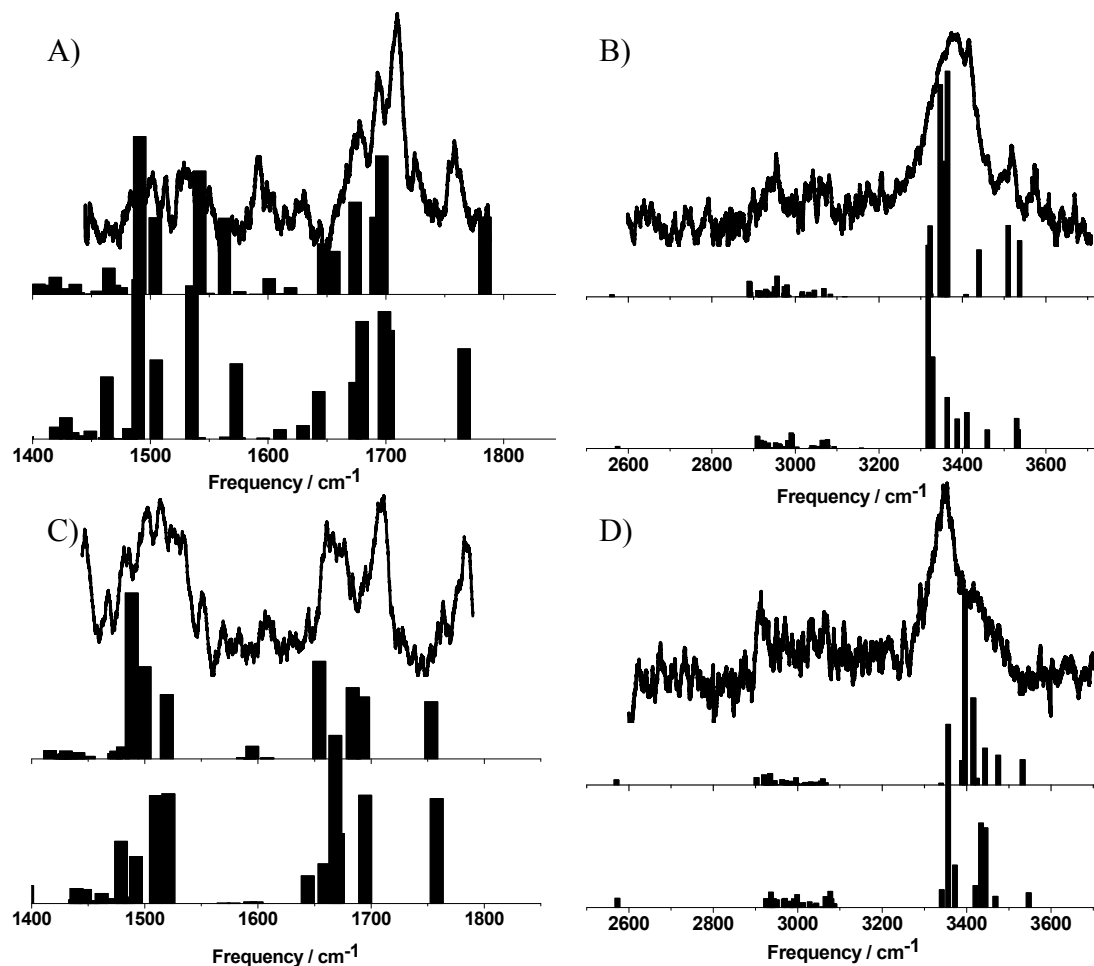


## Infrared Spectroscopy of 'Forbidden' Peptide Sequences

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### Supplementary Data



*Figure S1.* M05-2X/6-31G\* (upper stick spectra) and B3LYP/6-31G\* (lower stick spectra) frequencies, shown after scaling using recommended scaling factors (see ref 31) are compared for the 'best-fit' conformers, along with the experimental spectra. A) WCFNL, conformer W1, frequencies in the Amide I/II region. B) WCFNL, conformer W1, frequencies in the NH stretch region. C) FFMCT, conformer F4, frequencies in the Amide I/II region. D) FFMCT, conformer F4, frequencies in the NH stretch region.

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Cartesian coordinates of conformer **F1**, calculated at the M05-2X/6-31G\* level

atom	x	y	z
1	-1.530329	-3.576335	1.671272
7	-1.875531	-3.296789	2.58321
6	-1.395384	-4.208271	3.611156
6	0.125004	-4.202028	3.782215
8	0.649847	-3.790117	4.817066
6	-1.980182	-5.623164	3.399991
6	-1.854475	-6.193262	2.004446
6	-0.843711	-7.101333	1.674642
6	-2.779608	-5.837822	1.018374
6	-0.757419	-7.642977	0.396005
6	-2.706263	-6.384281	-0.25949
6	-1.697078	-7.295592	-0.574547
1	-1.758214	-3.853612	4.576201
1	-1.522601	-6.304605	4.121143
1	-3.041768	-5.550118	3.643005
1	-0.122766	-7.388184	2.431284
1	-3.561145	-5.130071	1.266225
1	0.026719	-8.352404	0.162819
1	-3.443405	-6.111658	-1.004976
1	-1.658566	-7.751054	-1.557878
1	0.417971	-4.765723	1.83447
7	0.861602	-4.661238	2.738497
6	2.307872	-4.5128	2.759505
6	2.624615	-3.072705	2.370166
8	2.829905	-2.717314	1.206338
6	3.006125	-5.505445	1.832198
6	4.50682	-5.355479	1.955273
6	5.26151	-4.758687	0.943978
6	5.151047	-5.766145	3.125252
6	6.632454	-4.573639	1.103332
6	6.520502	-5.584755	3.286013
6	7.26558	-4.985891	2.272752
1	2.627118	-4.673361	3.789184
1	2.693746	-6.510666	2.126469
1	2.684205	-5.340015	0.802388
1	4.771411	-4.440493	0.032122
1	4.574722	-6.238536	3.914185
1	7.20522	-4.107843	0.311347
1	7.005639	-5.915155	4.196023
1	8.333446	-4.848164	2.39134
1	2.129617	-2.492499	4.225352
7	2.601531	-2.184606	3.380236
6	2.619204	-0.772108	3.039408
6	1.437036	-0.510722	2.086605
8	0.370423	-1.097692	2.25204
6	3.988512	-0.31612	2.508368
6	5.138897	-0.902192	3.321603
16	6.702545	-0.168408	2.750404
6	7.840593	-1.258536	3.650397
1	2.397456	-0.230356	3.961374
1	4.10907	-0.630547	1.471793
1	4.031742	0.776671	2.549105
1	5.004837	-0.705396	4.388265
1	5.186524	-1.98193	3.172046

