

Novel acrylamide / acrylonitrile tethered carbazoles: synthesis, structural, biological and density functional theory studies

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Supplementary Information

Table S1. Experimental and calculated structural parameters of **6g**.

Bond length	Expt	Calc	Bond length	Expt	Calc
C1-C2	1.428(6)	1.413	C15-C20	1.413(5)	1.425
C1-N4	1.141(5)	1.158	C16-C17	1.363(5)	1.383
C3-C2	1.343(5)	1.356	C18-C17	1.411(5)	1.420
S5-C2	1.761(4)	1.822	C18-C19	1.393(5)	1.408
C18-C3	1.438(5)	1.447	C19-C20	1.379(5)	1.386
S5-O6	1.429(3)	1.467	C21-C20	1.442(5)	1.449
S5-O7	1.433(3)	1.462	C21-C22	1.390(5)	1.396
S5-C8	1.752(4)	1.801	C21-C26	1.395(5)	1.416
C8-C9	1.377(6)	1.393	C23-C22	1.382(6)	1.390
C13-C8	1.371(5)	1.394	C23-C24	1.380(6)	1.402
C10-C9	1.386(6)	1.393	C25-C24	1.366(5)	1.392
C11-C10	1.381(7)	1.394	C25-C26	1.395(5)	1.395
C12-C11	1.361(7)	1.395	C27-C28	1.512(6)	1.535
C13-C12	1.375(6)	1.391	C29-C28	1.492(6)	1.532
N14-C15	1.373(5)	1.377	C29-C30	1.448(7)	1.533
N14-C26	1.398(5)	1.397	C30-C31	1.528(12)	1.533
N14-C27	1.448(5)	1.457	C31-C32	1.209(14)	1.531
C16-C15	1.384(5)	1.400			
Bond angle	Expt	Calc	Bond angle	Expt	Calc
C3-C2-C1	126.5(4)	127.8	C17-C16-C15	119.1(4)	117.8
C1-C2-S5	113.0(3)	114.6	C16-C17-C18	121.7(4)	122.5
C3-C2-S5	120.5(3)	117.6	C17-C18-C3	123.3(4)	116.7
C2-C3-C18	132.0(4)	131.3	C19-C18-C3	118.3(3)	124.5
O6-S5-C2	107.3(19)	106.4	C19-C18-C17	118.4(4)	118.9
O7-S5-C2	108.5(18)	107.6	C20-C19-C18	121.1(4)	119.6
C8-S5-C2	102.5(17)	103.9	C19-C20-C15	118.7(4)	120.2
O6-S5-O7	120.3(18)	121.6	C15-C20-C21	106.5(3)	106.5
O6-S5-C8	108.2(19)	108.0	C19-C20-C21	134.8(4)	133.4
O7-S5-C8	108.4(2)	107.9	C22-C21-C20	134.0(4)	133.8
C9-C8-S5	118.5(3)	119.0	C26-C21-C20	107.0(3)	106.5

