.4536	2.2454
DELTA G solv	185.1231	18.8408	1.8841
DELTA TOTAL	-70.1303	5.6924	0.5692

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2365.0862	24.0405	2.4040
EEL	-19455.9444	79.2695	7.9269
EGB	-3328.7018	54.8367	5.4837
ESURF	84.9921	1.5940	0.1594
G gas	-21821.0306	79.6009	7.9601
G solv	-3243.7096	53.9540	5.3954
TOTAL	-25064.7403	47.3151	4.7315

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2296.9349	22.6356	2.2636
EEL	-18830.2014	77.3166	7.7317
EGB	-3273.6541	54.6295	5.4630
ESURF	86.0281	1.4853	0.1485
G gas	-21127.1363	78.1207	7.8121
G solv	-3187.6260	53.8202	5.3820
TOTAL	-24314.7623	45.7782	4.5778

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-27.8320	2.2793	0.2279
EEL	-432.0952	8.3616	0.8362
EGB	-226.3780	4.9662	0.4966
ESURF	6.7786	0.0937	0.0094
G gas	-459.9272	7.8451	0.7845
G solv	-219.5994	4.9246	0.4925
TOTAL	-679.5266	5.4744	0.5474

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-40.3192	4.3294	0.4329
EEL	-193.6479	20.2977	2.0298
EGB	171.3304	14.2423	1.4242
ESURF	-7.8146	0.2948	0.0295
DELTA G gas	-233.9671	19.1044	1.9104
DELTA G solv	163.5157	14.1251	1.4125
DELTA TOTAL	-70.4514	6.6106	0.6611

Peptide 1 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2387.6512	19.1768	1.9177
EEL	-19412.2893	68.1303	6.8130
EGB	-3837.9984	51.5100	5.1510
ESURF	87.8151	1.4902	0.1490
G gas	-21799.9405	68.8024	6.8802
G solv	-3750.1832	50.7985	5.0799
TOTAL	-25550.1237	48.5215	4.8521

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2300.2622	19.2031	1.9203
EEL	-18876.5771	63.8142	6.3814
EGB	-3251.7384	46.5225	4.6523
ESURF	87.5260	1.4371	0.1437
G gas	-21176.8392	63.5484	6.3548
G solv	-3164.2124	45.8408	4.5841
TOTAL	-24341.0516	49.1010	4.9101

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.6613	3.3212	0.3321
EEL	-360.9128	15.5495	1.5550
EGB	-757.6278	14.0959	1.4096
ESURF	9.0695	0.2591	0.0259
G gas	-399.5741	15.1298	1.5130
G solv	-748.5583	14.1607	1.4161
TOTAL	-1148.1324	6.3817	0.6382

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-48.7277	5.2304	0.5230
EEL	-174.7994	30.3503	3.0350
EGB	171.3678	26.6072	2.6607
ESURF	-8.7804	0.4273	0.0427
DELTA G gas	-223.5272	28.9961	2.8996
DELTA G solv	162.5874	26.5922	2.6592
DELTA TOTAL	-60.9398	5.6462	0.5646

Peptide 2 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2378.5549	20.7896	2.0790
EEL	-19339.8113	97.1504	9.7150
EGB	-3733.9895	69.9941	6.9994
ESURF	84.3201	1.6615	0.1662
G gas	-21718.3662	98.2870	9.8287
G solv	-3649.6694	69.0593	6.9059
TOTAL	-25368.0356	56.7181	5.6718

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2308.4386	20.9152	2.0915
EEL	-18938.8381	78.2528	7.8253
EGB	-3186.0391	56.1606	5.6161
ESURF	85.3106	1.5559	0.1556
G gas	-21247.2767	80.2170	8.0217
G solv	-3100.7285	55.3714	5.5371
TOTAL	-24348.0052	54.8478	5.4848

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-24.6937	2.8847	0.2885
EEL	-158.2946	16.4590	1.6459
EGB	-778.8312	13.7461	1.3746
ESURF	7.6617	0.1795	0.0179
G gas	-182.9883	17.4301	1.7430
G solv	-771.1695	13.7750	1.3775
TOTAL	-954.1578	6.0228	0.6023

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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VDWAALS	-45.4226	5.0439	0.5044
EEL	-242.6786	45.5502	4.5550
EGB	230.8808	40.7382	4.0738
ESURF	-8.6522	0.5012	0.0501
DELTA G gas	-288.1012	45.8605	4.5861
DELTA G solv	222.2286	40.4866	4.0487
DELTA TOTAL	-65.8726	7.9987	0.7999

Peptide 3 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2372.7968	22.2382	2.2238
EEL	-19414.3537	71.2354	7.1235
EGB	-3571.8338	54.9110	5.4911
ESURF	86.1181	1.6700	0.1670
G gas	-21787.1505	76.3810	7.6381
G solv	-3485.7156	54.1105	5.4110
TOTAL	-25272.8661	57.3637	5.7364

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2306.1603	21.6142	2.1614
EEL	-18900.0650	74.0593	7.4059
EGB	-3213.7560	59.1692	5.9169
ESURF	86.9758	1.6523	0.1652
G gas	-21206.2253	79.0220	7.9022
G solv	-3126.7802	58.3407	5.8341
TOTAL	-24333.0054	56.8839	5.6884

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean

VDWAALS	-26.7666	2.4583	0.2458
EEL	-316.0507	9.1415	0.9141
EGB	-546.9074	6.7563	0.6756
ESURF	6.9413	0.1029	0.0103
G gas	-342.8174	8.8522	0.8852
G solv	-539.9661	6.7513	0.6751
TOTAL	-882.7835	4.7902	0.4790

