SUPPLEMENTARY INFORMATION for

Amide-Derived Enols in Enol-Ugi Reactions: Expanding Horizons for Peptidomimetic Scaffold Synthesis

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Starting materials

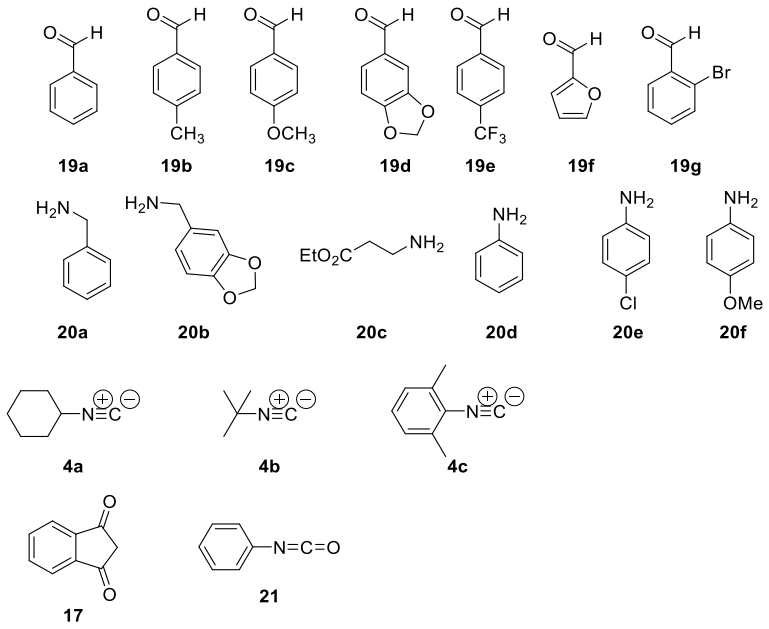


Figure S1. Aldehydes, amines, and isocyanide used as starting materials.

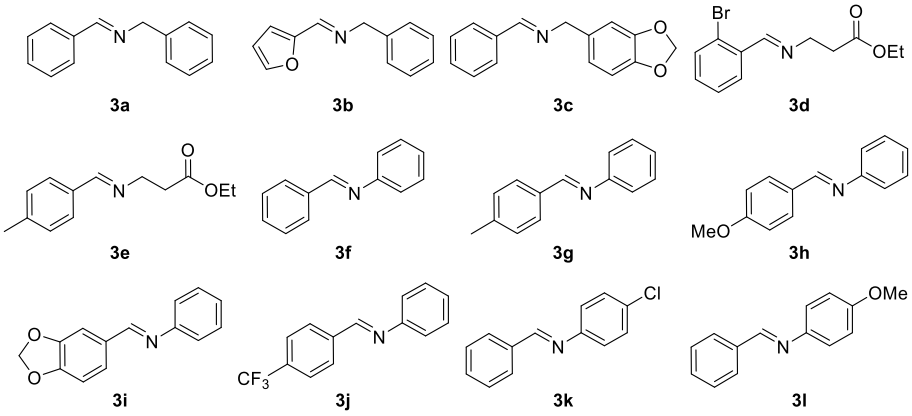
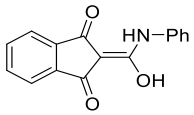


Figure S2. Imines used as starting materials.

Synthesis and spectroscopic data of 2-(Hydroxy(phenylamino)methylene)-1*H*-indene-1,3(2*H*)-dione (10)



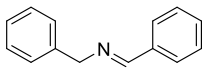
Enol (**10**) was synthesized following reported procedures.[1] A solution of 1,3-indandione (**17**, 13.7 mmol) in dry DMF (14 mL), cooled to -55ºC, was stirred for 10 minutes. Phenyl isocyanate (**21**, 25 mmol) was then added, and the stirring was continued while gradually warming to room temperature overnight. The reaction mixture was quenched with ice-cold 2 N HCl (250 mL), and the resulting precipitate was filtered and washed with cold water. The solid was recrystallized from EtOH.

Obtained as a green solid; 95%; mp 142-144 ºC (lit: 144-146 ºC);[2] IR (cm^{-1}) 3280, 3028, 1639, 1595, 1566, 1485, 1423, 1315, 1238, 1152, 941, 744, 681; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.53 (s, 1H), 7.66 (d, *J* = 6.9 Hz, 1H), 7.63 (d, *J* = 5.98 Hz, 1H), 7.57 (dt, *J* = 6.2, 1.4 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.21 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.94 (C), 190.54 (C), 165.42 (C), 137.66 (C), 137.48 (C), 135.74 (C), 133.64 (CH), 133.24 (CH), 129.47 (CH), 125.80 (CH), 122.14 (CH), 121.65 (CH), 121.23 (CH), 96.14 (C).

Synthesis of imines (3a-l) and spectroscopic data

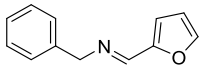
To a solution of aldehyde (**19**, 1 mmol) in CH_2Cl_2 (2 mL), anhydrous Na_2SO_4 (1 mmol) and amine (**20**, 1 mmol) were successively added. After 24 hours stirring at room temperature, the reaction went to completion, as judged by tlc. Then the Na_2SO_4 was filtered off, and the solvent was eliminated. In the case the amine was liberated from the corresponding hydrochloride, the crude was washed with 50 mL of H_2O and 3x20 mL of AcOEt, and the combined organic phases were dried over Na_2SO_4 and concentrated. The obtained imines **3a-l** were used without further purification in the enol-Ugi reactions.

(*E*)-*N*-Benzyl-1-phenylmethanimine (3a)[3]



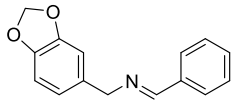
Obtained from benzaldehyde (**19a**, 1 mmol), and benzylamine (**20a**, 1 mmol) as a pale yellow oil; 99%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.39 (s, 1H), 7.79 – 7.74 (m, 2H), 7.45 – 7.37 (m, 3H), 7.35 – 7.32 (m, 4H), 7.29 – 7.20 (m, 1H).

(*E*)-*N*-benzyl-1-(furan-2-yl)methanimine (3b)[4]



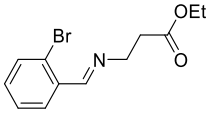
Obtained from furfural (**19f**, 1 mmol), and benzylamine (**20a**, 1 mmol) as a pale brown oil; 98%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.15 (s, 1H), 7.50 (d, *J* = 1.7 Hz, 1H), 7.37 – 7.29 (m, 4H), 7.28 – 7.22 (m, 1H), 6.77 (d, *J* = 3.4 Hz, 1H), 6.46 (dd, *J* = 3.5, 1.8 Hz, 1H), 4.78 (d, *J* = 1.4 Hz, 2H).

(*E*)-*N*-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-1-phenylmethanimine (3c)[5]



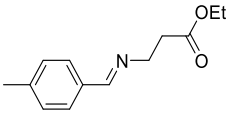
Obtained from benzaldehyde (**19a**, 1 mmol), and benzo[*d*][1,3]dioxol-5-ylmethanamine (**20b**, 1 mmol) as a white solid, mp 46-47 ºC; 99%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.36 (s, 1H), 7.80 – 7.70 (m, 2H), 7.50 – 7.32 (m, 3H), 6.86 – 6.71 (m, 3H), 5.93 (s, 2H), 4.73 (d, *J* = 1.4 Hz, 2H).

Ethyl (*E*)-3-((2-bromobenzylidene)amino)propanoate (3d)



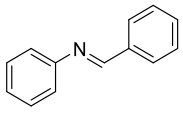
Obtained from 2-bromobenzaldehyde (**19g**, 1 mmol), and β-alanine ethyl ester hydrochloride (**20c**, 1 mmol) as a colourless liquid; 87%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.70 (s, 1H), 7.97 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.32 (t, *J* = 7.0 Hz, 1H), 7.25 (td, *J* = 7.0, 1.9 Hz, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.94 (td, *J* = 6.9, 1.5 Hz, 2H), 2.74 (t, *J* = 6.9 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H);^{13}C RNMR (126 MHz, $CDCl_3$) δ (ppm) 172.07 (C), 161.49 (CH), 134.57 (C), 133.14 (CH), 132.00 (CH), 128.93 (CH), 127.72 (CH), 125.16 (C), 60.65 (CH_2), 56.81 (CH_2), 35.64 (CH_2), 14.38 (CH_3); HRMS (qTOF) Calcd for $C_{12}H_{15}{}^{81}BrNO_2$: 286.0266. Found: 286.0244.

Ethyl (*E*)-3-((4-methylbenzylidene)amino)propanoate (3e)



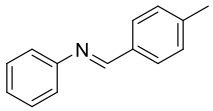
Obtained from 4-tolualdehyde (**19b**, 1 mmol), and β-alanine ethyl ester hydrochloride (**20c**, 1 mmol) as a colourless liquid; 89%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.29 (s, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.87 (td, *J* = 6.9, 1.4 Hz, 2H), 2.72 (t, *J* = 6.9 Hz, 2H), 2.37 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H);^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 172.26 (C), 162.43 (CH), 141.16 (C), 133.51 (C), 129.43 (CH), 128.27 (CH), 60.52 (CH_2), 56.80 (CH_2), 35.67 (CH_2), 21.61 (CH_3), 14.35 (CH_3); HRMS (qTOF) Calcd for $C_{13}H_{18}NO_2$: 220.1338. Found: 220.1341.

(*E*)-*N*,1-Diphenylmethanimine (3f)[6]



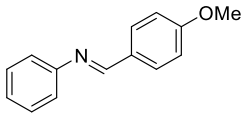
Obtained from benzaldehyde (**19a**, 1 mmol), and aniline (**20d**, 1 mmol) as a white solid, mp 49-50 ºC (lit: 49-51 ºC);[6] 97%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.45 (s, 1H), 7.93 – 7.87 (m, 2H), 7.49 – 7.44 (m, 3H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.25 – 7.19 (m, 3H).

(*E*)-*N*-Phenyl-1-(*p*-tolyl)methanimine (3g)[7]



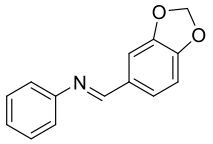
Obtained from *p*-methyl benzaldehyde (**19b**, 1 mmol), and aniline (**20d**, 1 mmol) as a white solid, mp 42-43 ºC (lit: 41-42 ºC);[7] 88%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.41 (s, 1H), 7.79 (d, J = 8.1 Hz, 2H), 7.38 (t, J = 7.8 Hz, 2H), 7.27 (d, J = 7.9 Hz, 2H), 7.25 – 7.17 (m, 3H), 2.41 (s, 3H).

(*E*)-1-(4-Methoxyphenyl)-*N*-phenylmethanimine (3h)[8]



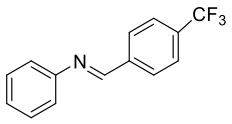
Obtained from *p*-methoxy benzaldehyde (**19c**, 1 mmol), and aniline (**20d**, 1 mmol) as a white solid, mp 51-53 ºC (lit: 49.5-50.1ºC); 96%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.38 (s, 1H), 7.86 (d, *J* = 8.7 Hz, 2H), 7.38 (t, *J* = 8.7 Hz, 2H), 7.23 – 7.18 (m, 3H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H).

(*E*)-1-(Benzo[*d*][1,3]dioxol-5-yl)-*N*-phenylmethanimine (3i)[9-10]



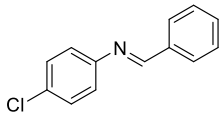
Obtained from benzo[*d*][1,3]dioxole-5-carbaldehyde (**19d**, 1 mmol), and aniline (**20d**, 1 mmol) as a white solid, mp 67-68 ºC (lit: 68-70 C);[10] 92%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.32 (s, 1H), 7.53 (s, 1H), 7.39 – 7.35 (m, 2H), 7.26 (dd, *J* = 6.4, 1.6 Hz, 1H), 7.23 – 7.17 (m, 3H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.03 (s, 2H).

(*E*)-*N*-Phenyl-1-(4-(trifluoromethyl)phenyl)methanimine (3j)[11]



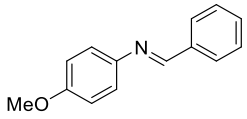
Obtained from *p*-trifluoro benzaldehyde (**19e**, 1 mmol), and aniline (**20d**, 1 mmol) as a white solid, mp 78-79 ºC (lit: 79 ºC);[11] 87%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.50 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.21 (m, 3H).

(*E*)-*N*-(4-Chlorophenyl)-1-phenylmethanimine (3k)[12]



Obtained from benzaldehyde (**19a**, 1 mmol), and *p*-chloro aniline (**20e**, 1 mmol) as a pale grey solid, mp 60-61 ºC (lit: 58-61 ºC);[12] 97%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.43 (s, 1H), 7.89 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.53 – 7.44 (m, 3H), 7.35 (d, *J* = 8.7 Hz, 2H), 7.15 (d, *J* = 8.6 Hz, 2H).

(*E*)-*N*-(4-Methoxyphenyl)-1-phenylmethanimine (3l)[13]



Obtained from benzaldehyde (**19a**, 1 mmol), and *p*-methoxy aniline (**20f**, 1 mmol) as a pale grey solid, mp 58-60 ºC (lit: 58-60 ºC);[13] 89%; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.48 (s, 1H), 7.90 – 7.87 (m, 2H), 7.48 – 7.44 (m, 3H), 7.27 – 7.21 (m, 2H), 6.97 – 6.90 (m, 2H), 3.83 (s, 3H).

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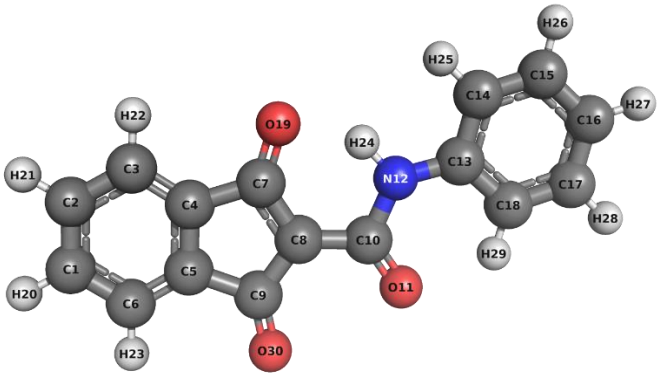
Computational methods.

Table S1. Fukui indices for enolate (12).

Atom	f-	f+
C 1	0,04358	0,08968
C 2	0,03288	0,06957
C 3	0,02928	0,01278
C 4	-0,01107	0,05782
C 5	-0,00017	0,05472
C 6	0,02206	0,00494
C 7	0,00454	0,06176
C 8	0,20753	0,00222
C 9	-0,01726	0,04692
C 10	-0,04708	0,00795
O 11	0,04761	0,03219
N 12	0,11605	0,02583
C 13	-0,00923	-0,08026
C 14	0,05063	0,03512
C 15	0,00858	0,05377
C 16	0,09785	0,12305
C 17	0,00475	0,01942
C 18	0,05736	0,03832
O 19	0,07839	0,07735
H 20	0,02306	0,02702
H 21	0,02275	0,02641
H 22	0,01532	0,02109
H 23	0,01727	0,02246
H 24	0,0068	-0,00177
H 25	0,01476	0,00456
H 26	0,02531	0,02385
H 27	0,02563	0,03246
H 28	0,02511	0,0172
H 29	0,00981	0,00283
O 30	0,09814	0,08844



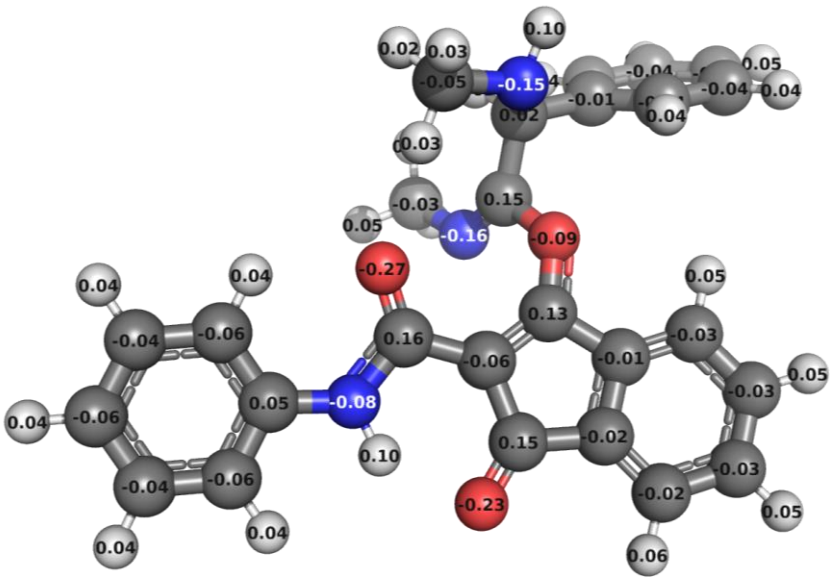


Figure S3. Natural Population Analysis (NPA) charges of primary adduct (15).

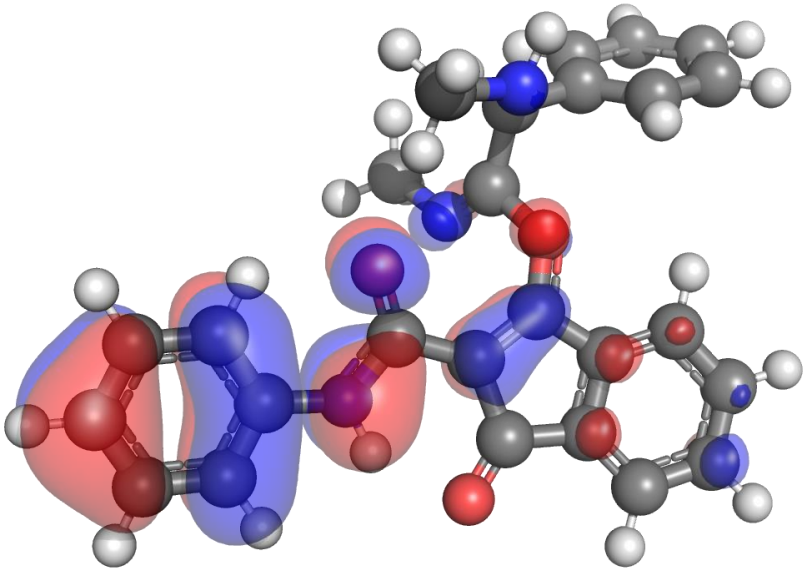
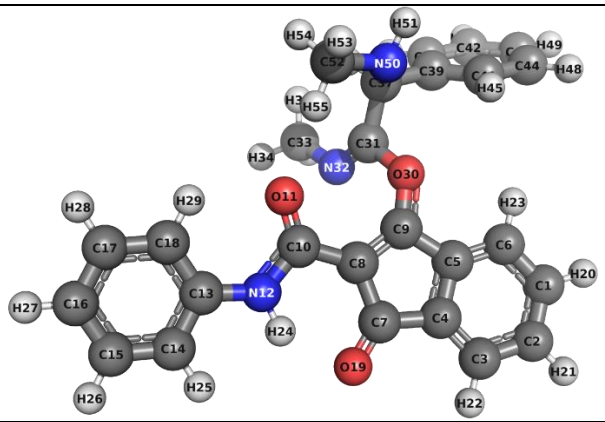


Figure S4. Representation of calculated HOMO for primary adduct (15).

Table S2. HOMO -1, HOMO and LUMO orbitals coefficients into the primary adduct (15).



ATOM	ATOMIC ORBITAL	HOMO - 1	HOMO	LUMO
	Energies (a.u.)	-0.23550	-0.21603	-0.10877
C1	1S	-0.00015	0.00013	0.00008
	2S	0.00027	-0.00023	0.00016
	2PX	0.00022	-0.00378	0.01382
	2PY	-0.00164	0.00391	-0.01016
	2PZ	0.00031	-0.04154	0.14575
	3S	0.00333	0.00188	-0.00371
	3PX	0.00014	-0.00252	0.01136
	3PY	-0.00054	0.00201	-0.00595
	3PZ	-0.00032	-0.02994	0.13948
	4S	-0.03214	0.02535	-0.14157
	4PX	0.01785	-0.02965	0.00455
	4PY	-0.01953	0.01575	0.04543
	4PZ	-0.00187	-0.00145	0.08146
	5XX	-0.00010	0.00034	0.00090
	5YY	-0.00006	0.00041	0.00115
	5ZZ	0.00016	-0.00063	-0.00197
	5XY	0.00009	-0.00030	-0.00118
	5XZ	-0.00025	0.00124	0.00462
	5YZ	0.00086	-0.00343	-0.00943
C2	1S	-0.00018	0.00037	0.00018
	2S	0.00041	-0.00041	-0.00033
	2PX	0.00049	-0.00539	-0.01429
	2PY	-0.00068	0.00493	0.01126
	2PZ	0.01312	-0.06170	-0.15089
	3S	0.00009	-0.00283	-0.00069
	3PX	0.00056	-0.00388	-0.01649
	3PY	0.00094	0.00464	0.01074
	3PZ	0.00925	-0.04609	-0.14175
	4S	0.09918	-0.19607	-0.05236
	4PX	0.00156	0.03041	-0.00708
	4PY	-0.01222	0.01611	0.00240

	4PZ	0.00154	-0.02838	-0.08688
	5XX	-0.00012	-0.00025	0.00160
	5YY	0.00008	-0.00003	0.00047
	5ZZ	0.00004	0.00045	-0.00204
	5XY	0.00015	0.00015	-0.00109
	5XZ	-0.00026	-0.00171	0.00919
	5YZ	-0.00010	0.00071	-0.00353
C3	1S	-0.00098	0.00015	0.00041
	2S	0.00196	-0.00048	-0.00095
	2PX	0.00088	0.00043	-0.00952
	2PY	-0.00570	0.00078	0.00934
	2PZ	0.00797	0.01145	-0.09354
	3S	0.01076	0.00110	-0.00249
	3PX	0.00165	0.00012	-0.01331
	3PY	-0.00706	0.00002	0.00826
	3PZ	0.00553	0.01213	-0.08918
	4S	0.29718	-0.24648	-0.25596
	4PX	-0.02851	0.07070	0.02940
	4PY	-0.06599	0.09347	0.07334
	4PZ	-0.00202	0.01772	-0.12128
	5XX	-0.00001	-0.00045	-0.00157
	5YY	-0.00016	0.00067	0.00152
	5ZZ	-0.00010	-0.00006	0.00012
	5XY	0.00042	-0.00034	-0.00054
	5XZ	0.00056	-0.00261	-0.00928
	5YZ	0.00038	-0.00351	-0.01059
C4	1S	0.00123	-0.00055	-0.00096
	2S	-0.00237	0.00156	0.00161
	2PX	-0.00719	0.00880	0.02030
	2PY	0.00756	-0.00726	-0.01773
	2PZ	-0.00602	0.06065	0.17793
	3S	-0.01155	-0.00563	0.01835
	3PX	-0.01137	0.01146	0.03153
	3PY	-0.00243	-0.00361	-0.02255
	3PZ	-0.00559	0.03871	0.17433
	4S	-0.07621	-0.05387	-0.07880
	4PX	0.00867	0.01831	-0.19586
	4PY	-0.23128	0.28152	0.19974
	4PZ	-0.02010	-0.00059	0.38554
	5XX	-0.00046	0.00041	-0.00250
	5YY	0.00058	-0.00039	0.00050
	5ZZ	0.00013	-0.00032	0.00177
	5XY	0.00028	-0.00008	0.00067
	5XZ	-0.00006	0.00258	-0.01474
	5YZ	0.00081	0.00050	-0.00557
C5	1S	-0.00186	0.00198	0.00129
	2S	0.00420	-0.00358	-0.00211

	2PX	0.00053	0.00681	-0.01455
	2PY	-0.01336	0.00502	0.01965
	2PZ	-0.00995	0.05395	-0.17342
	3S	0.00405	-0.02136	-0.01552
	3PX	-0.00177	0.00454	0.00201
	3PY	0.00136	0.00864	0.00849
	3PZ	-0.00510	0.03771	-0.16464
	4S	-0.03284	-0.00211	0.11989
	4PX	-0.06888	0.11400	0.10196
	4PY	-0.10593	0.12386	0.38524
	4PZ	0.00777	0.09728	-0.28131
	5XX	0.00026	0.00042	0.00001
	5YY	-0.00030	-0.00058	-0.00164
	5ZZ	-0.00022	0.00041	0.00177
	5XY	0.00087	-0.00019	0.00091
	5XZ	-0.00025	0.00198	0.00176
	5YZ	-0.00129	0.00490	0.01840
C6	1S	-0.00066	0.00003	0.00025
	2S	0.00176	-0.00056	-0.00095
	2PX	-0.00321	0.00240	0.00956
	2PY	0.00083	-0.00291	-0.00652
	2PZ	-0.01255	0.04149	0.09995
	3S	0.00256	0.00241	-0.00342
	3PX	-0.00160	0.00137	0.01256
	3PY	-0.00155	-0.00600	-0.00091
	3PZ	-0.00831	0.03092	0.08834
	4S	0.12862	-0.27683	-0.16502
	4PX	-0.04124	0.09053	0.09837
	4PY	-0.01290	0.03241	0.04540
	4PZ	-0.00334	-0.01787	0.12181
	5XX	-0.00017	-0.00034	0.00149
	5YY	0.00001	0.00027	-0.00125
	5ZZ	-0.00004	0.00010	-0.00023
	5XY	0.00051	-0.00017	0.00003
	5XZ	0.00047	-0.00282	0.00892
	5YZ	-0.00008	-0.00191	0.01076
C7	1S	0.00036	-0.00083	-0.00128
	2S	-0.00062	0.00252	0.00358
	2PX	-0.00108	-0.00295	0.03605
	2PY	0.00070	-0.00092	-0.02618
	2PZ	-0.00385	-0.02955	0.26954
	3S	-0.00615	0.00649	0.00939
	3PX	-0.00300	0.01180	0.02563
	3PY	-0.00356	0.00574	-0.00972
	3PZ	-0.00080	-0.02231	0.21769
	4S	-0.06567	0.15436	0.28769
	4PX	0.01274	0.02937	-0.10296

