

Data from Peptide Conformations

Conformation	HF 6-311G(2df,pd)	B3LYP 6-311G(2df,pd)	$\omega$ B97 6-311G(2df,pd)	$\omega$ B97X 6-311G(2df,pd)	$\omega$ B97X-D 6-311G(2df,pd)	LRC- $\omega$ PBEh 6-311G(2df,pd)	M06 6-311G(2df,pd)	M06-2X 6-311G(2df,pd)	M06-HF 6-311G(2df,pd)	HF cc-pVQZ	RI-MP2 Correlation cc-pVTZ	RI-MP2 Correlation cc-pVQZ	HF + RI-MP2 cc-pV(TQ)Z
<b>Linear</b>	-984.8879403920	-990.8451650913	-990.6872959797	-990.5982611122	-990.5332864235	-989.8594734327	-990.2077559975	-990.4273001843	-990.5564221297	-984.9999990000	-3.7375860000	-3.9965570000	-989.1855348378
<b>2</b>	-984.8867980414	-990.8448444754	-990.6871251292	-990.5976764321	-990.5327164491	-989.8590481619	-990.2054361869	-990.4278770772	-990.5637522544	-984.9985010000	-3.7392340000	-3.9980630000	-989.1854392162
<b>Globular</b>	-984.8871918196	-990.8478335736	-990.6937727466	-990.6040867708	-990.5413556720	-989.8623042723	-990.2117743815	-990.4338114083	-990.5676826754	-984.9962320000	-3.7475650000	-4.0062240000	-989.1912071622
<b>4</b>	-984.8843806594	-990.8418738700	-990.6840950982	-990.5949273064	-990.5305015724	-989.8560027283	-990.2037224054	-990.4248235756	-990.5580994003	-984.9960700000	-3.7393700000	-3.9981070000	-989.1829850811
<b>5</b>	-984.8844859818	-990.8413237376	-990.6843604379	-990.5949247409	-990.5304072557	-989.8558651120	-990.2044597646	-990.4253044150	-990.5588951418	-984.9961100000	-3.7398390000	-3.9987140000	-989.1837327838
<b>6</b>	-984.8859404922	-990.8441742810	-990.6908815335	-990.6008619280	-990.5370472043	-989.8594203753	-990.2095686815	-990.4316472773	-990.5660029657	-984.9952330000	-3.7447800000	-4.0034850000	-989.1875027297
<b>7</b>	-984.8778019024	-990.8368154967	-990.6840196097	-990.5937834891	-990.5299866372	-989.8519293457	-990.2036697365	-990.4253000074	-990.5565690670	-984.9872760000	-3.7469520000	-4.0055280000	-989.1814945946
<b>8</b>	-984.8809591175	-990.8394746455	-990.6867453027	-990.5963969035	-990.5332015374	-989.8546310937	-990.2064264051	-990.4284002878	-990.5609000277	-984.9899600000	-3.7475960000	-4.0061140000	-989.1847222703
<b>9</b>	-984.8754040920	-990.8382421530	-990.6822325731	-990.5924975964	-990.5292394478	-989.8517829570	-990.1998594112	-990.4216760458	-990.5541921049	-984.9857680000	-3.7464140000	-4.0050140000	-989.1794901081
<b>10</b>	-984.8755008861	-990.8358029297	-990.6830512583	-990.5927202159	-990.5291816651	-989.8509389803	-990.2012892006	-990.4238909349	-990.5554580497	-984.9844720000	-3.7479270000	-4.0065230000	-989.1797001892
<b>11</b>	-984.8869536011	-990.8464196011	-990.6948852573	-990.6045376767	-990.5418526897	-989.8616166420	-990.2127248037	-990.4350922981	-990.5708806676	-984.9958020000	-3.7487640000	-4.0075040000	-989.1921162703
<b>12</b>	-984.8848276346	-990.8440129607	-990.6930515056	-990.6027000759	-990.5404254637	-989.8601095135	-990.2130942316	-990.4345941431	-990.5675008915	-984.9939200000	-3.7499950000	-4.0088440000	-989.1916538108
<b>13</b>	-984.8862520476	-990.8450813789	-990.6884818260	-990.5991317182	-990.5348759812	-989.8594737421	-990.2070258324	-990.4288504026	-990.5635696401	-984.9973630000	-3.7415200000	-4.0001780000	-989.1862914324
