Supporting Information

Sustainable photocatalytic synthesis of 2-hydroxybenzofuran-3(2*H*)-ones by lead-free $Cs_2AgBiBr_6$ nanocrystals

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1. General information

All commercial reagents were used directly without further purification, unless otherwise stated. Unless otherwise specified, all reactions were carried out in a 10 mL quartz glass tube under air and then monitored by TLC. Products were purified by column chromatography on silica gel using petroleum ether and ethyl acetate as the eluent. DMSO-d_6 and $CDCl_3$ were purchased from Shanghai aladdin Biochemical Technology Co., Ltd. Chemical shifts for ^{1}H and ^{13}C NMR were referred to internal

Me_4Si (0 ppm) as the standard. The following abbreviations were used to describe NMR signals: s = singlet, d = doublet, t = triplet, m = mulitplet, dd = doublet of doublets, q = quartet.

Characterization. Transmission electron microscopy (TEM) images were obtained on a JEM F200 microscopy with an accelerating voltage of 200 kV. The energy dispersive X-ray (EDX) composition analysis was carried out using an accessory attached on TEM. Powder X-ray diffraction (XRD) patterns were collected on a Rigaku SmartLab diffractometer using a Cu Kα radiation at a scan rate of 10^{o} min^{-1}. UV-vis diffuse reflectance spectra (DRS) of the samples were obtained on a Lambda 1050 spectrometer (TU-1901, CN). Electron paramagnetic resonance (EPR) spin-trapping measurements were carried out on a Bruker EMX PLUS EPR spectrometer at X-band frequency (9.4 GHz) and at room temperature. The EPR signals of $\bullet O_2^-$ free radicals and $^1O_2$ were detected in the presence of 5,5-dimethyl-1-pyrroline N-oxide (DMPO) and 2,2,6,6-Tetramethylpiperidinooxy (TEMPO) under the illumination of 300 W Xe lamp with an optical cutoff filter ($\lambda \geq 420$ nm). ^1H NMR spectra were recorded at 500 MHz and ^{13}C NMR spectra were recorded at 126 MHz using a Bruker Avance 400 spectrometer at ambient temperature (25 ^{o}C) with TMS as an internal standard.

2. Preparation of $Cs_2AgBiBr_6$ NCs

Cs_2CO_3 (203.5 mg), ODE (10 mL) and OA (0.625 mL) were put into a three-neck round-bottom (RB) flask with the capacity of 100 mL, kept in vacuum for 1 h at 120 ℃, and then under N_2 environment was heated to 150 ℃ until the formation of Cs-oleate (clear solution). $BiBr_3$ (90 mg), $AgNO_3$ (34 mg), OA (2 mL), OLA (2 mL), ODE (8 mL) and HBr (0.2 mL) were put into a three-neck round-bottom flask with the capacity of 100 mL, and the reactant mixture heated to 120 ℃ for at least 1 h under vacuum to remove residual gases and water in solvents. After complete dissolution of the $AgNO_3$ and $BiBr_3$ salt, the reaction mixture was further heated to 200 ℃ under N_2 atmosphere and 1.6 mL preheated Cs-oleate was added rapidly into the flask under vigorous stirring. After 5 s, the mixture was cooled down to room temperature by putting the flask into the ice-water bath. Centrifuging the crude solution for 5 min at

7000 rpm to separate crude NCs from the solution. After centrifugation, the crude product was redispersed in dichloromethane and centrifuged again for 5 min at 8000 rpm, repeat it again, and then the precipitates were obtained and the upper solution were discarded. Drying at 70 ℃ for 30 min to obtain $Cs_2AgBiBr_6$ NCs.

3. Preparation of $Cs_2AgBiBr_6$ MCs

2.130 g CsBr (10.0 mmol), 0.940 g AgBr (5.0 mmol) and 2.245 g $BiBr_3$ (5.0 mmol) were added into a 100 mL round bottom flask with 50 mL of 48 % HBr. The mixture was heated to 110 °C for 2 h, then cooled to room temperature. An orange powder precipitated from solution, centrifuged at 8000 rpm for 5 min and dried at 70 ℃ under reduced pressure for 4 h to obtain the $Cs_2AgBiBr_6$ product. The $Cs_2AgBiBr_6$ product was dissolved in DMSO giving 50 mM the transparent solution. 1 mL $Cs_2AgBiBr_6$ transparent solution was added into 10 mL DCM, then precipitated, centrifuged at 8000 rpm for 5 min and dried at 70 ℃ under reduced pressure overnight to obtain the $Cs_2AgBiBr_6$ MCs.

4. Characterization of $Cs_2AgBiBr_6$

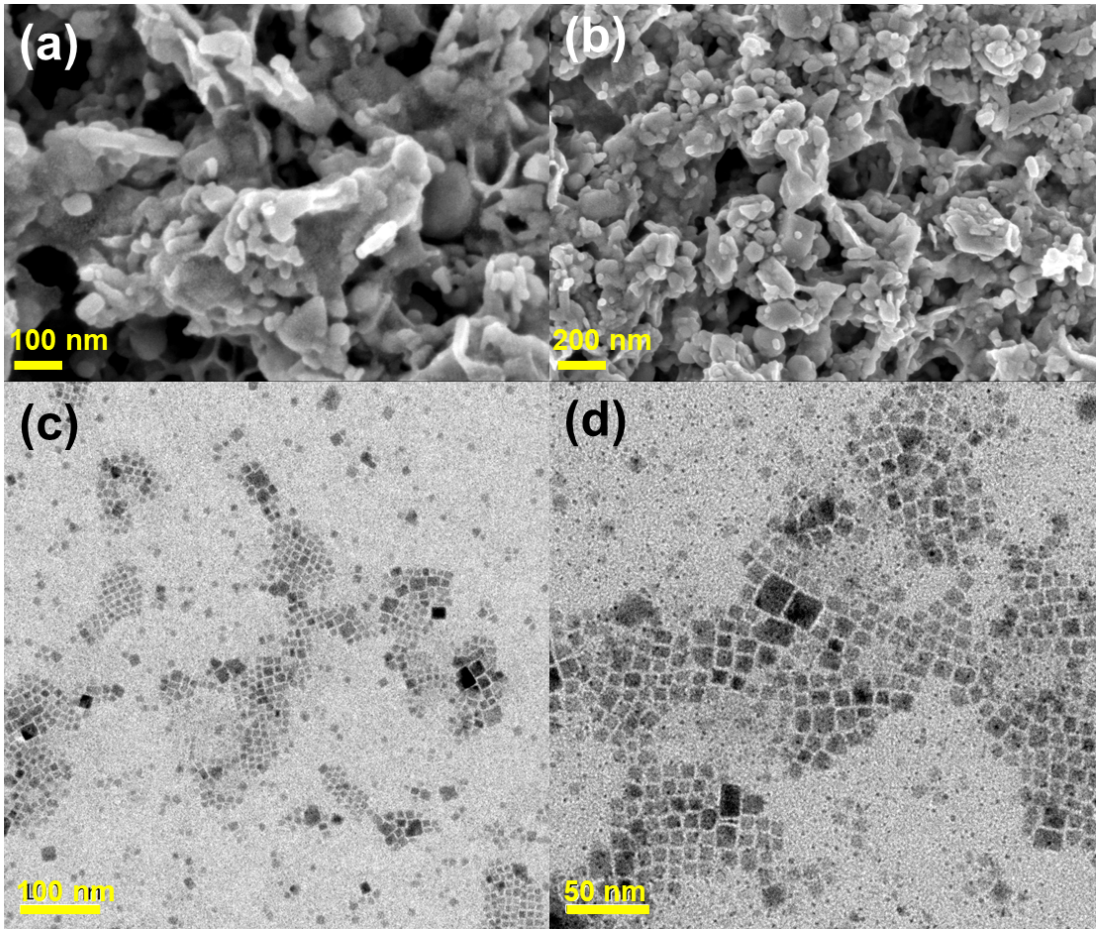


Figure S1 (a, b) SEM image of $Cs_2AgBiBr_6$ NCs. (c, d) TEM image of $Cs_2AgBiBr_6$ NCs.

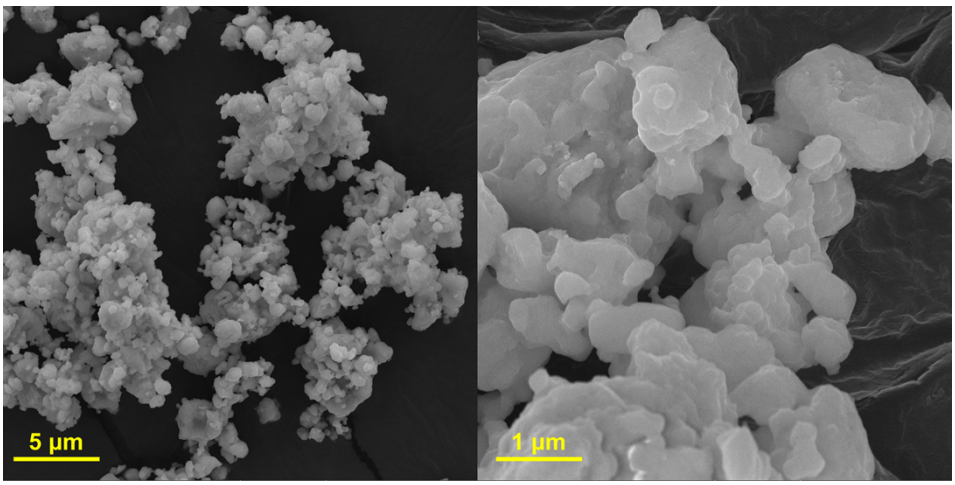


Figure S2 SEM image of $Cs_2AgBiBr_6$ MCs.

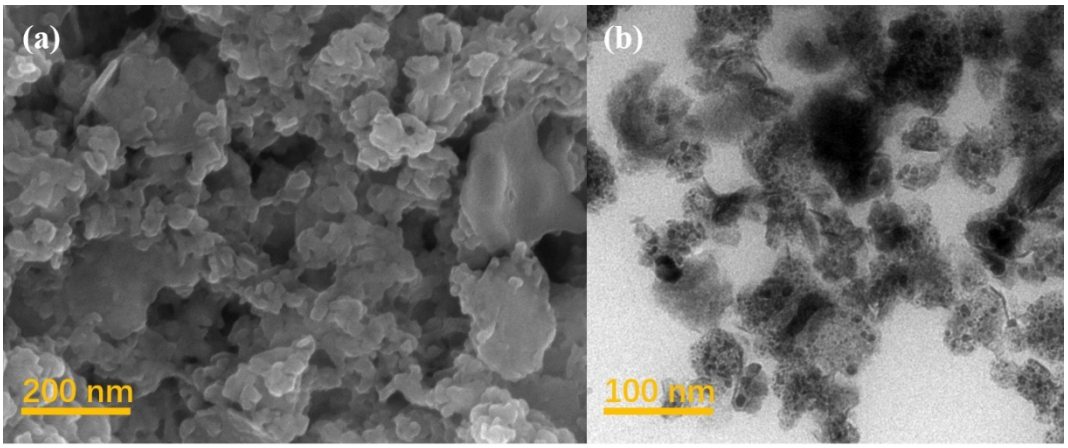


Figure S3 SEM image (a) and TEM image (b) of recycled $Cs_2AgBiBr_6$ NCs.

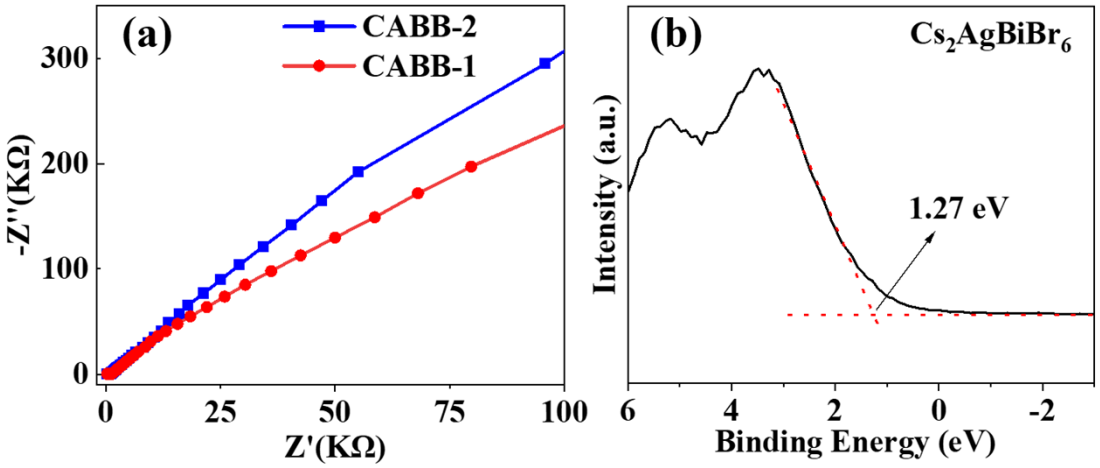
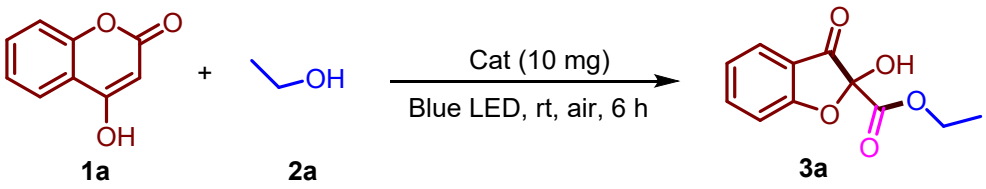


Figure S4 (a) Electrochemical impedance spectroscopy. (b) XPS valence spectra of $Cs_2AgBiBr_6$ NCs.

5. General Procedure for the reactions

A 10 mL quartz glass tube was charged with 4-hydroxycoumarins (**1**; 0.2 mmol), CABB (10 mol %), alcohol substrates (**2**; 2.0 ml) or amines (**4**; 0.3 mmol) dissolved in 2 mL of MeCN, and a magnetic stir bar in a sequential manner. and the resulting reaction mixture was stirred under irradiation of a 50 W 457 nm blue LED and an irradiation distance of about 5 cm under air atmosphere at room temperature. After total conversion of the 4-hydroxycoumarins (detected by TLC), the isolated photocatalyst was centrifuged, and the resulting mixture was purified by flash silica gel chromatography (EtOAc / PE = 1/4) to afford the desired products.

Table S1 Comparison between $Cs_2AgBiBr_6$ NCs and other photocatalysts[a]

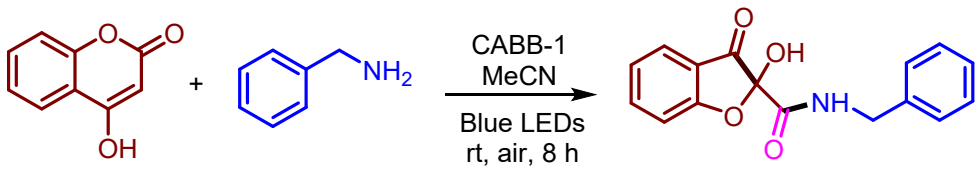


1a 2a 3a

Entry	Photocatalyst	Yield (%)[b]
1	**$Cs_2AgBiBr_6$**	**82**
2	Eosin Y	63
3	Eosin B	53
4	Rose Bengal	61
5	Rhodamine B	35
6	CBr_4	Trace
7	$Ru(bpy)_3Cl_2·6H_2O$	10

[a] Reaction conditions: 4-Hydroxycoumarin (**1a**, 0.2 mmol) and photocatalyst (10 mg) in 2.0 mL of ethanol, 457 nm Blue LED (50 W), under air atmosphere, rt, 6 h. [b] Isolated yields.

Table S2 Optimization of reaction conditions[a]



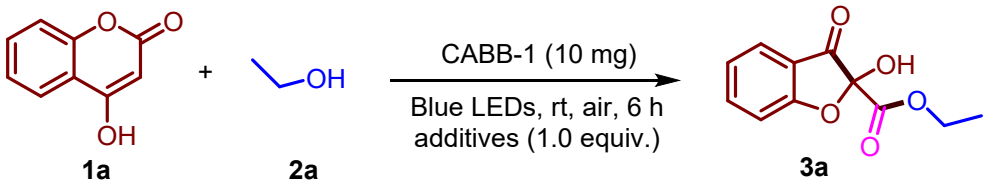
1a 4a 5a

Entry	Variation from the standard	Yield (%)[b]
1	**none**	**70**
2	DCE	46
3	EtOAc	65
4	THF	20
5	1,4-dioxane	60
6	**4a** (2 equiv.) was used	68

7	**4a** (1 equiv.) was used	55
8	Reaction time: 7 h	65
9	Reaction time: 9 h	69
10	CABB-1 (10 mg)	60
11	CABB-1 (20 mg)	71

[a] Standard reaction conditions: 4-Hydroxycoumarin (**1a**, 0.2 mmol), amines (**4a**, 0.3 mmol), MeCN (2.0 mL), CABB-1 (15 mg), 50 W 457 nm Blue LED, rt, air, 8 h, [b] Isolated yield.

Table S3 Free radical verification experiments[a]



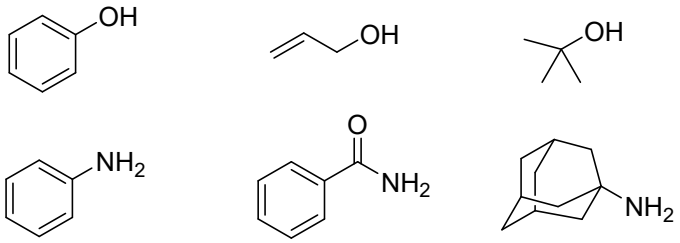
Entry	Scavenger	Inhibited species	Yield (%)[b]
1	none	/	82
2	TEMPO	$^1O_2$ and $\cdot O_2^-$	14
3	DABCO	$^1O_2$	NR
4	BQ	$O_2^{\cdot -}$	trace

[a] Reaction conditions: 4-Hydroxycoumarin (**1a**, 0.2 mmol) and CABB-1 (10 mg) in 2.0 mL of ethanol, 457 nm Blue LED (50 W), under air atmosphere, rt, 6 h. [b] Isolated yields.

6. General Procedure for the recycle experiments

0.2 mmol 4-hydroxycoumarins, 10 mg CABB, and 2.0 ml ethanol were added to a 10 ml glass tube and irradiated with a 50 W 457 nm blue LED in air at room temperature for 6 h. Upon completion of the reaction, the catalyst was collected by centrifuging the reaction solution, combined supernatant was purified by flash silica gel chromatography (EtOAc/PE = 1/3) to afford the desired products. The catalyst was dried under vacuum and was charged again with fresh reagents, repeating the process.

7. Inactive substrates



8. HRMS spectrums of the intermediates

HRMS (ESI) m/z: calcd for $C_{16}H_{16}O$ $[M + H]^+$: 225.1279, found: 225.1277.

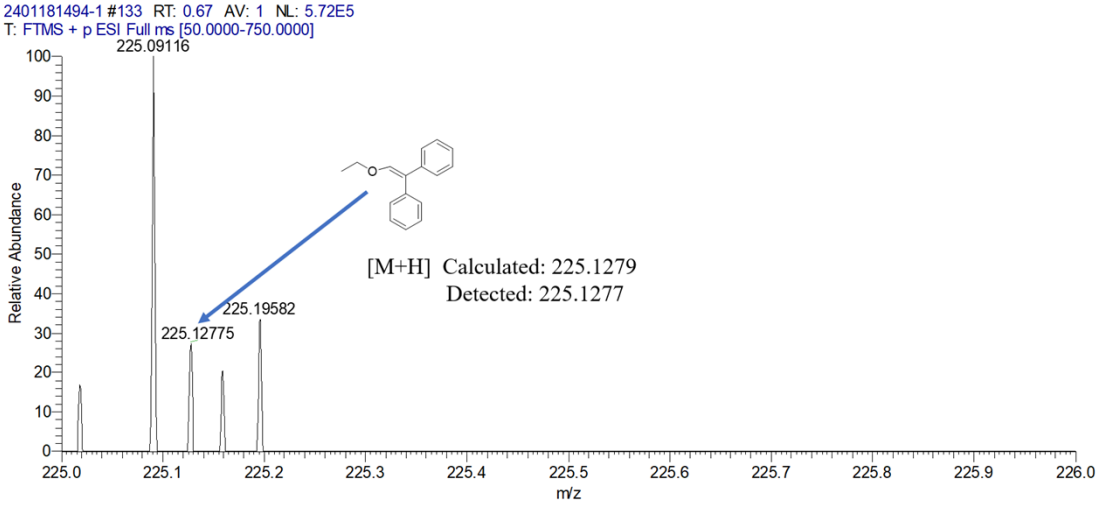


Figure S5. HRMS spectrums of free radical addition products

9. DFT calculations data

The transformation was initiated with **B** and singlet oxygen, leading to the formation of **C** via **TS1**, then undergoes a hydrogen transfer process, generate **D** through the **TS2** process, then loses one hydroxyl radical to generate **E**. The intermediate **4** then undergo radical addition, through a **TS4** process to produce **F**. Finally, after the α-ketol rearrangement reaction, the product **3** is produced after the **TS5** process.

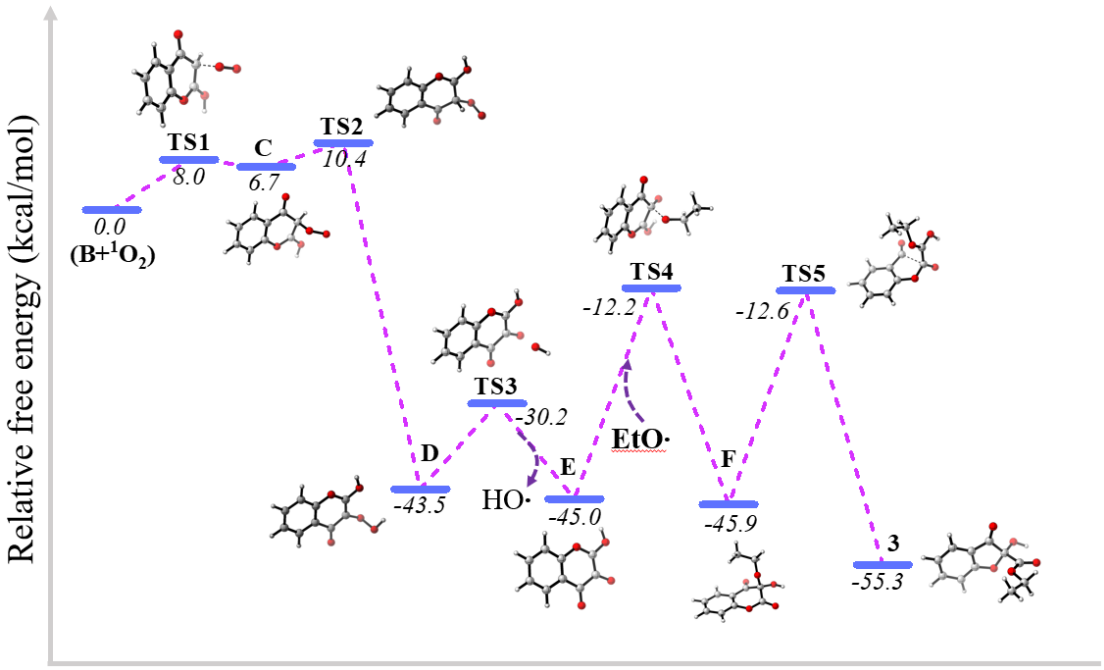


Figure S6. Gibbs energy profiles for model reaction of **1a** and **ethanol**

Cartesian coordination of 1

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#p opt freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.023406	-1.154509	0.322729
C	-1.795495	-1.675564	-0.058421
C	-0.750986	-0.807817	-0.342054
C	-0.920426	0.580979	-0.252877
C	-2.172156	1.082653	0.130562
C	-3.216193	0.226142	0.421514
H	-3.837803	-1.830486	0.548163
H	-1.635661	-2.741494	-0.143360
C	0.182422	1.491116	-0.576786
H	-2.293168	2.155392	0.197817
H	-4.176698	0.619973	0.724277
C	1.568879	0.796354	-0.631642
C	1.599433	-0.600211	-0.630905

H	2.462060	1.295584	-0.997730
O	0.060847	2.691168	-0.739800
O	0.421906	-1.378015	-0.790923
O	2.817444	-1.126374	-0.918372
H	2.753391	-2.093319	-0.953028
O	1.956272	-0.538152	1.812374
O	1.980462	0.721310	1.928114

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Cartesian coordination of TS1

#p opt(ts,calcfc,noeigen) freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.283484	-0.865537	0.518657
C	-2.087881	-1.541667	0.306443
C	-0.977475	-0.802912	-0.048531
C	-1.008275	0.582684	-0.203265
C	-2.227297	1.237424	0.009147
C	-3.354834	0.520654	0.369447
H	-4.164674	-1.426095	0.799905
H	-2.013826	-2.615075	0.408571
C	0.208471	1.318485	-0.566025
H	-2.259134	2.312000	-0.107370
H	-4.291524	1.033773	0.537979
C	1.501530	0.518183	-0.526732
C	1.300822	-0.935347	-0.622944
H	2.244248	0.905032	-1.220077
O	0.239954	2.505203	-0.820681
O	0.197066	-1.537029	-0.273599
O	2.322924	-1.682697	-0.860172
O	2.171140	0.619040	1.265400
O	3.558064	0.373426	1.294242
H	2.142256	-2.624975	-0.677707

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Cartesian coordination of 2

#p opt freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.237064	-0.952281	0.351230
C	-2.017519	-1.590310	0.169224
C	-0.903639	-0.810719	-0.081489
C	-0.960643	0.580781	-0.162118
C	-2.204262	1.197767	0.019059
C	-3.332079	0.439645	0.276606
H	-4.119542	-1.544986	0.551072
H	-1.923945	-2.666108	0.216682
C	0.256851	1.357861	-0.434363
H	-2.254272	2.276268	-0.041661
H	-4.288299	0.923139	0.422269
C	1.518455	0.577124	-0.396016
C	1.406287	-0.833957	-0.499380
H	2.379909	1.037193	-0.858562
O	0.268010	2.564394	-0.619766
O	0.296299	-1.499795	-0.275610
O	2.477188	-1.543373	-0.686864
O	1.877930	0.538652	0.997036
O	3.172791	0.274300	1.186400
H	2.310091	-2.494403	-0.555874

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Cartesian coordination of TS2

#p opt=(calcfc,ts,noeigen) freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	3.473672	-0.801985	0.054290
C	2.274415	-1.503927	0.028149
C	1.098894	-0.781493	-0.004024
C	1.067486	0.612700	-0.009161
C	2.289732	1.294435	0.025325
C	3.482823	0.594014	0.054229

H	4.406010	-1.349745	0.077224
H	2.245683	-2.584313	0.036205
C	-0.212588	1.328297	-0.061224
H	2.273925	2.375652	0.020026
H	4.423221	1.127235	0.074432
C	-1.432273	0.426146	-0.329408
C	-1.260396	-0.953412	-0.024545
H	-2.162014	0.526967	0.923389
O	-0.327323	2.533068	0.036268
O	-0.082508	-1.538647	-0.005667
O	-2.356561	-1.758812	0.029233
O	-2.810558	0.409998	-0.634312
O	-3.642655	0.519628	0.631528
H	-2.120583	-2.706328	0.010544

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Cartesian coordination of 3

#p opt freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.270867	-0.940115	0.380153
C	-2.049159	-1.581298	0.213000
C	-0.940125	-0.806253	-0.059292
C	-0.997180	0.582379	-0.174331
C	-2.241759	1.201642	-0.008878
C	-3.368697	0.447996	0.268467
H	-4.151553	-1.529498	0.596580
H	-1.953925	-2.655337	0.287120
C	0.218487	1.357226	-0.448457
H	-2.294092	2.278278	-0.095031
H	-4.325542	0.933692	0.401230
C	1.522147	0.540300	-0.367652
C	1.373258	-0.821511	-0.508036
O	0.234025	2.551719	-0.665460

O	0.262669	-1.505437	-0.242109
O	2.469551	-1.567483	-0.720282
O	1.942544	0.585747	0.979232
O	3.260712	0.382391	1.070784
H	2.303141	-2.518929	-0.575778
H	3.589319	0.034115	0.238725

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Cartesian coordination of TS3

#p opt=(calcfc,ts,noeigen) freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.544552	0.488607	0.203763
C	-2.435708	1.346843	0.166019
C	-1.184926	0.758227	0.032254
C	-0.959773	-0.621430	-0.068691
C	-2.098334	-1.453208	-0.021774
C	-3.372730	-0.897755	0.111580
H	-4.549629	0.913385	0.306054
H	-2.547381	2.432013	0.239147
C	0.375629	-1.213281	-0.210125
H	-1.968294	-2.539775	-0.092969
H	-4.247988	-1.554566	0.144674
C	1.548693	-0.226372	-0.405583
C	1.132296	1.265460	-0.166388
O	0.629074	-2.390964	-0.199820
O	-0.113177	1.702586	0.019923
O	2.035032	2.183343	-0.151954
O	2.762151	-0.499161	-0.702967
O	3.534440	-0.710846	1.128634
H	1.654431	3.162528	-0.074731
H	4.115126	-1.375807	0.880973

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Cartesian coordination of 4

#p opt freq b3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	3.084617	-0.869403	0.014835
C	1.869999	-1.544316	0.006424
C	0.711295	-0.793492	-0.005250
C	0.705276	0.598819	-0.012938
C	1.942223	1.252182	-0.002419
C	3.121045	0.525746	0.010092
H	4.005505	-1.436424	0.024884
H	1.816326	-2.623781	0.010665
C	-0.563874	1.349506	-0.014389
H	1.948942	2.333458	-0.005561
H	4.072291	1.039962	0.016725
C	-1.809793	0.515470	-0.030258
C	-1.643481	-0.930746	-0.004126
O	-0.626534	2.565912	-0.011253
O	-0.486857	-1.525410	-0.014185
O	-2.683552	-1.694626	-0.006000
O	-2.941510	0.991910	0.051991
H	-2.439284	-2.638103	0.017028

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Cartesian coordination of TS4

#p opt(calcfc,ts,noeigen) freq rb3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	-3.562188	-0.889363	0.668393
C	-2.432303	-1.556962	0.213666
C	-1.327290	-0.817721	-0.174817
C	-1.337625	0.579759	-0.120070
C	-2.493282	1.234054	0.324291
C	-3.599106	0.505809	0.721951
H	-4.425027	-1.463803	0.978721
H	-2.400678	-2.635621	0.149216
C	-0.165788	1.326953	-0.508481

H	-2.490276	2.315068	0.362577
H	-4.486461	1.011874	1.076267
C	1.150956	0.464647	-0.552944
C	0.910788	-0.887335	-1.066381
O	-0.090361	2.517468	-0.737138
O	-0.258319	-1.543466	-0.677304
O	1.779030	-1.595839	-1.806354
O	2.102350	1.061525	-1.314010
O	1.482836	0.365465	0.810856
C	2.668712	-0.404870	1.126666
C	2.989343	-0.161892	2.582958
H	3.484425	-0.082938	0.478233
H	2.470193	-1.464473	0.941973
H	3.871444	-0.740151	2.863449
H	3.196803	0.893624	2.763149
H	2.159306	-0.470434	3.220052
H	1.682682	-0.162858	-2.333422

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Cartesian coordination of 5

#p opt freq rb3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	3.698943	0.299132	0.683969
C	2.647733	1.207741	0.619031
C	1.438840	0.777754	0.113682
C	1.229598	-0.527176	-0.338213
C	2.305714	-1.415753	-0.268452
C	3.529625	-1.010794	0.240295
H	4.652370	0.620394	1.081000
H	2.759489	2.230791	0.949574
C	-0.081128	-0.967265	-0.869971
H	2.151996	-2.428599	-0.615170
H	4.351742	-1.711191	0.294333

C	-1.205030	0.042667	-0.687251
C	-0.745783	1.426918	-0.346616
O	-0.272391	-2.045464	-1.388242
O	0.433167	1.769866	0.050356
O	-1.605939	2.360998	-0.505042
O	-2.292530	0.007970	-1.317396
O	-1.284851	-0.066494	0.690327
C	-2.629065	-0.180427	1.129711
C	-2.908306	-1.587461	1.636732
H	-3.307608	0.050759	0.299699
H	-2.790891	0.563770	1.915540
H	-3.934418	-1.656743	2.006626
H	-2.781885	-2.314266	0.832501
H	-2.230311	-1.849239	2.450917
H	-2.376971	1.887311	-0.932541

****

Cartesian coordination of TS5

#p opt=(calcfc,ts,noeigen) freq rb3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	3.456324	0.936543	-0.594992
C	2.455156	0.404421	-1.395540
C	1.369822	-0.201024	-0.775663
C	1.283631	-0.252259	0.622426
C	2.312867	0.273428	1.416672
C	3.395878	0.873205	0.804491
H	4.306440	1.411704	-1.067490
H	2.510193	0.446947	-2.474422
C	0.070197	-0.842915	1.089465
H	2.233950	0.214069	2.494364
H	4.193535	1.297522	1.398625
C	-1.658265	-0.492292	-0.292501
C	-0.664117	-1.399740	-0.755077

O	-0.348556	-1.184196	2.148208
O	0.375631	-0.772389	-1.512496
O	-0.835715	-2.626860	-0.812943
O	-2.710561	-1.000681	0.301769
O	-1.599142	0.798253	-0.478514
C	-2.280338	1.708690	0.461404
C	-2.562592	2.975849	-0.304094
H	-1.594577	1.858454	1.295496
H	-3.193073	1.237100	0.813642
H	-3.036452	3.700849	0.358898
H	-1.644634	3.414537	-0.695575
H	-3.240021	2.772125	-1.135191
H	-2.659999	-1.969761	0.183916

****

Cartesian coordination of 6

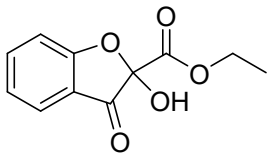
#p opt freq rb3lyp scrf=(solvent=ethanol) em=gd3bj tzvp

C	3.453157	0.817256	-0.448345
C	2.542867	0.221532	-1.310007
C	1.381105	-0.313268	-0.767905
C	1.137143	-0.245437	0.608275
C	2.074130	0.343717	1.468459
C	3.229349	0.881338	0.934748
H	4.361809	1.239808	-0.857649
H	2.723470	0.163605	-2.374326
C	-0.126807	-0.820290	0.983370
H	1.871676	0.380619	2.530770
H	3.959652	1.353665	1.577322
C	-1.618944	-0.463457	-0.311531
C	-0.562472	-1.396069	-0.558883
O	-0.653238	-1.096179	2.014251
O	0.467448	-0.939210	-1.555825

O	-0.734916	-2.631431	-0.549250
O	-2.722023	-0.926078	0.242566
O	-1.538734	0.808041	-0.598005
C	-2.411470	1.749435	0.122614
C	-1.998872	3.136714	-0.294872
H	-2.271641	1.580118	1.190315
H	-3.441685	1.523706	-0.146238
H	-2.631592	3.863831	0.216248
H	-0.960676	3.332682	-0.026172
H	-2.120143	3.272087	-1.369897
H	-2.634283	-1.900108	0.274192

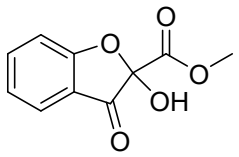
****

10. Data for the products.



ethyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

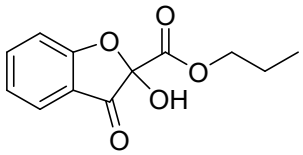
3a: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a faint yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.60 (m, 2H), 7.21 – 7.07 (m, 2H), 5.35 (s, 1H), 4.36 – 4.24 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.86, 171.43, 166.88, 139.17, 125.37, 123.11, 118.87, 113.50, 97.66, 64.06, 13.85.



methyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

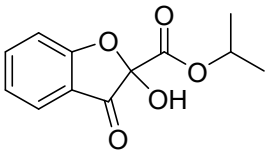
3b: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 14.2, 7.7 Hz, 2H), 7.20 –

7.11 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.65, 171.36, 167.40, 139.27, 125.42, 123.22, 118.81, 113.55, 97.59, 54.35.



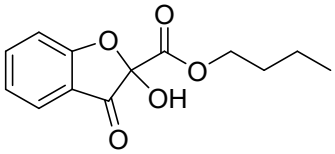
propyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3c: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.65 (m, 2H), 7.21 – 7.09 (m, 2H), 5.34 (s, 1H), 4.25 – 4.18 (m, 2H), 1.65 – 1.57 (m, 2H), 0.81 (dd, J = 10.6, 4.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.85, 171.38, 166.98, 139.17, 125.34, 123.11, 118.93, 113.45, 97.71, 69.33, 21.65, 9.88.



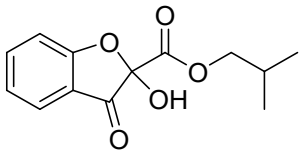
isopropyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3d: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.63 (m, 2H), 7.21 – 7.09 (m, 2H), 5.39 (s, 1H), 5.21 – 5.07 (m, 1H), 1.22 (dd, J = 6.3, 1.1 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.00, 171.48, 166.43, 139.11, 125.33, 123.03, 118.90, 113.45, 97.65, 72.72, 21.35 (d, J = 5.5 Hz).



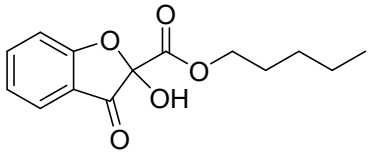
butyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3e: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 – 7.64 (m, 2H), 7.21 – 7.09 (m, 2H), 5.41 (s, 1H), 4.25 (qt, J = 10.7, 6.6 Hz, 2H), 1.62 – 1.51 (m, 2H), 1.23 (dt, J = 14.8, 7.4 Hz, 2H), 0.83 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.93, 171.38, 166.92, 139.19, 125.34, 123.10, 118.91, 113.45, 97.78, 67.73, 30.12, 18.68, 13.47.



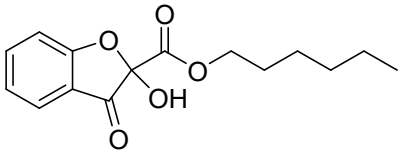
isobutyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3f: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.65 (m, 2H), 7.20 – 7.11 (m, 2H), 5.30 (s, 1H), 4.07 – 4.00 (m, 2H), 1.88 (dt, *J* = 13.4, 6.7 Hz, 1H), 0.82 – 0.77 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.83, 171.33, 166.93, 139.16, 125.29, 123.11, 119.02, 113.40, 97.79, 73.46, 27.56, 18.54.



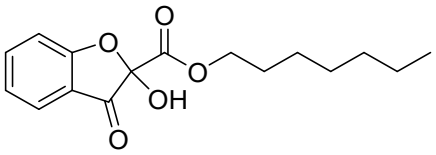
pentyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3g: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 – 7.65 (m, 2H), 7.19 – 7.10 (m, 2H), 5.28 (s, 1H), 4.29 – 4.19 (m, 2H), 1.58 (dt, *J* = 13.9, 6.8 Hz, 2H), 1.26 – 1.15 (m, 4H), 0.81 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.81, 171.37, 166.97, 139.16, 125.34, 123.11, 118.97, 113.45, 97.68, 68.06, 27.78, 27.52, 22.04, 13.86.



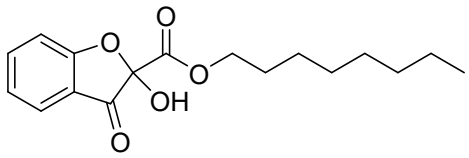
hexyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3h: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 17.2, 7.6 Hz, 2H), 7.16 – 6.92 (m, 2H), 5.31 (s, 1H), 4.16 (td, *J* = 6.7, 2. Hz, 2H), 1.56 – 1.41 (m, 2H), 1.18 – 1.00 (m, 6H), 0.74 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.09, 166.61, 162.17, 134.38, 120.57, 118.33, 114.21, 108.68, 93.01, 63.23, 26.29, 23.29, 20.24, 17.61, 9.11.



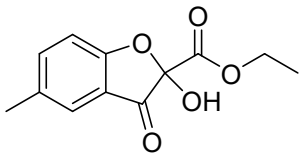
heptyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3i: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 16.7, 8.0 Hz, 2H), 7.21 – 7.10 (m, 2H), 5.29 (s, 1H), 4.24 (td, *J* = 6.6, 2.2 Hz, 2H), 1.58 (dd, *J* = 13.4, 6.6 Hz, 2H), 1.24 – 1.13 (m, 8H), 0.85 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.81, 171.37, 166.98, 139.15, 125.34, 123.11, 118.97, 113.45, 97.68, 68.04, 31.54, 28.58, 28.10, 25.29, 22.45, 14.07.



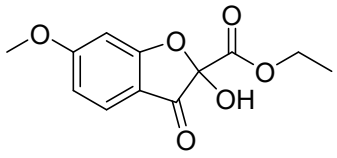
octyl 2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3j: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 17.8, 7.8 Hz, 2H), 7.22 – 7.07 (m, 2H), 5.28 (s, 1H), 4.29 – 4.19 (m, 2H), 1.65 – 1.50 (m, 2H), 1.22 (d, *J* = 32.2 Hz, 10H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.02, 166.61, 162.22, 134.36, 120.57, 118.34, 114.23, 108.68, 92.93, 63.28, 26.88, 24.27, 24.13, 23.36, 20.59, 17.86, 9.34.



ethyl 2-hydroxy-5-methyl-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

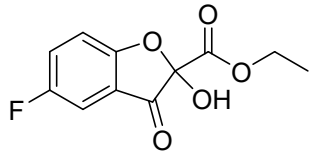
3k: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 1H), 4.34 – 4.26 (m, 2H), 2.37 (s, 3H), 1.23 (d, *J* = 7.1 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.97, 169.90, 167.04, 140.39, 132.89, 124.78, 118.74, 113.10, 97.90, 64.00, 20.65, 13.87.



ethyl 2-hydroxy-6-methoxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

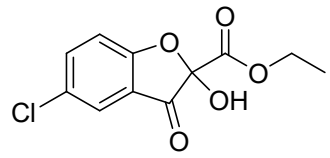
3l: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as

a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.6, 2.9 Hz, 1H), 6.70 (d, *J* = 8.6 Hz, 1H), 6.55 (t, *J* = 2.5 Hz, 1H), 5.42 (s, 1H), 4.36 – 4.24 (m, 2H), 3.90 (d, *J* = 2.9 Hz, 3H), 1.26 – 1.22 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.35, 174.02, 169.19, 167.00, 126.61, 112.41, 111.85, 98.68, 96.66, 63.99, 56.13, 13.89.



