

Supporting Information

Self-Assembly and Gelation Behavior of Tris(phenylisoxazoly)benzenes

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General: ^1H and ^{13}C NMR spectra were measured at 25 °C using the residual solvent signal as internal standard. All NMR spectra were recorded in CDCl_3 unless otherwise indicated. Mass spectra were recorded using a FAB mass spectrometer using 3-NBA matrix. Electronic absorption, fluorescence and infrared spectra were measured using a conventional quartz cell (light path 1cm) with temperature control. Elemental analyses were performed using a CHN analyzer.

All reactions were carried out under an argon atmosphere unless otherwise noted. Tetrahydrofuran (THF) was freshly distilled from Na-benzophenone. Dichloromethane (DCM) and dimethylformamide (DMF) were freshly distilled from CaH_2 .

Gelation tests: The gelators and the solvent were put in a screw-capped test tube and heated until the solid dissolved. The solution was cooled to 25 °C and left for 2 hours under ambient conditions. Gelation was determined by the absence of flow of the solvent when the test tube was inverted.

FESEM measurements: A piece of the gel was placed on a glass plate and removed after 30 s. Then it was dried overnight at low pressure. The obtained sample was shielded by Pt and measured with a field emission scanning electron microscope. An accelerating voltage of 20 kV was applied.

TEM measurements: A piece of the gel was placed on a carbon-coated copper grid and removed after 30 s. Then it was dried for overnight at low pressure without staining. The obtained sample was measured with a transmission electron microscope. The accelerating voltage of 200 kV was applied.

Analysis of self-association by ^1H NMR and UV/Vis titration experiments: Hyperbolic curves were obtained by plotting of the compound concentrations vs. ^1H NMR chemical shifts (δ) of the aromatic protons or ϵ . The curve-fitting analysis of the plots was carried out on the basis of an isodesmic association model, which is a type of unlimited self-association where the addition of

each successive monomer to polymer involves an equal association constant ($K_2 = K_3 = \dots K_i = K_E$). The fitting functions are given by equations 1 and 2 for NMR and UV/Vis titration experiments. ϵ denotes the apparent extinction coefficient obtained from the spectra; ϵ_m and ϵ_a are the extinction coefficients for the monomer and the self-assembled species, respectively; K_E is the association constant; and c is the total concentration of the compounds. δ denotes the apparent chemical shifts obtained from the spectra; δ_m and δ_a are the chemical shifts for the monomer and the self-assembled species, respectively.

$$\delta(c) = \delta_m + (\delta_a - \delta_m) \left(1 + \frac{1 - \sqrt{4K_E c + 1}}{2K_E c} \right) \text{-----} (1)$$

$$\epsilon(c) = \epsilon_a + \frac{2K_E c + 1 - \sqrt{4K_E c + 1}}{2K_E^2 c^2} (\epsilon_m - \epsilon_a) \text{-----} (2)$$

DFT calculations: Geometry optimizations of model compound **13** and **14** were carried out optimized using the B3LYP function of the G03W¹ software package with 6–31G(d) basis sets. The optical spectroscopic and electronic structures of **13** were studied using the TDDFT method.

Molecular Mechanics Calculations: A conformational exploration of the assembly of **4** as a model system was carried out with the low mode sampling method² using MMFF94s as implemented in MacroModel V.9.1.³ During the calculation, the C_3 axes of the six molecules were constrained along the principal anisotropic axis to ensure that each molecular center did not slip out of the principal axis, the horizontal rotation and shift along the axis are not fixed. 1000 Initial geometries were generated, and optimized by the PRCG method.

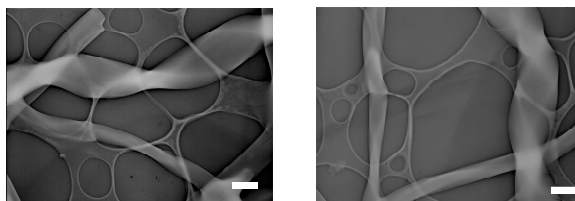


Figure S1. TEM images of xerogels of **2** prepared from DMSO. The bars represent 1 μm .

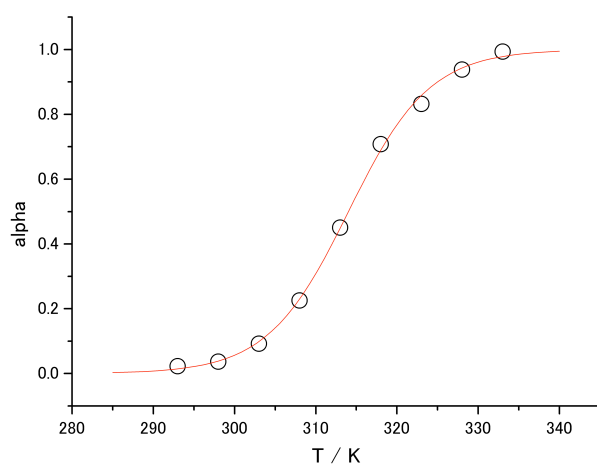


Figure S2. T -dependent plot of α_{agg} of **1** vs. T at 278 nm in MCH.

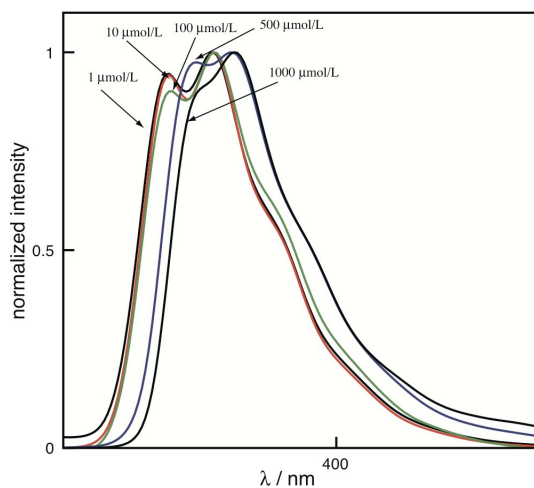


Figure S3. Fluorescence spectra (λ_{ex} =278 nm) of **1** at 298 K in MCH.

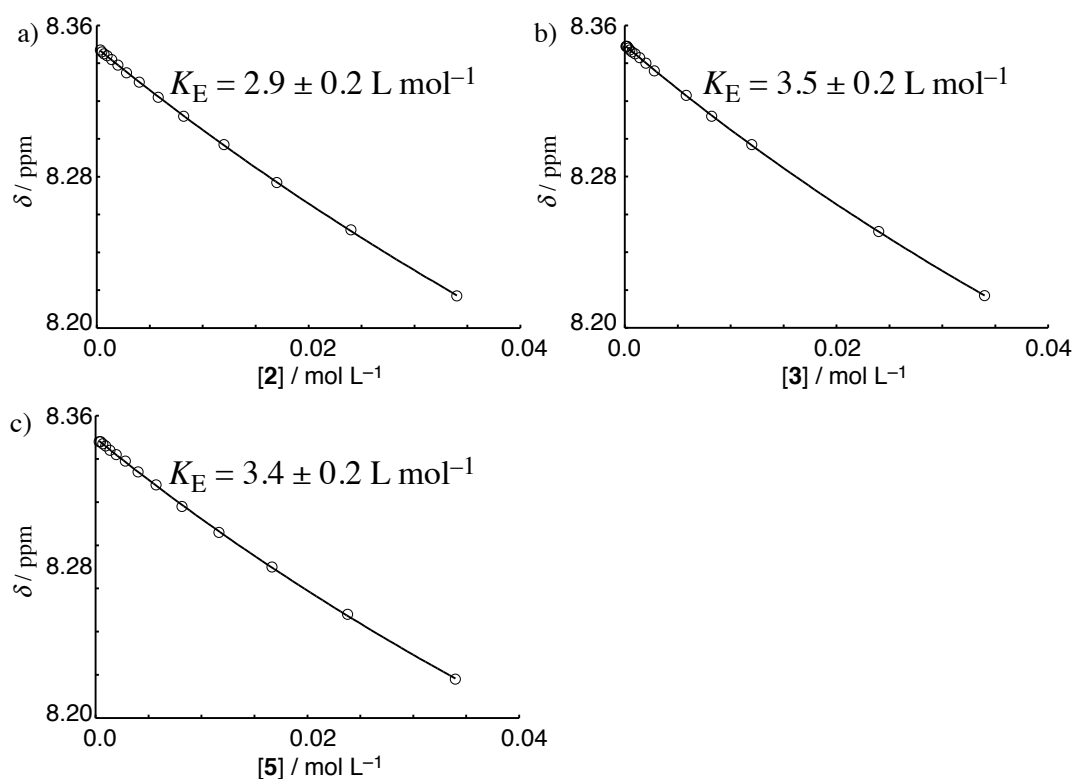


Figure S4. Concentration dependence of chemical shifts of the central aromatic protons for a) **2**, b) **3**, and c) **5** in chloroform- d_1 at 297 K.

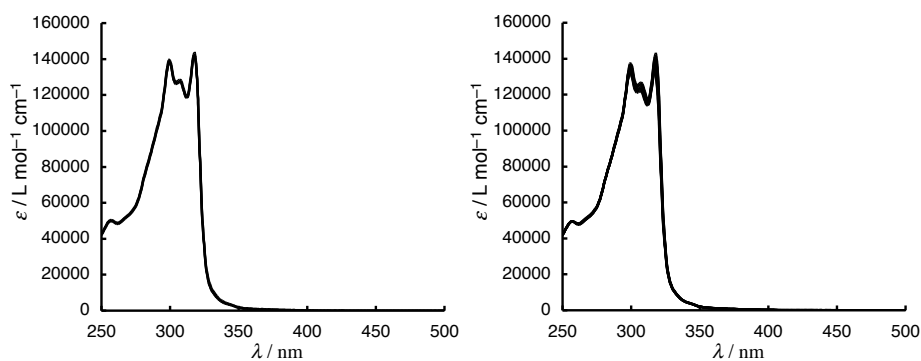


Figure S5. Electronic absorption spectra of **12** in MCH: (left) at the concentration of 1.0, 10.0 and 100.0 $\mu\text{mol L}^{-1}$ at 293K, and (right) at the concentration of 50.0 $\mu\text{mol L}^{-1}$ at 323, 318, 313, 308, 303, 298 and 293 K.

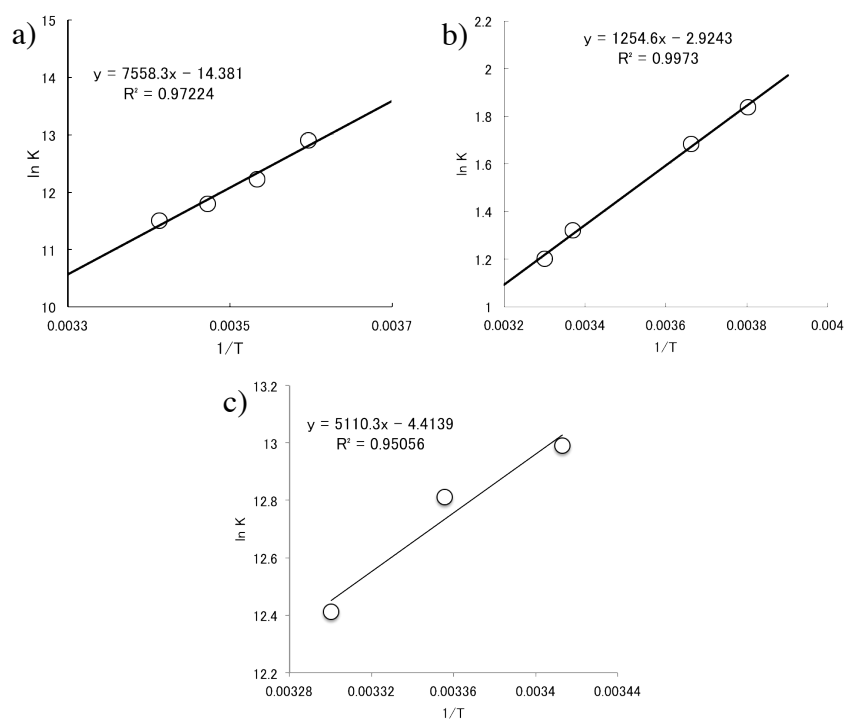
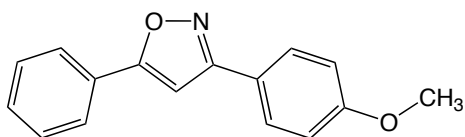


Figure S6. Van't Hoff plots of **1** (a) in MCH, (b) in CDCl_3 , and (c) in DMSO.

Calculated Structures of Isoxazole derivatives 13, 14 and the hexameric assembly of 4.

3-(4-Methoxyphenyl)-5-phenylisoxazole (**14**)

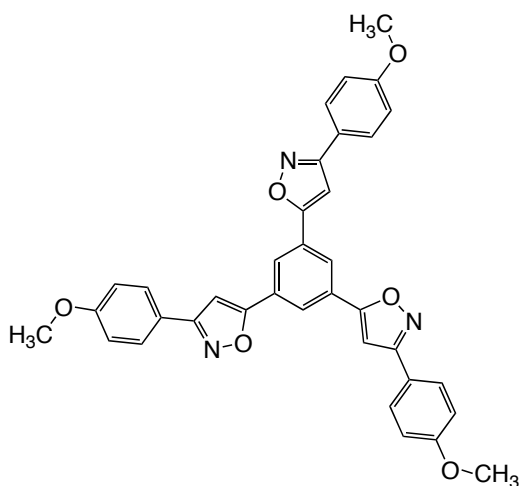


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.716093	-0.753677	-0.000175
2	6	0	4.350908	-1.030773	-0.000241
3	6	0	3.415206	0.017500	0.000108
4	6	0	3.878705	1.344048	0.000472
5	6	0	5.244031	1.614764	0.000515
6	6	0	6.168520	0.567241	0.000208
7	1	0	6.429008	-1.573655	-0.000425
8	1	0	4.000286	-2.057270	-0.000535
9	1	0	3.167707	2.165157	0.000741
10	1	0	5.587366	2.645656	0.000811
11	1	0	7.233992	0.779982	0.000248
12	6	0	1.980512	-0.263154	0.000040
13	6	0	0.863648	0.525483	0.000048
14	8	0	1.598537	-1.563071	-0.000553
15	6	0	-0.228188	-0.394159	-0.000098
16	1	0	0.821769	1.603325	0.000245
17	7	0	0.207014	-1.643322	-0.000371
18	6	0	-1.670861	-0.103854	-0.000091
19	6	0	-2.146858	1.218465	-0.000702
20	6	0	-2.611195	-1.143455	0.000542
21	6	0	-3.507017	1.491563	-0.000698
22	1	0	-1.446997	2.048989	-0.001239
23	6	0	-3.979825	-0.883444	0.000567

24	1	0	-2.260200	-2.170245	0.001045
25	6	0	-4.436868	0.441538	-0.000067
26	1	0	-3.876317	2.512192	-0.001181
27	1	0	-4.676149	-1.714188	0.001084
28	6	0	-6.737142	-0.207217	0.000444
29	1	0	-7.698424	0.309736	0.000243
30	1	0	-6.665371	-0.839649	-0.894103
31	1	0	-6.665276	-0.838809	0.895572
32	8	0	-5.748350	0.811424	-0.000090

1,3,5-Tris[3-(4-methoxyphenyl)isoxazol-5-yl]benzene (**13**)



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.716574	-0.794540	-0.008700
2	6	0	1.378707	0.565145	0.002671
3	6	0	0.036281	0.965441	-0.007293
4	6	0	-0.970386	-0.008582	-0.026946
5	6	0	-0.646417	-1.371019	-0.036315
6	6	0	0.700810	-1.759946	-0.028401

7	1	0	2.153964	1.322270	0.018045
8	1	0	-2.011556	0.296522	-0.036121
9	1	0	0.957361	-2.812188	-0.035843
10	6	0	-0.310274	2.386802	0.000854
11	6	0	-1.490784	3.072984	-0.041680
12	8	0	0.712184	3.272485	0.062249
13	6	0	-1.109268	4.449078	-0.000778
14	1	0	-2.487965	2.664361	-0.090440
15	7	0	0.206337	4.571583	0.059797
16	6	0	-1.972746	5.640011	-0.015677
17	6	0	-3.364354	5.528322	-0.178252
18	6	0	-1.425510	6.922262	0.131034
19	6	0	-4.176909	6.652420	-0.192679
20	1	0	-3.822229	4.551010	-0.300591
21	6	0	-2.229715	8.059358	0.117550
22	1	0	-0.352894	7.025806	0.258411
23	6	0	-3.616090	7.929661	-0.044608
24	1	0	-5.251587	6.568713	-0.319077
25	1	0	-1.770106	9.033944	0.235073
26	6	0	-3.986945	10.287729	0.069894
27	1	0	-4.854045	10.948440	0.019302
28	1	0	-3.482638	10.423643	1.035393
29	1	0	-3.290628	10.539720	-0.740413
30	8	0	-4.495420	8.969109	-0.071316
31	6	0	3.122660	-1.198635	0.000769
32	6	0	4.301359	-0.508206	0.019331
33	8	0	3.387894	-2.526103	-0.012328
34	6	0	5.309496	-1.519922	0.015615
35	1	0	4.436964	0.562015	0.024046
36	6	0	-1.707626	-2.378394	-0.050733
37	6	0	-3.071480	-2.313773	0.002798
38	8	0	-1.330496	-3.676001	-0.126426
39	6	0	-3.498037	-3.676017	-0.045104

40	1	0	-3.686518	-1.430869	0.079540
41	7	0	-2.459686	-4.491650	-0.123749
42	7	0	4.766594	-2.726195	-0.001276
43	6	0	-4.868827	-4.209163	-0.012650
44	6	0	-5.983572	-3.353409	-0.029247
45	6	0	-5.097608	-5.591362	0.035436
46	6	0	-7.275338	-3.858077	0.001723
47	1	0	-5.843702	-2.277110	-0.071624
48	6	0	-6.389349	-6.111419	0.065924
49	1	0	-4.247494	-6.265539	0.050240
50	6	0	-7.489915	-5.243465	0.049619
51	1	0	-8.137729	-3.199235	-0.012071
52	1	0	-6.526466	-7.185897	0.103919
53	6	0	6.771427	-1.355847	0.023936
54	6	0	7.360381	-0.089352	0.180695
55	6	0	7.616351	-2.464674	-0.122857
56	6	0	8.739092	0.063413	0.189375
57	1	0	6.735680	0.790530	0.304155
58	6	0	9.002242	-2.325386	-0.114929
59	1	0	7.176736	-3.449051	-0.246237
60	6	0	9.573053	-1.054658	0.041073
61	1	0	9.196399	1.040076	0.311531
62	1	0	9.623374	-3.205936	-0.232246
63	6	0	-9.073290	-7.031963	0.120859
64	1	0	-10.161302	-7.116215	0.133998
65	1	0	-8.679513	-7.549995	-0.763223
66	1	0	-8.662190	-7.497915	1.025831
67	6	0	11.806436	-1.894394	-0.087353
68	1	0	12.809465	-1.466564	-0.042350
69	1	0	11.687490	-2.626404	0.722102
70	1	0	11.669707	-2.398362	-1.052984
71	8	0	10.911686	-0.802022	0.061470
72	8	0	-8.792582	-5.640528	0.077413

Coordinate specifications in PDB format produced by MacroModel V9.1.

