

Supporting Information

A. Cartesian coordinates of acetylene-linked bimane oligomers optimized with B3LYP/6-31G*.

Dimer

C	-1.722325	0.250485	0.361951
C	-1.900504	1.544543	-0.055650
C	-0.646630	1.987907	-0.741518
C	1.504444	0.381908	-1.036431
C	1.529918	-1.001713	-0.531885
C	0.346309	-1.277958	0.072285
C	-5.127475	3.904140	0.381034
C	-5.305405	5.198365	-0.036141
C	-6.381413	3.460819	1.066802
C	-7.371377	6.729167	0.259590
C	-8.529675	5.069264	1.368060
C	-8.553468	6.454306	0.867345
C	-3.031500	2.358573	0.102610
C	-3.996614	3.089962	0.222553
H	-0.011515	-2.175608	0.557639
H	-2.395152	-0.410511	0.889548
H	-4.632347	5.859488	-0.563285
H	-7.012940	7.627298	-0.224421
H	-9.398259	7.115315	0.984539
H	2.376757	-1.660922	-0.644329
O	2.325569	1.041034	-1.631700
O	-0.357358	3.038695	-1.262420
O	-6.670554	2.410236	1.588186
O	-9.349998	4.410882	1.965256
N	-7.223136	4.608476	0.972382
N	-6.559970	5.619628	0.316935
N	-0.468141	-0.171053	0.007894
N	0.194693	0.839882	-0.648192

Trimer

C	-1.715749	0.264990	0.439227
C	-1.894564	1.558083	0.014456
C	-0.634309	2.007150	-0.651723

C	1.529772	0.428115	-0.891684
C	1.572672	-0.971932	-0.370428
C	0.359605	-1.249229	0.209071
C	-5.133920	3.909851	0.385772
C	-5.306713	5.201920	-0.041486
C	-6.398922	3.467817	1.051994
C	-7.387750	6.722935	0.188471
C	-8.563290	5.066683	1.284574
C	-8.585211	6.444275	0.762868
C	-3.030414	2.367699	0.150292
C	-3.999112	3.097659	0.251234
C	4.804599	-3.337810	-0.715899
C	4.858515	-4.739719	-0.195171
C	6.014554	-3.052128	-1.295553
C	7.053267	-6.297604	-0.418191
C	8.110307	-4.555915	-1.502589
C	8.290798	-5.827766	-1.065047
C	2.691957	-1.807528	-0.484691
C	3.681928	-2.505941	-0.601205
H	0.007487	-2.149161	0.692589
H	-2.392876	-0.398047	0.958395
H	-4.626015	5.861084	-0.561247
H	-7.023599	7.617383	-0.298063
H	-9.439811	7.098012	0.844432
H	6.360566	-2.148839	-1.777571
H	8.778607	-3.879899	-2.018074
H	9.180601	-6.431294	-1.156805
O	2.359681	1.088303	-1.468445
O	-0.337864	3.056509	-1.169628
O	-6.696421	2.418576	1.570844
O	-9.396374	4.407767	1.862745
O	4.031379	-5.401671	0.384704
O	6.764467	-7.346880	0.109169
N	-7.238314	4.615927	0.942028
N	-6.565658	5.624071	0.291484
N	-0.455456	-0.153624	0.105175
N	0.212033	0.860107	-0.544716
N	6.174172	-5.163480	-0.547927
N	6.833400	-4.144738	-1.195738

Tetramer

C	-0.117740	-0.450445	-0.885394
C	-0.144377	0.902905	-0.658610
C	1.265938	1.380656	-0.527788
C	3.386082	-0.263018	-0.725865
C	3.251929	-1.730219	-0.976449
C	1.914785	-2.026374	-1.075845
C	-3.325778	3.342452	-0.361538
C	-3.350415	4.695244	-0.135109
C	-4.738737	2.867073	-0.490375
C	-5.393778	6.272088	0.054566
C	-6.861600	4.524649	-0.290533
C	-6.712868	5.969744	-0.045119
C	-1.260628	1.744048	-0.557062
C	-2.208711	2.501528	-0.463457
C	6.405077	-4.204737	-1.272083
C	6.271187	-5.672030	-1.522282
C	7.742178	-3.908268	-1.173052
C	8.391674	-7.315229	-1.720799
C	9.775017	-5.483717	-1.363998
C	9.801917	-6.837082	-1.590663
C	10.918391	-7.677875	-1.692664
C	11.866732	-8.434954	-1.786891
C	12.984101	-9.275387	-1.889551
C	13.009199	-10.628252	-2.115501
C	14.396949	-8.799221	-1.762411
C	15.053369	-12.203287	-2.311564
C	16.520633	-10.454932	-1.968719
C	16.372511	-11.899690	-2.216439
C	4.343438	-2.602266	-1.081292
C	5.313436	-3.332856	-1.167224
H	1.421436	-2.971451	-1.252281
H	-0.929148	-1.148885	-1.031743
H	-2.537616	5.392610	0.009979
H	-4.891372	7.213558	0.229437
H	-7.547675	6.648597	0.036174
H	8.235362	-2.963039	-0.996968
H	10.586305	-4.785042	-1.218109
H	12.196624	-11.326054	-2.259745
H	14.551329	-13.144925	-2.486589
H	17.207723	-12.577479	-2.302321
O	4.360565	0.432437	-0.572502

O	1.717536	2.481634	-0.326035
O	-5.188327	1.764421	-0.691971
O	-7.837153	3.826713	-0.443975
O	5.296822	-6.367721	-1.675322
O	7.940281	-8.416342	-1.922267
O	14.846189	-7.696096	-1.562586
O	17.496051	-9.756124	-1.818381
N	-5.497265	4.062218	-0.314298
N	-4.649579	5.125510	-0.106583
N	1.182138	-0.881922	-0.912105
N	2.028278	0.184023	-0.702626
N	7.629083	-6.118791	-1.545656
N	8.475036	-5.052601	-1.336673
N	14.308519	-11.058052	-2.144036
N	15.155850	-9.994281	-1.937302

Pentamer

C	-1.751590	0.268800	0.410891
C	-1.911180	1.569295	0.002366
C	-0.658025	1.995943	-0.692305
C	1.465979	0.373850	-0.993852
C	1.491792	-1.029665	-0.480948
C	0.284997	-1.286689	0.121828
C	-5.079364	3.996056	0.486171
C	-5.230482	5.297077	0.077938
C	-6.335093	3.579731	1.185539
C	-7.249841	6.879578	0.414871
C	-8.434877	5.242663	1.529829
C	-8.428083	6.632516	1.040830
C	-3.023142	2.404299	0.175815
C	-3.970235	3.156863	0.310272
C	4.674659	-3.447860	-0.897317
C	4.712794	-4.851509	-0.384461
C	5.880702	-3.178467	-1.495451
C	6.865890	-6.442008	-0.651387
C	7.944229	-4.702694	-1.751257
C	8.123447	-5.995535	-1.325164
C	9.259285	-6.803706	-1.464303
C	10.232126	-7.528154	-1.568364
C	11.374255	-8.327513	-1.706920