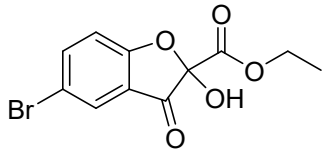
ethyl 5-fluoro-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

3m: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (td, *J* = 8.7, 2.6 Hz, 1H), 7.35 (dd, *J* = 6.4, 2.6 Hz, 1H), 7.11 (dd, *J* = 8.9, 3.5 Hz, 1H), 4.37 – 4.26 (m, 2H), 1.24 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.40 (d, *J* = 2.9 Hz), 167.06 (d, *J* = 124.8 Hz), 159.23, 157.29, 126.72 (d, *J* = 25.7 Hz), 119.40 (d, *J* = 8.2 Hz), 114.72 (d, *J* = 7.6 Hz), 110.55 (d, *J* = 24.1 Hz), 98.54, 64.24, 13.86; ^{19}F NMR ($CDCl_3$, 376 MHz, 298 K) δ = -119.09 (ddd, *J* = 8.7, 6.7, 3.7 Hz).



ethyl 5-chloro-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

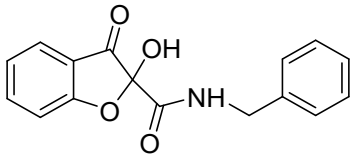
3n: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 2.2 Hz, 1H), 7.62 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 4.31 (dd, *J* = 8.9, 7.2 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.73, 169.69, 166.43, 138.96, 128.64, 124.70, 120.00, 114.88, 98.40, 64.28, 13.86.



ethyl 5-bromo-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxylate

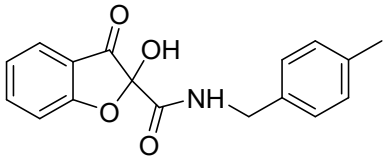
3o: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 2.1 Hz, 1H), 7.76 (dd,

J = 8.8, 2.2 Hz, 1H), 7.05 (d, J = 8.8 Hz, 1H), 5.43 (s, 1H), 4.31 (dd, J = 9.3, 7.2 Hz, 2H), 1.24 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.48, 170.11, 166.41, 141.67, 127.83, 120.54, 115.63, 115.32, 98.21, 64.32, 13.88.



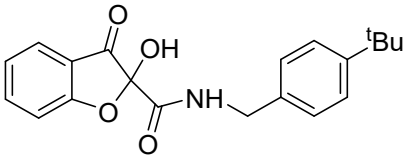
***N*-benzyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5a: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.02 (t, J = 6.3 Hz, 1H), 8.89 (s, 1H), 7.77 (t, J = 7.8 Hz, 1H), 7.66 (d, J = 7.4 Hz, 1H), 7.33 (t, J = 7.5 Hz, 2H), 7.30 – 7.22 (m, 4H), 7.18 (t, J = 7.4 Hz, 1H), 4.31 (d, J = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.67, 171.82, 165.66, 139.72, 139.39, 128.72, 127.58, 127.29, 124.96, 122.89, 119.49, 113.70, 101.15, 42.53.



2-hydroxy-*N*-(4-methylbenzyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

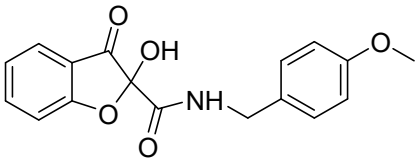
5b: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.97 (t, J = 6.3 Hz, 1H), 8.87 (s, 1H), 7.76 (dd, J = 11.4, 4.1 Hz, 1H), 7.65 (d, J = 7.5 Hz, 1H), 7.24 (d, J = 8.3 Hz, 1H), 7.20 – 7.10 (m, 5H), 4.25 (d, J = 6.3 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.66, 171.80, 165.54, 139.69, 136.37, 136.33, 129.24, 127.63, 124.93, 122.86, 119.50, 113.68, 101.13, 42.29, 21.15.



***N*-(4-(*tert*-butyl)benzyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

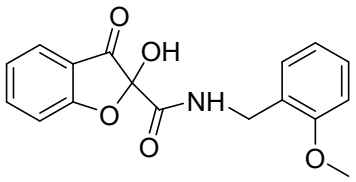
5c: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product

as a colorless liquid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.97 (t, J = 6.3 Hz, 1H), 8.86 (s, 1H), 7.79 – 7.72 (m, 1H), 7.67 – 7.61 (m, 1H), 7.33 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.3 Hz, 1H), 7.20 – 7.11 (m, 3H), 4.25 (d, J = 6.4 Hz, 2H), 1.26 (s, 9H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.67, 171.80, 165.53, 149.65, 139.69, 136.39, 127.41, 125.45, 124.93, 122.86, 119.50, 113.68, 101.13, 42.20, 34.64, 31.64.



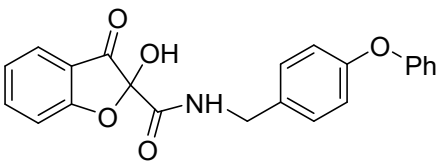
2-hydroxy-*N*-(4-methoxybenzyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

5d: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.94 (t, J = 6.3 Hz, 1H), 8.85 (s, 1H), 7.76 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.5 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.17 (t, J = 8.6 Hz, 3H), 6.88 (d, J = 8.5 Hz, 2H), 4.21 (d, J = 6.3 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.67, 171.79, 165.46, 158.69, 139.68, 131.37, 129.04, 124.93, 122.86, 119.50, 114.10, 113.68, 101.12, 55.51, 41.99.



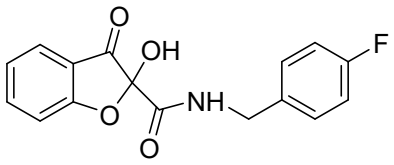
2-hydroxy-*N*-(2-methoxybenzyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

5e: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.94 (d, J = 1.5 Hz, 1H), 8.77 (t, J = 6.0 Hz, 1H), 7.81 – 7.74 (m, 1H), 7.70 – 7.64 (m, 1H), 7.25 (dd, J = 12.6, 4.8 Hz, 2H), 7.18 (t, J = 7.4 Hz, 1H), 7.13 (d, J = 7.4 Hz, 1H), 6.98 (d, J = 8.1 Hz, 1H), 6.93 (t, J = 7.4 Hz, 1H), 4.28 (t, J = 6.4 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.68, 171.84, 165.69, 156.87, 139.75, 128.45, 127.12, 126.44, 124.97, 122.91, 120.56, 119.46, 113.70, 110.81, 101.13, 55.76, 37.76.



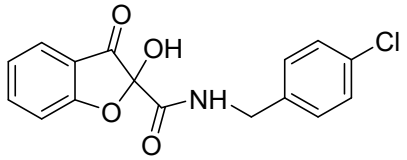
2-hydroxy-3-oxo-*N*-(4-phenoxybenzyl)-2,3-dihydrobenzofuran-2-carboxamide

5f: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.04 (t, J = 6.3 Hz, 1H), 8.90 (s, 1H), 7.76 (dd, J = 11.4, 4.2 Hz, 1H), 7.65 (d, J = 7.4 Hz, 1H), 7.38 (t, J = 7.9 Hz, 2H), 7.26 (dd, J = 19.4, 8.4 Hz, 3H), 7.15 (dt, J = 20.7, 7.4 Hz, 2H), 6.99 (dd, J = 7.9, 6.8 Hz, 4H), 4.28 (d, J = 6.3 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.66, 171.81, 165.62, 157.35, 155.87, 139.72, 134.61, 130.50, 129.43, 124.96, 123.76, 122.89, 119.48, 119.12, 118.83, 113.69, 101.13, 42.01.



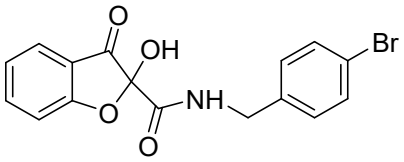
***N*-(4-fluorobenzyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5g: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (t, J = 7.5 Hz, 1H), 7.53 (d, J = 7.3 Hz, 1H), 7.22 – 7.13 (m, 2H), 7.12 – 6.93 (m, 5H), 6.44 (s, 1H), 4.30 (d, J = 5.3 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.96, 171.78, 165.19, 163.29, 139.50, 132.56 (d, J = 3.2 Hz), 129.48 (d, J = 8.2 Hz), 125.38, 123.09, 118.46, 115.67 (d, J = 21.5 Hz), 113.61, 99.60, 43.11; ^{19}F NMR ($CDCl_3$, 376 MHz, 298 K) δ = -114.23 – -114.45 (m).



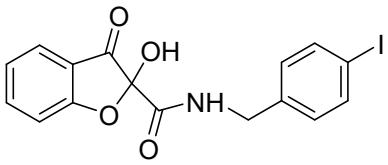
***N*-(4-chlorobenzyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5h: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.08 (t, J = 6.3 Hz, 1H), 8.91 (s, 1H), 7.76 (dd, J = 11.4, 4.1 Hz, 1H), 7.65 (d, J = 7.4 Hz, 1H), 7.39 (d, J = 8.3 Hz, 2H), 7.25 (dd, J = 15.6, 8.3 Hz, 3H), 7.17 (t, J = 7.4 Hz, 1H), 4.27 (d, J = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.59, 171.80, 165.75, 139.74, 138.45, 131.89, 129.51, 128.68, 124.96, 122.91, 119.44, 113.69, 101.11, 41.96.



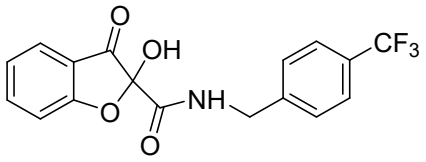
***N*-(4-bromobenzyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5i: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.10 (t, J = 6.2 Hz, 1H), 8.91 (s, 1H), 7.77 (t, J = 7.4 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.53 (d, J = 8.3 Hz, 2H), 7.28 – 7.13 (m, 4H), 4.25 (d, J = 6.2 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.59, 171.79, 165.73, 139.75, 138.88, 131.60, 129.89, 124.97, 122.92, 120.37, 119.43, 113.69, 101.09, 42.02.



2-hydroxy-*N*-(4-iodobenzyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

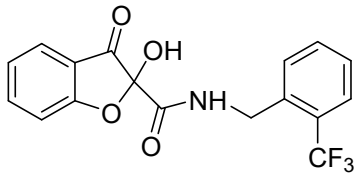
5j: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the titled thiocyanation indole as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.08 (s, 1H), 8.91 (d, J = 3.7 Hz, 1H), 7.77 (t, J = 7.7 Hz, 1H), 7.69 (d, J = 7.1 Hz, 2H), 7.65 (d, J = 7.5 Hz, 1H), 7.24 (d, J = 8.3 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 7.07 (d, J = 7.4 Hz, 2H), 4.23 (d, J = 5.7 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.59, 171.79, 165.71, 139.75, 139.27, 137.45, 130.06, 124.97, 122.92, 119.43, 113.69, 101.09, 93.15, 42.14.



2-hydroxy-3-oxo-*N*-(4-(trifluoromethyl)benzyl)-2,3-dihydrobenzofuran-2-carboxamide

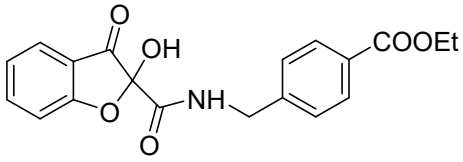
5k: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.18 (t, J = 6.3 Hz, 1H), 8.94 (s, 1H), 7.80 – 7.74 (m, 1H), 7.71 (d, J = 8.1 Hz, 2H), 7.67 – 7.63 (m, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.4 Hz, 1H), 7.18 (t, J = 7.4 Hz, 1H), 4.38 (d, J = 6.3 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.56, 171.80, 165.89, 144.26, 139.76, 128.25, 125.89, 125.65, 124.97, 123.72, 122.93, 119.41, 113.69, 101.11, 42.28; ^{19}F NMR (DMSO-d_6,

376 MHz, 298 K) δ = -60.81.



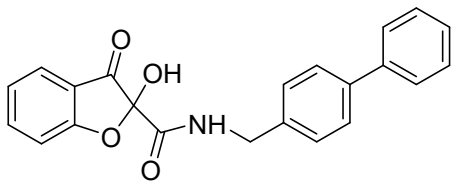
2-hydroxy-3-oxo-*N*-(2-(trifluoromethyl)benzyl)-2,3-dihydrobenzofuran-2-carboxamide

5l: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the titled thiocyanation indole as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.17 (t, J = 6.0 Hz, 1H), 7.77 (t, J = 7.8 Hz, 1H), 7.74 – 7.63 (m, 3H), 7.48 (t, J = 7.7 Hz, 2H), 7.25 (d, J = 8.4 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 4.50 (dd, J = 12.6, 5.3 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.53, 171.84, 166.08, 139.84, 137.34, 133.09, 127.81 (d, J = 3.6 Hz), 126.50, 126.25 (d, J = 4.2 Hz), 125.97, 125.02, 123.79, 122.99, 119.35, 113.72, 101.14, 39.09; ^{19}F NMR (DMSO-d_6, 376 MHz, 298 K) δ = -59.40.



ethyl 4-((2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamido)methyl)benzoate

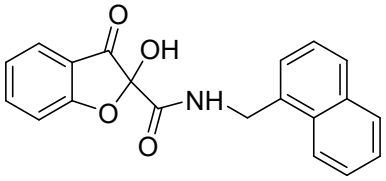
5m: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, J = 8.1 Hz, 2H), 7.56 (t, J = 7.5 Hz, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.24 (d, J = 8.1 Hz, 2H), 7.02 (dd, J = 15.7, 8.0 Hz, 2H), 6.76 (s, 1H), 4.44 – 4.36 (m, 2H), 4.29 (q, J = 7.2 Hz, 2H), 1.35 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.07, 171.81, 166.67, 165.45, 142.21, 139.37, 129.96, 129.46, 127.39, 125.22, 122.92, 118.51, 113.53, 99.80, 61.25, 43.23, 14.28.



***N*-([1,1'-biphenyl]-4-ylmethyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

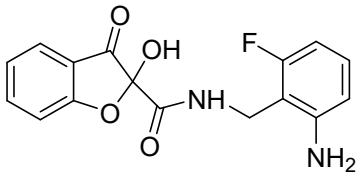
5n: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (t, J = 8.1 Hz, 2H), 7.53 (t, J = 8.3 Hz, 4H), 7.43 (t, J = 7.4 Hz, 2H), 7.37 – 7.32 (m, 1H), 7.31 – 7.25 (m, 2H), 7.15

– 7.02 (m, 2H), 6.94 (s, 1H), 4.43 (d, J = 5.4 Hz, 2H), 2.01 (s, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.69, 171.84, 165.72, 140.42, 139.73, 139.25, 138.65, 129.41, 128.28, 127.82, 127.08, 124.97, 122.91, 119.51, 113.71, 101.19, 56.54, 42.32.



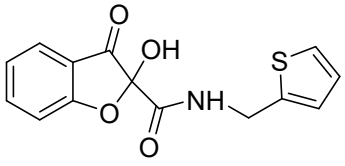
2-hydroxy-*N*-(naphthalen-1-ylmethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

5o: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 14.0, 8.1 Hz, 2H), 7.81 – 7.77 (m, 1H), 7.55 – 7.46 (m, 4H), 7.41 – 7.36 (m, 2H), 7.03 (d, J = 8.3 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 6.89 (s, 1H), 6.36 (s, 1H), 4.83 (d, J = 5.5 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.69, 171.85, 165.74, 139.75, 134.36, 133.69, 131.14, 128.98, 127.94, 126.72, 126.28, 125.84, 125.25, 124.99, 123.85, 122.93, 119.50, 113.72, 101.20, 40.62.



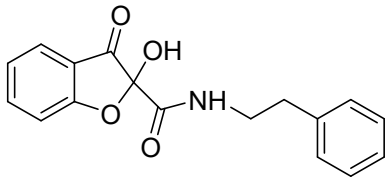
***N*-(2-amino-6-fluorobenzyl)-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5p: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.90 (s, 1H), 8.80 (t, J = 5.9 Hz, 1H), 7.77 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.22 (d, J = 8.4 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 6.98 (dd, J = 14.9, 8.0 Hz, 1H), 6.44 (d, J = 8.0 Hz, 1H), 6.29 (t, J = 8.9 Hz, 1H), 5.52 (s, 2H), 4.23 (ddd, J = 34.7, 14.5, 6.1 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.47, 171.69, 166.09, 161.28, 149.62, 139.72, 129.61, 124.94, 122.93, 119.49, 113.68, 111.09, 108.74, 102.42, 100.95, 60.26; ^{19}F NMR (DMSO-d_6, 376 MHz, 298 K) δ = -113.10 – -120.41 (m).



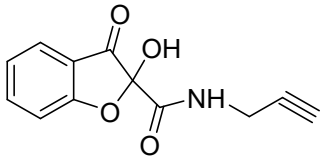
2-hydroxy-3-oxo-*N*-(thiophen-2-ylmethyl)-2,3-dihydrobenzofuran-2-carboxamide

5q: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.07 (t, J = 6.2 Hz, 1H), 8.86 (s, 1H), 7.76 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.5 Hz, 1H), 7.39 (dd, J = 4.6, 1.6 Hz, 1H), 7.23 (d, J = 8.3 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 6.99 – 6.90 (m, 2H), 4.43 (dd, J = 6.2, 1.8 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.47, 171.75, 165.47, 142.02, 139.71, 127.05, 126.11, 125.63, 124.95, 122.90, 119.47, 113.70, 101.04, 37.74.



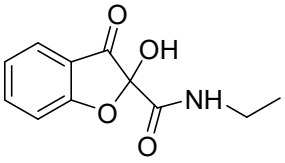
2-hydroxy-3-oxo-*N*-phenethyl-2,3-dihydrobenzofuran-2-carboxamide

5r: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 2H), 7.26 (t, J = 7.3 Hz, 3H), 7.12 (d, J = 7.1 Hz, 2H), 7.03 (t, J = 7.4 Hz, 2H), 6.66 (t, J = 5.7 Hz, 1H), 6.52 (s, 1H), 3.44 (dd, J = 13.4, 6.9 Hz, 2H), 2.76 (t, J = 7.1 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.01, 171.65, 165.10, 139.31, 138.20, 128.82, 128.70, 126.67, 125.24, 122.95, 118.63, 113.52, 99.73, 41.24, 35.27.



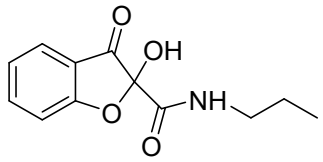
2-hydroxy-3-oxo-*N*-(prop-2-yn-1-yl)-2,3-dihydrobenzofuran-2-carboxamide

5s: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.90 (s, 1H), 7.80 – 7.75 (m, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.24 (d, J = 8.3 Hz, 1H), 7.18 (t, J = 7.4 Hz, 1H), 3.88 – 3.82 (m, 2H), 3.12 (s, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.35, 171.68, 165.47, 139.77, 124.96, 122.97, 119.43, 113.70, 100.89, 81.12, 73.36, 28.64.



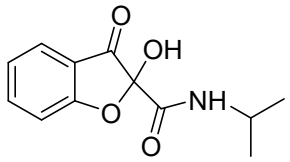
***N*-ethyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5aa: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.79 (s, 1H), 8.46 (t, J = 5.7 Hz, 1H), 7.76 (t, J = 7.8 Hz, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.23 (d, J = 8.3 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 3.20 – 3.03 (m, 2H), 1.03 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.80, 171.79, 165.20, 139.62, 124.88, 122.80, 119.59, 113.64, 101.00, 34.05, 15.04.



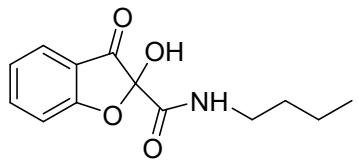
2-hydroxy-3-oxo-*N*-propyl-2,3-dihydrobenzofuran-2-carboxamide

5ab: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.56 (m, 2H), 7.09 (t, J = 8.0 Hz, 2H), 6.58 (s, 1H), 6.33 (s, 1H), 3.19 (dd, J = 13.5, 6.8 Hz, 2H), 1.56 – 1.47 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.37, 171.80, 165.20, 139.14, 125.08, 122.70, 118.66, 113.47, 99.81, 41.52, 22.38, 11.19.



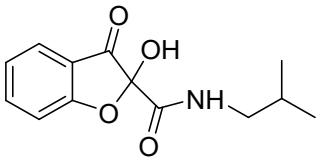
2-hydroxy-*N*-isopropyl-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

5ac: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.58 (m, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.07 (t, J = 8.2 Hz, 2H), 6.54 (s, 1H), 6.48 (d, J = 7.8 Hz, 1H), 3.95 (tt, J = 13.3, 6.6 Hz, 1H), 1.13 (d, J = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.24, 171.79, 164.17, 139.24, 125.21, 122.86, 118.66, 113.55, 99.58, 42.42, 22.29.



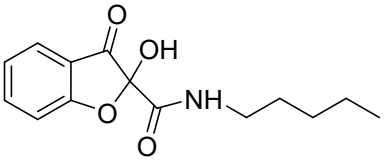
***N*-butyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5ad: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (t, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 8.2 Hz, 2H), 6.67 (s, 1H), 3.19 (dd, *J* = 13.4, 6.8 Hz, 2H), 1.45 (dd, *J* = 14.8, 7.4 Hz, 2H), 1.32 – 1.25 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.17, 171.79, 165.10, 139.32, 125.32, 122.91, 118.61, 113.59, 99.67, 39.17, 31.13, 19.88, 13.71.



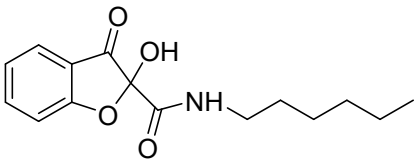
2-hydroxy-*N*-isobutyl-3-oxo-2,3-dihydrobenzofuran-2-carboxamide

5ae: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.58 (m, 2H), 7.15 – 7.06 (m, 2H), 6.59 (s, 1H), 6.29 (s, 1H), 3.05 (td, *J* = 6.7, 2.1 Hz, 2H), 1.81 – 1.71 (m, 1H), 0.87 (dd, *J* = 6.7, 0.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.18, 171.82, 165.22, 139.30, 125.31, 122.88, 118.61, 113.59, 99.74, 47.13, 28.31, 19.90 (d, *J* = 2.6 Hz).



2-hydroxy-3-oxo-*N*-pentyl-2,3-dihydrobenzofuran-2-carboxamide

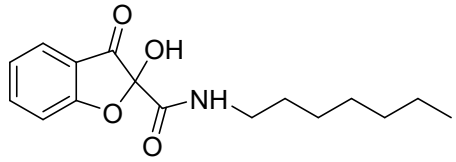
5af: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 – 7.59 (m, 2H), 7.13 (dd, *J* = 12.3, 5.1 Hz, 2H), 6.51 (s, 1H), 6.21 (s, 1H), 3.22 (dd, *J* = 13.7, 6.8 Hz, 2H), 1.49 (dt, *J* = 14.6, 7.4 Hz, 2H), 1.32 – 1.25 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.15, 171.78, 165.09, 139.29, 125.32, 122.89, 118.64, 113.59, 99.68, 40.05, 28.82, 28.77, 22.26, 13.97.



***N*-hexyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

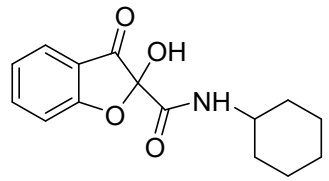
5ag: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product

as a colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 2H), 7.17 – 7.09 (m, 2H), 6.48 (s, 1H), 6.20 (s, 1H), 3.23 (dd, *J* = 13.8, 6.7 Hz, 2H), 1.48 (dd, *J* = 14.1, 7.0 Hz, 2H), 1.31 – 1.25 (m, 6H), 0.87 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.15, 171.78, 165.08, 139.27, 125.31, 122.88, 118.67, 113.58, 99.70, 40.08, 31.36, 29.05, 26.37, 22.51, 14.02.



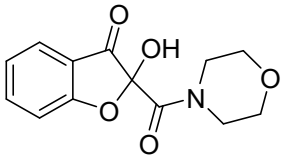
***N*-heptyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5ah: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 2H), 7.18 – 7.09 (m, 2H), 6.46 (s, 1H), 6.18 (s, 1H), 3.23 (dd, *J* = 13.8, 6.7 Hz, 2H), 1.53 – 1.45 (m, 2H), 1.28 (d, *J* = 18.3 Hz, 8H), 0.87 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.11, 171.77, 165.07, 139.30, 125.34, 122.91, 118.63, 113.59, 99.66, 40.10, 31.68, 29.08, 28.87, 26.66, 22.59, 14.10.



***N*-cyclohexyl-2-hydroxy-3-oxo-2,3-dihydrobenzofuran-2-carboxamide**

5ai: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 – 7.58 (m, 2H), 7.21 – 7.08 (m, 2H), 6.35 (d, *J* = 7.3 Hz, 1H), 3.69 (dd, *J* = 11.2, 7.3 Hz, 1H), 1.87 (d, *J* = 11.6 Hz, 2H), 1.69 (d, *J* = 12.8 Hz, 2H), 1.60 (d, *J* = 12.7 Hz, 1H), 1.38 – 1.24 (m, 3H), 1.21 – 1.08 (m, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 197.78, 171.79, 164.49, 139.57, 124.87, 122.78, 119.60, 113.64, 100.92, 48.48, 32.34, 25.48, 25.28.

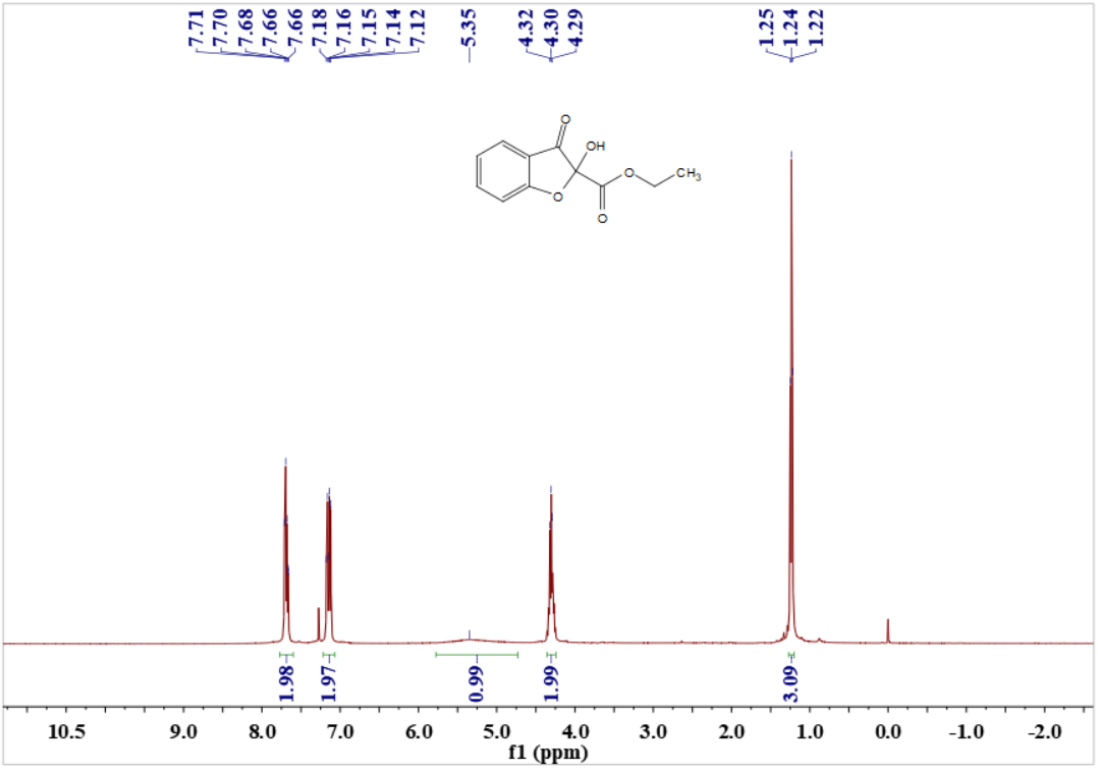


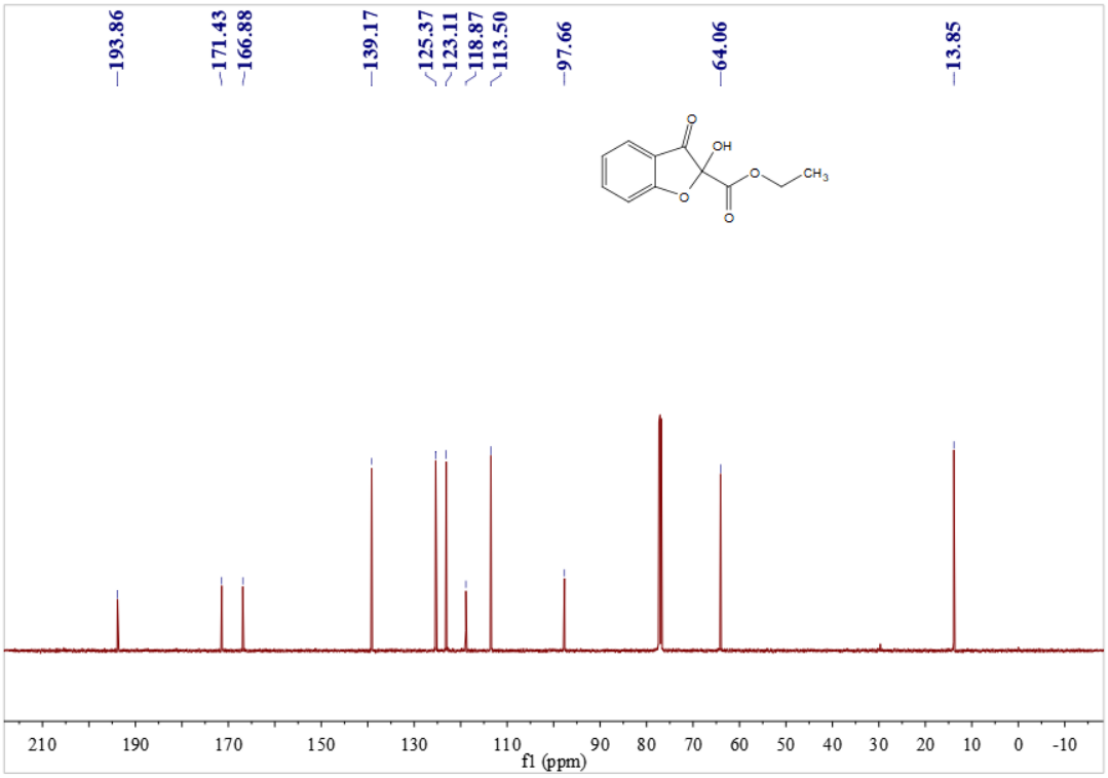
2-hydroxy-2-(morpholine-4-carbonyl)benzofuran-3(2*H*)-one

5aj: Flash column chromatography (petroleum/ethyl acetate 4:1) afforded the product

as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.26 (s, 1H), 7.61 – 7.54 (m, 2H), 7.07 – 7.02 (m, 1H), 6.97 (t, *J* = 7.6 Hz, 1H), 3.85 – 3.76 (m, 4H), 3.71 – 3.65 (m, 2H), 3.44 – 3.38 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.05, 163.55, 163.34, 138.22, 132.01, 119.96, 118.70, 116.79, 66.66 (d, *J* = 10.4 Hz), 46.39, 41.66.

11. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR for the products.

