

**Ethanolysis of N-substituted Norbornane Epoxyimides. Discovery of Diverse Pathways
Depending on Substituent of Character**

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Supplementary Information

Table of Contents

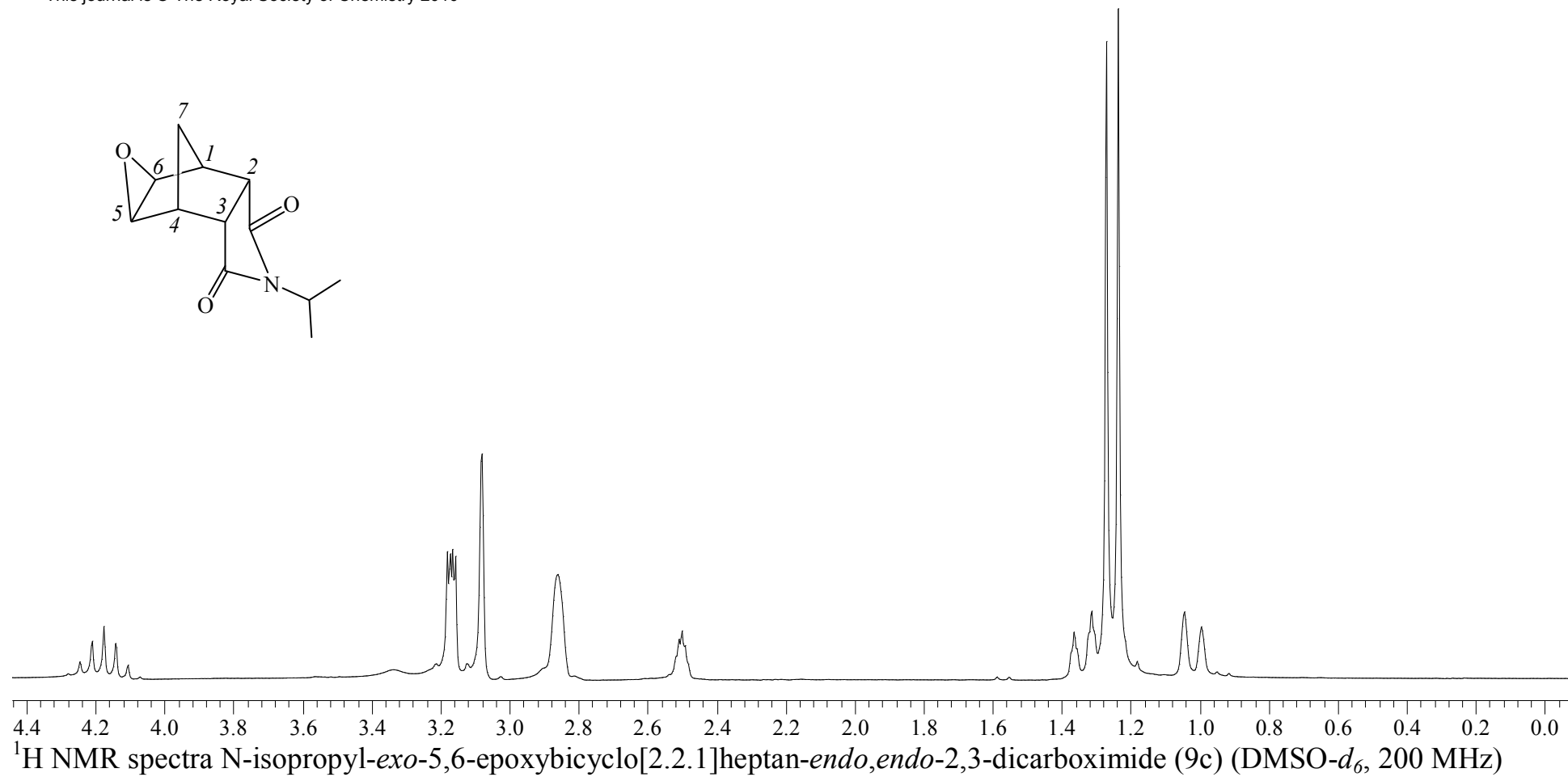
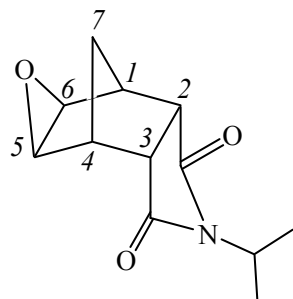
General Experimental	S 3-4
¹ H NMR Spectra for N-Isopropyl- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9c)	S 5
¹ H NMR Spectra for N-(<i>o,o'</i> -Dimethylphenyl)- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9f)	S 6
¹ H NMR Spectra for N-(<i>o,m'</i> -Dimethylphenyl)- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9g)	S 7
¹ H NMR Spectra for N-(<i>p</i> -Nitrophenyl)- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9l)	S 8
¹ H NMR Spectra for N-(<i>p</i> -Ethoxycarbonylphenyl)- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9m)	S 9
¹ H NMR Spectra for N-(2-Thiadiazolyl)- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9n)	S 10
¹ H NMR Spectra for N-Cyclohexyl- <i>exo</i> -5,6-epoxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (9o)	S 11
¹ H NMR Spectra for N-Methyl- <i>exo</i> -2, <i>endo</i> -3-dihydroxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (10a)	S 12
¹ H NMR Spectra for N- <i>n</i> -Propyl- <i>exo</i> -2, <i>endo</i> -3-dihydroxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (10b)	S 13
¹ H NMR Spectra for N- <i>i</i> -Propyl- <i>exo</i> -2, <i>endo</i> -3-dihydroxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (10c)	S 14
¹ H NMR Spectra for N-Benzyl- <i>exo</i> -2, <i>endo</i> -3-dihydroxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (10d)	S 15
¹ H NMR Spectra for N-Cyclohexyl- <i>exo</i> -2, <i>endo</i> -3-dihydroxybicyclo[2.2.1]heptan- <i>endo</i> , <i>endo</i> -2,3-dicarboximide (10e)	S 16
¹ H NMR Spectra for N- <i>n</i> -Tolyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11e)	S 17
¹ H NMR Spectra for N- <i>o,o'</i> -Dimethylphenyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11f)	S 18
¹ H NMR Spectra for N- <i>o,m'</i> -Dimethylphenyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11g)	S 19
¹ H NMR Spectra for N- <i>n</i> -Methoxyphenyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11h)	S 20
¹ H NMR Spectra for N- <i>n</i> -Bromphenyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11i)	S 21
¹ H NMR Spectra for N-Cyclohexyl- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11j)	S 22
¹ H NMR Spectra for N-(6-Quinolyl)- <i>exo</i> -2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxamide (11k)	S 23
¹ H NMR Spectra for N-Phenyl- <i>exo</i> -2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0 ^{3,7}]nonane- <i>endo</i> -9-carboxylic acid (12j)	S 24

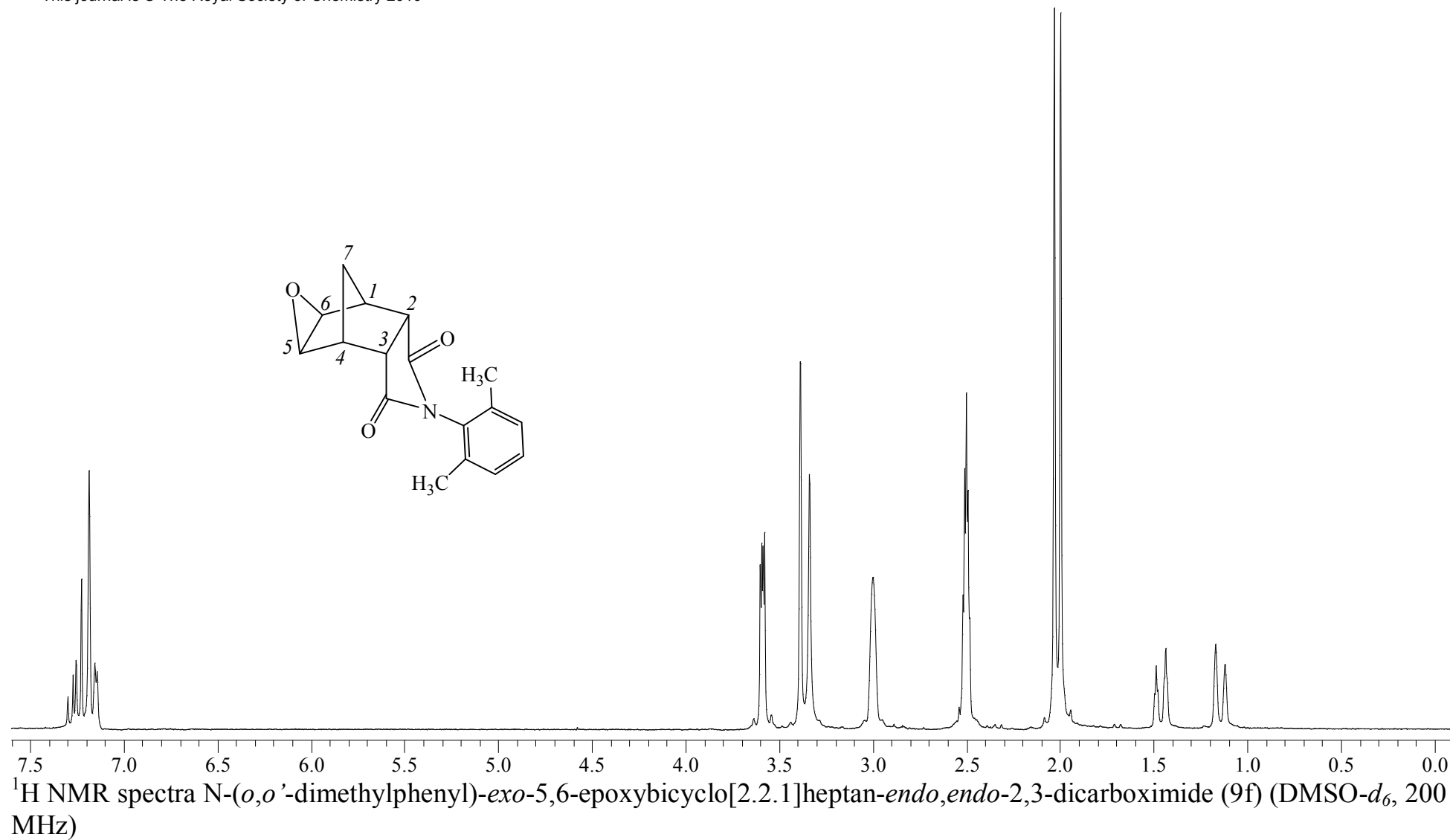
¹ H NMR Spectra for N-<i>m</i>-Nitrophenyl-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12k)	S 25
¹ H NMR Spectra for N-<i>p</i>-Nitrophenyl-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12l)	S 26
¹ H NMR Spectra for N-<i>p</i>-Ethoxycarbonylphenyl-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12m)	S 27
¹ H NMR Spectra for N-(2-Thiadiazolyl)-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12n)	S 28
¹ H NMR Spectra for N-(6-Quinolyl)-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12o)	S 29
Figure 1. The molecular structure of the compound 10a with numeration of the non-hydrogen atoms used in the structural investigation.	S 30
Figure 2. The molecular structure of the compound 11e with numeration of the non-hydrogen atoms used in the structural investigation.	S 31
Figure 3. The molecular structure of the compound 12k with numeration of the non-hydrogen atoms used in the structural investigation.	S 32
Mass Spectra for N-Methyl-<i>exo</i>-2,<i>endo</i>-3-dihydroxybicyclo[2.2.1]heptan-<i>endo</i>,<i>endo</i>-2,3-dicarboximide (10a)	S 33
Mass Spectra for N-<i>n</i>-Tolyl-<i>exo</i>-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxamide (11e)	S 34
Mass Spectra for N-<i>m</i>-Nitrophenyl-<i>exo</i>-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-<i>endo</i>-9-carboxylic acid (12k)	S 35
Cartezian coordinates for PCM/B3LYP/6-31+G(d) (solvent-ethanol) fully optimized geometries of the reagents, transition states and intermediates along the possible mechanisms for the ethanolysis for N-substituted epoxyimides	S 36-44
The reaction-coordinate vectors corresponding to the sole imaginary frequencies of transition states calculated at the PCM/B3LYP/6-31+G(d) level.	S 45-46

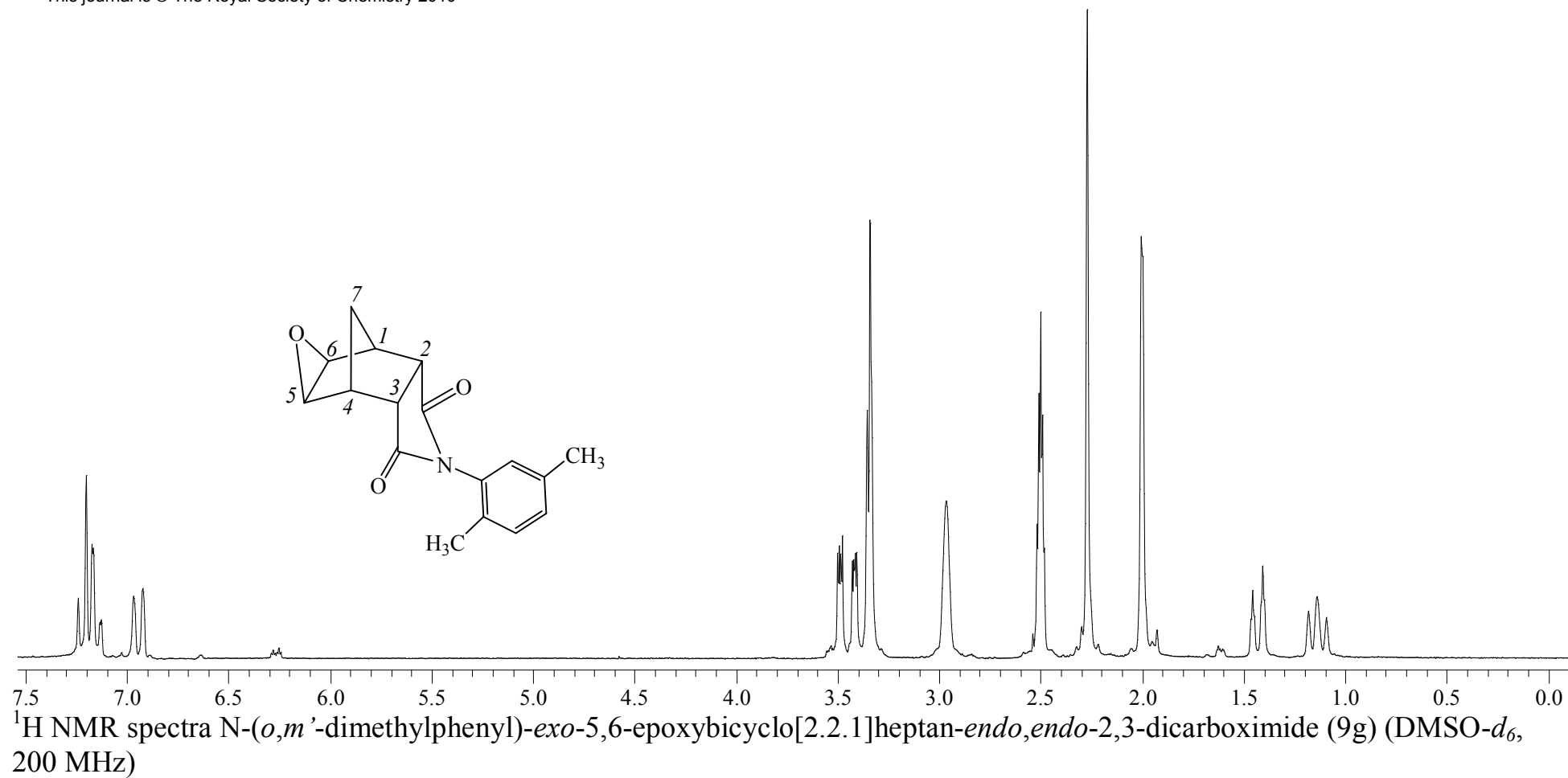
General Experimental. All solvents for reactions were dried and distilled immediately prior to use. Melting points were determined in capillary tubes and uncorrected. Infrared spectra were recorded on a UR-20 or Paragon 500 FT-IR (Perkin Elmer) spectrometer using KBr pellets. ¹H NMR spectra were recorded at 200 and 300 MHz on a Varian spectrometer. Chemical shifts (δ) are reported in ppm relative to TMS in the DMSO-*d*₆. EI mass spectra of compounds (**10a**, **11e**, **12k**) were recorded on an MX-1321 spectrometer (70eV). **The X-ray diffraction study** - All experiments were carried out on the «Xcalibur-3» diffractometer (graphite monochromated MoK_α radiation, CCD detector, ω-scanning). The structures were solved by direct method using SHELXTL package. The positions of the hydrogen atoms were located from electron density difference maps for all

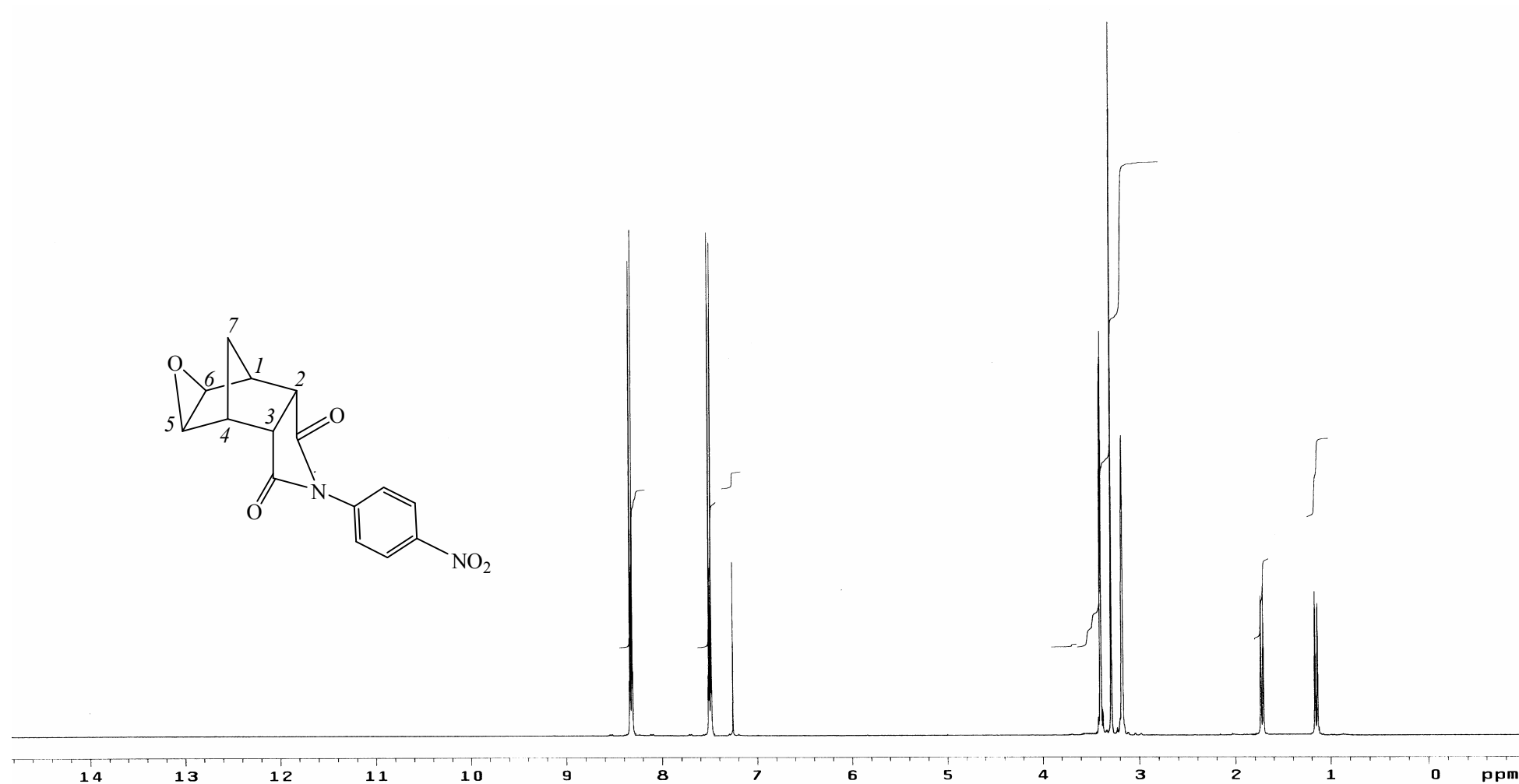
structures and refined by “riding” model with $U_{\text{iso}} = nU_{\text{eq}}$ of the carrier atom ($n = 1.5$ for methyl and hydroxyl groups and $n = 1.2$ for other hydrogen atoms) for the structure **11e**. The position of the hydrogen atoms in the structures **10a** and **12k** were refined in isotropic approximation. All non-hydrogen atoms were refined using anisotropic approximation. The final atomic coordinates, and crystallographic data have been deposited to with the Cambridge Crystallographic Data Centre, 12 Union Road, CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk). For thin-layer chromatography (TLC) analysis, TLC plates (Silufol UV-254) were used with diethyl ether or 2-propanol as an eluent and iodine vapor as a developer. Elemental analyses were carried out on a Carlo Erba analyzer.