C	11.566108	-9.619459	-1.282582
C	12.629571	-7.865672	-2.373695
C	13.658780	-11.110057	-1.506044
C	14.811753	-9.420212	-2.606346
C	14.870598	-10.818381	-2.080376
C	2.592297	-1.885250	-0.620636
C	3.568221	-2.599831	-0.758498
C	18.140819	-13.134201	-2.401365
C	19.349444	-12.829055	-2.974186
C	18.215367	-14.533748	-1.876928
C	21.472409	-14.296296	-3.163195
C	20.438535	-16.053404	-2.081095
C	21.672226	-15.563339	-2.720545
C	16.002246	-11.638062	-2.186377
C	17.003953	-12.320791	-2.295362
H	-0.074581	-2.182101	0.608292
H	-2.429839	-0.383345	0.942219
H	-4.547683	5.944516	-0.453711
H	-6.874357	7.771531	-0.067611
H	-9.251923	7.315727	1.178286
H	6.233782	-2.278602	-1.978392
H	8.620026	-4.040983	-2.273841
H	10.896147	-10.289104	-0.762547
H	13.316256	-12.012771	-1.020857
H	19.682932	-11.920986	-3.456093
H	22.132250	-13.609918	-3.675875
H	22.573223	-16.151213	-2.804028
O	2.297203	1.021327	-1.582642
O	-0.350666	3.043518	-1.206942
O	-6.642976	2.534223	1.705826
O	-9.262631	4.603214	2.136597
O	3.887491	-5.505957	0.204519
O	6.571951	-7.488924	-0.128018
O	12.915642	-6.812982	-2.890286
O	15.636168	-8.750784	-3.179869
O	17.396132	-15.208375	-1.300487
O	20.164889	-17.106002	-1.552500
N	-7.149645	4.748054	1.105880
N	-6.469432	5.746163	0.447617
N	-0.510235	-0.175956	0.039035
N	0.163255	0.828260	-0.619621

N	6.019034	-5.295181	-0.760228
N	6.685542	-4.283033	-1.413928
N	12.828986	-10.025566	-1.618695
N	13.486084	-9.005352	-2.269266
N	20.185894	-13.907120	-2.866869
N	19.540149	-14.935636	-2.220861

Hexamer

C	-1.702571	0.288832	0.480822
C	-1.904209	1.581950	0.067774
C	-0.641786	2.069914	-0.567274
C	1.558989	0.540669	-0.798783
C	1.621233	-0.867801	-0.302977
C	0.407096	-1.177082	0.259350
C	-5.217975	3.834318	0.393609
C	-5.421272	5.128461	-0.013762
C	-6.486016	3.337861	1.014035
C	-7.564615	6.567631	0.162996
C	-8.715375	4.851253	1.190980
C	-8.772656	6.232919	0.682385
C	-3.063299	2.360313	0.187925
C	-4.054657	3.060954	0.275802
C	4.876606	-3.196708	-0.663643
C	4.931897	-4.598602	-0.147135
C	6.085382	-2.908225	-1.246996
C	7.100917	-6.165640	-0.415056
C	8.164803	-4.411142	-1.504985
C	8.351419	-5.708060	-1.094436
C	9.483753	-6.516779	-1.256346
C	10.446976	-7.250721	-1.381295
C	11.570043	-8.071688	-1.546422
C	11.748061	-9.362600	-1.113698
C	12.810682	-7.645879	-2.263372
C	13.781511	-10.915849	-1.427012
C	14.932122	-9.267155	-2.591249
C	14.968456	-10.668125	-2.070748
C	2.753011	-1.684778	-0.422569
C	3.750794	-2.371746	-0.543254
C	18.093224	-13.142135	-2.586965
C	19.271520	-12.920516	-3.256545

C	18.123002	-14.532960	-2.040844
C	21.263283	-14.519254	-3.614332
C	20.200549	-16.199630	-2.413071
C	21.421497	-15.812940	-3.184403
C	22.506654	-16.673400	-3.398412
C	23.430274	-17.448049	-3.566515
C	24.510699	-18.314774	-3.782921
C	24.663208	-19.604511	-3.340761
C	25.726719	-17.947949	-4.574087
C	26.628584	-21.237877	-3.747181
C	27.770543	-19.663581	-4.990003
C	27.770104	-21.035303	-4.452144
C	16.056055	-11.533896	-2.244540
C	17.014259	-12.265577	-2.413472
H	0.065952	-2.092464	0.721327
H	-2.373878	-0.397342	0.976940
H	-4.748751	5.819412	-0.501961
H	-7.218133	7.481628	-0.299512
H	-9.656429	6.849900	0.734041
H	6.428706	-2.004557	-1.729856
H	8.833027	-3.742528	-2.028535
H	11.081239	-10.011834	-0.564575
H	13.432956	-11.807565	-0.926011
H	19.619755	-12.043637	-3.783352
H	21.922919	-13.892646	-4.197314
H	24.003835	-20.219529	-2.744914
H	26.268350	-22.105179	-3.211114
H	28.572038	-21.738645	-4.615227
O	2.381627	1.225086	-1.357004
O	-0.362068	3.131586	-1.068498
O	-6.763952	2.268104	1.500812
O	-9.544862	4.150602	1.723245
O	4.108465	-5.267291	0.428292
O	6.812989	-7.220705	0.095220
O	13.099452	-6.607599	-2.806470
O	15.744163	-8.629201	-3.215601
O	17.312455	-15.151924	-1.395322
O	19.902699	-17.229415	-1.858546
O	26.020615	-16.926513	-5.147563
O	28.570457	-19.061342	-5.667996
N	-7.357625	4.461865	0.906967

N	-6.700886	5.503925	0.294535
N	-0.424332	-0.094044	0.170079
N	0.231700	0.944014	-0.452792
N	6.252938	-5.017814	-0.497067
N	6.909717	-3.997322	-1.147689
N	12.991012	-9.799270	-1.485051
N	13.648240	-8.800812	-2.168590
N	20.052584	-14.042021	-3.185572
N	19.398190	-15.017940	-2.467740
N	25.866769	-20.091675	-3.773472
N	26.521975	-19.130340	-4.507472

Heptamer

C	-1.752248	0.326406	0.389378
C	-1.854794	1.666210	0.110281
C	-0.546441	2.126882	-0.447459
C	1.557654	0.484128	-0.776039
C	1.516284	-0.965712	-0.415952
C	0.265147	-1.248925	0.074330
C	-4.999575	4.116819	0.625231
C	-5.093250	5.458019	0.352087
C	-6.312713	3.663021	1.181024
C	-7.101103	7.050722	0.709606
C	-8.399916	5.336934	1.548128
C	-8.328867	6.770334	1.214599
C	-2.958728	2.509767	0.293229
C	-3.897537	3.270394	0.439830
C	4.663009	-3.422235	-0.879693
C	4.635428	-4.870282	-0.508860
C	5.909536	-3.131715	-1.375953
C	6.758653	-6.493440	-0.815416
C	7.944281	-4.687424	-1.670251
C	8.063801	-6.022296	-1.371226
C	9.182529	-6.849513	-1.534343
C	10.138089	-7.592698	-1.663393
C	11.261095	-8.413620	-1.828660
C	11.394832	-9.745526	-1.523136
C	12.558341	-7.933620	-2.395745
C	13.444949	-11.281955	-1.815905
C	14.696443	-9.536111	-2.701249

