Supporting Information

Facile and Eco-Friendly Synthesis of Hydrogen Bonding-Rich Bio-Based Bisbenzoxazine Resins with Low Surface Free Energy, Strong Adhesion Strength and High Thermal Stability

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S1. ^{1}H NMR Spectra

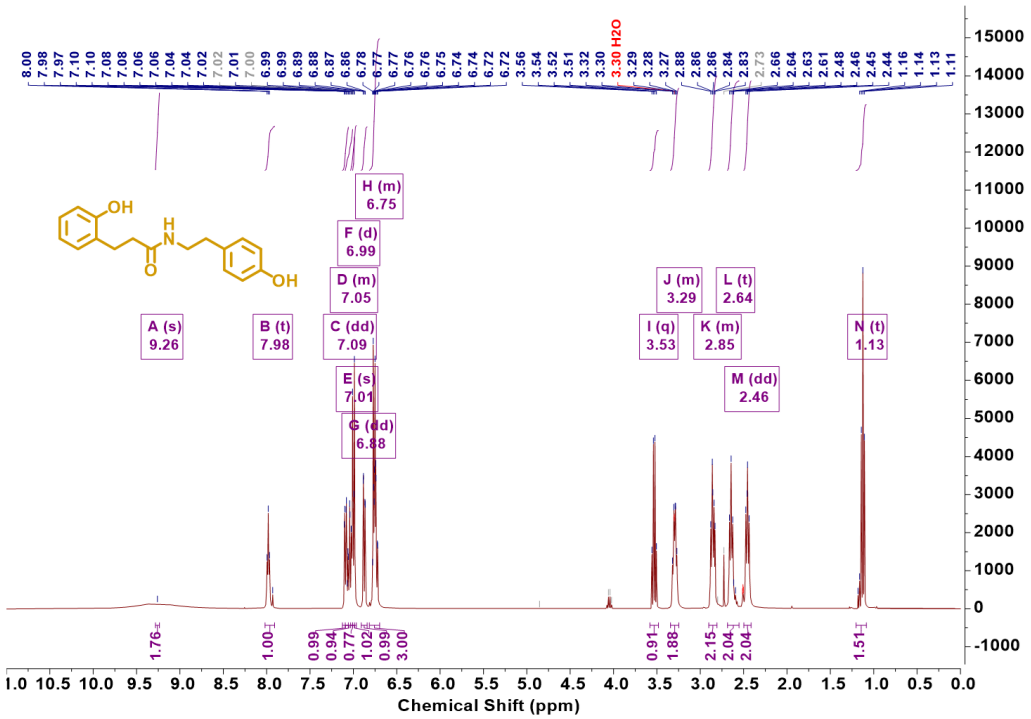


Figure S1. ^{1}H NMR spectrum of the product from the reaction between dihydrocoumarin and tyramine (DMSO-d_6).

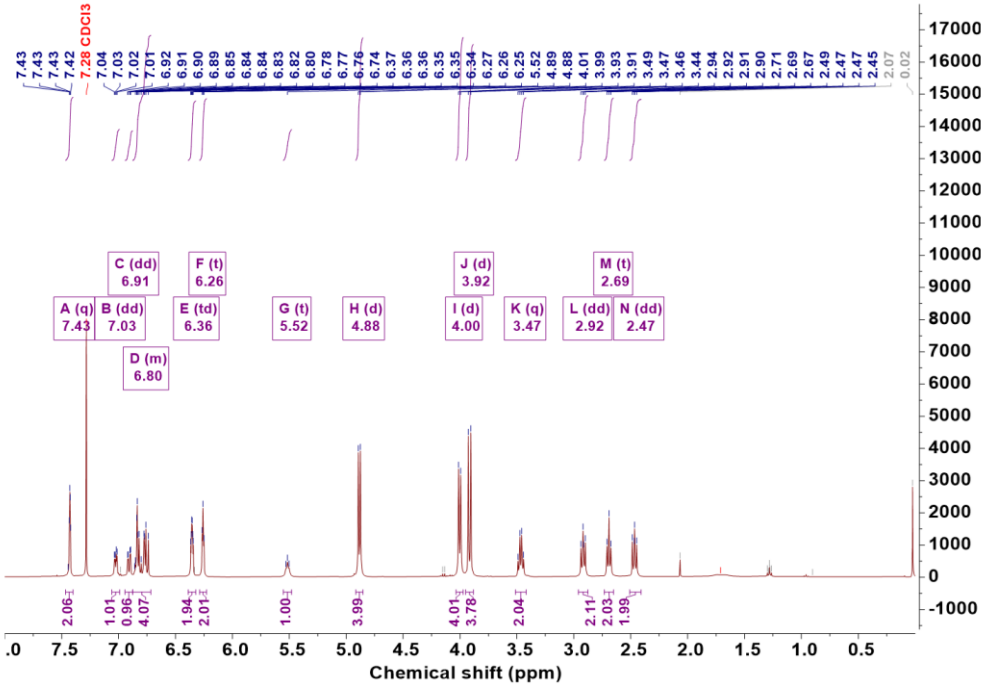


Figure S2. ^{1}H NMR spectrum of **DcTa-fa** ($CDCl_3$).

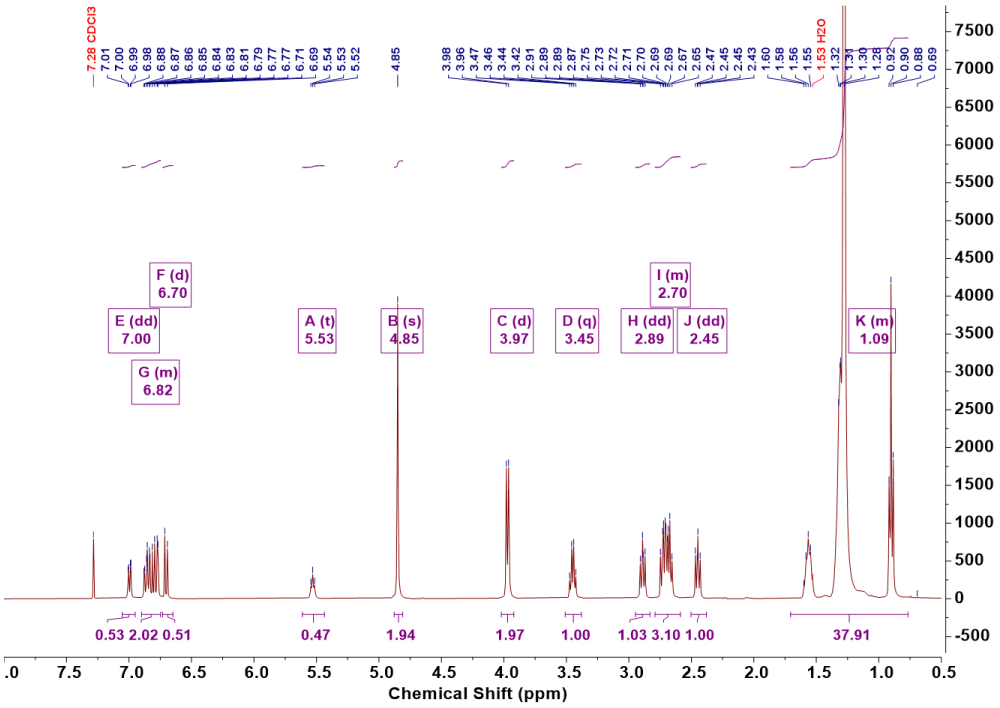


Figure S3. ^{1}H NMR spectrum of **DcTa-sa** ($CDCl_3$).

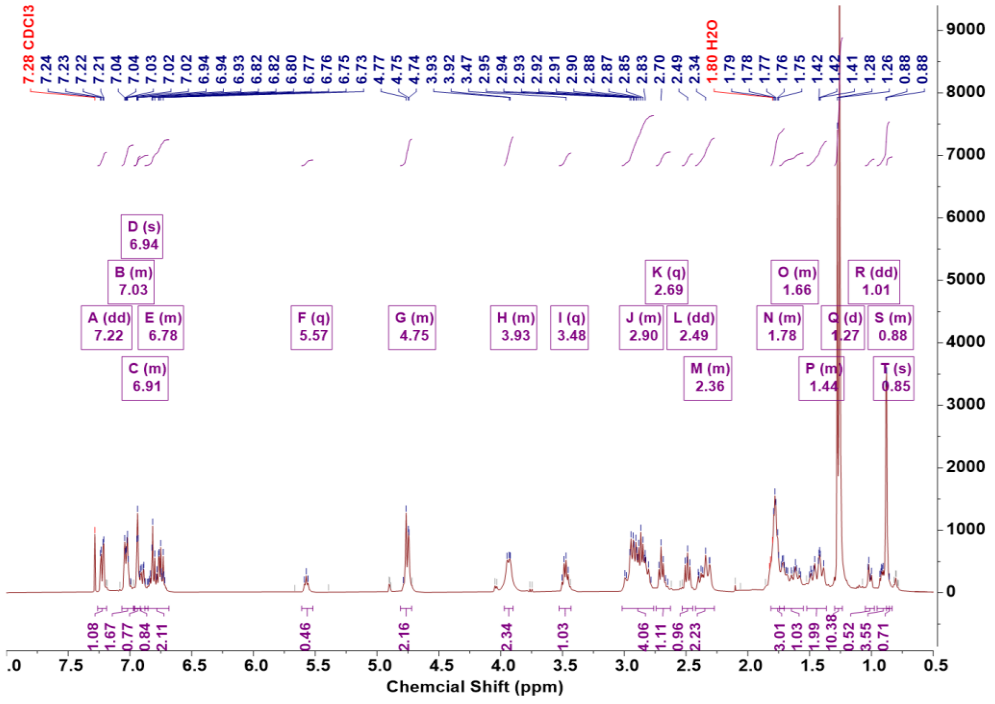


Figure S4. ^{1}H NMR spectrum of **DcTa-da** ($CDCl_3$).

