

Supplementary Materials

Structure – Selectivity Relationship in Ruthenium Catalyzed Regio- and Stereoselective Addition of Alkynes to Pyrazoles: An Experimental and Theoretical Investigation

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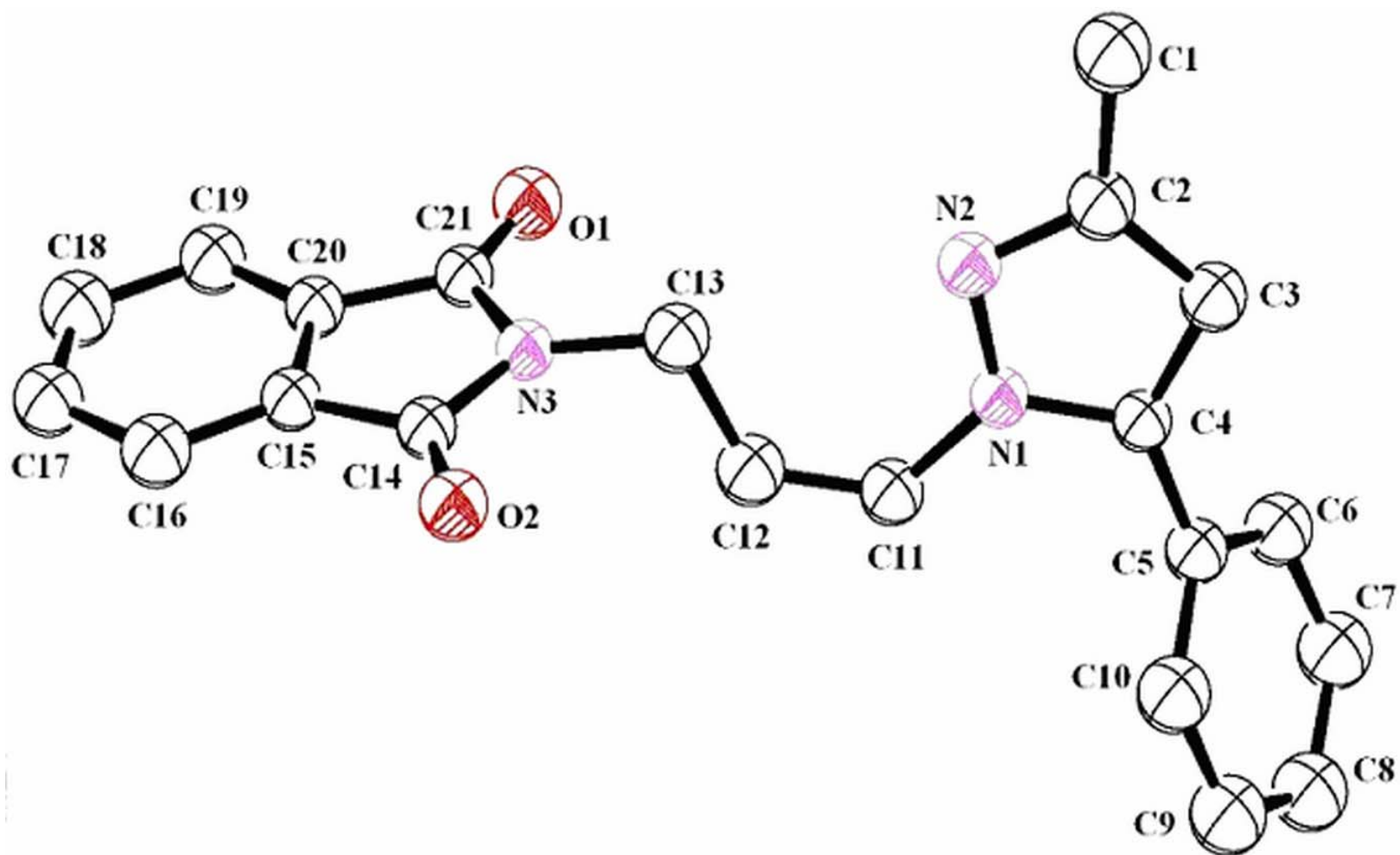


Figure S1 ORTEP view of **6z**, thermal ellipsoid drawn at 30% probability.