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.8698	4.5286	0.4529
EEL	-198.2380	24.0007	2.4001
EGB	188.8296	22.2794	2.2279
ESURF	-7.7990	0.2136	0.0214
DELTA G gas	-238.1078	23.9112	2.3911
DELTA G solv	181.0306	22.2565	2.2256
DELTA TOTAL	-57.0772	4.9676	0.4968

Peptide 4 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2365.9254	25.7022	2.5702
EEL	-19343.7624	92.2672	9.2267
EGB	-3568.0835	64.8595	6.4859
ESURF	85.3028	1.7374	0.1737
G gas	-21709.6878	96.1110	9.6111
G solv	-3482.7807	63.8492	6.3849
TOTAL	-25192.4685	53.2679	5.3268

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
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VDWAALS	-2300.4518	25.6403	2.5640
EEL	-18833.4582	91.2983	9.1298
EGB	-3210.6857	64.0533	6.4053
ESURF	85.9586	1.7713	0.1771
G gas	-21133.9099	96.0209	9.6021
G solv	-3124.7272	63.0258	6.3026
TOTAL	-24258.6371	52.0751	5.2075

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-26.3472	2.2845	0.2284
EEL	-305.1784	10.2894	1.0289
EGB	-554.5658	8.0586	0.8059
ESURF	7.0085	0.1049	0.0105
G gas	-331.5257	10.0801	1.0080
G solv	-547.5573	8.0733	0.8073
TOTAL	-879.0830	5.9685	0.5968

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.1264	4.6093	0.4609
EEL	-205.1258	23.6197	2.3620
EGB	197.1681	21.6982	2.1698
ESURF	-7.6643	0.2381	0.0238
DELTA G gas	-244.2522	23.4830	2.3483
DELTA G solv	189.5038	21.6415	2.1641
DELTA TOTAL	-54.7484	4.8695	0.4870

Peptide 5 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean

VDWAALS	-2410.7302	22.5309	2.2531
EEL	-19976.5849	69.9237	6.9924
EGB	-3366.1688	51.9427	5.1943
ESURF	91.1540	1.7170	0.1717
G gas	-22387.3151	70.2434	7.0243
G solv	-3275.0148	51.3961	5.1396
TOTAL	-25662.3299	47.5183	4.7518

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2319.8026	21.9843	2.1984
EEL	-19402.3346	66.7774	6.6777
EGB	-3203.2646	50.8421	5.0842
ESURF	91.8210	1.7732	0.1773
G gas	-21722.1372	67.2576	6.7258
G solv	-3111.4436	50.1558	5.0156
TOTAL	-24833.5807	46.3490	4.6349

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-37.5985	3.5105	0.3510
EEL	-432.5804	31.9942	3.1994
EGB	-323.5119	27.3982	2.7398
ESURF	7.8249	0.2990	0.0299
G gas	-470.1789	30.9907	3.0991
G solv	-315.6870	27.2636	2.7264
TOTAL	-785.8659	7.4441	0.7444

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-53.3292	4.2783	0.4278
EEL	-141.6698	31.7486	3.1749

EGB	160.6078	28.3868	2.8387
ESURF	-8.4920	0.4119	0.0412
DELTA G gas	-194.9990	31.7190	3.1719
DELTA G solv	152.1158	28.2257	2.8226
DELTA TOTAL	-42.8832	6.4195	0.6419

Peptide 6 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2428.5611	21.8551	2.1855
EEL	-20010.2669	96.1764	9.6176
EGB	-3464.1892	60.3228	6.0323
ESURF	89.0645	1.5383	0.1538
G gas	-22438.8280	92.3950	9.2395
G solv	-3375.1247	59.7928	5.9793
TOTAL	-25813.9527	58.1237	5.8124

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2342.0129	22.2165	2.2216
EEL	-19398.0455	90.5244	9.0524
EGB	-3242.8578	65.4153	6.5415
ESURF	90.4213	1.6801	0.1680
G gas	-21740.0584	88.4823	8.8482
G solv	-3152.4365	64.5890	6.4589
TOTAL	-24892.4948	57.6932	5.7693

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean

VDWAALS	-32.6770	2.4083	0.2408
EEL	-445.3235	9.9760	0.9976
EGB	-404.3625	8.0236	0.8024
ESURF	7.4127	0.1429	0.0143
G gas	-478.0005	10.2636	1.0264
G solv	-396.9499	8.0132	0.8013
TOTAL	-874.9504	4.9374	0.4937

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-53.8713	4.9699	0.4970
EEL	-166.8979	33.1336	3.3134
EGB	183.0311	29.2405	2.9240
ESURF	-8.7695	0.3383	0.0338
DELTA G gas	-220.7692	33.3965	3.3396
DELTA G solv	174.2617	29.1531	2.9153
DELTA TOTAL	-46.5075	6.3639	0.6364

Peptide 7 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2373.3748	19.5314	1.9531
EEL	-19513.0766	85.5949	8.5595
EGB	-3367.3294	62.7889	6.2789
ESURF	84.3971	1.7785	0.1778
G gas	-21886.4514	88.3930	8.8393
G solv	-3282.9323	61.7923	6.1792
TOTAL	-25169.3837	51.2235	5.1223

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2306.6445	19.6232	1.9623
EEL	-18863.9705	82.0675	8.2067
EGB	-3199.0725	62.1223	6.2122
ESURF	85.5950	1.8224	0.1822
G gas	-21170.6151	83.9460	8.3946
G solv	-3113.4774	61.1694	6.1169
TOTAL	-24284.0925	49.3688	4.9369