S2. ^{13}C NMR Spectra of Monomers

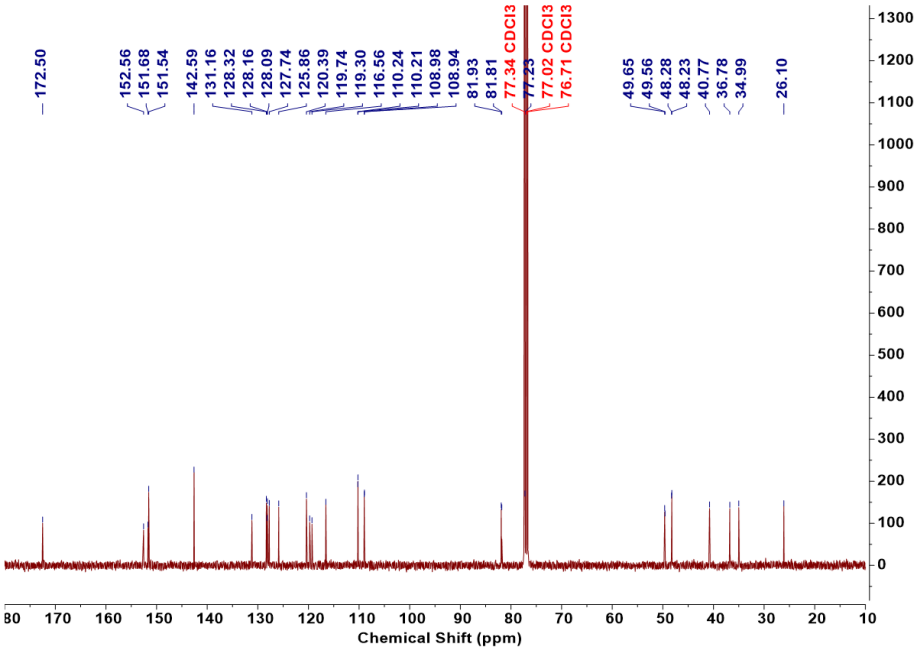


Figure S5. ^{13}C NMR spectrum of **DcTa-fa** ($CDCl_3$).

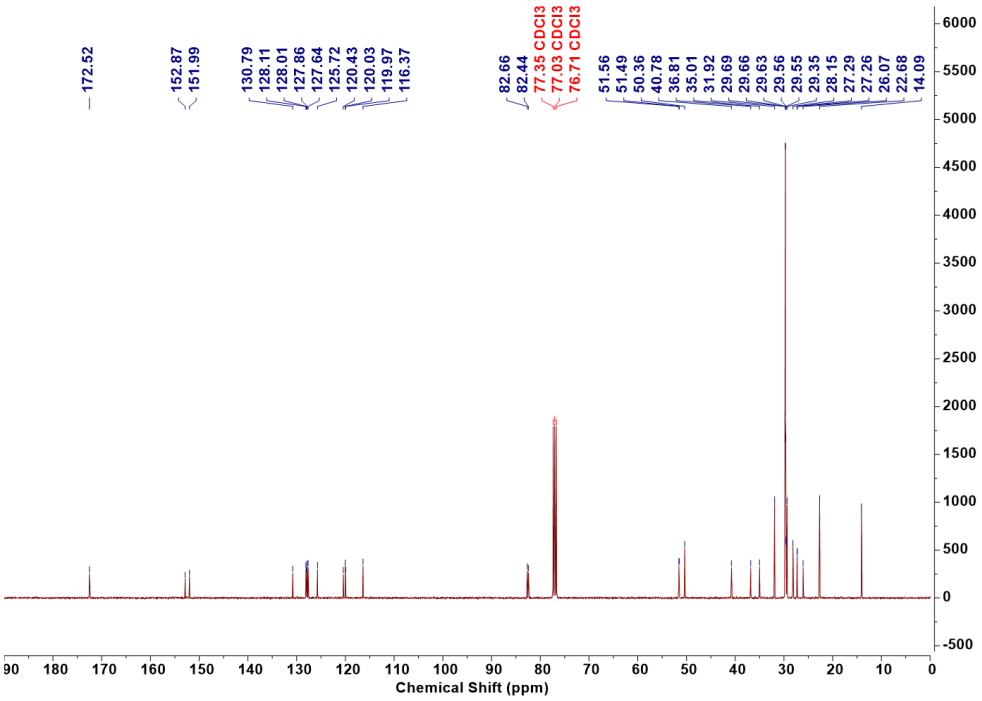


Figure S6. ^{13}C NMR spectrum of **DcTa-sa** ($CDCl_3$).

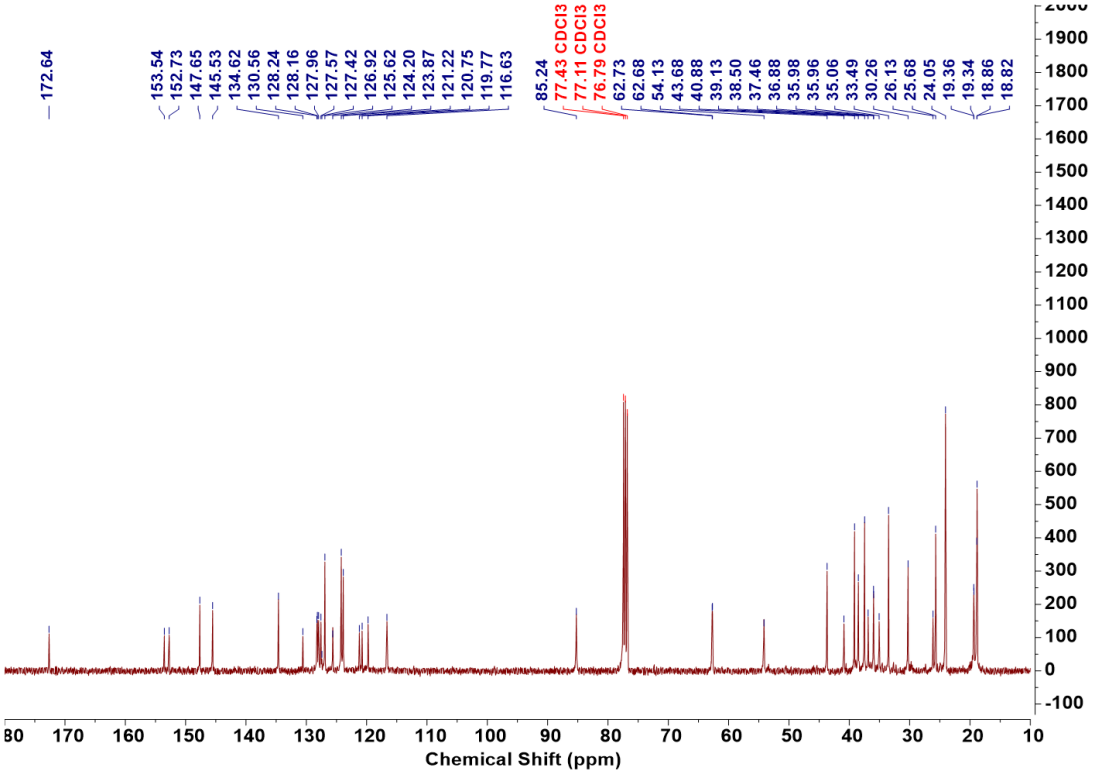


Figure S7. ^{13}C NMR spectrum of **DcTa-da** ($CDCl_3$).