C	14.686886	-10.981038	-2.317908
C	2.604008	-1.834435	-0.573432
C	3.570326	-2.559691	-0.722706
C	17.881383	-13.376759	-2.771901
C	19.116593	-13.066063	-3.284847
C	17.889155	-14.819501	-2.381029
C	21.180426	-14.582051	-3.583689
C	20.042749	-16.401182	-2.692339
C	21.330863	-15.910378	-3.271163
C	22.463536	-16.717145	-3.440681
C	23.432246	-17.441981	-3.575875
C	24.569779	-18.241066	-3.749225
C	24.735234	-19.567153	-3.432530
C	25.848517	-17.740612	-4.339048
C	26.812359	-21.064822	-3.739149
C	28.014225	-19.302555	-4.658864
C	28.040049	-20.743645	-4.261626
C	29.160221	-21.570312	-4.421440
C	30.152451	-22.258250	-4.575165
C	31.277292	-23.079319	-4.736057
C	31.321020	-24.520026	-4.333970
C	32.498846	-22.747411	-5.265008
C	33.520862	-26.055971	-4.641651
C	34.599185	-24.230795	-5.554492
C	34.771375	-25.534776	-5.221021
C	15.791466	-11.829072	-2.469972
C	16.771846	-12.535696	-2.616947
H	-0.147320	-2.179723	0.436569
H	-2.480250	-0.357863	0.800964
H	-4.359542	6.139482	-0.054508
H	-6.672499	7.978554	0.356355
H	-9.147781	7.457124	1.363176
H	6.313253	-2.199808	-1.745026
H	8.665984	-3.998822	-2.085778
H	10.682643	-10.438498	-1.098580
H	13.053267	-12.215103	-1.437091
H	19.495813	-12.130823	-3.671137
H	21.882234	-13.883970	-4.017044
H	24.043160	-20.270055	-2.991295
H	26.445385	-22.001948	-3.345771
H	32.854182	-21.807168	-5.662160

H	35.277455	-23.514747	-5.997867
H	35.663283	-26.129470	-5.344314
O	2.441690	1.164975	-1.236187
O	-0.181303	3.212978	-0.826554
O	-6.680116	2.576430	1.559042
O	-9.284382	4.659039	2.017588
O	3.759524	-5.554531	-0.038992
O	6.406752	-7.578305	-0.420954
O	12.897782	-6.847443	-2.797449
O	15.563424	-8.845445	-3.178397
O	17.032957	-15.516444	-1.893639
O	19.718123	-17.488373	-2.281445
O	26.160248	-16.651809	-4.756390
O	28.860020	-18.598947	-5.155064
O	30.482635	-25.227300	-3.828574
O	33.222140	-27.145324	-4.210016
N	-7.094895	4.855854	1.171929
N	-6.346975	5.899568	0.678322
N	-0.496902	-0.112440	0.059328
N	0.243001	0.935259	-0.441590
N	5.951717	-5.313643	-0.847875
N	6.681251	-4.262833	-1.357562
N	12.659720	-10.160567	-1.843118
N	13.375615	-9.105927	-2.364138
N	19.912957	-14.178968	-3.258007
N	19.211934	-15.238159	-2.726175
N	26.003157	-19.959298	-3.765729
N	26.689991	-18.895692	-4.307011
N	32.643651	-24.914213	-4.694560
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Octamer

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C	-5.122611	5.412372	0.550785

C	-6.377078	3.573116	1.213956
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C	-8.478938	5.226921	1.590217
C	-8.394272	6.677419	1.345480
C	-2.989283	2.467935	0.391979
C	-3.933476	3.219781	0.548932
C	4.675100	-3.390375	-0.870063
C	4.629638	-4.862141	-0.611171
C	5.942947	-3.068535	-1.286557
C	6.763191	-6.466501	-0.943949
C	7.987551	-4.606198	-1.606126
C	8.092457	-5.960241	-1.403494
C	9.216588	-6.777824	-1.577605
C	10.175709	-7.514304	-1.718132
C	11.302353	-8.328515	-1.891681
C	11.413485	-9.681733	-1.688192
C	12.629818	-7.816126	-2.350330
C	13.468341	-11.208093	-1.997636
C	14.773620	-9.408343	-2.672499
C	14.736569	-10.879209	-2.408167
C	2.605189	-1.822287	-0.537072
C	3.576989	-2.537781	-0.697454
C	17.929198	-13.273264	-2.883370
C	19.197356	-12.944217	-3.293980
C	17.892336	-14.744152	-2.619114
C	21.252450	-14.470241	-3.603360
C	20.036401	-16.336054	-2.941289
C	21.363822	-15.823427	-3.399811
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C	32.427766	-22.871775	-5.341347

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C	35.661691	-26.613318	-5.675785
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H	10.676749	-10.400025	-1.358131
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H	21.989078	-13.751808	-3.933355
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H	32.854675	-21.919270	-5.620997
H	35.202231	-23.717087	-6.009964
H	37.047229	-30.259465	-5.498455
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O	-9.383954	4.523561	1.975496
O	3.732823	-5.576167	-0.234284
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O	12.994903	-6.704234	-2.644734
O	15.668024	-8.689488	-3.046078
O	16.998055	-15.463114	-2.245451
O	19.671515	-17.448004	-2.646858

O	26.273106	-16.574003	-4.642535
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C	8.032363	-6.637153	-1.313269
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C	23.412371	-19.558059	-3.358922
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C	25.863100	-19.866878	-3.999949
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C	28.039752	-22.783032	-4.114741
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C	37.783796	-27.716809	-6.144349
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H	29.653031	-25.282876	-4.157100
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O	16.370426	-9.924170	-3.075131
O	19.046712	-11.906103	-3.473916
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O	23.045993	-20.668590	-3.061021

O	29.642502	-19.821043	-5.084137
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O	33.526614	-28.630069	-4.737970
O	36.153419	-30.665960	-5.183685
O	42.742077	-29.927428	-7.276583
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Decamer

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C	9.276465	-6.259075	-1.689687

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C	11.445056	-9.136489	-1.799297
C	12.574472	-9.947661	-1.968990
C	13.537047	-10.680237	-2.106217
C	14.666497	-11.491366	-2.275884
C	14.777955	-12.845473	-2.078220
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C	16.835228	-14.368672	-2.385593
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N	-3.161830	2.530715	0.322565
N	-3.924508	1.450753	0.707581
N	-10.355905	6.647763	1.756863
N	-9.584653	7.721320	1.371227
N	-16.946806	11.605950	2.961929
N	-16.168167	12.672159	2.575661