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-28.5069	2.5135	0.2514
EEL	-432.0760	9.5044	0.9504
EGB	-374.8029	6.2355	0.6235
ESURF	6.6085	0.1257	0.0126
G gas	-460.5828	8.9930	0.8993
G solv	-368.1944	6.2671	0.6267
TOTAL	-828.7773	6.1326	0.6133

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.2234	4.1597	0.4160
EEL	-217.0301	22.7958	2.2796
EGB	206.5460	19.1049	1.9105
ESURF	-7.8064	0.2085	0.0208
DELTA G gas	-255.2534	22.4536	2.2454
DELTA G solv	198.7395	19.0583	1.9058
DELTA TOTAL	-56.5139	5.7148	0.5715

Peptide 8 igb-2

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2365.0862	24.0405	2.4040
EEL	-19455.9444	79.2695	7.9269
EGB	-3276.2284	57.2828	5.7283
ESURF	84.9921	1.5940	0.1594
G gas	-21821.0306	79.6009	7.9601
G solv	-3191.2362	56.3507	5.6351
TOTAL	-25012.2669	47.3559	4.7356

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2296.9349	22.6356	2.2636
EEL	-18830.2014	77.3166	7.7317
EGB	-3226.8511	57.1244	5.7124
ESURF	86.0281	1.4853	0.1485
G gas	-21127.1363	78.1207	7.8121
G solv	-3140.8230	56.2720	5.6272
TOTAL	-24267.9593	45.6806	4.5681

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-27.8320	2.2793	0.2279
EEL	-432.0952	8.3616	0.8362
EGB	-234.3917	5.0876	0.5088
ESURF	6.7786	0.0937	0.0094
G gas	-459.9272	7.8451	0.7845
G solv	-227.6130	5.0450	0.5045
TOTAL	-687.5402	5.4754	0.5475

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-40.3192	4.3294	0.4329
EEL	-193.6479	20.2977	2.0298
EGB	185.0144	14.3825	1.4383
ESURF	-7.8146	0.2948	0.0295
DELTA G gas	-233.9671	19.1044	1.9104
DELTA G solv	177.1997	14.2551	1.4255
DELTA TOTAL	-56.7674	6.6094	0.6609

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2387.6512	19.1768	1.9177
EEL	-19412.2893	68.1303	6.8130
EGB	-3501.3327	50.5951	5.0595
ESURF	87.8151	1.4902	0.1490
G gas	-21799.9405	68.8024	6.8802
G solv	-3413.5176	49.9023	4.9902
TOTAL	-25213.4581	50.3001	5.0300

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2300.2622	19.2031	1.9203
EEL	-18876.5771	63.8142	6.3814
EGB	-2920.6617	45.5063	4.5506
ESURF	87.5260	1.4371	0.1437
G gas	-21176.8392	63.5484	6.3548
G solv	-2833.1357	44.8404	4.4840

TOTAL	-24009.9749	51.0301	5.1030
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Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.6613	3.3212	0.3321
EEL	-360.9128	15.5495	1.5550
EGB	-746.5294	14.1139	1.4114
ESURF	9.0695	0.2591	0.0259
G gas	-399.5741	15.1298	1.5130
G solv	-737.4599	14.1800	1.4180
TOTAL	-1137.0340	6.5020	0.6502

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-48.7277	5.2304	0.5230
EEL	-174.7994	30.3503	3.0350
EGB	165.8585	26.5058	2.6506
ESURF	-8.7804	0.4273	0.0427
DELTA G gas	-223.5272	28.9961	2.8996
DELTA G solv	157.0781	26.4885	2.6488
DELTA TOTAL	-66.4491	6.2731	0.6273

Peptide 2 igb-5

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2365.5123	25.4982	3.6060
EEL	-19366.8335	95.0269	13.4388
EGB	-3222.6742	70.3028	9.9423
ESURF	85.1095	1.7376	0.2457
G gas	-21732.3459	100.9640	14.2785
G solv	-3137.5646	68.8979	9.7436

TOTAL	-24869.9105	52.4306	7.4148
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Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2299.8150	25.3446	3.5843
EEL	-18851.7139	96.2538	13.6123
EGB	-2872.5120	72.1410	10.2023
ESURF	85.7902	1.7268	0.2442
G gas	-21151.5288	104.0846	14.7198
G solv	-2786.7218	70.7779	10.0095
TOTAL	-23938.2507	51.9886	7.3523

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-26.3514	2.3454	0.3317
EEL	-305.9267	8.8842	1.2564
EGB	-545.2512	6.8221	0.9648
ESURF	7.0009	0.0972	0.0137
G gas	-332.2781	8.8757	1.2552
G solv	-538.2503	6.8478	0.9684
TOTAL	-870.5284	6.4386	0.9106

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.3459	4.7580	0.6729
EEL	-209.1930	22.8592	3.2328
EGB	195.0891	20.6437	2.9195
ESURF	-7.6816	0.2110	0.0298
DELTA G gas	-248.5389	22.6256	3.1997
DELTA G solv	187.4075	20.5996	2.9132
DELTA TOTAL	-61.1314	5.6049	0.7927

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2363.2456	20.6895	2.9259
EEL	-19401.1634	78.5018	11.1018
EGB	-3261.8151	55.0917	7.7911
ESURF	86.8489	1.6805	0.2377
G gas	-21764.4090	78.9327	11.1628
G solv	-3174.9662	54.3932	7.6924
TOTAL	-24939.3752	59.3700	8.3962

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2297.0611	20.1991	2.8566
EEL	-18885.7205	83.2161	11.7685
EGB	-2906.9922	61.5992	8.7114
ESURF	87.6989	1.6535	0.2338
G gas	-21182.7816	83.9579	11.8734
G solv	-2819.2933	60.8461	8.6049
TOTAL	-24002.0749	59.1244	8.3615