	4PY	0.04208	-0.00138	-0.22644
	4PZ	0.00171	-0.01163	-0.13259
	5XX	0.00021	0.00033	0.00469
	5YY	-0.00056	-0.00138	0.00163
	5ZZ	0.00016	0.00122	-0.00625
	5XY	0.00006	0.00078	-0.00261
	5XZ	-0.00116	-0.00138	0.02285
	5YZ	0.00070	0.00523	-0.00839
C8	1S	0.00221	-0.00095	-0.00192
	2S	-0.00335	-0.00019	0.00582
	2PX	0.00616	-0.00322	0.01104
	2PY	0.00590	0.00914	-0.01410
	2PZ	-0.01361	-0.10833	0.12656
	3S	-0.00786	0.02619	-0.00414
	3PX	0.00570	-0.01261	-0.01199
	3PY	0.00479	-0.01172	-0.01011
	3PZ	-0.01555	-0.07338	0.12918
	4S	-0.30415	0.09190	-0.19823
	4PX	-0.10325	0.05776	0.34635
	4PY	-0.00460	0.05714	-0.23007
	4PZ	0.03186	0.00853	0.20308
	5XX	0.00108	-0.00225	-0.00369
	5YY	0.00025	0.00069	-0.00040
	5ZZ	-0.00066	0.00107	0.00382
	5XY	0.00068	0.00031	0.00206
	5XZ	0.00045	-0.00736	-0.01700
	5YZ	0.00031	-0.00253	0.01046
C9	1S	0.00163	0.00026	-0.00103
	2S	0.00177	-0.00074	0.00127
	2PX	-0.00958	-0.00576	-0.01730
	2PY	0.01455	-0.00009	0.00757
	2PZ	0.02535	-0.09064	-0.32292
	3S	-0.03343	0.00341	0.02759
	3PX	-0.00280	0.00377	-0.03711
	3PY	0.02687	0.01418	0.01126
	3PZ	0.01497	-0.06997	-0.25117
	4S	-0.25007	0.00899	0.06507
	4PX	-0.01170	0.10462	0.00115
	4PY	-0.06906	0.37701	0.42941
	4PZ	-0.03679	-0.12162	-0.11350
	5XX	-0.00039	0.00319	0.00137
	5YY	0.00287	-0.00139	-0.00040
	5ZZ	-0.00104	-0.00143	-0.00083
	5XY	0.00002	-0.00174	-0.00161
	5XZ	0.00272	0.00782	-0.00749
	5YZ	-0.00162	-0.00142	-0.01110
C10	1S	0.00029	0.00182	0.00129

	2S	0.00009	-0.00362	-0.00282
	2PX	0.00130	0.01249	0.00553
	2PY	0.01089	-0.02028	-0.01603
	2PZ	0.00052	0.06351	0.05036
	3S	0.00371	-0.01758	-0.01050
	3PX	0.00311	-0.00698	0.02044
	3PY	0.00625	-0.03282	-0.03129
	3PZ	-0.00203	0.03508	0.03001
	4S	0.02039	0.03529	0.07636
	4PX	0.17273	0.22687	-0.05574
	4PY	0.09699	-0.00187	-0.03989
	4PZ	-0.02371	0.03408	-0.05908
	5XX	0.00229	-0.00506	0.00077
	5YY	-0.00097	-0.00527	-0.00287
	5ZZ	-0.00114	0.01110	0.00250
	5XY	-0.00361	0.00769	-0.00007
	5XZ	-0.00162	-0.01740	0.00422
	5YZ	-0.00156	0.00997	0.00892
O11	1S	-0.00426	0.00124	-0.00022
	2S	0.01044	-0.00267	0.00063
	2PX	0.05699	-0.04565	-0.00838
	2PY	-0.00221	0.03423	0.02122
	2PZ	0.01536	-0.15067	-0.06470
	3S	0.01994	-0.00937	-0.00382
	3PX	0.03638	-0.02841	-0.00637
	3PY	0.00086	0.02297	0.01241
	3PZ	0.01054	-0.10779	-0.05145
	4S	-0.02068	-0.02826	-0.06196
	4PX	0.00396	-0.03175	-0.00750
	4PY	-0.02111	0.01015	-0.00073
	4PZ	-0.00059	-0.05581	-0.02685
	5XX	-0.00154	0.00082	0.00015
	5YY	0.00037	0.00156	-0.00011
	5ZZ	0.00020	-0.00183	-0.00040
	5XY	0.00255	-0.00131	-0.00024
	5XZ	0.00037	0.00073	0.00092
	5YZ	0.00012	-0.00407	-0.00085
N12	1S	-0.00234	-0.00173	0.00020
	2S	0.00586	0.00491	-0.00176
	2PX	0.01146	0.04315	-0.00795
	2PY	-0.00657	-0.06825	0.01254
	2PZ	-0.01022	0.30522	-0.05429
	3S	0.01263	0.00042	0.00976
	3PX	0.00791	0.03825	0.00747
	3PY	-0.00342	-0.05177	0.01524
	3PZ	-0.00776	0.25005	-0.04638
	4S	0.02521	-0.01785	0.02422

	4PX	-0.00047	0.02677	0.00735
	4PY	-0.01125	0.03232	0.02753
	4PZ	0.00099	0.06797	-0.01342
	5XX	0.00001	0.00272	0.00070
	5YY	-0.00062	-0.00090	-0.00048
	5ZZ	-0.00000	-0.00156	-0.00077
	5XY	0.00058	-0.00253	-0.00058
	5XZ	-0.00032	0.01113	0.00310
	5YZ	-0.00053	0.00427	0.00054
C13	1S	-0.00019	0.00054	-0.00028
	2S	0.00097	-0.00286	0.00041
	2PX	-0.00024	-0.03196	0.00117
	2PY	-0.00005	0.05025	0.00112
	2PZ	0.00706	-0.22666	-0.00145
	3S	0.00254	0.01117	0.00666
	3PX	-0.00237	-0.01459	0.00618
	3PY	-0.00305	0.04023	0.00780
	3PZ	0.00442	-0.16118	-0.00316
	4S	-0.38452	0.33495	-0.05932
	4PX	0.29059	0.28689	0.18915
	4PY	-0.15048	-0.22531	-0.11909
	4PZ	-0.07981	-0.14490	-0.04856
	5XX	0.00031	0.00397	-0.00068
	5YY	-0.00026	-0.00426	0.00099
	5ZZ	0.00014	0.00028	-0.00026
	5XY	-0.00024	-0.00275	0.00065
	5XZ	-0.00056	0.01724	-0.00342
	5YZ	-0.00013	0.01019	-0.00232
C14	1S	-0.00062	-0.00017	-0.00009
	2S	0.00150	-0.00002	-0.00010
	2PX	0.00427	-0.02343	0.00304
	2PY	-0.00182	0.04368	-0.00554
	2PZ	0.00723	-0.19436	0.02695
	3S	0.00144	0.00373	0.00150
	3PX	0.00255	-0.01872	0.00291
	3PY	0.00093	0.02884	-0.00639
	3PZ	0.00527	-0.13568	0.02352
	4S	0.61065	0.29420	0.59246
	4PX	0.15441	0.12977	-0.00661
	4PY	-0.07554	-0.00626	-0.08906
	4PZ	-0.03106	-0.05738	-0.02401
	5XX	0.00003	-0.00236	-0.00012
	5YY	-0.00003	-0.00145	0.00014
	5ZZ	-0.00009	0.00363	-0.00013
	5XY	-0.00021	0.00271	-0.00002
	5XZ	0.00017	-0.00954	-0.00040
	5YZ	-0.00013	0.00340	-0.00044

C15	1S	0.00020	0.00010	-0.00006
	2S	-0.00070	-0.00050	-0.00001
	2PX	-0.00173	0.01056	0.00019
	2PY	-0.00040	-0.02056	-0.00019
	2PZ	0.00001	0.08990	0.00102
	3S	0.00198	-0.00166	0.00015
	3PX	0.00066	0.00687	0.00073
	3PY	-0.00158	-0.01471	-0.00193
	3PZ	-0.00043	0.05840	0.00175
	4S	-0.13324	0.04797	-0.38361
	4PX	-0.00352	0.04115	-0.06048
	4PY	0.06827	0.05390	0.00750
	4PZ	0.01329	0.02645	0.02348
	5XX	0.00012	-0.00163	0.00021
	5YY	-0.00015	0.00537	-0.00067
	5ZZ	0.00011	-0.00382	0.00044
	5XY	-0.00014	-0.00001	-0.00000
	5XZ	0.00024	-0.00790	0.00128
	5YZ	0.00046	-0.01327	0.00180
C16	1S	-0.00040	0.00016	-0.00008
	2S	0.00103	-0.00061	0.00035
	2PX	0.00140	0.03245	-0.00345
	2PY	0.00106	-0.06032	0.00666
	2PZ	-0.00834	0.26406	-0.02913
	3S	-0.00048	-0.00099	-0.00100
	3PX	-0.00050	0.02353	-0.00377
	3PY	-0.00019	-0.04194	0.00498
	3PZ	-0.00554	0.18469	-0.02556
	4S	0.22574	0.00303	0.13352
	4PX	0.02089	-0.01596	0.01910
	4PY	0.04444	0.03861	0.05797
	4PZ	0.00967	0.07871	-0.01095
	5XX	-0.00017	0.00064	0.00001
	5YY	-0.00009	-0.00059	-0.00005
	5ZZ	0.00010	-0.00012	0.00001
	5XY	-0.00010	-0.00049	-0.00005
	5XZ	-0.00022	0.00289	0.00020
	5YZ	0.00011	0.00136	0.00009
C17	1S	0.00044	-0.00018	0.00000
	2S	-0.00084	0.00034	-0.00012
	2PX	-0.00403	0.01330	-0.00003
	2PY	0.00154	-0.02250	-0.00042
	2PZ	-0.00627	0.09829	0.00141
	3S	-0.00280	-0.00069	-0.00021
	3PX	-0.00349	0.00711	0.00035
	3PY	0.00206	-0.01443	-0.00031
	3PZ	-0.00407	0.06372	0.00282

	4S	-0.28550	-0.19279	-0.55420
	4PX	-0.04166	-0.10312	-0.13875
	4PY	-0.04042	-0.01463	-0.05796
	4PZ	-0.01299	0.04315	0.00036
	5XX	0.00031	-0.00351	0.00058
	5YY	-0.00012	-0.00020	-0.00013
	5ZZ	-0.00006	0.00362	-0.00046
	5XY	-0.00032	0.00367	-0.00054
	5XZ	0.00024	-0.01527	0.00219
	5YZ	-0.00011	0.00013	0.00018
C18	1S	-0.00061	0.00045	-0.00031
	2S	0.00223	-0.00149	0.00008
	2PX	0.00638	-0.02564	0.00429
	2PY	-0.00391	0.04322	-0.00680
	2PZ	0.00017	-0.18618	0.02705
	3S	-0.00247	0.00160	0.00589
	3PX	0.00198	-0.01897	0.00226
	3PY	-0.00643	0.03013	-0.00203
	3PZ	-0.00034	-0.12742	0.02313
	4S	0.11488	-0.26450	0.23052
	4PX	-0.10869	-0.16017	-0.24143
	4PY	-0.05727	-0.19309	-0.19757
	4PZ	0.01384	-0.08503	0.01011
	5XX	-0.00001	-0.00025	-0.00030
	5YY	-0.00003	0.00419	-0.00002
	5ZZ	0.00019	-0.00391	0.00007
	5XY	-0.00035	-0.00093	0.00014
	5XZ	0.00021	-0.00220	-0.00061
	5YZ	0.00041	-0.01034	0.00003
O19	1S	-0.00040	-0.00085	0.00026
	2S	0.00107	0.00085	-0.00069
	2PX	-0.00053	-0.00199	-0.03724
	2PY	-0.00860	-0.01138	0.02679
	2PZ	0.01324	0.01599	-0.27982
	3S	0.00128	0.01164	-0.00291
	3PX	0.00013	0.00046	-0.03126
	3PY	-0.00550	-0.00994	0.02063
	3PZ	0.00913	0.01336	-0.22609
	4S	0.00521	-0.01370	-0.01017
	4PX	-0.00110	0.00067	-0.01119
	4PY	-0.00331	0.00472	0.00803
	4PZ	0.00148	0.01499	-0.08267
	5XX	-0.00008	-0.00084	-0.00024
	5YY	0.00016	-0.00016	-0.00008
	5ZZ	-0.00013	-0.00024	0.00025
	5XY	-0.00026	-0.00075	0.00027
	5XZ	0.00036	-0.00048	-0.00036

	5YZ	-0.00009	-0.00054	0.00171
H20	1S	-0.00013	0.00048	0.00040
	2S	-0.00098	0.00023	0.00241
	3PX	0.00003	-0.00009	0.00046
	3PY	-0.00002	0.00013	-0.00040
	3PZ	0.00002	-0.00123	0.00491
H21	1S	0.00055	-0.00006	-0.00022
	2S	-0.00118	0.00079	0.00076
	3PX	0.00004	-0.00017	-0.00047
	3PY	-0.00002	0.00015	0.00039
	3PZ	0.00037	-0.00178	-0.00514
H22	1S	-0.00243	0.00142	0.00124
	2S	-0.00190	0.00050	-0.00006
	3PX	0.00001	0.00007	-0.00030
	3PY	-0.00007	0.00005	0.00033
	3PZ	0.00023	0.00023	-0.00306
H23	1S	-0.00175	0.00033	0.00081
	2S	-0.00379	0.00048	0.00318
	3PX	-0.00001	0.00009	0.00023
	3PY	0.00007	-0.00022	-0.00033
	3PZ	-0.00029	0.00112	0.00321
H24	1S	-0.00547	-0.00071	-0.00103
	2S	-0.00621	-0.00013	-0.00839
	3PX	0.00030	0.00114	-0.00049
	3PY	0.00017	-0.00169	0.00039
	3PZ	-0.00024	0.00954	-0.00294
H25	1S	0.00029	0.00012	-0.00005
	2S	-0.00310	0.00020	-0.00067
	3PX	0.00001	-0.00055	0.00002
	3PY	-0.00008	0.00117	-0.00018
	3PZ	0.00020	-0.00500	0.00063
H26	1S	0.00099	0.00040	-0.00017
	2S	0.00179	0.00054	0.00149
	3PX	-0.00001	0.00034	0.00004
	3PY	-0.00001	-0.00060	-0.00001
	3PZ	-0.00001	0.00262	0.00000
H27	1S	-0.00112	0.00029	-0.00012
	2S	-0.00319	0.00036	-0.00085
	3PX	-0.00002	0.00093	-0.00012
	3PY	0.00002	-0.00169	0.00023
	3PZ	-0.00023	0.00745	-0.00097
H28	1S	-0.00091	0.00028	-0.00019
	2S	0.00006	0.00066	0.00086
	3PX	-0.00004	0.00039	0.00000
	3PY	0.00003	-0.00063	0.00003
	3PZ	-0.00017	0.00285	0.00002
H29	1S	0.00375	-0.00073	-0.00003

	2S	0.00126	0.00170	0.00297
	3PX	-0.00040	-0.00049	-0.00005
	3PY	-0.00011	0.00128	-0.00011
	3PZ	0.00018	-0.00517	0.00051
O30	1S	-0.00551	0.00387	0.01194
	2S	0.00731	-0.00873	-0.02437
	2PX	-0.01673	0.02458	0.01886
	2PY	-0.04161	0.02569	0.03688
	2PZ	0.06391	0.06390	0.14322
	3S	0.06308	-0.01926	-0.07023
	3PX	-0.01372	0.01929	0.02290
	3PY	-0.04335	0.01430	0.03549
	3PZ	0.05067	0.05094	0.10766
	4S	0.11607	0.03690	-0.11289
	4PX	-0.03642	0.00909	0.03016
	4PY	-0.01949	-0.01406	0.04648
	4PZ	0.02208	0.03708	0.01477
	5XX	-0.00216	-0.00099	-0.00015
	5YY	-0.00587	0.00055	0.00193
	5ZZ	0.00221	0.00178	0.00386
	5XY	0.00232	-0.00062	-0.00353
	5XZ	-0.00379	0.00066	0.00484
	5YZ	0.00171	-0.00168	-0.01219
C31	1S	0.01765	-0.00183	-0.01304
	2S	-0.03637	0.00778	0.02889
	2PX	-0.06859	-0.01835	0.02811
	2PY	0.05241	0.00938	0.07411
	2PZ	0.08402	-0.02248	-0.00408
	3S	-0.14282	-0.01034	0.11117
	3PX	-0.03678	-0.01578	0.01054
	3PY	-0.01666	-0.00186	0.06500
	3PZ	0.05380	0.00200	0.01751
	4S	-0.21417	0.09888	0.26807
	4PX	-0.09860	-0.20676	-0.16598
	4PY	0.07133	0.19974	0.41767
	4PZ	0.07232	-0.01523	-0.10104
	5XX	-0.00606	0.00233	0.00242
	5YY	0.00511	0.00218	0.00461
	5ZZ	0.00090	-0.00485	-0.01070
	5XY	0.00435	0.00093	0.00293
	5XZ	0.00476	-0.00226	-0.00171
	5YZ	-0.01105	0.00172	0.00040
N32	1S	0.01930	-0.00387	0.00373
	2S	-0.03784	0.01021	-0.00592
	2PX	0.08493	-0.05801	-0.06716
	2PY	-0.12079	0.00453	-0.02677
	2PZ	-0.04823	-0.01661	-0.02659

	3S	-0.11012	0.01010	-0.04014
	3PX	0.05924	-0.04183	-0.06410
	3PY	-0.07363	0.00346	-0.02219
	3PZ	-0.03020	-0.01066	-0.01511
	4S	-0.07014	-0.04813	-0.08942
	4PX	0.01659	0.02398	0.01223
	4PY	-0.02328	-0.02722	-0.10628
	4PZ	-0.01416	0.01924	0.02670
	5XX	0.00141	-0.00308	-0.00111
	5YY	0.00333	0.00033	0.00126
	5ZZ	0.00129	0.00223	0.00138
	5XY	-0.00312	0.00184	0.00251
	5XZ	-0.00324	0.00010	-0.00106
	5YZ	0.00052	0.00017	-0.00116
C33	1S	-0.00281	0.00008	-0.00323
	2S	0.00672	0.00039	0.00934
	2PX	-0.03258	0.00765	0.00827
	2PY	0.07227	0.00023	0.01708
	2PZ	0.00709	0.00343	-0.00686
	3S	0.01393	-0.00056	0.00653
	3PX	-0.00987	-0.00099	0.00016
	3PY	0.03994	0.00271	0.01280
	3PZ	-0.00510	0.00415	-0.00430
	4S	-0.03858	-0.01811	-0.03375
	4PX	-0.01563	0.00639	0.01870
	4PY	0.01139	-0.00620	-0.00316
	4PZ	0.02008	0.00565	0.01357
	5XX	0.00154	-0.00139	-0.00179
	5YY	-0.00711	0.00042	-0.00094
	5ZZ	0.00508	0.00127	0.00255
	5XY	0.00557	-0.00244	-0.00296
	5XZ	-0.00210	0.00170	0.00233
	5YZ	-0.00274	-0.00002	-0.00071
H34	1S	0.02283	-0.01242	-0.01598
	2S	0.03500	-0.02411	-0.03038
	3PX	0.00029	-0.00012	-0.00008
	3PY	0.00130	0.00012	0.00081
	3PZ	0.00066	0.00007	-0.00037
H35	1S	-0.05368	0.00562	0.00106
	2S	-0.06419	0.01517	0.00518
	3PX	0.00137	0.00022	0.00043
	3PY	-0.00064	0.00013	0.00037
	3PZ	-0.00209	0.00009	-0.00012
H36	1S	0.01722	0.00728	0.01112
	2S	0.02592	0.00744	0.01621
	3PX	-0.00126	0.00015	0.00010
	3PY	0.00097	-0.00023	-0.00018

	3PZ	-0.00014	-0.00002	-0.00014
C37	1S	0.01122	-0.00122	0.00049
	2S	-0.03789	0.00193	-0.00020
	2PX	0.04192	-0.00428	-0.00254
	2PY	-0.09514	0.00427	-0.00499
	2PZ	0.07290	0.00774	-0.00161
	3S	0.00605	0.01417	-0.00002
	3PX	0.02527	-0.00717	-0.00933
	3PY	-0.00038	0.01137	0.00071
	3PZ	0.01453	-0.00085	-0.00145
	4S	0.50779	-0.01063	-0.49609
	4PX	-0.02317	-0.09641	-0.27899
	4PY	0.01327	-0.02016	-0.12497
	4PZ	0.01997	0.00810	0.14941
	5XX	-0.00551	0.00058	-0.00273
	5YY	0.00220	0.00029	0.00208
	5ZZ	0.00481	-0.00094	0.00102
	5XY	0.00433	-0.00030	0.00013
	5XZ	0.00072	0.00010	0.00045
	5YZ	-0.02695	-0.00164	0.00004
H38	1S	0.11625	0.00557	0.00989
	2S	0.21138	0.02249	0.03065
	3PX	0.00108	0.00004	0.00025
	3PY	0.00180	0.00022	-0.00005
	3PZ	0.00068	0.00012	-0.00018
C39	1S	0.00525	-0.00025	0.00234
	2S	-0.00726	-0.00029	-0.00772
	2PX	0.00188	-0.00058	0.01103
	2PY	0.04813	-0.00111	0.00475
	2PZ	0.01757	0.00005	0.00461
	3S	-0.07570	0.00360	-0.00317
	3PX	0.01153	-0.00523	-0.00858
	3PY	0.00402	-0.00356	0.01089
	3PZ	0.04095	0.00247	-0.00231
	4S	-0.06948	0.10768	114.488
	4PX	-0.00220	-0.01560	-0.12059
	4PY	-0.12525	-0.03029	0.01931
	4PZ	0.20884	0.04424	-0.11550
	5XX	-0.00104	0.00005	0.00021
	5YY	0.00230	-0.00018	-0.00004
	5ZZ	-0.00044	-0.00027	-0.00046
	5XY	0.00507	-0.00005	-0.00058
	5XZ	-0.00046	0.00000	-0.00057
	5YZ	-0.00051	-0.00011	-0.00006
C40	1S	0.00461	0.00001	-0.00016
	2S	-0.01076	0.00011	-0.00009
	2PX	0.00958	0.00063	0.00167