Dodecamer

C	1.503348	-2.827051	-0.018860
C	1.400641	-1.469151	-0.193680
C	2.737973	-0.951661	-0.616535
C	4.881457	-2.544830	-0.936718
C	4.834250	-4.021232	-0.706842
C	3.557807	-4.354190	-0.326292
C	0.273705	-0.654895	-0.022329
C	8.025800	-6.416893	-1.180965
C	7.978602	-7.893292	-0.951070
C	9.302238	-6.083934	-1.561532
C	10.122007	-9.486503	-1.271551
C	11.356626	-7.611116	-1.869249
C	11.459284	-8.969044	-1.694613
C	12.586135	-9.783347	-1.866286
C	13.545265	-10.519947	-2.006068
C	14.670049	-11.337057	-2.178070
C	14.767805	-12.695424	-2.003672
C	16.008810	-10.824536	-2.602230
C	16.814379	-14.231195	-2.319042
C	18.144429	-12.426980	-2.930734
C	18.090713	-13.903745	-2.704523
C	5.939667	-4.866323	-0.868835
C	6.920377	-5.571814	-1.018955
C	21.258993	-16.325387	-3.202221
C	22.537207	-16.006503	-3.589047
C	21.195357	-17.801800	-2.976965
C	24.569955	-17.558163	-3.918836
C	23.315896	-19.420306	-3.320377
C	24.656116	-18.918233	-3.752685
C	25.769866	-19.747103	-3.939535
C	26.716490	-20.497072	-4.092858

C 27.826277 -21.331065 -4.280666
C 27.903129 -22.691979 -4.114738
C 29.168795 -20.838620 -4.715924
C 29.919939 -24.260273 -4.460834
C 31.273387 -22.475035 -5.076491
C 31.197171 -23.952144 -4.858479
C 32.279924 -24.821091 -5.045948
C 33.239030 -25.550777 -5.218345
C 34.316869 -26.425728 -5.406319
C 34.230428 -27.901706 -5.188752
C 35.596121 -26.126698 -5.806422
C 36.318611 -29.554173 -5.567016
C 37.598019 -27.711369 -6.169704
C 37.662169 -29.073182 -6.012736
C 38.759195 -29.920626 -6.217927
C 39.691044 -30.685116 -6.387092
C 40.786202 -31.535623 -6.593412
C 40.842734 -32.897204 -6.435166
C 42.133184 -31.063687 -7.042906
C 42.842356 -34.494223 -6.819152
C 44.211459 -32.742495 -7.439077
C 44.101480 -34.196557 -7.227866
C 19.190058 -14.755191 -2.874495
C 20.163835 -15.468689 -3.031745
C -0.685487 0.081666 0.117245
C -1.810363 0.898700 0.288998
C -1.908206 2.257042 0.114448
C -3.149136 0.386115 0.713038
C -3.954867 3.792720 0.429701
C -5.284843 1.988463 1.041431
C -5.231164 3.465236 0.815277
C -6.330501 4.316668 0.985377
C -7.304255 5.030161 1.142788
C -8.399391 5.886855 1.313424
C -9.677564 5.567963 1.700377
C -8.335762 7.363284 1.088259
C -11.710226 7.119641 2.030607
C -10.456210 8.981809 1.432138
C -11.796369 8.479733 1.864638
C -12.910048 9.308627 2.051805
C -13.856593 10.058624 2.205486

C	-14.966280	10.892664	2.393666
C	-16.308713	10.400265	2.829225
C	-15.043070	12.253609	2.227945
C	-18.413216	12.036731	3.190115
C	-17.059788	13.821953	2.574365
C	-18.337022	13.513824	2.972011
C	-19.419780	14.382773	3.159444
C	-20.378884	15.112459	3.331855
C	-21.456698	15.987433	3.519853
C	-21.370183	17.463430	3.302408
C	-22.735967	15.688437	3.919920
C	-23.458329	19.115949	3.680649
C	-24.737833	17.273156	4.283168
C	-24.801941	18.634973	4.126227
C	-25.898958	19.482444	4.331360
C	-26.830785	20.246962	4.500530
C	-27.925904	21.097529	4.706822
C	-27.982294	22.459127	4.548629
C	-29.272922	20.625710	5.156286
C	-29.982189	24.056158	4.931181
C	-31.351491	22.304526	5.550943
C	-31.241637	23.758483	5.338880
H	3.133656	-5.315643	-0.074535
H	0.758219	-3.549748	0.281413
H	9.726380	-5.122483	-1.813313
H	12.101738	-6.888433	-2.169593
H	14.020070	-13.415346	-1.703198
H	16.386412	-15.191227	-2.068331
H	22.971362	-15.049439	-3.840484
H	25.321725	-16.843724	-4.222268
H	27.146468	-23.400937	-3.810547
H	29.478462	-25.214423	-4.211174
H	36.043584	-25.175682	-6.057551
H	38.358498	-27.008386	-6.478066
H	40.078065	-33.595243	-6.125247
H	42.381382	-35.439406	-6.567220
H	44.918282	-34.884052	-7.384561
H	-1.160485	2.976995	-0.185986
H	-3.526933	4.752772	0.179013
H	-10.111702	4.610891	1.951813
H	-12.461963	6.405192	2.334100

H	-14.286440	12.962544	1.923625
H	-16.618334	14.776094	2.324630
H	-23.183485	14.737423	4.170961
H	-25.498355	16.570177	4.591433
H	-27.217562	23.157081	4.238675
H	-29.521199	25.001272	4.679014
H	-32.058739	24.445892	5.494378
O	5.784993	-1.821433	-1.278053
O	3.112144	0.165148	-0.879115
O	7.075066	-8.616693	-0.609740
O	9.747807	-10.603325	-1.009069
O	16.386817	-9.709217	-2.865666
O	19.049879	-11.707391	-3.274970
O	20.284919	-18.515556	-2.633528
O	22.929077	-20.533646	-3.061377
O	29.562792	-19.728312	-4.977361
O	32.187059	-21.768794	-5.426569
O	33.311860	-28.602111	-4.838802
O	35.915359	-30.662279	-5.309925
O	42.538396	-29.956195	-7.303346
O	45.131812	-32.045035	-7.797829
O	-3.527071	-0.729198	0.976602
O	-6.190234	1.268855	1.385778
O	-7.425346	8.077052	0.744786
O	-10.069396	10.095170	1.173214
O	-16.702750	9.289943	3.090545
O	-19.326898	11.330484	3.540153
O	-20.451582	18.163812	2.952497
O	-23.055040	20.224050	3.423596
O	-29.678329	19.518226	5.416456
O	-32.272101	21.607080	5.909062
N	2.784719	-3.224783	-0.291487
N	3.543010	-2.132544	-0.649610
N	9.317078	-8.305556	-1.238061
N	10.075356	-7.213325	-1.596236
N	16.047397	-13.097823	-2.276957
N	16.809670	-12.008395	-2.635201
N	23.296617	-17.144810	-3.631189
N	22.527361	-18.228951	-3.271819
N	29.172607	-23.114091	-4.403392
N	29.949342	-22.035569	-4.763531

N	35.551452	-28.349801	-5.501465
N	36.334984	-27.277010	-5.863757
N	42.102482	-33.336087	-6.740889
N	42.891965	-32.270034	-7.104921
N	-3.187885	2.659355	0.387458
N	-3.950122	1.569896	0.745683
N	-10.436959	6.706275	1.742662
N	-9.667734	7.790429	1.383265
N	-17.089113	11.597291	2.877357
N	-16.312405	12.675795	2.517112
N	-22.691169	17.911572	3.615204
N	-23.474762	16.838787	3.977380
N	-29.241900	22.898168	4.854686
N	-30.031466	21.832197	5.218762

