

Supplementary Information

Design, Synthesis, and Cytotoxicity of Ibuprofen Appended Benzoxazole Analogues against Human Breast Adenocarcinoma

Vishnu Thumma,^a Veerabhadraiah Mallikanti,^b Raghavender Matta,^c Ravinder Dharavath,^d
Jalapathi Pochampally^{b*}

*^aDepartment of Sciences and Humanities, Matrusri Engineering College, Hyderabad,
500059, Telangana, India*

^bDepartment of Chemistry, Osmania University, Hyderabad - 500007, Telangana, India.

^cDepartment of Chemistry, Shyam Lal College, University of Delhi, Delhi – 110032, India

*^dDepartment of Chemistry, SRT Campus, Hemwati Nandan Bahuguna Garhwal University,
Tehri, 249199, Uttarakhand, India.*

*E-mail: pochampalli.ou.chemi@gmail.com

1. % Cell viabilities data
2. Spectral copies

Cell Viability Data

Table S1. % Cell viability of MCF-7 cell upon treatment of 7a-l.

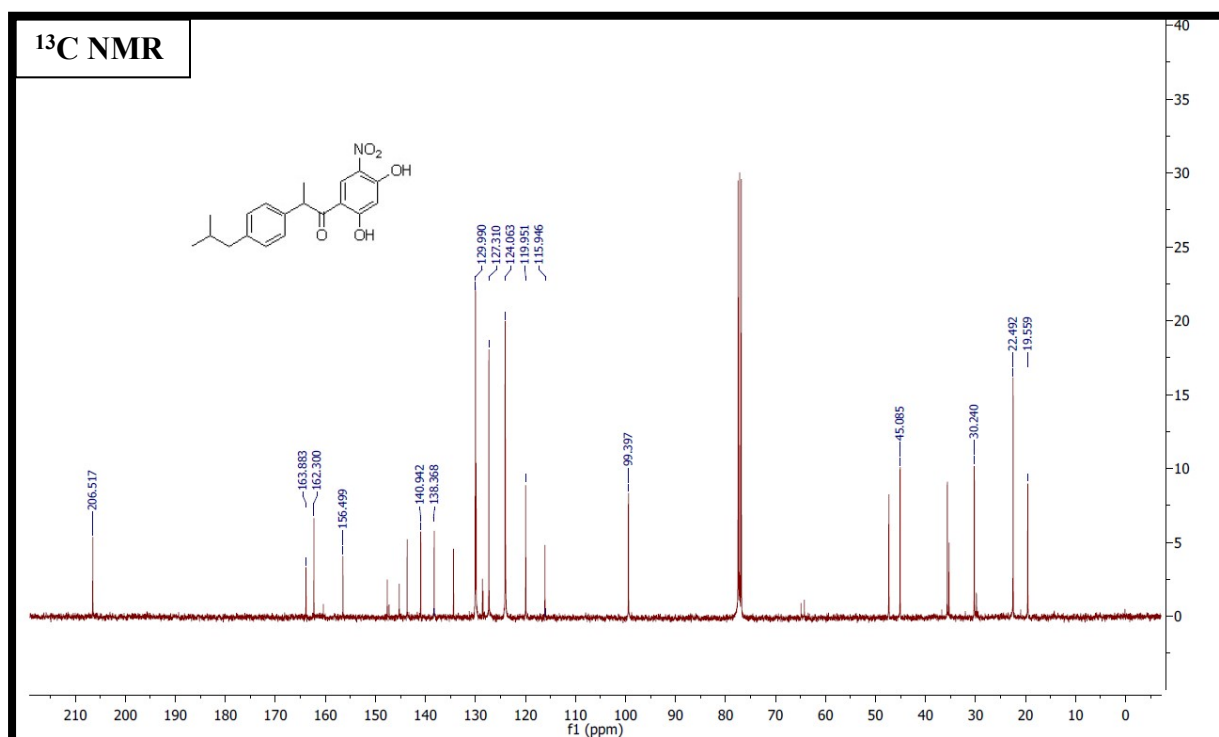
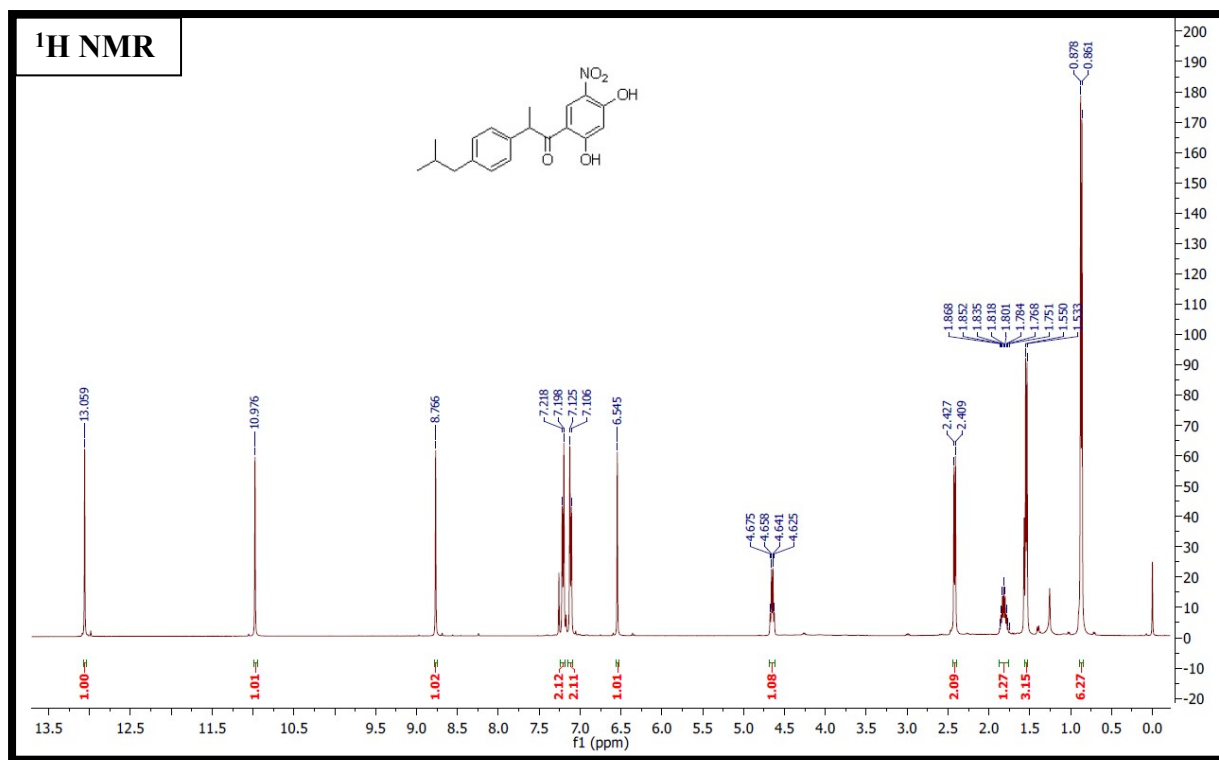
Entry	Conc. in μM						
	2	4	8	16	32	64	128
7a	95.36 $\pm$ 7.26	86.23 $\pm$ 10.26	71.34 $\pm$ 6.55	52.34 $\pm$ 6.05	42.03 $\pm$ 5.34	35.24 $\pm$ 3.96	31.07 $\pm$ 2.69
7b	96.54 $\pm$ 10.15	91.35 $\pm$ 10.14	82.34 $\pm$ 6.92	75.14 $\pm$ 6.94	65.35 $\pm$ 5.68	59.24 $\pm$ 6.04	47.12 $\pm$ 3.54
7c	89.36 $\pm$ 8.31	75.24 $\pm$ 8.24	63.21 $\pm$ 5.28	48.36 $\pm$ 5.07	40.08 $\pm$ 3.57	35.26 $\pm$ 2.96	29.33 $\pm$ 3.82
7d	88.26 $\pm$ 9.25	78.32 $\pm$ 7.12	65.42 $\pm$ 5.89	56.39 $\pm$ 5.12	48.28 $\pm$ 4.71	41.05 $\pm$ 3.48	38.33 $\pm$ 4.01
7e	93.25 $\pm$ 8.41	80.36 $\pm$ 6.35	62.14 $\pm$ 6.39	55.26 $\pm$ 4.86	46.29 $\pm$ 4.93	39.58 $\pm$ 4.15	33.21 $\pm$ 3.72
7f	92.04 $\pm$ 8.39	82.35 $\pm$ 6.98	63.58 $\pm$ 5.84	52.04 $\pm$ 4.33	41.06 $\pm$ 3.88	33.05 $\pm$ 4.63	24.18 $\pm$ 2.66