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64.06
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O
O
CH3
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150
130
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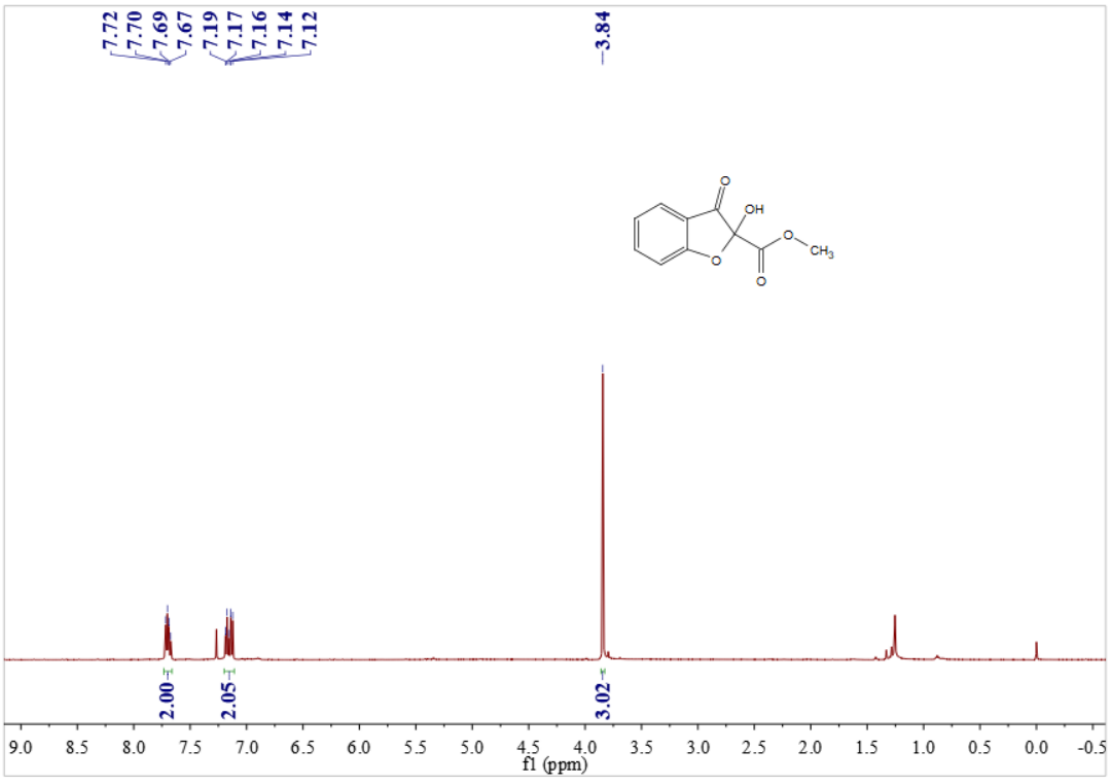
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.69
7.67
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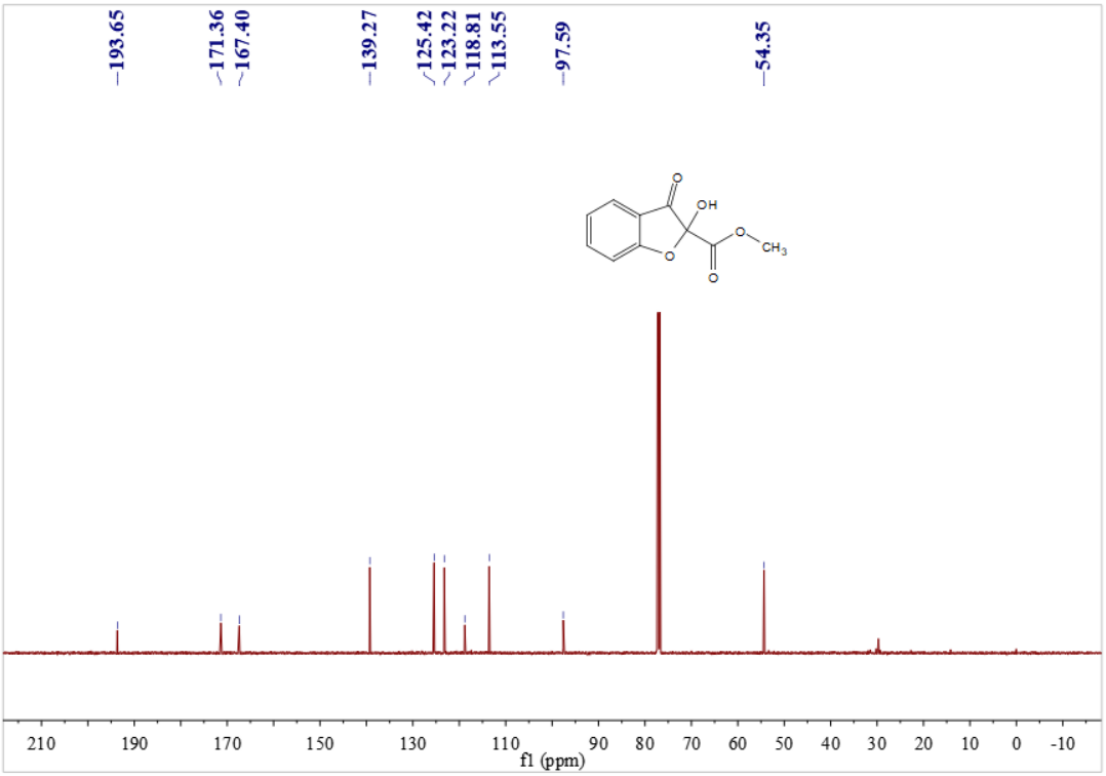
7.17
7.16
7.14
7.12
3.84
OH
O
O
O
CH3
2.00
2.05
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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113.55
97.59
54.35
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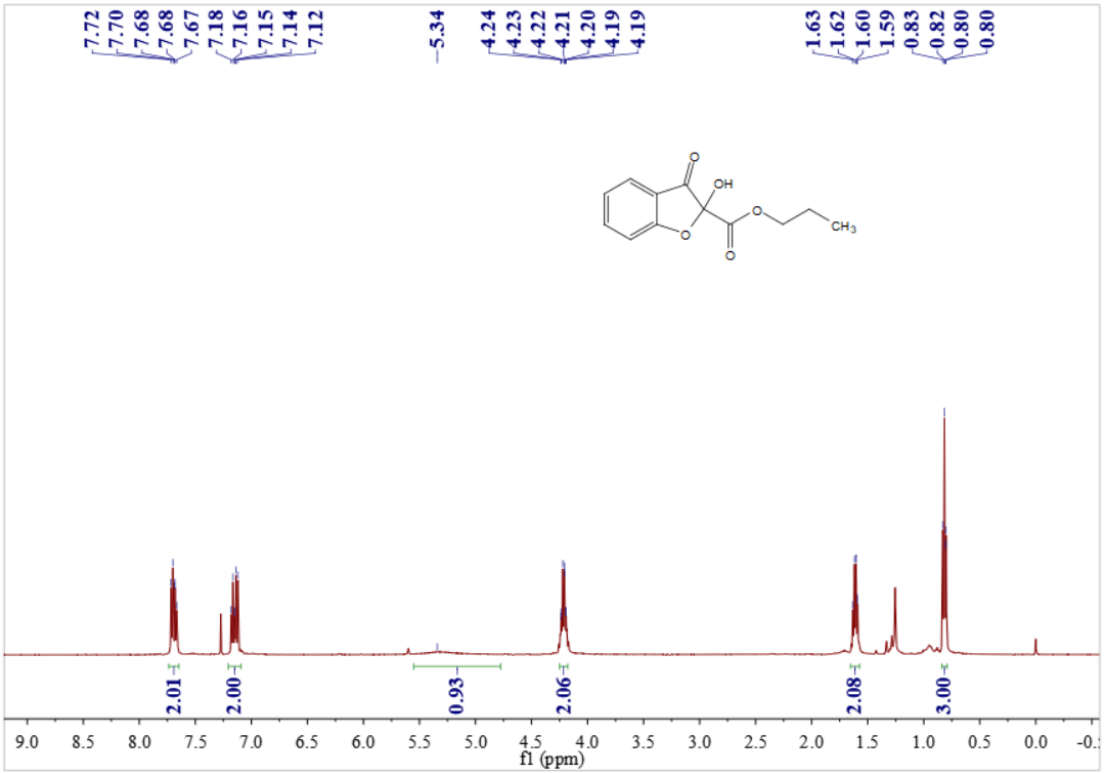
O
CH3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.12
5.34
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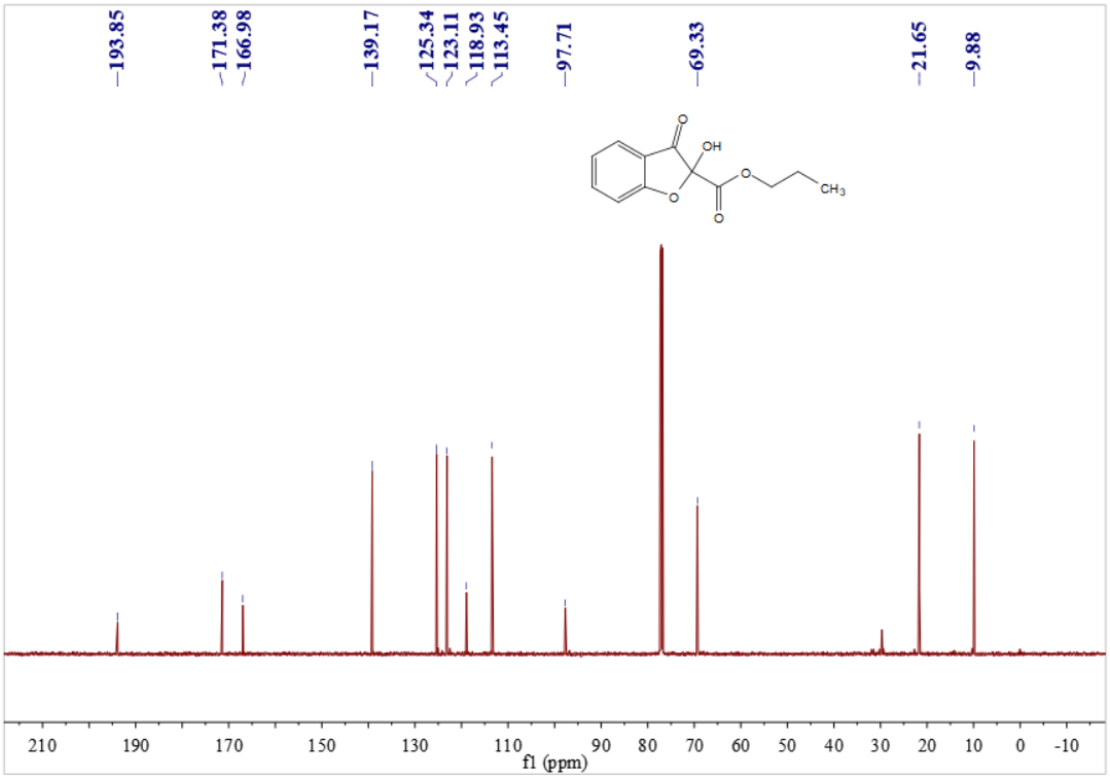
4.22
4.21
4.20
4.19
4.19
1.63
1.62
1.60
1.59
0.83
0.82
0.80
0.80
OH
O
CH3
2.01
2.00
0.93
2.06
2.08
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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113.45
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21.65
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O
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150
130
110
90
80
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60
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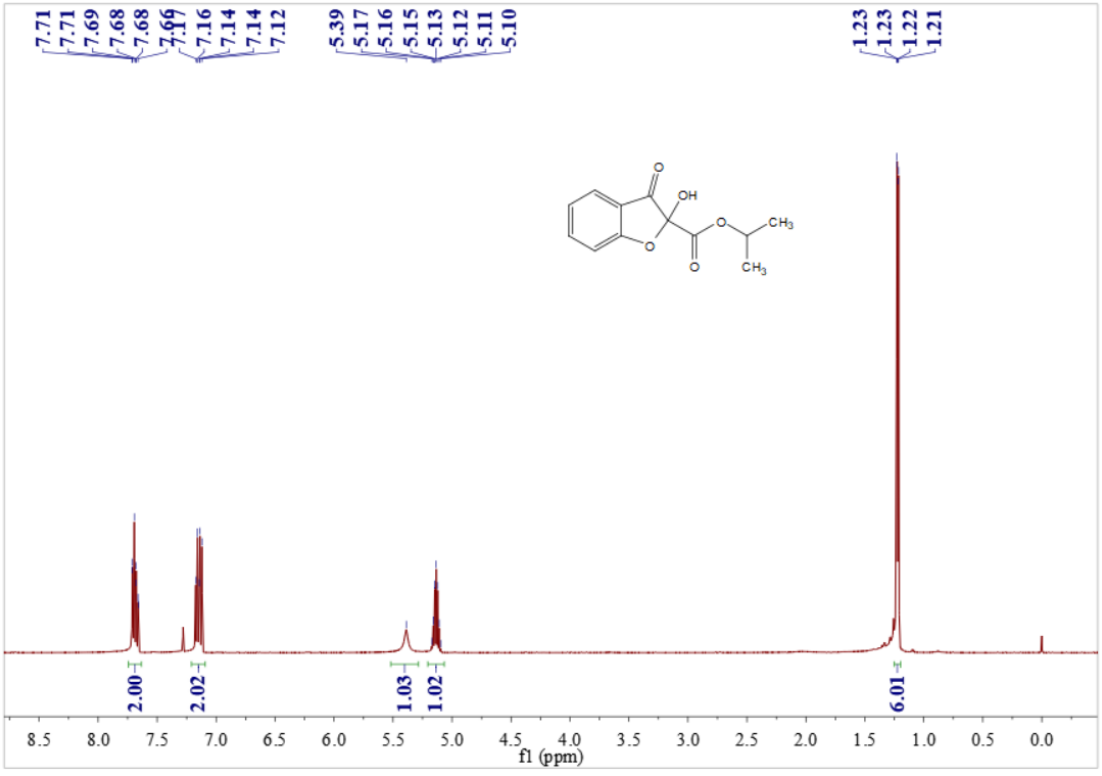
40
30
20
10
0
-10
f1 (ppm)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7.14
7.12
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5.17
5.16
5.15
5.13
5.12
5.11
5.10
1.23
1.23
1.22
1.21
OH
O
CH3
CH3
2.00
2.02
1.03
1.02
6.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.5
1.0
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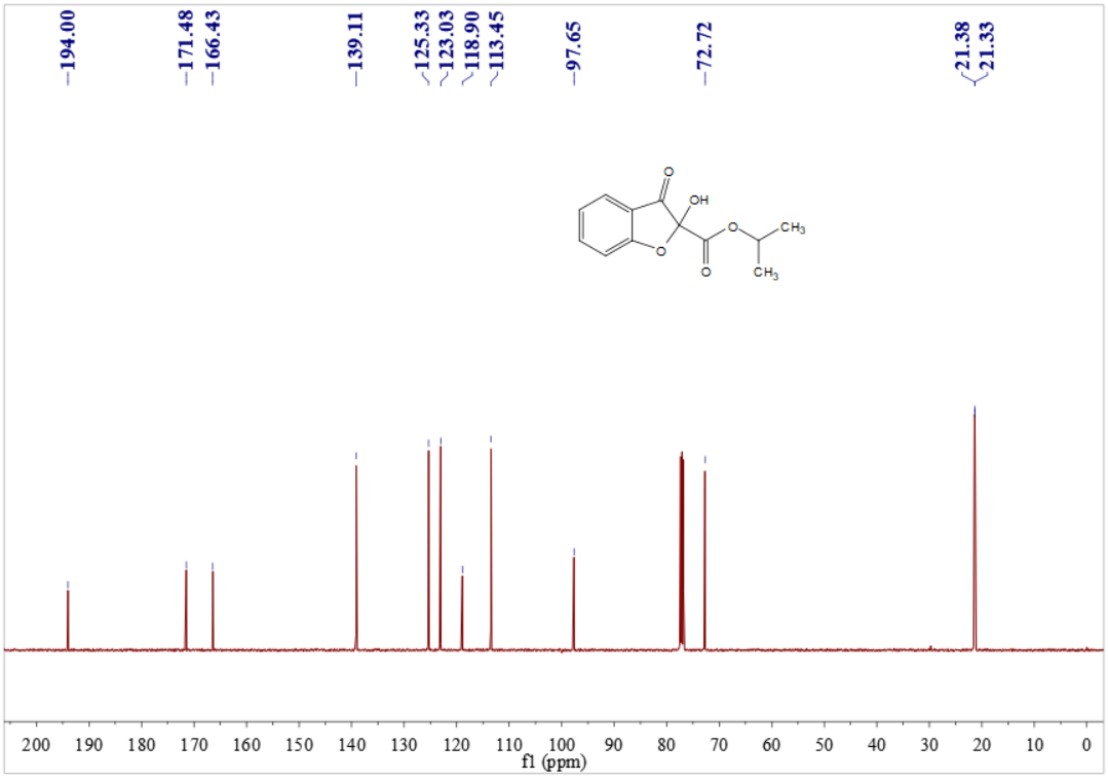
0.0
f1 (ppm)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113.45
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72.72
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21.33
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O
O
O
CH3
CH3
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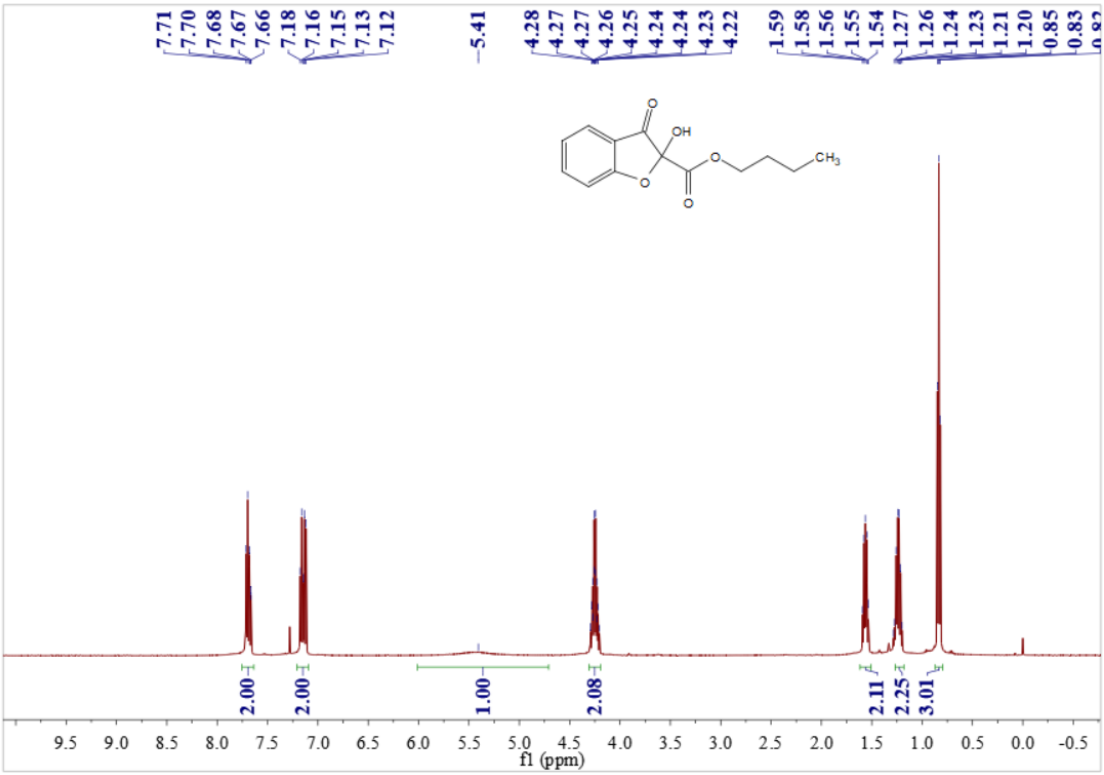
f1 (ppm)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4.24
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4.23
4.22
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1.58
1.56
1.55
1.54
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1.26
1.24
1.23
1.21
1.20
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0.83
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O
O
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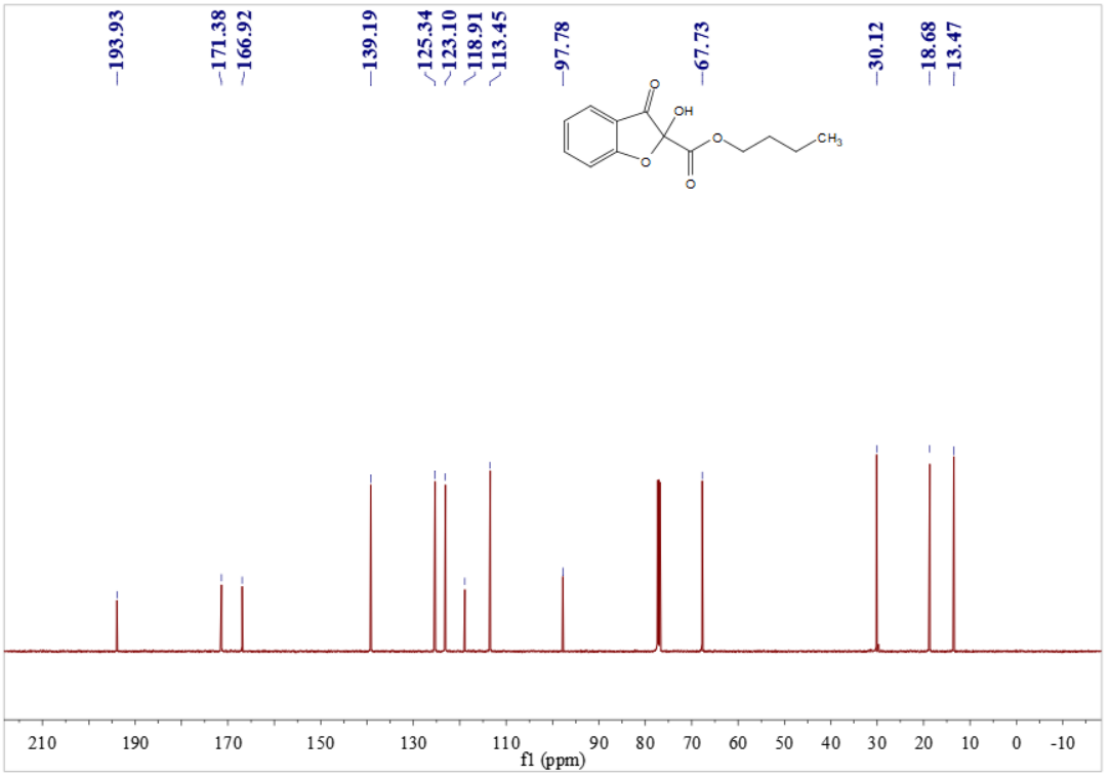
2.00
1.00
2.08
2.11
2.25
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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118.91
113.45
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CH3
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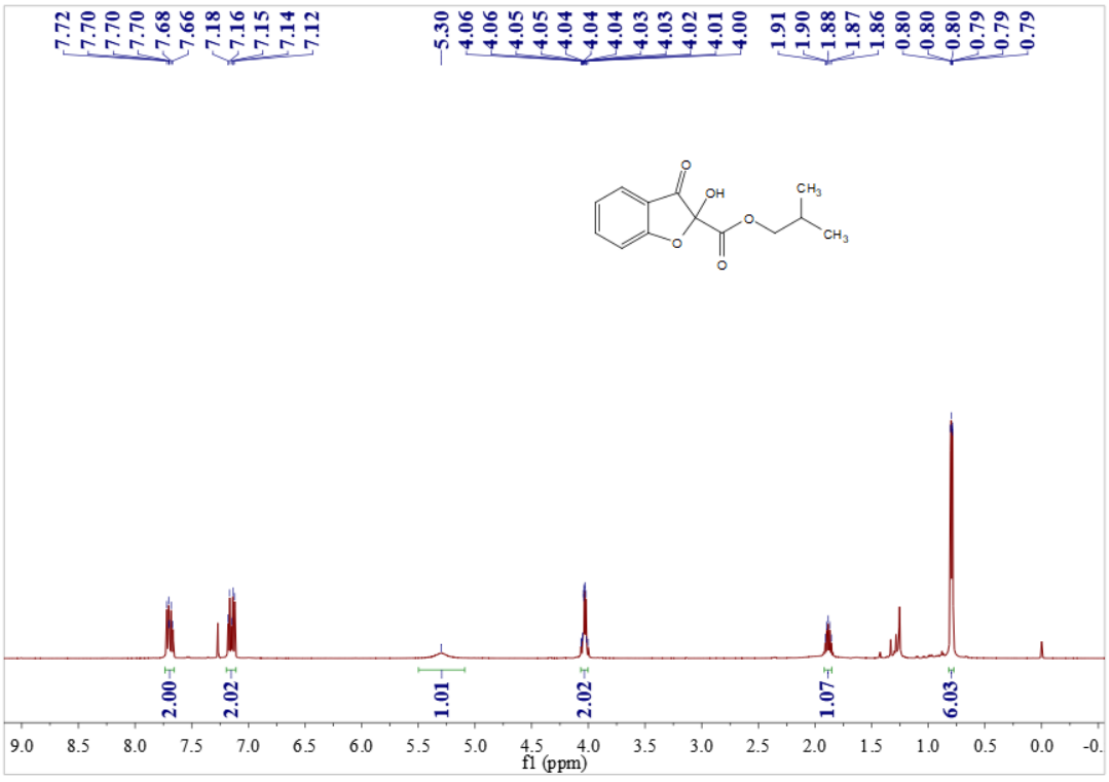
f1 (ppm)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7.16
7.15
7.14
7.12
5.30
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4.02
4.01
4.00
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1.87
1.86
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0.80
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0.79
0.79
0.79
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CH3
CH3
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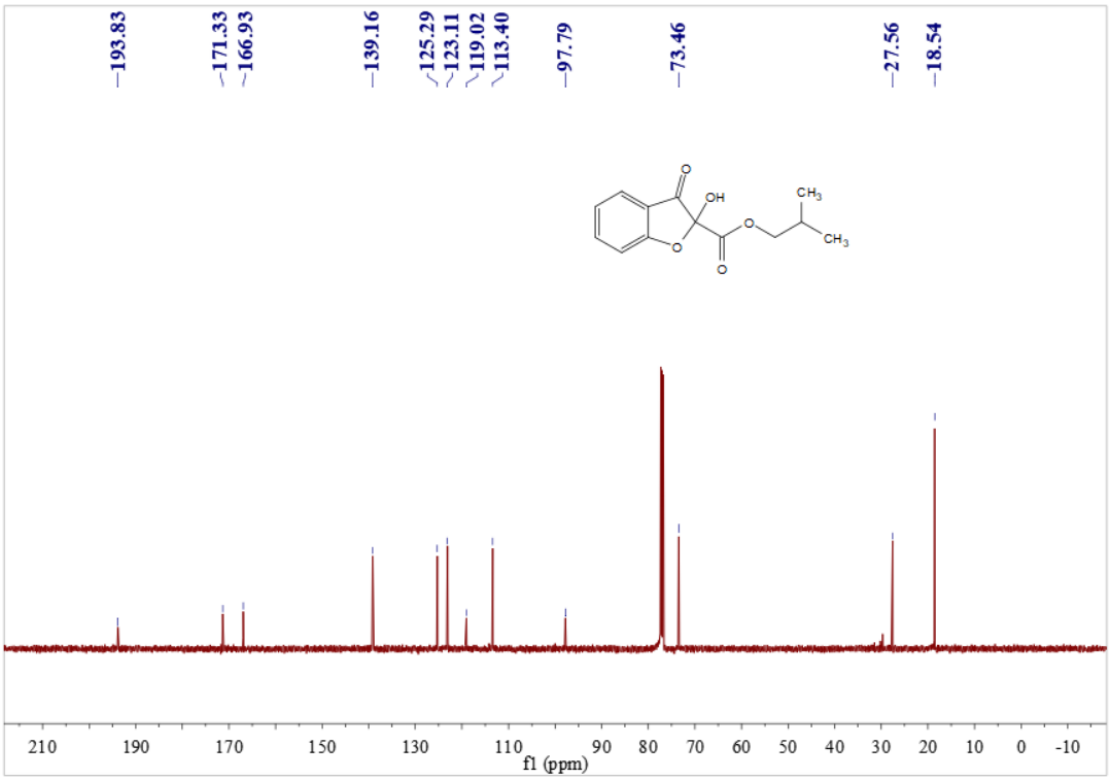
2.02
1.01
2.02
1.07
6.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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18.54
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40
30
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0
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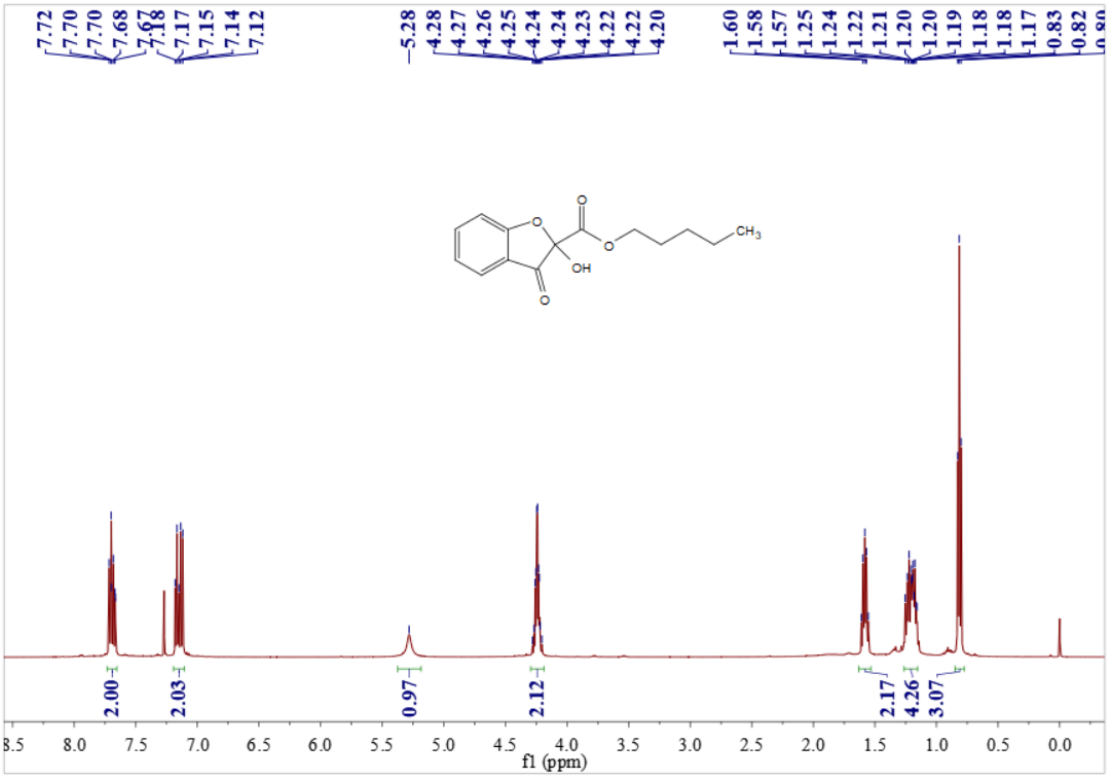
f1 (ppm)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4.27
4.26
4.25
4.24
4.24
4.23
4.22
4.22
4.20
1.60
1.58
1.57
1.25
1.24
1.22
1.21
1.20
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1.19
1.18
1.18
1.17
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OH
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CH3
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2.17
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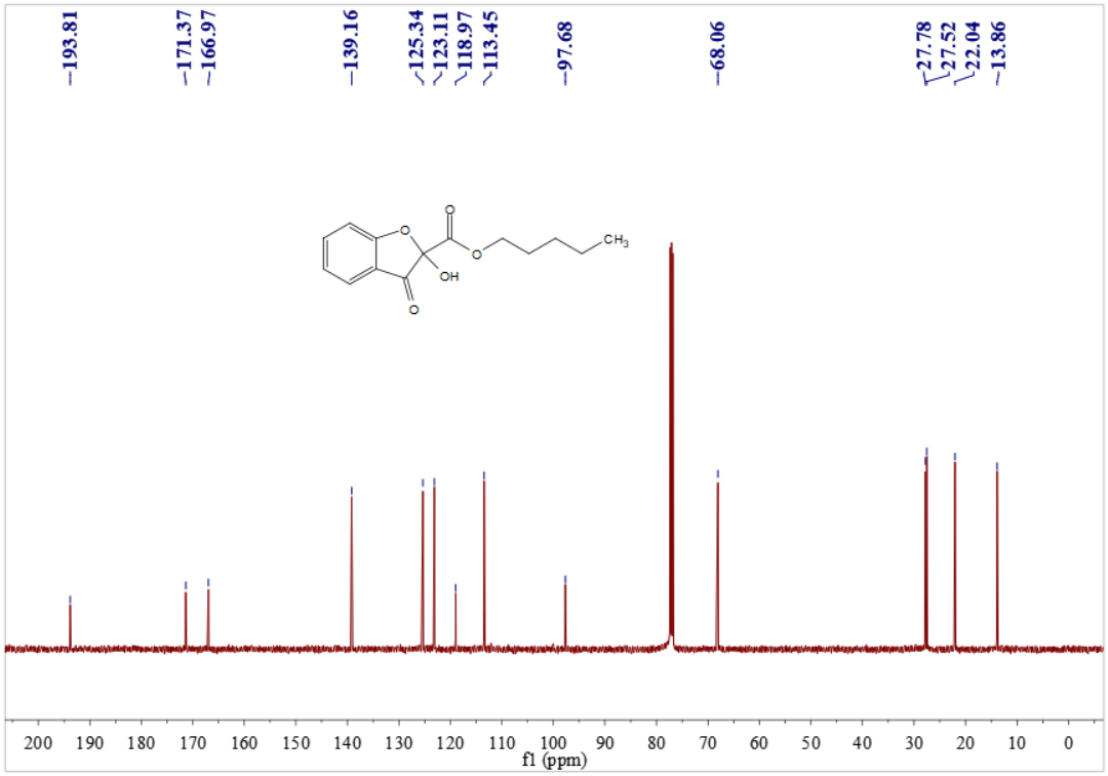
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113.45
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OH
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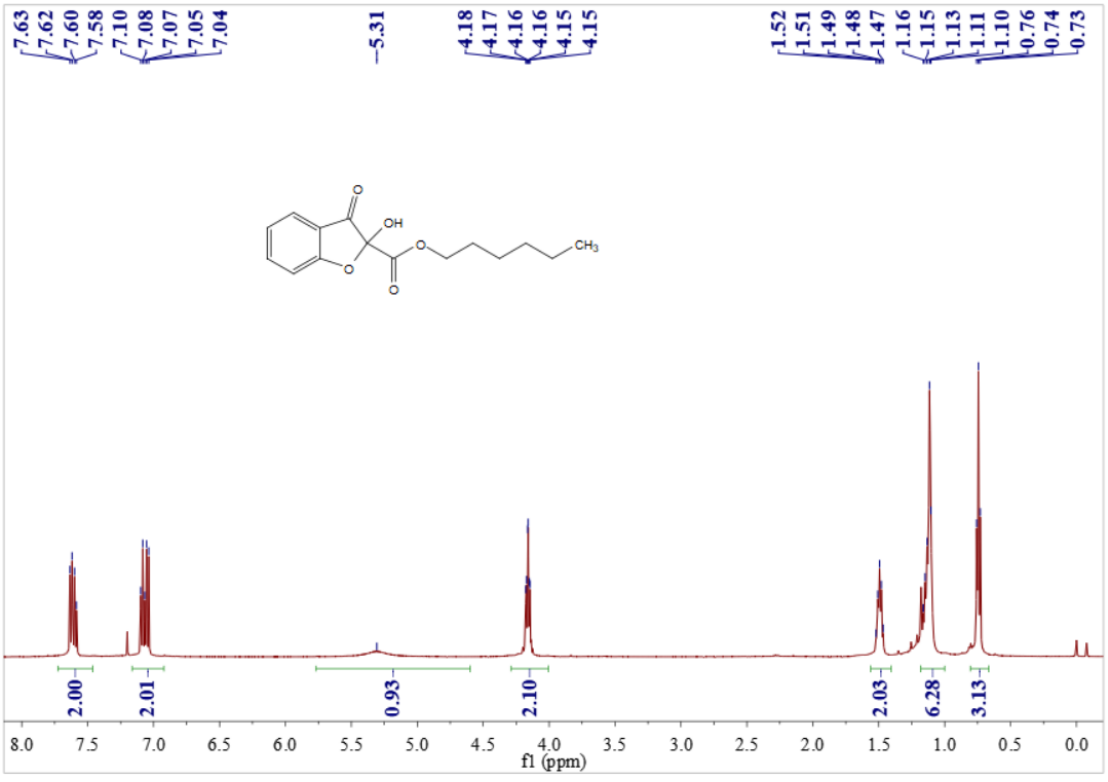
f1 (ppm)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7.05
7.04
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1.52
1.51
1.49
1.48
1.47
1.16
1.15
1.13
1.11
1.10
0.76
0.74
0.73
OH
CH3
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2.01
0.93
2.10
2.03
6.28
3.13
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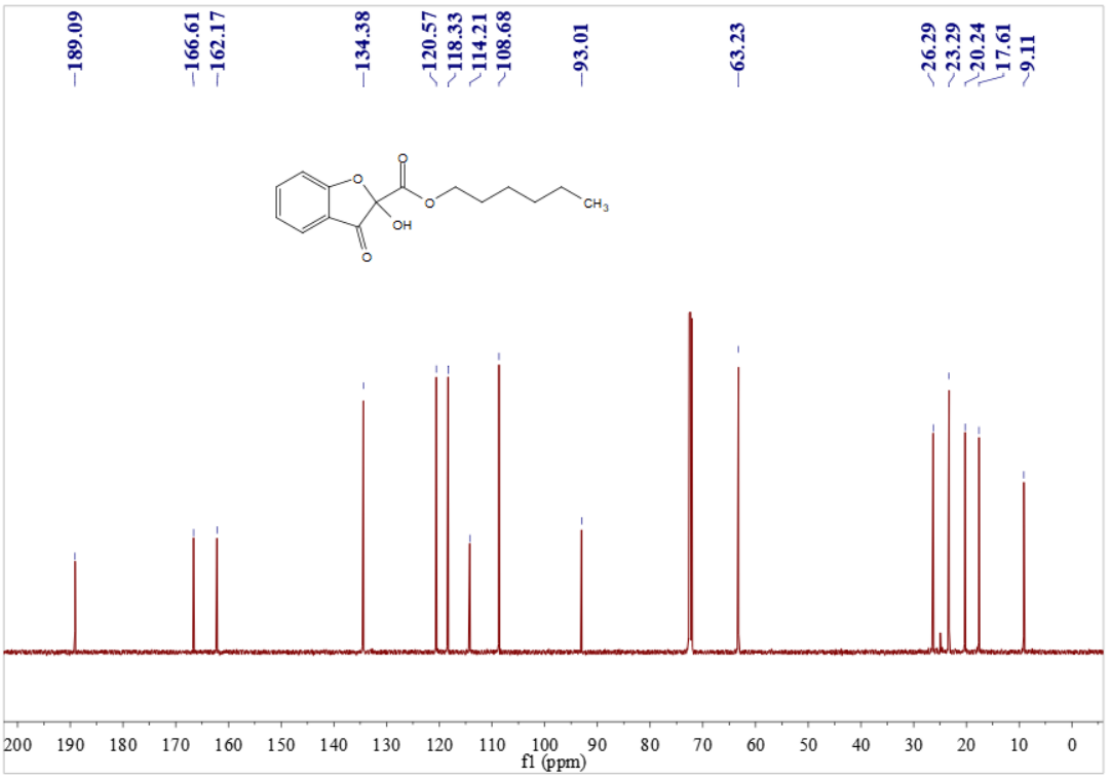
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17.61
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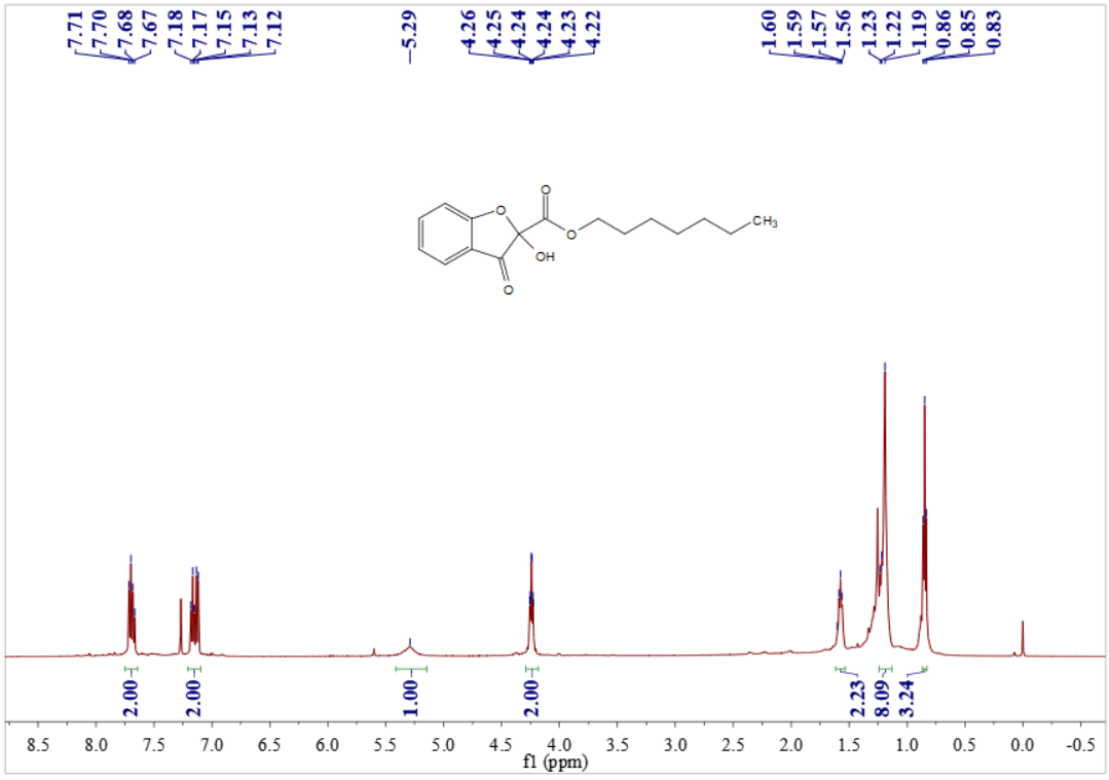
OH
CH3
f1 (ppm)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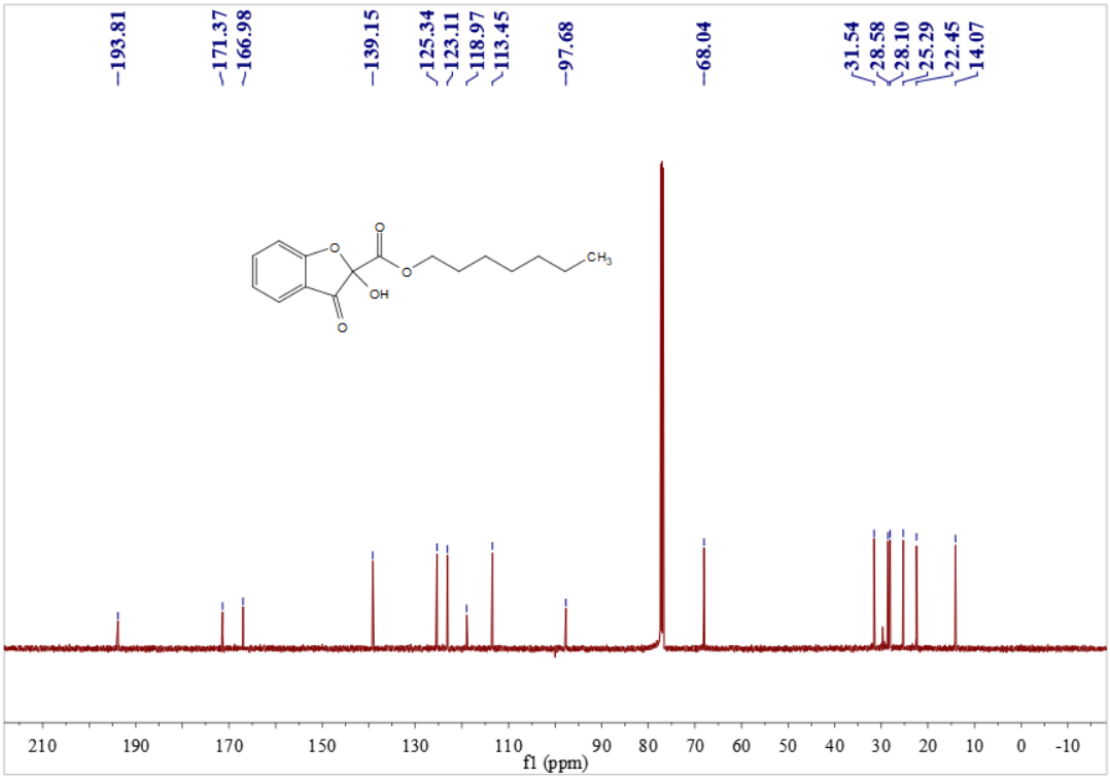
1.00
2.00
2.23
8.09
3.24
OH
CH3
f1 (ppm)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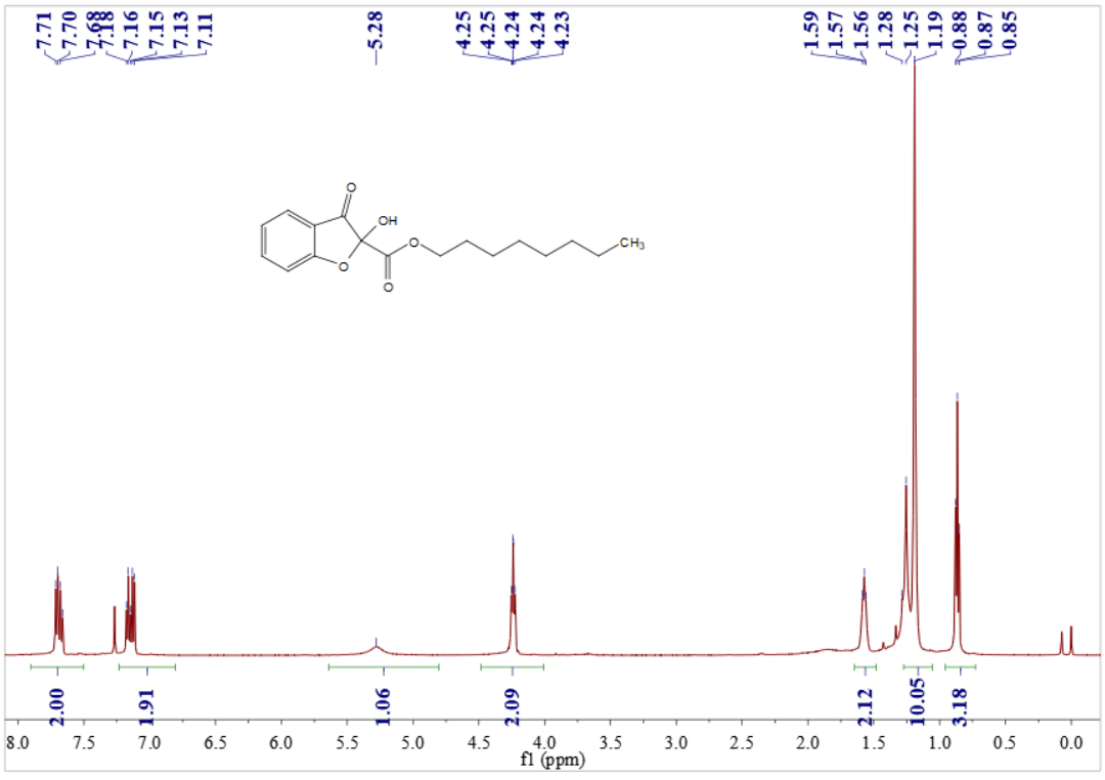
171.37
166.98
139.15
125.34
123.11
118.97
113.45
97.68
68.04
31.54
28.58
28.10
25.29
22.45
14.07
O
O
O
OH
O
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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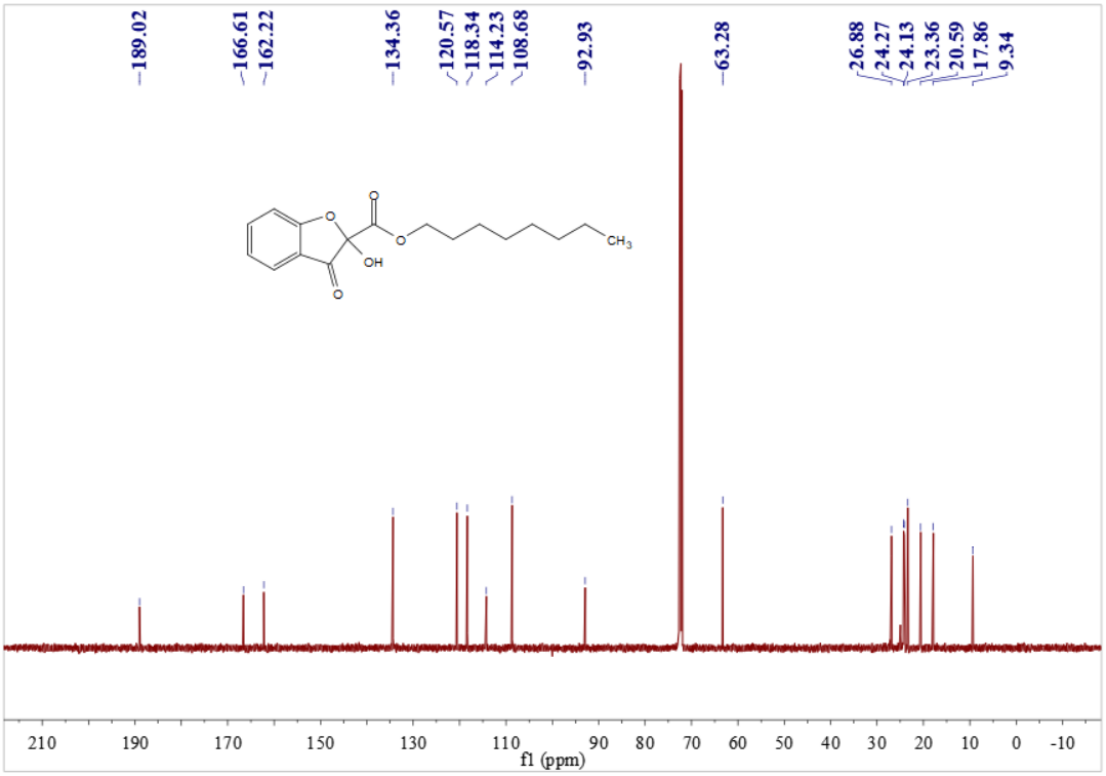
7.70
7.68
7.18
7.16
7.15
7.13
7.11
5.28
4.25
4.25
4.24
4.24
4.23
1.59
1.57
1.56
1.28
1.25
1.19
0.88
0.87
0.85
O
OH
O
O
O
CH3
2.00
1.91
1.06
2.09
2.12
10.05
3.18
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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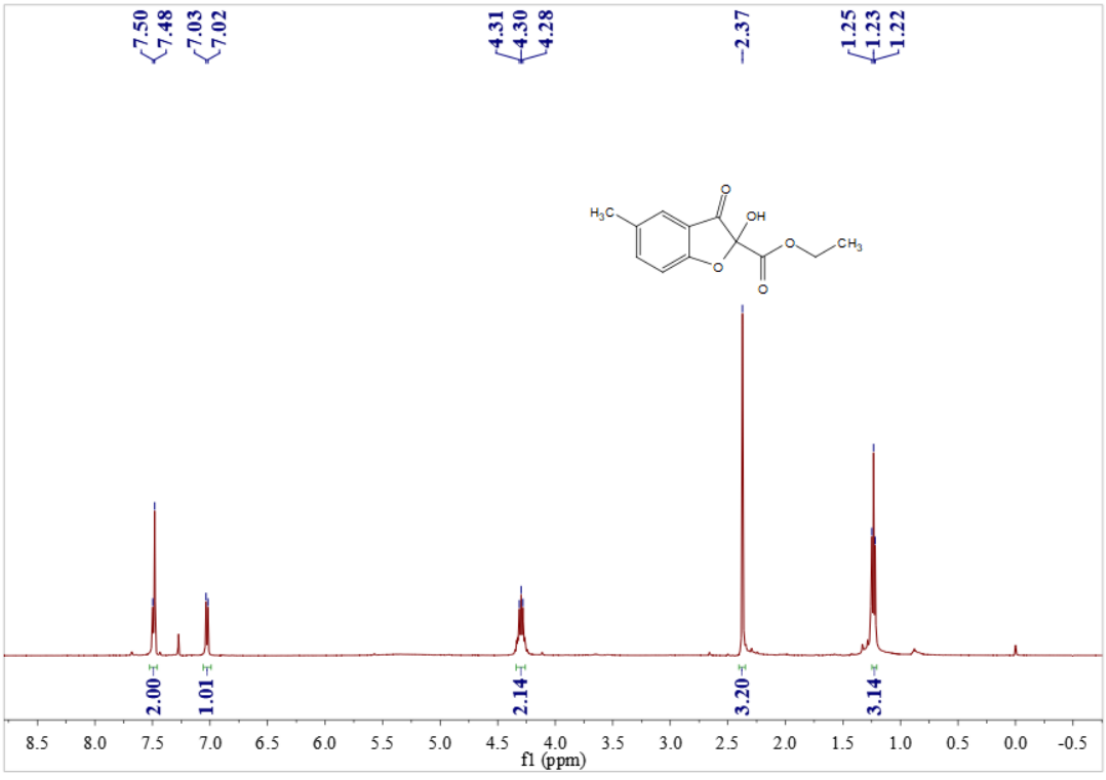
166.61
162.22
134.36
120.57
118.34
114.23
108.68
92.93
63.28
26.88
24.27
24.13
23.36
20.59
17.86
9.34
OH
CH3
f1 (ppm)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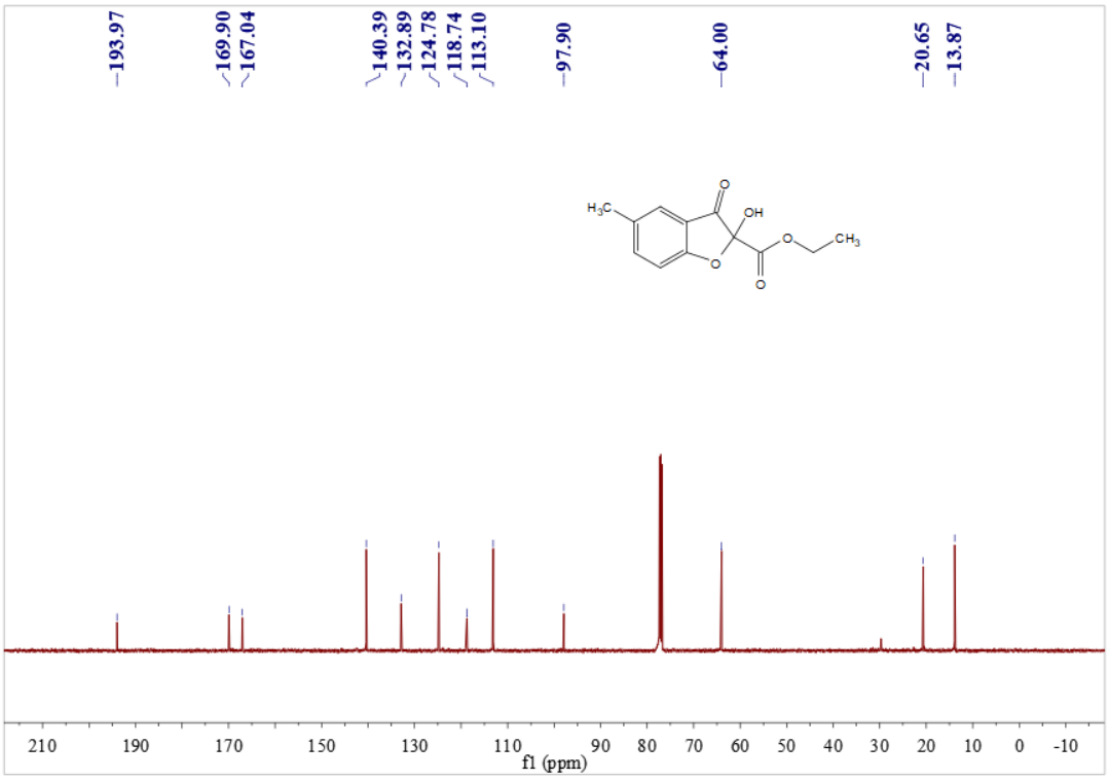
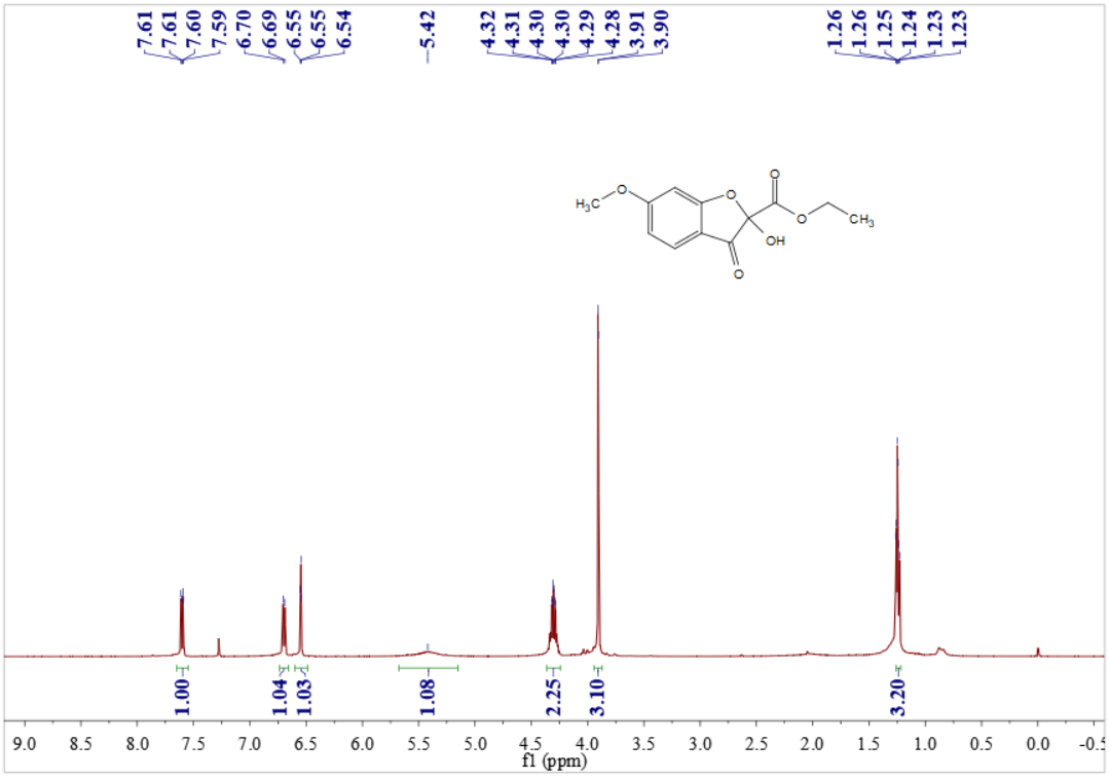
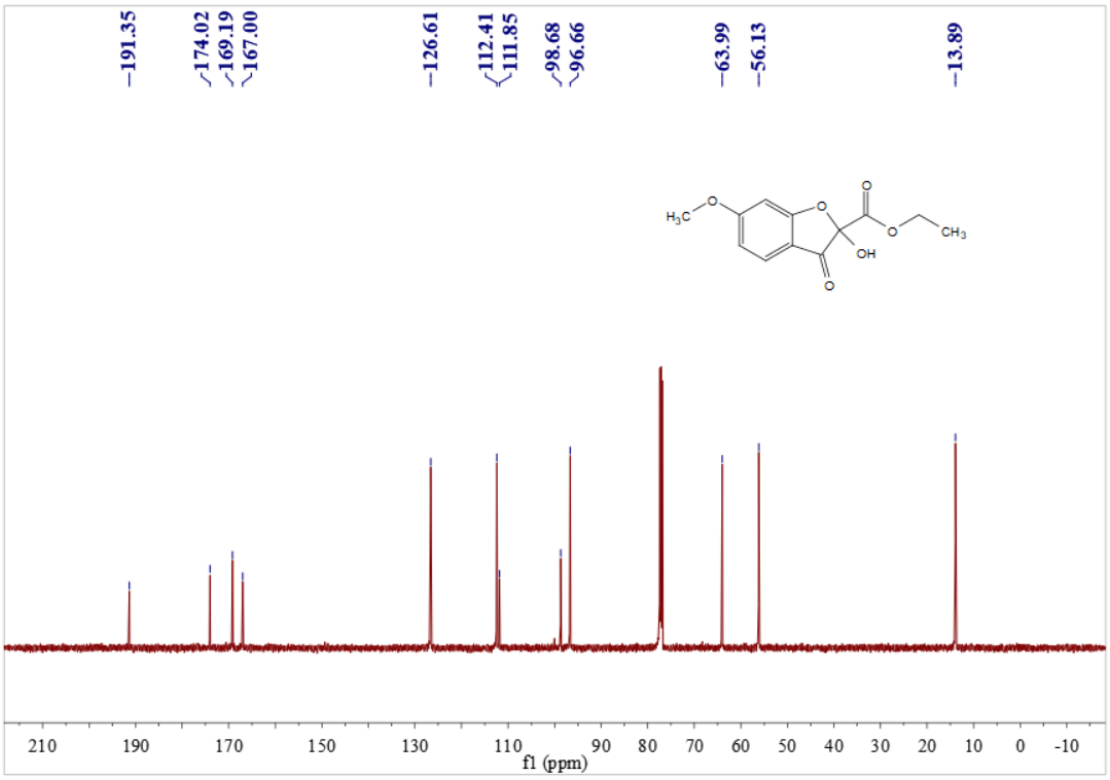
7.48
7.03
7.02
4.31
4.30
4.28
2.37
1.25
1.23
1.22
H3C
OH
CH3
2.00
1.01
2.14
3.20
3.14
f1 (ppm)