B. Cartesian coordinates of acetylene-linked bimane oligomers optimized with B3LYP/6-311G*.

Dimer

C	-1.726108	0.258474	0.354589
C	-1.904389	1.549494	-0.060976
C	-0.652964	1.993706	-0.749530
C	1.503609	0.383030	-1.037519
C	1.524034	-0.996974	-0.524356
C	0.339746	-1.269400	0.073183
C	-5.123441	3.899370	0.386323
C	-5.301624	5.190531	-0.028832
C	-6.374831	3.455084	1.074914
C	-7.365023	6.720552	0.258644
C	-8.528818	5.068004	1.369267
C	-8.547795	6.449379	0.859755
C	-3.032831	2.362351	0.099942
C	-3.995125	3.086407	0.225066
H	-0.018338	-2.163824	0.560791
H	-2.398034	-0.400252	0.883075
H	-4.629619	5.849406	-0.557032
H	-7.006483	7.615465	-0.227729
H	-9.392115	7.110109	0.968297
H	2.370221	-1.656043	-0.628378
O	2.323886	1.034239	-1.626875

O	-0.367011	3.038879	-1.265913
O	-6.660613	2.409986	1.591539
O	-9.348284	4.417425	1.960451
N	-7.215747	4.606163	0.985186
N	-6.552763	5.613628	0.328503
N	-0.475234	-0.164910	-0.003319
N	0.187617	0.842335	-0.660427

Trimer

C	-1.707014	0.273513	0.440296
C	-1.889709	1.562030	0.014936
C	-0.633735	2.013932	-0.656216
C	1.534520	0.431000	-0.898892
C	1.574232	-0.966807	-0.373010
C	0.365072	-1.238968	0.208589
C	-5.125447	3.899371	0.391221
C	-5.299775	5.186829	-0.038194
C	-6.387934	3.456982	1.060727
C	-7.377816	6.707268	0.182694
C	-8.557641	5.060444	1.285243
C	-8.574382	6.433997	0.754081
C	-3.024980	2.368003	0.152537
C	-3.992005	3.089476	0.256757
C	4.791060	-3.335308	-0.715023
C	4.844318	-4.734662	-0.188973
C	5.996851	-3.053019	-1.296842
C	7.046515	-6.292887	-0.412302
C	8.092546	-4.550847	-1.503650
C	8.278984	-5.817704	-1.063893
C	2.689694	-1.803550	-0.486972
C	3.671113	-2.503807	-0.600804
H	0.013804	-2.135999	0.694774
H	-2.381054	-0.388294	0.961938
H	-4.620365	5.843059	-0.560210
H	-7.013723	7.597780	-0.307595
H	-9.427265	7.088356	0.829226
H	6.340318	-2.152247	-1.782002
H	8.757210	-3.875897	-2.021935
H	9.169928	-6.416842	-1.155953

O	2.359882	1.082338	-1.476105
O	-0.344605	3.056656	-1.173688
O	-6.680694	2.414958	1.579082
O	-9.388451	4.410991	1.861104
O	4.022584	-5.389043	0.391319
O	6.766377	-7.335383	0.115313
N	-7.228799	4.606305	0.948905
N	-6.556695	5.609824	0.295231
N	-0.448126	-0.143574	0.103986
N	0.216387	0.866901	-0.548882
N	6.161144	-5.159815	-0.543611
N	6.815701	-4.143645	-1.195563

Tetramer

C	-0.102680	-0.444952	-0.884482
C	-0.131985	0.904940	-0.659293
C	1.276367	1.386849	-0.528568
C	3.400627	-0.261101	-0.727041
C	3.261040	-1.727411	-0.976840
C	1.926563	-2.019360	-1.074854
C	-3.312498	3.328070	-0.365380
C	-3.339480	4.677648	-0.140959
C	-4.723676	2.848943	-0.492991
C	-5.379103	6.253108	0.052856
C	-6.851042	4.510375	-0.288440
C	-6.696062	5.954231	-0.042362
C	-1.248031	1.742481	-0.558622
C	-2.195904	2.490551	-0.466788
C	6.396327	-4.206839	-1.273706
C	6.256890	-5.673205	-1.523227
C	7.730785	-3.914689	-1.176006
C	8.381348	-7.320921	-1.721684
C	9.760190	-5.488922	-1.365992
C	9.789654	-6.838810	-1.591179
C	10.905830	-7.676164	-1.691963
C	11.853861	-8.424015	-1.783952
C	12.970702	-9.261174	-1.885650
C	12.998094	-10.610814	-2.109652
C	14.381752	-8.781470	-1.758821

C	15.038334	-12.185002	-2.307300
C	16.509779	-10.441467	-1.967960
C	16.355309	-11.885128	-2.215586
C	4.348390	-2.600738	-1.082135
C	5.308932	-3.333567	-1.168413
H	1.432530	-2.962526	-1.250498
H	-0.912473	-1.143134	-1.029995
H	-2.527955	5.374461	0.002682
H	-4.876690	7.192918	0.226935
H	-7.527959	6.633945	0.042264
H	8.224716	-2.971416	-1.000651
H	10.569906	-4.790626	-1.220594
H	12.186785	-11.307962	-2.252871
H	14.536190	-13.124961	-2.481341
H	17.187568	-12.563982	-2.303508
O	4.371529	0.426394	-0.575890
O	1.721649	2.482286	-0.328851
O	-5.167324	1.751662	-0.691521
O	-7.822933	3.819928	-0.437623
O	5.286057	-6.360867	-1.674054
O	7.936194	-8.416415	-1.921374
O	14.825106	-7.683902	-1.561259
O	17.481544	-9.750304	-1.821322
N	-5.484491	4.045108	-0.318108
N	-4.637511	5.106596	-0.112430
N	1.196512	-0.874748	-0.911085
N	2.041540	0.189217	-0.702901
N	7.616037	-6.123371	-1.547392
N	8.460950	-5.059269	-1.339450
N	14.296239	-11.039446	-2.137647
N	15.142903	-9.977580	-1.932728

Pentamer

C	-1.739276	0.265449	0.415551
C	-1.897351	1.560157	0.000338
C	-0.649785	1.978545	-0.708170
C	1.468170	0.339364	-1.012110
C	1.485987	-1.058723	-0.485823
C	0.284247	-1.301004	0.124922

C	-5.042794	3.996446	0.494273
C	-5.191685	5.289109	0.070550
C	-6.290235	3.596526	1.216390
C	-7.195459	6.887454	0.399394
C	-8.382076	5.281427	1.553824
C	-8.368278	6.660304	1.036121
C	-3.002607	2.399368	0.177021
C	-3.942424	3.150357	0.315856
C	4.644405	-3.491339	-0.899666
C	4.676266	-4.895689	-0.389882
C	5.848355	-3.225223	-1.495170
C	6.833209	-6.490641	-0.661357
C	7.908142	-4.747762	-1.753686
C	8.089249	-6.038183	-1.332787
C	9.225608	-6.841231	-1.473514
C	10.199288	-7.553643	-1.580980
C	11.345223	-8.343068	-1.720664
C	11.541697	-9.635974	-1.313374
C	12.601940	-7.862645	-2.370230
C	13.641846	-11.110582	-1.532492
C	14.799703	-9.405844	-2.598963
C	14.856260	-10.808783	-2.087114
C	2.578291	-1.921022	-0.624480
C	3.543084	-2.640694	-0.759955
C	18.131464	-13.100937	-2.390576
C	19.343807	-12.779617	-2.937900
C	18.205940	-14.507558	-1.887233
C	21.478889	-14.223617	-3.121335
C	20.449539	-16.009195	-2.085712
C	21.684930	-15.493617	-2.700300
C	15.990744	-11.621059	-2.188044
C	16.990011	-12.297584	-2.289504
H	-0.077035	-2.188643	0.620955
H	-2.415265	-0.378599	0.956512
H	-4.512454	5.922537	-0.479171
H	-6.820402	7.766850	-0.102546
H	-9.186108	7.350087	1.164976
H	6.202914	-2.325952	-1.974788
H	8.583156	-4.084844	-2.272657
H	10.871882	-10.315230	-0.808958

