

Hydrazone integrated carbazoles: synthesis, computational, anticancer and molecular docking studies

Kannan Gokula Krishnan^a, Pathinettampadi Ashothai^b, Krishnaraj Padmavathy^a, Wei-Meng Lim^c, Chun-Wai Mai^{c,d}, Punniyakoti V Thanikachalam^c Chennan Ramalingan^{a,*}

^a*Department of Chemistry, School of Advanced Sciences (SAS), Kalasalingam Academy of Research and Education (Deemed to be University), Krishnankoil - 626 126, Tamilnadu, India*

^b*Department of Chemistry, Lady Doak College, Madurai - 625 002, Tamilnadu, India*

^c*School of Pharmacy, International Medical University, 126 Jalan Jalil Perkasa 19, 57000, Bukit Jalil, Kuala Lumpur, Malaysia.*

^d*Center for Cancer and Stem Cell Research, Institute for Research, Development and Innovation (IRDI), International Medical University, 126, Jalan Jalil Perkasa 19, 57000, Bukit Jalil, Kuala Lumpur, Malaysia.*

* *Corresponding author: ramalinganc@gmail.com; c.ramalingan@klu.ac.in (C. Ramalingan)*

SUPPLEMENTARY INFORMATION

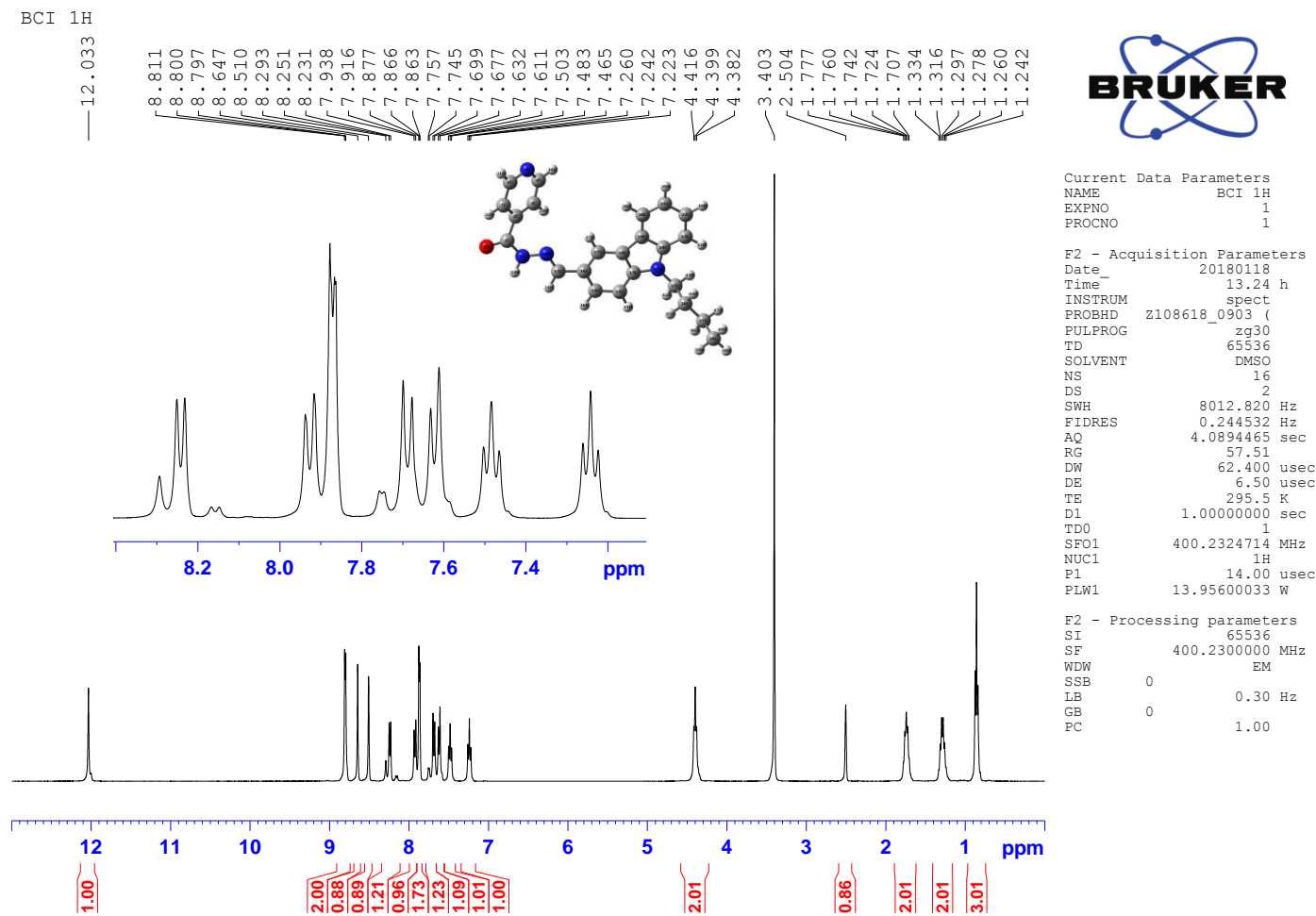


Figure S1. ^1H NMR spectrum of hydrazone integrated carbazole **6a**.

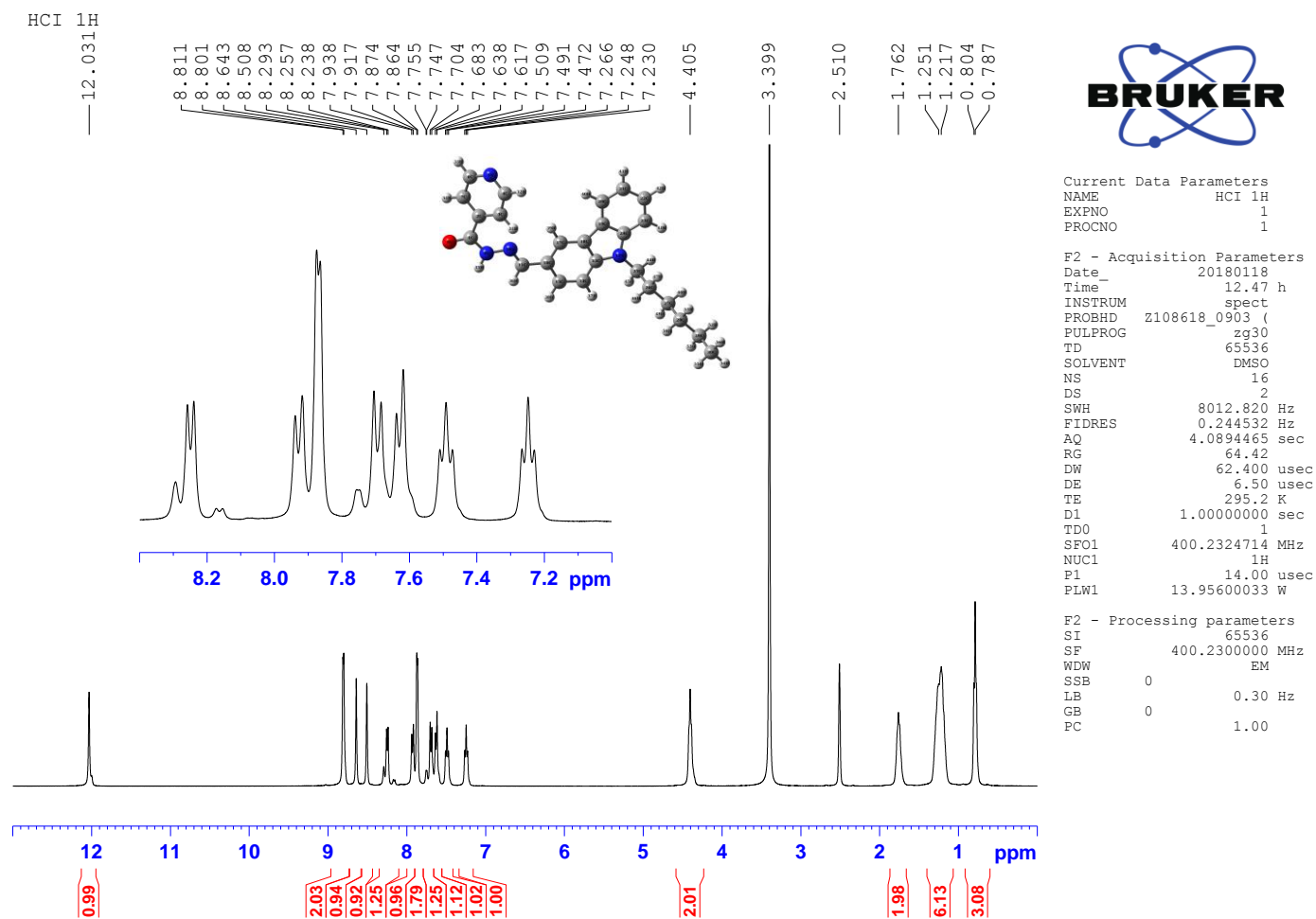


Figure S2. ^1H NMR spectrum of hydrazone integrated carbazole **6b**.

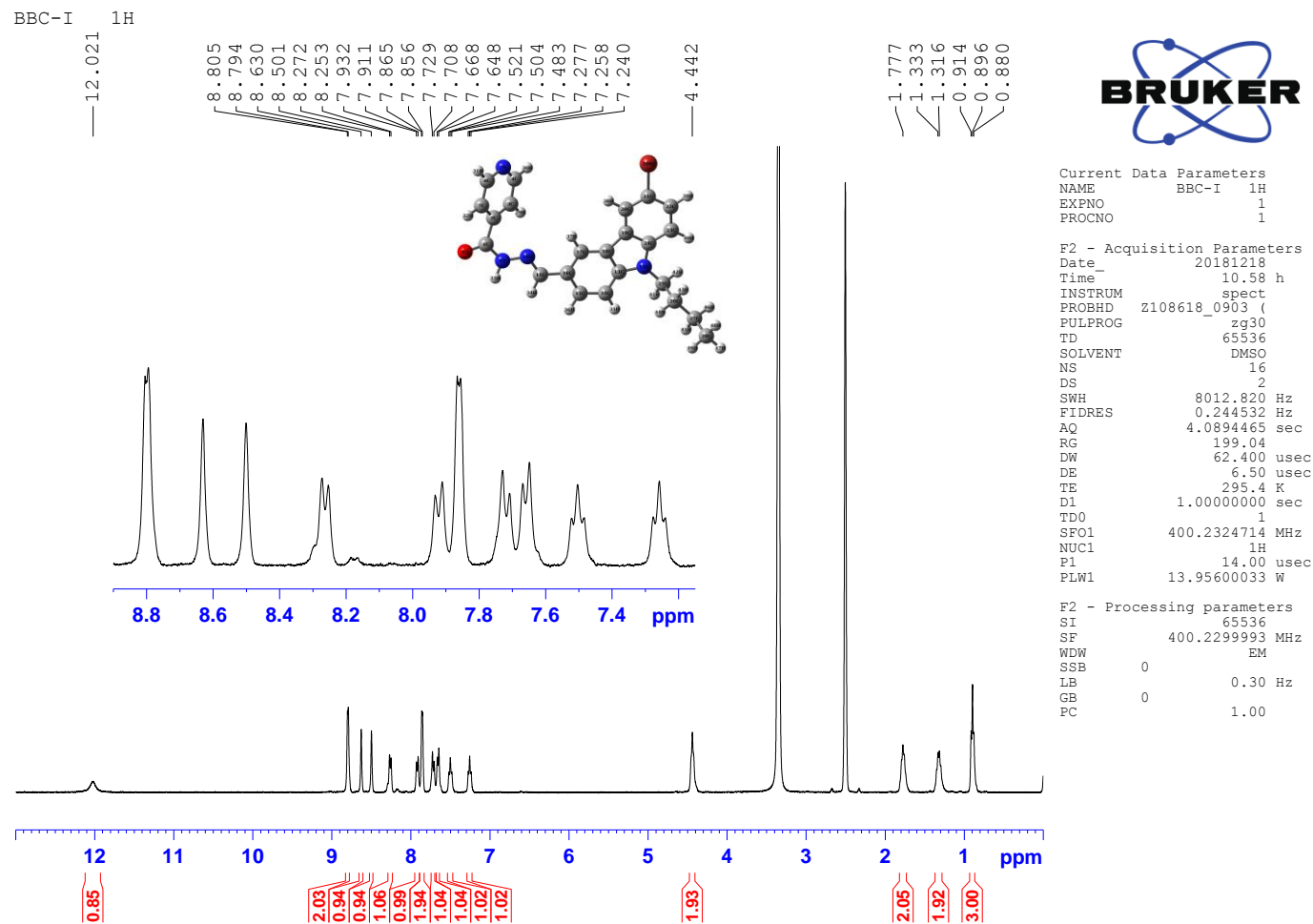


Figure S3. ¹H NMR spectrum of hydrazone integrated carbazole **6c**.