193.97
169.90
167.04
140.39
132.89
124.78
118.74
113.10
97.90
64.00
20.65
13.87
H3C
OH
O
CH3
f1 (ppm)


7.61
7.61
7.60
7.59
6.70
6.69
6.55
6.55
6.54
5.42
4.32
4.31
4.30
4.30
4.29
4.28
3.91
3.90
1.26
1.26
1.25
1.24
1.23
1.23
H3C
O
OH
CH3
1.00
1.04
1.03
1.08
2.25
3.10
3.20
f1 (ppm)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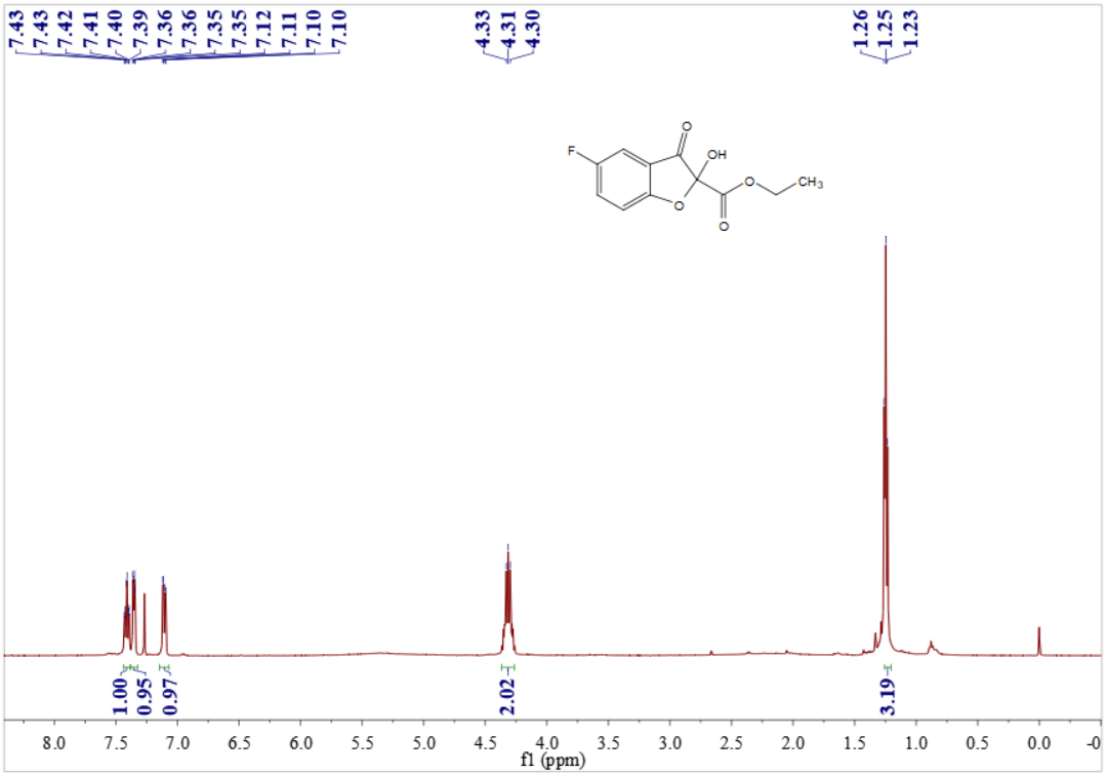
174.02
169.19
167.00
126.61
112.41
111.85
98.68
96.66
63.99
56.13
13.89
H3C
O
O
O
O
CH3
OH
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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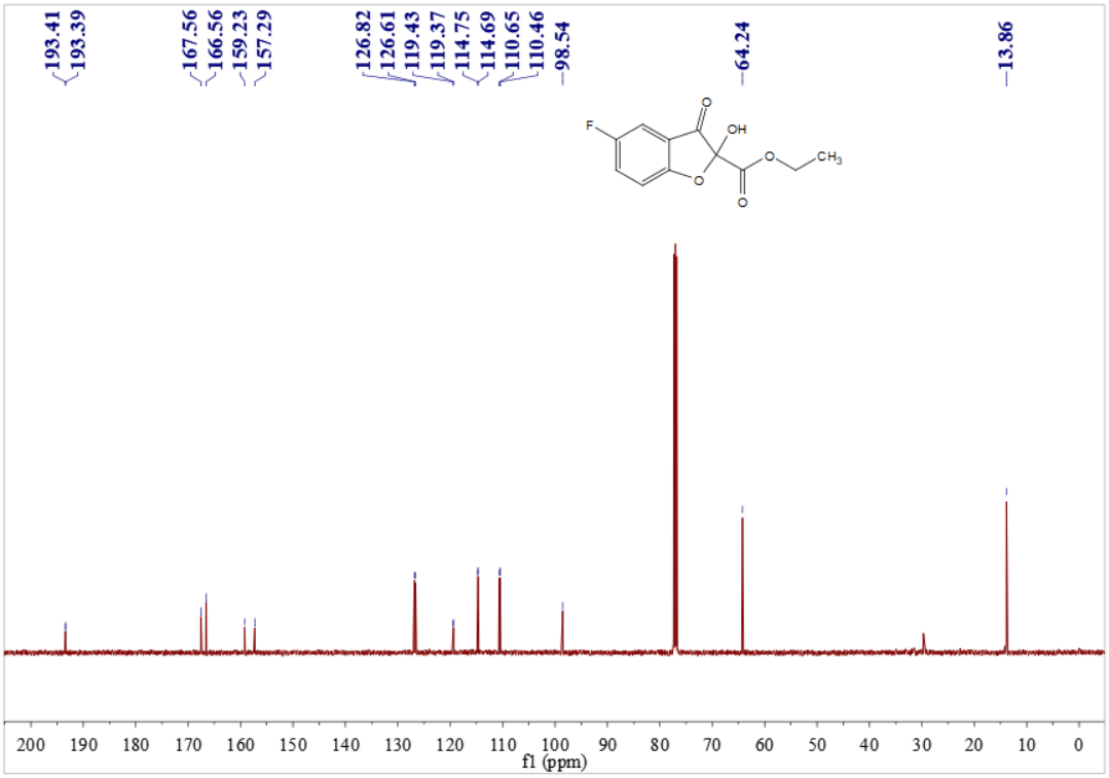
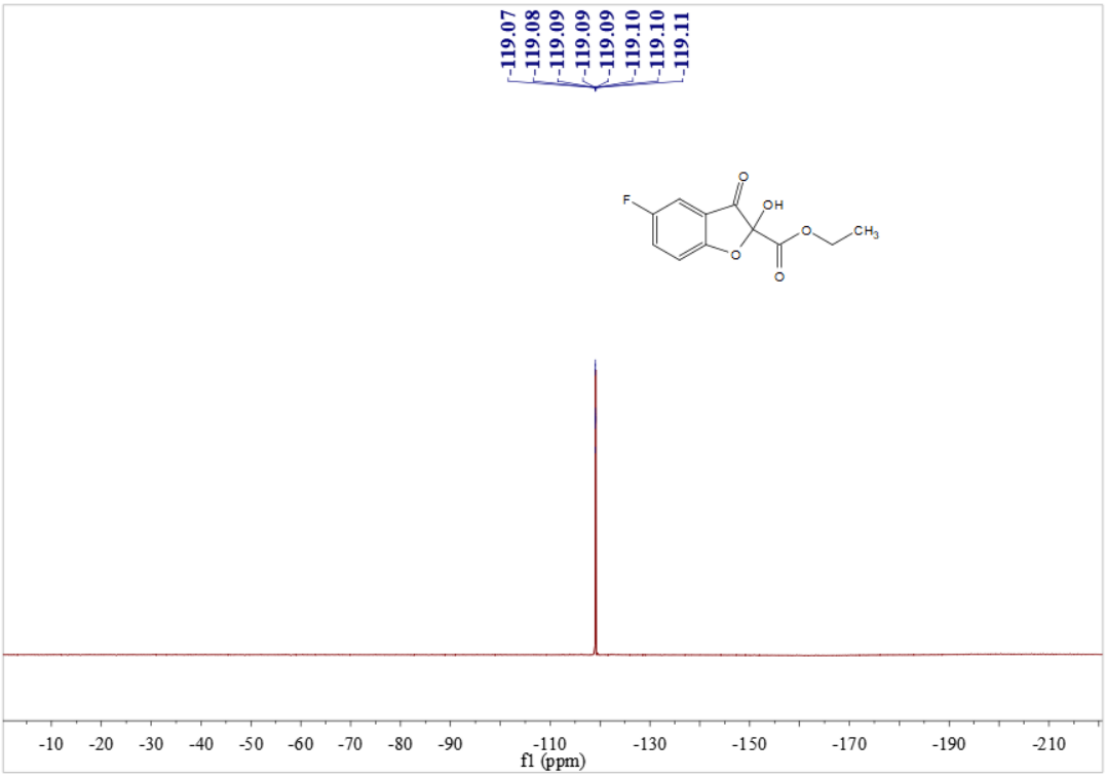
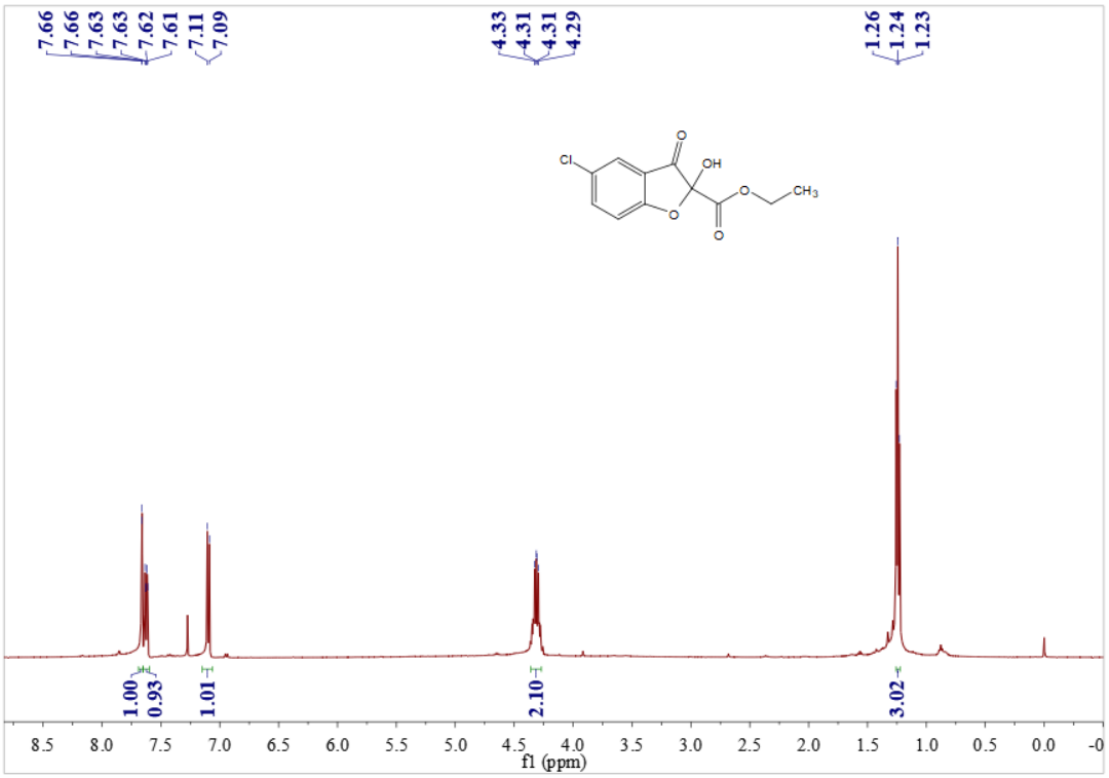
7.43
7.42
7.41
7.40
7.39
7.36
7.36
7.35
7.35
7.12
7.11
7.10
7.10
4.33
4.31
4.30
1.26
1.25
1.23
F
O
OH
O
O
CH3
1.00
0.95
0.97
2.02
3.19
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)


193.41
193.39
167.56
166.56
159.23
157.29
126.82
126.61
119.43
119.37
114.75
114.69
110.65
110.46
98.54
64.24
13.86
F
OH
O
O
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-119.07
-119.08
-119.09
-119.09
-119.09
-119.10
-119.10
-119.11
F
OH
O
O
O
CH3
-10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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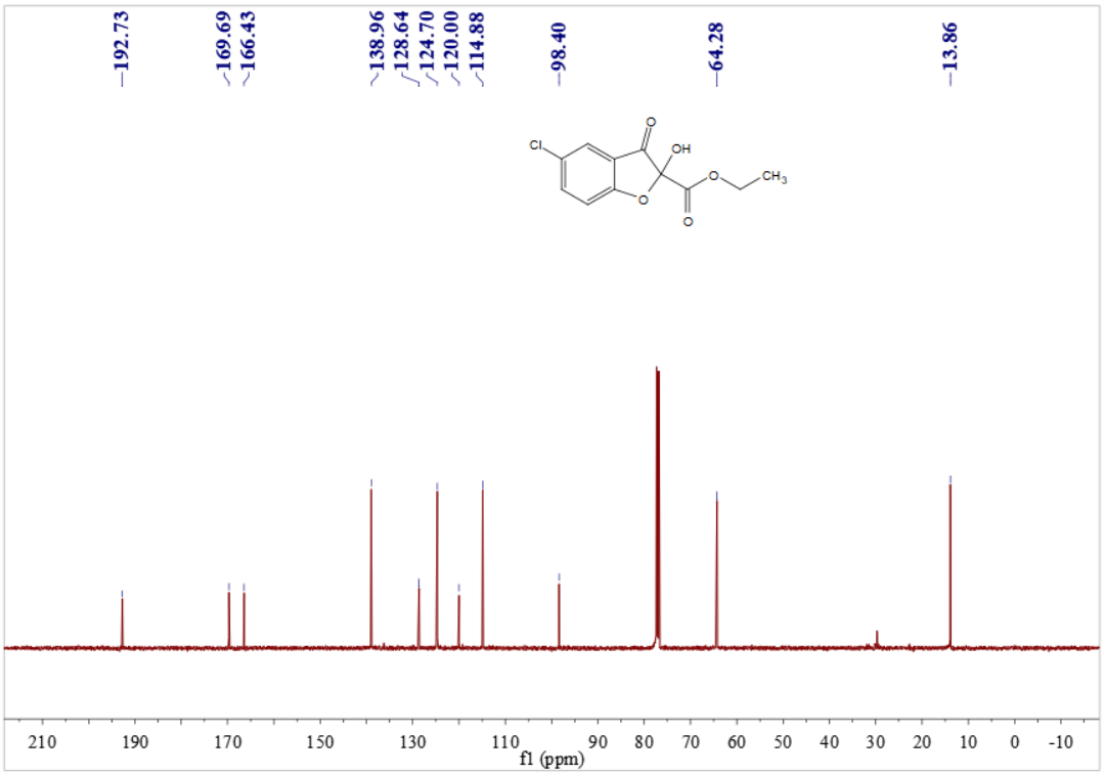
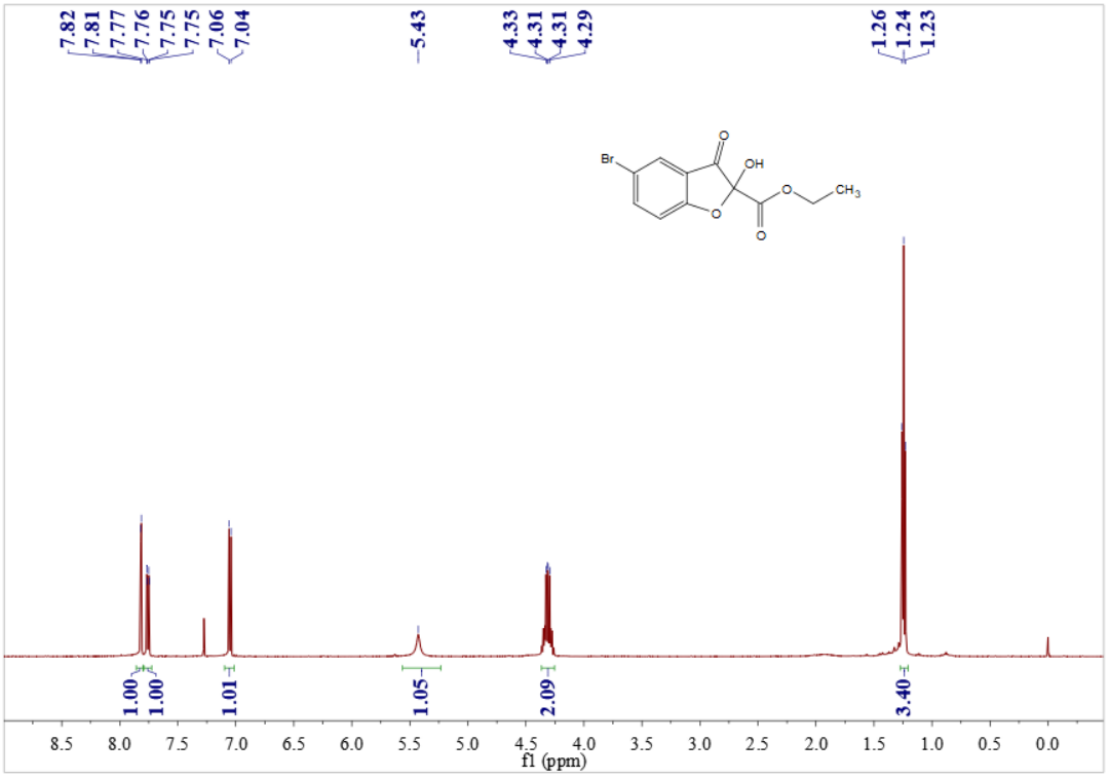
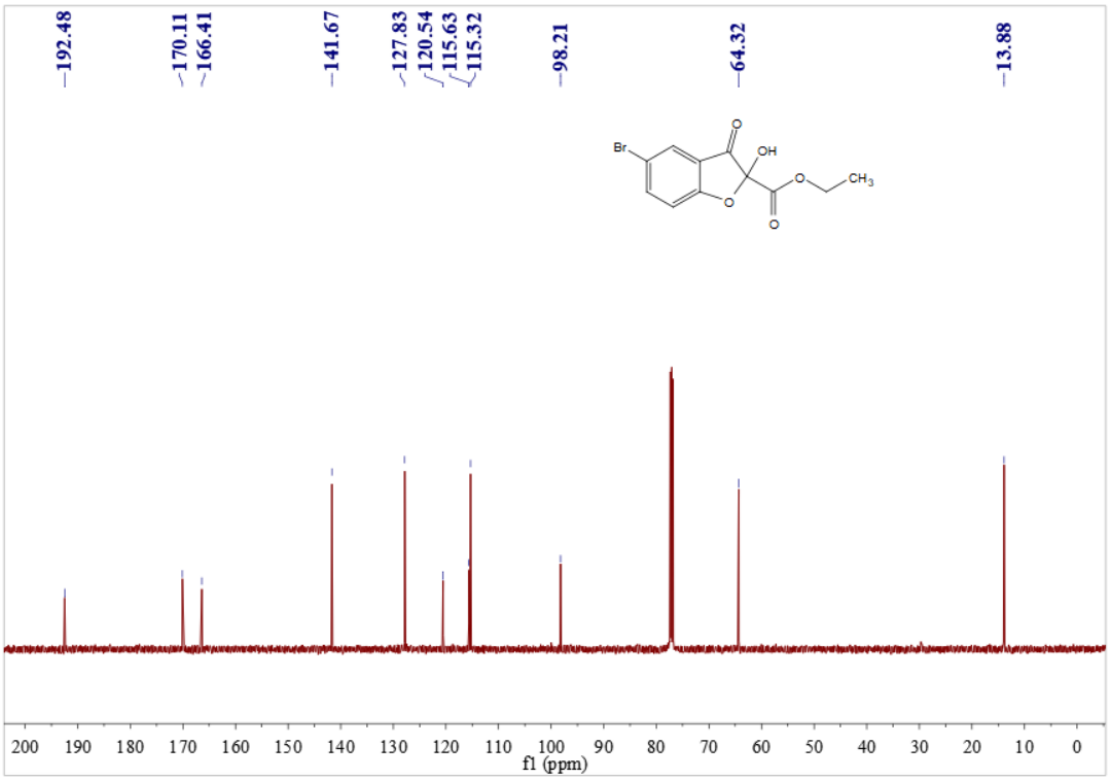
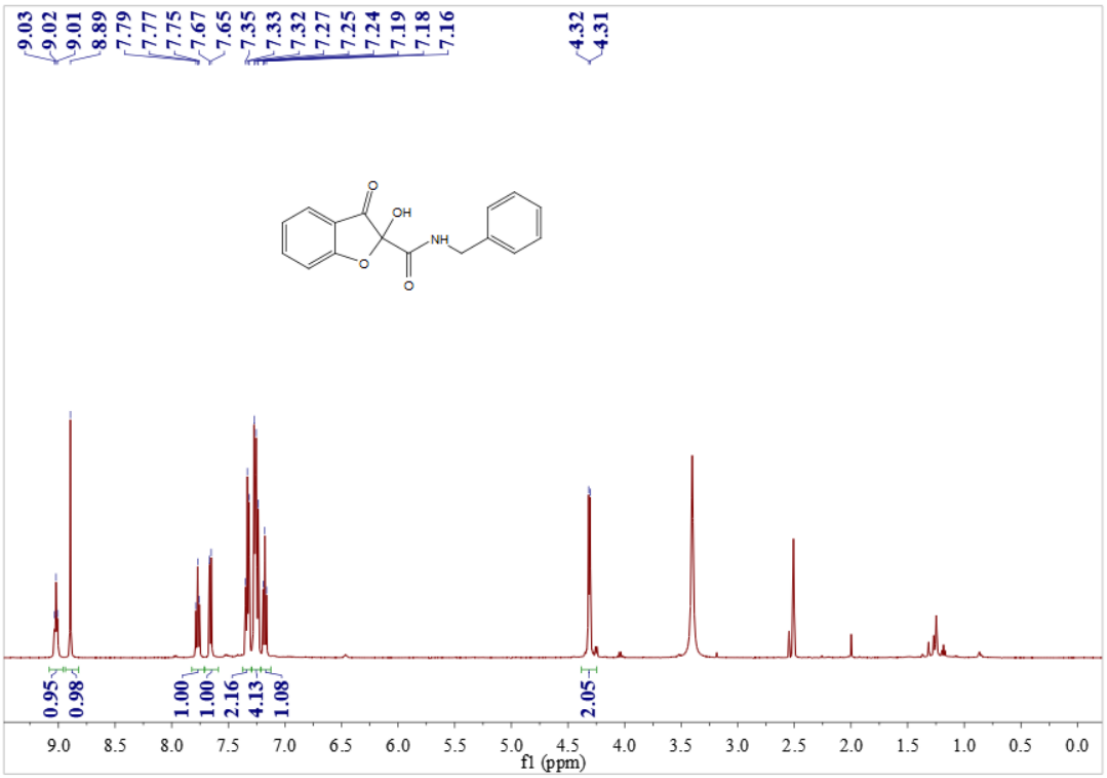
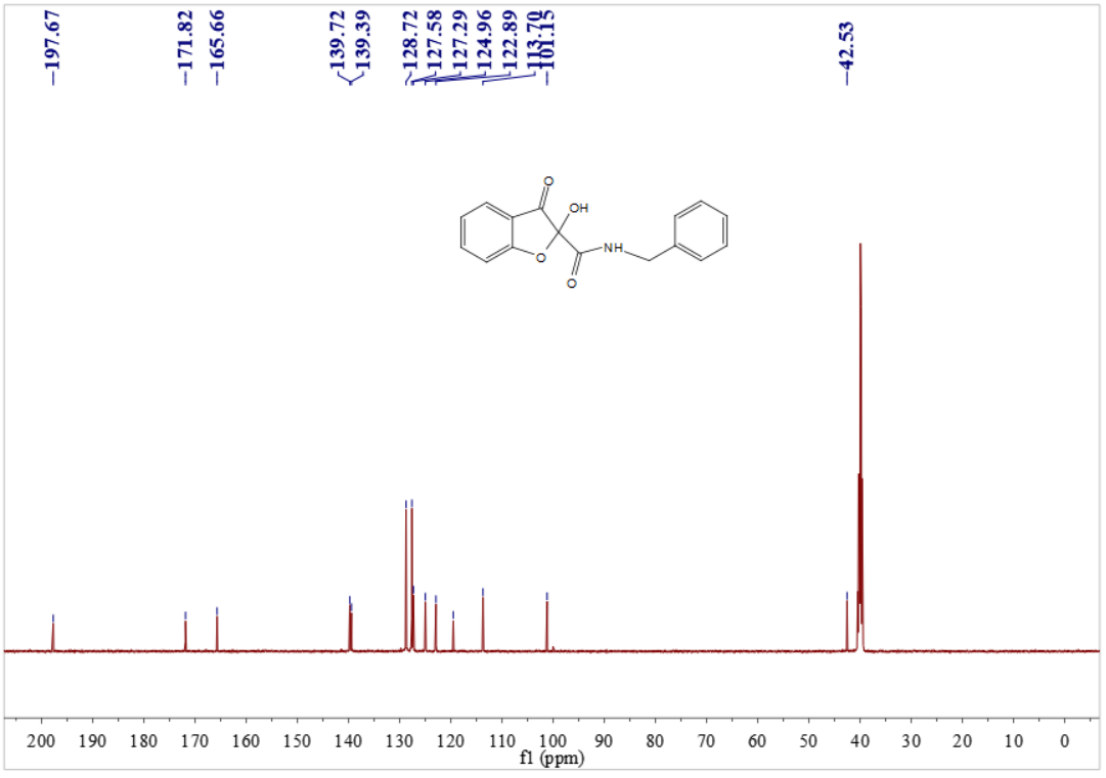
7.66
7.63
7.63
7.62
7.61
7.11
7.09
4.33
4.31
4.31
4.29
1.26
1.24
1.23
Cl
O
OH
O
O
O
CH3
1.00
0.93
1.01
2.10
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


192.73
169.69
166.43
138.96
128.64
124.70
120.00
114.88
98.40
64.28
13.86
Cl
O
OH
O
O
O
CH3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.82
7.81
7.77
7.76
7.75
7.75
7.06
7.04
5.43
4.33
4.31
4.31
4.29
1.26
1.24
1.23
Br
OH
O
O
O
O
CH3
1.00
1.00
1.01
1.05
2.09
3.40
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