1	8.853809	-0.963743	3.382244
1	7.713821	-1.14966	4.727412
1	7.679451	-2.296996	3.360345
1	2.542625	0.729409	0.876977
7	1.619945	0.382155	1.095848
6	0.579929	0.667617	0.124017
6	0.585356	-0.314062	-1.06566
8	0.439371	0.08615	-2.215414
6	0.69727	2.103325	-0.376101
16	2.336919	2.492874	-1.083591
1	2.176498	1.723934	-2.171513
1	-0.375536	0.539721	0.639214
1	-0.066878	2.291604	-1.124898
1	0.561111	2.789337	0.458833
1	0.731006	-1.901762	0.230143
7	0.734261	-1.61216	-0.740916
6	0.691046	-2.647679	-1.747129
6	0.030302	-3.860321	-1.133827
8	-0.142601	-3.99324	0.060433
6	2.092752	-3.107646	-2.230013
8	2.679216	-3.967204	-1.270396
6	2.996725	-1.928735	-2.55153
1	2.789055	-3.473538	-0.434291
1	0.116643	-2.282725	-2.599713
1	1.933597	-3.720298	-3.118453
1	3.941887	-2.301207	-2.946208
1	2.533451	-1.258997	-3.276843
1	3.201366	-1.363784	-1.638778
1	-1.497642	-2.369467	2.749053
8	-0.298834	-4.784731	-2.023914
1	-0.662745	-5.544099	-1.522925

Cartesian coordinates of conformer **F2**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-2.809282	-5.181456	0.935113
7	-1.85729	-4.935977	1.190117
6	-1.588916	-5.395629	2.555265
6	-0.184636	-5.022484	3.03117
8	0.233791	-5.444342	4.104094
6	-1.799556	-6.909224	2.771176
6	-0.852748	-7.756019	1.955574
6	-1.152196	-8.10086	0.634632
6	0.358528	-8.192044	2.503758
6	-0.260596	-8.852932	-0.127251
6	1.246264	-8.950389	1.74673
6	0.941897	-9.278911	0.427841
1	-2.275322	-4.862308	3.217634
1	-1.6604	-7.111315	3.832752
1	-2.835398	-7.148334	2.513972
1	-2.100326	-7.796463	0.203757
1	0.59879	-7.920932	3.52427
1	-0.510826	-9.112096	-1.14849
1	2.178618	-9.282692	2.185849
1	1.636605	-9.862862	-0.161979
1	0.188914	-3.874941	1.348044
7	0.543393	-4.228195	2.224586
6	1.88662	-3.84563	2.585377
6	2.173991	-2.521124	1.898865
8	1.595803	-2.219695	0.861166
6	2.922344	-4.913335	2.142127
6	2.969416	-5.078969	0.643604
6	3.915191	-4.38988	-0.118707
6	2.026194	-5.8713	-0.013323
6	3.910154	-4.468912	-1.506843
6	2.019107	-5.956253	-1.402764
6	2.956276	-5.252016	-2.153399
1	1.927815	-3.745687	3.67154
1	3.905508	-4.62695	2.525261
1	2.625403	-5.843667	2.631172
1	4.662768	-3.778171	0.373389
1	1.297335	-6.425788	0.564643
1	4.639189	-3.90626	-2.075185
1	1.273065	-6.568376	-1.893661
1	2.941832	-5.306117	-3.234562
1	3.380909	-1.911483	3.404702
7	3.142828	-1.749132	2.440498
6	3.420261	-0.431964	1.871986
6	2.085709	0.344014	1.787598
8	1.322141	0.319791	2.736402
6	4.24207	-0.549685	0.58343
6	5.624421	-1.126422	0.881124
16	6.505537	-1.450091	-0.676935
6	8.071708	-2.031367	0.028553
1	4.01147	0.102493	2.619589
1	3.706614	-1.174549	-0.137678
1	4.382409	0.440914	0.143358
1	6.205335	-0.418537	1.478691
1	5.534387	-2.056462	1.445825

1	8.729723	-2.280348	-0.802176
1	8.541052	-1.252344	0.629288
1	7.917499	-2.923892	0.635217
1	2.476857	0.947157	-0.138377
7	1.855991	1.044564	0.650268
6	0.571616	1.657935	0.373742
6	-0.23558	0.853736	-0.663748
8	-1.107097	1.394423	-1.334859
6	0.7242	3.097833	-0.103363
16	1.697034	3.226992	-1.646156
1	0.723682	2.742808	-2.434842
1	0.014146	1.640727	1.312756
1	-0.257286	3.53418	-0.2664
1	1.260532	3.67739	0.646165
1	0.855153	-0.804903	-0.17415
7	0.108026	-0.439458	-0.747656
6	-0.48777	-1.371219	-1.671589
6	-0.875716	-2.634642	-0.909048
8	-0.523532	-3.751329	-1.249571
6	0.490704	-1.713829	-2.805178
8	1.707552	-2.200311	-2.265095
6	0.831629	-0.486555	-3.629154
1	1.524869	-3.054727	-1.843795
1	-1.396342	-0.908512	-2.065208
1	0.01818	-2.473885	-3.436444
1	1.482553	-0.769596	-4.45602
1	-0.069341	-0.011505	-4.020774
1	1.365221	0.231807	-3.004548
1	-1.2512	-5.401196	0.51583
8	-1.618275	-2.39792	0.157921
1	-1.769796	-3.278173	0.62381