Calculations. All computations were carried out with the Gaussian 03 program package. Geometry optimizations of the local minima and transition state structures were performed using the B3LYP functional and the 6-31+G(d) basis set in the presence of ethanol as solvent (Polarizable Continuum Model (PCM)). The basis set includes diffuse functions on heavy atoms to ensure the appropriate description of the anionic reactants. Harmonic vibrational frequencies and zero-point vibrational energy (ZPVE) corrections were calculated at the same level of theory. The energies of optimized structures were corrected by (ZPVE) scaled by 0.98. The dielectric constant ($\epsilon = 24.55$) which formally corresponds to the bulk of ethanol has been used.

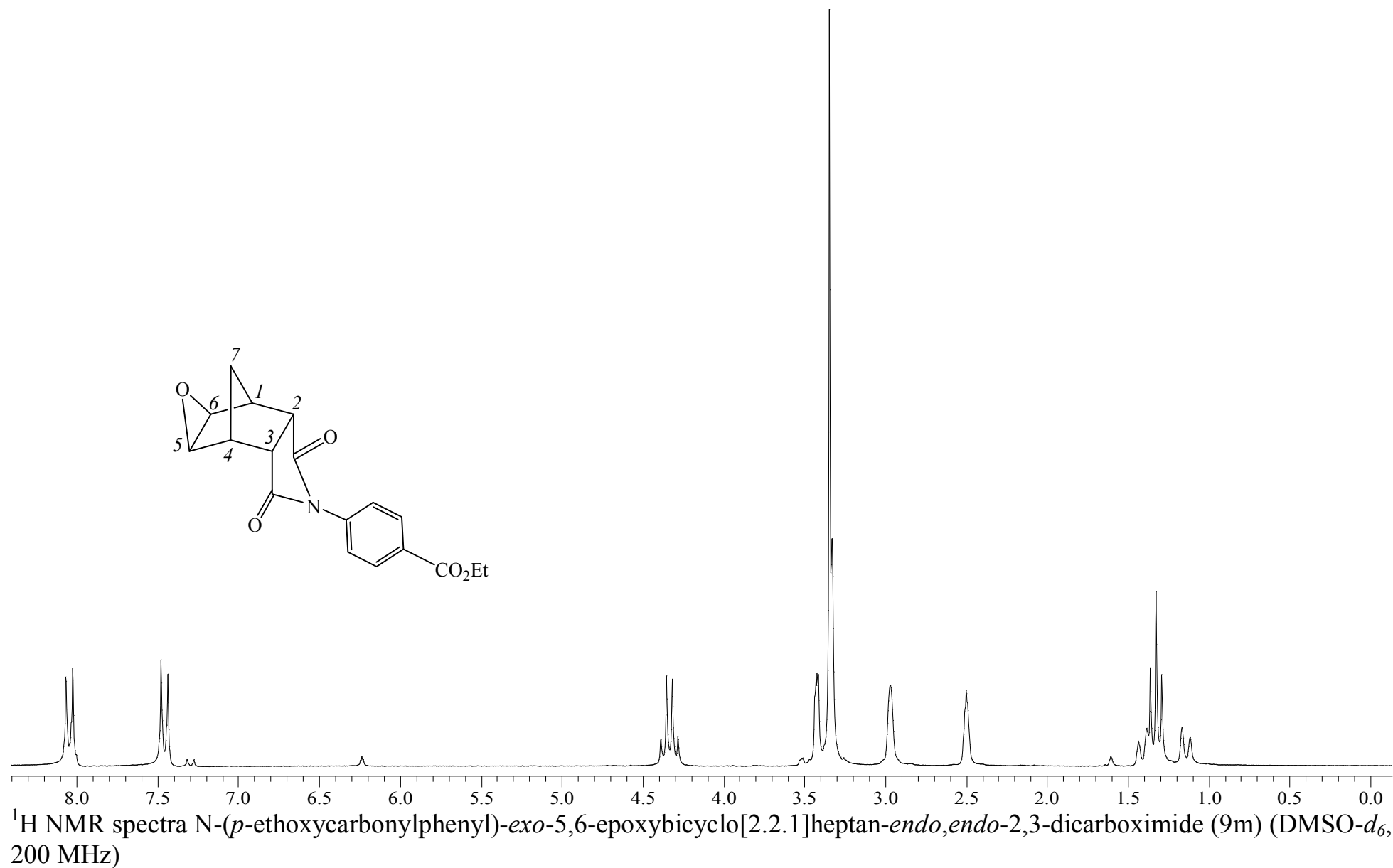


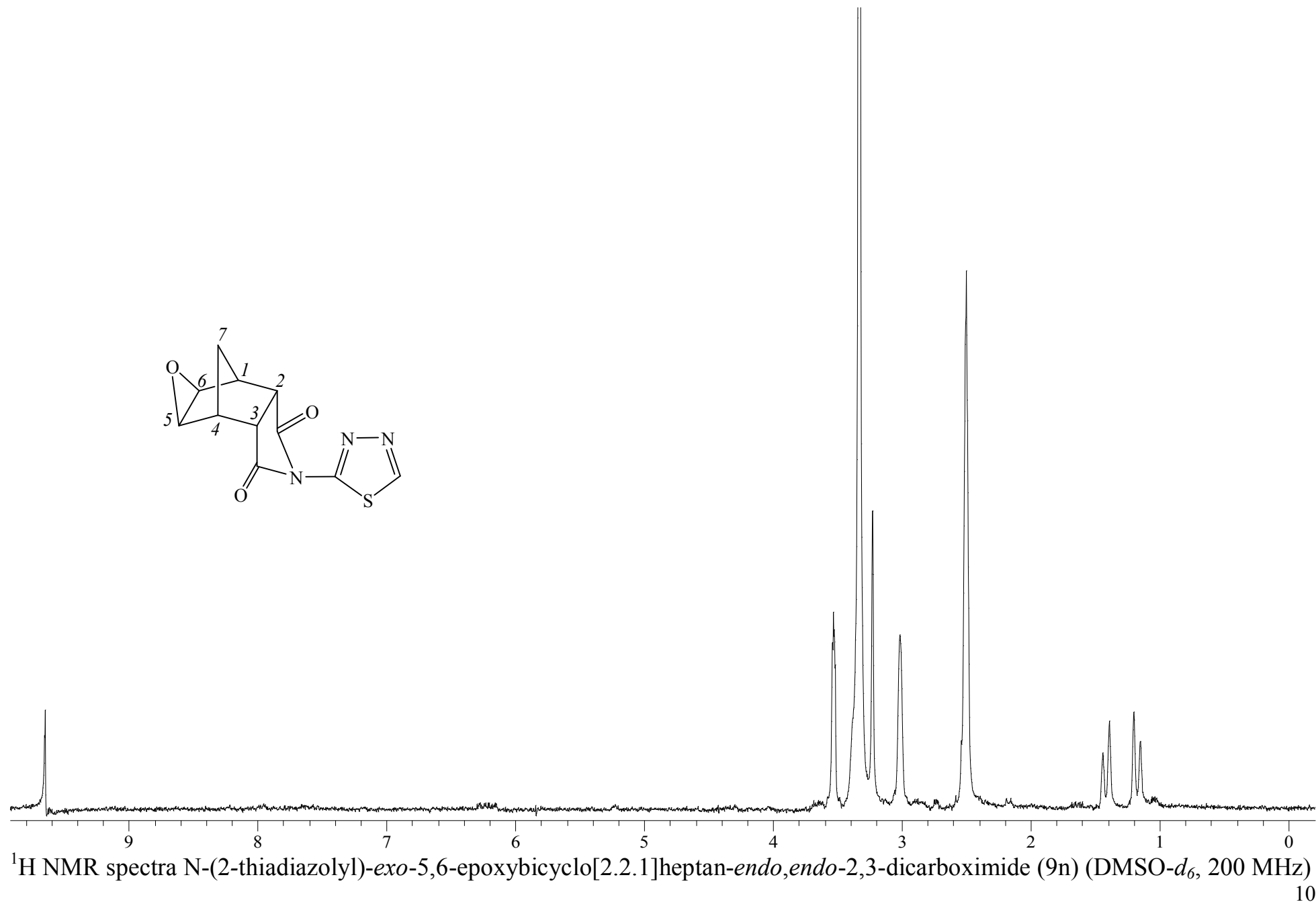


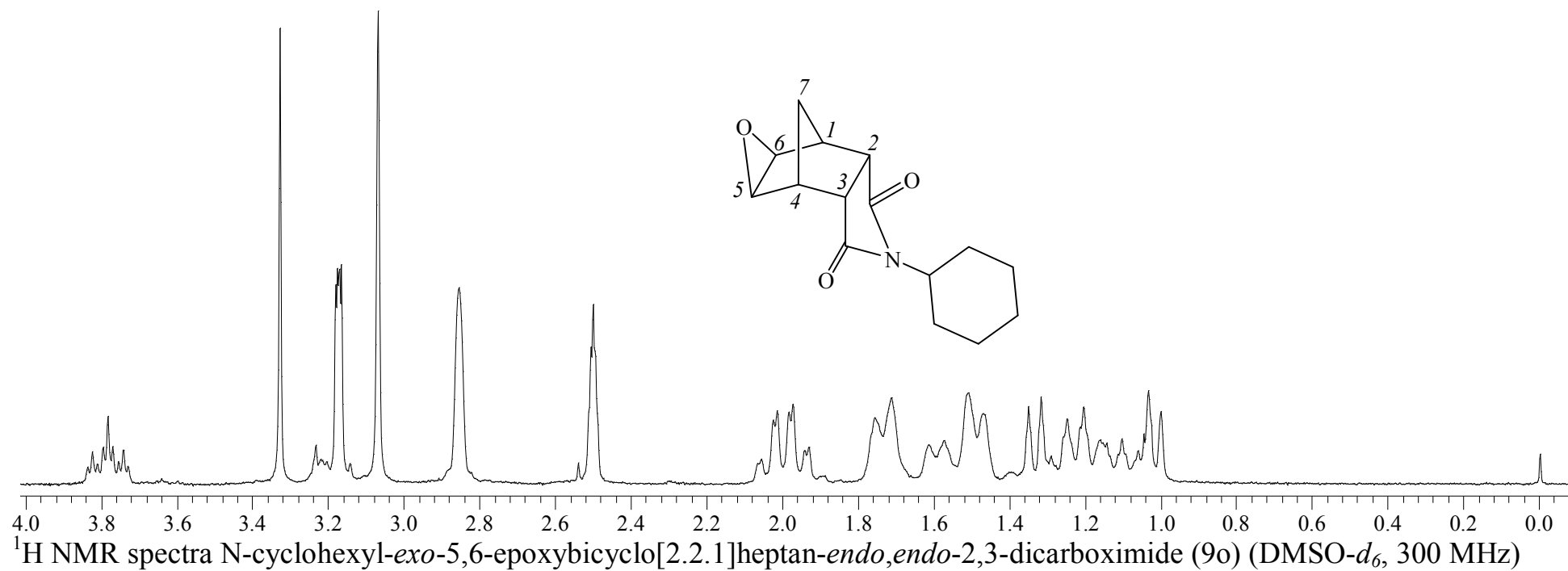


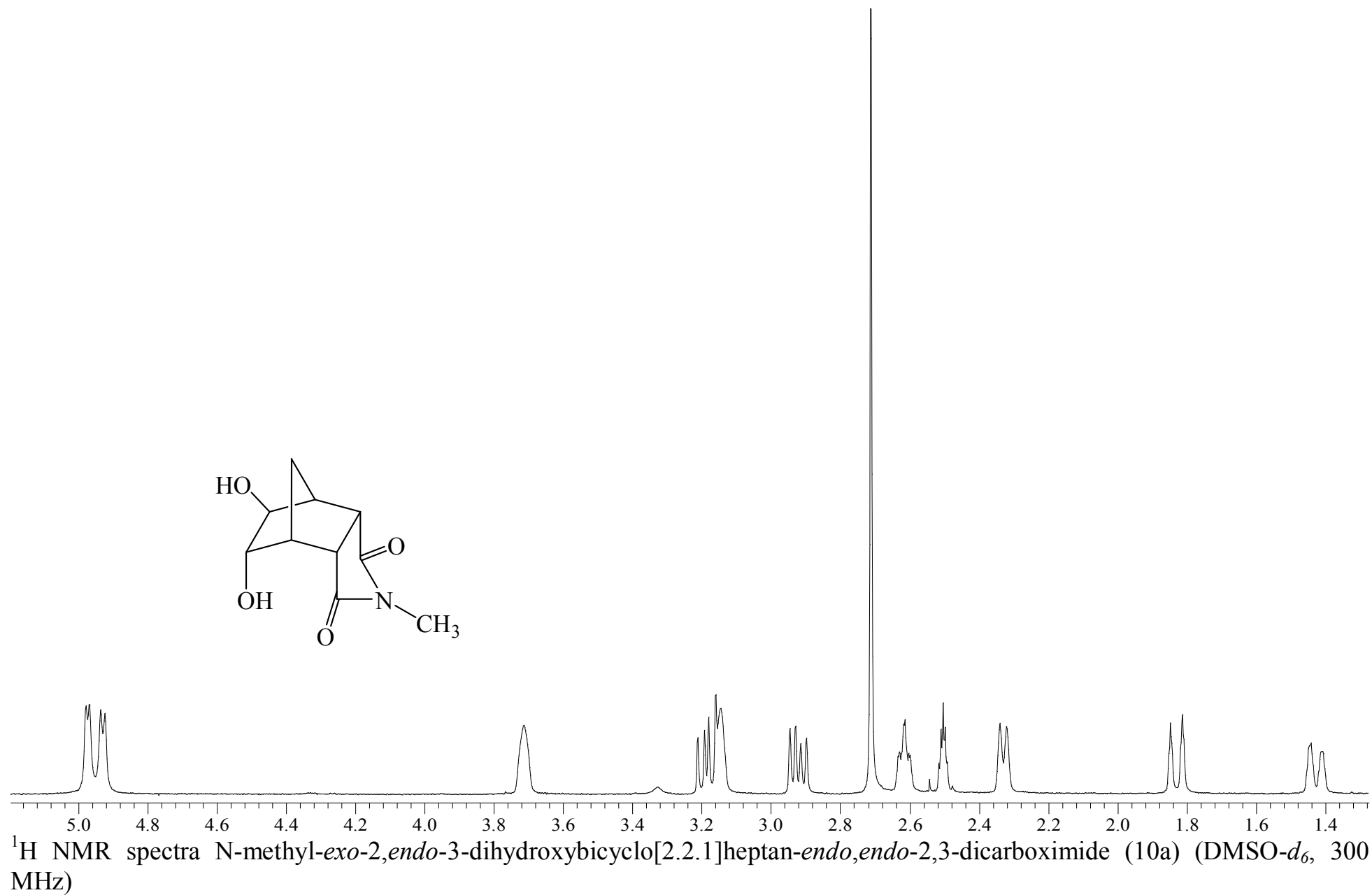


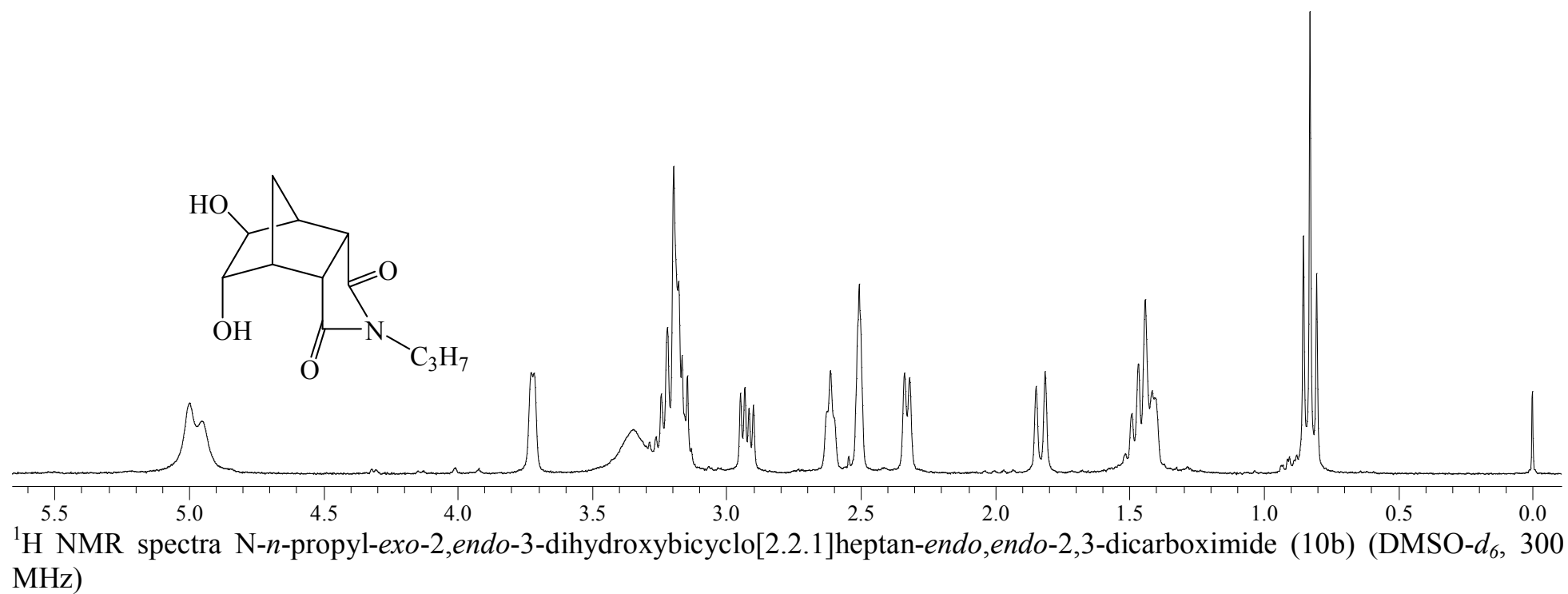
¹H NMR spectra N-(p-nitrophenyl)-exo-5,6-epoxybicyclo[2.2.1]heptan-endo,endo-2,3-dicarboximide (91) (300 MHz, CDCl₃)