Structure data of Conformer A

HETATM	1	C1	1	-4.652	2.552	-1.364	1.00	0.00	C
HETATM	2	C2	1	-5.002	2.721	-0.017	1.00	0.00	C
HETATM	3	C3	1	-4.170	3.412	0.877	1.00	0.00	C
HETATM	4	C4	1	-2.967	3.948	0.393	1.00	0.00	C
HETATM	5	C5	1	-2.586	3.802	-0.950	1.00	0.00	C
HETATM	6	C6	1	-3.442	3.104	-1.814	1.00	0.00	C
HETATM	7	C7	1	-4.529	3.565	2.282	1.00	0.00	C
HETATM	8	C8	1	-3.893	4.042	3.404	1.00	0.00	C
HETATM	9	C9	1	-4.834	3.905	4.460	1.00	0.00	C
HETATM	10	N1	1	-5.975	3.376	3.988	1.00	0.00	N
HETATM	11	O1	1	-5.780	3.163	2.641	1.00	0.00	O
HETATM	12	C10	1	-1.325	4.344	-1.442	1.00	0.00	C
HETATM	13	C11	1	-0.658	4.324	-2.644	1.00	0.00	C
HETATM	14	C12	1	0.547	5.046	-2.424	1.00	0.00	C
HETATM	15	N2	1	0.585	5.487	-1.156	1.00	0.00	N
HETATM	16	O2	1	-0.572	5.048	-0.552	1.00	0.00	O
HETATM	17	C13	1	-5.520	1.801	-2.265	1.00	0.00	C
HETATM	18	C14	1	-6.702	1.112	-2.131	1.00	0.00	C
HETATM	19	C15	1	-6.988	0.594	-3.425	1.00	0.00	C
HETATM	20	N3	1	-6.027	0.968	-4.286	1.00	0.00	N
HETATM	21	O3	1	-5.121	1.711	-3.563	1.00	0.00	O
HETATM	22	C16	1	-10.335	-1.768	-4.673	1.00	0.00	C
HETATM	23	C17	1	-9.544	-1.120	-5.618	1.00	0.00	C
HETATM	24	C18	1	-8.449	-0.353	-5.209	1.00	0.00	C
HETATM	25	C19	1	-8.132	-0.219	-3.848	1.00	0.00	C
HETATM	26	C20	1	-8.938	-0.880	-2.909	1.00	0.00	C
HETATM	27	C21	1	-10.032	-1.650	-3.319	1.00	0.00	C
HETATM	28	C22	1	3.714	5.865	-5.189	1.00	0.00	C
HETATM	29	C23	1	3.623	6.578	-3.996	1.00	0.00	C

HETATM	30	C24	1	2.590	6.308	-3.094	1.00	0.00	C
HETATM	31	C25	1	1.629	5.323	-3.372	1.00	0.00	C
HETATM	32	C26	1	1.735	4.615	-4.579	1.00	0.00	C
HETATM	33	C27	1	2.770	4.883	-5.480	1.00	0.00	C
HETATM	34	C28	1	-4.380	5.005	8.571	1.00	0.00	C
HETATM	35	C29	1	-5.652	4.859	8.022	1.00	0.00	C
HETATM	36	C30	1	-5.798	4.492	6.681	1.00	0.00	C
HETATM	37	C31	1	-4.675	4.272	5.869	1.00	0.00	C
HETATM	38	C32	1	-3.401	4.421	6.437	1.00	0.00	C
HETATM	39	C33	1	-3.255	4.784	7.780	1.00	0.00	C
HETATM	40	H1	1	-5.936	2.298	0.349	1.00	0.00	H
HETATM	41	H2	1	-2.312	4.489	1.073	1.00	0.00	H
HETATM	42	H3	1	-3.161	2.982	-2.858	1.00	0.00	H
HETATM	43	H4	1	-2.890	4.435	3.461	1.00	0.00	H
HETATM	44	H5	1	-0.984	3.846	-3.555	1.00	0.00	H
HETATM	45	H6	1	-7.279	0.987	-1.228	1.00	0.00	H
HETATM	46	H7	1	-9.775	-1.207	-6.677	1.00	0.00	H
HETATM	47	H8	1	-7.850	0.148	-5.967	1.00	0.00	H
HETATM	48	H9	1	-8.721	-0.826	-1.845	1.00	0.00	H
HETATM	49	H10	1	-10.639	-2.163	-2.577	1.00	0.00	H
HETATM	50	H11	1	4.355	7.348	-3.763	1.00	0.00	H
HETATM	51	H12	1	2.538	6.884	-2.171	1.00	0.00	H
HETATM	52	H13	1	1.027	3.830	-4.834	1.00	0.00	H
HETATM	53	H14	1	2.840	4.316	-6.405	1.00	0.00	H
HETATM	54	H15	1	-6.534	5.031	8.634	1.00	0.00	H
HETATM	55	H16	1	-6.803	4.388	6.273	1.00	0.00	H
HETATM	56	H17	1	-2.502	4.239	5.854	1.00	0.00	H
HETATM	57	H18	1	-2.260	4.885	8.206	1.00	0.00	H
HETATM	58	H19	1	-11.184	-2.368	-4.991	1.00	0.00	H
HETATM	59	H20	1	4.519	6.072	-5.888	1.00	0.00	H
HETATM	60	H21	1	-4.265	5.287	9.614	1.00	0.00	H
HETATM	61	C34	1	-3.425	-0.596	0.320	1.00	0.00	C
HETATM	62	C35	1	-3.028	-0.112	1.574	1.00	0.00	C

HETATM	63	C36	1	-1.810	0.563	1.751	1.00	0.00	C
HETATM	64	C37	1	-0.988	0.761	0.632	1.00	0.00	C
HETATM	65	C38	1	-1.356	0.293	-0.639	1.00	0.00	C
HETATM	66	C39	1	-2.576	-0.385	-0.776	1.00	0.00	C
HETATM	67	C40	1	-1.397	1.034	3.068	1.00	0.00	C
HETATM	68	C41	1	-0.290	1.669	3.580	1.00	0.00	C
HETATM	69	C42	1	-0.540	1.804	4.974	1.00	0.00	C
HETATM	70	N4	1	-1.744	1.289	5.269	1.00	0.00	N
HETATM	71	O4	1	-2.269	0.813	4.090	1.00	0.00	O
HETATM	72	C43	1	-0.500	0.500	-1.802	1.00	0.00	C
HETATM	73	C44	1	-0.618	0.261	-3.152	1.00	0.00	C
HETATM	74	C45	1	0.607	0.701	-3.721	1.00	0.00	C
HETATM	75	N5	1	1.411	1.182	-2.759	1.00	0.00	N
HETATM	76	O5	1	0.722	1.053	-1.573	1.00	0.00	O
HETATM	77	C46	1	-4.689	-1.306	0.174	1.00	0.00	C
HETATM	78	C47	1	-5.741	-1.607	1.008	1.00	0.00	C
HETATM	79	C48	1	-6.652	-2.352	0.212	1.00	0.00	C
HETATM	80	N6	1	-6.172	-2.477	-1.036	1.00	0.00	N
HETATM	81	O6	1	-4.956	-1.831	-1.053	1.00	0.00	O
HETATM	82	C49	1	-10.433	-4.017	1.322	1.00	0.00	C
HETATM	83	C50	1	-9.769	-4.483	0.190	1.00	0.00	C
HETATM	84	C51	1	-8.534	-3.938	-0.170	1.00	0.00	C
HETATM	85	C52	1	-7.945	-2.921	0.599	1.00	0.00	C
HETATM	86	C53	1	-8.627	-2.462	1.736	1.00	0.00	C
HETATM	87	C54	1	-9.864	-3.007	2.094	1.00	0.00	C
HETATM	88	C55	1	1.796	0.702	-7.830	1.00	0.00	C
HETATM	89	C56	1	2.757	0.769	-6.824	1.00	0.00	C
HETATM	90	C57	1	2.366	0.766	-5.482	1.00	0.00	C
HETATM	91	C58	1	1.009	0.691	-5.129	1.00	0.00	C
HETATM	92	C59	1	0.053	0.623	-6.154	1.00	0.00	C
HETATM	93	C60	1	0.446	0.629	-7.496	1.00	0.00	C
HETATM	94	C61	1	1.907	3.585	8.005	1.00	0.00	C
HETATM	95	C62	1	0.791	2.832	8.359	1.00	0.00	C

HETATM	96	C63	1	-0.003	2.250	7.367	1.00	0.00	C
HETATM	97	C64	1	0.309	2.409	6.006	1.00	0.00	C
HETATM	98	C65	1	1.439	3.169	5.666	1.00	0.00	C
HETATM	99	C66	1	2.231	3.754	6.660	1.00	0.00	C
HETATM	100	H22	1	-3.676	-0.270	2.434	1.00	0.00	H
HETATM	101	H23	1	-0.043	1.289	0.749	1.00	0.00	H
HETATM	102	H24	1	-2.875	-0.754	-1.755	1.00	0.00	H
HETATM	103	H25	1	0.589	1.974	3.033	1.00	0.00	H
HETATM	104	H26	1	-1.462	-0.179	-3.660	1.00	0.00	H
HETATM	105	H27	1	-5.835	-1.346	2.050	1.00	0.00	H
HETATM	106	H28	1	-10.209	-5.273	-0.414	1.00	0.00	H
HETATM	107	H29	1	-8.031	-4.319	-1.057	1.00	0.00	H
HETATM	108	H30	1	-8.214	-1.672	2.359	1.00	0.00	H
HETATM	109	H31	1	-10.382	-2.641	2.978	1.00	0.00	H
HETATM	110	H32	1	3.812	0.824	-7.080	1.00	0.00	H
HETATM	111	H33	1	3.133	0.819	-4.711	1.00	0.00	H
HETATM	112	H34	1	-1.009	0.573	-5.930	1.00	0.00	H
HETATM	113	H35	1	-0.306	0.578	-8.281	1.00	0.00	H
HETATM	114	H36	1	0.537	2.693	9.407	1.00	0.00	H
HETATM	115	H37	1	-0.869	1.664	7.669	1.00	0.00	H
HETATM	116	H38	1	1.723	3.323	4.629	1.00	0.00	H
HETATM	117	H39	1	3.104	4.338	6.382	1.00	0.00	H
HETATM	118	H40	1	-11.395	-4.441	1.602	1.00	0.00	H
HETATM	119	H41	1	2.100	0.706	-8.874	1.00	0.00	H
HETATM	120	H42	1	2.526	4.038	8.775	1.00	0.00	H
HETATM	121	C67	1	-1.487	-3.466	1.787	1.00	0.00	C
HETATM	122	C68	1	-0.536	-2.804	2.578	1.00	0.00	C
HETATM	123	C69	1	0.658	-2.307	2.030	1.00	0.00	C
HETATM	124	C70	1	0.891	-2.494	0.660	1.00	0.00	C
HETATM	125	C71	1	-0.036	-3.152	-0.163	1.00	0.00	C
HETATM	126	C72	1	-1.216	-3.638	0.420	1.00	0.00	C
HETATM	127	C73	1	1.628	-1.585	2.848	1.00	0.00	C
HETATM	128	C74	1	2.808	-0.924	2.600	1.00	0.00	C

HETATM	129	C75	1	3.244	-0.434	3.863	1.00	0.00	C
HETATM	130	N7	1	2.362	-0.789	4.812	1.00	0.00	N
HETATM	131	O7	1	1.365	-1.499	4.180	1.00	0.00	O
HETATM	132	C76	1	0.195	-3.298	-1.596	1.00	0.00	C
HETATM	133	C77	1	-0.529	-3.788	-2.658	1.00	0.00	C
HETATM	134	C78	1	0.292	-3.587	-3.801	1.00	0.00	C
HETATM	135	N8	1	1.453	-3.020	-3.435	1.00	0.00	N
HETATM	136	O8	1	1.388	-2.843	-2.071	1.00	0.00	O
HETATM	137	C79	1	-2.744	-3.923	2.369	1.00	0.00	C
HETATM	138	C80	1	-3.374	-3.765	3.582	1.00	0.00	C
HETATM	139	C81	1	-4.611	-4.457	3.460	1.00	0.00	C
HETATM	140	N9	1	-4.703	-5.011	2.241	1.00	0.00	N
HETATM	141	O9	1	-3.547	-4.679	1.570	1.00	0.00	O
HETATM	142	C82	1	-7.765	-4.839	6.329	1.00	0.00	C
HETATM	143	C83	1	-7.999	-5.133	4.989	1.00	0.00	C
HETATM	144	C84	1	-6.966	-5.012	4.056	1.00	0.00	C
HETATM	145	C85	1	-5.685	-4.590	4.448	1.00	0.00	C
HETATM	146	C86	1	-5.465	-4.298	5.803	1.00	0.00	C
HETATM	147	C87	1	-6.500	-4.423	6.737	1.00	0.00	C
HETATM	148	C88	1	-0.566	-4.498	-7.890	1.00	0.00	C
HETATM	149	C89	1	0.399	-3.545	-7.574	1.00	0.00	C
HETATM	150	C90	1	0.682	-3.254	-6.237	1.00	0.00	C
HETATM	151	C91	1	-0.002	-3.907	-5.199	1.00	0.00	C
HETATM	152	C92	1	-0.970	-4.865	-5.533	1.00	0.00	C
HETATM	153	C93	1	-1.249	-5.159	-6.871	1.00	0.00	C
HETATM	154	C94	1	6.774	1.805	4.806	1.00	0.00	C
HETATM	155	C95	1	5.901	1.415	5.818	1.00	0.00	C
HETATM	156	C96	1	4.748	0.689	5.506	1.00	0.00	C
HETATM	157	C97	1	4.451	0.339	4.178	1.00	0.00	C
HETATM	158	C98	1	5.340	0.743	3.170	1.00	0.00	C
HETATM	159	C99	1	6.493	1.472	3.483	1.00	0.00	C
HETATM	160	H43	1	-0.734	-2.654	3.638	1.00	0.00	H
HETATM	161	H44	1	1.806	-2.104	0.216	1.00	0.00	H

HETATM	162	H45	1	-1.953	-4.138	-0.206	1.00	0.00	H
HETATM	163	H46	1	3.291	-0.810	1.642	1.00	0.00	H
HETATM	164	H47	1	-1.522	-4.209	-2.623	1.00	0.00	H
HETATM	165	H48	1	-3.008	-3.207	4.430	1.00	0.00	H
HETATM	166	H49	1	-8.985	-5.456	4.663	1.00	0.00	H
HETATM	167	H50	1	-7.177	-5.244	3.012	1.00	0.00	H
HETATM	168	H51	1	-4.489	-3.980	6.159	1.00	0.00	H
HETATM	169	H52	1	-6.315	-4.197	7.785	1.00	0.00	H
HETATM	170	H53	1	0.933	-3.024	-8.364	1.00	0.00	H
HETATM	171	H54	1	1.437	-2.502	-6.014	1.00	0.00	H
HETATM	172	H55	1	-1.514	-5.407	-4.762	1.00	0.00	H
HETATM	173	H56	1	-1.999	-5.907	-7.118	1.00	0.00	H
HETATM	174	H57	1	6.115	1.673	6.852	1.00	0.00	H
HETATM	175	H58	1	4.080	0.399	6.317	1.00	0.00	H
HETATM	176	H59	1	5.158	0.504	2.126	1.00	0.00	H
HETATM	177	H60	1	7.173	1.778	2.691	1.00	0.00	H
HETATM	178	H61	1	-8.568	-4.934	7.056	1.00	0.00	H
HETATM	179	H62	1	-0.785	-4.726	-8.930	1.00	0.00	H
HETATM	180	H63	1	7.672	2.368	5.047	1.00	0.00	H
HETATM	181	C0	1	-8.198	12.861	-4.273	1.00	0.00	C
HETATM	182	C1	1	-9.419	12.175	-4.364	1.00	0.00	C
HETATM	183	C2	1	-10.261	12.020	-3.252	1.00	0.00	C
HETATM	184	C3	1	-9.857	12.575	-2.028	1.00	0.00	C
HETATM	185	C4	1	-8.644	13.268	-1.898	1.00	0.00	C
HETATM	186	C5	1	-7.828	13.402	-3.032	1.00	0.00	C
HETATM	187	C6	1	-11.524	11.296	-3.352	1.00	0.00	C
HETATM	188	C7	1	-12.501	10.912	-2.464	1.00	0.00	C
HETATM	189	C8	1	-13.474	10.226	-3.242	1.00	0.00	C
HETATM	190	N10	1	-13.096	10.209	-4.531	1.00	0.00	N
HETATM	191	O10	1	-11.888	10.869	-4.593	1.00	0.00	O
HETATM	192	C9	1	-8.226	13.833	-0.619	1.00	0.00	C
HETATM	193	C10	1	-7.103	14.479	-0.159	1.00	0.00	C
HETATM	194	C11	1	-7.361	14.762	1.211	1.00	0.00	C

HETATM	195	N11	1	-8.581	14.310	1.546	1.00	0.00	N
HETATM	196	O11	1	-9.110	13.734	0.412	1.00	0.00	O
HETATM	197	C12	1	-7.340	12.996	-5.446	1.00	0.00	C
HETATM	198	C13	1	-7.375	12.530	-6.739	1.00	0.00	C
HETATM	199	C14	1	-6.207	13.049	-7.363	1.00	0.00	C
HETATM	200	N12	1	-5.514	13.791	-6.483	1.00	0.00	N
HETATM	201	O12	1	-6.217	13.753	-5.298	1.00	0.00	O
HETATM	202	C15	1	-4.881	12.531	-11.400	1.00	0.00	C
HETATM	203	C16	1	-3.994	12.981	-10.425	1.00	0.00	C
HETATM	204	C17	1	-4.429	13.149	-9.107	1.00	0.00	C
HETATM	205	C18	1	-5.757	12.867	-8.746	1.00	0.00	C
HETATM	206	C19	1	-6.638	12.414	-9.741	1.00	0.00	C
HETATM	207	C20	1	-6.201	12.248	-11.059	1.00	0.00	C
HETATM	208	C21	1	-4.850	16.762	4.044	1.00	0.00	C
HETATM	209	C22	1	-5.925	15.993	4.483	1.00	0.00	C
HETATM	210	C23	1	-6.743	15.341	3.555	1.00	0.00	C
HETATM	211	C24	1	-6.496	15.446	2.177	1.00	0.00	C
HETATM	212	C25	1	-5.409	16.225	1.752	1.00	0.00	C
HETATM	213	C26	1	-4.592	16.879	2.680	1.00	0.00	C
HETATM	214	C27	1	-17.144	8.435	-1.955	1.00	0.00	C
HETATM	215	C28	1	-16.599	8.102	-3.192	1.00	0.00	C
HETATM	216	C29	1	-15.401	8.688	-3.610	1.00	0.00	C
HETATM	217	C30	1	-14.729	9.613	-2.795	1.00	0.00	C
HETATM	218	C31	1	-15.291	9.939	-1.551	1.00	0.00	C
HETATM	219	C32	1	-16.491	9.353	-1.135	1.00	0.00	C
HETATM	220	H64	1	-9.719	11.747	-5.319	1.00	0.00	H
HETATM	221	H65	1	-10.498	12.462	-1.155	1.00	0.00	H
HETATM	222	H66	1	-6.883	13.935	-2.948	1.00	0.00	H
HETATM	223	H67	1	-12.509	11.083	-1.399	1.00	0.00	H
HETATM	224	H68	1	-6.210	14.704	-0.722	1.00	0.00	H
HETATM	225	H69	1	-8.127	11.891	-7.175	1.00	0.00	H
HETATM	226	H70	1	-2.962	13.201	-10.686	1.00	0.00	H
HETATM	227	H71	1	-3.718	13.497	-8.361	1.00	0.00	H

HETATM	228	H72	1	-7.676	12.189	-9.512	1.00	0.00	H
HETATM	229	H73	1	-6.895	11.895	-11.819	1.00	0.00	H
HETATM	230	H74	1	-6.130	15.898	5.546	1.00	0.00	H
HETATM	231	H75	1	-7.575	14.741	3.921	1.00	0.00	H
HETATM	232	H76	1	-5.180	16.342	0.696	1.00	0.00	H
HETATM	233	H77	1	-3.751	17.477	2.336	1.00	0.00	H
HETATM	234	H78	1	-17.104	7.385	-3.835	1.00	0.00	H
HETATM	235	H79	1	-14.991	8.409	-4.579	1.00	0.00	H
HETATM	236	H80	1	-14.812	10.653	-0.887	1.00	0.00	H
HETATM	237	H81	1	-16.914	9.613	-0.167	1.00	0.00	H
HETATM	238	H82	1	-4.543	12.400	-12.425	1.00	0.00	H
HETATM	239	H83	1	-4.213	17.269	4.764	1.00	0.00	H
HETATM	240	H84	1	-18.076	7.980	-1.629	1.00	0.00	H
HETATM	241	C33	1	-6.901	9.348	-3.633	1.00	0.00	C
HETATM	242	C34	1	-8.111	8.824	-3.157	1.00	0.00	C
HETATM	243	C35	1	-8.503	8.978	-1.819	1.00	0.00	C
HETATM	244	C36	1	-7.655	9.682	-0.952	1.00	0.00	C
HETATM	245	C37	1	-6.437	10.220	-1.393	1.00	0.00	C
HETATM	246	C38	1	-6.078	10.047	-2.737	1.00	0.00	C
HETATM	247	C39	1	-9.752	8.408	-1.327	1.00	0.00	C
HETATM	248	C40	1	-10.367	8.321	-0.101	1.00	0.00	C
HETATM	249	C41	1	-11.579	7.612	-0.332	1.00	0.00	C
HETATM	250	N13	1	-11.682	7.304	-1.635	1.00	0.00	N
HETATM	251	O13	1	-10.549	7.795	-2.245	1.00	0.00	O
HETATM	252	C42	1	-5.547	10.929	-0.479	1.00	0.00	C
HETATM	253	C43	1	-4.297	11.492	-0.579	1.00	0.00	C
HETATM	254	C44	1	-4.011	12.015	0.712	1.00	0.00	C
HETATM	255	N14	1	-5.047	11.783	1.535	1.00	0.00	N
HETATM	256	O14	1	-5.993	11.108	0.795	1.00	0.00	O
HETATM	257	C45	1	-6.509	9.149	-5.024	1.00	0.00	C
HETATM	258	C46	1	-7.034	8.463	-6.094	1.00	0.00	C
HETATM	259	C47	1	-6.129	8.683	-7.168	1.00	0.00	C
HETATM	260	N15	1	-5.121	9.471	-6.757	1.00	0.00	N

HETATM	261	O15	1	-5.359	9.752	-5.430	1.00	0.00	O
HETATM	262	C48	1	-6.380	7.242	-11.192	1.00	0.00	C
HETATM	263	C49	1	-5.522	8.293	-10.877	1.00	0.00	C
HETATM	264	C50	1	-5.437	8.758	-9.561	1.00	0.00	C
HETATM	265	C51	1	-6.212	8.182	-8.542	1.00	0.00	C
HETATM	266	C52	1	-7.068	7.122	-8.876	1.00	0.00	C
HETATM	267	C53	1	-7.152	6.655	-10.192	1.00	0.00	C
HETATM	268	C54	1	-0.508	14.103	2.021	1.00	0.00	C
HETATM	269	C55	1	-1.674	14.145	2.781	1.00	0.00	C
HETATM	270	C56	1	-2.815	13.458	2.355	1.00	0.00	C
HETATM	271	C57	1	-2.808	12.722	1.160	1.00	0.00	C
HETATM	272	C58	1	-1.624	12.687	0.408	1.00	0.00	C
HETATM	273	C59	1	-0.482	13.372	0.835	1.00	0.00	C
HETATM	274	C60	1	-14.625	6.558	2.487	1.00	0.00	C
HETATM	275	C61	1	-14.887	6.502	1.121	1.00	0.00	C
HETATM	276	C62	1	-13.889	6.842	0.202	1.00	0.00	C
HETATM	277	C63	1	-12.616	7.245	0.636	1.00	0.00	C
HETATM	278	C64	1	-12.368	7.291	2.017	1.00	0.00	C
HETATM	279	C65	1	-13.366	6.950	2.936	1.00	0.00	C
HETATM	280	H85	1	-8.760	8.278	-3.839	1.00	0.00	H
HETATM	281	H86	1	-7.944	9.809	0.090	1.00	0.00	H
HETATM	282	H87	1	-5.134	10.456	-3.095	1.00	0.00	H
HETATM	283	H88	1	-9.994	8.702	0.837	1.00	0.00	H
HETATM	284	H89	1	-3.667	11.516	-1.455	1.00	0.00	H
HETATM	285	H90	1	-7.939	7.875	-6.103	1.00	0.00	H
HETATM	286	H91	1	-4.918	8.757	-11.653	1.00	0.00	H
HETATM	287	H92	1	-4.764	9.585	-9.342	1.00	0.00	H
HETATM	288	H93	1	-7.671	6.627	-8.119	1.00	0.00	H
HETATM	289	H94	1	-7.816	5.828	-10.431	1.00	0.00	H
HETATM	290	H95	1	-1.701	14.714	3.708	1.00	0.00	H
HETATM	291	H96	1	-3.715	13.513	2.965	1.00	0.00	H
HETATM	292	H97	1	-1.560	12.112	-0.513	1.00	0.00	H
HETATM	293	H98	1	0.429	13.327	0.242	1.00	0.00	H