S3. FT-IR Spectra of Monomers

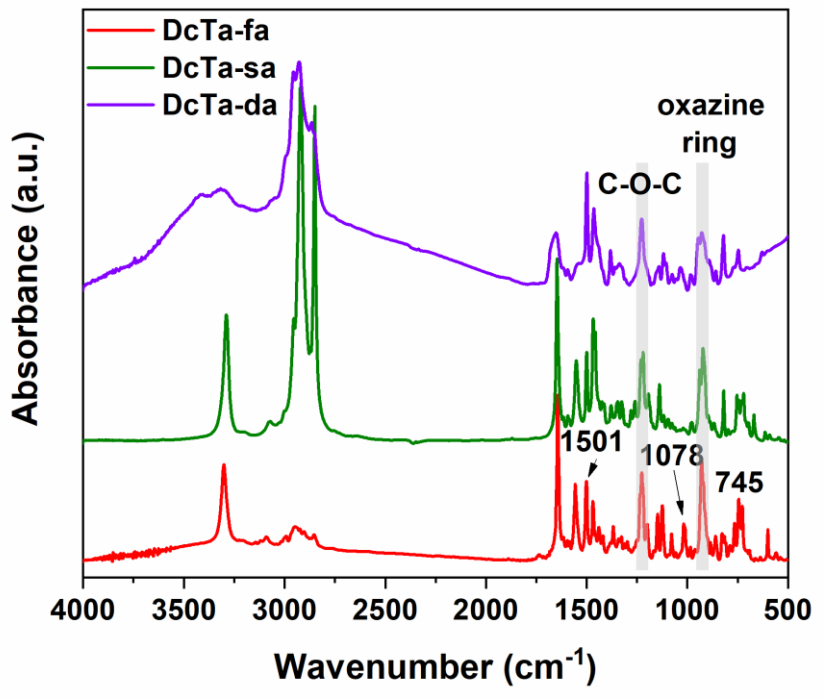


Figure S8. FT-IR spectra of **DcTa-fa, DcTa-sa** and **DcTa-da** .

S4. HR-MS Spectra of Monomers

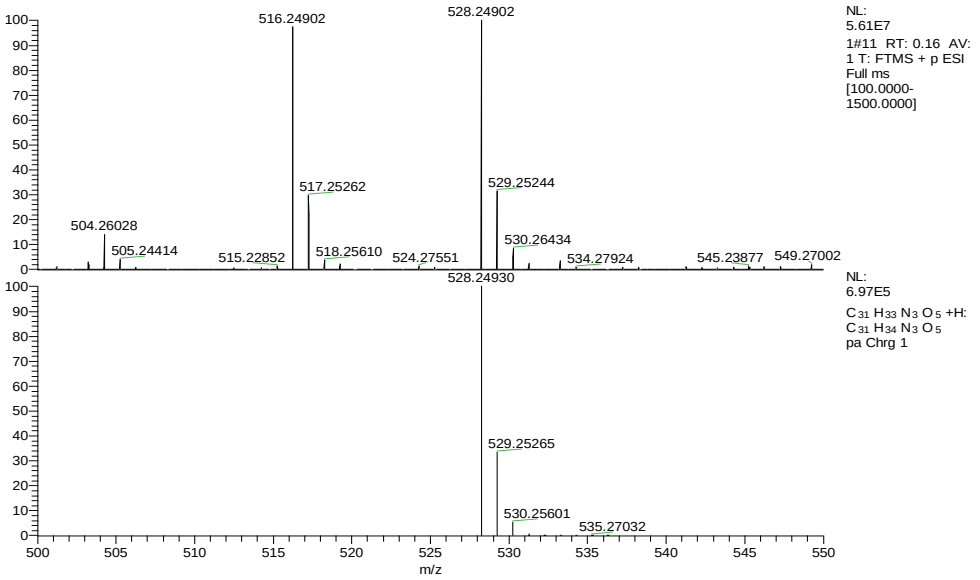


Figure S9. Experimental and theoretical HR-MS spectra of **DcTa-fa**.

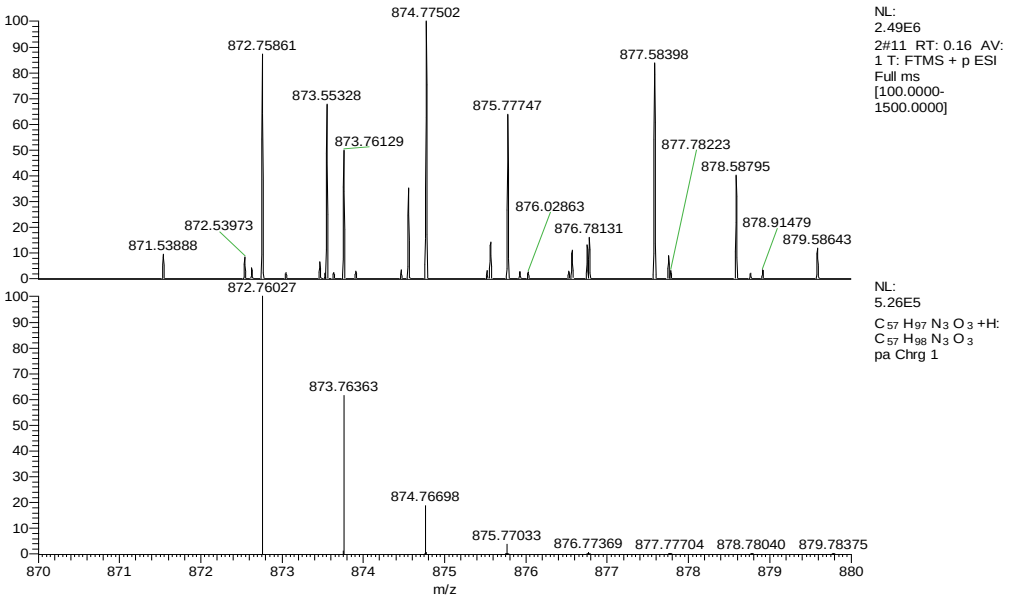


Figure S10. Experimental and theoretical HR-MS spectra of **DcTa-sa**.

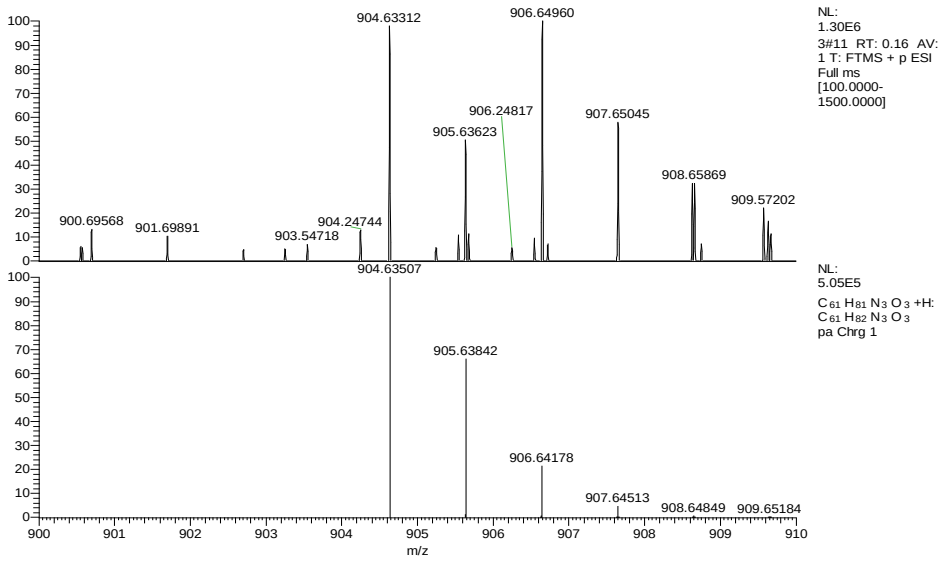


Figure S11. Experimental and theoretical HR-MS spectra of **DcTa-da**.