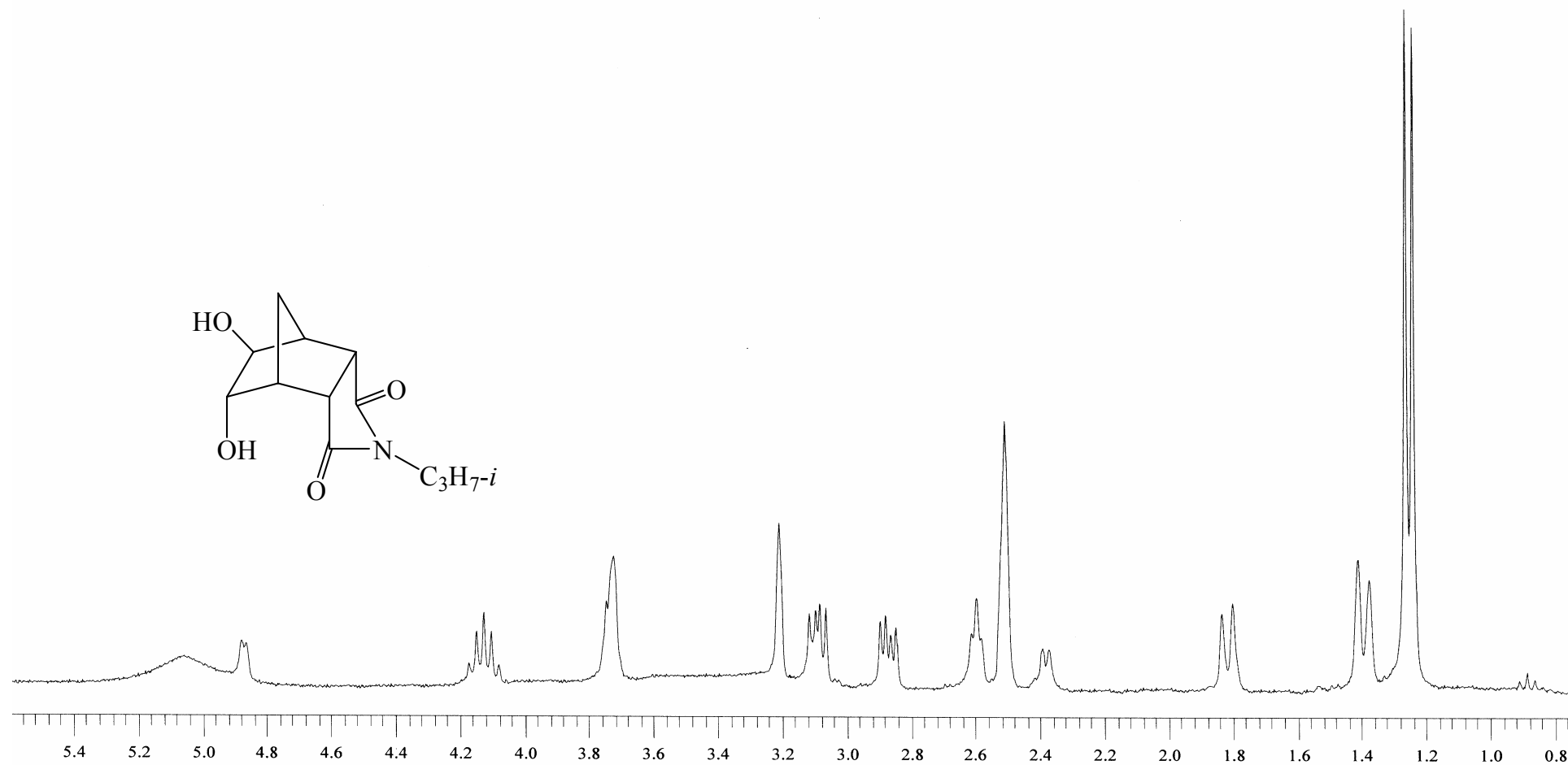




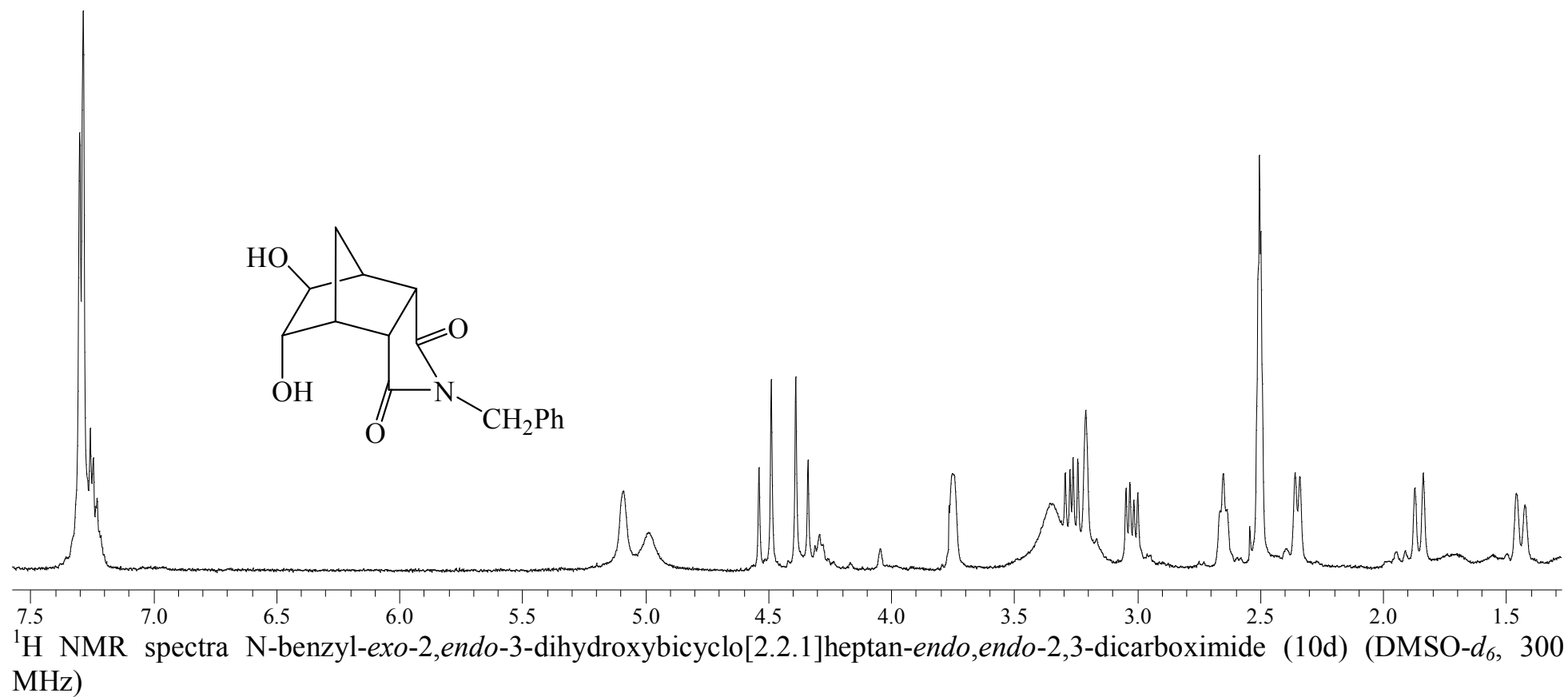


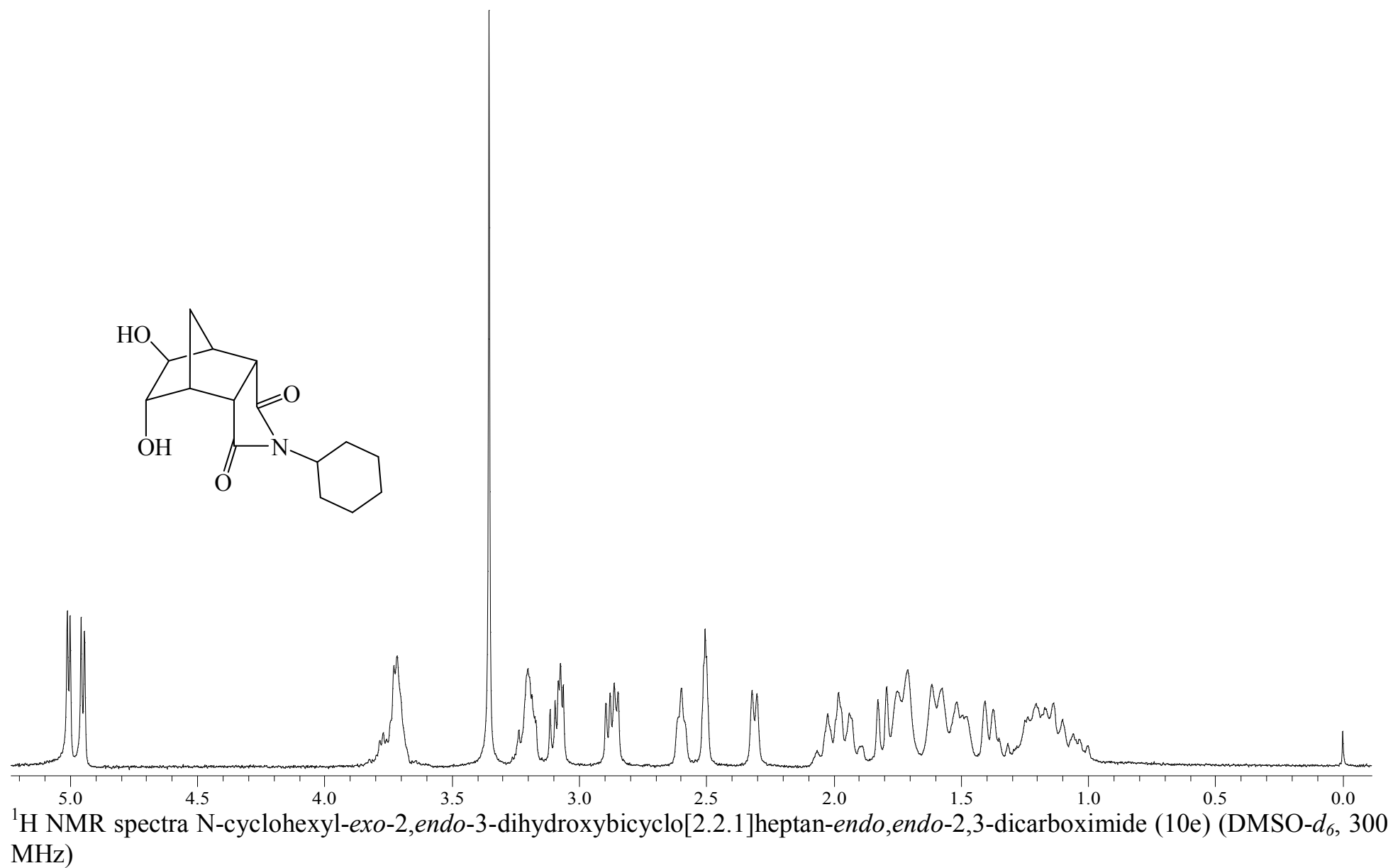


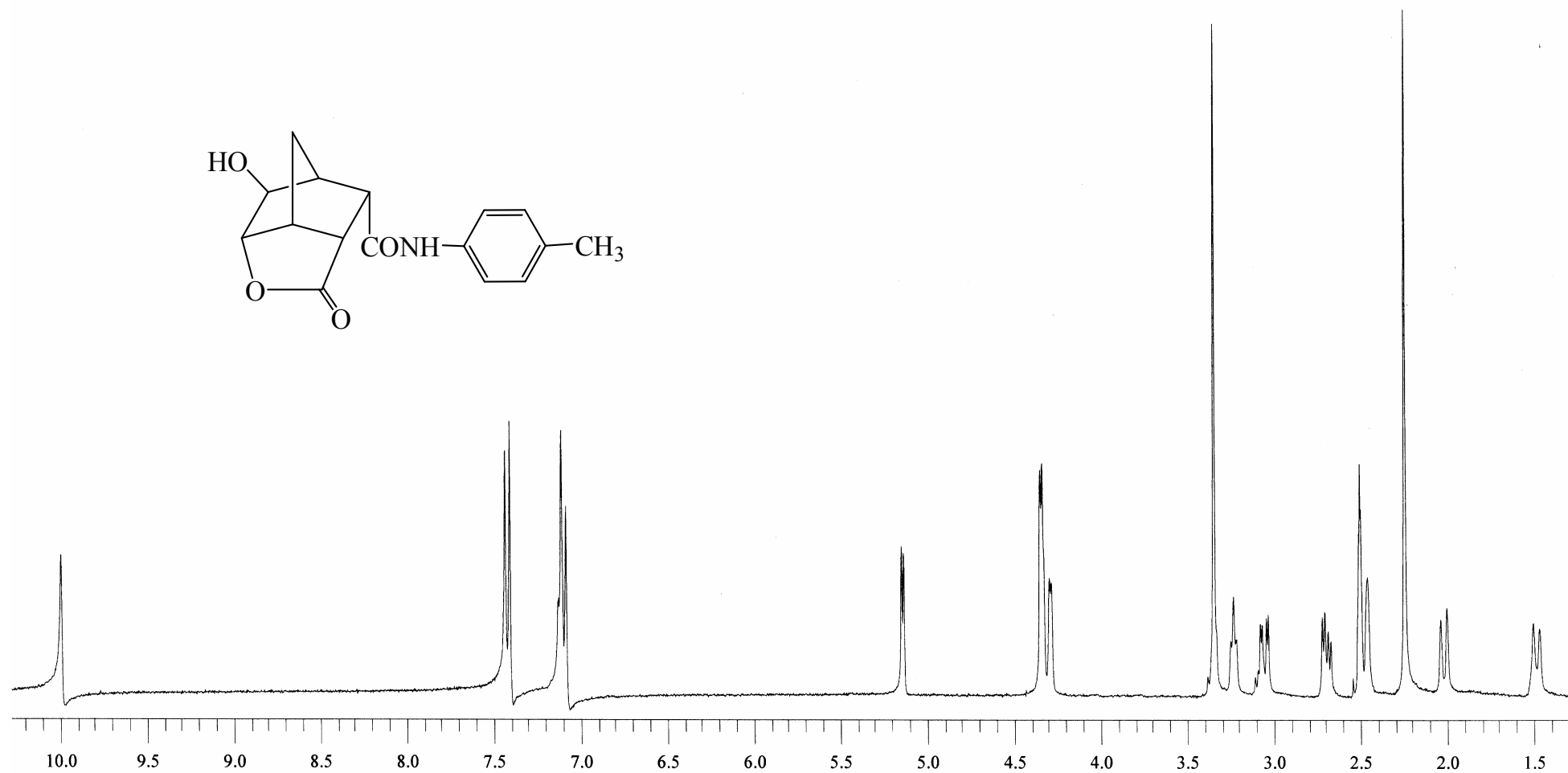




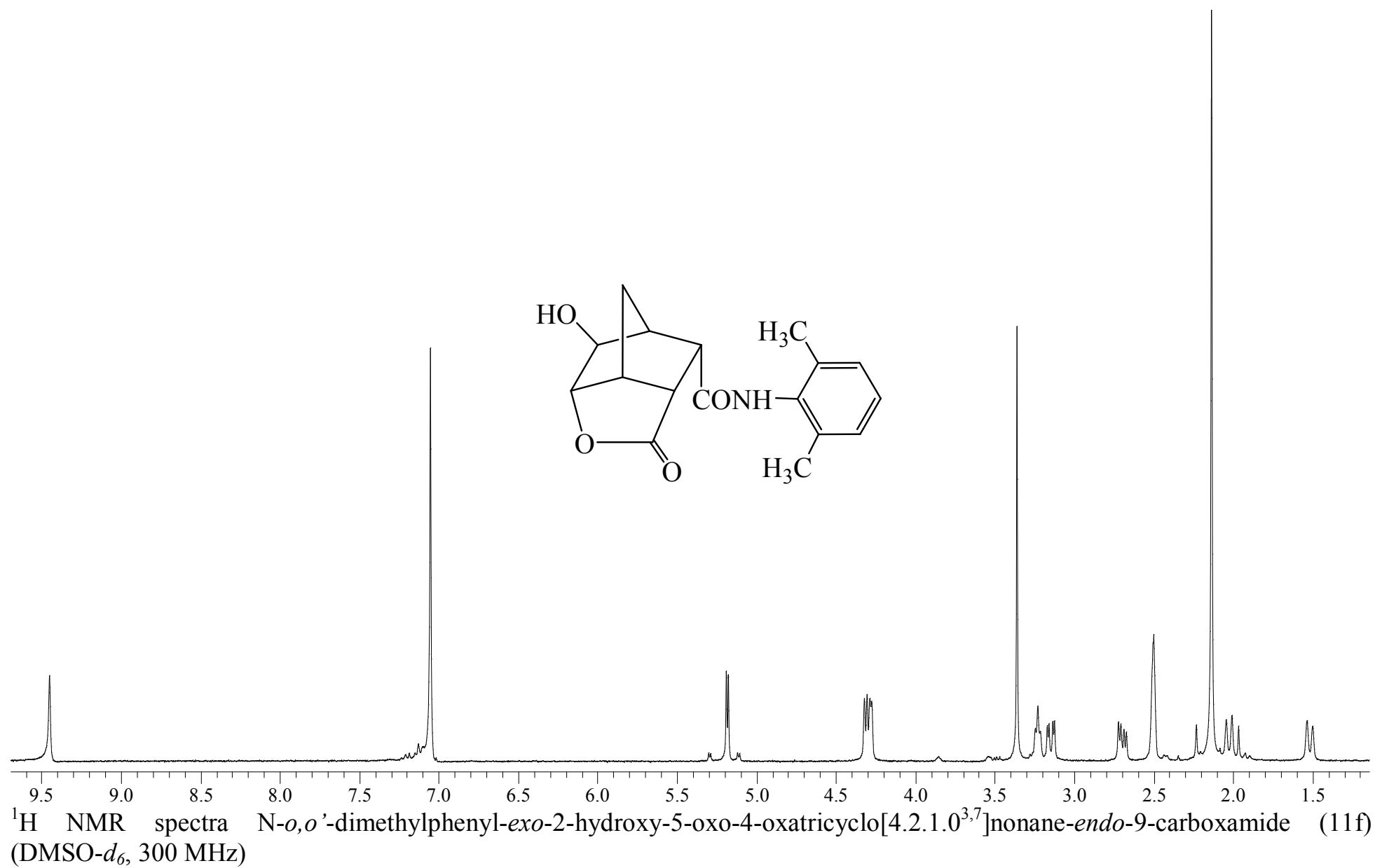
¹H NMR spectra N-*i*-propyl-exo-2,endo-3-dihydroxybicyclo[2.2.1]heptan-endo,endo-2,3-dicarboximide (10c) (DMSO-*d*₆, 300 MHz)

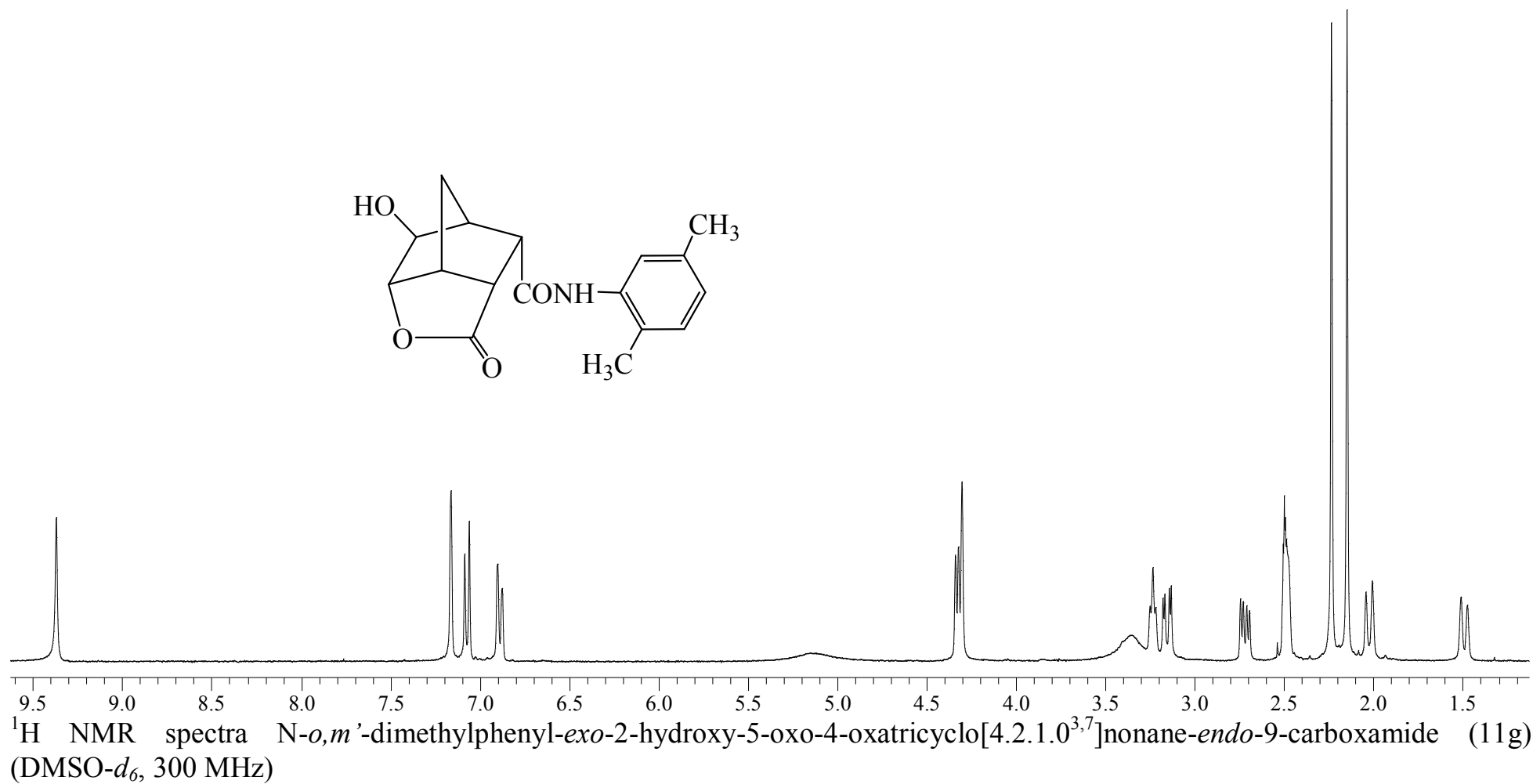
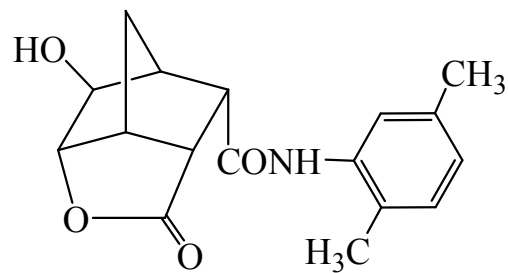