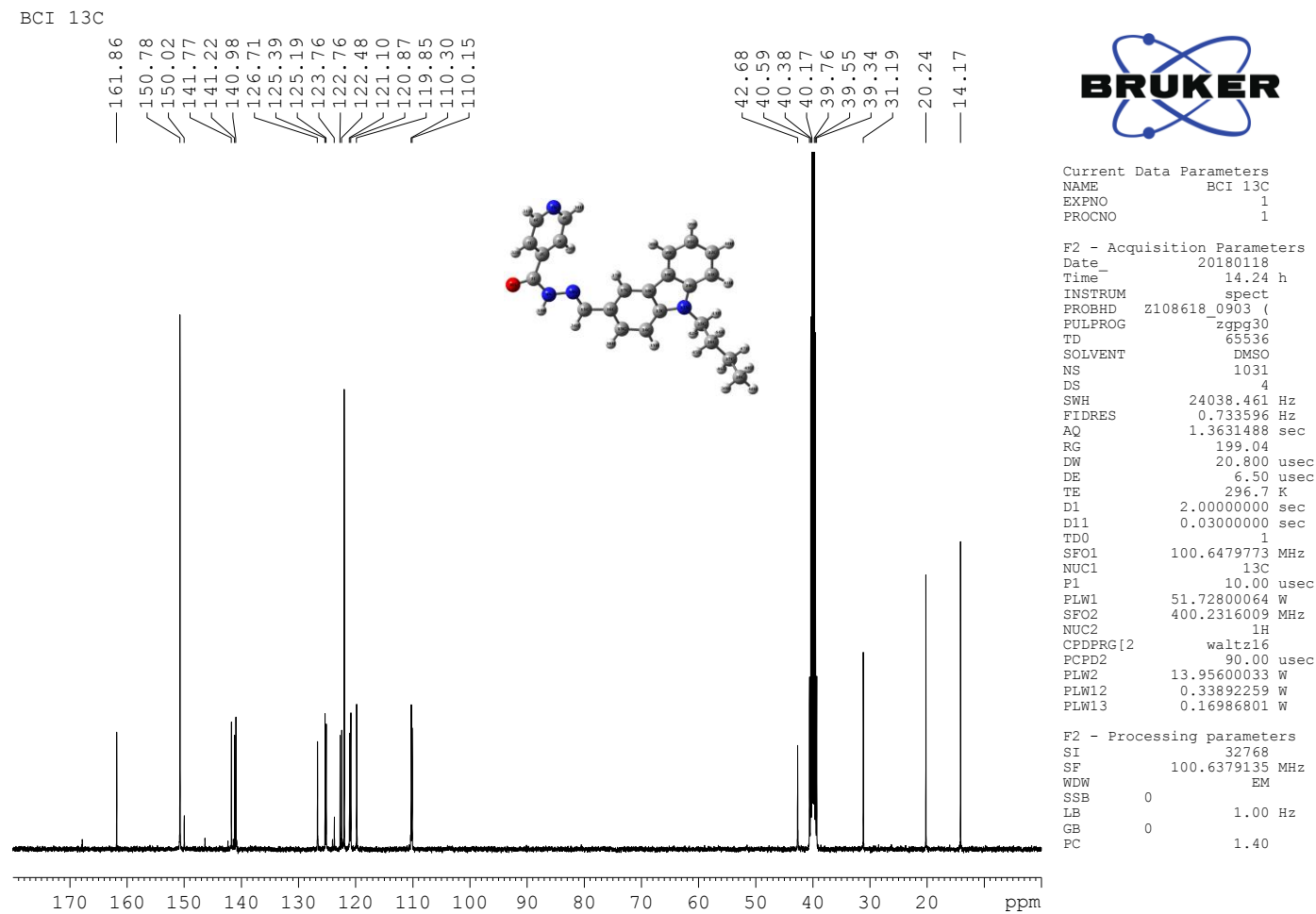


Figure S4. ^{13}C NMR spectrum of hydrazone integrated carbazole **6a**.

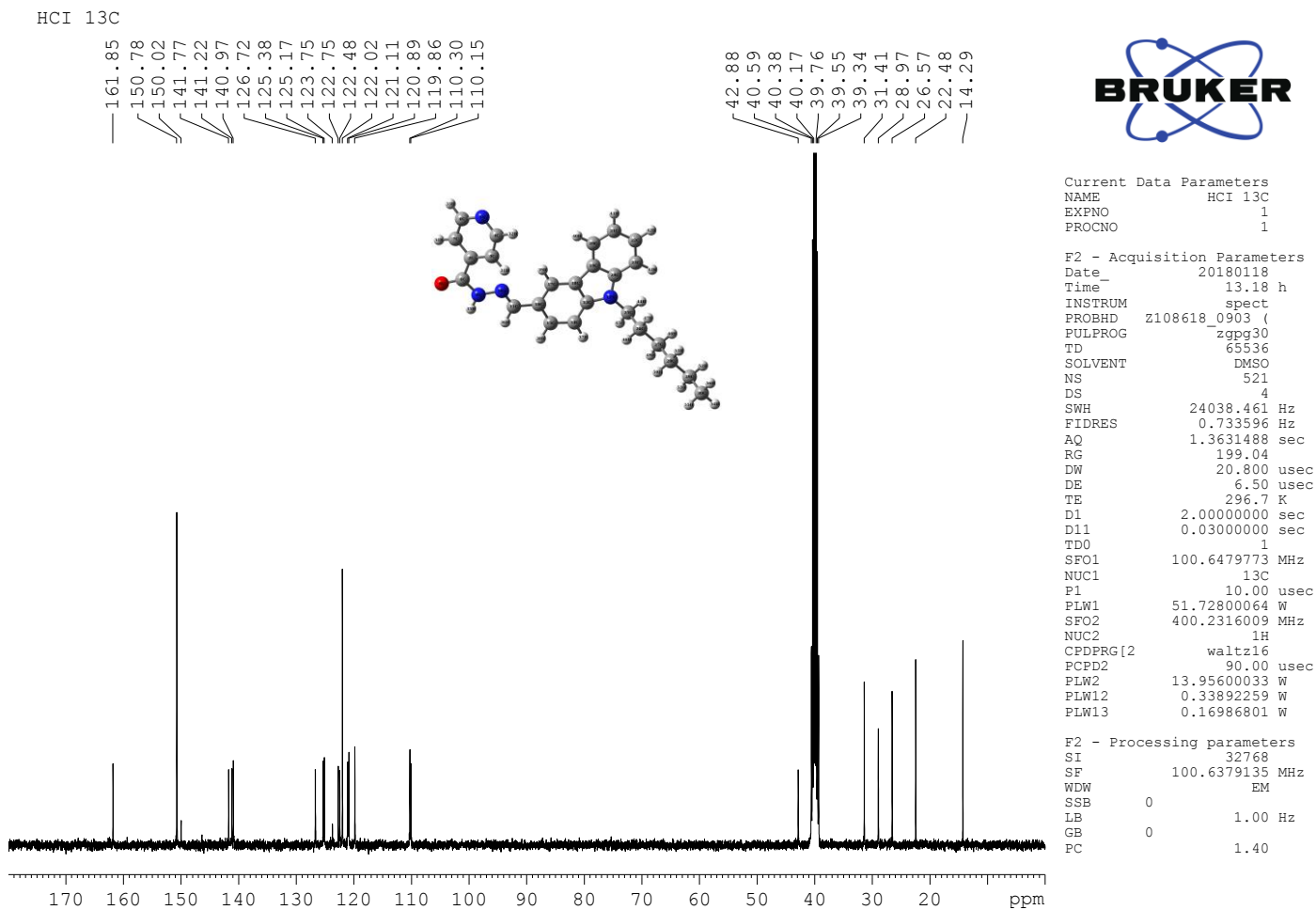
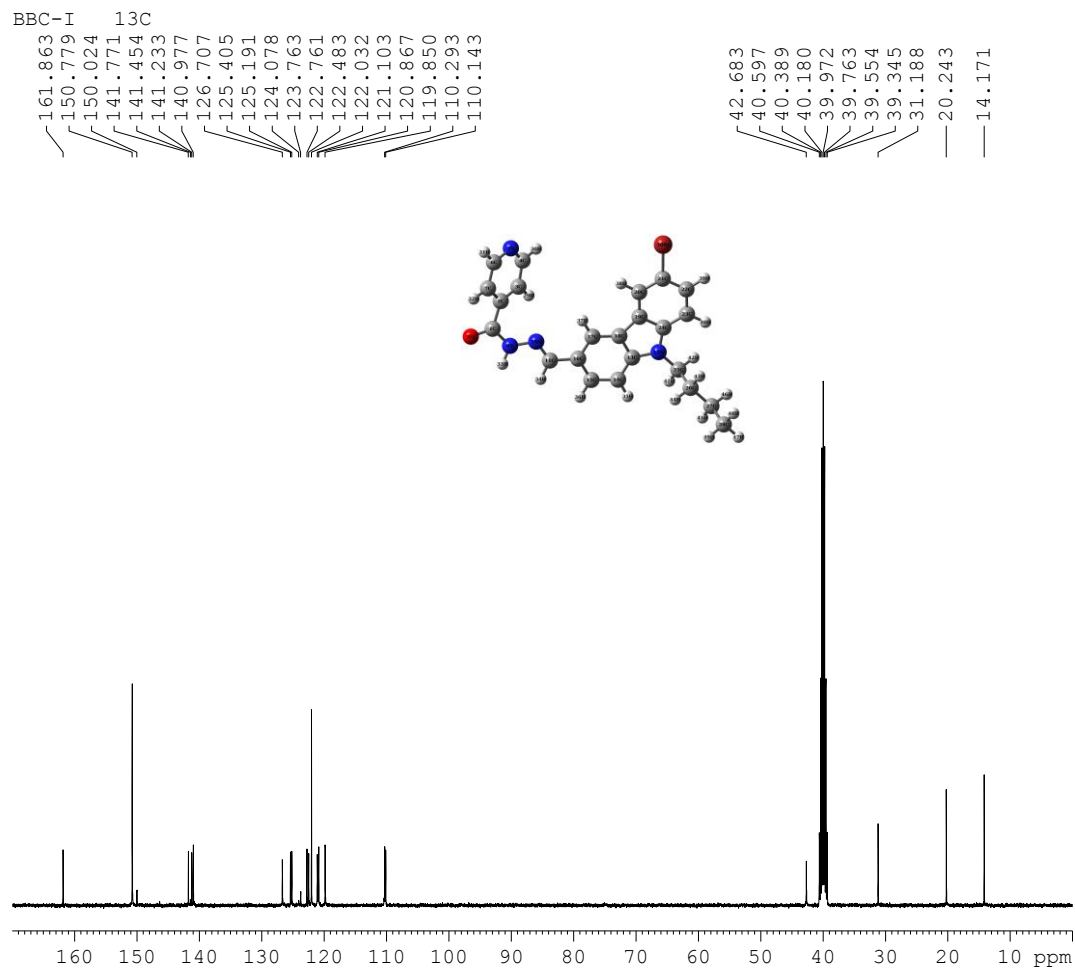


Figure S5. ^{13}C NMR spectrum of hydrazide integrated carbazole **6b**.



Current Data Parameters
 NAME BBC-I 13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181218
 Time_ 11.28 h
 INSTRUM spect
 PROBHD Z108618_0903 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 425
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 199.04
 DW 20.800 usec
 DE 6.50 usec
 TE 296.6 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SF01 100.6479773 MHz
 NUC1 13C
 F1 10.00 usec
 PLW1 51.72800064 W
 SF02 400.2316009 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 13.95600033 W
 PLW12 0.33892259 W
 PLW13 0.16986801 W

F2 - Processing parameters
 SI 32768
 SF 100.6379135 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S6. ¹³C NMR spectrum of hydrazone integrated carbazole **6c**.