S5. DSC Analysis at different temperature ramp rates

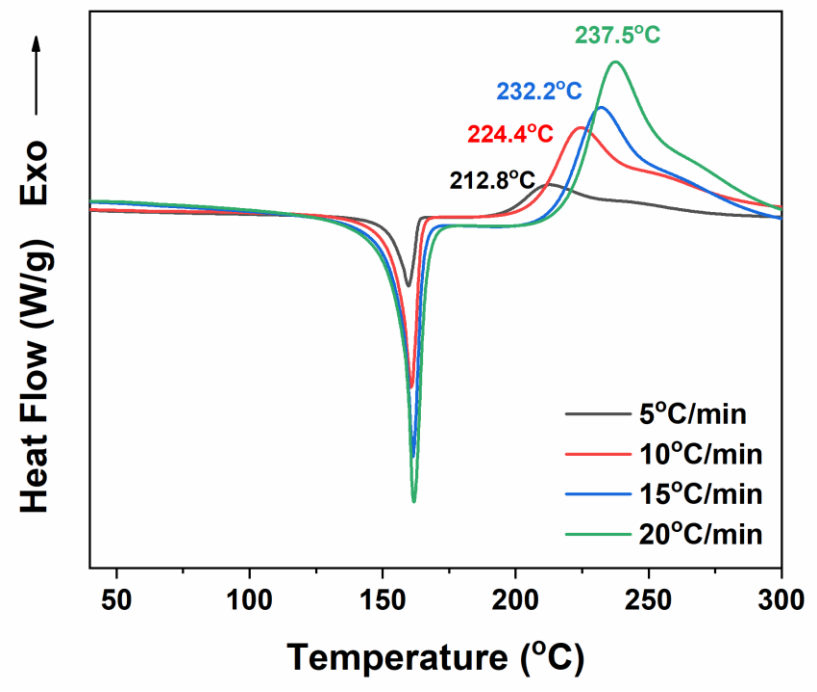


Figure S12.DSC thermograms of **DcTa-fa** at different heating rates

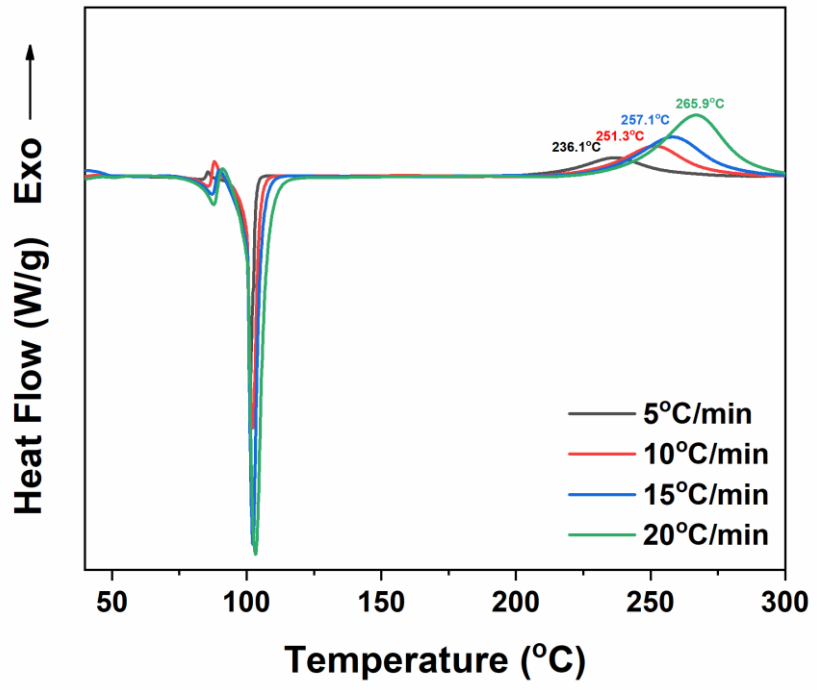


Figure S13.DSC thermograms of **DcTa-sa** at different heating rates

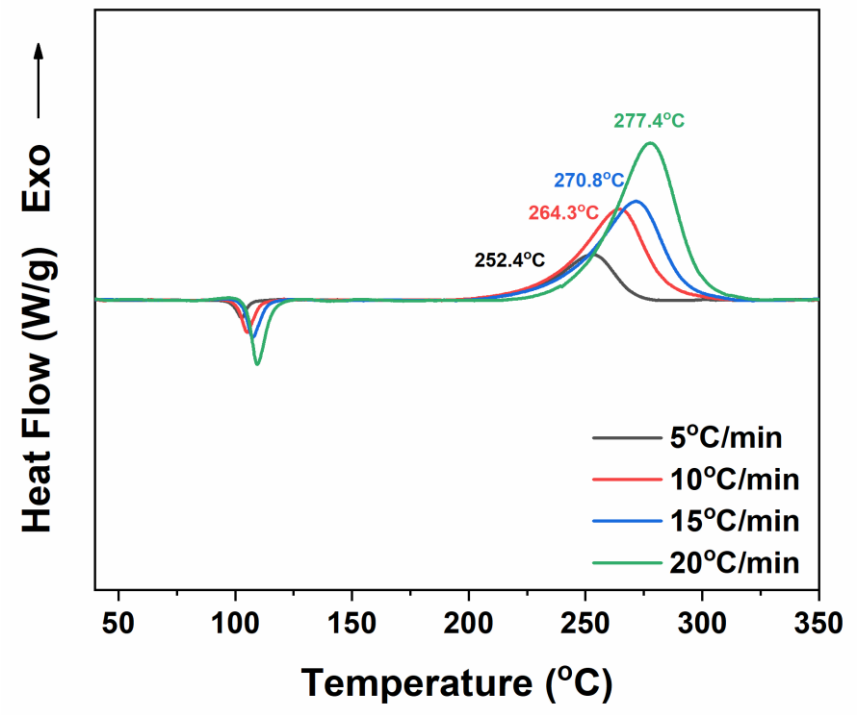


Figure S14.DSC thermograms of **DcTa-da** at different heating rates

S6. Structures of BA-a and poly(BA-a)

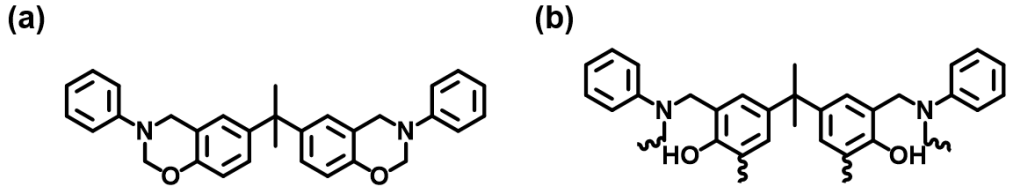
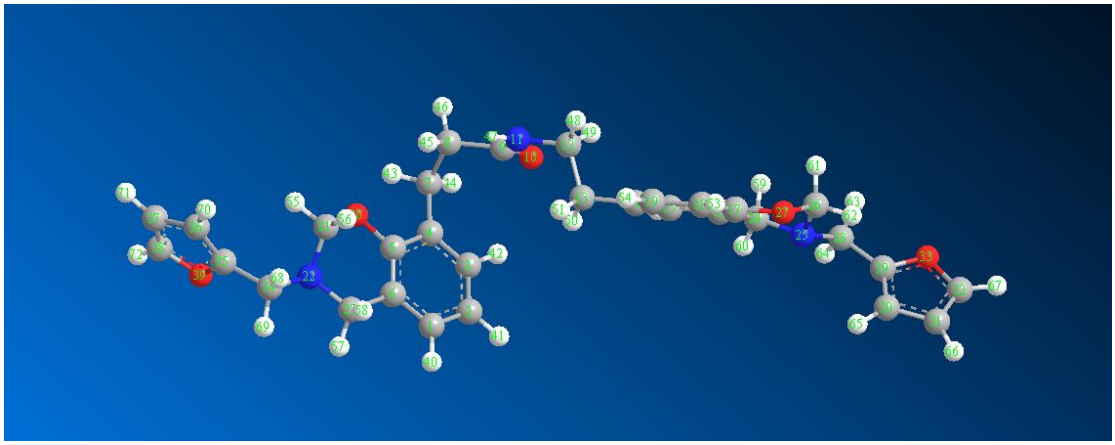


Figure S15. Structure of BA-a (a) and poly(BA-a) (b).

S7. Detailed DFT optimized structure

1. DcTa-fa



Atomic Coordinates of the Atoms.

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7	C	4	3	2	1.512979	121.6098	179.4822	-3.3001	1.373754	-2.37276
8	C	7	4	3	1.541855	113.3427	-97.5002	-2.76988	2.483218	-1.44256
9	C	8	7	4	1.527489	111.6201	68.18475	-1.26857	2.343081	-1.1983
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13	C	12	11	9	1.54476	113.3026	-84.6905	0.914537	0.96529	0.841378
14	C	13	12	11	1.51244	112.0851	176.7596	2.383879	0.821947	1.169951
15	C	14	13	12	1.399165	120.5641	-82.5168	3.330642	0.680701	0.149485