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-26.9922	2.3282	0.3293
EEL	-314.4086	10.1483	1.4352
EGB	-538.4494	7.1837	1.0159
ESURF	6.9554	0.1021	0.0144
G gas	-341.4009	9.8030	1.3864
G solv	-531.4939	7.1694	1.0139
TOTAL	-872.8948	4.9088	0.6942

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-39.1923	4.6300	0.6548
EEL	-201.0342	20.8491	2.9485
EGB	183.6265	20.0581	2.8366
ESURF	-7.8054	0.2094	0.0296
DELTA G gas	-240.2266	20.9836	2.9675
DELTA G solv	175.8210	20.0662	2.8378
DELTA TOTAL	-64.4055	5.3636	0.7585

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2378.5549	20.7896	2.0790
EEL	-19339.8113	97.1504	9.7150
EGB	-3400.2558	69.1389	6.9139
ESURF	84.3201	1.6615	0.1662
G gas	-21718.3662	98.2870	9.8287
G solv	-3315.9357	68.2142	6.8214
TOTAL	-25034.3019	58.1654	5.8165

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2308.4386	20.9152	2.0915
EEL	-18938.8381	78.2528	7.8253
EGB	-2857.2877	55.6432	5.5643
ESURF	85.3106	1.5559	0.1556
G gas	-21247.2767	80.2170	8.0217
G solv	-2771.9771	54.8639	5.4864
TOTAL	-24019.2539	56.1570	5.6157

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-24.6937	2.8847	0.2885
EEL	-158.2946	16.4590	1.6459
EGB	-768.2275	13.7867	1.3787
ESURF	7.6617	0.1795	0.0179
G gas	-182.9883	17.4301	1.7430
G solv	-760.5659	13.8159	1.3816
TOTAL	-943.5542	6.1758	0.6176

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-45.4226	5.0439	0.5044
EEL	-242.6786	45.5502	4.5550
EGB	225.2595	40.6741	4.0674
ESURF	-8.6522	0.5012	0.0501
DELTA G gas	-288.1012	45.8605	4.5861
DELTA G solv	216.6073	40.4285	4.0429
DELTA TOTAL	-71.4939	8.8496	0.8850

Peptide 5 igb-5

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2419.4652	18.4236	2.6055
EEL	-20041.0592	96.3658	13.6282
EGB	-3113.1780	60.5239	8.5594
ESURF	89.9446	1.4362	0.2031
G gas	-22460.5244	94.4350	13.3551
G solv	-3023.2335	59.7646	8.4520
TOTAL	-25483.7579	50.3830	7.1252

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2332.6030	18.5759	2.6270
EEL	-19413.6987	98.4606	13.9244
EGB	-2913.1980	65.5967	9.2768
ESURF	91.4357	1.5855	0.2242
G gas	-21746.3018	99.0142	14.0027
G solv	-2821.7623	64.6168	9.1382
TOTAL	-24568.0641	52.0092	7.3552

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-32.2077	2.1156	0.2992
EEL	-442.1916	5.9706	0.8444
EGB	-397.5752	5.3047	0.7502
ESURF	7.3331	0.1059	0.0150
G gas	-474.3994	6.5059	0.9201
G solv	-390.2421	5.3260	0.7532
TOTAL	-864.6415	4.6020	0.6508

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-54.6545	5.6027	0.7923
EEL	-185.1688	20.4409	2.8908
EGB	197.5952	16.3736	2.3156
ESURF	-8.8242	0.3489	0.0493
DELTA G gas	-239.8233	19.6579	2.7800
DELTA G solv	188.7710	16.2888	2.3036
DELTA TOTAL	-51.0524	6.5209	0.9222

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2413.6468	23.1955	3.2480
EEL	-19978.9178	60.0506	8.4088
EGB	-3021.2282	58.6880	8.2180
ESURF	91.5505	1.5972	0.2237
G gas	-22392.5647	63.7437	8.9259
G solv	-2929.6777	58.2244	8.1530
TOTAL	-25322.2423	46.0277	6.4452

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2322.5753	23.1036	3.2352
EEL	-19406.7270	72.0863	10.0941
EGB	-2865.3578	67.9339	9.5127
ESURF	92.2786	1.6104	0.2255
G gas	-21729.3022	74.2512	10.3972
G solv	-2773.0792	67.5278	9.4558
TOTAL	-24502.3814	46.7162	6.5416

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-38.2285	3.3306	0.4664
EEL	-420.1897	27.9186	3.9094
EGB	-325.1664	24.6367	3.4498
ESURF	7.7915	0.2669	0.0374
G gas	-458.4181	28.0128	3.9226
G solv	-317.3749	24.4618	3.4253
TOTAL	-775.7931	5.8969	0.8257

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-52.8431	3.7932	0.5312
EEL	-152.0012	22.1725	3.1048
EGB	169.2960	18.7154	2.6207
ESURF	-8.5196	0.4002	0.0560
DELTA G gas	-204.8443	23.3209	3.2656
DELTA G solv	160.7764	18.5583	2.5987
DELTA TOTAL	-44.0679	7.5771	1.0610

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GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2373.3782	16.5330	2.3381
EEL	-19562.3052	72.7860	10.2935
EGB	-2997.0937	49.5179	7.0029
ESURF	83.9177	1.6415	0.2321
G gas	-21935.6834	75.2708	10.6449
G solv	-2913.1761	48.6466	6.8797
TOTAL	-24848.8595	44.9353	6.3548

Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2306.6137	18.0609	2.5542
EEL	-18906.1957	75.9149	10.7360
EGB	-2836.7560	51.0321	7.2170
ESURF	85.1688	1.6978	0.2401
G gas	-21212.8095	77.0334	10.8942
G solv	-2751.5872	50.2576	7.1075
TOTAL	-23964.3967	44.6311	6.3118