H	13.298670	-12.019107	-1.062164
H	19.676662	-11.862425	-3.399139
H	22.138892	-13.524037	-3.612180
H	22.591503	-16.070319	-2.782603
O	2.295773	0.970348	-1.608053
O	-0.346433	3.015081	-1.229361
O	-6.594565	2.565930	1.750640
O	-9.205499	4.663597	2.173247
O	3.853273	-5.543551	0.193707
O	6.544151	-7.533504	-0.145108
O	12.882191	-6.807424	-2.866409
O	15.624009	-8.732309	-3.151178
O	17.386600	-15.191630	-1.338711
O	20.182301	-17.067579	-1.583880
N	-7.098162	4.771672	1.133322
N	-6.420297	5.752317	0.451363
N	-0.504088	-0.187261	0.037040
N	0.168718	0.806272	-0.633351
N	5.983381	-5.342783	-0.767657
N	6.649646	-4.331051	-1.417128
N	12.808724	-10.029909	-1.643294
N	13.465985	-9.000116	-2.273175
N	20.186131	-13.851552	-2.834769
N	19.541105	-14.894417	-2.216213

Hexamer

C	-1.675247	0.269678	0.445893
C	-1.886805	1.563656	0.053157
C	-0.623488	2.078765	-0.556870
C	1.600404	0.571679	-0.783887
C	1.665080	-0.843310	-0.309105
C	0.448773	-1.169640	0.229685
C	-5.229220	3.753735	0.376561
C	-5.447253	5.049110	-0.006839
C	-6.496554	3.223662	0.968544
C	-7.608564	6.455050	0.170550
C	-8.753314	4.707053	1.147406
C	-8.816326	6.098054	0.667036
C	-3.055183	2.323926	0.171432

C	-4.054662	3.001927	0.260253
C	4.925322	-3.148946	-0.654002
C	4.977165	-4.554310	-0.148115
C	6.136492	-2.853433	-1.220065
C	7.159873	-6.113073	-0.410398
C	8.221774	-4.343344	-1.471980
C	8.412012	-5.640087	-1.074947
C	9.547047	-6.440859	-1.236536
C	10.509536	-7.165215	-1.363245
C	11.630390	-7.985148	-1.528579
C	11.806318	-9.272685	-1.096462
C	12.870017	-7.560428	-2.246786
C	13.829575	-10.832874	-1.410379
C	14.988516	-9.195290	-2.577087
C	15.014090	-10.595193	-2.054613
C	2.802040	-1.649494	-0.424939
C	3.797498	-2.330104	-0.538734
C	18.101653	-13.098989	-2.566545
C	19.274059	-12.899834	-3.246049
C	18.117477	-14.483239	-2.004854
C	21.240654	-14.522578	-3.609680
C	20.176222	-16.180751	-2.384160
C	21.390076	-15.811486	-3.173964
C	22.460945	-16.683942	-3.395638
C	23.370581	-17.463469	-3.572883
C	24.434720	-18.344203	-3.797486
C	24.578496	-19.627542	-3.344637
C	25.640084	-18.000617	-4.613838
C	26.514657	-21.289249	-3.754800
C	27.661397	-19.751370	-5.035528
C	27.648122	-21.112843	-4.473566
C	16.092583	-11.468520	-2.228425
C	17.035947	-12.209906	-2.394275
H	0.110055	-2.094049	0.671550
H	-2.344581	-0.430898	0.920855
H	-4.778952	5.758487	-0.470444
H	-7.268294	7.381708	-0.267023
H	-9.705700	6.704177	0.720840
H	6.481176	-1.945669	-1.690782
H	8.890263	-3.667257	-1.982345

H	11.138694	-9.918683	-0.547429
H	13.476999	-11.720909	-0.908871
H	19.627171	-12.033813	-3.784379
H	21.899325	-13.909161	-4.204889
H	23.922141	-20.225206	-2.730814
H	26.152201	-22.142572	-3.201261
H	28.438453	-21.827780	-4.633224
O	2.421007	1.265623	-1.316028
O	-0.353316	3.145697	-1.032871
O	-6.760517	2.146813	1.427803
O	-9.576915	3.992702	1.652228
O	4.153668	-5.224390	0.409104
O	6.877144	-7.168749	0.082956
O	13.156908	-6.529155	-2.786993
O	15.799562	-8.569118	-3.199668
O	17.308850	-15.080245	-1.350724
O	19.877569	-17.197437	-1.822768
O	25.934338	-16.994745	-5.198496
O	28.457256	-19.174651	-5.726480
N	-7.386015	4.336692	0.868424
N	-6.735939	5.398201	0.287951
N	-0.389856	-0.093385	0.146355
N	0.262849	0.959151	-0.449874
N	6.305157	-4.967192	-0.488061
N	6.962833	-3.939595	-1.121278
N	13.046931	-9.712254	-1.467420
N	13.706427	-8.719168	-2.151750
N	20.042405	-14.028234	-3.169162
N	19.385510	-14.988394	-2.437104
N	25.765350	-20.136302	-3.793533
N	26.420342	-19.195519	-4.549915

Heptamer

C	-1.566220	0.441738	0.716833
C	-1.841843	1.636441	0.108305
C	-0.721576	1.951936	-0.829337
C	1.408591	0.330746	-1.146422
C	1.560465	-0.953754	-0.398872
C	0.468337	-1.107561	0.413355
C	-5.020664	4.028727	0.603251

C	-5.294329	5.222039	-0.008287
C	-6.142401	3.719196	1.543229
C	-7.334093	6.778146	0.302480
C	-8.273664	5.358188	1.858482
C	-8.407179	6.621322	1.112656
C	-2.955162	2.464267	0.287920
C	-3.907394	3.200121	0.423218
C	4.714566	-3.386171	-0.845390
C	4.867651	-4.671375	-0.098047
C	5.806819	-3.230239	-1.656069
C	7.003054	-6.287071	-0.409039
C	7.846085	-4.773771	-1.953752
C	8.125052	-5.967332	-1.342756
C	9.243217	-6.788808	-1.517651
C	10.200598	-7.519189	-1.648430
C	11.319824	-8.339195	-1.823405
C	11.601073	-9.532369	-1.213011
C	12.441591	-8.016496	-2.756589
C	13.646490	-11.068557	-1.507118
C	14.583233	-9.624296	-3.063780
C	14.740484	-10.907891	-2.314799
C	2.656258	-1.809968	-0.547369
C	3.617589	-2.531527	-0.696708
C	17.914228	-13.315970	-2.753005
C	19.006372	-13.150142	-3.562396
C	18.077395	-14.599970	-2.006252
C	21.058141	-14.676711	-3.860661
C	20.226128	-16.198020	-2.317880
C	21.345835	-15.868767	-3.251461
C	22.470032	-16.681593	-3.428542
C	23.433624	-17.402959	-3.563669
C	24.560528	-18.210792	-3.746159
C	24.856593	-19.404092	-3.142161
C	25.674814	-17.872714	-4.682147
C	26.915075	-20.920121	-3.453845
C	27.829382	-19.459065	-5.007487
C	28.002336	-20.745546	-4.266688
C	29.111685	-21.583224	-4.423746
C	30.084053	-22.287445	-4.582153
C	31.195877	-23.121888	-4.743362