C13-C8-S5	120.2(4)	119.2	C22-C21-C26	119.0(4)	119.7
C13-C8-C9	121.2(4)	121.9	C23-C22-C21	118.8(4)	118.9
C8-C9-C10	118.7(5)	118.7	C24-C23-C22	120.9(4)	120.7
C11-C10-C9	119.8(5)	120.2	C25-C24-C23	121.8(4)	121.5
C12-C11-C10	120.7(5)	120.4	C24-C25-C26	117.3(4)	117.6
C11-C12-C13	119.9(5)	120.1	C21-C26-N14	109.0(3)	109.1
C8-C13-C12	119.7(5)	118.8	C25-C26-N14	128.9(4)	129.4
C15-N14-C26	108.5(3)	108.7	C21-C26-C25	122.1(4)	121.6
C15-N14-C27	126.8(3)	125.7	N14-C27-C28	113.4(3)	113.7
C26-N14-C27	124.8(3)	125.5	C29-C28-C27	114.4(4)	112.4
N14-C15-C16	129.8(4)	129.7	C30-C29-C28	116.8(5)	113.3
N14-C15-C20	109.1(3)	109.2	C29-C30-C31	112.8(6)	113.5
C16-C15-C20	121.0(4)	121.1	C32-C31-C30	118.4(11)	113.2
Dihedral angle	Expt	Calc	Dihedral angle	Expt	Calc
C18-C3-C2-C1	2.33	-0.5	C26-N14-C27-C28	84.25	89.3
C18-C3-C2-S5	-176.2	177.5	C17-C16-C15-N14	-179.98	-179.5
O6-S5-C2-C1	170.53	179.4	C17-C16-C15-C20	-0.26	0.3
O7-S5-C2-C1	38.99	47.6	N14-C15-C20-C19	179.69	179.5
C8-S5-C2-C1	-75.54	-66.7	N14-C15-C20-C21	0.66	-0.4
O6-S5-C2-C3	-10.76	1.1	C16-C15-C20-C19	-0.08	-0.4
O7-S5-C2-C3	-142.3	-130.6	C16-C15-C20-C21	-179.12	179.7
C8-S5-C2-C3	103.18	115.1	C15-C16-C17-C18	0.33	-0.1
C17-C18-C3-C2	0.83	-178.8	C3-C18-C17-C16	178.97	-179.8
C19-C18-C3-C2	179.85	1.3	C19-C18-C17-C16	-0.06	0.0
C2-S5-C8-C9	82	90.2	C3-C18-C19-C20	-179.37	179.7
C2-S5-C8-C13	-93.62	-90.3	C17-C18-C19-C20	-0.29	-0.1
O6-S5-C8-C9	-164.78	-157.1	C18-C19-C20-C15	0.36	0.3
O6-S5-C8-C13	19.6	22.4	C18-C19-C20-C21	179.06	-179.8
O7-S5-C8-C9	-32.65	-23.9	C22-C21-C20-C15	179.12	179.8
O7-S5-C8-C13	151.72	155.6	C26-C21-C20-C15	-0.45	0.0
S5-C8-C9-C10	-176.11	179.9	C22-C21-C20-C19	0.31	-0.1
C13-C8-C9-C10	-0.53	-178.8	C26-C21-C20-C19	-179.26	-179.9
C12-C13-C8-S5	176.36	-179.7	C20-C21-C22-C23	-178.63	-180.0

C12-C13-C8-C9	0.85	-0.2	C26-C21-C22-C23	0.9	-0.1
C11-C10-C9-C8	0.65	-0.2	C20-C21-C26-N14	0.09	0.5
C12-C11-C10-C9	-1.13	-0.2	C20-C21-C26-C25	179.58	-179.8
C13-C12-C11-C10	1.45	0.3	C22-C21-C26-N14	-179.56	-179.4
C8-C13-C12-C11	-1.3	-0.1	C22-C21-C26-C25	-0.06	0.3
C26-N14-C15-C16	179.14	-179.4	C24-C23-C22-C21	-1.53	0.0
C26-N14-C15-C20	-0.61	0.7	C22-C23-C24-C25	1.32	0.0
C27-N14-C15-C16	0.78	-1.8	C26-C25-C24-C23	-0.45	0.1
C27-N14-C15-C20	-178.97	178.3	C24-C25-C26-N14	179.21	179.3
C15-N14-C26-C21	0.32	-0.8	C24-C25-C26-C21	-0.18	-0.3
C15-N14-C26-C25	-179.13	179.6	N14-C27-C28-C29	64.44	-179.9
C27-N14-C26-C21	178.71	-178.4	C30-C29-C28-C27	179.63	-179.1
C27-N14-C26-C25	-0.73	2.0	C28-C29-C30-C31	174.4	180.0
C15-N14-C27-C28	-97.65	-87.9	C29-C30-C31-C32	-172.05	-179.6

Table S2. Experimental and calculated vibrational frequencies along with their proposed assignment of **6g**