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18	C	17	16	15	1.397482	120.4936	1.09436	4.203518	0.772199	2.785809
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42	H	3	2	1	1.086375	120.2969	-179.843	-1.41829	-0.58118	-2.65164
43	H	7	4	3	1.09461	109.7976	141.1058	-4.32567	1.625227	-2.66111
44	H	7	4	3	1.093858	109.3584	22.81708	-2.68559	1.373724	-3.27769
45	H	8	7	4	1.096075	110.2305	-56.567	-3.33433	2.492002	-0.50305
46	H	8	7	4	1.098453	108.9933	-173.79	-2.92831	3.458366	-1.92275
47	H	11	9	8	1.010031	118.3362	10.59544	-1.55372	2.655671	0.806821
48	H	12	11	9	1.095734	108.5997	152.3643	0.740144	3.086606	1.322973
49	H	12	11	9	1.092528	107.0896	36.07807	1.150492	2.751868	-0.36521
50	H	13	12	11	1.095637	107.7106	54.94707	0.646998	0.329149	-0.0096
51	H	13	12	11	1.097651	109.1706	-60.8941	0.302803	0.637538	1.691788
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53	H	18	17	16	1.085675	118.7226	179.1437	4.567421	0.80088	3.808278
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57	H	23	22	21	1.097103	108.3804	-168.286	-5.77116	-3.12371	0.334048
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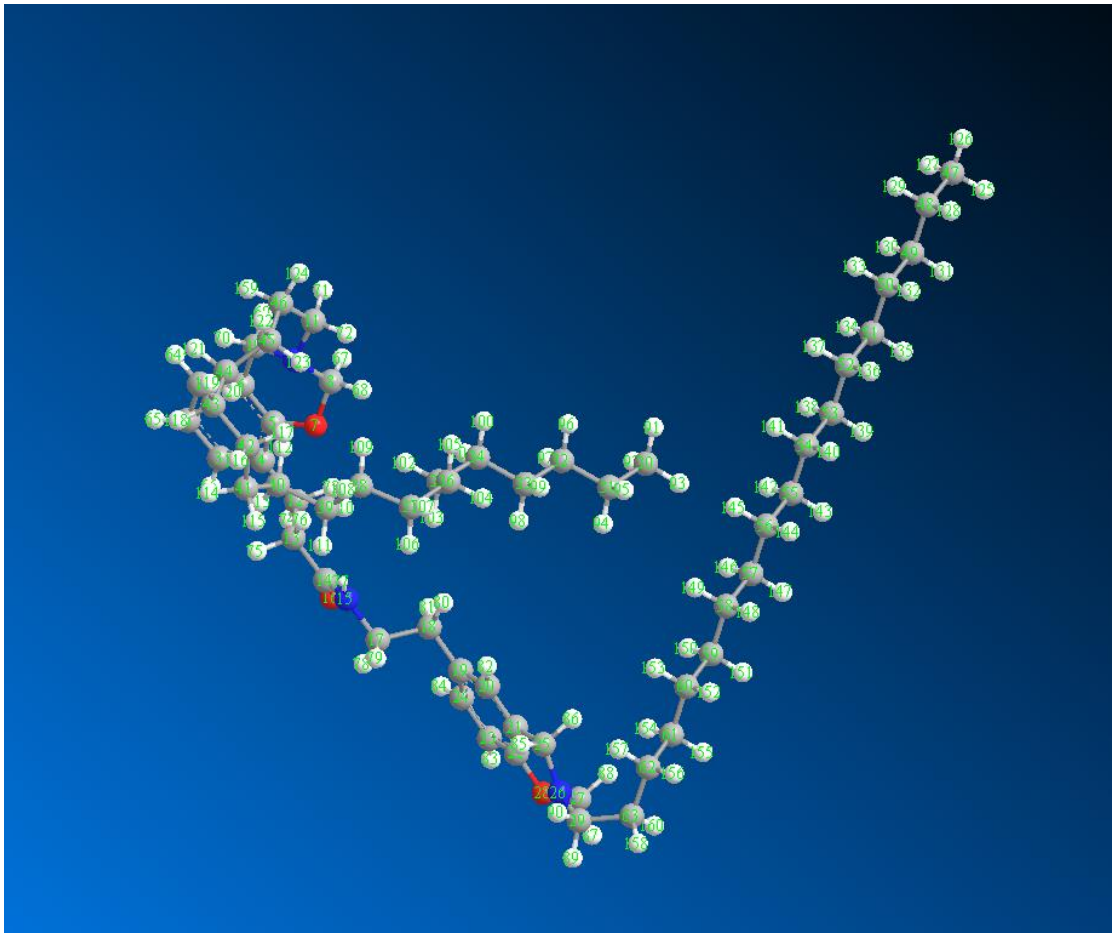
65	H	30	29	28	1.080463	125.7021	-2.60381	8.49204	-2.50781	0.689221
66	H	31	30	29	1.081277	127.2609	179.6776	11.14238	-3.25284	0.661174
67	H	32	31	30	1.079296	133.9903	179.915	12.32856	-1.4513	-1.05272

68	H	34	22	21	1.107611	112.3696	-55.918	-7.42861	-1.2524	2.381191
69	H	34	22	21	1.097176	106.6438	-172.317	-7.84517	-2.58287	1.295163
70	H	36	35	34	1.081742	126.0602	1.194898	-9.44581	0.638251	2.566777
71	H	37	36	35	1.081032	127.4639	-179.963	-11.6496	1.105028	0.996245
72	H	38	37	36	1.079461	133.7319	-179.729	-11.3272	-0.60538	-1.13819

Total Energy: -1741.487245 au

2. DcTa-sa



Atomic Coordinates of the Atoms.

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							-8.46662	3.690855	-2.49133
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14	C	13	12	4	1.526991	111.8849	176.451	-4.90475	-1.84106	-2.16418
15	N	14	13	12	1.367599	115.2837	143.9748	-4.31379	-2.36503	-1.04769
16	O	14	13	12	1.227699	122.4073	-37.9058	-4.74206	-2.32514	-3.28062
17	C	15	14	13	1.456357	121.9002	179.0935	-3.43338	-3.52321	-1.11454
18	C	17	15	14	1.544439	113.4201	84.37841	-1.97291	-3.16462	-1.46631
19	C	18	17	15	1.512504	112.2162	-178.223	-1.09243	-4.38999	-1.57072
20	C	19	18	17	1.397391	121.3637	-94.9948	-0.33013	-4.83236	-0.48633
21	C	20	19	18	1.398733	122.3402	177.749	0.455096	-5.98837	-0.54569
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23	C	22	21	20	1.39973	120.3082	-1.1895	-0.27819	-6.29695	-2.84253
24	C	23	22	21	1.389484	120.0132	0.704001	-1.05743	-5.15016	-2.75128
25	C	21	20	19	1.517746	121.3654	-178.393	1.246393	-6.46849	0.65717
26	N	25	21	20	1.453347	109.2424	167.0243	1.70907	-7.82491	0.415743
27	C	26	25	21	1.431017	113.055	44.61314	2.249998	-8.00729	-0.89649
28	O	22	21	20	1.369604	122.3786	178.871	1.242318	-7.84457	-1.90056

29	C	26	25	21	1.454357	120.1603	-167.375	2.252306	-8.61691	1.507885
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43	C	42	41	40	1.543464	115.4539	86.96605	-8.08127	3.097957	3.949754
44	C	43	42	41	1.539889	117.5515	-74.4082	-7.71848	4.039145	2.786223
45	C	44	43	42	1.536812	113.6125	-69.5214	-6.4989	4.929503	3.072029
46	C	11	9	8	1.535442	115.2191	-166.596	-6.1695	5.963146	1.976698
47	C	30	18	17	11.92471	171.6159	16.23146	12.79405	9.64644	-1.58487
48	C	47	30	18	1.532134	44.07397	58.87631	12.0879	8.744684	-0.56721
49	C	48	47	30	1.534148	113.2661	32.88103	11.65951	7.392045	-1.1507
50	C	49	48	47	1.534045	113.6234	179.9918	10.95166	6.482343	-0.13844
51	C	50	49	48	1.534207	113.5978	179.9747	10.52298	5.130075	-0.72272
52	C	51	50	49	1.534221	113.5959	179.9746	9.815598	4.220058	0.289856
53	C	52	51	50	1.534217	113.5761	179.9411	9.385838	2.868489	-0.29529
54	C	53	52	51	1.534224	113.5946	179.959	8.679294	1.957725	0.717211

55	C	54	53	52	1.534188	113.5727	179.9169	8.247968	0.60714	0.131029
56	C	55	54	53	1.534166	113.6	179.9745	7.541926	-0.30435	1.143135
57	C	56	55	54	1.534218	113.5856	-179.842	7.114159	-1.65639	0.557613
58	C	57	56	55	1.534178	113.5702	179.8887	6.410563	-2.56866	1.570729
59	C	58	57	56	1.534222	113.5785	-179.746	5.988211	-3.92319	0.987033
60	C	59	58	57	1.534234	113.5316	179.813	5.288771	-4.8364	2.002272
61	C	60	59	58	1.533885	113.5992	-179.86	4.868857	-6.19244	1.421206
62	C	61	60	59	1.535903	113.3717	178.0525	4.211954	-7.12062	2.453656
63	C	62	61	60	1.545217	114.7772	178.5709	3.744561	-8.48324	1.894634
64	H	1	2	3	1.088241	120.1478	-179.412	-9.1556	4.518769	-2.336
65	H	2	1	6	1.086228	120.2149	-179.899	-9.72742	2.698437	-3.92793
66	H	3	2	1	1.087591	119.8541	-179.788	-8.14982	0.807636	-4.25845
67	H	8	7	5	1.109065	108.2532	-71.0769	-4.43811	4.416523	-1.61063
68	H	8	7	5	1.091997	106.0435	172.0736	-3.87908	3.529631	-0.15729
69	H	10	9	8	1.110328	110.8424	-76.9054	-6.66321	5.700631	-1.36099
70	H	10	9	8	1.09497	108.9634	166.0704	-7.76746	4.993197	-0.17468
71	H	11	9	8	1.109134	110.8427	69.60572	-4.98171	6.334707	0.209106
72	H	11	9	8	1.097896	107.1304	-46.3283	-4.31356	5.117564	1.306239
73	H	12	4	3	1.095774	109.7873	138.0803	-4.70294	0.765511	-3.11851
74	H	12	4	3	1.093691	110.2013	20.37392	-5.93752	-0.12648	-4.00221
75	H	13	12	4	1.098709	109.209	57.62714	-6.84511	-1.0171	-1.84629
76	H	13	12	4	1.095143	110.0439	-59.3322	-5.58715	-0.15898	-0.96077
77	H	15	14	13	1.010353	118.8389	-7.48689	-4.41311	-1.87649	-0.1689
78	H	17	15	14	1.093119	107.4679	-36.5221	-3.83364	-4.19603	-1.87744
79	H	17	15	14	1.09557	108.4141	-152.885	-3.47351	-4.04446	-0.15175
80	H	18	17	15	1.098044	109.0251	59.39962	-1.57936	-2.4786	-0.7046