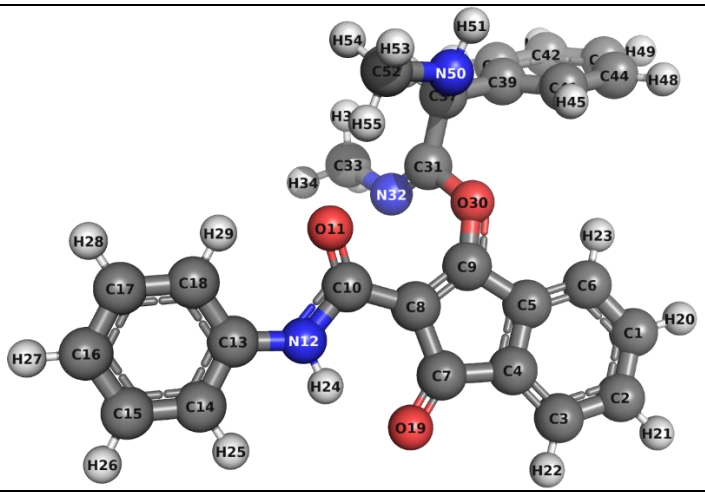
	2PY	0.02297	0.00027	-0.00411
	2PZ	0.01956	-0.00057	-0.00650
	3S	-0.03811	-0.00360	0.00585
	3PX	-0.01068	-0.00250	0.00223
	3PY	0.01202	0.00063	-0.00131
	3PZ	0.01086	-0.00168	-0.01228
	4S	-0.09273	-0.23756	-0.26364
	4PX	0.18473	-0.11524	-0.03669
	4PY	-0.00384	-0.00623	-0.02892
	4PZ	0.12892	-0.02687	0.02715
	5XX	0.00160	-0.00015	-0.00028
	5YY	0.00095	-0.00000	0.00021
	5ZZ	-0.00225	0.00007	0.00018
	5XY	-0.00055	0.00010	-0.00002
	5XZ	-0.00073	0.00011	-0.00024
	5YZ	-0.00112	0.00001	-0.00032
C41	1S	0.00285	0.00033	-0.00062
	2S	-0.00780	-0.00105	0.00110
	2PX	0.00382	0.00214	0.00013
	2PY	0.00542	-0.00212	-0.00599
	2PZ	0.06434	-0.00092	-0.00554
	3S	-0.00759	0.00296	0.00531
	3PX	-0.05710	0.00041	0.01166
	3PY	-0.02667	-0.00314	-0.00280
	3PZ	0.04580	0.00195	-0.00435
	4S	0.30738	0.10066	-0.28310
	4PX	-0.07643	-0.03258	0.08648
	4PY	-0.06562	-0.01319	0.09555
	4PZ	0.08360	0.01283	-0.07479
	5XX	0.00133	0.00021	-0.00032
	5YY	-0.00227	-0.00002	-0.00013
	5ZZ	0.00045	-0.00006	0.00045
	5XY	0.00116	0.00002	-0.00051
	5XZ	-0.00085	-0.00002	0.00011
	5YZ	0.00077	0.00004	-0.00017
C42	1S	-0.00179	-0.00006	0.00031
	2S	0.00227	0.00009	-0.00097
	2PX	-0.00072	-0.00131	0.00164
	2PY	-0.02230	0.00169	0.00042
	2PZ	-0.01704	0.00138	0.00014
	3S	0.02848	0.00204	-0.00307
	3PX	-0.00552	-0.00219	0.00034
	3PY	-0.01262	0.00014	-0.00120
	3PZ	-0.01827	0.00088	0.00228
	4S	-0.15340	0.18850	0.19534
	4PX	0.12342	-0.07081	-0.03586
	4PY	0.06702	-0.04563	-0.00205

	4PZ	-0.03605	-0.00261	-0.02532
	5XX	0.00143	0.00007	-0.00027
	5YY	-0.00222	0.00006	0.00036
	5ZZ	0.00009	-0.00003	-0.00007
	5XY	-0.00057	0.00006	0.00014
	5XZ	-0.00118	0.00010	0.00048
	5YZ	0.00006	0.00000	0.00006
H43	1S	-0.00463	-0.00038	0.00064
	2S	-0.00005	0.00197	0.00936
	3PX	-0.00079	-0.00002	-0.00003
	3PY	-0.00015	-0.00003	-0.00021
	3PZ	0.00049	-0.00003	-0.00019
C44	1S	-0.00235	-0.00012	0.00058
	2S	0.00204	0.00062	-0.00148
	2PX	-0.00994	-0.00032	0.00354
	2PY	-0.00301	-0.00146	-0.00099
	2PZ	-0.01504	-0.00123	-0.00111
	3S	0.05277	-0.00129	-0.00854
	3PX	-0.02935	0.00062	0.00814
	3PY	-0.00738	-0.00033	-0.00019
	3PZ	-0.01297	-0.00127	0.00140
	4S	-0.11323	0.07043	0.02170
	4PX	-0.04348	0.01786	0.04294
	4PY	0.01313	-0.01175	-0.02402
	4PZ	-0.06901	0.00716	0.04794
	5XX	0.00193	-0.00009	-0.00037
	5YY	0.00038	0.00004	-0.00001
	5ZZ	-0.00273	0.00009	0.00037
	5XY	-0.00008	0.00010	0.00038
	5XZ	-0.00237	0.00003	0.00008
	5YZ	-0.00141	0.00009	0.00025
H45	1S	-0.02322	-0.00078	0.00229
	2S	-0.00501	0.00051	0.00089
	3PX	-0.00299	-0.00006	0.00014
	3PY	-0.00032	-0.00016	-0.00042
	3PZ	-0.00121	-0.00012	-0.00021
C46	1S	0.00351	0.00014	0.00008
	2S	-0.00771	-0.00018	-0.00082
	2PX	0.02643	-0.00021	-0.00249
	2PY	-0.03713	0.00128	0.00590
	2PZ	-0.01439	0.00109	0.00382
	3S	-0.01815	-0.00032	0.00185
	3PX	0.02442	0.00044	-0.00428
	3PY	-0.01978	0.00083	0.00400
	3PZ	-0.01511	0.00090	0.00495
	4S	-0.00296	-0.00525	-0.14069
	4PX	-0.00487	0.00605	0.01599

	4PY	0.05008	-0.01334	-0.00508
	4PZ	-0.07965	0.03856	0.02488
	5XX	0.00084	0.00009	-0.00021
	5YY	0.00067	-0.00011	-0.00006
	5ZZ	-0.00072	0.00012	0.00005
	5XY	0.00069	0.00003	0.00006
	5XZ	0.00055	-0.00001	-0.00005
	5YZ	0.00038	0.00007	0.00001
H47	1S	-0.00313	-0.00001	0.00084
	2S	-0.00150	-0.00034	0.00021
	3PX	0.00019	-0.00000	0.00008
	3PY	-0.00057	0.00006	0.00001
	3PZ	-0.00043	0.00005	0.00000
H48	1S	0.00779	-0.00012	0.00057
	2S	0.01230	0.00020	0.00068
	3PX	0.00025	-0.00001	0.00004
	3PY	-0.00023	-0.00004	-0.00009
	3PZ	0.00002	-0.00003	-0.00004
H49	1S	0.00722	0.00025	-0.00047
	2S	0.00741	0.00042	0.00062
	3PX	0.00048	-0.00000	-0.00010
	3PY	-0.00109	0.00004	0.00021
	3PZ	-0.00048	0.00003	0.00010
N50	1S	-0.05392	-0.00267	-0.00522
	2S	0.11558	0.00656	0.01300
	2PX	-0.00690	-0.00211	-0.00149
	2PY	0.46376	0.02759	0.02488
	2PZ	-0.17343	-0.01671	-0.00184
	3S	0.24935	0.00758	0.02941
	3PX	0.00563	0.00017	0.00274
	3PY	0.34410	0.01683	0.01285
	3PZ	-0.12660	-0.01468	-0.00614
	4S	-0.16872	0.04829	0.13312
	4PX	0.04259	0.01345	0.04557
	4PY	0.14141	0.00999	0.00322
	4PZ	-0.13733	0.00164	-0.00352
	5XX	0.00111	0.00029	0.00022
	5YY	-0.01512	-0.00083	-0.00167
	5ZZ	0.00046	0.00035	0.00080
	5XY	0.00416	0.00048	0.00085
	5XZ	0.00050	-0.00022	0.00041
	5YZ	0.00775	0.00083	-0.00041
H51	1S	-0.07040	-0.00330	-0.00731
	2S	-0.05547	-0.00617	-0.02830
	3PX	0.00291	0.00017	0.00029
	3PY	0.01242	0.00078	0.00084
	3PZ	-0.00788	-0.00072	-0.00026

C52	1S	0.01307	0.00164	0.00056
	2S	-0.03652	-0.00407	-0.00145
	2PX	-0.02312	0.00410	-0.00315
	2PY	-0.12487	-0.01047	-0.00178
	2PZ	0.02339	0.00128	-0.00014
	3S	-0.00344	-0.00273	0.00056
	3PX	0.01052	-0.00055	-0.00791
	3PY	-0.03383	-0.00236	0.00458
	3PZ	0.02088	-0.00043	0.00085
	4S	0.01506	-0.03729	-0.02003
	4PX	-0.00685	0.00068	-0.00140
	4PY	-0.04486	-0.01158	-0.00508
	4PZ	0.03114	-0.01125	-0.00890
	5XX	-0.01286	-0.00060	-0.00047
	5YY	0.01982	0.00138	0.00082
	5ZZ	-0.00563	-0.00041	-0.00029
	5XY	0.01486	0.00090	0.00084
	5XZ	-0.00739	-0.00060	-0.00009
	5YZ	-0.00714	-0.00047	-0.00026
H53	1S	-0.03897	-0.00350	-0.00142
	2S	-0.03384	-0.00269	0.00077
	3PX	0.00041	0.00020	-0.00003
	3PY	-0.00246	-0.00024	-0.00003
	3PZ	-0.00054	-0.00013	0.00003
H54	1S	0.12521	0.00873	0.00414
	2S	0.20527	0.01585	0.01408
	3PX	-0.00089	0.00014	-0.00003
	3PY	0.00076	0.00001	-0.00000
	3PZ	-0.00098	-0.00008	-0.00002
H55	1S	-0.06724	-0.00491	-0.00138
	2S	-0.07057	-0.01408	-0.01196
	3PX	-0.00187	-0.00078	-0.00051
	3PY	-0.00054	0.00044	-0.00001
	3PZ	0.00188	0.00007	-0.00022

Table S3. Fukui indices for primary adduct (15).



Atom	f-	f+	Atom	f-3	f+4
C 1	0,02012	0,05906	H 29	0,01492	-0,00195
C 2	0,03899	0,06518	O 30	0,02046	0,02426
C 3	0,01099	0,02853	C 31	-0,00526	-0,02294
C 4	0,01043	0,01574	N 32	0,01049	0,02903
C 5	-0,00261	0,01923	C 33	-0,00484	-0,00573
C 6	0,02187	0,03193	H 34	0,001	0,01119
C 7	-0,00436	0,11929	H 35	0,00881	0,01626
C 8	0,03047	0,00231	H 36	0,01548	0,01481
C 9	0,03258	0,15038	C 37	-0,00711	-0,00526
C 10	-0,01215	0,00441	H 38	0,01908	0,01269
O 11	0,04142	0,04572	C 39	-0,01787	-0,02344
N 12	0,10627	0,01624	C 40	0,00251	0,00996
C 13	0,03904	-0,01923	C 41	-0,00666	-0,00474
C 14	0,05336	0,00903	C 42	0,00938	0,00971
C 15	0,00939	0,00987	H 43	0,00229	0,00363
C 16	0,11815	0,03199	C 44	0,00566	0,00192
C 17	0,00896	0,00851	H 45	-0,00577	-0,00654
C 18	0,05307	0,01145	C 46	0,01492	0,01313
O 19	0,01367	0,12553	H 47	0,01033	0,01076
H 20	0,0163	0,02895	H 48	0,00783	0,00534
H 21	0,01697	0,02944	H 49	0,01095	0,01057
H 22	0,01261	0,02319	N 50	0,08501	-0,00416
H 23	0,00974	0,02575	H 51	0,01837	0,01355
H 24	0,01507	-0,00577	C 52	-0,00872	-0,00168
H 25	0,02239	-0,00127	H 53	0,01587	0,01164
H 26	0,02813	0,01268	H 54	0,02531	0,01186
H 27	0,02617	0,01468	H 55	-0,0062	-0,01353
H 28	0,02671	0,01224			

Table S4. Relative energies of the intermediates of the Michael-retro-Michael rearrangement affording product (11), calculated at B3LYP/6-31+g(d) level of theory.

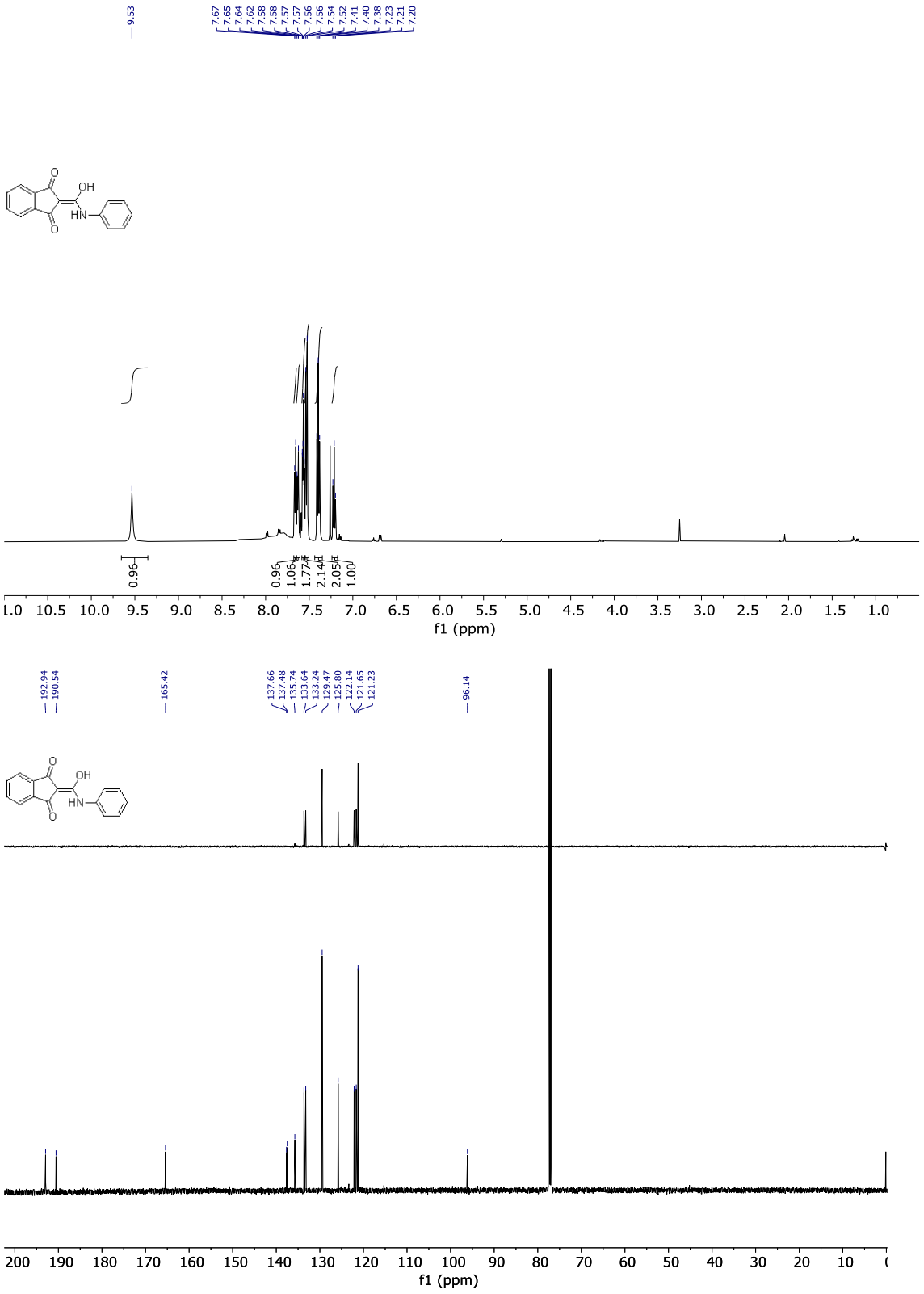
	Primary adduct (15)	**Spirane-*SR* (16a)**	**Spirane-*SS* (16b)**	**Product (11)**
ΔG (kcal/mol)	0.0	0.48	-2.81	-22.82

Matrices XYZ for computationally derived structures.

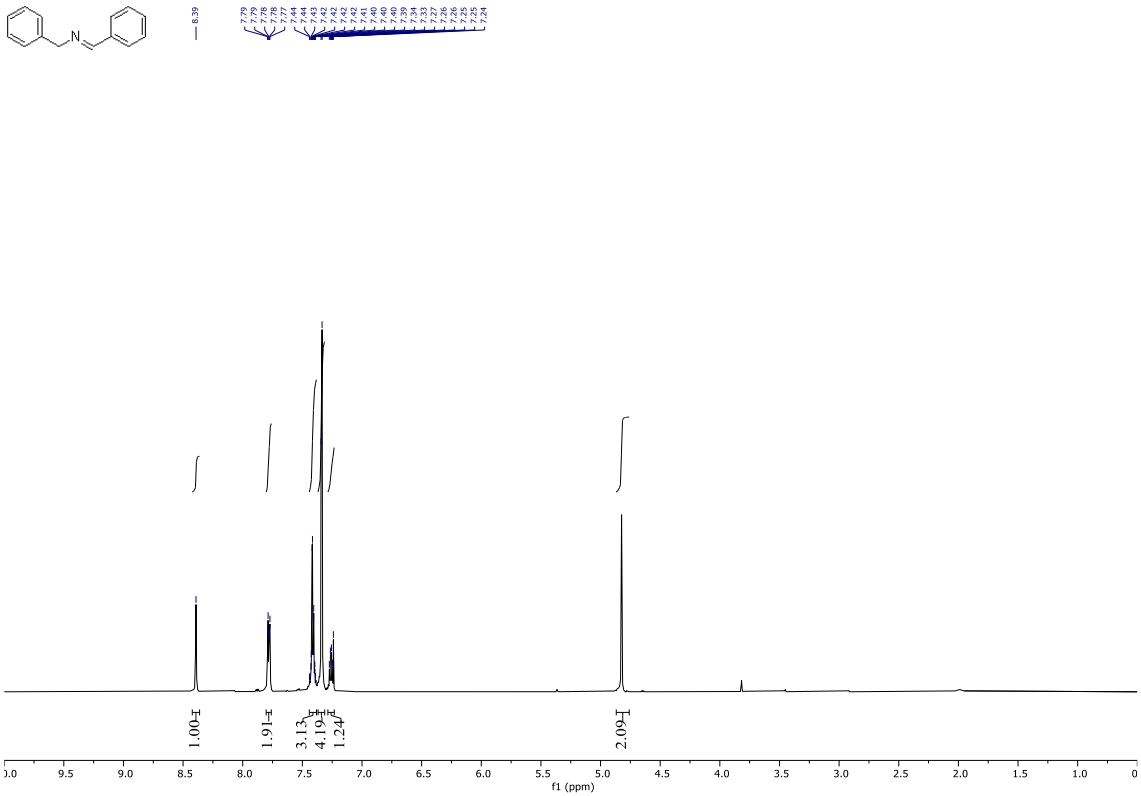
The xyz matrices for the computationally derived structures of primary adduct (**15**), spirane-*SR* (**16a**) spirane-*SS* and indandione derivative (**11**) can be founded in the zip folder.

Spectra

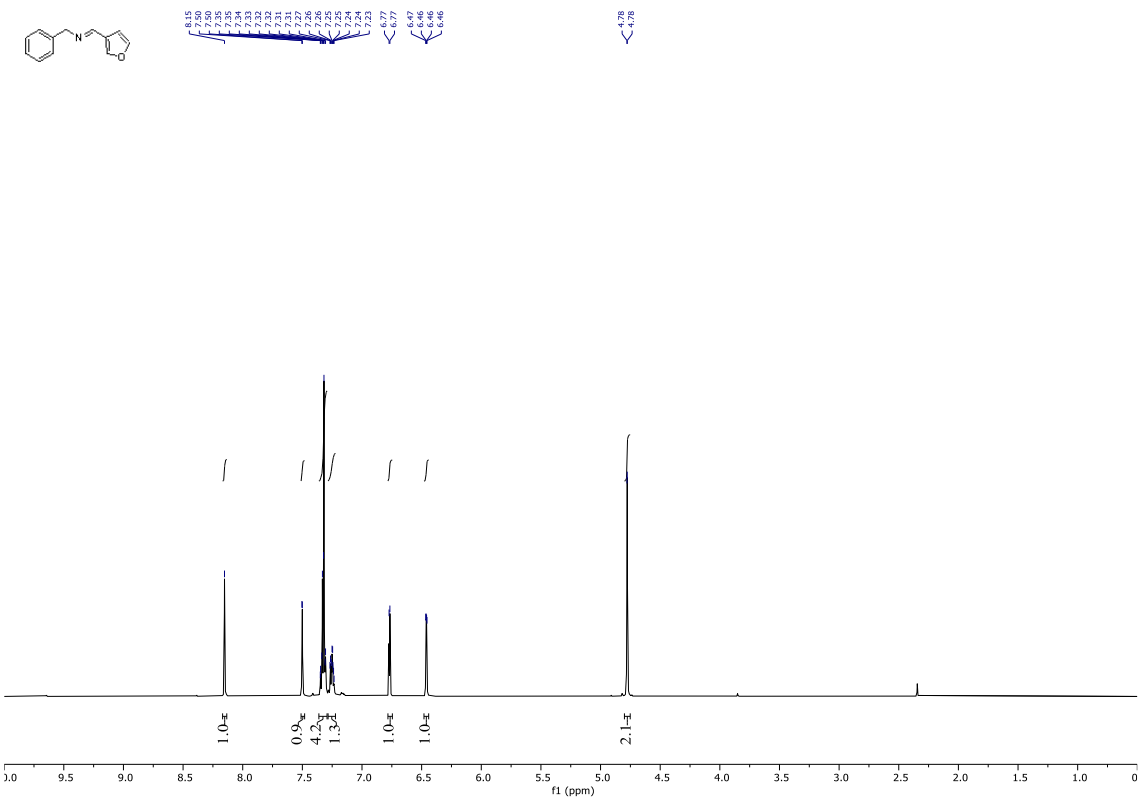
2-(Hydroxy(phenylamino)methylene)-1*H*-indene-1,3(2*H*)-dione (10)



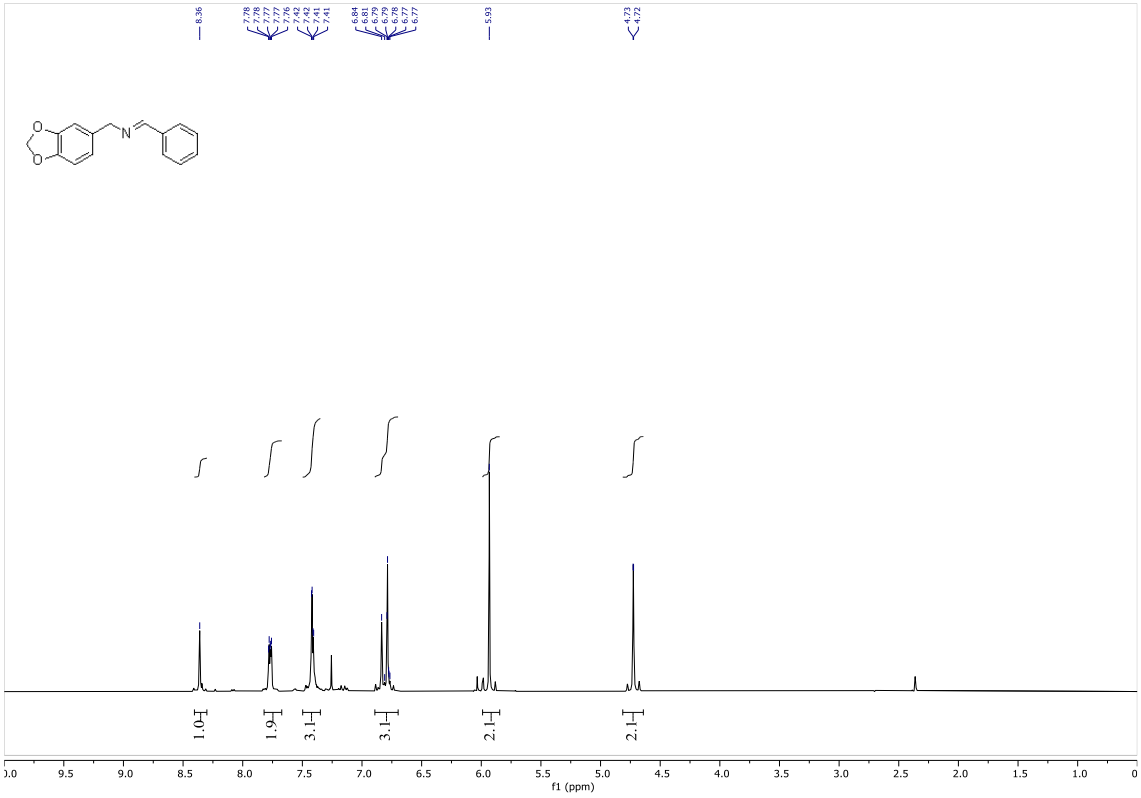
(*E*)-*N*-benzyl-1-phenylmethanimine (3a)