Mode	Expt	Unscaled	Scale	I_{IR}	Assignment
1		14	14	3.8	$\Gamma C2C3C18C17$ [35]; $\Gamma C3C2S5C8$ [27]
2		15	15	3.37	$\Gamma C15N14C27C28$ [23]; $\Gamma C18C3C2S5$ [10]; $\Gamma C29C28C27N14$ [18]
3		20	19	3.43	$\Gamma C18C3C2S5$ [33]; $\tau C3C17C19C18$ [10]
4		27	26	3.38	$\Gamma C2S5C8C9$ [47]; $\Gamma C3C2S5C8$ [11]; $\tau C27C15C26N14$ [17]
5		32	31	3.03	$\Gamma C2S5C8C9$ [33]; $\Gamma C3C2S5C8$ [22]; $\tau C27C15C26N14$ [18]
6		46	45	4.4	$\Gamma C2C3C18C17$ [16]; $\Gamma C3C2S5C8$ [17]
7		58	56	1.08	$\Gamma C29C28C27N14$ [24]; $\Gamma C28C29C30C31$ [10]
8		59	57	2.89	$\Gamma C27C28C29C30$ [38]
9		67	65	2.03	$\Gamma C15N14C27C28$ [13]; $\Gamma C28C29C30C31$ [23]
10		74	72	3.95	$\beta C2C3C18$ [14]; $\beta C3C18C19$ [14]; $\Gamma C29C30C31C32$ [10]
11		105	102	1	$\tau C27C15C26N14$ [15]; $\beta C28C29C30$ [17]; $\beta C29C30C31$ [13]
12		114	111	6.17	$\tau C20C21C26C22$ [20]; $\tau C21C15C19C20$ [12]
13		133	129	6.02	$\Gamma C29C28C27N14$ [10]; $\Gamma C28C29C30C31$ [10]; $\Gamma C29C30C31C32$ [10]; $\beta C1C2C3$ [17]
14		136	132	7.14	$\Gamma C29C28C27N14$ [15]; $\Gamma C28C29C30C31$ [17]
15		141	137	1.86	$\Gamma C27C28C29C30$ [13]; $\Gamma C29C30C31C32$ [16]; $\beta C3C2S5$ [13]
16		142	138	3.88	$\beta C3C2S5$ [21]
17		149	145	4.8	$\beta C3C2S5$ [35]
18		165	160	8.45	$\beta C2C1N4$ [12]; $\beta C1C2C3$ [23]
19		184	178	4.38	$\beta C9C8S5$ [50]; $\beta C8S5O7$ [12]
20		195	189	3.51	$\tau C1C3S5C2$ [11]; $\beta C8S5O7$ [11]
21		219	212	2.46	$\beta C27C28C29$ [10]; $\beta C30C31C32$ [11]
22		246	239	1.91	$\Gamma H56C32C31C30$ [27]; $\Gamma H58C32C31C30$ [23]
23		249	242	2.67	$\Gamma H57C32C31C30$ [15]; $\beta C27C28C29$ [16]; $\beta C30C31C32$ [16]