81	H	18	17	15	1.095673	107.5767	-56.5422	-1.98567	-2.62034	-2.41715
82	H	20	19	18	1.09001	119.1691	-1.87645	-0.34879	-4.26367	0.443382
83	H	23	22	21	1.085727	118.5396	-179.881	-0.23562	-6.88157	-3.75643
84	H	24	23	22	1.087686	119.4967	179.6868	-1.6426	-4.83052	-3.61062
85	H	25	21	20	1.097872	109.6081	48.60931	0.598843	-6.47942	1.54367
86	H	25	21	20	1.107289	109.5848	-67.8414	2.062613	-5.75246	0.874357
87	H	27	26	25	1.092642	109.875	177.415	2.622467	-9.02862	-1.00609
88	H	27	26	25	1.106928	113.5129	55.17592	3.065476	-7.29958	-1.14028
89	H	29	26	25	1.100019	107.1051	152.7347	2.073605	-9.6739	1.261112
90	H	29	26	25	1.098147	106.756	39.25326	1.638543	-8.39977	2.392233
91	H	30	18	17	1.097112	134.5743	5.099988	4.361605	2.472841	-1.62463
92	H	30	18	17	1.09698	79.97681	-99.6553	3.775283	1.507426	-2.98672
93	H	30	18	17	1.096367	112.4197	155.2809	5.085075	0.892992	-1.9664
94	H	31	30	18	1.099225	109.447	40.44006	2.933345	-0.24818	-1.3746
95	H	31	30	18	1.099581	109.4461	156.2599	3.519776	0.705045	-0.0207
96	H	32	31	30	1.100532	109.201	-57.9831	1.947603	2.564278	-0.64652
97	H	32	31	30	1.100231	109.1902	57.46245	1.364575	1.61524	-2.00567
98	H	33	32	31	1.100473	109.183	-58.1258	0.550394	-0.16039	-0.42389
99	H	33	32	31	1.098836	108.9412	57.35704	1.144437	0.781517	0.936255
100	H	34	33	32	1.100801	109.2542	-60.0938	-0.43582	2.644348	0.338883
101	H	34	33	32	1.099108	108.4943	55.02811	-0.97208	1.73989	-1.06854
102	H	35	34	33	1.097862	108.2707	-169.356	-2.65683	1.470375	0.599517
103	H	35	34	33	1.100915	109.0112	-54.6398	-1.85063	-0.08001	0.443855
104	H	36	35	34	1.098112	109.2472	-55.3055	-0.46815	0.473356	2.503616
105	H	36	35	34	1.100854	108.712	59.76082	-1.34743	1.983519	2.659402
106	H	37	36	35	1.100572	109.3457	61.10733	-2.54483	-0.8344	2.886074

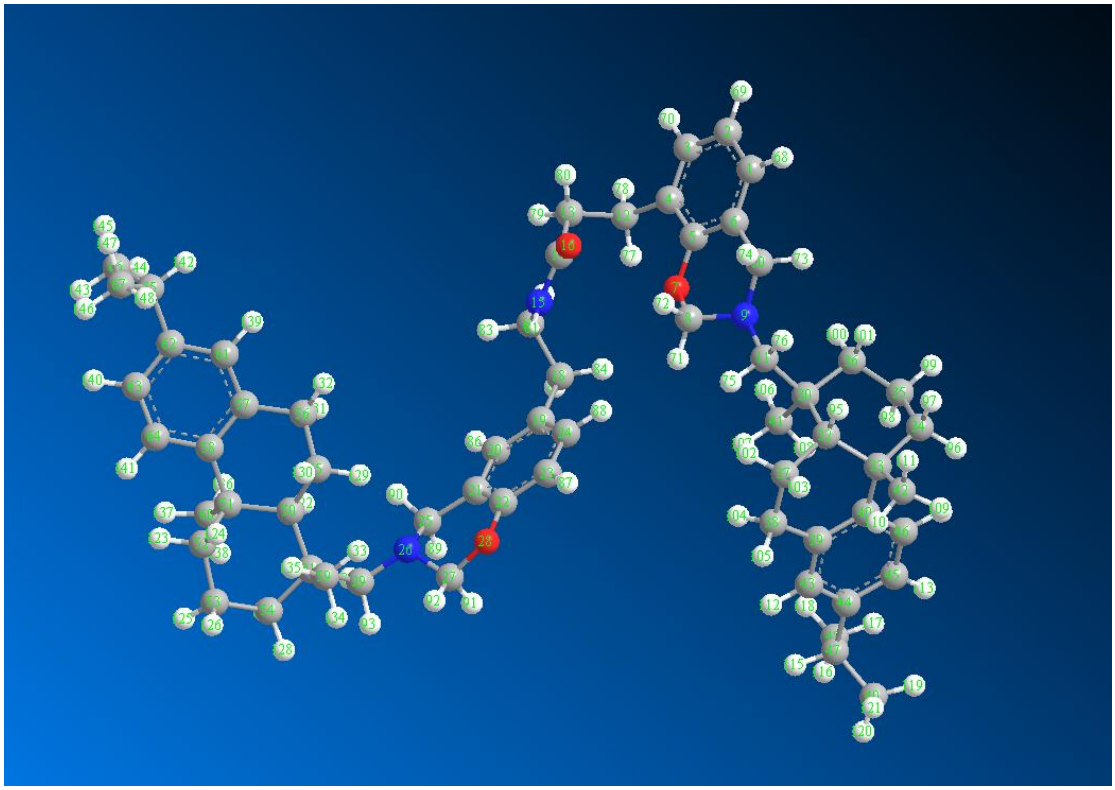
107	H	37	36	35	1.097917	107.2633	175.1281	-2.11967	0.227725	4.211452
108	H	38	37	36	1.097109	108.8675	-144.33	-4.35941	0.72601	4.157499
109	H	38	37	36	1.100488	109.3659	-29.1885	-3.84909	1.913383	2.973714
110	H	39	38	37	1.098262	108.9402	-52.9177	-4.38802	0.210127	1.144972
111	H	39	38	37	1.102066	108.3078	62.35689	-4.99872	-0.86862	2.39612
112	H	40	39	38	1.096268	109.0172	60.69287	-6.1245	1.893707	1.685731
113	H	40	39	38	1.098031	107.2417	174.226	-6.7695	0.357887	1.167916
114	H	41	40	39	1.098918	108.9615	-143.602	-8.19484	0.622661	2.940602
115	H	41	40	39	1.099685	108.0441	-29.825	-6.89156	-0.16764	3.793134
116	H	42	41	40	1.098554	107.8441	-153.624	-7.38518	1.547018	5.247363
117	H	42	41	40	1.09712	110.3633	-38.8036	-6.08821	2.314696	4.361356
118	H	43	42	41	1.099495	108.0088	49.04309	-9.07646	2.670079	3.761559
119	H	43	42	41	1.100262	108.2501	163.083	-8.1862	3.708587	4.858983
120	H	44	43	42	1.094633	110.8035	54.84377	-7.55932	3.472734	1.863147
121	H	44	43	42	1.100369	107.8763	170.7457	-8.58251	4.69455	2.599944
122	H	45	44	43	1.099469	107.9072	-54.2049	-6.68638	5.468063	4.01205
123	H	45	44	43	1.098892	110.1857	60.90605	-5.61057	4.308776	3.254052
124	H	46	11	9	1.098283	105.6867	-176.763	-5.65048	6.816652	2.43317
125	H	47	30	18	1.097077	106.8935	162.1268	13.7019	9.169361	-1.97447
126	H	47	30	18	1.09609	143.7625	0.141274	13.08679	10.60345	-1.13782
127	H	47	30	18	1.097082	71.42807	-94.6333	12.14299	9.863973	-2.44067
128	H	48	47	30	1.099413	109.4496	155.0017	12.75111	8.573959	0.292859
129	H	48	47	30	1.099417	109.4472	-89.2367	11.20384	9.263545	-0.1698
130	H	49	48	47	1.10039	109.1974	-57.7099	10.99627	7.563208	-2.01191
131	H	49	48	47	1.100385	109.1951	57.69697	12.54439	6.873382	-1.54924
132	H	50	49	48	1.100303	109.2495	-57.7617	11.61558	6.311756	0.722251