192.48
170.11
166.41
141.67
127.83
120.54
115.63
115.32
98.21
64.32
13.88
Br
OH
O
O
O
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.03
9.02
9.01
8.89
7.79
7.77
7.75
7.67
7.65
7.35
7.33
7.32
7.27
7.25
7.24
7.19
7.18
7.16
4.32
4.31
O
OH
O
NH
O
0.95
0.98
1.00
1.00
2.16
4.13
1.08
2.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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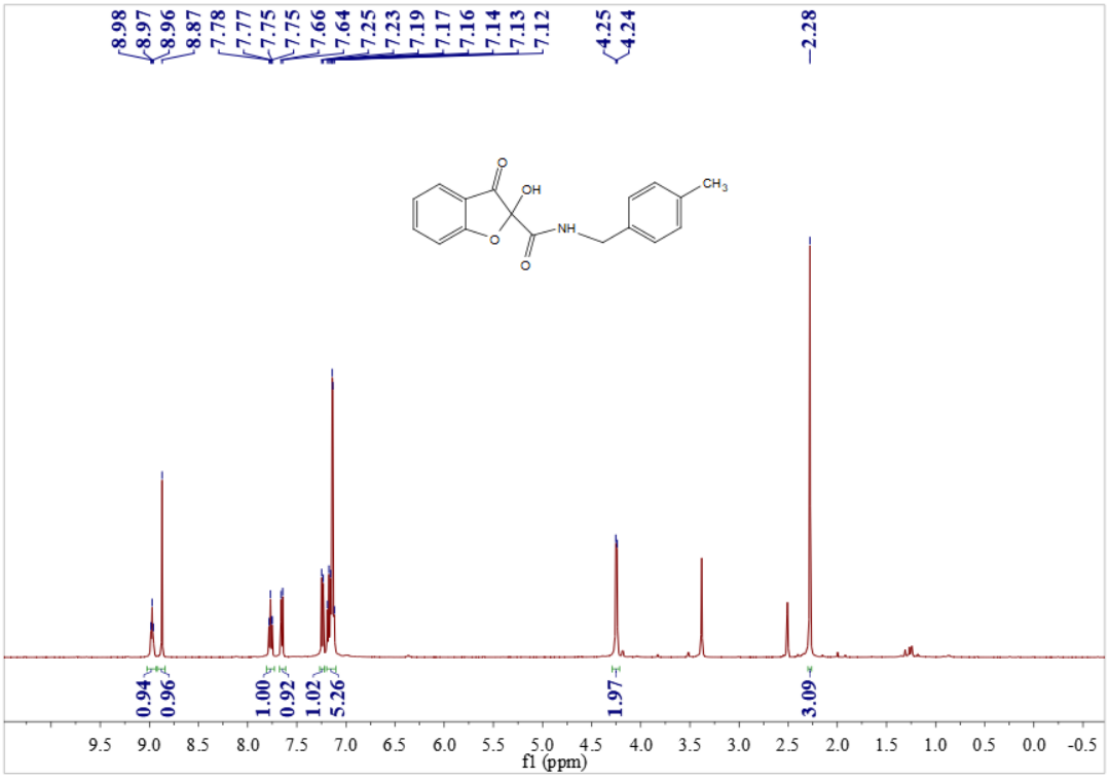
127.29
124.96
122.89
113.70
101.15
42.53
O
OH
O
NH
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.96
8.87
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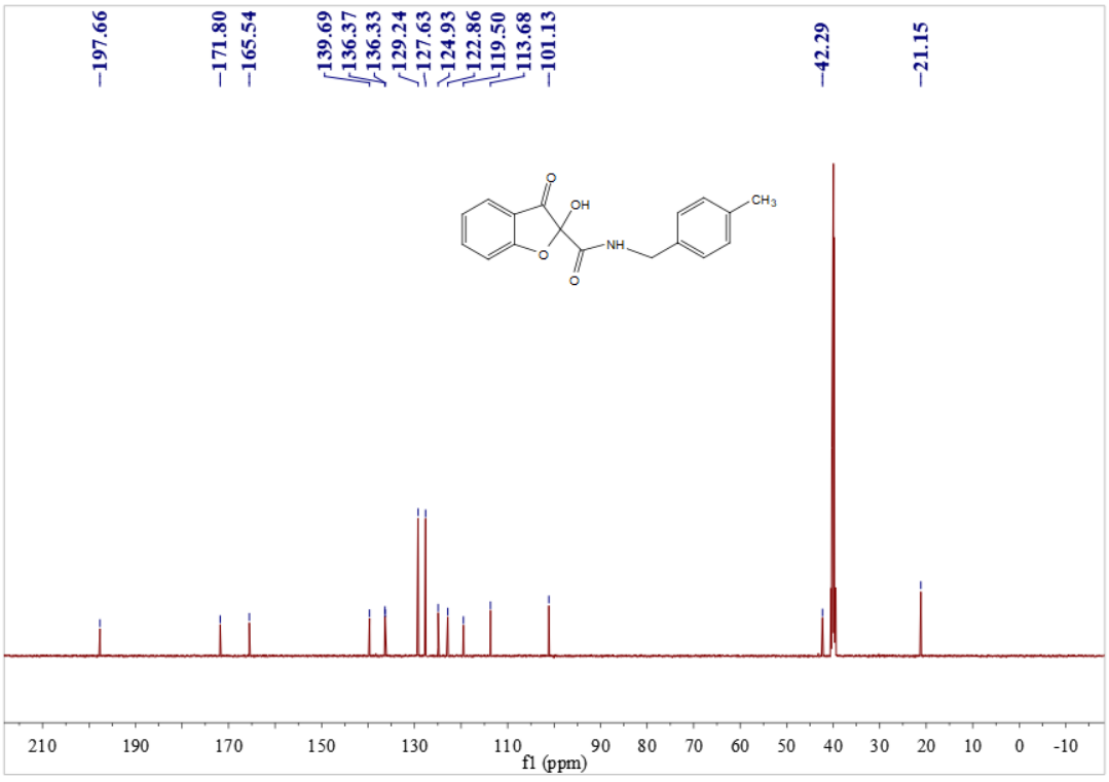
7.77
7.75
7.75
7.66
7.64
7.25
7.23
7.19
7.17
7.16
7.14
7.13
7.12
4.25
4.24
2.28
OH
NH
O
CH3
0.94
0.96
1.00
0.92
1.02
5.26
1.97
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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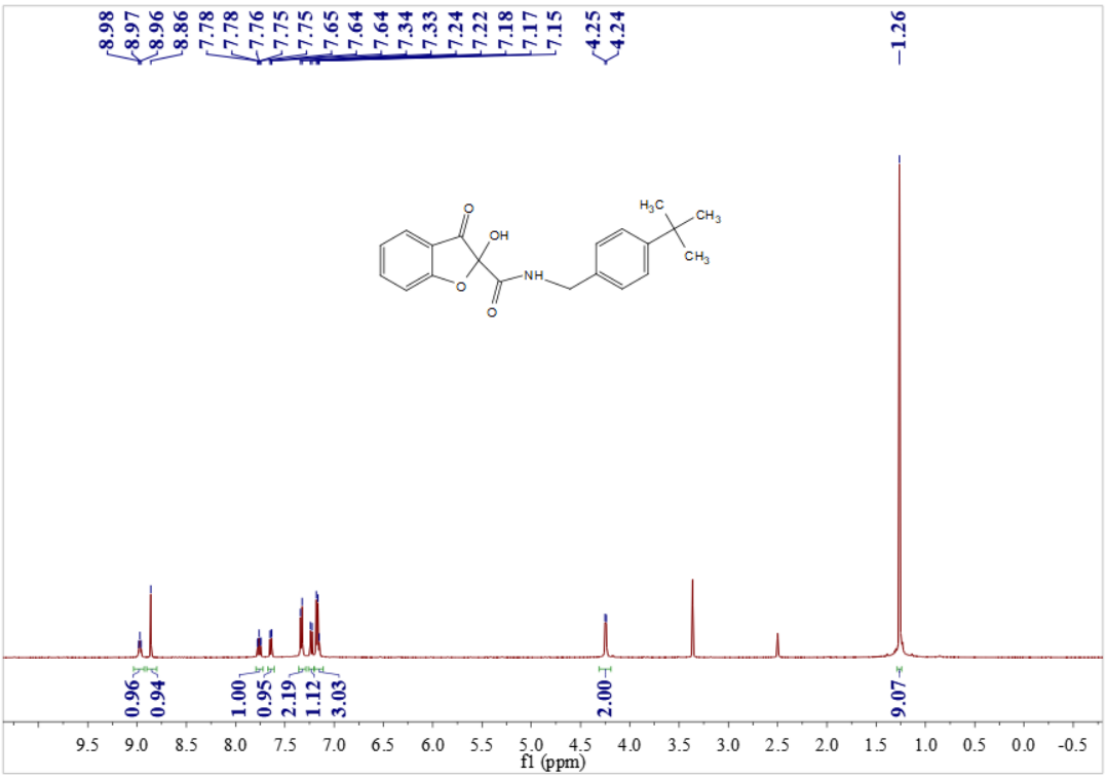
136.33
129.24
127.63
124.93
122.86
119.50
113.68
101.13
42.29
21.15
OH
NH
O
CH3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.96
8.86
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7.78
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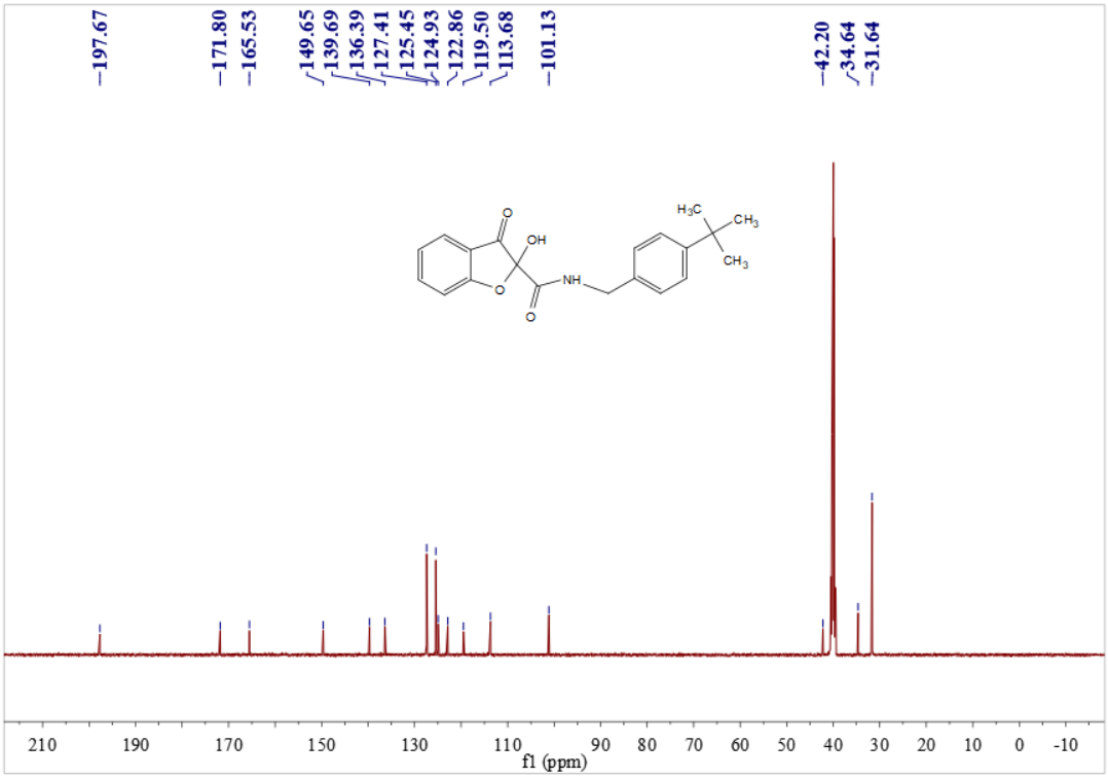
7.75
7.75
7.65
7.64
7.64
7.34
7.33
7.24
7.22
7.18
7.17
7.15
4.25
4.24
1.26
O
OH
O
NH
O
H3C
CH3
CH3
0.96
0.94
1.00
0.95
2.19
1.12
3.03
2.00
9.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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165.53
149.65
139.69
136.39
127.41
125.45
124.93
122.86
119.50
113.68
101.13
42.20
34.64
31.64
O
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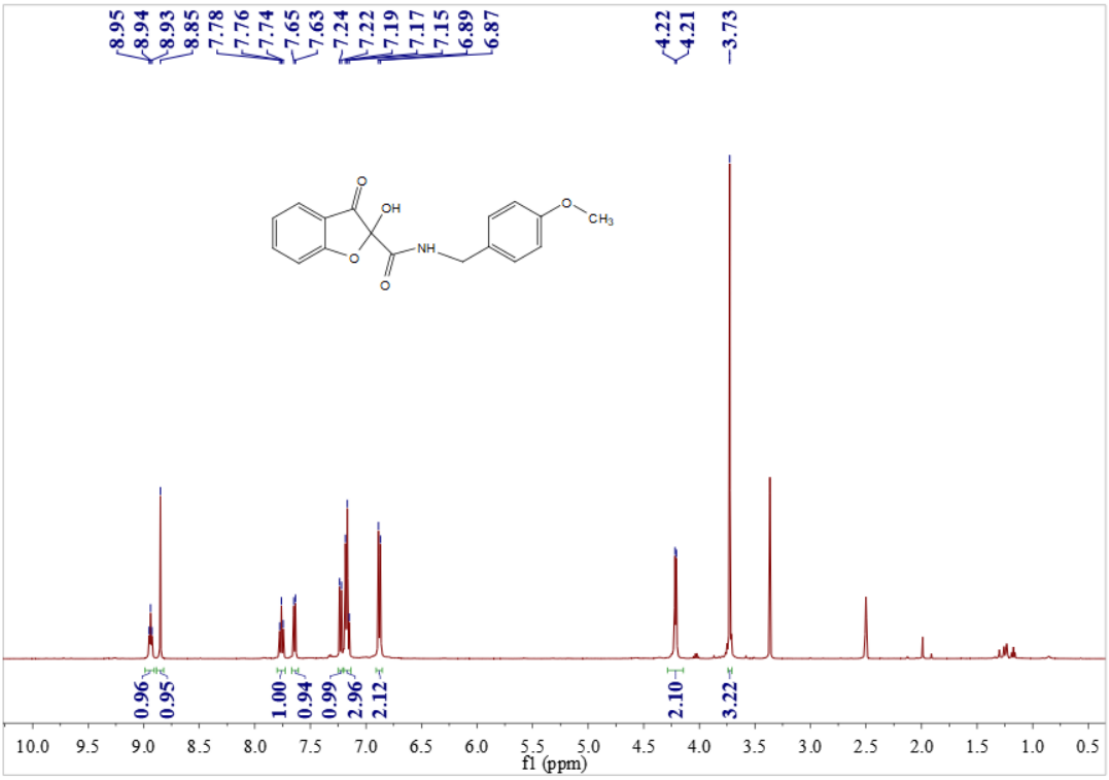
O
NH
O
H3C
CH3
CH3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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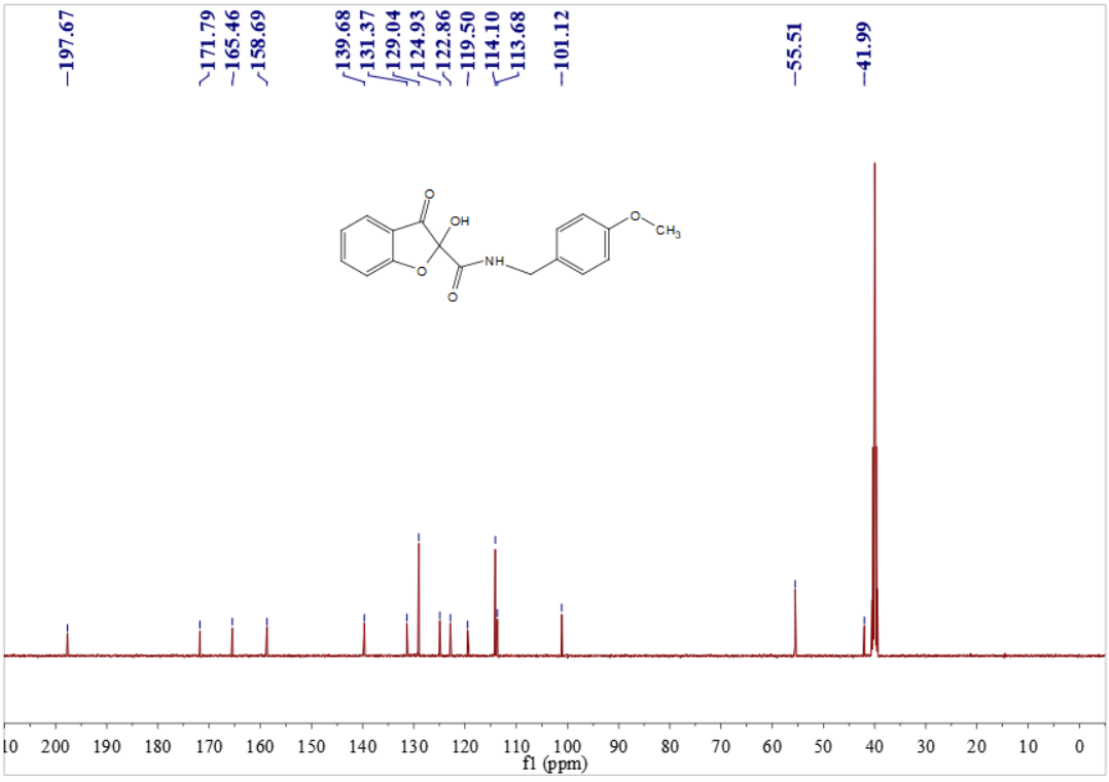
7.76
7.74
7.65
7.63
7.24
7.22
7.19
7.17
7.15
6.89
6.87
4.22
4.21
3.73
OH
O
NH
O
O
CH3
0.96
0.95
1.00
0.94
0.99
2.96
2.12
2.10
3.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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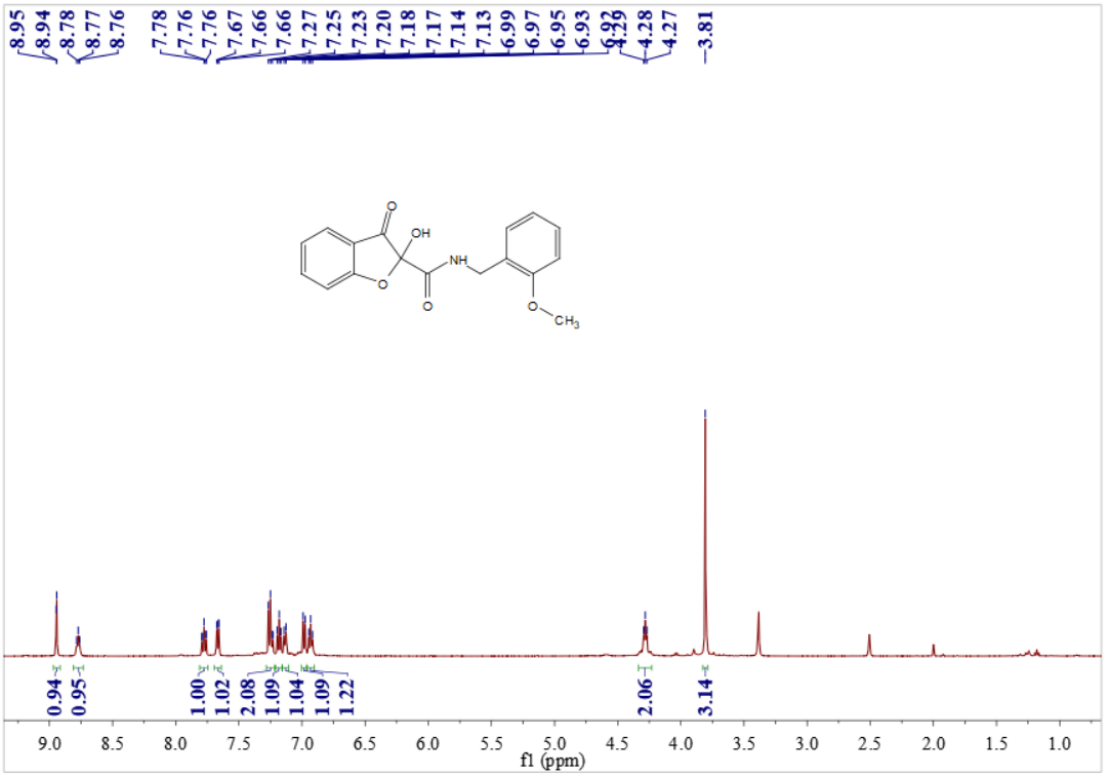
139.68
131.37
129.04
124.93
122.86
119.50
114.10
113.68
101.12
55.51
41.99
OH
O
NH
O
O
CH3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.94
8.78
8.77
8.76
7.78
7.76
7.76
7.67
7.66
7.66
7.27
7.25
7.23
7.20
7.18
7.17
7.14
7.13
6.99
6.97
6.95
6.93
6.92
4.29
4.28
4.27
3.81
OH
NH
O
CH3
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0.95
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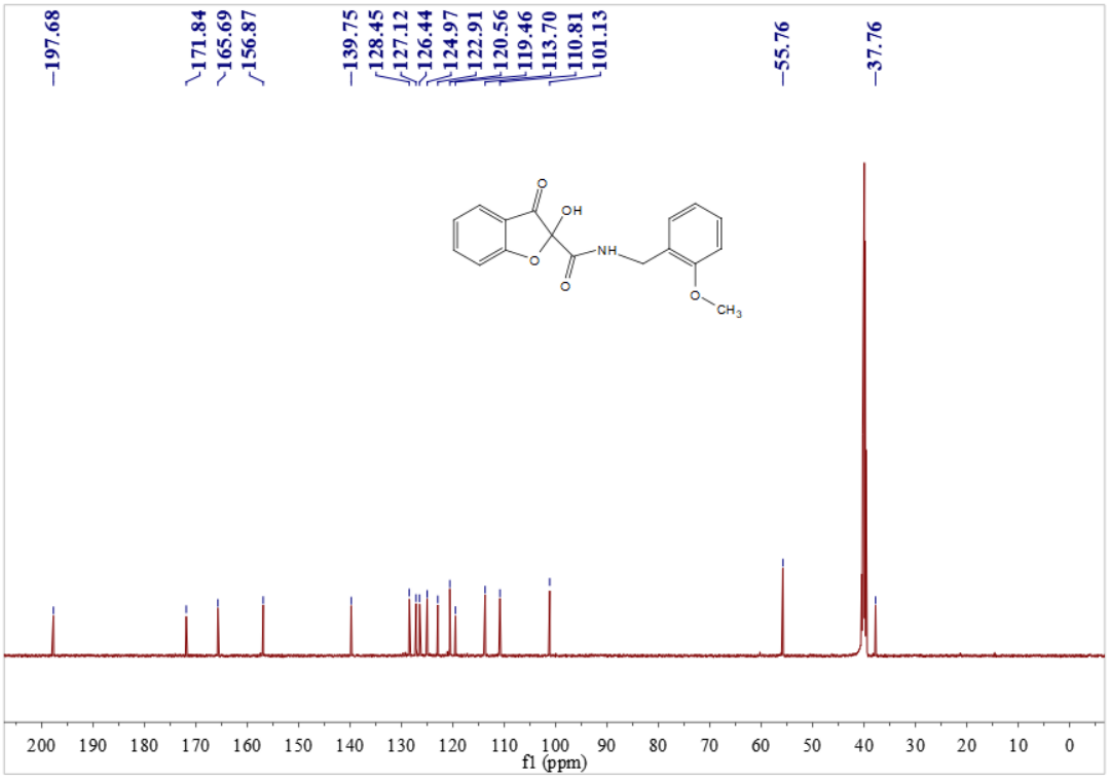
1.02
2.08
1.09
1.04
1.09
1.22
2.06
3.14
f1 (ppm)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126.44
124.97
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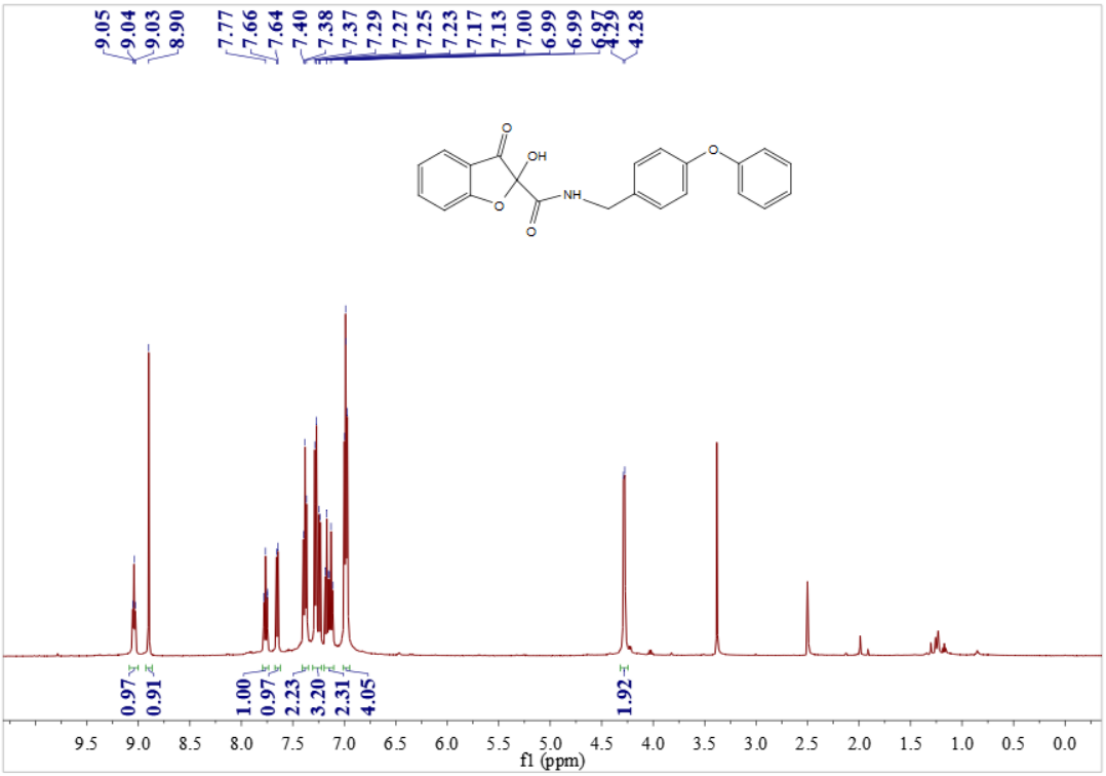
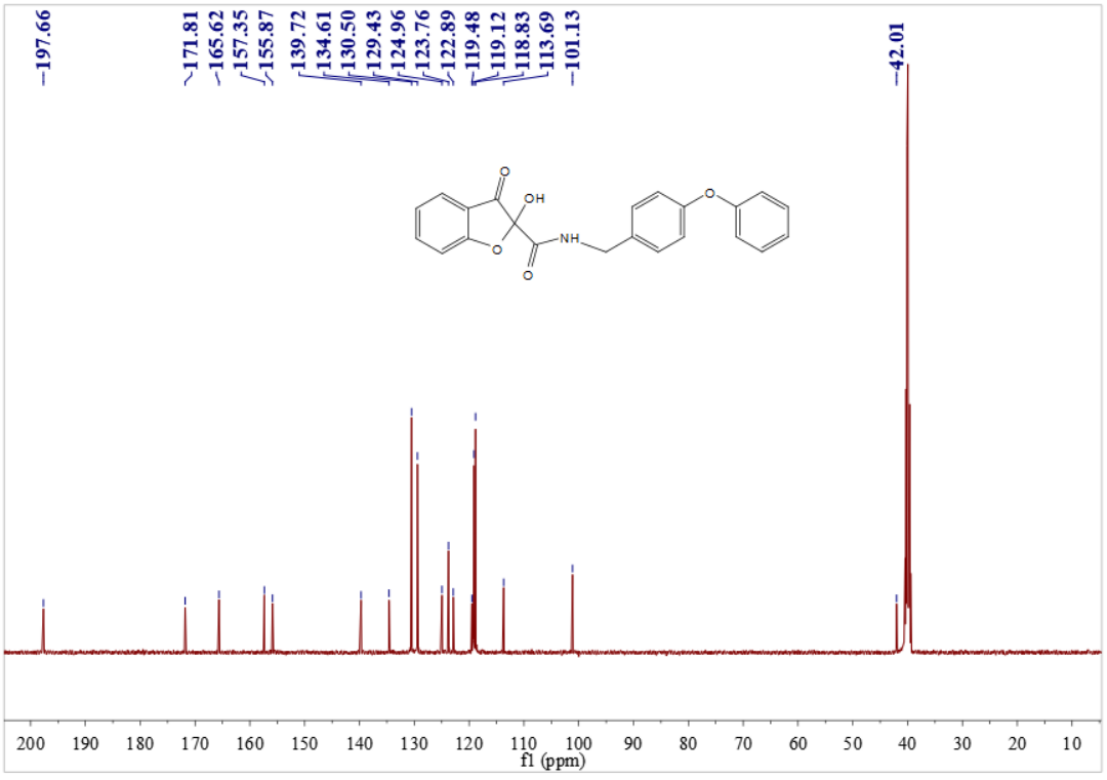
113.70
110.81
101.13
55.76
37.76
OH
NH
O
CH3
f1 (ppm)


9.05
9.04
9.03
8.90
7.77
7.66
7.64
7.40
7.38
7.37
7.29
7.27
7.25
7.23
7.17
7.13
7.00
6.99
6.97
4.29
4.28
OH
NH
O
0.97
0.91
1.00
0.97
2.23
3.20
2.31
4.05
1.92
f1 (ppm)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157.35
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134.61
130.50
129.43
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123.76
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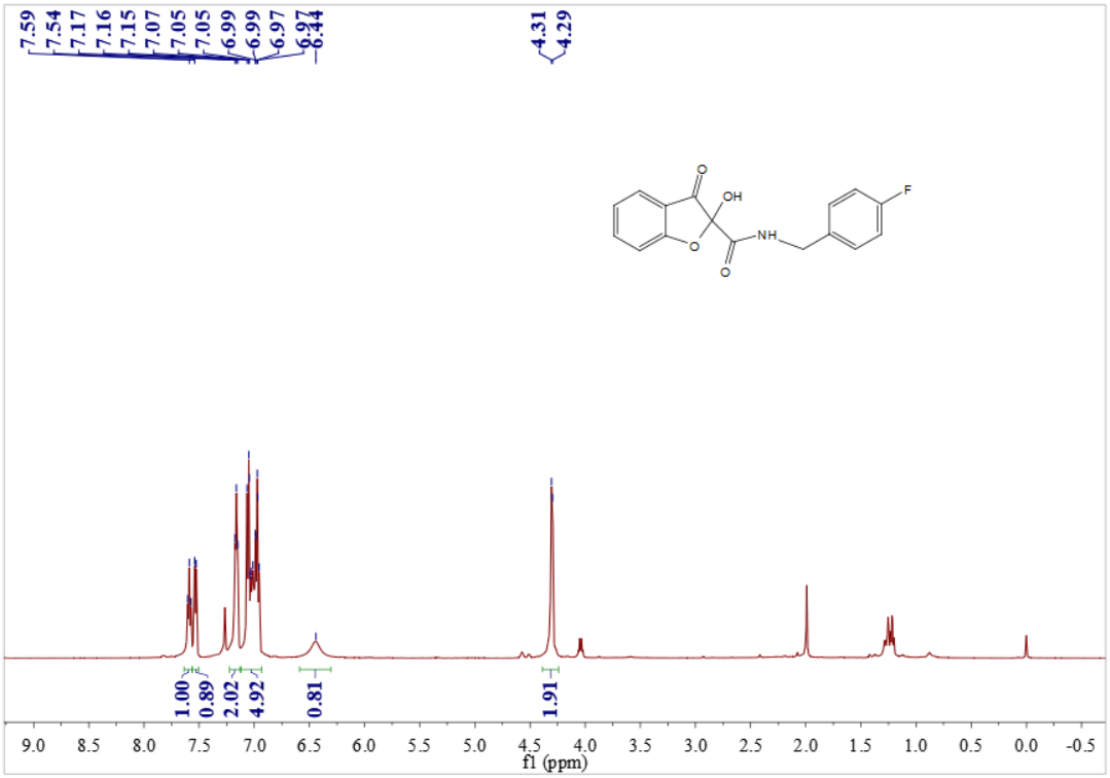
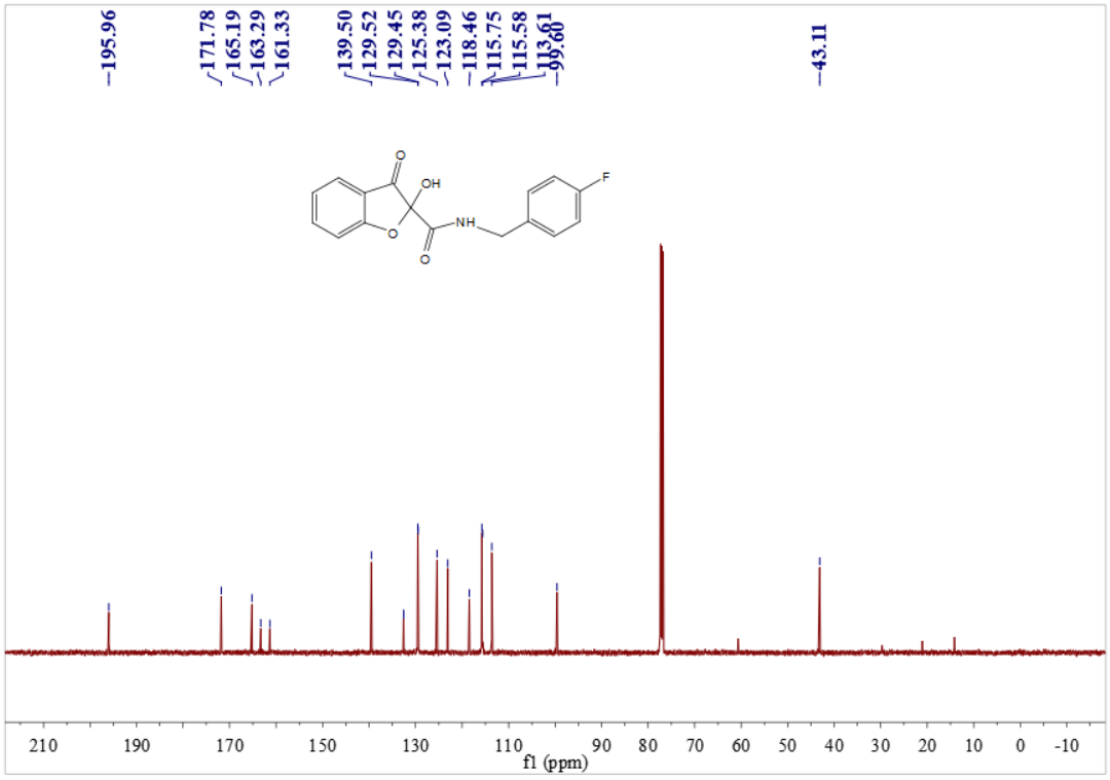
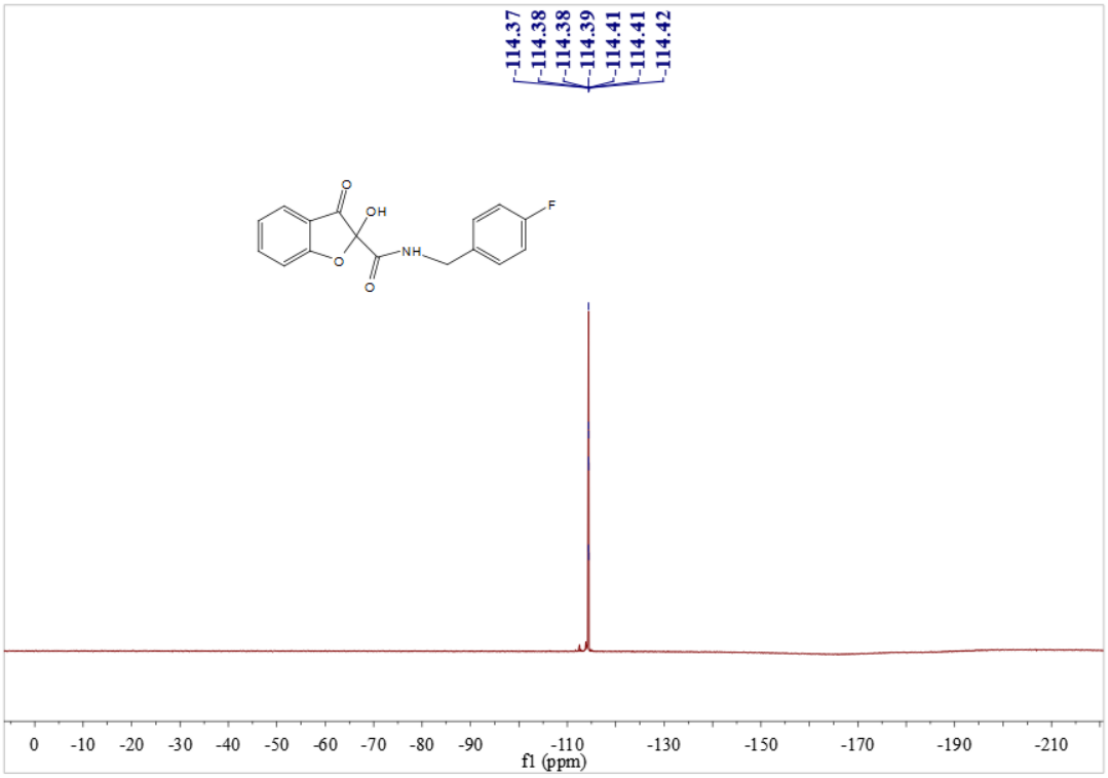
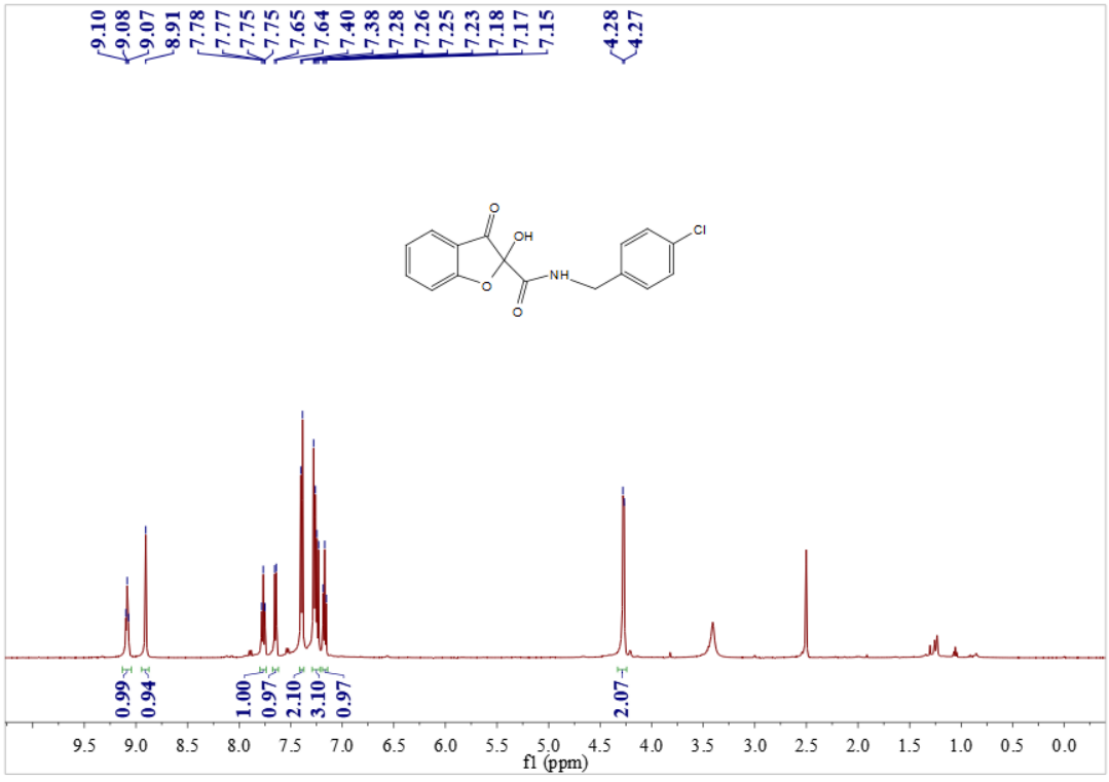
119.12
118.83
113.69
101.13
42.01
OH
NH
O
f1 (ppm)


7.59
7.54
7.17
7.16
7.15
7.07
7.05
7.05
6.99
6.99
6.97
6.44
4.31
4.29
O
OH
O
NH
F
1.00
0.89
2.02
4.92
0.81
1.91
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


195.96
171.78
165.19
163.29
161.33
139.50
129.52
129.45
125.38
123.09
118.46
115.75
115.58
113.61
99.60
43.11
O
OH
O
NH
F
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-114.37
-114.38
-114.38
-114.39
-114.41
-114.41
-114.42
O
OH
O
NH
O
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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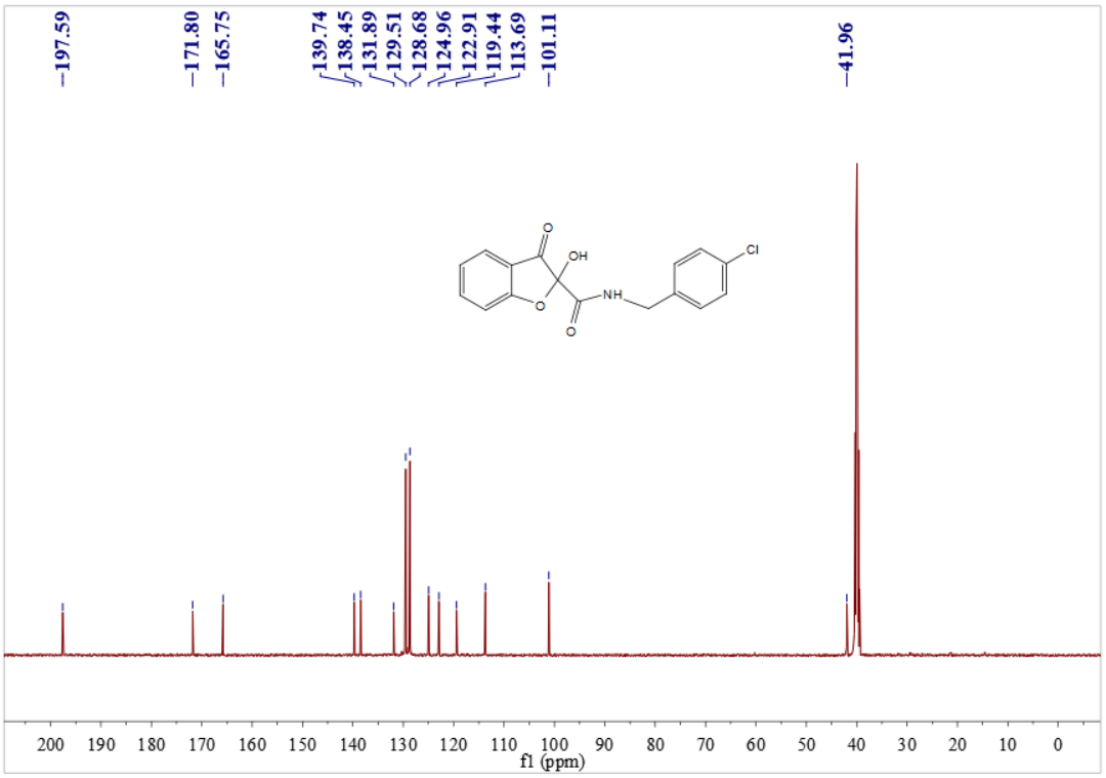
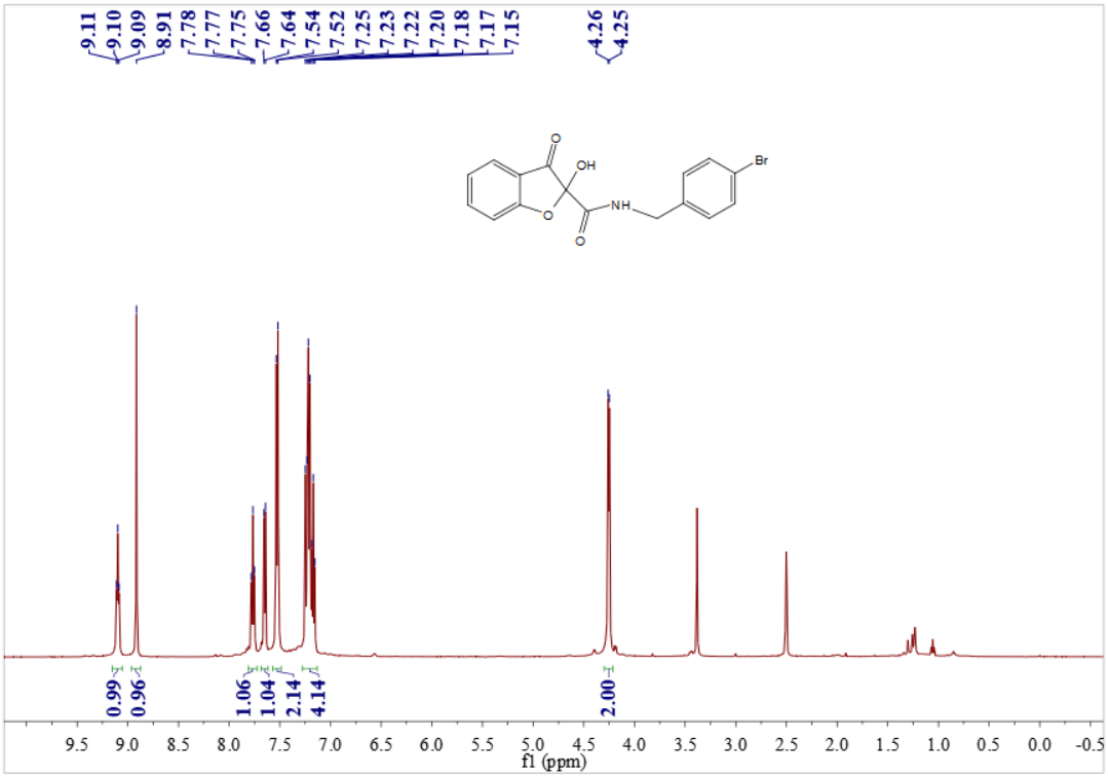
9.08
9.07
8.91
7.78
7.77
7.75
7.75
7.65
7.64
7.40
7.38
7.28
7.26
7.25
7.23
7.18
7.17
7.15
4.28
4.27
O
OH
O
NH
O
Cl
0.99
0.94
1.00
0.97
2.10
3.10
0.97
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