HETATM	294	H99	1	-15.867	6.197	0.764	1.00	0.00	H
HETATM	295	H0	1	-14.120	6.796	-0.861	1.00	0.00	H
HETATM	296	H1	1	-11.392	7.573	2.403	1.00	0.00	H
HETATM	297	H2	1	-13.153	6.985	4.001	1.00	0.00	H
HETATM	298	H3	1	-6.445	6.879	-12.214	1.00	0.00	H
HETATM	299	H4	1	0.380	14.634	2.353	1.00	0.00	H
HETATM	300	H5	1	-15.400	6.292	3.202	1.00	0.00	H
HETATM	301	C66	1	-5.960	5.823	-2.631	1.00	0.00	C
HETATM	302	C67	1	-6.760	5.707	-1.486	1.00	0.00	C
HETATM	303	C68	1	-6.373	6.267	-0.259	1.00	0.00	C
HETATM	304	C69	1	-5.151	6.951	-0.194	1.00	0.00	C
HETATM	305	C70	1	-4.324	7.088	-1.319	1.00	0.00	C
HETATM	306	C71	1	-4.744	6.517	-2.528	1.00	0.00	C
HETATM	307	C72	1	-7.218	6.161	0.924	1.00	0.00	C
HETATM	308	C73	1	-7.111	6.554	2.238	1.00	0.00	C
HETATM	309	C74	1	-8.321	6.141	2.858	1.00	0.00	C
HETATM	310	N16	1	-9.111	5.537	1.955	1.00	0.00	N
HETATM	311	O16	1	-8.422	5.546	0.762	1.00	0.00	O
HETATM	312	C75	1	-3.063	7.817	-1.246	1.00	0.00	C
HETATM	313	C76	1	-2.041	8.091	-2.124	1.00	0.00	C
HETATM	314	C77	1	-1.106	8.869	-1.386	1.00	0.00	C
HETATM	315	N17	1	-1.558	9.054	-0.135	1.00	0.00	N
HETATM	316	O17	1	-2.764	8.397	-0.051	1.00	0.00	O
HETATM	317	C78	1	-6.394	5.244	-3.897	1.00	0.00	C
HETATM	318	C79	1	-7.466	4.488	-4.309	1.00	0.00	C
HETATM	319	C80	1	-7.265	4.271	-5.700	1.00	0.00	C
HETATM	320	N18	1	-6.134	4.878	-6.094	1.00	0.00	N
HETATM	321	O18	1	-5.596	5.472	-4.976	1.00	0.00	O
HETATM	322	C81	1	-9.724	2.131	-8.475	1.00	0.00	C
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HETATM	324	C83	1	-7.625	3.186	-7.915	1.00	0.00	C
HETATM	325	C84	1	-8.111	3.534	-6.643	1.00	0.00	C
HETATM	326	C85	1	-9.423	3.166	-6.308	1.00	0.00	C

HETATM	327	C86	1	-10.224	2.468	-7.219	1.00	0.00	C
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HETATM	329	C88	1	2.312	10.477	-1.323	1.00	0.00	C
HETATM	330	C89	1	1.098	9.926	-0.904	1.00	0.00	C
HETATM	331	C90	1	0.166	9.440	-1.836	1.00	0.00	C
HETATM	332	C91	1	0.482	9.524	-3.200	1.00	0.00	C
HETATM	333	C92	1	1.697	10.076	-3.619	1.00	0.00	C
HETATM	334	C93	1	-9.565	6.655	6.921	1.00	0.00	C
HETATM	335	C94	1	-10.216	5.737	6.101	1.00	0.00	C
HETATM	336	C95	1	-9.807	5.571	4.775	1.00	0.00	C
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CONNECT	334	335		
CONNECT	335	334	336	354

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CONNECT 335 334
CONNECT 336 335 337 355
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CONNECT 354 335
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CONNECT 356 338
CONNECT 357 339
CONNECT 358 322
CONNECT 359 328
CONNECT 360 334
ENDMDL
END

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Structure data of Conformer B

HETATM	1	C1	1	-4.591	6.524	-2.393	1.00	0.00	C
HETATM	2	C2	1	-5.794	5.822	-2.556	1.00	0.00	C
HETATM	3	C3	1	-6.698	5.662	-1.496	1.00	0.00	C
HETATM	4	C4	1	-6.383	6.235	-0.256	1.00	0.00	C
HETATM	5	C5	1	-5.192	6.951	-0.060	1.00	0.00	C
HETATM	6	C6	1	-4.309	7.087	-1.140	1.00	0.00	C
HETATM	7	C7	1	-7.933	4.907	-1.664	1.00	0.00	C
HETATM	8	C8	1	-9.065	4.710	-0.908	1.00	0.00	C
HETATM	9	C9	1	-9.890	3.850	-1.682	1.00	0.00	C
HETATM	10	N1	1	-9.269	3.532	-2.829	1.00	0.00	N
HETATM	11	O1	1	-8.060	4.193	-2.815	1.00	0.00	O
HETATM	12	C10	1	-4.870	7.545	1.232	1.00	0.00	C
HETATM	13	C11	1	-3.902	8.405	1.693	1.00	0.00	C

HETATM	14	C12	1	-4.202	8.608	3.066	1.00	0.00	C
HETATM	15	N2	1	-5.271	7.873	3.415	1.00	0.00	N
HETATM	16	O2	1	-5.683	7.220	2.274	1.00	0.00	O
HETATM	17	C13	1	-3.649	6.638	-3.499	1.00	0.00	C
HETATM	18	C14	1	-3.694	6.385	-4.849	1.00	0.00	C
HETATM	19	C15	1	-2.395	6.700	-5.336	1.00	0.00	C
HETATM	20	N3	1	-1.614	7.103	-4.320	1.00	0.00	N
HETATM	21	O3	1	-2.396	7.070	-3.187	1.00	0.00	O
HETATM	22	C16	1	-0.900	6.464	-9.341	1.00	0.00	C
HETATM	23	C17	1	-0.193	7.169	-8.370	1.00	0.00	C
HETATM	24	C18	1	-0.685	7.246	-7.064	1.00	0.00	C
HETATM	25	C19	1	-1.891	6.620	-6.710	1.00	0.00	C
HETATM	26	C20	1	-2.592	5.916	-7.700	1.00	0.00	C
HETATM	27	C21	1	-2.099	5.838	-9.006	1.00	0.00	C
HETATM	28	C22	1	-2.217	11.174	5.851	1.00	0.00	C
HETATM	29	C23	1	-3.548	10.818	6.054	1.00	0.00	C
HETATM	30	C24	1	-4.191	9.970	5.148	1.00	0.00	C
HETATM	31	C25	1	-3.514	9.475	4.023	1.00	0.00	C
HETATM	32	C26	1	-2.174	9.841	3.832	1.00	0.00	C
HETATM	33	C27	1	-1.529	10.683	4.743	1.00	0.00	C
HETATM	34	C28	1	-13.784	2.346	-0.748	1.00	0.00	C
HETATM	35	C29	1	-13.347	2.383	-2.070	1.00	0.00	C
HETATM	36	C30	1	-12.074	2.874	-2.373	1.00	0.00	C
HETATM	37	C31	1	-11.222	3.337	-1.357	1.00	0.00	C
HETATM	38	C32	1	-11.678	3.296	-0.031	1.00	0.00	C
HETATM	39	C33	1	-12.950	2.801	0.271	1.00	0.00	C
HETATM	40	H1	1	-6.021	5.370	-3.520	1.00	0.00	H
HETATM	41	H2	1	-7.070	6.112	0.579	1.00	0.00	H
HETATM	42	H3	1	-3.374	7.628	-1.001	1.00	0.00	H
HETATM	43	H4	1	-9.279	5.137	0.059	1.00	0.00	H
HETATM	44	H5	1	-3.106	8.853	1.118	1.00	0.00	H
HETATM	45	H6	1	-4.543	6.028	-5.410	1.00	0.00	H
HETATM	46	H7	1	0.743	7.658	-8.626	1.00	0.00	H

HETATM	47	H8	1	-0.116	7.806	-6.323	1.00	0.00	H
HETATM	48	H9	1	-3.520	5.396	-7.472	1.00	0.00	H
HETATM	49	H10	1	-2.645	5.273	-9.758	1.00	0.00	H
HETATM	50	H11	1	-4.089	11.199	6.916	1.00	0.00	H
HETATM	51	H12	1	-5.234	9.709	5.320	1.00	0.00	H
HETATM	52	H13	1	-1.604	9.464	2.986	1.00	0.00	H
HETATM	53	H14	1	-0.486	10.948	4.589	1.00	0.00	H
HETATM	54	H15	1	-13.995	2.029	-2.868	1.00	0.00	H
HETATM	55	H16	1	-11.754	2.899	-3.413	1.00	0.00	H
HETATM	56	H17	1	-11.045	3.623	0.790	1.00	0.00	H
HETATM	57	H18	1	-13.282	2.759	1.305	1.00	0.00	H
HETATM	58	H19	1	-0.516	6.397	-10.355	1.00	0.00	H
HETATM	59	H20	1	-1.714	11.830	6.557	1.00	0.00	H
HETATM	60	H21	1	-14.771	1.958	-0.510	1.00	0.00	H
HETATM	61	C34	1	-8.311	8.760	-2.749	1.00	0.00	C
HETATM	62	C35	1	-7.155	9.173	-3.426	1.00	0.00	C
HETATM	63	C36	1	-6.148	9.905	-2.778	1.00	0.00	C
HETATM	64	C37	1	-6.313	10.217	-1.422	1.00	0.00	C
HETATM	65	C38	1	-7.457	9.819	-0.716	1.00	0.00	C
HETATM	66	C39	1	-8.443	9.086	-1.391	1.00	0.00	C
HETATM	67	C40	1	-4.962	10.352	-3.497	1.00	0.00	C
HETATM	68	C41	1	-3.732	10.847	-3.134	1.00	0.00	C
HETATM	69	C42	1	-3.053	11.110	-4.356	1.00	0.00	C
HETATM	70	N4	1	-3.850	10.800	-5.394	1.00	0.00	N
HETATM	71	O4	1	-5.026	10.324	-4.857	1.00	0.00	O
HETATM	72	C43	1	-7.640	10.172	0.685	1.00	0.00	C
HETATM	73	C44	1	-8.425	9.699	1.709	1.00	0.00	C
HETATM	74	C45	1	-8.131	10.530	2.825	1.00	0.00	C
HETATM	75	N5	1	-7.226	11.461	2.474	1.00	0.00	N
HETATM	76	O5	1	-6.917	11.227	1.150	1.00	0.00	O
HETATM	77	C46	1	-9.357	8.033	-3.457	1.00	0.00	C
HETATM	78	C47	1	-9.461	7.431	-4.688	1.00	0.00	C
HETATM	79	C48	1	-10.789	6.929	-4.755	1.00	0.00	C

HETATM	80	N6	1	-11.445	7.225	-3.619	1.00	0.00	N
HETATM	81	O6	1	-10.551	7.902	-2.817	1.00	0.00	O
HETATM	82	C49	1	-12.684	4.815	-7.960	1.00	0.00	C
HETATM	83	C50	1	-13.282	4.861	-6.703	1.00	0.00	C
HETATM	84	C51	1	-12.660	5.550	-5.657	1.00	0.00	C
HETATM	85	C52	1	-11.433	6.203	-5.854	1.00	0.00	C
HETATM	86	C53	1	-10.846	6.148	-7.128	1.00	0.00	C
HETATM	87	C54	1	-11.468	5.458	-8.173	1.00	0.00	C
HETATM	88	C55	1	-9.752	10.334	6.782	1.00	0.00	C
HETATM	89	C56	1	-8.622	11.107	6.527	1.00	0.00	C
HETATM	90	C57	1	-8.096	11.171	5.234	1.00	0.00	C
HETATM	91	C58	1	-8.690	10.461	4.178	1.00	0.00	C
HETATM	92	C59	1	-9.831	9.691	4.452	1.00	0.00	C
HETATM	93	C60	1	-10.358	9.628	5.746	1.00	0.00	C
HETATM	94	C61	1	0.885	12.687	-4.937	1.00	0.00	C
HETATM	95	C62	1	0.193	12.124	-6.006	1.00	0.00	C
HETATM	96	C63	1	-1.092	11.607	-5.813	1.00	0.00	C
HETATM	97	C64	1	-1.703	11.648	-4.549	1.00	0.00	C
HETATM	98	C65	1	-0.992	12.221	-3.484	1.00	0.00	C
HETATM	99	C66	1	0.294	12.736	-3.677	1.00	0.00	C
HETATM	100	H22	1	-7.041	8.936	-4.482	1.00	0.00	H
HETATM	101	H23	1	-5.547	10.795	-0.907	1.00	0.00	H
HETATM	102	H24	1	-9.342	8.783	-0.857	1.00	0.00	H
HETATM	103	H25	1	-3.370	10.996	-2.129	1.00	0.00	H
HETATM	104	H26	1	-9.108	8.866	1.663	1.00	0.00	H
HETATM	105	H27	1	-8.689	7.363	-5.439	1.00	0.00	H
HETATM	106	H28	1	-14.234	4.365	-6.534	1.00	0.00	H
HETATM	107	H29	1	-13.145	5.570	-4.683	1.00	0.00	H
HETATM	108	H30	1	-9.908	6.656	-7.337	1.00	0.00	H
HETATM	109	H31	1	-11.005	5.434	-9.157	1.00	0.00	H
HETATM	110	H32	1	-8.151	11.664	7.332	1.00	0.00	H
HETATM	111	H33	1	-7.212	11.781	5.058	1.00	0.00	H
HETATM	112	H34	1	-10.340	9.140	3.666	1.00	0.00	H

HETATM	113	H35	1	-11.247	9.033	5.941	1.00	0.00	H
HETATM	114	H36	1	0.649	12.088	-6.991	1.00	0.00	H
HETATM	115	H37	1	-1.612	11.169	-6.663	1.00	0.00	H
HETATM	116	H38	1	-1.428	12.295	-2.491	1.00	0.00	H
HETATM	117	H39	1	0.828	13.185	-2.843	1.00	0.00	H
HETATM	118	H40	1	-13.170	4.285	-8.775	1.00	0.00	H
HETATM	119	H41	1	-10.166	10.288	7.786	1.00	0.00	H
HETATM	120	H42	1	1.882	13.095	-5.087	1.00	0.00	H
HETATM	121	C67	1	-9.612	11.965	-3.999	1.00	0.00	C
HETATM	122	C68	1	-10.271	11.985	-2.760	1.00	0.00	C
HETATM	123	C69	1	-9.700	12.595	-1.633	1.00	0.00	C
HETATM	124	C70	1	-8.443	13.204	-1.769	1.00	0.00	C
HETATM	125	C71	1	-7.755	13.203	-2.992	1.00	0.00	C
HETATM	126	C72	1	-8.357	12.586	-4.098	1.00	0.00	C
HETATM	127	C73	1	-10.375	12.583	-0.340	1.00	0.00	C
HETATM	128	C74	1	-10.145	13.166	0.884	1.00	0.00	C
HETATM	129	C75	1	-11.210	12.730	1.721	1.00	0.00	C
HETATM	130	N7	1	-12.023	11.914	1.029	1.00	0.00	N
HETATM	131	O7	1	-11.503	11.826	-0.244	1.00	0.00	O
HETATM	132	C76	1	-6.433	13.808	-3.116	1.00	0.00	C
HETATM	133	C77	1	-5.613	14.152	-4.164	1.00	0.00	C
HETATM	134	C78	1	-4.447	14.707	-3.568	1.00	0.00	C
HETATM	135	N8	1	-4.561	14.671	-2.229	1.00	0.00	N
HETATM	136	O8	1	-5.791	14.115	-1.955	1.00	0.00	O
HETATM	137	C79	1	-10.217	11.295	-5.144	1.00	0.00	C
HETATM	138	C80	1	-11.461	10.781	-5.425	1.00	0.00	C
HETATM	139	C81	1	-11.370	10.265	-6.747	1.00	0.00	C
HETATM	140	N9	1	-10.124	10.443	-7.218	1.00	0.00	N
HETATM	141	O9	1	-9.415	11.080	-6.223	1.00	0.00	O
HETATM	142	C82	1	-14.443	8.465	-9.123	1.00	0.00	C
HETATM	143	C83	1	-13.246	8.863	-9.713	1.00	0.00	C
HETATM	144	C84	1	-12.242	9.445	-8.934	1.00	0.00	C
HETATM	145	C85	1	-12.421	9.638	-7.554	1.00	0.00	C

HETATM	146	C86	1	-13.631	9.227	-6.975	1.00	0.00	C
HETATM	147	C87	1	-14.636	8.645	-7.756	1.00	0.00	C
HETATM	148	C88	1	-0.999	16.370	-5.487	1.00	0.00	C
HETATM	149	C89	1	-1.192	16.549	-4.120	1.00	0.00	C
HETATM	150	C90	1	-2.317	16.001	-3.495	1.00	0.00	C
HETATM	151	C91	1	-3.263	15.267	-4.229	1.00	0.00	C
HETATM	152	C92	1	-3.050	15.092	-5.605	1.00	0.00	C
HETATM	153	C93	1	-1.925	15.641	-6.229	1.00	0.00	C
HETATM	154	C94	1	-11.999	13.757	5.804	1.00	0.00	C
HETATM	155	C95	1	-12.930	13.022	5.075	1.00	0.00	C
HETATM	156	C96	1	-12.668	12.684	3.744	1.00	0.00	C
HETATM	157	C97	1	-11.471	13.076	3.123	1.00	0.00	C
HETATM	158	C98	1	-10.542	13.812	3.874	1.00	0.00	C
HETATM	159	C99	1	-10.805	14.151	5.205	1.00	0.00	C
HETATM	160	H43	1	-11.240	11.496	-2.665	1.00	0.00	H
HETATM	161	H44	1	-7.980	13.672	-0.901	1.00	0.00	H
HETATM	162	H45	1	-7.829	12.567	-5.051	1.00	0.00	H
HETATM	163	H46	1	-9.326	13.819	1.141	1.00	0.00	H
HETATM	164	H47	1	-5.829	14.033	-5.215	1.00	0.00	H
HETATM	165	H48	1	-12.323	10.790	-4.775	1.00	0.00	H
HETATM	166	H49	1	-13.090	8.718	-10.779	1.00	0.00	H
HETATM	167	H50	1	-11.316	9.749	-9.418	1.00	0.00	H
HETATM	168	H51	1	-13.810	9.333	-5.908	1.00	0.00	H
HETATM	169	H52	1	-15.564	8.324	-7.291	1.00	0.00	H
HETATM	170	H53	1	-0.468	17.111	-3.536	1.00	0.00	H
HETATM	171	H54	1	-2.446	16.155	-2.425	1.00	0.00	H
HETATM	172	H55	1	-3.740	14.513	-6.213	1.00	0.00	H
HETATM	173	H56	1	-1.768	15.489	-7.294	1.00	0.00	H
HETATM	174	H57	1	-13.861	12.708	5.541	1.00	0.00	H
HETATM	175	H58	1	-13.413	12.110	3.196	1.00	0.00	H
HETATM	176	H59	1	-9.591	14.121	3.448	1.00	0.00	H
HETATM	177	H60	1	-10.071	14.713	5.776	1.00	0.00	H
HETATM	178	H61	1	-15.222	8.008	-9.727	1.00	0.00	H

HETATM	179	H62	1	-0.121	16.789	-5.972	1.00	0.00	H
HETATM	180	H63	1	-12.199	14.015	6.841	1.00	0.00	H
HETATM	181	C0	1	-0.499	-2.760	2.391	1.00	0.00	C
HETATM	182	C1	1	-1.443	-3.518	1.682	1.00	0.00	C
HETATM	183	C2	1	-1.282	-3.805	0.317	1.00	0.00	C
HETATM	184	C3	1	-0.138	-3.319	-0.336	1.00	0.00	C
HETATM	185	C4	1	0.828	-2.559	0.341	1.00	0.00	C
HETATM	186	C5	1	0.633	-2.292	1.704	1.00	0.00	C
HETATM	187	C6	1	-2.277	-4.579	-0.418	1.00	0.00	C
HETATM	188	C7	1	-2.398	-5.030	-1.712	1.00	0.00	C
HETATM	189	C8	1	-3.637	-5.728	-1.759	1.00	0.00	C
HETATM	190	N10	1	-4.224	-5.689	-0.550	1.00	0.00	N
HETATM	191	O10	1	-3.380	-4.976	0.274	1.00	0.00	O
HETATM	192	C9	1	2.009	-2.047	-0.347	1.00	0.00	C
HETATM	193	C10	1	3.158	-1.400	0.043	1.00	0.00	C
HETATM	194	C11	1	3.902	-1.189	-1.151	1.00	0.00	C
HETATM	195	N11	1	3.219	-1.676	-2.201	1.00	0.00	N
HETATM	196	O11	1	2.049	-2.205	-1.699	1.00	0.00	O
HETATM	197	C12	1	-0.702	-2.465	3.806	1.00	0.00	C
HETATM	198	C13	1	-1.629	-2.832	4.753	1.00	0.00	C
HETATM	199	C14	1	-1.229	-2.179	5.953	1.00	0.00	C
HETATM	200	N12	1	-0.125	-1.447	5.722	1.00	0.00	N
HETATM	201	O12	1	0.195	-1.627	4.394	1.00	0.00	O
HETATM	202	C15	1	-3.042	-2.364	9.833	1.00	0.00	C
HETATM	203	C16	1	-1.886	-1.614	9.635	1.00	0.00	C
HETATM	204	C17	1	-1.296	-1.556	8.369	1.00	0.00	C
HETATM	205	C18	1	-1.856	-2.243	7.279	1.00	0.00	C
HETATM	206	C19	1	-3.023	-2.993	7.497	1.00	0.00	C
HETATM	207	C20	1	-3.611	-3.053	8.765	1.00	0.00	C
HETATM	208	C21	1	7.750	0.642	-1.614	1.00	0.00	C
HETATM	209	C22	1	7.114	0.062	-2.708	1.00	0.00	C
HETATM	210	C23	1	5.859	-0.534	-2.555	1.00	0.00	C
HETATM	211	C24	1	5.218	-0.557	-1.305	1.00	0.00	C