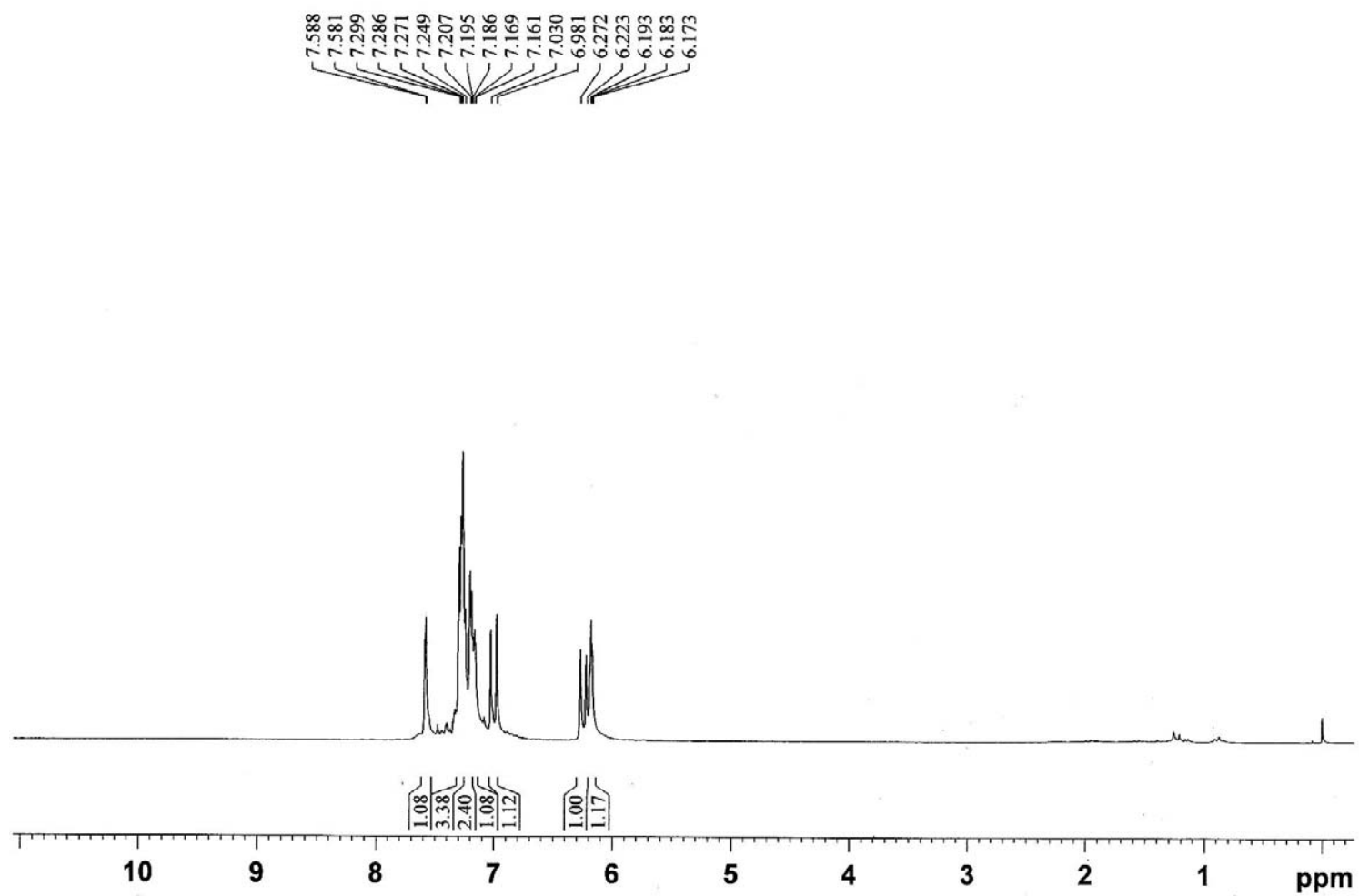


Figure S2 ^1H NMR spectrum of **6a**

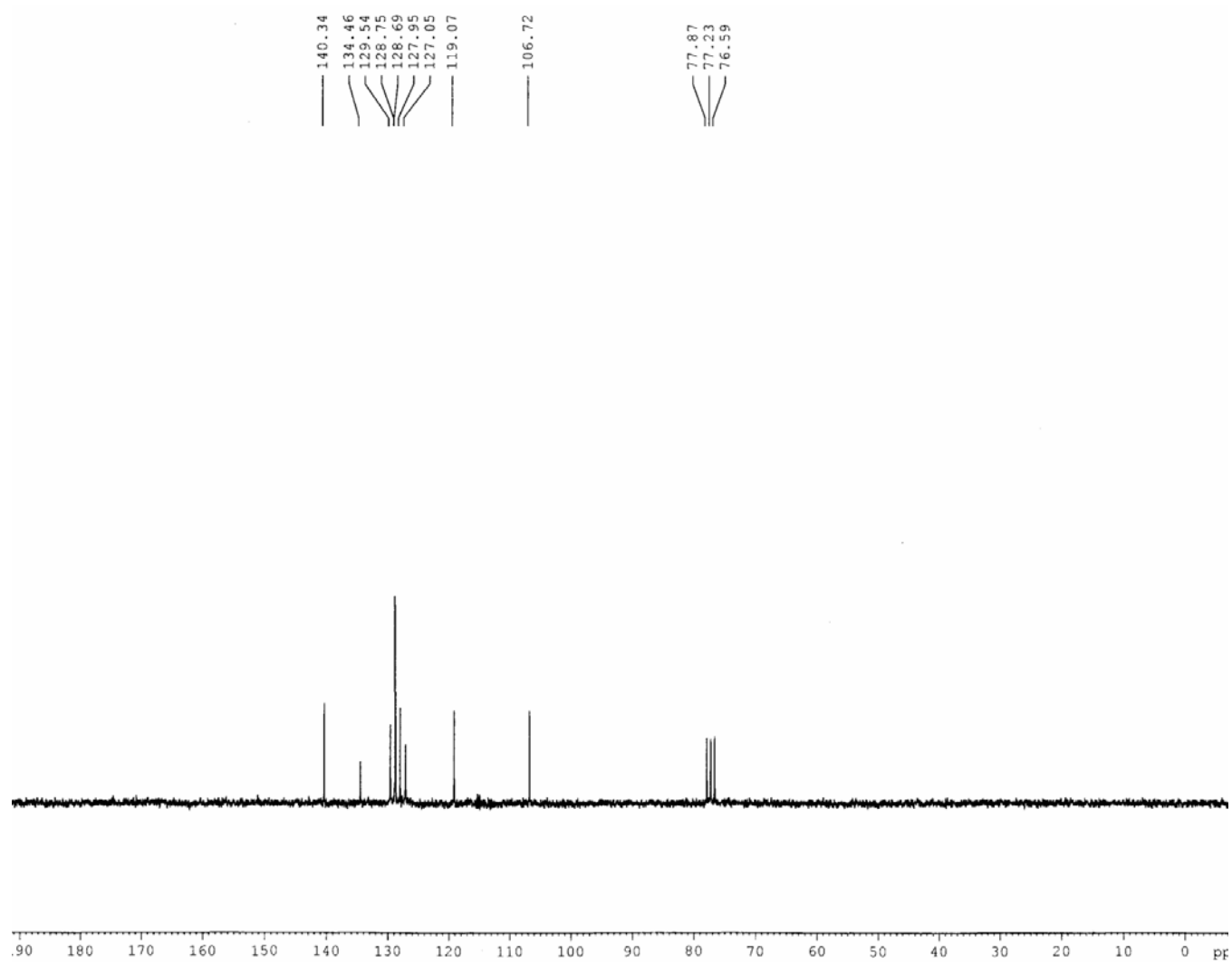


Figure S3 ^{13}C NMR spectrum of **6a**

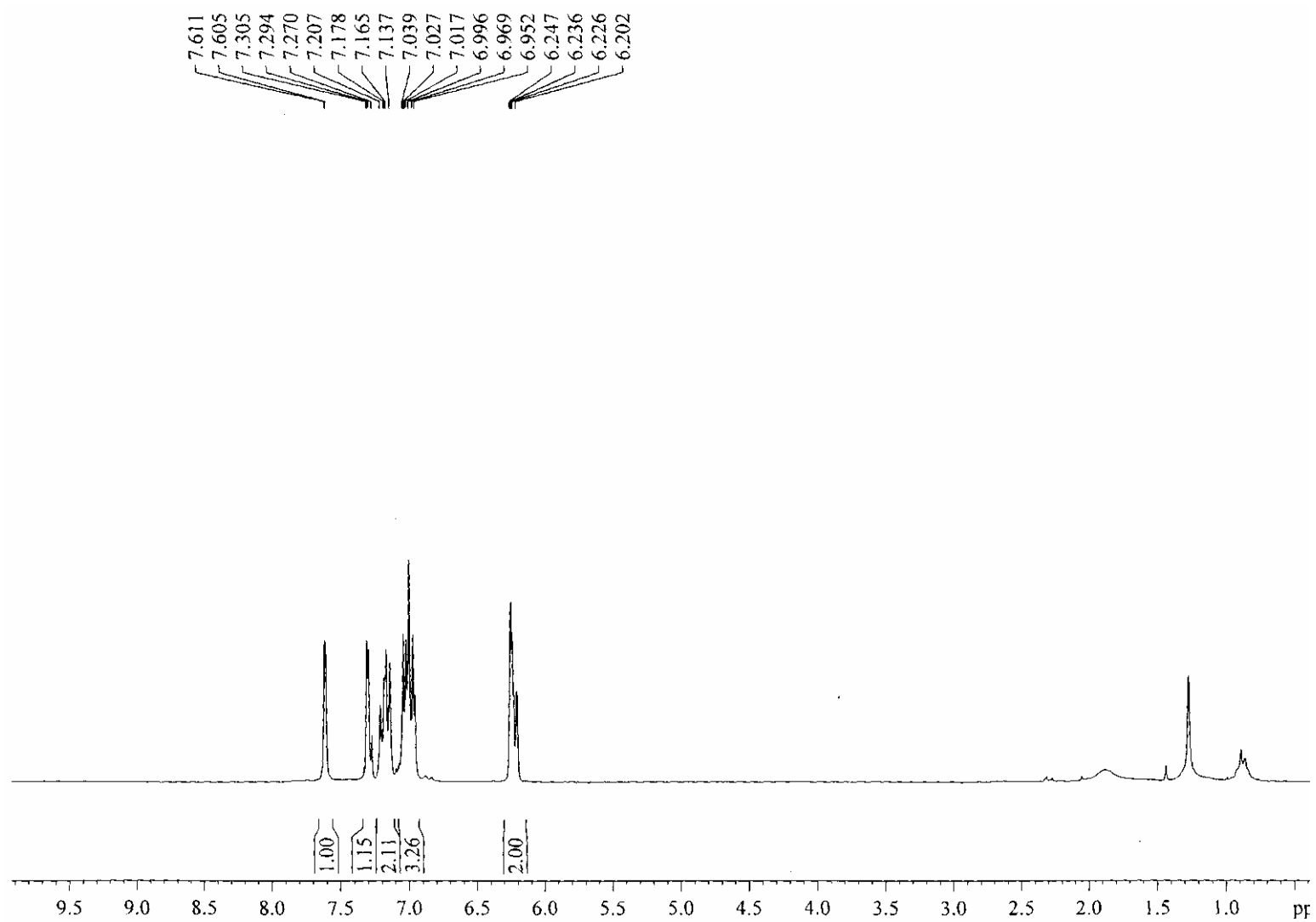


Figure S4 ¹H NMR spectrum of **6b**

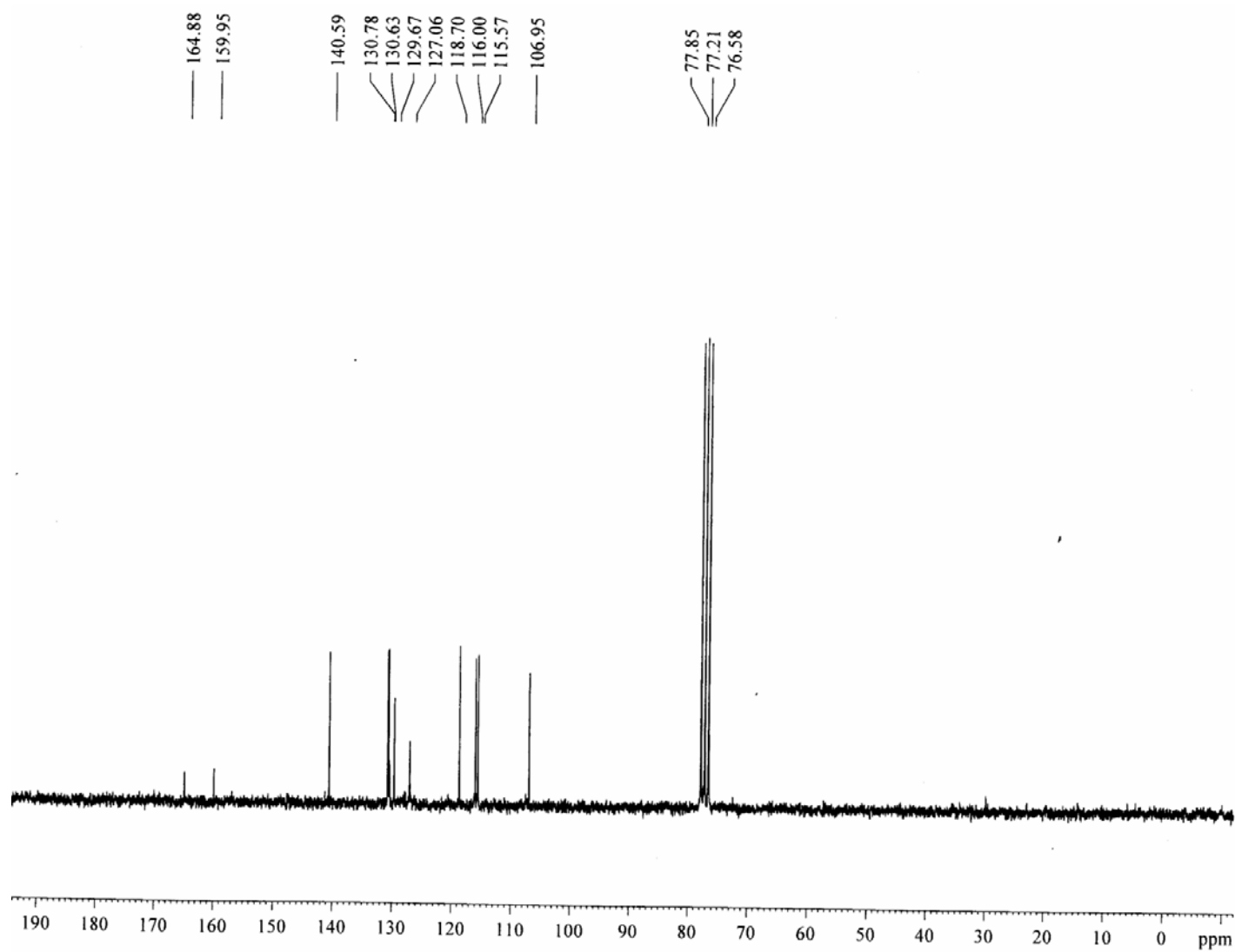


Figure S5 ¹³C NMR spectrum of **6b**

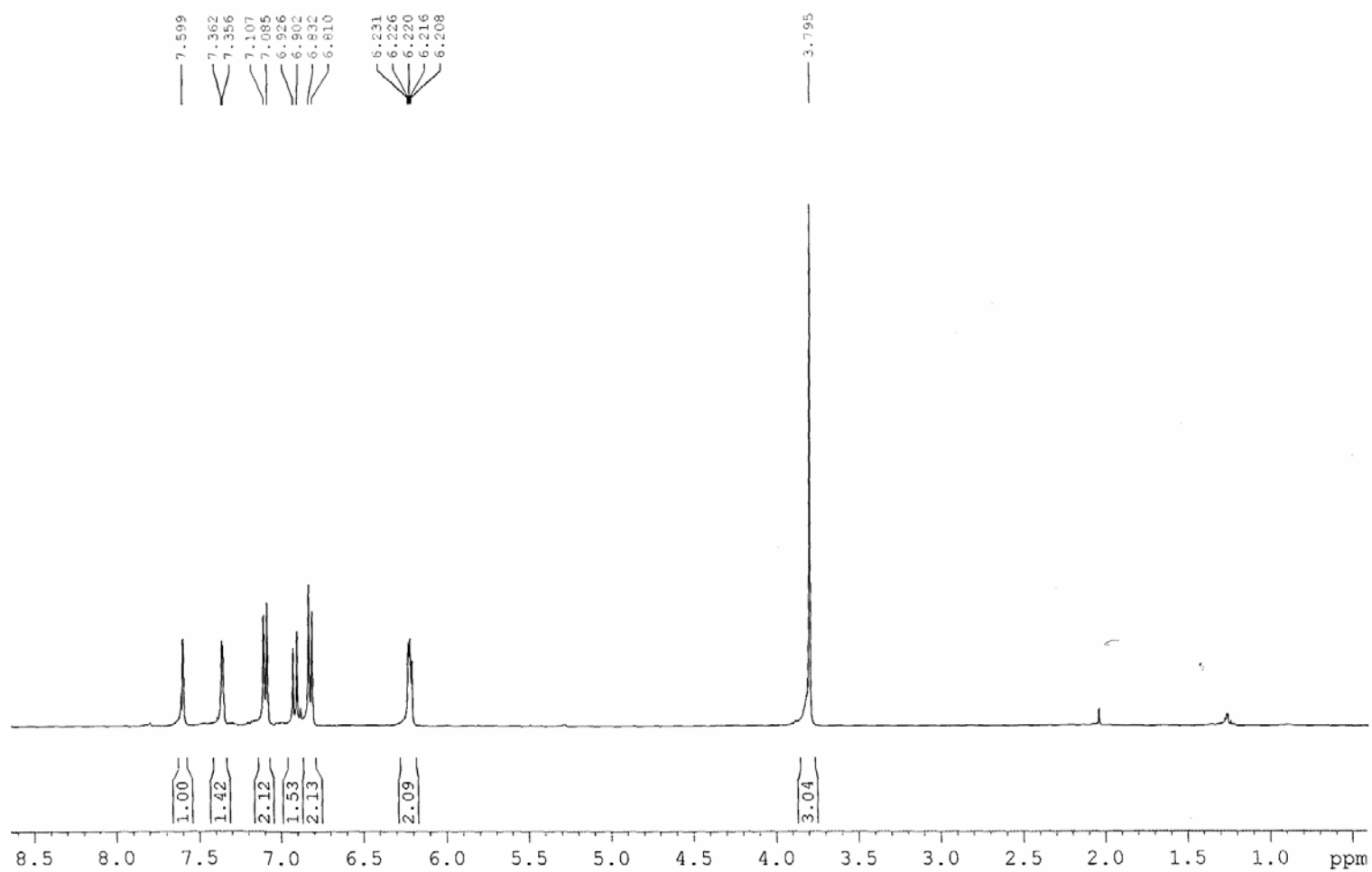


Figure S6 ¹H NMR spectrum of **6c**

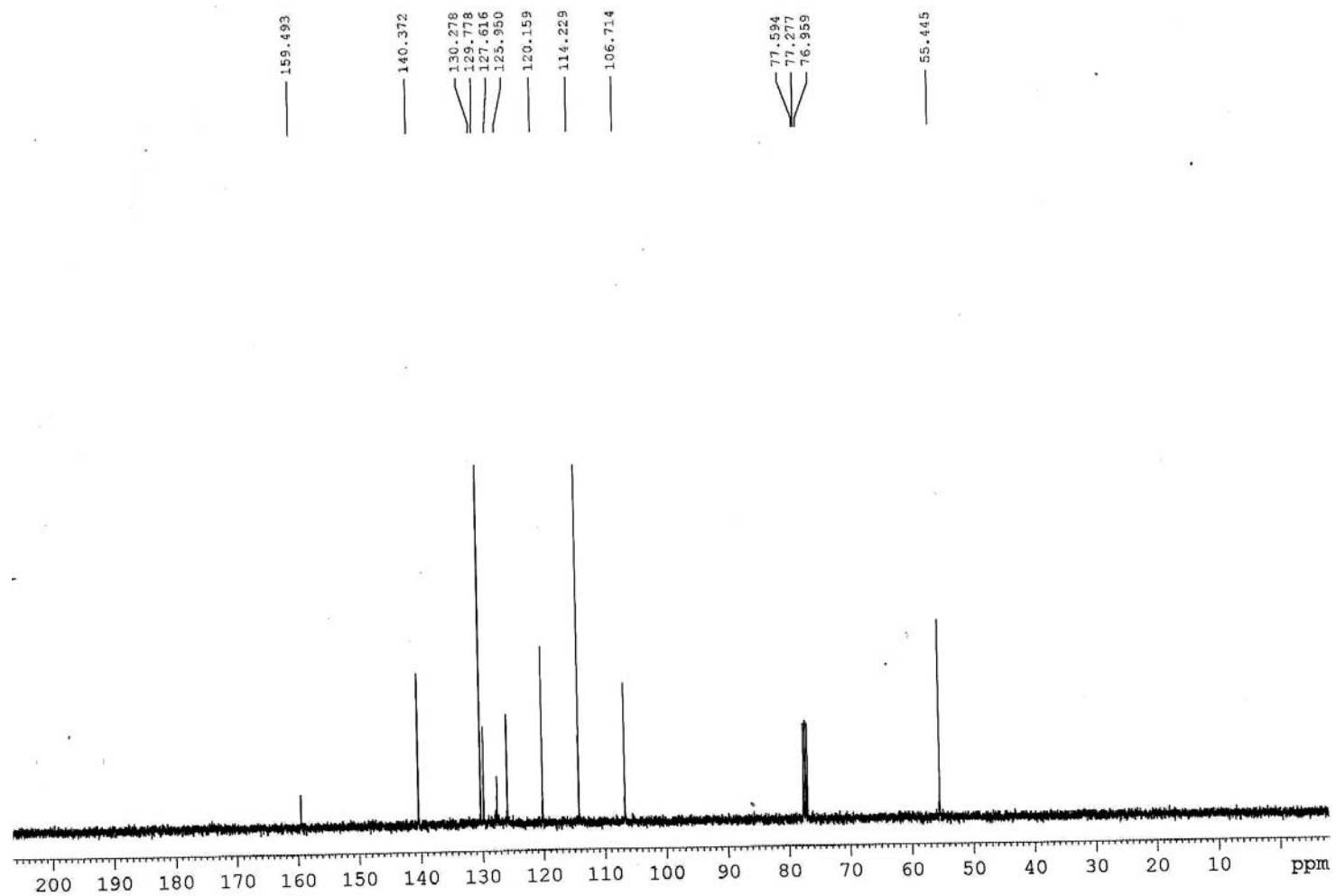


Figure S7 ¹³C NMR spectrum of **6c**

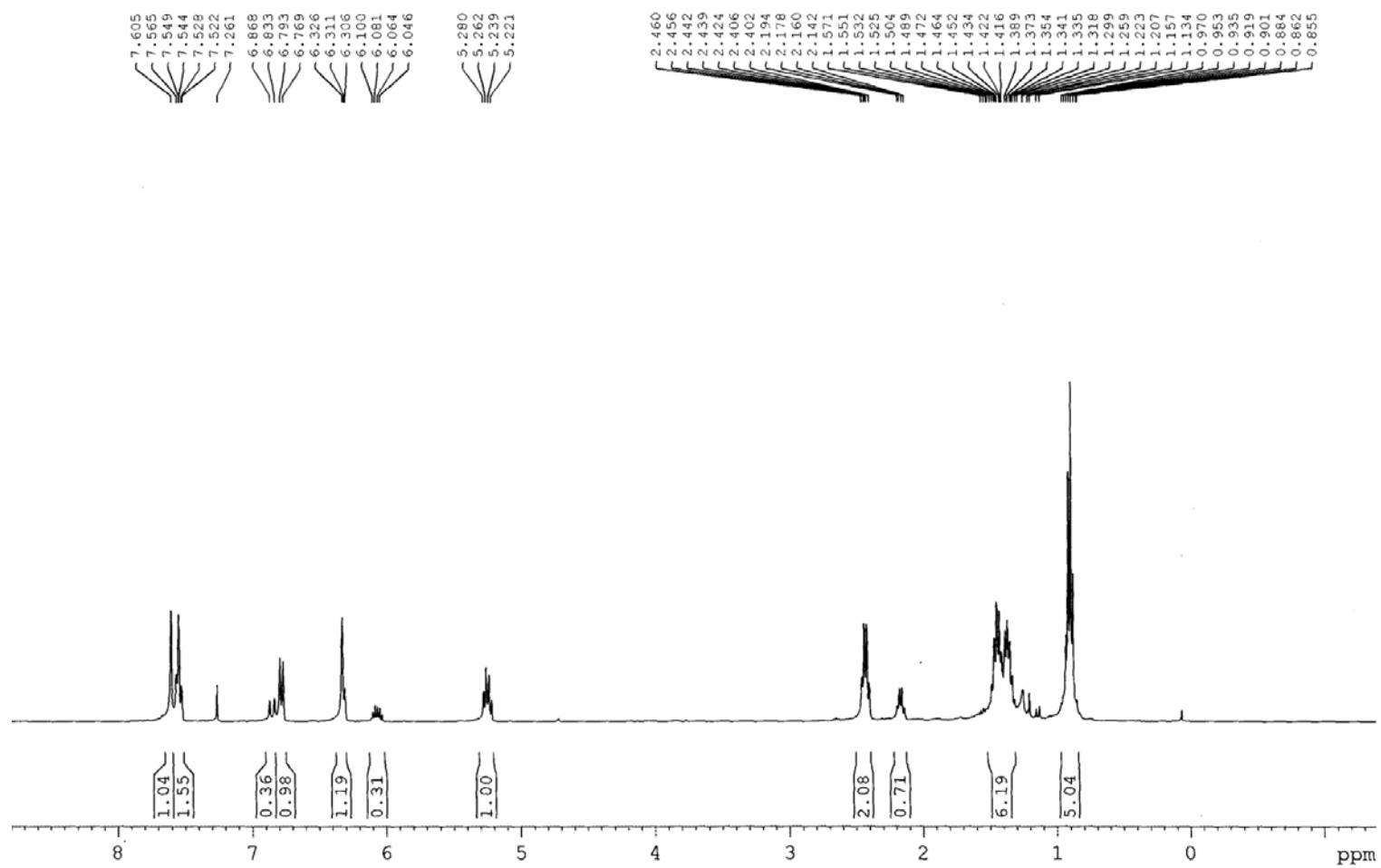


Figure S8 ^1H NMR spectrum of **6d**

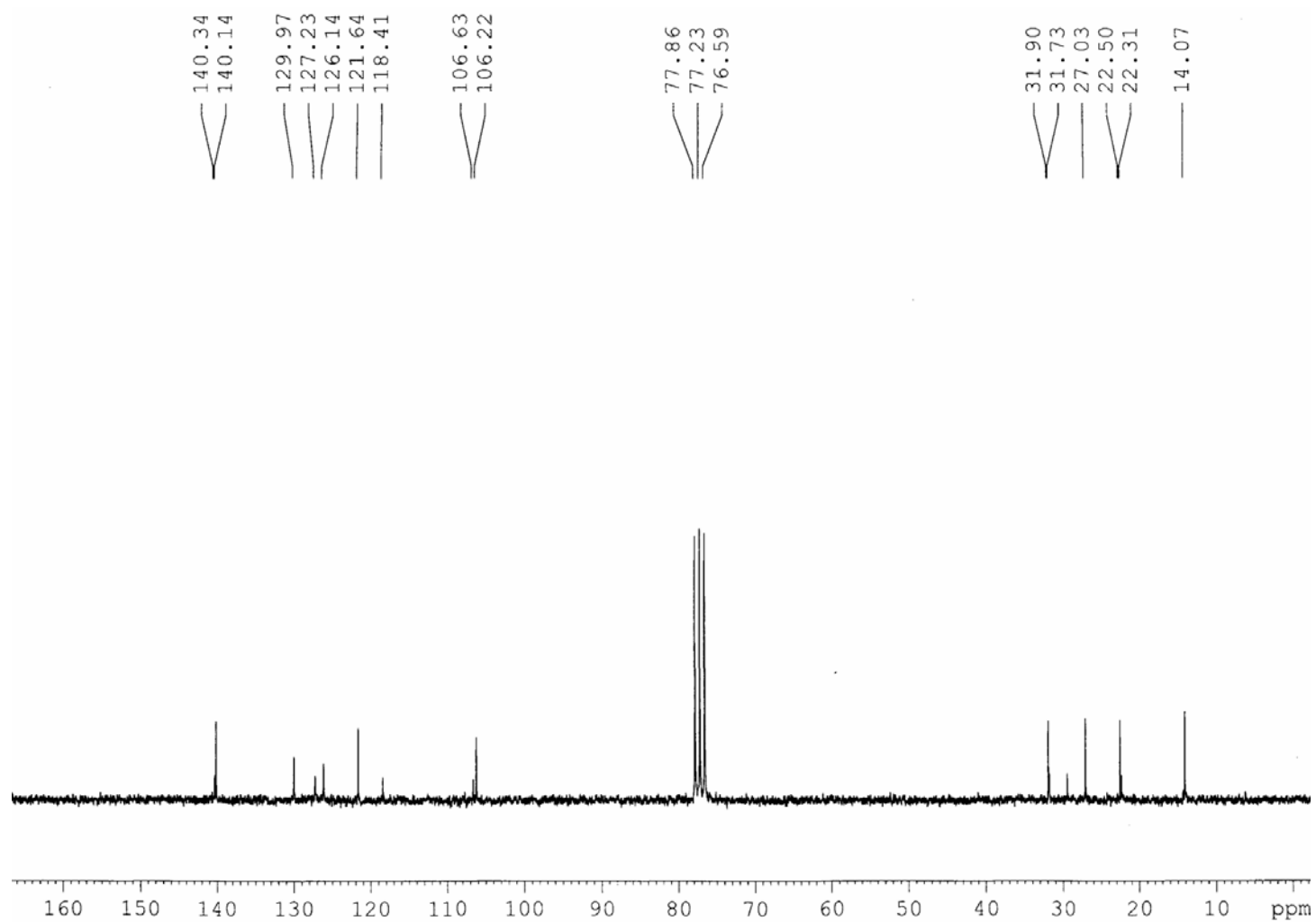


Figure S9 ¹³C NMR spectrum of **6d**

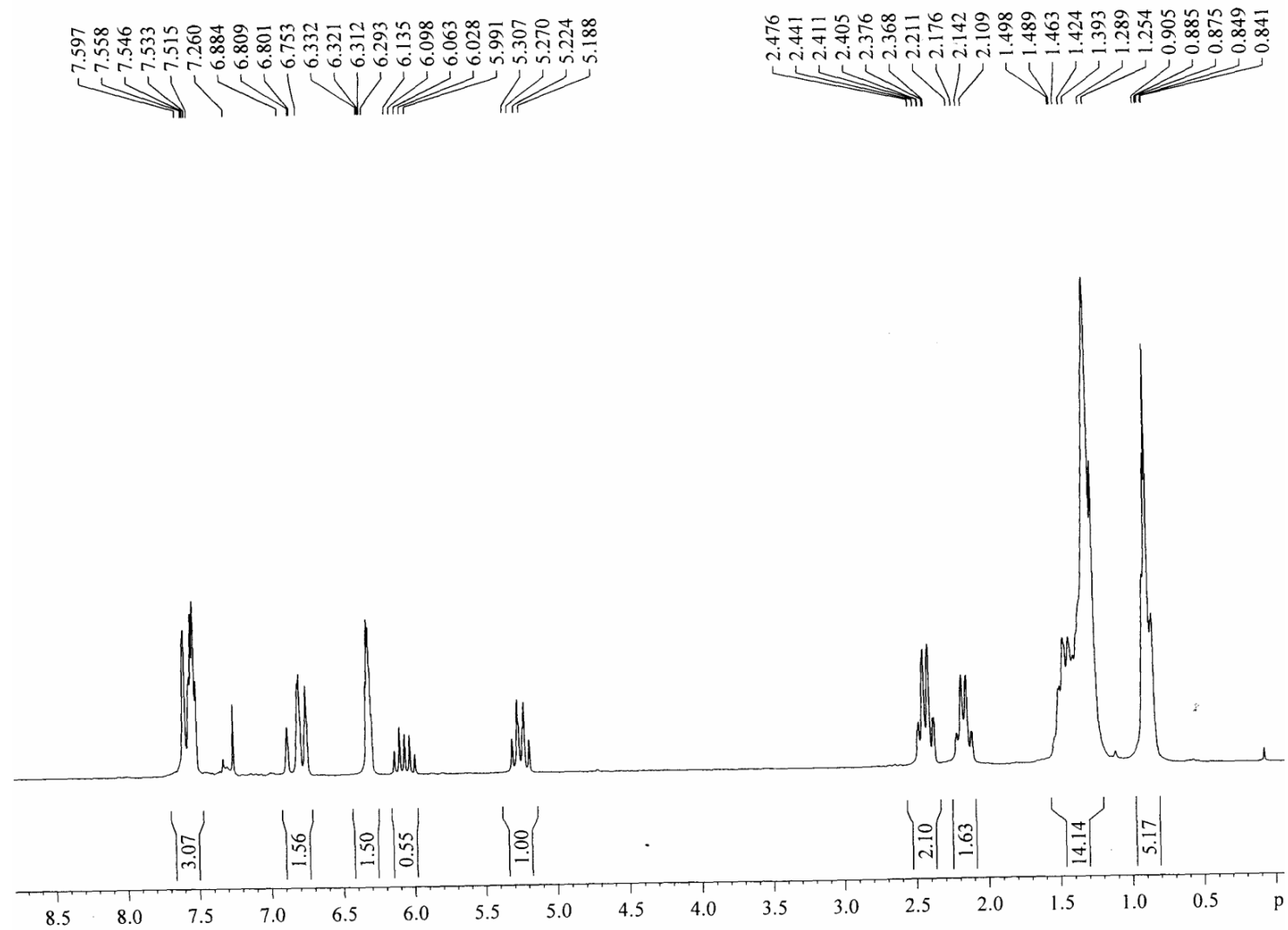


Figure S10 ^1H NMR spectrum of **6e**

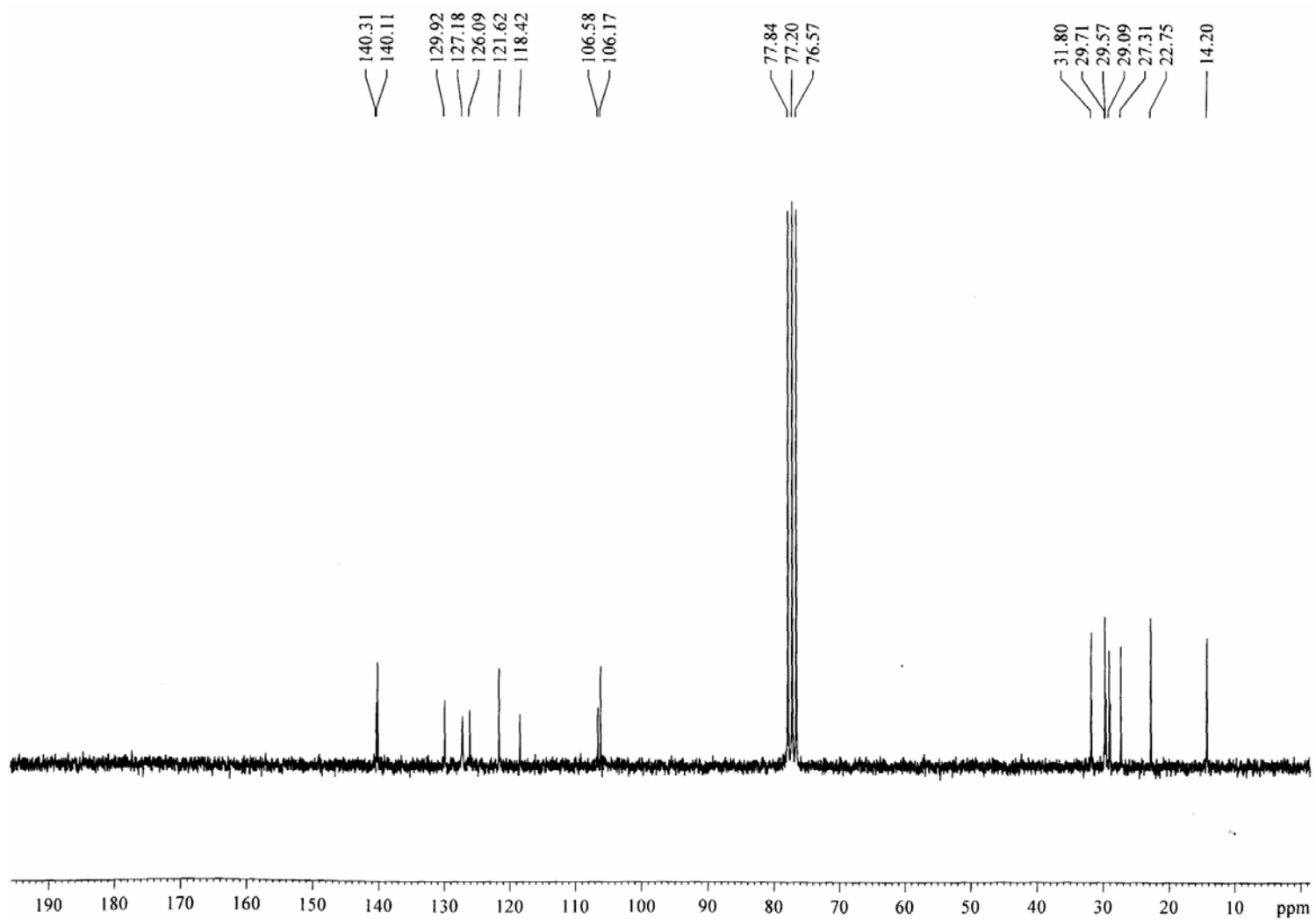


Figure S11 ¹³C NMR spectrum of **6e**

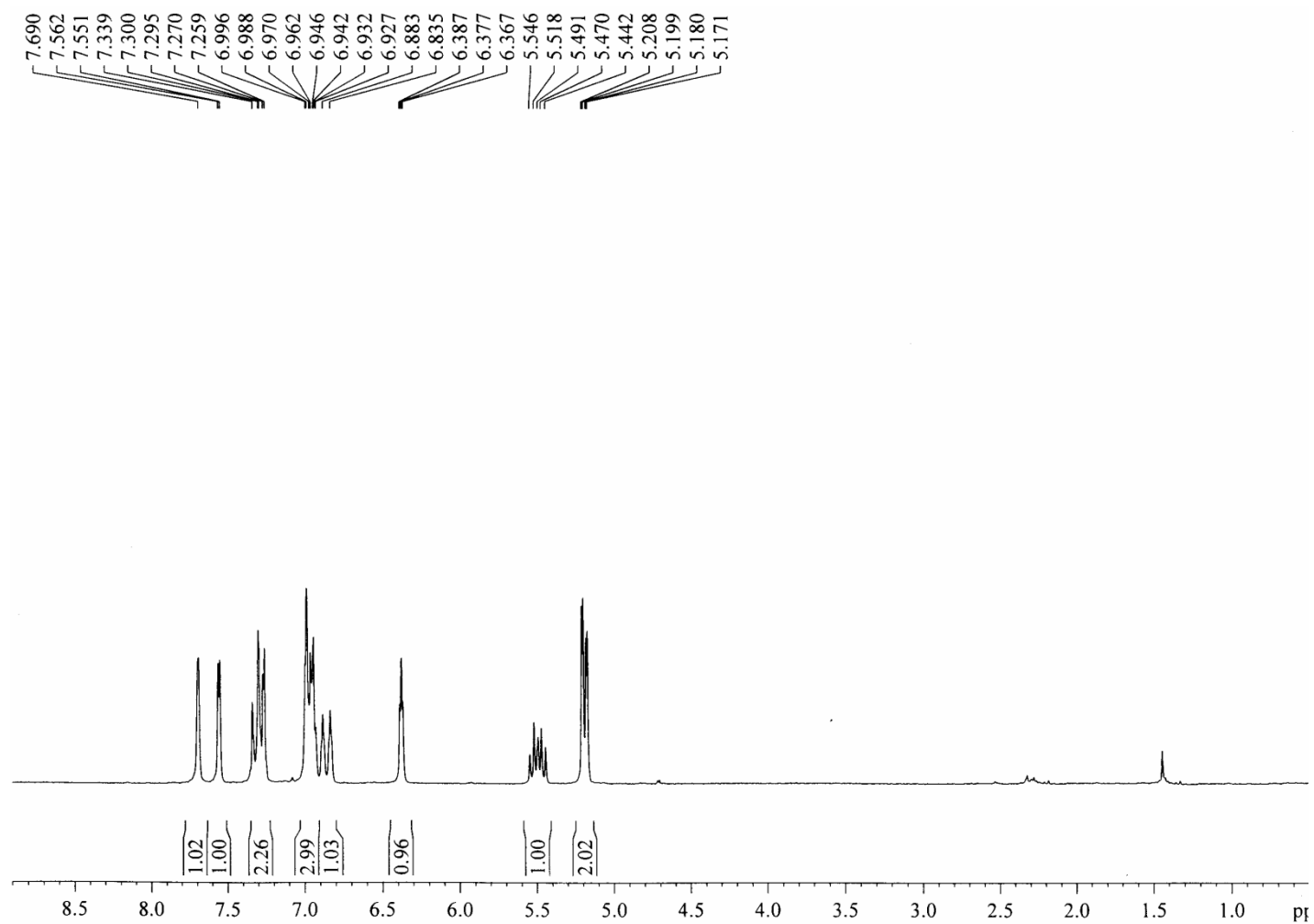


Figure S12 ¹H NMR spectrum of **6f**

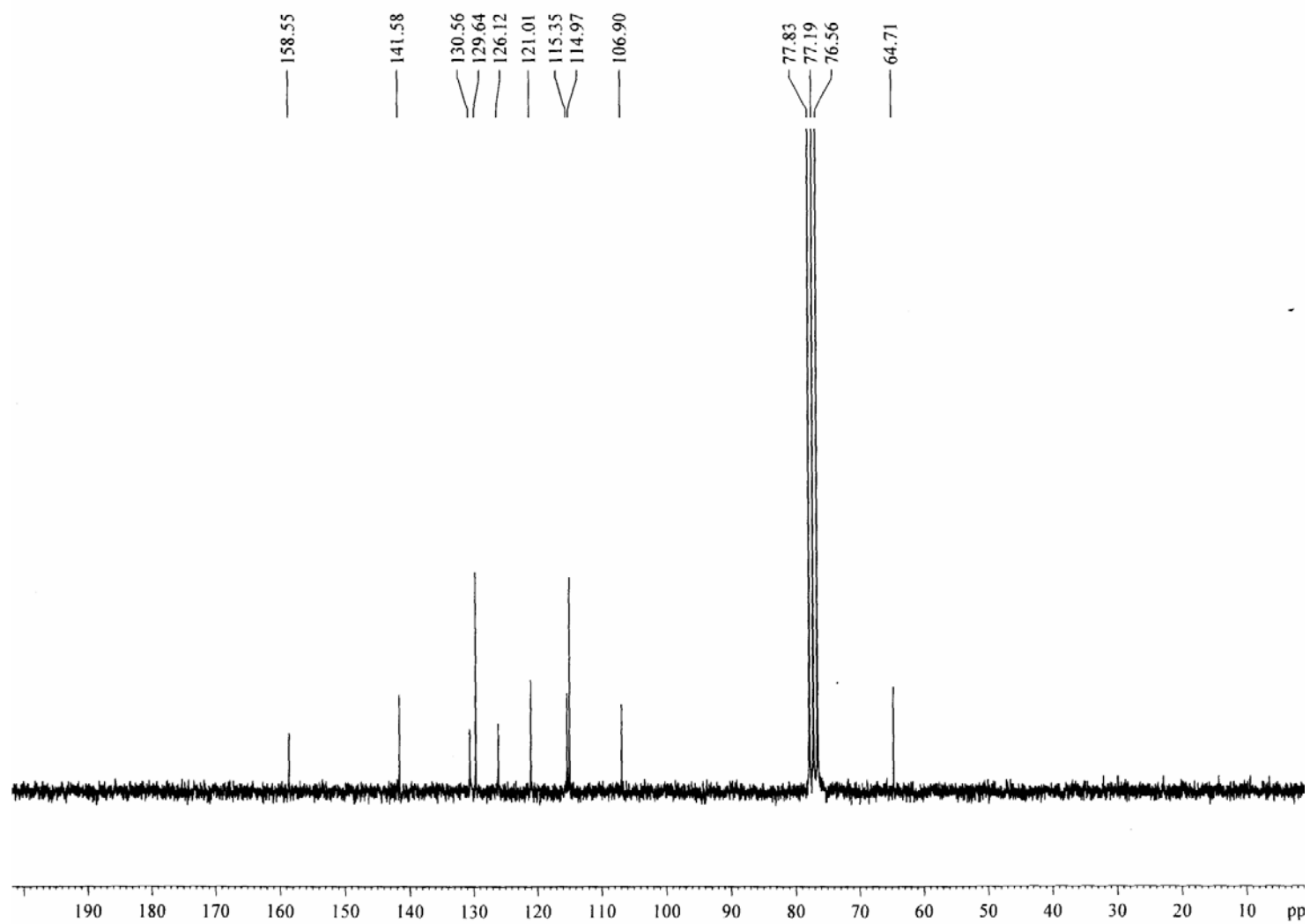


Figure S13 ^{13}C NMR spectrum of **6f**

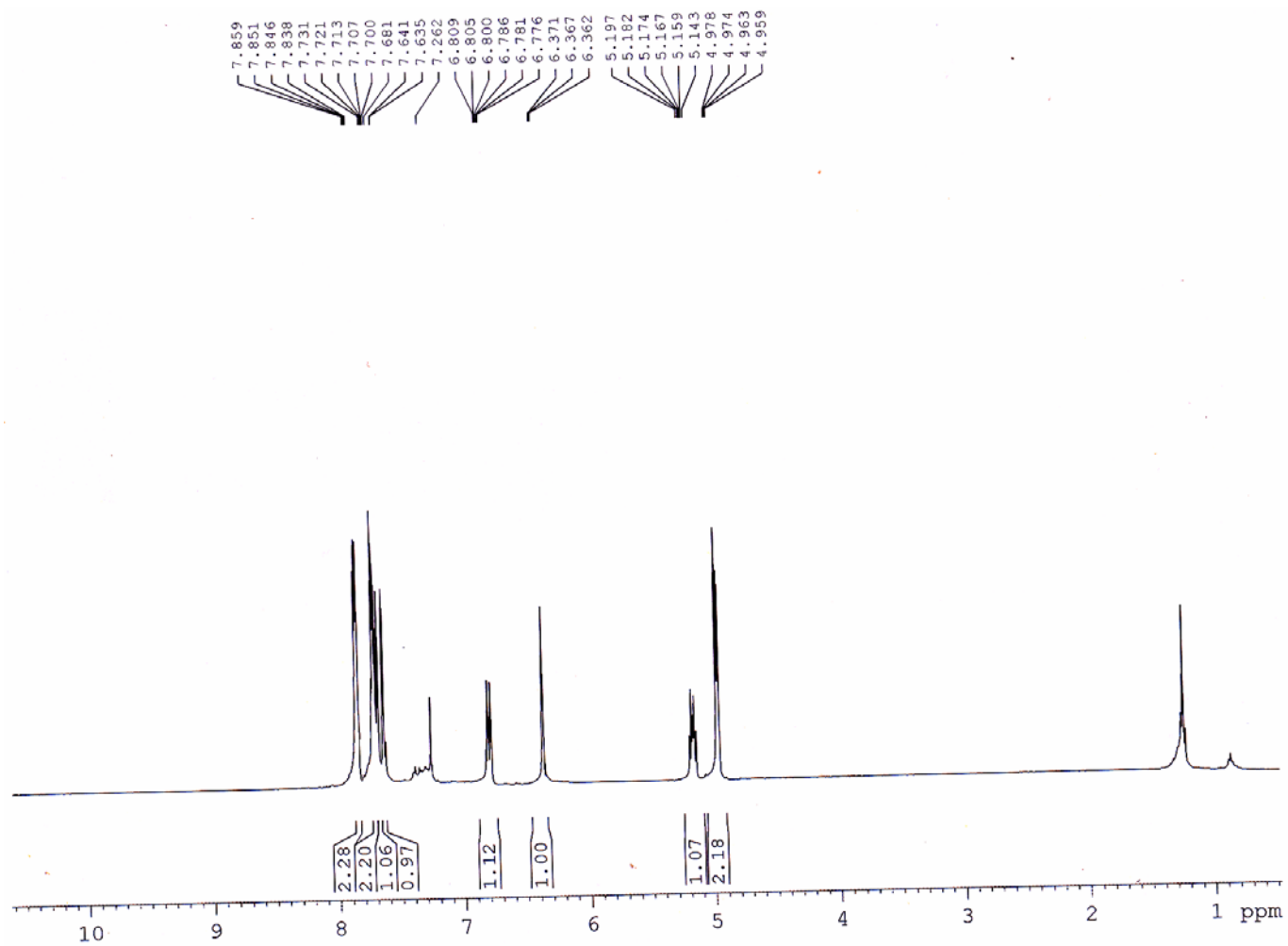


Figure S14 ¹H NMR spectrum of **6g**

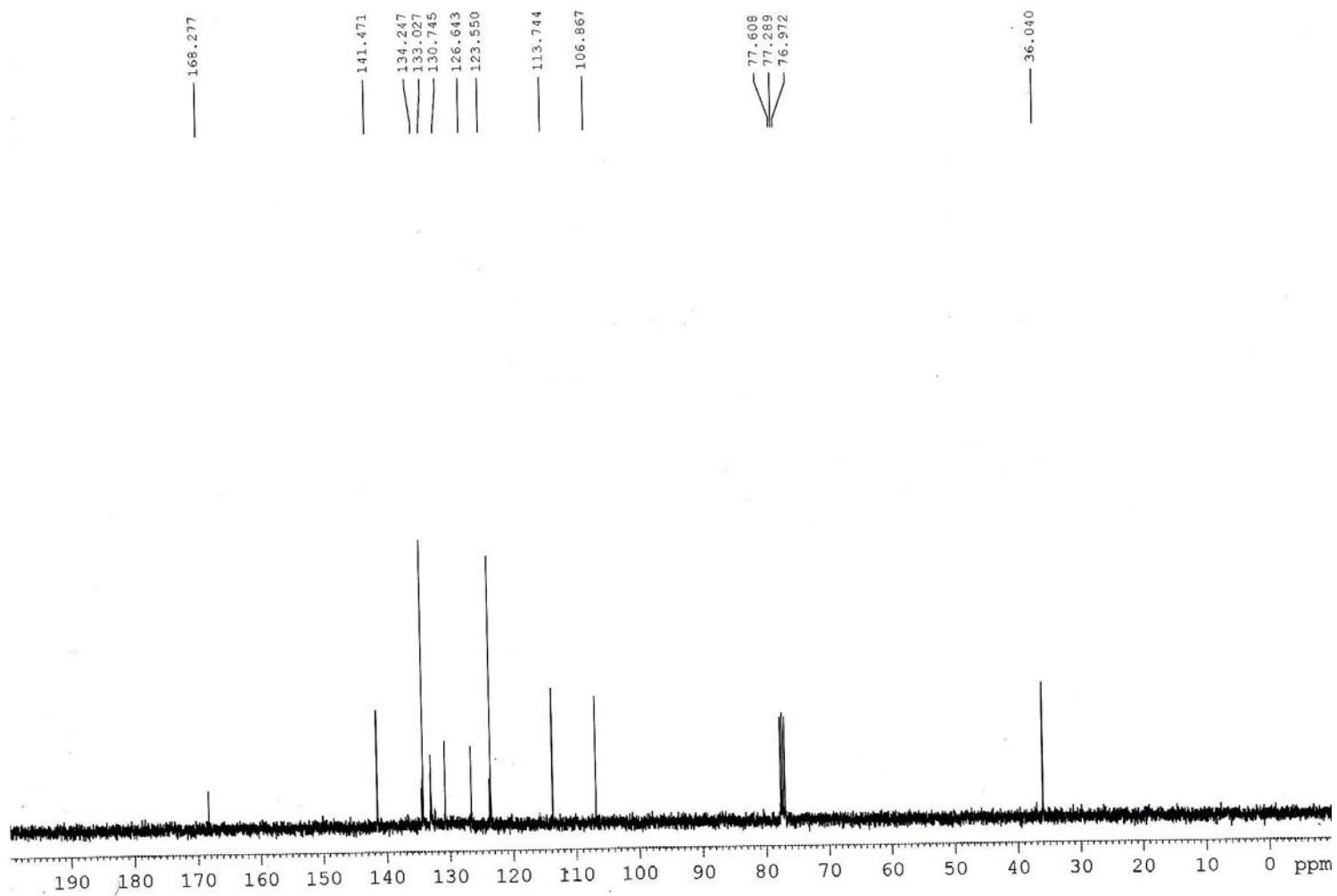


Figure S15 ¹³C NMR spectrum of **6g**

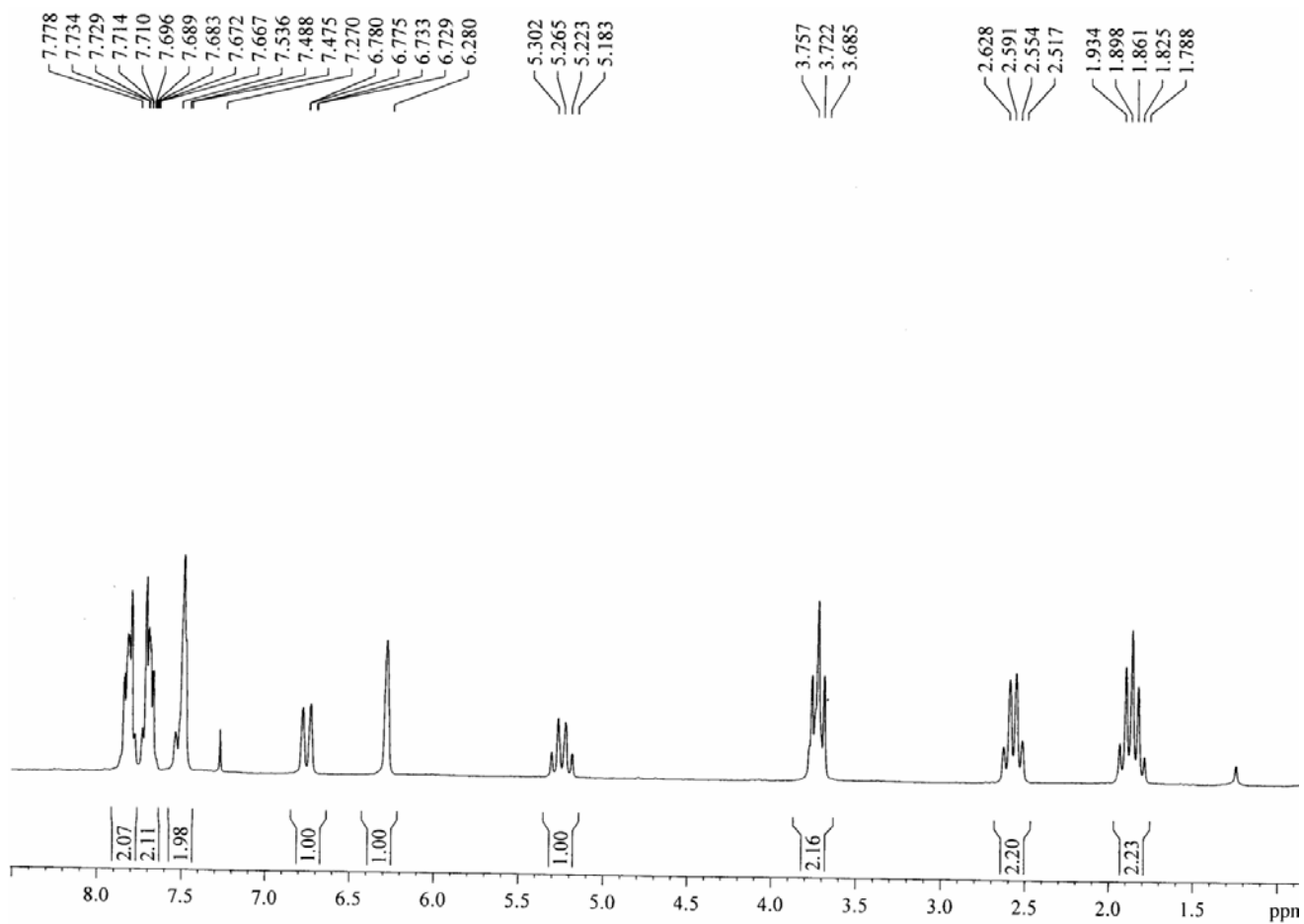


Figure S16 ^1H NMR spectrum of **6h**

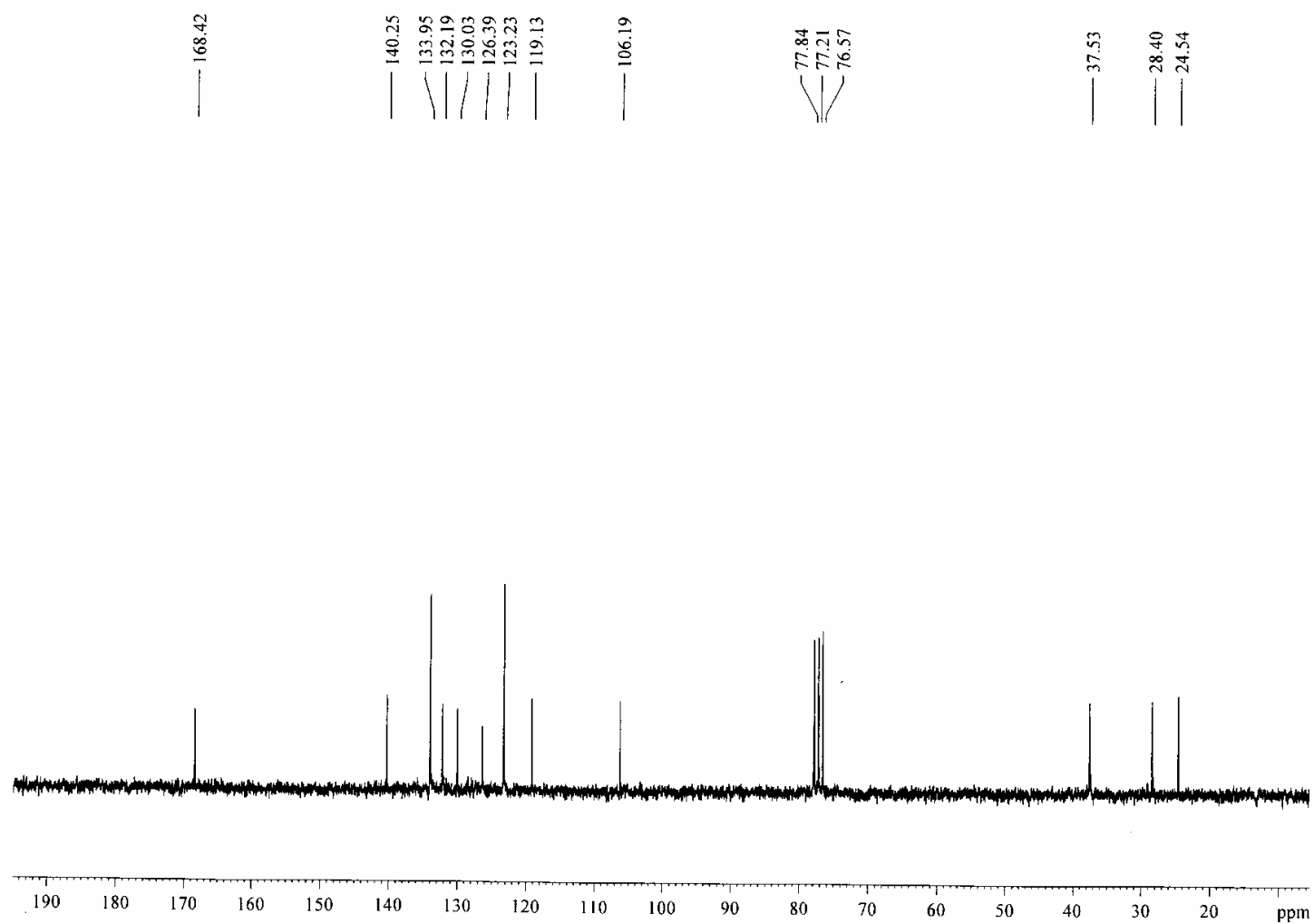


Figure S17 ¹³C NMR spectrum of **6h**

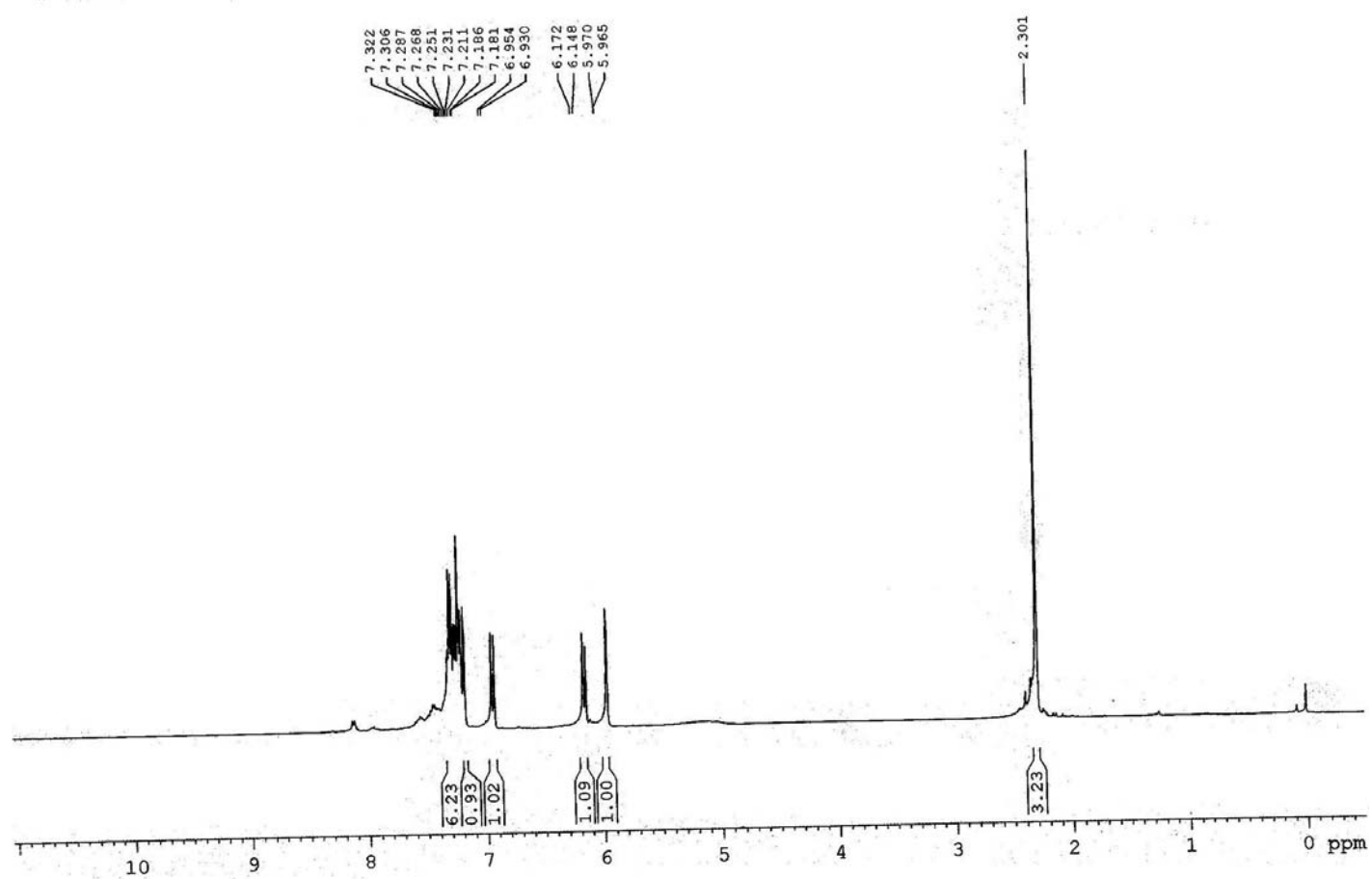


Figure S18 ¹H NMR spectrum of **6i**

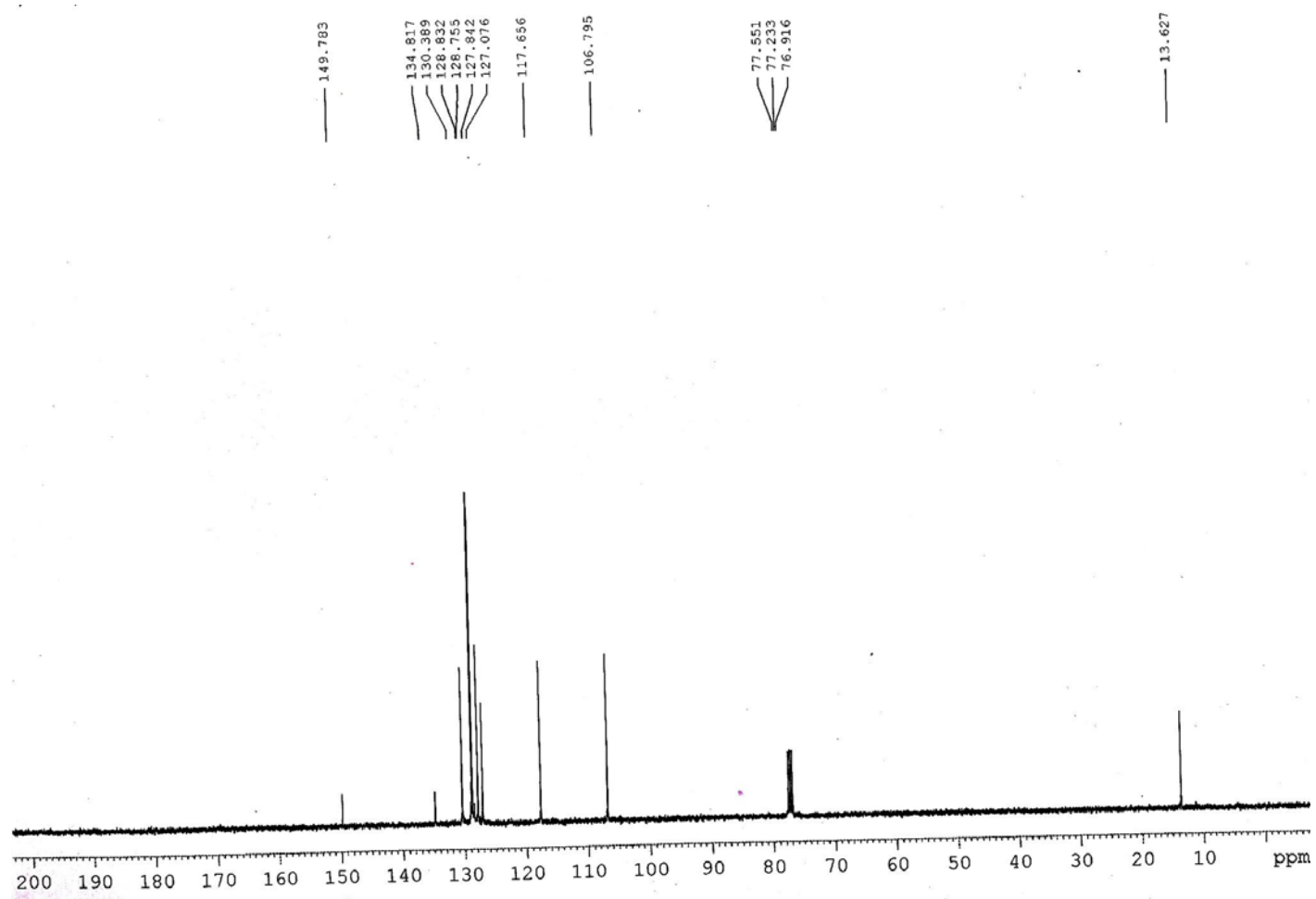


Figure S19 ^{13}C NMR spectrum of **6i**

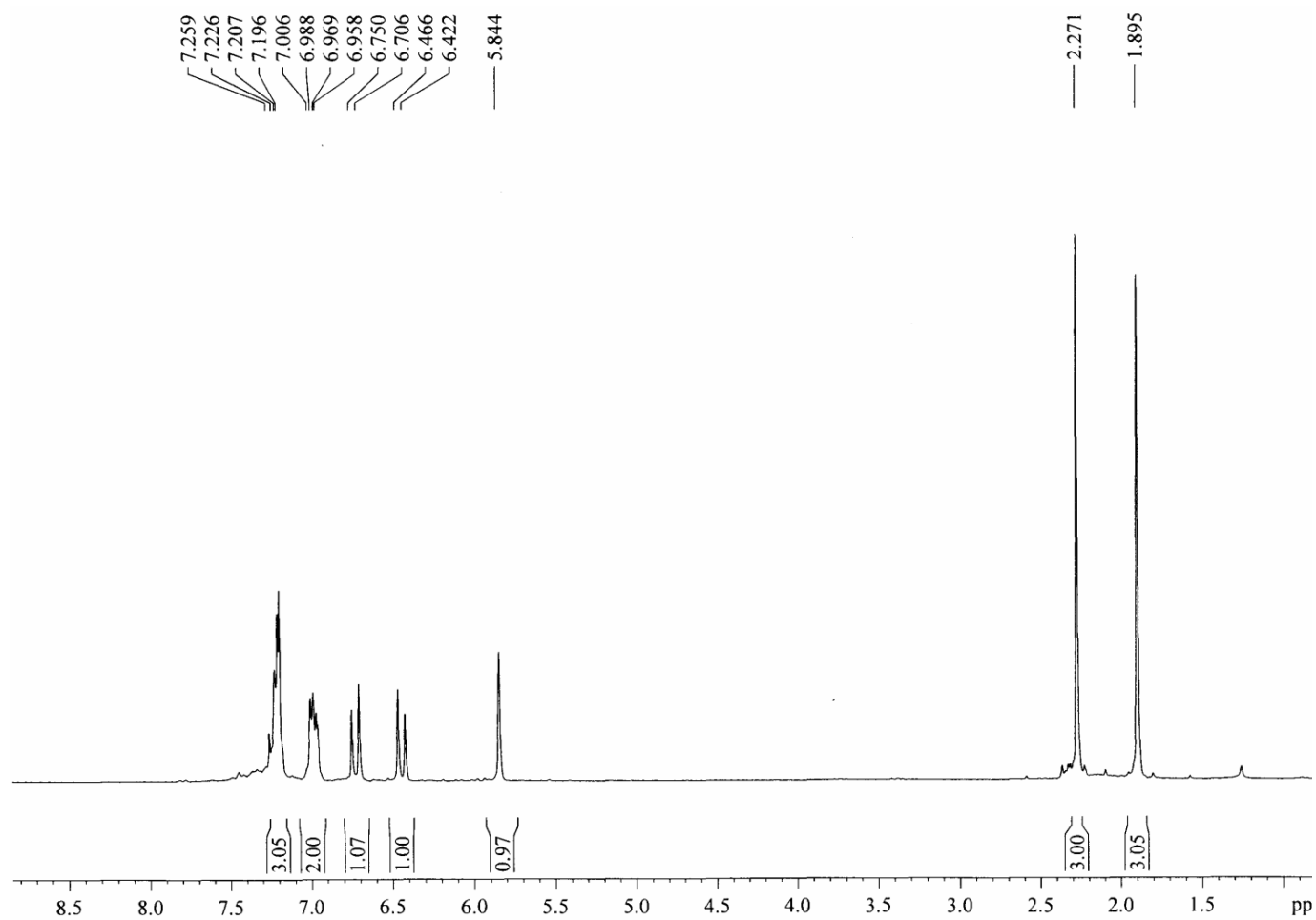


Figure S20 ¹H NMR spectrum of **6j**

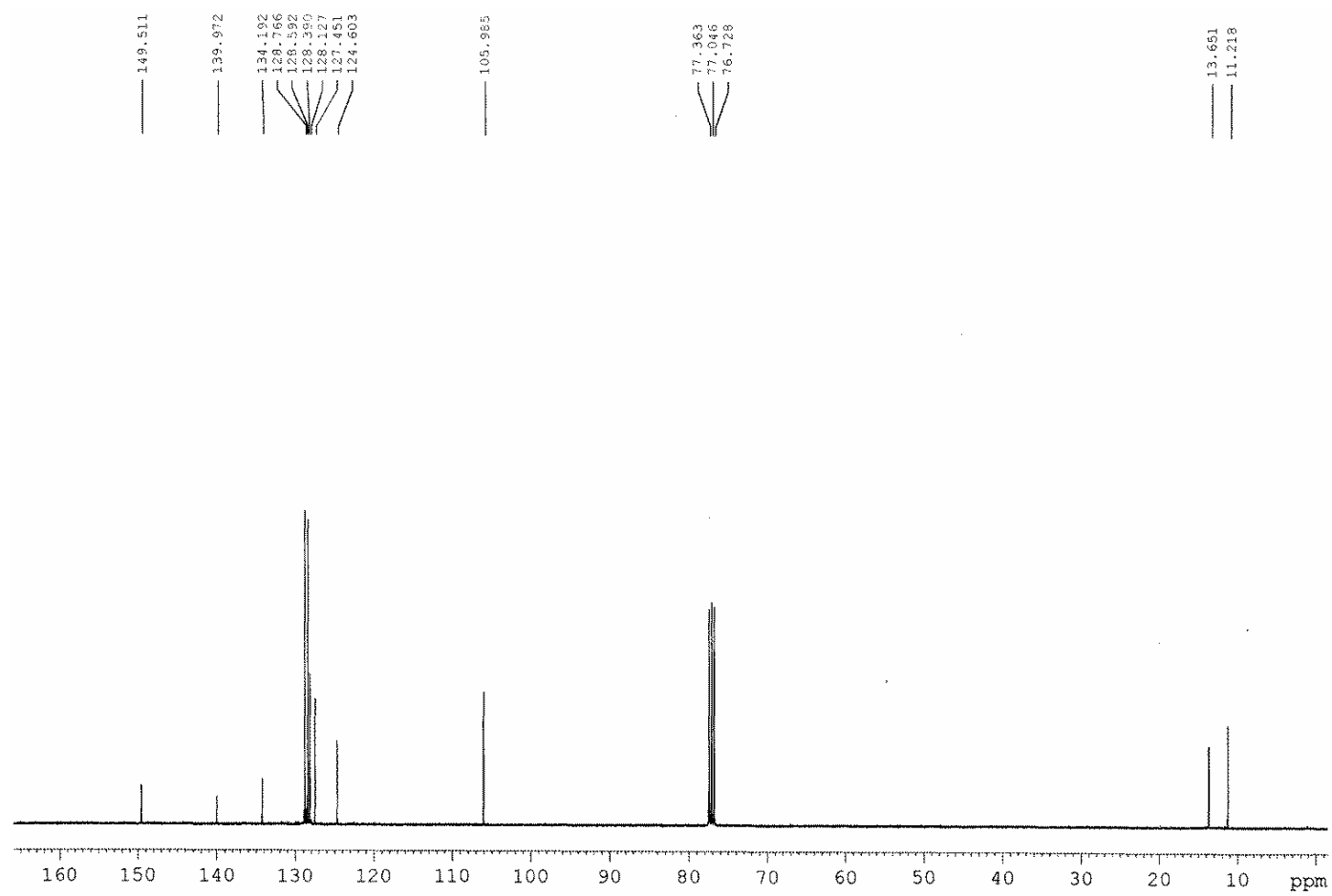


Figure S21 ¹³C NMR spectrum of **6j**

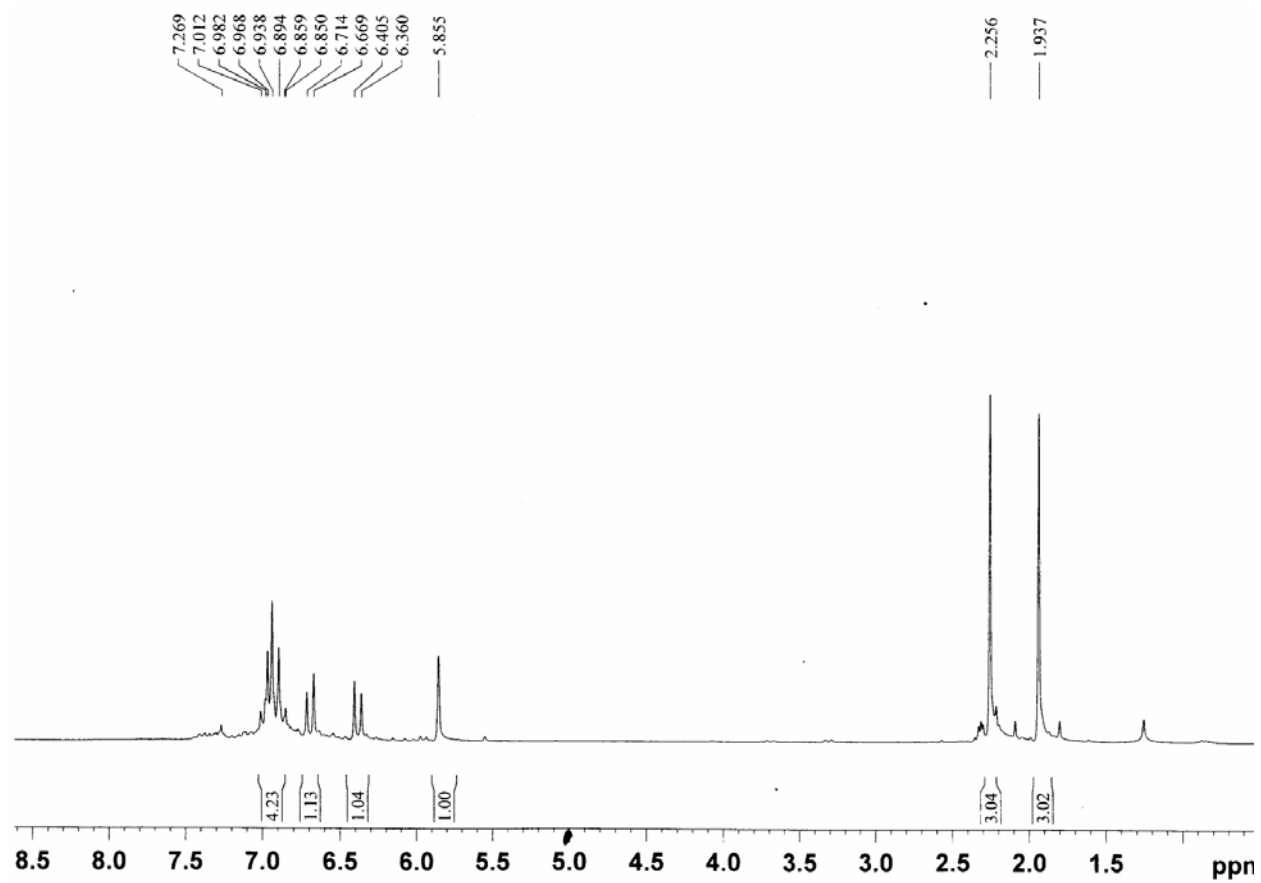


Figure S22 ^1H NMR spectrum of **6k**

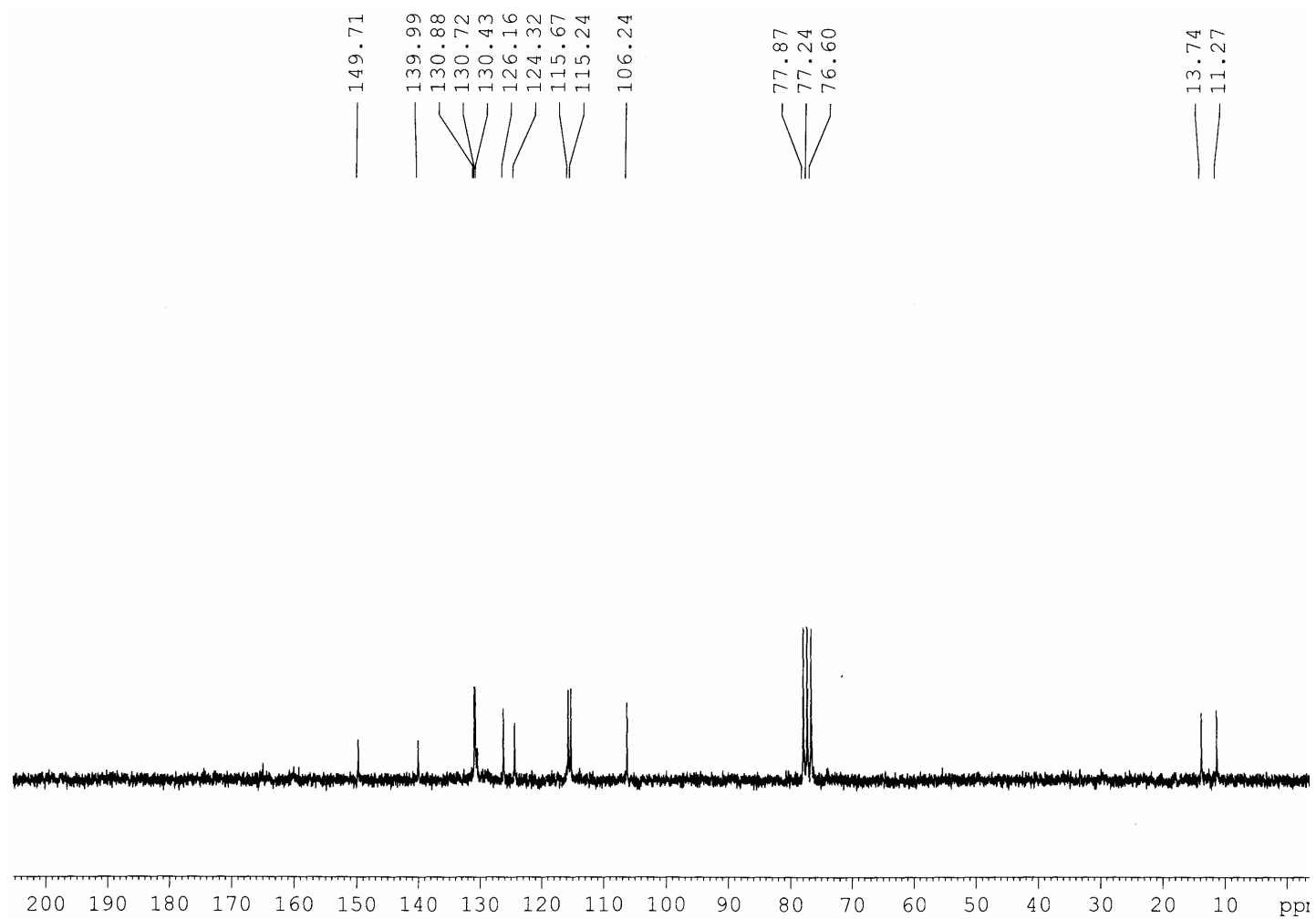


Figure S23 ¹³C NMR spectrum of **6k**

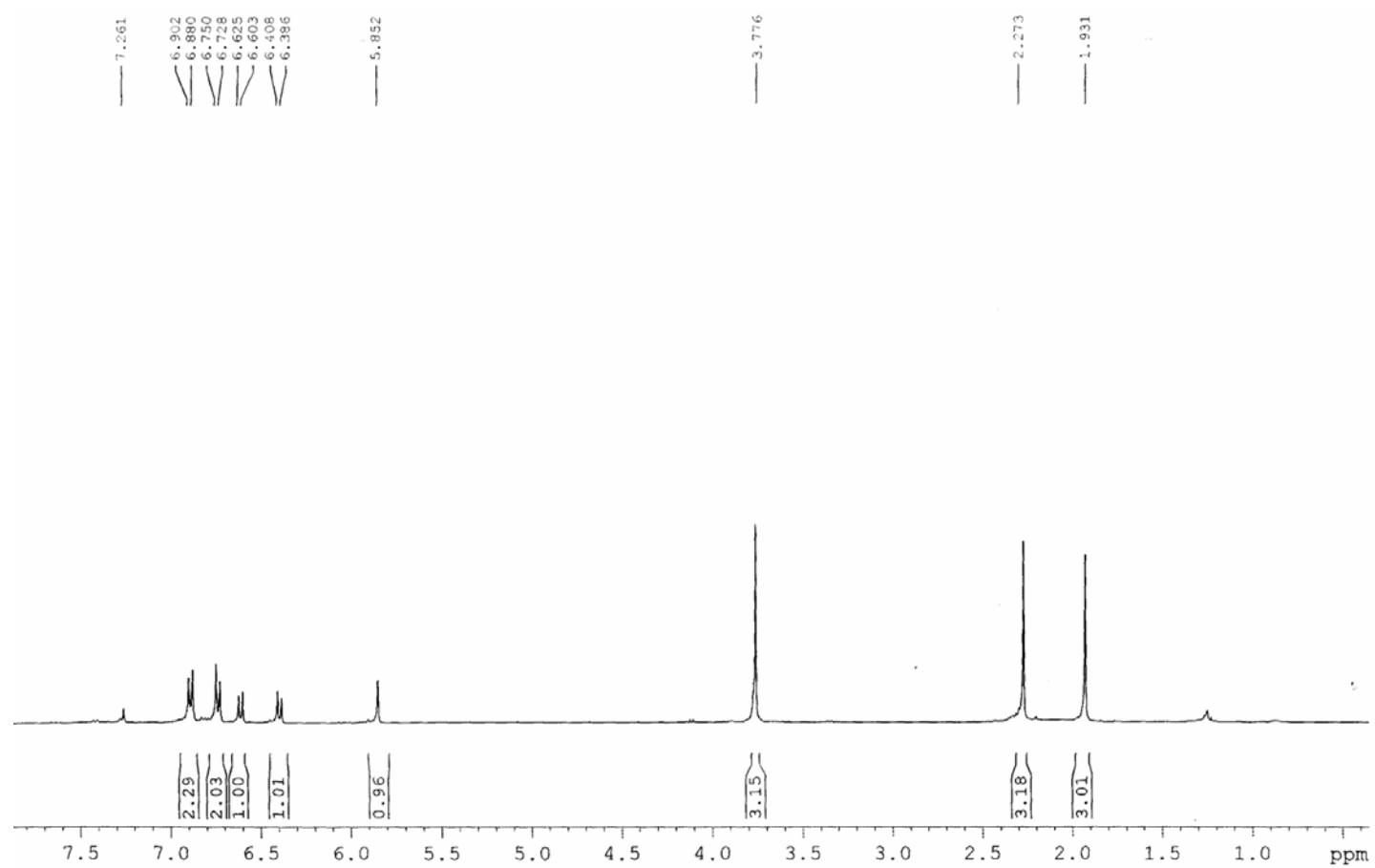


Figure S24 ¹H NMR spectrum of **6l**

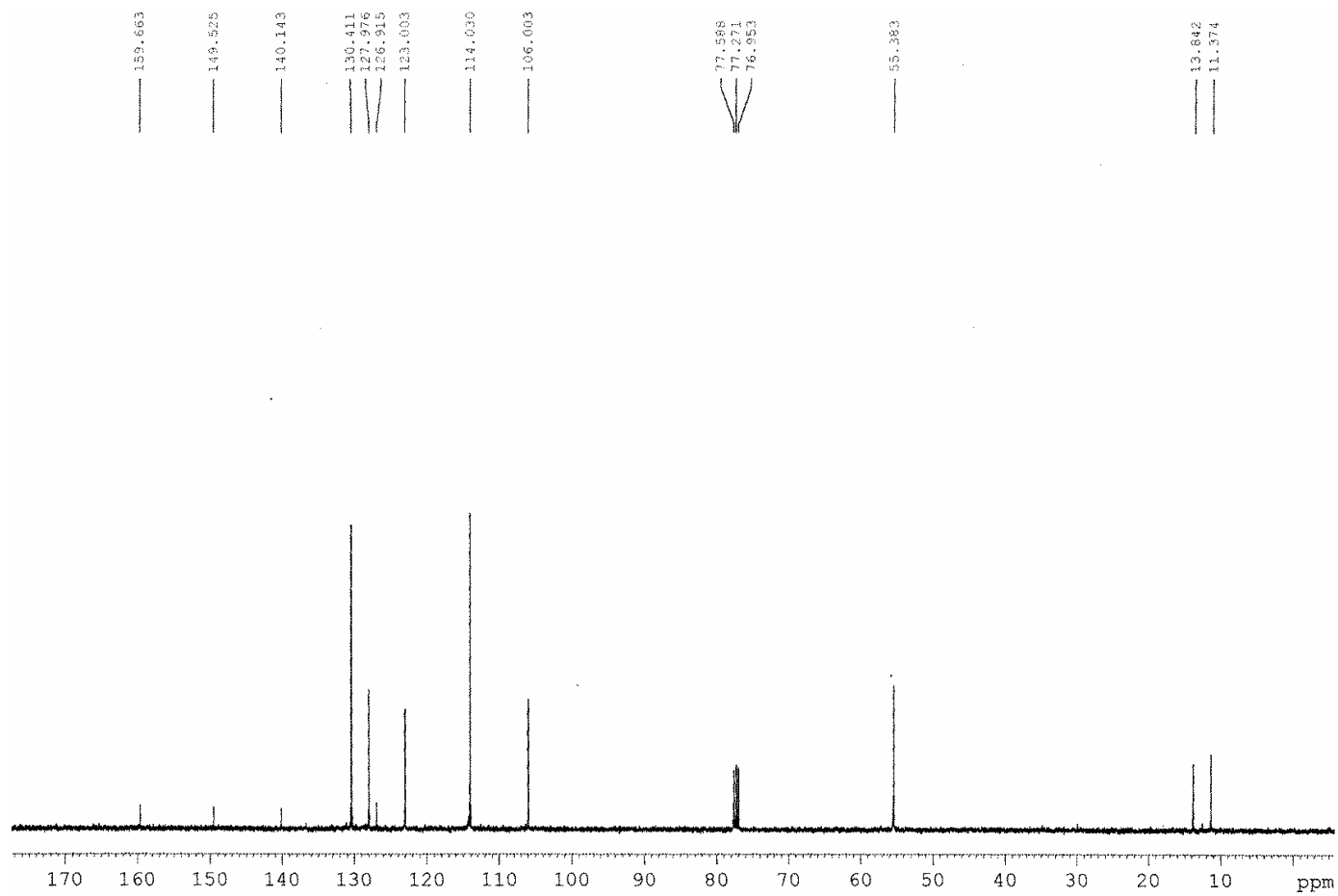


Figure S25 ¹³C NMR spectrum of **6l**

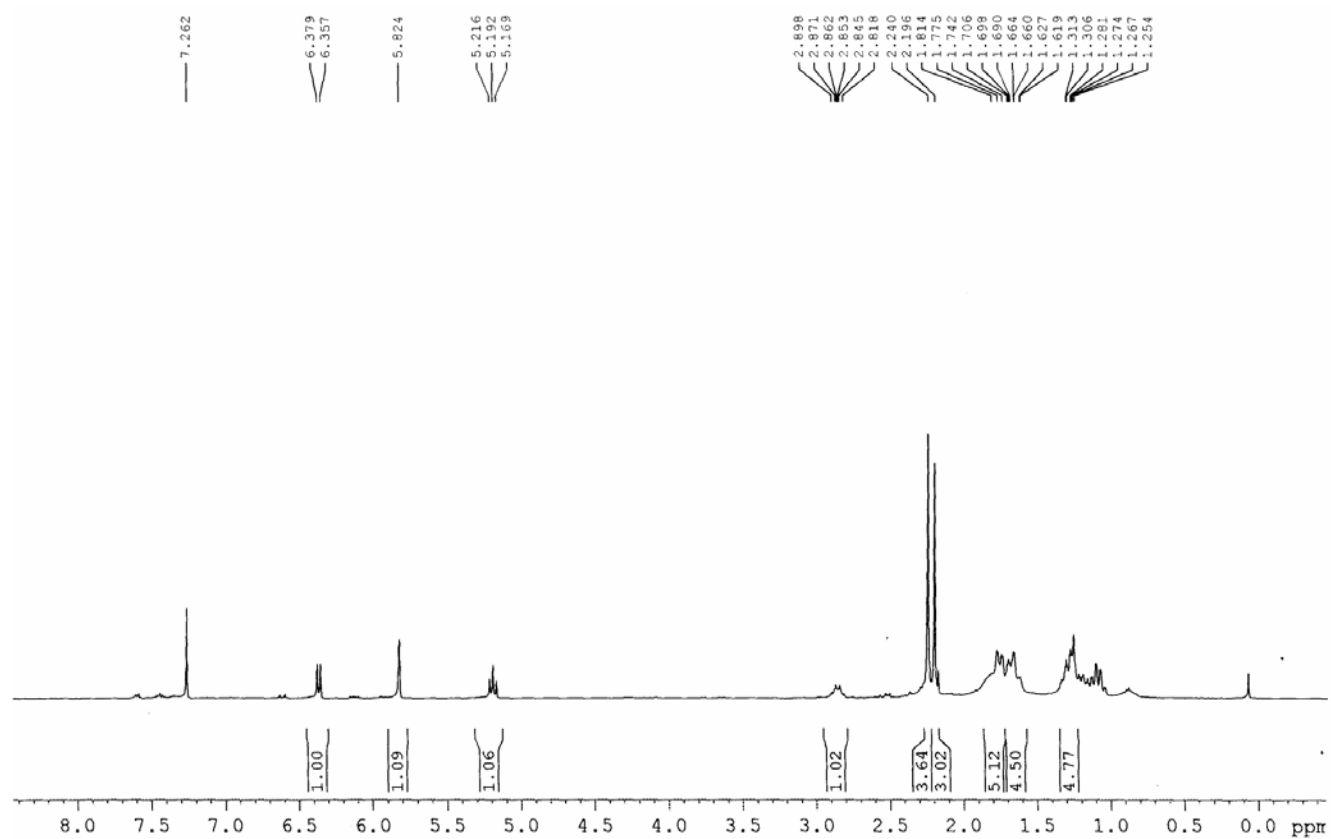


Figure S26 ^1H NMR spectrum of **6m**

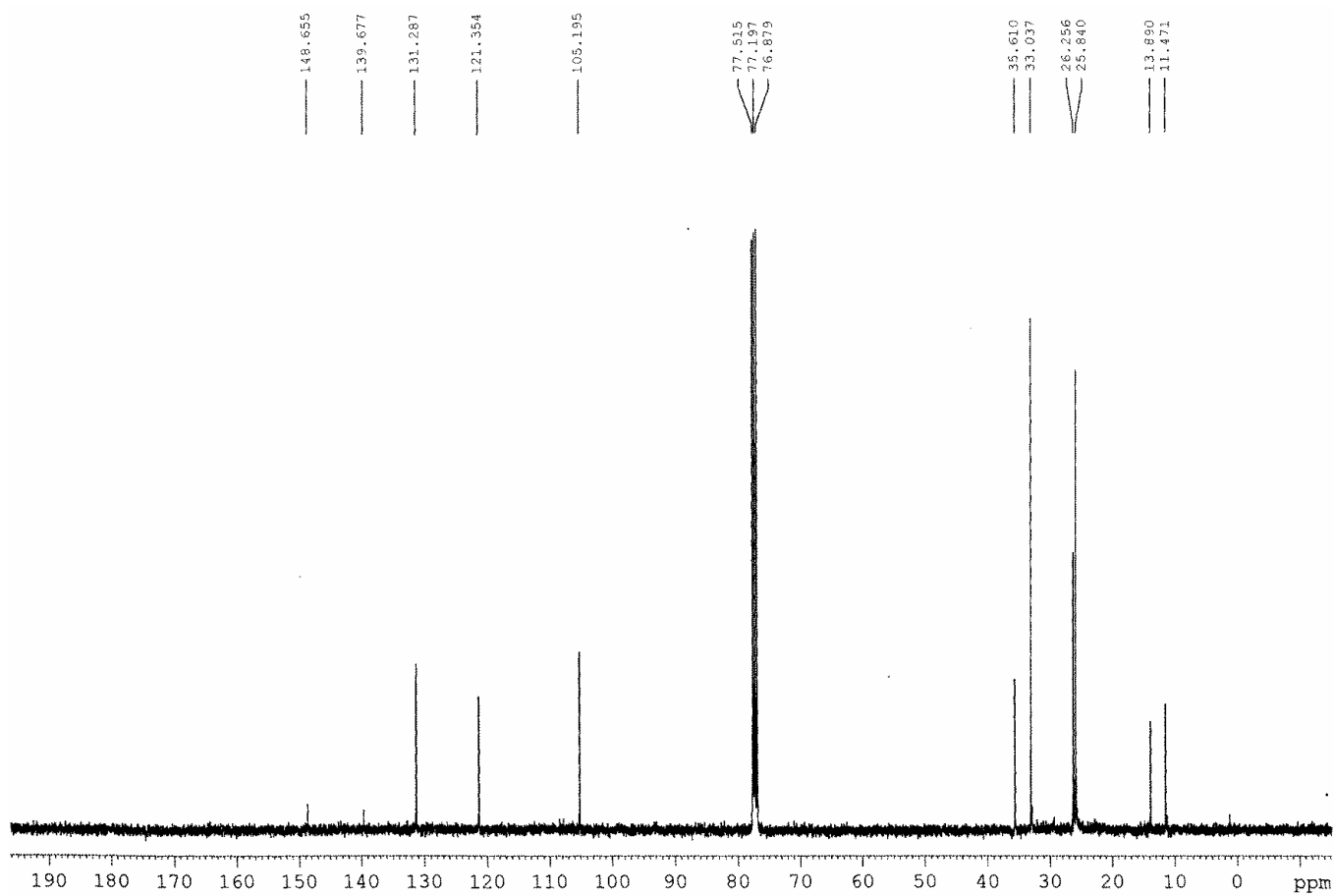


Figure S27 ¹³C NMR spectrum of **6m**

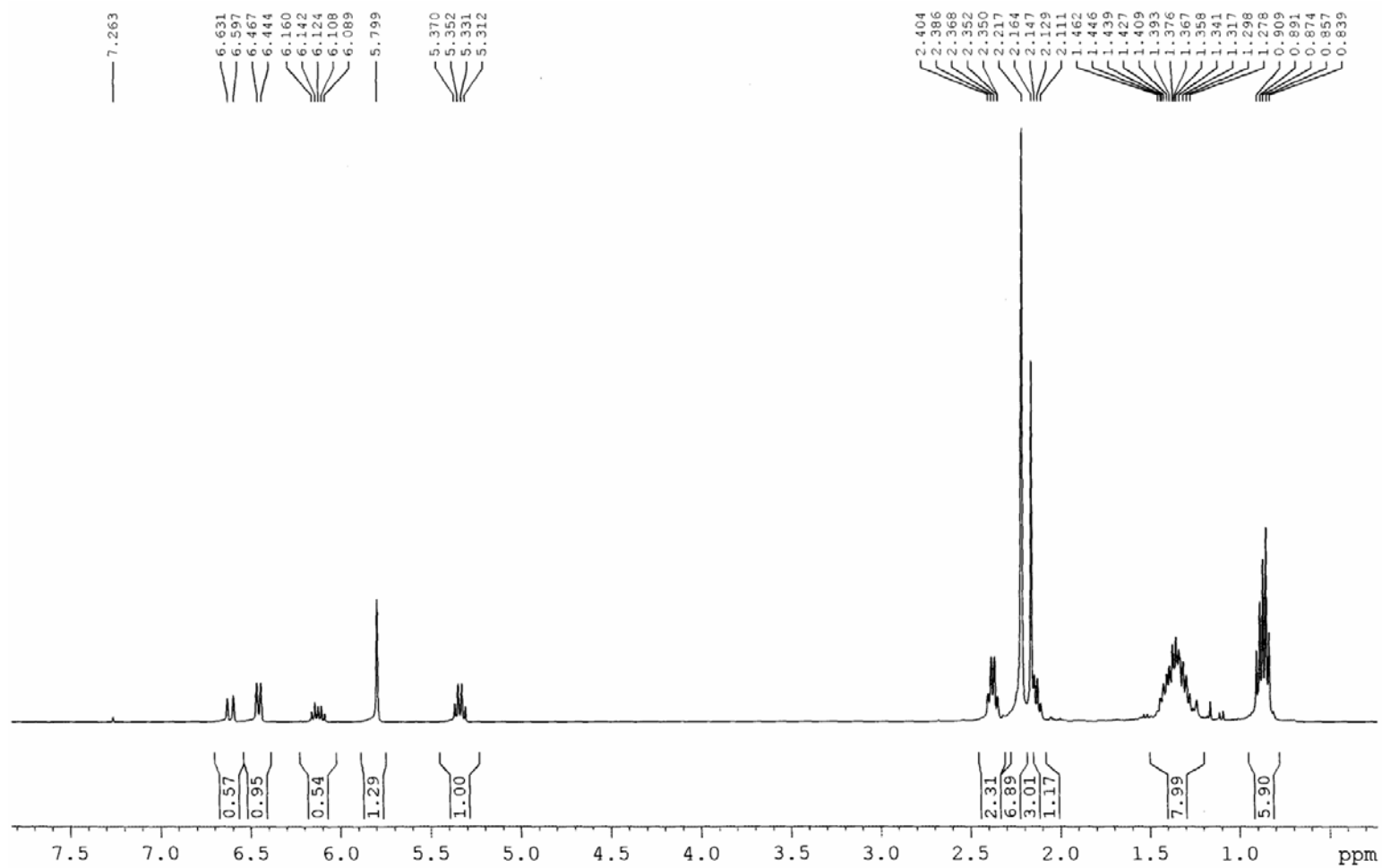


Figure S28 ^1H NMR spectrum of **6n**

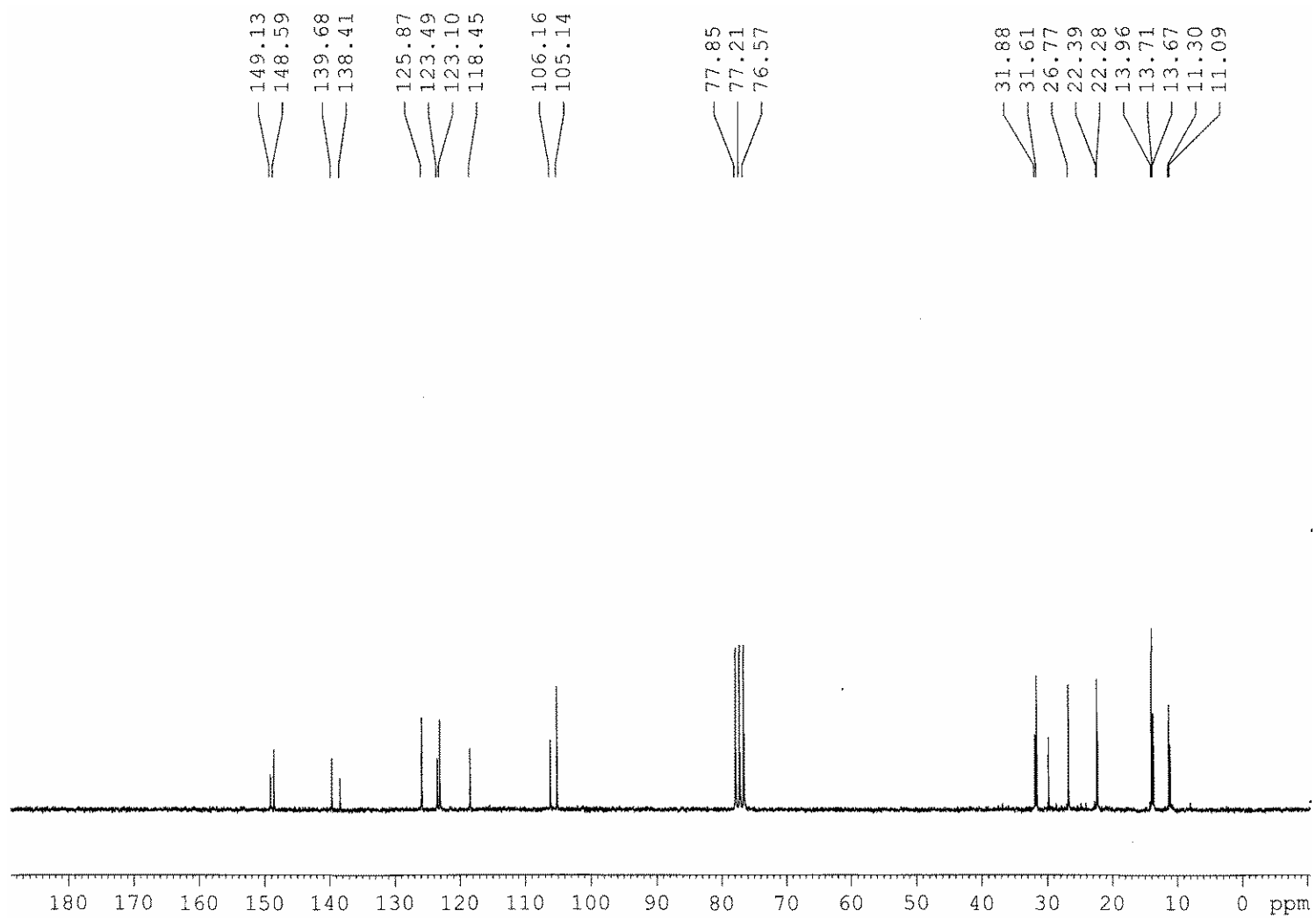


Figure S29 ¹³C NMR spectrum of **6n**

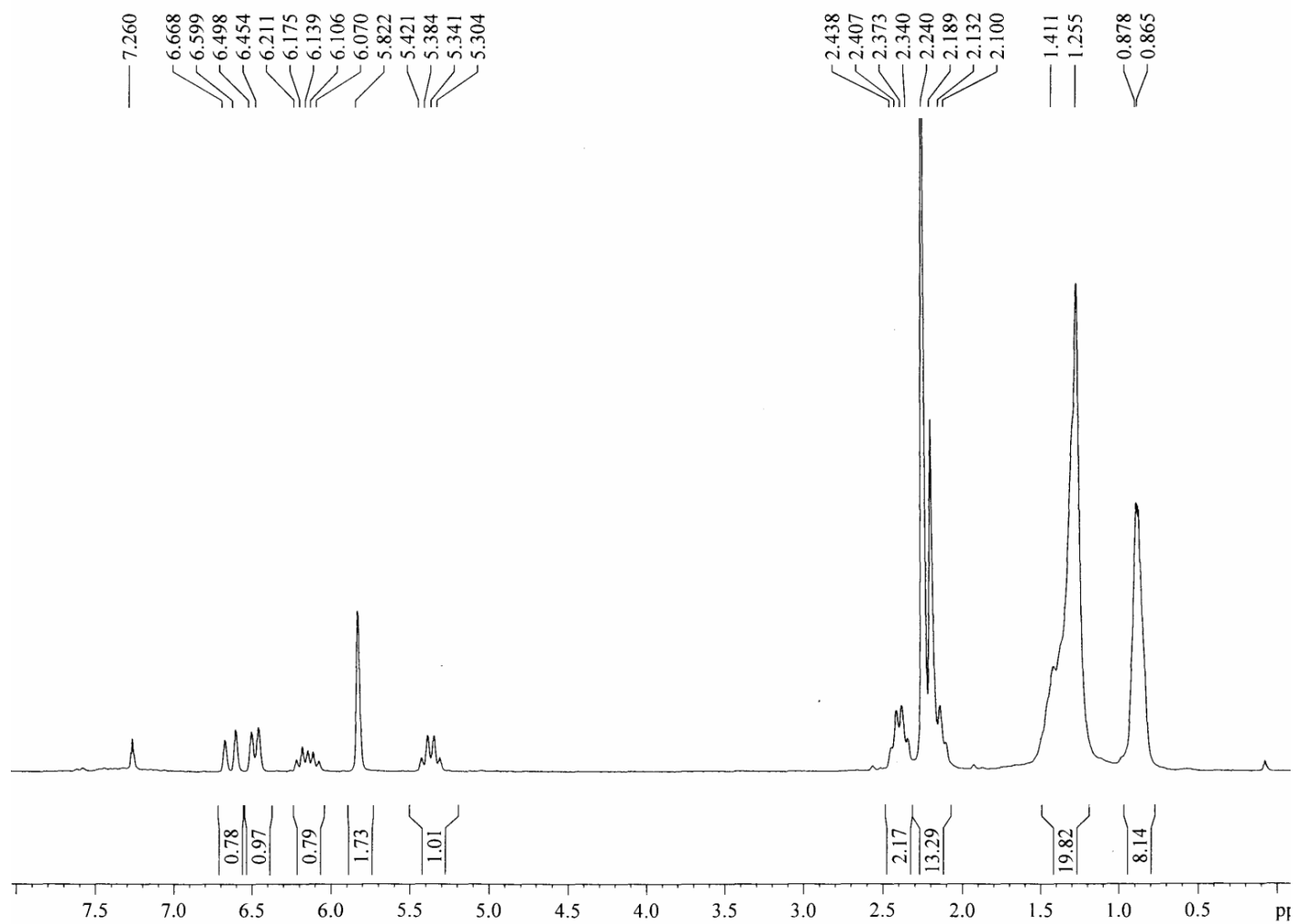


Figure S30 ¹H NMR spectrum of **6o**

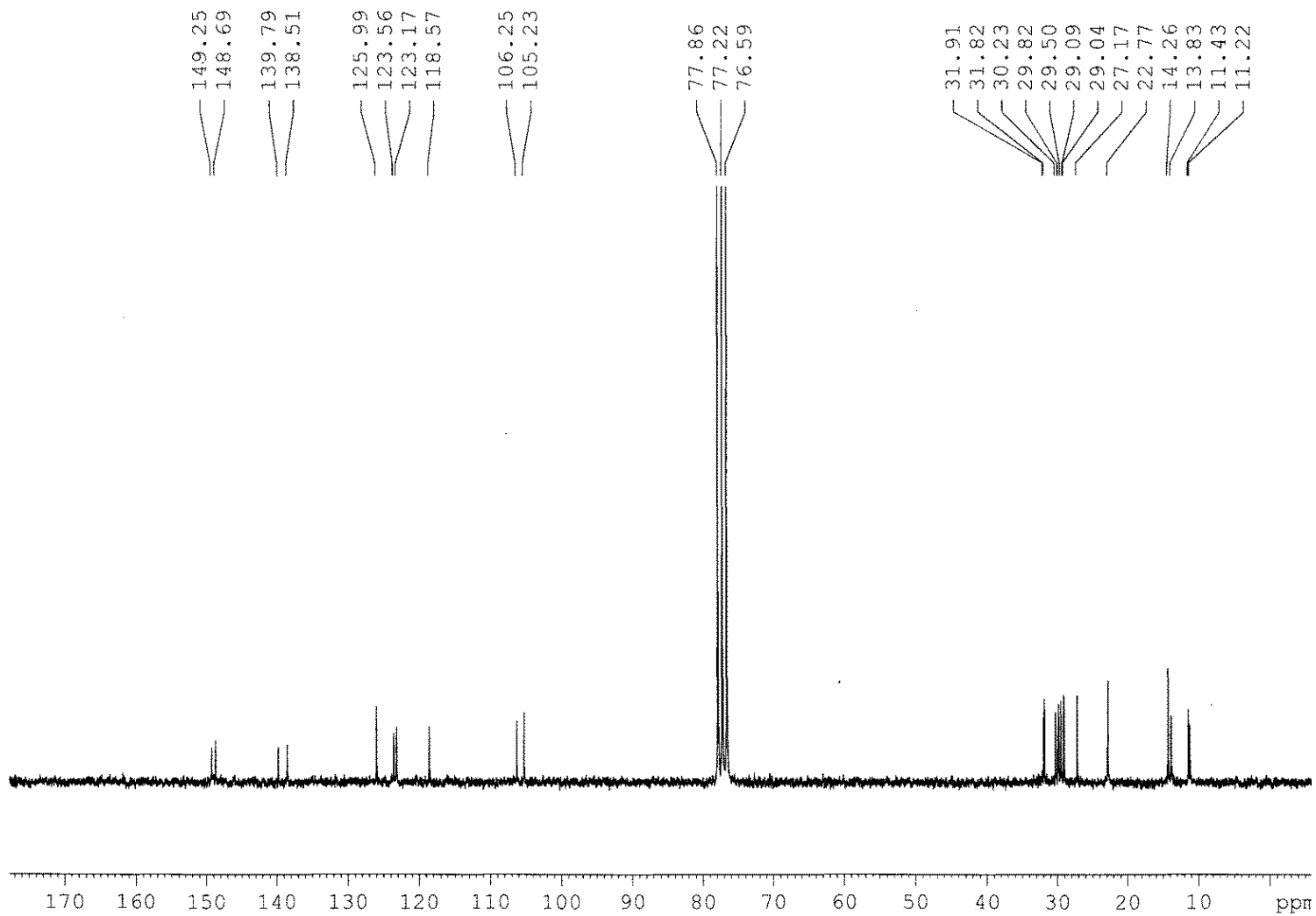


Figure S31 ¹³C NMR spectrum of **6o**

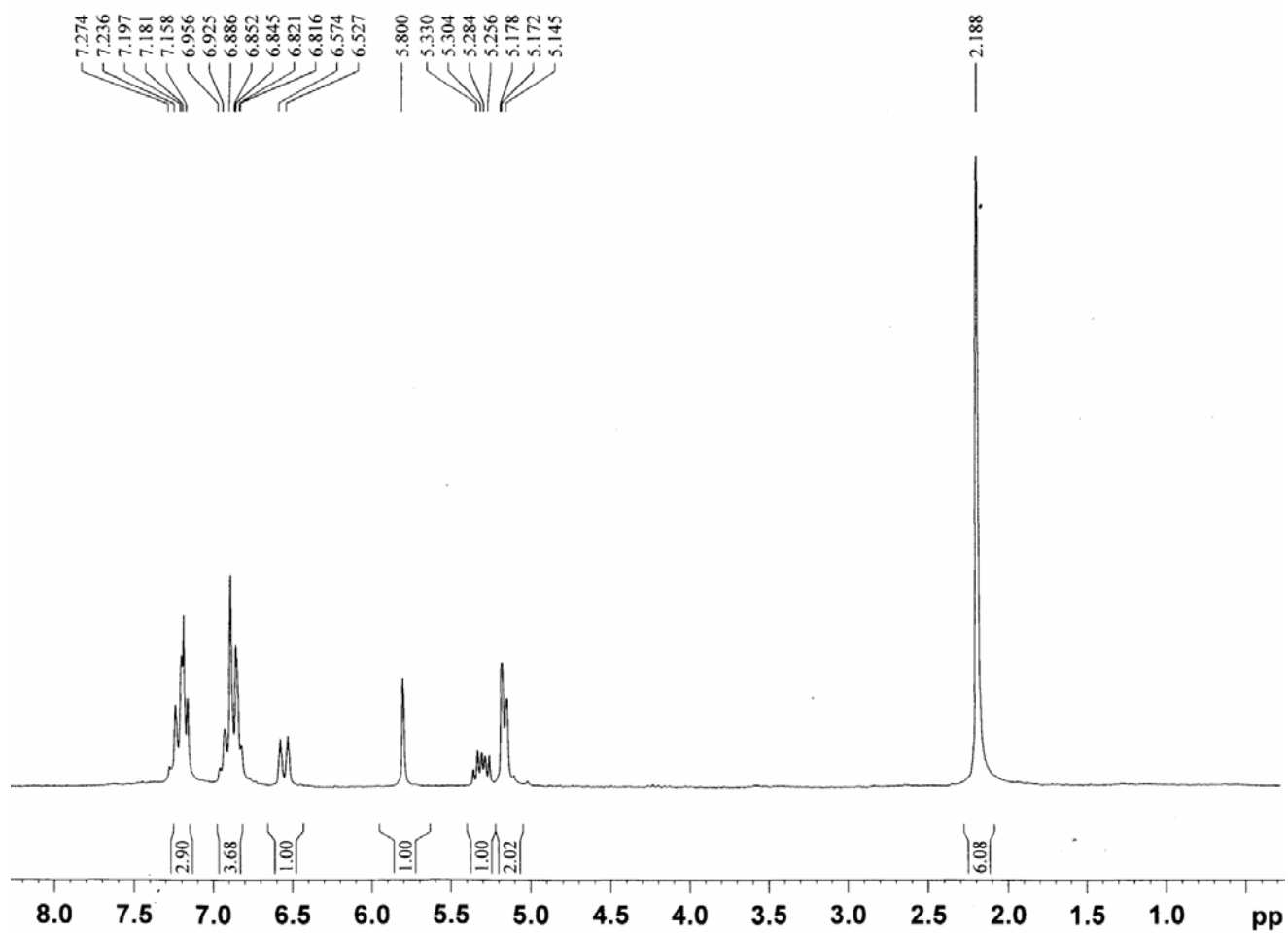


Figure S32 ¹H NMR spectrum of **6p**

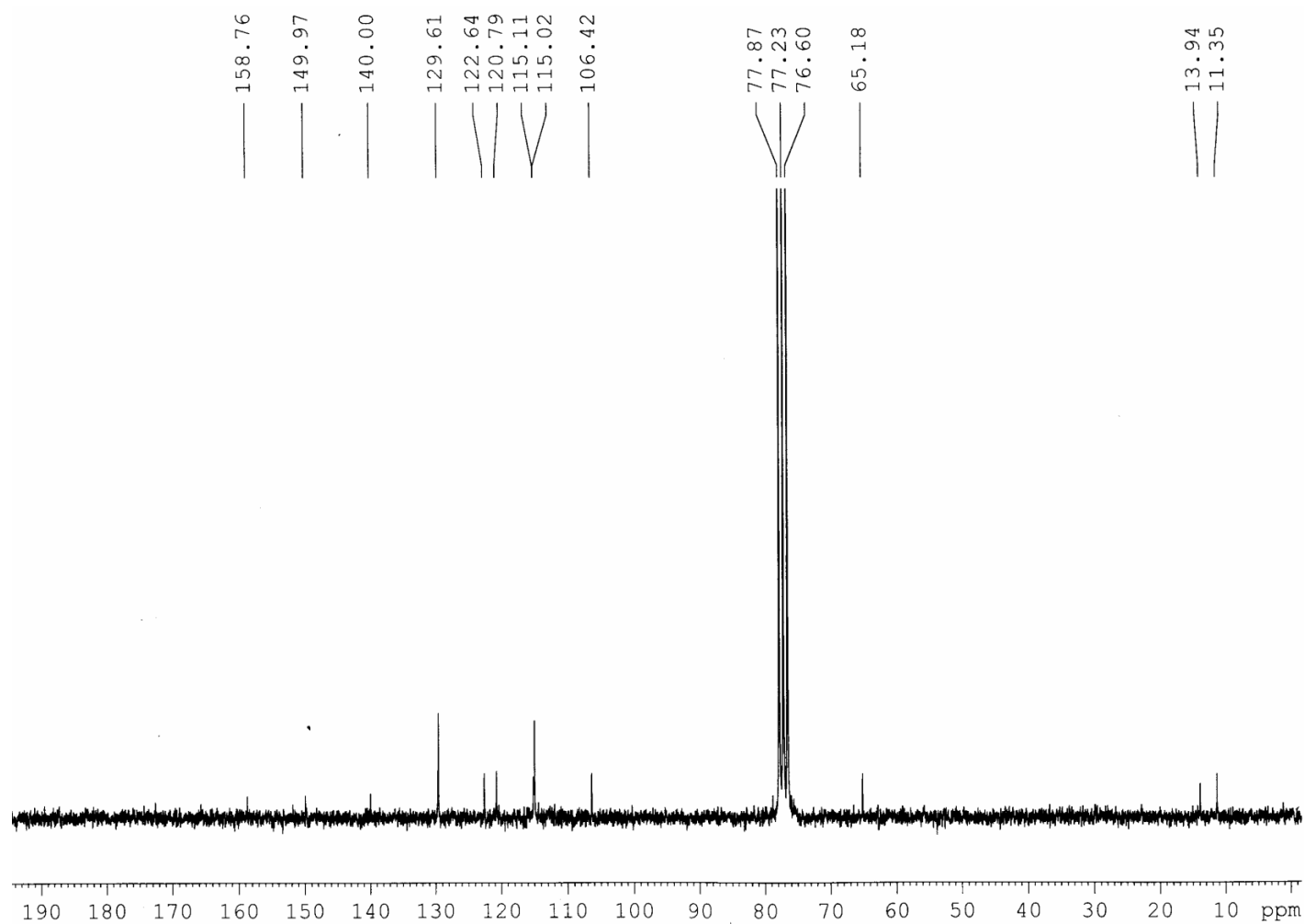


Figure S33 ¹³C NMR spectrum of **6p**

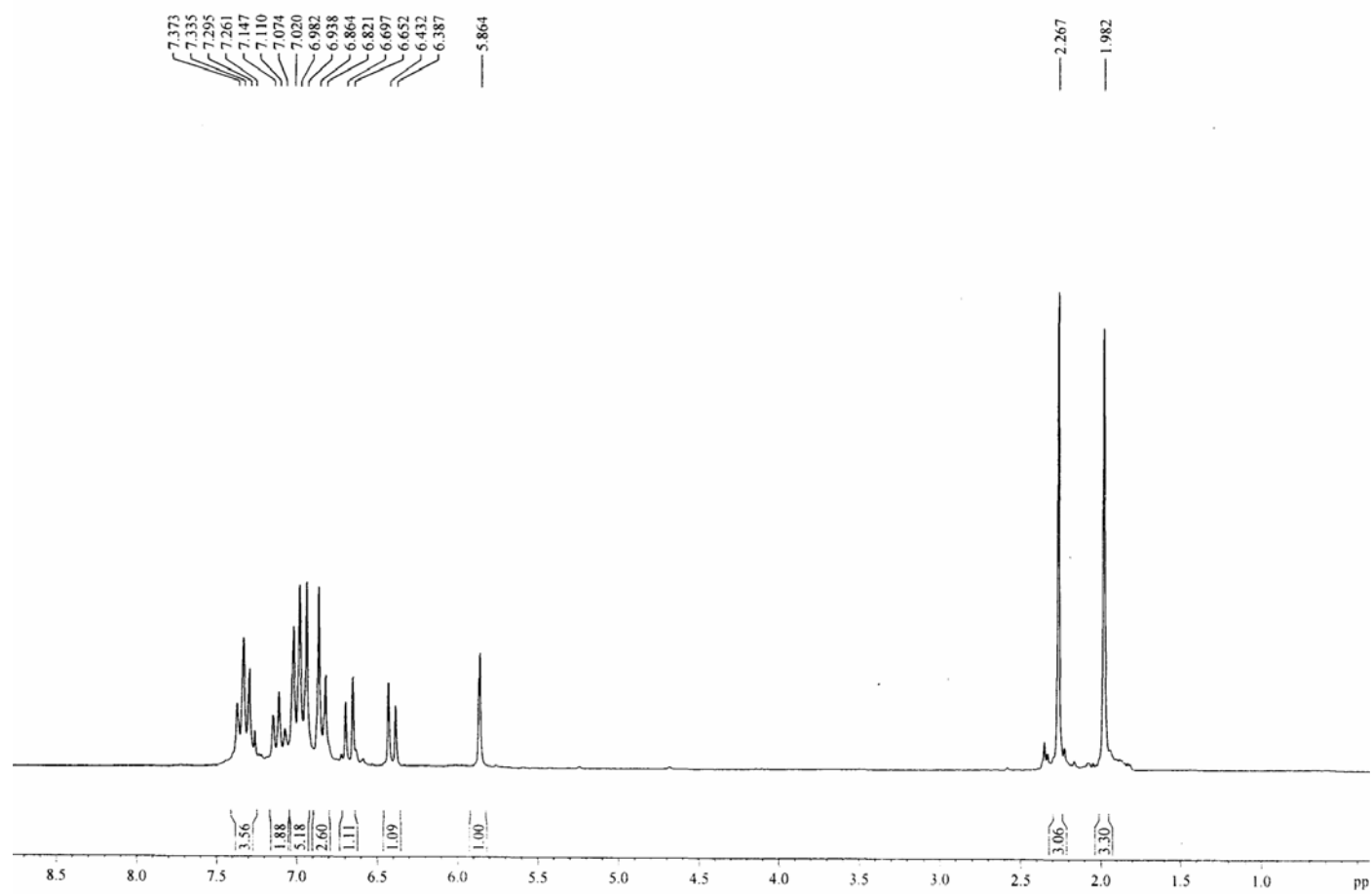


Figure S34 ¹H NMR spectrum of **6q**

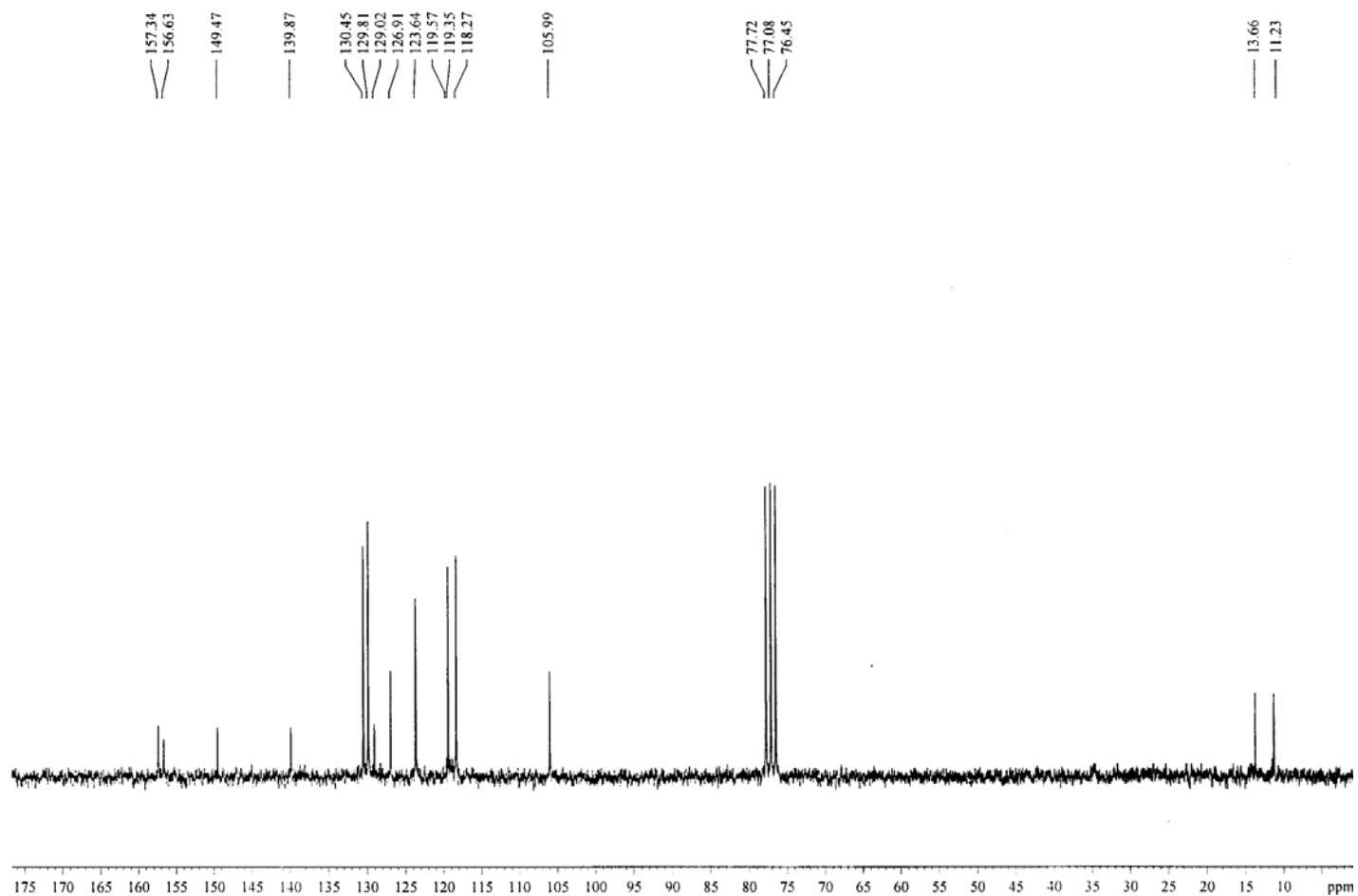


Figure S35 ¹³C NMR spectrum of **6q**

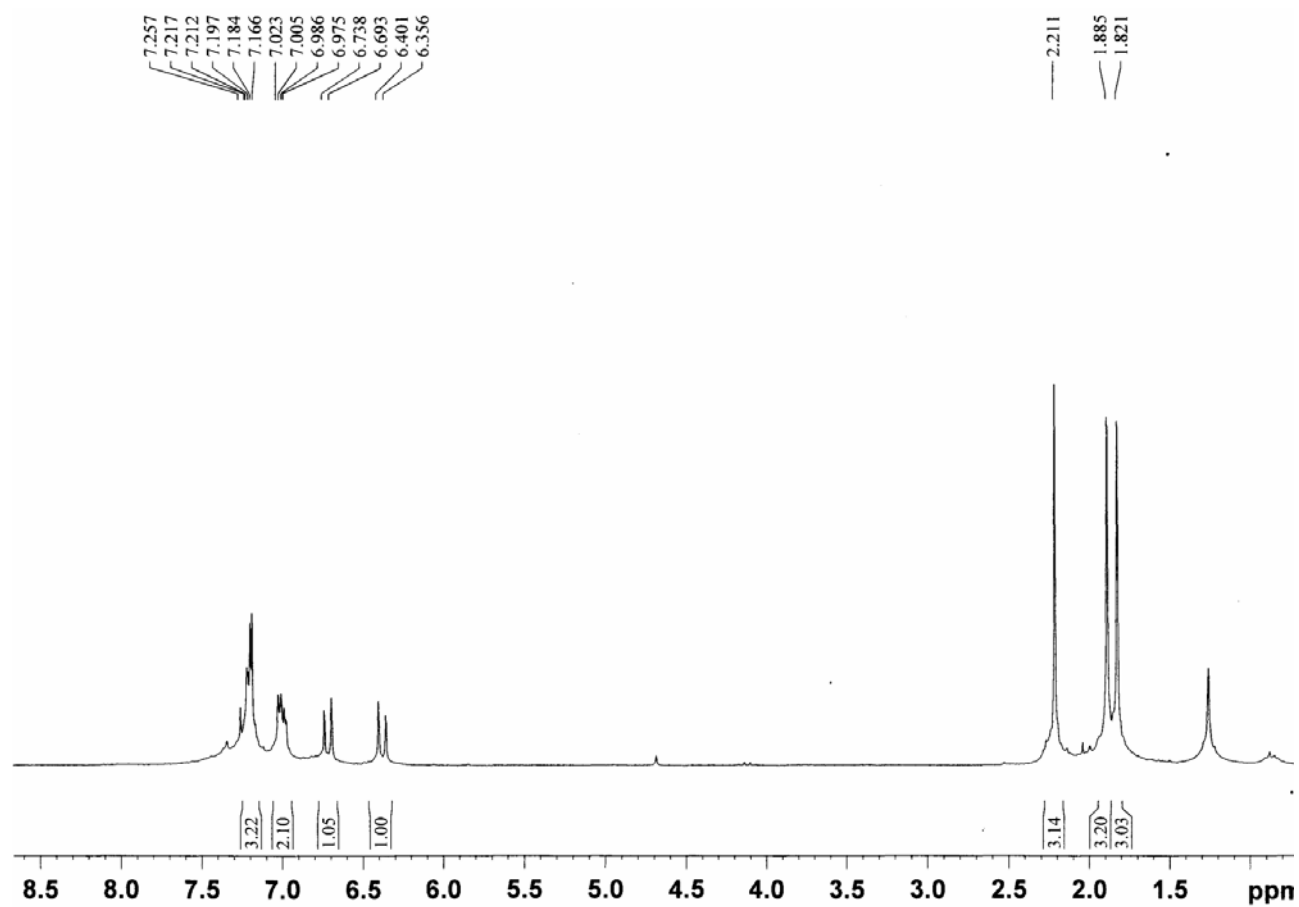


Figure S36 ¹H NMR spectrum of **6r**

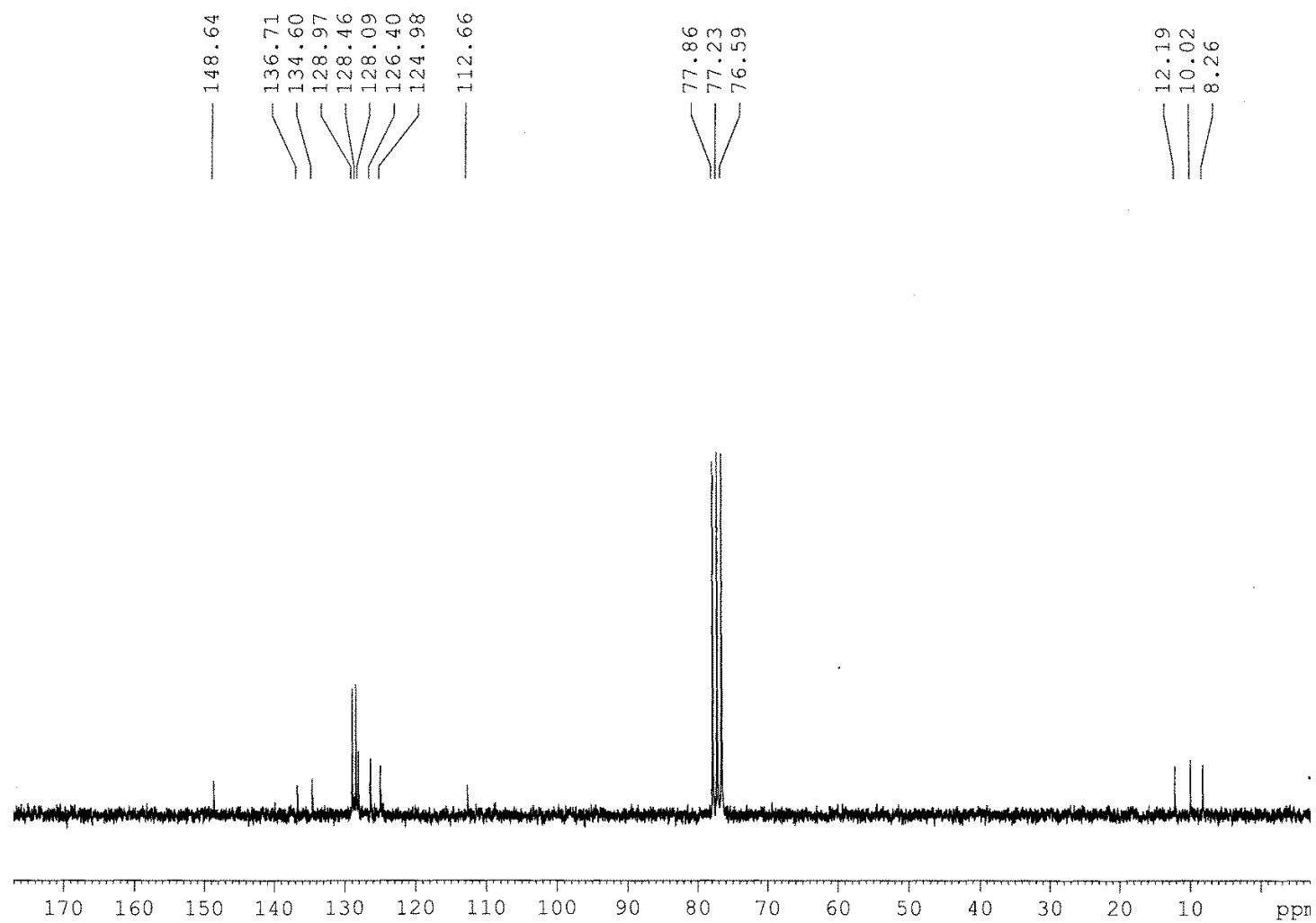


Figure S37 ¹³C NMR spectrum of **6r**

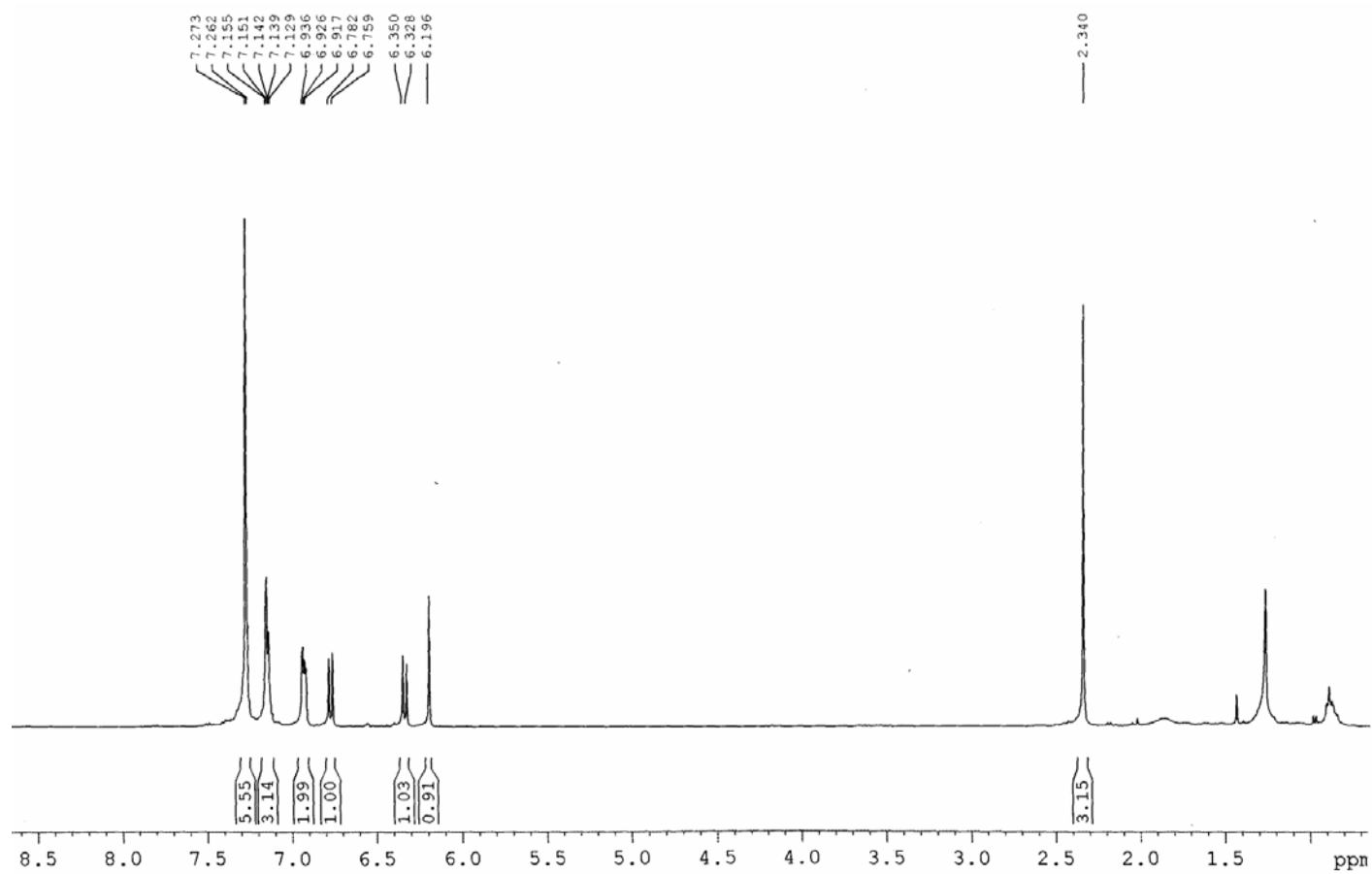


Figure S38 ^1H NMR spectrum of **6s**

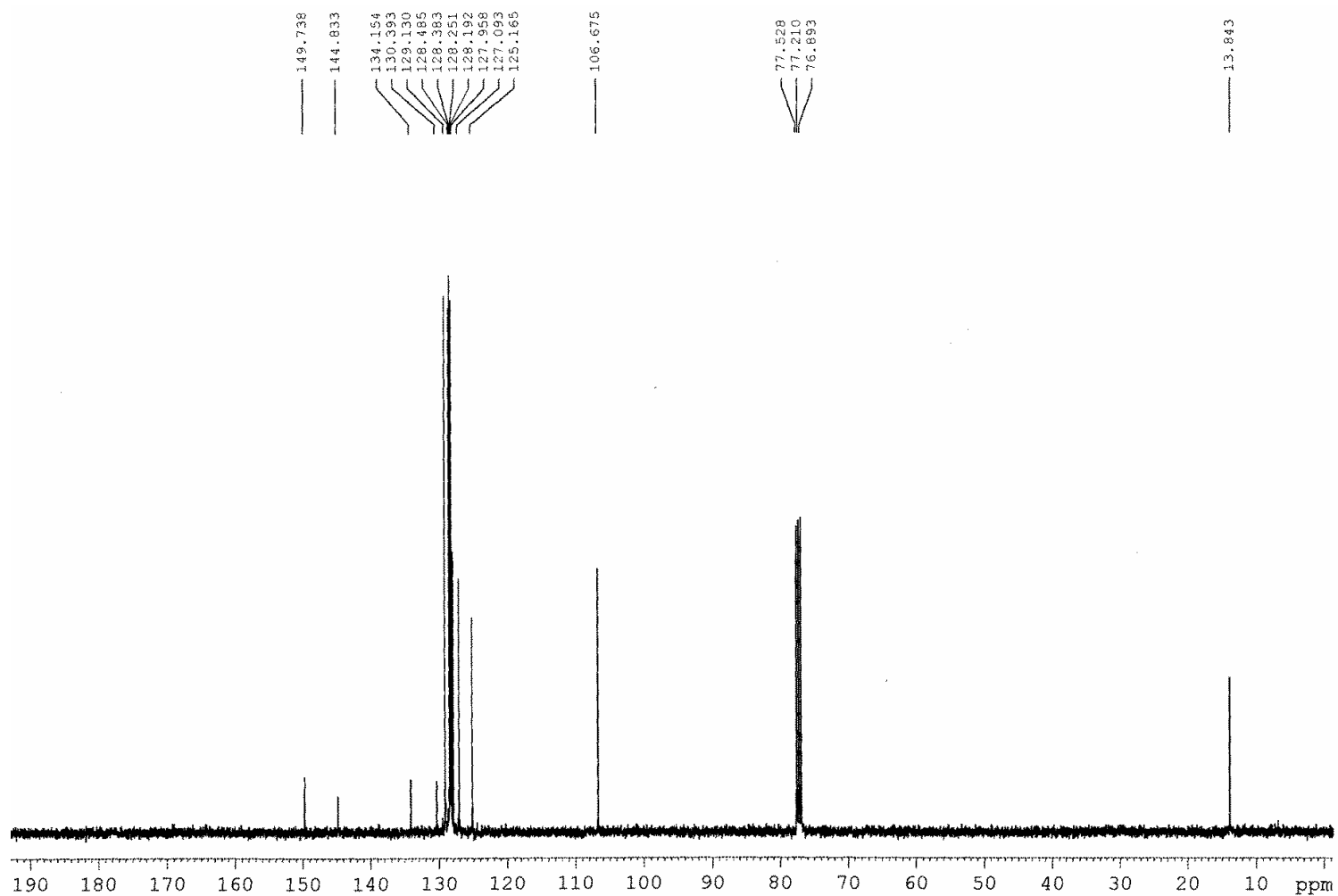


Figure S39 ¹³C NMR spectrum of 6s

mb / ukd / 859a

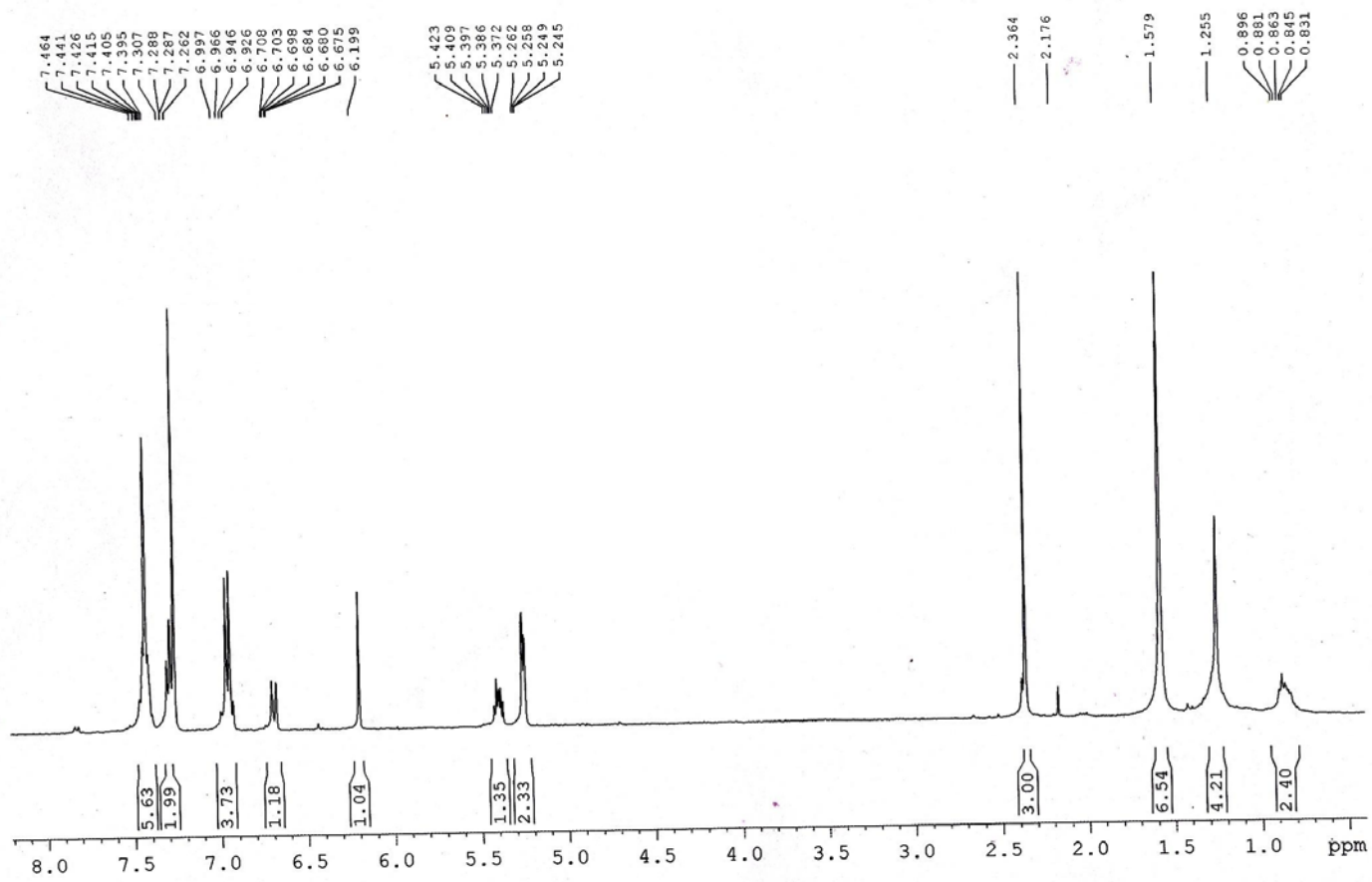


Figure S40 ¹H NMR spectrum of 6t

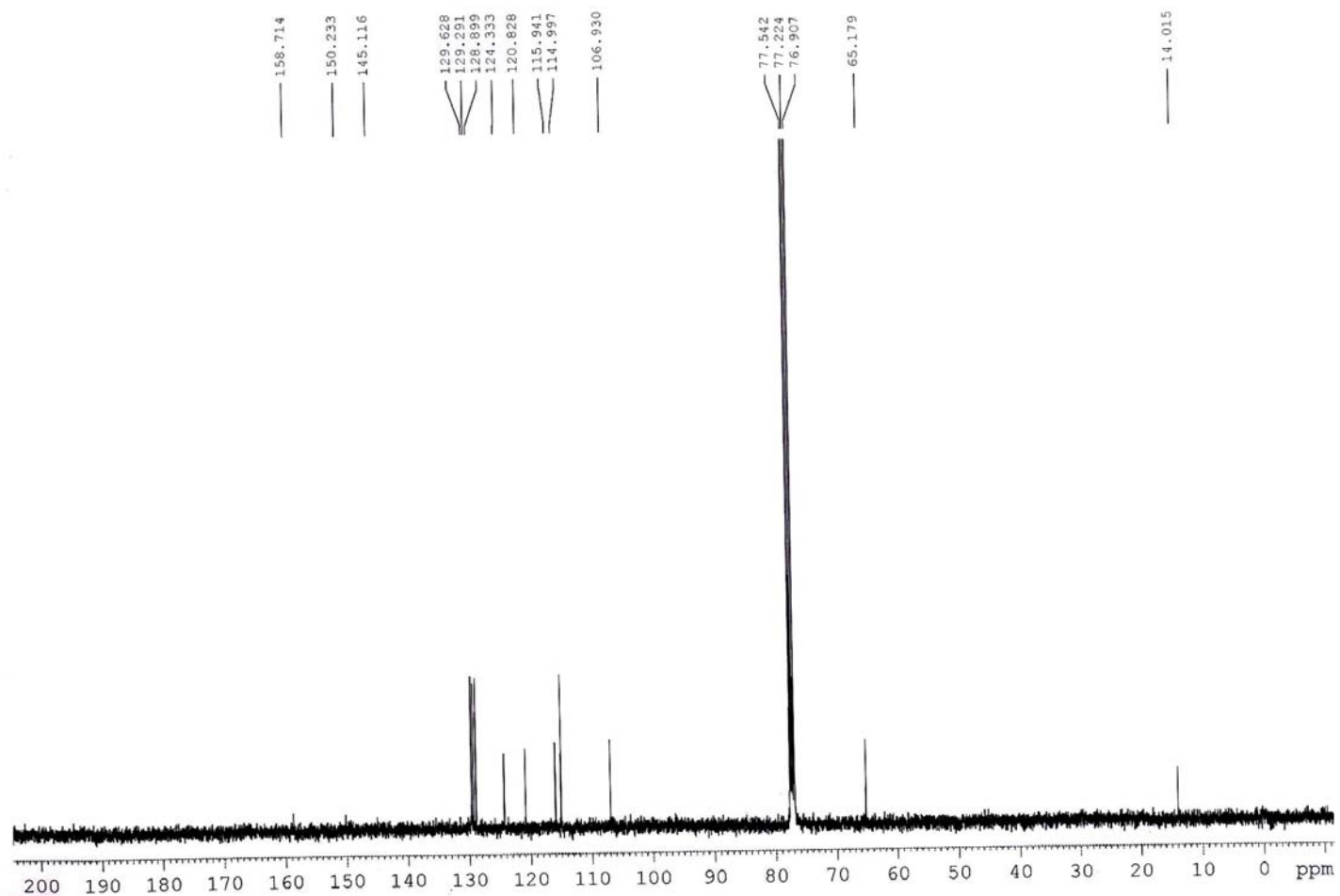


Figure S41 ¹³C NMR spectrum of **6t**

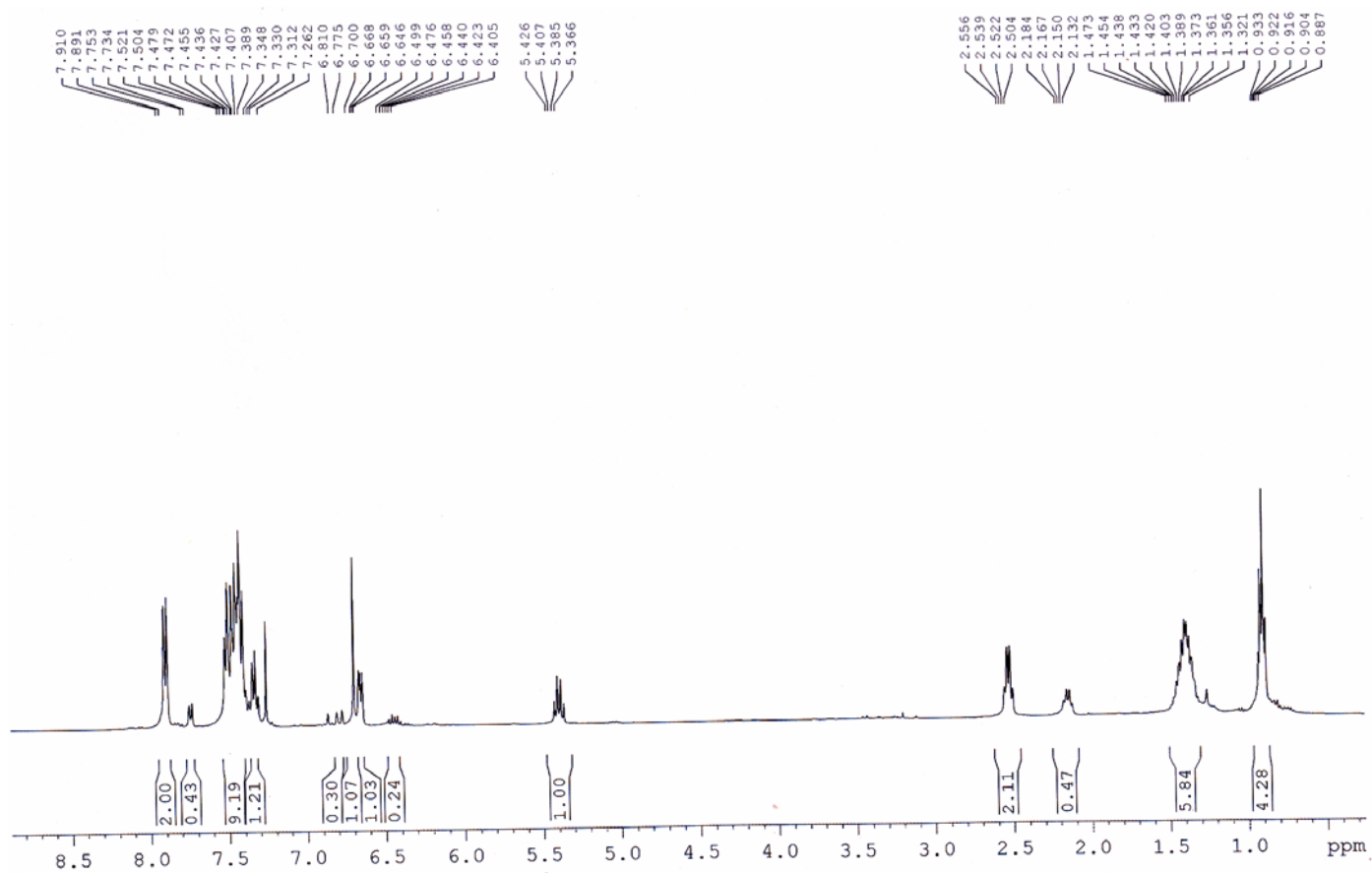


Figure S42 ^1H NMR spectrum of **6u**

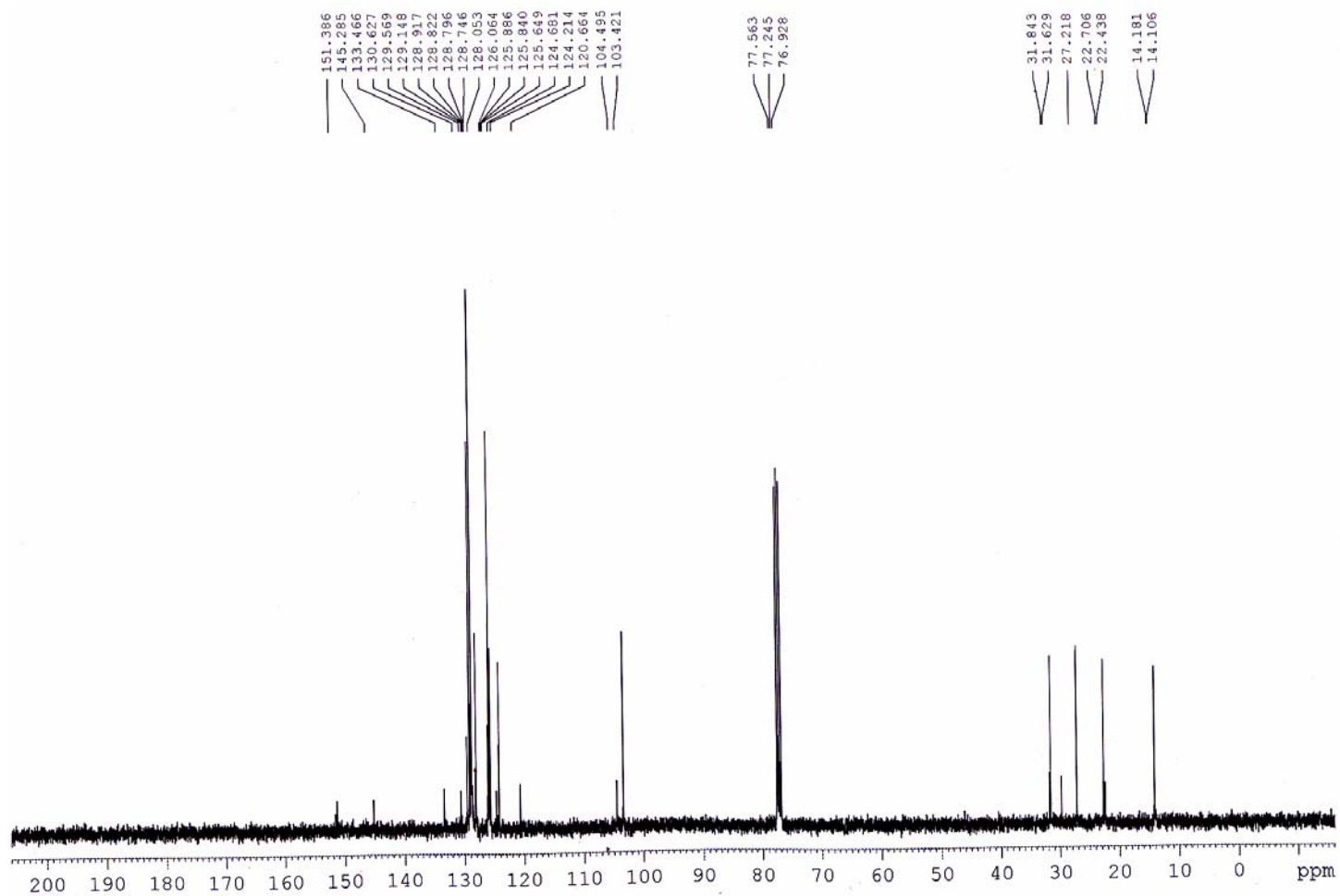


Figure S43 ^{13}C NMR spectrum of **6u**

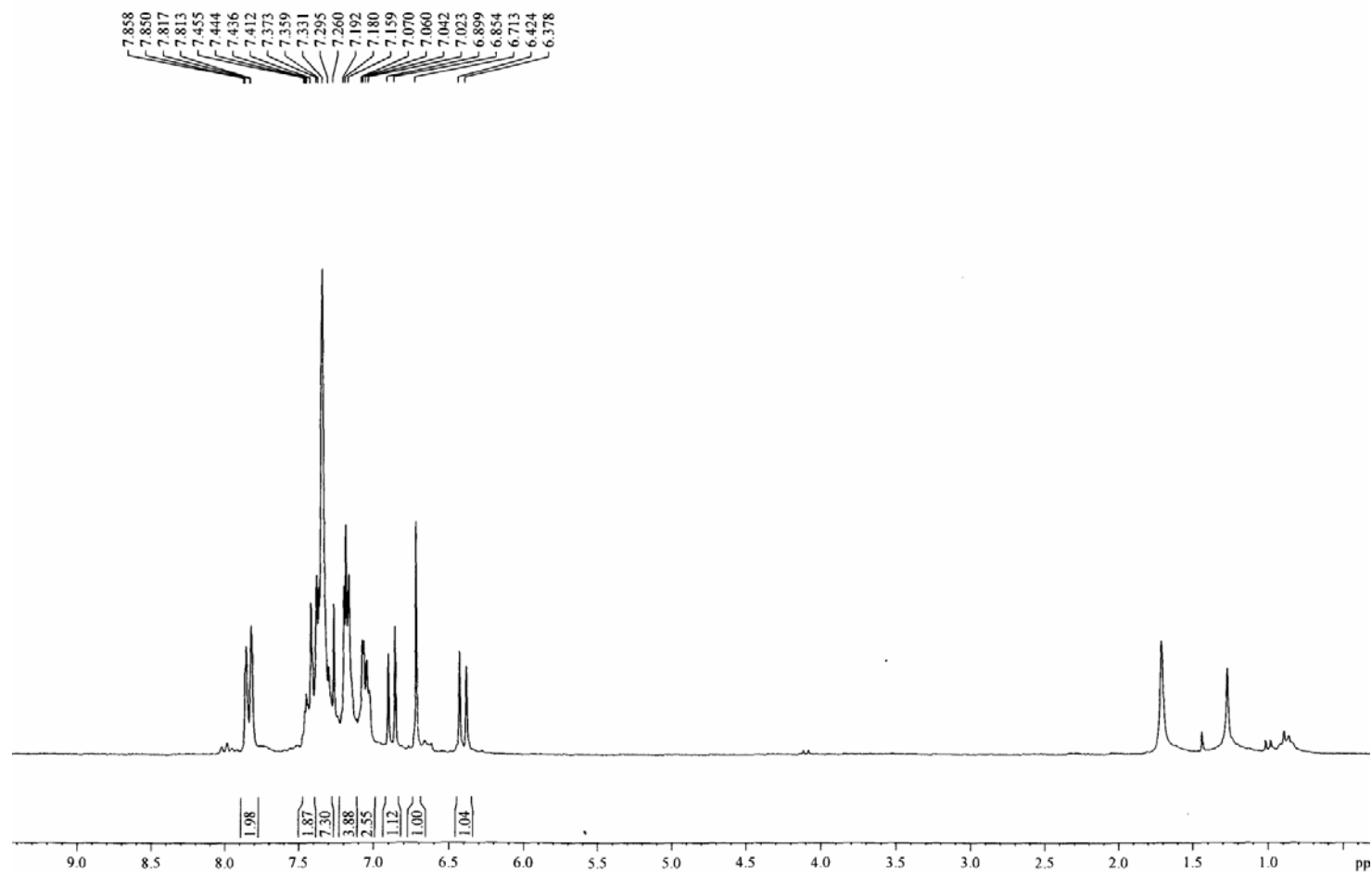


Figure S44 ¹H NMR spectrum of **6v**

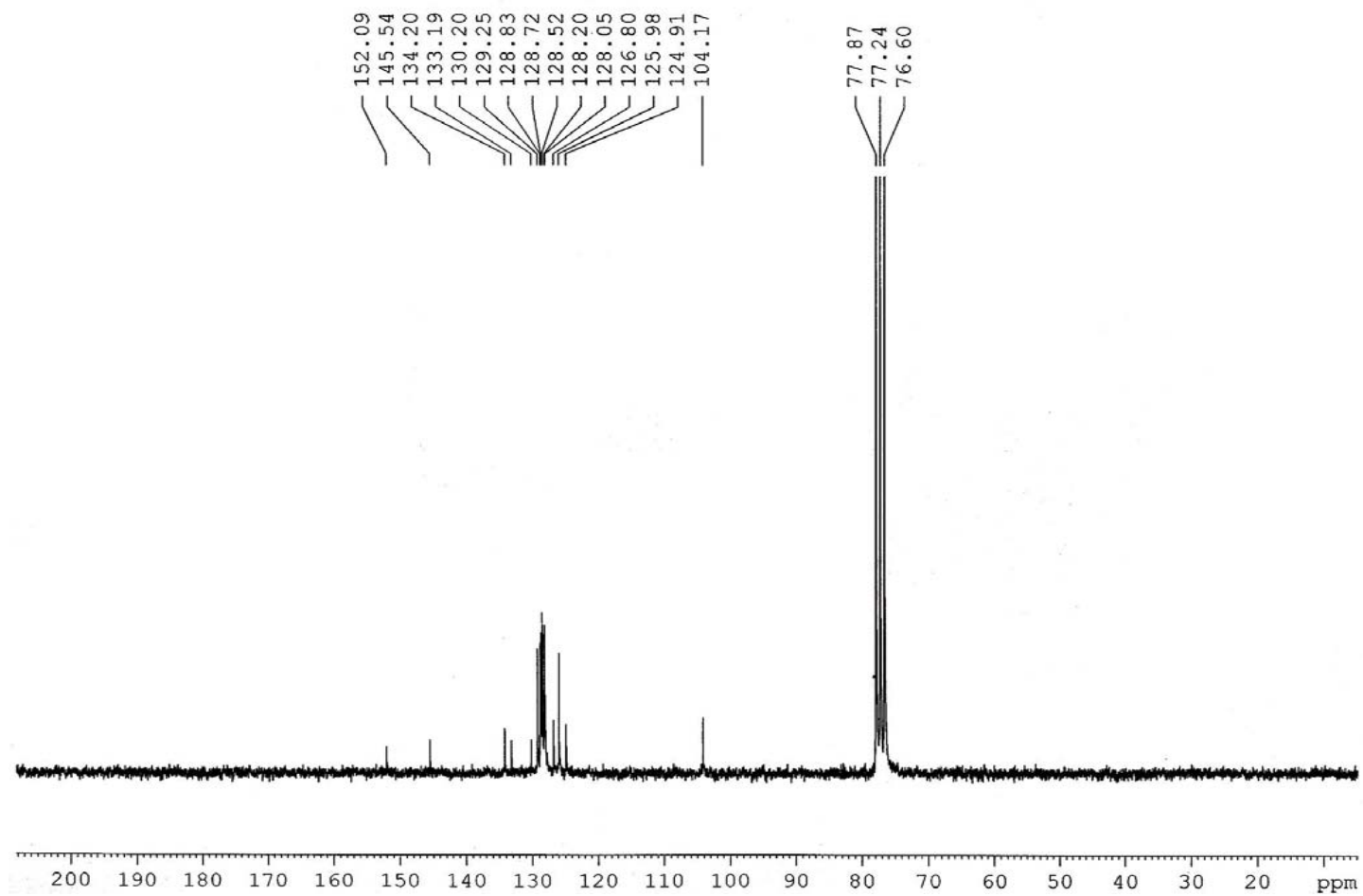


Figure S45 ¹³C NMR spectrum of **6v**

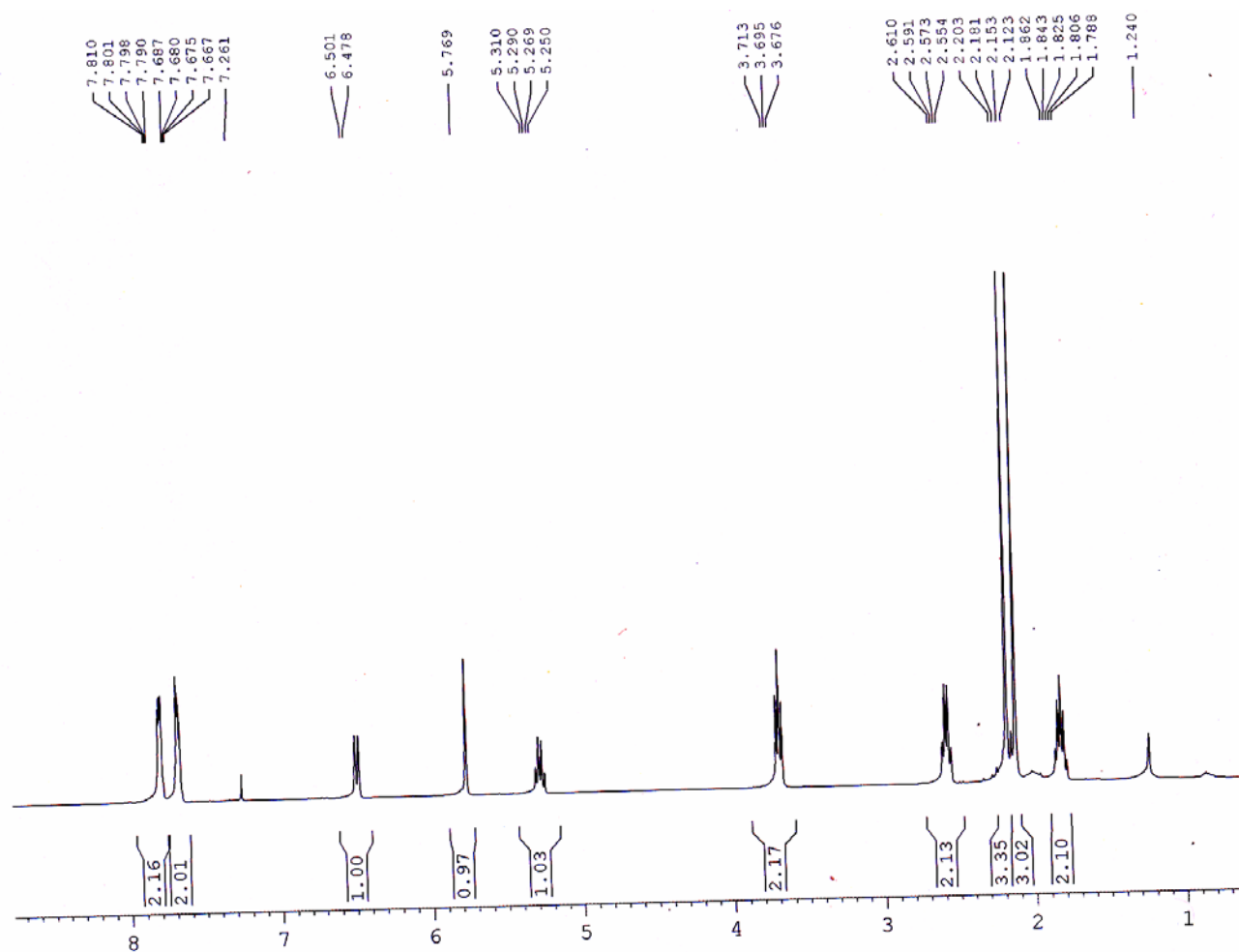


Figure S46 ^1H NMR spectrum of **6w**

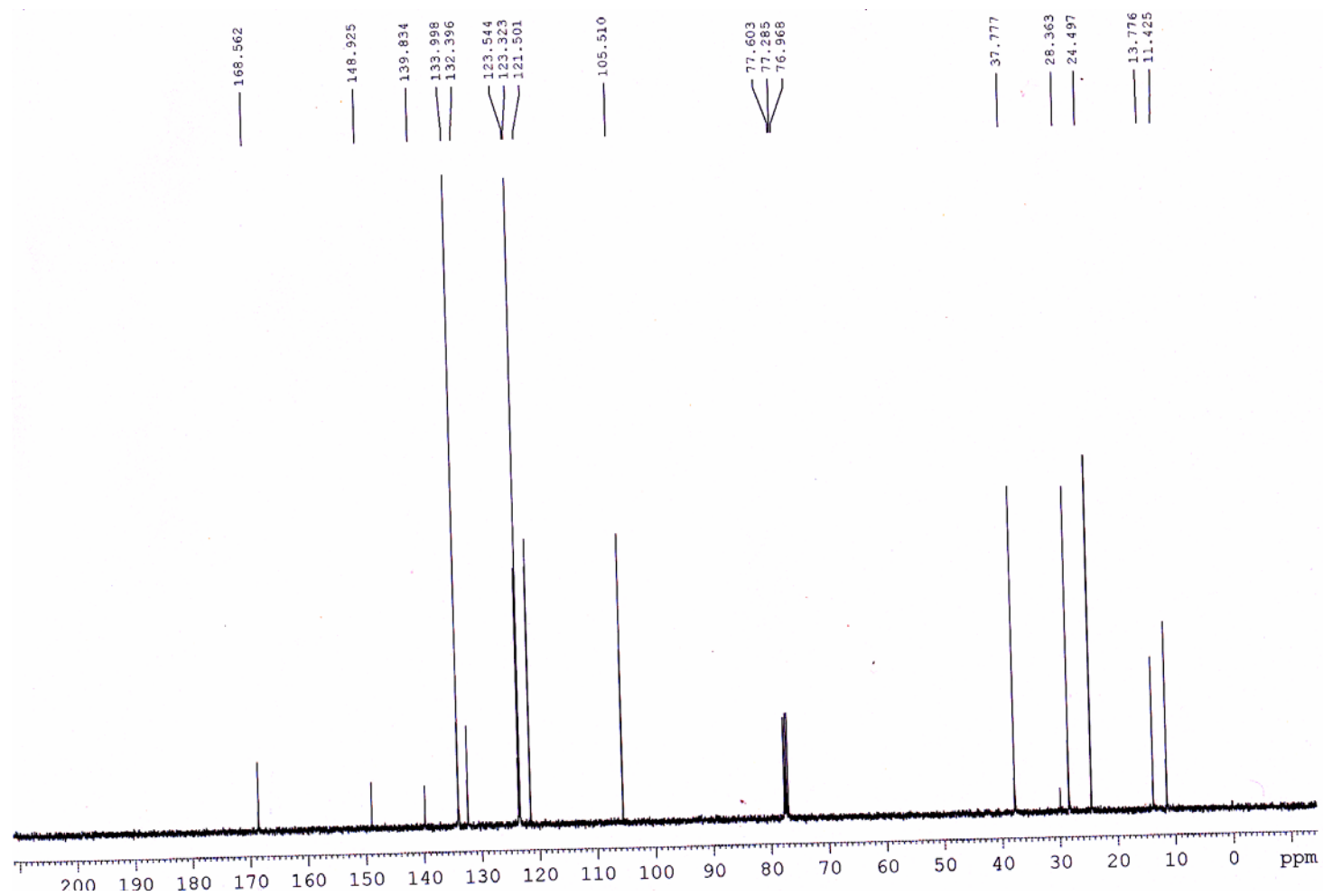


Figure S47 ¹³C NMR spectrum of **6w**

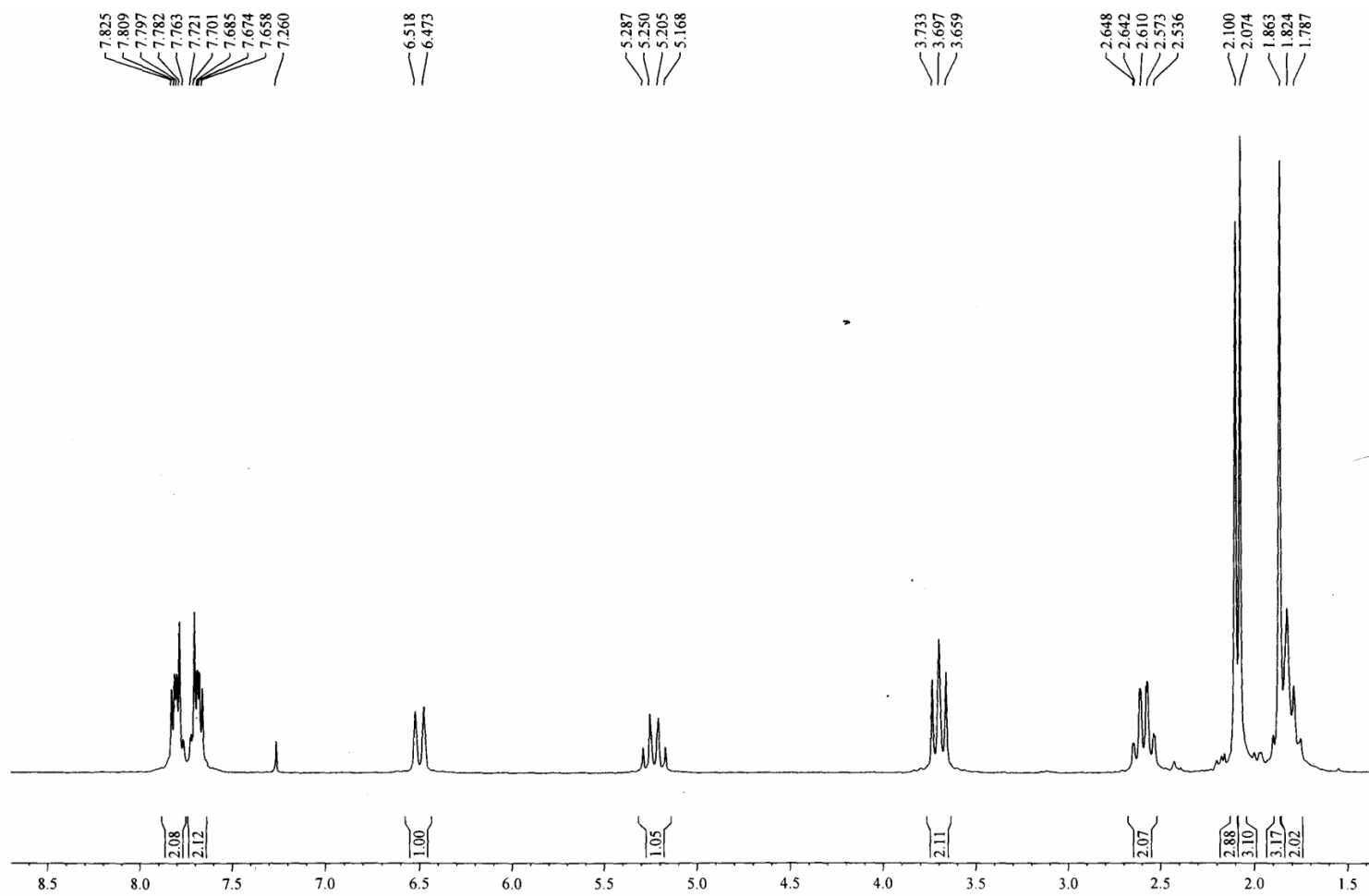


Figure S48 ¹H NMR spectrum of **6x**

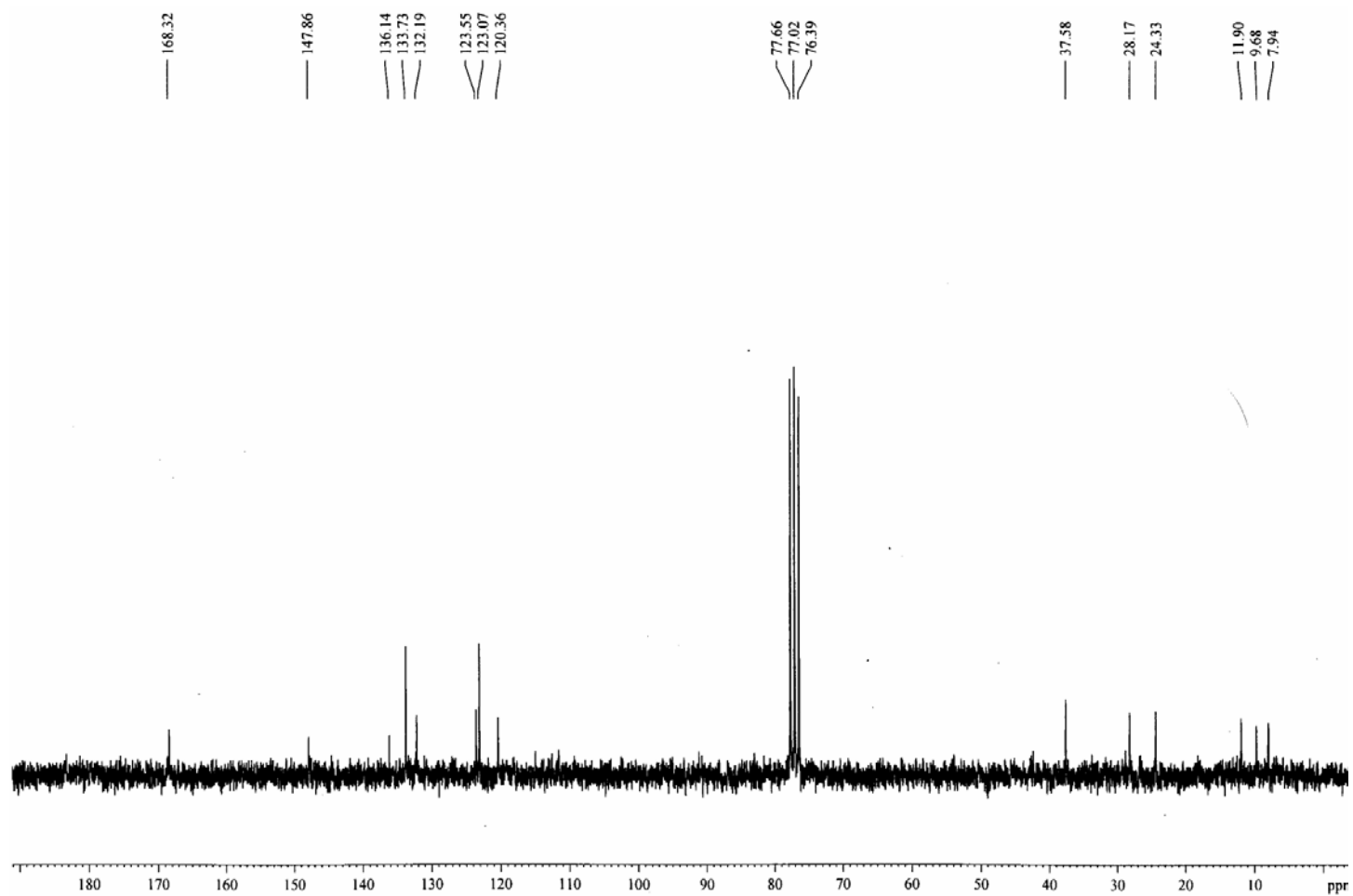


Figure S49 ¹³C NMR spectrum of 6x

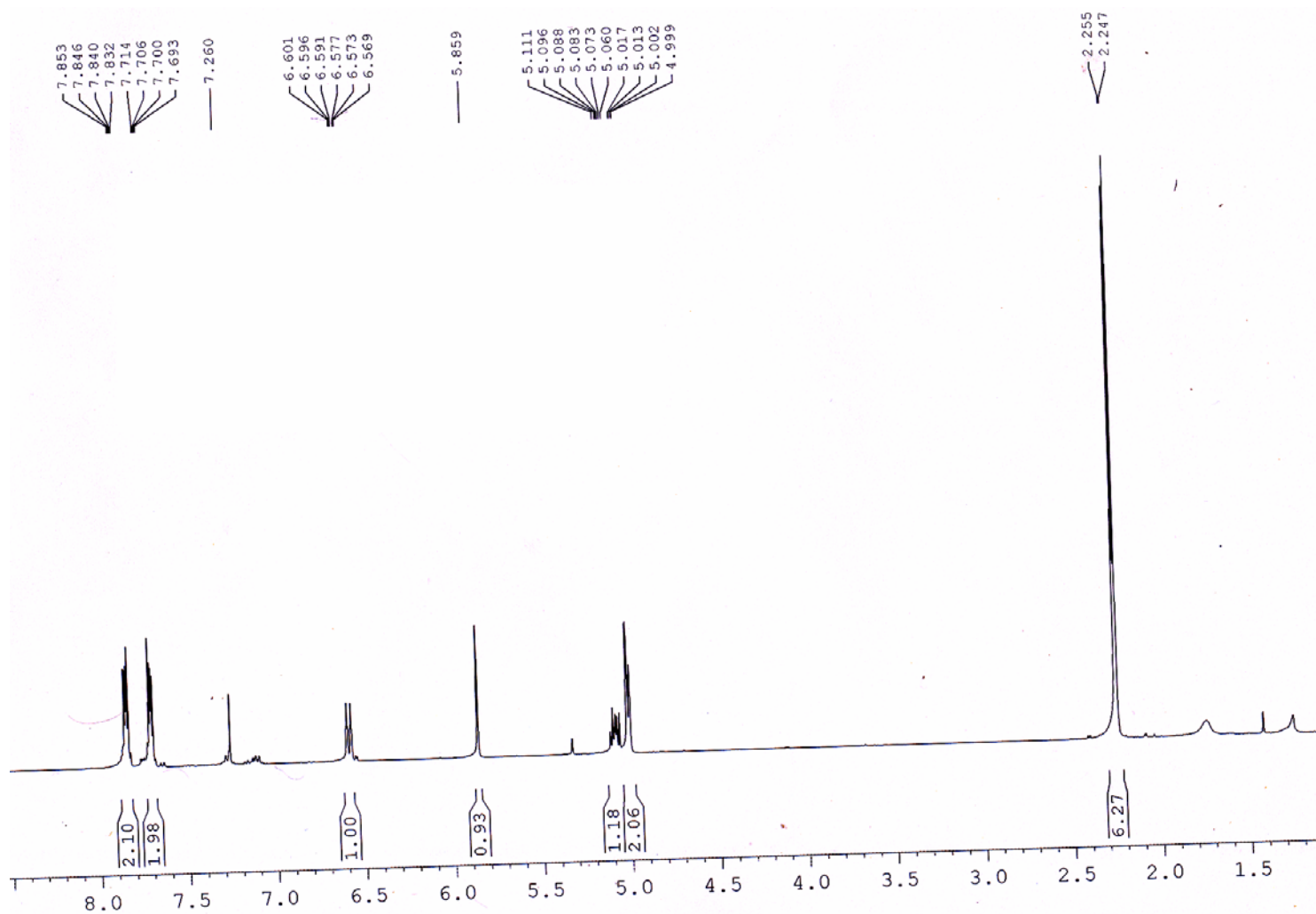


Figure S50 ¹H NMR spectrum of **6y**

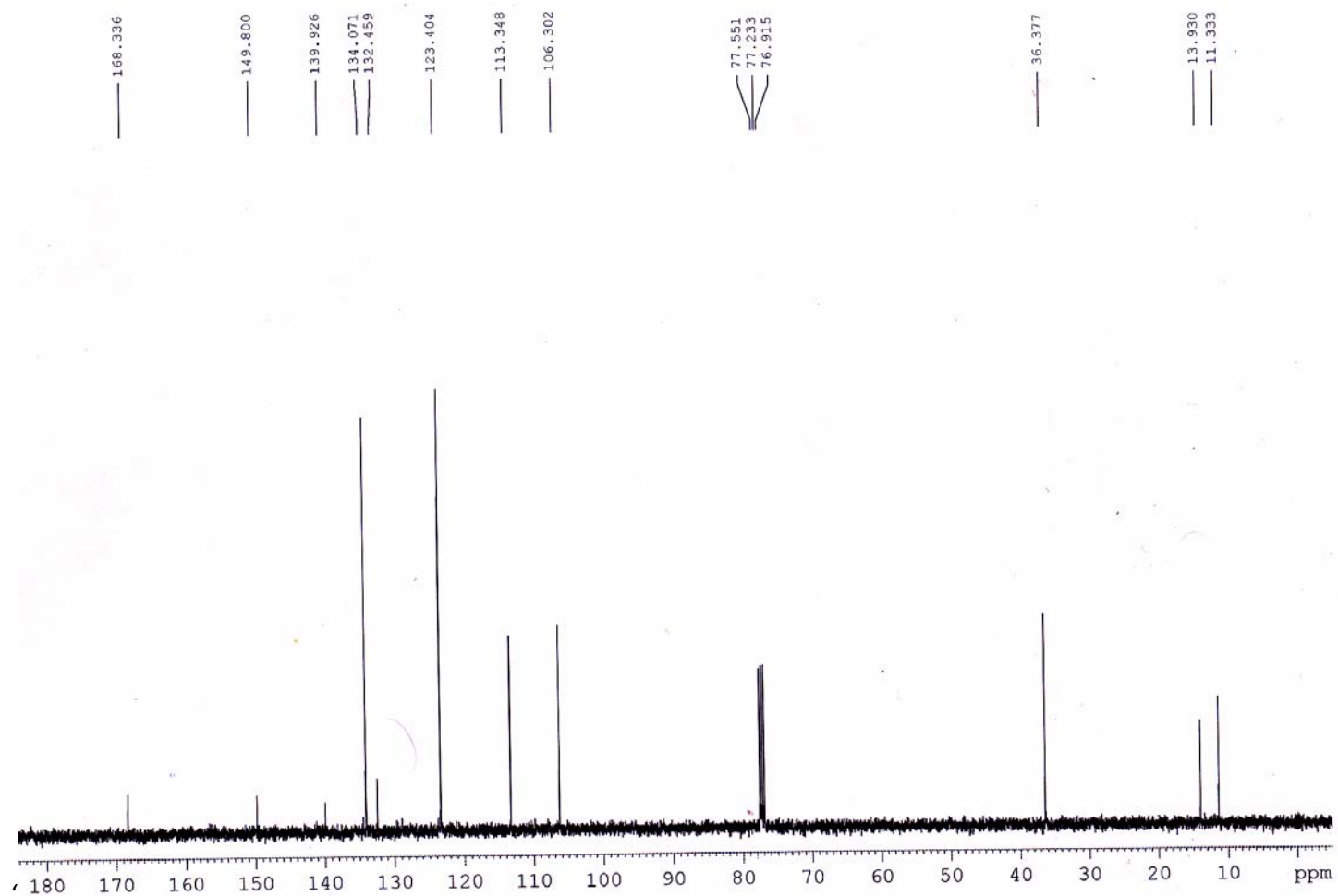


Figure S51 ¹³C NMR spectrum of **6y**

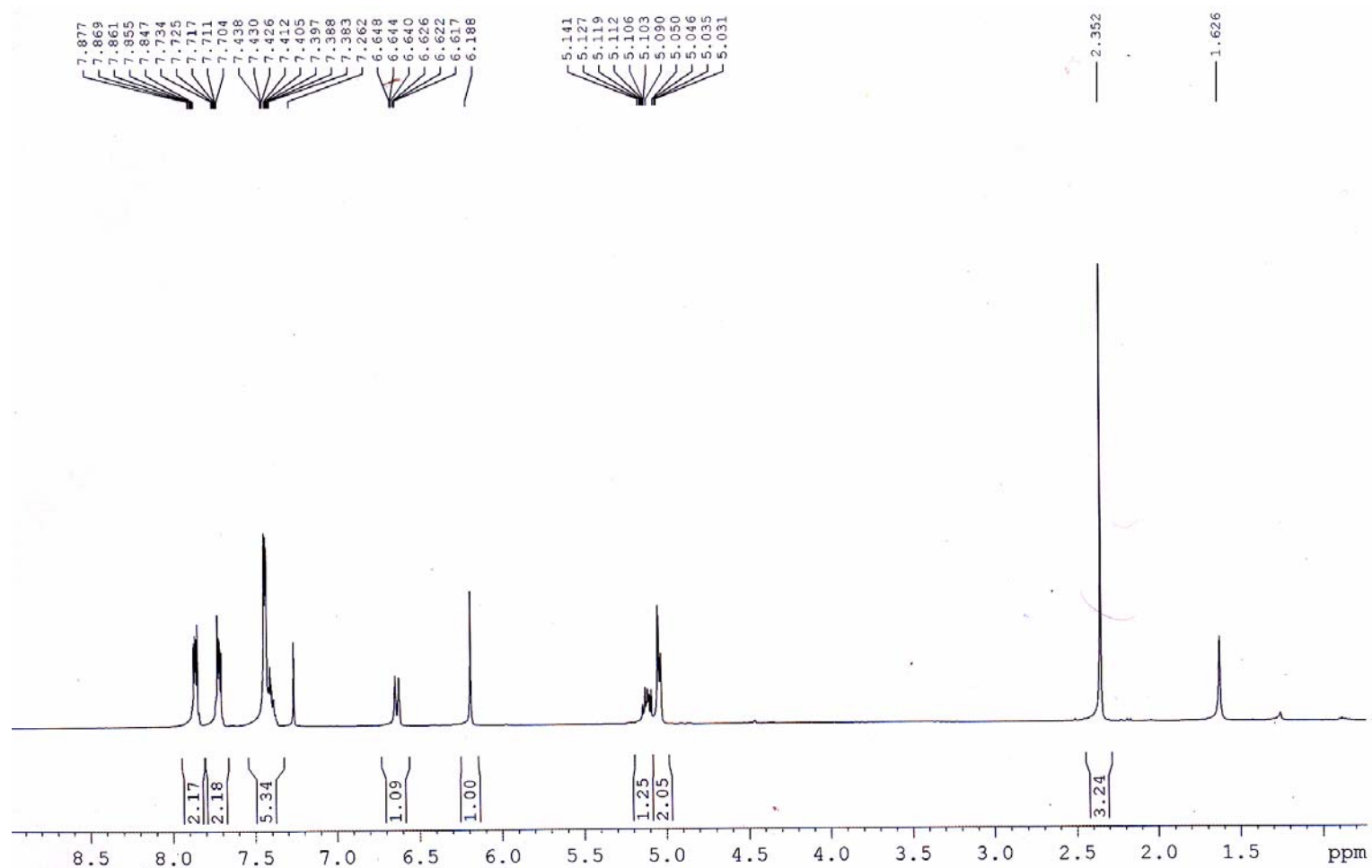


Figure S52 ^1H NMR spectrum of **6z**

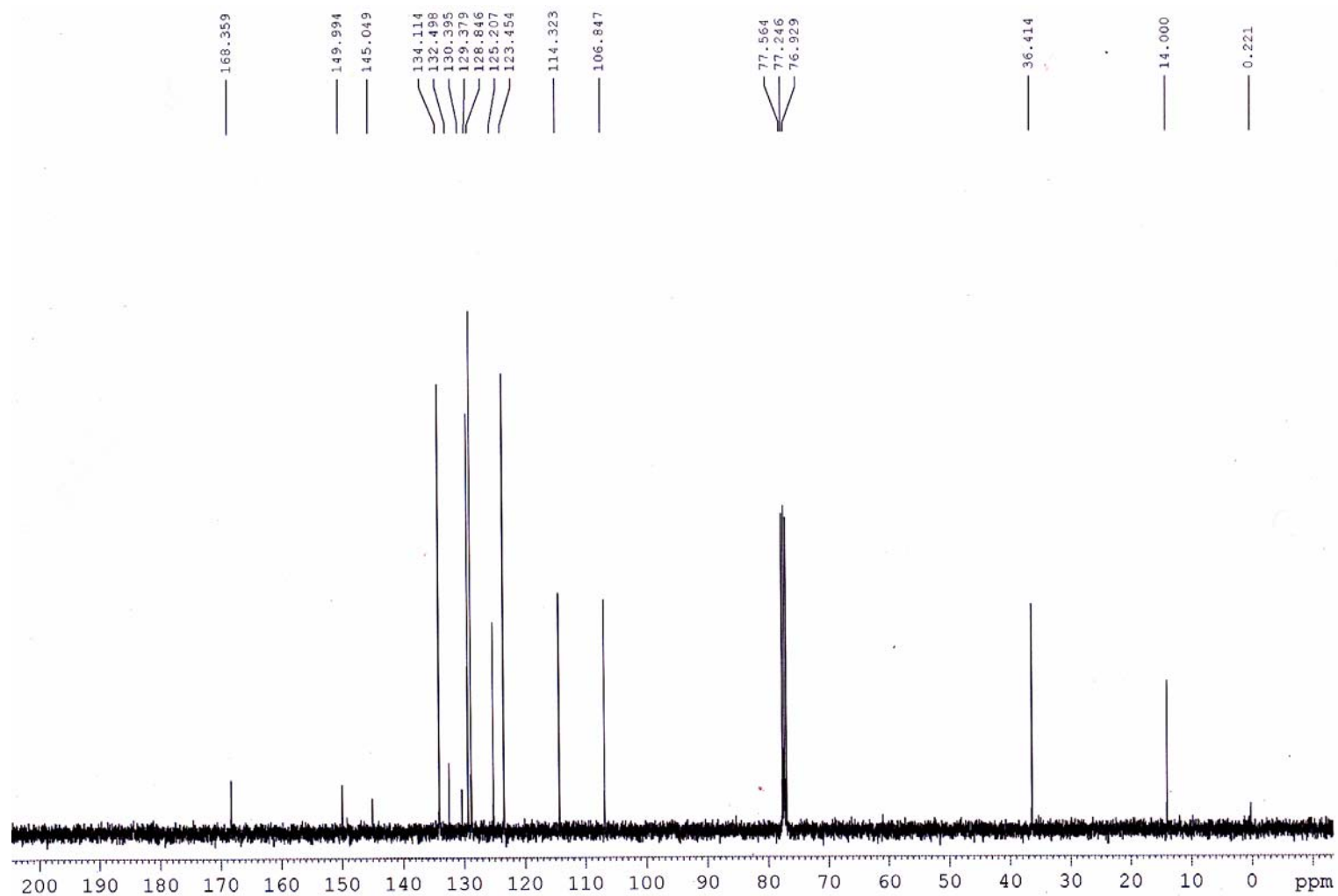


Figure S53 ¹³C NMR spectrum of **6z**

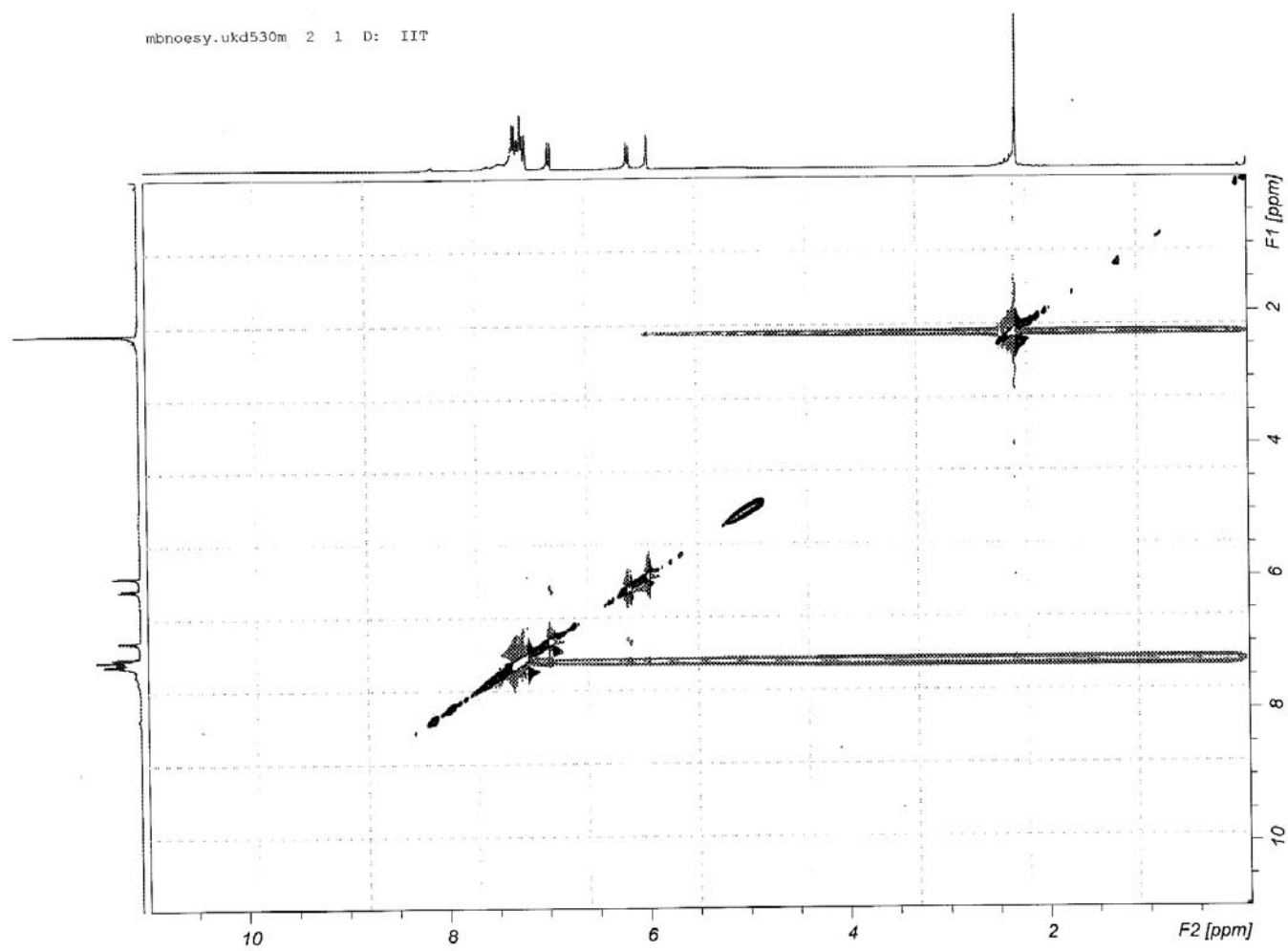


Figure S54 NOESY spectrum of **6i**

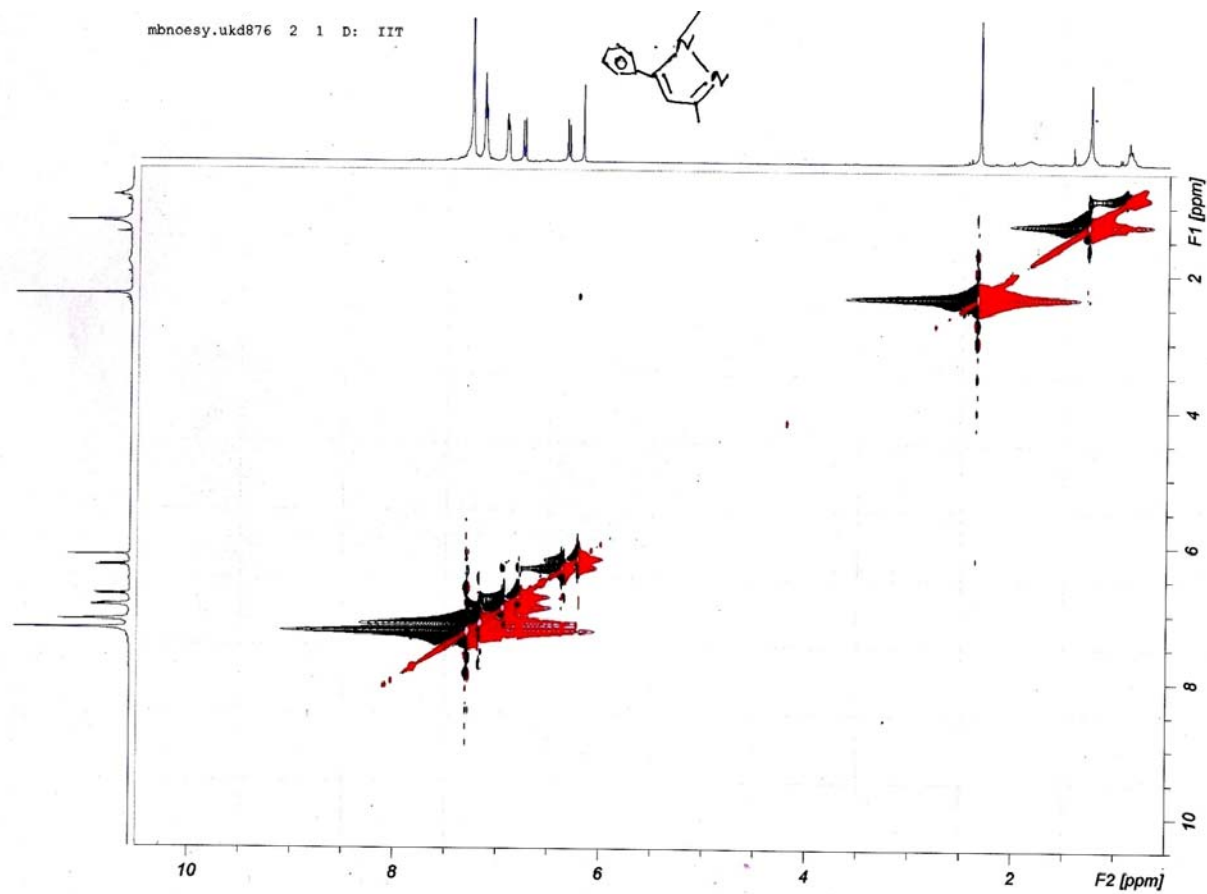


Figure S55 NOESY spectrum of **6s**

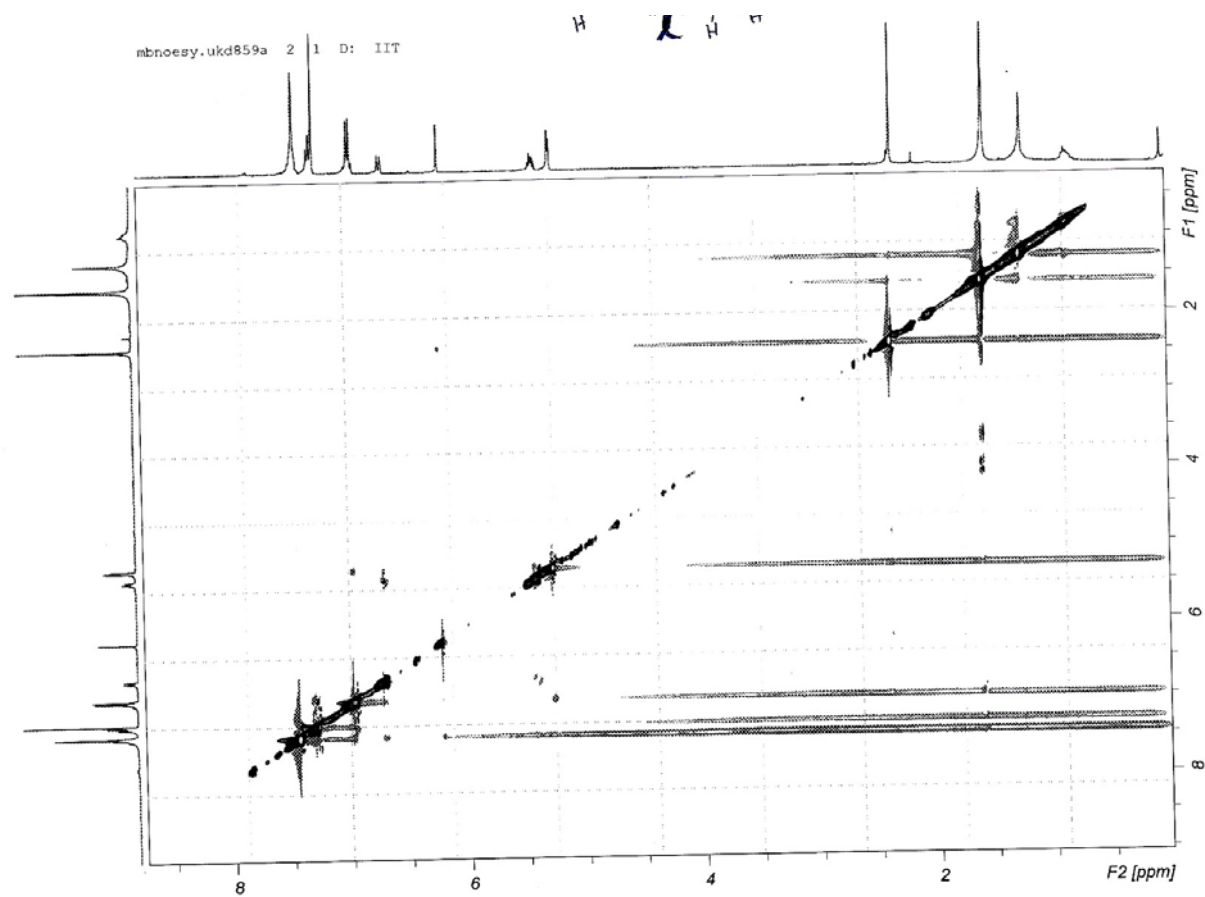


Figure S56 NOESY spectrum of **6t**

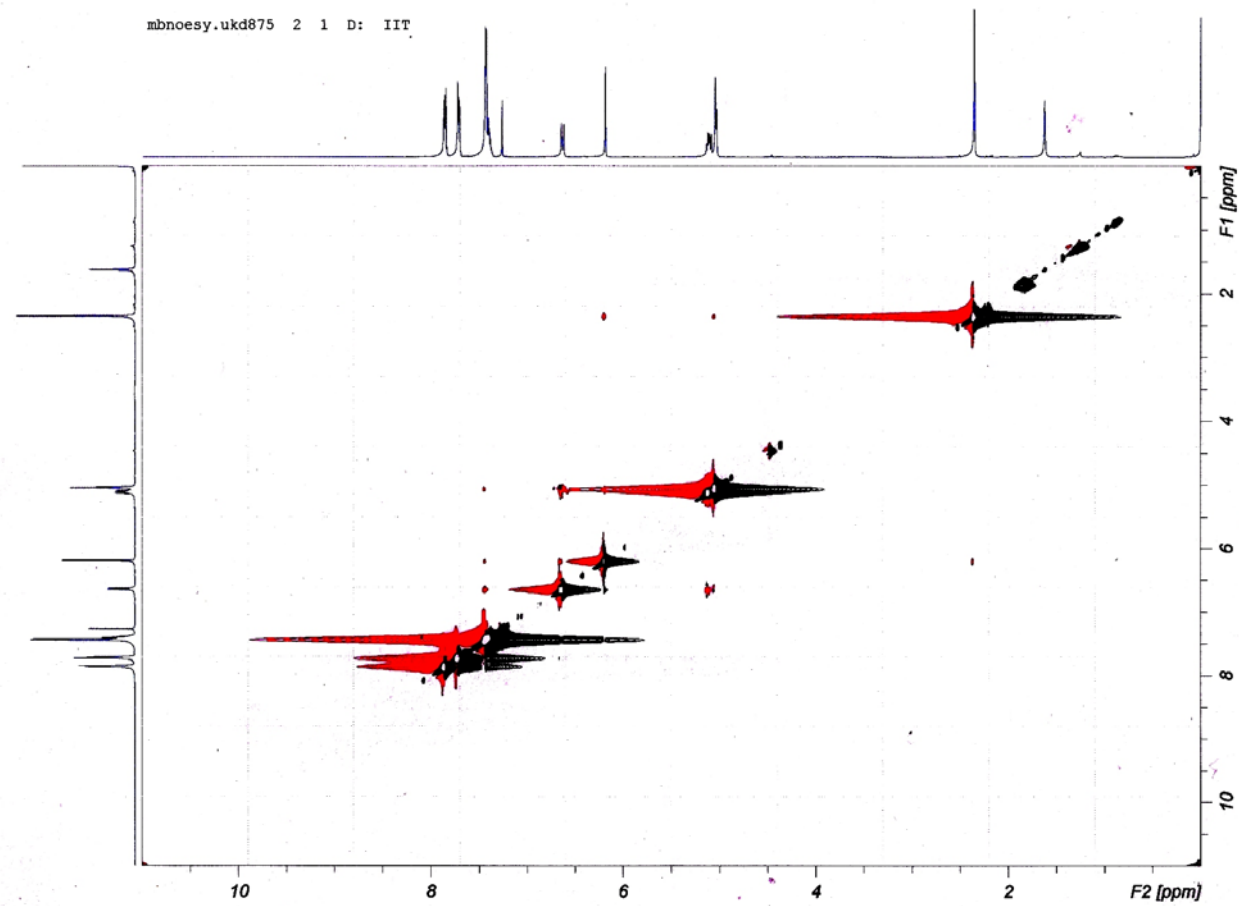


Figure S57 NOESY spectrum of **6z**

1. Relative free energies in kcal/mol for the vinylation of pyrazoles catalyzed by **1** [Ru(dppe)(PPh₃)(CH₃CN)₂Cl][BPh₄]

1.1. BP(RI,D3-BJ)/def2-SVP

Orientation	1_a	1_TS-a_c (AN1)	1_c (AN1)	1_TS-c_d	1_d	1_TS-d_e	1_e	1_f	1_TS-f_g	1_g	1_h	1_i