<b>14</b>	-984.8834011006	-990.8413215500	-990.6855792882	-990.5960665544	-990.5326815213	-989.8563185609	-990.2047626748	-990.4270420067	-990.5610325548	-984.9941710000	-3.7429140000	-4.0016680000	-989.1846594865
<b>15</b>	-984.8833464052	-990.8417695958	-990.6913225862	-990.6006826939	-990.5376629128	-989.8577255005	-990.2111697147	-990.4328990890	-990.5652056320	-984.9914230000	-3.7500780000	-4.0085690000	-989.1886205676
<b>16</b>	-984.8827823487	-990.8418427158	-990.6874244103	-990.5977036047	-990.5346883931	-989.8561498167	-990.2059502265	-990.4280538013	-990.5633415859	-984.9929310000	-3.7461210000	-4.0047790000	-989.1864604324
<b>17</b>	-984.8824140148	-990.8427733662	-990.6906787023	-990.6001774395	-990.5371222388	-989.8575752187	-990.2091435086	-990.4302068769	-990.5618357741	-984.9911160000	-3.7482000000	-4.0068270000	-989.1866708108
<b>18</b>	-984.8876461655	-990.8479594411	-990.6918059058	-990.6021668600	-990.5378103526	-989.8623228308	-990.2104005643	-990.4318542107	-990.5643717413	-984.9981080000	-3.7437960000	-4.0023120000	-989.1890668108
<b>19</b>	-984.8836998435	-990.8447740619	-990.6886125949	-990.5988060856	-990.5346487520	-989.8588329431	-990.2066644325	-990.4288116291	-990.5632147068	-984.9942430000	-3.7445330000	-4.0031050000	-989.1860356757
<b>20</b>	-984.8865837312	-990.8458872863	-990.6901583615	-990.6004960759	-990.5369700046	-989.8605363608	-990.2084307916	-990.4316260586	-990.5663423452	-984.9972250000	-3.7446380000	-4.0033250000	-989.1893215946
<b>21</b>	-984.8851943820	-990.8434323504	-990.6896045139	-990.5995717872	-990.5362428838	-989.8578880823	-990.2094571564	-990.4301503961	-990.5611298333	-984.9948330000	-3.7455210000	-4.0040080000	-989.1874666486
<b>22</b>	-984.8791243044	-990.8394400927	-990.6857564687	-990.5955781083	-990.5318530458	-989.8541742483	-990.2035627794	-990.4261741334	-990.5597227124	-984.9882300000	-3.7473130000	-4.0059040000	-989.1828355405
<b>23</b>	-984.8791135723	-990.8390067758	-990.6852066021	-990.5950874712	-990.5315021847	-989.8535476125	-990.2036706379	-990.4258148720	-990.5585072430	-984.9885460000	-3.7469530000	-4.0055780000	-989.1828503514
<b>24</b>	-984.8826721451	-990.8415225577	-990.6878786648	-990.5976425045	-990.5333574456	-989.8565365219	-990.2060653949	-990.4290763400	-990.5643247664	-984.9920460000	-3.7464760000	-4.0050470000	-989.1857799459
<b>25</b>	-984.8849790411	-990.8440682947	-990.6892013662	-990.5993754771	-990.5357723541	-989.8589140677	-990.2075692641	-990.4302083328	-990.5651617054	-984.9955310000	-3.7450660000	-4.0038020000	-989.1881403514
<b>26</b>	-984.8864812223	-990.8449448025	-990.6910896306	-990.6011612623	-990.5381457875	-989.8602346341	-990.2096908303	-990.4325379111	-990.5673381171	-984.9968580000	-3.7465130000	-4.0053230000	-989.1910423514
<b>27</b>	-984.8819962837	-990.8416427534	-990.6865216336	-990.5965837462	-990.5331401829	-989.8561531912	-990.2048764769	-990.4274711630	-990.5621004554	-984.9926410000	-3.7455420000	-4.0042690000	-989.1857107838