Table S1a. Selected bond lengths, bond angles and dihedral angles of hydrazides **6a-c**

Hydrazide 6a		Hydrazide 6b		Hydrazide 6c	
Bond length	[Å]	Bond length	[Å]	Bond length	[Å]
C1-C2	1.503	C1-C2	1.503	C1-C2	1.502
C1-O8	1.220	C1-O8	1.220	C1-O8	1.219
C1-N9	1.380	C1-N9	1.380	C1-N9	1.382
C2-C3	1.397	C2-C3	1.397	C2-C3	1.396
C2-C7	1.397	C2-C7	1.397	C2-C7	1.397
C3-C4	1.394	C3-C4	1.394	C3-C4	1.393
C4-N5	1.336	C4-N5	1.336	C4-N5	1.336
N5-C6	1.337	N5-C6	1.337	N5-C6	1.337
C6-C7	1.390	C6-C7	1.390	C6-C7	1.390
N9-N10	1.360	N9-N10	1.360	N9-N10	1.359
N10-C11	1.282	N10-C11	1.282	N10-C11	1.282
C11-C16	1.459	C11-C16	1.459	C11-C16	1.460
N12-C13	1.384	N12-C13	1.383	N12-C13	1.384
N12-C24	1.393	N12-C24	1.393	N12-C24	1.391
N12-C25	1.455	N12-C25	1.455	N12-C25	1.456
C13-C14	1.397	C13-C14	1.397	C13-C14	1.397
C13-C18	1.424	C13-C18	1.424	C13-C18	1.423
C14-C15	1.388	C14-C15	1.388	C14-C15	1.387
C15-C16	1.411	C15-C16	1.411	C15-C16	1.412
C16-C17	1.402	C16-C17	1.402	C16-C17	1.401
C17-C18	1.389	C17-C18	1.389	C17-C18	1.389
C18-C19	1.448	C18-C19	1.448	C18-C19	1.448
C19-C20	1.397	C19-C20	1.397	C19-C20	1.397
C19-C24	1.417	C19-C24	1.418	C19-C24	1.417
C20-C21	1.390	C20-C21	1.390	C20-C21	1.387
C21-C22	1.403	C21-C22	1.403	C21-C22	1.401
C22-C23	1.391	C22-C23	1.391	C21-Br50	1.921
C23-C24	1.396	C23-C24	1.396	C22-C23	1.391
C25-C26	1.535	C25-C26	1.535	C23-C24	1.395
C26-C27	1.533	C26-C27	1.533	C25-C26	1.535
C27-C28	1.531	C27-C28	1.533	C26-C27	1.533
		C28-C29	1.533	C27-C28	1.531
		C29-C30	1.531		

Bond angle	[°]	Bond angle	[°]	Bond angle	[°]
C2-C1-O8	121.2	C2-C1-O8	121.2	C2-C1-O8	121.4
C2-C1-N9	120.1	C2-C1-N9	120.1	C2-C1-N9	119.9
O8-C1-N9	118.7	O8-C1-N9	118.7	O8-C1-N9	118.7
C1-C2-C3	125.4	C1-C2-C3	125.4	C1-C2-C3	125.2
C1-C2-C7	116.6	C1-C2-C7	116.6	C1-C2-C7	116.8
C3-C2-C7	117.8	C3-C2-C7	117.8	C3-C2-C7	117.9
C2-C3-C4	118.5	C2-C3-C4	118.5	C2-C3-C4	118.5
C3-C4-N5	124.1	C3-C4-N5	124.1	C3-C4-N5	124.0
C4-N5-C6	116.9	C4-N5-C6	116.9	C4-N5-C6	117.0
N5-C6-C7	123.7	N5-C6-C7	123.7	N5-C6-C7	123.7
C2-C7-C6	119.0	C2-C7-C6	119.0	C2-C7-C6	118.9
C1-N9-N10	125.7	C1-N9-N10	125.7	C1-N9-N10	125.5
N9-N10-C11	117.0	N9-N10-C11	117.0	N9-N10-C11	117.1
N10-C11-C16	122.9	N10-C11-C16	122.9	N10-C11-C16	122.7
C13-N12-C24	108.7	C13-N12-C24	108.7	C13-N12-C24	108.6
C13-N12-C25	125.8	C13-N12-C25	125.7	C13-N12-C25	125.8
C24-N12-C25	125.5	C24-N12-C25	125.6	C24-N12-C25	125.6
N12-C13-C14	129.8	N12-C13-C14	129.7	N12-C13-C14	129.7
N12-C13-C18	109.2	N12-C13-C18	109.2	N12-C13-C18	109.2
C14-C13-C18	121.1	C14-C13-C18	121.1	C14-C13-C18	121.1
C13-C14-C15	117.9	C13-C14-C15	117.9	C13-C14-C15	117.8
C14-C15-C16	122.1	C14-C15-C16	122.1	C14-C15-C16	122.1
C11-C16-C15	118.7	C11-C16-C15	118.6	C11-C16-C15	118.7
C11-C16-C17	121.9	C11-C16-C17	121.9	C11-C16-C17	121.9
C15-C16-C17	119.5	C15-C16-C17	119.5	C15-C16-C17	119.5
C16-C17-C18	119.5	C16-C17-C18	119.5	C16-C17-C18	119.4
C13-C18-C17	119.9	C13-C18-C17	119.9	C13-C18-C17	120.0
C13-C18-C19	106.5	C13-C18-C19	106.5	C13-C18-C19	106.4
C17-C18-C19	133.6	C17-C18-C19	133.6	C17-C18-C19	133.6
C18-C19-C20	133.8	C18-C19-C20	133.8	C18-C19-C20	133.3
C18-C19-C24	106.5	C18-C19-C24	106.6	C18-C19-C24	106.6
C20-C19-C24	119.6	C20-C19-C24	119.6	C20-C19-C24	120.1
C19-C20-C21	119.1	C19-C20-C21	119.1	C19-C20-C21	118.1
C20-C21-C22	120.6	C20-C21-C22	120.6	C20-C21-C22	122.0
C21-C22-C23	121.4	C21-C22-C23	121.5	C20-C21-Br50	119.2

C22-C23-C24	117.8	C22-C23-C24	117.8	C22-C21-Br50	118.7
N12-C24-C19	109.1	N12-C24-C19	109.1	C21-C22-C23	120.4
N12-C24-C23	129.4	N12-C24-C23	129.4	C22-C23-C24	118.2
C19-C24-C23	121.5	C19-C24-C23	121.4	N12-C24-C19	109.2
N12-C25-C26	113.8	N12-C25-C26	113.8	N12-C24-C23	129.6
C25-C26-C27	112.5	C25-C26-C27	112.5	C19-C24-C23	121.2
C26-C27-C28	113.0	C26-C27-C28	113.3	N12-C25-C26	113.8
		C27-C28-C29	113.6	C25-C26-C27	112.4
		C28-C29-C30	113.2	C26-C27-C28	113.0
Dihedral angle	[°]	Dihedral angle	[°]	Dihedral angle	[°]
O8-C1-C2-C3	-149.6	O8-C1-C2-C3	149.3	O8-C1-C2-C3	-148.0
O8-C1-C2-C7	25.7	O8-C1-C2-C7	-26.0	O8-C1-C2-C7	27.1
N9-C1-C2-C3	29.8	N9-C1-C2-C3	-30.0	N9-C1-C2-C3	31.1
N9-C1-C2-C7	-154.9	N9-C1-C2-C7	154.7	N9-C1-C2-C7	-153.8
C2-C1-N9-N10	12.0	C2-C1-N9-N10	-12.0	C2-C1-N9-N10	13.2
O8-C1-N9-N10	-168.6	O8-C1-N9-N10	168.6	O8-C1-N9-N10	-167.7
C1-C2-C3-C4	175.8	C1-C2-C3-C4	-175.7	C1-C2-C3-C4	175.5
C7-C2-C3-C4	0.5	C7-C2-C3-C4	-0.5	C7-C2-C3-C4	0.5
C1-C2-C7-C6	-177.2	C1-C2-C7-C6	177.2	C1-C2-C7-C6	-177.0
C3-C2-C7-C6	-1.5	C3-C2-C7-C6	1.5	C3-C2-C7-C6	-1.5
C2-C3-C4-N5	0.8	C2-C3-C4-N5	-0.8	C2-C3-C4-N5	0.9
C3-C4-N5-C6	-1.0	C3-C4-N5-C6	1.0	C3-C4-N5-C6	-1.0
C4-N5-C6-C7	0.0	C4-N5-C6-C7	0.1	C4-N5-C6-C7	-0.1
N5-C6-C7-C2	1.3	N5-C6-C7-C2	-1.3	N5-C6-C7-C2	1.4
C1-N9-N10-C11	174.2	C1-N9-N10-C11	-174.3	C1-N9-N10-C11	174.1
N9-N10-C11-C16	-179.6	N10-C11-C16-C15	176.3	N9-N10-C11-C16	-179.3
N10-C11-C16-C15	-176.6	N10-C11-C16-C17	-3.7	N10-C11-C16-C15	-176.1
N10-C11-C16-C17	3.5	C24-N12-C13-C14	-179.8	N10-C11-C16-C17	4.1
C24-N12-C13-C14	-179.3	C24-N12-C13-C18	0.7	C24-N12-C13-C14	-179.1
C24-N12-C13-C18	0.8	C25-N12-C13-C14	-2.1	C24-N12-C13-C18	0.9
C25-N12-C13-C14	-1.9	C25-N12-C13-C18	178.4	C25-N12-C13-C14	-1.8
C25-N12-C13-C18	178.2	C13-N12-C24-C19	-0.8	C25-N12-C13-C18	178.2
C13-N12-C24-C19	-0.7	C13-N12-C24-C23	179.6	C13-N12-C24-C19	-0.8
C13-N12-C24-C23	179.6	C25-N12-C24-C19	-178.5	C13-N12-C24-C23	179.5
C25-N12-C24-C19	-178.2	C25-N12-C24-C23	1.8	C25-N12-C24-C19	-178.2
C25-N12-C24-C23	2.1	C13-N12-C25-C26	-89.1	C25-N12-C24-C23	2.1

C13-N12-C25-C26	-90.0	C24-N12-C25-C26	88.2	C13-N12-C25-C26	-88.8
C24-N12-C25-C26	87.1	N12-C13-C14-C15	-179.2	C24-N12-C25-C26	88.1
N12-C13-C14-C15	-179.3	C18-C13-C14-C15	0.2	N12-C13-C14-C15	-179.5
C18-C13-C14-C15	0.5	N12-C13-C18-C17	179.3	C18-C13-C14-C15	0.5
N12-C13-C18-C17	179.4	N12-C13-C18-C19	-0.4	N12-C13-C18-C17	179.5
N12-C13-C18-C19	-0.5	C14-C13-C18-C17	-0.2	N12-C13-C18-C19	-0.6
C14-C13-C18-C17	-0.5	C14-C13-C18-C19	-179.9	C14-C13-C18-C17	-0.5
C14-C13-C18-C19	179.6	C13-C14-C15-C16	-0.3	C14-C13-C18-C19	179.4
C13-C14-C15-C16	-0.1	C14-C15-C16-C11	-179.6	C13-C14-C15-C16	0.0
C14-C15-C16-C11	179.8	C14-C15-C16-C17	0.4	C14-C15-C16-C11	179.9
C14-C15-C16-C17	-0.4	C11-C16-C17-C18	179.7	C14-C15-C16-C17	-0.4
C11-C16-C17-C18	-179.7	C15-C16-C17-C18	-0.3	C11-C16-C17-C18	-179.9
C15-C16-C17-C18	0.4	C16-C17-C18-C13	0.2	C15-C16-C17-C18	0.4
C16-C17-C18-C13	0.0	C16-C17-C18-C19	179.9	C16-C17-C18-C13	0.1
C16-C17-C18-C19	179.9	C13-C18-C19-C20	179.8	C16-C17-C18-C19	-179.8
C13-C18-C19-C20	179.9	C13-C18-C19-C24	-0.1	C13-C18-C19-C20	180.0
C13-C18-C19-C24	0.1	C17-C18-C19-C20	0.1	C13-C18-C19-C24	0.1
C17-C18-C19-C20	-0.1	C17-C18-C19-C24	-179.8	C17-C18-C19-C20	-0.1
C17-C18-C19-C24	-179.8	C18-C19-C20-C21	-180.0	C17-C18-C19-C24	-180.0
C18-C19-C20-C21	-179.8	C24-C19-C20-C21	-0.2	C18-C19-C20-C21	-180.0
C24-C19-C20-C21	-0.1	C18-C19-C24-N12	0.5	C24-C19-C20-C21	-0.1
C18-C19-C24-N12	0.4	C18-C19-C24-C23	-179.8	C18-C19-C24-N12	0.4
C18-C19-C24-C23	-179.9	C20-C19-C24-N12	-179.4	C18-C19-C24-C23	-179.8
C20-C19-C24-N12	-179.4	C20-C19-C24-C23	0.3	C20-C19-C24-N12	-179.5
C20-C19-C24-C23	0.3	C19-C20-C21-C22	0.0	C20-C19-C24-C23	0.3
C19-C20-C21-C22	0.0	C20-C21-C22-C23	0.0	C19-C20-C21-C22	0.0
C20-C21-C22-C23	0.0	C21-C22-C23-C24	0.2	C19-C20-C21-Br50	-179.9
C21-C22-C23-C24	0.2	C22-C23-C24-N12	179.3	C20-C21-C22-C23	0.0
C22-C23-C24-N12	179.3	C22-C23-C24-C19	-0.3	Br50-C21-C22-C23	179.8
C22-C23-C24-C19	-0.3	N12-C25-C26-C27	-179.5	C21-C22-C23-C24	0.2
N12-C25-C26-C27	-179.7	C25-C26-C27-C28	180.0	C22-C23-C24-N12	179.4
C25-C26-C27-C28	179.6	C26-C27-C28-C29	-179.7	C22-C23-C24-C19	-0.3
		C27-C28-C29-C30	179.9	C25-C26-C27-C28	179.9

Table S1b. Cartesian coordinates of atoms obtained from geometry optimization of hydrazide integrated carbazole **6a-c**.