Cartesian coordinates of conformer **F3**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-0.169762	-8.790781	3.355693
7	-0.383157	-8.715631	2.365134
6	-0.638	-7.304873	2.06381
6	0.540887	-6.462333	2.547203
8	0.733987	-6.239765	3.736933
6	-1.926204	-6.880598	2.772696
6	-2.426619	-5.513734	2.371829
6	-3.412143	-5.383366	1.387556
6	-1.926932	-4.356949	2.974224
6	-3.911252	-4.129122	1.037571
6	-2.407873	-3.100969	2.613848
6	-3.411089	-2.982881	1.655906
1	-0.759559	-7.19521	0.984077
1	-2.676343	-7.639194	2.545073
1	-1.734564	-6.904261	3.848202
1	-3.806402	-6.273829	0.910936
1	-1.148781	-4.447656	3.721352
1	-4.687612	-4.047449	0.286857
1	-1.990108	-2.214581	3.07387
1	-3.788943	-2.00709	1.379469
1	1.084417	-5.995704	0.648083
7	1.439947	-6.094542	1.591833
6	2.507844	-5.206327	1.984614
6	1.92335	-3.83502	2.342194
8	0.857618	-3.451881	1.862723
6	3.517104	-5.085993	0.827804
6	4.735721	-4.253286	1.148603
6	5.073639	-3.167638	0.336439
6	5.551062	-4.557981	2.24346
6	6.187329	-2.382115	0.635694
6	6.664195	-3.775899	2.538791
6	6.980108	-2.677785	1.740269
1	2.984468	-5.628245	2.870245
1	3.812475	-6.102711	0.55547
1	3.012604	-4.649093	-0.036374
1	4.477547	-2.969697	-0.550961
1	5.324516	-5.42156	2.860409
1	6.441956	-1.544609	-0.002231
1	7.286123	-4.023009	3.39007
1	7.837023	-2.061464	1.9787
1	3.50617	-3.421196	3.555112
7	2.667436	-3.044766	3.141264
6	2.187148	-1.741704	3.575824
6	1.887578	-0.788133	2.416695
8	1.099941	0.129763	2.576784
6	3.203079	-1.097366	4.529081
6	4.565261	-0.863232	3.8755
16	5.811074	-0.192278	5.016156
6	5.222254	1.523944	5.108735
1	1.228563	-1.859151	4.084625
1	2.774532	-0.150014	4.859166
1	3.317752	-1.731647	5.411933
1	4.995023	-1.795651	3.504505
1	4.480819	-0.185451	3.023558

1	5.15001	1.949662	4.108081
1	4.259682	1.593407	5.61324
1	5.958679	2.084248	5.682449
1	3.268152	-1.732175	1.23709
7	2.560052	-1.010725	1.259712
6	2.284727	-0.251569	0.065108
6	1.897339	-1.172745	-1.099397
8	2.071456	-0.833214	-2.268391
6	3.425626	0.671564	-0.358468
16	3.896202	1.849204	0.956308
1	2.645015	2.110356	1.370412
1	1.404611	0.354408	0.297843
1	4.322265	0.090772	-0.579219
1	3.137299	1.198803	-1.263485
1	1.136775	-2.517706	0.237457
7	1.347656	-2.346453	-0.741508
6	0.784781	-3.234452	-1.745531
6	-0.229078	-4.120388	-1.027017
8	-0.118734	-5.321547	-0.892331
6	1.835234	-4.082615	-2.495718
8	3.067073	-3.400488	-2.623125
6	1.282696	-4.506986	-3.849665
1	2.872465	-2.498809	-2.930556
1	0.240154	-2.616078	-2.467109
1	2.04556	-4.973389	-1.905595
1	2.012339	-5.131423	-4.363895
1	0.355954	-5.073232	-3.733598
1	1.083569	-3.626655	-4.46641
1	0.442776	-9.029208	1.866514
8	-1.236739	-3.406871	-0.553533
1	-1.819696	-3.97009	-0.004876

Cartesian coordinates of conformer **F4**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-1.928717	-3.758031	1.808399
7	-2.140775	-3.481982	2.760315
6	-1.751679	-4.484569	3.733086
6	-0.251331	-4.756491	3.917685
8	0.165497	-5.479975	4.814674
6	-2.452588	-5.822479	3.428783
6	-2.084992	-6.35244	2.06397
6	-0.878014	-7.035096	1.869471
6	-2.912291	-6.12825	0.960755
6	-0.505712	-7.474616	0.600783
6	-2.549103	-6.576627	-0.30798
6	-1.343253	-7.247742	-0.492922
1	-2.093803	-4.157086	4.717651
1	-2.164148	-6.534512	4.202812
1	-3.528546	-5.654754	3.485959
1	-0.233881	-7.218574	2.72188
1	-3.843672	-5.592311	1.101676
1	0.438221	-7.985916	0.461362
1	-3.202017	-6.391128	-1.151264
1	-1.047115	-7.581428	-1.478721
1	0.170708	-3.634976	2.258981
7	0.565404	-4.153667	3.028333
6	2.008289	-4.267306	3.102527
6	2.500969	-3.038345	2.364035
8	2.297361	-2.939345	1.150439
6	2.547199	-5.541851	2.433031
6	4.051213	-5.491034	2.324402
6	4.65785	-5.211356	1.097294
6	4.855715	-5.655475	3.454305
6	6.042672	-5.106753	1.000032
6	6.240657	-5.548333	3.359778
6	6.837426	-5.271405	2.131569
1	2.297117	-4.252758	4.155227
1	2.217048	-6.390016	3.035753
1	2.101255	-5.622065	1.440378
1	4.031771	-5.084986	0.22103
1	4.394209	-5.885239	4.408904
1	6.500414	-4.899061	0.040832
1	6.853671	-5.691885	4.241433
1	7.915027	-5.193143	2.056704
1	3.154154	-2.123259	4.063751
7	3.057522	-2.045471	3.065325
6	3.245117	-0.751977	2.42974
6	1.885276	-0.339086	1.826458
8	0.847987	-0.600912	2.416404
6	4.435549	-0.752321	1.459117
6	5.666444	-1.434019	2.051201
16	6.139568	-0.668908	3.637376
6	7.4925	-1.799069	4.068388
1	3.441175	-0.04232	3.235364
1	4.165537	-1.284395	0.544655
1	4.675968	0.282464	1.200472
1	5.463023	-2.492557	2.219991
1	6.500355	-1.351041	1.352578