7g	86.91 $\pm$ 9.25	65.34 $\pm$ 5.39	39.54 $\pm$ 4.12	15.06 $\pm$ 2.04	8.04 $\pm$ 5.27	3.69 $\pm$ 0.69	2.15 $\pm$ 2.41
7h	85.97 $\pm$ 8.54	64.36 $\pm$ 6.08	33.06 $\pm$ 3.58	13.57 $\pm$ 1.87	7.86 $\pm$ 8.27	2.77 $\pm$ 0.38	1.67 $\pm$ 0.26
7i	86.91 $\pm$ 10.04	69.35 $\pm$ 5.87	49.25 $\pm$ 3.74	36.27 $\pm$ 1.92	30.05 $\pm$ 2.64	22.15 $\pm$ 1.69	18.34 $\pm$ 1.89
7j	86.33 $\pm$ 9.87	67.34 $\pm$ 6.93	32.07 $\pm$ 3.08	12.59 $\pm$ 1.35	7.66 $\pm$ 1.03	2.74 $\pm$ 0.39	1.81 $\pm$ 0.29
7k	92.35 $\pm$ 7.66	85.36 $\pm$ 7.14	69.35 $\pm$ 5.27	51.34 $\pm$ 5.87	32.15 $\pm$ 3.65	24.18 $\pm$ 2.97	15.22 $\pm$ 1.63
7l	93.58 $\pm$ 8.18	85.34 $\pm$ 6.48	69.84 $\pm$ 6.27	55.27 $\pm$ 4.76	46.25 $\pm$ 3.41	41.08 $\pm$ 3.74	35.27 $\pm$ 4.08
Doxorubicin	86.23 $\pm$ 8.74	63.48 $\pm$ 7.04	34.07 $\pm$ 3.11	14.96 $\pm$ 1.22	8.15 $\pm$ 1.36	1.52 $\pm$ 0.25	0.98 $\pm$ 0.08