6a				6b				6c			
E = -1184.22657168 a.u.				E = -1262.87510908 a.u.				E = -3757.76795231 a.u.			
Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-5.140	-1.684	0.168	C	-5.740	-1.925	-0.005	C	-5.529	-1.998	0.270
C	-5.310	-0.191	0.166	C	-5.961	-0.514	0.461	C	-5.556	-0.501	0.150
C	-4.570	0.707	-0.607	C	-5.083	0.222	1.259	C	-4.769	0.250	-0.725
C	-4.909	2.058	-0.563	C	-5.474	1.491	1.683	C	-4.974	1.627	-0.789
N	-5.893	2.559	0.188	N	-6.638	2.062	1.360	N	-5.871	2.284	-0.048
C	-6.599	1.690	0.920	C	-7.473	1.347	0.599	C	-6.621	1.554	0.784
C	-6.359	0.320	0.933	C	-7.192	0.065	0.141	C	-6.515	0.174	0.909
O	-6.081	-2.427	0.391	O	-6.677	-2.683	-0.196	O	-6.530	-2.630	0.564
N	-3.905	-2.241	-0.097	N	-4.458	-2.392	-0.213	N	-4.357	-2.688	0.028
N	-2.725	-1.566	-0.147	N	-3.333	-1.628	-0.258	N	-3.121	-2.132	-0.074
C	-1.660	-2.265	-0.295	C	-2.240	-2.220	-0.573	C	-2.126	-2.933	-0.186
N	3.436	0.081	-0.544	N	2.646	0.525	-0.933	N	3.159	-1.075	-0.594
C	2.268	-0.659	-0.504	C	1.541	-0.305	-0.872	C	1.929	-1.702	-0.510
C	2.075	-2.033	-0.669	C	1.453	-1.688	-1.047	C	1.610	-3.059	-0.604
C	0.778	-2.520	-0.593	C	0.200	-2.276	-0.947	C	0.276	-3.420	-0.493
C	-0.327	-1.674	-0.355	C	-0.961	-1.523	-0.671	C	-0.746	-2.468	-0.290
C	-0.119	-0.299	-0.182	C	-0.859	-0.135	-0.498	C	-0.413	-1.111	-0.188
C	1.170	0.213	-0.254	C	0.384	0.477	-0.594	C	0.917	-0.724	-0.296
C	1.724	1.545	-0.128	C	0.834	1.849	-0.476	C	1.593	0.555	-0.236
C	1.170	2.804	0.112	C	0.187	3.060	-0.221	C	1.149	1.866	-0.050
C	2.008	3.911	0.171	C	0.936	4.229	-0.173	C	2.094	2.882	-0.049
C	3.392	3.770	-0.006	C	2.323	4.198	-0.377	C	3.459	2.626	-0.227
C	3.970	2.527	-0.246	C	2.993	3.005	-0.634	C	3.913	1.324	-0.412
C	3.124	1.419	-0.308	C	2.236	1.833	-0.684	C	2.973	0.293	-0.419
C	4.775	-0.452	-0.740	C	4.018	0.098	-1.164	C	4.443	-1.738	-0.773
C	5.488	-0.830	0.565	C	4.782	-0.252	0.121	C	5.120	-2.144	0.543
C	6.898	-1.381	0.326	C	6.225	-0.685	-0.155	C	6.467	-2.838	0.319
C	7.623	-1.752	1.622	C	7.007	-1.038	1.115	C	7.155	-3.246	1.625
H	-3.754	0.371	-1.229	C	8.454	-1.466	0.847	H	-4.019	-0.216	-1.346
H	-4.355	2.774	-1.164	C	9.226	-1.815	2.122	H	-4.383	2.232	-1.471
H	-7.400	2.110	1.521	H	-4.122	-0.174	1.548	H	-7.349	2.102	1.376
H	-6.973	-0.352	1.518	H	-4.814	2.079	2.314	H	-7.164	-0.382	1.573

H	-3.908	-3.261	-0.080	H	-8.418	1.822	0.349	H	-4.454	-3.699	0.120
H	-1.716	-3.358	-0.382	H	-7.909	-0.492	-0.448	H	-2.281	-4.019	-0.206
H	2.903	-2.707	-0.847	H	-4.424	-3.365	-0.517	H	2.372	-3.814	-0.755
H	0.607	-3.584	-0.720	H	-2.228	-3.296	-0.788	H	0.008	-4.470	-0.564
H	-0.967	0.345	0.014	H	2.327	-2.293	-1.252	H	-1.197	-0.383	-0.018
H	0.100	2.917	0.251	H	0.110	-3.349	-1.079	H	0.099	2.088	0.092
H	1.591	4.894	0.359	H	-1.754	0.442	-0.298	H	4.164	3.447	-0.217
H	4.028	4.647	0.047	H	-0.885	3.088	-0.062	H	4.971	1.135	-0.542
H	5.041	2.434	-0.375	H	0.447	5.176	0.025	H	4.282	-2.617	-1.404
H	4.699	-1.323	-1.397	H	2.889	5.121	-0.333	H	5.091	-1.067	-1.343
H	5.358	0.294	-1.289	H	4.065	2.997	-0.784	H	5.260	-1.251	1.163
H	5.540	0.053	1.212	H	4.532	0.897	-1.706	H	4.448	-2.806	1.101
H	4.884	-1.571	1.100	H	3.994	-0.763	-1.838	H	6.319	-3.726	-0.308
H	6.839	-2.263	-0.324	H	4.246	-1.049	0.647	H	7.129	-2.172	-0.249
H	7.490	-0.639	-0.223	H	4.775	0.618	0.786	H	8.112	-3.737	1.432
H	8.625	-2.140	1.420	H	6.751	0.116	-0.691	H	7.349	-2.376	2.258
H	7.729	-0.882	2.278	H	6.225	-1.551	-0.830	H	6.534	-3.941	2.198
H	7.075	-2.519	2.177	H	6.485	-1.842	1.650	Br	1.520	4.697	0.208
				H	7.005	-0.174	1.792				
				H	8.975	-0.662	0.313				
				H	8.455	-2.330	0.171				
				H	10.253	-2.114	1.897				
				H	8.750	-2.641	2.659				
				H	9.271	-0.960	2.804				

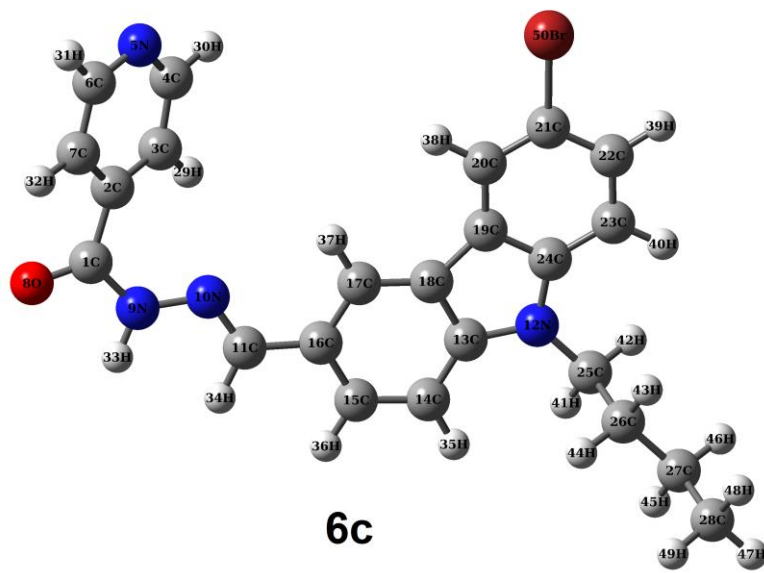
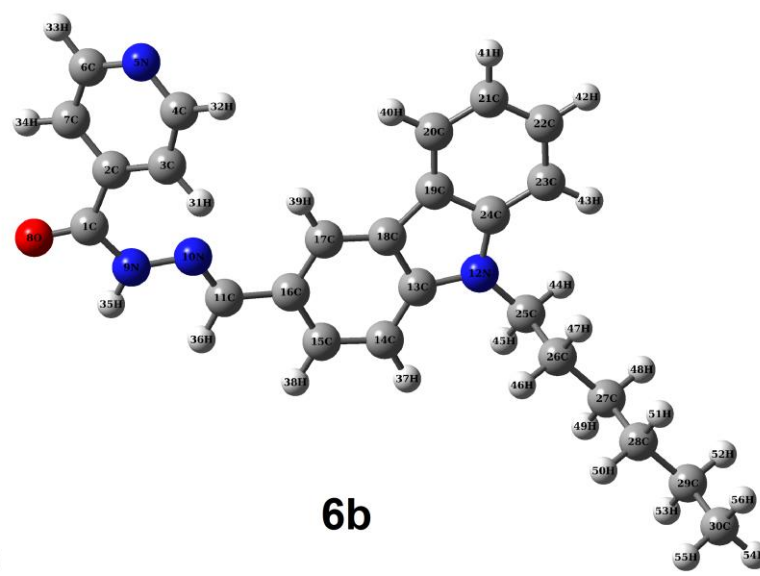
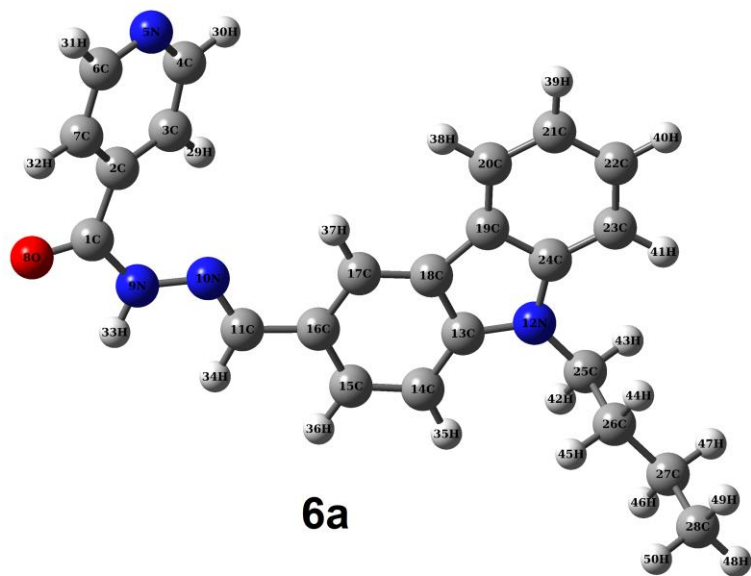


Table S2. Experimental and calculated vibrational frequencies along with their proposed assignment of hydrazide **6a**