1	8.293953	-1.736368	3.332597
1	7.877227	-1.494752	5.040093
1	7.125477	-2.823383	4.126873
1	2.727679	0.201763	0.060382
7	1.918369	0.345519	0.651065
6	0.672983	0.618892	-0.064292
6	0.487487	-0.466661	-1.138403
8	0.352647	-0.19272	-2.326007
6	0.698527	1.996773	-0.708383
16	0.723075	3.342718	0.518295
1	1.811044	2.899749	1.169508
1	-0.126778	0.55572	0.673915
1	1.544431	2.083327	-1.389821
1	-0.204962	2.131669	-1.299788
1	0.830619	-1.848106	0.302528
7	0.554327	-1.729969	-0.661983
6	1.003356	-2.779878	-1.545686
6	0.76858	-4.148443	-0.930829
8	1.430674	-5.123336	-1.199597
6	2.510069	-2.636732	-1.936032
8	2.932508	-1.277091	-1.901638
6	2.772729	-3.245607	-3.304
1	2.415942	-0.798959	-2.568755
1	0.394924	-2.725676	-2.453927
1	3.103887	-3.133958	-1.172778
1	3.830863	-3.158039	-3.551152
1	2.487553	-4.296836	-3.315143
1	2.193473	-2.714095	-4.065343
1	-1.717585	-2.580039	2.943662
8	-0.27298	-4.195421	-0.086162
1	-0.370229	-5.133684	0.176619

Cartesian coordinates of conformer **F5**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-2.123028	-4.923819	1.946201
7	-2.313939	-5.030028	2.935626
6	-1.410151	-5.968188	3.569971
6	0.090285	-5.654883	3.517588
8	0.917054	-6.417836	4.009655
6	-1.617246	-7.380874	2.990337
6	-1.267525	-7.449183	1.523788
6	0.033226	-7.764284	1.118989
6	-2.224941	-7.169214	0.545405
6	0.370673	-7.793065	-0.230676
6	-1.891216	-7.203977	-0.805677
6	-0.591881	-7.514976	-1.197515
1	-1.656583	-6.014923	4.634077
1	-0.992767	-8.071832	3.55591
1	-2.665045	-7.643828	3.140912
1	0.776286	-7.988336	1.875649
1	-3.23709	-6.929666	0.851058
1	1.38216	-8.04013	-0.528708
1	-2.647022	-6.991237	-1.551974
1	-0.331007	-7.546762	-2.24817
1	-0.224551	-3.894927	2.474028
7	0.454094	-4.503184	2.908212
6	1.850981	-4.171988	2.788961
6	1.979557	-2.654202	2.729511
8	1.032399	-1.938147	2.398603
6	2.469447	-4.873644	1.551653
6	3.941045	-4.602115	1.37942
6	4.852364	-4.931402	2.389349
6	4.412363	-3.973932	0.223996
6	6.196114	-4.587133	2.269567
6	5.760048	-3.636192	0.10121
6	6.65117	-3.925547	1.130057
1	2.349776	-4.547239	3.68422
1	2.28513	-5.939086	1.70201
1	1.928734	-4.565724	0.655023
1	4.505695	-5.465561	3.268372
1	3.710575	-3.769095	-0.580691
1	6.890245	-4.844677	3.059921
1	6.117441	-3.148761	-0.797531
1	7.694722	-3.654773	1.036853
1	3.945621	-2.780002	3.246527
7	3.190442	-2.144268	3.033885
6	3.438725	-0.71182	3.067968
6	3.309707	-0.012763	1.717537
8	3.160731	1.199006	1.67757
6	4.829795	-0.434499	3.637832
6	4.945947	-0.674694	5.143517
16	3.718794	0.221304	6.149943
6	3.95662	1.9026	5.501485
1	2.681225	-0.242214	3.698449
1	5.564907	-1.053704	3.109932
1	5.076518	0.60216	3.408337
1	4.795086	-1.72761	5.390554
1	5.949834	-0.402128	5.473381

1	3.369608	2.56499	6.135423
1	5.004778	2.196579	5.564103
1	3.602185	1.991922	4.474222
1	3.640094	-1.776526	0.74864
7	3.377747	-0.808311	0.626621
6	3.14025	-0.311219	-0.704112
6	1.935641	-1.025177	-1.332231
8	1.812675	-1.13278	-2.551132
6	4.352158	-0.429116	-1.628313
16	5.862579	0.29938	-0.91417
1	5.313262	1.481368	-0.587962
1	2.875272	0.742772	-0.58494
1	4.587051	-1.478432	-1.811785
1	4.114372	0.022033	-2.58788
1	1.200255	-1.383624	0.544349
7	1.044026	-1.503897	-0.449533
6	-0.174743	-2.14514	-0.893115
6	-1.188148	-2.019782	0.233309
8	-1.749839	-2.942595	0.777664
6	0.008541	-3.619106	-1.322809
8	1.28605	-3.827503	-1.896201
6	-1.106372	-4.013227	-2.280844
1	1.435976	-3.122087	-2.547771
1	-0.552172	-1.570913	-1.74644
1	-0.031573	-4.25543	-0.437871
1	-0.96626	-5.04594	-2.593396
1	-2.082241	-3.923243	-1.799351
1	-1.08473	-3.372067	-3.166618
1	-2.278163	-4.112133	3.359853
8	-1.392547	-0.744534	0.570736
1	-1.995572	-0.741167	1.33244