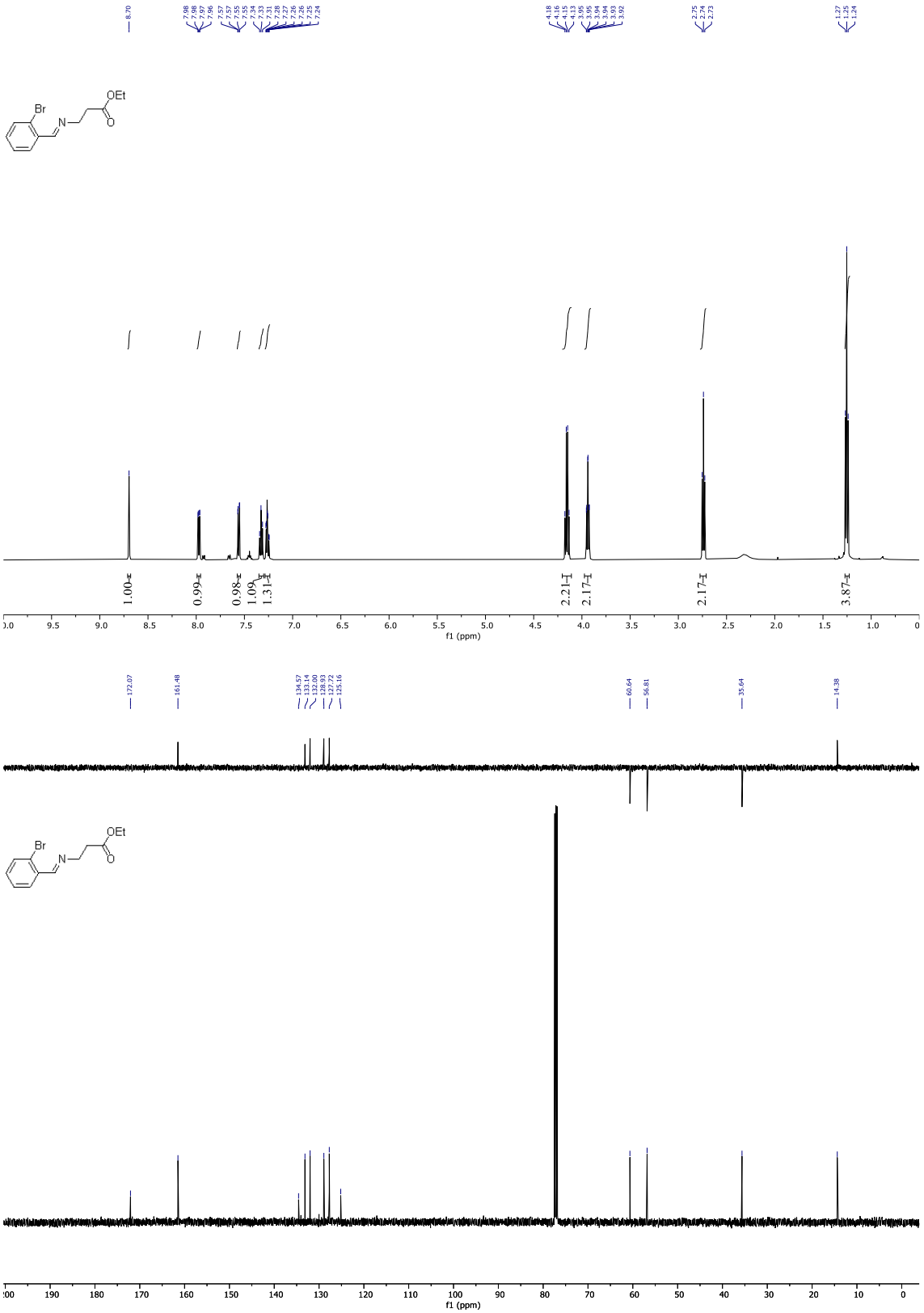
(*E*)-*N*-benzyl-1-(furan-2-yl)methanimine (3b)



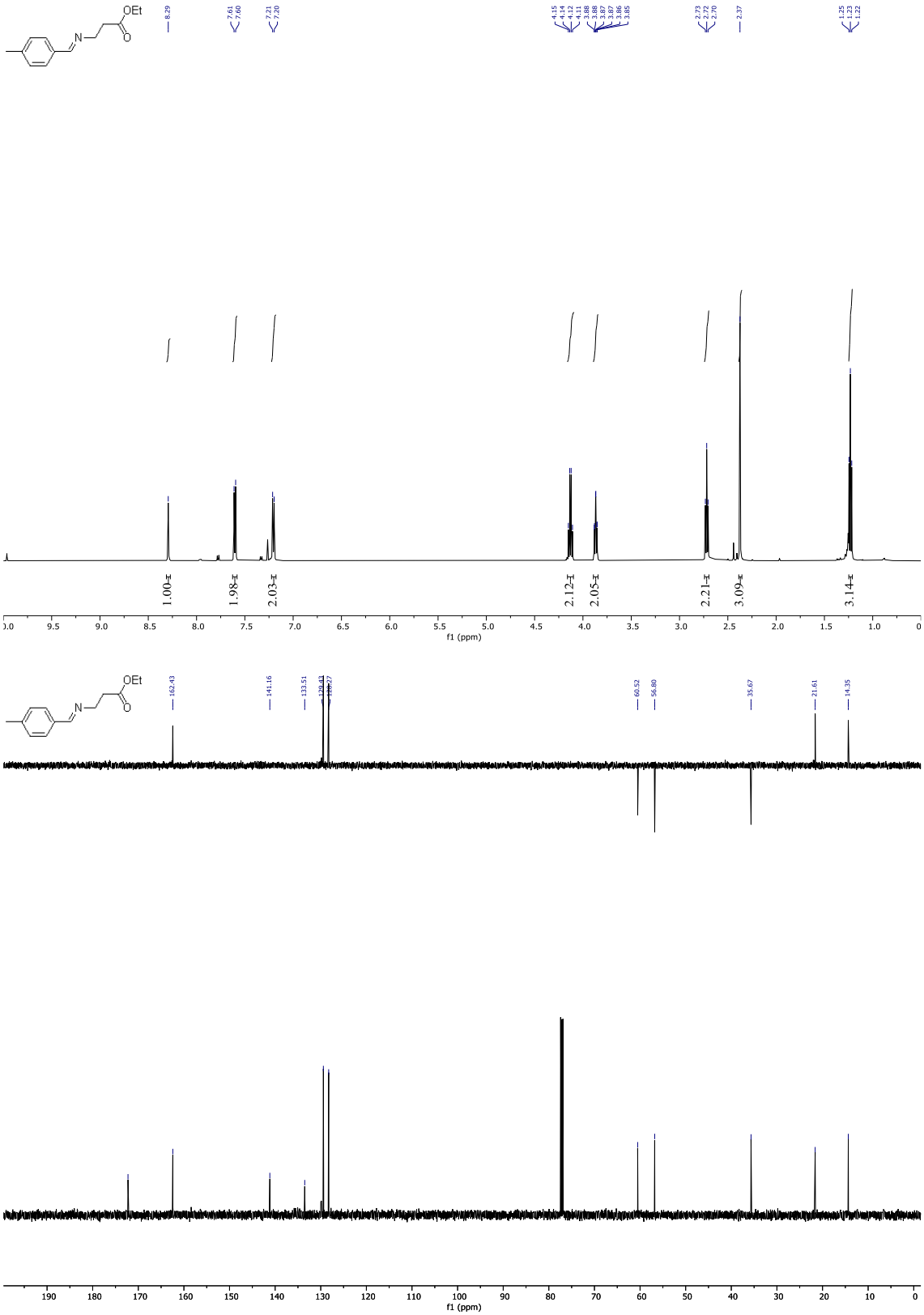
(E)-*N*-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-1-phenylmethanimine (3c)



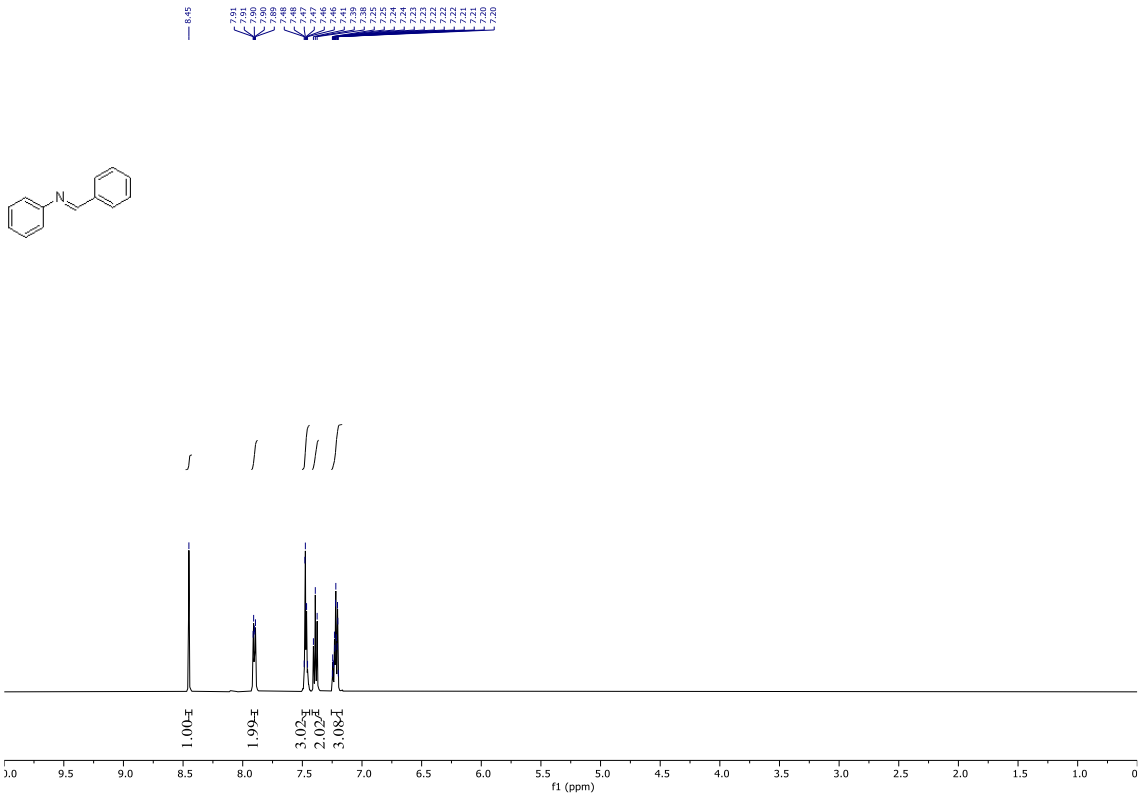
Ethyl (*E*)-3-((2-bromobenzylidene)amino)propanoate (3d)



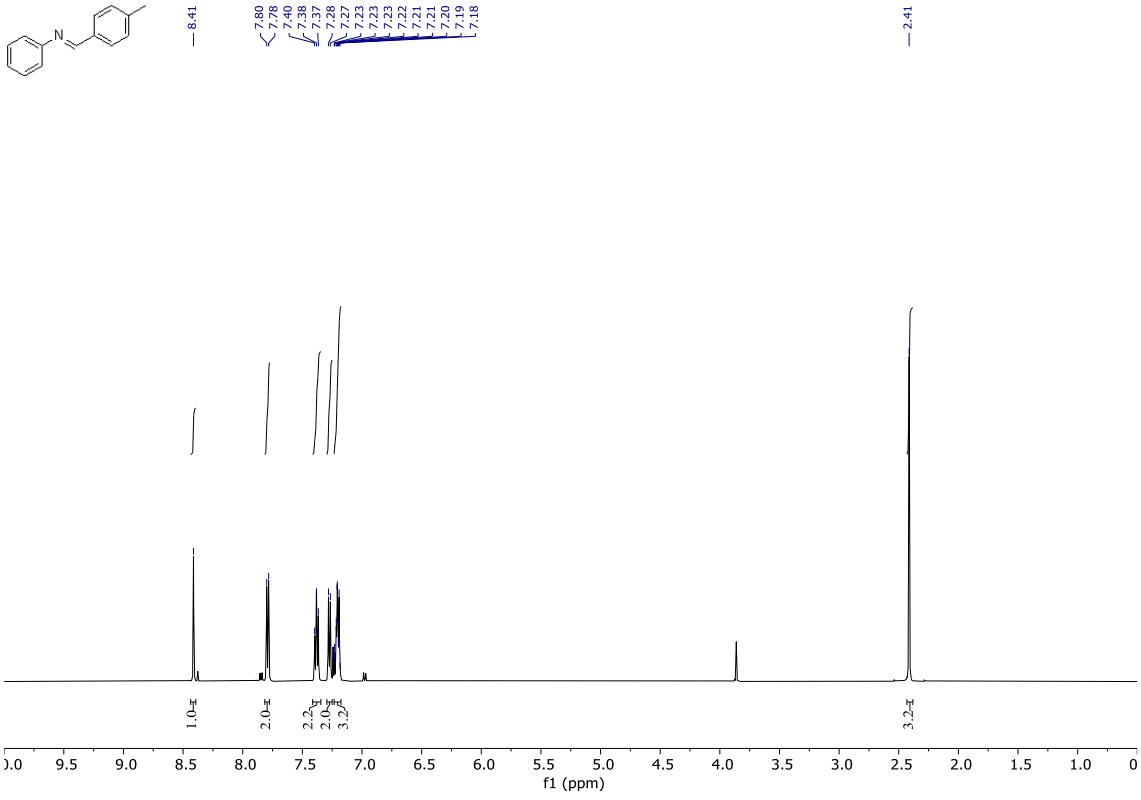
Ethyl (*E*)-3-((4-methylbenzylidene)amino)propanoate (3e)



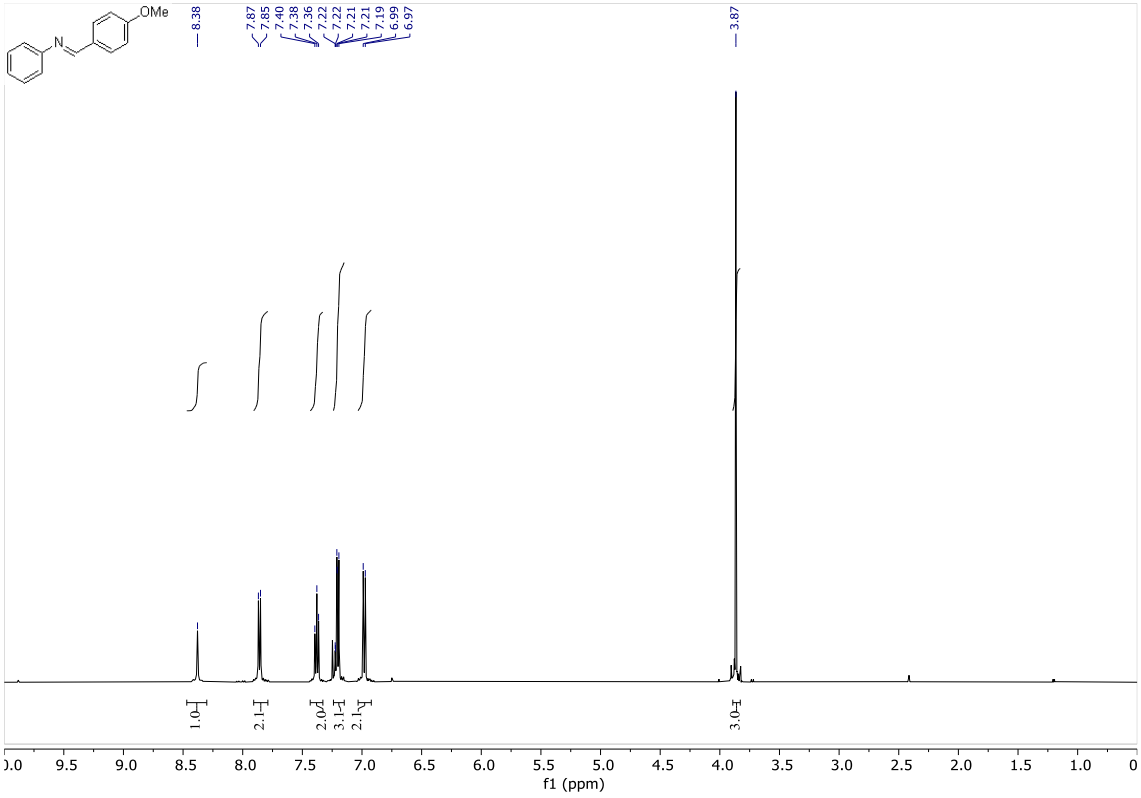
(*E*)-*N*,1-Diphenylmethanimine (3f)



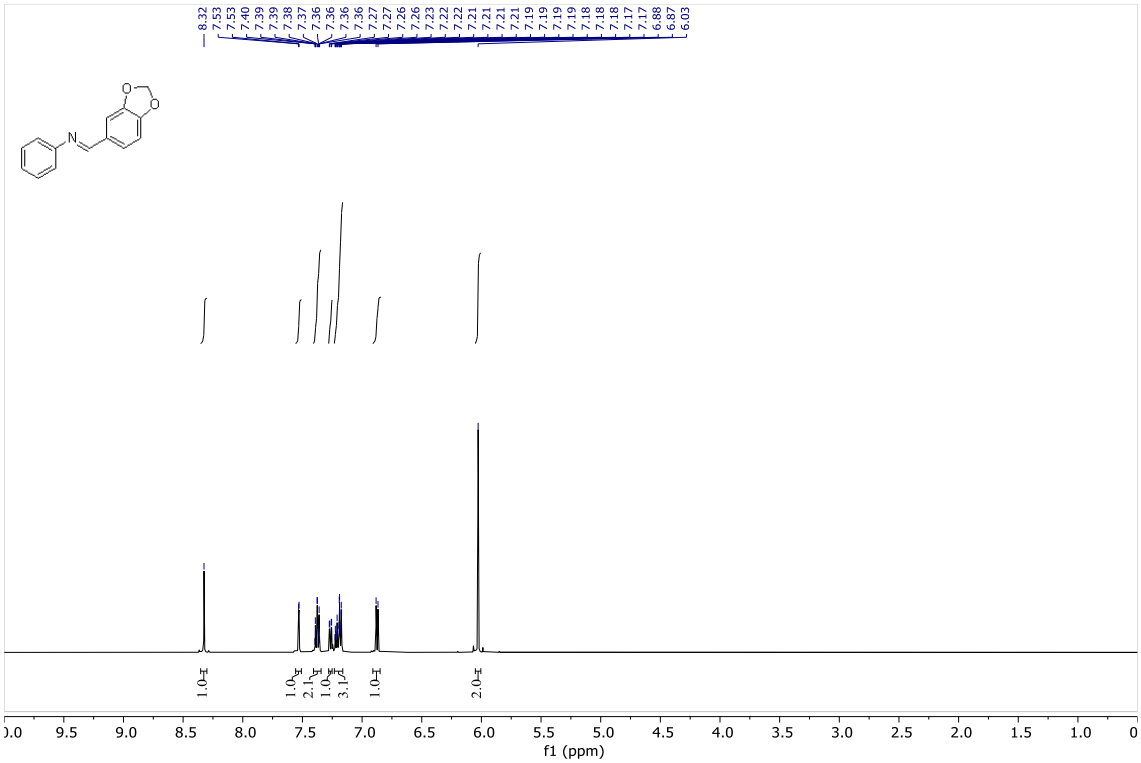
(*E*)-*N*-Phenyl-1-(*p*-tolyl)methanimine (3g)



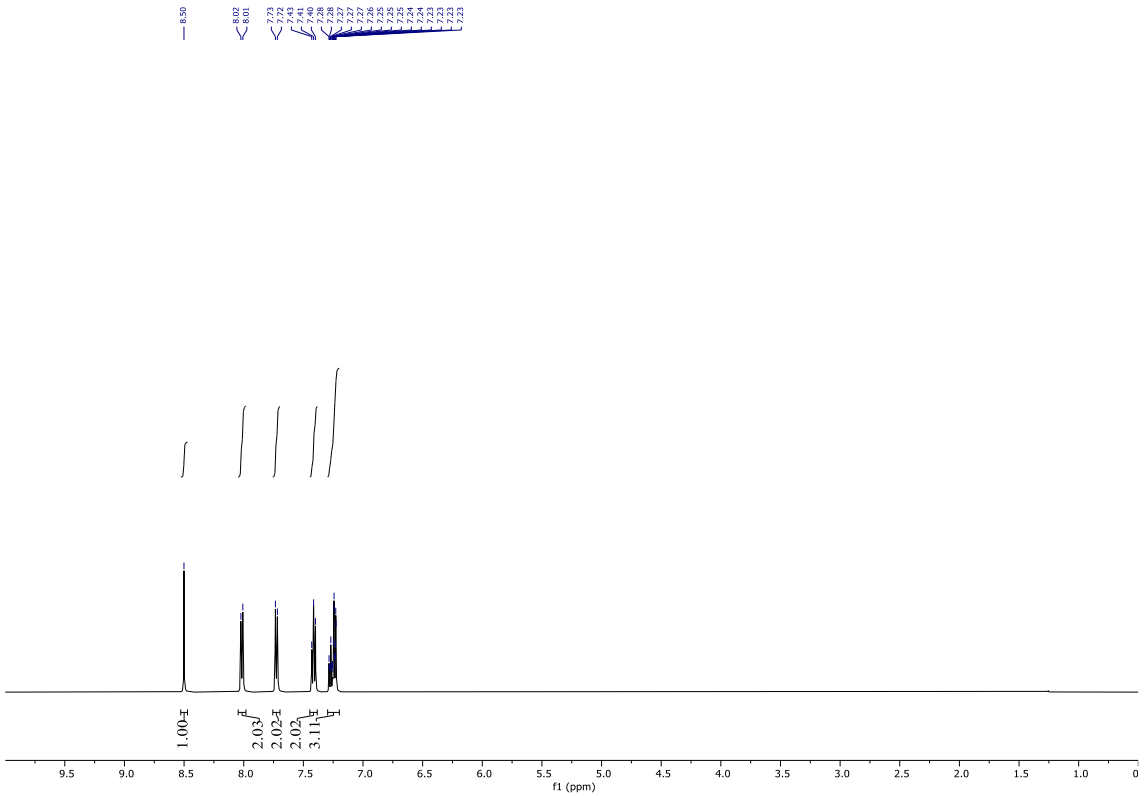
(*E*)-1-(4-Methoxyphenyl)-*N*-phenylmethanimine (3h)



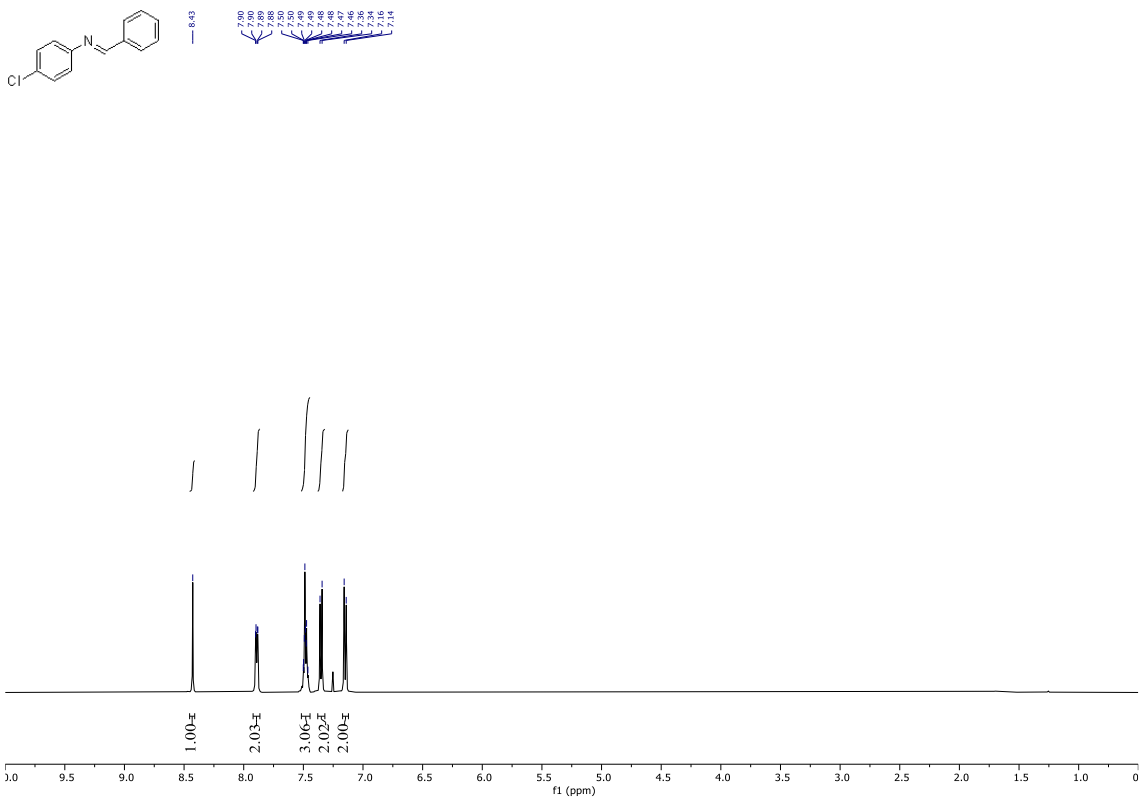
(*E*)-1-(Benzo[*d*][1,3]dioxol-5-yl)-*N*-phenylmethanimine (3i)