Mode	Expt. Freq.	Calc. Freq.			Vibrational Assignment with PED (%)
		Unscaled	Scaled	I_{IR}	
1		12	12	0.15	τ C15C16C11N10 (47); τ C1N9N10C11 (28)
2		21	20	2.11	β C16C11N10 (14); β C11N10N9 (11); τ C13N12C25C26 (17); β C1N9N10 (10)
3		24	23	1.78	β C1N9N10 (11); τ C2C1N9N10 (10)
4		30	29	0.81	τ C13N12C25C26 (14); τ C2C1N9N10 (12); Γ C25C13C24N12 (13)
5		41	40	1.03	Γ C25C13C24N12 (24); τ C7C2C1N9 (27)
6		59	57	1.9	Γ C25C13C24N12 (22); τ C7C2C1N9 (22)
7		74	72	0.62	τ C27C26C25N12 (59); τ C25C26C27C28 (11)
8		88	85	3.11	τ C2C1N9N10 (12)
9		105	102	5.65	τ C7C2C1N9 (15)
10		113	110	2.6	τ C1N9N10C11 (17); Γ C18C19C24C20 (20)
11		115	112	0.36	τ C27C26C25N12 (10); τ C25C26C27C28 (53)
12		158	153	3.49	Γ C1C2C7C3 (25); τ C7C4C6N5 (12)
13		163	158	3.42	τ C19C24C22C23 (24)
14		179	174	6.2	β C25C26C27 (23); β C26C27C28 (12)
15		197	191	2.31	β C1C2C7 (16)
16		220	213	10.08	β C11C16C17 (10); τ C13C18C16C17 (20)
17		233	226	8.81	τ C2C7N5C6 (16); τ C4C3N5C6 (30)
18		245	238	5.23	τ H49C28C27C26 (15); τ H50C28C27C26 (17); τ H48C28C27C26 (32)
19		252	244	11.5	β C1C2C7 (27); τ C1N9N10C11 (10); τ C2C1N9N10 (15)
20		278	270	7.55	τ C19C24C22C23 (10); τ C16C11N10N9 (10)
21		291	282	5.6	τ C16C11N10N9 (15); β C24N12C25 (11); τ C22C21C23C24 (11)
22		301	292	7.38	β C24N12C25 (27)
23		336	326	2.58	τ C15C14C16C17 (10); β C26C27C28 (11)
24		367	356	9.55	β N9C1O8 (15); β C4N5C6 (12); ν C1C2 (23)
25		391	379	2.23	τ H29C3C4N5 (10); τ H32C7C6N5 (10); τ C7C4C6N5 (16)
26		398	386	5.3	β C26C27C28 (18); τ C17C18C19C24 (17)

27		413	401	11.42	β C2C1N9 (11); β C16C17C18 (12); τ C7C4C6N5 (11)
28		434	421	8.19	Γ C18C19C24C20 (10); τ C13C18C16C17 (17); τ C22C21C23C24 (16); τ C13C18C14C15 (10)
29	426	440	427	7.22	β C26C25N12 (20); β C26C27C28 (20); τ C17C18C19C24 (10)
30		457	443	11.84	τ C13C18C14C15 (19)
31		461	447	13.47	τ C13C18C14C15 (10)
32		494	479	24.34	β C16C11N10 (10)
33		531	515	17.3	β C17C18C19 (14)
34		578	561	8.33	τ C22C21C23C24 (17); τ C21C20C22C23 (33); Γ N12C19C23C24 (12)
35		591	573	20.46	β N9C1O8 (12)
36		615	597	19.74	τ H33N9N10C11 (43)
37		620	601	8.98	τ H33N9N10C11 (17); Γ C11C15C17C16 (11)
38	611	629	610	19.29	τ C15C14C16C17 (13); Γ C11C15C17C16 (20)
39		641	622	8.47	τ H33N9N10C11 (11); β C16C17C18 (16); β C21C22C23 (12); β C14C15C16 (15)
40		652	632	28	β C14C13C18 (16)
41		678	658	7.49	β C1N9N10 (10); β C7C6N5 (11)
42	680	686	665	4.53	β C3C4N5 (26); β C7C6N5 (13)
43		725	703	29.36	τ C2C7N5C6 (21); τ C4C3N5C6 (11); Γ O8C2N9C1 (34)
44		740	718	5.55	τ H44C26C27C28 (19); τ H46C27C26C25 (20); β H44C26C27 (15); β H46C27C28 (12)
45		743	721	16.14	τ H39C21C22C23 (10)
46		747	725	19.33	τ H39C21C22C23 (10)
47		749	727	4.84	ν C13C18 (10)
48		764	741	20.72	Γ N12C19C23C24 (24); τ H40C22C23C24 (11); τ H38C20C21C22 (10)
49	748	773	750	19.47	τ C7C4C6N5 (10); τ C2C7N5C6 (28); τ C4C3N5C6 (13); Γ O8C2N9C1 (15); τ H29C3C4N5 (14); τ H32C7C6N5 (14)
50		782	759	4.07	Γ C19C13C17C18 (19);
51		794	770	4.79	τ H46C27C26C25 (10); τ H45C26C27C28 (11); τ H48C28C27C26 (15)
52		803	779	7.99	β C14C15C16 (11); β C11N10N9 (12); ν C1C2 (10)
53	798	812	788	22.31	τ C13C18C14C15 (12); τ H35C14C15C16 (39); τ H36C15C16C11 (31)
54		858	832	1.55	τ H41C23C24N12 (42); τ H38C20C21C22 (19);

					τ H39C21C22C23 (17)
55		864	838	19.96	Γ O8C2N9C1 (19); Γ C1C2C7C3 (18); τ H29C3C4N5 (18)
56	842	880	854	10.72	τ H42C25N12C13 (10)
57		900	873	7.74	τ H29C3C4N5 (29); τ H31C6N5C4 (21); τ H32C7C6N5 (38)
58		911	884	6.14	τ H49C28C27C26 (16); τ H50C28C27C26 (16); ν C26C27 (26); ν C27C28 (16)
59	891	924	896	5.65	τ C13C18C16C17 (11); τ H37C17C18C13 (58); τ H34C11N10N9 (11)
60		936	908	7.4	τ H30C4N5C6 (19); τ H31C6N5C4 (11)
61		937	909	10.64	τ H35C14C15C16 (23); τ H37C17C18C13 (11); ν C16C17 (17); τ H36C15C16C11 (36)
62		940	912	1.5	τ H38C20C21C22 (36); τ H39C21C22C23 (10); τ H40C22C23C24 (20)
63	931	961	932	2.24	τ H48C28C27C26 (10); β H46C27C28 (11); β H44C26C27 (19)
64		969	940	14.18	τ H36C15C16C11 (12); τ H34C11N10N9 (75)
65		979	950	0.43	τ H38C20C21C22 (12); τ H39C21C22C23 (34); τ H40C22C23C24 (35)
66		993	963	5.07	τ H29C3C4N5 (24); τ C4C3N5C6 (10); τ H30C4N5C6 (35); τ H32C7C6N5 (15)
67	975	1005	975	5.88	ν C25C26 (49); ν C27C28 (30)
68		1007	977	7.66	τ H30C4N5C6 (18); τ H31C6N5C4 (36); τ H32C7C6N5 (14)
69		1013	983	8.11	β C4N5C6 (13); β C3C4N5 (14); β C7C6N5 (16); ν N5C4 (15); ν N5C6 (17)
70		1031	1000	5.09	ν C21C22 (10)
71		1046	1015	9.59	β H38C20C21 (12); ν C21C22 (29); β H41C23C24 (12)
72		1056	1024	2.21	ν C25C26 (17); ν C27C28 (36); ν C26C27 (37)
73		1080	1048	12.37	β C22C23C24 (25); β C20C21C22 (11); ν N12C25 (22)
74		1094	1061	15.96	β C3C4N5 (19); β C7C6N5 (25); β H32C7C6 (17)
75		1111	1078	1.92	β H29C3C4 (22); β H32C7C6 (15); ν C3C4 (23); ν C6C7 (16)
76		1128	1094	14.04	τ H49C28C27C26 (15); τ H50C28C27C26 (15)
77		1131	1097	15.81	ν N9N10 (23); ν C2C7 (12)
78		1144	1110	17.79	ν C20C21 (12); β H39C21C22 (12)
79		1162	1127	41.27	ν C26C27 (15); β C25C26C27 (10)
80		1169	1134	33.68	ν N9N10 (20)

81		1178	1143	10.98	β H35C14C15 (11); vN9N10 (10); β H36C15C16 (23); vC14C15 (13)
82	1147	1181	1146	4.77	β H40C22C23 (32); β H39C21C22 (16); β H41C23C24 (12)
83		1216	1180	28.37	vC11C16 (20); β H37C17C18 (10)
84		1237	1200	33.93	β H42C25C26 (13); β H44C26C27 (11)
85		1244	1207	11.57	β H30C4N5 (23); vN5C4 (10); vN5C6 (12); β H31C6N5 (21)
86	1211	1250	1213	28.63	β H37C17C18 (12)
87		1273	1235	28.34	β H44C26C27 (11)
88	1240	1274	1236	8.44	vN5C4 (27); vN5C6 (24); vC2C3 (15); vC6C7 (10); vC2C7 (12)
89		1294	1255	9.13	τ H44C26C27C28 (20); τ H45C26C27C28 (24)
90		1303	1264	31.79	β H36C15C16 (14); β H37C17C18 (23); β H34C11N10 (12)
91	1278	1321	1281	15.38	β H42C25C26 (19); β H46C27C28 (27)
92		1332	1292	7.12	β H44C26C27 (33); β H46C27C28 (19)
93	1298	1344	1304	76.05	vN9C1 (20); vC1C2 (11); β H29C3C4 (14)
94		1353	1312	23.96	β H29C3C4 (10); β H32C7C6 (10)
95		1358	1317	54.2	β H32C7C6 (11); β H31C6N5 (13)
96	1328	1367	1326	20.48	vC23C24 (10)
97		1376	1335	47.66	vN12C25 (19); vN12C13 (16); vN12C24 (14)
98		1384	1342	3.79	τ H46C27C26C25 (13); τ H47C27C26C25 (25); τ H43C25N12C13 (10)
99	1352	1390	1348	38.64	β H34C11N10 (38); β H33N9N10 (22)
100		1407	1365	15.18	τ H42C25N12C13 (13); τ H43C25N12C13 (18); β H42C25H43 (11)
101		1418	1375	22.54	vN12C13 (11); vN12C24 (10); β H42C25C26 (16)
102	1381	1420	1377	7.72	β H48C28H50 (29); β H48C28H49 (28); β H49C28H50 (24)
103	1408	1439	1396	21.74	vC6C7 (14); vC3C4 (14); β H30C4N5 (28); β H31C6N5 (23)
104		1470	1426	20.92	vC14C15 (17); vC17C18 (14); β H38C20C21 (10); β H41C23C24 (12)
105	1438	1488	1443	34.18	τ H44C26C27C28 (10); τ H45C26C27C28 (12)
106		1492	1447	8.45	β H46C27H47 (55); β H44C26H45 (18)
107		1497	1452	25.64	β H44C26H45 (38); β H49C28H50 (13); β H42C25H43 (10)
108		1503	1458	11.97	β H48C28H50 (38); β H48C28H49 (38); τ H48C28C27C26 (14)

109		1505	1460	30.83	β H33N9N10 (26)
110	1465	1507	1462	7.53	β H49C28H50 (26); β H42C25H43 (27);
111		1517	1471	14.3	β H42C25H43 (21); β H44C26H45 (22); β H46C27H47 (25)
112		1518	1472	29.89	vC22C23 (10); β H39C21C22 (11)
113		1521	1475	20.77	β H30C4N5 (11); β H31C6N5 (12)
114	1489	1525	1479	20.03	β H33N9N10 (12)
115		1594	1546	22.69	vN5C4 (15); vN5C6 (16); vC2C3 (24); vC2C7 (24)
116	1554	1606	1558	12.65	vC13C14 (25); vC15C16 (10); vC13C18 (17)
117		1617	1568	3.89	vC21C22 (19); vC19C24 (20); vC19C20 (11)
118		1633	1584	24.36	vC6C7 (16); vC2C7 (10); vC3C4 (14);
119		1635	1586	40.49	vC17C18 (13)
120		1657	1607	26.92	vC19C20 (14); vC23C24 (11); vN10C11 (18)
121	1587	1674	1624	14.98	vN10C11 (70)
122	1641	1741	1689	100	vO8C1 (88)
123	2868	3005	3035	18.33	vC27H46 (47); vC27H47 (47)
124	2953	3019	3049	33.57	vC11H34 (100)
125		3022	3052	12.54	vC26H44 (22); vC26H45 (29); vC28H48 (10); vC28H49 (17); vC28H50 (16)
126		3026	3056	23.39	vC26H45 (24); vC28H48 (15); vC26H44 (11); vC28H49 (17); vC28H50 (23)
127		3028	3058	11.42	vC27H46 (36); vC27H47 (42); vC26H44 (14)
128	3070	3044	3074	31.61	vC25H43 (50); vC25H42 (41)
129		3056	3087	9.41	vC26H44 (35); vC26H45 (30); vC25H42 (12)
130		3083	3114	3.08	vC25H42 (26); vC25H43 (22); vC28H49 (22); vC28H50 (22)
131		3088	3119	34.31	vC25H42 (16); vC25H43 (14); vC28H49 (22); vC28H50 (25)
132		3092	3123	27.54	vC28H48 (73); vC28H49 (15); vC28H50 (10)
133		3147	3178	21.87	vC4H30 (85); vC6H31 (13)
134		3152	3184	17.91	vC4H30 (13); vC6H31 (84)
135		3163	3195	12.64	vC14H35 (10); vC15H36 (90)
136		3166	3198	2.78	vC20H38 (20); vC21H39 (30); vC22H40 (41); vC23H41 (10)
137		3174	3206	8.88	vC20H38 (53); vC22H40 (26); vC23H41 (16)
138		3185	3217	19.38	vC20H38 (17); vC21H39 (25); vC23H41 (52)
139	3221	3190	3222	18.61	vC14H35 (86); vC15H36 (10)
140		3193	3225	8.39	vC17H37 (96)