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-29.0495	2.3147	0.3273
EEL	-431.8080	8.8445	1.2508
EGB	-367.7632	4.8998	0.6929
ESURF	6.5553	0.0997	0.0141
G gas	-460.8575	8.2551	1.1675
G solv	-361.2079	4.8920	0.6918
TOTAL	-822.0654	5.8503	0.8274

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-37.7150	4.2461	0.6005
EEL	-224.3015	18.9697	2.6827
EGB	207.4256	16.8716	2.3860
ESURF	-7.8064	0.1852	0.0262
DELTA G gas	-262.0165	18.6553	2.6383
DELTA G solv	199.6191	16.8605	2.3844
DELTA TOTAL	-62.3973	5.6928	0.8051

Peptide 8 igb-5

GENERALIZED BORN:

Complex:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2364.6323	21.7895	3.0815
EEL	-19438.7549	82.6823	11.6930
EGB	-2965.1546	53.8186	7.6111
ESURF	85.4195	1.4982	0.2119
G gas	-21803.3872	81.2950	11.4969
G solv	-2879.7351	53.2301	7.5279

TOTAL	-24683.1223	49.3948	6.9855
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Receptor:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-2296.0542	20.4278	2.8889
EEL	-18819.2632	77.6933	10.9875
EGB	-2916.1518	51.2393	7.2463
ESURF	86.3401	1.2951	0.1832
G gas	-21115.3174	76.4907	10.8174
G solv	-2829.8117	50.7752	7.1807
TOTAL	-23945.1291	47.5595	6.7259

Ligand:

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-27.9791	2.5583	0.3618
EEL	-433.7503	9.3564	1.3232
EGB	-225.6354	5.9577	0.8425
ESURF	6.7511	0.0946	0.0134
G gas	-461.7294	8.6582	1.2245
G solv	-218.8844	5.9084	0.8356
TOTAL	-680.6138	5.1290	0.7254

Differences (Complex - Receptor - Ligand):

Energy Component	Average	Std. Dev.	Std. Err. of Mean
VDWAALS	-40.5990	4.2385	0.5994
EEL	-185.7414	20.5281	2.9031
EGB	176.6326	14.2019	2.0085
ESURF	-7.6716	0.3352	0.0474
DELTA G gas	-226.3404	19.3254	2.7330
DELTA G solv	168.9610	14.0647	1.9890
DELTA TOTAL	-57.3794	7.5969	1.0744

results of p62 peptide

Keapl

	van der Waals				Electrostatic				Polar Solvation				Non-Polar Solv.				TOTAL	
	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	of Mean	
Tyr334	-2.65058	0.280258	0.008863		-0.94057	0.951044	0.030075		1.510675	0.924913	0.029248		-0.17905	0.032329	0.001022		-2.25953 0.330992 0.010467	
Ser363	0.649794	0.776431	0.024553		-11.3075	1.402307	0.044345		8.833485	0.923345	0.029199		-0.0865	0.009468	0.000299		-1.91072 0.520511 0.01646	
Arg380	0.353109	1.041189	0.032925		-103.525	3.933393	0.124385		98.13044	2.586803	0.081802		-0.35508	0.041128	0.001301		-5.39702 1.515585 0.047927	
Asn382	-0.43361	0.692361	0.021894		-13.4133	2.368797	0.074908		9.310144	1.286696	0.040689		-0.13811	0.040496	0.001281		-4.67483 1.43588 0.045406	
Arg415	-1.37147	0.716226	0.022649		-76.6484	5.939867	0.187835		76.94577	4.675546	0.147854		-0.45368	0.059617	0.001885		-1.52778 1.82005 0.057555	
Arg483	-0.45577	0.220326	0.006967		-44.0776	3.822158	0.120867		44.64422	3.907286	0.123559		-0.12699	0.071678	0.002267		-0.01617 0.333723 0.010553	
Ser508	-0.68112	0.213004	0.006736		-1.29826	1.00484	0.031776		1.591844	1.191633	0.037683		-0.03083	0.012624	0.000399		-0.41837 0.452926 0.014323	
Gly509	-0.60992	0.164503	0.005202		-0.35605	0.501837	0.015869		0.486334	0.467403	0.014781		-0.01163	0.013728	0.000434		-0.49126 0.252277 0.007978	
Tyr525	-2.68036	0.33577	0.010618		0.353259	0.363219	0.011486		-0.02325	0.443772	0.014033		-0.28445	0.040504	0.001281		-2.63481 0.409334 0.012944	
Gln530	-0.37133	0.530156	0.016765		-7.99996	0.673199	0.021288		6.665035	0.454279	0.014366		-0.09515	0.020427	0.000646		-1.80139 0.46531 0.014714	
Ser555	-0.94944	0.709786	0.022445		-3.63758	3.466157	0.10961		3.418941	3.341223	0.105659		-0.07433	0.013651	0.000432		-1.24241 0.739379 0.023381	
Ala556	-0.92107	0.285512	0.009029		0.384824	0.524893	0.016599		-0.20717	0.508568	0.016082		-0.1285	0.023756	0.000751		-0.87192 0.308143 0.009744	
Tyr572	-4.09445	0.424951	0.013438		-0.27906	0.643104	0.020337		0.48624	0.709168	0.022426		-0.40197	0.039675	0.001255		-4.28923 0.462366 0.014621	
Phe577	-1.01681	0.273473	0.008648		-2.3989	0.260949	0.008252		2.274724	0.227469	0.007193		-0.13681	0.028311	0.000895		-1.27781 0.270809 0.008564	
Ser602	-0.28284	0.493612	0.015609		-4.4404	1.052518	0.033284		4.955878	0.913365	0.028883		-0.11057	0.015589	0.000493		0.122064 0.391706 0.012387	