Cartesian coordinates of conformer **W1**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-0.436785	3.681812	0.451404
7	0.044986	3.974495	-0.389705
6	-0.577548	3.349564	-1.558908
6	0.409156	3.364146	-2.729225
8	0.063277	3.203986	-3.900271
6	-1.941996	3.949091	-1.974944
6	-2.848534	2.949237	-2.618815
6	-3.047876	2.739826	-3.954285
6	-3.612126	1.938524	-1.939745
7	-3.884803	1.673268	-4.157765
6	-4.237595	1.151354	-2.94019
6	-3.813793	1.613423	-0.590227
6	-5.044357	0.054745	-2.622467
6	-4.612062	0.527455	-0.272068
6	-5.219184	-0.245941	-1.281282
1	-4.024571	1.253993	-5.071577
1	-0.731611	2.291989	-1.322417
1	-2.411069	4.331377	-1.062506
1	-1.779991	4.802541	-2.637487
1	-2.632213	3.280228	-4.788021
1	-3.352688	2.204138	0.194146
1	-5.515542	-0.53634	-3.397822
1	-4.777036	0.266063	0.765543
1	-5.838011	-1.089267	-1.002333
1	1.900382	3.63926	-1.388155
7	1.703135	3.531431	-2.376674
6	2.739052	3.710653	-3.366453
6	3.276328	2.41318	-3.976873
8	4.248629	2.448006	-4.719913
6	3.896293	4.546518	-2.830995
16	4.745169	3.779516	-1.407952
1	5.28532	2.772431	-2.113736
1	2.29326	4.238303	-4.216548
1	4.610623	4.711312	-3.633174
1	3.527078	5.509412	-2.480171
1	1.812189	1.333514	-3.049142
7	2.588234	1.288054	-3.693027
6	2.787236	0.072996	-4.446605
6	1.95544	0.02645	-5.729649
8	2.116951	-0.908139	-6.516947
6	2.445629	-1.162711	-3.592983
6	1.050386	-1.073335	-3.020605
6	-0.068224	-1.331067	-3.820969
6	0.851767	-0.669379	-1.698331
6	-1.353312	-1.178413	-3.311943
6	-0.436608	-0.53491	-1.182548
6	-1.542615	-0.784302	-1.988433
1	3.830079	0.03412	-4.760273
1	2.551341	-2.037919	-4.234709
1	3.178154	-1.234232	-2.787255
1	0.075996	-1.665169	-4.842764
1	1.713036	-0.477698	-1.066388
1	-2.211832	-1.369482	-3.944326
1	-0.578172	-0.239923	-0.149509

1	-2.542629	-0.677386	-1.590582
1	0.907645	1.723671	-5.226584
7	1.043867	0.995803	-5.921993
6	0.084316	0.913809	-7.020959
6	0.719333	1.519037	-8.286619
8	0.305774	2.562111	-8.797161
6	-1.189411	1.643652	-6.590726
6	-2.431116	1.321177	-7.410025
8	-3.446569	0.860752	-6.89046
7	-2.347463	1.572432	-8.72847
1	-3.17551	1.432475	-9.283221
1	-1.55632	2.087128	-9.094349
1	-0.110966	-0.146422	-7.202371
1	-1.410381	1.358722	-5.563676
1	-1.000573	2.719587	-6.624119
1	2.053702	-0.008732	-8.263061
7	1.764825	0.830417	-8.758476
6	2.58798	1.373274	-9.823263
6	3.511788	0.312659	-10.391619
8	4.402495	0.546978	-11.167634
6	3.373624	2.631388	-9.406597
6	4.031954	2.552946	-8.026401
6	4.964669	1.350603	-7.873655
6	4.794707	3.850335	-7.755854
1	1.927517	1.655046	-10.649383
1	4.128543	2.811094	-10.176342
1	2.674547	3.46869	-9.418037
1	3.244738	2.467454	-7.271264
1	4.42631	0.400628	-7.933062
1	5.4501	1.386831	-6.897016
1	5.735072	1.357851	-8.650088
1	5.182302	3.850809	-6.736476
1	5.634652	3.951804	-8.449264
1	4.147126	4.721908	-7.881933
1	-0.053257	4.983466	-0.447113
8	3.221474	-0.93393	-9.974317
1	3.871161	-1.521253	-10.393811

Cartesian coordinates of conformer **W2**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	4.626077	25.00781	-0.954438
7	3.914718	24.650104	-0.326587
6	3.283841	23.461362	-0.900887
6	2.524693	23.842188	-2.169139
8	1.481672	24.504126	-2.108156
6	2.304252	22.881535	0.121344
6	1.640645	21.617098	-0.333708
6	0.436986	21.505659	-0.976025
6	2.13049	20.27319	-0.17774
7	0.132271	20.185596	-1.205847
6	1.152812	19.403779	-0.727518
6	3.297045	19.722517	0.373975
6	1.318209	18.012327	-0.743815
6	3.46543	18.347655	0.357527
6	2.487412	17.501292	-0.201486
1	-0.655542	19.892573	-1.765743
1	4.057005	22.728283	-1.134067
1	2.859248	22.716041	1.046556
1	1.547001	23.64275	0.321331
1	-0.247445	22.283106	-1.275955
1	4.058458	20.366239	0.797825
1	0.55957	17.358035	-1.15799
1	4.363804	17.912596	0.776185
1	2.646104	16.430478	-0.199286
7	3.094449	23.506565	-3.344122
6	2.575879	24.005074	-4.613137
6	1.437213	23.107255	-5.125626
8	1.542493	22.441826	-6.160023
6	3.714574	24.110716	-5.619568
16	3.260762	24.984479	-7.154407
1	2.5721	23.961515	-7.680158
1	2.151898	24.993474	-4.422033
1	4.514736	24.698636	-5.170544
1	4.100808	23.123302	-5.860142
1	3.207093	25.373607	-0.238621
7	0.34207	23.127684	-4.345201
6	-0.9309	22.476548	-4.641818
6	-0.849881	20.956278	-4.456437
8	-1.465066	20.398698	-3.550866
6	-1.514183	22.876769	-6.01275
6	-1.721746	24.368191	-6.090896
6	-0.723537	25.191499	-6.612672
6	-2.885097	24.95289	-5.588682
6	-0.881716	26.573652	-6.630802
6	-3.049356	26.334364	-5.609747
6	-2.046227	27.148201	-6.129785
1	-1.621687	22.808163	-3.868237
1	-0.847209	22.545649	-6.807458
1	-2.465179	22.350551	-6.128005
1	0.18315	24.747607	-7.005811
1	-3.668356	24.320834	-5.183299
1	-0.093131	27.195975	-7.034797
1	-3.959302	26.774568	-5.221677
1	-2.173042	28.223243	-6.144874