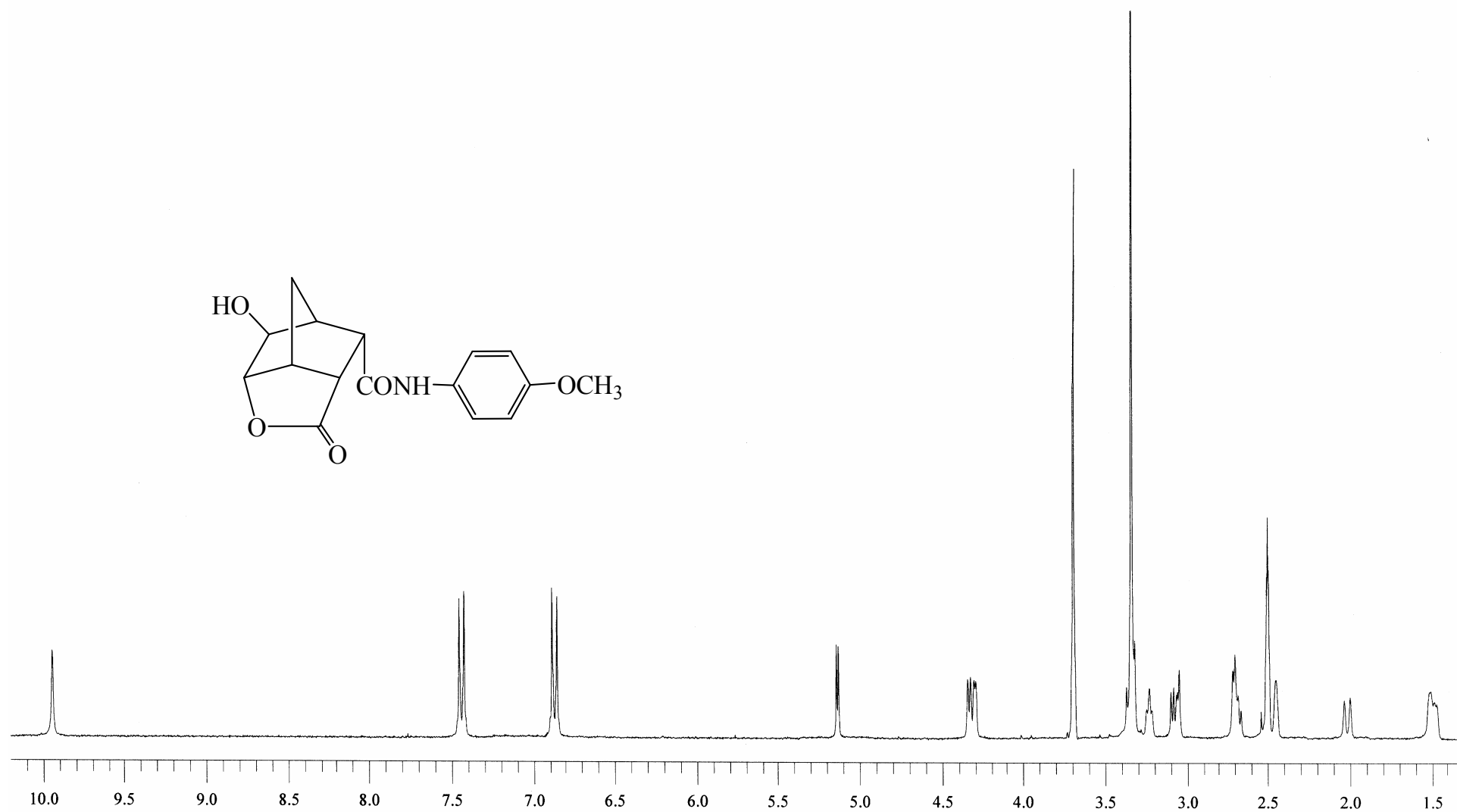




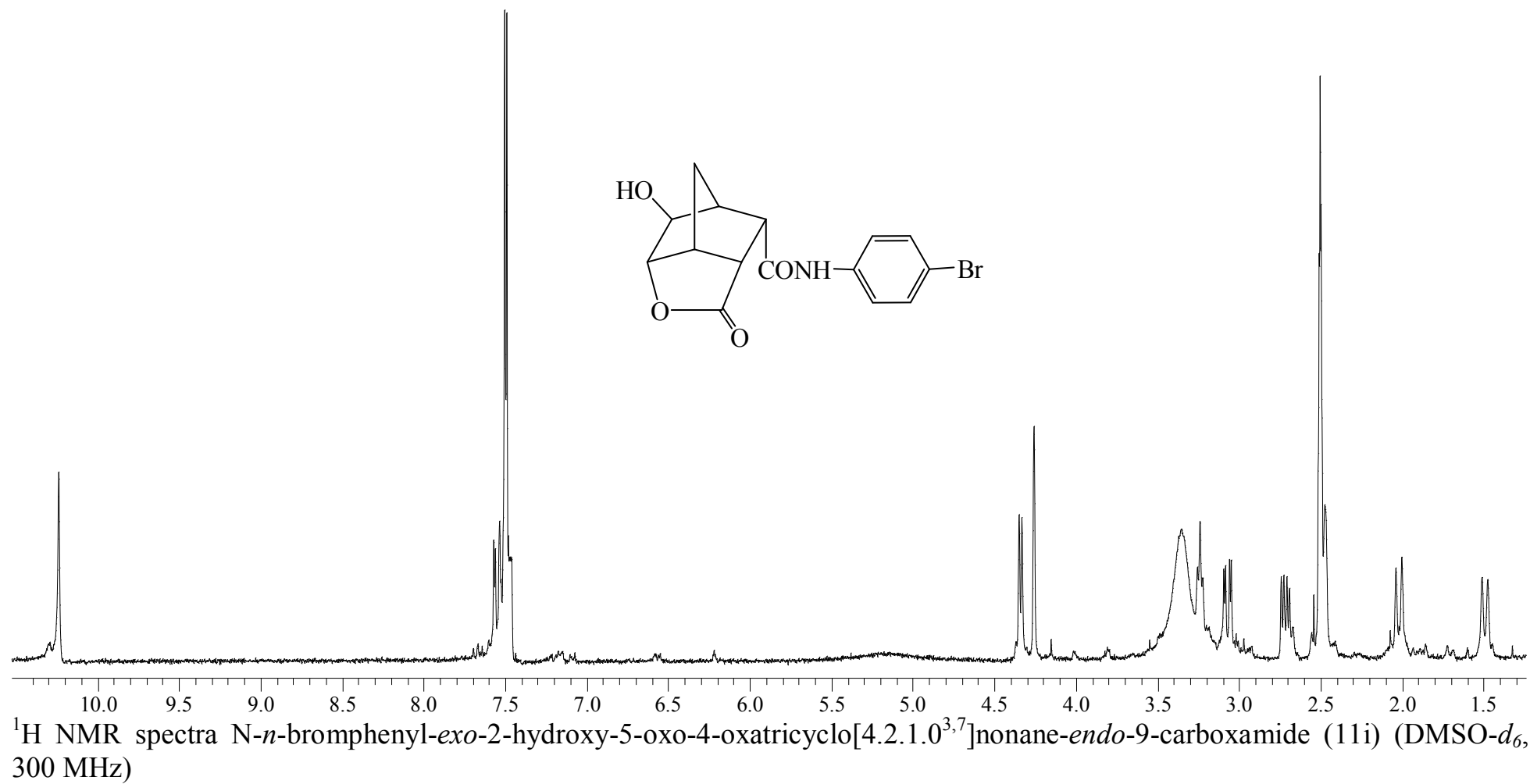
¹H NMR spectra N-*n*-tolyl-*exo*-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxamide (11e) (DMSO-*d*₆, 300 MHz)

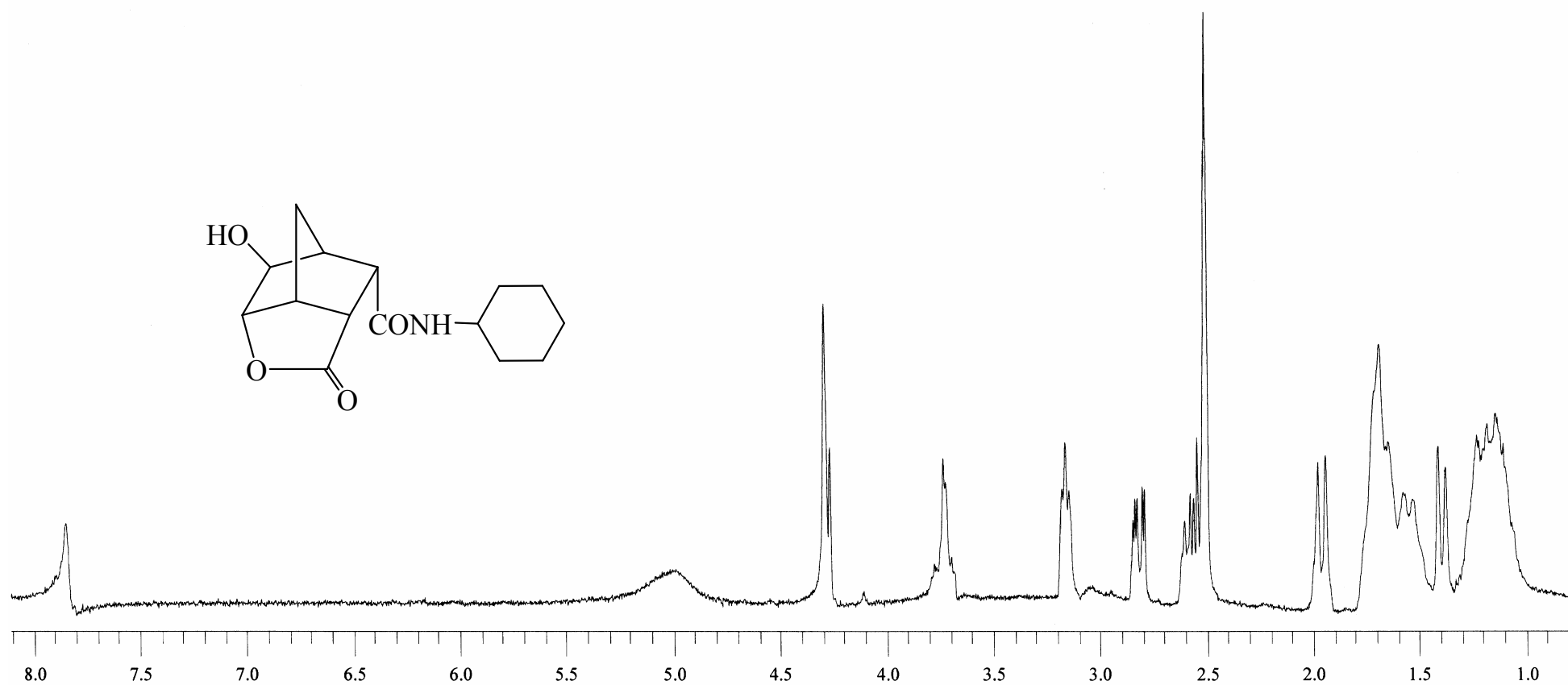




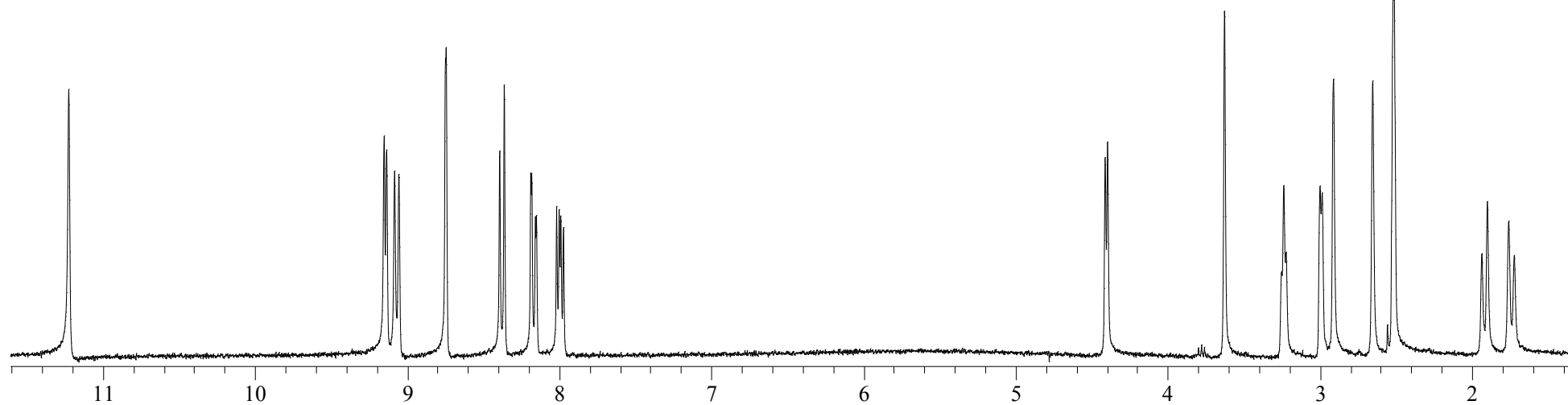
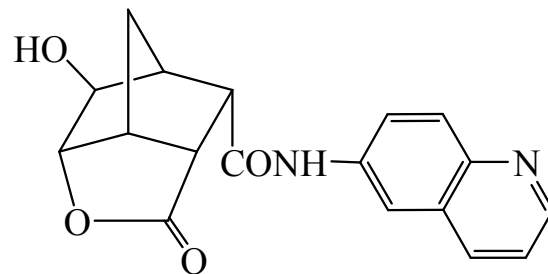


¹H NMR spectra *N*-*n*-methoxyphenyl-*exo*-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxamide (11h) (DMSO-*d*₆, 300 MHz)

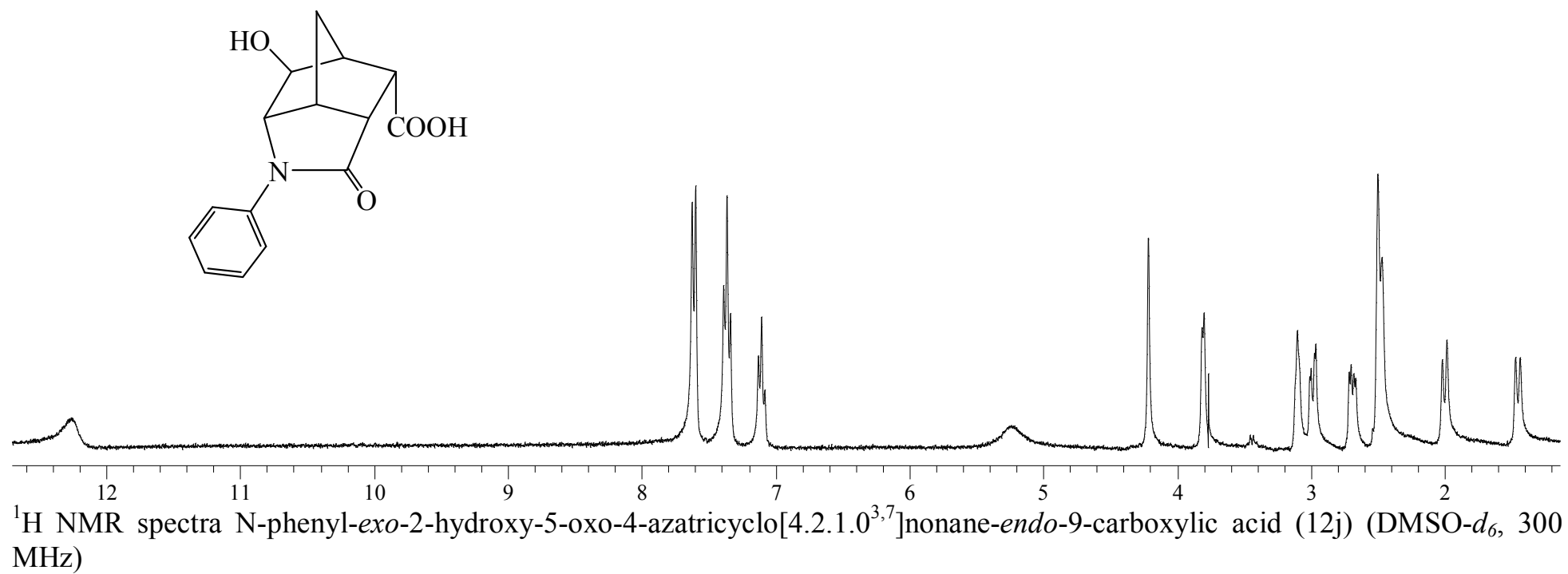


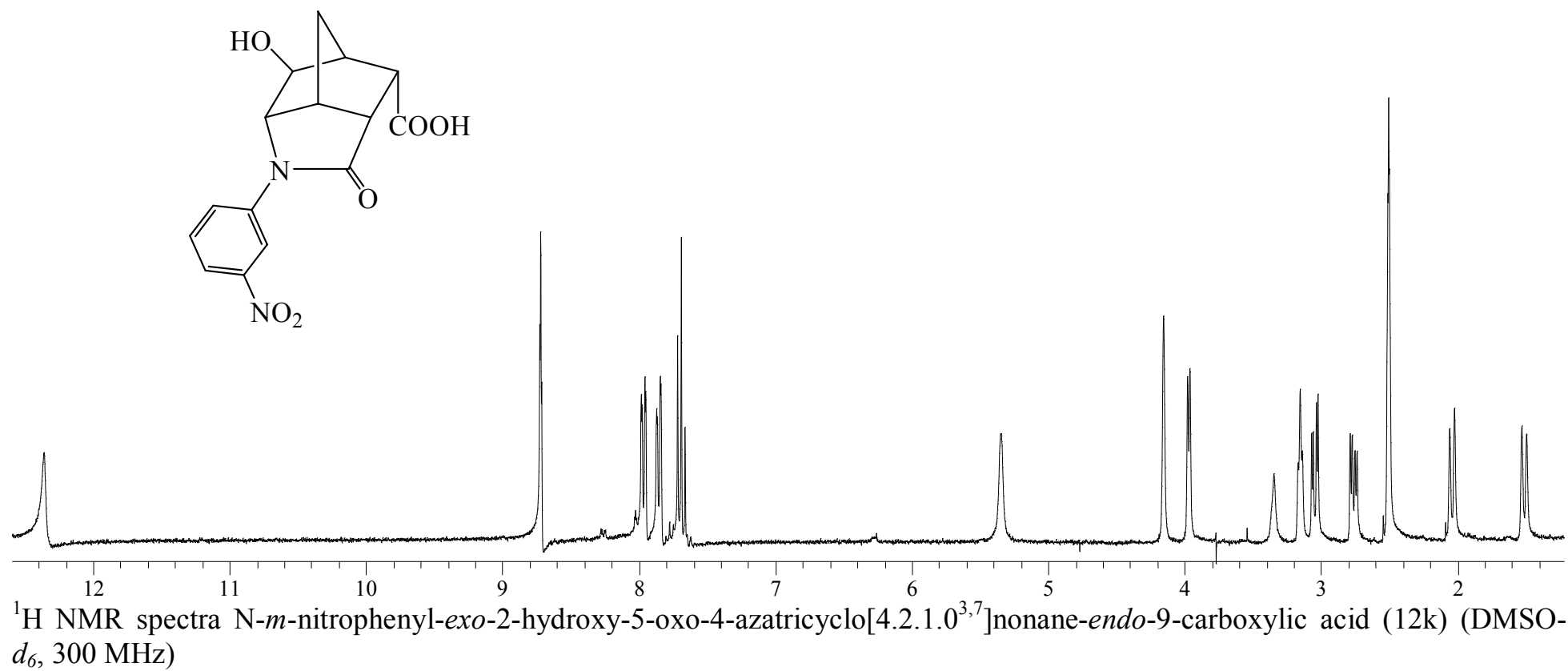


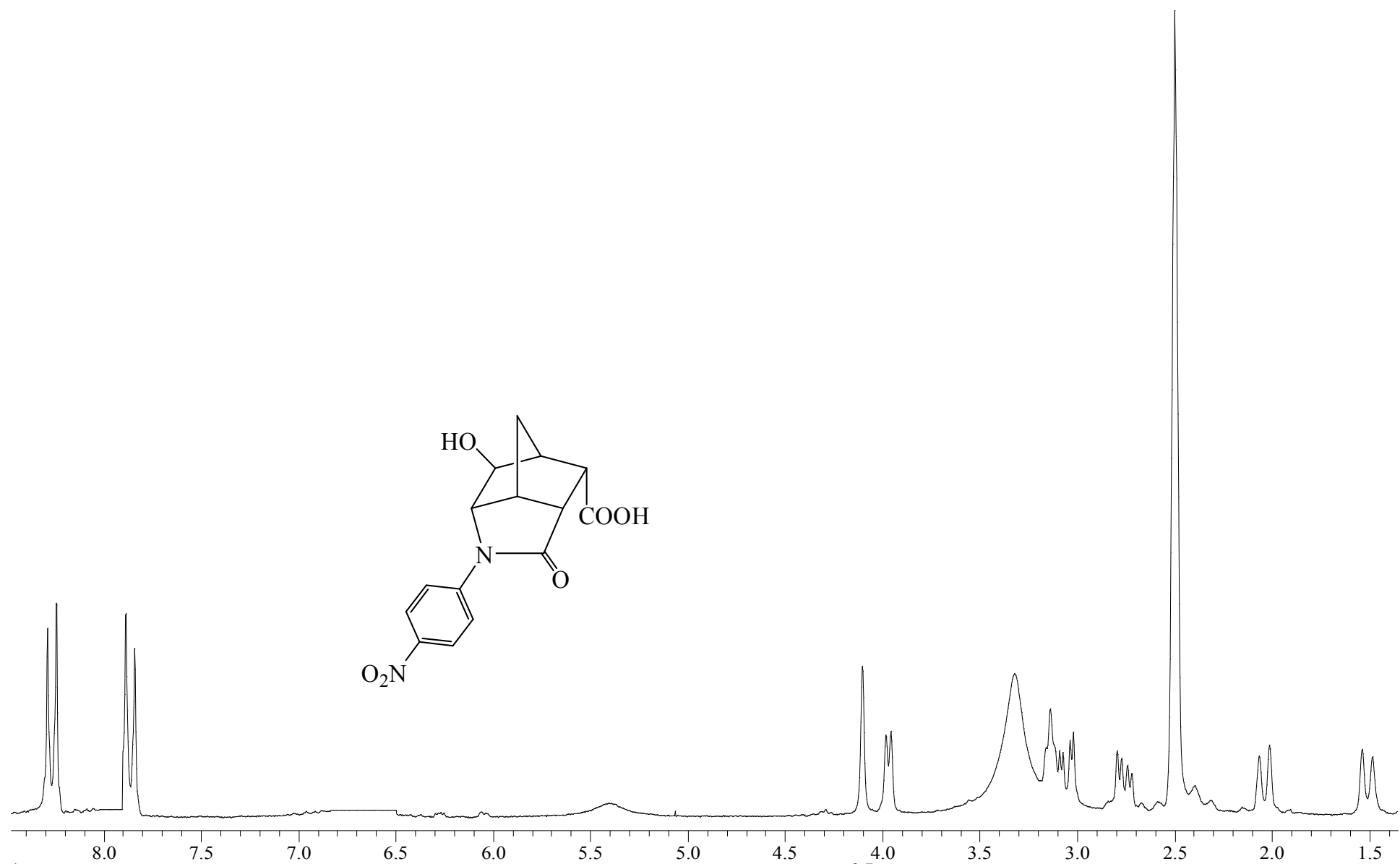
¹H NMR spectra N-cyclohexyl-*exo*-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxamide (11j) (DMSO-*d*₆, 300 MHz)