p62 peptide

	van der Waals				Electrostatic				Polar Solvation				Non-Polar Solv.				TOTAL	
	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Std. Err.	of Mean	
Val348	-0.94706	0.233214	0.007375		1.788465	0.469953	0.014861		-1.31211	0.484323	0.015316		-0.13213	0.056721	0.001794		-0.60284 0.359786 0.011377	
Asp349	-1.52502	0.426956	0.013502		-13.9999	6.477325	0.204831		15.71222	5.793069	0.183193		-0.16115	0.063019	0.001993		0.02612 1.445804 0.04572	
Pro350	-3.26167	0.68117	0.02154		-1.7535	1.02766	0.032497		1.966444	0.764361	0.024171		-0.69581	0.050967	0.001612		-3.74454 0.698248 0.022081	
Sep351	-4.42535	0.863501	0.027306		-7.64366	2.413237	0.076313		7.054475	1.427245	0.045133		-0.73804	0.029227	0.000924		-5.75258 1.668907 0.052775	
Thr352	-4.17615	0.68668	0.021715		-2.6872	1.809814	0.057231		3.569311	1.953447	0.061773		-0.68133	0.039797	0.001258		-3.97537 0.83241 0.026323	
Gly353	-2.52571	0.338459	0.010703		-0.42207	0.583747	0.01846		1.730788	0.753551	0.023829		-0.36233	0.025194	0.000797		-1.57932 0.491978 0.015558	
Glu354	-2.98516	1.187353	0.037547		-36.0111	4.255578	0.134573		39.35636	3.52245	0.11139		-0.83134	0.028411	0.000898		-0.4712 1.547749 0.048944	
Leu355	-0.59535	0.835368	0.026417		-26.6378	4.925408	0.155755		24.70902	4.45759	0.140961		-0.35044	0.068272	0.002159		-2.87454 1.337757 0.042304	

results of phosphorylated p62 peptide

Keap1

	van der Waals			Electrostatic			Polar Solvation			Non-Polar Solv.			TOTAL		
	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	of Mean		
Tyr334	-3.27298	0.42249	0.01336	-1.80152	1.154713	0.036515	2.003712	1.111736	0.035156	-0.33199	0.036321	0.001149	-3.40277	0.571062	0.018059
Ser363	0.425135	0.943537	0.029837	-10.7273	5.019354	0.158726	9.121015	3.284334	0.10386	-0.08802	0.017825	0.000564	-1.26921	1.196768	0.037845
Arg380	-0.20596	0.585983	0.01853	-109.65	3.685418	0.116543	105.3911	3.183255	0.100663	-0.11531	0.045414	0.001436	-4.58031	0.792467	0.02506
Asn382	-0.94287	0.548595	0.017348	-9.47946	2.555914	0.080825	7.048486	1.458144	0.046111	-0.18947	0.032258	0.00102	-3.56332	1.531424	0.048428
Arg415	-1.44914	0.960874	0.030386	-146.744	9.693614	0.306539	136.1236	7.126017	0.225344	-0.67484	0.090783	0.002871	-12.7441	3.239217	0.102433
Arg483	0.366532	0.876819	0.027727	-121.026	3.623173	0.114575	107.2378	2.55411	0.080768	-0.13002	0.035895	0.001135	-13.5512	1.349629	0.042679
Ser508	0.740992	0.864295	0.027331	-15.3957	2.451926	0.077537	10.38405	1.837035	0.058092	-0.06777	0.024046	0.00076	-4.33848	1.01958	0.032242
Ser509	-0.29188	0.164434	0.0052	0.155978	1.426037	0.045095	0.245532	1.2423	0.039285	-0.03586	0.017481	0.000553	0.073769	0.367862	0.011633
Tyr525	-2.90513	0.404003	0.012776	1.396184	1.164136	0.036813	-0.85738	0.970995	0.030706	-0.32787	0.034485	0.001091	-2.69419	0.54241	0.017153
Gln530	-0.47484	0.417529	0.013203	-12.2097	1.275091	0.040322	10.06422	1.421375	0.044948	-0.07853	0.026483	0.000837	-2.69882	0.652159	0.020623
Ser555	-0.13645	0.664052	0.020999	-12.3761	2.02267	0.063962	11.59449	1.567941	0.049583	-0.09251	0.019956	0.000631	-1.01054	0.620053	0.019608
Ala556	-0.88698	0.186599	0.005901	-2.57115	0.813501	0.025725	2.80465	0.784062	0.024794	-0.15701	0.021543	0.000681	-0.81049	0.21728	0.006871
Tyr572	-4.41325	0.489677	0.015485	0.978753	0.816302	0.025814	-0.26548	0.858765	0.027157	-0.44383	0.03835	0.001213	-4.1438	0.517318	0.016359
Phe577	-1.19196	0.238595	0.007545	-2.55334	0.348968	0.011035	2.4883	0.308107	0.009743	-0.11558	0.028117	0.000889	-1.37257	0.24164	0.007641
Ser602	-0.29327	0.542435	0.017153	-7.93122	1.882468	0.059529	8.091667	1.688612	0.053399	-0.1167	0.020354	0.000644	-0.24952	0.500374	0.015823