141		3194	3226	16.4	ν C21H39 (30); ν C22H40 (21); ν C23H41 (15)
142		3208	3240	7.9	ν C7H32 (98)
143		3231	3263	5.04	ν C3H29 (99)
144	3405	3464	3499	10.27	ν N9H33 (100)

ν - stretching, β - in-plane bending, τ - torsional vibrations, Γ - out of plane bending

Table S3. Experimental and calculated vibrational frequencies along with their proposed assignment of hydrazide **6b**

Mode	Expt. Freq	Calc. Freq.			Vibrational Assignment with PED (%)
		Unscaled	Scaled	I_{IR}	
1		10	10	0.93	τ C15C16C11N10 (44); τ C1N9N10C11 (20); Γ C25C13C24N12 (15)
2		17	16	1.72	τ C13N12C25C26 (25); τ C27C26C25N12 (25)
3		23	22	2.09	β C16C11N10 (14); β C1N9N10 (15); β C11N10N9 (12)
4		25	24	1.33	τ C16C11N10N9 (10); Γ C25C13C24N12 (21); τ C2C1N9N10 (15)
5		38	37	0.87	Γ C25C13C24N12 (18)
6		53	51	0.62	τ C27C26C25N12 (29); τ C25C26C27C28 (12); τ C26C27C28C29 (19)
7		55	53	1.11	τ C7C2C1N9 (32)
8		73	71	0.45	τ C25C26C27C28 (30); τ C26C27C28C29 (16); τ C27C28C29C30 (24)
9		87	84	3.48	β C11C16C17 (10); τ C1N9N10C11 (13); τ C2C1N9N10 (13)
10		102	99	4.07	Γ C25C13C24N12 (10); β C26C27C28 (13); β C25C26C27 (10); β C27C28C29 (12)
11		104	101	4.29	Γ C19C13C17C18 (12); Γ N12C19C23C24 (10); Γ C18C19C24C20 (18)
12		118	114	2.49	Γ C18C19C24C20 (12); τ C1N9N10C11 (16)
13		134	130	0.38	τ C27C26C25N12 (26); τ C26C27C28C29 (30)
14		147	143	1.45	τ C25C26C27C28 (24); τ C27C28C29C30 (29)
15		157	152	4.93	Γ C1C2C7C3 (17)
16		168	163	3.54	τ C15C16C11N10 (17); τ C1N9N10C11 (10); τ C17C18C19C24 (12); β C1C2C7 (10)
17		174	169	2.5	τ C19C24C22C23 (14)
18		217	210	8.63	β C1C2C7 (19)
19		232	225	9.65	τ C7C2C1N9 (13); τ C2C1N9N10 (13)
20		236	229	10.5	τ C22C21C23C24 (15); τ C13C18C14C15 (11)
21		249	242	3.39	τ H54C30C29C28 (33); τ H55C30C29C28 (23)
22		251	243	6.71	β C25C26C27 (11); β C28C29C30 (12); τ C2C1N9N10 (10)
23		270	262	6.73	β C1C2C7 (14)
24		292	283	9.23	τ C16C11N10N9 (22); τ C2C1N9N10 (10)
25		297	288	6.44	β C24N12C25 (36)

26		321	311	3.86	β C27C28C29 (10); τ C15C14C16C17 (15)
27		367	356	9.05	ν C1C2 (23); β N9C1O8 (15); β C4N5C6 (12)
28		391	379	1.89	τ H31C3C4N5 (10); τ H34C7C6N5 (10); τ C4C3N5C6 (31)
29		403	391	3.15	τ C17C18C19C24 (19)
30		412	400	11.34	β C2C1N9 (11); β C16C17C18 (12); τ C7C4C6N5 (11)
31		435	422	8.68	Γ C18C19C24C20 (13); τ C13C18C16C17 (17)
32		436	423	3.97	β C25C26C27 (10); β C27C28C29 (14); β C28C29C30 (36)
33		448	435	9.74	β C26C27C28 (14); β C26C25N12 (14)
34		458	444	7.91	τ C13C18C14C15 (20)
35		466	452	12.61	β C26C25N12 (10)
36		495	480	26.15	β C16C11N10 (10)
37	522	532	516	17.24	β C17C18C19 (14)
38		578	561	5.09	τ C22C21C23C24 (18); τ C21C20C22C23 (33); Γ N12C19C23C24 (12)
39		592	574	22.07	β N9C1O8 (12)
40		614	596	16.93	τ H35N9N10C11 (49)
41		625	606	19.96	τ H35N9N10C11 (19); β C21C22C23 (10)
42	611	629	610	12.58	τ C15C14C16C17 (13); Γ C11C15C17C16 (12); τ H38C15C16C17 (10)
43		641	622	7.61	β C16C17C18 (17); β C21C22C23 (14); β C14C15C16 (16)
44		655	635	26.67	β C14C13C18 (17)
45		678	658	7.31	β C1N9N10 (10); β C7C6N5 (11)
46	688	686	665	4.32	β C3C4N5 (25); β C7C6N5 (13)
47		725	703	28.93	τ C2C7N5C6 (21); τ C4C3N5C6 (10); Γ O8C2N9C1 (34)
48		734	712	7.74	τ H52C29C28C27 (12); τ H50C28C29C30 (18); τ H48C27C28C29 (16); β H48C27C28 (10)
49		744	722	18.7	τ H41C21C22C23 (12)
50		746	724	7.42	τ C7C4C6N5 (16); τ C2C7N5C6 (16)
51		749	727	14.91	τ H31C3C4N5 (14); τ H34C7C6N5 (14)
52		751	728	3.57	τ C13C18C16C17 (22); τ C22C21C23C24 (13)
53		764	741	20.65	τ C19C24C22C23 (11); Γ N12C19C23C24 (24); τ H42C22C23C24 (11)
54	750	773	750	18.88	τ C7C4C6N5 (10); τ C2C7N5C6 (27); τ C4C3N5C6 (13); Γ O8C2N9C1 (15)
55		782	759	3.99	Γ C19C13C17C18 (19); τ H37C14C15C16 (10);

					τ H39C17C18C13 (10)
56		796	772	8.59	τ H54C30C29C28 (11); β H48C27C28 (10)
57		804	780	6.73	β C14C15C16 (11); β C11N10N9 (12)
58	798	812	788	22.47	τ C13C18C14C15 (14); τ H37C14C15C16 (42); τ H38C15C16C17 (26)
59		858	832	1.31	τ H40C20C21C22 (19); τ H41C21C22C23 (17); τ H43C23C24N12 (41)
60		863	837	20.18	Γ O8C2N9C1 (19); Γ C1C2C7C3 (18); τ H31C3C4N5 (18)
61	846	867	841	5.69	τ H32C4N5C6 (18); τ H33C6N5C4 (11)
62		899	872	5	τ H55C30C29C28 (13); τ H56C30C29C28 (15); ν C28C29 (30); ν C29C30 (17)
63		900	873	7.75	τ H31C3C4N5 (28); τ H33C6N5C4 (22); τ H34C7C6N5 (39)
64	891	919	891	5.76	τ H42C22C23C24 (19); τ H43C23C24N12 (18)
65		924	896	5.8	τ C13C18C16C17 (10); τ H39C17C18C13 (54); τ H36C11N10N9 (11)
66		936	908	7.55	τ H37C14C15C16 (20); τ H38C15C16C17 (37); τ H39C17C18C13 (15)
67		938	910	10.25	ν C16C17 (17)
68		940	912	2.19	τ H40C20C21C22 (35); τ H41C21C22C23 (10)
69		968	939	14.18	τ H36C11N10N9 (76)
70		979	950	0.21	τ H40C20C21C22 (12); τ H41C21C22C23 (33); τ H42C22C23C24 (36); τ H43C23C24N12 (10)
71		993	963	4.92	τ H31C3C4N5 (23); τ C4C3N5C6 (10); τ H32C4N5C6 (35); τ H34C7C6N5 (15)
72		1001	971	3.89	ν C25C26 (26); ν C27C28 (29); ν C29C30 (25)
73	975	1007	977	7.68	τ H32C4N5C6 (18); τ H33C6N5C4 (36); τ H34C7C6N5 (13)
74		1011	981	3.86	β H48C27C28 (16); β H50C28C29 (10); τ H51C28C29C30 (11); β H46C26C27 (14)
75		1013	983	8.01	β C4N5C6 (13); β C3C4N5 (14); β C7C6N5 (16); ν N5C4 (15); ν N5C6 (16)
76		1031	1000	5.27	ν C21C22 (10)
77		1034	1003	6.35	ν C25C26 (29); ν C26C27 (15)
78		1046	1015	9.36	β H40C20C21 (12); ν C21C22 (28); β H43C23C24 (11)
79		1048	1017	2.55	ν C26C27 (42); ν C29C30 (23)
80		1065	1033	2.93	ν C27C28 (35); ν C29C30 (13); ν C28C29 (28)
81		1080	1048	12.66	β C22C23C24 (24); β C20C21C22 (11); ν N12C25 (21)

82	1066	1094	1061	15.77	β C3C4N5 (19); β C7C6N5 (25); β H34C7C6 (17)
83		1111	1078	2.15	β H31C3C4 (22); β H34C7C6 (15); vC3C4 (23); vC6C7 (16)
84		1131	1097	16.38	vN9N10 (23); vC2C7 (12)
85		1136	1102	12.92	τ H55C30C29C28 (11); τ H56C30C29C28 (12); vC28C29 (12)
86		1145	1111	17.17	vC20C21 (12); β H41C21C22 (12)
87		1162	1127	44.08	β H37C14C15 (11)
88		1170	1135	28.53	vN9N10 (19)
89	1149	1178	1143	12.97	vN9N10 (10); β H37C14C15 (11); β H38C15C16 (21); vC14C15 (12)
90		1182	1147	5.66	β H41C21C22 (15); β H42C22C23 (30); β H43C23C24 (11)
91		1215	1179	27.19	vC11C16 (20); β H39C17C18 (10)
92		1223	1186	25.66	β H31C3C4 (10); β H34C7C6 (11)
93		1244	1207	12.39	β H32C4N5 (23); vN5C4 (10); vN5C6 (12); β H33C6N5 (21)
94	1217	1248	1211	19.94	vC19C24 (11); vC18C19 (10)
95		1259	1221	8.68	β H39C17C18 (16)
96		1260	1222	49.77	τ H47C26C27C28 (13); τ H48C27C28C29 (11); τ H51C28C29C30 (10); τ H49C27C28C29 (16)
97		1274	1236	9.3	vN5C4 (27); vN5C6 (24); vC2C3 (15); vC6C7 (10); vC2C7 (12)
98	1247	1290	1251	6.62	β H46C26C27 (13); β H52C29C30 (14)
99		1303	1264	30.39	β H38C15C16 (11); β H39C17C18 (18); β H36C11N10 (11)
100	1280	1325	1285	13.56	β H44C25C26 (19); β H52C29C30 (13)
101		1326	1286	3.2	τ H46C26C27C28 (12)
102		1334	1294	7.22	β H48C27C28 (42); β H46C26C27 (11); τ H49C27C28C29 (12)
103		1339	1299	12.66	β H52C29C30 (20); β H50C28C29 (23); β H46C26C27 (14)
104	1303	1345	1305	76.32	vN9C1 (20); vC1C2 (11)
105		1354	1313	22.86	β H31C3C4 (14)
106		1358	1317	53.77	β H34C7C6 (10); β H33C6N5 (12)
107	1327	1367	1326	20.1	vC23C24 (10)
108		1376	1335	48.68	vN12C25 (19); vN12C13 (15); vN12C24 (13)
109		1382	1341	3.31	τ H53C29C28C27 (16); τ H49C27C28C29 (10)
110	1354	1391	1349	39.58	β H36C11N10 (38); β H35N9N10 (22)
111		1405	1363	3.3	τ H48C27C28C29 (11); τ H49C27C28C29 (14);