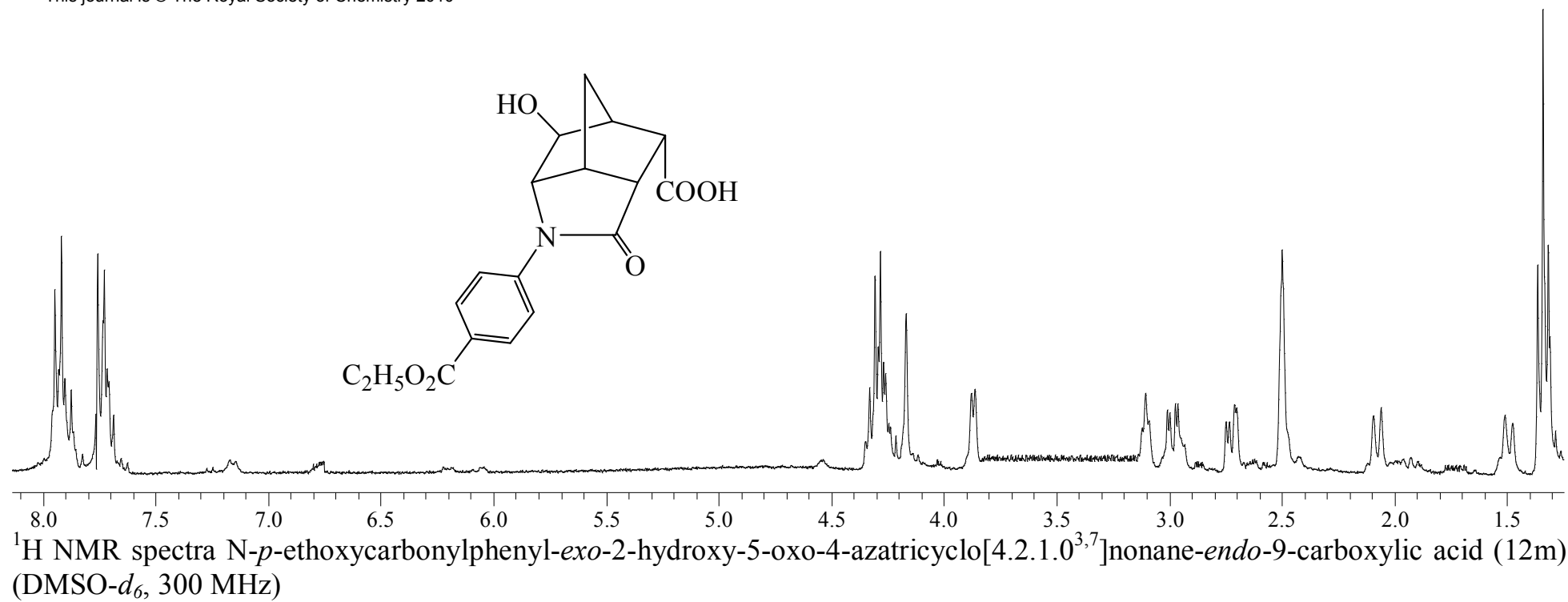
^1H NMR spectra N-(6-quinolyl)-*exo*-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxamide (11k) (DMSO-*d*₆, 300 MHz)

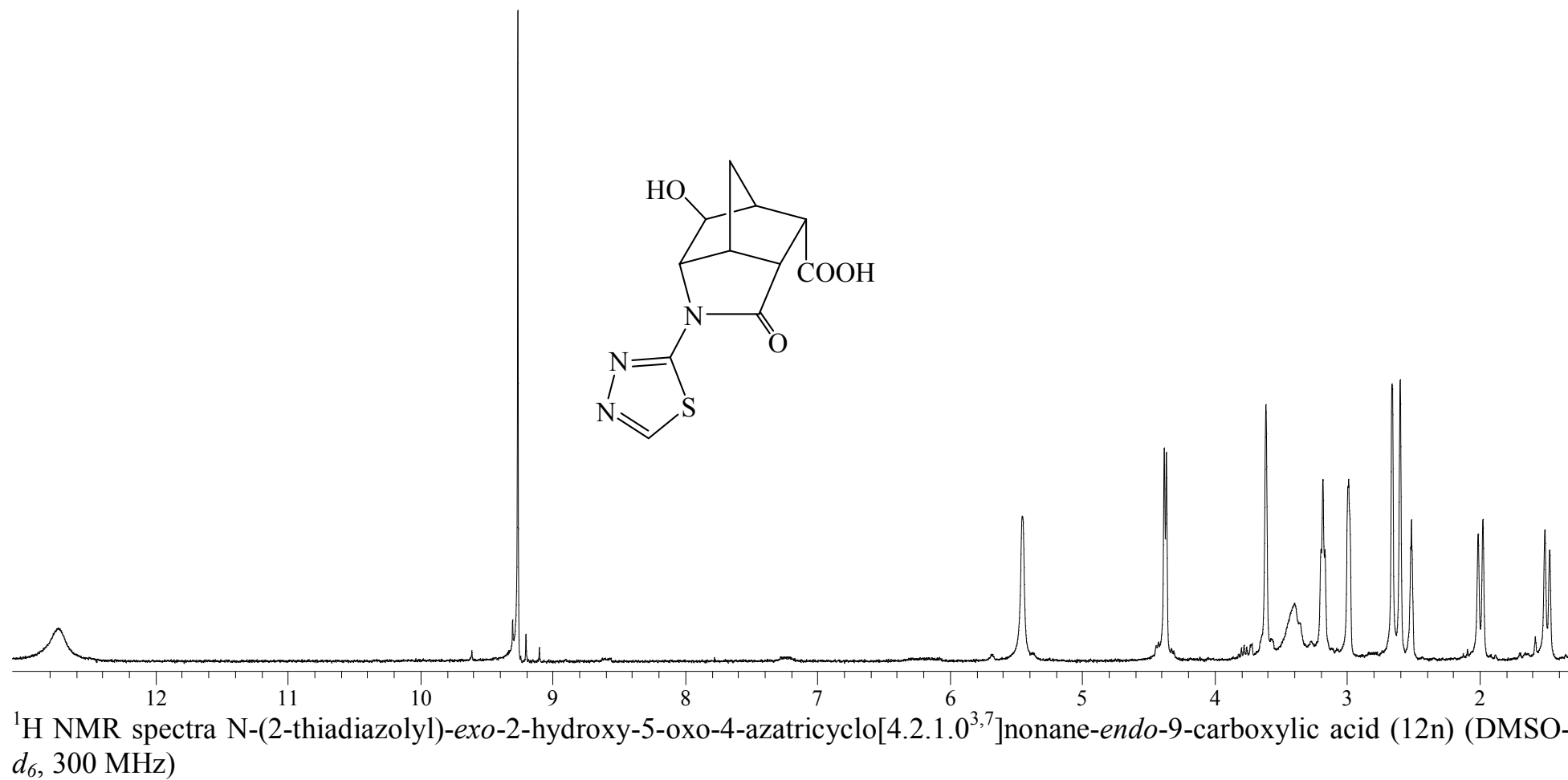


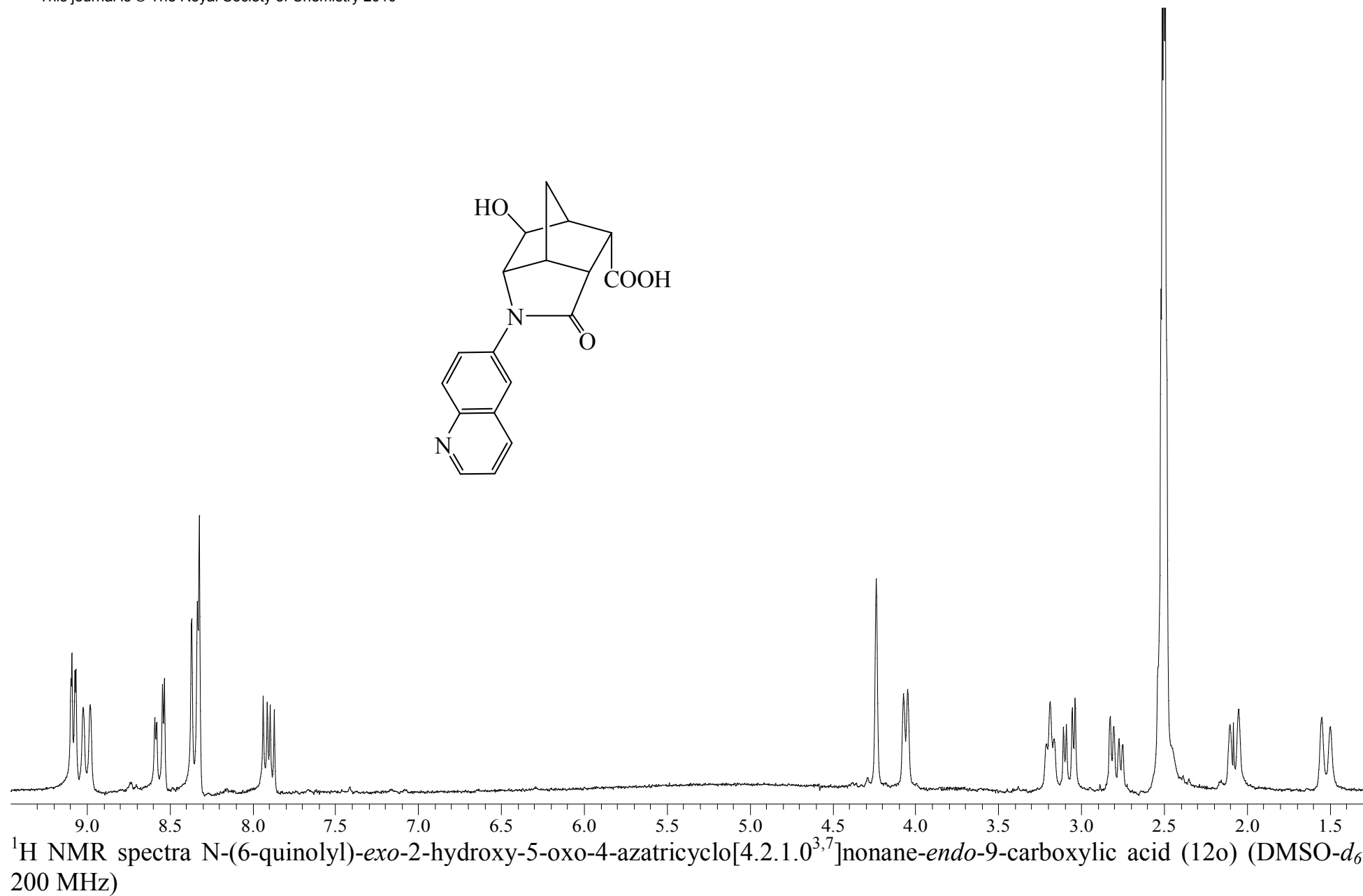
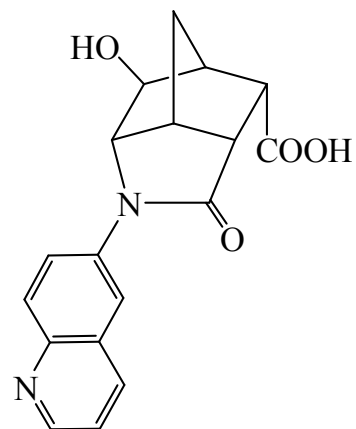




¹H NMR spectra N-*p*-nitrophenyl-*exo*-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxylic acid (12l) (DMSO-*d*₆, 200 MHz)







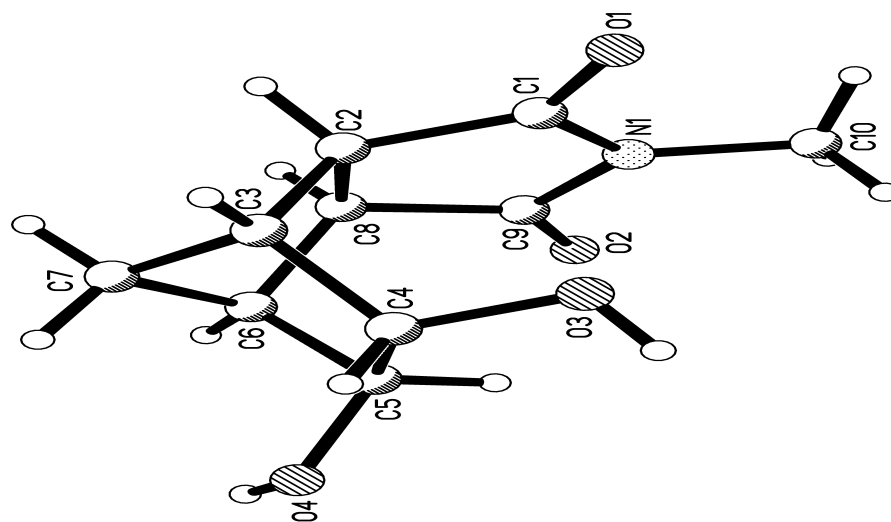


Figure 1. The molecular structure of the compound **10a** with numeration of the non-hydrogen atoms used in the structural investigation.

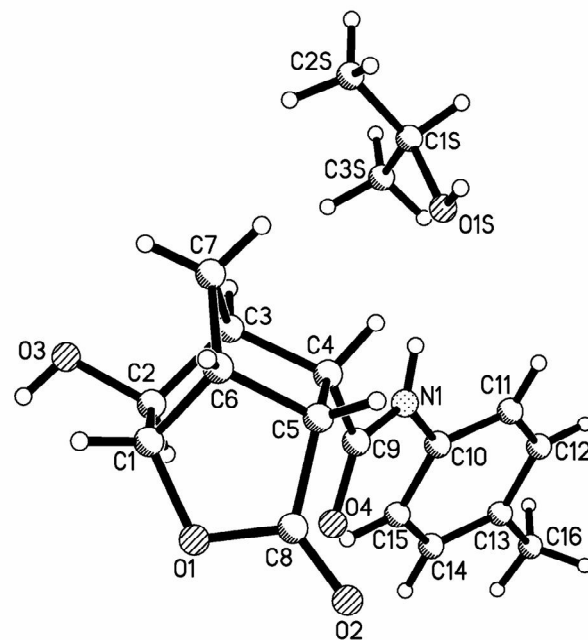


Figure 2. The molecular structure of the compound **11e** with numeration of the non-hydrogen atoms used in the structural investigation.

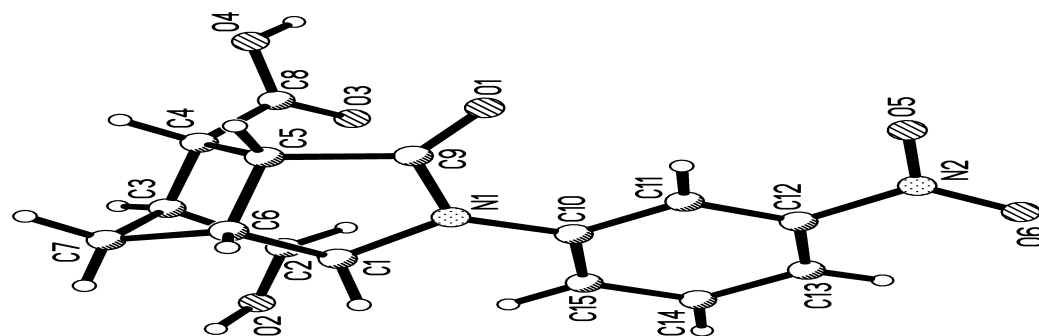
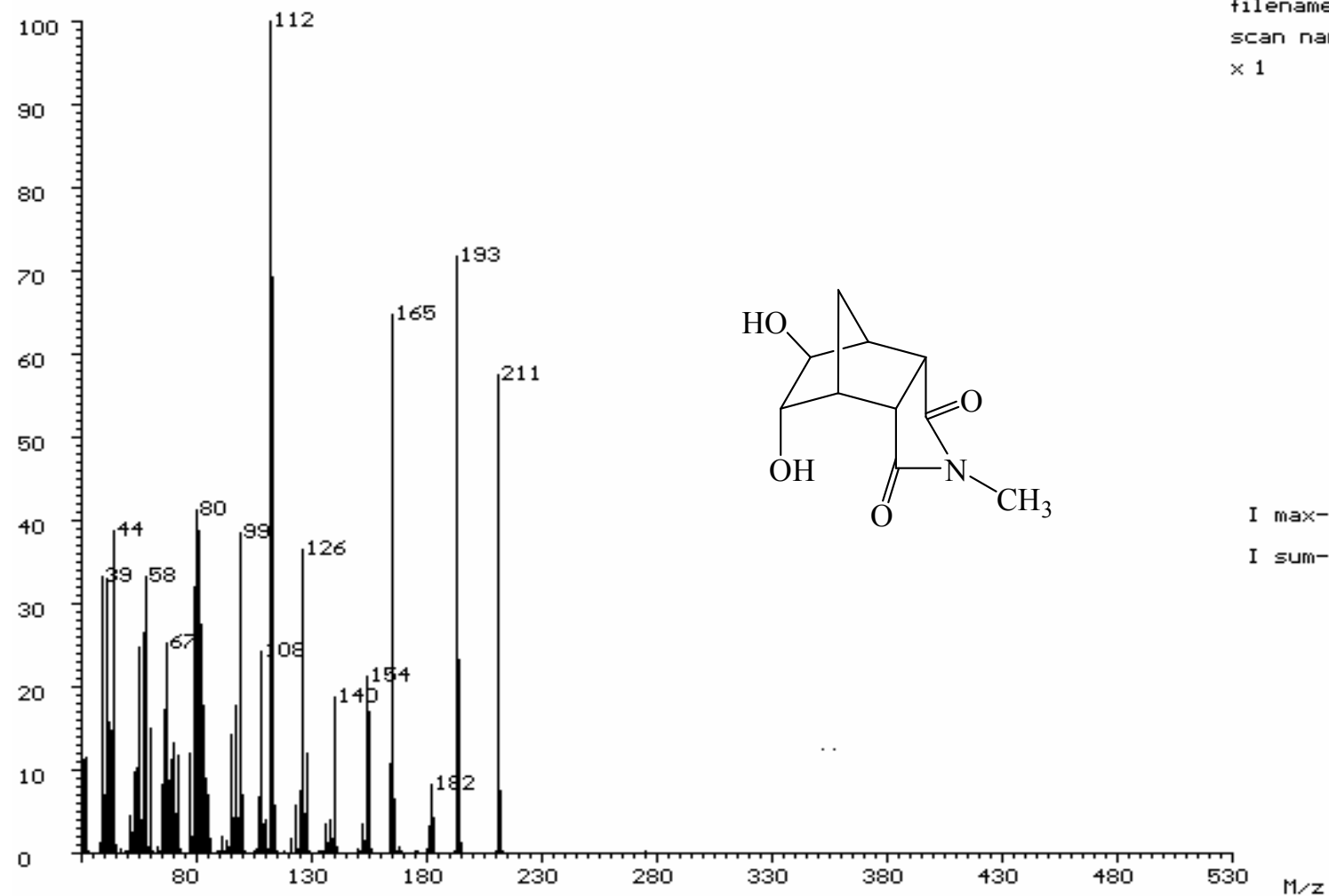
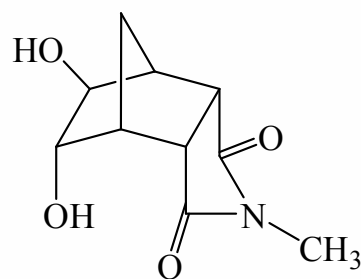


Figure 3. The molecular structure of the compound **12k** with numeration of the non-hydrogen atoms used in the structural investigation.