phosphorylated p62 peptide

	van der Waals			Electrostatic			Polar Solvation			Non-Polar Solv.			TOTAL		
	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	Avg.	Std. Dev.	Std. Err.	of Mean		
Val348	-0.88901	0.190498	0.006024	0.541256	0.28318	0.008955	-0.6346	0.327902	0.010369	-0.12353	0.04336	0.001371	-1.10589	0.282598	0.008937
Asp349	-1.16958	0.595048	0.018817	-23.7219	6.748379	0.213402	25.17676	5.646622	0.178562	-0.11322	0.02977	0.000941	0.172048	1.614726	0.051062
Pro350	-2.79617	0.553152	0.017492	-0.67741	1.284224	0.040611	0.862109	1.137102	0.035958	-0.5673	0.050652	0.001602	-3.17877	0.668469	0.021139
Sep351	-3.34182	1.601164	0.050633	-84.2029	8.59228	0.271712	107.1729	7.394285	0.233828	-1.19669	0.050141	0.001586	18.43145	2.773987	0.087721
Thr352	-4.50282	0.765324	0.024202	-2.09675	1.599919	0.050594	1.786989	1.314057	0.041554	-0.62766	0.036851	0.001165	-5.44024	0.78789	0.024915
Gly353	-2.5714	0.349543	0.011054	-0.13713	0.566716	0.017921	0.846111	0.667677	0.021114	-0.33036	0.02785	0.000881	-2.19278	0.458198	0.01449
Glu354	-3.43288	1.061362	0.033563	-44.9448	5.746092	0.181707	48.09714	4.268524	0.134983	-0.83332	0.051855	0.00164	-1.11389	2.053662	0.064943
Leu355	-2.755	0.78098	0.024697	-0.74826	5.479978	0.173292	3.01935	5.404865	0.170917	-0.55946	0.163192	0.005161	-1.04337	1.101574	0.034835

Peptide Synthesis and Purification.

All linear peptides were synthesized manually using a standard solid phase peptide synthesis approach with Fmoc chemistry. Peptide couplings were carried out using HATU and DIPEA in DMF. The N-terminal acetyl group was attached using acetic anhydride and DIPEA in DMF. Fmoc removal was achieved with 20% piperidine in DMF for 20 min. Peptides were cleaved from the resin and side chain deprotected using TFA–TIS–H₂O (95: 2.5: 2.5). All reactions were carried out at room temperature. Cyclization was carried out in solution with 0.1 M ammonium bicarbonate, pH 8.0, for 24 h at a peptide concentration of 0.5 mM. The crude peptide was purified by semi-preparative reverse-phase high performance liquid chromatography (RP-HPLC). The purity and molecular mass of the synthesized and cyclized peptide were confirmed with liquid chromatography-mass spectroscopy (LC-MS).