C	31.379624	-24.412684	-4.010069
C	32.279348	-22.937130	-5.558607
C	33.555892	-25.985623	-4.351797
C	34.351639	-24.448156	-5.876145
C	34.644104	-25.626645	-5.277489
C	15.842788	-11.756261	-2.459449
C	16.810059	-12.470370	-2.606236
H	0.218687	-1.902401	1.099207
H	-2.131845	-0.111616	1.450496
H	-4.727516	5.771857	-0.743949
H	-7.076678	7.567785	-0.387553
H	-9.245395	7.289397	1.223626
H	6.056409	-2.434644	-2.341008
H	8.412240	-4.218487	-2.685595
H	11.036125	-10.089183	-0.481409
H	13.399011	-11.864592	-0.821904
H	19.249664	-12.352014	-4.246688
H	21.619947	-14.116343	-4.591951
H	24.300112	-19.969897	-2.410937
H	26.678449	-21.722115	-2.771790
H	32.508779	-22.129589	-6.236848
H	34.898037	-23.869224	-6.605686
H	35.520653	-26.235465	-5.426603
O	2.115115	0.862490	-1.956490
O	-0.542439	2.884519	-1.561573
O	-6.319276	2.786947	2.277960
O	-8.978846	4.827591	2.673681
O	4.161254	-5.203874	0.711233
O	6.825568	-7.219319	0.323856
O	12.617537	-7.083153	-3.488424
O	15.289660	-9.088718	-3.871081
O	17.374537	-15.139286	-1.198301
O	20.055526	-17.132648	-1.586519
O	25.838376	-16.934503	-5.410993
O	28.526302	-18.913021	-5.816237
O	30.685613	-24.963973	-3.201014
O	33.397686	-26.928074	-3.623677
N	-7.017394	4.835488	1.374990
N	-6.487583	5.704365	0.452770
N	-0.370473	-0.039633	0.255781

N	0.157869	0.834316	-0.664122
N	6.119133	-5.173620	-0.579788
N	6.647449	-4.298277	-1.498486
N	12.800896	-10.005441	-1.668738
N	13.327423	-9.128476	-2.586940
N	19.855755	-14.210216	-3.404117
N	19.334115	-15.090641	-2.486460
N	26.058778	-19.862464	-3.604231
N	26.572674	-18.976114	-4.520435
N	32.633786	-24.885115	-4.504275
N	33.138559	-23.991017	-5.416341

Octamer

C	-1.757748	0.265985	0.360933
C	-1.844501	1.621098	0.189168
C	-0.509517	2.121057	-0.259681
C	1.608543	0.491981	-0.613948
C	1.538927	-0.981417	-0.377222
C	0.265640	-1.290831	0.021692
C	-5.001403	4.030439	0.738731
C	-5.076575	5.386014	0.567144
C	-6.341263	3.543312	1.191393
C	-7.090836	6.962403	0.935698
C	-8.443316	5.205936	1.572889
C	-8.343847	6.658233	1.347882
C	-2.953842	2.451034	0.383074
C	-3.895815	3.195101	0.542945
C	4.684175	-3.414538	-0.878600
C	4.628321	-4.888705	-0.639070
C	5.954376	-3.093695	-1.276290
C	6.767005	-6.496313	-0.971830
C	7.996462	-4.628951	-1.594902
C	8.099636	-5.982077	-1.410565
C	9.224034	-6.795297	-1.584199
C	10.182875	-7.521826	-1.725231
C	11.310199	-8.331123	-1.898085
C	11.420496	-9.683332	-1.712707
C	12.640669	-7.809884	-2.335803
C	13.474059	-11.205926	-2.019982
C	14.790848	-9.403836	-2.656669

C	14.744524	-10.877170	-2.411111
C	2.627086	-1.842802	-0.549817
C	3.589801	-2.560825	-0.707045
C	17.923613	-13.272695	-2.877941
C	19.194040	-12.943833	-3.269114
C	17.877408	-14.746045	-2.632444
C	21.247736	-14.466217	-3.576432
C	20.027704	-16.339818	-2.953507
C	21.358162	-15.818422	-3.391127
C	22.485551	-16.627625	-3.563975
C	23.444451	-17.354078	-3.705001
C	24.568934	-18.167173	-3.878678
C	24.672232	-19.520296	-3.694375
C	25.901509	-17.652801	-4.317389
C	26.714532	-21.055315	-4.012831
C	28.040395	-19.260160	-4.650032
C	27.984732	-20.734307	-4.410393
C	29.079247	-21.587876	-4.581788
C	30.042152	-22.305713	-4.738703
C	31.130514	-23.166891	-4.911045
C	31.061170	-24.640286	-4.674237
C	32.403813	-22.857226	-5.309738
C	33.179786	-26.268852	-5.027581
C	34.427743	-24.413535	-5.648027
C	34.514843	-25.768577	-5.475901
C	35.624513	-26.598235	-5.669097
C	36.566810	-27.342049	-5.828233
C	37.672742	-28.177121	-6.023216
C	37.748198	-29.532628	-5.851205
C	39.012710	-27.689747	-6.475273
C	39.762649	-31.108761	-6.219700
C	41.114965	-29.352110	-6.856733
C	41.015501	-30.804498	-6.632292
C	15.847573	-11.721801	-2.571067
C	16.820521	-12.428133	-2.717919
H	-0.168659	-2.243466	0.283149
H	-2.506588	-0.444319	0.675720
H	-4.321258	6.089294	0.251450
H	-6.640712	7.908787	0.675544
H	-9.165250	7.339141	1.499225

H	6.380249	-2.137369	-1.537987
H	8.739547	-3.911315	-1.906817
H	10.681311	-10.404853	-1.400530
H	13.053876	-12.164227	-1.756253
H	19.614154	-11.985492	-3.532812
H	21.986849	-13.744585	-3.888525
H	23.929201	-20.237994	-3.382473
H	26.288787	-22.011691	-3.751107
H	32.837961	-21.904512	-5.571157
H	35.176502	-23.703054	-5.962607
H	36.992877	-30.236034	-5.535799
H	39.312558	-32.055232	-5.959808
H	41.836810	-31.485386	-6.784233
O	2.514117	1.194003	-0.967896
O	-0.128322	3.226253	-0.526481
O	-6.727615	2.439616	1.461106
O	-9.351755	4.509309	1.937336
O	3.729571	-5.598053	-0.283374
O	6.398053	-7.603825	-0.698024
O	13.003929	-6.700388	-2.609022
O	15.686755	-8.689092	-3.008928
O	16.981571	-15.460875	-2.280198
O	19.664558	-17.449365	-2.680363
O	26.270370	-16.545243	-4.591149
O	28.939086	-18.550690	-5.005638
O	30.155701	-25.342482	-4.320380
O	32.798837	-27.374106	-4.760666
O	39.398845	-26.586054	-6.745309
O	42.023229	-28.655420	-7.221493
N	-7.117299	4.741634	1.239574
N	-6.341080	5.811243	0.865756
N	-0.488476	-0.151215	0.062205
N	0.278551	0.926826	-0.310442
N	5.962200	-5.312175	-0.942743
N	6.719520	-4.227322	-1.315669
N	12.700174	-10.078421	-1.991461
N	13.451612	-8.989600	-2.364778
N	19.968002	-14.071276	-3.297711
N	19.216660	-15.160176	-2.924457
N	25.949196	-19.921808	-3.973674