HETATM	212	C25	1	5.872	0.036	-0.214	1.00	0.00	C
HETATM	213	C26	1	7.130	0.629	-0.367	1.00	0.00	C
HETATM	214	C27	1	-5.446	-7.742	-5.082	1.00	0.00	C
HETATM	215	C28	1	-6.020	-7.825	-3.816	1.00	0.00	C
HETATM	216	C29	1	-5.428	-7.167	-2.733	1.00	0.00	C
HETATM	217	C30	1	-4.254	-6.415	-2.900	1.00	0.00	C
HETATM	218	C31	1	-3.691	-6.339	-4.184	1.00	0.00	C
HETATM	219	C32	1	-4.283	-6.999	-5.266	1.00	0.00	C
HETATM	220	H64	1	-2.328	-3.884	2.199	1.00	0.00	H
HETATM	221	H65	1	0.001	-3.531	-1.394	1.00	0.00	H
HETATM	222	H66	1	1.371	-1.700	2.242	1.00	0.00	H
HETATM	223	H67	1	-1.695	-4.875	-2.515	1.00	0.00	H
HETATM	224	H68	1	3.428	-1.122	1.050	1.00	0.00	H
HETATM	225	H69	1	-2.475	-3.485	4.605	1.00	0.00	H
HETATM	226	H70	1	-1.445	-1.065	10.463	1.00	0.00	H
HETATM	227	H71	1	-0.397	-0.957	8.241	1.00	0.00	H
HETATM	228	H72	1	-3.502	-3.538	6.688	1.00	0.00	H
HETATM	229	H73	1	-4.516	-3.636	8.916	1.00	0.00	H
HETATM	230	H74	1	7.589	0.080	-3.686	1.00	0.00	H
HETATM	231	H75	1	5.382	-0.975	-3.428	1.00	0.00	H
HETATM	232	H76	1	5.417	0.057	0.773	1.00	0.00	H
HETATM	233	H77	1	7.622	1.086	0.488	1.00	0.00	H
HETATM	234	H78	1	-6.935	-8.393	-3.669	1.00	0.00	H
HETATM	235	H79	1	-5.902	-7.242	-1.757	1.00	0.00	H
HETATM	236	H80	1	-2.793	-5.757	-4.372	1.00	0.00	H
HETATM	237	H81	1	-3.836	-6.927	-6.255	1.00	0.00	H
HETATM	238	H82	1	-3.503	-2.405	10.816	1.00	0.00	H
HETATM	239	H83	1	8.724	1.109	-1.734	1.00	0.00	H
HETATM	240	H84	1	-5.909	-8.249	-5.924	1.00	0.00	H
HETATM	241	C33	1	-0.880	0.695	-0.257	1.00	0.00	C
HETATM	242	C34	1	-1.717	-0.040	-1.107	1.00	0.00	C
HETATM	243	C35	1	-2.916	-0.605	-0.649	1.00	0.00	C
HETATM	244	C36	1	-3.269	-0.423	0.695	1.00	0.00	C

HETATM	245	C37	1	-2.455	0.306	1.576	1.00	0.00	C
HETATM	246	C38	1	-1.264	0.856	1.083	1.00	0.00	C
HETATM	247	C39	1	-3.786	-1.362	-1.541	1.00	0.00	C
HETATM	248	C40	1	-5.007	-1.982	-1.416	1.00	0.00	C
HETATM	249	C41	1	-5.284	-2.537	-2.695	1.00	0.00	C
HETATM	250	N13	1	-4.273	-2.267	-3.537	1.00	0.00	N
HETATM	251	O13	1	-3.349	-1.540	-2.818	1.00	0.00	O
HETATM	252	C42	1	-2.834	0.499	2.971	1.00	0.00	C
HETATM	253	C43	1	-2.279	1.144	4.051	1.00	0.00	C
HETATM	254	C44	1	-3.193	0.947	5.122	1.00	0.00	C
HETATM	255	N14	1	-4.234	0.210	4.701	1.00	0.00	N
HETATM	256	O14	1	-4.007	-0.065	3.370	1.00	0.00	O
HETATM	257	C45	1	0.352	1.284	-0.768	1.00	0.00	C
HETATM	258	C46	1	0.976	1.326	-1.992	1.00	0.00	C
HETATM	259	C47	1	2.154	2.096	-1.791	1.00	0.00	C
HETATM	260	N15	1	2.233	2.480	-0.506	1.00	0.00	N
HETATM	261	O15	1	1.116	1.975	0.123	1.00	0.00	O
HETATM	262	C48	1	5.101	3.227	-4.680	1.00	0.00	C
HETATM	263	C49	1	5.000	3.920	-3.476	1.00	0.00	C
HETATM	264	C50	1	4.041	3.545	-2.531	1.00	0.00	C
HETATM	265	C51	1	3.169	2.472	-2.778	1.00	0.00	C
HETATM	266	C52	1	3.288	1.780	-3.993	1.00	0.00	C
HETATM	267	C53	1	4.248	2.156	-4.938	1.00	0.00	C
HETATM	268	C54	1	-2.945	2.438	9.125	1.00	0.00	C
HETATM	269	C55	1	-4.165	1.996	8.618	1.00	0.00	C
HETATM	270	C56	1	-4.242	1.502	7.312	1.00	0.00	C
HETATM	271	C57	1	-3.101	1.446	6.496	1.00	0.00	C
HETATM	272	C58	1	-1.879	1.890	7.024	1.00	0.00	C
HETATM	273	C59	1	-1.802	2.383	8.330	1.00	0.00	C
HETATM	274	C60	1	-8.746	-4.721	-3.939	1.00	0.00	C
HETATM	275	C61	1	-7.913	-4.132	-4.887	1.00	0.00	C
HETATM	276	C62	1	-6.780	-3.423	-4.479	1.00	0.00	C
HETATM	277	C63	1	-6.465	-3.293	-3.117	1.00	0.00	C

HETATM	278	C64	1	-7.311	-3.898	-2.175	1.00	0.00	C
HETATM	279	C65	1	-8.445	-4.607	-2.584	1.00	0.00	C
HETATM	280	H85	1	-1.434	-0.173	-2.150	1.00	0.00	H
HETATM	281	H86	1	-4.197	-0.854	1.067	1.00	0.00	H
HETATM	282	H87	1	-0.622	1.426	1.753	1.00	0.00	H
HETATM	283	H88	1	-5.620	-2.029	-0.529	1.00	0.00	H
HETATM	284	H89	1	-1.348	1.689	4.069	1.00	0.00	H
HETATM	285	H90	1	0.632	0.873	-2.909	1.00	0.00	H
HETATM	286	H91	1	5.667	4.752	-3.268	1.00	0.00	H
HETATM	287	H92	1	3.979	4.102	-1.597	1.00	0.00	H
HETATM	288	H93	1	2.653	0.926	-4.216	1.00	0.00	H
HETATM	289	H94	1	4.333	1.607	-5.872	1.00	0.00	H
HETATM	290	H95	1	-5.058	2.031	9.236	1.00	0.00	H
HETATM	291	H96	1	-5.205	1.163	6.936	1.00	0.00	H
HETATM	292	H97	1	-0.964	1.841	6.438	1.00	0.00	H
HETATM	293	H98	1	-0.848	2.719	8.728	1.00	0.00	H
HETATM	294	H99	1	-8.140	-4.226	-5.946	1.00	0.00	H
HETATM	295	H0	1	-6.142	-2.972	-5.237	1.00	0.00	H
HETATM	296	H1	1	-7.092	-3.848	-1.111	1.00	0.00	H
HETATM	297	H2	1	-9.087	-5.076	-1.843	1.00	0.00	H
HETATM	298	H3	1	5.849	3.517	-5.413	1.00	0.00	H
HETATM	299	H4	1	-2.885	2.820	10.141	1.00	0.00	H
HETATM	300	H5	1	-9.625	-5.276	-4.257	1.00	0.00	H
HETATM	301	C66	1	-5.023	2.821	0.098	1.00	0.00	C
HETATM	302	C67	1	-4.778	2.547	-1.254	1.00	0.00	C
HETATM	303	C68	1	-3.621	3.012	-1.897	1.00	0.00	C
HETATM	304	C69	1	-2.691	3.750	-1.153	1.00	0.00	C
HETATM	305	C70	1	-2.907	4.043	0.202	1.00	0.00	C
HETATM	306	C71	1	-4.072	3.562	0.815	1.00	0.00	C
HETATM	307	C72	1	-3.400	2.767	-3.316	1.00	0.00	C
HETATM	308	C73	1	-2.317	2.825	-4.160	1.00	0.00	C
HETATM	309	C74	1	-2.819	2.471	-5.443	1.00	0.00	C
HETATM	310	N16	1	-4.142	2.249	-5.366	1.00	0.00	N

HETATM	311	O16	1	-4.494	2.424	-4.047	1.00	0.00	O
HETATM	312	C75	1	-1.966	4.861	0.955	1.00	0.00	C
HETATM	313	C76	1	-1.730	5.099	2.288	1.00	0.00	C
HETATM	314	C77	1	-0.662	6.038	2.320	1.00	0.00	C
HETATM	315	N17	1	-0.305	6.362	1.066	1.00	0.00	N
HETATM	316	O17	1	-1.108	5.624	0.225	1.00	0.00	O
HETATM	317	C78	1	-6.258	2.374	0.728	1.00	0.00	C
HETATM	318	C79	1	-7.245	1.471	0.412	1.00	0.00	C
HETATM	319	C80	1	-8.186	1.552	1.477	1.00	0.00	C
HETATM	320	N18	1	-7.788	2.478	2.364	1.00	0.00	N
HETATM	321	O18	1	-6.591	2.977	1.902	1.00	0.00	O
HETATM	322	C81	1	-11.799	-0.670	2.055	1.00	0.00	C
HETATM	323	C82	1	-11.264	0.079	3.100	1.00	0.00	C
HETATM	324	C83	1	-10.084	0.804	2.906	1.00	0.00	C
HETATM	325	C84	1	-9.423	0.789	1.666	1.00	0.00	C
HETATM	326	C85	1	-9.977	0.031	0.625	1.00	0.00	C
HETATM	327	C86	1	-11.158	-0.693	0.819	1.00	0.00	C
HETATM	328	C87	1	1.334	7.735	5.707	1.00	0.00	C
HETATM	329	C88	1	1.871	7.884	4.431	1.00	0.00	C
HETATM	330	C89	1	1.215	7.331	3.328	1.00	0.00	C
HETATM	331	C90	1	0.012	6.621	3.484	1.00	0.00	C
HETATM	332	C91	1	-0.518	6.484	4.775	1.00	0.00	C
HETATM	333	C92	1	0.140	7.037	5.879	1.00	0.00	C
HETATM	334	C93	1	-0.718	2.075	-9.155	1.00	0.00	C
HETATM	335	C94	1	-2.046	1.672	-9.057	1.00	0.00	C
HETATM	336	C95	1	-2.728	1.803	-7.844	1.00	0.00	C
HETATM	337	C96	1	-2.092	2.341	-6.711	1.00	0.00	C
HETATM	338	C97	1	-0.754	2.744	-6.828	1.00	0.00	C
HETATM	339	C98	1	-0.072	2.611	-8.043	1.00	0.00	C
HETATM	340	H6	1	-5.513	1.984	-1.828	1.00	0.00	H
HETATM	341	H7	1	-1.794	4.130	-1.642	1.00	0.00	H
HETATM	342	H8	1	-4.258	3.792	1.863	1.00	0.00	H
HETATM	343	H9	1	-1.304	3.079	-3.888	1.00	0.00	H

HETATM	344	H10		1	-2.248	4.652	3.122	1.00	0.00	H
HETATM	345	H11		1	-7.281	0.837	-0.460	1.00	0.00	H
HETATM	346	H12		1	-11.762	0.102	4.066	1.00	0.00	H
HETATM	347	H13		1	-9.683	1.379	3.739	1.00	0.00	H
HETATM	348	H14		1	-9.517	0.004	-0.360	1.00	0.00	H
HETATM	349	H15		1	-11.581	-1.268	-0.001	1.00	0.00	H
HETATM	350	H16		1	2.802	8.428	4.291	1.00	0.00	H
HETATM	351	H17		1	1.658	7.455	2.341	1.00	0.00	H
HETATM	352	H18		1	-1.454	5.960	4.949	1.00	0.00	H
HETATM	353	H19		1	-0.286	6.928	6.873	1.00	0.00	H
HETATM	354	H20		1	-2.555	1.254	-9.922	1.00	0.00	H
HETATM	355	H21		1	-3.765	1.477	-7.792	1.00	0.00	H
HETATM	356	H22		1	-0.221	3.184	-5.990	1.00	0.00	H
HETATM	357	H23		1	0.962	2.939	-8.121	1.00	0.00	H
HETATM	358	H24		1	-12.719	-1.231	2.202	1.00	0.00	H
HETATM	359	H25		1	1.842	8.166	6.566	1.00	0.00	H
HETATM	360	H26		1	-0.187	1.977	-10.098	1.00	0.00	H
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CONECT	41	4								
CONECT	42	6								
CONECT	7	3	8	11						

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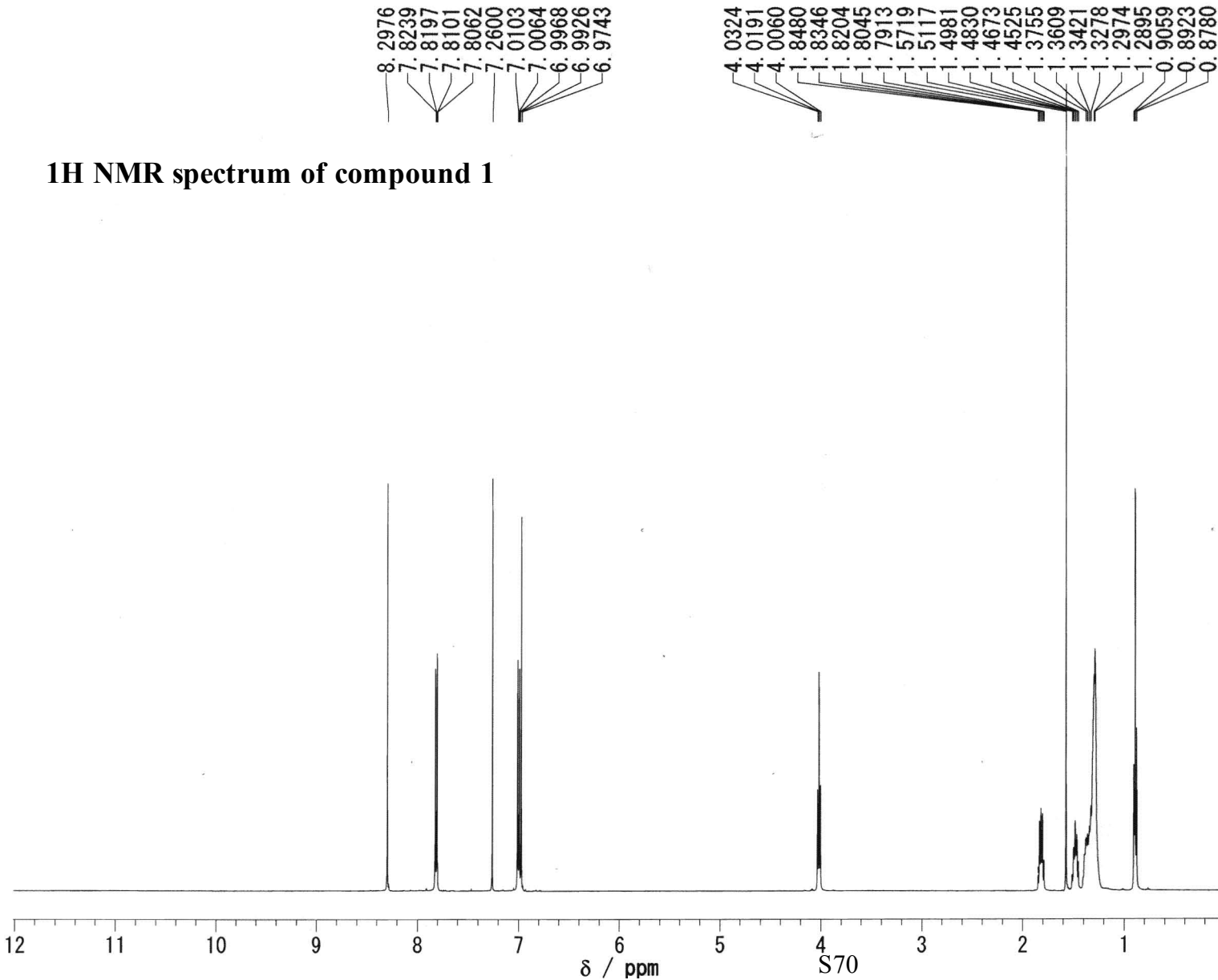
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- (1)Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, J. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *R. C. Gaussian 03, Gaussian, Inc., Wallingford CT 2004.*
- (2)Kolossvary, I.; Guida, W. C. *J. Am. Chem. Soc.* **1996**, *118*, 5011-5019.
- (3)Mohamadi, F.; Richards, N. G. J.; Guida, W. C.; Liskamp, R.; Lipton, M.; Caufield, C.; Chang, G.; Hendrickson, T.; Still, W. C. *J. Comput. Chem.* **1990**, *11*, 440-467.

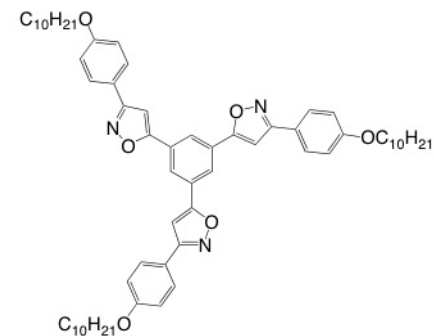
¹H NMR spectrum of compound 1



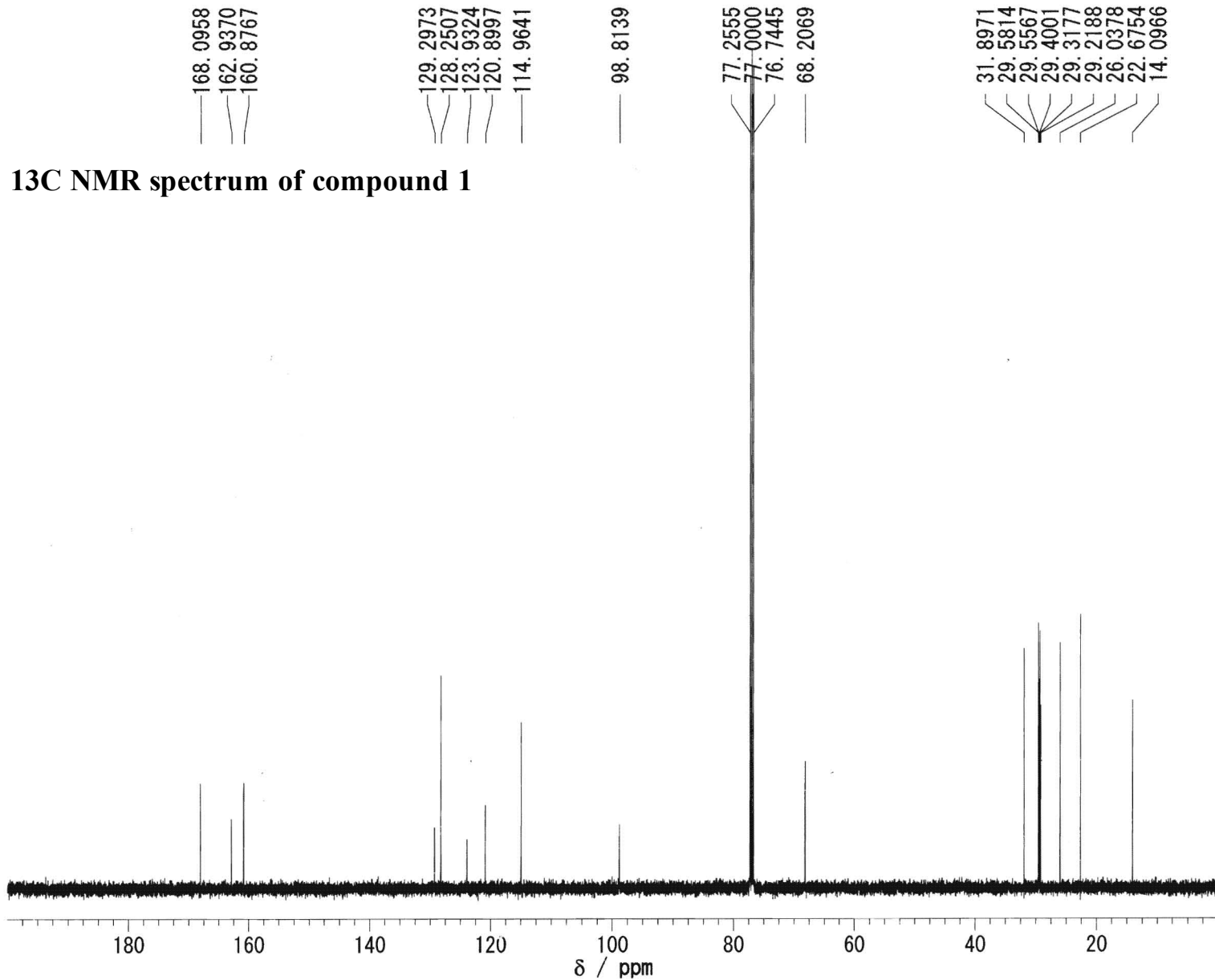
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Date Wed Jun 14 21:54:53 2006
Comment