<i>Cis</i>	0.00	17.19	11.01	19.06	15.75	19.61	-3.95	-8.16	38.05	35.06	-49.67	-28.49
<i>Trans</i>	0.00	17.19	11.01	19.06	15.75	19.61	-3.95	-12.42	16.67	15.52	-61.54	-32.85

1.2. B3LYP(D3-BJ)/def2-SVP//BP(RI,D3-BJ)/def2-SVP

Orientation	1_a	1_TS-a_c (AN1)	1_c (AN1)	1_TS-c_d	1_d	1_TS-d_e	1_e	1_f	1_TS-f_g	1_g	1_h	1_i
<i>Cis</i>	0.00	22.43	18.60	23.59	21.85	25.82	1.55	-1.77	49.43	46.46	-36.25	-25.97
<i>Trans</i>	0.00	22.43	18.60	23.59	21.85	25.82	1.55	-5.35	28.73	27.34	-47.35	-30.62

1.3 Solvation correction with COSMO model. Solvent: Toluene ($\epsilon = 2.38$) [//BP(RI,D3-BJ)/def2-SVP]

Orientation	1_a	1_TS-a_c (AN1)	1_c (AN1)	1_TS-c_d	1_d	1_TS-d_e	1_e	1_f	1_TS-f_g	1_g	1_h	1_i
<i>Cis</i>	0.00	17.25	10.75	18.76	15.20	19.58	-4.56	-5.85	40.65	37.08	-36.33	-26.25
<i>Trans</i>	0.00	17.25	10.75	18.76	15.20	19.58	-4.56	-9.60	20.24	18.96	-46.94	-30.93

2. Relative free energies in kcal/mol for the vinylation of pyrazoles catalyzed by **2** [Ru(dppp)₂(CH₃CN)Cl][BPh₄].

2.1. BP(RI,D3-BJ)/def2-SVP

Orientation	2_a	2_b	2_c	2_TS-b_d	2_d	2_TS-d_e	2_e	2_f	2_TS-f_g	2_g	2_h	2_i
<i>Cis</i>	0.00	3.71	17.04	24.47	9.67	14.85	5.37	-10.25	32.01	30.88	-54.65	-28.49
<i>Trans</i>	0.00	3.71	17.04	24.47	9.67	14.85	5.37	-0.16	62.20	57.62	-37.17	-32.85

2.2. B3LYP(D3-BJ)/def2-SVP//BP(RI,D3-BJ)/def2-SVP

Orientation	2_a	2_b	2_c	2_TS-b_d	2_d	2_TS-d_e	2_e	2_f	2_TS-f_g	2_g	2_h	2_i
<i>Cis</i>	0.00	2.13	23.97	28.38	16.54	22.18	13.02	-3.04	45.71	43.85	-41.17	-25.97
<i>Trans</i>	0.00	2.13	23.97	28.38	16.54	22.18	13.02	8.38	78.41	73.03	-22.63	-30.62

2.3 Solvation correction with COSMO model. Solvent: Toluene ($\epsilon = 2.38$) [//BP(RI,D3-BJ)/def2-SVP]

Orientation	2_a	2_b	2_c	2_TS-b_d	2_d	2_TS-d_e	2_e	2_f	2_TS-f_g	2_g	2_h	2_i
<i>Cis</i>	0.00	3.07	17.04	24.23	9.48	14.42	5.12	-7.68	34.52	32.90	-40.59	-26.25
<i>Trans</i>	0.00	3.07	17.04	24.23	9.48	14.42	5.12	2.50	64.73	59.83	-22.98	-30.93

3. Cartesian coordinates of BP(RI,D3-BJ)/def2-SVP optimized geometries.

Acetonitrile

C	-0.0000000	0.0000000	0.9714200
N	0.0000000	0.0000000	2.1421388
C	0.0000000	0.0000000	-0.4883695
H	-0.5192315	-0.8993354	-0.8750631
H	-0.5192315	0.8993354	-0.8750631
H	1.0384631	0.0000000	-0.8750631

Phenylacetylene

C	0.0000000	0.0000000	0.7342496
C	0.0000000	0.0000000	2.1648741
C	1.2214380	0.0000000	0.0135762
C	1.2159488	0.0000000	-1.3869768
C	0.0000000	0.0000000	-2.0919493
C	-1.2159488	0.0000000	-1.3869768
C	-1.2214380	0.0000000	0.0135762
H	2.1698965	0.0000000	0.5699450
H	2.1704984	0.0000000	-1.9347626
H	0.0000000	0.0000000	-3.1923053
H	-2.1704984	0.0000000	-1.9347626
H	-2.1698965	0.0000000	0.5699450
C	0.0000000	0.0000000	3.3905388
H	0.0000000	0.0000000	4.4710286

Pyrazole

N	-0.8069423	1.3408169	0.3671878
C	-1.1984478	0.0992273	0.0324083
C	-0.0699427	-0.7440113	-0.2023917
C	1.0502649	0.0609095	0.0105017
N	0.5437681	1.2898053	0.3467830
H	1.0740103	2.1319590	0.5709505
C	2.5171441	-0.2221997	-0.0730996
H	-0.0661913	-1.8012420	-0.4892217
C	-2.6555024	-0.2439002	-0.0517451
H	3.0231791	0.4216775	-0.8236354
H	3.0282718	-0.0619655	0.9001309
H	2.6852723	-1.2743503	-0.3682923
H	-2.9277994	-1.0479510	0.6634117
H	-3.2630425	0.6504863	0.1826866
H	-2.9340421	-0.5992619	-1.0656746

Structures related to catalyst 1, [Ru(dppe)(PPh₃)(CH₃CN)₂Cl][BPh₄]

1_a

C	-2.4284311	1.5339110	-1.4943250
C	-2.2912328	2.6940365	-0.5097215
C	-1.5698196	-1.1559721	-2.1625782
C	-1.8105300	-2.5395666	-2.0246517
C	-1.1171968	-0.6653579	-3.4087499
C	-1.5950165	-3.4096844	-3.1043892
C	2.6000282	-0.9979335	2.9591893
C	2.4033934	-1.9307236	-0.8745832
C	2.1931113	-1.9812826	2.0357259
C	1.9030448	-2.2474159	-2.1566189
C	3.7809214	-1.6905273	-0.7017710
C	-0.9009994	-1.5380268	-4.4848918
C	-1.1337685	-2.9156551	-4.3347206
Cl	2.5509458	1.4684322	0.8437011
N	-0.1394022	0.5836156	2.1480068
N	1.0613703	0.7603516	-1.5813557
C	1.6855222	4.1183674	-1.0756572
C	3.2877574	-1.3687707	4.1272009
C	2.7801451	-2.3591911	-3.2449081
C	4.6520250	-1.7906215	-1.7988381
C	4.1567817	-2.1311140	-3.0692143
C	-1.6011858	5.4972468	2.9806633
C	3.5809930	-2.7172571	4.3827761
C	2.4960383	-3.3370657	2.2948566
C	3.1891910	-3.7002541	3.4580211
C	-0.2197294	0.6447973	3.3148093
C	1.6498978	0.9310613	-2.5752052
C	2.4090275	1.1702554	-3.7842934
C	-0.2617318	0.7374140	4.7605762
Ru	0.3199339	0.6068712	0.2312381
P	-0.5145985	2.8015219	0.0342421
P	1.2451605	-1.5797092	0.4941949
P	-1.6923164	-0.0126835	-0.7268755
C	-0.5332933	3.8419015	1.5425748
C	0.3278714	3.7819873	-1.2701434
C	0.0373146	-2.9673442	0.5258551
C	-3.1483291	-0.5862947	0.2440872
C	-4.2002632	-1.3180657	-0.3472962
C	0.5364455	3.7438284	2.4586386
C	-3.2625619	-0.1846183	1.5907776
C	-1.0875204	-2.7968282	1.3588983
C	-1.8955415	-5.0051877	0.7478404
C	0.5311600	4.5234903	3.6258817

C	-4.3880854	-0.5458014	2.3473162
C	0.4362610	4.7247701	-3.5201386
C	-0.2914927	4.0912484	-2.4989453
C	-5.3190095	-1.6864508	0.4149372
C	0.2078124	-4.1813937	-0.1682801