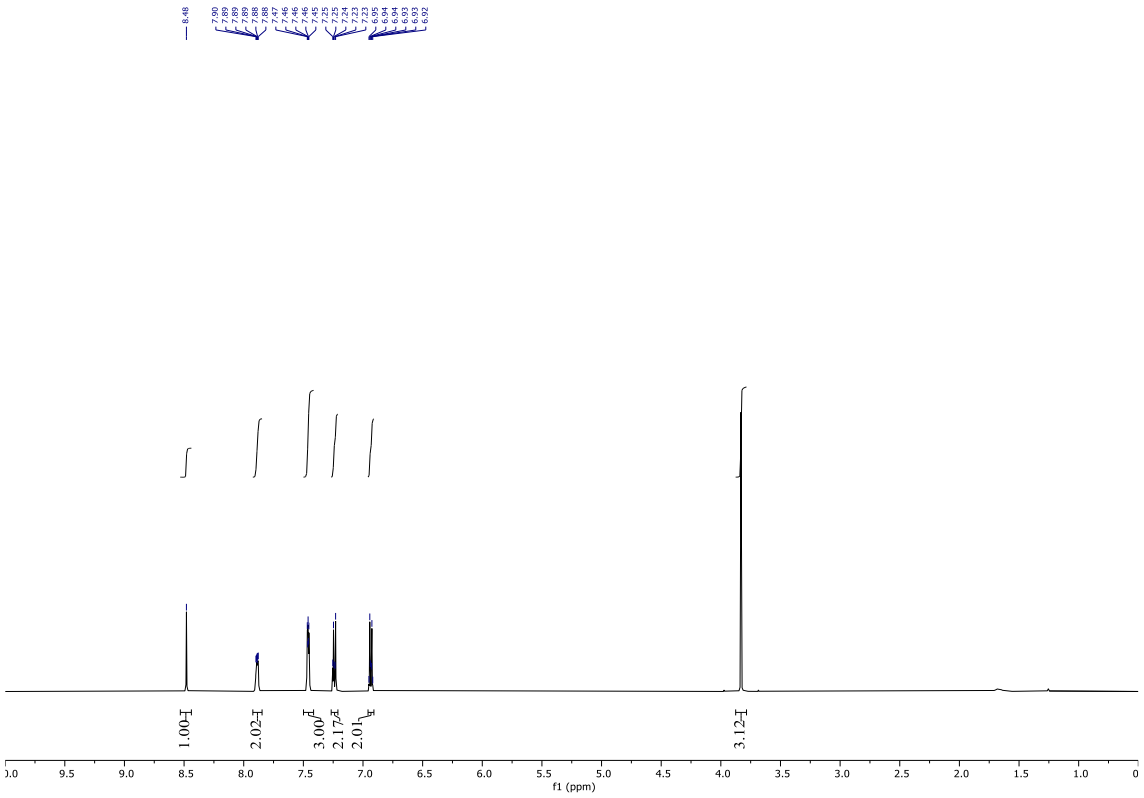
(*E*)-*N*-Phenyl-1-(4-(trifluoromethyl)phenyl)methanimine (3j)



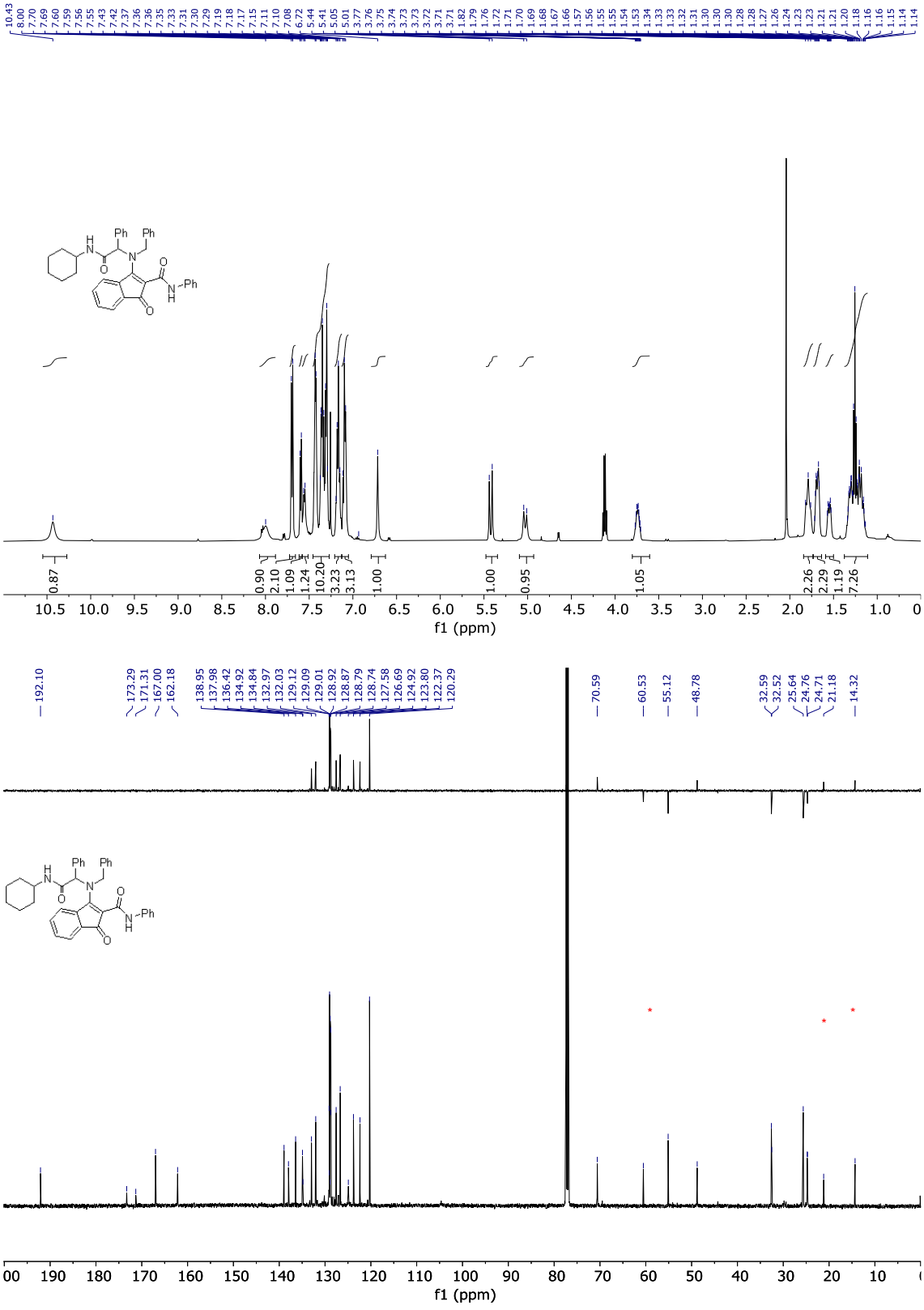
(*E*)-*N*-(4-Chlorophenyl)-1-phenylmethanimine (3k)



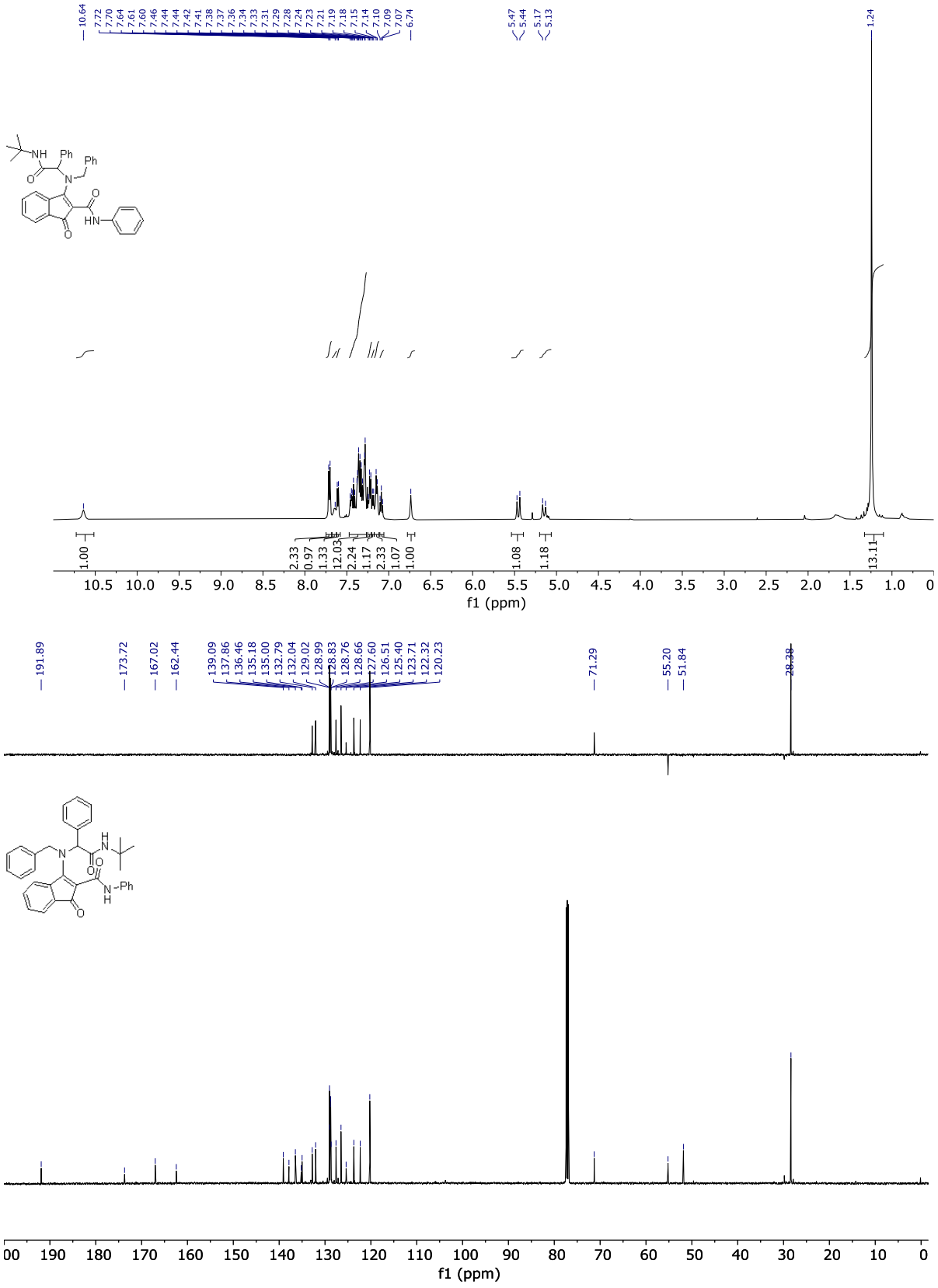
(*E*)-*N*-(4-Methoxyphenyl)-1-phenylmethanimine (3l)



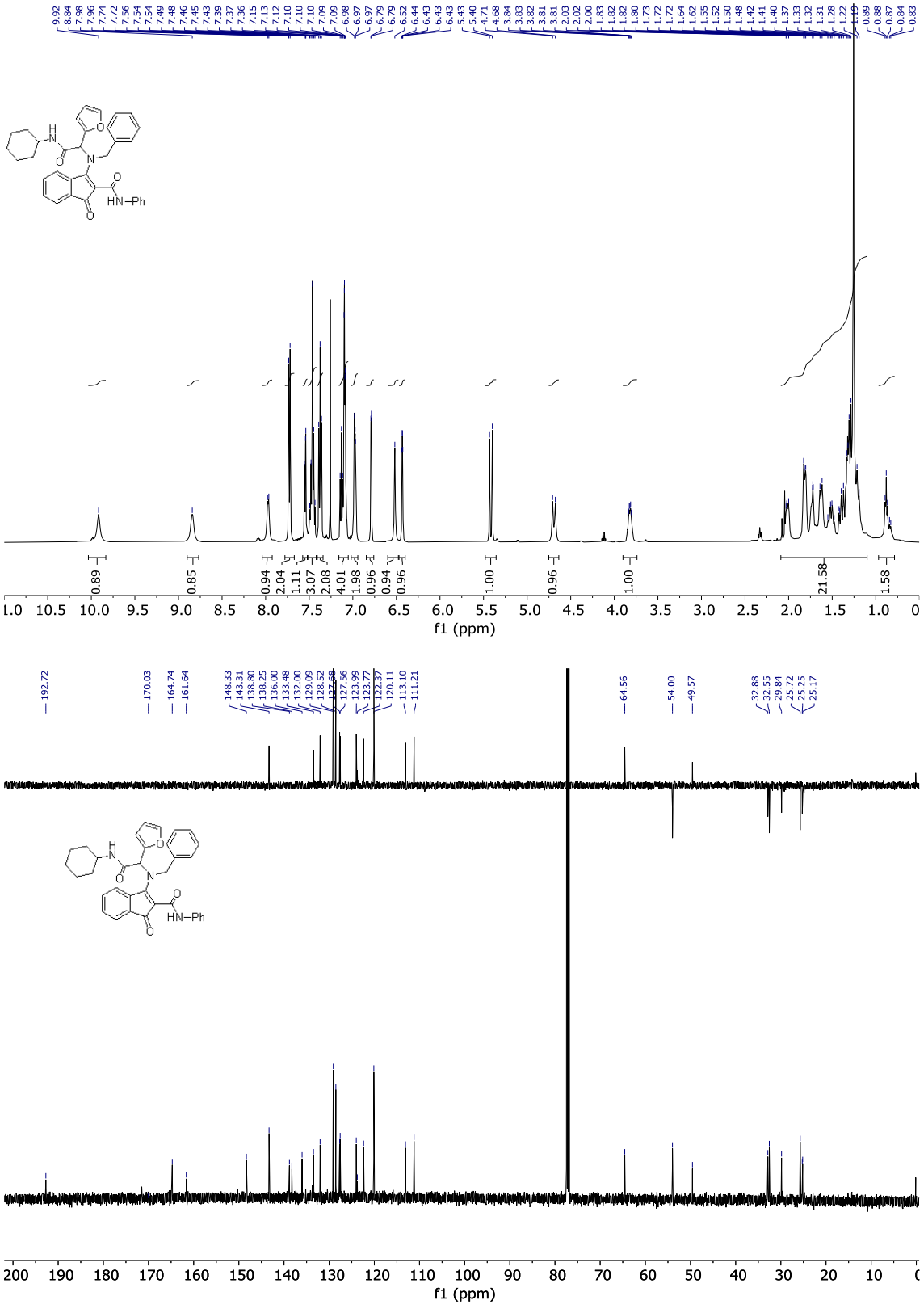
3-(Benzyl(2-(cyclohexylamino)-2-oxo-1-phenylethyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11a)



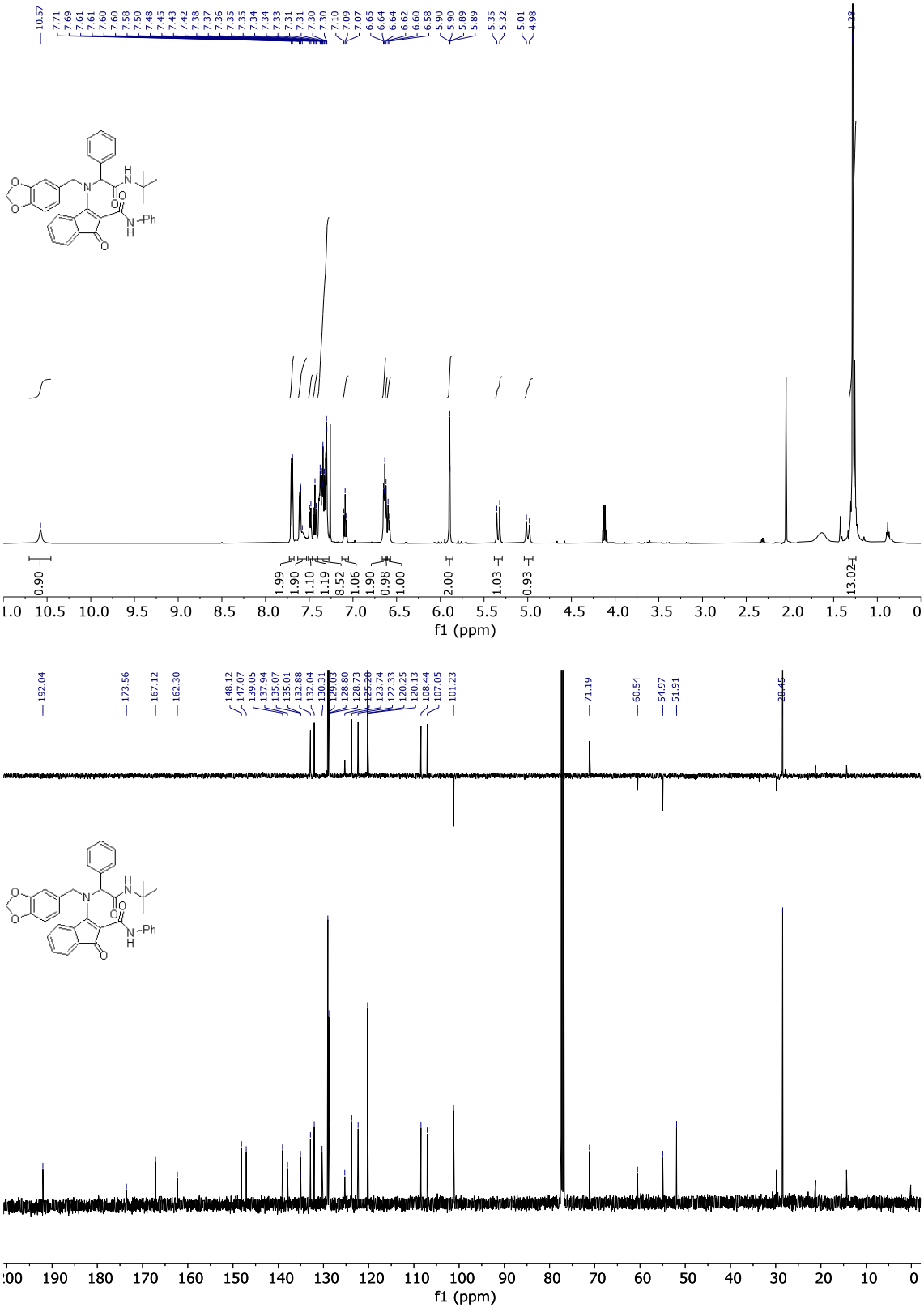
3-(Benzyl(2-(*tert*-butylamino)-2-oxo-1-phenylethyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11b)



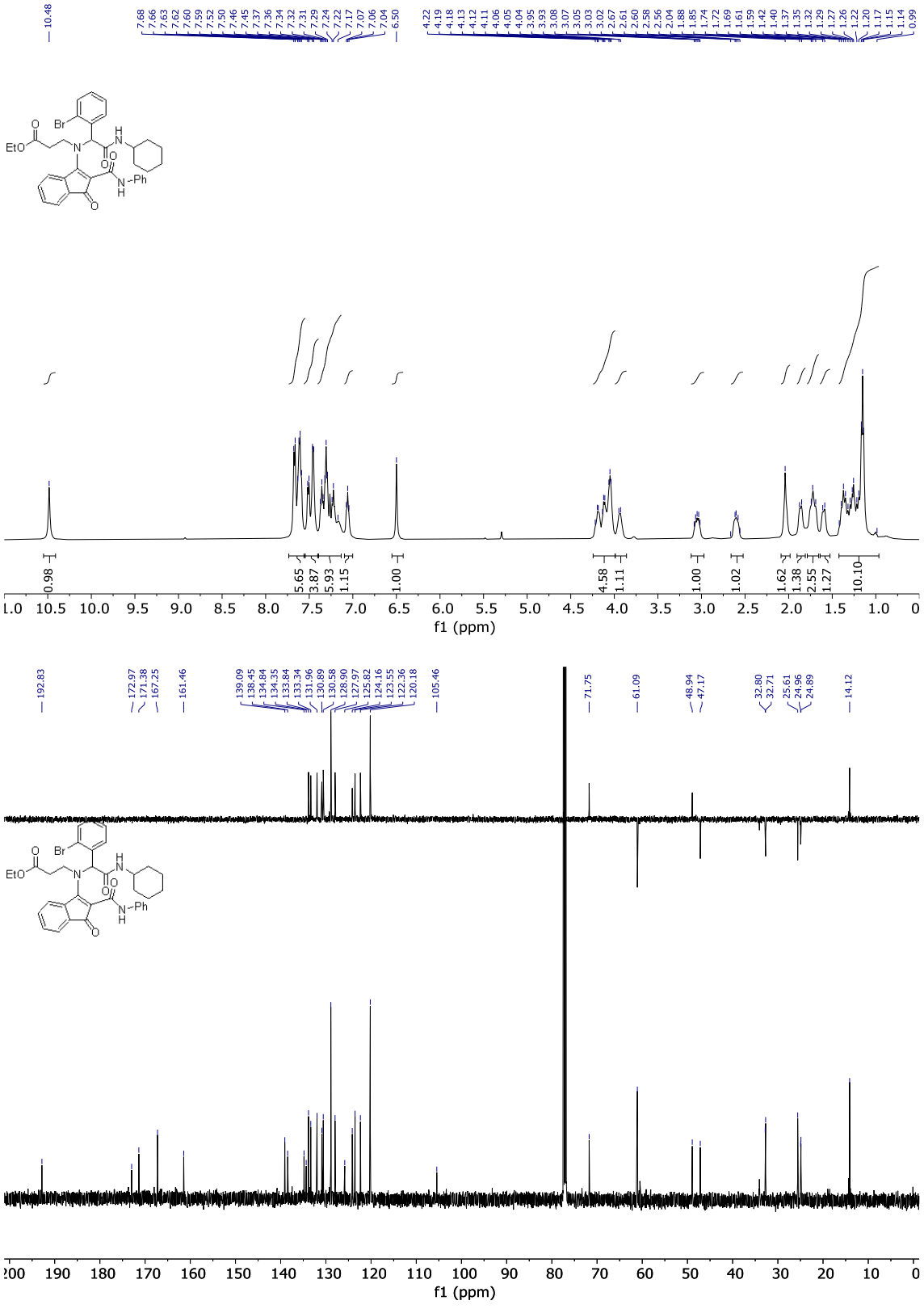
3-(Benzyl(2-(cyclohexylamino)-1-(furan-2-yl)-2-oxoethyl)amino)-1-oxo-*N*-phenyl-1H-indene-2-carboxamide (11c)



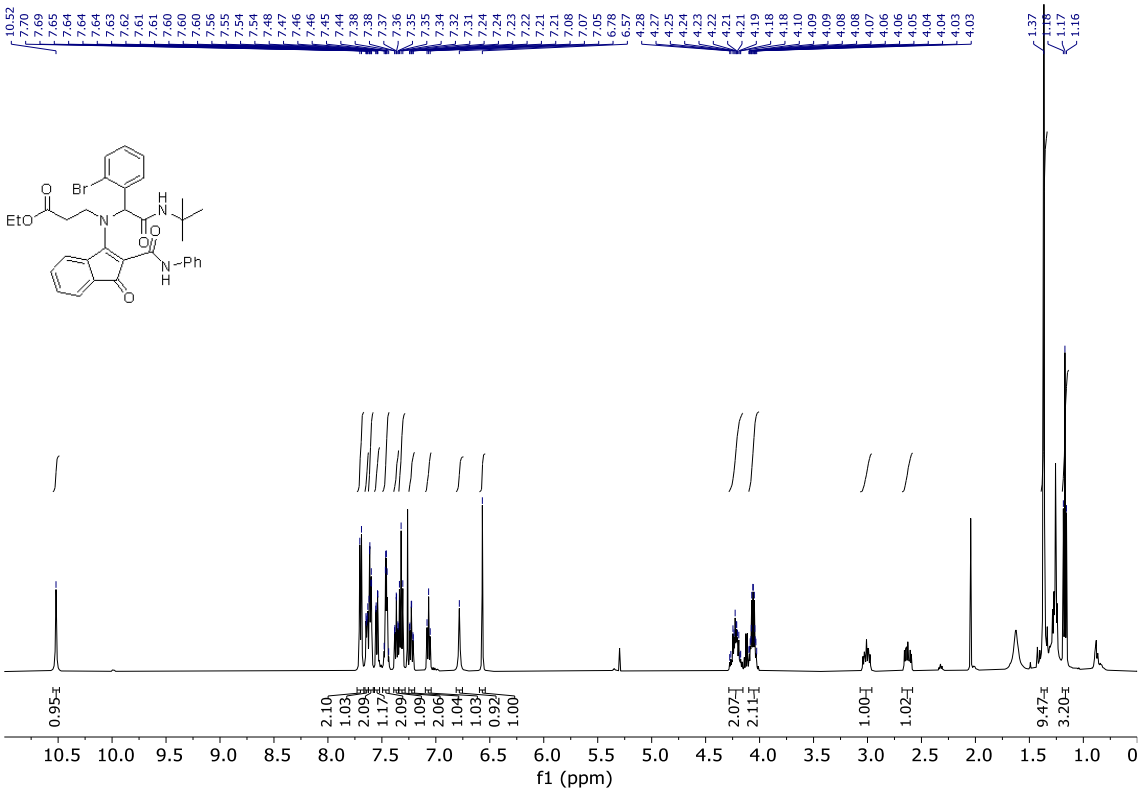
3-((Benzo[*d*][1,3]dioxol-5-ylmethyl)(2-(*tert*-butylamino)-2-oxo-1-phenylethyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11d)