197.59
171.80
165.75
139.74
138.45
131.89
129.51
128.68
124.96
122.91
119.44
113.69
101.11
41.96
OH
NH
O
Cl
f1 (ppm)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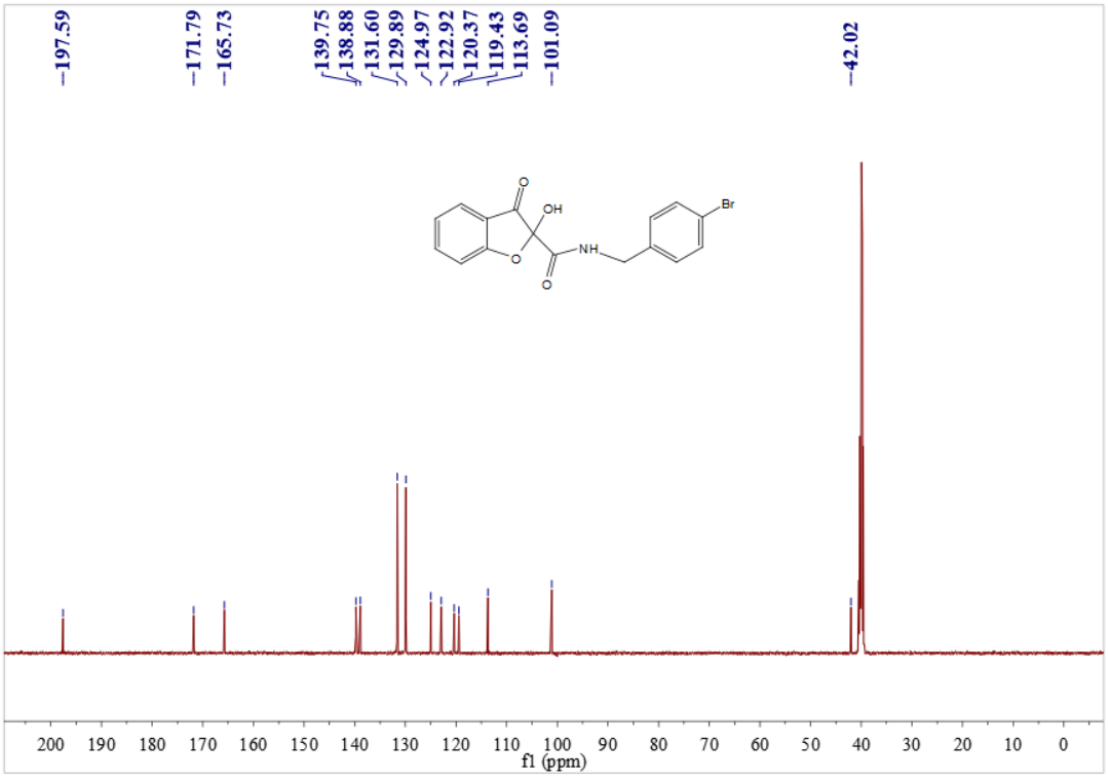
9.10
9.09
8.91
7.78
7.77
7.75
7.66
7.64
7.54
7.52
7.25
7.23
7.22
7.20
7.18
7.17
7.15
4.26
4.25
OH
NH
O
Br
0.99
0.96
1.06
1.04
2.14
4.14
2.00
f1 (ppm)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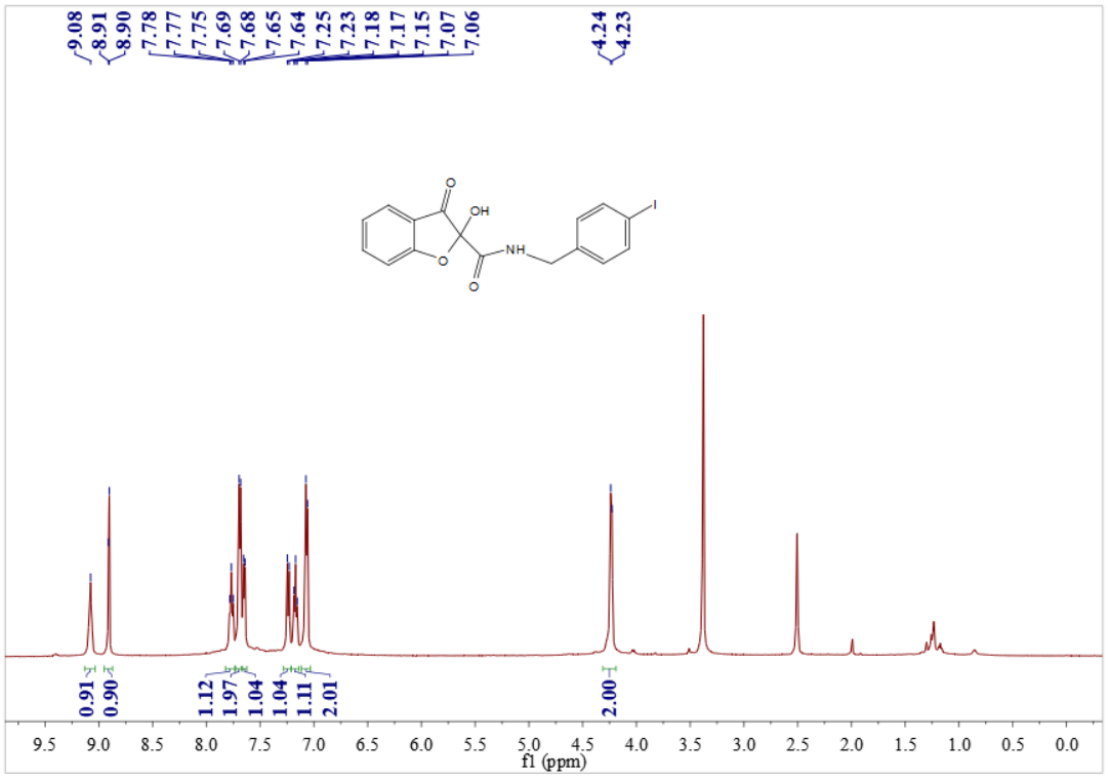
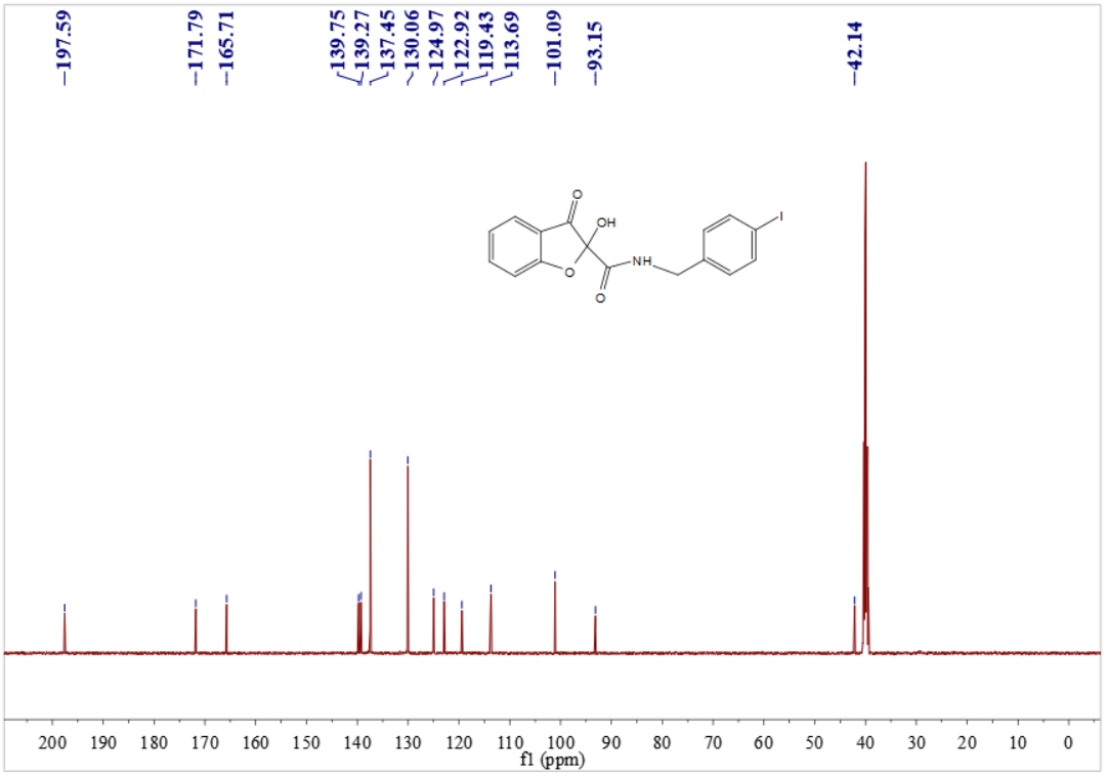
139.75
138.88
131.60
129.89
124.97
122.92
120.37
119.43
113.69
101.09
42.02
O
OH
O
NH
O
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.08
8.91
8.90
7.78
7.77
7.75
7.69
7.68
7.65
7.64
7.25
7.23
7.18
7.17
7.15
7.07
7.06
4.24
4.23
O
OH
O
NH
O
I
0.91
0.90
1.12
1.97
1.04
1.04
1.11
2.01
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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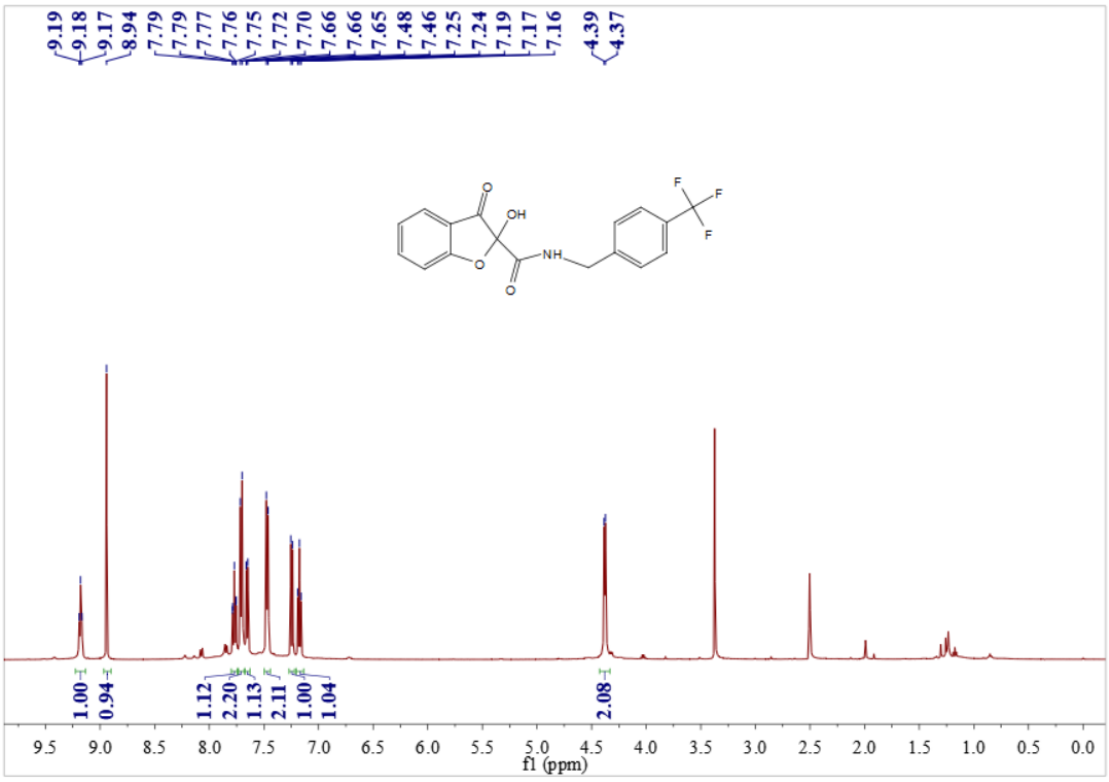
137.45
130.06
124.97
122.92
119.43
113.69
101.09
93.15
42.14
O
OH
O
NH
O
I
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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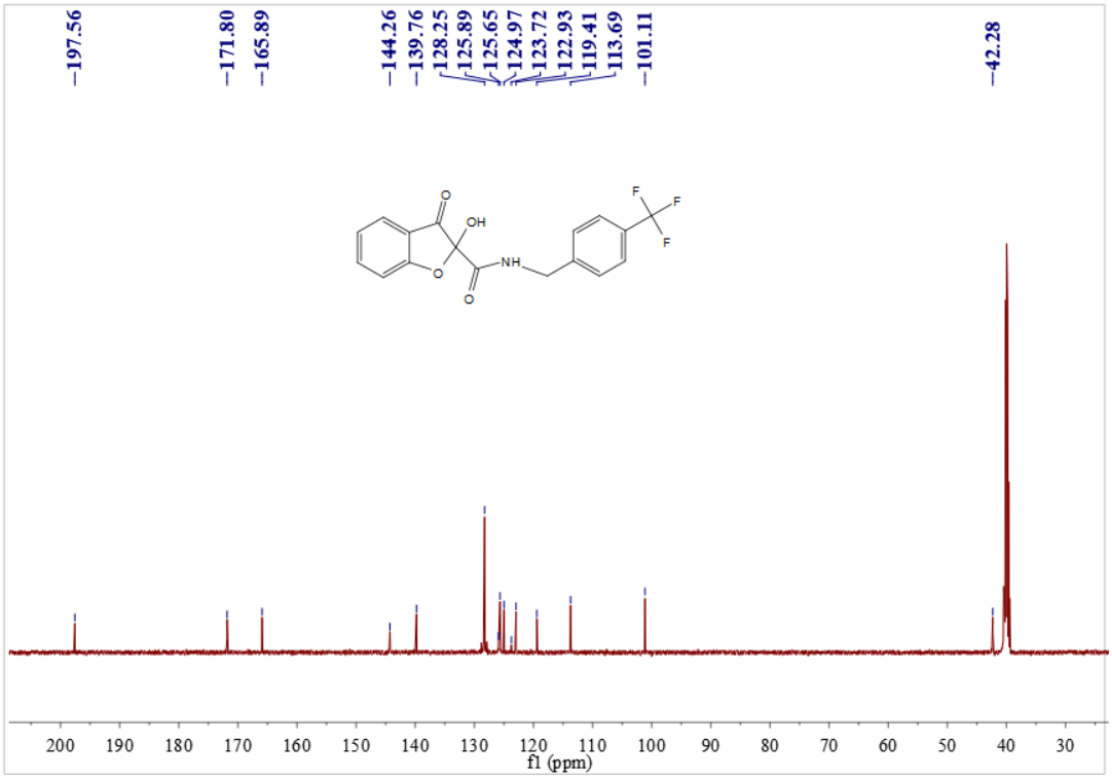
9.18
9.17
8.94
7.79
7.79
7.77
7.76
7.75
7.72
7.70
7.66
7.65
7.48
7.46
7.25
7.24
7.19
7.17
7.16
4.39
4.37
O
OH
O
NH
O
F
F
F
1.00
0.94
1.12
2.20
1.13
2.11
1.00
1.04
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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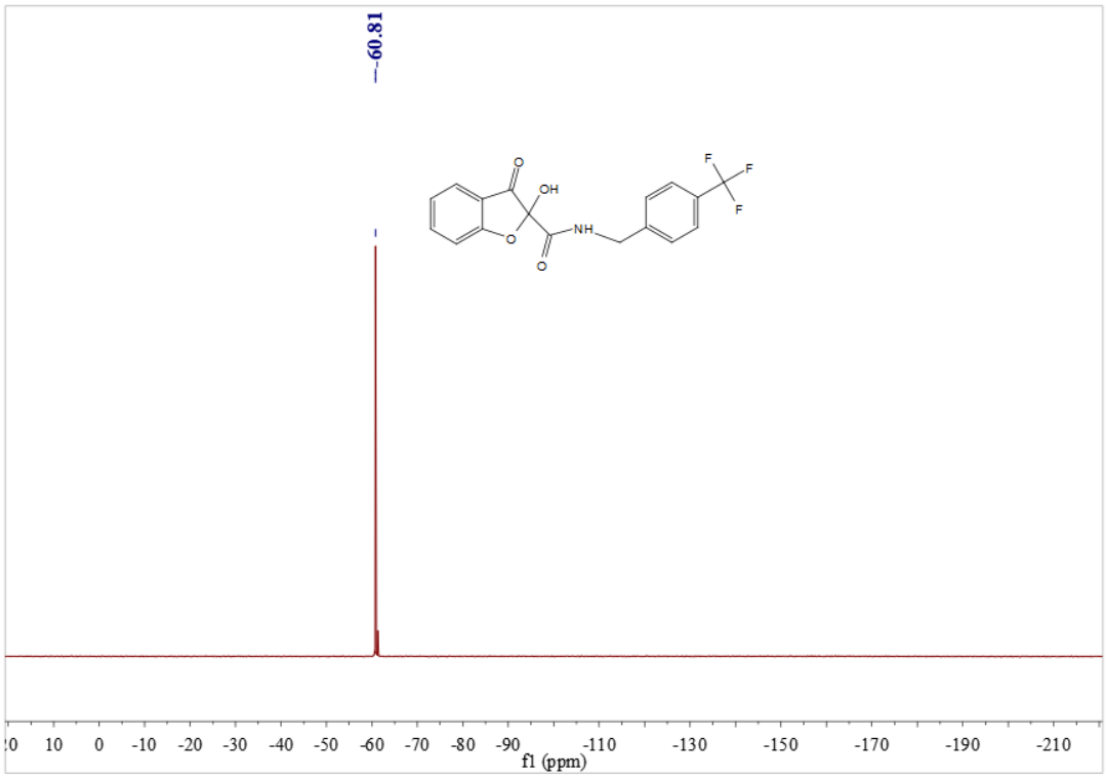
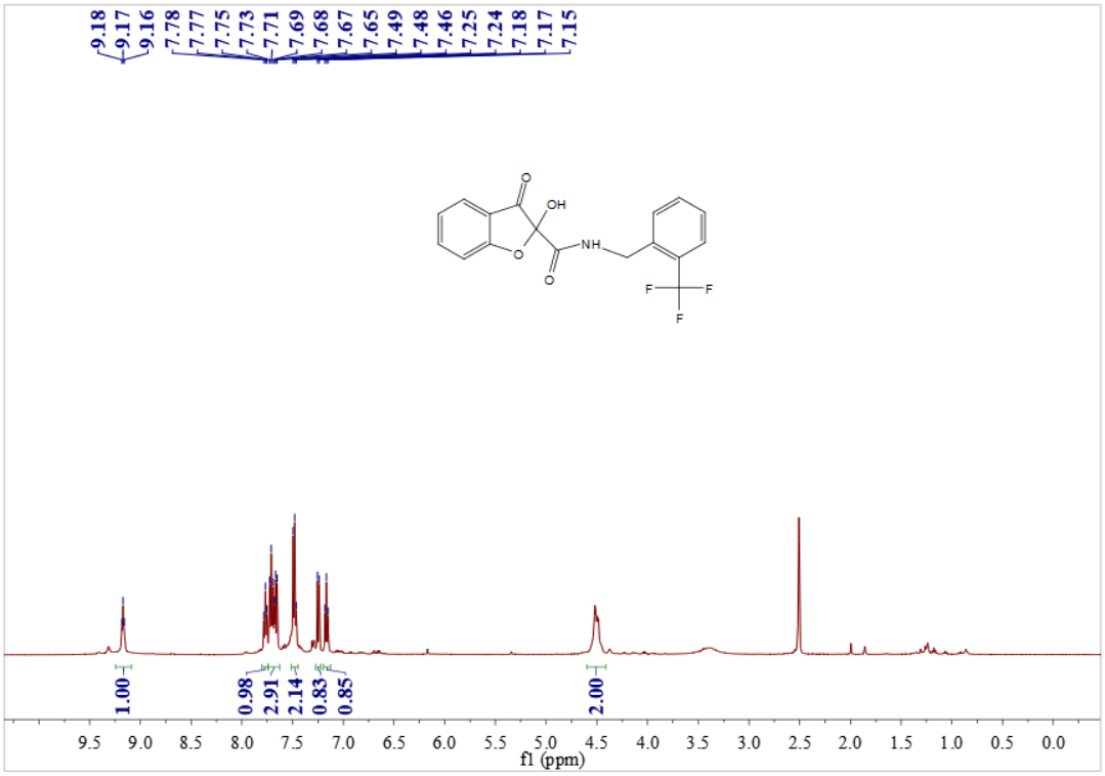
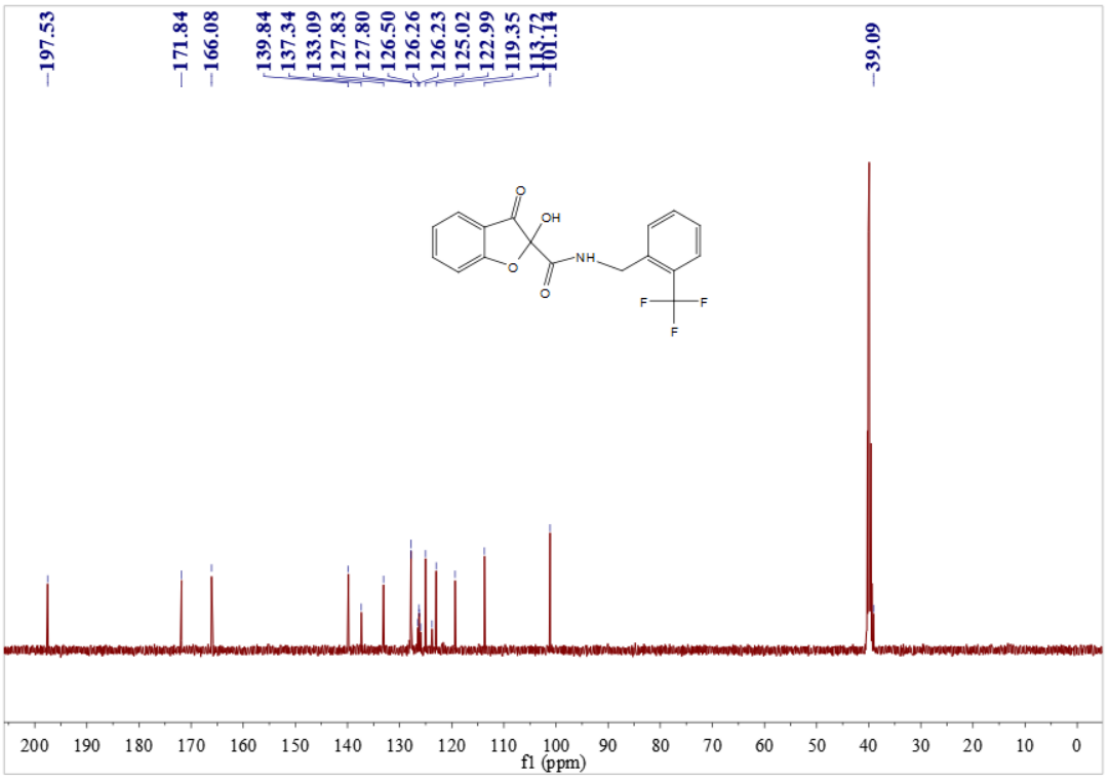
171.80
165.89
144.26
139.76
128.25
125.89
125.65
124.97
123.72
122.93
119.41
113.69
101.11
42.28
OH
NH
F
F
F
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)