C	1.7861699	5.0573796	-3.3223444
C	-0.5372665	5.3965393	3.8925209
C	2.4051736	4.7555560	-2.0963899
C	-0.7571032	-5.1954163	-0.0538902
C	-5.4121898	-1.3106526	1.7655182
C	-1.6002971	4.7269892	1.8072553
C	-2.0556180	-3.8047657	1.4624336
H	2.4238017	0.0617852	2.7315868
H	0.8265817	-2.4001914	-2.3089583
H	4.1690309	-1.4167034	0.2896260
H	3.6118507	-0.5895366	4.8339524
H	2.3809853	-2.6254011	-4.2353606
H	5.7274130	-1.6065416	-1.6566619
H	4.8452850	-2.2232569	-3.9227919
H	4.1214393	-3.0042100	5.2972881
H	2.1831066	-4.1195357	1.5890059
H	3.4203062	-4.7596946	3.6444972
H	-1.2097737	-1.8616556	1.9210698
H	-2.6556515	-5.7971109	0.8228883
H	1.0885203	-4.3338319	-0.8082189
H	-0.6205318	-6.1401591	-0.6012020
H	-2.9414658	-3.6457408	2.0950866
H	-2.1687780	-2.9466076	-1.0709779
H	-0.9256914	0.4071981	-3.5477341
H	-1.7856359	-4.4848466	-2.9736113
H	-0.5557757	-1.1379087	-5.4499975
H	-0.9637104	-3.6009834	-5.1781615
H	-4.1495749	-1.6070062	-1.4067324
H	-2.4597381	0.4077418	2.0461675
H	-4.4662096	-0.2278414	3.3978802
H	-6.1270997	-2.2685619	-0.0526785
H	-6.2900187	-1.6030856	2.3606943
H	2.1886255	3.8430495	-0.1378764
H	-2.4362691	6.1853538	3.1798736
H	1.3701492	3.0554365	2.2437100
H	1.3751546	4.4518964	4.3289871
H	-0.0605394	4.9680779	-4.4714626
H	-1.3498850	3.8528056	-2.6758020
H	2.3530280	5.5609871	-4.1198358
H	-0.5380938	6.0067356	4.8081794
H	3.4612288	5.0167422	-1.9311373
H	-2.4361238	4.8304119	1.1001498
H	1.9186186	0.6878942	-4.6529556
H	3.4236298	0.7386056	-3.6706043
H	2.4883369	2.2619729	-3.9644341

H	-1.2491431	0.4209202	5.1519699
H	-0.0730118	1.7857935	5.0703974
H	0.5211577	0.0829366	5.1961594
H	-3.4832125	1.3344934	-1.7685036
H	-1.8682627	1.7441417	-2.4263850
H	-2.6435342	3.6517557	-0.9418489
H	-2.8894861	2.5037355	0.4058023

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C	-2.0660467	1.2325333	-2.0877222
C	-1.8614881	2.4133096	-1.1416269
C	-1.2045917	-1.4583930	-2.7568989
C	-1.4429427	-2.8421526	-2.6159682
C	-0.7461502	-0.9709216	-4.0021446
C	-1.2205616	-3.7153501	-3.6917824
C	2.9344488	-1.3124522	2.3976829
C	2.7595878	-2.3275419	-1.3908056
C	2.4795004	-2.3119994	1.5148645
C	2.2796171	-2.6359108	-2.6831305
C	4.1420220	-2.1577055	-1.1810445
C	-0.5212789	-1.8470085	-5.0738736
C	-0.7528321	-3.2246073	-4.9208868
Cl	2.9418827	1.1128125	0.2306863
N	0.2185275	0.2571409	1.5415537
N	1.4588102	0.3592020	-2.1859541
C	2.1384172	3.6445290	-1.9243927
C	3.5900731	-1.6683245	3.5886082
C	3.1803576	-2.8122196	-3.7430133
C	5.0375412	-2.3197155	-2.2507959
C	4.5616824	-2.6540461	-3.5299286
C	-0.8711193	5.6000236	1.9358638
C	3.8054836	-3.0182182	3.9072092
C	2.7036683	-3.6696534	1.8379430
C	3.3664848	-4.0182865	3.0230161
C	0.1190822	0.1943095	2.7068410
C	2.0537432	0.4735544	-3.1839980
C	2.8160053	0.6418819	-4.4029249
C	0.0451047	0.0305151	4.1433445
Ru	0.6987187	0.2823981	-0.3780587
P	-0.0642106	2.4911396	-0.6628160
P	1.5759168	-1.9230162	-0.0579475
P	-1.3275094	-0.3138672	-1.3206114
C	0.0035701	3.6617710	0.7438737
C	0.7587091	3.3698188	-2.0516221
C	0.3522941	-3.2974284	-0.0323966
C	-2.7812702	-0.9004037	-0.3518058
C	-3.8300362	-1.6296352	-0.9530905
C	0.9946072	3.5014784	1.7361203
C	-2.8911889	-0.5318804	1.0040221

C	-0.7758920	-3.1151260	0.7933239	H	2.3119229	0.1325177	-5.2479960
C	-1.6079814	-5.3119927	0.1735485	H	3.8209545	0.1929743	-4.2723513
C	1.0431297	4.3901228	2.8213513	H	2.9190598	1.7225157	-4.6312410
C	-4.0006573	-0.9344190	1.7634651	H	-0.9818912	-0.2502578	4.4503785
C	0.8076381	4.2661773	-4.3221196	H	0.3071474	0.9774359	4.6591854
C	0.0985236	3.6853608	-3.2566968	H	0.7548475	-0.7647406	4.4519840
C	-4.9362076	-2.0336350	-0.1908496	H	-3.1356748	1.0473438	-2.3088138
C	0.5134788	-4.5139196	-0.7246255	H	-1.5474604	1.4110073	-3.0495997
C	2.1786481	4.5397547	-4.1909264	H	-2.2109804	3.3667615	-1.5852632
C	0.1085706	5.4327239	2.9288746	H	-2.4226826	2.2625990	-0.1964299
C	2.8392993	4.2299286	-2.9882761	C	-2.1120776	2.6713266	4.8689692
C	-0.4648344	-5.5162960	-0.6180502	C	-0.9096955	2.9830104	5.5789300
C	-5.0180915	-1.7002759	1.1720371	C	-2.1344373	2.6907324	3.4511507
C	-0.9225735	4.7229259	0.8419592	C	-3.3221553	2.4134031	2.7651892
C	-1.7580135	-4.1103567	0.8883658	C	-4.4975132	2.0984794	3.4682562
H	2.8119318	-0.2556599	2.1256084	C	-4.4791153	2.0603787	4.8736014
H	1.2010983	-2.7330165	-2.8652433	C	-3.2990904	2.3463622	5.5735425
H	4.5158408	-1.8921650	-0.1819710	H	-1.2188271	2.9376040	2.9012343
H	3.9482357	-0.8769466	4.2647880	H	-3.3333431	2.4521870	1.6662560
H	2.7965360	-3.0723250	-4.7411607	H	-5.4277524	1.8864851	2.9208192
H	6.1166340	-2.1900784	-2.0798774	H	-5.3959276	1.8167230	5.4308762
H	5.2686798	-2.7956280	-4.3613614	H	-3.2840101	2.3323466	6.6727223
H	4.3213001	-3.2930750	4.8395799	C	0.1240164	3.2359722	6.1885119
H	2.3513758	-4.4646828	1.1655745	H	1.0205126	3.4803033	6.7413618
H	3.5360308	-5.0795643	3.2585829				
H	-0.8906442	-2.1801062	1.3563229	l_c			