24		277	269	5.4	τ S5C8C9C13 [23]; τ O6C2O7S5 [11]
25		281	273	3.7	β C26N14C27 [19]
26		294	285	5.91	β C26N14C27 [12]; β C8S5O7 [10]; Γ C15C20C18C19 [13]
27		302	293	6.36	ν S5C8 [38]; τ O6C2O7S5 [11]
28		314	305	4.5	β C2S5C8 [17]; Γ N4C1C2S5 [11]
29		330	320	4.93	Γ C21C26C24C25 [10]
30		349	339	2.74	β C3C18C19 [14]; β C8S5O7 [15]
31		401	389	7.38	Γ C19C20C21C26 [15]
32		413	401	3	Γ C10C9C11C12 [38]; Γ C11C10C12C13 [20]; Γ H34C9C10C11 [11]; Γ H38C13C12C11 [12]
33		415	403	19.39	Γ C15C20C18C19 [13]; Γ C15C20C16C17 [18]; β O6S5O7 [18]
34		423	410	6.11	β C9C8S5 [13]; τ O7C2C8S5 [30]
35	420	435	422	9.82	τ C20C21C26C22 [10]; Γ C15C20C18C19 [14]; Γ C15C20C16C17 [10]
36		438	425	9.74	β C27C28C29 [11]; β C28C29C30 [12]; β C29C30C31 [11]; β C30C31C32 [33]
37		450	437	8.04	Γ C15C20C16C17 [12]
38		458	444	10.19	Γ C15C20C16C17 [11]; β O6S5O7 [14]
39		465	451	8.31	τ N14C21C25C26 [12]
40		488	473	7.82	β C2C1N4 [16]
41		529	513	33.16	β O6S5O7 [11]; τ O6C2O7S5 [18]
42		544	528	25.57	β O6S5O7 [10]; τ O6C2O7S5 [11]
43		580	563	11.6	Γ C24C23C25C26 [18]; Γ C23C22C24C25 [34]
44		588	570	63.39	Γ C17C16C18C19 [26]
45	596	610	592	25.28	β C19C20C21 [12]; β C16C15C20 [21]
46		619	600	32.54	τ C3C17C19C18 [10]
47		628	609	1.84	β C9C10C11 [31]; β C11C12C13 [43]
48		632	613	30.11	β C20C21C26 [14]
49	626	642	623	11.95	β C18C19C20 [19]; β C23C24C25 [11]; β C16C17C18 [22]
50		649	630	30.89	Γ N4C1C2S5 [16]; τ C1C3S5C2 [26]; τ C3C17C19C18 [13]
51	686	702	681	27.42	Γ C10C9C11C12 [18]; Γ C11C10C12C13 [14]; Γ C8C13C11C12 [39]; Γ H36C11C12C13 [10]

52		718	696	35.86	vS5C8 [24]; β C10C11C12 [29]
53		736	714	10.8	ГH54C31C30C29 [12]; ГH50C29C30C31 [16]; ГH52C30C31C32 [18]; β H50C29C30 [11]
54		745	723	11.57	ГC8C13C11C12 [21]
55		746	724	15.37	ГH43C23C24C25 [11]
56		749	727	11.37	ГH48C28C29C30 [11]
57		753	730	22.93	β H34C9C10 [16]; β H35C10C11 [13]
58		764	741	17.44	ГH36C11C12C13 [14]; ГH35C10C11C12 [18]; ГH37C12C11C10 [19]
59	746	767	744	18.77	τ N14C21C25C26 [24]; ГC21C26C24C25 [11]; ГH44C24C25C26 [11]
60		782	759	6.18	ГC21C26C24C25 [10]; τ C21C15C19C20 [18]; ГH41C19C20C15 [10]
61		794	770	24.05	ГH49C28C29C30 [11]; β H46C27H47 [11]
62		799	775	20.78	β C1C2C3 [13]; vC1C2 [10]
63	798	818	793	24.69	ГC15C20C16C17 [11]; ГH39C16C17C18 [42]; ГH40C17C18C3 [31]
64		858	832	0.21	ГH34C9C10C11 [24]; ГH35C10C11C12 [25]; ГH37C12C11C10 [23]; ГH38C13C12C11 [27]
65		863	837	0.71	ГH43C23C24C25 [18]; ГH45C25C26N14 [42]; ГH42C22C23C24 [19]
66	848	867	841	15.47	vC16C17 [11]; β H40C17C18 [11]
67		896	869	21.74	vC30C31 [16]
68		899	872	19.01	vC30C31 [13]
69		919	891	9.84	ГH41C19C20C15 [68]; ГC15C20C18C19 [15]
70		920	892	4.07	β H52C30C31 [13]; ГH53C30C31C32 [10]
71		943	915	1.66	ГH34C9C10C11 [26]; ГH36C11C12C13 [29]; ГH38C13C12C11 [28]
72		945	917	5.6	ГH45C25C26N14 [19]; ГH42C22C23C24 [31]; ГH44C24C25C26 [22]
73	921	947	919	4.33	ГH39C16C17C18 [22]; ГH33C3C2S5 [18]; ГH40C17C18C3 [31]
74		977	948	9.88	ГH33C3C2S5 [60]; ГH40C17C18C3 [20]
75		984	954	0.69	ГH42C22C23C24 [14]; ГH43C23C24C25 [36]; ГH44C24C25C26 [32]
76		992	962	0.69	ГH34C9C10C11 [21]; ГH38C13C12C11 [18]; ГH35C10C11C12 [21]; ГH37C12C11C10 [30]