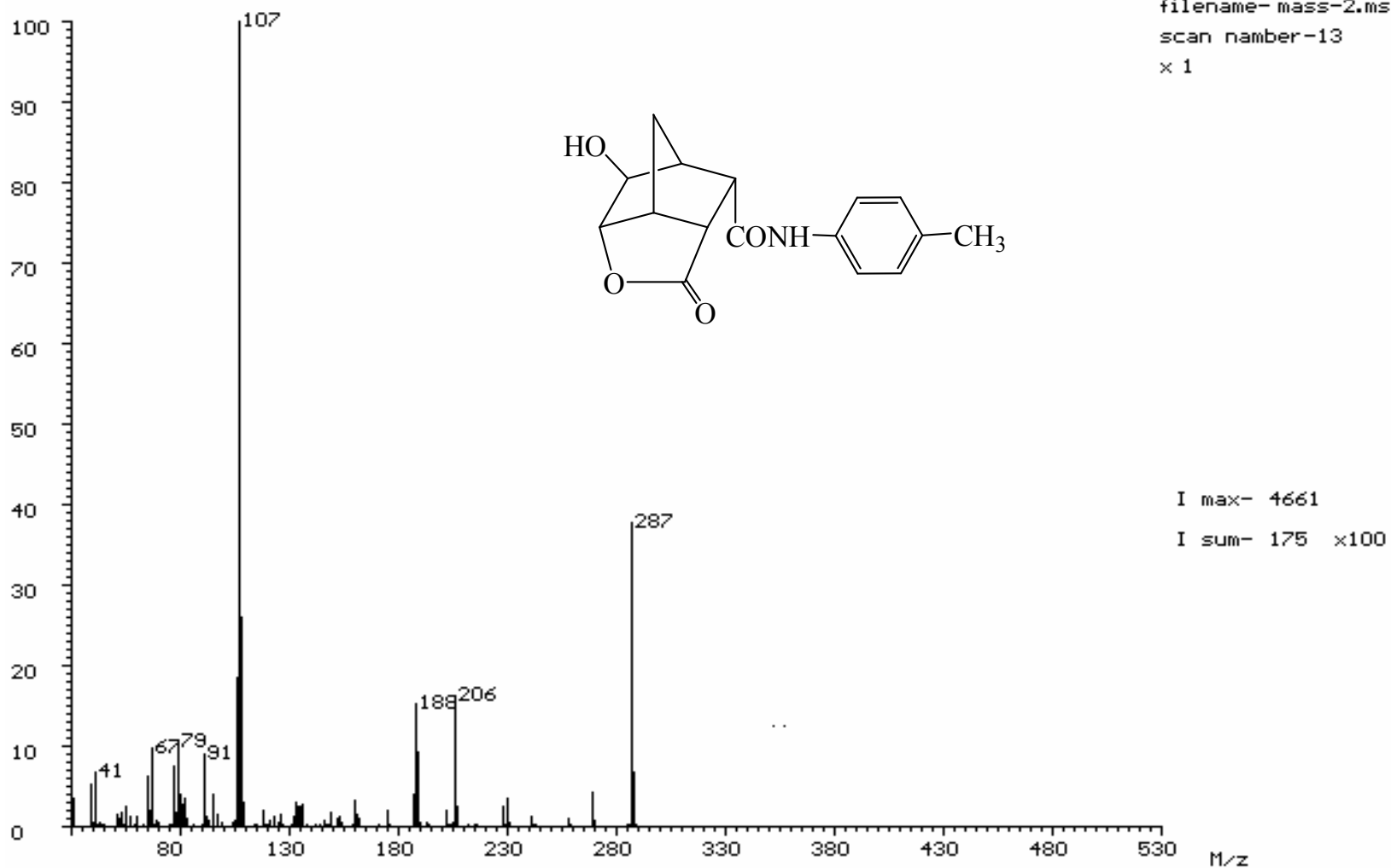


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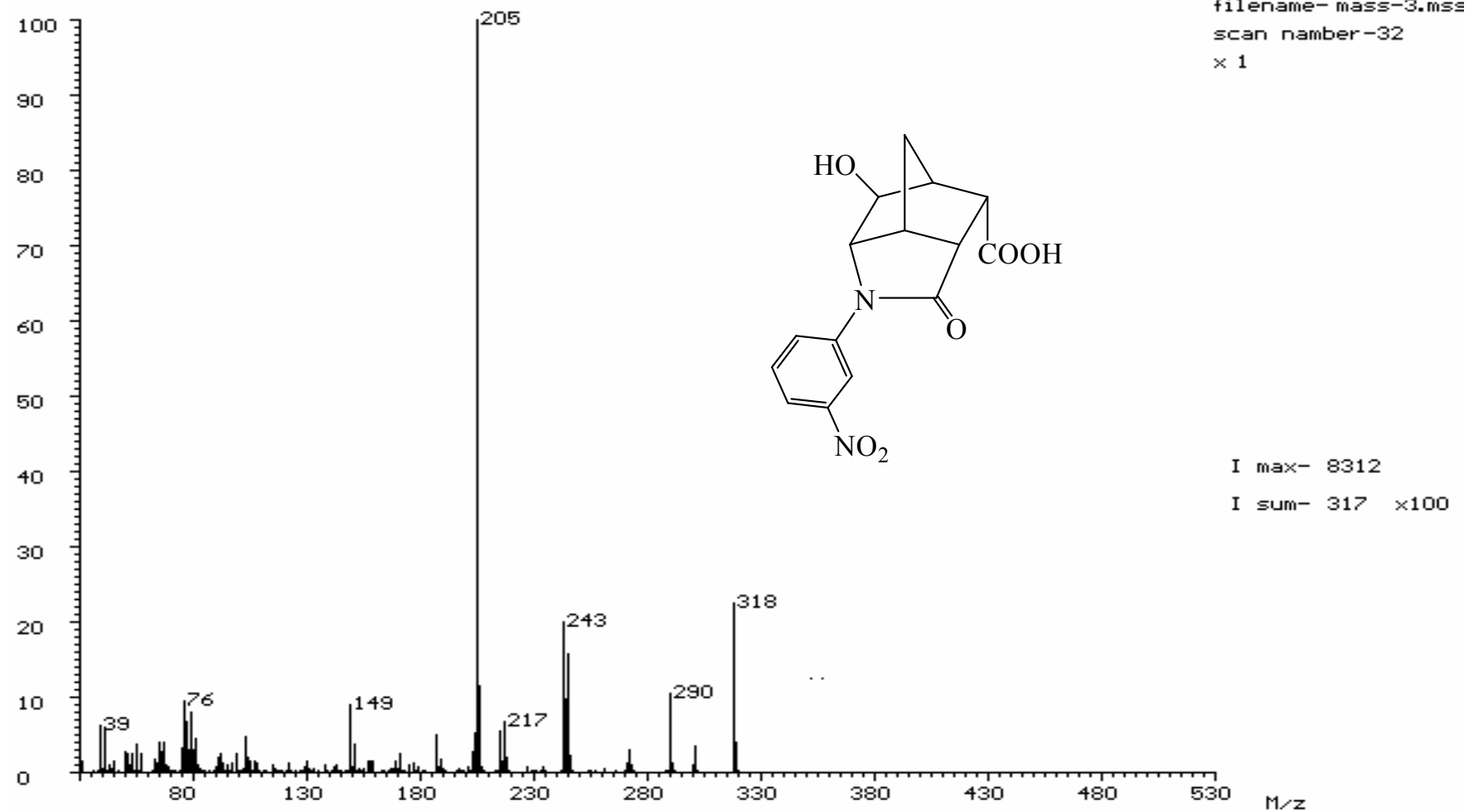


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Mass Spectra for N-Methyl-*exo*-2,*endo*-3-dihydroxybicyclo[2.2.1]heptan-*endo,endo*-2,3-dicarboximide (10a)



Mass Spectra for N-*n*-Tolyl-*exo*-2-hydroxy-5-oxo-4-oxatricyclo[4.2.1.0^{3,7}]nonane-*endo*-9-carboxamide (11e)



Mass Spectra for **N-m-Nitrophenyl-exo-2-hydroxy-5-oxo-4-azatricyclo[4.2.1.0^{3,7}]nonane-endo-9-carboxylic acid (12k)**

Cartezian coordinates for PCM/B3LYP/6-31+G(d) (solvent-ethanol) optimized geometries

9a					9e					9l				
6	0	1.364809	-0.738204	1.049138	6	0	-2.566380	-1.471221	-0.162240	6	0	-3.073801	-1.445637	-0.486555
6	0	1.364568	0.734966	1.051633	6	0	-2.558200	-0.608969	-1.357310	6	0	-3.063301	-0.368193	-1.492612
6	0	1.474668	-1.143978	-0.424966	6	0	-3.085002	-0.585943	0.976335	6	0	-3.646636	-0.810765	0.785659
6	0	1.473749	1.146300	-0.420933	6	0	-3.073602	0.754155	-0.881146	6	0	-3.631652	0.863521	-0.777197
6	0	0.097204	0.780553	-1.075613	6	0	-1.937828	1.357284	0.014291	6	0	-2.536500	1.311484	0.250558
6	0	-1.159475	1.165158	-0.317306	6	0	-0.519344	1.281054	-0.518127	6	0	-1.107291	1.380939	-0.246382
6	0	0.097592	-0.777079	-1.077792	6	0	-1.944033	0.446533	1.276092	6	0	-2.545770	0.174832	1.311658
6	0	-1.158028	-1.164448	-0.319128	6	0	-0.526987	-0.085802	1.383092	6	0	-1.119965	-0.336158	1.359123
6	0	2.337524	0.002542	-1.007619	6	0	-4.071815	0.346130	0.230671	6	0	-4.642716	0.223902	0.206139
8	0	-1.569556	2.291080	-0.071454	8	0	-0.067512	1.834597	-1.507141	8	0	-0.649888	2.119105	-1.100537
7	0	-1.816519	-0.000412	0.074281	7	0	0.230521	0.452283	0.331288	7	0	-0.347643	0.420187	0.453077
8	0	-1.566612	-2.291292	-0.074775	8	0	-0.079831	-0.842348	2.229924	8	0	-0.670879	-1.230625	2.053787
6	0	-3.071215	-0.002298	0.817816	6	0	1.631705	0.187207	0.144442	6	0	1.056282	0.236266	0.264302
8	0	2.495879	-0.002394	1.572026	8	0	-3.503013	-1.699028	-1.241391	8	0	-3.976439	-1.483264	-1.616264
1	0	0.832479	-1.349070	1.778116	6	0	3.415552	-1.289270	-0.532717	6	0	2.920245	-1.200622	-0.275704
1	0	0.833309	1.343396	1.783365	6	0	2.049718	-1.044995	-0.359074	6	0	1.550622	-1.022450	-0.097982
1	0	1.804535	-2.168288	-0.621226	6	0	4.373839	-0.315427	-0.215611	6	0	3.769935	-0.107051	-0.094172
1	0	1.802808	2.171588	-0.613395	6	0	5.850218	-0.579743	-0.404187	7	0	5.210433	-0.290293	-0.284337
1	0	0.036272	1.212530	-2.082948	6	0	3.927342	0.918354	0.288425	6	0	3.290175	1.155336	0.263562
1	0	0.035729	-1.206229	-2.086279	6	0	2.567984	1.172542	0.472179	6	0	1.920534	1.322741	0.447476
1	0	2.340869	0.004492	-2.102623	1	0	-1.857835	-2.280459	0.012482	8	0	5.951836	0.685276	-0.127706
1	0	3.366169	0.002333	-0.642828	1	0	-1.841251	-0.702457	-2.172745	8	0	5.623579	-1.412671	-0.593364
1	0	-3.923988	-0.010348	0.130463	1	0	-3.460577	-1.107298	1.861525	1	0	-2.346882	-2.256626	-0.450940
1	0	-3.113410	0.897062	1.434592	1	0	-3.438641	1.431374	-1.658628	1	0	-2.324886	-0.284333	-2.289775
1	0	-3.105191	-0.894803	1.445040	1	0	-2.159469	2.408340	0.241351	1	0	-4.025611	-1.502535	1.543182
EtO (anion)					1	0	-2.170369	0.993851	2.200455	1	0	-3.998354	1.669460	-1.419072
6	0	-1.183475	-0.211295	0.000000	1	0	-4.382599	1.198756	0.843571	1	0	-2.796218	2.292763	0.669405
6	0	0.188167	0.496482	0.000078	1	0	-4.956089	-0.169999	-0.146778	1	0	-2.811178	0.526804	2.317180
8	0	1.272022	-0.360248	0.000030	1	0	3.735778	-2.254437	-0.924994	1	0	-4.991892	0.933636	0.963276
1	0	-1.283681	-0.851576	0.887964	1	0	1.318554	-1.811074	-0.613440	1	0	-5.502481	-0.230532	-0.288768
1	0	-1.281594	-0.854032	-0.886368	1	0	6.302725	0.158724	-1.078038	1	0	3.318140	-2.170948	-0.558033
1	0	-2.016142	0.510266	-0.002137	1	0	6.026889	-1.574647	-0.825545	1	0	0.874314	-1.860722	-0.245670
1	0	0.188980	1.182920	-0.884997	1	0	6.388861	-0.516900	0.550082	1	0	3.972325	1.988656	0.404339
1	0	0.188110	1.183291	0.884826	1	0	4.651969	1.692094	0.543741	1	0	1.526555	2.293691	0.739126
					1	0	2.232261	2.131053	0.866114					

TS1a					INT1a					INT2a				
6	0	-2.715246	0.502194	0.202819	6	0	-2.599193	0.448303	0.417718	6	0	-2.360007	0.506158	-0.797178
6	0	-2.221928	-0.498268	1.160754	6	0	-1.971574	-0.637775	1.180280	6	0	-2.102976	0.870588	0.666606
6	0	-2.309810	-0.025215	-1.178294	6	0	-2.367098	0.092512	-1.054786	6	0	-0.561488	0.710286	0.912930
6	0	-1.554603	-1.585437	0.313118	6	0	-1.415833	-1.608896	0.135550	6	0	-0.396959	-0.872174	0.853124
6	0	-0.233219	-0.974778	-0.266008	6	0	-0.186497	-0.927664	-0.538427	6	0	-1.837230	-1.388433	0.551173
6	0	0.681043	-0.229068	0.697386	6	0	0.949396	-0.361447	0.371839	6	0	-2.188733	-0.945796	-0.873175
6	0	-0.748342	0.117227	-1.250687	6	0	-0.826452	0.278837	-1.293406	6	0	-2.644893	-0.378834	1.399898
6	0	-0.166322	1.419356	-0.725509	6	0	-0.215456	1.520584	-0.660394	8	0	-3.515305	-0.358230	-1.025505
6	0	-2.418164	-1.556080	-0.973518	6	0	-2.443089	-1.452514	-1.016024	6	0	0.705303	-1.418337	-0.028020
8	0	1.103934	-0.628490	1.785380	8	0	1.083054	-0.786303	1.585680	7	0	0.805530	2.655241	0.535048
7	0	0.546419	1.165210	0.408952	7	0	0.671233	1.159428	0.274587	6	0	0.341295	1.545532	-0.013906
8	0	-0.319630	2.542839	-1.221067	8	0	-0.526934	2.697020	-0.961790	8	0	0.561177	-2.164525	-0.987710
6	0	1.273792	2.192179	1.130398	6	0	1.341711	2.112401	1.132008	8	0	0.543194	1.122408	-1.204007
8	0	-3.648950	-0.327432	0.939927	8	0	-3.424344	-0.481066	1.167484	6	0	1.634493	3.460384	-0.352976
1	0	-2.778720	1.568467	0.416595	1	0	-2.644111	1.481433	0.758103	8	0	1.915745	-1.087184	0.462173
1	0	-1.880910	-0.257266	2.166092	1	0	-1.499992	-0.502462	2.148098	1	0	-2.122364	1.180595	-1.614159
1	0	-2.842683	0.403898	-2.032255	1	0	-3.005753	0.606923	-1.779657	1	0	-2.493214	1.841395	0.990943
1	0	-1.423766	-2.556611	0.800489	1	0	-1.227121	-2.626333	0.492171	1	0	-0.363836	1.039313	1.937668
1	0	0.345269	-1.753979	-0.763752	1	0	0.262360	-1.643748	-1.232975	1	0	-0.129746	-1.206744	1.865840
1	0	-0.404045	-0.030900	-2.281109	1	0	-0.614905	0.280902	-2.370613	1	0	-1.985166	-2.451001	0.772171
1	0	-1.956911	-2.117162	-1.793192	1	0	-2.091469	-1.907957	-1.948185	1	0	-1.812627	-1.464708	-1.748986
1	0	-3.441909	-1.906104	-0.826679	1	0	-3.438346	-1.835822	-0.780796	1	0	-3.725926	-0.505901	1.319233
1	0	2.160551	2.504019	0.566972	1	0	2.221829	2.554152	0.645766	1	0	-2.356306	-0.396967	2.456523
1	0	1.583698	1.774512	2.089712	1	0	1.656434	1.581405	2.034379	1	0	1.966805	4.363441	0.175407
1	0	0.628536	3.060322	1.290108	1	0	0.656101	2.923153	1.399791	1	0	1.102796	3.780411	-1.266905
8	0	2.402883	-0.534003	-0.710324	8	0	2.170579	-0.574305	-0.496773	1	0	2.533005	2.918581	-0.697003
6	0	3.572729	-0.325059	-0.010565	6	0	3.424966	-0.322016	0.121489	6	0	3.073962	-1.489672	-0.309568
6	0	4.743264	-1.225603	-0.454488	6	0	4.509790	-1.140643	-0.570352	6	0	4.302801	-0.902150	0.359217
1	0	3.931820	0.732044	-0.088418	1	0	3.676244	0.750016	0.052466	1	0	3.112318	-2.584398	-0.340888
1	0	3.418434	-0.499593	1.080016	1	0	3.362603	-0.585881	1.184745	1	0	2.949484	-1.116801	-1.331027
1	0	5.651545	-1.022699	0.134029	1	0	4.562770	-0.902838	-1.640263	1	0	5.197787	-1.177884	-0.211192
1	0	4.480538	-2.285322	-0.329651	1	0	5.490614	-0.927135	-0.125303	1	0	4.238995	0.190494	0.397570
1	0	4.978583	-1.062094	-1.515391	1	0	4.311230	-2.214663	-0.469623	1	0	4.417395	-1.281577	1.381112

TS2a					TS3a					INT3a				
6	0	2.529457	0.446140	0.515549	6	0	-2.357244	-0.064935	0.905489	6	0	-2.053747	-0.304096	1.040730
6	0	2.319154	0.280622	-0.992007	6	0	-1.413200	-1.202160	0.995615	6	0	-0.900671	-1.353585	0.757180
6	0	0.769533	0.419532	-1.209189	6	0	-2.457566	0.200653	-0.623985	6	0	-2.436098	0.097861	-0.429846
6	0	0.215850	-0.931928	-0.633177	6	0	-1.147605	-1.655345	-0.426973	6	0	-0.997186	-1.632378	-0.759704
6	0	1.488592	-1.624242	-0.054471	6	0	-0.174139	-0.563552	-0.985468	6	0	-0.204528	-0.405963	-1.265360
6	0	1.981103	-0.771546	1.118382	6	0	0.900875	-0.160186	0.062566	6	0	0.828547	-0.089519	-0.167886
6	0	2.497625	-1.244677	-1.166760	6	0	-1.086796	0.681203	-1.179681	6	0	-1.227511	0.758965	-1.169971
8	0	3.420919	-0.520772	1.139405	6	0	-0.386302	1.819249	-0.460699	6	0	-0.498517	1.855136	-0.416189
6	0	-0.983560	-0.790795	0.315505	6	0	-2.446657	-1.250169	-1.169248	6	0	-2.454142	-1.283469	-1.119339
7	0	-0.693582	1.284653	0.429734	8	0	0.703497	-0.709422	1.247570	8	0	0.451061	-0.839025	0.969021
6	0	0.143179	1.631458	-0.515867	7	0	0.742640	1.361871	0.109598	7	0	0.671905	1.355234	0.072166
8	0	-1.016235	-1.236655	1.473644	8	0	-0.797400	2.999666	-0.428612	8	0	-0.890421	3.021887	-0.265463
8	0	0.485585	2.809447	-0.881136	6	0	1.566180	2.179201	0.979638	6	0	1.543736	2.098015	0.965190
6	0	-1.338371	2.289272	1.242612	8	0	-3.286741	-1.019351	1.332774	8	0	-3.094802	-0.842569	1.751141
8	0	-2.143979	-0.771631	-0.457350	1	0	-2.238308	0.825037	1.539636	1	0	-1.592635	0.570776	1.554757
1	0	2.501987	1.422271	0.995180	1	0	-1.213362	-1.713714	1.921987	1	0	-1.003394	-2.218252	1.418640
1	0	2.922295	0.930385	-1.633601	1	0	-3.310348	0.826932	-0.907254	1	0	-3.357734	0.687184	-0.482236
1	0	0.575094	0.496663	-2.287482	1	0	-0.796992	-2.684228	-0.544321	1	0	-0.609936	-2.603699	-1.085628
1	0	-0.141896	-1.554350	-1.463642	1	0	0.290573	-0.891358	-1.920566	1	0	0.270501	-0.509670	-2.245090
1	0	1.362561	-2.691819	0.154292	1	0	-1.206428	0.964139	-2.233898	1	0	-1.545709	1.142048	-2.147565
1	0	1.505831	-0.801602	2.093330	1	0	-2.324315	-1.289458	-2.257871	1	0	-2.624340	-1.239255	-2.203074
1	0	3.515093	-1.594090	-0.978961	1	0	-3.318372	-1.834356	-0.873165	1	0	-3.185801	-1.960368	-0.666598
1	0	2.174744	-1.591353	-2.154514	1	0	1.032902	3.104930	1.210837	1	0	1.165282	3.119785	1.034612
1	0	-1.763550	1.811559	2.134274	1	0	2.520359	2.432100	0.501382	1	0	2.565801	2.119149	0.573154
1	0	-2.159227	2.797642	0.708689	1	0	1.764080	1.630120	1.905783	1	0	1.548523	1.648771	1.965657
1	0	-0.635849	3.071626	1.571046	8	0	2.198667	-0.440112	-0.542511	8	0	2.143300	-0.388277	-0.561164
6	0	-3.381342	-0.672381	0.261462	6	0	4.414214	-1.346473	-0.436189	6	0	4.433614	-0.977640	-0.235299
6	0	-4.521477	-0.717557	-0.743029	6	0	3.306009	-0.644807	0.336900	6	0	3.068758	-0.888890	0.426700
1	0	-3.454550	-1.496455	0.980495	1	0	5.285543	-1.501651	0.212635	1	0	5.164192	-1.378159	0.477643
1	0	-3.388368	0.269299	0.824105	1	0	4.076720	-2.323975	-0.800871	1	0	4.402494	-1.643217	-1.105637
1	0	-5.482236	-0.639774	-0.219489	1	0	4.733612	-0.750070	-1.299549	1	0	4.778667	0.008783	-0.565826
1	0	-4.452326	0.110439	-1.458150	1	0	3.672315	0.318056	0.723662	1	0	3.100607	-0.220131	1.295369
1	0	-4.513303	-1.659508	-1.304287	1	0	2.982738	-1.247915	1.192825	1	0	2.733513	-1.873139	0.771146