ObsNuc ¹H
ExMode non
ObsFreq 499.1 MHz
ObsSet 128.0 kHz
ObsFine 250.0 Hz
Point 32768
Frequency (Span) 9980.04 Hz
Scan 16
AcqTime 3.2834 s
PD 3.7166 s
Pulse1 7.1 μs
IrrNuc ¹H
ProbeHead TH5ATFG2
Instrument JEOL LAMBDA
Pulse Program
Gradient Program
Temperature 27.7 °C
Solvent CDCl₃
Reference 7.26 ppm
Broad.Factor 0.25 Hz
Window Exponential
RGain 23

Operator



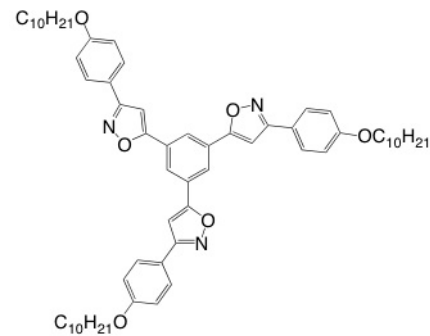
¹³C NMR spectrum of compound 1



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Date Wed Jun 14 23:40:48 2006
Comment

ObsNuc ¹³C
ExMode bcm
ObsFreq 125.4 MHz
ObsSet 143.0 kHz
ObsFine 41.0 Hz
Point 32768
Frequency (Span) 33898.3 Hz
Scan 2048
AcqTime 0.9667 s
PD 2.0333 s
Pulse1 6.0 μs
IrrNuc ¹H
ProbeHead TH5ATFG2
Instrument JEOL LAMBDA
Pulse Program
Gradient Program
Temperature 29.6 °C
Solvent CDCL₃
Reference 77.0 ppm
Broad. Factor 0.5172 Hz
Window Exponential
RGain 16

Operator _____

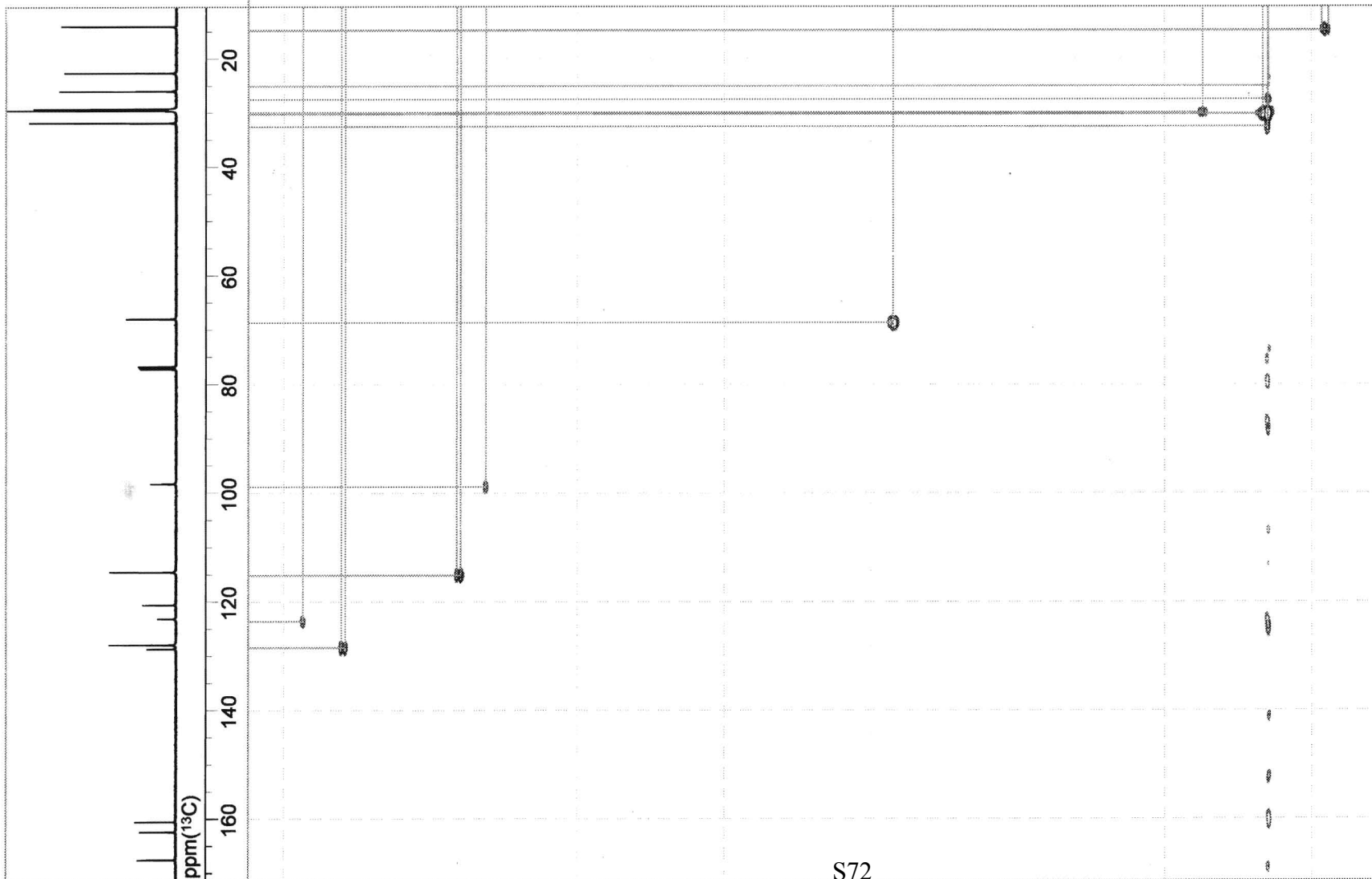
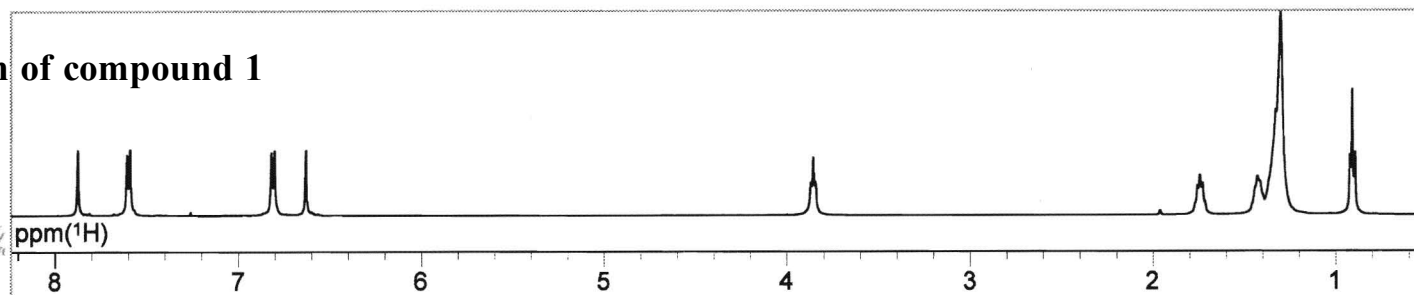


1H₂

OC₁₀H₂₁

10 m M

HMOC spectrum of compound 1



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Date Thu Oct 20 21:55:56 2
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Comment
PHPC10-200M-1-HMQC

ExMode hmqc_bird

-----F2 Parameter-----

F2-Nucleus ^1H

F2-ObsFreq 499.227

0002 MHz

F2-Point 1024 (Zer

ill: $\times 2$)

F2-Resol 3.771

8 Hz

F2-Ref. 0.510

ppm

F2 Ref_Point 0

-----F1 Parameter-----

F1-Nucleus ^{13}C

F1-ObsFreq 125.541

1159 MHz

F1-Point 256 (Zer

ill: $\times 2$)

F1-Resol 79.234

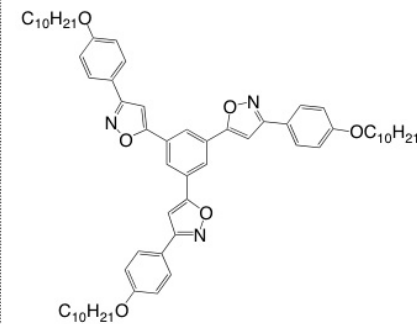
Hz

F1-Ref. 10.444

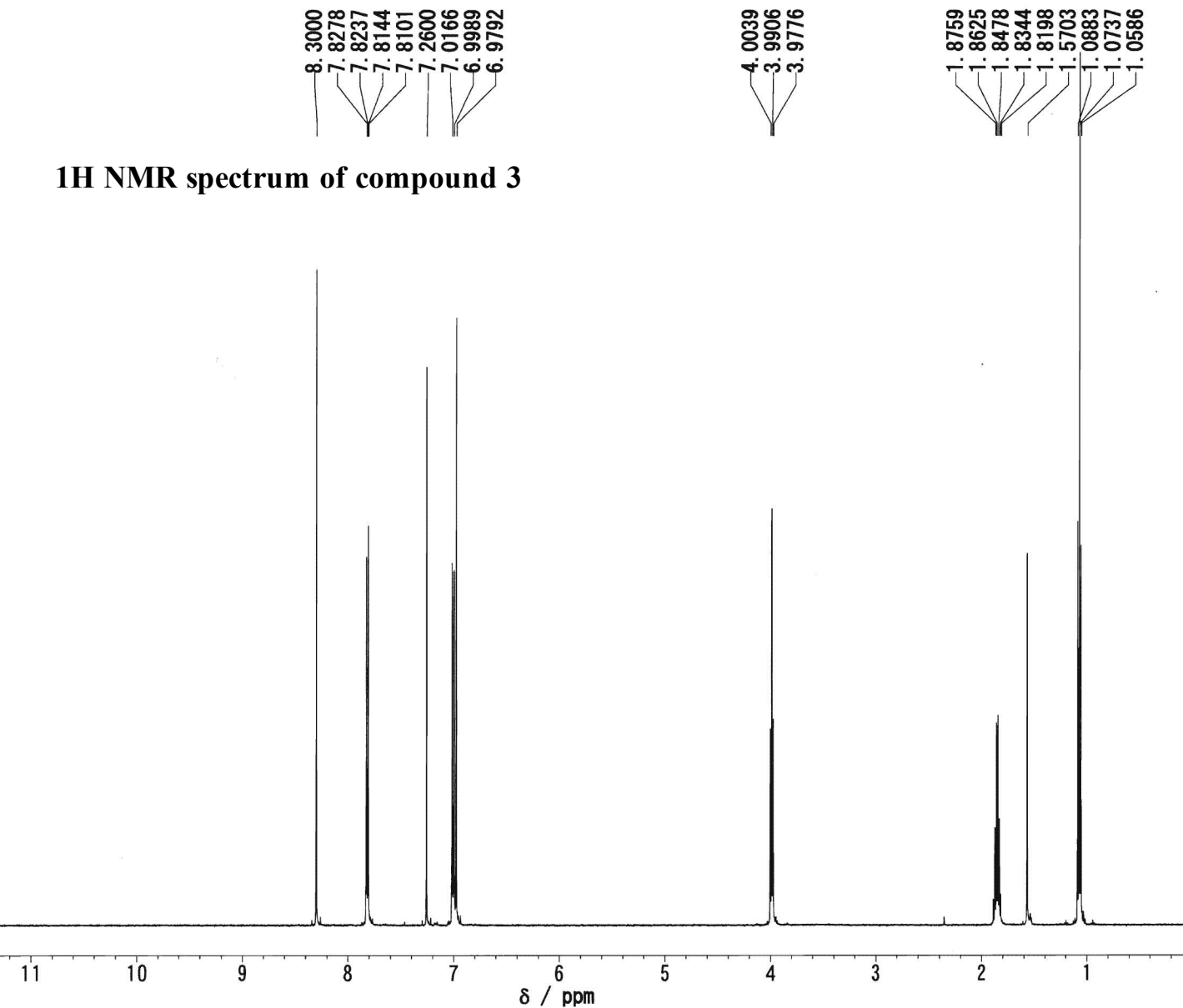
ppm

F1 Ref_Point 0

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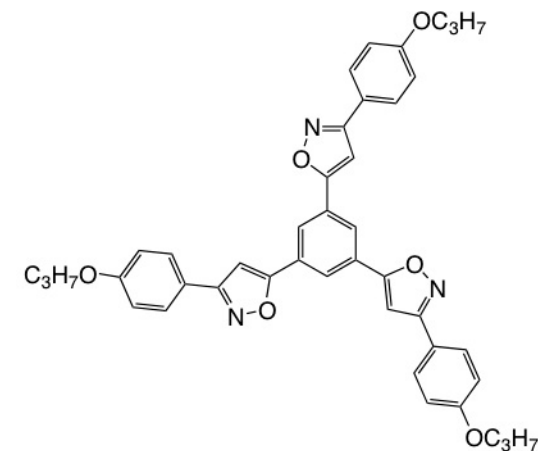


¹H NMR spectrum of compound 3

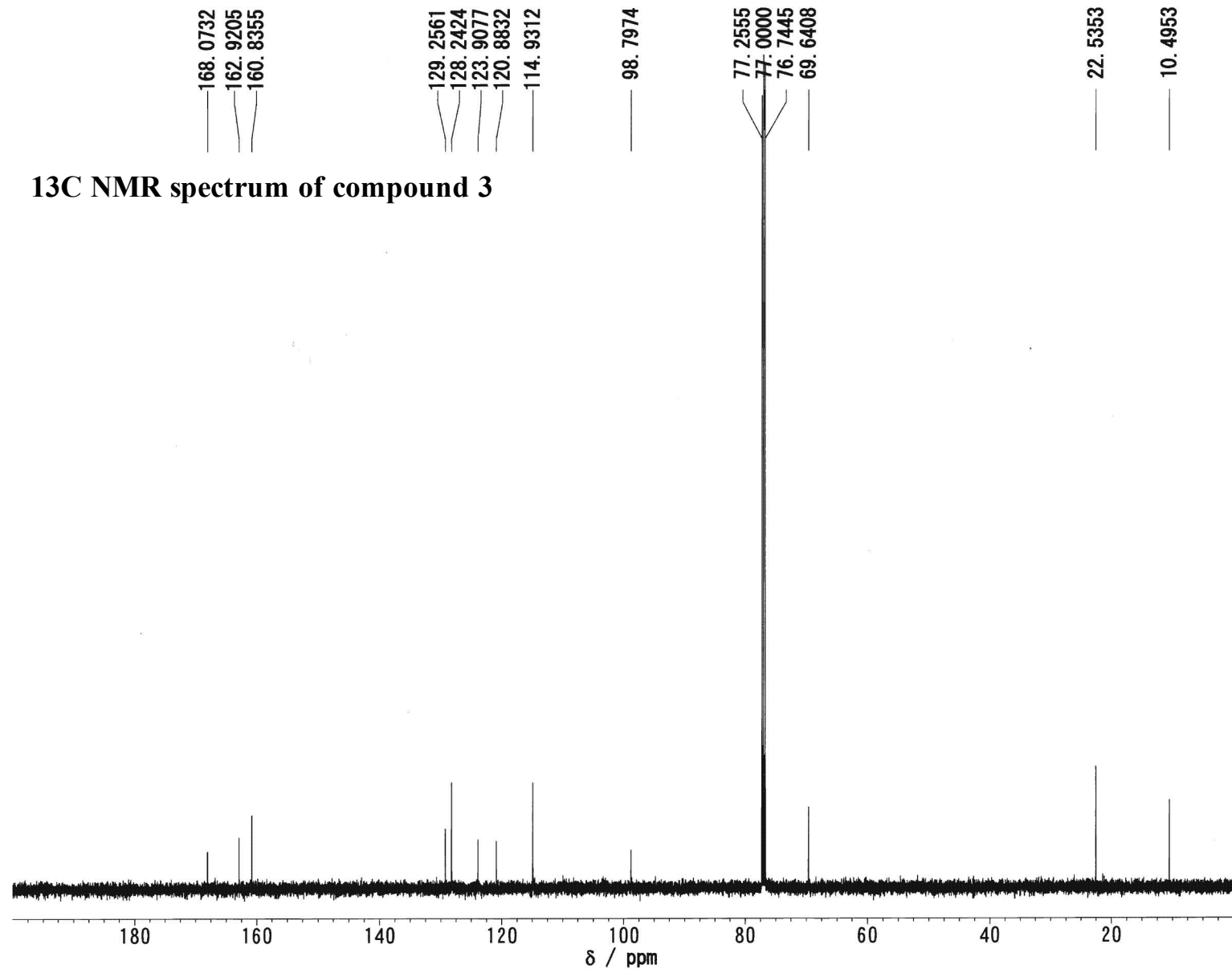


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ExMode	non
ObsFreq	499.1 MHz
ObsSet	128.0 kHz
ObsFine	250.0 Hz
Point	32768
Frequency (Span)	9980.04 Hz
Scan	16
AcqTime	3.2834 s
PD	3.7166 s
Pulse1	7.1 μs
IrrNuc	¹ H
ProbeHead	TH5ATFG2
Instrument	JEOL LAMBDA
Pulse Program	
Gradient Program	
Temperature	24.3 °C
Solvent	CDCl ₃
Reference	7.26 ppm
Broad. Factor	0.25 Hz
Window	Exponential
RGain	30