7	-0.08539	20.303303	-5.358885
6	0.326354	18.924359	-5.152904
6	1.839875	18.983456	-4.982047
8	2.543	19.17682	-5.986677
6	-0.022171	18.046252	-6.34581
6	0.441216	16.625776	-6.073612
8	1.034607	16.331986	-5.046864
7	0.139544	15.718579	-7.032648
1	0.489029	14.781279	-6.924452
1	-0.264563	15.988788	-7.911398
1	-0.164462	18.557127	-4.254715
1	-1.099413	18.073475	-6.52169
1	0.483783	18.431478	-7.234278
7	2.306386	18.972784	-3.733714
6	3.71668	19.051104	-3.34786
6	4.281287	20.438918	-3.643997
8	4.792248	21.128295	-2.786025
6	4.561967	17.934849	-3.975503
6	6.049504	18.019508	-3.614994
6	6.27727	18.00898	-2.101882
6	6.791205	16.858312	-4.278514
1	3.727681	18.95971	-2.264296
1	4.147213	16.985207	-3.622897
1	4.44223	17.955942	-5.05984
1	6.450786	18.956113	-4.01943
1	7.345005	17.95542	-1.878915
1	5.880254	18.905262	-1.623086
1	5.793613	17.135897	-1.652478
1	7.863875	16.920972	-4.085996
1	6.432417	15.904228	-3.8824
1	6.637017	16.85472	-5.359664
8	4.196075	20.873209	-4.895497
1	3.687743	20.233741	-5.470308
1	1.661084	18.787902	-2.980829
1	0.499273	20.877675	-5.966507
1	0.401271	23.721073	-3.520392
1	3.888672	22.873947	-3.34299

Cartesian coordinates of conformer **W3**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	0.276701	4.137331	-5.070183
7	0.186911	4.77613	-4.285773
6	-0.216884	4.056154	-3.08225
6	1.005954	3.711147	-2.224244
8	0.897021	3.022351	-1.203004
6	-0.951569	2.72597	-3.319346
6	-2.16508	2.810771	-4.19093
6	-2.860112	3.896132	-4.644632
6	-2.834485	1.659602	-4.737672
7	-3.935121	3.495006	-5.411587
6	-3.916011	2.128931	-5.518382
6	-2.591015	0.282007	-4.652361
6	-4.735018	1.258121	-6.24582
6	-3.403915	-0.585698	-5.36279
6	-4.461566	-0.100809	-6.156931
1	-4.431702	4.101758	-6.039765
1	-0.846992	4.706916	-2.469342
1	-0.245821	2.027793	-3.783999
1	-1.199042	2.298346	-2.345713
1	-2.695046	4.946951	-4.471915
1	-1.772058	-0.093066	-4.050367
1	-5.549504	1.627586	-6.855958
1	-3.22262	-1.651987	-5.318739
1	-5.075202	-0.80073	-6.709356
1	2.083646	4.724629	-3.539662
7	2.175477	4.156254	-2.703942
6	3.482607	3.90888	-2.12045
6	4.025589	2.515655	-2.474088
8	5.161646	2.374196	-2.892379
6	3.559566	4.107681	-0.599567
16	2.984915	5.744801	-0.05001
1	1.677463	5.454015	-0.14288
1	4.171674	4.607418	-2.590208
1	2.99833	3.341292	-0.074553
1	4.608553	4.03643	-0.311579
1	2.25825	1.668971	-1.84746
7	3.16284	1.481574	-2.270225
6	3.54539	0.12578	-2.598329
6	3.068937	-0.317405	-3.982392
8	3.338808	-1.446825	-4.397989
6	3.052557	-0.88538	-1.54642
6	1.545926	-0.961493	-1.472495
6	0.844436	-1.882782	-2.25713
6	0.824028	-0.091366	-0.654273
6	-0.545809	-1.923364	-2.230192
6	-0.568146	-0.121588	-0.634087
6	-1.257219	-1.038061	-1.421467
1	4.635315	0.102439	-2.636551
1	3.463589	-1.857683	-1.817565
1	3.468644	-0.59299	-0.580543
1	1.399489	-2.571421	-2.883456
1	1.348247	0.622755	-0.029888
1	-1.075677	-2.648888	-2.836159
1	-1.106835	0.573965	-0.003385



1	-2.339703	-1.06464	-1.407715
1	2.201282	1.509995	-4.355224
7	2.343702	0.565541	-4.686361
6	1.93381	0.265696	-6.033481
6	1.28889	1.513993	-6.629298
8	1.183141	2.549024	-5.973908
6	0.943071	-0.929665	-6.108666
6	1.401834	-1.802641	-7.256215
8	1.087029	-1.554353	-8.417878
7	2.244835	-2.79334	-6.898111
1	2.728702	-3.275196	-7.638966
1	2.688844	-2.725913	-5.989961
1	2.823368	0.023357	-6.624739
1	0.96515	-1.467481	-5.164185
1	-0.073757	-0.587726	-6.30451
1	0.83204	0.43018	-8.287261
7	0.859599	1.372363	-7.893788
6	0.026324	2.388814	-8.502836
6	-1.415868	2.31063	-8.019209
8	-2.15742	3.262307	-7.966627
6	0.034034	2.242129	-10.029098
6	1.431189	2.304811	-10.656434
6	1.303425	2.199507	-12.176727
6	2.173899	3.582506	-10.266169
1	0.397827	3.367523	-8.208015
1	-0.443125	1.291589	-10.29081
1	-0.589502	3.042303	-10.439676
1	2.006733	1.445431	-10.299093
1	2.287227	2.183961	-12.64966
1	0.77169	1.291125	-12.467932
1	0.752454	3.057113	-12.573321
1	3.122706	3.650714	-10.801935
1	1.579404	4.464514	-10.523104
1	2.394971	3.617044	-9.197685
1	-0.482098	5.489025	-4.534612
8	-1.777711	1.054857	-7.737191
1	-2.701053	1.059703	-7.416213