					τ H50C28C29C30 (16); τ H51C28C29C30 (18)
112		1409	1367	15.13	τ H44C25N12C13 (14); τ H45C25N12C13 (25); τ H47C26C27C28 (10); β H44C25H45 (14)
113		1417	1374	21.4	β H44C25C26 (17); ν N12C13 (10); ν N12C24 (10)
114		1420	1377	6.39	β H54C30H56 (30); β H54C30H55 (31); β H55C30H56 (27)
115	1386	1439	1396	21.81	β H32C4N5 (28); β H33C6N5 (22); ν C6C7 (14); ν C3C4 (14)
116		1471	1427	20.88	ν C14C15 (16); ν C17C18 (14); β H43C23C24 (12); β H40C20C21 (10)
117	1436	1487	1442	28.79	β H46C26H47 (12)
118		1489	1444	14.43	β H50C28H51 (52); β H52C29H53 (16); β H48C27H49 (20)
119		1490	1445	19.32	β H48C27H49 (37); β H52C29H53 (22)
120		1497	1452	17.24	β H46C26H47 (36); β H52C29H53 (12); β H55C30H56 (12)
121		1503	1458	18.77	β H48C27H49 (11); β H54C30H55 (14); β H55C30H56 (16); β H44C25H45 (22)
122		1504	1459	12.66	β H54C30H56 (43); β H54C30H55 (28); τ H54C30C29C28 (14)
123		1506	1461	30.17	β H35N9N10 (25)
124	1465	1511	1466	3.36	β H55C30H56 (16); β H44C25H45 (20); β H52C29H53 (22)
125		1517	1471	13.56	β H50C28H51 (13); β H44C25H45 (11)
126		1518	1472	44.7	β H46C26H47 (16); β H48C27H49 (16); β H52C29H53 (11)
127		1521	1475	20.1	β H32C4N5 (12); β H33C6N5 (13)
128	1490	1526	1480	20.51	β H35N9N10 (13)
129	1548	1594	1546	22.63	ν N5C4 (15); ν N5C6 (16); ν C2C3 (24); ν C2C7 (24)
130		1606	1558	12.63	ν C13C14 (25); ν C15C16 (10); ν C13C18 (17)
131		1617	1568	3.97	ν C19C24 (19); ν C21C22 (19); ν C19C20 (11)
132		1633	1584	23.07	ν C6C7 (17); ν C2C7 (10); ν C3C4 (15)
133		1636	1587	41.15	ν C17C18 (14)
134		1657	1607	27.72	ν C19C20 (14); ν C23C24 (11); ν N10C11 (18)
135	1587	1674	1624	15.69	ν N10C11 (70)
136	1637	1741	1689	100	ν O8C1 (88)
137	2935	2995	3025	8.22	ν C27H48 (39); ν C27H49 (38); ν C28H51 (11); ν C28H50 (11)
138	2960	3000	3030	9.08	ν C28H51 (26); ν C28H50 (29); ν C29H52 (15);

				vC29H53 (15)	
139		3010	3040	30.94	vC28H50 (13); vC29H52 (31); vC29H53 (36)
140		3013	3043	4.9	vC27H48 (24); vC27H49 (21); vC28H50 (18); vC28H51 (25)
141		3020	3050	33.39	vC11H36 (100)
142		3022	3052	24.11	vC30H54 (25); vC30H55 (36); vC30H56 (35)
143		3025	3055	19.3	vC26H46 (46); vC26H47 (36)
144		3026	3056	4	vC27H48 (18); vC27H49 (16); vC29H52 (23); vC29H53 (23)
145		3044	3074	32.17	vC25H44 (46); vC25H45 (45)
146		3046	3076	20.51	vC28H50 (18); vC28H51 (19); vC29H52 (16); vC29H53 (16); vC26H47 (10)
147		3059	3090	20.59	vC25H44 (11); vC25H45 (11); vC26H46 (24); vC26H47 (27)
148		3083	3114	28.44	vC30H55 (44); vC30H56 (43)
149		3086	3117	27.7	vC25H44 (36); vC25H45 (38); vC26H46 (10); vC26H47 (11)
150		3088	3119	27.61	vC30H54 (74); vC30H55 (12); vC30H56 (13)
151		3147	3178	21.29	vC4H32 (89); vC6H33 (10)
152		3152	3184	18.54	vC4H32 (10); vC6H33 (87)
153		3162	3194	12.67	vC15H38 (90); vC14H37 (10)
154		3166	3198	2.74	vC20H40 (20); vC21H41 (30); vC22H42 (41)
155		3174	3206	9.22	vC20H40 (53); vC22H42 (28); vC23H43 (14)
156	3213	3186	3218	19.27	vC20H40 (17); vC21H41 (28); vC23H43 (51)
157		3189	3221	18.87	vC14H37 (87)
158		3193	3225	6.37	vC17H39 (97)
159		3194	3226	17.17	vC21H41 (31); vC22H42 (23); vC23H43 (21)
160		3208	3240	7.9	vC7H34 (98)
161		3230	3262	5.06	vC3H31 (99)
162	3587	3465	3500	10.24	vN9H35 (100)

v - stretching, β - in-plane bending, τ - torsional vibrations, Γ - out of plane bending

Table S4. Experimental and calculated vibrational frequencies along with their proposed assignment of hydrazide **6c**

Mode	Expt. Freq.	Calc. Freq.			Vibrational Assignment with PED (%)
		Unscaled	Scaled	I_{IR}	
1	12	12	0.22	τ C15C16C11N10 (50); τ C1N9N10C11 (24)	
2	17	16	1.18	τ C13N12C25C26 (29); β C16C11N10 (10)	
3	20	19	1.94	β C1N9N10 (14); β C11C16C17 (10); β C11N10N9 (11); τ C13N12C25C26 (15); β C16C11N10 (14)	
4	25	24	0.62	Γ C25C13C24N12 (37)	
5	39	38	1.03	Γ C25C13C24N12 (18); τ C7C2C1N9 (22); τ C2C1N9N10 (17)	
6	49	48	0.93	τ C7C2C1N9 (25)	
7	69	67	0.47	τ C27C26C25N12 (44)	
8	71	69	1.27	τ C27C26C25N12 (18)	
9	86	83	1.85	Γ Br50C20C22C21 (11); Γ C18C19C24C20 (16)	
10	98	95	5.8	τ C7C2C1N9 (16); τ C1N9N10C11 (13); τ C2C1N9N10 (12)	
11	109	106	0.4	τ C27C26C25N12 (14); τ C25C26C27C28 (54)	
12	124	120	2.75	τ C19C24C22C23 (13); τ C1N9N10C11 (10)	
13	135	131	2.96	Γ C1C2C7C3 (24); β C22C21Br50 (14)	
14	169	164	3.98	τ C15C16C11N10 (12)	
15	187	181	4.16	β C25C26C27 (13)	
16	203	197	3.2	β C25C26C27 (14)	
17	213	207	6.74	β C1C2C7 (18)	
18	217	210	9.67	Γ Br50C20C22C21 (10)	
19	228	221	4.43	ν Br50C21 (10); β C24N12C25 (12); τ H47C28C27C26 (11)	
20	242	235	4.19	ν Br50C21 (10); τ H48C28C27C26 (10); τ H47C28C27C26 (23)	
21	251	243	11.83	β C1C2C7 (15)	
22	262	254	8.1	β C1C2C7 (12); β C22C21Br50 (10)	
23	289	280	11.63	τ C16C11N10N9 (24); τ C2C1N9N10 (11); τ C13C18C16C17 (10)	
24	314	305	5.36	ν Br50C21 (15); β C24N12C25 (14)	
25	326	316	0.76	β C24N12C25 (12); β C22C21Br50 (14)	
26	353	342	2.77	Γ Br50C20C22C21 (13); τ C15C14C16C17 (12); β C26C27C28 (12)	

27		369	358	7.7	β N9C1O8 (14); β C4N5C6 (12); ν C1C2 (22)
28		391	379	1.43	τ C7C4C6N5 (17); τ C2C7N5C6 (15); τ C4C3N5C6 (31); τ H29C3C4N5 (10); τ H32C7C6N5 (10)
29		399	387	5.5	β C26C27C28 (21); τ C17C18C19C24 (14)
30		419	406	14.56	β C2C1N9 (11); τ C7C4C6N5 (15); β C16C17C18 (10)
31	426	433	420	9.39	τ C22C21C23C24 (20); Γ C18C19C24C20 (14); τ C13C18C16C17 (16)
32		445	432	6.3	β C26C25N12 (18); β C26C27C28 (15); τ C17C18C19C24 (10)
33		460	446	7.3	τ C13C18C14C15 (26); Γ C11C15C17C16 (11)
34		477	463	16.08	β C16C17C18 (11)
35		498	483	25.96	β C16C11N10 (10)
36		554	537	18.21	β C17C18C19 (17)
37		581	564	12.37	τ C22C21C23C24 (19); τ C21C20C22C23 (32)
38		594	576	18.51	β N9C1O8 (11); β C14C15C16 (10)
39		616	598	22.57	τ H33N9N10C11 (69)
40		628	609	13.45	τ C15C14C16C17 (17); Γ C11C15C17C16 (29); Γ C19C13C17C18 (13)
41		649	630	10.92	β C16C17C18 (10)
42		651	631	18.07	β C14C13C18 (36)
43		655	635	30.49	β C21C22C23 (13); β C18C19C24 (10)
44		679	659	8.46	β C7C6N5 (14)
45		687	666	5.33	β C3C4N5 (21)
46	683	726	704	29.66	τ C2C7N5C6 (22); τ C4C3N5C6 (10); Γ O8C2N9C1 (33)
47		739	717	5.87	τ H43C26C27C28 (20); τ H45C27C26C25 (20); β H43C26C27 (16); β H45C27C28 (12)
48		745	723	7.42	Γ C18C19C24C20 (12); Γ N12C19C23C24 (19)
49		751	728	11.42	Γ N12C19C23C24 (11)
50		755	732	3.34	ν C1C2 (11)
51		773	750	19.76	τ C7C4C6N5 (10); τ C2C7N5C6 (27); τ C4C3N5C6 (12); Γ O8C2N9C1 (14); τ H29C3C4N5 (14); τ H32C7C6N5 (13)
52		775	752	3.04	τ C13C18C14C15 (11); Γ C19C13C17C18 (23); τ C13C18C16C17 (11)
53		793	769	4.31	τ H41C25N12C13 (10); τ H45C27C26C25 (10); τ H47C28C27C26 (16); τ H44C26C27C28 (11)
54		808	784	16.93	τ H39C22C23C24 (35); τ H40C23C24N12 (44)