H	-2.3784162	-6.0943510	0.2416093	C	-2.4427587	1.1186452	-1.3262873
H	1.3983974	-4.6779545	-1.3553692	C	-2.1713684	2.3931335	-0.5339192
H	-0.3340904	-6.4631905	-1.1631931	C	-1.4937285	-1.5134022	-1.9991692
H	-2.6461941	-3.9394821	1.5145001	C	-1.7400210	-2.8965224	-1.8698263
H	-1.8055958	-3.2464282	-1.6630863	C	-1.0763644	-1.0132750	-3.2537727
H	-0.5557739	0.1016380	-4.1440986	C	-1.5620175	-3.7570049	-2.9640772
H	-1.4103636	-4.7902915	-3.5583846	C	3.1578378	-1.3088038	2.6849239
H	-0.1715688	-1.4494538	-6.0385752	C	2.5252506	-2.1620515	-1.0470178
H	-0.5777028	-3.9120584	-5.7616223	C	2.6244641	-2.2834176	1.8181642
H	-3.7848626	-1.8910065	-2.0198728	C	1.9635252	-2.5921983	-2.2685086
H	-2.1010976	0.0681090	1.4699475	C	3.8971746	-1.8467455	-0.9830557
H	-4.0684941	-0.6392720	2.8207048	C	-0.9010907	-1.8752109	-4.3463265
H	-5.7414359	-2.6127811	-0.6670638	C	-1.1377489	-3.2528743	-4.2038506
H	-5.8830166	-2.0264613	1.7687654	Cl	2.6126008	1.3378170	0.8612995
H	2.6669512	3.3616053	-1.0018850	N	1.1348505	0.3768584	-1.5211299
H	-1.6036452	6.4168565	2.0144482	C	1.7474733	3.4969722	-1.7740654
H	1.7284264	2.6860131	1.6388307	C	4.0512481	-1.6854620	3.7016082
H	1.8122985	4.2583311	3.5959802	C	2.7789223	-2.7565628	-3.3976396
H	0.2800894	4.5151490	-5.2551768	C	4.7041732	-1.9936101	-2.1232056
H	-0.9770160	3.4945457	-3.3797604	C	4.1518009	-2.4612676	-3.3275339
H	2.7305611	5.0031888	-5.0225267	C	-1.0759559	6.0618690	1.8501851
H	0.1385317	6.1131241	3.7923100	C	4.4238546	-3.0285243	3.8606472
H	3.9125034	4.4454977	-2.8757734	C	3.0013061	-3.6358136	1.9824619
H	-1.6909975	4.8717964	0.0694053				

C	3.8980889	-4.0027241	2.9950761	H	-2.2125420	-0.7255691	2.3813301
C	1.6659593	0.4601590	-2.5572129	H	-4.1923871	-1.6126274	3.5986737
C	2.3117165	0.5954818	-3.8440900	H	-6.1309263	-2.4737443	-0.1899587
Ru	0.4167207	0.3221994	0.3211591	H	-6.1595130	-2.5119631	2.3198431
P	-0.3578033	2.5404430	-0.1881364	H	2.3672965	3.2575965	-0.8971486
P	1.4708445	-1.8683381	0.4240796	H	-1.9292200	6.7368745	2.0124746
P	-1.6182473	-0.3819301	-0.5426368	H	1.9160667	3.6011483	1.3316600
C	-0.1759694	4.0090667	0.8985481	H	2.2487802	5.7244315	2.6122404
C	0.3647485	3.2069886	-1.7515852	H	-0.4327373	4.1895407	-4.9451501
C	0.3413537	-3.3264116	0.4925292	H	-1.4883525	3.2451871	-2.9147695
C	-3.0412034	-1.0881925	0.4055061	H	2.0165019	4.7378824	-4.9649838
C	-4.1602480	-1.5770620	-0.3069982	H	0.3231667	7.2989256	2.9628864
C	1.0863679	4.3137278	1.4513628	H	3.4090949	4.2787752	-2.9228021
C	-3.0707034	-1.1037981	1.8138372	H	-2.2541545	4.6690426	0.6958396
C	-0.7571999	-3.2627791	1.3709277	H	1.9699560	-0.2043336	-4.5297086
C	-1.4245014	-5.5165568	0.7567157	H	3.4094310	0.5097293	-3.7219351
C	1.2610747	5.4948600	2.1852294	H	2.0694527	1.5904531	-4.2694866
C	-4.1874450	-1.6102073	2.4985463	H	-3.5273188	0.9138884	-1.4153308
C	0.1859447	3.9928972	-4.0567434	H	-2.0407326	1.2077679	-2.3531135
C	-0.4091039	3.4519630	-2.9026699	H	-2.5443586	3.2913887	-1.0642918
C	-5.2711113	-2.0888678	0.3784528	H	-2.6654834	2.3666086	0.4566256
C	0.5700734	-4.5182854	-0.2272001	C	-1.1323759	1.9585921	2.9815761
C	1.5555682	4.2991836	-4.0673675	C	-0.4089489	0.8767510	2.3493472
C	0.1835768	6.3731719	2.3850254	C	-0.4142075	2.8609890	3.8029630
C	2.3335075	4.0465177	-2.9224680	C	-1.0839761	3.8946750	4.4666893
C	-0.3103075	-5.6036242	-0.0947813	C	-2.4743396	4.0446544	4.3265557
C	-5.2870389	-2.1095376	1.7839091	C	-3.1961209	3.1468362	3.5243177
C	-1.2585055	4.8882555	1.1031704	C	-2.5330336	2.1100394	2.8527694
C	-1.6414821	-4.3429767	1.4977854	H	0.6728267	2.7389310	3.8998657
H	2.8989452	-0.2502633	2.5416633	H	-0.5135780	4.5943901	5.0943457
H	0.8889475	-2.8012320	-2.3415227	H	-2.9959028	4.8610247	4.8475091
H	4.3331554	-1.4852512	-0.0409923	H	-4.2871165	3.2480645	3.4246118
H	4.4612055	-0.9138060	4.3702360	H	-3.1074441	1.3924298	2.2516166
H	2.3333090	-3.1179135	-4.3368321	C	0.2211995	-0.2228179	2.3969283
H	5.7761452	-1.7533333	-2.0634162	H	0.5997744	-1.0513047	2.9935015
H	4.7919228	-2.5957603	-4.2124884				
H	5.1234687	-3.3190992	4.6586478	1_TS-c_d			
H	2.5904903	-4.4131914	1.3236859				
H	4.1823030	-5.0592410	3.1109662	C	-2.4459157	1.0704874	-1.4422652
H	-0.9353790	-2.3514803	1.9516563	C	-2.1671877	2.2820269	-0.5569722
H	-2.1181044	-6.3654554	0.8486119	C	-1.4787310	-1.5587409	-2.2053551
H	1.4331474	-4.6042333	-0.9009039	C	-1.6443630	-2.9507185	-2.0467503
H	-0.1228422	-6.5249531	-0.6663125	C	-1.1479428	-1.0529678	-3.4830319
H	-2.5080626	-4.2568749	2.1696839	C	-1.4659337	-3.8164054	-3.1368189
H	-2.0796816	-3.3086163	-0.9109215	C	2.9894867	-1.1420047	2.6146081
H	-0.8860148	0.0597987	-3.3916348	C	2.6504439	-2.2689353	-1.1141738
H	-1.7578700	-4.8318261	-2.8390980	C	2.5204133	-2.1926831	1.7986344
H	-0.5876253	-1.4655351	-5.3184067	C	2.1160967	-2.6174784	-2.3751980
H	-1.0028619	-3.9296192	-5.0605592	C	4.0383405	-2.0810239	-0.9720285
H	-4.1614782	-1.5725437	-1.4074297	C	-0.9692696	-1.9211738	-4.5700143