Cartesian coordinates of conformer **W4**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	5.844679	24.267389	-1.095432
7	4.999424	24.17054	-0.544649
6	4.055932	23.270517	-1.210426
6	3.574919	23.915027	-2.507756
8	2.738829	24.826943	-2.496973
6	2.868104	23.030973	-0.275363
6	1.828709	22.102875	-0.829736
6	0.748351	22.445364	-1.598529
6	1.746023	20.676809	-0.646815
7	-0.011554	21.336126	-1.885414
6	0.582742	20.234608	-1.325922
6	2.542926	19.73561	0.021613
6	0.209088	18.886683	-1.371385
6	2.177146	18.400052	-0.017843
6	1.025497	17.978107	-0.713571
1	-0.758166	21.321385	-2.566164
1	4.568191	22.328878	-1.415755
1	3.271463	22.641961	0.660631
1	2.416669	24.002309	-0.061657
1	0.448776	23.423635	-1.939853
1	3.445143	20.042503	0.534568
1	-0.669862	18.559403	-1.911936
1	2.787228	17.664793	0.492194
1	0.767817	16.926709	-0.735068
7	4.187862	23.526998	-3.64661
6	3.949613	24.224144	-4.900139
6	2.710296	23.660402	-5.611877
8	2.791373	23.032075	-6.671452
6	5.17523	24.199712	-5.809111
16	5.89478	22.551537	-6.117838
1	4.822375	22.065166	-6.758744
1	3.728863	25.262796	-4.640039
1	4.92301	24.668537	-6.758481
1	5.971199	24.776968	-5.33989
1	4.575359	25.090648	-0.476675
7	1.556283	23.894571	-4.967852
6	0.24539	23.413188	-5.386486
6	0.032034	21.923774	-5.08922
8	-1.015336	21.537662	-4.571883
6	-0.108211	23.731966	-6.854244
6	-0.011019	25.209918	-7.139099
6	-1.030218	26.074438	-6.73606
6	1.111365	25.739645	-7.776663
6	-0.932243	27.442734	-6.965011
6	1.210979	27.108619	-8.009251
6	0.190542	27.963267	-7.6032
1	-0.47952	23.921647	-4.751627
1	0.549025	23.172326	-7.516156
1	-1.132204	23.381304	-7.006578
1	-1.910097	25.669629	-6.246762
1	1.904278	25.070304	-8.089683
1	-1.73254	28.100861	-6.650761
1	2.084189	27.507309	-8.510554
1	0.267248	29.027647	-7.785635

7	1.041044	21.101403	-5.42655
6	1.111554	19.739073	-4.944188
6	2.574238	19.506249	-4.570479
8	3.458593	19.988268	-5.30146
6	0.64741	18.733385	-6.000348
6	0.485839	17.344072	-5.40371
8	0.44303	17.151717	-4.197517
7	0.373508	16.340548	-6.304914
1	0.198309	15.41036	-5.963518
1	0.372441	16.507348	-7.295199
1	0.471456	19.645902	-4.069827
1	-0.326894	19.067336	-6.367412
1	1.341131	18.723721	-6.844774
7	2.813053	18.810721	-3.462166
6	4.138395	18.450213	-2.949914
6	4.928153	19.67431	-2.471404
8	5.375586	19.761529	-1.35639
6	4.951605	17.614443	-3.949104
6	6.361488	17.26739	-3.454891
6	6.33784	16.545982	-2.105884
6	7.066242	16.413975	-4.50993
1	3.947721	17.874288	-2.049111
1	4.390644	16.691587	-4.131304
1	5.015944	18.148001	-4.899037
1	6.924038	18.200577	-3.33865
1	7.341606	16.210074	-1.838049
1	5.98271	17.197307	-1.306368
1	5.691989	15.663573	-2.156719
1	8.093174	16.197178	-4.210197
1	6.544943	15.460967	-4.638279
1	7.092784	16.919254	-5.477834
8	5.139491	20.631913	-3.381857
1	4.695664	20.412107	-4.242017
1	2.010103	18.470763	-2.941689
1	1.85584	21.465528	-5.911998
1	1.634836	24.389758	-4.082987
1	4.777218	22.700892	-3.649806

Cartesian coordinates of conformer **W5**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	4.48749	25.307265	0.457937
7	3.658029	24.899883	0.876508
6	3.252036	23.719774	0.123917
6	2.813018	24.101814	-1.287715
8	1.93044	24.948117	-1.46864
6	2.085836	23.030419	0.840612
6	1.623031	21.817844	0.095922
6	0.523619	21.734122	-0.715032
6	2.296909	20.551215	-0.017961
7	0.456544	20.500563	-1.307964
6	1.534355	19.75322	-0.914096
6	3.474859	20.019193	0.530857
6	1.929392	18.458295	-1.280859
6	3.869311	18.742839	0.170014
6	3.106756	17.973116	-0.730202
1	-0.240067	20.27679	-2.003531
1	4.099823	23.032264	0.069767
1	2.414524	22.790298	1.853722
1	1.268171	23.751391	0.918479
1	-0.230523	22.474111	-0.930054
1	4.069023	20.603522	1.223395
1	1.34829	17.863811	-1.975826
1	4.779881	18.326895	0.580886
1	3.439789	16.976841	-0.993857
7	3.471662	23.522726	-2.307437
6	3.317903	23.988728	-3.670877
6	2.143928	23.28767	-4.371621
8	2.318719	22.462019	-5.270013
6	4.605	23.80478	-4.467552
16	6.00242	24.754799	-3.782636
1	5.488955	25.971534	-4.032561
1	3.066922	25.050197	-3.602367
1	4.924008	22.762863	-4.459927
1	4.43567	24.080468	-5.506129
1	2.918988	25.59109	0.783808
7	0.934549	23.685791	-3.935852
6	-0.332083	23.278714	-4.543034
6	-0.594281	21.782476	-4.321312
8	-1.200585	21.40863	-3.319284
6	-0.449526	23.749128	-6.003126
6	-1.800084	23.413186	-6.594416
6	-2.948822	24.055952	-6.128349
6	-1.925962	22.449911	-7.597189
6	-4.200278	23.741094	-6.64707
6	-3.177935	22.135907	-8.119749
6	-4.317715	22.777791	-7.645213
1	-1.112154	23.761115	-3.956109
1	-0.298454	24.831615	-5.996732
1	0.353242	23.322787	-6.605979
1	-2.863026	24.81674	-5.359452
1	-1.043722	21.939527	-7.967413
1	-5.080932	24.249958	-6.276153
1	-3.2599	21.392157	-8.902914
1	-5.290518	22.533426	-8.052659