60.81
OH
NH
F
F
F
O
O
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


9.18
9.17
9.16
7.78
7.77
7.75
7.73
7.71
7.69
7.68
7.67
7.65
7.49
7.48
7.46
7.25
7.24
7.18
7.17
7.15
O
OH
NH
O
O
F
F
F
1.00
0.98
2.91
2.14
0.83
0.85
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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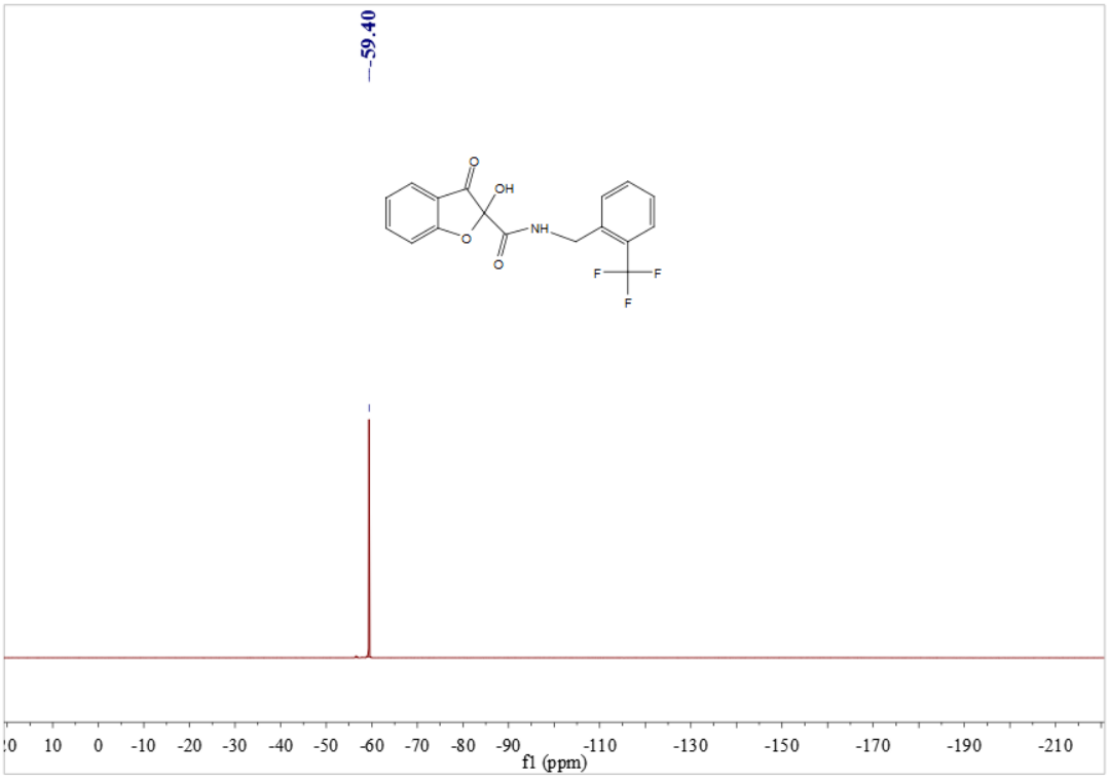
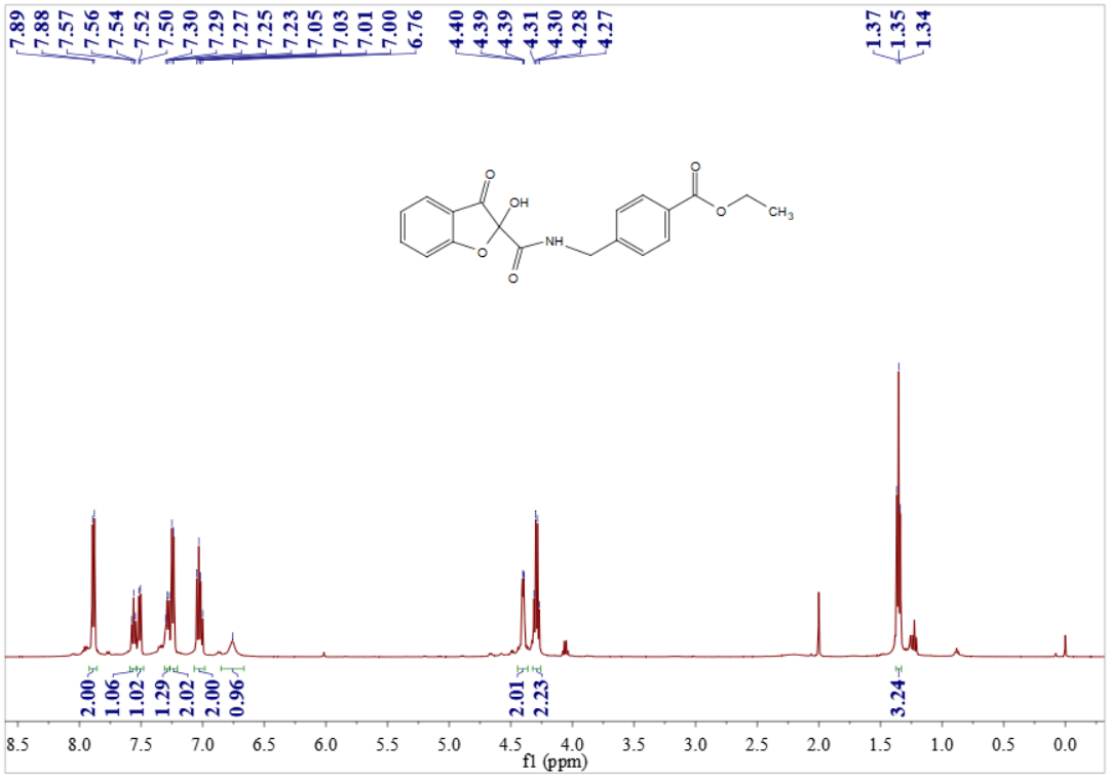
171.84
166.08
139.84
137.34
133.09
127.83
127.80
126.50
126.26
126.23
125.02
122.99
119.35
39.09
O
OH
NH
O
O
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-59.40
OH
O
NH
F
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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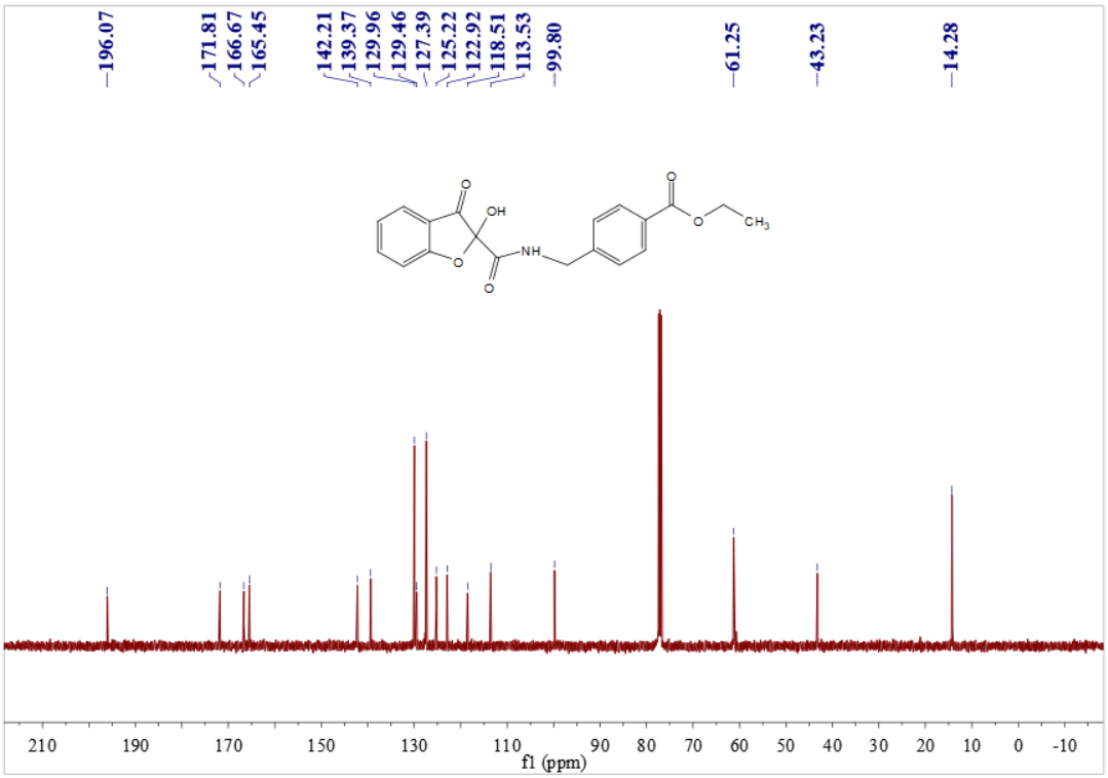
7.88
7.57
7.56
7.54
7.52
7.50
7.30
7.29
7.27
7.25
7.23
7.05
7.03
7.01
7.00
6.76
4.40
4.39
4.39
4.31
4.30
4.28
4.27
1.37
1.35
1.34
OH
NH
CH3
2.00
1.06
1.02
1.29
2.02
2.00
0.96
2.01
2.23
3.24
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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171.81
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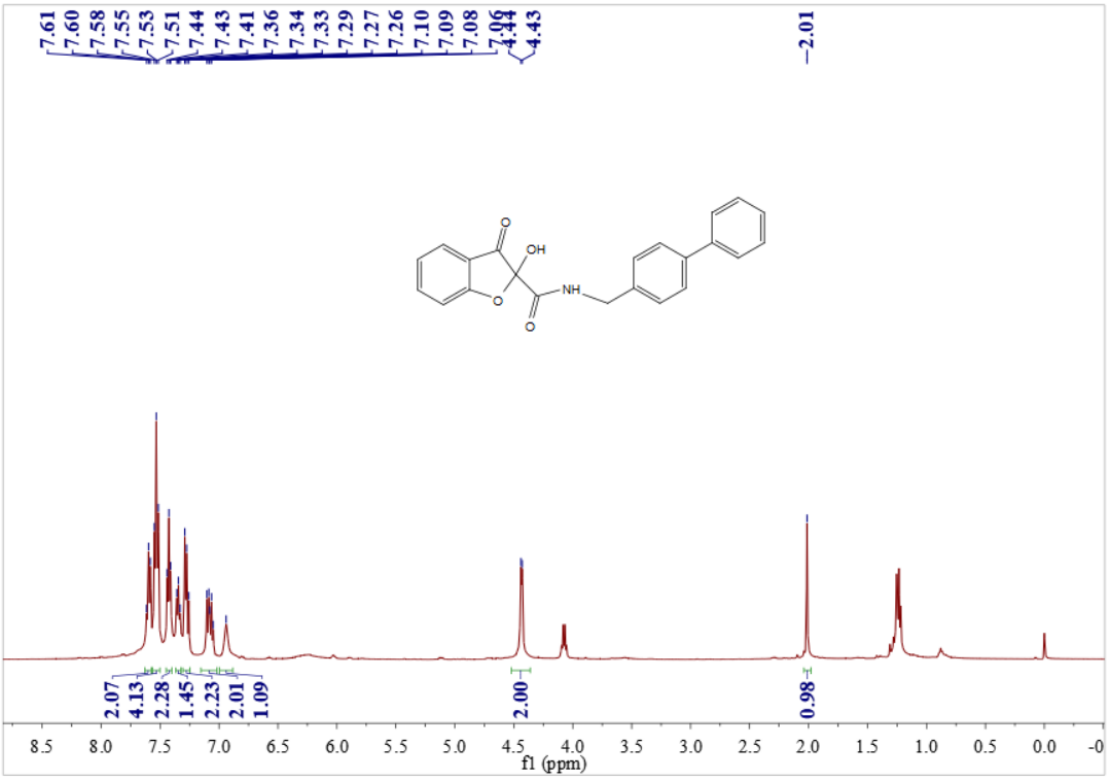
139.37
129.96
129.46
127.39
125.22
122.92
118.51
113.53
99.80
61.25
43.23
14.28
OH
NH
O
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.51
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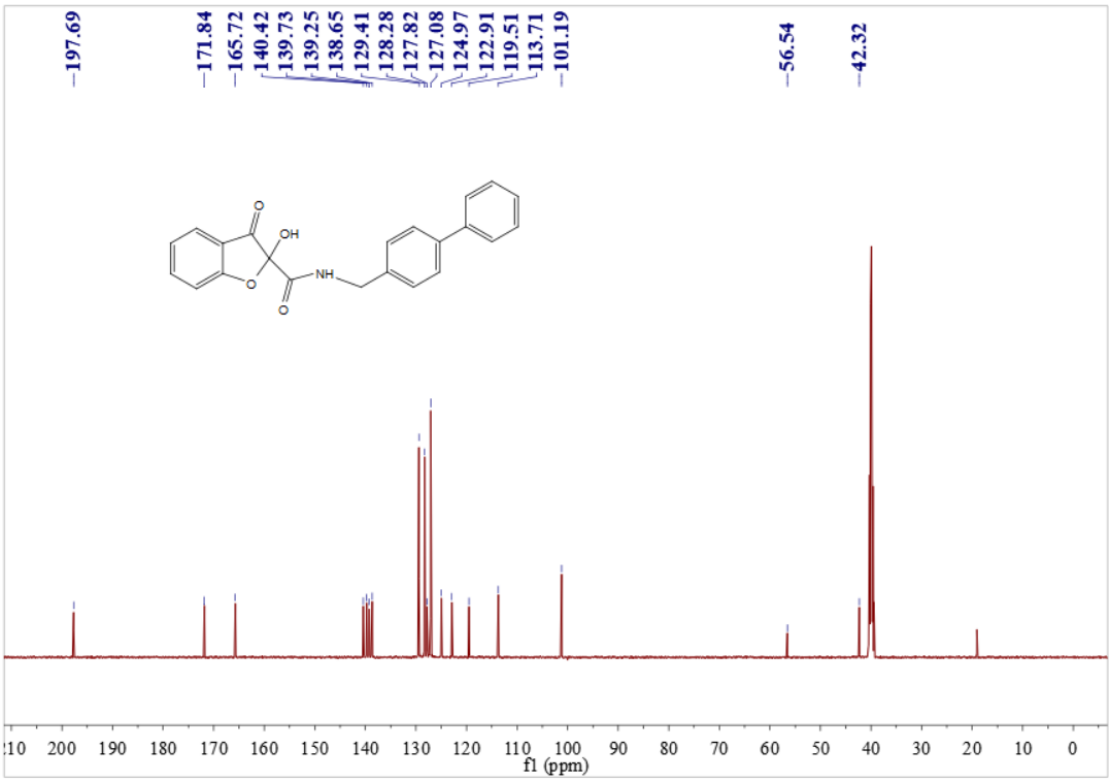
7.43
7.41
7.36
7.34
7.33
7.29
7.27
7.26
7.10
7.09
7.08
7.06
4.44
4.43
2.01
OH
NH
O
2.07
4.13
2.28
1.45
2.23
2.01
1.09
2.00
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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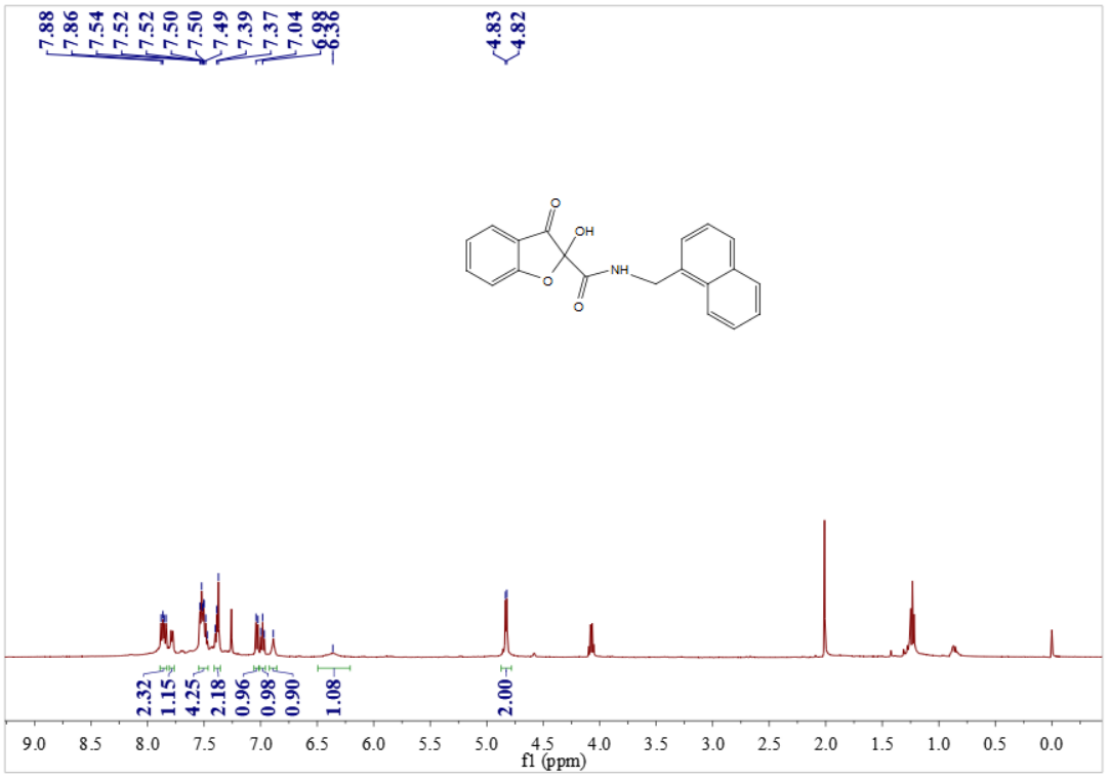
140.42
139.73
139.25
138.65
129.41
128.28
127.82
127.08
124.97
122.91
119.51
113.71
101.19
56.54
42.32
O
OH
NH
O
O
f1 (ppm)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7.86
7.54
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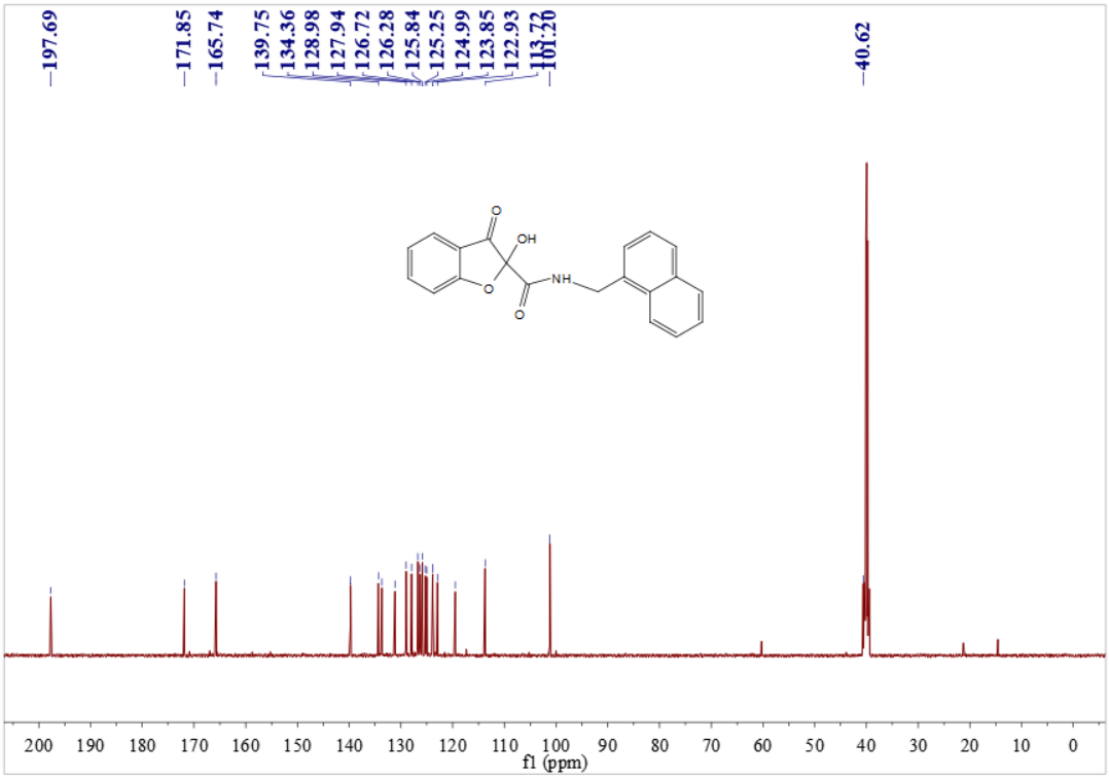
7.52
7.50
7.50
7.49
7.39
7.37
7.04
6.98
6.96
4.83
4.82
O
OH
NH
O
O
2.32
1.15
4.25
2.18
0.96
0.98
0.90
1.08
2.00
f1 (ppm)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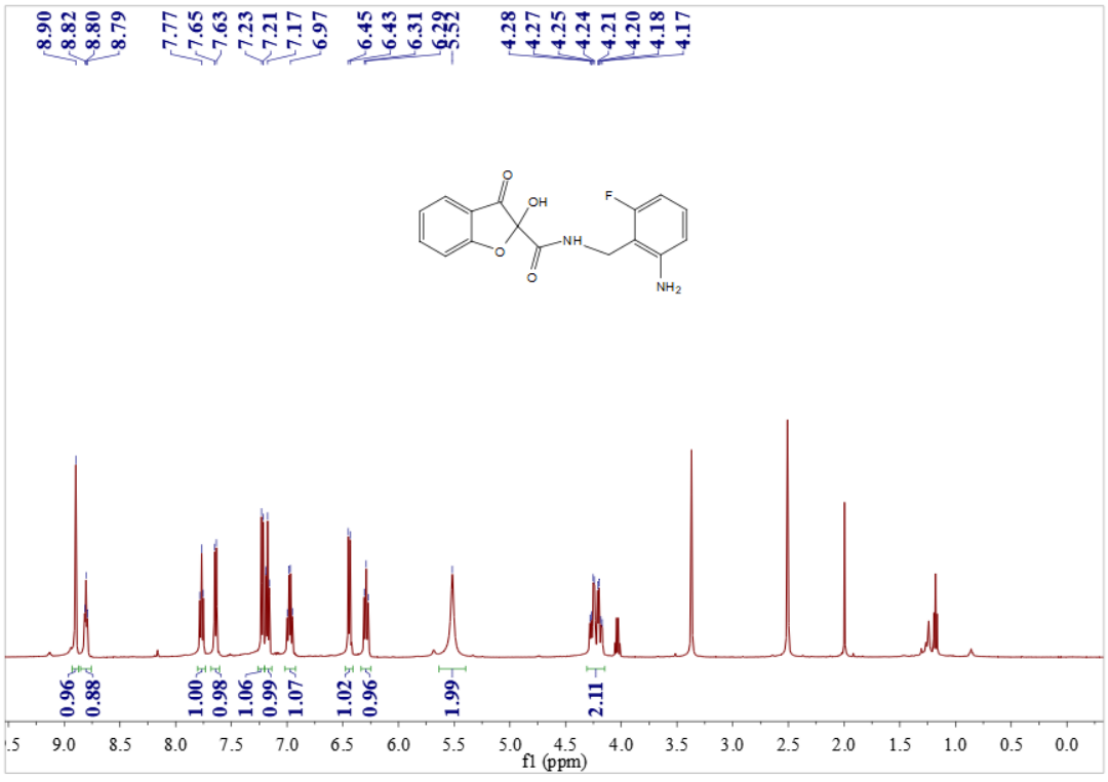
127.94
126.72
126.28
125.84
125.25
124.99
123.85
122.93
113.72
101.20
40.62
OH
NH
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.80
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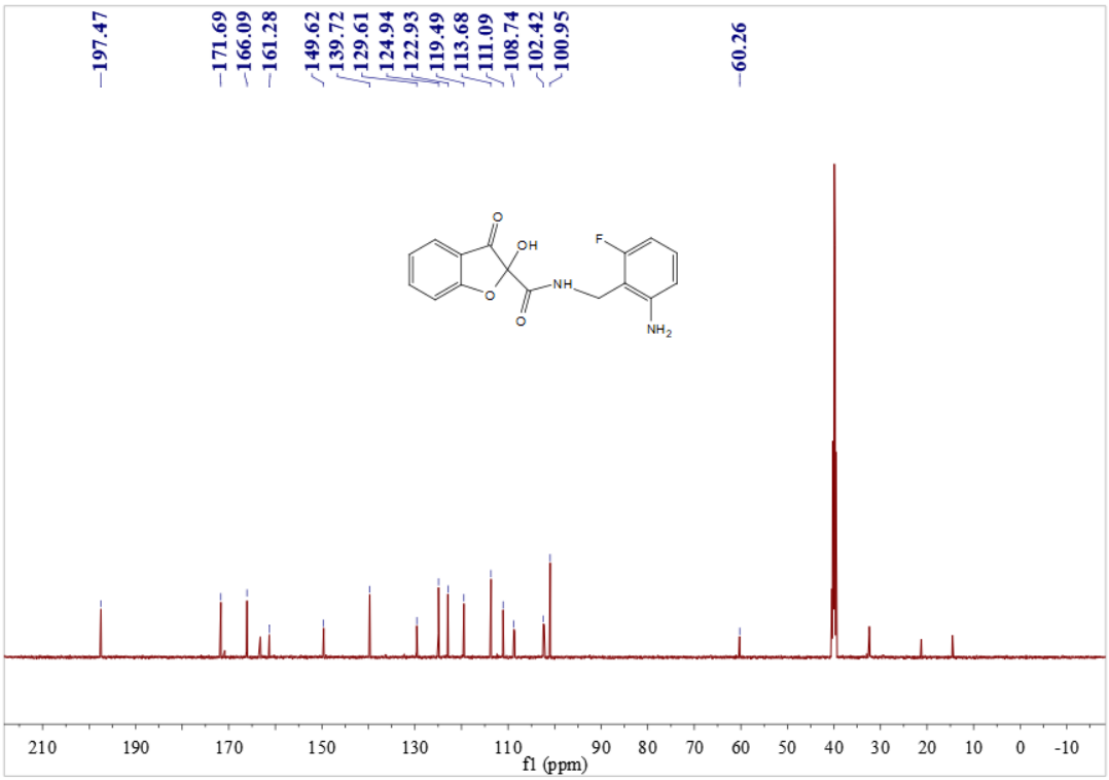
7.65
7.63
7.23
7.21
7.17
6.97
6.45
6.43
6.31
6.29
5.52
4.28
4.27
4.25
4.24
4.21
4.20
4.18
4.17
OH
NH
F
NH2
O
O
O
0.96
0.88
1.00
0.98
1.06
0.99
1.07
1.02
0.96
1.99
2.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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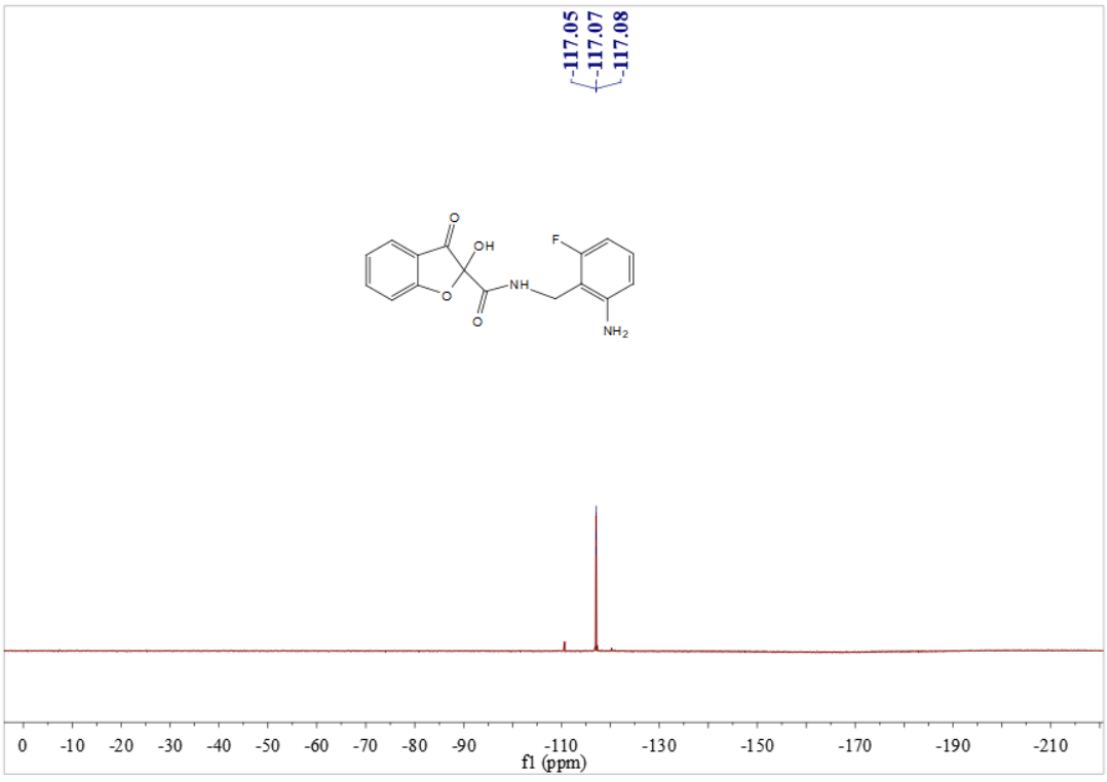
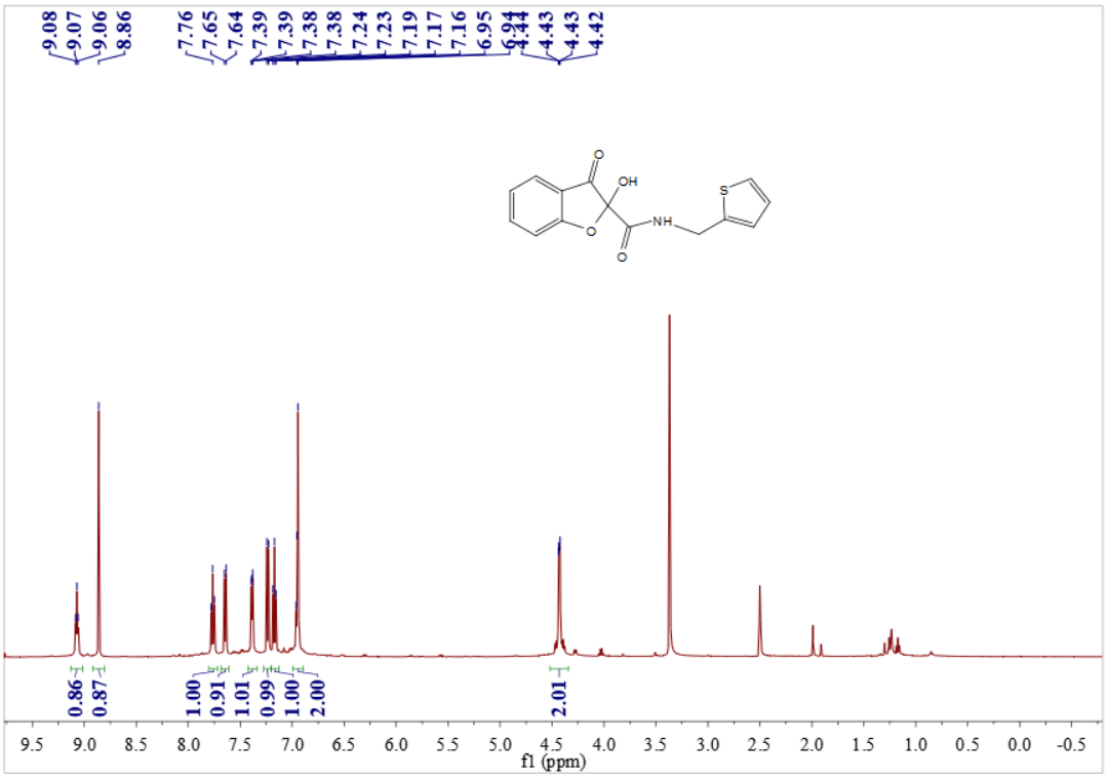
161.28
149.62
139.72
129.61
124.94
122.93
119.49
113.68
111.09
108.74
102.42
100.95
60.26
O
OH
O
NH
O
F
NH2
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-117.05
-117.07
-117.08
O
OH
O
NH
O
F
NH2
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)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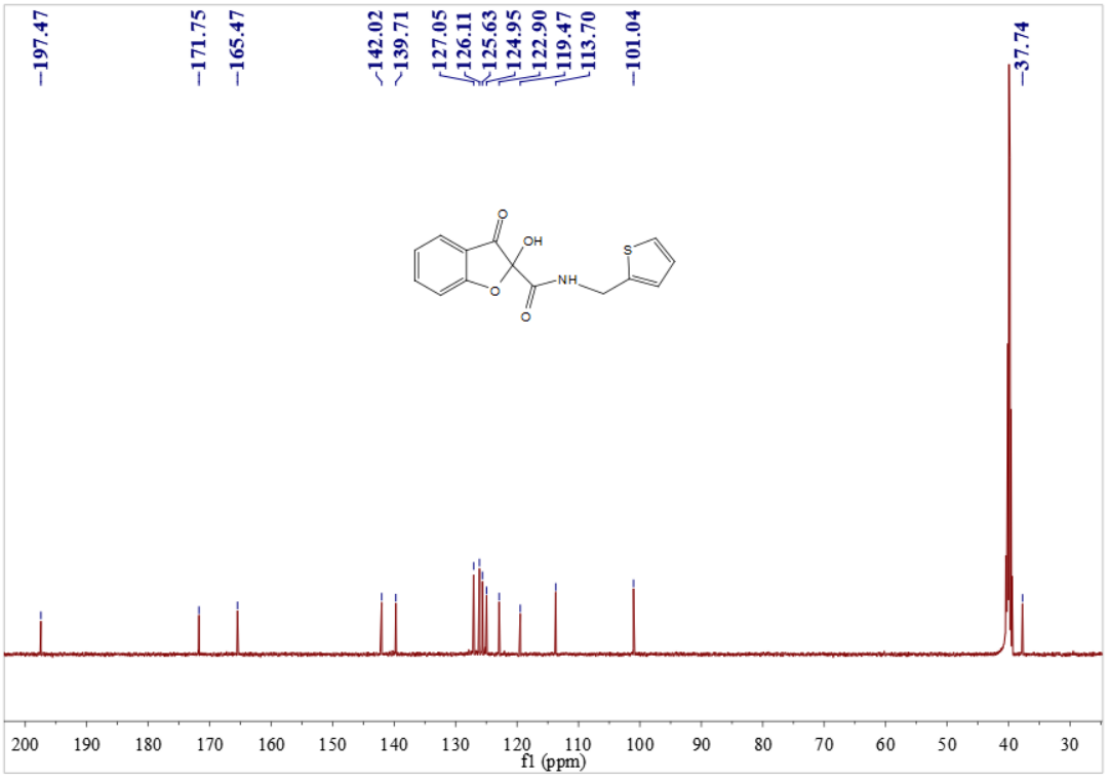
7.39
7.38
7.38
7.24
7.23
7.19
7.17
7.16
6.95
6.94
4.44
4.43
4.43
4.42
OH
O
NH
S
0.86
0.87
1.00
0.91
1.01
0.99
1.00
2.00
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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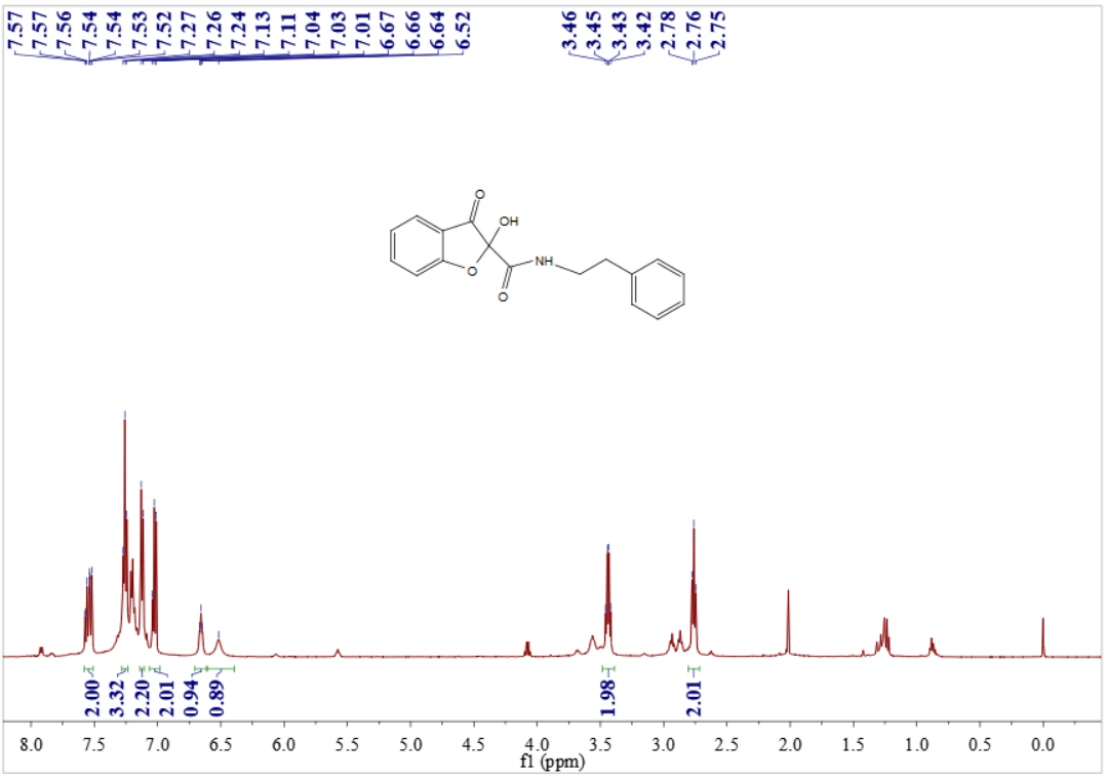
125.63
124.95
122.90
119.47
113.70
101.04
37.74
OH
O
NH
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)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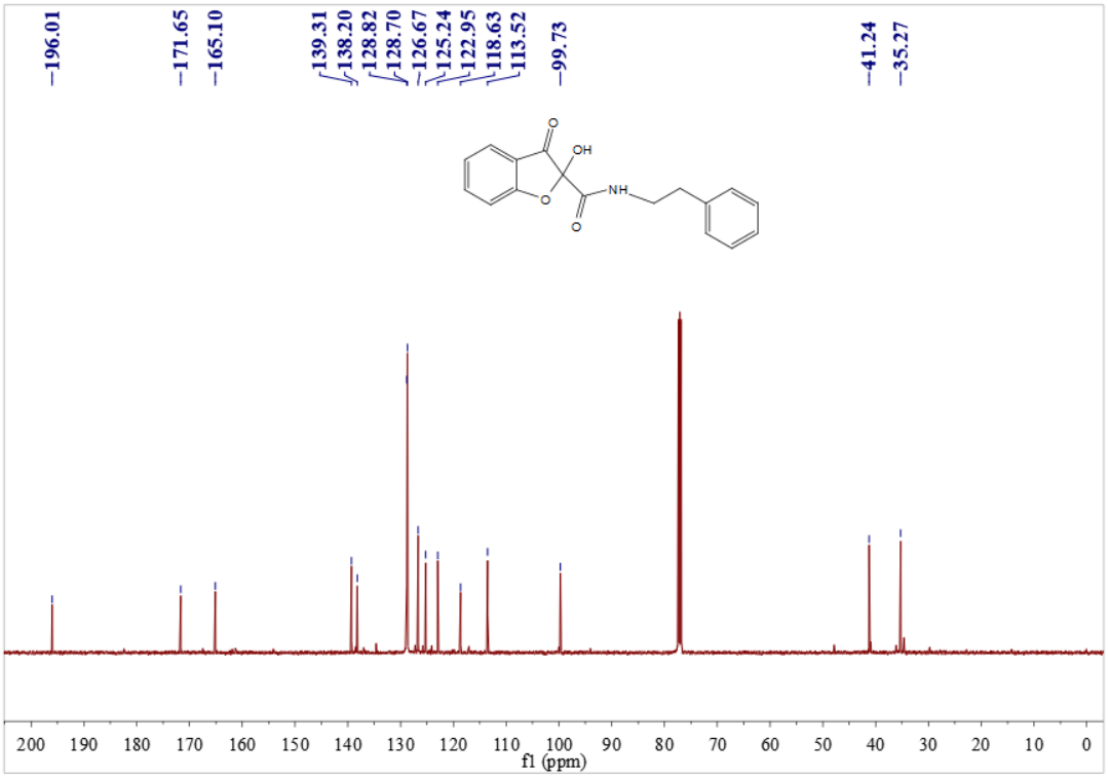
7.54
7.53
7.52
7.27
7.26
7.24
7.13
7.11
7.04
7.03
7.01
6.67
6.66
6.64
6.52
3.46
3.45
3.43
3.42
2.78
2.76
2.75
OH
NH
O
2.00
3.32
2.20
2.01
0.94
0.89
1.98
2.01
f1 (ppm)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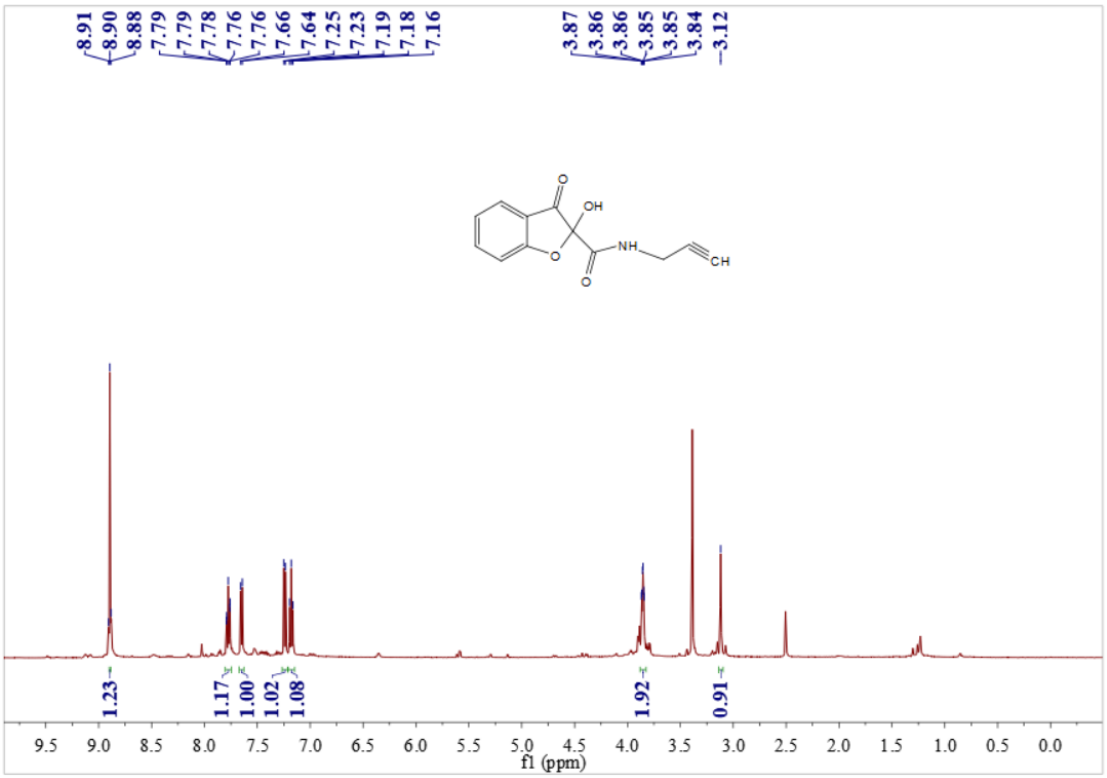
138.20
128.82
128.70
126.67
125.24
122.95
118.63
113.52
99.73
41.24
35.27
OH
NH
O
f1 (ppm)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8.90
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7.78
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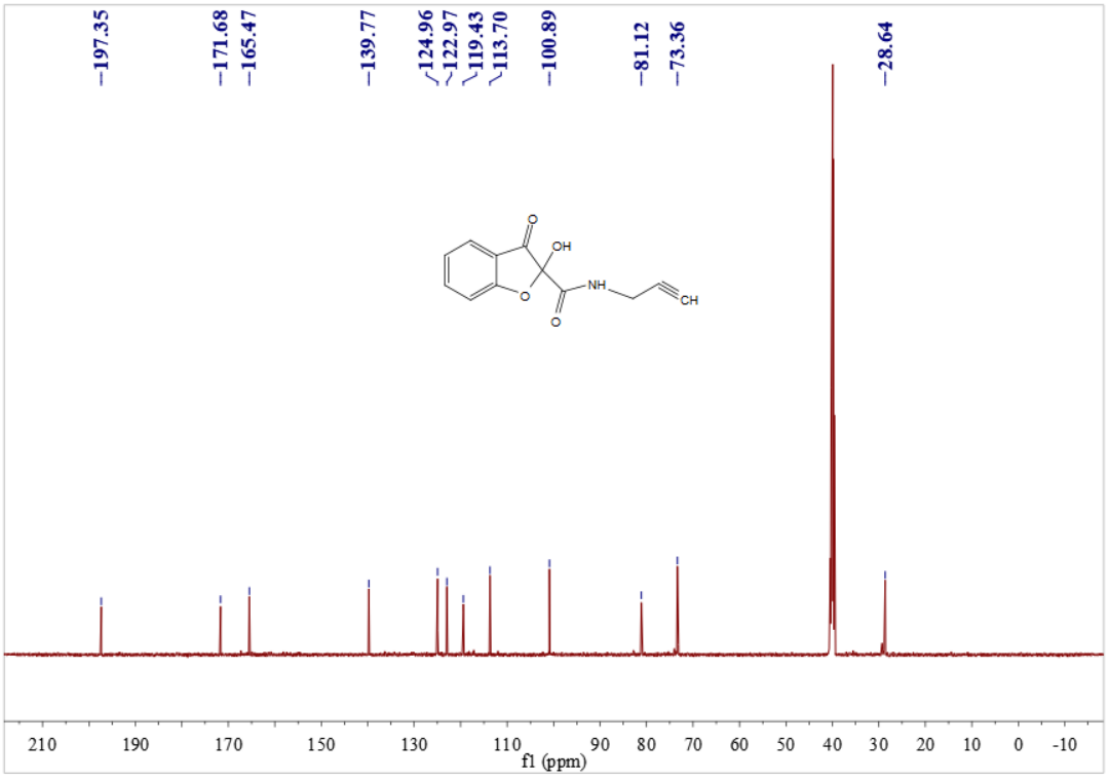
7.76
7.66
7.64
7.25
7.23
7.19
7.18
7.16
3.87
3.86
3.86
3.85
3.85
3.84
3.12
OH
O
NH
CH
1.23
1.17
1.00
1.02
1.08
1.92
0.91
f1 (ppm)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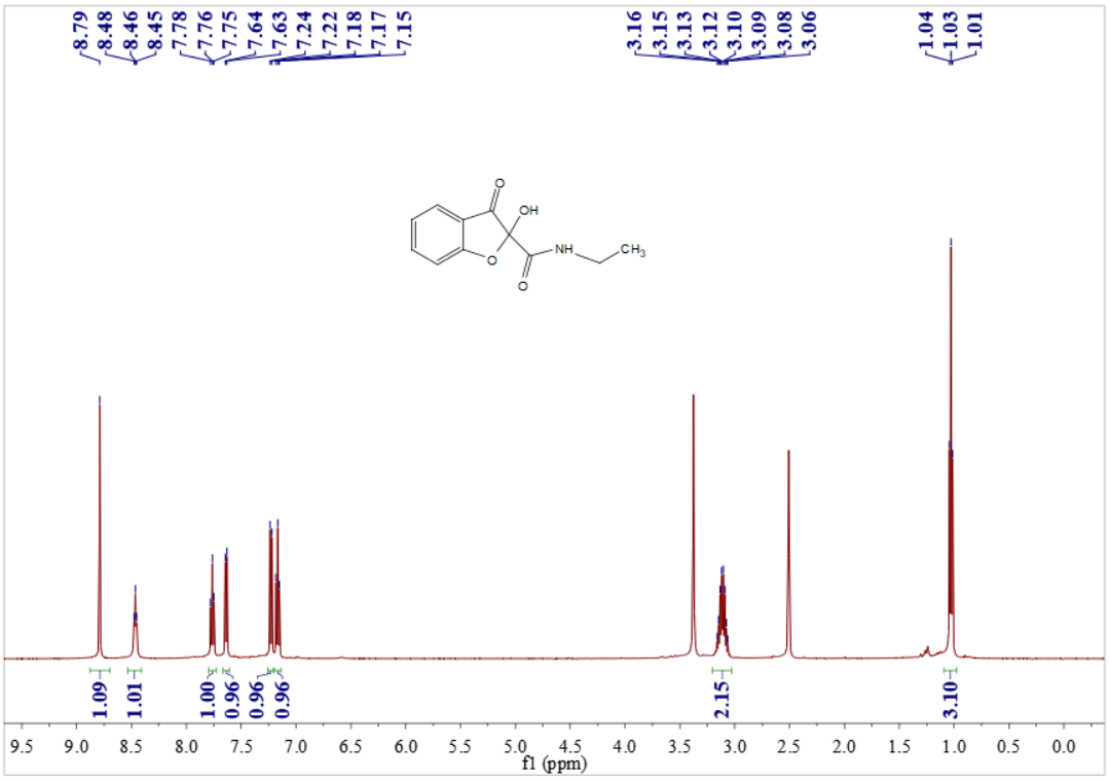
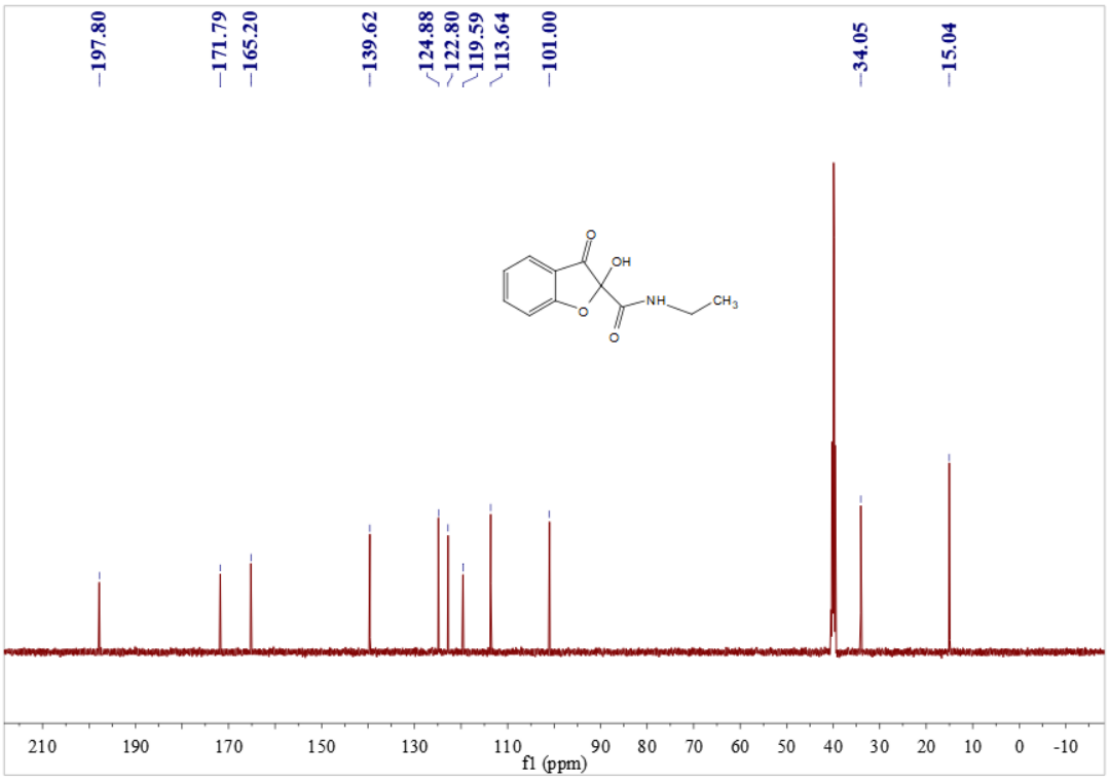
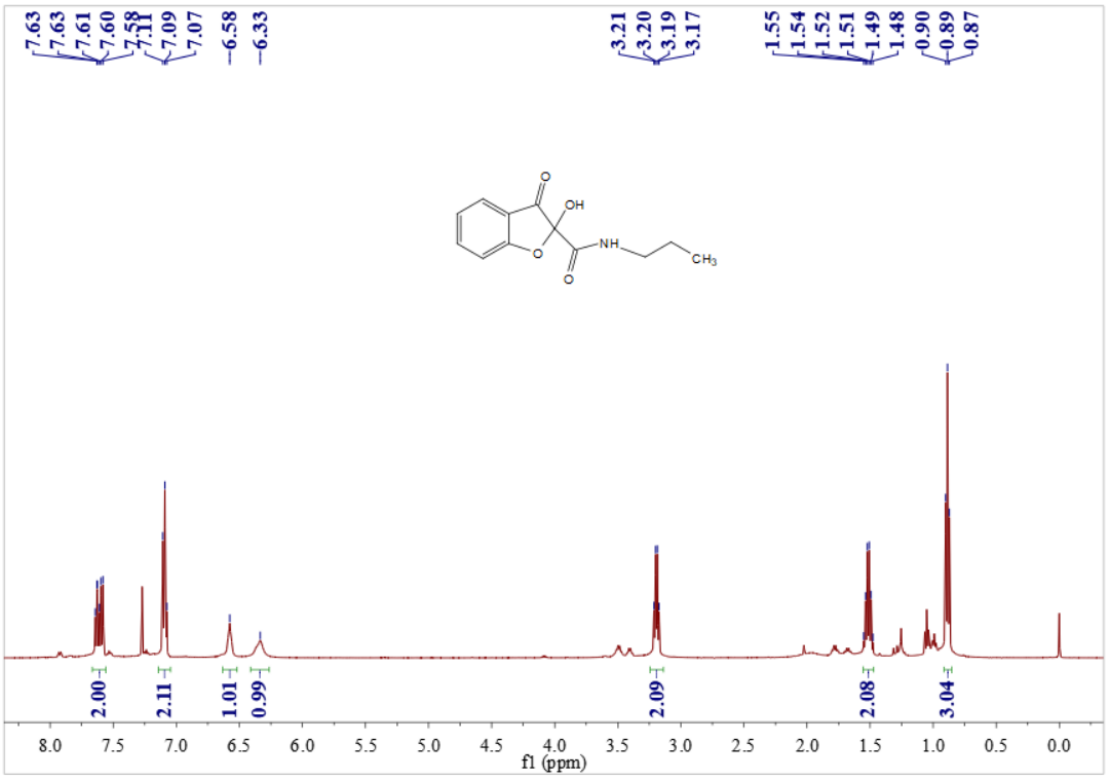
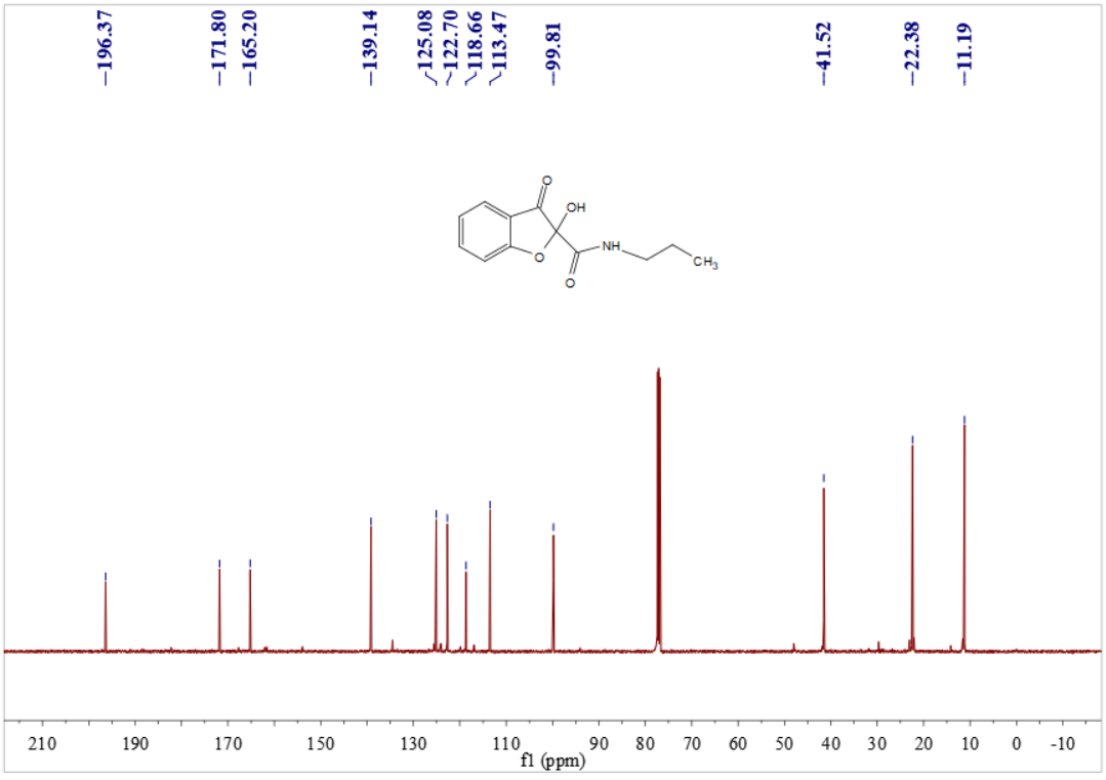
122.97
119.43
113.70
100.89
81.12
73.36
28.64
OH
O
NH
CH
f1 (ppm)


8.79
8.48
8.46
8.45
7.78
7.76
7.75
7.64
7.63
7.24
7.22
7.18
7.17
7.15
3.16
3.15
3.13
3.12
3.10
3.09
3.08
3.06
1.04
1.03
1.01
OH
O
NH
CH3
1.09
1.01
1.00
0.96
0.96
0.96
2.15
3.10
f1 (ppm)


197.80
171.79
165.20
139.62
124.88
122.80
119.59
113.64
101.00
34.05
15.04
OH
O
NH
CH3
f1 (ppm)