Operator _____



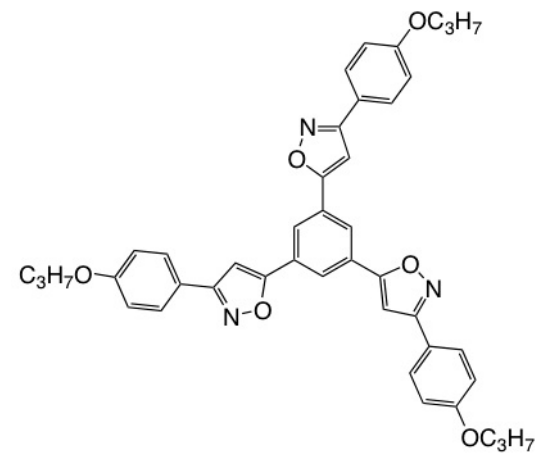
¹³C NMR spectrum of compound 3



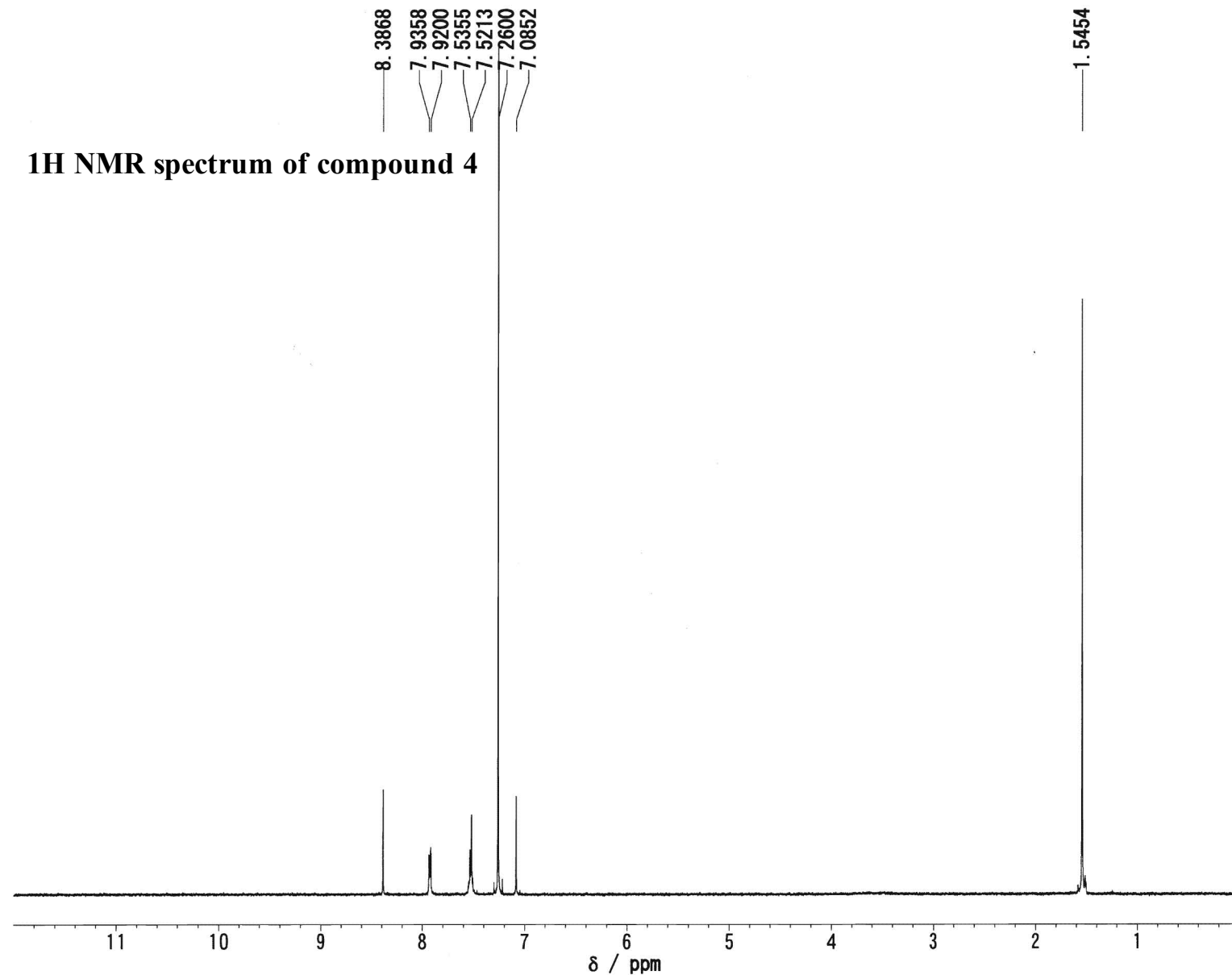
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ObsNuc      13C
ExMode      bcm
ObsFreq      125.4 MHz
ObsSet       143.0 kHz
ObsFine      41.0 Hz
Point        32768
Frequency (Span) 33898.3 Hz
Scan         2024
AcqTime      0.9667 s
PD           2.0333 s
Pulse1       6.0  $\mu$ s
IrrNuc       1H
ProbeHead    TH5ATFG2
Instrument    JEOL LAMBDA
Pulse Program
Gradient Program
Temperature   26.0  $^{\circ}$ C
Solvent       CDCL3
Reference     77.0 ppm
Broad. Factor 0.25 Hz
Window        Exponential
RGain         32
  
```

Operator _____



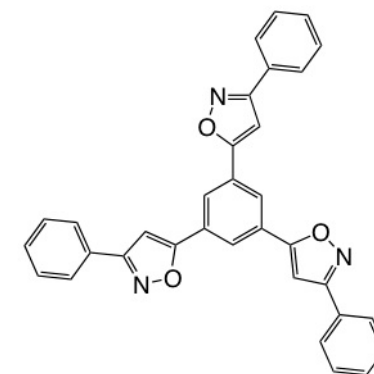
¹H NMR spectrum of compound 4



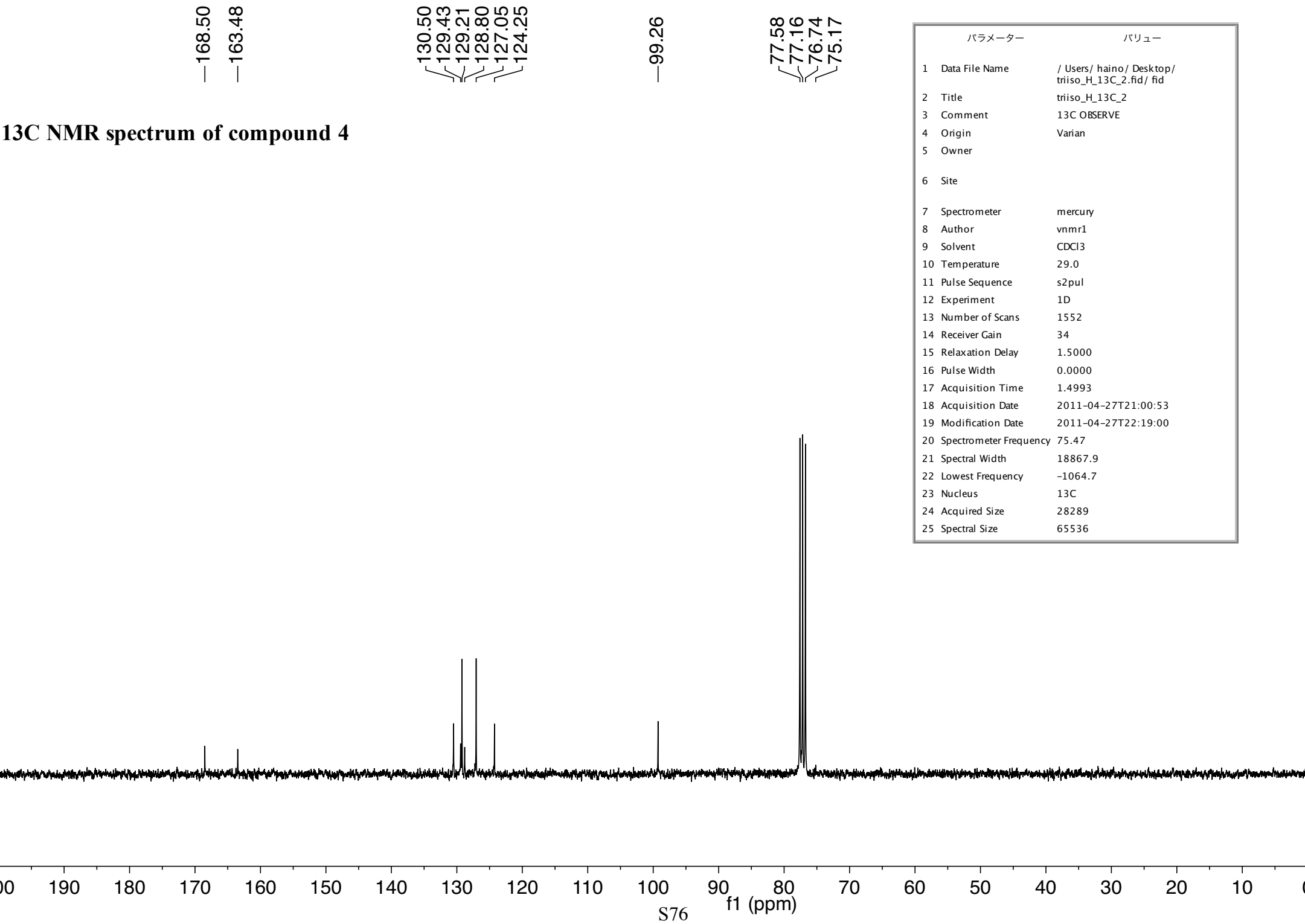
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ExMode      non
ObsFreq     499.1 MHz
ObsSet      128.0 kHz
ObsFine     250.0 Hz
Point       32768
Frequency (Span) 9980.04 Hz
Scan        16
AcqTime     3.2834 s
PD          3.7166 s
Pulse1      7.1 μs
IrrNuc      1H
ProbeHead   TH5ATFG2
Instrument   JEOL LAMBDA
Pulse Program
Gradient Program
Temperature  25.3 °C
Solvent      CDCL3
Reference    7.26 ppm
Broad. Factor 0.25 Hz
Window      Exponential
RGain       35
  
```

Operator _____



13C NMR spectrum of compound 4



¹H NMR spectrum of compound (R)-4-(3,7-dimethyloctoxy)benzaldehyde oxime

STANDARD ¹H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

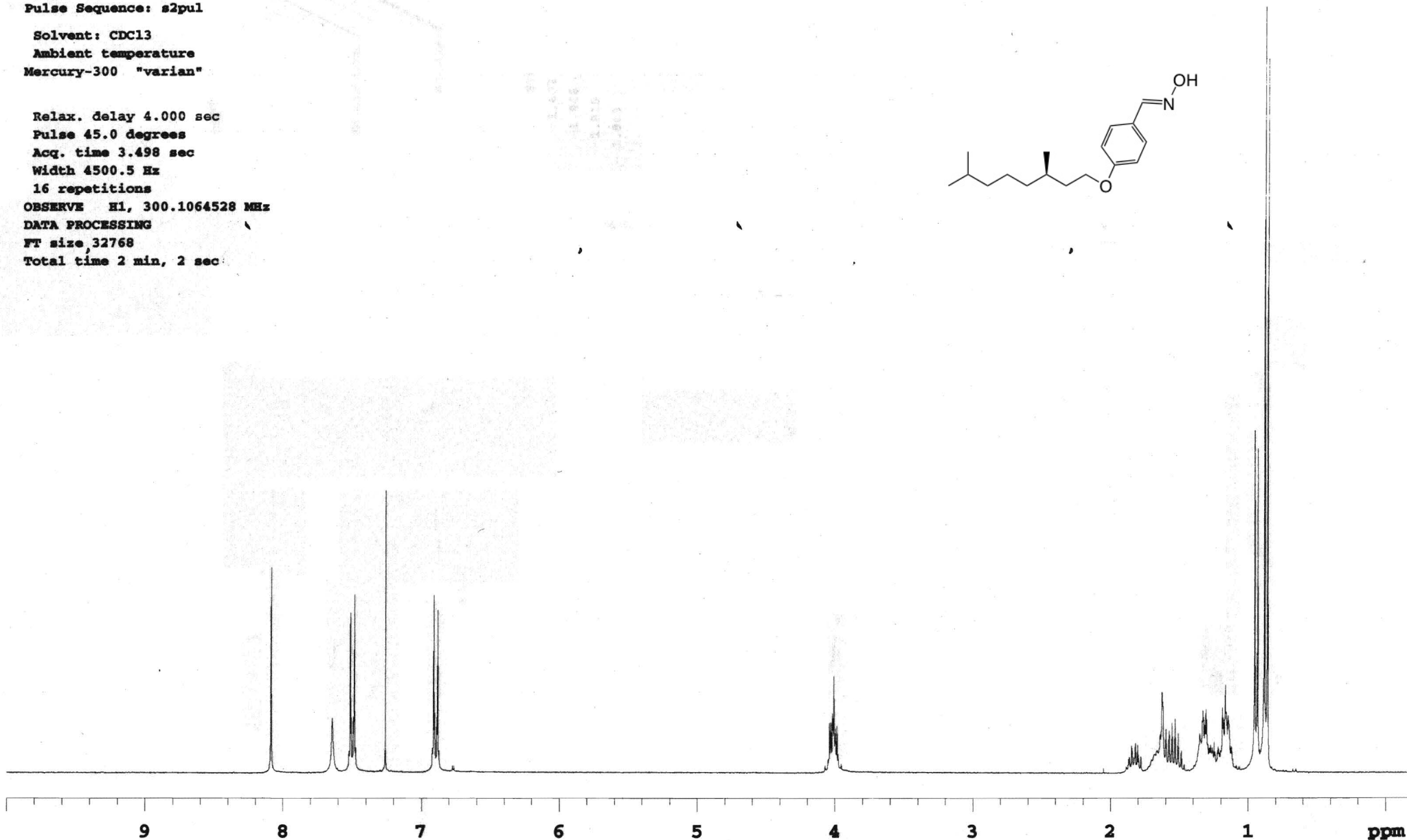
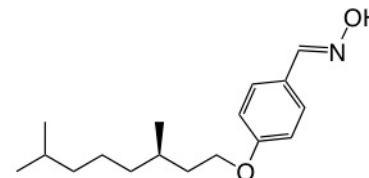
16 repetitions

OBSERVE H1, 300.1064528 MHz

DATA PROCESSING

FT size, 32768

Total time 2 min, 2 sec



¹³C NMR spectrum of compound (R)-4-(3,7-dimethyloctoxy)benzaldoxime

¹³C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 1.499 sec

Width 18867.9 Hz

944 repetitions

OBSERVE C13, 75.4618277 MHz

DECOUPLE H1, 300.1079971 MHz

Power 44 dB

continuously on

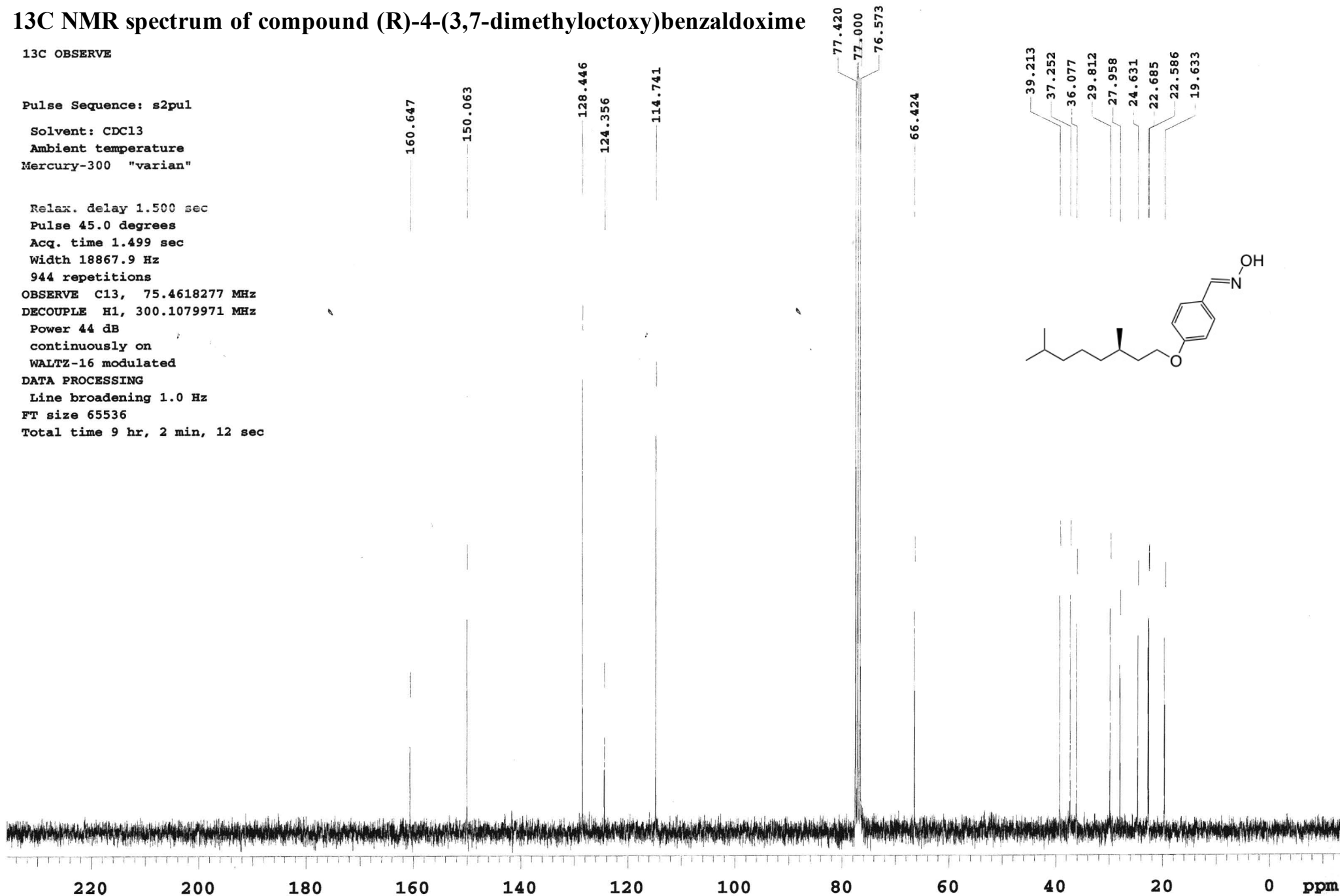
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 9 hr, 2 min, 12 sec



¹H NMR spectrum of compound (S)-4-(3,7-dimethyloctoxy)benzaldehyde oxime

STANDARD ¹H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

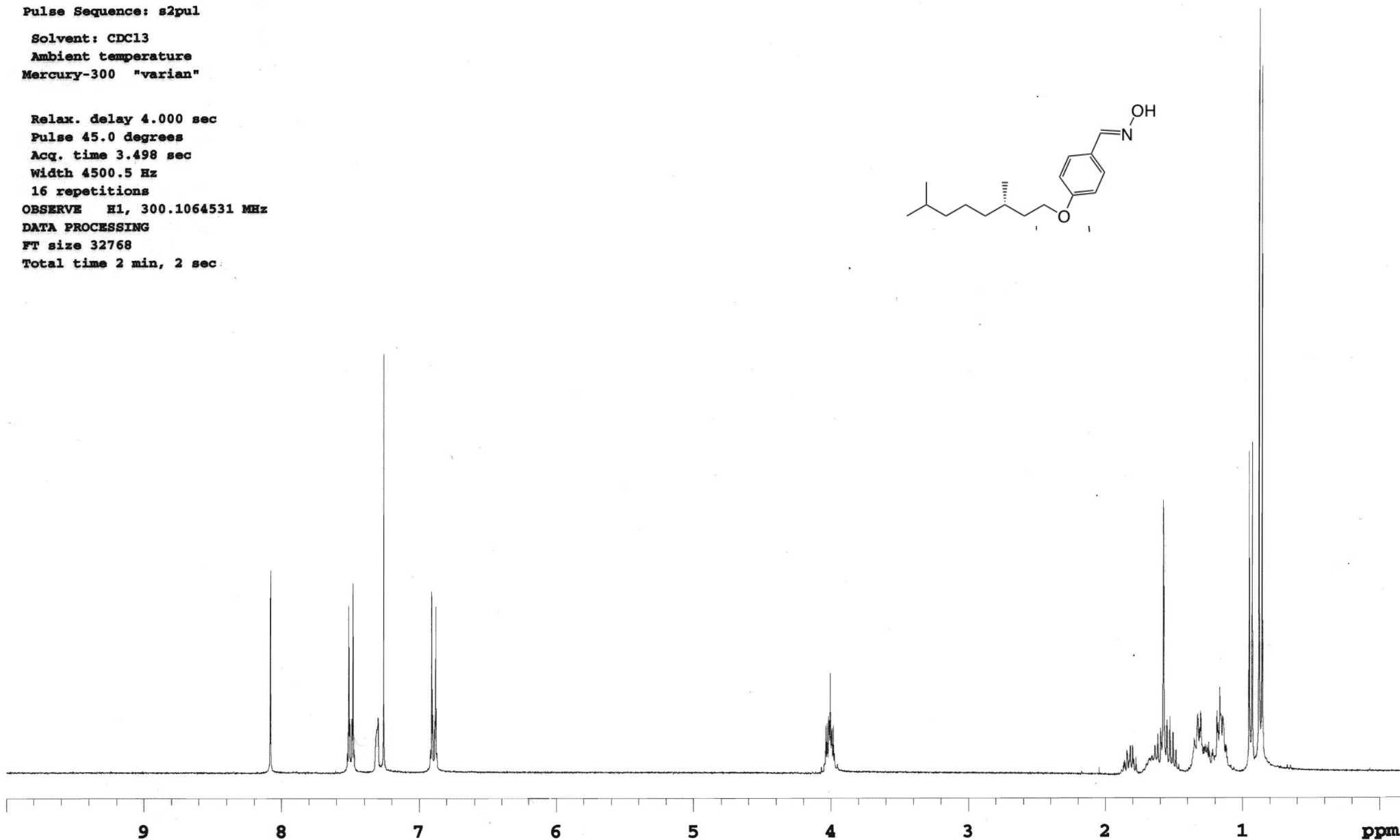
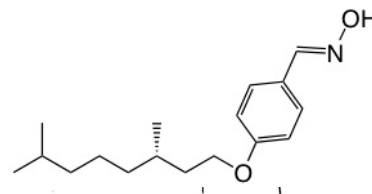
16 repetitions

OBSERVE H1, 300.1064531 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec



13C NMR spectrum of compound (S)-4-(3,7-dimethyloctoxy)benzaldehyde oxime

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Mercury-300 "varian"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 1.499 sec

Width 18867.9 Hz

5072 repetitions

OBSERVE C13, 75.4618271 MHz

DECOUPLE H1, 300.1079971 MHz

Power 44 dB

continuously on

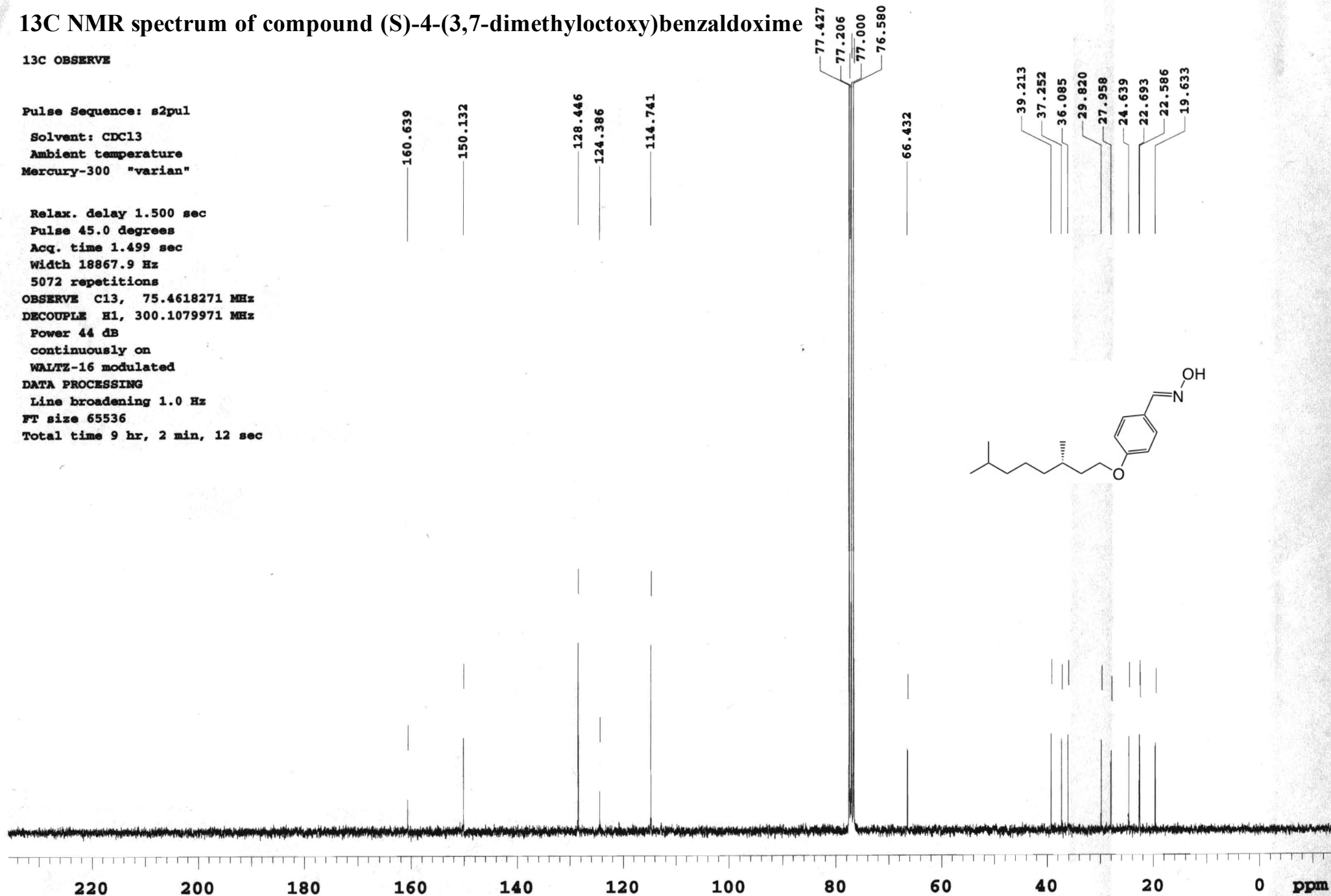
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 9 hr, 2 min, 12 sec