INT1e

6	0	2.354121	-2.140483	-0.107686
6	0	3.008066	-1.262815	0.964128
6	0	1.962593	-0.130540	1.270230
6	0	2.012914	0.776080	0.005534
6	0	2.994496	0.009729	-0.932139
6	0	2.328216	-1.312738	-1.320001
6	0	4.028450	-0.457228	0.125686
8	0	3.194049	-2.486356	-1.239821
6	0	0.536649	1.013154	-0.457815
7	0	-0.221937	-0.037652	0.408183
6	0	0.520125	-0.595857	1.389027
8	0	0.261693	0.986732	-1.715141
8	0	0.116408	-1.385109	2.266674
8	0	0.093153	2.273942	0.255562
1	0	1.595311	-2.880044	0.141049
1	0	3.386396	-1.784339	1.848768
1	0	2.240944	0.391494	2.194734
1	0	2.459254	1.747882	0.234055
1	0	3.377519	0.605762	-1.766432
1	0	1.544379	-1.362773	-2.069707
1	0	4.838832	-1.066931	-0.280051
1	0	4.453881	0.382315	0.686221
6	0	0.375871	3.465010	-0.459467
6	0	-0.183631	4.655385	0.311031
1	0	1.465930	3.587792	-0.594292
1	0	-0.068903	3.415461	-1.462562
1	0	0.033287	5.590565	-0.221480
1	0	-1.271135	4.569459	0.424128
1	0	0.259182	4.720607	1.312511
6	0	-1.595877	-0.335065	0.202537
6	0	-2.567544	0.671343	0.292248
6	0	-1.999493	-1.640144	-0.108245
6	0	-3.915998	0.369068	0.086758
1	0	-2.249562	1.681757	0.523992
6	0	-3.351784	-1.934603	-0.305240
1	0	-1.254234	-2.428007	-0.190784
6	0	-4.334848	-0.937417	-0.212621
1	0	-4.656445	1.166057	0.166479
1	0	-3.643841	-2.958860	-0.539174
6	0	-5.795010	-1.251640	-0.451519
1	0	-6.443051	-0.688965	0.231500
1	0	-6.098390	-0.987685	-1.474757
1	0	-6.002113	-2.319116	-0.314346

INT1f

6	0	2.522432	-2.320580	-0.266258
6	0	3.362731	-1.571411	0.774121
6	0	2.495697	-0.326962	1.193245
6	0	2.568276	0.607724	-0.047096
6	0	3.371184	-0.239585	-1.080765
6	0	2.513548	-1.452325	-1.451519
6	0	4.412188	-0.870484	-0.120310
8	0	3.224143	-2.726851	-1.467973
6	0	1.117370	1.052786	-0.403088
7	0	0.266264	0.019762	0.486608
6	0	1.025491	-0.629053	1.419269
8	0	0.769158	1.114433	-1.633177
8	0	0.605753	-1.364873	2.326193
8	0	0.848011	2.288054	0.401598
1	0	1.695934	-2.968507	0.021062
1	0	3.734472	-2.166958	1.613523
1	0	2.905949	0.120452	2.107555
1	0	3.151339	1.507525	0.173032
1	0	3.763245	0.336553	-1.924403
1	0	1.678163	-1.378463	-2.141009
1	0	5.103005	-1.563877	-0.604412
1	0	4.984228	-0.112807	0.426133
6	0	1.237653	3.492087	-0.248530
6	0	0.881745	4.671097	0.647616
1	0	2.322883	3.487196	-0.449568
1	0	0.727801	3.576137	-1.217451
1	0	1.169475	5.613839	0.165101
1	0	-0.197012	4.700344	0.842709
1	0	1.401534	4.606100	1.611173
6	0	-1.109088	-0.131643	0.325282
6	0	-1.873368	0.933308	-0.206754
6	0	-1.765285	-1.346364	0.637762
6	0	-3.237777	0.796257	-0.410381
1	0	-1.378900	1.863972	-0.445211
6	0	-3.130525	-1.488089	0.436891
1	0	-1.200205	-2.179251	1.037275
6	0	-3.865271	-0.414998	-0.085906
1	0	-3.817556	1.623399	-0.810031
1	0	-3.623311	-2.426758	0.673390
7	0	-5.285930	-0.559592	-0.294833
8	0	-5.832769	-1.630633	0.018672
8	0	-5.919970	0.391037	-0.783158

INT2e

6	0	2.507476	-1.408294	-1.343529
6	0	2.101174	-2.192990	-0.174741
6	0	3.308912	-0.228370	-0.783814
6	0	2.660899	-1.436402	1.032365
6	0	1.777080	-0.141666	1.151976
6	0	0.278150	-0.467882	1.275789
6	0	2.296983	0.724639	-0.071268
6	0	1.324696	1.416914	-1.016680
6	0	3.972992	-0.858377	0.462682
8	0	-0.063767	-1.025281	2.373313
7	0	-0.454412	-0.134156	0.228090
8	0	1.259726	1.165278	-2.213547
8	0	3.094720	-2.721356	-1.097080
6	0	-2.662715	-1.028902	1.058823
6	0	-4.035521	-1.176807	0.817877
6	0	-1.828186	-0.349529	0.136206
6	0	-2.462137	0.163461	-1.025275
6	0	-3.827649	0.011273	-1.250327
6	0	-6.135604	-0.828543	-0.580871
6	0	-4.651913	-0.665273	-0.331189
1	0	1.920888	-1.328436	-2.252743
1	0	1.174577	-2.760191	-0.121554
1	0	3.968546	0.280001	-1.494538
1	0	2.727974	-2.003807	1.965300
1	0	2.060063	0.363491	2.084833
1	0	2.899672	1.542719	0.351084
1	0	4.419197	-0.106414	1.122670
1	0	4.720640	-1.617059	0.223791
1	0	-2.222681	-1.436104	1.960346
1	0	-4.640993	-1.709279	1.554102
1	0	-1.842873	0.689196	-1.749135
1	0	-4.265933	0.425794	-2.160408
1	0	-6.333642	-1.370050	-1.516098
1	0	-6.644067	0.142083	-0.662425
1	0	-6.615382	-1.385644	0.231985
6	0	0.612618	2.927216	0.790971
6	0	-0.068835	4.283164	0.853012
8	0	0.698828	2.547433	-0.602390
1	0	0.032989	2.165356	1.317505
1	0	1.618851	2.980573	1.222969
1	0	0.508833	5.041050	0.311679
1	0	-0.158102	4.600076	1.898942
1	0	-1.074258	4.235351	0.420642

INT21					TS4e					TS51				
6	0	3.417909	-1.730762	0.803468	6	0	-1.891648	-1.983118	1.181304	6	0	2.808107	-1.844107	0.704013
6	0	3.787494	-0.397664	1.291338	6	0	-1.472723	-2.239065	-0.303880	6	0	3.739516	-0.847014	1.284596
6	0	3.432082	-1.625432	-0.724163	6	0	-1.074314	-0.914130	-1.023377	6	0	2.981401	-1.794535	-0.804570
6	0	3.998315	0.450308	0.031361	6	0	-2.436843	-0.114422	-1.039162	6	0	4.200844	-0.061501	0.019598
6	0	2.583101	0.685263	-0.614068	6	0	-3.466152	-1.160844	-0.480403	6	0	2.996592	0.649481	-0.649670
6	0	1.579569	1.343082	0.313117	6	0	-3.139187	-1.148072	1.002971	6	0	2.306833	1.709165	0.187707
6	0	2.203600	-0.766372	-1.143186	6	0	-2.847131	-2.493261	-0.957737	6	0	2.110712	-0.554965	-1.209878
6	0	0.809857	-1.299061	-0.788235	8	0	-2.566061	-3.059577	1.715652	6	0	0.759872	-0.728313	-0.550081
6	0	4.562952	-0.596031	-0.957705	6	0	-2.507457	1.041424	-0.080858	6	0	4.407117	-1.222416	-0.977314
8	0	1.160617	0.881461	1.362849	7	0	1.327926	-0.729981	-0.815950	8	0	2.713285	2.138726	1.257743
7	0	-0.184090	-0.494397	-1.235078	6	0	0.133301	-0.197815	-0.424126	7	0	-0.330241	-0.547395	-1.279717
8	0	0.687374	-2.426255	-0.256452	8	0	-2.859582	0.803344	1.089847	8	0	0.842616	-1.131893	0.663234
6	0	-1.459285	-0.576056	-0.787747	8	0	0.025966	0.752172	0.359195	6	0	-1.594148	-0.556339	-0.741772
8	0	4.710494	-1.510257	1.442479	8	0	-2.311119	2.245131	-0.556713	8	0	4.595532	-1.899405	1.608729
8	0	1.224505	2.564667	-0.138241	6	0	2.640738	-0.383586	-0.413724	8	0	1.219050	2.197506	-0.430006
6	0	0.267646	3.307901	0.663196	6	0	2.941910	0.634837	0.502718	6	0	0.493817	3.268413	0.235033
6	0	-0.009452	4.619895	-0.046365	6	0	4.277235	0.894382	0.834482	6	0	-0.637251	3.695667	-0.680795
6	0	-1.869334	-1.120951	0.475704	6	0	5.338263	0.167958	0.280298	6	0	-1.927897	-0.201564	0.598867
6	0	-3.187589	-1.089966	0.877749	6	0	5.017776	-0.846893	-0.637820	6	0	-3.244538	-0.168201	1.024245
6	0	-4.175796	-0.526236	0.039028	6	0	3.696424	-1.120942	-0.980562	6	0	-4.278937	-0.497316	0.129276
7	0	-5.528063	-0.510247	0.449827	6	0	6.775038	0.450748	0.657176	7	0	-5.637773	-0.470919	0.574021
8	0	-6.395625	0.003465	-0.298822	1	0	1.279441	-1.497934	-1.494135	8	0	-6.546707	-0.753367	-0.233183
6	0	-3.808043	0.024424	-1.210019	6	0	-2.371019	3.372665	0.380157	6	0	-3.986154	-0.849226	-1.202183
8	0	-5.844243	-1.009134	1.557862	6	0	-2.148794	4.638971	-0.419863	8	0	-5.884287	-0.166020	1.758719
6	0	-2.487787	0.004066	-1.601038	1	0	-1.086119	-1.553142	1.801341	6	0	-2.670185	-0.867325	-1.622367
1	0	2.750194	-2.404307	1.330896	1	0	-0.728094	-3.035319	-0.408385	1	0	2.420389	-2.662974	1.293121
1	0	3.429177	0.027748	2.224059	1	0	-0.833178	-1.164474	-2.065229	1	0	3.403040	-0.219909	2.119747
1	0	3.510291	-2.573837	-1.264856	1	0	-2.677532	0.215627	-2.055225	1	0	2.726331	-2.708503	-1.349553
1	0	4.576023	1.371665	0.163639	1	0	-4.505305	-0.948209	-0.747750	1	0	5.061920	0.592528	0.192530
1	0	2.711502	1.355452	-1.468888	1	0	-3.852777	-1.086653	1.815756	1	0	3.365853	1.200872	-1.528050
1	0	2.208041	-0.699424	-2.239840	1	0	-3.357105	-3.367575	-0.552654	1	0	2.012774	-0.475185	-2.295850
1	0	4.585056	-0.225677	-1.988169	1	0	-2.805079	-2.556089	-2.051103	1	0	4.586329	-0.884072	-2.004533
1	0	5.555033	-0.957496	-0.683003	1	0	2.147088	1.217428	0.949095	1	0	5.189431	-1.916388	-0.671254
1	0	0.696348	3.464932	1.658860	1	0	4.487853	1.690903	1.548839	1	0	1.192032	4.088247	0.433721
1	0	-0.635287	2.699129	0.769813	1	0	5.813803	-1.436054	-1.094671	1	0	0.124530	2.889728	1.193957
1	0	-0.731129	5.203861	0.536859	1	0	3.474760	-1.915042	-1.695255	1	0	-1.206168	4.501449	-0.202048
1	0	0.905845	5.213096	-0.152068	1	0	6.851000	1.336954	1.296206	1	0	-0.251085	4.068992	-1.635877
1	0	-0.431918	4.448534	-1.042683	1	0	7.218451	-0.392735	1.203185	1	0	-1.318899	2.862620	-0.880250
1	0	-1.121871	-1.557160	1.127716	1	0	7.397283	0.620307	-0.230720	1	0	-1.137509	0.045592	1.297435
1	0	-3.474373	-1.498562	1.842926	1	0	-1.593565	3.210100	1.132233	1	0	-3.482004	0.109599	2.047515
1	0	-4.567930	0.459627	-1.852940	1	0	-3.351551	3.352777	0.865292	1	0	-4.789635	-1.100944	-1.888522
1	0	-2.196348	0.434904	-2.557589	1	0	-2.184966	5.499873	0.257579	1	0	-2.431363	-1.127252	-2.652336
					1	0	-2.925990	4.768183	-1.180897					
					1	0	-1.170029	4.629370	-0.911272					

INT4e					6	0	2.237190	-0.603798	-0.287605	6	0	2.678505	-0.171798	4.357776
6	0	-1.970965	2.001749	-1.652299	6	0	1.930705	-1.798736	-0.982274	1	0	3.362551	0.441153	2.384432
6	0	-1.168118	2.659181	-0.526607	6	0	2.939718	-2.698180	-1.346078	1	0	1.960667	1.359508	2.992622
6	0	-0.764200	1.518497	0.476835	6	0	4.290346	-2.467015	-1.051780	1	0	3.155215	-1.156852	4.320648
6	0	-2.168687	1.159021	1.131885	6	0	4.597128	-1.285596	-0.355898	1	0	3.340864	0.509591	4.905839
6	0	-3.171490	2.104866	0.406289	6	0	3.601963	-0.383914	0.017316	1	0	1.738055	-0.254993	4.913857
6	0	-3.256866	1.639680	-1.051795	1	0	0.899872	-2.012960	-1.227787	6	0	-0.845036	2.351011	-0.381841
6	0	-2.282152	3.363188	0.283066	1	0	2.658433	-3.609279	-1.877991	6	0	0.262953	3.126178	-0.765471
8	0	-3.186046	2.710243	-2.038599	1	0	5.634435	-1.067541	-0.095752	6	0	0.121681	4.507608	-0.922610
6	0	-2.570327	-0.299460	1.197067	1	0	3.872842	0.517470	0.563907	6	0	-1.099845	5.162454	-0.706120
7	0	1.333231	0.374418	0.166247	6	0	-3.749833	-3.628456	-3.167439	6	0	-2.195294	4.374066	-0.323411
6	0	0.028732	0.359816	-0.147404	6	0	-2.902347	-2.952746	-2.099821	6	0	-2.075672	2.993577	-0.161571
8	0	-3.604706	-0.771511	0.748382	8	0	-2.211696	-1.846509	-2.682517	1	0	1.219045	2.652786	-0.938992
8	0	-0.580548	-0.447559	-0.903131	1	0	-4.288683	-4.484821	-2.743451	1	0	0.995854	5.086562	-1.223828
8	0	-1.685675	-1.006445	1.924535	1	0	-4.486426	-2.927569	-3.578817	1	0	-3.164213	4.842383	-0.147857
1	0	-1.500632	1.434833	-2.448665	1	0	-3.123278	-3.990280	-3.991914	1	0	-2.941261	2.405361	0.132858
1	0	-0.318769	3.273728	-0.835021	1	0	-2.180577	-3.674807	-1.684137	6	0	6.350379	0.856973	-1.368987
1	0	-0.135828	1.971567	1.246027	1	0	-3.537787	-2.604571	-1.273256	6	0	4.969627	0.754488	-0.739856
1	0	-2.117170	1.472782	2.184639	1	0	-1.681906	-1.401680	-1.985599	8	0	3.990612	0.688260	-1.782061
1	0	-4.127287	2.222298	0.927499	6	0	5.373730	-3.429373	-1.488643	1	0	7.121610	0.911313	-0.590967
1	0	-3.838127	0.774244	-1.349379	1	0	6.206410	-3.447196	-0.775109	1	0	6.556074	-0.017568	-1.997771
1	0	-2.759653	4.186206	-0.251058	1	0	4.987607	-4.451213	-1.582960	1	0	6.427557	1.755334	-1.993326
1	0	-1.926338	3.721806	1.255085	1	0	5.792977	-3.150504	-2.466297	1	0	4.781489	1.631213	-0.100004
6	0	-1.905993	-2.431155	2.084175						1	0	4.903800	-0.140971	-0.106495
6	0	-2.687726	-2.728706	3.355390						1	0	3.107978	0.579664	-1.377200
1	0	-2.420130	-2.807929	1.197613	INT5e					1	0	-1.695504	0.539830	0.131027
1	0	-0.899815	-2.856268	2.125327	6	0	1.221358	-2.148151	-2.092103	6	0	-2.844177	0.262964	3.093382
1	0	-3.694766	-2.301002	3.308980	6	0	-0.161166	-2.262361	-1.440213	6	0	-3.807549	-0.390568	2.115600
1	0	-2.781248	-3.814465	3.482490	6	0	-0.140013	-1.379936	-0.137589	8	0	-3.334136	-0.188504	0.774811
1	0	-2.174265	-2.324735	4.235033	6	0	0.838193	-2.208378	0.803866	1	0	-3.196805	0.115515	4.121211
6	0	3.340221	4.263802	-2.270698	6	0	1.247098	-3.425986	-0.075556	1	0	-3.196805	0.115515	4.121211
6	0	2.771091	2.926119	-1.822002	6	0	2.127727	-2.892170	-1.210789	1	0	-1.841681	-0.172523	3.010538
8	0	2.475038	2.985561	-0.426022	6	0	-0.093749	-3.671086	-0.805585	1	0	-2.768445	1.340633	2.908235
1	0	3.576536	4.239314	-3.341668	8	0	1.794043	-3.410350	-2.528367	1	0	-4.811223	0.045824	2.219350
1	0	2.619457	5.071556	-2.094891	6	0	1.972006	-1.458542	1.476107	1	0	-3.885461	-1.468147	2.321986
1	0	4.259696	4.499263	-1.720874	7	0	-0.814452	0.947256	-0.199823	1	0	-4.013093	-0.516496	0.140358
1	0	3.494942	2.121017	-2.021495	6	0	0.221369	0.083170	-0.377281	6	0	-5.412915	-3.306888	-0.429084
1	0	1.858408	2.696127	-2.394218	8	0	3.152842	-1.759710	1.417108	6	0	-5.593445	-2.288512	-1.541022
1	0	2.079479	2.117968	-0.156561	8	0	1.355766	0.431903	-0.737619	8	0	-5.324629	-0.974599	-1.010705
6	0	1.716337	0.317340	5.133326	8	0	1.491451	-0.451595	2.227510	1	0	-5.618491	-4.314753	-0.808484
6	0	1.663846	-0.051204	3.657448	1	0	1.518307	-1.284323	-2.678249	1	0	-4.387077	-3.291058	-0.043064
8	0	1.963101	1.103458	2.872103	1	0	-1.012843	-2.050061	-2.093777	1	0	-6.099858	-3.105207	0.400951
1	0	1.517128	-0.563481	5.756637	1	0	-1.142724	-1.417924	0.293986	1	0	-6.621690	-2.317394	-1.926393
1	0	2.705221	0.709680	5.401300	1	0	0.231081	-2.587008	1.639209	1	0	-4.908119	-2.496954	-2.374292
1	0	0.968573	1.084059	5.370010	1	0	1.658793	-4.263451	0.496529	1	0	-5.454347	-0.302792	-1.720866
1	0	0.667331	-0.434389	3.396242	1	0	3.171779	-2.640262	-1.062489	6	0	-1.223273	6.660937	-0.869840
1	0	2.392856	-0.850961	3.447013	1	0	-0.052337	-4.476451	-1.539717	1	0	-2.269892	6.980792	-0.824776
1	0	1.758294	0.893390	1.922637	1	0	-0.918691	-3.858609	-0.110392	1	0	-0.678509	7.195721	-0.080063
					6	0	2.436756	0.376278	2.960123	1	0	-0.807981	6.994614	-1.828844

INT4I

6	0	2.768976	-1.143925	-1.949910
6	0	2.265420	-2.179055	-0.938924
6	0	1.589043	-1.386341	0.240532
6	0	2.847856	-0.707254	0.935056
6	0	4.050184	-1.175906	0.063044
6	0	3.913115	-0.494485	-1.303010
6	0	3.581713	-2.614564	-0.254717
8	0	4.118125	-1.375830	-2.444473
6	0	2.776455	0.779004	1.222228
7	0	-0.780486	-0.908936	0.144935
6	0	0.454536	-0.450536	-0.189001
8	0	3.591744	1.612586	0.859238
8	0	0.732187	0.593153	-0.821902
8	0	1.732267	1.058060	2.025036
1	0	2.108291	-0.642740	-2.649957
1	0	1.630739	-2.974208	-1.337634
1	0	1.170678	-2.123355	0.928341
1	0	2.952273	-1.171732	1.926395
1	0	5.021938	-1.068654	0.555784
1	0	4.188837	0.542089	-1.463486
1	0	4.257449	-3.160257	-0.914832
1	0	3.403992	-3.206743	0.649448
6	0	1.511015	2.438915	2.417041
6	0	2.204883	2.754271	3.733519
1	0	1.855973	3.091600	1.612524
1	0	0.425002	2.521337	2.508912
1	0	3.292626	2.672180	3.636868
1	0	1.963860	3.780482	4.037319
1	0	1.869519	2.075677	4.525675
6	0	-1.685268	-4.751891	-2.965203
6	0	-1.430361	-3.413843	-2.288860
8	0	-1.147125	-3.637125	-0.904721
1	0	-1.900952	-4.605843	-4.030663
1	0	-0.808523	-5.404734	-2.877280
1	0	-2.541118	-5.261984	-2.506943
1	0	-2.311155	-2.762469	-2.395143
1	0	-0.582321	-2.904382	-2.772776
1	0	-1.008546	-2.762137	-0.471473
6	0	-0.986725	-1.799250	5.093863
6	0	-0.963428	-1.185477	3.702320
8	0	-0.967371	-2.232669	2.728170
1	0	-0.989576	-1.012580	5.858439
1	0	-1.882738	-2.416419	5.232662
1	0	-0.105833	-2.432645	5.254426
1	0	-0.067507	-0.560152	3.577843
1	0	-1.843323	-0.537373	3.563795
1	0	-0.903328	-1.821626	1.830620