7.63
7.63
7.61
7.60
7.58
7.11
7.09
7.07
6.58
6.33
3.21
3.20
3.19
3.17
1.55
1.54
1.52
1.51
1.49
1.48
0.90
0.89
0.87
OH
NH
CH3
O
2.00
2.11
1.01
0.99
2.09
2.08
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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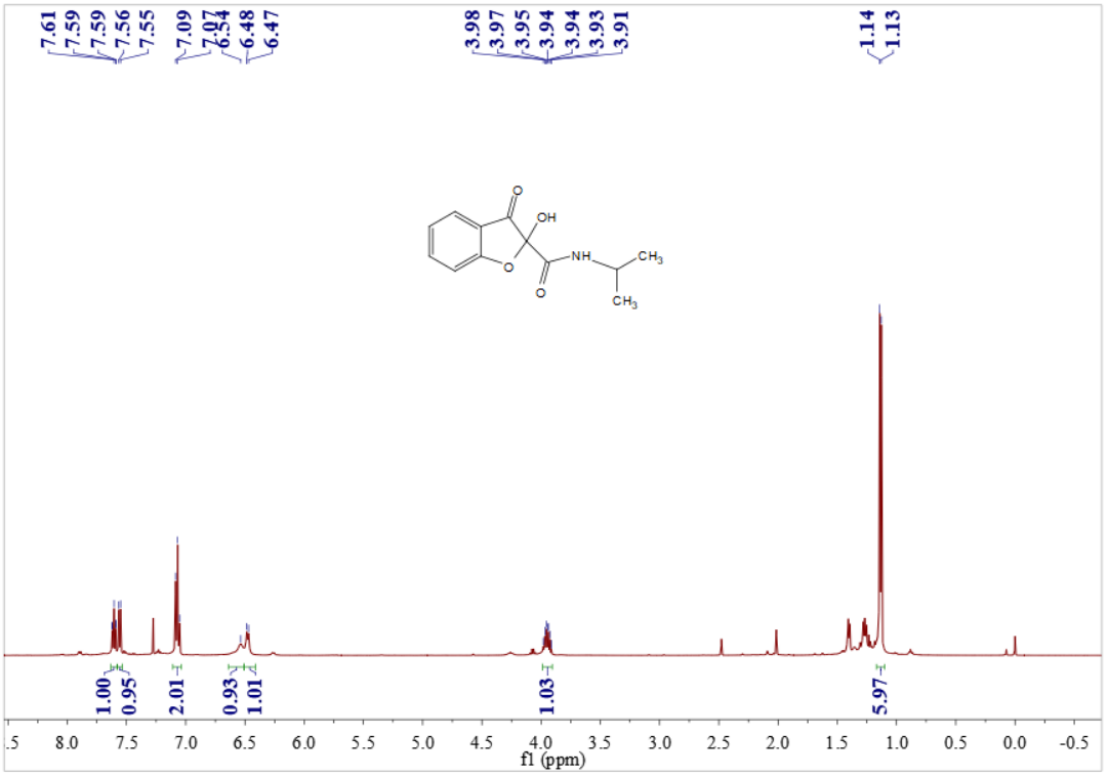
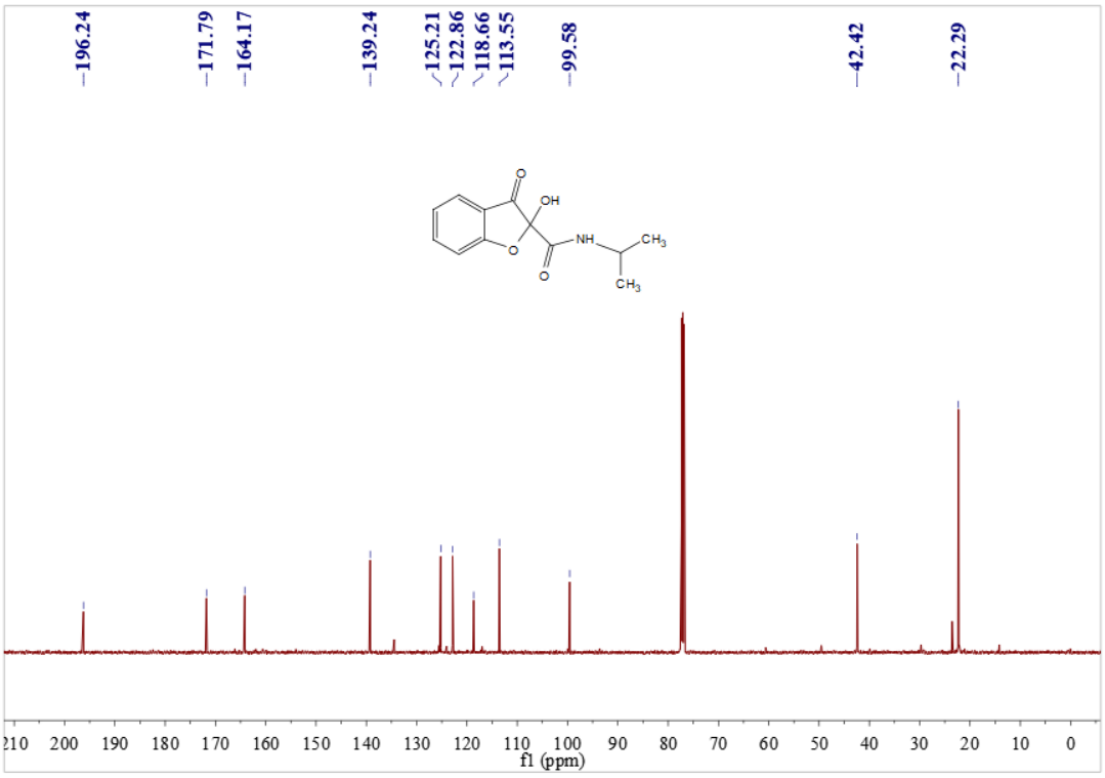
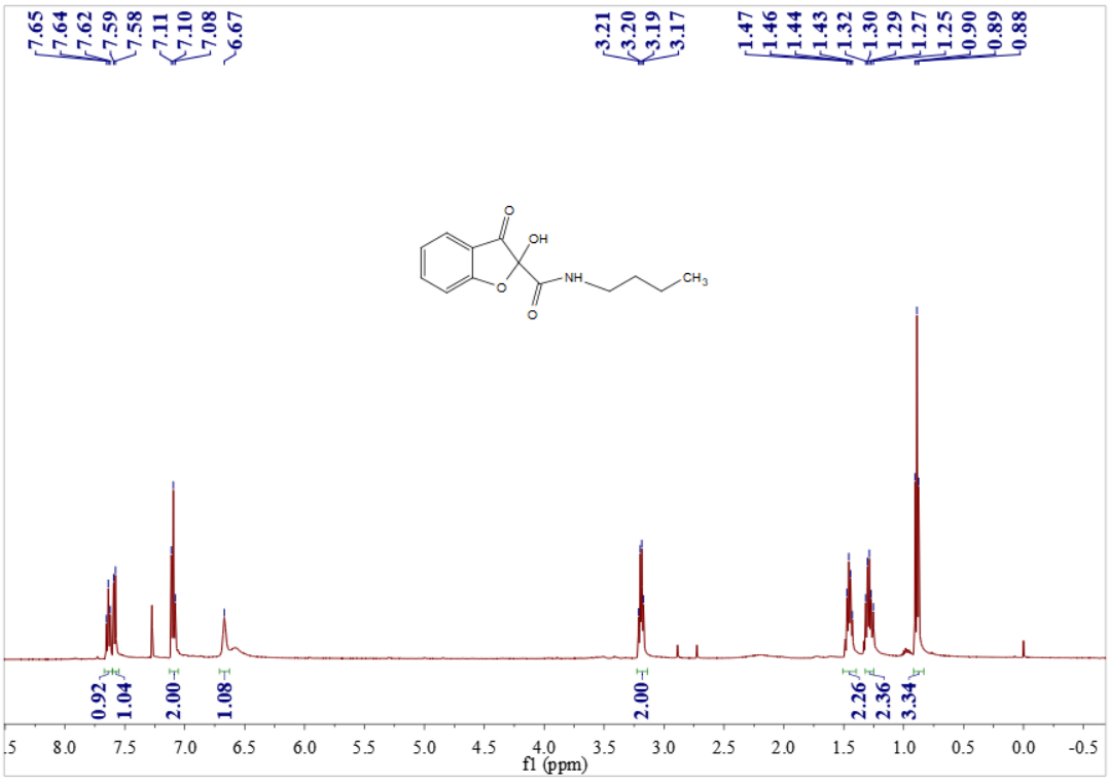
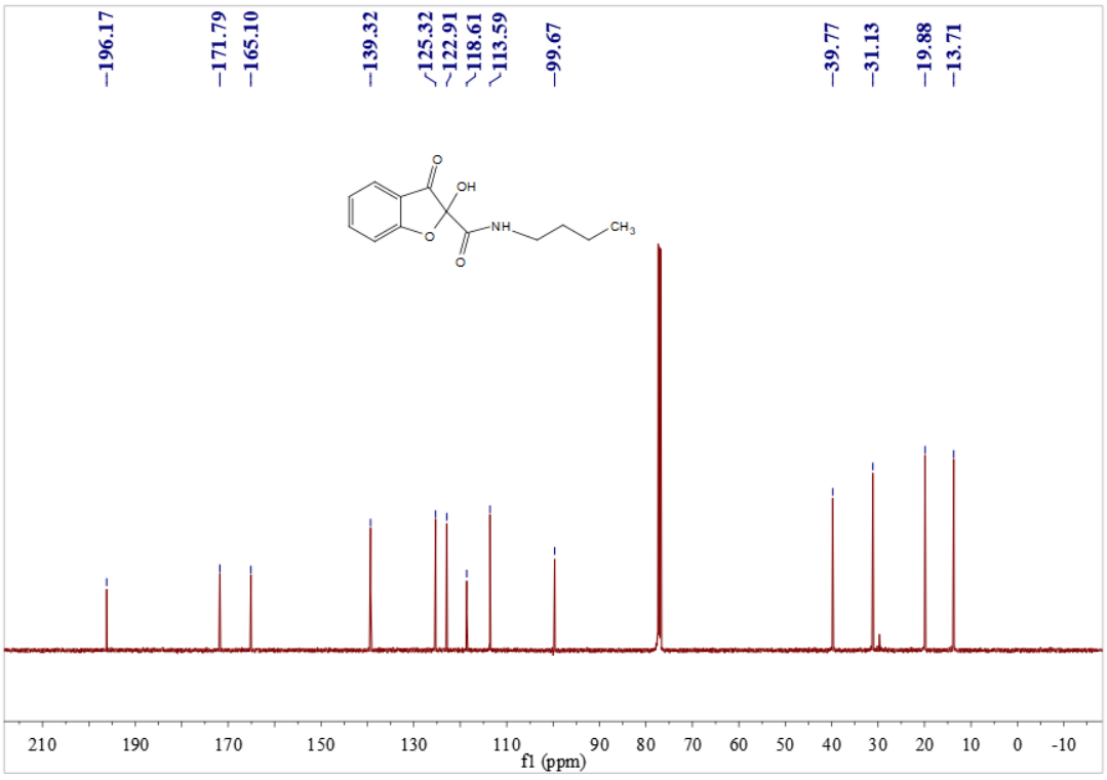
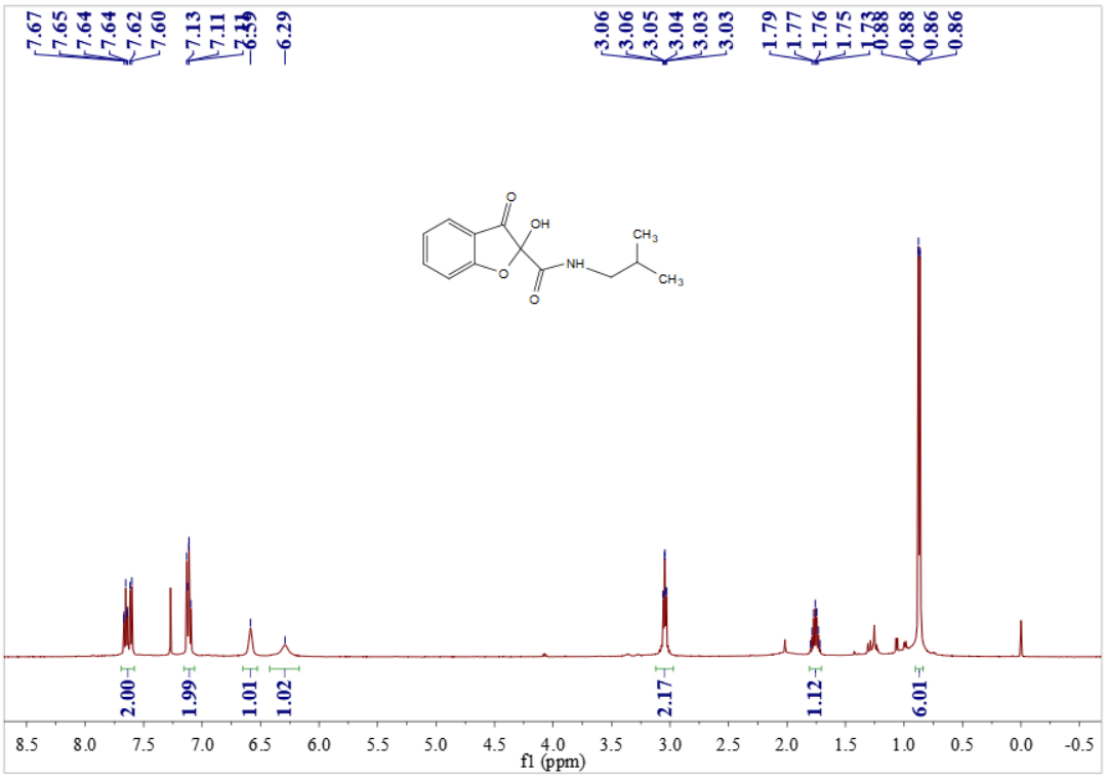
171.80
165.20
139.14
125.08
122.70
118.66
113.47
99.81
41.52
22.38
11.19
OH
NH
CH3
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

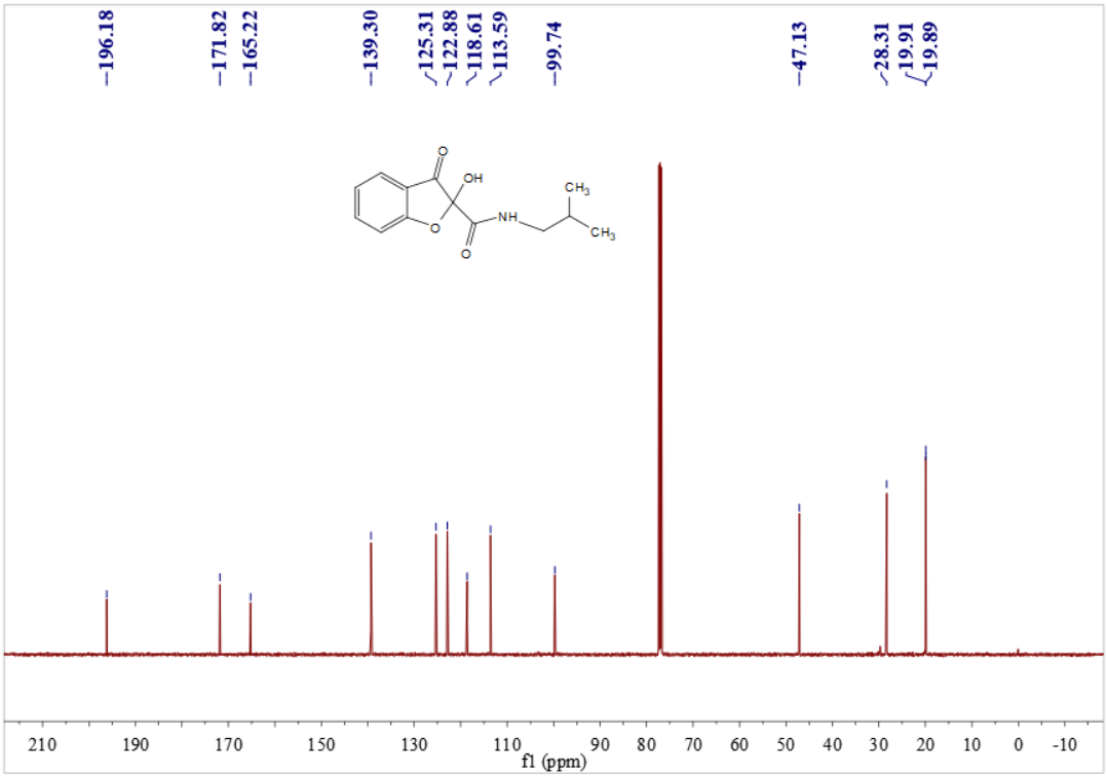

7.61
7.59
7.59
7.56
7.55
7.09
7.07
6.54
6.48
6.47
3.98
3.97
3.95
3.94
3.94
3.93
3.91
1.14
1.13
OH
NH
CH3
CH3
O
O
O
1.00
0.95
2.01
0.93
1.01
1.03
5.97
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

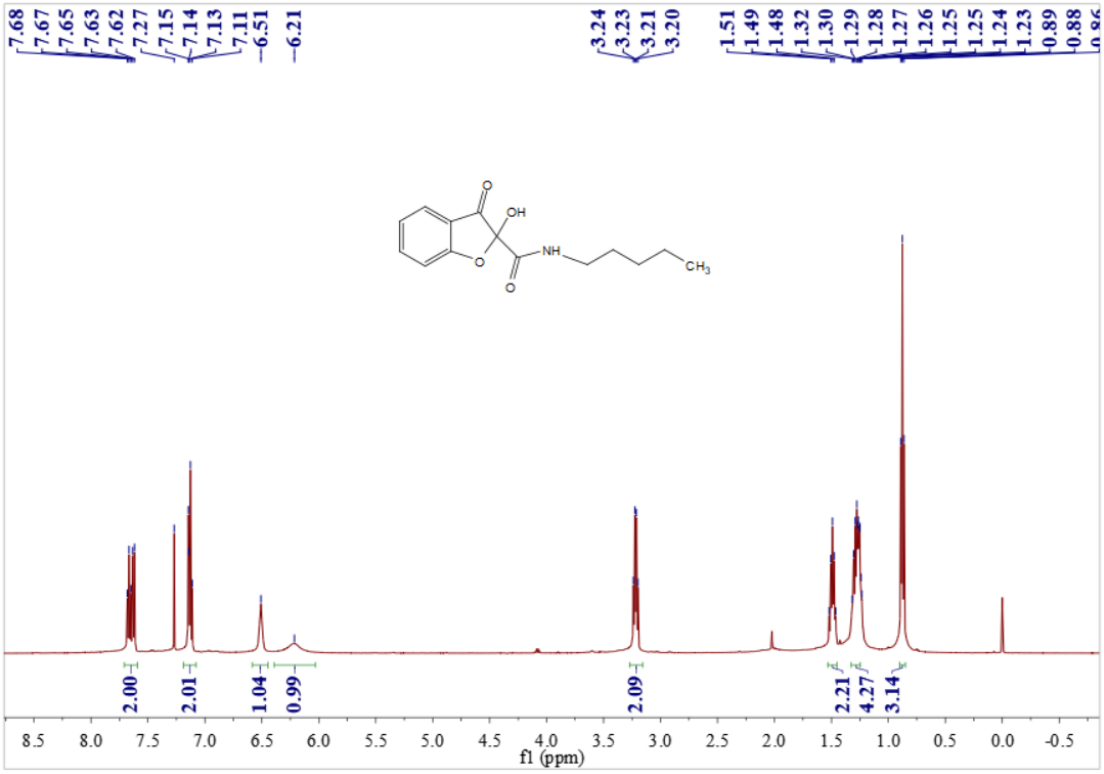

196.24
171.79
164.17
139.24
125.21
122.86
118.66
113.55
99.58
42.42
22.29
OH
NH
CH3
CH3
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

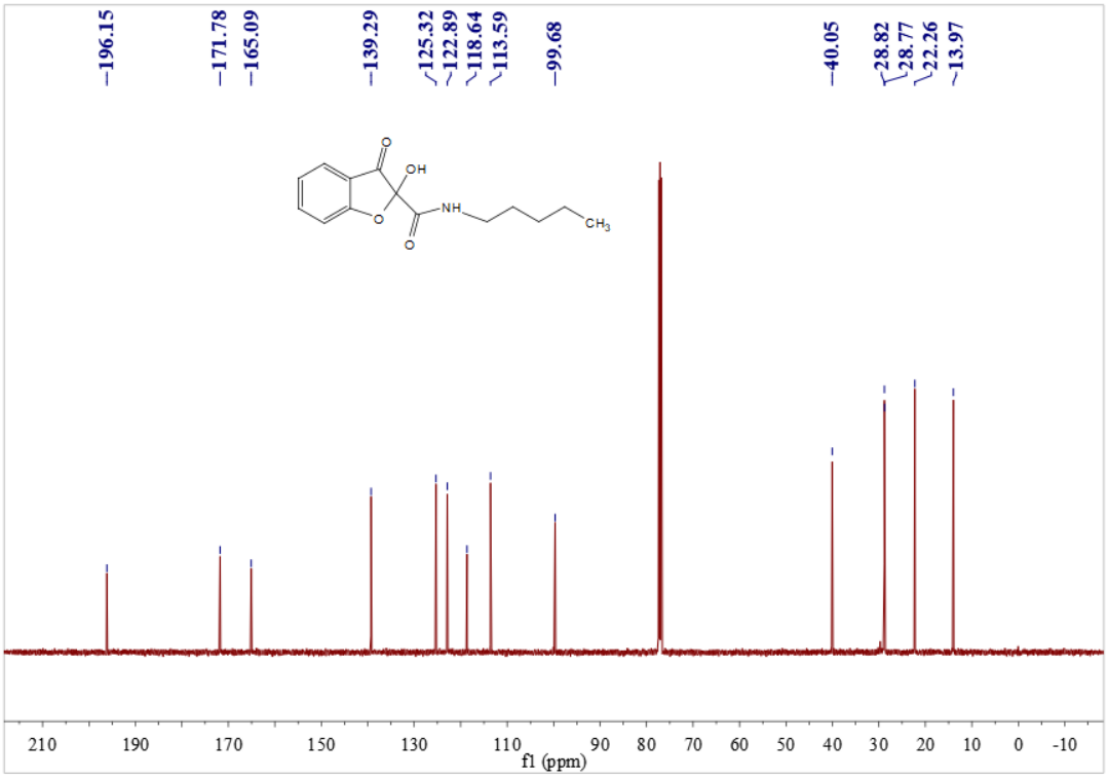

7.65
7.64
7.62
7.59
7.58
7.11
7.10
7.08
6.67
3.21
3.20
3.19
3.17
1.47
1.46
1.44
1.43
1.32
1.30
1.29
1.27
1.25
0.90
0.89
0.88
OH
NH
CH3
O
0.92
1.04
2.00
1.08
2.00
2.26
2.36
3.34
f1 (ppm)

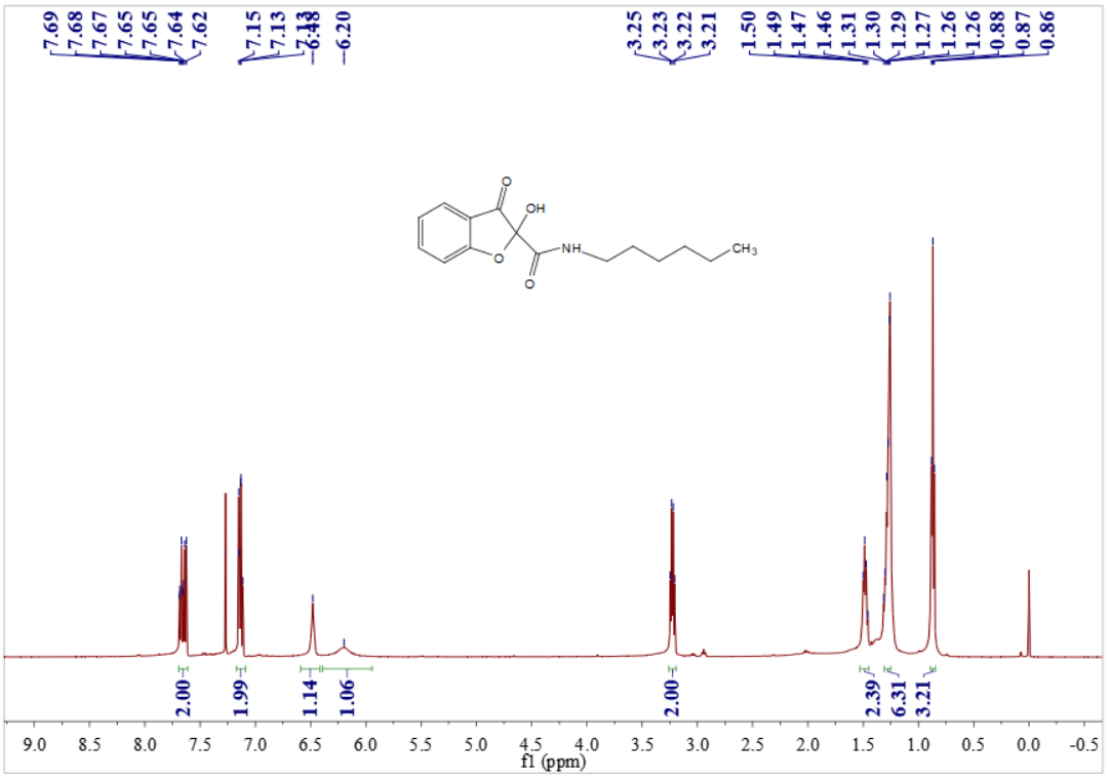

196.17
171.79
165.10
139.32
125.32
122.91
118.61
113.59
99.67
39.77
31.13
19.88
13.71
OH
NH
CH3
O
f1 (ppm)


7.67
7.65
7.64
7.64
7.62
7.60
7.13
7.11
6.29
3.06
3.06
3.05
3.04
3.03
3.03
1.79
1.77
1.76
1.75
0.88
0.86
0.86
OH
NH
CH3
CH3
2.00
1.99
1.01
1.02
2.17
1.12
6.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.18
171.82
165.22
139.30
125.31
122.88
118.61
113.59
99.74
47.13
28.31
19.91
19.89
OH
NH
CH3
CH3
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.68
7.67
7.65
7.63
7.62
7.27
7.15
7.14
7.13
7.11
6.51
6.21
3.24
3.23
3.21
3.20
1.51
1.49
1.48
1.32
1.30
1.29
1.28
1.27
1.26
1.25
1.25
1.24
1.23
0.89
0.88
OH
NH
CH3
2.00
2.01
1.04
0.99
2.09
2.21
4.27
3.14
f1 (ppm)


196.15
171.78
165.09
139.29
125.32
122.89
118.64
113.59
99.68
40.05
28.82
28.77
22.26
13.97
OH
NH
CH3
f1 (ppm)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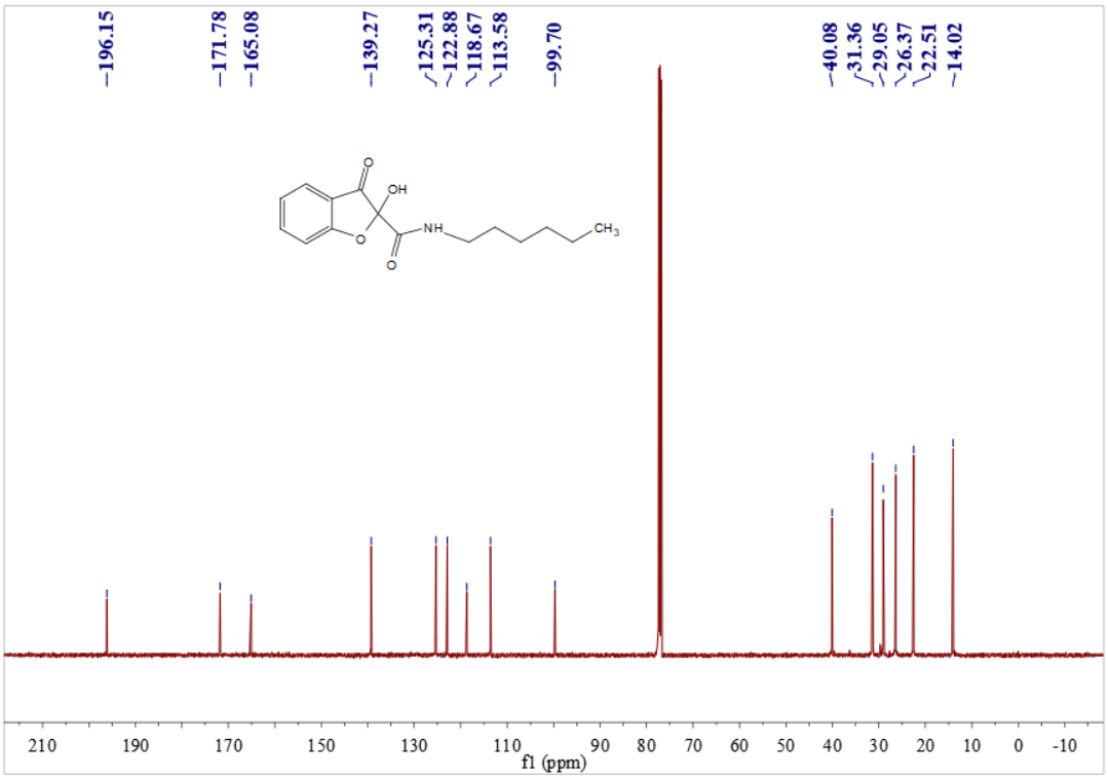
7.68
7.67
7.65
7.65
7.64
7.62
7.15
7.13
6.20
3.25
3.23
3.22
3.21
1.50
1.49
1.47
1.46
1.31
1.30
1.29
1.27
1.26
1.26
0.88
0.87
0.86
OH
NH
CH3
2.00
1.99
1.14
1.06
2.00
2.39
6.31
3.21
f1 (ppm)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171.78
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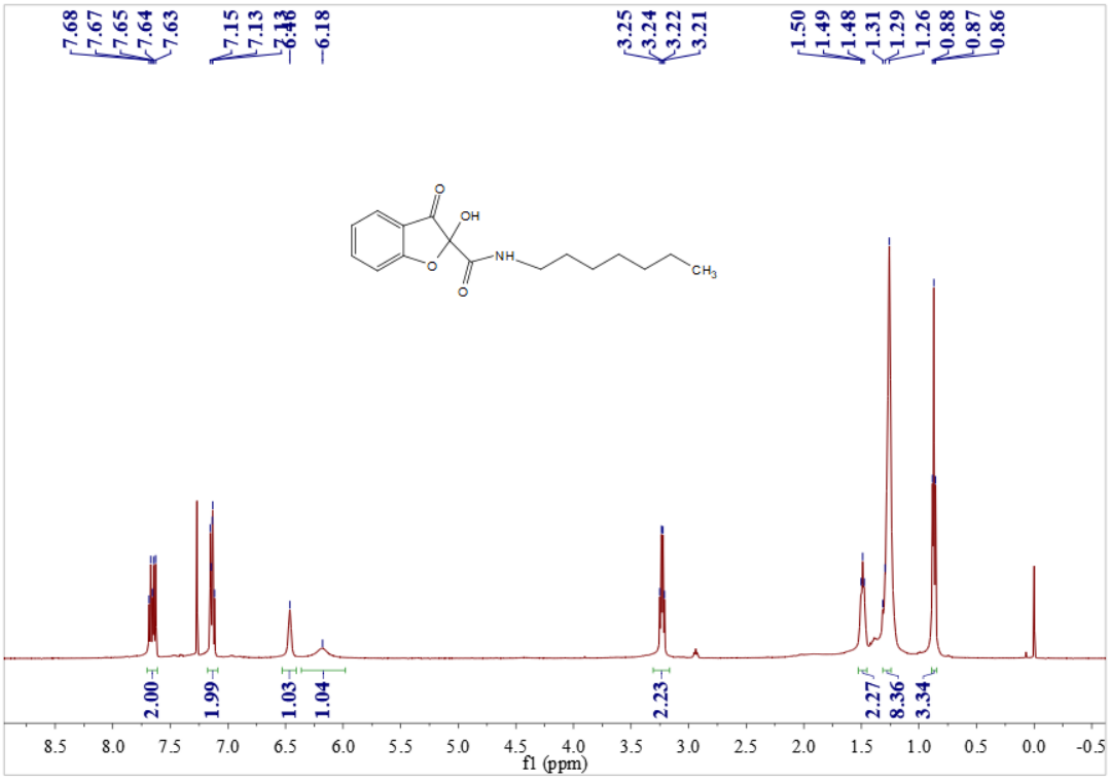
139.27
125.31
122.88
118.67
113.58
99.70
40.08
31.36
29.05
26.37
22.51
14.02
OH
NH
CH3
f1 (ppm)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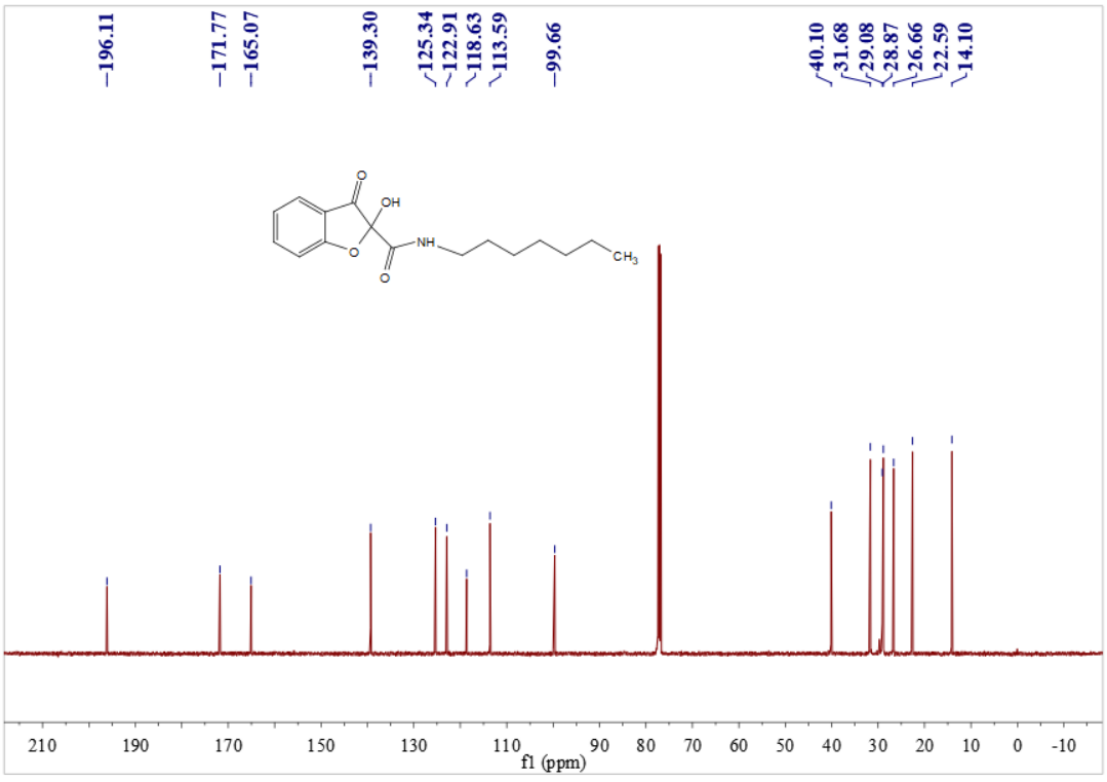
7.67
7.65
7.64
7.63
7.15
7.13
6.18
3.25
3.24
3.22
3.21
1.50
1.49
1.48
1.31
1.29
1.26
0.88
0.87
0.86
OH
NH
CH3
2.00
1.99
1.03
1.04
2.23
2.27
8.36
3.34
f1 (ppm)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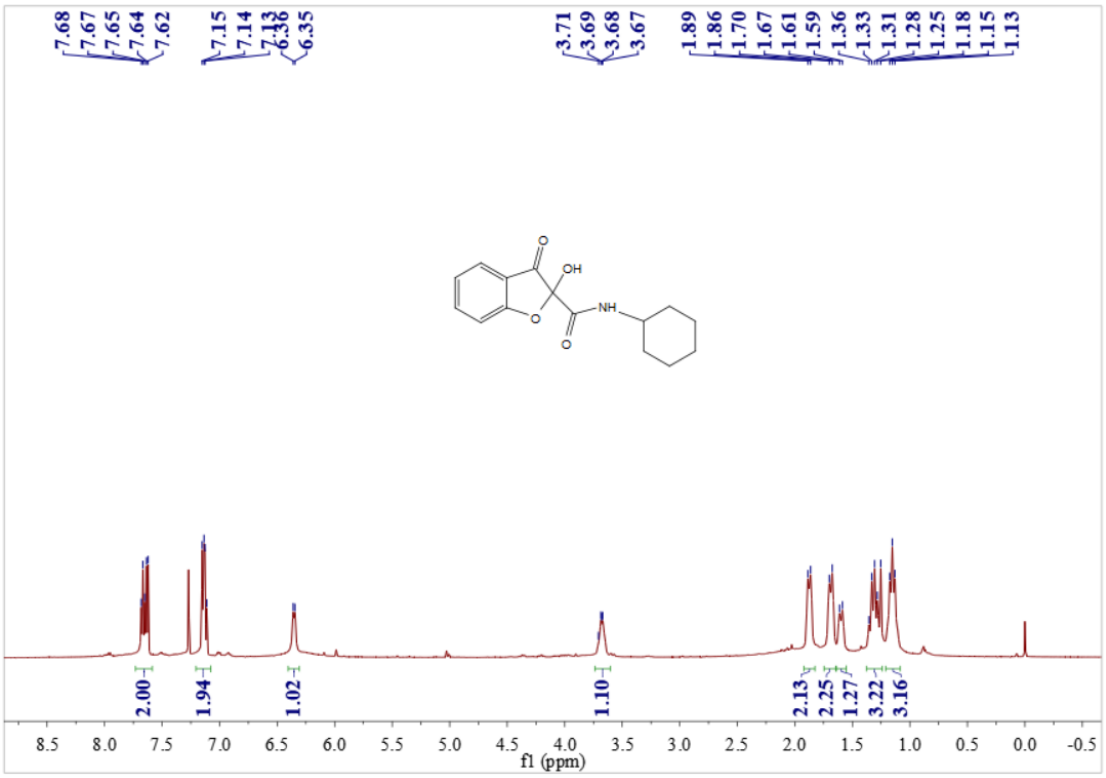
171.77
165.07
139.30
125.34
122.91
118.63
113.59
99.66
40.10
31.68
29.08
28.87
26.66
22.59
14.10
OH
NH
CH3
f1 (ppm)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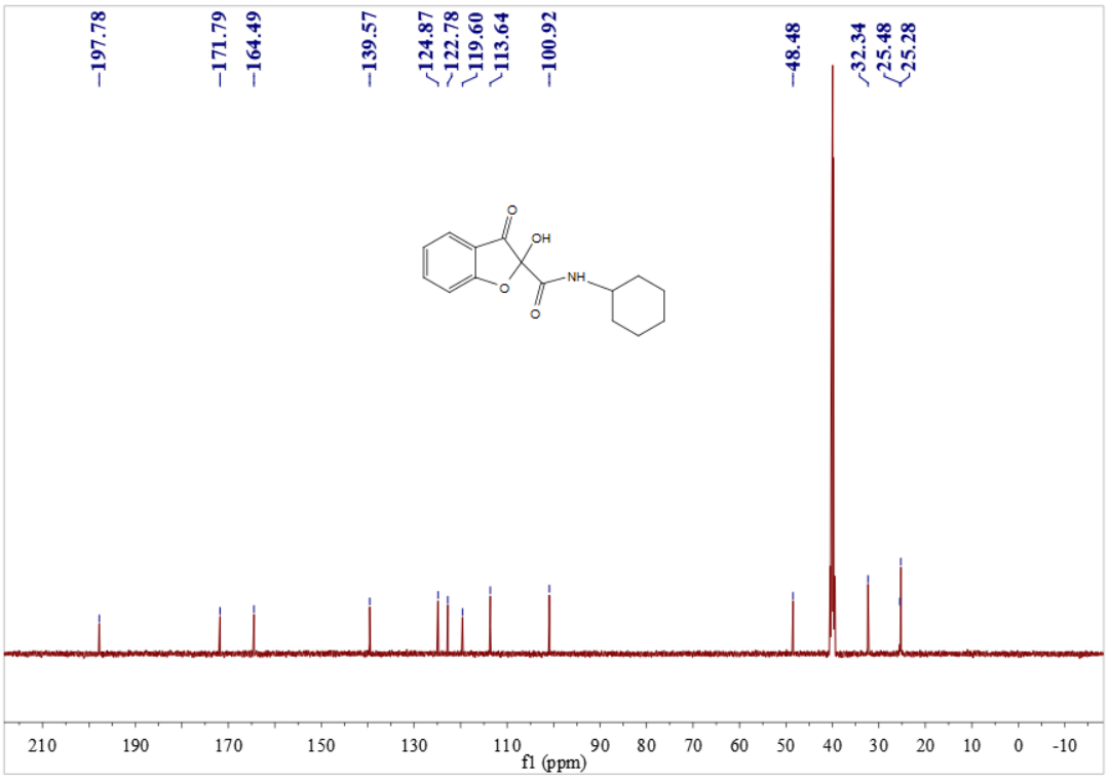
7.67
7.65
7.64
7.62
7.15
7.14
7.13
6.36
6.35
3.71
3.69
3.68
3.67
1.89
1.86
1.70
1.67
1.61
1.59
1.36
1.33
1.31
1.28
1.25
1.18
1.15
1.13
OH
NH
2.00
1.94
1.02
1.10
2.13
2.25
1.27
3.22
3.16
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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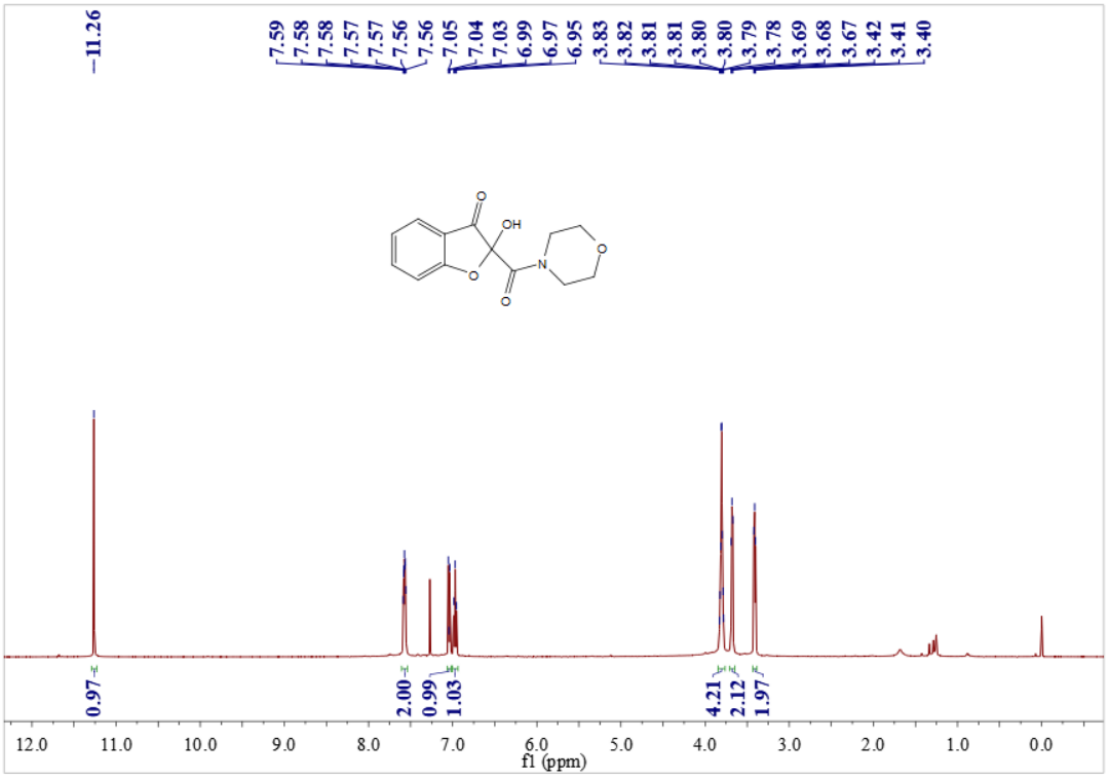
122.78
119.60
113.64
100.92
48.48
32.34
25.48
25.28
OH
NH
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.26
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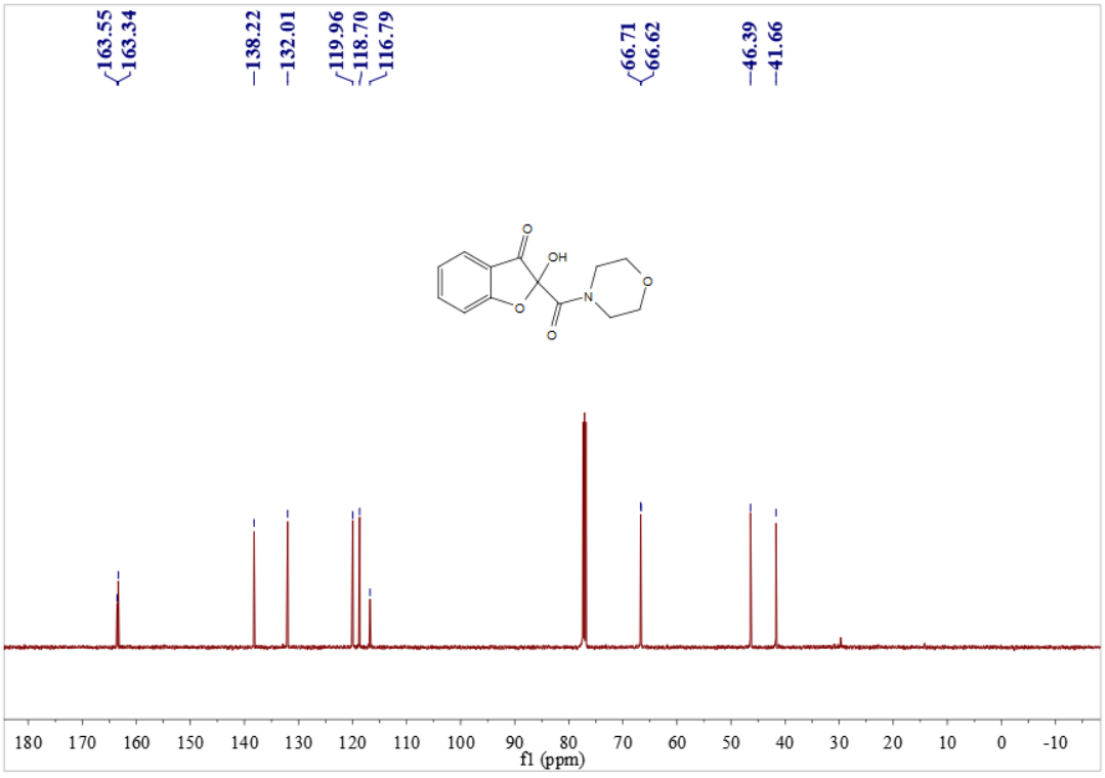
7.58
7.58
7.57
7.57
7.56
7.56
7.05
7.04
7.03
6.99
6.97
6.95
3.83
3.82
3.81
3.81
3.80
3.80
3.79
3.78
3.69
3.68
3.67
3.42
3.41
3.40
OH
O
N
0.97
2.00
0.99
1.03
4.21
2.12
1.97
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


163.55
163.34
138.22
132.01
119.96
118.70
116.79
66.71
66.62
46.39
41.66
OH
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)