C	-1.1195685	-3.3080708	-4.3986182	H	-0.7827669	-2.3479629	1.9011451
Cl	2.8090816	1.1880522	0.3456682	H	-2.1176831	-6.3232973	0.8195367
N	1.1537355	0.2820957	-1.8937901	H	1.4085701	-4.6373375	-1.0596995
C	1.6363889	3.4362833	-2.0772594	H	-0.1817041	-6.5319098	-0.7620986
C	3.7226511	-1.4262413	3.7798747	H	-2.4046733	-4.2148974	2.1654385
C	2.9708643	-2.8203470	-3.4678801	H	-1.9182333	-3.3658717	-1.0684211
C	4.8871293	-2.2660589	-2.0758888	H	-1.0235267	0.0277525	-3.6383138
C	4.3586589	-2.6441217	-3.3213697	H	-1.5957164	-4.8985266	-2.9901629
C	-0.9136680	5.7782035	2.0284332	H	-0.7222743	-1.5106256	-5.5608725
C	4.0062968	-2.7530466	4.1345446	H	-0.9796989	-3.9892947	-5.2510010
C	2.8118182	-3.5280266	2.1605732	H	-4.0471292	-1.8788850	-1.3766988
C	3.5547467	-3.8034818	3.3162797	H	-1.9773986	-0.4626345	2.1603329
C	1.6521936	0.3566759	-2.9479987	H	-3.8513132	-1.2916140	3.5938528
C	2.2777975	0.4619993	-4.2494246	H	-5.9007116	-2.7298142	0.0469093
Ru	0.5411595	0.2860266	-0.0357470	H	-5.8146640	-2.4519532	2.5389559
P	-0.3257535	2.4449593	-0.3607695	H	2.3245809	3.1104628	-1.2812298
P	1.5149465	-1.8837677	0.2684882	H	-1.7341730	6.4724086	2.2630242
P	-1.5314391	-0.4217080	-0.7555142	H	1.9748373	3.2600394	1.2269883
C	-0.0993656	3.8004059	0.8587004	H	2.3973063	5.2227385	2.7318349
C	0.2465978	3.2342379	-1.9243535	H	-0.8048063	4.4443910	-4.9621251
C	0.3942467	-3.3451793	0.3730458	H	-1.7112196	3.4630253	-2.8745879
C	-2.8751263	-1.1224947	0.3034873	H	1.6620681	4.8198542	-5.2204890
C	-3.9940861	-1.7509460	-0.2854034	H	0.5423769	6.8328076	3.2522352
C	1.1730107	3.9856945	1.4396622	H	3.2216385	4.1720493	-3.3583345
C	-2.8441181	-0.9530345	1.7004065	H	-2.1442708	4.5706872	0.7259832
C	-0.6631212	-3.2579593	1.3000210	H	1.7656315	-0.2013589	-4.9743947
C	-1.4077867	-5.4909597	0.7031998	H	3.3377587	0.1470026	-4.1769811
C	1.3990797	5.0769705	2.2919381	H	2.2275403	1.5108524	-4.6067234
C	-3.8960106	-1.4245458	2.5022517	H	-3.5258095	0.8346600	-1.5091740
C	-0.1144791	4.1596807	-4.1539239	H	-2.0751185	1.2495921	-2.4703073
C	-0.6243954	3.5988711	-2.9699366	H	-2.6226811	3.2066675	-0.9637780
C	-5.0407063	-2.2297515	0.5169505	H	-2.5756054	2.1322611	0.4644397
C	0.5714685	-4.5382027	-0.3552920	C	-1.1714554	2.3005695	3.5471058
C	1.2660149	4.3693364	-4.2979961	C	-0.4341512	1.3635837	2.8080385
C	0.3608417	5.9766580	2.5851982	C	-0.5073737	3.2614691	4.3624038
C	2.1381719	4.0087014	-3.2546712	C	-1.2555769	4.1832610	5.0971720
C	-0.3269969	-5.6048594	-0.1873279	C	-2.6594360	4.1846113	5.0067641
C	-4.9936280	-2.0721422	1.9127732	C	-3.3284551	3.2458838	4.1958778
C	-1.1440625	4.6989886	1.1625918	C	-2.5980887	2.2939200	3.4844947
C	-1.5686680	-4.3154463	1.4575779	H	0.5895458	3.2603215	4.3993693
H	2.8304188	-0.0987713	2.3043203	H	-0.7442392	4.9200635	5.7330307
H	1.0306603	-2.7274767	-2.5066102	H	-3.2415145	4.9247999	5.5760767
H	4.4539606	-1.7859333	0.0018328	H	-4.4265204	3.2540929	4.1352495
H	4.0842332	-0.5964237	4.4056403	H	-3.1052306	1.5407811	2.8645637
H	2.5465894	-3.1149393	-4.4398215	C	0.1504413	0.5066201	2.0785789
H	5.9713128	-2.1212096	-1.9575318	H	0.6644904	-0.3851161	2.4889500
H	5.0294163	-2.8049262	-4.1788862				
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H	2.4504913	-4.3604058	1.5402216				
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C	-2.2021486	2.1962001	-1.0729008	C	-1.7358474	-4.2212086	1.3472790
C	-1.2329386	-1.7113951	-2.4438701	H	1.7498658	-0.1529919	2.8304935
C	-1.3919878	-3.0947390	-2.2111135	H	1.2032322	-2.9960727	-2.3544726
C	-0.7530829	-1.2819317	-3.7015824	H	4.3397486	-1.3611691	0.1708314
C	-1.0732757	-4.0240157	-3.2131052	H	2.8716781	-0.5954363	5.0107830
C	2.2961126	-1.0924100	2.9799190	H	2.8336535	-3.2871874	-4.2055905
C	2.6777650	-2.2055039	-0.9529649	H	5.9748662	-1.6282457	-1.7021490
C	2.3877272	-2.0356918	1.9391349	H	5.2359089	-2.6066800	-3.8916408
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C	4.0169182	-1.7982818	-0.7844979	H	3.2059477	-3.9644941	1.3215438
C	-0.4320241	-2.2143355	-4.6991339	H	4.3734954	-4.3725008	3.4844220
C	-0.5873066	-3.5897322	-4.4568716	H	-1.0602449	-2.2013452	1.7062742
Cl	2.5832006	1.1994328	0.6679091	H	-2.1643095	-6.2911307	0.8281301
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C	1.7798280	3.4440519	-1.9319427	H	-0.0195836	-6.5963993	-0.4359184
C	2.9443650	-1.3370879	4.2015136	H	-2.6654078	-4.0767696	1.9171835
C	3.1724571	-2.8673770	-3.2464535	H	-1.7695154	-3.4533600	-1.2451595
C	4.9289863	-1.9394418	-1.8429001	H	-0.6286358	-0.2109898	-3.9135385
C	4.5134599	-2.4827459	-3.0707018	H	-1.2034012	-5.0970184	-3.0107916
C	-1.6346976	5.4609073	1.9966658	H	-0.0690346	-1.8634161	-5.6769588
C	3.6907291	-2.5108188	4.3866452	H	-0.3390051	-4.3209083	-5.2403276
C	3.1349363	-3.2193485	2.1282657	H	-3.8421720	-2.1576616	-1.9033729
C	3.7886728	-3.4510442	3.3456635	H	-2.4351623	-0.1394117	1.6826523
C	1.8976294	0.3816233	-2.8307482	H	-4.4565189	-0.9128523	2.9088713
C	2.6603641	0.5183741	-4.0524570	H	-5.8541523	-2.9365096	-0.6693884
Ru	0.4233592	0.2813825	-0.0731811	H	-6.1685893	-2.3392770	1.7472879
P	-0.4349354	2.4457702	-0.5660706	H	2.3331243	3.1038988	-1.0417060
P	1.4607881	-1.8417027	0.3611578	H	-2.5545880	6.0259306	2.2069294
P	-1.5104461	-0.4875400	-1.0992634	H	1.6013502	3.3757234	1.2971064
C	-0.4663936	3.7449866	0.7216064	H	1.6124071	5.1590999	3.0503982
C	0.3834738	3.2403325	-2.0074021	H	-0.1723828	4.4939346	-5.1561311
C	0.3507712	-3.3066501	0.4647350	H	-1.3988469	3.4795118	-3.2545233
C	-2.9787891	-1.1216473	-0.1838391	H	2.3020895	4.8779155	-5.0086520
C	-3.9630253	-1.8903485	-0.8436419	H	-0.4733702	6.4701698	3.5300691
C	0.7055932	3.9927194	1.4680577	H	3.5466728	4.2012146	-2.9323258
C	-3.1773068	-0.7608101	1.1642669	H	-2.5607989	4.3069250	0.4207381
C	-0.8313322	-3.1586130	1.2182997	H	2.2853780	-0.1881237	-4.8189365
C	-1.4543309	-5.4558167	0.7368555	H	3.7241286	0.2836328	-3.8500516
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C	-4.3198907	-1.1958424	1.8543986	H	-3.3201164	0.7196404	-2.2654561
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C	-0.3110842	3.6182111	-3.1738245	H	-2.6217850	3.1028927	-1.5518272
C	-5.1002707	-2.3275143	-0.1485139	H	-2.7674184	2.0221540	-0.1335935
C	0.6470018	-4.5575087	-0.1127345	C	-1.2542569	2.3117831	3.7934024
C	1.7653350	4.4114511	-4.1689278	C	-0.7766569	1.4664324	2.7637049
C	-0.4692202	5.7097979	2.7355614	C	-0.3659693	2.8263811	4.7753184
C	2.4612127	4.0351997	-3.0054132	C	-0.8380644	3.7000486	5.7599135
C	-0.2552390	-5.6246885	0.0234670	C	-2.1925261	4.0780685	5.7809264
C	-5.2779352	-1.9898869	1.2040378	C	-3.0816643	3.5737367	4.8147201
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H	-0.1292893	-0.3099083	1.5909767

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C	-2.8118004	2.2908124	-0.3442039
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C	-0.9324062	0.4733336	-4.1365252
C	-0.6973241	-2.2545650	-4.7395935
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C	2.5129294	-1.7560895	0.9697743
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C	-2.1952609	3.1525248	4.1173513
C	3.7809329	-2.7819462	3.2785345
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Ru	0.2423811	0.8132096	-0.2392641
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C	-3.7142535	-1.8087645	-1.6081954
C	-0.1926784	4.1509086	2.4154407
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H	4.2675962	-3.1851563	4.1792789
H	2.6246399	-3.8046643	0.2193106
H	3.7608302	-4.6950713	2.2393922
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H	0.8837849	-5.3789513	-3.1424168
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H	-0.6107343	-3.3271499	-4.9663509
H	-0.2937687	0.8294802	-6.1794121
H	-0.0566642	-1.6116258	-6.7173933
H	-3.6525208	-1.6836459	-2.6989646
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H	-5.3660621	-3.2089687	-1.7340722
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H	0.3599285	7.3102368	-3.0167913
H	-1.2162758	4.2899459	5.6892079
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H	-2.9545704	2.1013784	2.3874688
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H	-1.7247989	-0.5461891	5.0620845
C	-0.1813089	0.2947603	1.6147452
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C	1.0227223	-2.3523999	-5.0677031
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C	0.4202136	3.1791957	-3.8412377
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C	3.5233362	0.2994047	1.1387487
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C	-2.7568372	2.0827773	1.8065903
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C	0.0259963	0.0040829	1.7676511
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H	-4.8670797	1.7857139	1.3010662
H	-1.6030257	3.1413290	4.8523327
H	-5.6837846	2.4094361	3.5654112
H	-4.0574385	3.0645304	5.3579486
H	3.0567123	0.4548407	-5.1161554
H	4.2586723	2.6510750	-4.8657943
H	2.2618081	-0.7678845	-3.1051359
H	4.6562910	3.5979269	-2.5762551
H	4.3874888	-4.3145783	-2.0394914
H	4.0850733	-1.8428994	-1.9793729
H	3.8789680	2.3546308	-0.5503285
H	3.0658210	-5.7892939	-0.5005719
H	1.4730129	-4.7585584	1.1529036
H	1.2083508	-2.2821059	1.2443443
H	5.1363617	-0.7661515	0.1178356
H	6.8089039	-0.3420343	1.9076512
H	2.1562406	1.4574532	2.3660090
H	6.1574926	0.9401986	3.9658320
H	3.8199758	1.8244553	4.1939123

H	1.5076063	-2.6054271	-6.0221149
H	-0.0199461	-0.6180586	-5.8696202
H	1.9061830	-4.0227018	-3.9855434
H	-1.1027191	-0.0374358	-3.7170261
H	0.8051052	-3.4648475	-1.8344045
H	-1.8327393	-3.8378036	-2.0580277
H	-2.4851059	-5.9703468	-0.9576647
H	-2.3940311	-6.1869151	1.5399767
H	-0.9638797	-2.1094623	1.8322384
H	-1.6566751	-4.2253899	2.9343351
H	-2.5704282	-0.0219276	-2.3818961
H	-3.2786823	-1.5381874	-1.7528606
H	-4.2999222	0.5474664	-0.6185502
H	-3.4553120	-0.4985524	0.5564406
H	0.4475328	2.6357029	-4.8057889
H	1.3712915	3.7343030	-3.7194016
H	-0.4294866	3.8919820	-3.8348602
C	-1.0449188	-0.4514628	3.9959372
H	1.1058983	-0.4123780	3.4667935
C	-2.3785657	-0.6071061	3.5463244
C	-3.4375811	-0.6804016	4.4562896
C	-3.1903622	-0.6107893	5.8384190
C	-1.8697714	-0.4766447	6.2990868
C	-0.8060963	-0.4014442	5.3892378
H	-2.5813827	-0.6627618	2.4692631
H	-4.4665804	-0.7896978	4.0838148
H	-4.0238839	-0.6666452	6.5538814
H	-1.6648450	-0.4298174	7.3792415
H	0.2252847	-0.2853886	5.7559073

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C	3.7131321	-3.1053874	-3.1626570
C	2.9636390	-2.0590265	-3.7266779
C	3.3725324	-3.5959827	-1.8917427
C	5.4383154	0.3765259	-2.1159575
C	2.9183539	2.6028848	-3.6134702
C	1.8858930	-1.5044748	-3.0211919
C	6.0338263	1.6437937	-1.9884819
C	2.2935109	-3.0453137	-1.1839148
C	4.5086851	-0.0647150	-1.1629018
C	1.5374168	-1.9923495	-1.7418854
C	2.2482423	1.8972585	-2.5438286
C	5.6924377	2.4703764	-0.9041655
C	-0.2844226	4.4073781	-4.5589567
C	4.3438971	-3.5552436	1.6173591
C	-0.7187592	3.0917477	-4.7917857
C	-0.1825315	4.8862573	-3.2406495
C	4.2517705	-2.2050310	1.2432429
C	4.1855412	0.7534827	-0.0601835

C	-0.6515476	-3.8668234	-0.4294309
C	4.7718304	2.0301783	0.0600522
C	3.2602198	-4.1943190	2.2432659
C	-1.1190787	-0.8669255	-2.0817275
C	-1.3114921	-4.9067039	0.2425060
C	-1.0474011	2.2569220	-3.7102837
C	-0.5105040	4.0586172	-2.1574823
C	3.0668164	-1.4856536	1.4957671
C	-0.9462282	2.7355954	-2.3878651
C	-0.5784565	-2.5800373	0.1486690
C	2.0879015	-3.4703054	2.5227174
C	-2.1319603	0.1634453	-1.5888774
C	1.9966577	-2.1199528	2.1584839
C	-1.9222399	-4.6717202	1.4880755
C	-1.1903976	-2.3522091	1.3947078
C	4.5455470	0.6415497	3.2725299
C	3.3287788	1.0621761	2.6901874
C	-1.8651716	-3.3892031	2.0599541
C	-2.4861722	2.5489212	0.0843452
C	4.9540156	1.1643435	4.5065074
C	2.5313782	2.0118124	3.3547145
C	-2.0857709	3.2341793	1.2481427
C	-3.8509485	2.4922433	-0.2698744
C	-0.6597377	0.7292007	2.9582762
C	4.1497407	2.1046321	5.1744365
C	2.9429545	2.5261225	4.5960252
C	-3.0548959	3.8232013	2.0737253
C	-4.8099943	3.0845064	0.5618110
C	-4.4148960	3.7381245	1.7414201
N	1.6971012	1.3666479	-1.6640837
C	-0.1051888	0.7120512	1.7465341
P	0.1915718	-1.1868605	-0.7790374
P	2.8405653	0.2912135	1.0878423
P	-1.2603944	1.6638396	-0.9353046
Cl	1.3078111	3.2330675	0.6030582
Ru	0.7249684	0.8869442	0.1297684
H	-0.0358520	5.0642886	-5.4061065
H	-0.8164734	2.7142213	-5.8208190
H	0.1498935	5.9182307	-3.0527132
H	-1.3960011	1.2344209	-3.9133983
H	-0.4081678	4.4269640	-1.1272299
H	-1.0185589	3.2918287	1.5046983
H	-4.1733496	1.9702731	-1.1808907
H	-2.7411485	4.3385221	2.9929180
H	-5.8747590	3.0285108	0.2915170
H	-5.1728016	4.1838442	2.4021359
H	5.6961474	-0.2790813	-2.9612800
H	6.7684238	1.9863511	-2.7330051
H	4.0304107	-1.0443661	-1.2850312
H	6.1527971	3.4643950	-0.8009484

H	5.2699957	-4.1134174	1.4133669
H	5.1019341	-1.7190526	0.7441947
H	4.4981416	2.6818719	0.9020388
H	3.3333392	-5.2556083	2.5237782
H	1.2360910	-3.9576021	3.0198459
H	1.0858131	-1.5489242	2.3866134
H	5.1759738	-0.1027027	2.7643760
H	5.9039165	0.8318012	4.9508152
H	1.6158081	2.3847658	2.8781078
H	4.4700407	2.5117277	6.1451899
H	2.3159638	3.2724525	5.1065275
H	4.5586870	-3.5410698	-3.7152560
H	3.2180133	-1.6732515	-4.7251791
H	3.9516565	-4.4129683	-1.4374219
H	1.3214718	-0.6791547	-3.4755640
H	2.0407198	-3.4414515	-0.1916049
H	-0.1873594	-4.0633734	-1.4068302
H	-1.3542164	-5.9072087	-0.2131776
H	-2.4447140	-5.4875459	2.0093539
H	-1.1313824	-1.3617418	1.8575495
H	-2.3471951	-3.1836389	3.0269361
H	-0.5914056	-0.5060909	-2.9860953
H	-1.6095714	-1.8247523	-2.3413401
H	-2.8528676	0.4312913	-2.3852072
H	-2.7369962	-0.2371388	-0.7494318
H	3.6525653	1.9414774	-4.1127557
H	3.4553995	3.4731245	-3.1873573
H	2.1654727	2.9631120	-4.3432578
C	-2.0898540	0.7034139	3.2973882
H	0.0667624	0.8165650	3.7892099
C	-3.0804108	0.3027249	2.3690461
C	-4.4348816	0.3144503	2.7153636
C	-4.8335217	0.7379973	3.9947240
C	-3.8605822	1.1320265	4.9296433
C	-2.5010989	1.1068773	4.5899388
H	-2.8024547	-0.0289906	1.3605919
H	-5.1612286	-0.0351524	1.9682417
H	-5.8991975	0.7507705	4.2676577
H	-4.1625387	1.4561139	5.9370918
H	-1.7428987	1.4154242	5.3260567
N	-4.6820244	-1.3882116	-0.1918829
C	-5.3952282	-1.0634045	-1.2869646
C	-5.1356350	-1.9830323	-2.3447114
C	-4.2264788	-2.9091598	-1.8261923
N	-3.9886883	-2.4982338	-0.5415341
H	-3.3902976	-2.9483063	0.1568551
C	-3.5936018	-4.1195180	-2.4343175
H	-5.5754222	-1.9955538	-3.3477134
C	-6.3362382	0.1020892	-1.2745945
H	-2.5143254	-3.9662951	-2.6483693

H	-3.6680825	-4.9992480	-1.7642322
H	-4.0927282	-4.3716332	-3.3879336
H	-7.3864922	-0.2311840	-1.4046447
H	-6.2633223	0.6395570	-0.3116310
H	-6.1222487	0.8155782	-2.0968575

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C	1.0741955	-2.8368594	-5.6441705
C	0.0877595	-1.8391207	-5.5771530
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C	2.5636579	0.7496663	-5.1139563
C	-0.6730239	2.7274585	-4.4895314
C	-0.4941361	-1.5064612	-4.3453805
C	2.8022954	2.1334405	-5.1280381
C	0.8788365	-3.1851363	-3.2409884
C	2.4447814	0.0639306	-3.8945070
C	-0.1068949	-2.1776839	-3.1653249
C	-0.4817709	1.8397593	-3.3632739
C	2.9130560	2.8337133	-3.9129618
C	-3.8318672	4.2351003	-3.0028120
C	4.2725259	-3.5290878	-2.0503127
C	-4.2722868	2.9298107	-3.2768046
C	-2.9903826	4.4702393	-1.9004379
C	3.8356437	-2.1955122	-2.0718378
C	2.5753429	0.7588848	-2.6761801
C	-1.4116336	-4.4652393	-1.3843444
C	2.7967298	2.1545877	-2.6914684
C	3.7507328	-4.4326386	-1.1081000
C	-2.6362329	-1.4143653	-1.9770728
C	-1.5615877	-5.6969602	-0.7337411
C	-3.8743812	1.8627857	-2.4522977
C	-2.5923156	3.4103127	-1.0737172
C	2.8568426	-1.7646098	-1.1545579
C	-3.0361241	2.0969555	-1.3435107
C	-0.9549133	-3.3349014	-0.6670230
C	2.8096814	-3.9912337	-0.1622593
C	-3.3522905	-0.7682784	-0.7920339
C	2.3715607	-2.6596581	-0.1814540
C	-1.2665440	-5.8137703	0.6368780
C	-0.6602654	-3.4604896	0.7005971
C	4.7797761	0.9916796	-0.4334901
C	3.4881740	0.7003244	0.0571593
C	-0.8198006	-4.6934000	1.3526664
C	-3.0259940	1.1486756	1.4137885
C	5.7700823	1.4607528	0.4417293
C	3.2128953	0.8634876	1.4241433
C	-4.3206585	0.7638477	1.8236610
C	-2.1551359	1.7729264	2.3275145
C	-0.0254254	-0.5251426	2.4994501

C	5.4841891	1.6333530	1.8075111	H	-3.3636080	-1.4533381	0.0801810
C	4.2046387	1.3302565	2.2987409	H	-1.7294476	3.0637754	-4.5174620
C	-4.7150612	0.9593399	3.1545907	H	-0.4075055	2.2154211	-5.4349014
C	-2.5522515	1.9554064	3.6600446	H	-0.0122704	3.6082374	-4.3707869
C	-3.8250811	1.5358654	4.0769158	C	-1.0519974	-1.0992618	3.3760468
N	-0.3408102	1.1487177	-2.4342587	H	0.8231145	-0.0246084	3.0429603
C	-0.0208964	-0.3305086	1.1876504	C	-2.2531881	-1.6634472	2.8856168
P	-0.8379323	-1.7226414	-1.5407978	C	-3.2246033	-2.1573577	3.7626459
P	2.2343363	-0.0410377	-1.0631667	C	-3.0210336	-2.0998938	5.1519425
P	-2.4172613	0.7507676	-0.2584377	C	-1.8294532	-1.5479869	5.6528498
Cl	0.5336983	2.5558929	0.0926790	C	-0.8545310	-1.0550205	4.7767825
Ru	-0.1008537	0.2550191	-0.5583531	H	-2.4261784	-1.7044915	1.8033439
H	-4.1499323	5.0707481	-3.6440259	H	-4.1540195	-2.5853705	3.3580173
H	-4.9404748	2.7381133	-4.1299080	H	-3.7868201	-2.4855117	5.8410161
H	-2.6439766	5.4906767	-1.6784627	H	-1.6576835	-1.5010882	6.7388145
H	-4.2395956	0.8516088	-2.6811685	H	0.0715699	-0.6144743	5.1689112
H	-1.9128640	3.5931877	-0.2289741	N	1.4437912	1.6400234	4.0619992
H	-5.0206235	0.2945079	1.1168363	C	1.2163943	2.0679456	5.3216656
H	-1.1561661	2.0815104	1.9977919	C	0.6253881	3.3633032	5.3024349
H	-5.7180248	0.6439595	3.4774990	C	0.5046022	3.7019240	3.9487787
H	-1.8463567	2.4037468	4.3753967	N	1.0096158	2.6378641	3.2609711
H	-4.1266583	1.6562940	5.1276342	H	1.0513200	2.5432710	2.2291309
H	2.4736999	0.1900965	-6.0569658	C	-0.0703315	4.8945131	3.2534889
H	2.9068285	2.6671894	-6.0848443	H	0.3385051	3.9807265	6.1603595
H	2.2464992	-1.0145698	-3.8998458	C	1.5844019	1.2231819	6.5026755
H	3.0992926	3.9183770	-3.9146951	H	-1.1558246	4.7612007	3.0569373
H	5.0285644	-3.8643281	-2.7761457	H	0.0481456	5.8053362	3.8698041
H	4.2542207	-1.4966070	-2.8090407	H	0.4234903	5.0650447	2.2767920
H	2.8600600	2.7076148	-1.7436266	H	0.6886985	0.9263967	7.0870273
H	4.0902175	-5.4790608	-1.1019160	H	2.1062471	0.3053636	6.1714764
H	2.4061554	-4.6856875	0.5893862	H	2.2556489	1.7695521	7.1959809
H	1.6470473	-2.3040005	0.5630530	1_TS-f_g-cisoid			
H	5.0135660	0.8573838	-1.4997174	C	1.6370780	-2.4346184	-5.1930343
H	6.7729096	1.6926386	0.0529443	C	0.8521531	-1.3353541	-5.5762203
H	2.2197044	0.6267074	1.8169444	C	1.6134783	-2.8802745	-3.8605393
H	6.2636674	2.0048939	2.4895262	C	3.8086878	0.5792768	-4.1121236
H	3.9489589	1.4609456	3.3599475	C	2.3692669	4.0241251	-2.7667318
H	1.5327567	-3.0970406	-6.6096828	C	0.0445134	-0.6787334	-4.6327817
H	-0.2327236	-1.3157622	-6.4902486	C	5.2025806	0.6242373	-3.9504138
H	2.2373870	-4.2899787	-4.5134761	C	0.8255853	-2.2157097	-2.9128265
H	-1.2575583	-0.7175775	-4.3129192	C	2.9766423	0.3663476	-3.0014638
H	1.1878835	-3.7262127	-2.3363630	C	0.0360771	-1.1092882	-3.2900426
H	-1.6385798	-4.3890107	-2.4587094	C	1.5739473	2.9962095	-2.1270081
H	-1.9127015	-6.5723247	-1.3001214	C	5.7580554	0.4466337	-2.6714440
H	-1.3886897	-6.7819373	1.1451980	C	-0.6380687	6.7477867	-0.6239105
H	-0.2912919	-2.5932896	1.2605097	C	3.7419818	-4.0938066	-0.8374867
H	-0.5951764	-4.7673786	2.4266953	C	-0.7295895	5.9495358	-1.7755961
H	-2.6516014	-0.7401586	-2.8564076	C	-0.9005265	6.1833201	0.6349726
H	-3.1054907	-2.3716779	-2.2783320				
H	-4.4075790	-0.5264751	-1.0278670				

C	3.4918914	-2.7257213	-1.0249744	H	1.8933259	0.3252509	-3.1428497
C	3.5218754	0.1965166	-1.7156030	H	6.8495556	0.4712586	-2.5343665
C	-2.4720260	-2.5882739	-2.5257726	H	4.3219352	-4.6464479	-1.5921466
C	4.9266664	0.2317469	-1.5622444	H	3.8782563	-2.2228861	-1.9210159
C	3.2768687	-4.7525045	0.3130735	H	5.3728713	0.0861786	-0.5683122
C	-1.7901241	1.1420708	-2.8568112	H	3.4924998	-5.8205674	0.4651386
C	-3.5892731	-3.4277792	-2.3861131	H	2.1784421	-4.5351734	2.1794340
C	-1.0723755	4.5925464	-1.6652779	H	1.6641334	-2.1207039	1.8021549
C	-1.2404584	4.8273457	0.7486856	H	3.4344929	-1.1743003	2.4603542
C	2.7482939	-1.9975641	-0.0704521	H	4.6757879	-0.0276626	4.2697626
C	-1.3275436	4.0181761	-0.4016678	H	3.7018096	2.4076077	0.0126394
C	-2.3658932	-1.3995800	-1.7701398	H	5.4809924	2.3299055	3.9605756
C	2.5431700	-4.0343483	1.2694831	H	4.9938057	3.5355748	1.8117643
C	-2.6549016	1.9081222	-1.8509613	H	2.2685552	-2.9457368	-5.9345930
C	2.2671078	-2.6730480	1.0716608	H	0.8625965	-0.9871049	-6.6198814
C	-4.6199443	-3.0996662	-1.4903847	H	2.2235043	-3.7407946	-3.5502630
C	-3.4258511	-1.0674376	-0.8915405	H	-0.5680234	0.1752981	-4.9525521
C	3.7524175	-0.1349312	2.3104882	H	0.8360064	-2.5475821	-1.8653814
C	3.4742396	0.5356501	1.1058834	H	-1.6752899	-2.8636345	-3.2295384
C	-4.5351755	-1.9139073	-0.7442007	H	-3.6493120	-4.3498765	-2.9832690
C	-2.8782963	2.0963786	1.1248548	H	-5.4878375	-3.7656075	-1.3764598
C	4.4655666	0.5119176	3.3343047	H	-3.3910783	-0.1670542	-0.2613417
C	3.9203216	1.8667948	0.9438684	H	-5.3287327	-1.6367665	-0.0353261
C	-2.3432517	2.0686133	2.4310319	H	-1.0006503	1.7920054	-3.2869691
C	-4.2738345	2.0153917	0.9383419	H	-2.4035861	0.7351058	-3.6852215
C	0.2890146	-0.2808359	2.6465432	H	-3.0060030	2.8737754	-2.2611564
C	4.9171666	1.8279196	3.1602377	H	-3.5600494	1.3206429	-1.6111388
C	4.6484649	2.5011767	1.9567459	H	1.7900660	4.5335662	-3.5616374
C	-3.2021130	1.9777614	3.5338817	H	3.2774402	3.5685647	-3.2126558
C	-5.1239403	1.8917324	2.0480627	H	2.6668020	4.7806250	-2.0131093
C	-4.5894703	1.8793904	3.3469497	C	-0.0718131	-1.0038645	3.8808135
N	0.9882472	2.1469161	-1.5767556	H	1.0379993	0.5343820	2.7632865
C	-0.1652046	-0.2637973	1.3841903	C	0.0745990	-2.3986284	4.0287542
P	-0.9040583	-0.2526153	-1.9708113	C	-0.2765044	-3.0360362	5.2291853
P	2.4469583	-0.1820444	-0.2515293	C	-0.7673361	-2.2874904	6.3103508
P	-1.6954047	2.2168547	-0.2636453	C	-0.8878867	-0.8913309	6.1880447
Cl	0.9889695	2.5188017	1.3517310	C	-0.5340432	-0.2569894	4.9902655
Ru	0.2096646	0.8208550	-0.2431071	H	0.4647303	-2.9961343	3.1953733
H	-0.3745395	7.8125605	-0.7088633	H	-0.1559741	-4.1259459	5.3232490
H	-0.5474015	6.3878995	-2.7687958	H	-1.0368622	-2.7864819	7.2532035
H	-0.8412591	6.8037533	1.5413634	H	-1.2534779	-0.2930412	7.0362867
H	-1.1435195	3.9874026	-2.5806429	H	-0.6172082	0.8354935	4.8961345
H	-1.4451638	4.3993667	1.7384489	N	-2.6479533	-1.0236459	2.2703569
H	-1.2516704	2.1110477	2.5642122	C	-3.0349541	-2.0944731	2.9369527
H	-4.7135930	2.0602463	-0.0690934	C	-2.4115336	-3.3016009	2.4198296
H	-2.7818972	1.9606885	4.5499039	C	-1.5929141	-2.9025945	1.3985985
H	-6.2117673	1.8252053	1.8959577	N	-1.6905883	-1.4771059	1.3512782
H	-5.2599046	1.7978198	4.2157291	H	-1.9139226	-1.1339600	0.4063372
H	3.3579802	0.7007337	-5.1084803	C	-0.7923989	-3.6417919	0.3884231
H	5.8573043	0.7900620	-4.8191033	H	-2.5610682	-4.3247037	2.7812292

C	-3.9701817	-1.9846403	4.0927143
H	0.0937798	-3.0565617	0.0832023
H	-0.4454576	-4.6135377	0.7841089
H	-1.4005191	-3.8370811	-0.5191830
H	-3.4081443	-2.1410265	5.0370302
H	-4.4231323	-0.9771366	4.1173925
H	-4.7663028	-2.7538358	4.0441274

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C	2.5497249	-2.0885114	-4.9701628
C	1.2855492	-1.4746602	-4.9691855
C	3.0822924	-2.5781995	-3.7672274
C	3.0637205	1.7269446	-4.4492504
C	-0.3005808	2.6029537	-4.3124670
C	0.5657013	-1.3479698	-3.7726466
C	3.2079521	3.1227060	-4.5284901
C	2.3600030	-2.4596818	-2.5693710
C	2.8663571	1.1069940	-3.2077493
C	1.0915318	-1.8433246	-2.5575271
C	-0.1553668	1.8406543	-3.0913340
C	3.1455051	3.8894992	-3.3540306
C	-3.9983248	2.8910620	-3.8430931
C	5.6076274	-1.6267348	-1.3633964
C	-3.8021817	1.5145894	-4.0425068
C	-3.6773125	3.4672346	-2.6010145
C	4.7563743	-0.5108232	-1.3883438
C	2.8311487	1.8685062	-2.0191973
C	0.7583024	-4.3486733	-0.6061132
C	2.9614841	3.2680515	-2.1067849
C	5.4066776	-2.6547745	-0.4261596
C	-1.5744344	-2.1488481	-1.5770688
C	1.1573669	-5.4728029	0.1314169
C	-3.2973727	0.7167682	-3.0019082
C	-3.1772910	2.6726249	-1.5589086
C	3.6830837	-0.4195162	-0.4771992
C	-2.9952287	1.2868813	-1.7484190
C	0.6978153	-3.0775727	0.0075161
C	4.3667689	-2.5447992	0.5118535
C	-2.7127566	-1.4688225	-0.8265914
C	3.5198241	-1.4274541	0.4904932
C	1.4903976	-5.3427687	1.4908245
C	1.0262977	-2.9578021	1.3709814
C	4.7196410	1.7206296	1.2822804
C	3.4718555	2.1311739	0.7652116
C	1.4169257	-4.0848803	2.1089588
C	-3.4358122	0.6829824	1.0052343
C	5.4120384	2.5246152	2.1985941
C	2.9477487	3.3779612	1.1737556
C	-4.6352768	-0.0372474	1.1783566

C	-3.1400015	1.7638204	1.8596180
C	-0.7857404	-0.4025279	2.8235251
C	4.8728720	3.7511139	2.6203326
C	3.6416624	4.1754676	2.0990859
C	-5.5250480	0.3173761	2.2028950
C	-4.0384176	2.1170593	2.8772444
C	-5.2302516	1.3946014	3.0533036
N	-0.0421739	1.2453812	-2.0938184
C	-0.1478173	0.1183523	1.7459628
P	0.1433665	-1.6213704	-0.9823755
P	2.5280419	1.0177852	-0.4016896
P	-2.2913620	0.2828670	-0.3712740
Cl	-0.2476763	2.9446745	0.3792165
Ru	0.0226483	0.5301850	-0.1881358
H	-4.4046637	3.5145095	-4.6535744
H	-4.0507562	1.0542807	-5.0106903
H	-3.8253288	4.5452365	-2.4379162
H	-3.1508398	-0.3582738	-3.1793322
H	-2.9191017	3.1327073	-0.5949601
H	-4.8852979	-0.8838730	0.5248589
H	-2.2042438	2.3218044	1.7124406
H	-6.4535221	-0.2565677	2.3370080
H	-3.8085803	2.9681182	3.5362882
H	-5.9320086	1.6720153	3.8539696
H	3.1079719	1.1069243	-5.3570956
H	3.3709451	3.6104670	-5.5013637
H	2.7469122	0.0192656	-3.1657158
H	3.2578194	4.9830985	-3.4007255
H	6.4368718	-1.6912387	-2.0838213
H	4.9367323	0.2875736	-2.1207100
H	2.9377573	3.8851055	-1.2000565
H	6.0692735	-3.5331913	-0.4184389
H	4.2014280	-3.3349397	1.2593665
H	2.7377366	-1.2993076	1.2443928
H	5.1506530	0.7568499	0.9836865
H	6.3833568	2.1839322	2.5879232
H	1.9772672	3.7196057	0.7880236
H	5.4152085	4.3763670	3.3452535
H	3.2113488	5.1397386	2.4090515
H	3.1154986	-2.1892025	-5.9081734
H	0.8550803	-1.0930147	-5.9071932
H	4.0712279	-3.0584064	-3.7516476
H	-0.4128455	-0.8492754	-3.7928402
H	2.7917590	-2.8522636	-1.6396190
H	0.5090451	-4.4637496	-1.6723122
H	1.2076842	-6.4563710	-0.3591233
H	1.7993405	-6.2266401	2.0686266
H	0.9503586	-1.9774672	1.8600719
H	1.6585450	-3.9759577	3.1766181
H	-1.6085512	-1.8964492	-2.6535281

H	-1.6421854	-3.2522584	-1.5061025
H	-3.6547363	-1.4901209	-1.4083955
H	-2.9076600	-1.9707165	0.1381092
H	-1.3584718	2.9105094	-4.4342137
H	0.0130828	1.9955252	-5.1838432
H	0.3475926	3.4997473	-4.2612099
C	-1.9085560	-1.3533976	2.9229828
H	-0.4870540	-0.0338965	3.8189358
C	-2.0760637	-2.5085715	2.1284998
C	-3.1697173	-3.3676949	2.3218593
C	-4.1229268	-3.0939055	3.3145520
C	-3.9561268	-1.9627091	4.1332818
C	-2.8598353	-1.1140219	3.9472411
H	-1.3210961	-2.7620336	1.3792017
H	-3.2667939	-4.2674881	1.6952903
H	-4.9793720	-3.7676261	3.4645160
H	-4.6877745	-1.7410785	4.9242694
H	-2.7408555	-0.2279851	4.5880430
N	2.2159602	0.4796766	2.6955797
C	2.5740338	0.5073920	3.9621893
C	1.7018264	1.3786514	4.7387606
C	0.7861092	1.8871604	3.8553108
N	1.0734988	1.2860726	2.5987334
H	1.0473854	1.9625715	1.7977883
C	-0.3451976	2.8385064	3.9966009
H	1.7781618	1.6030380	5.8086668
C	3.7527859	-0.2669338	4.4486144
H	-1.3124338	2.2942311	3.9568566
H	-0.2826176	3.3843514	4.9549607
H	-0.3580493	3.5576164	3.1524410
H	3.4728374	-0.9454551	5.2796166
H	4.1897164	-0.8591398	3.6242134
H	4.5292526	0.4242908	4.8364914

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C	0.5037544	-2.7254008	-5.3540239
C	-0.6502108	-1.9432252	-5.5200766
C	1.0499368	-2.8983726	-4.0710565
C	1.9675788	0.7858456	-5.1630332
C	0.0913618	4.1274339	-3.5915442
C	-1.2637389	-1.3391204	-4.4096092
C	3.3089321	1.0119178	-5.5065940
C	0.4557948	-2.2754178	-2.9665437
C	1.6012526	0.6373278	-3.8153346
C	-0.7079970	-1.4947598	-3.1236327
C	-0.1125914	3.0286868	-2.6677350
C	4.2814911	1.0919946	-4.4937569
C	-2.7129593	6.2538321	-0.7236243
C	4.1291757	-3.1539304	-1.3911114

C	-2.9418480	5.3252435	-1.7520290
C	-2.4013921	5.7968665	0.5671436
C	3.4616363	-1.9524033	-1.6758438
C	2.5656905	0.7095593	-2.7957890
C	-2.2810820	-3.4288702	-1.4414703
C	3.9141991	0.9459860	-3.1489717
C	4.4328557	-3.5003005	-0.0642286
C	-2.8614803	0.2883704	-2.2657583
C	-2.9894100	-4.4942845	-0.8631667
C	-2.8484878	3.9485763	-1.4903838
C	-2.3082676	4.4226133	0.8315083
C	3.0568268	-1.0882331	-0.6347543
C	-2.5305437	3.4844189	-0.1963576
C	-2.3483303	-2.1304756	-0.8883282
C	4.0562257	-2.6374471	0.9772573
C	-3.5831084	0.9536701	-1.0904905
C	3.3620393	-1.4498968	0.6982259
C	-3.7829787	-4.2902700	0.2777425
C	-3.1716801	-1.9364194	0.2494854
C	4.3500674	1.5341761	0.5544932
C	3.2673705	1.7795870	-0.3081763
C	-3.8736875	-3.0048499	0.8313738
C	-3.0354833	1.4488665	1.7991987
C	5.1635897	2.5938974	0.9945806
C	3.0195191	3.1045231	-0.7314601
C	-2.1840495	1.6973306	2.8972890
C	-4.3611674	1.0238087	2.0265570
C	1.0036663	0.0430704	2.3581240
C	4.9101838	3.9050636	0.5694212
C	3.8371990	4.1555733	-0.3034138
C	-2.6643527	1.5361575	4.2037055
C	-4.8227946	0.8294453	3.3378562
C	-3.9766165	1.0915263	4.4285112
N	-0.2263103	2.1485154	-1.9041370
C	0.1290795	-0.2696576	1.3674950
P	-1.3945558	-0.6880070	-1.6217901
P	2.1417584	0.4766774	-0.9999684
P	-2.3362606	1.6771350	0.1203102
Cl	0.4883417	2.7855671	0.9402547
Ru	-0.1997542	0.8218314	-0.3670263
H	-2.7900782	7.3326239	-0.9254301
H	-3.2112482	5.6716902	-2.7617792
H	-2.2292610	6.5168110	1.3808485
H	-3.0317632	3.2401249	-2.3110414
H	-2.0657597	4.0800475	1.8453447
H	-1.1442104	2.0062431	2.7059169
H	-5.0512736	0.8523449	1.1872015
H	-2.0002881	1.7393813	5.0564363
H	-5.8570958	0.4940073	3.5073615
H	-4.3467813	0.9560919	5.4560955

H	1.1957594	0.7158863	-5.9441140	C	0.5950494	-3.3687964	0.6248696
H	3.5998146	1.1276216	-6.5615430	H	-0.5911865	-4.4862157	3.1793135
H	0.5547231	0.4583290	-3.5587471	C	-2.2759320	-2.6140943	4.8356596
H	5.3354682	1.2728787	-4.7527788	H	1.2902919	-2.5852032	0.2732755
H	4.4353251	-3.8135028	-2.2173472	H	1.1790530	-4.2528680	0.9375753
H	3.2632530	-1.6768318	-2.7199248	H	-0.0491529	-3.6660323	-0.2279488
H	4.6808655	1.0161063	-2.3634866	H	-1.5320096	-2.7557884	5.6466803
H	4.9747244	-4.4323415	0.1551725	H	-2.8778662	-1.7139073	5.0543964
H	4.3046790	-2.8859102	2.0201620	H	-2.9286717	-3.5093792	4.8177597
H	3.0419567	-0.8038037	1.5238065				
H	4.5921936	0.5135182	0.8752329	l_g-transoid			
H	6.0083149	2.3827157	1.6672244	C	1.0772388	-1.9237532	-5.4045798
H	2.1777704	3.3104192	-1.4042260	C	0.0439631	-0.9963769	-5.1863653
H	5.5494587	4.7320875	0.9126742	C	1.5306032	-2.7174161	-4.3392438
H	3.6277419	5.1810348	-0.6423874	C	2.7152903	1.5081569	-4.4794311
H	0.9791320	-3.1990611	-6.2255019	C	-0.2526563	3.2087925	-3.8932829
H	-1.0833635	-1.8060210	-6.5222258	C	-0.5240335	-0.8635028	-3.9116041
H	1.9537967	-3.5094774	-3.9315280	C	3.2282112	2.8130025	-4.3812037
H	-2.1715917	-0.7394185	-4.5612592	C	0.9587938	-2.5900803	-3.0632458
H	0.9101875	-2.3763302	-1.9716574	C	2.4292363	0.7727003	-3.3208844
H	-1.6708300	-3.6107955	-2.3366946	C	-0.0769981	-1.6614729	-2.8333206
H	-2.9190402	-5.4960922	-1.3129452	C	-0.2439159	2.2632659	-2.7975291
H	-4.3311804	-5.1302859	0.7291549	C	3.4465624	3.3745147	-3.1131754
H	-3.2557702	-0.9545183	0.7369610	C	-3.6873734	4.3741830	-3.0860022
H	-4.4907466	-2.8162005	1.7221270	C	4.3999029	-2.8472977	-2.1450139
H	-2.4419015	1.0447842	-2.9604734	C	-3.9077234	3.0354142	-3.4489494
H	-3.5465087	-0.3717162	-2.8340399	C	-3.1226256	4.6706080	-1.8326887
H	-4.2738701	1.7494164	-1.4268619	C	3.8859465	-1.5572135	-1.9403364
H	-4.2026448	0.2079997	-0.5608433	C	2.6767918	1.3194207	-2.0428544
H	-0.1243813	3.8126507	-4.6320031	C	-0.9179013	-4.2410222	-1.1333704
H	1.1464422	4.4655666	-3.5425875	C	3.1770709	2.6324754	-1.9504844
H	-0.5703154	4.9745440	-3.3182878	C	3.9958374	-3.9136395	-1.3233309
C	1.1748366	-0.5955016	3.6852243	C	-2.6469100	-1.3998008	-1.6196658
H	1.5594751	0.9830431	2.1882419	C	-0.7829709	-5.5132830	-0.5580928
C	1.7552149	-1.8703737	3.8548434	C	-3.5773649	1.9999158	-2.5577523
C	1.8544030	-2.4549814	5.1278889	C	-2.7961944	3.6391466	-0.9403323
C	1.3874419	-1.7665028	6.2587742	C	2.9490284	-1.3227754	-0.9120399
C	0.8424263	-0.4778024	6.1100693	C	-3.0347925	2.2935767	-1.2904137
C	0.7475573	0.1037390	4.8391645	C	-0.6011203	-3.0843254	-0.3874616
H	2.1313191	-2.4128319	2.9776624	C	3.0987354	-3.6747107	-0.2689753
H	2.3094529	-3.4512390	5.2378358	C	-3.4984939	-0.5236770	-0.7099850
H	1.4682914	-2.2216555	7.2573591	C	2.5906319	-2.3844271	-0.0607393
H	0.4937768	0.0781018	6.9936310	C	-0.3413633	-5.6437242	0.7701445
H	0.3241487	1.1112533	4.7197403	C	-0.1677512	-3.2238247	0.9443609
N	-1.5728249	-1.2979015	2.9146667	C	4.6838136	0.1758700	0.9431885
C	-1.5580318	-2.4466622	3.5404429	C	3.5419638	0.9587771	0.6641622
C	-0.7579794	-3.4545266	2.8508866	C	-0.0411987	-4.4961047	1.5211132
C	-0.2347741	-2.8703331	1.7435774	C	-3.4713608	1.4900834	1.3977524
N	-0.7599626	-1.4881812	1.7275594	C	5.6351131	0.6064769	1.8791510
H	-1.4744372	-1.5117303	0.9595313				