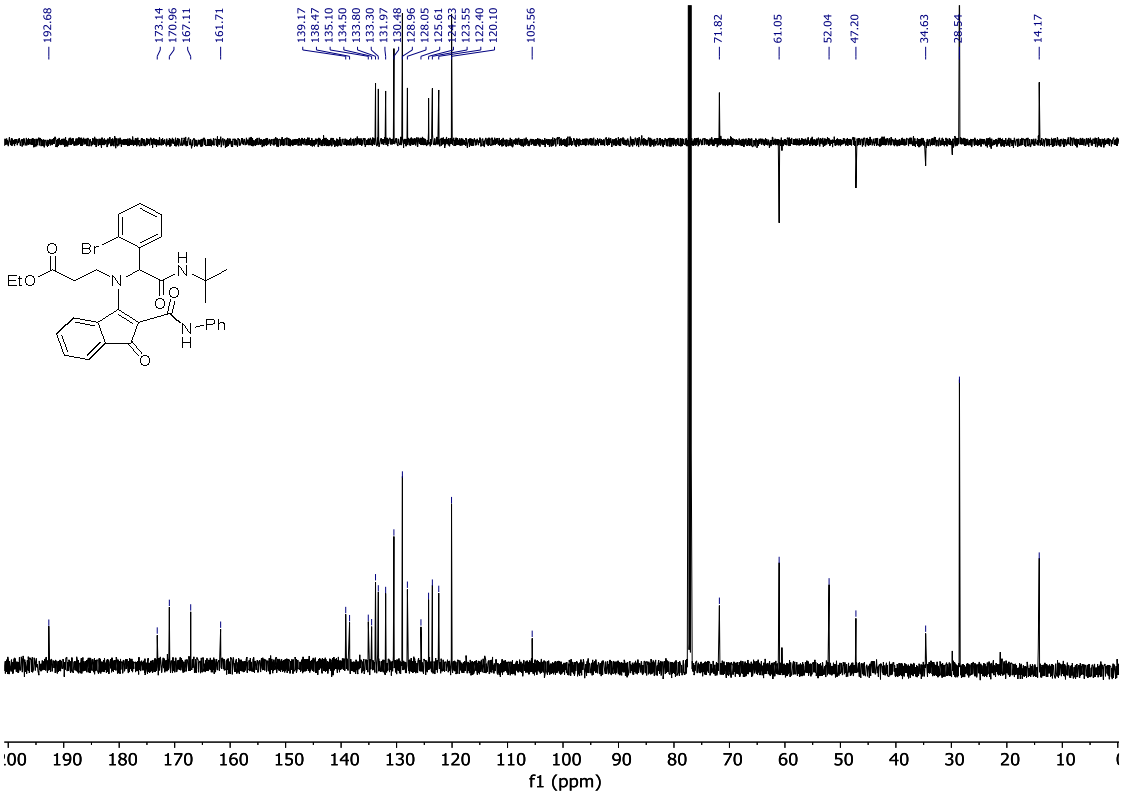


Ethyl 3-((1-(2-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl)(1-oxo-2-(phenylcarbamoyl)-1*H*-inden-3-yl)amino)propanoate (11e)

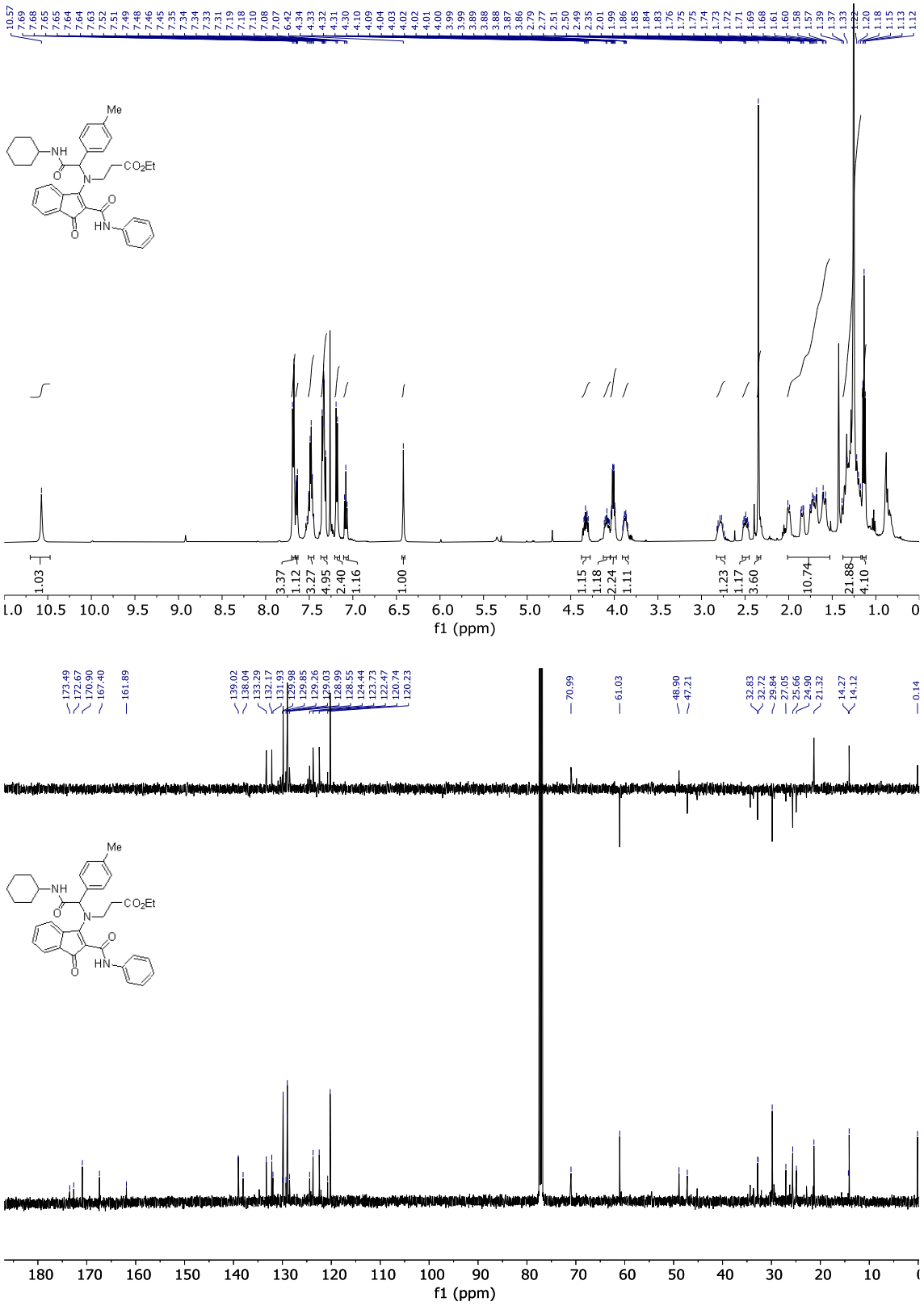


Ethyl 3-((1-(2-bromophenyl)-2-(*tert*-butylamino)-2-oxoethyl)(1-oxo-2-(phenylcarbamoyl)-1*H*-inden-3-yl)amino)propanoate (11f)

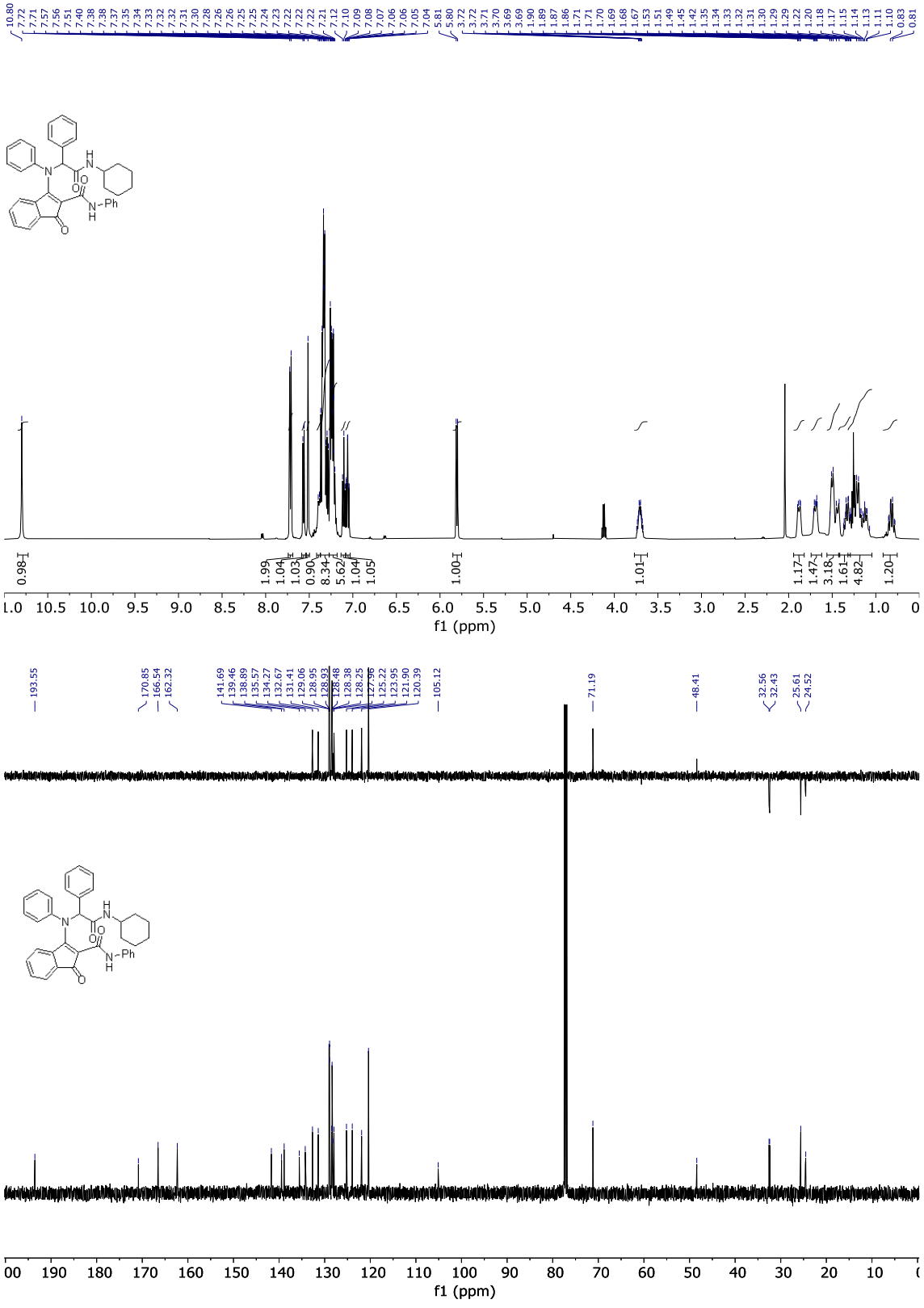




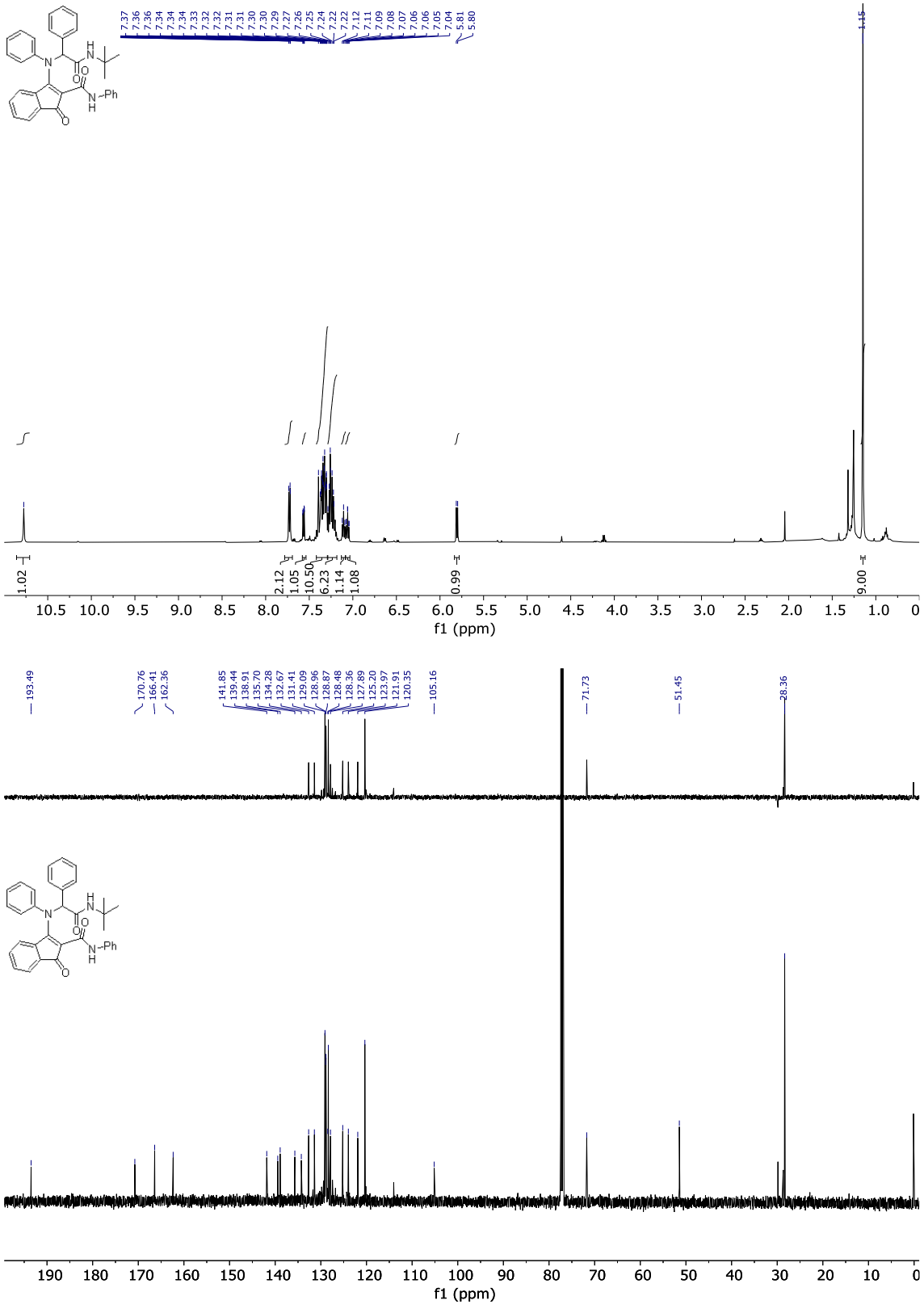
Ethyl 3-((2-(cyclohexylamino)-2-oxo-1-(*p*-tolyl)ethyl)(1-oxo-2-(phenylcarbamoyl)-1*H*-inden-3-yl)amino)propanoate (11g)



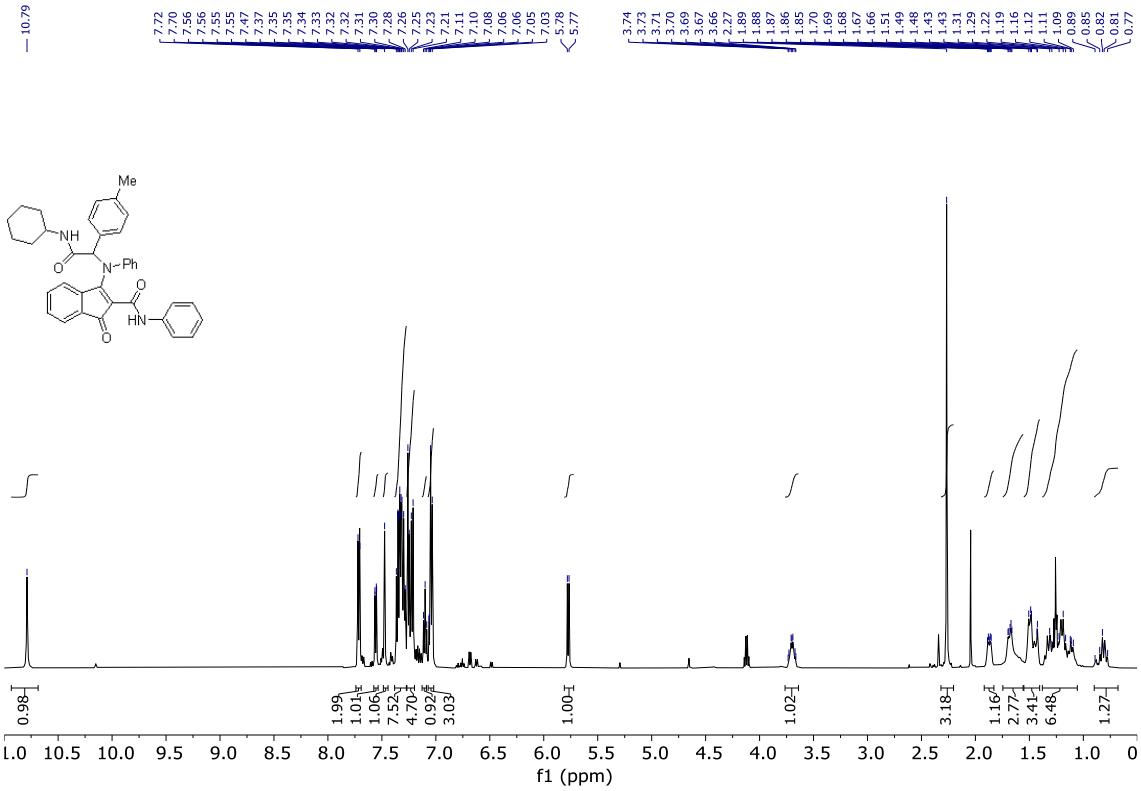
3-((2-(Cyclohexylamino)-2-oxo-1-phenylethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11h)

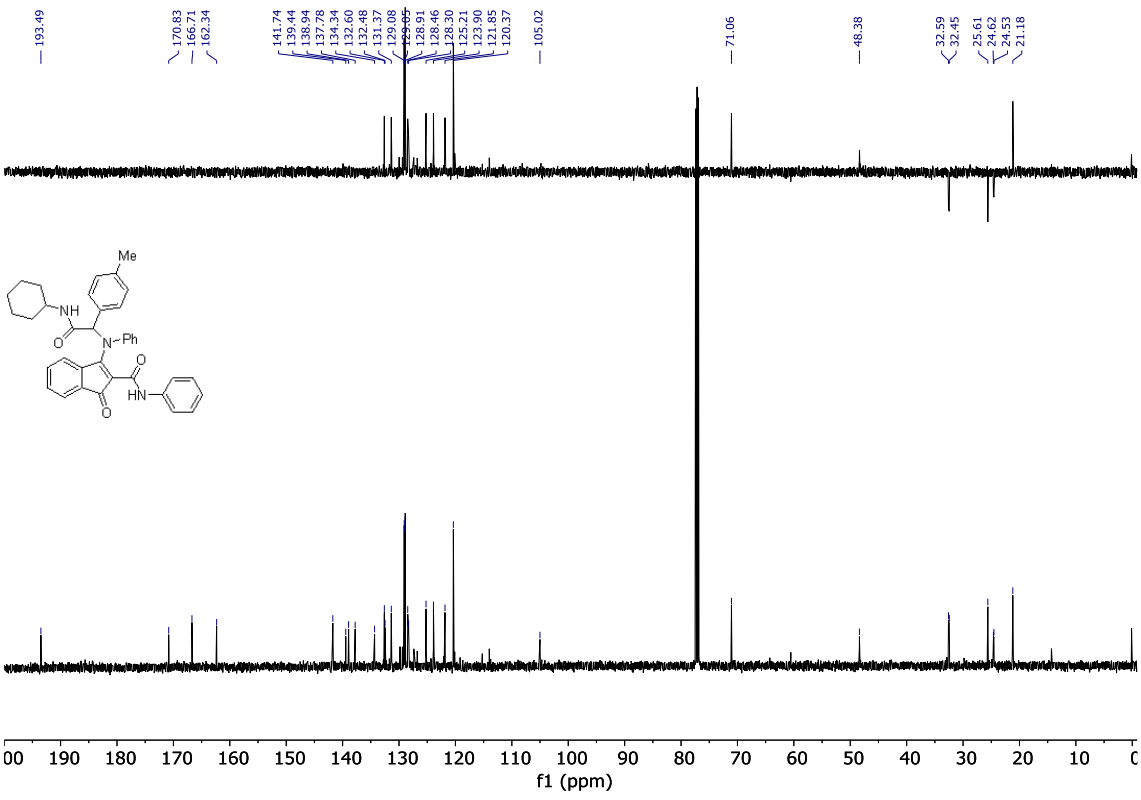


3-((2-(*tert*-Butylamino)-2-oxo-1-phenylethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11i)

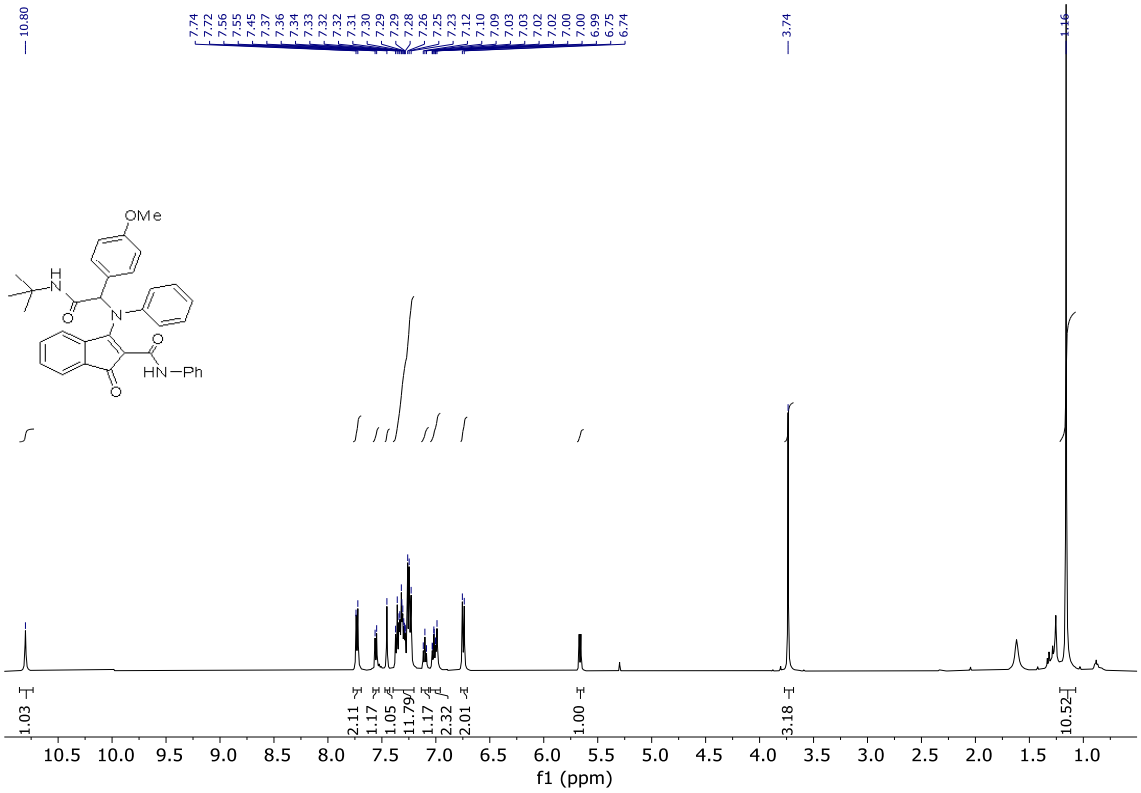


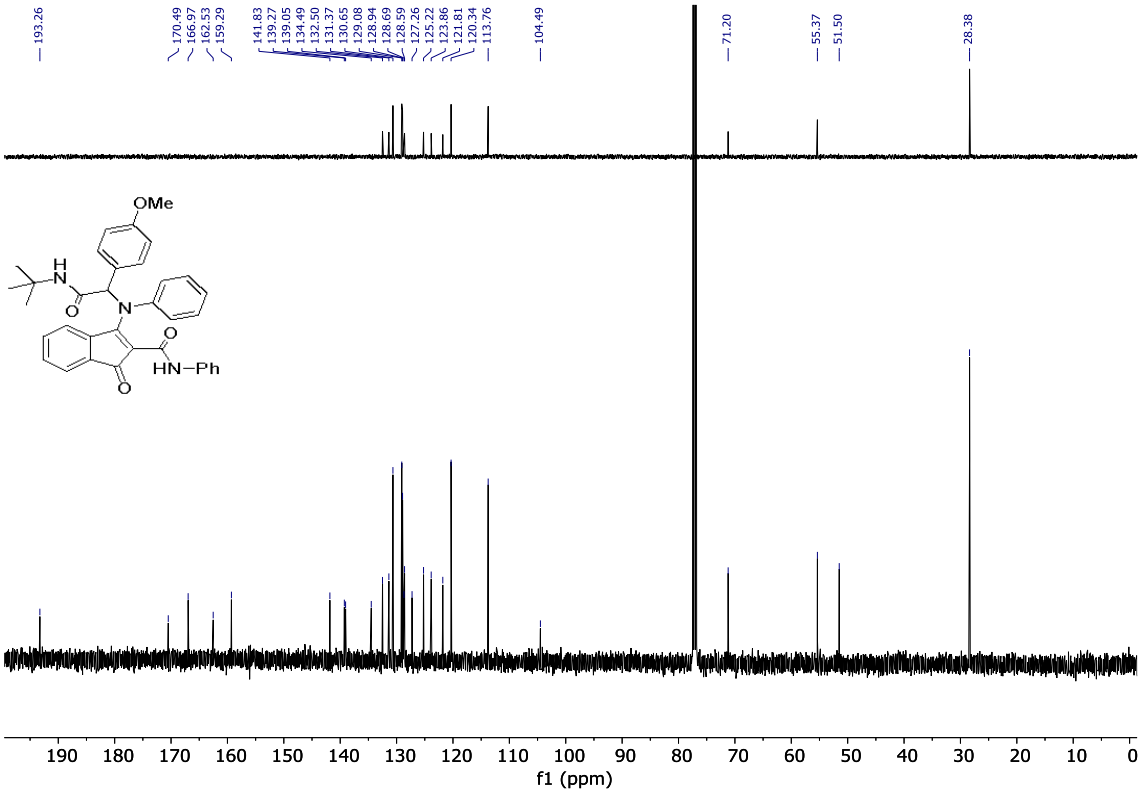
3-((2-(Cyclohexylamino)-2-oxo-1-(*p*-tolyl)ethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11j)