133	H	50	49	48	1.100311	109.2484	57.71866	10.06752	7.002094	0.260097
134	H	51	50	49	1.100244	109.2561	-57.7655	9.858767	5.300717	-1.5831
135	H	51	50	49	1.100243	109.2552	57.71859	11.40698	4.610572	-1.1217
136	H	52	51	50	1.100281	109.2574	-57.795	10.48017	4.048558	1.149824
137	H	52	51	50	1.10029	109.2559	57.6936	8.932026	4.739855	0.689543
138	H	53	52	51	1.100206	109.2572	-57.7856	8.72069	3.040156	-1.15468
139	H	53	52	51	1.100248	109.2555	57.70549	10.26925	2.349074	-0.69571
140	H	54	53	52	1.100292	109.2611	-57.8289	9.344963	1.784649	1.576031
141	H	54	53	52	1.100261	109.2593	57.67477	7.796535	2.477486	1.118658
142	H	55	54	53	1.100392	109.2208	-57.798	7.581538	0.780948	-0.72718
143	H	55	54	53	1.100242	109.2668	57.69398	9.130375	0.08762	-0.27145
144	H	56	55	54	1.100295	109.2532	-57.5926	8.206869	-0.47538	2.002931
145	H	56	55	54	1.100322	109.2487	57.9076	6.657573	0.214082	1.542956
146	H	57	56	55	1.100247	109.2746	-57.8685	6.447519	-1.4858	-0.3009
147	H	57	56	55	1.100233	109.2522	57.65208	7.998213	-2.17391	0.156208
148	H	58	57	56	1.100298	109.2504	-57.5182	7.075599	-2.73609	2.431165
149	H	58	57	56	1.100253	109.257	57.99005	5.524181	-2.05279	1.969174
150	H	59	58	57	1.100091	109.2912	-57.8964	5.321371	-3.75677	0.128064
151	H	59	58	57	1.100186	109.2453	57.63911	6.874488	-4.43793	0.587076
152	H	60	59	58	1.100365	109.2849	-57.6263	5.955286	-5.00157	2.862086
153	H	60	59	58	1.100424	109.2767	57.86279	4.401646	-4.32262	2.402236
154	H	61	60	59	1.098583	109.1578	-58.6441	4.19044	-6.02677	0.573156
155	H	61	60	59	1.100148	109.2688	56.65151	5.752489	-6.69805	1.00422
156	H	62	61	60	1.098498	107.7424	-59.9204	4.940144	-7.29614	3.257166
157	H	62	61	60	1.099753	109.7815	54.48632	3.365533	-6.60605	2.931406
158	H	63	62	61	1.098965	109.105	142.9202	3.920703	-9.26154	2.650242

159	H	46	11	9	1.098529	110.4566	-63.2377	-7.09835	6.375614	1.559703
160	H	63	62	61	1.099677	109.5167	28.06809	4.372409	-8.76306	1.036266

Total Energy: -2620.474156 au

3. DcTa-da



Atomic Coordinates of the Atoms.

Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z

1	C							4.904107	6.482341	0.327668
2	C	1			1.391912			4.320673	7.422479	-0.51682
3	C	2	1		1.396423	119.4574		3.299708	7.027043	-1.38357
4	C	3	2	1	1.396348	121.4184	0.292219	2.844974	5.707277	-1.41853
5	C	4	3	2	1.40526	117.9765	-0.90226	3.459837	4.775346	-0.56518
6	C	1	2	3	1.39802	120.8474	0.381447	4.486335	5.148287	0.312658
7	O	5	4	3	1.372963	117.2174	-178.581	3.021048	3.476195	-0.63373
8	C	7	5	4	1.424287	113.6454	-159.798	3.334299	2.70569	0.522469
9	N	8	7	5	1.447218	110.7178	-53.8462	4.751125	2.768033	0.810841
10	C	9	8	7	1.461367	109.9925	67.68394	5.116826	4.119588	1.229357
11	C	9	8	7	1.468832	114.668	-161.068	5.246758	1.69595	1.684026
12	C	4	3	2	1.512379	120.9785	177.441	1.700041	5.302023	-2.31975
13	C	12	4	3	1.555192	113.8746	-92.0607	0.30486	5.375476	-1.63659
14	C	13	12	4	1.52757	114.8593	-70.0568	0.060034	4.318713	-0.56106
15	N	14	13	12	1.372934	118.0063	-88.1487	-0.45765	3.108741	-0.95211
16	O	14	13	12	1.22732	121.5462	93.36546	0.288941	4.543235	0.623641
17	C	15	14	13	1.452738	130.1129	8.450781	-0.68027	2.572291	-2.28369
18	C	17	15	14	1.545886	112.5774	121.6665	0.072227	1.243022	-2.5215
19	C	18	17	15	1.514423	113.4128	64.7217	-0.4116	0.11142	-1.63896
20	C	19	18	17	1.399751	120.7756	82.51364	-1.54567	-0.63236	-1.98534
21	C	20	19	18	1.396839	122.2918	-178.052	-2.04277	-1.65602	-1.17529
22	C	21	20	19	1.402806	118.4792	-0.41482	-1.37121	-1.94811	0.021182
23	C	22	21	20	1.397275	120.4479	0.948235	-0.24324	-1.21427	0.39741
24	C	23	22	21	1.391592	119.8033	-0.77152	0.22706	-0.19717	-0.42774
25	C	21	20	19	1.514945	121.7644	178.8214	-3.28653	-2.43603	-1.54904
26	N	25	21	20	1.462515	109.861	-163.342	-3.7985	-3.14609	-0.37744

27	C	26	25	21	1.446514	109.7517	-48.3123	-2.71841	-3.85084	0.277642
28	O	22	21	20	1.368688	121.9628	-179.301	-1.78786	-2.94523	0.861104
29	C	26	25	21	1.470291	114.7146	-178.457	-4.98997	-3.96975	-0.62991
30	C	11	9	8	1.559545	113.9823	116.4922	6.286947	0.754103	1.003503
31	C	29	26	25	1.556893	116.0987	-122.491	-6.24513	-3.64038	0.230318
32	C	30	11	9	1.576684	107.7413	175.0272	6.812542	-0.25177	2.097986
33	C	32	30	11	1.571317	116.0069	-164.95	8.120391	-1.04344	1.734894
34	C	33	32	30	1.547998	109.1052	48.06936	9.178434	-0.05229	1.19225
35	C	34	33	32	1.528159	113.9748	-52.7314	8.676555	0.826269	0.047032
36	C	35	34	33	1.529841	109.5593	58.76349	7.464563	1.634267	0.51461
37	C	32	30	11	1.546789	115.8566	64.91776	5.763758	-1.2338	2.670899
38	C	37	32	30	1.542445	115.3238	80.86367	5.474356	-2.47268	1.798801
39	C	38	37	32	1.518609	115.8318	25.92685	6.597203	-2.90737	0.873362
40	C	39	38	37	1.407102	122.655	-1.50066	7.818061	-2.21364	0.782909
41	C	30	11	9	1.542573	107.914	-59.9595	5.607866	0.100957	-0.21788
42	C	33	32	30	1.554918	109.5931	163.9754	8.728569	-1.66488	3.023966
43	C	39	38	37	1.402054	117.734	-179.797	6.375151	-4.02697	0.05915
44	C	43	39	38	1.395076	122.8809	178.5684	7.320521	-4.50141	-0.85048
45	C	44	43	39	1.401291	117.1326	-0.18301	8.533537	-3.80473	-0.93328
46	C	45	44	43	1.391475	120.748	0.179393	8.770707	-2.69161	-0.13271
47	C	44	43	39	1.522519	120.9789	-179.978	7.033377	-5.72185	-1.71426
48	C	47	44	43	1.540467	111.8464	117.0279	7.022559	-5.37257	-3.21457
49	C	47	44	43	1.540426	111.8829	-117.753	8.013071	-6.87446	-1.42338
50	C	31	29	26	1.588773	109.664	64.46418	-6.75957	-2.17694	-0.11303
51	C	50	31	29	1.586938	115.3401	141.3001	-8.33646	-2.00457	-0.15854
52	C	51	50	31	1.549765	108.981	30.20831	-8.98196	-3.00784	0.830694