Table S2. % Cell viability of MDA-MB-231 cells upon treatment of 7a-l

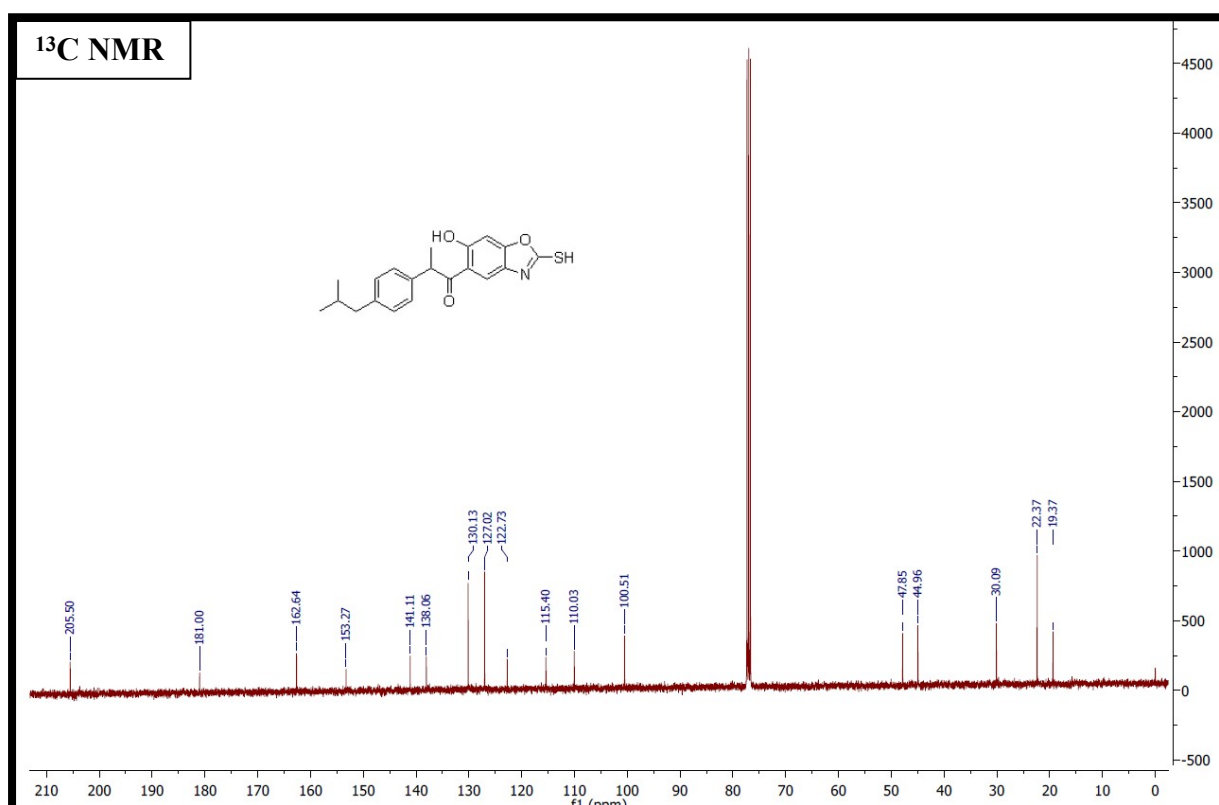
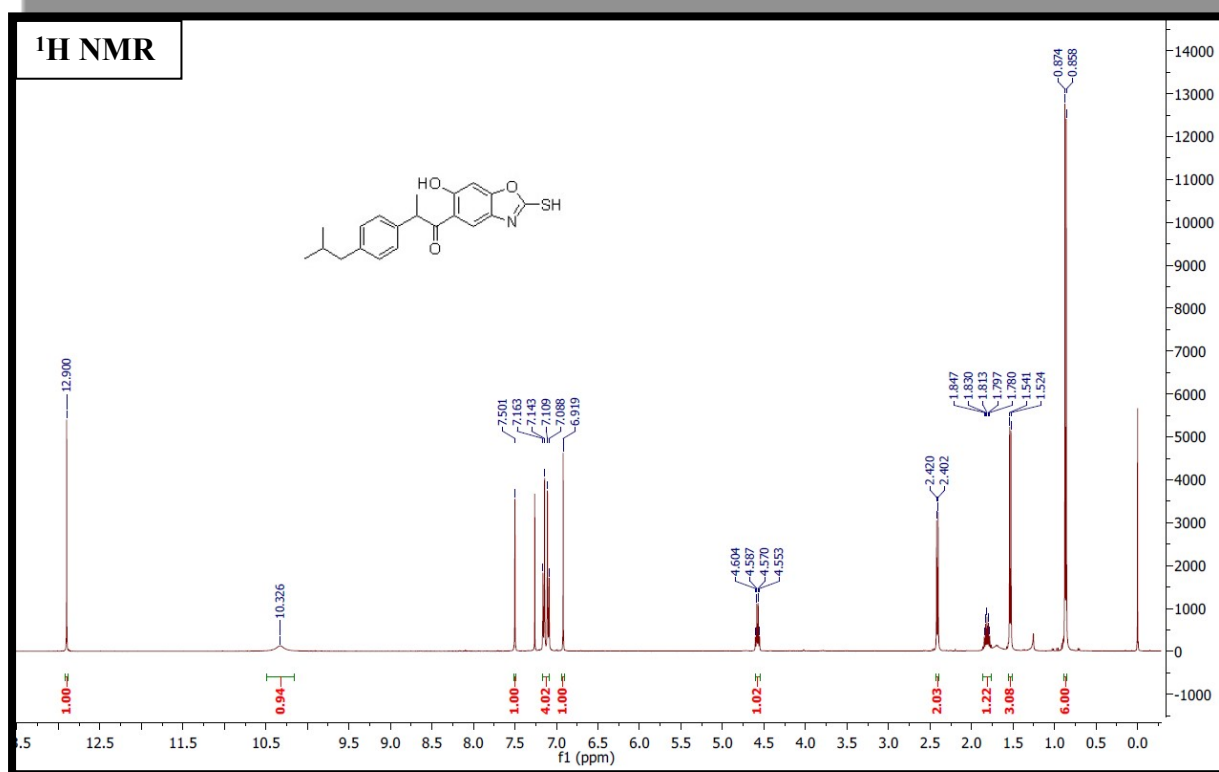
Entry	Conc. in μM						
	2	4	8	16	32	64	128
7a	95.66 $\pm$ 9.15	89.35 $\pm$ 9.23	73.25 $\pm$ 6.89	56.35 $\pm$ 4.86	45.12 $\pm$ 4.15	39.36 $\pm$ 3.59	34.21 $\pm$ 3.17
7b	92.35 $\pm$ 10.33	84.26 $\pm$ 8.29	74.12 $\pm$ 8.22	65.39 $\pm$ 5.93	58.24 $\pm$ 5.23	43.12 $\pm$ 4.58	35.69 $\pm$ 2.98
7c	90.36 $\pm$ 8.56	79.35 $\pm$ 8.56	62.55 $\pm$ 7.35	51.38 $\pm$ 6.23	42.15 $\pm$ 5.07	30.48 $\pm$ 3.61	21.33 $\pm$ 1.89
7d	95.36 $\pm$ 10.71	82.35 $\pm$ 9.47	62.14 $\pm$ 7.17	52.39 $\pm$ 6.17	42.17 $\pm$ 4.69	32.15 $\pm$ 3.48	22.98 $\pm$ 2.11
7e	91.25 $\pm$ 9.24	83.26 $\pm$ 8.61	66.35 $\pm$ 7.59	53.26 $\pm$ 4.82	42.18 $\pm$ 4.22	36.25 $\pm$ 3.27	25.15 $\pm$ 2.47
7f	93.55 $\pm$ 8.99	83.45 $\pm$ 9.48	65.24 $\pm$ 6.78	56.29 $\pm$ 4.66	41.05 $\pm$ 3.75	32.08 $\pm$ 2.95	21.36 $\pm$ 1.96
