Supporting Information

Table S1.The nuclear coordinates (in Å) of optimized dimer shown in Figure 6.

atoms	x	y	z
O	-2.32475	0.34615	0.01565
C	-3.55773	0.57555	-0.32291
O	-4.46948	-0.25072	-0.19937
C	-3.83734	1.96746	-0.89259
C	-5.26143	2.16848	-1.40556
O	2.32457	-0.34612	0.01585
C	3.55748	-0.57552	-0.32296
O	4.46924	0.25083	-0.19981
C	3.83705	-1.96751	-0.89246
C	5.26113	-2.16869	-1.40535
H	5.39670	-3.18809	-1.77881
H	5.48633	-1.47446	-2.21788
H	5.99259	-1.98888	-0.61519
H	3.60905	-2.68938	-0.09850
H	3.10183	-2.15719	-1.68106
H	-5.39707	3.18787	-1.77902
H	-5.48651	1.47423	-2.21810
H	-5.99289	1.98861	-0.61542
H	-3.60943	2.68943	-0.09871
H	-3.10210	2.15708	-1.68119
N	2.17912	2.14856	0.75697
C	0.81442	2.57747	1.20893
C	-0.16708	2.87995	0.07622
O	-0.25555	1.84363	-0.86323
H	-0.98417	1.23200	-0.59419
C	3.12356	2.12958	1.90977
C	2.73549	2.95375	-0.36656
H	2.14793	1.09865	0.40170
H	2.80000	4.00456	-0.07494
H	3.72208	2.55204	-0.59118
H	2.09080	2.83547	-1.23442
H	2.68735	1.53215	2.71068
H	4.05024	1.66852	1.57170
H	3.29299	3.14927	2.26186
H	0.43311	1.76392	1.83052
H	0.93172	3.46610	1.83962
H	-1.13522	3.09424	0.54800
H	0.13753	3.79388	-0.44514
N	-2.17892	-2.14842	0.75711
C	-0.81409	-2.57720	1.20890
C	0.16716	-2.88012	0.07609

O	0.25572	-1.84408	-0.86367
H	0.98389	-1.23206	-0.59439
C	-3.12314	-2.12935	1.91007
C	-2.73546	-2.95370	-0.36627
H	-2.14783	-1.09856	0.40173
H	-2.79997	-4.00448	-0.07454
H	-3.72209	-2.55199	-0.59076
H	-2.09089	-2.83551	-1.23423
H	-2.68682	-1.53182	2.71084
H	-4.04991	-1.66836	1.57213
H	-3.29246	-3.14902	2.26228
H	-0.43263	-1.76344	1.83010
H	-0.93126	-3.46561	1.83992
H	1.13533	-3.09449	0.54777
H	-0.13770	-3.79409	-0.44503
O	-2.32475	0.34615	0.01565
C	-3.55773	0.57555	-0.32291
O	-4.46948	-0.25072	-0.19937
C	-3.83734	1.96746	-0.89259
C	-5.26143	2.16848	-1.40556
O	2.32457	-0.34612	0.01585
C	3.55748	-0.57552	-0.32296
O	4.46924	0.25083	-0.19981
C	3.83705	-1.96751	-0.89246
C	5.26113	-2.16869	-1.40535
H	5.39670	-3.18809	-1.77881
H	5.48633	-1.47446	-2.21788
H	5.99259	-1.98888	-0.61519
H	3.60905	-2.68938	-0.0985
H	3.10183	-2.15719	-1.68106
H	-5.39707	3.18787	-1.77902
H	-5.48651	1.47423	-2.21810
H	-5.99289	1.98861	-0.61542
H	-3.60943	2.68943	-0.09871
H	-3.10210	2.15708	-1.68119
N	2.17912	2.14856	0.75697
C	0.81442	2.57747	1.20893
C	-0.16708	2.87995	0.07622
O	-0.25555	1.84363	-0.86323
H	-0.98417	1.23200	-0.59419
C	3.12356	2.12958	1.90977
C	2.73549	2.95375	-0.36656
H	2.14793	1.09865	0.40170
H	2.80000	4.00456	-0.07494
H	3.72208	2.55204	-0.59118
H	2.09080	2.83547	-1.23442

H	2.68735	1.53215	2.71068
H	4.05024	1.66852	1.57170
H	3.29299	3.14927	2.26186
H	0.43311	1.76392	1.83052
H	0.93172	3.46610	1.83962
H	-1.13522	3.09424	0.54800
H	0.13753	3.79388	-0.44514
N	-2.17892	-2.14842	0.75711
C	-0.81409	-2.57720	1.20890
C	0.16716	-2.88012	0.07609
O	0.25572	-1.84408	-0.86367
H	0.98389	-1.23206	-0.59439
C	-3.12314	-2.12935	1.91007
C	-2.73546	-2.95370	-0.36627
H	-2.14783	-1.09856	0.40173
H	-2.79997	-4.00448	-0.07454
H	-3.72209	-2.55199	-0.59076
H	-2.09089	-2.83551	-1.23423
H	-2.68682	-1.53182	2.71084
H	-4.04991	-1.66836	1.57213
H	-3.29246	-3.14902	2.26228
H	-0.43263	-1.76344	1.83010
H	-0.93126	-3.46561	1.83992
H	1.13533	-3.09449	0.54777
H	-0.13770	-3.79409	-0.44503