53	C	52	51	50	1.543112	113.957	-60.29	-8.67441	-4.48635	0.513515
54	C	53	52	51	1.541987	113.5768	30.79957	-7.30103	-4.70121	-0.15387
55	C	50	31	29	1.538766	111.884	-88.7109	-6.08067	-1.10996	0.763584
56	C	55	50	31	1.525825	110.8177	171.4652	-6.42965	0.293593	0.277382
57	C	56	55	50	1.508942	110.3028	60.41062	-7.92084	0.514779	0.343113
58	C	57	56	55	1.405302	120.1173	-29.6022	-8.80193	-0.56916	0.189411
59	C	31	29	26	1.545553	108.377	-59.8345	-5.87818	-3.8289	1.719795
60	C	51	50	31	1.554726	109.3743	-90.6832	-8.84222	-2.26502	-1.60545
61	C	57	56	55	1.402016	119.8521	148.7029	-8.42555	1.798623	0.593426
62	C	61	57	56	1.394741	122.7307	-178.774	-9.79085	2.066315	0.691447
63	C	62	61	57	1.401882	117.065	0.240264	-10.6663	0.982911	0.532867
64	C	63	62	61	1.390515	120.778	-0.04959	-10.1786	-0.29604	0.288024
65	C	62	61	57	1.522349	121.036	179.936	-10.2966	3.475707	0.965964
66	C	65	62	61	1.540484	111.855	117.7558	-11.1597	4.011017	-0.19233
67	C	65	62	61	1.540443	111.8809	-117.023	-11.0542	3.563241	2.304359
68	H	1	2	3	1.088306	120.0918	179.8537	5.702205	6.778723	1.005612
69	H	2	1	6	1.086217	120.3002	-179.398	4.658867	8.454634	-0.50469
70	H	3	2	1	1.088123	119.773	179.8152	2.837936	7.758384	-2.04382
71	H	8	7	5	1.091032	105.8513	-172.355	3.057949	1.678488	0.279905
72	H	8	7	5	1.105893	107.4971	70.61169	2.699703	3.07441	1.349713
73	H	10	9	8	1.095741	108.7828	-165.815	6.207839	4.215929	1.196834
74	H	10	9	8	1.109608	111.6017	76.83186	4.811797	4.319298	2.277357
75	H	11	9	8	1.098015	109.0623	-6.27406	4.394942	1.103742	2.04366
76	H	11	9	8	1.100173	109.1648	-121.409	5.701197	2.141949	2.581217
77	H	12	4	3	1.095156	110.1401	144.0301	1.868693	4.294149	-2.71359
78	H	12	4	3	1.096555	108.514	27.34545	1.677524	5.980777	-3.18069

79	H	13	12	4	1.096262	108.8579	165.2292	-0.47109	5.328102	-2.40955
80	H	13	12	4	1.093246	108.917	48.3284	0.20746	6.340628	-1.13243
81	H	15	14	13	1.014328	112.8668	-179.288	-0.59926	2.471242	-0.17596
82	H	17	15	14	1.091378	108.8318	0.787129	-0.34533	3.305517	-3.01942
83	H	17	15	14	1.1002	110.1359	-116.362	-1.75556	2.411995	-2.45254
84	H	18	17	15	1.096218	108.2431	-58.0707	1.141965	1.4208	-2.36103
85	H	18	17	15	1.097855	107.655	-173.718	-0.05808	0.970876	-3.57707
86	H	20	19	18	1.089706	119.1944	1.686671	-2.06542	-0.4067	-2.91614
87	H	23	22	21	1.08556	118.7118	179.8055	0.252775	-1.46216	1.330659
88	H	24	23	22	1.08718	119.3156	-179.197	1.113054	0.360037	-0.13364
89	H	25	21	20	1.109855	110.1197	73.20105	-3.06448	-3.1307	-2.38565
90	H	25	21	20	1.09583	109.6711	-43.8816	-4.05943	-1.7476	-1.90895
91	H	27	26	25	1.109345	112.2884	-53.5285	-2.16319	-4.51147	-0.41946
92	H	27	26	25	1.089983	110.042	-175.244	-3.10801	-4.44898	1.101361
93	H	29	26	25	1.102462	109.6664	114.7353	-4.74367	-5.03399	-0.48104
94	H	29	26	25	1.09814	108.5556	-0.05619	-5.26086	-3.87674	-1.69005
95	H	32	30	11	1.1019	103.9907	-50.7301	7.105869	0.398072	2.93813
96	H	34	33	32	1.095753	110.4482	-178.89	10.09443	-0.58499	0.913208
97	H	34	33	32	1.100152	107.1121	66.91258	9.466352	0.603252	2.027537
98	H	35	34	33	1.097112	110.3999	-63.5375	8.421654	0.210147	-0.82422
99	H	35	34	33	1.097824	109.8586	179.4069	9.473942	1.50754	-0.27741
100	H	36	35	34	1.095597	111.1316	178.2718	7.101838	2.297116	-0.27873
101	H	36	35	34	1.101621	107.8229	61.75005	7.791054	2.283127	1.342833
102	H	37	32	30	1.09495	110.9033	-43.6884	4.821321	-0.71855	2.883602
103	H	37	32	30	1.094991	107.3053	-157.768	6.129527	-1.56774	3.647476
104	H	38	37	32	1.097365	110.0454	-96.4993	4.582748	-2.29925	1.183037

105	H	38	37	32	1.098806	108.8376	149.1142	5.205255	-3.31275	2.453974
106	H	41	30	11	1.095385	108.872	59.32335	5.280849	0.888933	-0.90492
107	H	41	30	11	1.095209	111.8258	-59.3933	4.722257	-0.47609	0.068827
108	H	41	30	11	1.091904	112.7318	179.3947	6.274606	-0.57096	-0.76216
109	H	42	33	32	1.096128	109.727	-172.639	9.706445	-2.10491	2.796763
110	H	42	33	32	1.093508	112.6595	68.21485	8.107323	-2.46245	3.440732
111	H	42	33	32	1.097825	110.9439	-53.4483	8.873507	-0.89975	3.797787
112	H	43	39	38	1.090007	118.2896	-1.21108	5.419158	-4.5441	0.141414
113	H	45	44	43	1.08753	120.1974	-179.82	9.304665	-4.12969	-1.62789
114	H	46	45	44	1.084996	118.0436	179.7742	9.726545	-2.18753	-0.23015
115	H	47	44	43	1.098828	107.066	-0.3516	6.025855	-6.07302	-1.45157
116	H	48	47	44	1.096777	110.7142	-176.765	6.757889	-6.25107	-3.8155
117	H	48	47	44	1.09656	111.2544	63.55907	8.007436	-5.02524	-3.54896
118	H	48	47	44	1.095482	111.1733	-56.4674	6.298626	-4.57936	-3.43095
119	H	49	47	44	1.09656	111.2705	-63.5957	9.0425	-6.59537	-1.67799
120	H	49	47	44	1.096764	110.7067	176.7386	7.753674	-7.76205	-2.01311
121	H	49	47	44	1.095488	111.1818	56.44974	7.995459	-7.15097	-0.36351
122	H	50	31	29	1.100482	105.6064	25.69611	-6.41896	-1.97677	-1.14015
123	H	52	51	50	1.094417	110.4012	176.9259	-10.0675	-2.87149	0.858317
124	H	52	51	50	1.096764	107.782	62.24699	-8.63049	-2.75723	1.838939
125	H	53	52	51	1.096688	109.9351	-91.314	-9.45262	-4.89823	-0.14029
126	H	53	52	51	1.096558	108.5469	153.4847	-8.73307	-5.06236	1.444756
127	H	54	53	52	1.096973	109.8544	-93.62	-7.41408	-4.7085	-1.24498
128	H	54	53	52	1.098328	109.583	151.1038	-6.91766	-5.69732	0.105177
129	H	55	50	31	1.093228	109.1499	49.45905	-4.9987	-1.26529	0.744217
130	H	55	50	31	1.09781	110.4436	-68.2222	-6.40513	-1.20836	1.807724

131	H	56	55	50	1.102074	109.4658	-61.3261	-6.06573	0.425903	-0.75443
132	H	56	55	50	1.096981	110.6576	-177.803	-5.91346	1.051298	0.879711
133	H	59	31	29	1.092794	111.8656	58.54224	-5.04288	-3.19011	2.017168
134	H	59	31	29	1.098114	109.6654	-61.0673	-5.58469	-4.87179	1.898955
135	H	59	31	29	1.09361	112.4907	179.8578	-6.71621	-3.61133	2.387886
136	H	60	51	50	1.096094	110.1313	-64.5553	-8.44548	-1.50339	-2.28658
137	H	60	51	50	1.095293	111.0945	176.6401	-9.93501	-2.21163	-1.65666
138	H	60	51	50	1.093161	112.7797	55.72634	-8.54047	-3.24293	-1.9897
139	H	61	57	56	1.08947	118.2339	0.832496	-7.71604	2.615345	0.721879
140	H	63	62	61	1.087565	120.1762	179.9133	-11.7411	1.134076	0.600969
141	H	64	63	62	1.0863	117.9574	-179.384	-10.8981	-1.10011	0.162501
142	H	65	62	61	1.098729	107.0534	0.375437	-9.41388	4.125105	1.045118
143	H	66	65	62	1.096613	111.279	63.59436	-12.0703	3.413387	-0.31926
144	H	66	65	62	1.095504	111.1793	-56.4632	-10.6102	3.986121	-1.1397
145	H	66	65	62	1.09673	110.6975	-176.738	-11.4656	5.046738	-0.00124
146	H	67	65	62	1.096609	111.2624	-63.5585	-11.9599	2.945036	2.289848
147	H	67	65	62	1.096739	110.7051	176.7613	-11.3598	4.596271	2.510158
148	H	67	65	62	1.09544	111.1711	56.48784	-10.4294	3.21945	3.135875

Total Energy: -2763.227827 au