INT5I

6	0	-1.934746	-0.190543	-0.089170
6	0	-2.034456	1.152284	-0.565108
6	0	-3.265052	1.769848	-0.716310
6	0	-4.446982	1.075270	-0.407579
6	0	-4.388675	-0.250536	0.061981
6	0	-3.159014	-0.858732	0.216156
7	0	-5.714053	1.718187	-0.568625
1	0	-1.130448	1.689120	-0.810920
1	0	-3.318926	2.793894	-1.076006
1	0	-5.302999	-0.785780	0.301683
1	0	-3.112558	-1.880044	0.586759
8	0	-6.754300	1.088087	-0.288678
8	0	-5.751483	2.894626	-0.983463
6	0	2.427513	4.978321	-2.628383
6	0	1.921167	3.897942	-1.685158
8	0	1.733899	2.687381	-2.423611
1	0	2.576847	5.919937	-2.085861
1	0	3.383654	4.684439	-3.078012
1	0	1.708263	5.157297	-3.436752
1	0	0.969904	4.214990	-1.228022
1	0	2.644282	3.732186	-0.873589
1	0	1.440935	1.988613	-1.803520
6	0	-2.688714	0.416296	-2.197640
6	0	-1.958673	1.616062	-1.582049
6	0	-1.336654	1.138419	-0.216086
6	0	-2.633337	0.925617	0.679327
6	0	-3.803231	1.295544	-0.278627
6	0	-3.872908	0.207802	-1.355913
6	0	-3.139145	2.461104	-1.048785
8	0	-4.012871	0.712652	-2.712070
6	0	-2.764301	-0.389606	1.422800
7	0	0.923564	0.244484	-0.138182
6	0	-0.399932	-0.055823	-0.349810
8	0	-3.729773	-1.133302	1.375818
8	0	-0.796781	-1.183704	-0.656445
8	0	-1.697893	-0.591565	2.217448
1	0	-2.164230	-0.377877	-2.719029
1	0	-1.237820	2.120852	-2.233638
1	0	-0.767286	1.975740	0.192678
1	0	-2.599600	1.684815	1.474572
1	0	-4.741287	1.516964	0.239908
1	0	-4.324953	-0.760721	-1.172811
1	0	-3.764230	2.876763	-1.839630
1	0	-2.813040	3.268517	-0.384855
6	0	-1.660683	-1.794179	3.036953
6	0	-2.261868	-1.539221	4.410185

1	0	-2.184058	-2.593598	2.508211
1	0	-0.597605	-2.038394	3.104086
1	0	-3.326553	-1.293741	4.337637
1	0	-2.159504	-2.442029	5.024765
1	0	-1.743828	-0.718827	4.919010
6	0	2.038487	-0.594284	-0.239344
6	0	1.974622	-1.956877	-0.599098
6	0	3.140647	-2.709516	-0.679517
6	0	4.373879	-2.111881	-0.400794
6	0	4.458980	-0.760454	-0.040573
6	0	3.296313	-0.011718	0.038551
7	0	5.585545	-2.903442	-0.485442
1	0	1.020315	-2.414641	-0.812353
1	0	3.090191	-3.758509	-0.958036
1	0	5.421637	-0.304984	0.173676
1	0	3.350683	1.037122	0.316177
8	0	6.670627	-2.355918	-0.240835
8	0	5.495036	-4.097848	-0.803928
6	0	-3.579075	-5.436127	-1.257451
6	0	-2.813221	-4.285847	-0.623804
8	0	-2.245849	-3.479402	-1.664414
1	0	-4.021078	-6.072320	-0.481082
1	0	-4.387163	-5.059801	-1.896069
1	0	-2.914208	-6.054989	-1.871975
1	0	-2.015364	-4.677814	0.026430
1	0	-3.483509	-3.676283	-0.001661
1	0	-1.788448	-2.721656	-1.254779
1	0	1.132390	1.203386	0.167686
6	0	1.401802	2.292309	3.128066
6	0	1.533953	3.438598	2.138333
8	0	1.517681	2.917345	0.798517
1	0	1.394149	2.683027	4.152589
1	0	0.470440	1.736601	2.969006
1	0	2.241652	1.593793	3.035770
1	0	2.473301	3.983555	2.306160
1	0	0.703460	4.148178	2.264982
1	0	1.731761	3.642405	0.166250
6	0	0.409589	6.407426	-0.646985
6	0	1.574630	6.037855	-1.547847
8	0	2.278654	4.927173	-0.955978
1	0	-0.139067	7.254949	-1.074168
1	0	-0.286978	5.567637	-0.542262
1	0	0.762276	6.694051	0.350552
1	0	2.264225	6.886243	-1.654252
1	0	1.217884	5.755440	-2.547902
1	0	3.044074	4.676395	-1.524515

EtO (anion+first solvation sphere)

6	0	1.207046	-1.283029	2.679057
6	0	0.024426	-1.521571	1.729280
8	0	0.065498	-0.716825	0.583466
1	0	1.140056	-1.929845	3.566297
1	0	2.157517	-1.492434	2.172051
1	0	1.227454	-0.238514	3.015621
1	0	-0.913726	-1.347679	2.295591
1	0	0.014050	-2.596290	1.453874
6	0	-0.689345	3.994300	0.088061
6	0	-0.446555	2.506774	-0.134162
8	0	-0.190638	1.867527	1.107415
1	0	-0.885037	4.501760	-0.865228
1	0	-1.553104	4.152546	0.745871
1	0	0.184931	4.465013	0.554894
1	0	0.406862	2.370550	-0.820297
1	0	-1.326671	2.057333	-0.623469
1	0	-0.070749	0.874195	0.933107
6	0	4.285747	-0.362724	-1.705895
6	0	3.080585	-0.130216	-0.803407
8	0	2.132729	-1.171389	-0.986035
1	0	5.027509	0.435798	-1.575908
1	0	4.767037	-1.320590	-1.472007
1	0	3.983289	-0.382539	-2.760377
1	0	2.627179	0.848148	-1.035913
1	0	3.408771	-0.088429	0.248841
1	0	1.341476	-1.001553	-0.368753
6	0	-4.357921	-1.176039	-1.253934
6	0	-3.151821	-0.794745	-0.404895
8	0	-1.971060	-1.346010	-0.969334
1	0	-5.278968	-0.755346	-0.830496
1	0	-4.246286	-0.798387	-2.277977
1	0	-4.468592	-2.266468	-1.303335
1	0	-3.294792	-1.162250	0.625517
1	0	-3.073670	0.303805	-0.345618
1	0	-1.179745	-1.091748	-0.381019

EtOH (neutral molecule+first solvation sphere)

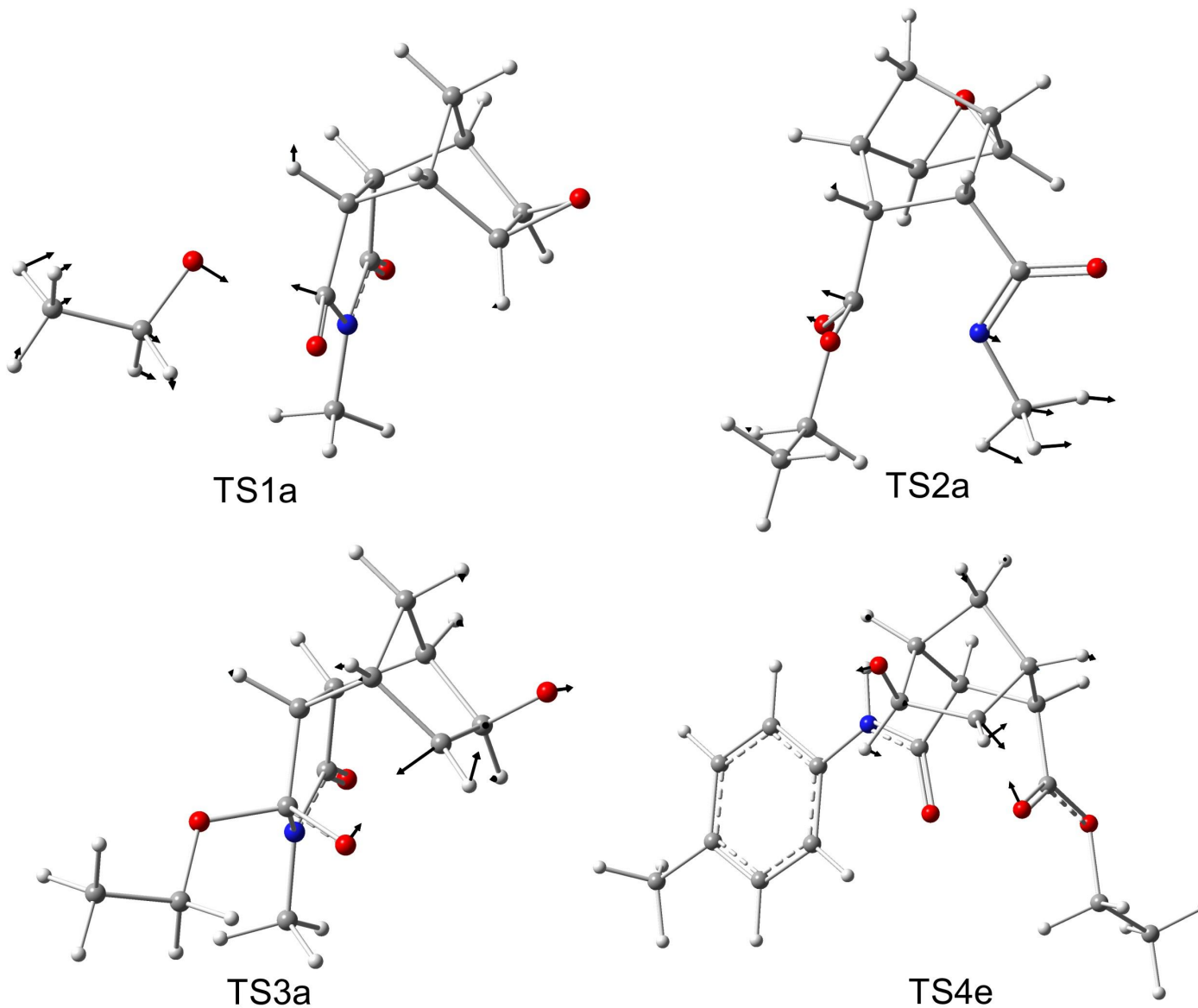
6	0	-0.362173	-0.195798	2.822866
6	0	0.824754	-0.512014	1.929019
8	0	0.450588	-0.302980	0.548995
1	0	-0.084401	-0.341070	3.873477
1	0	-0.683870	0.844297	2.696356
1	0	-1.210497	-0.853261	2.601049
1	0	1.142950	-1.554889	2.059551
1	0	1.673421	0.140452	2.174071
1	0	1.216041	-0.550819	-0.030795
6	0	-3.816432	-2.587246	-0.915621
6	0	-2.820566	-1.549074	-0.423362
8	0	-1.519401	-2.143191	-0.368225
1	0	-4.822932	-2.154844	-0.968541
1	0	-3.541994	-2.945063	-1.915128
1	0	-3.846528	-3.448593	-0.237681
1	0	-3.115688	-1.187755	0.573885
1	0	-2.812601	-0.682959	-1.102928
1	0	-0.876805	-1.476848	-0.038615
6	0	-1.780203	4.042976	-0.678075
6	0	-1.522497	2.596492	-0.286192
8	0	-0.110837	2.390446	-0.172637
1	0	-2.857271	4.225946	-0.774429
1	0	-1.380690	4.727677	0.079548
1	0	-1.303807	4.275738	-1.637907
1	0	-1.943900	1.920255	-1.045968
1	0	-2.017949	2.372221	0.671195
1	0	0.055441	1.457446	0.087025
6	0	4.446598	-0.285849	0.003056
6	0	3.724617	-0.380758	-1.329081
8	0	2.483247	-1.094989	-1.134568
1	0	5.400938	0.237688	-0.128033
1	0	3.853714	0.272263	0.736998
1	0	4.652792	-1.283406	0.407476
1	0	4.335832	-0.925009	-2.060739
1	0	3.512860	0.619386	-1.731516
1	0	2.061583	-1.255524	-2.012541

TS61

6	0	-1.625165	-2.000044	0.008424
6	0	-2.375523	-1.637204	-1.206991
6	0	-2.532732	-1.704873	1.196921
6	0	-3.609350	-0.884957	-0.627998
6	0	-3.157761	0.400352	0.116109
6	0	-2.453830	1.438504	-0.736061
6	0	-2.403146	-0.157427	1.405653
6	0	-0.934290	0.216487	1.563487
6	0	-3.949190	-1.783973	0.582144
8	0	-2.400912	1.423257	-1.956871
7	0	-0.212292	-0.384353	0.592113
8	0	-0.543339	0.939581	2.504237
6	0	1.142592	-0.336790	0.443967
8	0	-2.589748	-3.016138	-1.321078
8	0	-1.981509	2.452325	0.011085
6	0	-1.336562	3.567903	-0.666542
6	0	0.134142	3.287911	-0.933922
6	0	2.064405	0.295158	1.335911
6	0	3.425978	0.266893	1.091574
6	0	3.926394	-0.389039	-0.048310
7	0	5.331818	-0.414591	-0.294241
8	0	5.761478	-1.001890	-1.309653
6	0	3.045724	-1.018545	-0.950479
8	0	6.102682	0.150027	0.510436
6	0	1.688224	-0.987665	-0.704913
1	0	-0.757709	-2.640492	-0.013233
1	0	-1.873501	-1.148461	-2.049048
1	0	-2.337703	-2.286877	2.102960
1	0	-4.411851	-0.718236	-1.354255
1	0	-4.057867	0.922456	0.476650
1	0	-2.944191	0.148168	2.306472
1	0	-4.702574	-1.344019	1.245842
1	0	-4.245742	-2.793263	0.298999
1	0	-1.463508	4.401965	0.028416
1	0	-1.883900	3.780157	-1.589084
1	0	0.596816	4.179853	-1.374631
1	0	0.660885	3.048060	-0.004772
1	0	0.259381	2.454530	-1.631654
1	0	1.682342	0.803412	2.211325
1	0	4.112836	0.751000	1.780487
1	0	3.435429	-1.518016	-1.832949
1	0	1.005480	-1.461053	-1.405721

PR1					PR2					PR e				
6	0	1.51169	-2.3634	0.5316	6	0	-0.979148	-1.825687	-0.056243	6	0	-1.998520	-1.747939	1.280540
6	0	2.5221	-1.54102	1.4279	6	0	-1.597493	-1.156741	-1.370798	6	0	-1.554091	-2.237631	-0.148908
6	0	2.18441	-2.44085	-0.85561	6	0	-2.211156	-2.155060	0.819865	6	0	-1.056410	-1.056906	-1.044778
6	0	3.52483	-1.04638	0.3236	6	0	-3.091478	-0.992740	-0.909644	6	0	-2.352325	-0.174161	-1.211680
6	0	2.83493	-0.10213	-0.71889	6	0	-3.235632	-0.016332	0.309009	6	0	-3.462738	-1.106912	-0.622139
6	0	2.37768	1.22308	-0.15066	6	0	-2.980160	1.438607	-0.026145	6	0	-3.220002	-0.828474	0.875329
6	0	1.74988	-1.03809	-1.37943	6	0	-2.430582	-0.753273	1.453061	6	0	-2.911659	-2.527215	-0.814042
6	0	0.35293	-0.91541	-0.82768	6	0	-1.012986	-0.273725	1.720268	8	0	-2.394140	-2.761060	2.099788
6	0	3.68078	-2.31157	-0.54079	6	0	-3.345977	-2.331689	-0.195251	6	0	-2.419835	0.974493	-0.256684
8	0	1.30815	1.45254	0.39046	8	0	-3.865323	2.174289	-0.447092	7	0	1.347712	-0.852865	-0.799037
7	0	-0.61365	-0.30141	-1.41191	7	0	-0.184827	-0.911410	0.800656	6	0	0.143930	-0.298249	-0.499369
8	0	0.23758	-1.65462	0.28898	8	0	-0.656919	0.477312	2.624006	8	0	-2.888003	0.655976	0.899650
6	0	-1.88066	-0.15814	-0.85823	6	0	1.154717	-0.626572	0.548844	8	0	-0.001113	0.725151	0.186315
8	0	3.12032	-2.31301	2.38902	8	0	-1.452990	-1.937529	-2.480729	8	0	-2.231089	2.196744	-0.595855
8	0	3.34719	2.15338	-0.27803	8	0	-1.714125	1.837063	0.143901	6	0	2.648231	-0.451593	-0.404535
6	0	3.08464	3.46567	0.29123	6	0	-1.363630	3.211019	-0.188387	6	0	3.722889	-1.227676	-0.871326
6	0	4.30155	4.33283	0.03059	6	0	-1.037826	3.365236	-1.665835	6	0	5.033590	-0.901383	-0.528735
6	0	-2.11509	0.14465	0.50501	6	0	1.970803	0.056508	1.484218	6	0	5.320624	0.206230	0.285615
6	0	-3.40432	0.35455	0.97207	6	0	3.303936	0.309244	1.200097	6	0	4.237727	0.966854	0.746776
6	0	-4.48456	0.26027	0.08177	6	0	3.849711	-0.117909	-0.018459	6	0	2.914865	0.655904	0.415097
7	0	-5.82687	0.46868	0.56977	7	0	5.237571	0.146515	-0.309492	6	0	6.745453	0.576223	0.630216
8	0	-6.77437	0.38765	-0.23017	8	0	5.712353	-0.260696	-1.382624	1	0	1.321510	-1.687830	-1.395249
6	0	-4.2814	-0.02868	-1.27623	6	0	3.062815	-0.798655	-0.957139	6	0	-2.366396	3.262165	0.424610
8	0	-5.99469	0.72035	1.77485	8	0	5.915024	0.773602	0.522341	6	0	-2.157020	4.583135	-0.280136
6	0	-2.98825	-0.22196	-1.7365	6	0	1.728653	-1.048171	-0.675836	1	0	-1.209836	-1.101641	1.722530
1	0	1.24149	-3.31096	1.00286	1	0	-0.378782	-2.697613	-0.328511	1	0	-0.842936	-3.069252	-0.105839
1	0	1.96791	-0.6755	1.84814	1	0	-1.135184	-0.152442	-1.482550	1	0	-0.806882	-1.461271	-2.035541
1	0	1.8634	-3.27695	-1.48686	1	0	-2.052249	-2.954840	1.552293	1	0	-2.495933	0.162022	-2.243113
1	0	4.44291	-0.62018	0.74227	1	0	-3.763796	-0.738919	-1.736488	1	0	-4.472906	-0.889595	-0.985380
1	0	3.57806	0.1272	-1.4919	1	0	-4.291088	-0.037853	0.607270	1	0	-4.062320	-0.922721	1.561296
1	0	1.74398	-0.92108	-2.4665	1	0	-2.996307	-0.739403	2.389958	1	0	-3.489640	-3.278224	-0.267932
1	0	4.29914	-2.16886	-1.43594	1	0	-4.334890	-2.409540	0.273700	1	0	-2.843486	-2.816546	-1.869615
1	0	4.06714	-3.16003	0.03221	1	0	-3.190967	-3.188562	-0.858388	1	0	3.526811	-2.095432	-1.502959
1	0	2.88983	3.34453	1.36204	1	0	-0.490464	3.413543	0.436509	1	0	5.846548	-1.524556	-0.902687
1	0	2.18371	3.87156	-0.18067	1	0	-2.186845	3.862526	0.116956	1	0	4.421834	1.829500	1.388116
1	0	4.13053	5.33233	0.44746	1	0	-0.662743	4.380030	-1.847485	1	0	2.102202	1.262574	0.791689
1	0	5.19564	3.91203	0.50377	1	0	-0.261902	2.654755	-1.970667	1	0	7.380798	-0.312863	0.715049
1	0	4.48988	4.43699	-1.04378	1	0	-1.924175	3.209550	-2.288620	1	0	7.188204	1.218828	-0.143678
1	0	-1.27756	0.22335	1.18971	1	0	1.554302	0.379123	2.428147	1	0	6.797897	1.124248	1.577539
1	0	-3.5775	0.58836	2.01875	1	0	3.924129	0.828282	1.925298	1	0	-1.607427	3.059417	1.185164
1	0	-5.12593	-0.09272	-1.95628	1	0	3.489168	-1.118721	-1.903756	1	0	-3.364194	3.167740	0.861763
1	0	-2.80925	-0.43186	-2.78965	1	0	1.121009	-1.552356	-1.419999	1	0	-2.245620	5.389786	0.456561
										1	0	-2.912431	4.742378	-1.056668
										1	0	-1.161313	4.637818	-0.732094

The reaction-coordinate vectors corresponding to the sole imaginary frequencies of transition states calculated at the PCM/B3LYP/6-31+G(d) level.



The reaction-coordinate vectors corresponding to the sole imaginary frequencies of transition states calculated at the PCM/B3LYP/6-31+G(d) level.