C	3.3969812	2.1968634	1.3300642	H	0.2881969	-4.5877387	2.5668040
C	-4.8128781	1.1096114	1.6034213	H	-2.6842780	-1.0362778	-2.6636317
C	-2.8417336	2.3486442	2.3202596	H	-3.0073277	-2.4470350	-1.6339817
C	-1.1094600	-0.4547283	2.8909786	H	-4.4308947	-0.1974801	-1.2103347
C	5.4642578	1.8211131	2.5642228	H	-3.7897981	-1.0668124	0.2055177
C	4.3438257	2.6156570	2.2801410	H	-1.2779382	3.6052760	-4.0350550
C	-5.5108291	1.5755440	2.7273137	H	0.0945993	2.7181176	-4.8235737
C	-3.5473204	2.8160691	3.4387376	H	0.4370022	4.0451020	-3.6655592
C	-4.8814338	2.4286232	3.6473691	C	-2.4432297	-1.0681907	2.9446166
N	-0.2425633	1.5141412	-1.9010516	H	-0.7110572	-0.3184476	3.9131644
C	-0.3229700	0.0080845	1.8726246	C	-2.9441000	-2.0205052	2.0310664
P	-0.8116686	-1.4142599	-1.1485472	C	-4.2175400	-2.5865489	2.1985715
P	2.2401731	0.3408843	-0.5342110	C	-5.0266184	-2.2102705	3.2812911
P	-2.5555402	0.9604386	-0.1036951	C	-4.5353789	-1.2808816	4.2152969
Cl	0.2076037	2.8514023	0.7496259	C	-3.2591621	-0.7328145	4.0561414
Ru	-0.2640909	0.5511321	-0.1260073	H	-2.3145093	-2.3532667	1.2017556
H	-3.9569908	5.1862245	-3.7778232	H	-4.5736502	-3.3386426	1.4778634
H	-4.3475270	2.7917852	-4.4278939	H	-6.0253719	-2.6531398	3.4100529
H	-2.9421979	5.7164740	-1.5424615	H	-5.1528089	-0.9840667	5.0760120
H	-3.7588740	0.9593665	-2.8632461	H	-2.8838093	-0.0063479	4.7927676
H	-2.3449465	3.8804501	0.0321274	N	1.9747685	-0.5261287	2.4711658
H	-5.3261814	0.4417342	0.8983992	C	2.5523518	-0.5668488	3.6443713
H	-1.7987971	2.6467138	2.1431347	C	2.0313004	0.4545213	4.5527343
H	-6.5541673	1.2650703	2.8845948	C	1.0641976	1.1325380	3.8818821
H	-3.0538672	3.4948786	4.1513188	N	1.0093594	0.5384492	2.5346011
H	-5.4328465	2.7945697	4.5263354	H	1.2681057	1.3251072	1.8680081
H	2.5336298	1.0504101	-5.4635655	C	0.2240684	2.3029903	4.2180240
H	3.4584667	3.3894906	-5.2898094	H	2.3716830	0.6489188	5.5762710
H	2.0157135	-0.2372221	-3.4156861	C	3.6215629	-1.5612224	3.9416192
H	3.8472737	4.3952737	-3.0218024	H	-0.8490389	2.0218359	4.2341136
H	5.1234467	-3.0186695	-2.9561534	H	0.5109248	2.7162754	5.2013714
H	4.2217774	-0.7351861	-2.5858272	H	0.3260553	3.0799260	3.4310730
H	3.3737750	3.0838557	-0.9697171	H	3.3527985	-2.1735926	4.8264009
H	4.3908183	-4.9257995	-1.4971774	H	3.7889108	-2.2202454	3.0711038
H	2.7786808	-4.4949277	0.3909953	H	4.5682274	-1.0341746	4.1772623
H	1.9267809	-2.1761178	0.7825955	1_h-cis-precursor			
H	4.8296545	-0.7872344	0.4380379	C	-0.8213640	-3.7598949	-4.6446285
H	6.5194659	-0.0188775	2.0750167	C	-2.1138219	-3.4221665	-4.2143625
H	2.5293930	2.8370844	1.1160820	C	0.2739980	-3.5231755	-3.7976540
H	6.2088861	2.1521426	3.3035627	C	-0.7677516	-0.2062919	-5.5082206
H	4.2032024	3.5798687	2.7916660	C	-3.4898102	2.2965604	-3.4793056
H	1.5240339	-2.0304146	-6.4042224	C	-2.3126532	-2.8495562	-2.9464112
H	-0.3238812	-0.3721854	-6.0144920	C	0.0908820	0.3814599	-6.4486524
H	2.3395690	-3.4459474	-4.4944264	C	0.0788638	-2.9408056	-2.5391427
H	-1.3192865	-0.1208934	-3.7599910	C	-0.4874329	-0.1032537	-4.1349514
H	1.3258024	-3.2214427	-2.2440029	C	-1.2163043	-2.5951607	-2.0961087
H	-1.2567793	-4.1530977	-2.1769585	C	-2.7082051	1.5439645	-2.5161459
H	-1.0255684	-6.4080491	-1.1505708	C	1.2345049	1.0729698	-6.0085778
H	-0.2403828	-6.6424518	1.2207579				
H	0.0499826	-2.3224273	1.5336511				

C	-5.5766908	3.9340492	0.1638332	H	-2.8014452	-0.4586891	6.1402151
C	4.1185895	-1.9332790	-2.8569032	H	-1.1158300	1.2923674	6.7572909
C	-5.6608333	2.6749467	-0.4523381	H	-1.6595300	-0.7613510	-5.8360052
C	-4.5890650	4.1639861	1.1359034	H	-0.1256892	0.3010707	-7.5250345
C	2.9411191	-1.1691862	-2.8872965	H	-1.1554554	-0.5732815	-3.4087018
C	0.6492552	0.5887472	-3.6848105	H	1.9161258	1.5353250	-6.7387291
C	-1.0826659	-4.4612014	0.3141230	H	4.3346445	-2.6277966	-3.6834031
C	1.5108953	1.1778141	-4.6389106	H	2.2561768	-1.2696063	-3.7396516
C	5.0244038	-1.8009290	-1.7916292	H	2.4045194	1.7221709	-4.3000898
C	-3.2678461	-1.6392130	-0.2674262	H	5.9537647	-2.3903506	-1.7770899
C	-1.0761879	-5.4965036	1.2621722	H	5.4114966	-0.8080624	0.1125451
C	-4.7536716	1.6597506	-0.1054146	H	3.2918976	0.4525757	0.1089075
C	-3.6825833	3.1513641	1.4824223	H	3.5848351	2.1688778	-0.8636579
C	2.6366974	-0.2711104	-1.8401632	H	4.1836512	4.5668033	-0.8317335
C	-3.7537571	1.8874786	0.8630096	H	-0.1372358	3.1173758	-2.8848192
C	-1.1557329	-3.1148349	0.7305537	H	2.6491447	6.2742413	-1.8560952
C	4.7282122	-0.9153631	-0.7432253	H	0.4836338	5.5294349	-2.8908339
C	-3.5715343	-0.9694396	1.0742165	H	-0.6673746	-4.2031696	-5.6397752
C	3.5386840	-0.1725360	-0.7563643	H	-2.9792975	-3.6076427	-4.8690285
C	-1.1656193	-5.2019450	2.6336635	H	1.2931459	-3.7805223	-4.1227293
C	-1.2194117	-2.8272258	2.1090097	H	-3.3330557	-2.5943429	-2.6309678
C	2.8917361	2.8925710	-1.3080121	H	0.9463170	-2.7374807	-1.8990551
C	1.6824845	2.4691311	-1.8854422	H	-1.0300214	-4.7036164	-0.7569532
C	-1.2395904	-3.8650711	3.0522561	H	-1.0085496	-6.5420723	0.9245061
C	-2.1431529	0.7931839	3.0142118	H	-1.1660982	-6.0160291	3.3744716
C	3.2347303	4.2557064	-1.2941943	H	-1.2068205	-1.7890502	2.4676262
C	0.8181868	3.4359324	-2.4457064	H	-1.2840674	-3.6137905	4.1219964
C	-1.1878757	1.7720182	3.3630500	H	-3.6578033	-1.0361584	-1.1129420
C	-2.7240421	-0.0054984	4.0195253	H	-3.7036981	-2.6574372	-0.3209343
C	1.5927144	1.3597446	1.4164969	H	-4.6414967	-0.7068332	1.1826721
C	2.3781155	5.2074523	-1.8661073	H	-3.3148127	-1.6584959	1.8999974
C	1.1693527	4.7906505	-2.4493328	H	-3.8886071	1.6357757	-4.2751649
C	-0.8330252	1.9560186	4.7052092	H	-2.8551338	3.0711650	-3.9553694
C	-2.3501039	0.1731886	5.3599891	H	-4.3343645	2.7988949	-2.9637305
C	-1.4084959	1.1571803	5.7047151	C	2.7680049	1.5512250	2.2728225
N	-2.0376605	0.9911771	-1.7289139	H	1.3288453	2.2695674	0.8587603
C	0.7760476	0.2834430	1.1800920	C	3.5423051	0.5267183	2.8824484
P	-1.3952682	-1.7249279	-0.4776960	C	4.6920796	0.8391084	3.6204428
P	1.0682759	0.7188323	-1.8756947	C	5.1079692	2.1721386	3.7846680
P	-2.5106992	0.5702912	1.2359834	C	4.3619413	3.1993232	3.1810133
Cl	-0.7814846	2.9116621	0.0902588	C	3.2195244	2.8901371	2.4325021
Ru	-0.7299430	0.4489696	-0.2702030	H	3.2624113	-0.5274686	2.7686177
H	-6.2864579	4.7311582	-0.1050108	H	5.2717039	0.0223906	4.0789555
H	-6.4454014	2.4736723	-1.1986972	H	6.0091526	2.4072547	4.3715109
H	-4.5187288	5.1449657	1.6296113	H	4.6763650	4.2491807	3.2904579
H	-4.8353290	0.6817203	-0.6004134	H	2.6434161	3.6943326	1.9479655
H	-2.9144899	3.3433125	2.2427447	N	0.7626135	-0.6315790	3.4043574
H	-0.7125917	2.3648253	2.5673708	C	1.2273171	-1.7200301	4.0404726
H	-3.4709190	-0.7722940	3.7672932	C	1.7894633	-2.6375706	3.1135735
H	-0.0735086	2.7084292	4.9633312	C	1.6177483	-2.0540473	1.8555122

N	1.0036221	-0.8382525	2.0778434
C	1.9674405	-2.5900593	0.5116808
H	2.2238312	-3.6233187	3.3134768
C	1.1092394	-1.8261819	5.5305515
H	1.5564292	-1.9323417	-0.2712256
H	3.0615902	-2.6412296	0.3534844
H	1.5522172	-3.6084930	0.3833663
H	2.1029184	-1.7697052	6.0229475
H	0.4875454	-0.9931070	5.9084692
H	0.6452995	-2.7857562	5.8406126

l_h-trans-precursor

C	1.0909018	-1.8981481	-5.2763177
C	0.0407584	-0.9899433	-5.0562672
C	1.5420632	-2.7018982	-4.2173834
C	2.7393941	1.5282722	-4.2856462
C	-0.2207626	3.2146123	-3.7934065
C	-0.5450598	-0.8859446	-3.7868617
C	3.2314256	2.8385515	-4.1534381
C	0.9523479	-2.6016814	-2.9468428
C	2.4359974	0.7707071	-3.1459499
C	-0.0996143	-1.6916968	-2.7141344
C	-0.2271800	2.2411265	-2.7215544
C	3.4044771	3.3816658	-2.8704806
C	-3.6821152	4.3165966	-3.1318306
C	4.4488406	-2.7810763	-2.0896935
C	-3.8398255	2.9661953	-3.4845324
C	-3.1720842	4.6461548	-1.8635136
C	3.9121856	-1.5130509	-1.8150052
C	2.6462846	1.2944275	-1.8515899
C	-0.9517581	-4.2771521	-1.0340203
C	3.1182869	2.6151631	-1.7274400
C	4.0639098	-3.8975591	-1.3282266
C	-2.6740136	-1.4542289	-1.4856661
C	-0.8070666	-5.5564562	-0.4776348
C	-3.5035725	1.9552129	-2.5679400
C	-2.8416664	3.6380899	-0.9458587
C	2.9700922	-1.3440213	-0.7771311
C	-3.0190961	2.2803398	-1.2849501
C	-0.6084287	-3.1296415	-0.2856743
C	3.1671187	-3.7263797	-0.2610807
C	-3.5253314	-0.4993291	-0.6543920
C	2.6376568	-2.4578101	0.0172391
C	-0.3256373	-5.7029607	0.8355036
C	-0.1336253	-3.2841726	1.0300318
C	4.7319195	0.3858221	0.9407150
C	3.4517649	0.9703311	0.8352318
C	0.0051502	-4.5648281	1.5871014
C	-3.5043262	1.5813015	1.3938751

C	5.7106394	0.9656417	1.7600701
C	3.1703499	2.1415872	1.5656591
C	-4.8951229	1.3689000	1.4780787
C	-2.8493959	2.3244955	2.3944784
C	-1.2029335	-0.5108835	2.9000407
C	5.4280363	2.1368603	2.4840598
C	4.1573374	2.7191134	2.3810501
C	-5.6214486	1.8866438	2.5602828
C	-3.5831276	2.8469335	3.4698340
C	-4.9677822	2.6276916	3.5581366
N	-0.2301103	1.4838305	-1.8310794
C	-0.2989383	-0.0796334	1.9596889
P	-0.8268997	-1.4435506	-1.0207034
P	2.1912570	0.2924910	-0.3506535
P	-2.5479326	0.9731325	-0.0570783
Cl	0.0473478	2.8857073	0.7244453
Ru	-0.2757307	0.5225477	-0.0396791
H	-3.9539561	5.1103768	-3.8442779
H	-4.2313216	2.6938457	-4.4768104
H	-3.0347848	5.7011464	-1.5814121
H	-3.6306506	0.9043699	-2.8658132
H	-2.4249936	3.8994367	0.0365962
H	-5.4233008	0.7927935	0.7051927
H	-1.7668413	2.4904260	2.3090240
H	-6.7047633	1.7046301	2.6253468
H	-3.0637802	3.4262574	4.2485787
H	-5.5394458	3.0331796	4.4070167
H	2.5837394	1.0851590	-5.2813845
H	3.4739840	3.4348150	-5.0465463
H	2.0336521	-0.2413086	-3.2680003
H	3.7802662	4.4095270	-2.7512586
H	5.1755653	-2.8942244	-2.9088741
H	4.2359597	-0.6550008	-2.4181390
H	3.2711249	3.0509926	-0.7311103
H	4.4757027	-4.8926463	-1.5565385
H	2.8647874	-4.5822938	0.3612991
H	1.9972368	-2.2885664	0.8901520
H	4.9671837	-0.5331671	0.3869566
H	6.7034884	0.4951683	1.8323263
H	2.1756576	2.6029542	1.4817115
H	6.1982284	2.5900331	3.1269686
H	3.9182548	3.6323050	2.9475577
H	1.5552160	-1.9784460	-6.2707985
H	-0.3225251	-0.3537882	-5.8776551
H	2.3675271	-3.4124850	-4.3700138
H	-1.3492752	-0.1547164	-3.6290259
H	1.3223498	-3.2355240	-2.1305770
H	-1.3179263	-4.1742485	-2.0673238
H	-1.0697484	-6.4440850	-1.0731650
H	-0.2139987	-6.7073507	1.2720050

H	0.1216613	-2.3951268	1.6244469
H	0.3759437	-4.6645852	2.6182586
H	-2.7136735	-1.1872860	-2.5589048
H	-3.0403394	-2.4965190	-1.4040914
H	-4.4178772	-0.1570073	-1.2132474
H	-3.8821660	-0.9902922	0.2669090
H	-1.2461019	3.6039176	-3.9527843
H	0.1593080	2.7562727	-4.7274396
H	0.4528551	4.0516567	-3.5233447
C	-2.5881999	-1.0089352	2.8801926
H	-0.8098439	-0.5269620	3.9352475
C	-3.0496526	-2.0263108	2.0165388
C	-4.3489505	-2.5486697	2.1315960
C	-5.2262271	-2.0630926	3.1122795
C	-4.7733999	-1.0738291	4.0046259
C	-3.4726868	-0.5730836	3.9008404
H	-2.3662463	-2.4422796	1.2694492
H	-4.6704044	-3.3500599	1.4477337
H	-6.2463087	-2.4671844	3.1982954
H	-5.4429747	-0.6909687	4.7899138
H	-3.1263098	0.1955138	4.6073289
N	1.8931732	-0.9052238	2.4974347
C	2.8331242	-0.7149889	3.4420343
C	2.5120121	0.4240977	4.2235743
C	1.3117276	0.9207925	3.6992494
N	0.9891202	0.0934353	2.6504598
C	0.4980187	2.1034902	4.1076337
H	3.0934030	0.8649146	5.0402868
C	4.0070439	-1.6396533	3.5465383
H	-0.4979233	1.8065595	4.4965199
H	1.0271261	2.6674125	4.8981036
H	0.3229173	2.7684632	3.2373061
H	3.9406527	-2.2854982	4.4479290
H	4.0568987	-2.2942810	2.6556766
H	4.9567304	-1.0723533	3.6095365

1_i-cis-pyrazole

N	0.9114391	-1.3323157	0.2902580
N	2.0911363	-1.3623860	0.9773055
C	1.7654461	-1.0913440	2.2483136
C	0.3558247	-0.9062284	2.3842304
C	-0.1780733	-1.0761982	1.1096775
C	-1.5967750	-1.0646940	0.6418472
H	-0.2104658	-0.7096535	3.3012440
C	2.8217431	-1.0294017	3.3092414
H	2.8686019	-0.0246942	3.7785003
H	2.6242581	-1.7603669	4.1206679
H	3.8101399	-1.2550456	2.8669339
H	-2.2675275	-1.3575598	1.4719771

H	-1.9100757	-0.0616577	0.2858653
H	-1.7500994	-1.7681720	-0.1997820
C	0.9397570	-1.5874967	-1.0967652
C	0.3132228	-0.8451460	-2.0428134
H	1.5384479	-2.4705663	-1.3695871
H	0.3333308	-1.2563146	-3.0659357
C	-0.3661697	0.4494061	-1.8765461
C	0.0656120	1.4021694	-0.9194685
C	-0.5954339	2.6292829	-0.7887285
C	-1.6968296	2.9373267	-1.6081547
C	-2.1207807	2.0119848	-2.5757984
C	-1.4558642	0.7846756	-2.7136071
H	0.9332338	1.1760170	-0.2839731
H	-0.2443619	3.3575711	-0.0419648
H	-2.2158743	3.9015297	-1.4991241
H	-2.9734515	2.2482168	-3.2304505
H	-1.7904112	0.0610614	-3.4733630

1_i-trans-pyrazole

C	-0.6056160	0.1851675	0.7476286
C	0.0843503	0.1122634	-0.4183048
C	-1.7621253	1.0406128	1.0109776
C	-2.3764153	0.9821336	2.2873958
C	-3.4883482	1.7766158	2.5980600
C	-4.0188587	2.6548666	1.6394380
C	-3.4222633	2.7277795	0.3667420
C	-2.3124499	1.9346380	0.0563770
H	-0.2586385	-0.4630621	1.5669292
H	-1.9644626	0.2950901	3.0430350
H	-3.9446230	1.7095966	3.5975585
H	-4.8916263	3.2805420	1.8793518
H	-3.8293999	3.4131795	-0.3924534
H	-1.8644630	2.0115682	-0.9459263
N	1.6487526	-1.5335749	0.3746491
C	2.6928117	-2.1833931	-0.1514116
C	2.9113854	-1.7877468	-1.5093924
C	1.9277604	-0.8461751	-1.7877614
N	1.1874721	-0.7243930	-0.6195190
C	1.6312044	-0.0705624	-3.0303851
H	3.6866450	-2.1423278	-2.1972462
C	3.4642759	-3.1754668	0.6633431
H	0.6151766	-0.2841102	-3.4249702
H	1.7023057	1.0257894	-2.8676324
H	2.3584039	-0.3386672	-3.8187003
H	3.4390026	-4.1847695	0.2025478
H	4.5312920	-2.8835044	0.7523923
H	3.0327930	-3.2422919	1.6795371
H	-0.1743415	0.7102023	-1.3022599

Structures related with catalyst 2,
[Ru(dppp)₂(CH₃CN)Cl][BPh₄]

2_a

Ru	0.0276234	0.2032252	-0.3840992
Cl	0.2428486	1.2820127	-2.5682643
P	-1.6203519	1.6976177	0.6074918
P	-1.6174796	-1.1876522	-1.4275348
P	1.6707435	-1.3215077	-1.2141321
P	1.6992670	1.7491356	0.4085532
C	4.4851652	2.1893389	0.0509284
H	4.6280718	1.6705066	1.0076120
C	-5.3189001	0.0017152	1.4378656
H	-6.2740864	-0.1266991	0.9083033
C	6.1896135	-0.2473878	-1.6051792
H	7.2607281	-0.0317866	-1.7327307
C	-0.1624994	-1.1559765	2.4055424
N	-0.0976470	-0.6573204	1.3441636
C	-3.0443070	-3.6146097	1.5770468
H	-3.4203622	-3.4572070	2.5994260
C	3.4456711	-0.8260033	-1.2963943
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C	-5.6443637	-0.4845235	-2.1620479
H	-6.5969432	-1.0247623	-2.0535337
C	3.0486641	2.9257606	-1.7735468
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C	-0.8570180	2.5434514	2.0862205
C	-3.0368471	0.8700450	1.4548895
C	2.6754108	-0.0656008	2.3202736
H	2.4266871	-0.8269358	1.5712969
C	4.1535443	3.5181521	-2.4004149
H	4.0168775	4.0359306	-3.3617283
C	-2.4190958	3.1356904	-0.2213038
C	-3.2236791	-0.4156519	-1.9046969
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C	4.3775785	-1.2378663	-0.3216655
H	4.0511014	-1.8304455	0.5433795
C	-4.2773281	0.6984582	0.8076499
H	-4.4402154	1.1279242	-0.1878514
C	5.4243862	3.4568869	-1.8054314
H	6.2889403	3.9299562	-2.2947160
C	5.2648639	0.1878150	-2.5676227
H	5.6051775	0.7566110	-3.4444447
C	3.2070826	2.2599367	-0.5371490
C	-3.2082086	0.8798703	-2.4586938
H	-2.2483845	1.3949808	-2.5978901
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H	4.0077320	0.2242096	5.4682394
C	-4.4097454	1.5035810	-2.8261752
H	-4.3865733	2.5280048	-3.2262158
C	-4.1080752	4.8968570	-0.2297887
H	-4.9838955	5.3747383	0.2339655
C	2.7467895	2.2616119	3.0111700
H	2.5921229	3.3296618	2.8033677
C	-1.1500216	-1.8256762	-3.1097292
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H	0.1178053	-5.2051911	1.5691440
C	-2.4392571	4.8088782	-1.9950268
H	-2.0053250	5.2132181	-2.9217479
C	0.8286426	-3.5144782	0.4151316
H	-0.0112200	-2.8845164	0.7138923
C	1.8010688	-3.0127217	-0.4685658
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C	-0.1855126	-1.8632268	3.6709109
C	-2.9888330	-4.9087554	1.0309877
H	-3.3053056	-5.7769695	1.6281656
C	3.8998681	-0.0877334	-2.4107273
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C	-3.9297726	-0.3205655	3.3998131
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C	-5.1461715	-0.5244589	2.7272951
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H	3.7269801	-5.8481738	-0.7594072
C	3.2518339	-0.4485758	3.5405881
H	3.4636665	-1.5113208	3.7345678
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H	0.3202258	-1.2694094	4.4593322
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H	1.9165273	4.1655001	0.7198176
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H	-1.6761146	2.8561960	2.7628393
H	-0.2554065	1.7753901	2.6152320
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H	-0.6383124	4.5853271	1.4017221
H	-2.0224628	-2.4089757	-3.4674464
H	-1.1028948	-0.9080406	-3.7300082
H	1.3777971	-0.8494978	-3.5743510
H	2.3172510	-2.3566454	-3.3016997
H	0.1531263	-3.5125209	-2.5861910
H	0.1979582	-3.0122611	-4.2840193

2_b

Ru	0.1556238	0.4106814	-0.5693798
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H	-0.0806908	-2.2802634	-7.2018444
C	-1.3996842	-3.6956913	5.1130660
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H	1.0059099	6.2945238	-1.8721570
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C	-0.5235492	1.6265418	3.2037166
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H	-0.6731488	-0.5275203	2.8646715
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H	-1.9664138	-3.2563917	0.7626577
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2_TS-b_d

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C	0.5489673	2.5452979	2.4859108
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H	1.2363761	4.2179082	0.0467396
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H	0.4594724	-2.4548357	-1.3105251	H	-2.2898219	0.2807554	-4.5204368
C	1.8370629	-1.4725835	-2.6691376	H	-1.6218387	1.7565174	-3.7797248
C	-4.3252079	4.7681582	2.2431770	H	0.8666914	2.1059929	-3.5768539
H	-4.8804155	5.6899442	2.4728313	H	1.9982104	0.9755543	-4.3821850
C	-2.0789542	-1.7937709	-2.4074909	H	0.0926942	-0.6909875	-4.6378744
C	-2.4010359	-4.5966004	-2.5902989	H	-0.1215964	0.8101090	-5.5496898
H	-2.5189538	-5.6881352	-2.6619272	C	1.1238476	-3.1163180	2.5694827
C	3.3784619	2.3213020	-2.2164062	C	0.4722313	-2.3752336	1.5544851
H	2.5261732	2.9754209	-2.4449819	C	1.9277502	-4.2375176	2.2303331
C	-2.5280431	3.6257033	1.0623068	C	2.5956311	-4.9458578	3.2328182
H	-1.6890350	3.6492059	0.3510411	C	2.4811699	-4.5448522	4.5771950
C	-2.5640686	-2.5370485	-1.3087963	C	1.6869075	-3.4372844	4.9214685
H	-2.8484724	-2.0252687	-0.3799762	C	1.0044590	-2.7266415	3.9287421
C	-3.9004963	-2.7076656	2.0899609	H	2.0194557	-4.5286883	1.1742414
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C	-5.1519762	-2.5255698	1.4786521	H	3.0134814	-5.1023404	5.3622411
H	-5.8984522	-3.3335511	1.4934194	H	1.6013349	-3.1259954	5.9727705
C	1.0714527	1.0373539	-3.7800792	H	0.3898775	-1.8531500	4.1866924
C	5.5629683	0.6845273	-1.5582934	C	-0.0579785	-1.6880799	0.6716743
H	6.4151480	0.0392769	-1.2976620	H	-0.8653932	-1.5097540	-0.0630792
C	-1.9457882	-3.8624408	-3.6966702				
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C	2.3452386	-4.0748480	-3.6524682				
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C	3.0112745	-2.9668211	-4.2082568	P	-2.3572804	0.3564926	-1.0363502
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C	3.8964378	-1.6538201	1.9539226	P	2.3981081	0.3931396	0.0806215
H	4.3559810	-2.4606514	1.3647530	C	4.3368562	-1.5246389	-0.7642879
C	2.7619333	-1.6771033	-3.7214169	H	4.1402679	-2.0580462	0.1749166
H	3.3034034	-0.8239925	-4.1563551	C	-3.7372122	3.9031048	2.1233482
C	-0.0971384	0.3956498	-4.5194297	H	-4.5963385	4.4705364	1.7371737
C	-0.3899083	1.8736361	3.4965528	C	3.6144243	-4.2191675	-3.1733835
C	-4.6504474	-0.1010594	-2.3499735	H	4.4329780	-4.7844143	-3.6432246
H	-4.5307863	-1.1413118	-2.6845490	C	-0.0281753	-1.0971162	1.4449822
C	4.9768877	3.5380216	0.9211435	C	-0.8598396	-0.1445467	1.6077280
H	6.0321502	3.3358794	1.1572426	C	-4.8571460	-0.2518078	2.1939537
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C	-1.7881584	-2.4698641	-3.6091768	H	-5.9241964	3.9062719	-1.0863868
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C	3.1921359	-2.9993664	-3.7268893	H	-0.4365164	-4.7332450	-2.3356743
H	3.6836605	-2.5994956	-4.6248978	C	-2.3710949	-1.6960487	-3.1431884
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C	4.6647449	-0.1745089	4.1539556	C	5.3763295	-1.9697639	-1.5912404
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H	1.1963574	5.4848721	-3.2550940	H	-2.8454560	-2.4730076	-2.5092167
C	-1.9302694	-3.1919671	0.3386627	H	-2.7509238	-1.8741192	-4.1718825
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2_d

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H	3.1329349	2.2786610	-0.9117152
H	1.1356920	3.4416805	2.3492887
H	1.3981154	1.6704517	2.2596763
H	3.5552534	2.8184578	2.0604477
H	2.9568231	3.8904960	0.7844623
C	-0.4844315	-0.9277491	3.7758630
C	0.2590005	-0.2497149	4.7822515

C	0.0533311	-0.5590951	6.1297124
C	-0.9090788	-1.5189755	6.4953658
C	-1.6543679	-2.1904198	5.5076791
C	-1.4364069	-1.9149254	4.1545993
H	1.0137013	0.4911913	4.4816088
H	0.6406587	-0.0453978	6.9048830
H	-1.0772286	-1.7485250	7.5581002
H	-2.4018087	-2.9429076	5.7994426
H	-1.9952807	-2.4453125	3.3716348
H	-1.3591781	0.0062071	1.3703738

2_e

Ru	0.0857613	0.3539196	-0.5020885
Cl	0.9835143	0.9856012	-2.7648775
P	0.3730466	2.5592308	0.5407473
P	-2.1541967	0.8712881	-1.3338727
P	-0.4029363	-1.7900608	-1.6110687
P	2.5162907	0.1606268	-0.1508345
C	4.0186111	-0.5656955	-2.4390806
H	3.6985980	0.3911932	-2.8716240
C	-2.9056510	3.7619268	2.7835077
H	-3.7985477	4.3854918	2.6290022
C	2.7119876	-5.0935754	-2.6833487
H	3.3868758	-5.9055861	-2.9919518
C	-0.5975912	-0.8728417	2.3096959
C	-0.3598649	-0.3212153	1.1104804
C	-4.6986768	-1.4512748	0.9580141
H	-4.6747561	-1.9309973	1.9468482
C	0.9349872	-3.0329959	-1.9279835
C	3.2820907	1.8185404	-0.5496581
C	-4.5692023	4.1041795	-0.3706853
H	-5.4753626	4.2902042	0.2247806
C	3.8815653	-2.2424374	-0.6756369
H	3.4852808	-2.5821144	0.2909319
C	0.1763216	5.3655132	0.2954463
H	-0.0980457	5.3613797	1.3598195
C	1.9668824	2.8038023	1.4669521
C	-0.8307315	2.8240503	1.9074681
C	4.7403274	-0.2902313	1.5240479
H	5.3221932	-0.2842631	0.5915410
C	4.8109500	-3.0350794	-1.3597785
H	5.1117990	-4.0049494	-0.9384431
C	0.3964173	4.1519316	-0.3933433
C	-2.8635822	2.5631907	-1.1769271
C	3.3337965	-0.1467373	1.4900108
C	1.0635973	-4.1930099	-1.1364573
H	0.4367527	-4.3343141	-0.2470927
C	-1.9816869	3.6175476	1.7378041
H	-2.1471098	4.1502454	0.7951555

C	5.3618373	-2.5907685	-2.5739308
H	6.1055509	-3.2077156	-3.0998521
C	2.6135911	-3.9256231	-3.4568021
H	3.2219739	-3.8109034	-4.3650625
C	3.5017712	-0.9865011	-1.1965636
C	-2.2808530	3.6115292	-1.9171961
H	-1.4040393	3.4203485	-2.5476126
C	4.6822573	-0.4874324	3.9515106
H	5.2070780	-0.6335656	4.9073417
C	-2.8158806	4.9061043	-1.8537330
H	-2.3344691	5.7185886	-2.4171651
C	0.2978482	6.5906964	-0.3756509
H	0.1101545	7.5281847	0.1687532
C	2.6262961	-0.1469227	2.7036817
H	1.5409077	-0.0114893	2.6929688
C	-2.2207634	0.7060008	-3.1849686
C	-3.7665286	-4.1932603	-1.1276807
H	-4.6050503	-4.5341501	-1.7526876
C	0.9209410	5.4199582	-2.4096162
H	1.2227189	5.4333136	-3.4676069
C	-2.7965690	-3.3463689	-1.6837068
H	-2.8958236	-3.0656368	-2.7378568
C	-1.7189394	-2.8769837	-0.9022032
C	0.6641910	6.6223300	-1.7321745
H	0.7600861	7.5854442	-2.2555721
C	-3.5776623	-0.1413638	-0.7636985
C	-5.8408734	-1.5518312	0.1500107
H	-6.7208834	-2.1092137	0.5037837
C	1.7475221	-2.8923870	-3.0753168
H	1.7044217	-1.9779804	-3.6798139
C	0.7893183	4.1897712	-1.7453805
H	0.9674742	3.2489505	-2.2874770
C	-3.5721128	-0.7502474	0.5019759
H	-2.6725349	-0.6956440	1.1224210
C	-1.5311100	2.3522236	4.2011311
H	-1.3381558	1.8676209	5.1699825
C	-2.6900324	3.1238482	4.0144081
H	-3.4148928	3.2408479	4.8337971
C	-0.9414514	-1.5418010	-3.3817065
C	1.9535929	-5.2123822	-1.5095904
H	2.0274708	-6.1178443	-0.8890830
C	-5.8584708	-0.9369704	-1.1133413
H	-6.7536751	-1.0037851	-1.7491230
C	-3.6651917	-4.6122974	0.2079227
H	-4.4263873	-5.2802295	0.6377317
C	-0.6056872	2.2048753	3.1577900
H	0.2963362	1.6043061	3.3293914
C	-2.5797631	-4.1793863	0.9830137
H	-2.4681715	-4.5077052	2.0272088
C	5.4060154	-0.4588225	2.7467402

H	6.5001750	-0.5730720	2.7559973
C	-1.6243277	-3.3140888	0.4335883
H	-0.7904172	-2.9977645	1.0624203
C	-2.2027302	-0.7325297	-3.6932011
C	3.2272999	2.8417190	0.5954713
C	-4.0188725	2.8137642	-0.4075970
H	-4.4862515	2.0032501	0.1676674
C	4.9487813	-1.3665365	-3.1206902
H	5.3605842	-1.0211532	-4.0806518
C	-3.9606709	5.1553500	-1.0773212
H	-4.3863107	6.1688536	-1.0332161
C	3.2898445	-0.3253806	3.9271232
H	2.7066136	-0.3500008	4.8591337
C	-4.7376670	-0.2281703	-1.5667548
H	-4.7820772	0.2739669	-2.5431386
H	-3.1370635	1.2295124	-3.5200508
H	-1.3474618	1.2717719	-3.5640438
H	-0.0735661	-1.0422049	-3.8496552
H	-1.0137270	-2.5590855	-3.8148819
H	-3.1074574	-1.2555938	-3.3272689
H	-2.3004229	-0.7011770	-4.7994393
H	4.3329728	1.6302878	-0.8422209
H	2.7492730	2.1777670	-1.4498872
H	1.8522560	3.7492961	2.0330816
H	2.0377844	1.9893435	2.2077347
H	4.0958938	2.6923848	1.2679797
H	3.3391418	3.8510420	0.1493901
C	0.1655917	-1.9730617	2.9090118
C	-0.0483312	-2.3330068	4.2594898
C	0.7094551	-3.3515081	4.8566391
C	1.6870526	-4.0399702	4.1176203
C	1.8974054	-3.7033534	2.7687811
C	1.1500109	-2.6834696	2.1730199
H	-1.4147497	-0.4265902	2.9041566
H	-0.8109933	-1.7970732	4.8453841
H	0.5322807	-3.6125280	5.9109273
H	2.2777425	-4.8383872	4.5898197
H	2.6548470	-4.2386049	2.1761330
H	1.3350041	-2.4142116	1.1225561

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Ru	0.1107505	0.7740395	-0.9894546
Cl	1.0658727	1.0293109	-3.2832439
P	-0.1212675	3.2056391	-0.5153867
P	-2.0314131	0.6024001	-2.0961553
P	0.3559847	-1.5762141	-1.4369058
P	2.4102058	1.0162610	-0.2253420
C	4.6940554	-0.6613973	-0.2270330
H	4.4211361	-0.9148102	0.8054596

C	-3.9997414	4.6264502	-0.1115750	H	0.1956008	-4.5018335	-1.4860041
H	-4.7859895	4.9877881	-0.7899416	C	-0.7400850	-2.7644041	-0.5392747
C	4.3103777	-3.9765843	-1.1123262	C	0.9346939	6.7329817	-3.3852825
H	5.2084594	-4.6100509	-1.0603870	H	1.1904728	7.5733068	-4.0479334
C	-1.2916184	0.6469902	1.8173241	C	-3.4567022	0.0658582	-1.0757039
C	-0.6092607	0.5731623	0.6745871	C	-5.5781762	-0.7077480	0.6167644
C	-5.2472823	-1.4885696	-0.5015631	H	-6.4006538	-1.0130852	1.2806137
H	-5.8108850	-2.4072884	-0.7213642	C	2.8489383	-2.5011418	-2.3802321
C	1.9866980	-2.4007171	-1.2675350	H	2.6224168	-1.9668321	-3.3122700
C	3.0320791	2.7557780	-0.4958866	C	1.0275938	4.3570649	-2.8571534
C	-4.5291621	3.5741795	-3.5701128	H	1.3393880	3.3363282	-3.1212563
H	-5.6019564	3.8180807	-3.5461100	C	-4.1926143	-1.1051693	-1.3449612
C	4.2124249	0.4580295	-2.3364210	H	-3.9480604	-1.7373337	-2.2081836
H	3.5483502	1.0729669	-2.9577728	C	-3.2010168	4.1246747	2.1227494
C	-0.1478301	5.8888515	-1.3747850	H	-3.3544058	4.0987905	3.2120169
H	-0.7375197	6.0815901	-0.4671485	C	-4.2349799	4.5431957	1.2701416
C	1.0273374	3.6283932	0.8855470	H	-5.2120008	4.8320797	1.6848841
C	-1.7312785	3.7724725	0.1943198	C	-0.0729015	-2.0429080	-3.1871014
C	1.9434901	-0.2687374	2.2300525	C	3.4773311	-3.8400176	0.0082050
H	1.1856459	-0.8380848	1.6778376	H	3.7059197	-4.3677158	0.9450855
C	5.4139121	-0.0323539	-2.8673575	C	-4.8653237	0.4749265	0.8761898
H	5.6898051	0.2184374	-3.9026304	H	-5.1304107	1.1068424	1.7361627
C	0.2614100	4.5751493	-1.6955793	C	-2.5252935	-4.6334409	0.5968093
C	-2.6892206	2.1167700	-2.9209311	H	-3.2231538	-5.3618544	1.0366154
C	2.7026212	0.7047853	1.5580876	C	-1.9541129	3.7532659	1.5919371
C	2.3224049	-3.0470840	-0.0623991	H	-1.1517108	3.4657522	2.2832899
H	1.6796801	-2.9761067	0.8283131	C	-2.6406176	-3.2709663	0.9054225
C	-2.7589923	4.2505403	-0.6456241	H	-3.4182150	-2.9119140	1.5935386
H	-2.5806220	4.3585813	-1.7208218	C	2.1551738	-0.5282777	3.5919120
C	6.2626980	-0.8297773	-2.0829375	H	1.5515271	-1.3000380	4.0873672
H	7.2097785	-1.2060417	-2.4976029	C	-1.7605539	-2.3400678	0.3225435
C	4.0040137	-3.2901683	-2.2991730	H	-1.8827950	-1.2740395	0.5421354
H	4.6685206	-3.3684011	-3.1716400	C	-1.5589909	-1.9228738	-3.5125638
C	3.8473415	0.1514485	-1.0064694	C	2.4715014	3.8418546	0.4304152
C	-1.7990949	2.9275469	-3.6526885	C	-4.0633079	2.4328604	-2.8988830
H	-0.7378304	2.6512992	-3.7055149	H	-4.7689058	1.8009013	-2.3416336
C	3.1375428	0.1864871	4.2939145	C	5.8936406	-1.1484604	-0.7670052
H	3.3000679	-0.0075729	5.3647347	H	6.5440367	-1.7838265	-0.1477967
C	-2.2665748	4.0775153	-4.3057970	C	-3.6315462	4.4085441	-4.2589474
H	-1.5542384	4.7197470	-4.8445695	H	-3.9987720	5.3125093	-4.7673232
C	0.1851006	6.9585592	-2.2182886	C	3.9265134	1.1387756	3.6245723
H	-0.1445542	7.9760757	-1.9603290	H	4.7139557	1.6842791	4.1657279
C	3.7179929	1.3921099	2.2613987	C	-3.8140990	0.8611316	0.0348055
H	4.3648763	2.1134072	1.7427102	H	-3.2872082	1.8042778	0.2204763
C	-2.0626482	-0.4829459	-3.6084660	H	-3.1081531	-0.4424417	-3.9762727
C	-1.5083714	-5.0683251	-0.2784836	H	-1.4450581	0.0823195	-4.3354790
H	-1.4082869	-6.1363134	-0.5215181	H	0.5309395	-1.3932377	-3.8495244
C	1.3587074	5.4317816	-3.6974253	H	0.2715973	-3.0872709	-3.3140507
H	1.9499360	5.2444910	-4.6063979	H	-2.1512623	-2.5131385	-2.7834148
C	-0.6129226	-4.1454236	-0.8308894	H	-1.7319411	-2.4021924	-4.4996123

H	4.1381460	2.7286496	-0.4519147
H	2.7745206	2.9576383	-1.5544104
H	0.6484665	4.5460654	1.3760704
H	0.9560173	2.7936802	1.6147627
H	3.0970313	3.9212581	1.3414434
H	2.5525074	4.8173474	-0.0918849
C	-1.6286465	-0.1974842	2.9603299
C	-2.6448527	0.2638526	3.8367905
C	-3.0551901	-0.5001238	4.9352875
C	-2.4531658	-1.7437110	5.1945111
C	-1.4387306	-2.2070249	4.3404525
C	-1.0344376	-1.4515774	3.2322425
H	-1.8324729	1.6153226	1.8148735
H	-3.1162041	1.2395936	3.6401575
H	-3.8476481	-0.1207846	5.5980896
H	-2.7668961	-2.3423862	6.0625389
H	-0.9379391	-3.1668742	4.5367132
H	-0.2340959	-1.8528732	2.5984428
N	1.2162592	-3.7040103	2.8567456
C	2.3023506	-4.3910163	3.2669130
C	2.0684370	-5.7920770	3.1724328
C	0.7672202	-5.9276545	2.6769079
N	0.3121125	-4.6498785	2.5134402
C	-0.0474866	-7.1316545	2.3283084
H	2.7542645	-6.6034122	3.4384748
C	3.5343769	-3.6839730	3.7482934
H	0.0816237	-7.4183074	1.2631451
H	0.2582737	-7.9985083	2.9434784
H	-1.1280302	-6.9560381	2.4996495
H	3.7500232	-2.7916863	3.1292631
H	3.4214212	-3.3345873	4.7957745
H	4.4117973	-4.3575756	3.7170720
H	-0.5979814	-4.3646275	2.1387848

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Ru	0.8581189	0.7478156	-0.4517141
Cl	1.7099538	2.5825028	-1.9420692
P	-0.3096304	2.1848438	1.1656213
P	-1.0560408	0.7260302	-1.9917017
P	1.9431590	-0.7083842	-2.0942421
P	2.8437488	1.3999508	0.7964003
C	5.1850360	2.3105398	-0.5216377
H	4.6262781	3.2219455	-0.7720420
C	-3.7728280	0.1665146	2.2026826
H	-4.7422746	-0.0373246	1.7298929
C	6.4676145	-1.1679418	-3.0653237
H	7.5117167	-1.2906218	-3.3896361
C	-0.4302041	-1.5146770	1.3108847
C	0.2447556	-0.6189953	0.5787520

C	-2.2888147	-3.2411377	-2.0326400
H	-1.9408012	-4.1866949	-1.5933664
C	3.7798069	-0.8619758	-2.2763885
C	2.8130898	3.2393759	1.1215895
C	-4.5663319	2.9170228	-1.5753920
H	-5.6117265	2.7268822	-1.2894953
C	5.2631291	0.0424828	0.3622391
H	4.7676212	-0.8129387	0.8449639
C	-2.3508817	4.1787196	1.1375965
H	-2.9860491	3.4788495	1.6973376
C	0.6981544	2.8481046	2.5836516
C	-1.5881030	1.2586691	2.1177922
C	4.2834051	1.1193822	3.2066350
H	5.0486488	1.7429614	2.7209470
C	6.6226912	-0.0358093	0.0371582
H	7.1789368	-0.9616585	0.2428438
C	-1.0873270	3.7744142	0.6634965
C	-2.3033608	2.0770427	-1.8921705
C	3.1263499	0.7273545	2.4953399
C	4.4387567	-2.0936966	-2.0927539
H	3.9019917	-2.9551186	-1.6737205
C	-2.8275114	0.9507824	1.5239506
H	-3.0690587	1.3288187	0.5243066
C	7.2744479	1.0659471	-0.5423722
H	8.3468274	1.0077956	-0.7802595
C	5.8213921	0.0694167	-3.2244370
H	6.3601974	0.9220696	-3.6621697
C	4.5411972	1.2277646	0.1111779
C	-1.8944430	3.3671252	-2.2973723
H	-0.8438493	3.5532909	-2.5613833
C	3.5058437	-0.1064101	5.1636865
H	3.6583137	-0.4338871	6.2029265
C	-2.8236480	4.4138502	-2.3559511
H	-2.4938773	5.4114995	-2.6779752
C	-2.7983067	5.4892125	0.9058641
H	-3.7899332	5.7937218	1.2722125
C	2.1691883	-0.0755605	3.1354059
H	1.2527610	-0.3511024	2.5989914
C	-0.5643681	0.9879586	-3.7733536
C	0.7896801	-4.6041039	-2.9849180
H	0.4982670	-5.1870100	-3.8711144
C	-0.7282607	6.0052086	-0.2548685
H	-0.0915924	6.7133500	-0.8061609
C	1.1128280	-3.2459874	-3.1277982
H	1.0740762	-2.7934373	-4.1267247
C	1.4769474	-2.4828236	-2.0000013
C	-1.9856943	6.4084293	0.2239361
H	-2.3360864	7.4380938	0.0584450
C	-2.0507740	-0.8142963	-2.2275534
C	-3.3603063	-3.2203284	-2.9373427

H	-3.8733106	-4.1537204	-3.2122139
C	4.4893846	0.2293026	-2.8235690
H	3.9931871	1.2044481	-2.9373696
C	-0.2830673	4.6923424	-0.0477257
H	0.6758467	4.3625747	-0.4708840
C	-1.6369338	-2.0446658	-1.6815586
H	-0.7981653	-2.0787837	-0.9816987
C	-2.2451357	-0.0588255	4.0710183
H	-1.9982874	-0.4601182	5.0650074
C	-3.4811512	-0.3499587	3.4745371
H	-4.2206813	-0.9744762	3.9972563
C	1.6450524	-0.2644534	-3.8793630
C	5.7795885	-2.2411878	-2.4822536
H	6.2803871	-3.2113032	-2.3443354
C	-3.7852285	-1.9958938	-3.4825447
H	-4.6360436	-1.9659647	-4.1785408
C	0.8344911	-5.2167949	-1.7215174
H	0.5751543	-6.2807817	-1.6146770
C	-1.3108398	0.7481036	3.4050505
H	-0.3561981	0.9520741	3.9035247
C	1.2220623	-4.4688789	-0.5970897
H	1.2726370	-4.9315678	0.3998273
C	4.4674595	0.7041079	4.5328425
H	5.3718413	1.0132058	5.0780153
C	1.5462587	-3.1133473	-0.7442260
H	1.8640694	-2.5326467	0.1291001
C	0.2091248	-0.1716368	-4.3852374
C	1.8904431	3.7394982	2.2435852
C	-3.6497744	1.8538592	-1.5375599
H	-4.0348002	0.8621852	-1.2470360
C	6.5504071	2.2310124	-0.8351670
H	7.0489115	3.0879817	-1.3121614
C	-4.1606383	4.1945843	-1.9880948
H	-4.8853282	5.0214392	-2.0265500
C	2.3560154	-0.4969504	4.4620513
H	1.5994627	-1.1399652	4.9349673
C	-3.1364689	-0.8031996	-3.1364311
H	-3.4869376	0.1423747	-3.5738742
H	-1.5177557	1.1617209	-4.3093301
H	0.0271088	1.9227629	-3.8092622
H	2.1440022	0.7166612	-3.9999574
H	2.2381466	-0.9972015	-4.4612776
H	-0.3414092	-1.1234376	-4.2341304
H	0.2504888	-0.0183320	-5.4845089
H	3.8568258	3.5374691	1.3322551
H	2.5388512	3.6708449	0.1390284
H	-0.0216332	3.3893982	3.2296102
H	1.0543200	1.9706184	3.1484021
H	2.4790252	3.8509855	3.1768288
H	1.5380115	4.7559711	1.9765081