77		1001	971	3.96	vC27C28 [24]; vC29C30 [30]; vC31C32 [26]
78		1011	981	5.18	β H50C29C30 [16]; β H52C30C31 [10]; β H48C28C29 [13]; Γ H53C30C31C32 [11]
79		1012	982	20.5	β C10C11C12 [12]; β C9C10C11 [15]; β C11C12C13 [13]; vC1C2 [10]
80		1016	986	3.13	Γ H35C10C11C12 [22]; Γ H36C11C12C13 [36]; Γ H37C12C11C10 [13]; Γ C11C10C12C13 [10]
81		1018	987	18.25	vC1C2 [16]
82		1032	1001	8.17	vC9C10 [18]; vC12C13 [19]
83		1034	1003	3.68	vC27C28 [24]; vC28C29 [12]
84		1043	1012	15.99	β C9C10C11 [13]; β C11C12C13 [14]; vC10C11 [15]; vC11C12 [15]
85		1048	1017	11.98	β H42C22C23 [10]; β H45C25C26 [11]; vC23C24 [24]
86		1049	1018	3.64	vC28C29 [39]; vC31C32 [22]
87		1067	1035	3.09	vC29C30 [35]; vC31C32 [13]; vC30C31 [28]
88		1075	1043	57.12	vS5O7 [17]; vS5O6 [19]; vC8C9 [12]; vC8C13 [11]
89		1084	1051	12.72	β C24C25C26 [25]; vN14C27 [18]
90		1102	1069	12.15	β H34C9C10 [14]; β H36C11C12 [12]; β H38C13C12 [12]
91		1122	1088	56.46	vS5C8 [12]; vS5O7 [20]; vS5O6 [24]; vC8C9 [10]; vC8C13 [11]
92		1136	1102	13.75	Γ H57C32C31C30 [13]; Γ H58C32C31C30 [11]; vC30C31 [12]
93		1147	1113	16.52	β H43C23C24 [12]; vC24C25 [11]; vC22C23 [14]
94		1165	1130	42.98	β H42C22C23 [10]
95		1181	1146	21.35	β H39C16C17 [14]; β H44C24C25 [20]; β H45C25C26 [12]
96		1184	1148	7.59	β H44C24C25 [14]
97		1186	1150	1.43	vC11C12 [10]; β H36C11C12 [37]; β H35C10C11 [18]; β H37C12C13 [20]
98	1159	1201	1165	11.62	β H34C9C10 [17]; β H38C13C12 [16]; β H35C10C11 [19]; β H37C12C13 [18]
99		1214	1178	40.57	vC3C18 [23]
100	1197	1225	1188	23.56	β H50C29C30 [10]
101		1254	1216	40.22	vC20C21 [12]; vC21C26 [11]
102		1261	1223	7.8	Γ H50C29C30C31 [11]; Γ H51C29C30C31 [16]
103		1262	1224	47.07	Γ H49C28C29C30 [11]; Γ H53C30C31C32 [11]