7	-0.11771	20.938413	-5.253318
6	-0.245475	19.507271	-5.13391
6	1.055417	18.80525	-4.716245
8	1.05939	17.589904	-4.544268
6	-0.700951	18.883177	-6.464425
6	0.392232	19.086028	-7.496832
8	0.68821	20.204493	-7.905287
7	1.035809	17.967477	-7.89921
1	1.859911	18.086947	-8.467184
1	0.933581	17.110418	-7.381487
1	-0.992252	19.303423	-4.367813
1	-0.916306	17.828915	-6.300903
1	-1.600441	19.39794	-6.803674
7	2.148942	19.585535	-4.612331
6	3.469172	18.986596	-4.437295
6	4.380664	20.086294	-3.898804
8	5.36514	20.486425	-4.462948
6	4.008123	18.378405	-5.728933
6	5.30127	17.567384	-5.576
6	5.15822	16.457571	-4.530422
6	5.669638	16.966807	-6.93354
1	3.362718	18.214949	-3.672285
1	3.225432	17.71592	-6.109424
1	4.156076	19.184595	-6.452388
1	6.099318	18.246244	-5.269553
1	6.027294	15.796813	-4.554146
1	5.078228	16.852027	-3.514961
1	4.26719	15.854249	-4.729946
1	6.618843	16.430343	-6.879542
1	4.902158	16.256669	-7.25752
1	5.760935	17.742359	-7.697156
8	3.989177	20.641521	-2.740033
1	3.21129	20.187879	-2.359991
1	2.094935	20.557553	-4.905507
1	0.371257	21.296766	-6.064049
1	0.929476	24.298721	-3.123622
1	4.080366	22.733535	-2.140714

Cartesian coordinates of conformer **W6**, calculated at the M05-2X/6-31G\* level

atomic #	x	y	z
1	-0.282454	1.263165	-0.836207
7	-0.800867	2.08124	-1.143664
6	-1.156116	1.947929	-2.557675
6	0.045148	2.3224	-3.412426
8	0.213714	1.904044	-4.557784
6	-2.309749	2.92707	-2.864937
6	-2.831877	2.824274	-4.26037
6	-2.584983	3.670501	-5.303741
6	-3.662787	1.771919	-4.782562
7	-3.207329	3.213665	-6.441449
6	-3.872743	2.048177	-6.154851
6	-4.234553	0.617097	-4.224013
6	-4.626457	1.205772	-6.977968
6	-4.983856	-0.217387	-5.034399
6	-5.175532	0.074622	-6.398668
1	-3.160743	3.65492	-7.34177
1	-1.431183	0.934615	-2.8688
1	-3.117094	2.709515	-2.1568
1	-1.964124	3.942318	-2.651795
1	-1.995767	4.573953	-5.324319
1	-4.074542	0.37244	-3.181119
1	-4.771536	1.426008	-8.028154
1	-5.419396	-1.116891	-4.620031
1	-5.758681	-0.603212	-7.008324
1	0.706187	3.489049	-1.895455
7	0.9295	3.161456	-2.827337
6	2.092233	3.602036	-3.557918
6	3.043049	2.443334	-3.892365
8	3.835674	2.538382	-4.819722
6	2.888032	4.638656	-2.76768
16	1.946072	6.139663	-2.337284
1	1.708402	6.521878	-3.603013
1	1.797075	4.007438	-4.528923
1	3.207566	4.213688	-1.814146
1	3.780398	4.898219	-3.333627
1	2.249274	1.345569	-2.36868
7	2.971704	1.373109	-3.073004
6	3.739147	0.173113	-3.319674
6	3.216143	-0.683173	-4.483106
8	3.842132	-1.678808	-4.813471
6	3.877394	-0.658649	-2.033249
6	2.594574	-0.783285	-1.23787
6	1.408341	-1.233067	-1.827672
6	2.571978	-0.428469	0.11356
6	0.238752	-1.347263	-1.081308
6	1.407899	-0.551567	0.868101
6	0.238008	-1.01817	0.273476
1	4.733074	0.47531	-3.652484
1	4.245538	-1.641365	-2.334264
1	4.639676	-0.197881	-1.402909
1	1.366602	-1.496607	-2.876106
1	3.479408	-0.063933	0.581709
1	-0.658695	-1.686262	-1.5814
1	1.417023	-0.284194	1.917535

1	-0.667351	-1.119858	0.859645
1	1.516462	0.469839	-4.697921
7	2.099941	-0.249502	-5.1139
6	1.58233	-0.962855	-6.258778
6	1.17432	-0.008745	-7.384718
8	0.405397	-0.375849	-8.272417
6	0.443916	-1.931254	-5.902638
6	-0.725513	-1.21577	-5.245427
8	-0.838104	-1.153952	-4.02226
7	-1.601445	-0.660405	-6.101987
1	-2.322431	-0.063145	-5.725783
1	-1.369651	-0.605601	-7.082778
1	2.413291	-1.558418	-6.644077
1	0.12619	-2.434346	-6.815409
1	0.830529	-2.663818	-5.195591
1	2.296891	1.500932	-6.574726
7	1.751131	1.204529	-7.373629
6	1.484574	2.152789	-8.44275
6	2.625651	3.148035	-8.469462
8	3.323599	3.406194	-9.415017
6	0.144064	2.884578	-8.264989
6	-0.0688	4.004575	-9.292333
6	0.053792	3.496398	-10.731453
6	-1.432039	4.663028	-9.081865
1	1.497288	1.608724	-9.384431
1	-0.645594	2.13291	-8.355707
1	0.104682	3.279117	-7.245624
1	0.69822	4.771046	-9.131002
1	-0.225634	4.280419	-11.438632
1	1.07337	3.18882	-10.965667
1	-0.611592	2.642764	-10.891086
1	-1.569844	5.506325	-9.761081
1	-2.229977	3.941204	-9.288245
1	-1.538114	5.034096	-8.058407
1	-1.644066	2.11622	-0.582443
8	2.758263	3.742039	-7.266581
1	3.580597	4.257575	-7.275723