C	-0.0554483	-2.5804105	2.2384100
C	-1.0965984	-3.2552590	2.9259894
C	-0.8208580	-4.2928193	3.8242677
C	0.5069046	-4.6859409	4.0682305
C	1.5521314	-4.0195412	3.4057957
C	1.2786142	-2.9810649	2.5061204
H	-1.5229214	-1.3562970	1.1991229
H	-2.1347831	-2.9365691	2.7531408
H	-1.6497964	-4.7983301	4.3423058
H	0.7256769	-5.5014745	4.7729681
H	2.5974524	-4.3063438	3.5958207
H	2.1181364	-2.4623822	2.0251708
N	-5.3797743	-0.7039860	-0.5276327
C	-6.5130131	-0.8701359	0.1838560
C	-6.4395647	-2.0605975	0.9662005
C	-5.1879915	-2.6189409	0.6844113
N	-4.6073754	-1.7629964	-0.2066643
C	-4.5208039	-3.8816063	1.1280845
H	-7.2029230	-2.4687978	1.6370246
C	-7.6239410	0.1315087	0.1008351
H	-4.8390444	-4.7487523	0.5116455
H	-3.4184398	-3.8064353	1.0488211
H	-4.7738508	-4.1147000	2.1797898
H	-7.7373094	0.6951499	1.0502573
H	-7.4212361	0.8560995	-0.7101430
H	-8.5964263	-0.3585696	-0.1057711
H	-3.6784398	-1.8560599	-0.6280063

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Ru	0.4159101	0.4079528	-0.6211298
Cl	1.2588230	1.0394710	-2.9004904
P	0.4727400	2.6280659	0.3642160
P	-1.7358847	0.8587151	-1.6683690
P	0.3393113	-1.7752211	-1.6735537
P	2.8361673	0.2602627	0.0179274
C	5.1766314	-1.2031333	-0.8298740
H	5.1167993	-1.7742652	0.1031441
C	-2.9735362	4.8732107	1.0026907
H	-3.5817768	5.5761721	0.4153309
C	4.2505447	-4.1652840	-2.5480420
H	5.1533432	-4.7447894	-2.7918121
C	-1.5467401	0.0598550	1.7696003
C	-0.4092467	-0.1871393	1.0747709
C	-5.2268418	-1.0112606	-0.3880407
H	-5.7868172	-1.9229951	-0.6444966
C	1.9209222	-2.6912187	-1.9378520
C	3.6128760	1.9273165	0.3823643
C	-3.6230116	4.4400283	-2.6851958
H	-4.6501745	4.8349951	-2.6906355

C	4.3512333	0.4844512	-2.3625344	H	-3.7345327	-1.3705154	-1.9044567
H	3.6013123	1.2306377	-2.6487390	C	-2.5055819	3.6914291	3.0671691
C	1.0315443	5.4002686	0.1709867	H	-2.7414201	3.4757893	4.1200872
H	0.4505807	5.4954827	1.0993789	C	-3.3143722	4.5720918	2.3310526
C	1.5892727	2.5954996	1.8661236	H	-4.1941269	5.0381507	2.7989202
C	-1.0457138	3.3723602	1.1286690	C	-0.2215243	-1.7324698	-3.4621142
C	3.3359190	-2.1422555	1.4403653	C	3.4366517	-4.5481781	-1.4705292
H	3.0013909	-2.6302614	0.5175853	H	3.6968199	-5.4308497	-0.8666294
C	5.4405128	0.2437838	-3.2120449	C	-4.9664084	1.0051099	0.9304938
H	5.5343074	0.8244267	-4.1419160	H	-5.3172553	1.6882964	1.7173052
C	1.1748980	4.1416244	-0.4559704	C	-2.7962004	-5.0598442	-0.5706885
C	-2.0799326	2.6074623	-2.2098276	H	-3.5552475	-5.8223685	-0.3399670
C	3.3476538	-0.7280116	1.5139857	C	-1.3835681	3.0929541	2.4711392
C	2.2745157	-3.8200131	-1.1706569	H	-0.7705791	2.4020468	3.0646748
H	1.6229397	-4.1312589	-0.3441007	C	-2.9102464	-3.7645659	-0.0434198
C	-1.8449505	4.2882550	0.4100360	H	-3.7602198	-3.4952694	0.6009051
H	-1.5716000	4.5723142	-0.6116205	C	3.7283901	-2.9254837	2.5324724
C	6.4034265	-0.7218856	-2.8791635	H	3.7073202	-4.0218316	2.4440652
H	7.2598641	-0.9073787	-3.5443806	C	-1.9366842	-2.7953270	-0.3341881
C	3.9066066	-3.0402442	-3.3131269	H	-2.0202040	-1.7889016	0.0913468
H	4.5434272	-2.7257039	-4.1518487	C	-1.6873641	-1.3535159	-3.6421274
C	4.1928989	-0.2503788	-1.1653155	C	3.0534856	2.8251628	1.4985282
C	-1.0255588	3.3984590	-2.7050841	C	-3.3916178	3.1295653	-2.2395827
H	-0.0189739	2.9711745	-2.7603096	H	-4.2419096	2.5227122	-1.9028852
C	4.1501990	-2.3162692	3.7255689	C	6.2664492	-1.4391076	-1.6821833
H	4.4569292	-2.9305533	4.5849914	H	7.0153671	-2.1932286	-1.3980013
C	-1.2566133	4.7112574	-3.1422536	C	-2.5551213	5.2441321	-3.1186096
H	-0.4080950	5.3176867	-3.4923022	H	-2.7390691	6.2765200	-3.4520324
C	1.6224018	6.5432678	-0.3867508	C	4.1863913	-0.9160881	3.8091489
H	1.4962117	7.5170520	0.1097525	H	4.5296647	-0.4263336	4.7326661
C	3.7949733	-0.1288380	2.7139286	C	-3.8053565	1.3213418	0.2152695
H	3.8488264	0.9607342	2.8050559	H	-3.2816224	2.2599634	0.4376096
C	-1.9846378	0.1209073	-3.3710430	H	-3.0312318	0.3761472	-3.6330869
C	-1.7112359	-5.3739018	-1.4080593	H	-1.3283503	0.7479116	-4.0061269
H	-1.6186508	-6.3822544	-1.8389554	H	0.4314818	-1.0256422	-4.0051197
C	2.5328710	5.1963992	-2.1890416	H	-0.0335800	-2.7529664	-3.8496933
H	3.1184906	5.1071932	-3.1163840	H	-2.3292309	-2.0261785	-3.0367759
C	-0.7457579	-4.4003827	-1.7091109	H	-1.9651019	-1.5527636	-4.6989881
H	0.0881565	-4.6605596	-2.3770597	H	4.6937026	1.7343447	0.5268858
C	-0.8419892	-3.1038601	-1.1570181	H	3.5225603	2.4413417	-0.5937524
C	2.3716971	6.4465033	-1.5717436	H	1.2571635	3.3797891	2.5736483
H	2.8304522	7.3455310	-2.0100160	H	1.4320393	1.6117724	2.3545420
C	-3.3194797	0.4620730	-0.7976631	H	3.6653156	2.7324773	2.4187743
C	-5.6751003	-0.1731221	0.6419351	H	3.1781599	3.8790322	1.1782366
H	-6.5807995	-0.4284286	1.2113637	C	-2.3713290	-0.6092533	2.7798275
C	2.7581574	-2.2984683	-3.0049778	C	-3.1885813	0.1817632	3.6287694
H	2.5132177	-1.4048574	-3.5947581	C	-4.0538087	-0.4040503	4.5600890
C	1.9419162	4.0505515	-1.6331823	C	-4.1457496	-1.8034790	4.6583803
H	2.0436263	3.0783694	-2.1369431	C	-3.3696319	-2.6027081	3.8033734
C	-4.0610200	-0.6937742	-1.1059024	C	-2.4986774	-2.0147415	2.8764103

H	-2.0225684	0.9744387	1.3930238
H	-3.1422778	1.2749403	3.5398477
H	-4.6708301	0.2357300	5.2090873
H	-4.8306980	-2.2665866	5.3840172
H	-3.4541250	-3.6995529	3.8460048
H	-1.9438276	-2.6504487	2.1803122
N	0.4919491	-2.7026596	1.3773163
C	0.3526026	-3.5822057	2.3499591
C	0.3501767	-2.9425708	3.6532452
C	0.4556512	-1.5993379	3.4288000
N	0.5301414	-1.4368540	1.9937138
C	0.5386240	-0.4291905	4.3360567
H	0.2475314	-3.4346500	4.6264768
C	0.1861423	-5.0360787	2.0574875
H	-0.2909866	0.2757390	4.1320540
H	0.4800737	-0.7563879	5.3892626
H	1.4947442	0.1153820	4.1920378
H	-0.7074141	-5.4341512	2.5786980
H	0.0609971	-5.2030708	0.9718718
H	1.0599354	-5.6157373	2.4212578
H	1.4506839	-1.0041280	1.7548388

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Ru	-0.0569852	0.1026341	-0.4581048
Cl	-0.0336421	0.8232634	-2.8442842
P	-1.3785694	2.2044569	0.0518463
P	-1.9092825	-1.2438984	-1.2693897
P	1.3025989	-1.8190728	-0.8830075
P	1.9807967	1.6625826	-0.6675378
C	2.9450692	0.9880491	-3.3814463
H	2.0948921	0.3095397	-3.4871244
C	-5.1774249	1.6269859	1.5887334
H	-6.1769138	1.4408050	1.1686869
C	6.0134163	-1.8927753	-0.9099053
H	7.1131806	-1.9143816	-0.9209037
C	0.3084311	0.3690004	2.6441519
C	-0.1875382	-0.1035029	1.4524318
C	-2.2666872	-4.6840026	1.0376030
H	-1.7996859	-5.0732193	1.9532925
C	3.1754911	-1.8148844	-0.8734540
C	1.3942103	3.4259099	-0.9196329
C	-5.8844121	-0.0430762	-1.6057577
H	-6.8636150	-0.3731604	-1.2263572
C	4.1849045	2.6325989	-2.1252389
H	4.3550142	3.2284049	-1.2179898
C	-2.9788679	4.4443822	-0.5547861
H	-3.2731466	4.3916125	0.5027450
C	-0.2697435	3.3202517	1.0528738
C	-2.8024762	2.0487859	1.2225979

C	4.5423584	1.1294356	0.3917770
H	4.6667293	0.4795551	-0.4823692
C	5.0665757	2.7995427	-3.2012966
H	5.8913603	3.5224356	-3.1140438
C	-2.0988948	3.4812376	-1.1025502
C	-3.4642235	-0.3485348	-1.7160466
C	3.3224513	1.8096165	0.6009387
C	3.9049146	-2.2250592	0.2648807
H	3.3831707	-2.5587234	1.1697469
C	-4.0936818	1.7968647	0.7188879
H	-4.2562324	1.7566395	-0.3635709
C	4.8958715	2.0543153	-4.3792146
H	5.5851012	2.1855609	-5.2267179
C	5.2994801	-1.5291836	-2.0616391
H	5.8287022	-1.2614049	-2.9880029
C	3.1123156	1.7073924	-2.1863139
C	-3.3827216	0.7646837	-2.5781715
H	-2.4044217	1.0753048	-2.9656588
C	5.4980722	2.1691446	2.3709057
H	6.3467320	2.3184981	3.0545879
C	-4.5374266	1.4823261	-2.9266280
H	-4.4450833	2.3659027	-3.5753153
C	-3.4976489	5.4745350	-1.3519491
H	-4.1847144	6.2095986	-0.9065214
C	3.1966064	2.6357080	1.7363309
H	2.2505452	3.1426641	1.9569141
C	-1.4794333	-1.9406732	-2.9588773
C	1.1616801	-5.7084462	0.5600219
H	1.2069381	-6.7253066	0.1429116
C	-2.2531768	4.6305256	-3.2527905
H	-1.9571664	4.6960639	-4.3105785
C	1.1847208	-4.6038389	-0.3053709
H	1.2678626	-4.7792454	-1.3861458
C	1.1104814	-3.2946872	0.2092998
C	-3.1426676	5.5683043	-2.7078754
H	-3.5538945	6.3746126	-3.3334864
C	-2.4891476	-2.8661933	-0.5794996
C	-3.2004405	-5.4523543	0.3264949
H	-3.4754633	-6.4583776	0.6769376
C	3.8964980	-1.5080909	-2.0449943
H	3.3726496	-1.2506281	-2.9681230
C	-1.7311235	3.5974833	-2.4573927
H	-1.0440313	2.8642344	-2.8984691
C	-1.9178675	-3.4050302	0.5812213
H	-1.1999828	-2.8091675	1.1477056
C	-3.7153349	1.9622810	3.4952542
H	-3.5627245	2.0472932	4.5816475
C	-4.9894589	1.6795330	2.9800134
H	-5.8388663	1.5267719	3.6621148
C	1.0223458	-2.4705822	-2.6043755

C	5.3068896	-2.2575488	0.2473336
H	5.8493912	-2.5874909	1.1459058
C	-3.7867412	-4.9256852	-0.8378605
H	-4.5273779	-5.5139648	-1.3999844
C	1.0931815	-5.5186643	1.9492474
H	1.0881973	-6.3863275	2.6256803
C	-2.6297722	2.1684663	2.6215647
H	-1.6537285	2.4460637	3.0426490
C	1.0347497	-4.2153086	2.4702046
H	0.9888253	-4.0553352	3.5574726
C	5.6204857	1.3127517	1.2654232
H	6.5640795	0.7804878	1.0739158
C	1.0346406	-3.1122239	1.6049150
H	0.9590197	-2.0930209	2.0079629
C	-0.3783189	-3.0001044	-2.9299829
C	0.6605479	4.1718167	0.1948287
C	-4.7275737	-0.7475278	-1.2405658
H	-4.8071926	-1.6106318	-0.5753477
C	3.8255433	1.1547252	-4.4639821
H	3.6602312	0.5735435	-5.3838704
C	-5.7935569	1.0830273	-2.4416022
H	-6.6987081	1.6446918	-2.7164728
C	4.2785725	2.8200325	2.6098210
H	4.1611426	3.4723003	3.4870974
C	-3.4329886	-3.6451216	-1.2901276
H	-3.9089799	-3.2538924	-2.2007219
H	-2.4182594	-2.3769447	-3.3496373
H	-1.2047761	-1.0936691	-3.6116640
H	1.2515918	-1.6137315	-3.2685594
H	1.7924561	-3.2447206	-2.7899707
H	-0.6569975	-3.8206983	-2.2359855
H	-0.3255905	-3.4636323	-3.9381820
H	2.2734550	4.0089360	-1.2494231
H	0.7478621	3.3111806	-1.8123385
H	-0.9099760	3.9770827	1.6730934
H	0.2930754	2.6464742	1.7326863
H	1.3905239	4.6758838	0.8600811
H	0.0724599	4.9842495	-0.2802066
C	1.6528148	0.3781278	3.2124367
C	1.8251072	0.9293691	4.5089171
C	3.0312642	0.7803780	5.2041545
C	4.0912136	0.0598835	4.6293007
C	3.9399888	-0.4742690	3.3376716
C	2.7459600	-0.3018212	2.6337326
H	-0.4137329	0.6121317	3.4390123
H	0.9840760	1.4631445	4.9808945
H	3.1389629	1.2140039	6.2098030
H	5.0333072	-0.0770759	5.1798440
H	4.7692672	-1.0181414	2.8640711
H	2.6433197	-0.6931137	1.6179151

N	-3.0464890	-0.8835615	1.5336585
C	-3.7299358	-1.7945352	2.2032661
C	-3.0042211	-2.2531259	3.3603319
C	-1.8296965	-1.5518655	3.4002277
N	-1.8507719	-0.6682577	2.2484243
C	-0.7570208	-1.6573172	4.4311072
H	-3.3255147	-3.0211034	4.0724468
C	-5.0744134	-2.2880956	1.7822231
H	0.2491166	-1.7664781	3.9875882
H	-0.7045468	-0.7682951	5.0921275
H	-0.9682731	-2.5358198	5.0695283
H	-5.6104418	-2.7287160	2.6430013
H	-5.6827623	-1.4673343	1.3609873
H	-4.9704647	-3.0806172	1.0114213
H	-1.9373793	0.3376757	2.5265578

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Ru	-0.3352635	0.4916363	-0.6249713
Cl	-1.3687659	1.5561105	-2.6599692
P	-0.2832169	2.4549008	0.7789139
P	-2.6781807	0.0990807	-0.0692342
P	-0.4786100	-1.4622406	-2.0473938
P	1.8282212	1.2811286	-1.5255049
C	3.4090212	0.9675611	-3.9298727
H	4.1173951	0.3639208	-3.3518963
C	-2.9642281	3.0665898	3.9058975
H	-3.9643352	3.5097296	4.0184611
C	2.4545737	-1.9875922	-5.6439271
H	3.1153138	-2.1248493	-6.5127195
C	-0.1403162	-0.8183581	2.1828511
C	0.4059414	-0.5523286	0.9611977
C	-3.9103787	-3.1107462	2.2840391
H	-4.2303440	-4.1496255	2.1144387
C	0.7434893	-1.6476899	-3.4211012
C	2.1848957	3.0905489	-1.1773243
C	-5.6665248	2.6764241	1.3040266
H	-6.5178464	2.6243287	1.9994104
C	1.3667387	2.2555610	-4.1397022
H	0.4303004	2.6376966	-3.7169786
C	-0.7630941	5.2250730	1.1707381
H	-0.6189051	5.0138754	2.2400511
C	1.4823580	2.7974463	1.3037912
C	-1.0943037	2.4621099	2.4487105
C	3.7628114	-0.8010857	-1.4598496
H	3.0709332	-1.3167662	-2.1368819
C	1.6875886	2.5443353	-5.4734659
H	1.0040657	3.1704965	-6.0664337
C	-0.7151408	4.1777282	0.2229424
C	-3.7523286	1.5906841	0.2427861

C	3.4203782	0.4797761	-0.9593726	C	-0.4086064	1.9660756	3.5788161
C	1.7938012	-2.5879939	-3.3800140	H	0.5953975	1.5356236	3.4709737
H	1.9266190	-3.2055673	-2.4827416	C	-1.2302537	-4.7013018	0.4316758
C	-2.3725579	3.0326556	2.6347575	H	-1.5084176	-4.8391471	1.4870451
H	-2.9025171	3.4817320	1.7879101	C	4.9700181	-1.4178229	-1.1045866
C	2.8678880	2.0455167	-6.0462994	H	5.2118485	-2.4075731	-1.5202554
H	3.1207359	2.2753770	-7.0921878	C	-0.9905793	-3.4043010	-0.0495515
C	1.4118963	-1.0493742	-5.6920761	H	-1.0634705	-2.5465699	0.6284878
H	1.2576325	-0.4392570	-6.5930779	C	-3.3081794	-1.7625631	-2.2928556
C	2.2155505	1.4454573	-3.3514234	C	2.2448751	3.6174153	0.2658106
C	-3.5226931	2.7695308	-0.4923063	C	-4.8600052	1.5429977	1.1175539
H	-2.7170028	2.7865848	-1.2335540	H	-5.0953126	0.6251498	1.6714779
C	5.8668809	-0.7728538	-0.2382869	C	3.7266674	1.2596412	-5.2652768
H	6.8154944	-1.2552122	0.0403616	H	4.6612703	0.8662765	-5.6920636
C	-4.3243263	3.9046807	-0.2992825	C	-5.3905421	3.8687198	0.6132731
H	-4.0994643	4.8224964	-0.8628054	H	-6.0153075	4.7599729	0.7746237
C	-1.0021481	6.5448995	0.7606923	C	5.5473610	0.4994212	0.2614885
H	-1.0426397	7.3480194	1.5118224	H	6.2475108	1.0219836	0.9302097
C	4.3429919	1.1228817	-0.1005428	C	-3.1268867	-0.4543698	2.6810240
H	4.1340221	2.1262861	0.2850157	H	-2.8541366	0.5947326	2.8522887
C	-3.7456743	-0.5553793	-1.4643286	H	-4.7382430	-0.7240846	-0.9998713
C	-0.7829854	-5.5992698	-1.7779988	H	-3.8429467	0.3256274	-2.1288200
H	-0.7079116	-6.4551015	-2.4657907	H	-2.0970219	-0.5907904	-3.6669265
C	-1.1230264	5.8076669	-1.5484419	H	-1.8661787	-2.3665423	-3.8067050
H	-1.2656498	6.0260904	-2.6174775	H	-3.2064125	-2.6777252	-1.6739741
C	-0.5580140	-4.3002682	-2.2611872	H	-4.1291353	-1.9810497	-3.0089399
H	-0.3135044	-4.1584311	-3.3240034	H	3.1121879	3.3333286	-1.7318333
C	-0.6404617	-3.1896295	-1.3927699	H	1.3632573	3.5913845	-1.7249706
C	-1.1877558	6.8407223	-0.6005288	H	1.4695930	3.3368325	2.2706012
H	-1.3799636	7.8760719	-0.9195827	H	1.9518179	1.8076655	1.4757127
C	-3.1763515	-0.9667796	1.3631405	H	3.2976027	3.7202120	0.6008475
C	-3.8209474	-2.6020628	3.5870885	H	1.8438788	4.6507451	0.2653607
H	-4.0573652	-3.2411841	4.4504342	C	0.0879414	-1.8154947	3.2359010
C	0.5698058	-0.8685416	-4.5860979	C	-0.2177791	-1.4742897	4.5795673
H	-0.2252870	-0.1119283	-4.6245127	C	-0.0803920	-2.4023438	5.6178665
C	-0.8838626	4.4856345	-1.1404463	C	0.3454446	-3.7142851	5.3439133
H	-0.8652096	3.6743276	-1.8825986	C	0.6144733	-4.0835890	4.0162109
C	-3.5968818	-2.2977210	1.1808663	C	0.4838595	-3.1501523	2.9787263
H	-3.6756422	-2.7241086	0.1739928	H	-0.9991324	-0.1775353	2.4013795
C	-0.9959515	2.0156632	4.8534179	H	-0.5764381	-0.4602701	4.7972860
H	-0.4369688	1.6426734	5.7247503	H	-0.3182191	-2.1047015	6.6504104
C	-2.2827259	2.5521548	5.0203735	H	0.4461819	-4.4478812	6.1575041
H	-2.7424393	2.5883646	6.0191646	H	0.9114692	-5.1171592	3.7807535
C	-2.0322505	-1.5341578	-3.0952204	H	0.6332793	-3.4751893	1.9443522
C	2.6485242	-2.7515291	-4.4821533	N	1.7759479	-2.4247586	-0.0624673
H	3.4596636	-3.4942364	-4.4377207	C	2.6288039	-3.2697388	0.4651619
C	-3.4414227	-1.2628596	3.7799331	C	3.2898079	-2.7257055	1.6433859
H	-3.3905019	-0.8385803	4.7931156	C	2.7627025	-1.4939304	1.8689898
C	-1.1158737	-5.8049399	-0.4275402	N	1.8131995	-1.2513745	0.7645938
H	-1.2975879	-6.8230849	-0.0517444	C	3.0423598	-0.4517105	2.8827611

H	4.0480235	-3.2265865	2.2550761
C	2.8159147	-4.6301774	-0.1162593
H	2.1200318	-0.1961899	3.4402139
H	3.8047642	-0.8141471	3.5948958
H	3.4225633	0.4732820	2.4031487
H	2.7328545	-5.3988903	0.6779664
H	2.0498578	-4.8317387	-0.8874951
H	3.8268603	-4.7306113	-0.5625709
H	2.3157861	-0.5456913	0.1543368

2_g-transoid

Ru	-0.1422395	0.3985504	-0.4119960
Cl	-0.7442939	1.6350607	-2.5311686
P	-0.0350374	2.4382354	1.0754185
P	-2.4994821	0.1828013	-0.3230799
P	-0.1495645	-1.5226001	-1.9504001
P	2.0854371	1.3958714	-1.2124473
C	2.2480291	1.8791292	-4.0170239
H	1.3728077	2.5282991	-3.8878640
C	-1.2194599	2.3962654	5.1099944
H	-2.0345963	2.8072500	5.7248387
C	2.7882504	-2.4560621	-5.4645073
H	3.4082925	-2.7214776	-6.3336404
C	1.5238989	-1.2574076	1.6925421
C	0.3511287	-0.6937316	1.2164019
C	-3.2144277	-3.5699441	1.2315279
H	-2.6502935	-4.5134312	1.2812973
C	1.1619710	-1.7981095	-3.2494686
C	1.8008265	3.2544621	-1.3426496
C	-4.2199691	3.3202792	1.7971135
H	-4.1447631	3.7212225	2.8198120
C	3.8125703	0.2413438	-3.1431791
H	4.2083824	-0.3485070	-2.3091200
C	-1.0058734	5.0436861	1.6719732
H	-0.4506541	4.9647337	2.6179146
C	1.6194451	3.3155420	1.2058880
C	-0.1425945	2.1887202	2.9231237
C	4.8374233	2.1039732	-0.9801632
H	4.7370628	2.4882257	-2.0050580
C	4.4496257	0.1826716	-4.3893491
H	5.3100028	-0.4887582	-4.5264475
C	-1.0366813	3.9632458	0.7603944
C	-3.5295226	1.6642643	0.1302189
C	3.7427523	1.4744919	-0.3462212
C	2.0674027	-2.8752192	-3.1788967
H	2.1185488	-3.5017688	-2.2795224
C	-1.1729554	2.6944076	3.7388040
H	-1.9568929	3.3222674	3.2998027
C	4.0051637	0.9891545	-5.4492340

H	4.5186210	0.9582540	-6.4218485
C	1.8951802	-1.3750764	-5.5380698
H	1.8187696	-0.7822192	-6.4602820
C	2.7167414	1.1028755	-2.9350321
C	-4.3738844	2.3020099	-0.8061715
H	-4.4444407	1.9476564	-1.8400675
C	6.2264910	1.7433534	0.9886093
H	7.1956033	1.8369594	1.5009819
C	-5.1280667	3.4278576	-0.4414376
H	-5.7709058	3.9113525	-1.1920656
C	-1.6786608	6.2382894	1.3792813
H	-1.6544864	7.0672095	2.1026320
C	3.9086749	1.0188423	0.9727500
H	3.0597352	0.5519254	1.4824694
C	-3.3571109	-0.2074522	-1.9401802
C	-1.2008273	-5.5526724	-1.5481206
H	-1.9097085	-6.2420208	-2.0306490
C	-2.3636196	5.3257073	-0.7618914
H	-2.8822168	5.4319684	-1.7260386
C	-1.1657636	-4.2099736	-1.9539441
H	-1.8442871	-3.8997725	-2.7559583
C	-0.2781247	-3.2896762	-1.3517194
C	-2.3658876	6.3809324	0.1620171
H	-2.8907604	7.3200476	-0.0686427
C	-3.2943895	-1.2085758	0.6046136
C	-4.5389369	-3.4999983	1.6858511
H	-5.0319688	-4.3914614	2.1017321
C	1.1020505	-1.0334556	-4.4356061
H	0.4276496	-0.1698175	-4.5011951
C	-1.7034542	4.1228618	-0.4676702
H	-1.6932290	3.3063883	-1.2022773
C	-2.5930424	-2.4230570	0.7114654
H	-1.5500297	-2.4740837	0.3787395
C	0.8284307	1.1174750	4.9100316
H	1.6349412	0.5217974	5.3642587
C	-0.2406406	1.5791353	5.6972974
H	-0.2879869	1.3329814	6.7681590
C	-1.5616824	-1.4881637	-3.1684005
C	2.8857502	-3.1916931	-4.2751610
H	3.5811475	-4.0415285	-4.2022853
C	-5.2433983	-2.2833056	1.5954438
H	-6.2863842	-2.2261994	1.9427453
C	-0.3307516	-6.0191700	-0.5503618
H	-0.3494790	-7.0758817	-0.2447215
C	0.8910675	1.4413810	3.5415919
H	1.7532026	1.1051522	2.9503639
C	0.5751804	-5.1230432	0.0356717
H	1.2876532	-5.4717190	0.7988446
C	6.0673009	2.2353718	-0.3177067
H	6.9089136	2.7250576	-0.8302662

C	0.5897747	-3.7735786	-0.3528960
H	1.3083210	-3.0975681	0.1147739
C	-2.9701875	-1.5248761	-2.5898177
C	2.0703140	4.0363472	-0.0584784
C	-3.4580696	2.2036761	1.4276319
H	-2.7702612	1.7356814	2.1373993
C	2.8947608	1.8261993	-5.2613737
H	2.5273312	2.4527427	-6.0880773
C	-5.0603004	3.9413219	0.8622173
H	-5.6494803	4.8264099	1.1430645
C	5.1386811	1.1382661	1.6359178
H	5.2448880	0.7503944	2.6598100
C	-4.6339631	-1.1471751	1.0421768
H	-5.1987709	-0.2069311	0.9510562
H	-4.4366202	-0.2075182	-1.6937674
H	-3.1414368	0.6300616	-2.6298030
H	-1.4238613	-0.5465569	-3.7300677
H	-1.3751725	-2.3175657	-3.8760585
H	-3.1076635	-2.3652891	-1.8781488
H	-3.6784607	-1.7176572	-3.4237173
H	2.4474386	3.6270240	-2.1588038
H	0.7526930	3.3676899	-1.6776164
H	1.5281302	4.0204131	2.0543501
H	2.3609733	2.5566126	1.5051260
H	3.1543647	4.2499820	0.0415806
H	1.5555038	5.0162771	-0.1359533
C	2.7780718	-1.7134422	1.1058488
C	3.7456149	-2.2364947	2.0079153
C	4.9764241	-2.7286717	1.5646661
C	5.2707555	-2.7462527	0.1903147
C	4.3202217	-2.2556295	-0.7181545
C	3.1025944	-1.7282216	-0.2715201
H	1.5499791	-1.4811008	2.7735714
H	3.5176803	-2.2390078	3.0864744
H	5.7068162	-3.1122922	2.2926211
H	6.2293433	-3.1472341	-0.1698015
H	4.5253249	-2.2912564	-1.7977451
H	2.3851652	-1.3234472	-0.9945570
N	-1.7673982	-0.0144967	2.6175919
C	-2.5394591	-0.6242655	3.4899525
C	-2.0259172	-1.9237912	3.8575317
C	-0.8645232	-2.1197725	3.1779970
N	-0.5898418	-0.8278141	2.4735300
C	-0.0232794	-3.3373181	3.1047942
H	-2.5166901	-2.6503700	4.5135220
C	-3.7850241	-0.0044050	4.0274945
H	0.2366391	-3.5656284	2.0545249
H	0.9273151	-3.2573325	3.6684226
H	-0.6013301	-4.1823782	3.5237251
H	-4.5201209	-0.7833939	4.2997210

H	-3.5365104	0.5737484	4.9431121
H	-4.2401116	0.6908340	3.3014795
H	0.0395466	-0.2908794	3.1463906

2_h-cis-precursor

Ru	-0.3442285	0.4827994	-0.6150720
Cl	-1.4224623	1.5540667	-2.6796860
P	-0.2639072	2.4321390	0.7796705
P	-2.6661173	0.1019965	-0.0488332
P	-0.4839685	-1.4857713	-1.9898731
P	1.8646009	1.1613679	-1.4422308
C	3.4738614	0.9149645	-3.8582019
H	4.2006253	0.3363435	-3.2777131
C	-2.9364599	3.0886468	3.9169321
H	-3.9347791	3.5365965	4.0291573
C	2.4466637	-2.0307497	-5.5854927
H	3.1178893	-2.1618594	-6.4478266
C	-0.1360706	-0.7702467	2.1800233
C	0.4534315	-0.5893030	0.9513759
C	-3.9646886	-3.0812593	2.3096902
H	-4.2794699	-4.1221731	2.1412033
C	0.7238402	-1.6913088	-3.3727862
C	2.2410403	2.9874810	-1.1505327
C	-5.6516726	2.7117828	1.3070351
H	-6.5041885	2.6717055	2.0026412
C	1.3934320	2.1303078	-4.0633754
H	0.4381410	2.4676319	-3.6426828
C	-0.7361082	5.2220160	1.1412283
H	-0.6072316	5.0230541	2.2149218
C	1.4930416	2.7890543	1.3160192
C	-1.0727367	2.4723306	2.4555741
C	3.8614195	-0.8499160	-1.4437954
H	3.2048664	-1.3651542	-2.1532536
C	1.7068396	2.4452959	-5.3929186
H	1.0005094	3.0511167	-5.9813501
C	-0.6824615	4.1597389	0.2113362
C	-3.7457652	1.5999543	0.2548713
C	3.4417733	0.3651936	-0.8632699
C	1.7601265	-2.6432051	-3.3325285
H	1.8803169	-3.2582317	-2.4347435
C	-2.3451514	3.0526484	2.6452051
H	-2.8746820	3.5030614	1.7989433
C	2.9040705	1.9926521	-5.9690988
H	3.1512827	2.2388270	-7.0132160
C	1.4131239	-1.0825201	-5.6342644
H	1.2769016	-0.4572083	-6.5279881
C	2.2633763	1.3428079	-3.2758945
C	-3.4995106	2.7770114	-0.4777967
H	-2.6885879	2.7813216	-1.2150507

C	5.9768732	-0.7509158	-0.2418971	C	3.7847743	1.2286645	-5.1910434
H	6.9627375	-1.1804842	-0.0082824	H	4.7337362	0.8688133	-5.6169653
C	-4.2885686	3.9218324	-0.2910632	C	-5.3591020	3.9004739	0.6168248
H	-4.0458222	4.8366408	-0.8526210	H	-5.9719348	4.8006047	0.7776801
C	-0.9604605	6.5376159	0.7090750	C	5.5587547	0.4401152	0.3691854
H	-1.0056907	7.3522979	1.4480252	H	6.2122758	0.9544921	1.0901347
C	4.3094837	0.9959595	0.0528350	C	-3.1590300	-0.4317059	2.7013821
H	4.0257045	1.9409277	0.5263011	H	-2.8682923	0.6128159	2.8710068
C	-3.7520021	-0.5521636	-1.4338474	H	-4.7460856	-0.7120494	-0.9686015
C	-0.8629471	-5.6123868	-1.6705640	H	-3.8380245	0.3245225	-2.1053035
H	-0.8104753	-6.4775426	-2.3494367	H	-2.0914360	-0.6152412	-3.6260563
C	-1.0526251	5.7667133	-1.5898486	H	-1.8762594	-2.3952218	-3.7533668
H	-1.1773884	5.9687599	-2.6646712	H	-3.2256611	-2.6788843	-1.6275365
C	-0.6340985	-4.3213918	-2.1740638	H	-4.1401747	-1.9852514	-2.9717389
H	-0.4070848	-4.1926885	-3.2426816	H	3.1840463	3.1977416	-1.6917867
C	-0.6774124	-3.2021518	-1.3159832	H	1.4369488	3.4768912	-1.7324897
C	-1.1247089	6.8148366	-0.6589403	H	1.4728453	3.3467107	2.2723678
H	-1.3053430	7.8468732	-0.9962718	H	1.9484075	1.7966017	1.5035287
C	-3.1899231	-0.9519832	1.3872276	H	3.3308187	3.6629310	0.6193543
C	-3.9073366	-2.5602472	3.6091603	H	1.8944773	4.6076098	0.2278418
H	-4.1676243	-3.1899042	4.4728170	C	0.0616092	-1.7972872	3.2115929
C	0.5640049	-0.9033723	-4.5334301	C	-0.3890740	-1.5270189	4.5309508
H	-0.2212299	-0.1353514	-4.5688977	C	-0.3032960	-2.4826626	5.5513091
C	-0.8284466	4.4491635	-1.1584449	C	0.2297308	-3.7548791	5.2850871
H	-0.8077062	3.6236496	-1.8862458	C	0.6680615	-4.0495490	3.9819846
C	-3.6176745	-2.2808391	1.2077329	C	0.5878823	-3.0934022	2.9619037
H	-3.6696213	-2.7175507	0.2037225	H	-0.9622653	-0.0970003	2.4139106
C	-0.9796741	2.0119971	4.8581214	H	-0.8177440	-0.5395160	4.7460772
H	-0.4271172	1.6149931	5.7228209	H	-0.6614234	-2.2334328	6.5626743
C	-2.2604367	2.5620399	5.0288115	H	0.2964120	-4.5115929	6.0816758
H	-2.7220237	2.5930996	6.0273808	H	1.0748975	-5.0461097	3.7493045
C	-2.0361104	-1.5559199	-3.0486117	H	0.9078719	-3.3724500	1.9519524
C	2.6203625	-2.8079547	-4.4295331	N	1.7422341	-2.3568963	-0.1113792
H	3.4264308	-3.5565368	-4.3800578	C	2.8018125	-3.1122165	0.2254110
C	-3.5152781	-1.2246319	3.7985527	C	3.4646697	-2.5553599	1.3510917
H	-3.4782035	-0.7925543	4.8091276	C	2.7237532	-1.4303130	1.7102132
C	-1.1614332	-5.7983580	-0.3097086	N	1.6772810	-1.3588931	0.8079389
H	-1.3384093	-6.8107203	0.0847724	C	2.9453555	-0.4928624	2.8487130
C	-0.3917768	1.9638794	3.5838884	H	4.3781249	-2.9126277	1.8374849
H	0.6008940	1.5082103	3.4746359	C	3.1529845	-4.3446077	-0.5502798
C	-1.2355120	-4.6835663	0.5404768	H	2.3529406	-0.7845508	3.7408516
H	-1.4689553	-4.8044857	1.6088726	H	4.0172007	-0.4943272	3.1232734
C	5.1206078	-1.3908148	-1.1497710	H	2.6628687	0.5432707	2.5881979
H	5.4316638	-2.3277185	-1.6363390	H	3.7061916	-5.0622335	0.0857066
C	-0.9926047	-3.3966273	0.0387794	H	2.2374335	-4.8440548	-0.9235285
H	-1.0228406	-2.5316757	0.7117676	H	3.7984455	-4.1182523	-1.4264981
C	-3.3198227	-1.7677270	-2.2536362				
C	2.2818171	3.5694261	0.2699756				
C	-4.8583643	1.5681972	1.1233914				
H	-5.1037957	0.6543350	1.6801859				
				2_h-trans-precursor			
				Ru	-0.3017813	0.2667102	-0.4107818

Cl	-1.0496818	1.3744035	-2.5932495	H	3.3993243	0.6155119	1.1446186
P	-0.0730410	2.4160760	0.7912114	C	-3.6758613	-0.1513724	-1.3709683
P	-2.5776513	0.0563367	0.1444433	C	-1.7986278	-5.6105816	-0.7318593
P	-0.6415927	-1.7250724	-1.7173344	H	-2.5677630	-6.3269613	-1.0579781
P	1.9548871	1.0226216	-1.5038119	C	-1.5474282	5.6027833	-1.4802812
C	1.7571872	1.3544988	-4.3309914	H	-1.8686863	5.7603425	-2.5215103
H	0.9926777	2.1114394	-4.1176432	C	-1.7426180	-4.3399773	-1.3239869
C	-1.7577006	3.0720160	4.5351869	H	-2.4657809	-4.0965080	-2.1114343
H	-2.6674459	3.5434828	4.9380313	C	-0.7790991	-3.3947395	-0.9147719
C	1.6668158	-3.1923567	-5.5140096	C	-1.5216314	6.6762834	-0.5770053
H	2.1322437	-3.5761693	-6.4346607	H	-1.8262182	7.6840738	-0.8984281
C	1.7572789	-0.9841342	1.5681639	C	-3.3492344	-1.3531197	1.0866256
C	0.4421652	-0.6046930	1.2838958	C	-4.5657688	-3.5929208	2.3242595
C	-3.1853135	-3.5835524	2.0737425	H	-5.0381275	-4.4597687	2.8112635
H	-2.5555740	-4.4403070	2.3538607	C	0.3021756	-1.5256023	-4.3797102
C	0.4378258	-2.2258656	-3.1605154	H	-0.2726280	-0.5900684	-4.4111222
C	1.8231563	2.8842940	-1.6914734	C	-1.1687856	4.3157802	-1.0672946
C	-4.8613774	2.7551003	2.3692561	H	-1.2058418	3.4801550	-1.7818571
H	-5.3919238	2.7719308	3.3338542	C	-2.5899632	-2.4737784	1.4592371
C	3.2360909	-0.4189318	-3.5865452	H	-1.5139530	-2.4746106	1.2817934
H	3.6810161	-1.0117167	-2.7794988	C	0.3481658	1.9135943	4.8702795
C	-0.6983703	5.1694638	1.1500169	H	1.0940680	1.4589037	5.5391535
H	-0.3471494	5.0247074	2.1809725	C	-0.8132439	2.4983212	5.4014288
C	1.6980197	3.0145206	0.8739030	H	-0.9791941	2.5095381	6.4893515
C	-0.3969290	2.4549234	2.6103028	C	-2.2021909	-1.6823435	-2.7528895
C	4.7450488	1.5323222	-1.8518842	C	1.8475206	-3.8647997	-4.2969421
H	4.4825875	1.7072475	-2.9036458	H	2.4555415	-4.7815580	-4.2529687
C	3.6630643	-0.6208139	-4.9050190	C	-5.3428777	-2.4854384	1.9432910
H	4.4079477	-1.4017149	-5.1181930	H	-6.4283076	-2.4811275	2.1272365
C	-0.7594759	4.0749925	0.2583418	C	-0.8791763	-5.9680813	0.2663473
C	-3.4618243	1.5568733	0.7676814	H	-0.9188021	-6.9673516	0.7259280
C	3.7591947	1.0978204	-0.9344190	C	0.5650693	1.9082655	3.4860884
C	1.2240905	-3.3940383	-3.1294330	H	1.4738219	1.4402143	3.0839686
H	1.3324688	-3.9600477	-2.1951635	C	0.0918912	-5.0390603	0.6719700
C	-1.5575793	3.0411482	3.1477530	H	0.8242372	-5.3061901	1.4484321
H	-2.3066321	3.4880525	2.4833269	C	6.0692124	1.7500612	-1.4435914
C	3.1521773	0.1747843	-5.9431532	H	6.8141330	2.0815754	-2.1832878
H	3.4967119	0.0255757	-6.9778601	C	0.1341920	-3.7615815	0.0932043
C	0.8940666	-2.0201253	-5.5486071	H	0.8780126	-3.0335461	0.4339699
H	0.7603923	-1.4733449	-6.4927469	C	-3.5383898	-1.5139900	-2.0394327
C	2.2934234	0.5833350	-3.2784557	C	2.2092523	3.6460713	-0.4214327
C	-3.5134553	2.6771214	-0.0848454	C	-4.1513157	1.6060989	1.9911500
H	-3.0026682	2.6367009	-1.0556508	H	-4.1302611	0.7372986	2.6506070
C	6.4416293	1.5498395	-0.1042762	C	2.1879161	1.1518080	-5.6519507
H	7.4820198	1.7138776	0.2150294	H	1.7672097	1.7718759	-6.4583717
C	-4.2006277	3.8382215	0.3011190	C	-4.8759035	3.8830187	1.5313122
H	-4.1939185	4.7151442	-0.3629407	H	-5.4152139	4.7933963	1.8338260
C	-1.0879137	6.4533431	0.7399610	C	5.4694554	1.1445659	0.8203514
H	-1.0439780	7.2867499	1.4578170	H	5.7362854	0.9843196	1.8756780
C	4.1452211	0.9299657	0.4073838	C	-4.7430833	-1.3792949	1.3214060

H	-5.3741787	-0.5299547	1.0219915
H	-4.7135359	0.0127969	-1.0212388
H	-3.4149101	0.6580804	-2.0787682
H	-2.0423995	-0.8179643	-3.4226345
H	-2.1801057	-2.5914255	-3.3839027
H	-3.7122957	-2.3249696	-1.3009576
H	-4.3414433	-1.6195198	-2.8016518
H	2.4747403	3.1875693	-2.5335012
H	0.7786933	3.0834656	-1.9888836
H	1.7637150	3.7358406	1.7116416
H	2.3021731	2.1352339	1.1554794
H	3.3137898	3.7220263	-0.3517816
H	1.8194981	4.6814970	-0.5063939
C	2.8240321	-1.6342934	0.8279570
C	3.9740611	-2.0308794	1.5736787
C	5.0326550	-2.7317707	0.9937696
C	4.9794496	-3.0981926	-0.3636913
C	3.8509769	-2.7360733	-1.1145817
C	2.8025297	-2.0040619	-0.5404207
H	1.9994489	-0.9688696	2.6433510
H	4.0227410	-1.7610984	2.6412436
H	5.9062398	-3.0033679	1.6064264
H	5.8024353	-3.6627285	-0.8262973
H	3.7781463	-3.0296742	-2.1722237
H	1.9465063	-1.7113658	-1.1581061
N	-1.4726944	-0.0916543	2.7742307
C	-1.9312376	-0.5494171	3.9501846
C	-1.1146332	-1.6050915	4.4241888
C	-0.1155902	-1.7827598	3.4778592
N	-0.3453105	-0.8109462	2.4889404
C	0.8959705	-2.8875874	3.4986766
H	-1.2599235	-2.2017631	5.3313391
C	-3.1811311	-0.0748331	4.6248765
H	1.1509586	-3.2412566	2.4866090
H	1.8542218	-2.5961885	3.9767674
H	0.4779559	-3.7345564	4.0785023
H	-3.1422282	-0.3283649	5.7016832
H	-3.3084630	1.0171060	4.5334909
H	-4.0781691	-0.5752292	4.1999992

2_i-cis-pyrazole

N	0.9114391	-1.3323157	0.2902580
N	2.0911363	-1.3623860	0.9773055
C	1.7654461	-1.0913440	2.2483136
C	0.3558247	-0.9062284	2.3842304
C	-0.1780733	-1.0761982	1.1096775
C	-1.5967750	-1.0646940	0.6418472
H	-0.2104658	-0.7096535	3.3012440
C	2.8217431	-1.0294017	3.3092414

H	2.8686019	-0.0246942	3.7785003
H	2.6242581	-1.7603669	4.1206679
H	3.8101399	-1.2550456	2.8669339
H	-2.2675275	-1.3575598	1.4719771
H	-1.9100757	-0.0616577	0.2858653
H	-1.7500994	-1.7681720	-0.1997820
C	0.9397570	-1.5874967	-1.0967652
C	0.3132228	-0.8451460	-2.0428134
H	1.5384479	-2.4705663	-1.3695871
H	0.3333308	-1.2563146	-3.0659357
C	-0.3661697	0.4494061	-1.8765461
C	0.0656120	1.4021694	-0.9194685
C	-0.5954339	2.6292829	-0.7887285
C	-1.6968296	2.9373267	-1.6081547
C	-2.1207807	2.0119848	-2.5757984
C	-1.4558642	0.7846756	-2.7136071
H	0.9332338	1.1760170	-0.2839731
H	-0.2443619	3.3575711	-0.0419648
H	-2.2158743	3.9015297	-1.4991241
H	-2.9734515	2.2482168	-3.2304505
H	-1.7904112	0.0610614	-3.4733630

2_i-trans-pyrazole

C	-0.6056160	0.1851675	0.7476286
C	0.0843503	0.1122634	-0.4183048
C	-1.7621253	1.0406128	1.0109776
C	-2.3764153	0.9821336	2.2873958
C	-3.4883482	1.7766158	2.5980600
C	-4.0188587	2.6548666	1.6394380
C	-3.4222633	2.7277795	0.3667420
C	-2.3124499	1.9346380	0.0563770
H	-0.2586385	-0.4630621	1.5669292
H	-1.9644626	0.2950901	3.0430350
H	-3.9446230	1.7095966	3.5975585
H	-4.8916263	3.2805420	1.8793518
H	-3.8293999	3.4131795	-0.3924534
H	-1.8644630	2.0115682	-0.9459263
N	1.6487526	-1.5335749	0.3746491
C	2.6928117	-2.1833931	-0.1514116
C	2.9113854	-1.7877468	-1.5093924
C	1.9277604	-0.8461751	-1.7877614
N	1.1874721	-0.7243930	-0.6195190
C	1.6312044	-0.0705624	-3.0303851
H	3.6866450	-2.1423278	-2.1972462
C	3.4642759	-3.1754668	0.6633431
H	0.6151766	-0.2841102	-3.4249702
H	1.7023057	1.0257894	-2.8676324
H	2.3584039	-0.3386672	-3.8187003
H	3.4390026	-4.1847695	0.2025478

H	4.5312920	-2.8835044	0.7523923
H	3.0327930	-3.2422919	1.6795371
H	-0.1743415	0.7102023	-1.3022599