104		1292	1253	15.95	βH48C28C29 [12]; βH54C31C32 [13]
105	1232	1295	1256	43.79	vS5O7 [44]; vS5O6 [36]
106		1313	1274	28.95	βH41C19C20 [32]; βH40C17C18 [13]
107		1325	1285	3.13	βH54C31C32 [20]; βH46C27C28 [15]
108		1327	1287	3.26	ГH48C28C29C30 [11]; ГH49C28C29C30 [14]; ГH55C31C30C29 [12]
109		1331	1291	2.2	vC8C9 [21]; βH35C10C11 [13]; βH37C12C13 [14]; vC8C13 [17]
110		1333	1293	7.52	βH50C29C30 [38]; ГH51C29C30C31 [11]; βH48C28C29 [10]
111		1339	1299	10.49	βH48C28C29 [19]; βH52C30C31 [21]; βH54C31C32 [18]
112		1347	1307	4.63	βH34C9C10 [24]; βH38C13C12 [24]; vC9C10 [14]; vC12C13 [14]
113		1354	1313	32.08	βH46C27C28 [12]
114		1366	1325	15.48	vC25C26 [11]; vC23C24 [10]
115	1334	1379	1338	42.55	vN14C27 [11]
116		1383	1342	32.18	vN14C26 [10]
117		1402	1360	41.98	βH33C3C2 [47]
118		1405	1363	3.62	ГH52C30C31C32 [16]; ГH53C30C31C32 [18]; ГH55C31C30C29 [11]
119		1407	1365	12.51	ГH46C27N14C15 [11]; ГH47C27N14C15 [18]; ГH48C28C29C30 [11]
120		1416	1374	6.63	βH56C32H58 [30]; βH56C32H57 [29]; βH57C32H58 [25]
121	1390	1420	1377	18.98	βH46C27C28 [18]
122		1474	1430	33.52	βH42C22C23 [11]; βH45C25C26 [14]; vC16C17 [13]; vC19C20 [11]
123		1478	1434	16.72	βH35C10C11 [14]; βH36C11C12 [30]; βH37C12C13 [11]; vC9C10 [12]; vC12C13 [12]
124		1489	1444	2.14	βH52C30H53 [49]; βH54C31H55 [28]
125		1490	1445	8.82	βH50C29H51 [47]; βH48C28H49 [19]
126		1492	1447	25.95	βH54C31H55 [16]
127		1498	1453	16.3	βH48C28H49 [27]; βH57C32H58 [14]
128		1502	1457	11.88	βH56C32H58 [40]; βH56C32H57 [35]; ГH56C32C31C30 [15]; βH57C32H58 [15]
129		1503	1458	17.09	βH46C27H47 [25]; βH50C29H51 [10]

130		1508	1463	8.92	β H37C12C13 [15]; β H38C13C12 [16]; vC8C13 [10]
131	1465	1511	1466	7.31	β H46C27H47 [18]; β H57C32H58 [15]; β H48C28H49 [10]; β H54C31H55 [22]
132		1513	1468	18.66	β H40C17C18 [10]; vC18C19 [12]
133		1518	1472	15.01	β H48C28H49 [20]; β H50C29H51 [21]; β H52C30H53 [17]; β H54C31H55 [15]
134		1525	1479	52.06	vN14C15 [13]
135	1514	1593	1545	68.35	vC15C16 [24]; vC15C20 [15]; vC2C3 [14]
136		1613	1565	100	vC2C3 [24]; vC19C20 [11]
137		1620	1571	23.66	vC23C24 [18]; vC21C26 [19]; vC21C22 [10]
138	1577	1625	1576	11.01	vC8C9 [16]; vC9C10 [20]; vC12C13 [20]
139		1628	1579	9.65	vC8C13 [23]; vC10C11 [23]; vC11C12 [12]; β H36C11C12 [10]
140		1644	1595	22.84	vC2C3 [15]; vC22C23 [10]; vC25C26 [13]; vC21C22 [12]
141	1627	1665	1615	18.82	vC19C20 [14]; vC21C22 [10]
142	2208	2308	2331	27.32	vN4C1 [89]; vC1C2 [11]
143	2862	2995	3025	8.11	vC29H50 [34]; vC29H51 [40]; vC30H53 [13]; vC30H52 [12]
144	2951	3000	3030	9.96	vC30H53 [25]; vC30H52 [27]; vC31H54 [15]; vC31H55 [15]
145		3011	3041	33.33	vC30H52 [12]; vC31H54 [31]; vC31H55 [36]
146		3015	3045	4.99	vC29H50 [25]; vC29H51 [18]; vC30H52 [20]; vC30H53 [24]
147		3022	3052	26.97	vC32H56 [25]; vC32H57 [35]; vC32H58 [36]
148		3026	3056	19.63	vC31H54 [21]; vC31H55 [22]; vC28H48 [48]; vC28H49 [32]
149	3059	3027	3057	6.47	vC29H50 [20]; vC29H51 [13]; vC28H49 [12]
150		3046	3076	32.21	vC27H47 [53]; vC27H46 [30]
151		3047	3077	25.11	vC30H52 [17]; vC30H53 [16]; vC31H54 [14]; vC31H55 [14]; vC28H49 [11]
152		3061	3092	22.16	vC27H46 [14]; vC28H48 [25]; vC28H49 [30]
153		3083	3114	33.44	vC32H57 [43]; vC32H58 [45]
154		3088	3119	25.97	vC27H46 [43]; vC27H47 [34]; vC28H48 [10]; vC28H49 [10]
155		3089	3120	56.3	vC32H56 [74]; vC32H57 [13]; vC32H58 [11]
156	3176	3151	3183	9.07	vC3H33 [98]