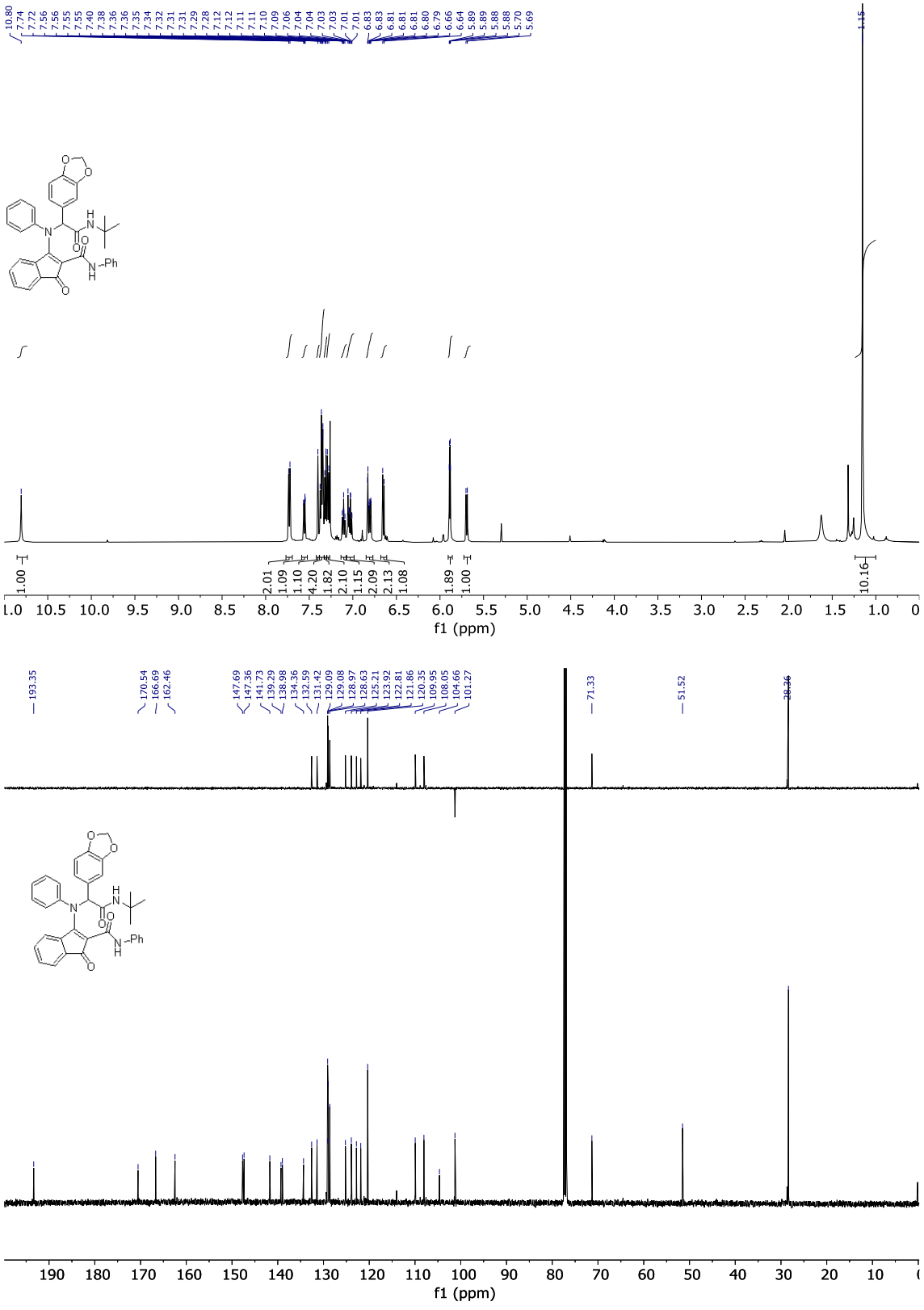


3-((2-(*tert*-Butylamino)-1-(4-methoxyphenyl)-2-oxoethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11k)

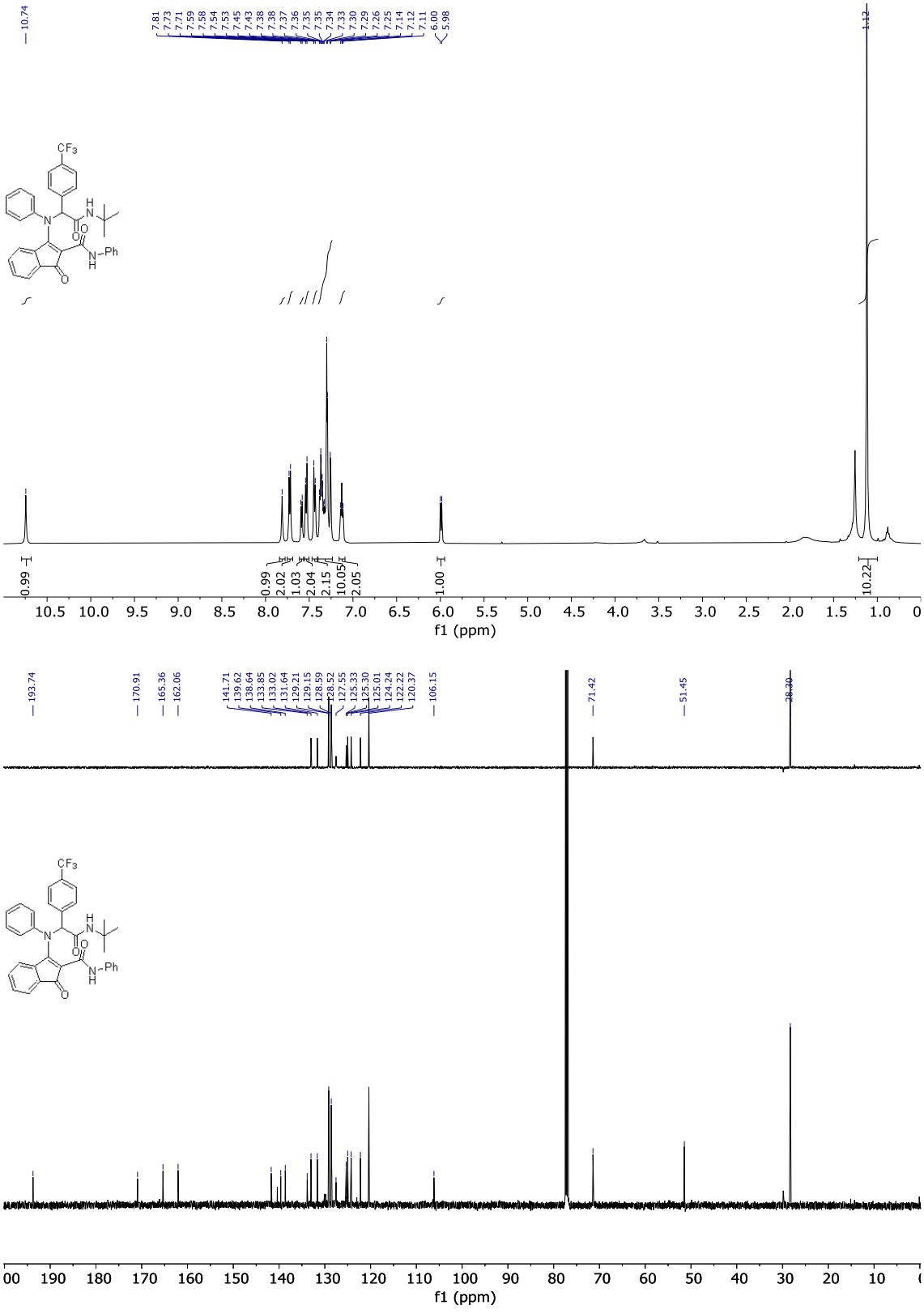




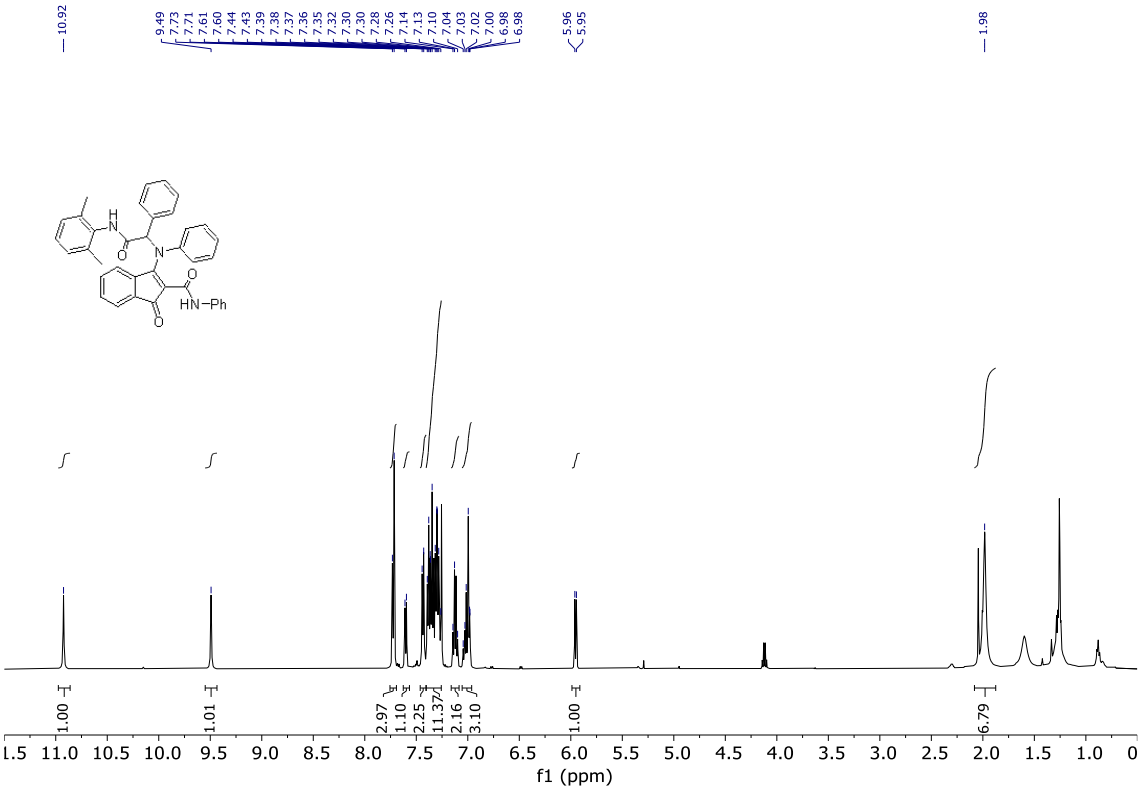
3-((1-(Benzo[*d*][1,3]dioxol-5-yl)-2-(*tert*-butylamino)-2-oxoethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11l)

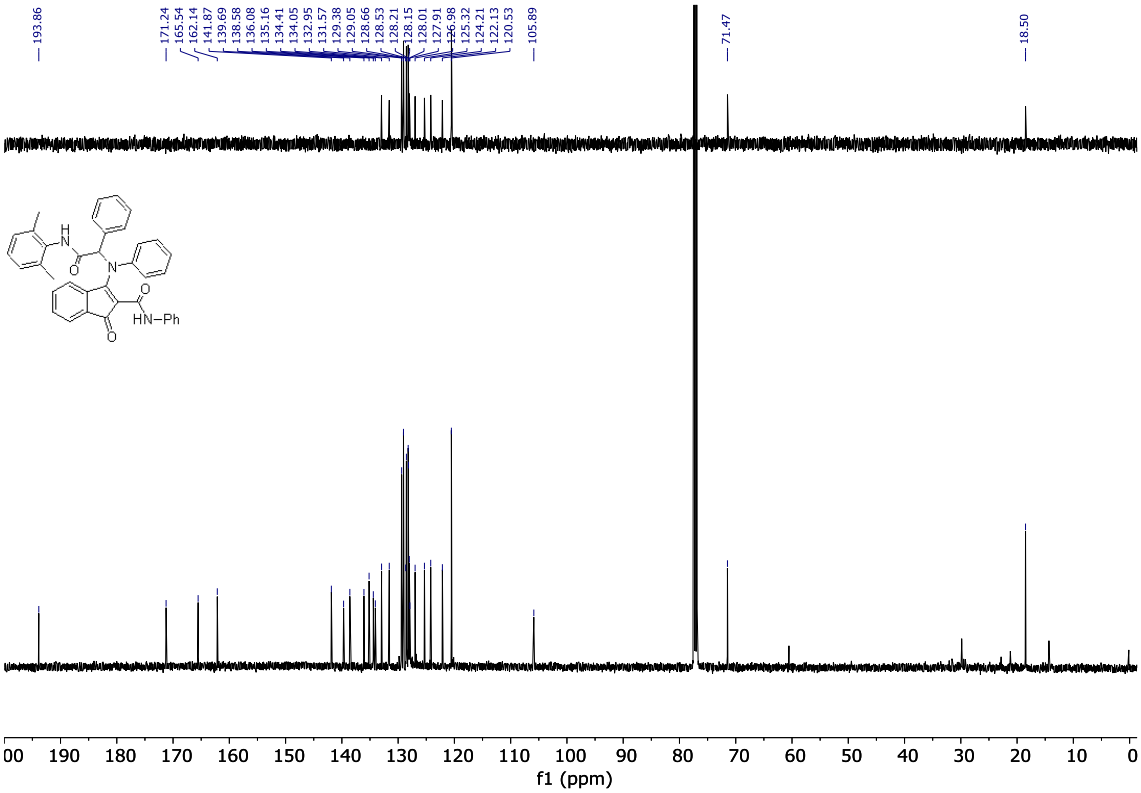


3-(Benzyl(1-(*tert*-butylamino)-3-methyl-1-oxobutan-2-yl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11m)

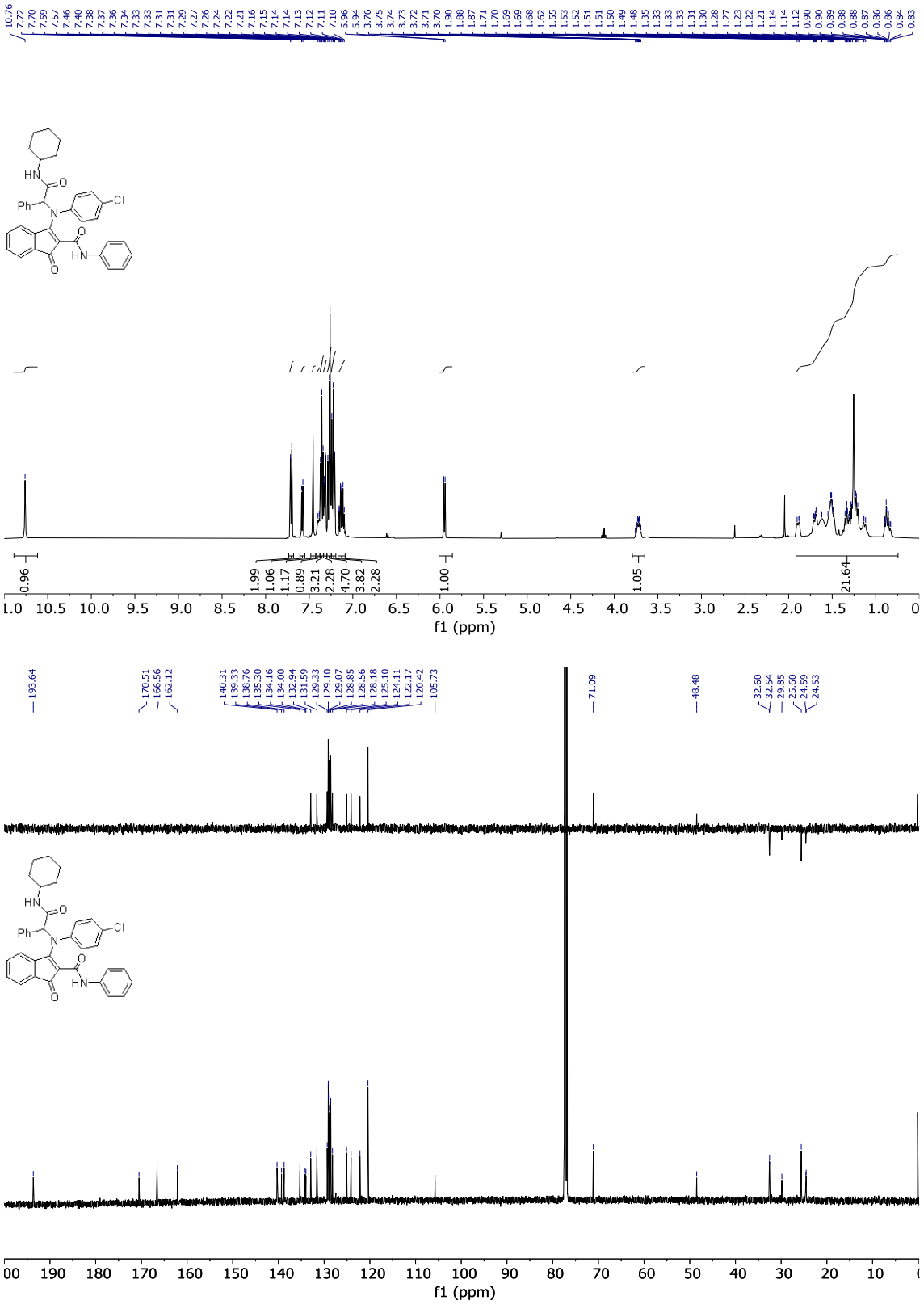


3-((2-((2,6-Dimethylphenyl)amino)-2-oxo-1-phenylethyl)(phenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11n)

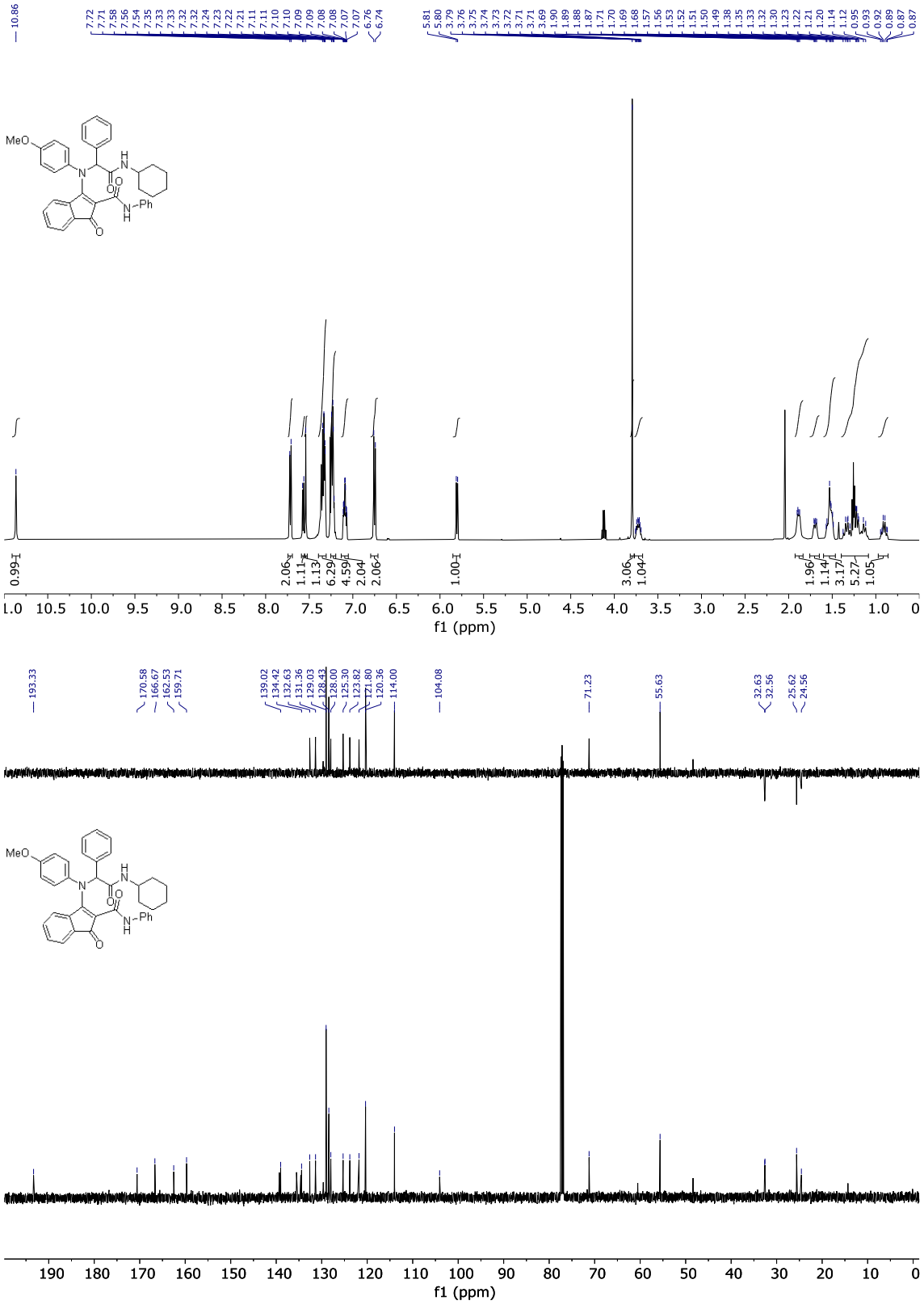




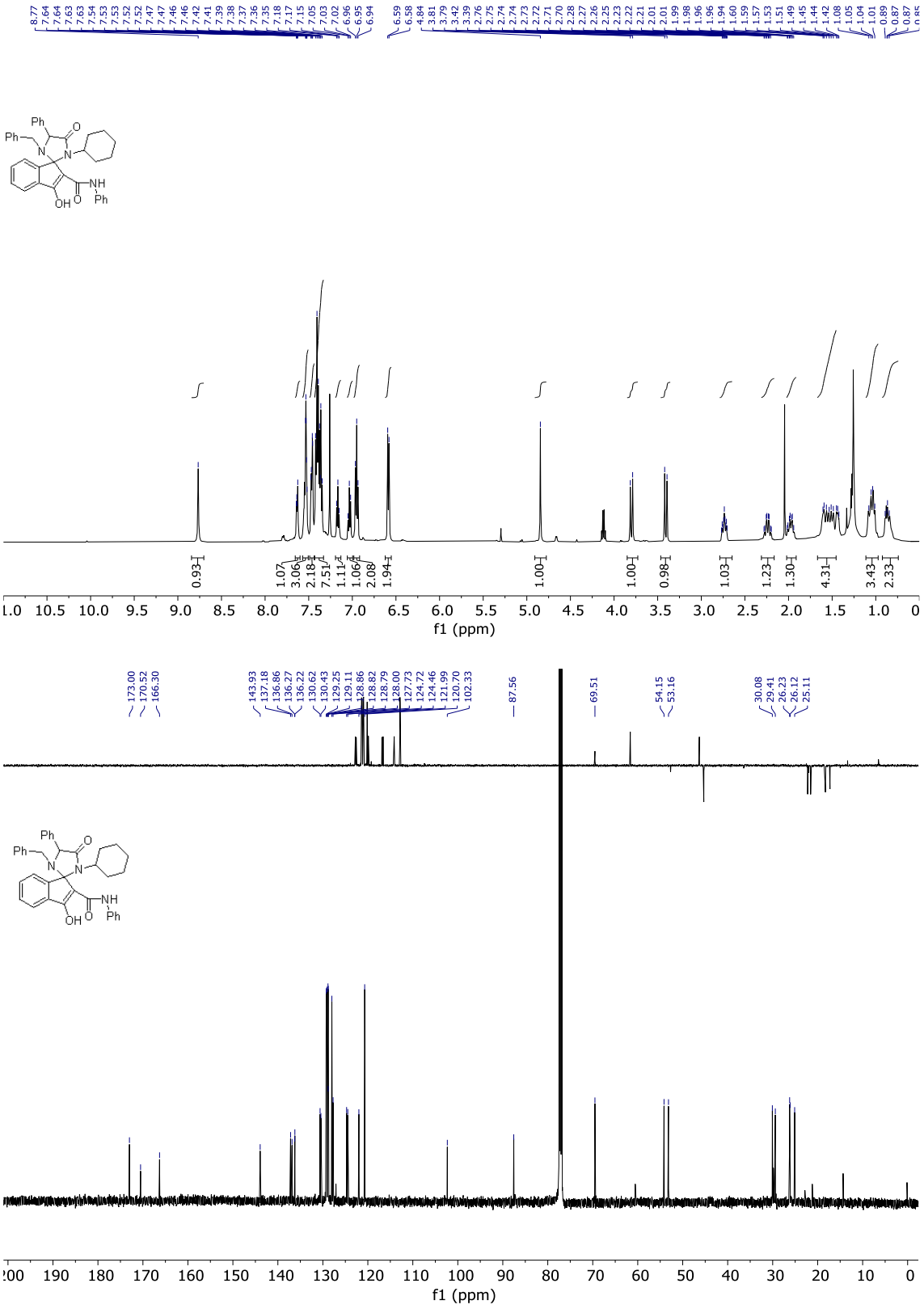
3-((4-Chlorophenyl)(2-(cyclohexylamino)-2-oxo-1-phenylethyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11o)