N	26.706403	-18.836872	-4.346588
N	32.391287	-25.074885	-4.977612
N	33.158157	-23.996689	-5.350127
N	39.013089	-29.957539	-6.148630
N	39.789234	-28.887810	-6.522279

C. Cartesian coordinates of acetylene-linked bimane oligomers optimized with MP2P/6-31G*.

Dimer

C	-1.656962	0.316317	0.561676
C	-1.847710	1.587177	0.086446
C	-0.577184	2.051929	-0.529298
C	1.472821	0.439238	-0.959700
C	1.445465	-0.984372	-0.598222
C	0.333418	-1.234049	0.139430
C	-5.178389	3.863260	0.243382
C	-5.369102	5.134108	-0.231929
C	-6.448965	3.398499	0.859016
C	-7.360013	6.684322	0.189194
C	-8.499378	5.011207	1.288661
C	-8.472354	6.434627	0.926416
C	-3.001485	2.383686	0.174054
C	-4.024632	3.066730	0.155790
H	-0.035721	-2.150661	0.582448
H	-2.342224	-0.349095	1.072893
H	-4.683811	5.799506	-0.743123
H	-6.990955	7.600831	-0.254104
H	-9.229504	7.145187	1.225569
H	2.202192	-1.695052	-0.898164
O	2.238335	1.093102	-1.645310
O	-0.300418	3.085567	-1.109614
O	-6.725821	2.364803	1.439192
O	-9.265076	4.357407	1.974132
N	-7.349376	4.479072	0.601998
N	-6.683376	5.499734	-0.043041
N	0.323339	0.971448	-0.272190
N	-0.342648	-0.049314	0.372793

Trimer

C	-1.808866	0.160693	0.204887
C	-1.944160	1.479216	-0.151606
C	-0.723280	1.895157	-0.889257
C	1.417418	0.336550	-1.123566
C	1.491892	-1.022539	-0.527738
C	0.257256	-1.343661	-0.021329
C	-5.049833	3.964429	0.530119
C	-5.186757	5.281640	0.177175
C	-6.277717	3.543969	1.254979
C	-7.291478	6.730911	0.306657
C	-8.446783	5.052206	1.381332
C	-8.525207	6.375477	0.747711
C	-3.042181	2.327284	0.059948
C	-3.950618	3.117098	0.316184
C	4.857696	-3.248945	-0.554367
C	4.928266	-4.614720	0.028372
C	6.092055	-2.930060	-1.057402
C	7.014774	-6.204506	-0.310837
C	8.104187	-4.477831	-1.378315
C	8.197709	-5.799433	-1.082363
C	2.648791	-1.816243	-0.563006
C	3.700755	-2.453704	-0.521323
H	-0.082272	-2.240203	0.482897
H	-2.483042	-0.492179	0.745772
H	-4.508104	5.937316	-0.355009
H	-6.948163	7.619898	-0.207648
H	-9.439590	6.943801	0.655001
H	6.434072	-2.029301	-1.552737
H	8.768655	-3.822629	-1.927735
H	8.992898	-6.475577	-1.361976
O	2.266280	1.032252	-1.648797
O	-0.392997	2.968388	-1.357790
O	-6.609848	2.463507	1.706351
O	-9.297177	4.326521	1.864436
O	4.070762	-5.312662	0.537306
O	6.650757	-7.284236	0.119112
N	-7.037681	4.752430	1.334236
N	-6.370916	5.768324	0.682864
N	-0.620739	-0.321240	-0.289086
N	0.038870	0.684947	-0.955821
N	6.306318	-4.962838	-0.126471

N 6.975070 -3.948408 -0.778056

Tetramer

C -0.098607 -0.437718 -1.162919
C -0.112502 0.899049 -0.852039
C 1.290714 1.385872 -0.802625
C 3.386629 -0.240321 -0.994580
C 3.250917 -1.710747 -1.160491
C 1.923485 -2.006910 -1.348222
C -3.292135 3.297317 -0.201285
C -3.310031 4.631850 0.110488
C -4.695940 2.812432 -0.264707
C -5.329079 6.202580 0.172903
C -6.774364 4.447336 -0.198992
C -6.627927 5.904966 -0.086556
C -1.223970 1.734091 -0.660499
C -2.177934 2.464641 -0.394020
C 6.407289 -4.222036 -1.091561
C 6.271589 -5.692468 -1.257417
C 7.734719 -3.925851 -0.903839
C 8.367559 -7.318599 -1.449485
C 9.756850 -5.495008 -1.089080
C 9.770780 -6.831773 -1.399949
C 10.882226 -7.666852 -1.591438
C 11.836084 -8.397568 -1.857839
C 12.950137 -9.230417 -2.050662
C 12.967802 -10.564991 -2.362274
C 14.354021 -8.745715 -1.987526
C 14.986634 -12.136001 -2.424897
C 16.432206 -10.380921 -2.053355
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D. Vertical excitation energies ($S_0 \rightarrow S_1$) for bimane oligomers in A and B evaluated with various exchange correlation functionals within TD-DFT.

Table S1 Vertical excitation energies (eV) for $S_0 \rightarrow S_1$ in bimane oligomers ($n=2-8$) calculated at various levels of theory using the 6-311+G* basis set. All molecular structures were optimized in the electronic ground state using B3LYP/6-31G*.

n	B3LYP	LC-BLYP	ω B97X	CAM-B3LYP
2	2.74	3.50	3.36	3.17
3	2.45	3.18	3.04	2.82
4	2.43	3.04	2.90	2.67
5	2.41	2.97	2.82	2.59
6	2.40	2.92	2.77	2.54
7	2.40	2.89	2.74	2.50
8	2.39	2.87	2.72	2.48

Table S2 Vertical excitation energies (eV) for $S_0 \rightarrow S_1$ in bimane oligomers ($n=2-8$) calculated at various levels of theory using the 6-31+G* basis set. All molecular structures were optimized in the electronic ground state using B3LYP/6-311G*.

n	B3LYP	LC-BLYP	ω B97X	CAM-B3LYP
2	2.76	3.51	3.38	3.19
3	2.45	3.20	3.06	2.84
4	2.43	3.06	2.91	2.69
5	2.42	2.98	2.84	2.60

6	2.41	2.93	2.78	2.55
7	2.40	2.91	2.75	2.52
8	2.40	2.88	2.74	2.49