P62 peptide

Analysis Report

Inj. Date: 12/23/2014 15:24:20

Operator: Kai Yuan

Product Name: P105037

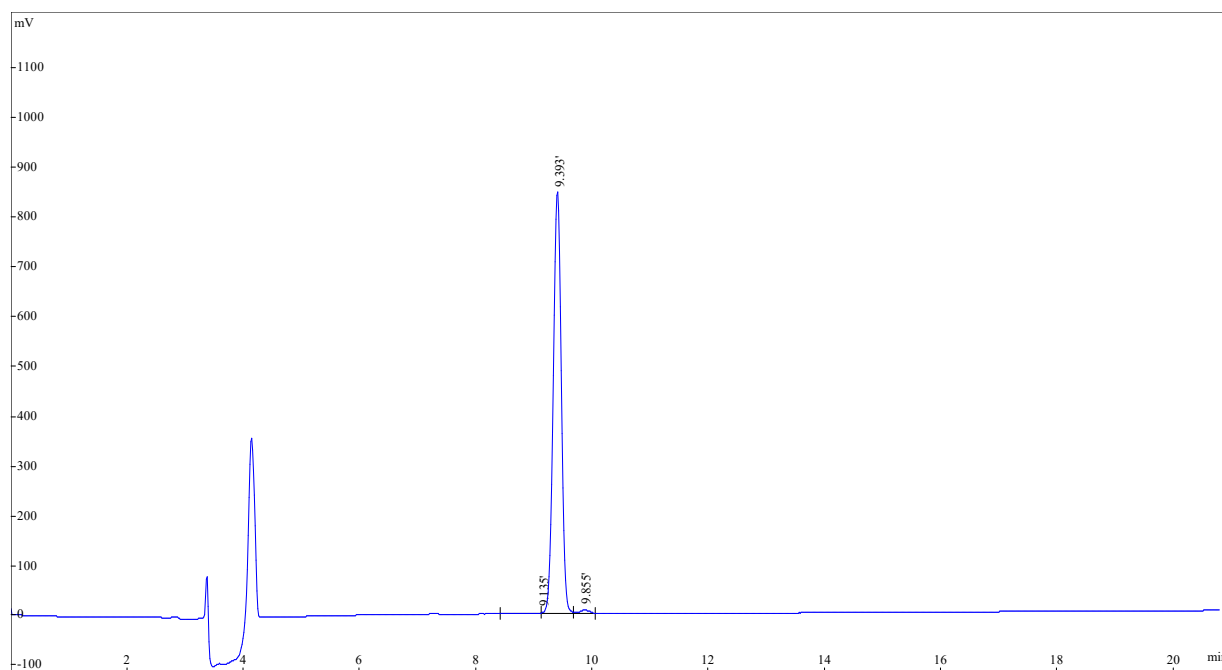
Lot: ON121614LJ-02B

Mobile Phase: A: 0.1% TFA in H2O

B: 0.1% TFA in 100% ACN

Grads: 25%-45%B in 20 min Flow : 1.0 ml/min

Column : 4.6×250mm, Welchrom C18



Rank	Time	Name	Conc.	Area
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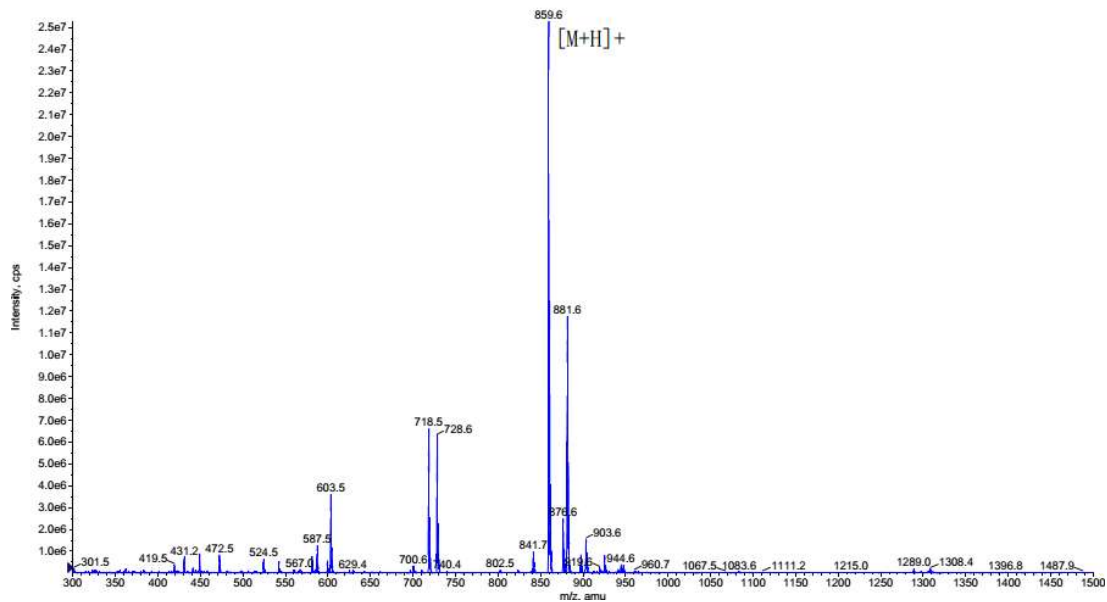
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Product Name: P105037

Lot: 0N121614LJ-02B

MW: 858.87

Date: 2014-12-23



Phosphorylated p62 peptide

Analysis Report

Inj. Date: 12/23/2014 09:46:09

Operator: Kai Yuan

Product Name: P105038

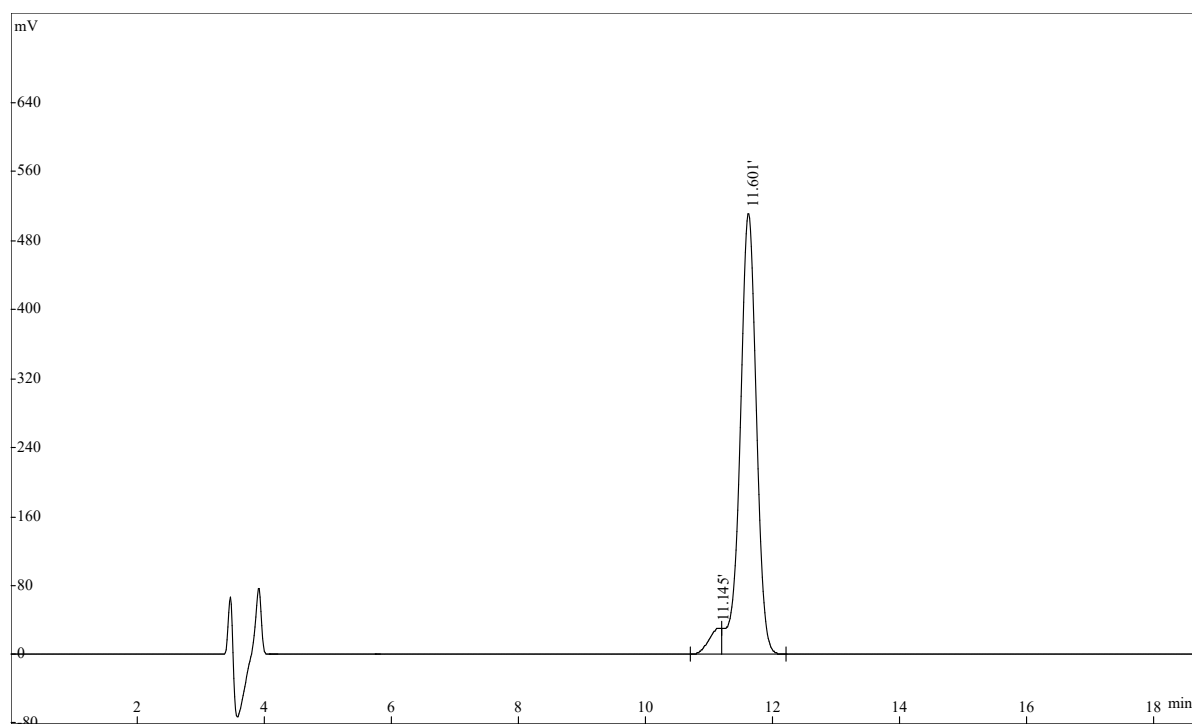
Lot: ON121614LJ-02C

Mobile Phase: A: 0.1% TFA in H2O

B: 0.1% TFA in 100% ACN

Grads: 16%-36%B in 20 min Flow : 1.0 ml/min

Column : 4.6×250mm, Welchrom C18



Time	Quantity	Area	Height	Resolut.	T.PlateNum	Asymmetry
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11.601	95.24	9106342	512779	0.00	9957	0.99
	100	9561083	544157			

Product Name: P105038

Lot: 0N121614LJ-02C

MW: 938.87

Date: 2014-12-23