Table S2.The nuclear coordinates (in Å) of optimized tetramer shown in **Figure 6.**

atoms	x	y	z
O	-3.40466	1.64312	-2.03485
C	-3.11565	2.8604	-2.29142
O	-2.64099	3.65243	-1.44089
C	-3.36094	3.34264	-3.71766
C	-2.05068	3.62919	-4.46769
H	-2.25929	3.96532	-5.48693
H	-1.47637	4.41074	-3.96645
1	-1.43041	2.73058	-4.53201
1	-3.94501	2.58670	-4.24520
1	-3.95537	4.26034	-3.66402
O	1.15905	5.21516	2.20637
C	0.98012	4.02750	2.62345
O	1.07515	2.98759	1.92734
C	0.63500	3.84605	4.10504
H	-0.17747	3.11482	4.16000
H	1.50039	3.35170	4.56252
C	0.28294	5.12109	4.86888

H	-0.59691	5.60855	4.44172
H	0.06942	4.89547	5.91808
H	1.10293	5.84057	4.83217
N	1.65490	6.22309	-0.10445
C	0.56298	5.97471	-1.10775
C	2.96412	5.72926	-0.61966
C	1.75517	7.64942	0.30787
C	-0.84580	6.37110	-0.63999
H	0.80958	6.52643	-2.01960
H	1.90158	8.2797	-0.57186
H	2.60124	7.75453	0.98549
H	0.85005	7.94333	0.83293
H	2.87884	4.66934	-0.85732
H	3.71575	5.86395	0.15835
H	3.24340	6.30272	-1.50614
H	0.58554	4.90756	-1.33335
O	-1.75517	6.17216	-1.69374
H	-1.11578	5.79823	0.25526
H	-0.87826	7.43292	-0.37805
H	-2.1125	5.25139	-1.64878
H	1.42925	5.66212	0.82086
N	-3.00445	1.02132	0.40411
C	-3.10179	-0.46772	0.52611
C	-4.09718	1.70710	1.13825
C	-1.68145	1.55064	0.83738
C	-2.34422	-1.21843	-0.57852
H	-2.72266	-0.76774	1.50748
H	-1.54106	1.38376	1.90624
H	-1.64445	2.61068	0.60004
H	-0.89075	1.04686	0.28814
H	-5.05603	1.36599	0.74864
H	-4.00211	2.77938	0.96991
H	-4.03127	1.48510	2.20598
H	-4.15777	-0.7373	0.46776
O	-2.41445	-2.60997	-0.34714
H	-2.79902	-1.01092	-1.54886
H	-1.30116	-0.88212	-0.62867
H	-1.90176	-2.81432	0.47827
H	-3.14922	1.30834	-0.69271
O	3.40466	-1.64312	-2.03485
C	3.11565	-2.86040	-2.29142
O	2.64099	-3.65243	-1.44089
C	3.36094	-3.34264	-3.71766
C	2.05068	-3.62919	-4.46769
H	2.25929	-3.96532	-5.48693
H	1.47637	-4.41074	-3.96645

H	1.43041	-2.73058	-4.53201
H	3.94501	-2.5867	-4.2452
H	3.95537	-4.26034	-3.66402
O	-1.15905	-5.21516	2.20637
C	-0.98012	-4.02750	2.62345
O	-1.07515	-2.98759	1.92734
C	-0.63500	-3.84605	4.10504
H	0.17747	-3.11482	4.16000
H	-1.50039	-3.35170	4.56252
C	-0.28294	-5.12109	4.86888
H	0.59691	-5.60855	4.44172
H	-0.06942	-4.89547	5.91808
H	-1.10293	-5.84057	4.83217
N	-1.65490	-6.22309	-0.10445
C	-0.56298	-5.97471	-1.10775
C	-2.96412	-5.72926	-0.61966
C	-1.75517	-7.64942	0.30787
C	0.84580	-6.37110	-0.63999
H	-0.80958	-6.52643	-2.01960
H	-1.90158	-8.27970	-0.57186
H	-2.60124	-7.75453	0.98549
H	-0.85005	-7.94333	0.83293
H	-2.87884	-4.66934	-0.85732
H	-3.71575	-5.86395	0.15835
H	-3.24340	-6.30272	-1.50614
H	-0.58554	-4.90756	-1.33335
O	1.75517	-6.17216	-1.69374
H	1.11578	-5.79823	0.25526
H	0.87826	-7.43292	-0.37805
H	2.11250	-5.25139	-1.64878
H	-1.42925	-5.66212	0.82086
N	3.00445	-1.02132	0.40411
C	3.10179	0.46772	0.52611
C	4.09718	-1.70710	1.13825
C	1.68145	-1.55064	0.83738
C	2.34422	1.21843	-0.57852
H	2.72266	0.76774	1.50748
H	1.54106	-1.38376	1.90624
H	1.64445	-2.61068	0.60004
H	0.89075	-1.04686	0.28814
H	5.05603	-1.36599	0.74864
H	4.00211	-2.77938	0.96991
H	4.03127	-1.48510	2.20598
H	4.15777	0.73730	0.46776
O	2.41445	2.60997	-0.34714
H	2.79902	1.01092	-1.54886

H	1.30116	0.88212	-0.62867
H	1.90176	2.81432	0.47827
H	3.14922	-1.30834	-0.69271