¹H NMR spectrum of compound R-9

STANDARD ¹H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

16 repetitions

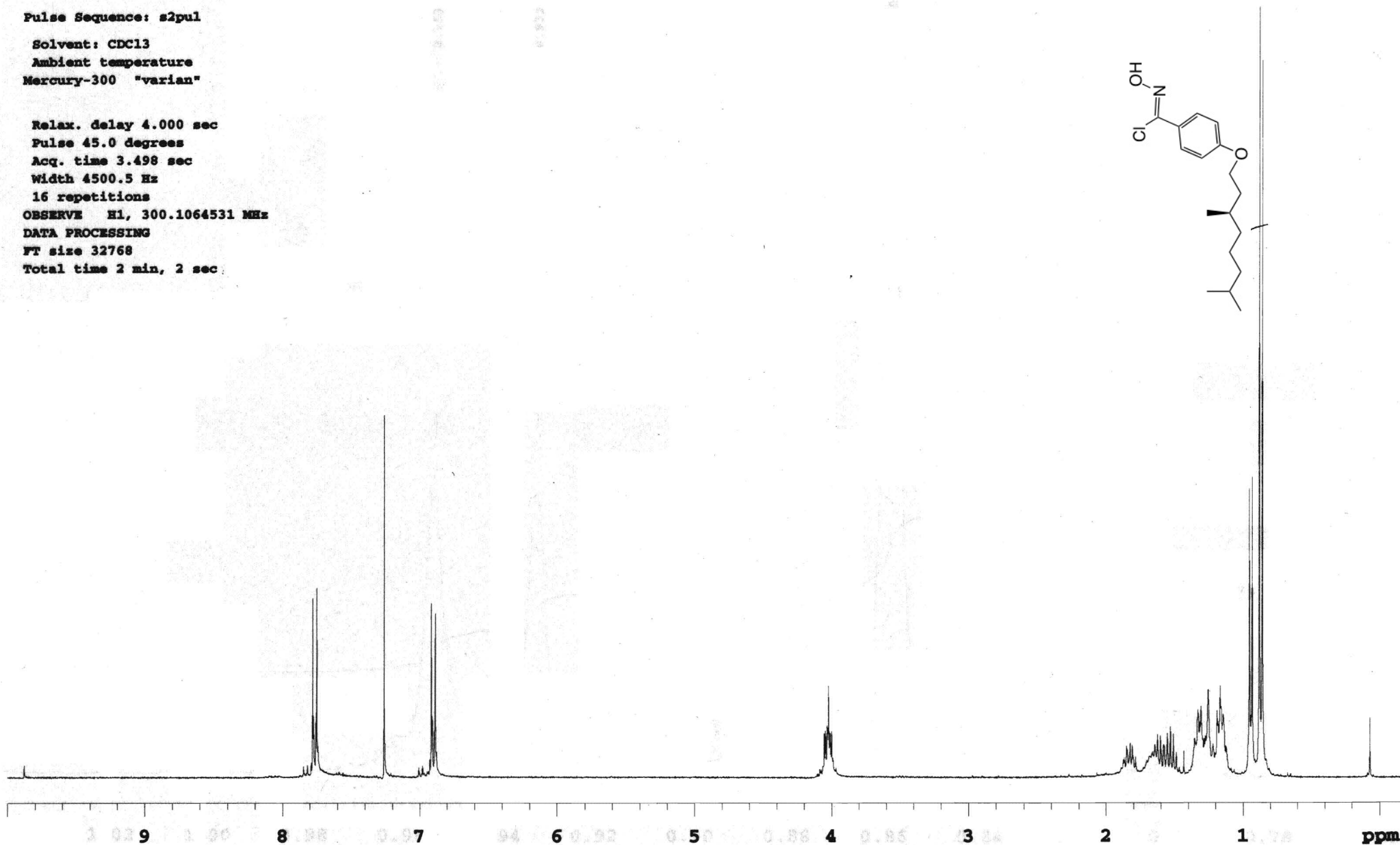
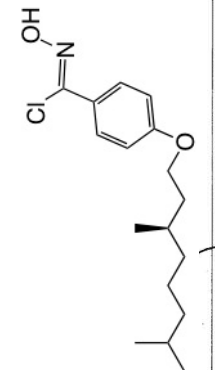
OBSERVE H1, 300.1064531 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec

R-59-1



¹H NMR spectrum of compound S-9

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

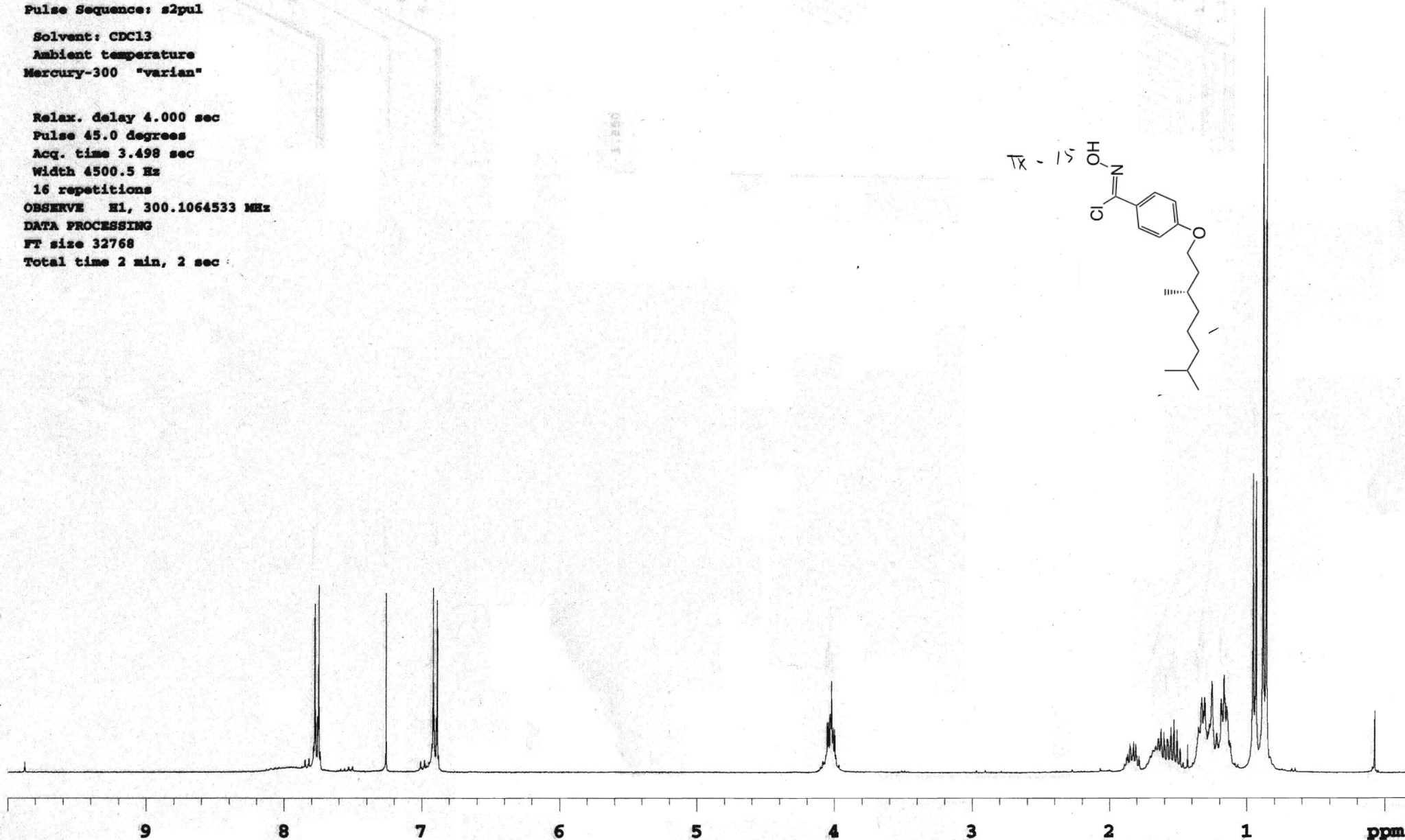
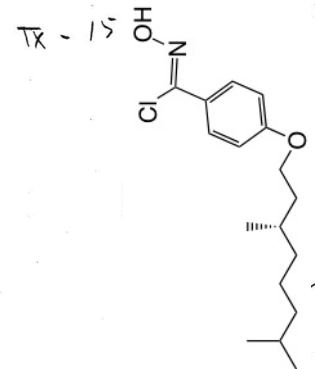
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OBSERVE H1, 300.1064533 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec



STANDARD 1H OBSERVE

1H NMR spectrum of compound R-5

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Mercury-300 "varian"

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

16 repetitions

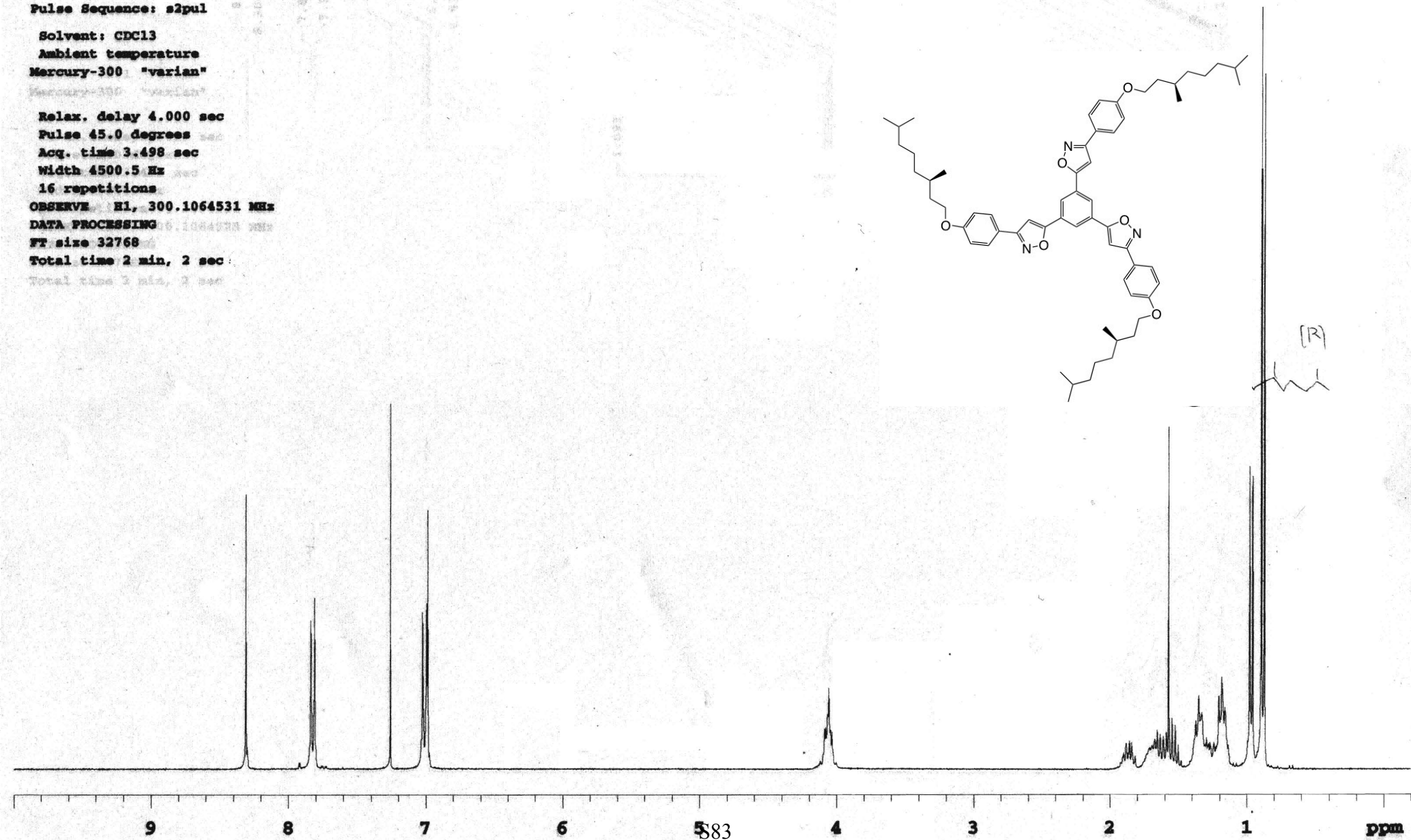
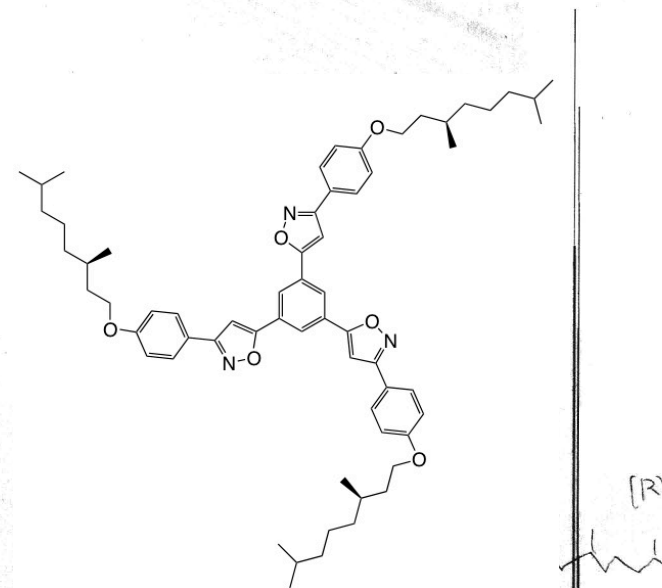
OBSERVE E1, 300.1064531 MHz

DATA PROCESSING 6.1084928 MHz

FF size 32768

Total time 2 min, 2 sec

Total time 2 min, 2 sec



¹³C OBSERVE ¹³C NMR spectrum of compound R-5

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Mercury-300 "varian"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 1.499 sec

Width 18867.9 Hz

10000 repetitions

OBSERVE C13, 75.4618283 MHz

DECOUPLE H1, 300.1079971 MHz

Power 44 dB

continuously on

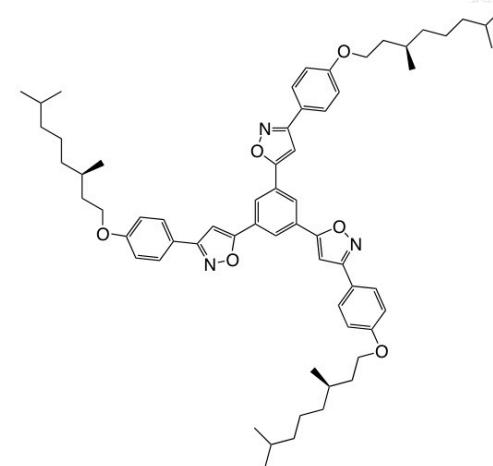
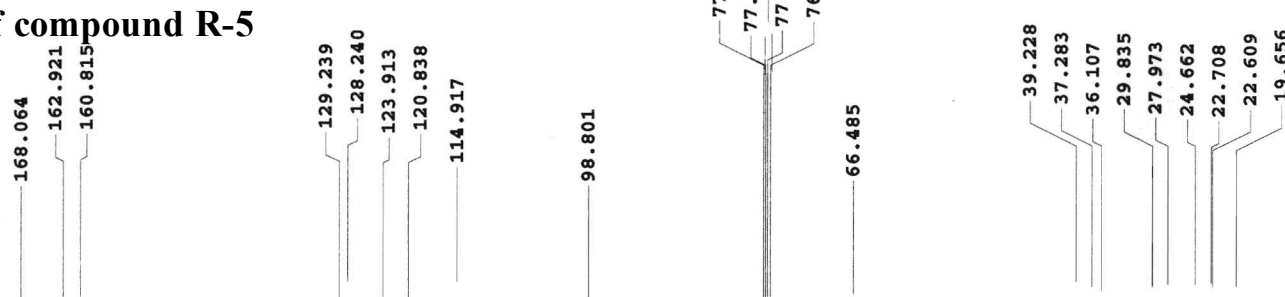
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 9 hr, 2 min, 12 sec



220 200 180 160 140 120 100 80 60 40 20 0 ppm

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

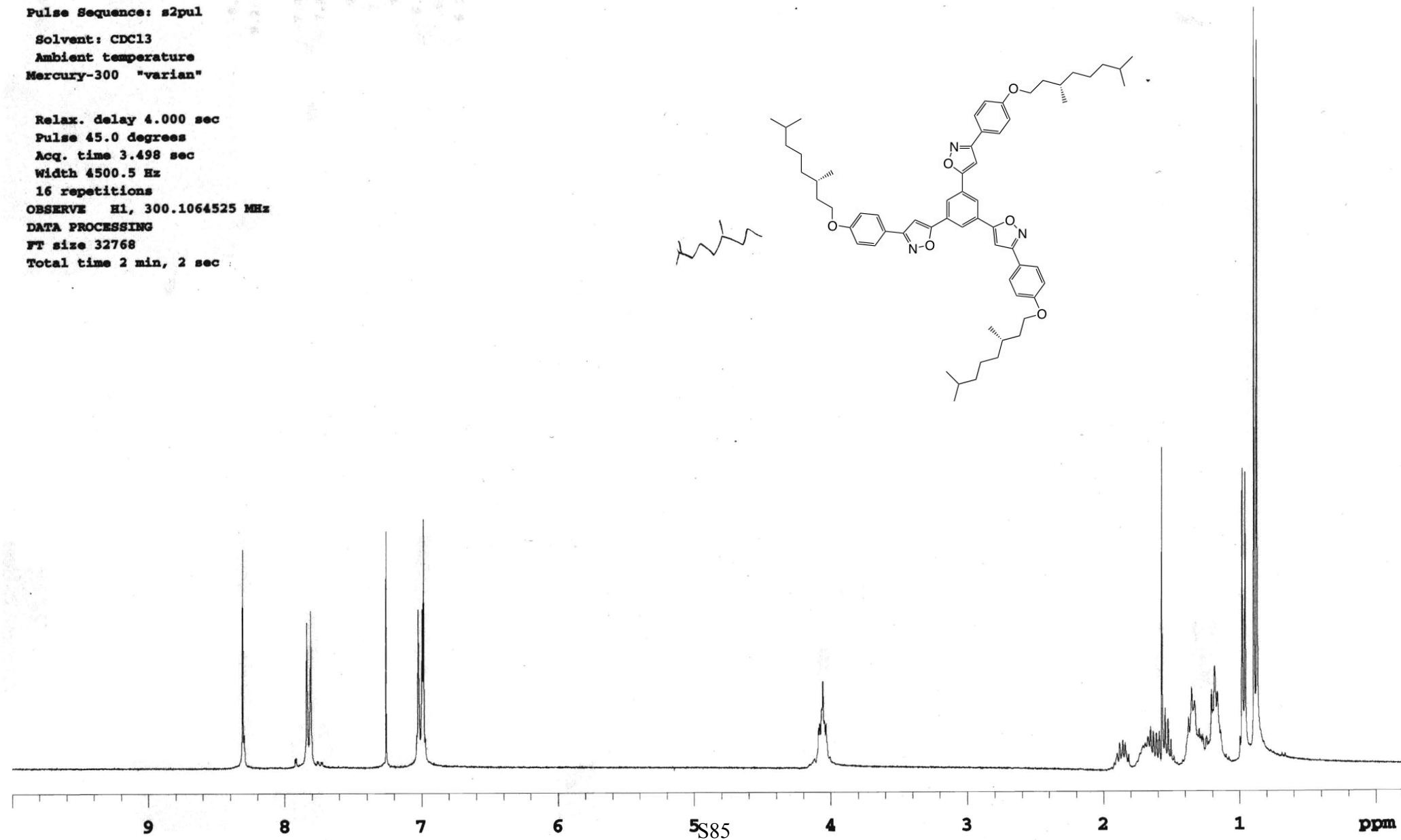
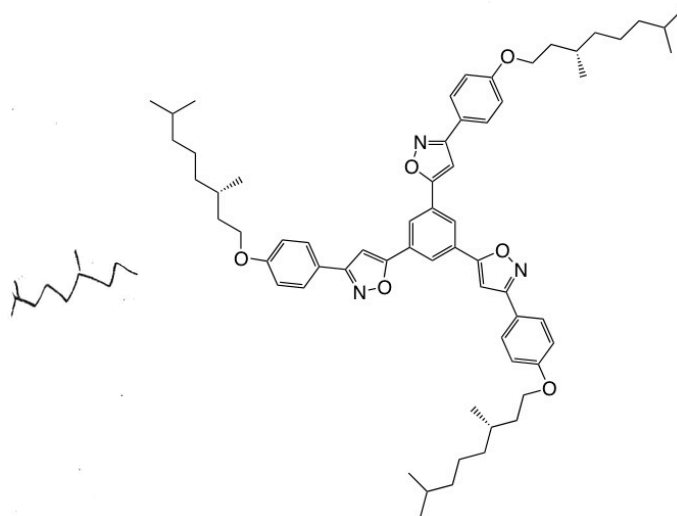
16 repetitions

OBSERVE H1, 300.1064525 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec



13C OBSERVE 13C NMR spectrum of compound S-5

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Mercury-300 "varian"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 1.499 sec