157		3169	3201	3.25	vC23H43 [29]; vC24H44 [46]; vC22H42 [14]; vC25H45 [11]
158		3171	3203	3.35	vC11H36 [51]; vC10H35 [16]; vC12H37 [30]
159		3174	3206	7.01	vC16H39 [18]; vC17H40 [81]
160		3177	3209	9.1	vC24H44 [21]; vC22H42 [54]; vC25H45 [15]
161		3183	3215	14.63	vC10H35 [43]; vC12H37 [47]
162		3188	3220	19.47	vC22H42 [19]; vC23H43 [23]; vC25H45 [53]
163		3193	3225	17.33	vC10H35 [32]; vC11H36 [43]; vC12H37 [12]
164		3194	3226	17.27	vC16H39 [81]; vC17H40 [17]
165		3196	3228	19.38	vC22H42 [11]; vC23H43 [39]; vC24H44 [27]; vC25H45 [21]
166		3206	3238	8.59	vC12H37 [10]; vC13H38 [86]
167		3211	3243	8.75	vC9H34 [89]
168		3215	3247	6.09	vC19H41 [99]

Table S3. Experimental and calculated ^1H and ^{13}C chemical shift values of **6g**

Atom	Calc.	Expt.	Atom	Calc.	Expt.
H33	9.16	8.65	C1	113.2	114.4
H34	7.74	7.68	C2	107.5	109.5
H35	7.52	7.56	C3	149.9	152.7
H36	7.58	7.58	C8	141.3	141.0
H37	7.43	7.44	C9	125.7	128.3
H38	7.50	7.54	C10	126.9	128.7
H39	7.28	7.33	C11	132.1	134.1
H40	7.44	7.46	C12	127.7	129.5
H41	8.01	8.37	C13	124.3	128.3
H42	7.89	8.13	C15	142.3	143.7
H43	7.21	7.31	C16	106.6	108.9
H44	7.44	7.45	C17	132.8	134.1
H45	7.30	7.35	C18	118.9	120.7
H46	3.98	4.33	C19	119.0	122.5
H47	3.98	4.29	C20	122.4	127.1
H48	1.57	1.90	C21	120.9	123.5
H49	1.59	1.83	C22	118.9	121.1
H50	1.36	1.36	C23	118.5	120.8
H51	1.35	1.34	C24	125.2	128.3
H52	1.16	1.24	C25	106.9	109.5
H53	1.16	1.26	C26	139.5	139.0
H54	1.28	1.29	C27	43.1	43.4
H55	1.28	1.28	C28	30.1	28.8
H56	1.03	0.87	C29	29.4	26.8
H57	0.76	0.85	C30	34.4	31.4
H58	0.76	0.83	C31	25.9	22.4
			C32	14.0	13.9