55		814	790	21.8	τ H35C14C15C16 (22); τ H36C15C16C11 (17)
56	799	816	792	16.63	τ H35C14C15C16 (21); τ H36C15C16C11 (15)
57	843	863	837	19.89	Γ O8C2N9C1 (19); Γ C1C2C7C3 (19); τ H29C3C4N5 (18); τ H30C4N5C6 (18); τ H31C6N5C4 (11)
58		879	853	8.61	β C20C21C22 (10)
59		892	865	12.09	τ H38C20C21C22 (78)
60		898	871	7.18	τ H29C3C4N5 (29); τ H31C6N5C4 (21); τ H32C7C6N5 (39)
61		911	884	5.84	τ H48C28C27C26 (16); τ H49C28C27C26 (16); ν C26C27 (26); ν C27C28 (15)
62		924	896	5.67	τ H37C17C18C13 (62); τ C13C18C16C17 (11); τ H34C11N10N9 (11)
63		940	912	6.37	τ H35C14C15C16 (19); τ H36C15C16C11 (30); τ H39C22C23C24 (12); τ H40C23C24N12 (10)
64		942	914	3.46	τ H39C22C23C24 (37); τ H40C23C24N12 (30)
65		946	918	21.02	ν C16C17 (18)
66	932	961	932	2.89	τ H47C28C27C26 (10); β H43C26C27 (19); β H45C27C28 (10)
67		968	939	14.34	τ H36C15C16C11 (14); τ H34C11N10N9 (71)
68		992	962	4.58	τ H29C3C4N5 (22); τ C4C3N5C6 (10); τ H30C4N5C6 (34); τ H31C6N5C4 (10); τ H32C7C6N5 (16)
69	976	1005	975	6.43	ν C25C26 (49); ν C27C28 (30)
70		1007	977	7.32	τ H30C4N5C6 (19); τ H31C6N5C4 (35); τ H32C7C6N5 (12)
71		1013	983	7.6	β C4N5C6 (12); β C3C4N5 (14); β C7C6N5 (16); ν N5C4 (15); ν N5C6 (16)
72		1039	1008	13.41	ν C21C22 (29)
73		1055	1023	2.49	ν C25C26 (16); ν C27C28 (37); ν C26C27 (37)
74		1071	1039	15.43	ν C20C21 (16); β H38C20C21 (10)
75		1083	1051	14.23	β C22C23C24 (18); β C20C21C22 (17); ν N12C25 (20)
76		1094	1061	15.8	β C3C4N5 (19); β C7C6N5 (25); β H32C7C6 (18)
77		1111	1078	2.21	β H32C7C6 (15); ν C3C4 (23); β H29C3C4 (22); ν C6C7 (16)
78		1129	1095	12.98	τ H48C28C27C26 (16); τ H49C28C27C26 (16); ν C26C27 (15); β C25C26C27 (10)
79		1132	1098	14.82	ν N9N10 (21); ν C2C7 (12)
80		1153	1118	35.36	β H35C14C15 (16)
81		1169	1134	43.09	ν N9N10 (20); β H39C22C23 (10)

82		1172	1137	13.21	β H39C22C23 (17); vC22C23 (14);
83	1148	1178	1143	12.83	β H36C15C16 (24); vN9N10 (10); β H35C14C15 (11); vC14C15 (12)
84		1210	1174	26.96	vC11C16 (18); vC18C19 (14)
85		1237	1200	31.21	β H43C26C27 (10); β H41C25C26 (14)
86		1243	1206	11.44	β H32C7C6 (11); β H29C3C4 (10); β H30C4N5 (23); vN5C4 (11); vN5C6 (12); β H31C6N5 (20)
87	1213	1249	1212	29.53	vC18C19 (10); β H37C17C18 (12)
88		1271	1233	20.6	β H38C20C21 (16); β H43C26C27 (10)
89	1244	1275	1237	10.18	vN5C4 (27); vN5C6 (24); vC6C7 (10); vC2C7 (12); vC2C3 (15)
90		1293	1254	20.75	β H37C17C18 (12); β H38C20C21 (18); β H34C11N10 (10)
91		1296	1257	13.99	τ H43C26C27C28 (19); τ H44C26C27C28 (23)
92		1310	1271	40.75	β H45C27C28 (12)
93	1281	1328	1288	26.72	β H45C27C28 (24); β H41C25C26 (14)
94	1298	1334	1294	14.13	β H43C26C27 (30); β H45C27C28 (16); β H41C25C26 (11); τ H44C26C27C28 (10)
95		1344	1304	80.2	vC1C2 (11); β H29C3C4 (13); vN9C1 (20)
96		1354	1313	19.21	β H29C3C4 (12); β H32C7C6 (11); β H31C6N5 (10)
97		1360	1319	48.76	vN9C1 (11); β H31C6N5 (11)
98	1329	1374	1333	44.51	vN12C25 (20); vN12C13 (16); vN12C24 (15)
99		1384	1342	3.44	τ H41C25N12C13 (10); τ H45C27C26C25 (12); τ H46C27C26C25 (23); τ H42C25N12C13 (13)
100	1352	1390	1348	35.54	β H34C11N10 (40); β H33N9N10 (22)
101		1406	1364	16.5	τ H42C25N12C13 (13); τ H43C26C27C28 (11); τ H44C26C27C28 (13)
102		1414	1372	19.71	β H41C25C26 (11); vN12C13 (10); vN12C24 (10)
103	1383	1417	1374	8.44	β H47C28H49 (27); β H47C28H48 (28); β H48C28H49 (24)
104		1440	1397	21.59	β H30C4N5 (28); β H31C6N5 (22); vC6C7 (15); vC3C4 (14)
105	1408	1453	1409	8.07	β H35C14C15 (10); β H40C23C24 (11); vC14C15 (13); vC22C23 (15); vC19C20 (10)
106	1439	1474	1430	42.11	β H39C22C23 (13); vC20C21 (21)
107		1492	1447	6.58	β H45C27H46 (44); β H43C26H44 (37)
108		1494	1449	11.23	β H45C27H46 (13); β H43C26H44 (15); β H48C28H49 (13); β H41C25H42 (24)
109		1500	1455	15.28	β H47C28H49 (34); β H47C28H48 (40);

					τ H47C28C27C26 (14)
110		1502	1457	47.85	β H43C26H44 (12); β H33N9N10 (10)
111		1505	1460	29.52	β H33N9N10 (19); β H41C25H42 (11)
112		1507	1462	19.3	β H41C25H42 (14); β H48C28H49 (11)
113	1468	1516	1471	18.24	β H41C25H42 (15); β H43C26H44 (21); β H45C27H46 (29); β H48C28H49 (11)
114		1520	1474	13.48	β H30C4N5 (12); β H31C6N5 (13)
115	1491	1525	1479	24.09	β H33N9N10 (12)
116		1595	1547	22.14	vN5C4 (15); vN5C6 (16); vC2C7 (25); vC2C3 (24)
117	1555	1603	1555	10.69	vC21C22 (17); vC19C24 (23); vC19C20 (12)
118		1606	1558	12.11	vC13C14 (25); vC15C16 (10); vC13C18 (17)
119		1631	1582	29.91	vC19C20 (10); vC23C24 (15); vC17C18 (12)
120		1634	1585	14.3	vC6C7 (19); vC2C7 (13); vC2C3 (11); vC3C4 (18)
121		1653	1603	31.12	vC17C18 (11); vN10C11 (19)
122	1589	1675	1625	21.35	vN10C11 (52)
123	1643	1744	1692	100	vO8C1 (79)
124	2870	3006	2916	18.15	vC27H45 (48); vC27H46 (46)
125		3021	2930	12.09	vC11H34 (100)
126		3022	2931	36.33	vC26H44 (28); vC26H43 (25); vC28H48 (17); vC28H49 (15)
127		3026	2935	23.23	vC26H44 (21); vC28H47 (16); vC26H43 (12); vC28H48 (18); vC28H49 (23)
128		3028	2937	11.32	vC27H45 (36); vC27H46 (43); vC26H43 (13)
129	2953	3043	2952	31.9	vC25H41 (42); vC25H42 (48)
130		3056	2964	9.34	vC26H43 (32); vC26H44 (31); vC25H41 (12); vC25H42 (10)
131		3083	2991	0.85	vC25H41 (29); vC25H42 (26); vC28H48 (18); vC28H49 (18)
132		3088	2995	34.56	vC25H41 (12); vC25H42 (11); vC28H48 (26); vC28H49 (29)
133		3092	2999	27.47	vC28H47 (74); vC28H48 (14); vC28H49 (11)
134		3148	3054	21.71	vC4H30 (84); vC6H31 (15)
135		3153	3058	17.3	vC4H30 (15); vC6H31 (83)
136		3164	3069	12.53	vC15H36 (91)
137		3186	3090	11.13	vC22H39 (16); vC23H40 (84)
138		3192	3096	17.2	vC14H35 (83)
139		3194	3098	3.64	vC17H37 (90)

140		3200	3104	2.13	vC20H38 (97)
141		3206	3110	8.17	vC22H39 (83); vC23H40 (16)
142		3207	3111	7.89	vC7H32 (97)
143	3221	3227	3130	5.73	vC3H29 (99)
144	3400	3465	3361	10.04	vN9H33 (100)

v - stretching, β - in-plane bending, τ - torsional vibrations, Γ - out of plane bending

Table S5. Experimental and calculated ¹H chemical shift values of hydrazides **6a-c**

Hydrazide 6a			Hydrazide 6b			Hydrazide 6c		
Atom	Calc.	Expt.	Atom	Calc.	Expt.	Atom	Calc.	Expt.
H29	8.28	8.79	H31	8.31	8.64	H29	8.15	8.50
H30	8.80	8.81	H32	8.75	8.81	H30	8.69	8.80
H31	8.74	8.80	H33	8.73	8.80	H31	8.58	8.79
H32	7.84	8.64	H34	7.83	8.50	H32	7.73	7.91
H33	8.13	12.03	H35	8.17	12.03	H33	7.99	12.02
H34	7.72	7.87	H36	7.73	7.91	H34	7.60	7.85
H35	7.32	7.46	H37	7.42	7.49	H35	7.21	7.48
H36	7.44	7.67	H38	7.43	7.86	H36	7.28	7.64
H37	8.68	8.29	H39	8.69	8.25	H37	8.63	8.63
H38	8.08	8.23	H40	8.05	8.23	H38	7.98	8.25
H39	7.18	7.22	H41	7.17	7.23	H39	7.29	7.70
H40	7.45	7.86	H42	7.41	7.68	H40	7.09	7.24
H41	7.35	7.61	H43	7.41	7.61	H41	3.95	4.44
H42	4.15	4.41	H44	4.11	4.40	H42	3.96	4.44
H43	4.14	4.38	H45	4.12	4.40	H43	1.50	1.77
H44	1.62	1.77	H46	1.64	1.76	H44	1.45	1.77
H45	1.53	1.70	H47	1.63	1.76	H45	1.33	1.33
H46	1.44	1.33	H48	1.41	1.25	H46	1.33	1.31
H47	1.46	1.24	H49	1.38	1.25	H47	1.09	0.91
H48	1.15	0.90	H50	1.15	1.25	H48	0.75	0.88
H49	0.78	0.87	H51	1.16	1.21	H49	0.76	0.89
H50	0.77	0.86	H52	1.29	1.21			
			H53	1.30	1.21			
			H54	1.10	0.80			
			H55	0.70	0.78			
			H56	0.71	0.78			

Table S6. Experimental and calculated ^{13}C chemical shift values of hydrazides **6a-c**

Hydrazide 6a			Hydrazide 6b			Hydrazide 6a		
Atom	Calc.	Expt.	Atom	Calc.	Expt.	Atom	Calc.	Expt.
C1	162.1	161.8	C1	162.5	161.8	C1	161.8	161.1
C2	138.0	140.9	C2	138.2	140.9	C2	137.9	126.7
C3	123.3	123.7	C3	123.4	123.7	C3	123.2	123.7
C4	147.2	150.7	C4	147.4	150.7	C4	147.2	141.7
C6	148.4	150.7	C6	148.5	150.7	C6	148.1	150.7
C7	122.6	122.7	C7	122.5	122.7	C7	122.2	122.0
C11	141.4	150.0	C11	141.3	150.0	C11	140.8	141.4
C13	140.3	141.7	C13	140.5	141.7	C13	140.0	141.2
C14	105.6	110.1	C14	105.9	110.1	C14	106.3	110.1
C15	126.8	126.7	C15	126.7	126.7	C15	127.0	125.1
C16	123.3	125.1	C16	122.8	125.1	C16	122.8	122.7
C17	114.0	119.8	C17	114.2	119.8	C17	114.5	119.8
C18	122.9	122.7	C18	123.2	122.7	C18	121.3	121.1
C19	122.1	122.4	C19	122.2	122.4	C19	122.7	122.4
C20	118.4	121.1	C20	118.9	121.1	C20	121.0	120.8
C21	117.0	120.8	C21	117.0	120.8	C21	127.2	125.4
C22	123.8	125.3	C22	123.8	125.3	C22	126.5	124.0
C23	106.3	110.3	C23	106.3	110.3	C23	107.5	110.2
C24	139.9	141.2	C24	140.2	141.2	C24	138.5	140.9
C25	43.7	42.6	C25	43.7	42.8	C25	43.5	42.6
C26	31.6	31.1	C26	30.4	31.4	C26	31.0	31.1
C27	22.3	20.2	C27	30.1	28.9	C27	21.6	20.2
C28	13.5	14.1	C28	34.2	26.5	C28	13.2	14.1
			C29	26.1	22.4			
			C30	13.8	14.2			