Width 18867.9 Hz

7488 repetitions

OBSERVE C13, 75.4618277 MHz

DECOUPLE H1, 300.1079971 MHz

Power 44 dB

continuously on

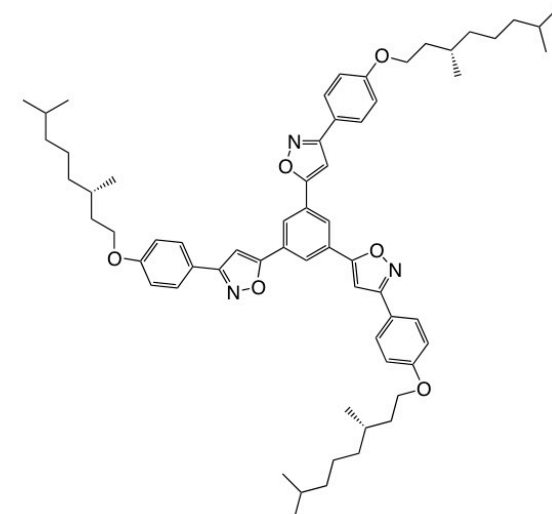
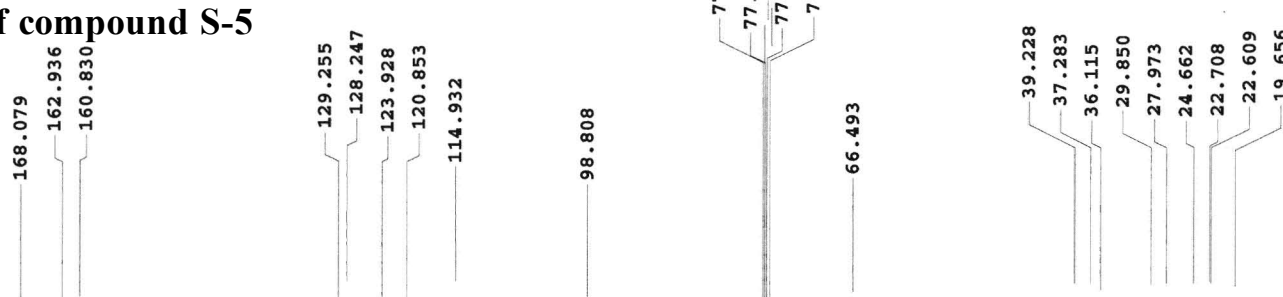
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 9 hr, 2 min, 12 sec



220 200 180 160 140 120 100 80 60 40 20 0 ppm

STANDARD 1H OBSERVE 1H NMR spectrum of compound 11

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4860.5 Hz

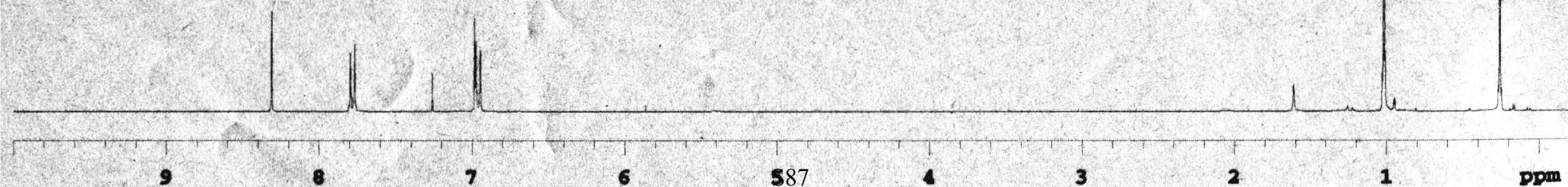
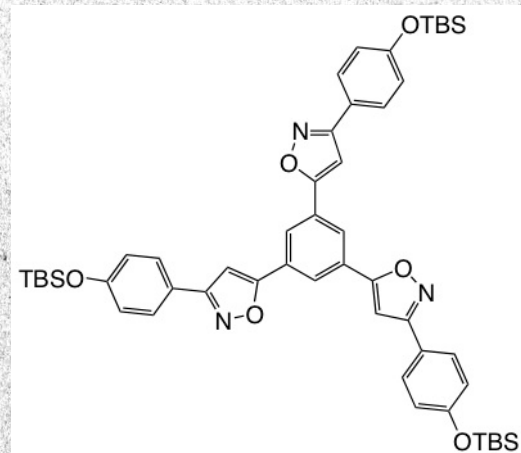
16 repetitions

OBSERVE H1, 300.1064528 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec



13C OBSERVE

13C NMR spectrum of compound 11

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Mercury-300 "varian"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 1.499 sec

Width 18867.9 Hz

784 repetitions

OBSERVE C13, 75.4618271 MHz

DECOUPLE H1, 300.1079971 MHz

Power 42 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 903 hr, 41 min, 29 sec

168.117
162.967
157.686

129.270
128.270
123.951
121.754
120.662

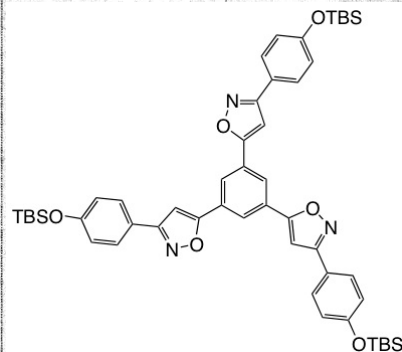
98.869

77.4
77.000
76.1

25.646

18.252

-4.373



220 200 180 160 140 120 S88 100 80 60 40 20 0 ppm

STANDARD 1H OBSERVE

¹H NMR spectrum of compound 2

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Mercury-300 "varian"

Relax. delay 4.000 sec

Pulse 45.0 degrees

Acq. time 3.498 sec

Width 4500.5 Hz

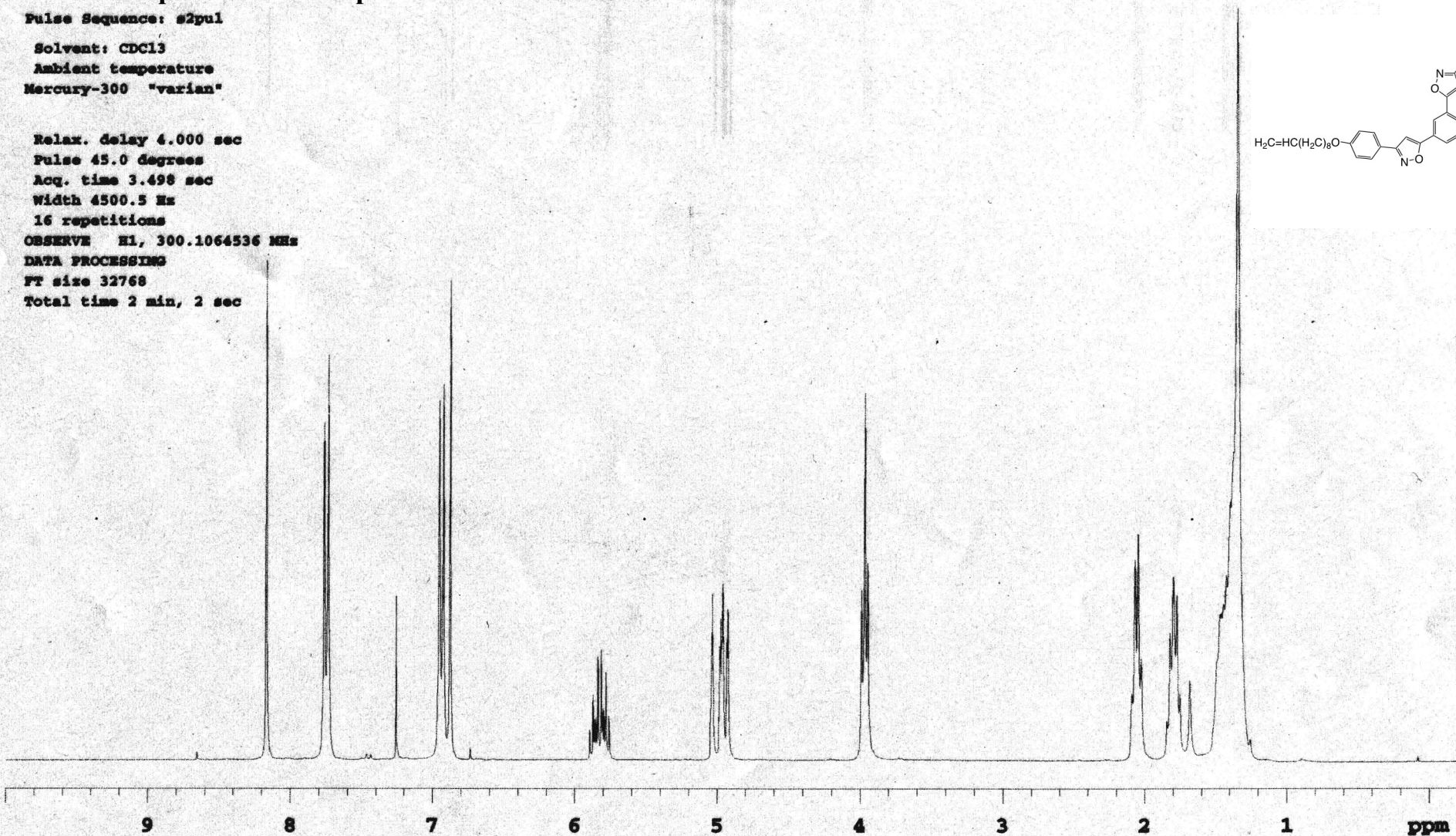
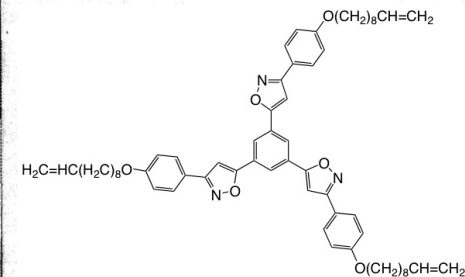
16 repetitions

OBSERVE H1, 300.1064536 MHz

DATA PROCESSING

FT size 32768

Total time 2 min, 2 sec



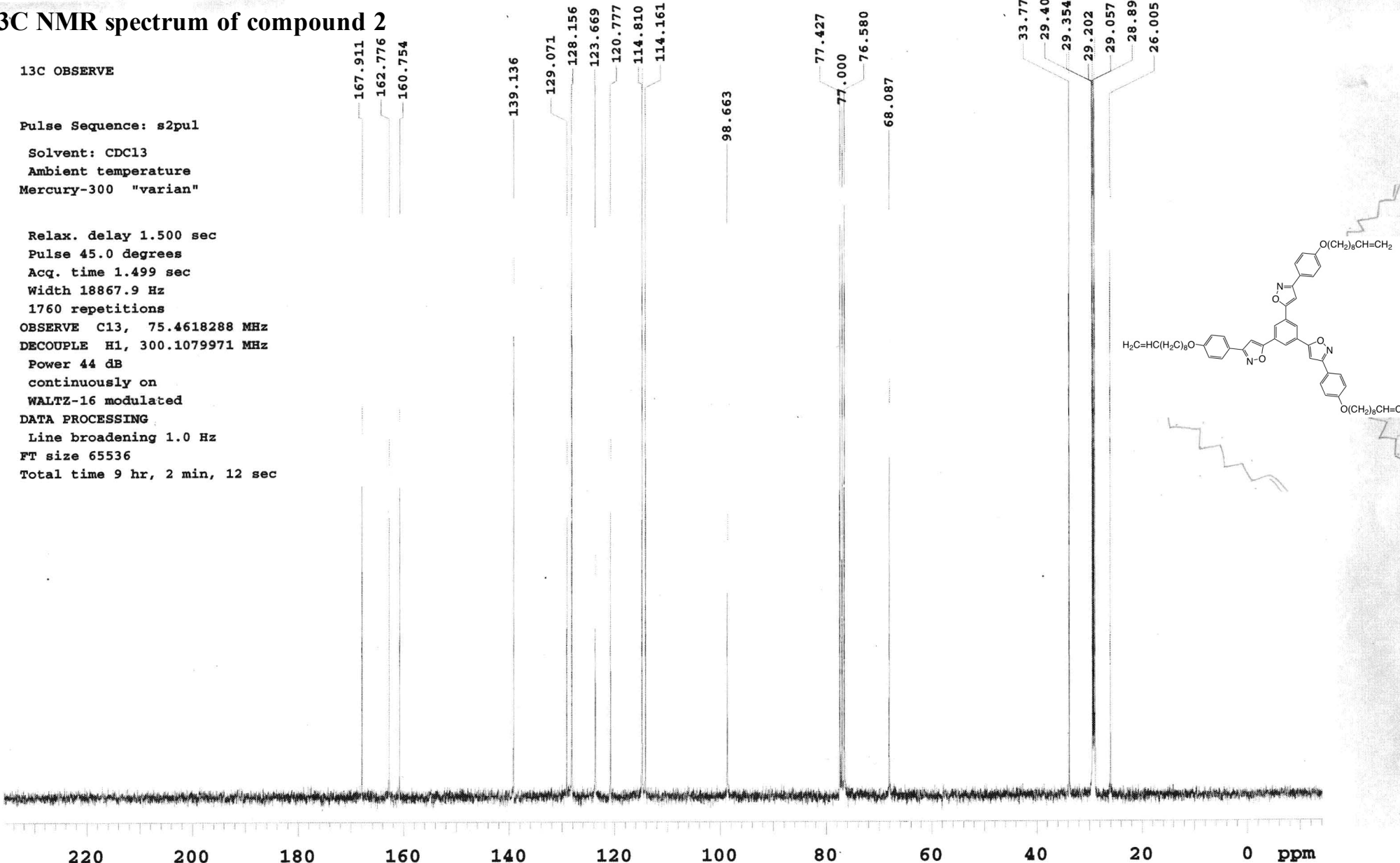
13C NMR spectrum of compound 2

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
Mercury-300 "varian"

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 1.499 sec
Width 18867.9 Hz
1760 repetitions
OBSERVE C13, 75.4618288 MHz
DECOUPLE H1, 300.1079971 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 2 min, 12 sec

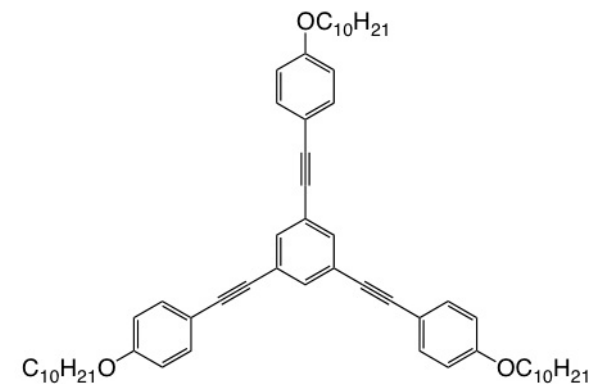
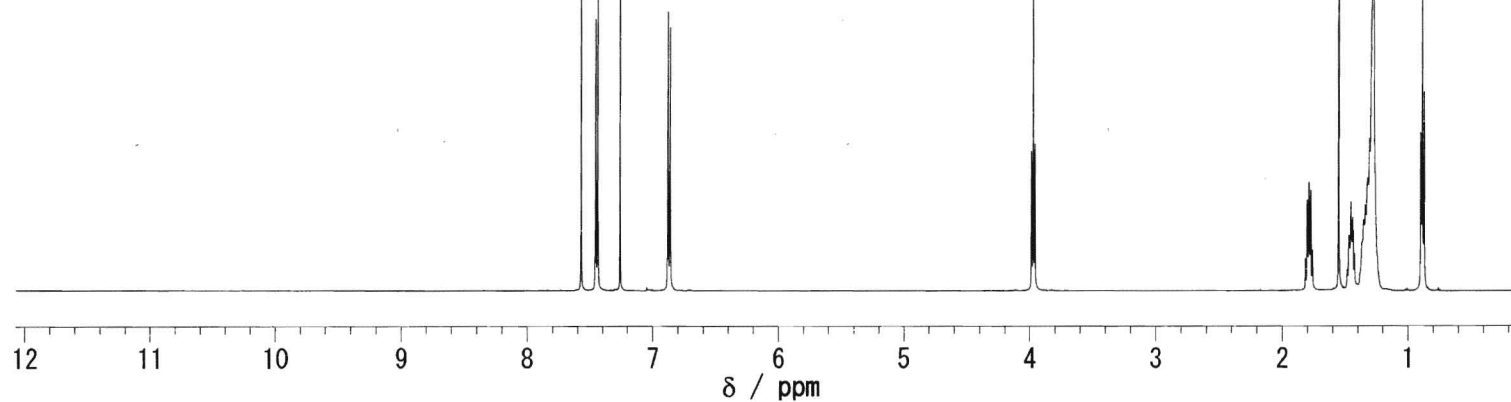


¹H NMR spectrum of compound 12

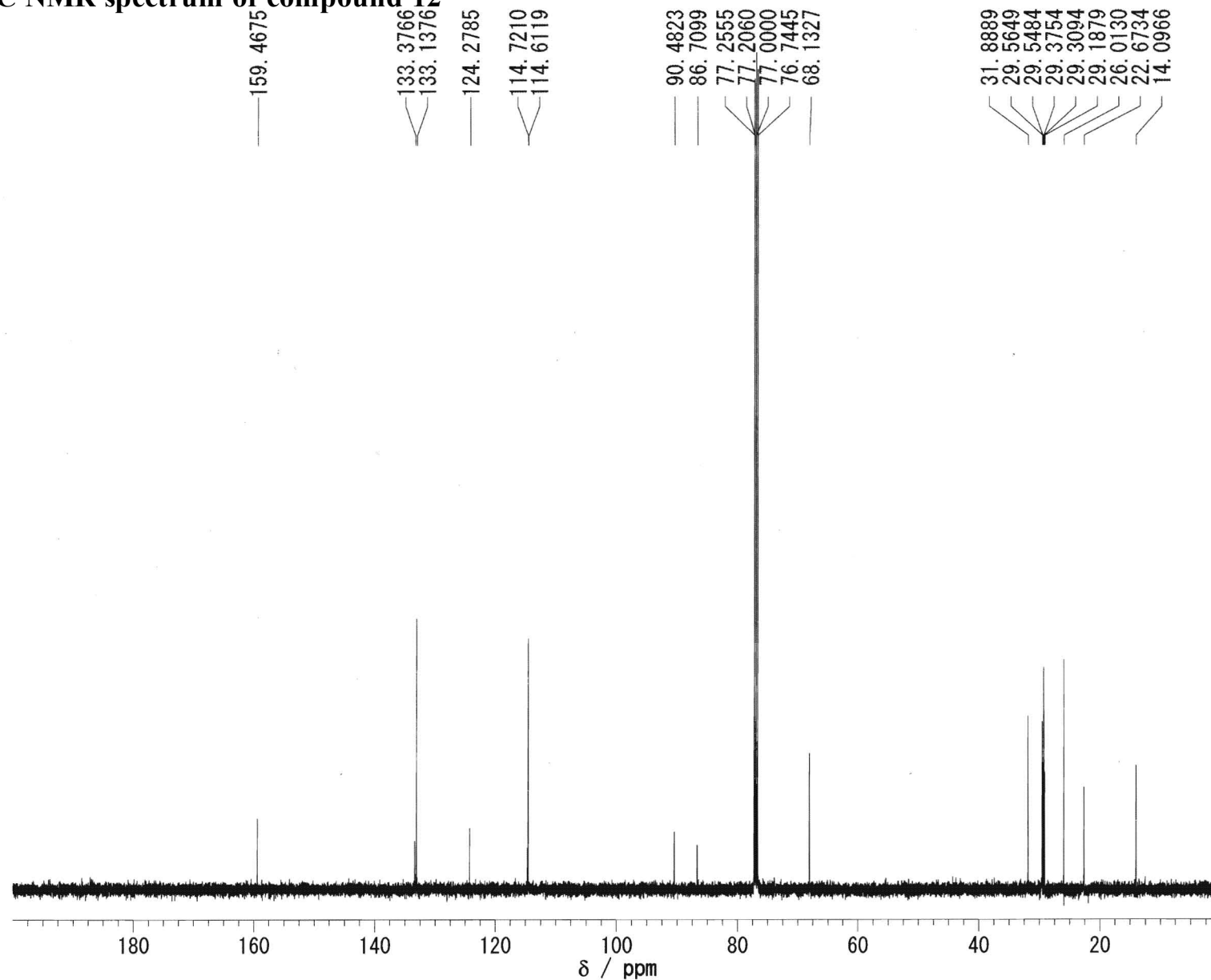
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10-10MM-1H\PHACE10-10MM-1H. ALS
Date Tue Jun 20 12:40:42 2006
Comment

ObsNuc ¹H
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ObsFreq 499.1 MHz
ObsSet 128.0 kHz
ObsFine 250.0 Hz
Point 32768
Frequency (Span) 9980.04 Hz
Scan 16
AcqTime 3.2834 s
PD 3.7166 s
Pulse1 7.1 μs
IrrNuc ¹H
ProbeHead TH5ATFG2
Instrument JEOL LAMBDA
Pulse Program
Gradient Program
Temperature 27.0 °C
Solvent CDCL₃
Reference 7.26 ppm
Broad. Factor 0.25 Hz
Window Exponential
RGain 23

Operator _____



¹³C NMR spectrum of compound 12



File H:\STUDENTSYD1_2005\TANAKA\DATA\PHACE
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Date Tue Jun 20 14:24:41 2006
Comment

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ObsSet 143.0 kHz
ObsFine 41.0 Hz
Point 32768
Frequency (Span) 33898.3 Hz
Scan 2024
AcqTime 0.9667 s
PD 2.0333 s
Pulse1 6.0 μs
IrrNuc ¹H
ProbeHead TH5ATFG2
Instrument JEOL LAMBDA
Pulse Program
Gradient Program
Temperature 29.1 °C
Solvent CDCL₃
Reference 77.0 ppm
Broad. Factor 0.5172 Hz
Window Exponential
RGain 16

Operator _____