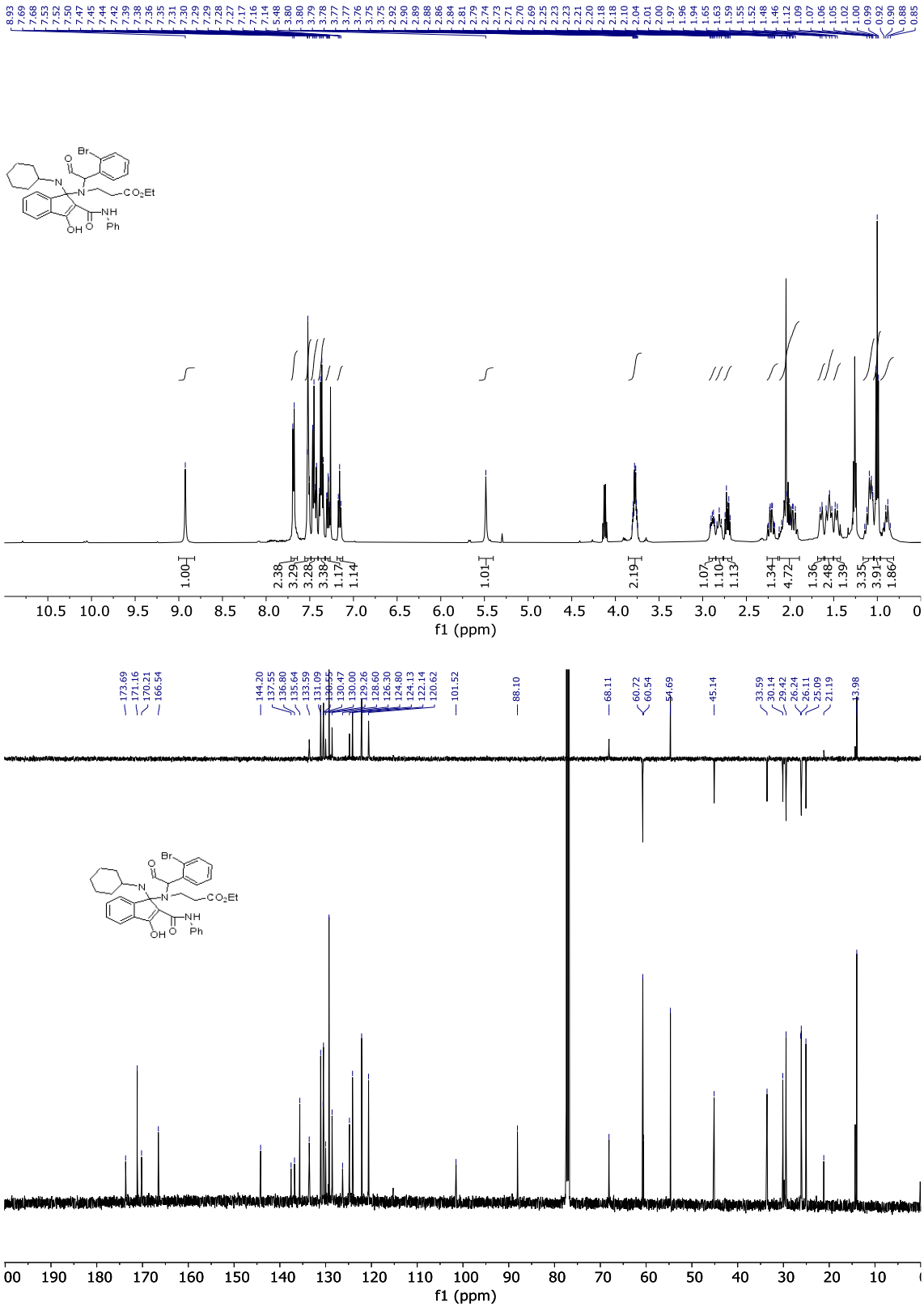
3-((2-(Cyclohexylamino)-2-oxo-1-phenylethyl)(4-methoxyphenyl)amino)-1-oxo-*N*-phenyl-1*H*-indene-2-carboxamide (11p)



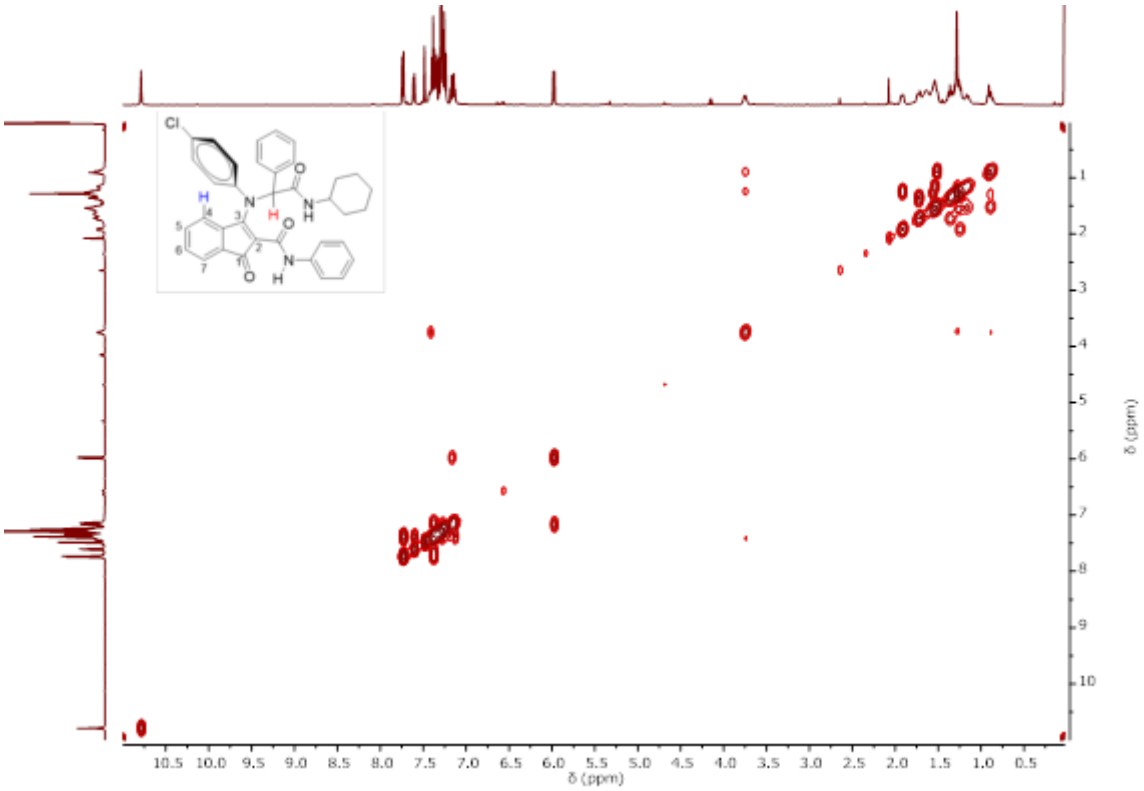
1-Benzyl-3-cyclohexyl-3'-hydroxy-4-oxo-*N*,5-diphenylspiro[imidazolidine-2,1'-indene]-2'-carboxamide (18a)

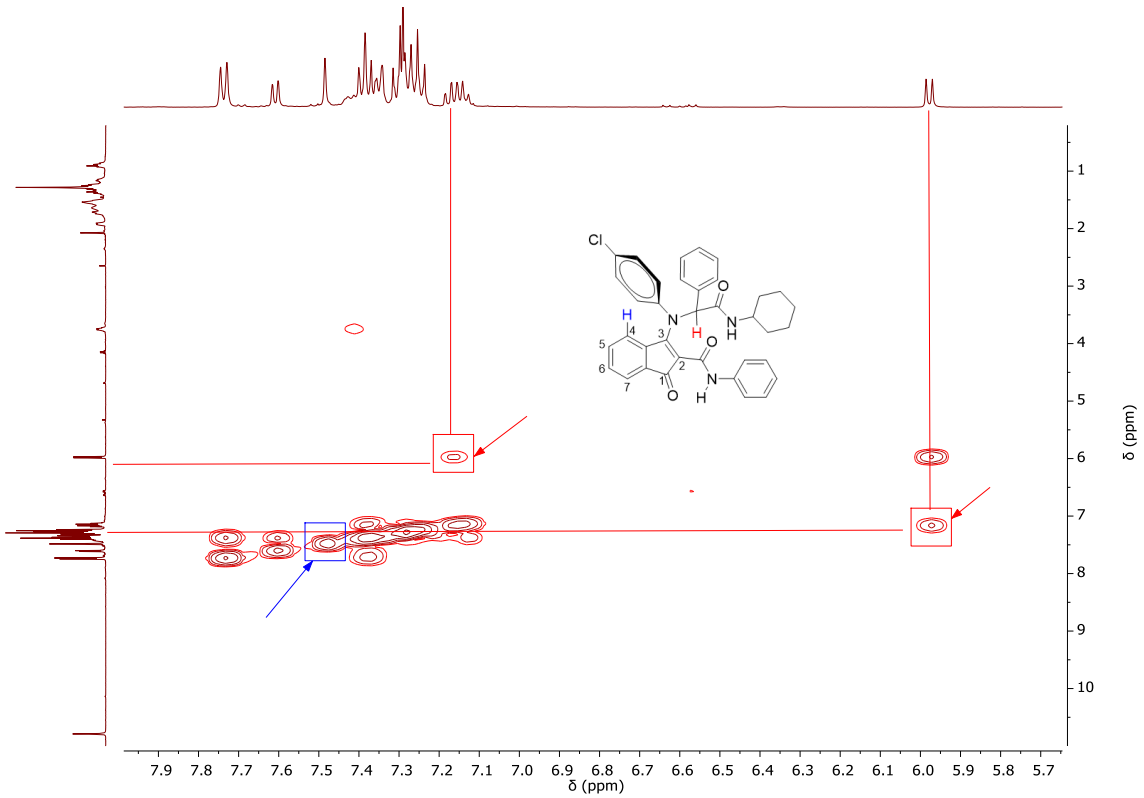


Ethyl 3-(4-(2-bromophenyl)-1-cyclohexyl-3'-hydroxy-5-oxo-2'-(phenylcarbamoyl)spiro[imidazolidine-2,1'-inden]-3-yl)propanoate (18e)

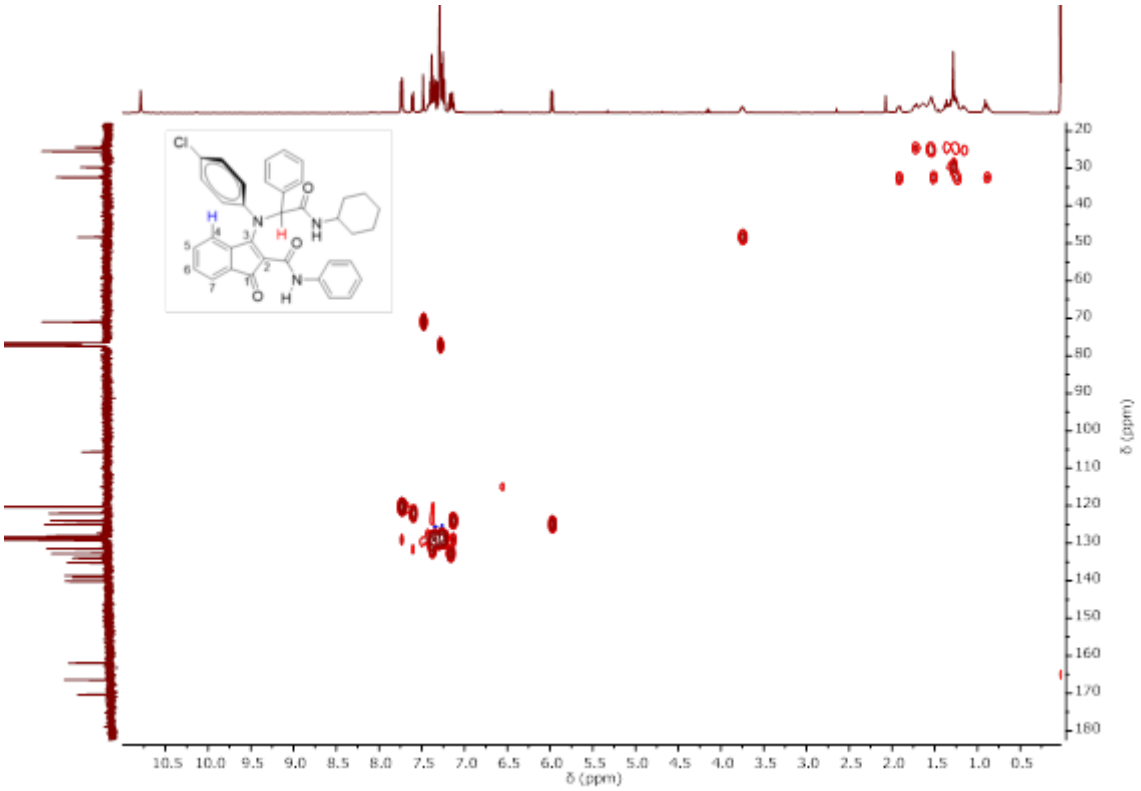


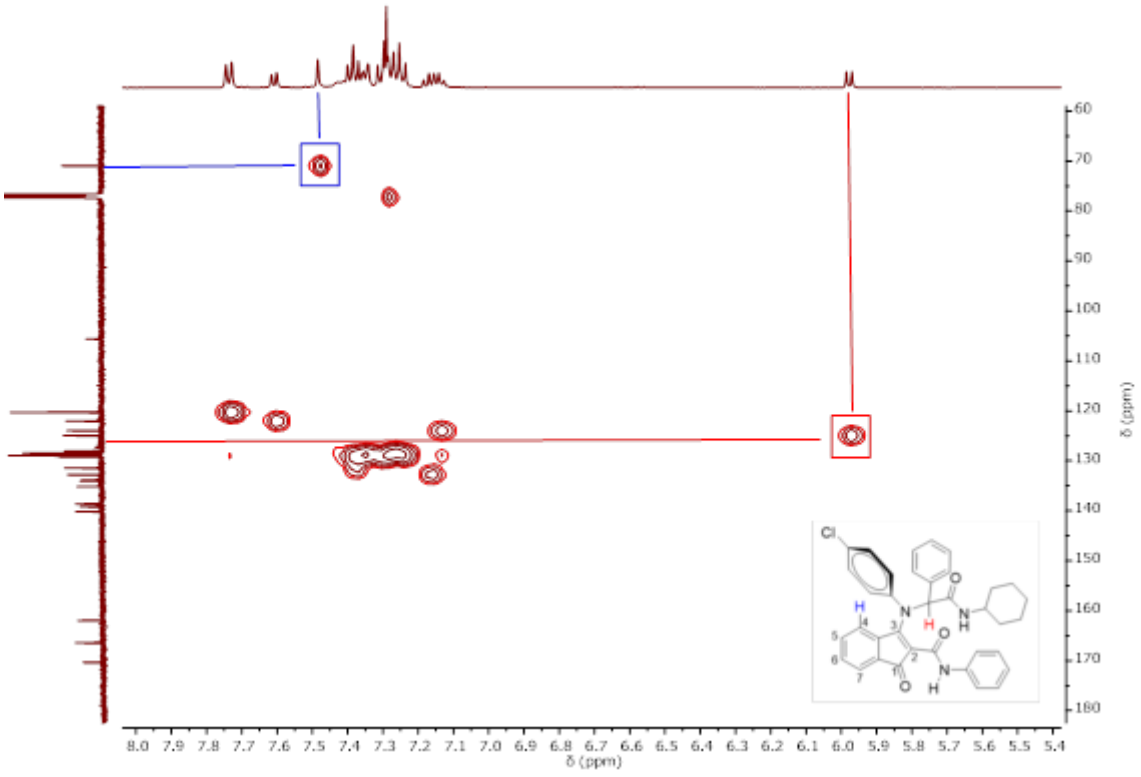
Compound 11o: COSY and COSY ampliation spectra



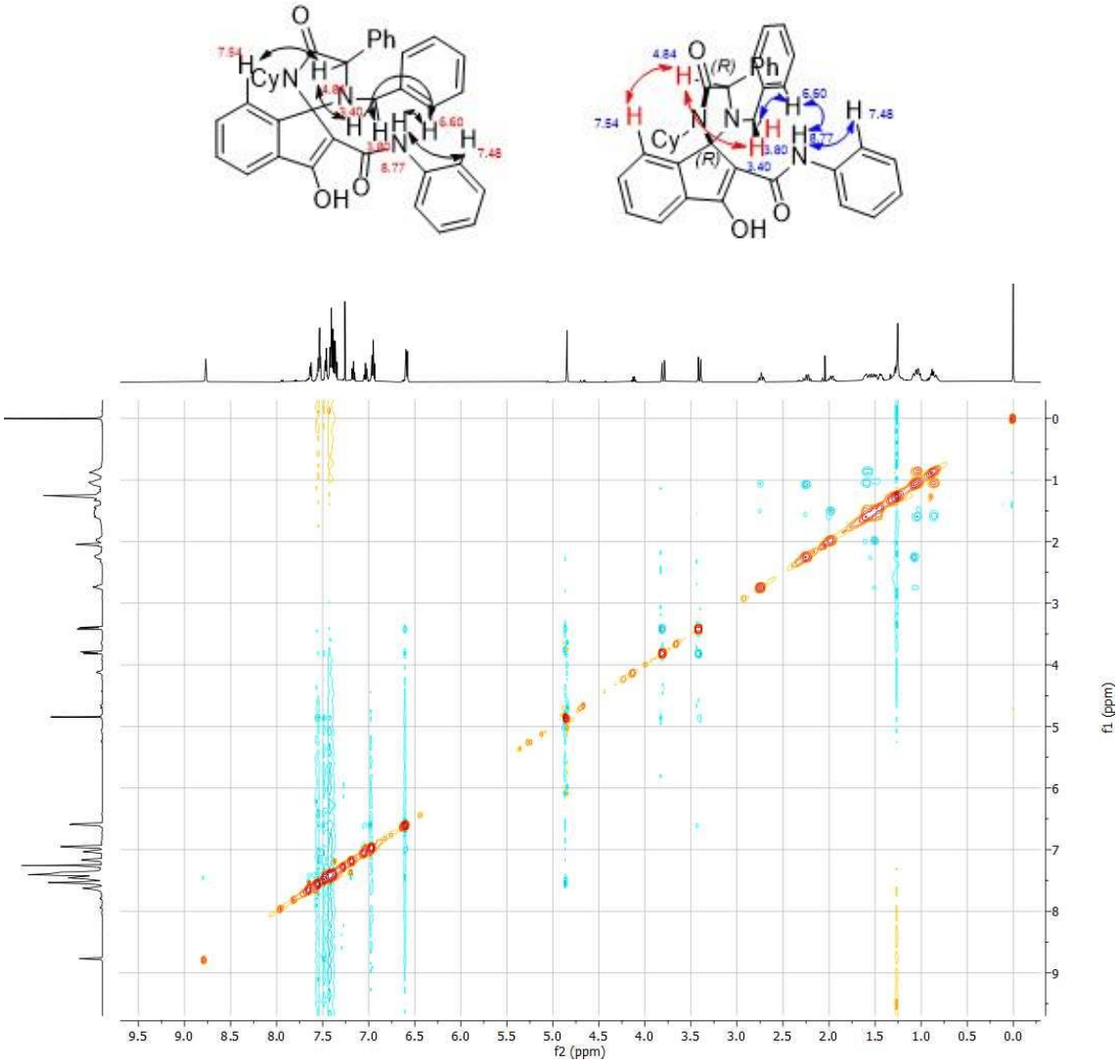


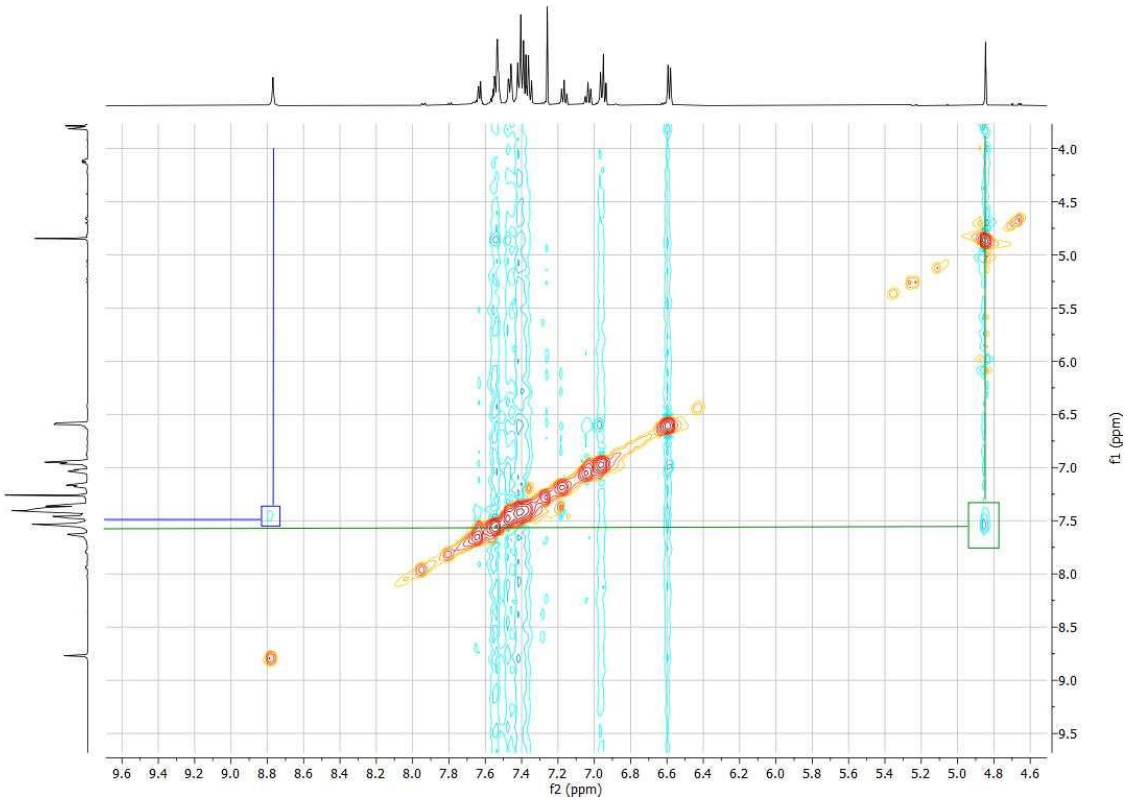
Compound 11o: HSQC and HSQC ampliation spectra





Compound 18a: ROESY and ROESY ampliation spectra




f1 (ppm)
f2 (ppm)