7g	87.24 $\pm$ 7.25	68.25 $\pm$ 6.88	35.24 $\pm$ 4.12	15.34 $\pm$ 2.31	9.35 $\pm$ 1.31	5.24 $\pm$ 0.93	3.47 $\pm$ 0.53
7h	88.62 $\pm$ 8.18	65.38 $\pm$ 7.15	34.28 $\pm$ 3.86	11.39 $\pm$ 1.54	8.16 $\pm$ 1.24	2.23 $\pm$ 0.35	1.39 $\pm$ 0.26
7i	87.86 $\pm$ 8.63	65.23 $\pm$ 6.35	33.47 $\pm$ 3.44	13.48 $\pm$ 1.69	8.65 $\pm$ 1.32	4.28 $\pm$ 0.69	2.11 $\pm$ 0.34
7j	87.91 $\pm$ 9.51	68.24 $\pm$ 5.98	42.15 $\pm$ 4.28	25.98 $\pm$ 3.05	13.69 $\pm$ 1.59	7.96 $\pm$ 0.95	3.15 $\pm$ 0.51
7k	92.35 $\pm$ 8.24	86.25 $\pm$ 6.17	69.35 $\pm$ 5.93	52.39 $\pm$ 4.78	39.41 $\pm$ 4.14	27.45 $\pm$ 2.11	21.06 $\pm$ 1.94
7l	93.58 $\pm$ 7.92	82.36 $\pm$ 7.49	65.47 $\pm$ 4.28	52.49 $\pm$ 4.92	41.09 $\pm$ 3.62	33.27 $\pm$ 3.17	28.41 $\pm$ 2.54
Doxorubicin	85.22 $\pm$ 9.26	61.35 $\pm$ 7.35	33.01 $\pm$ 3.54	12.39 $\pm$ 1.65	8.27 $\pm$ 1.09	2.69 $\pm$ 0.59	1.23 $\pm$ 0.31

Spectral Copies

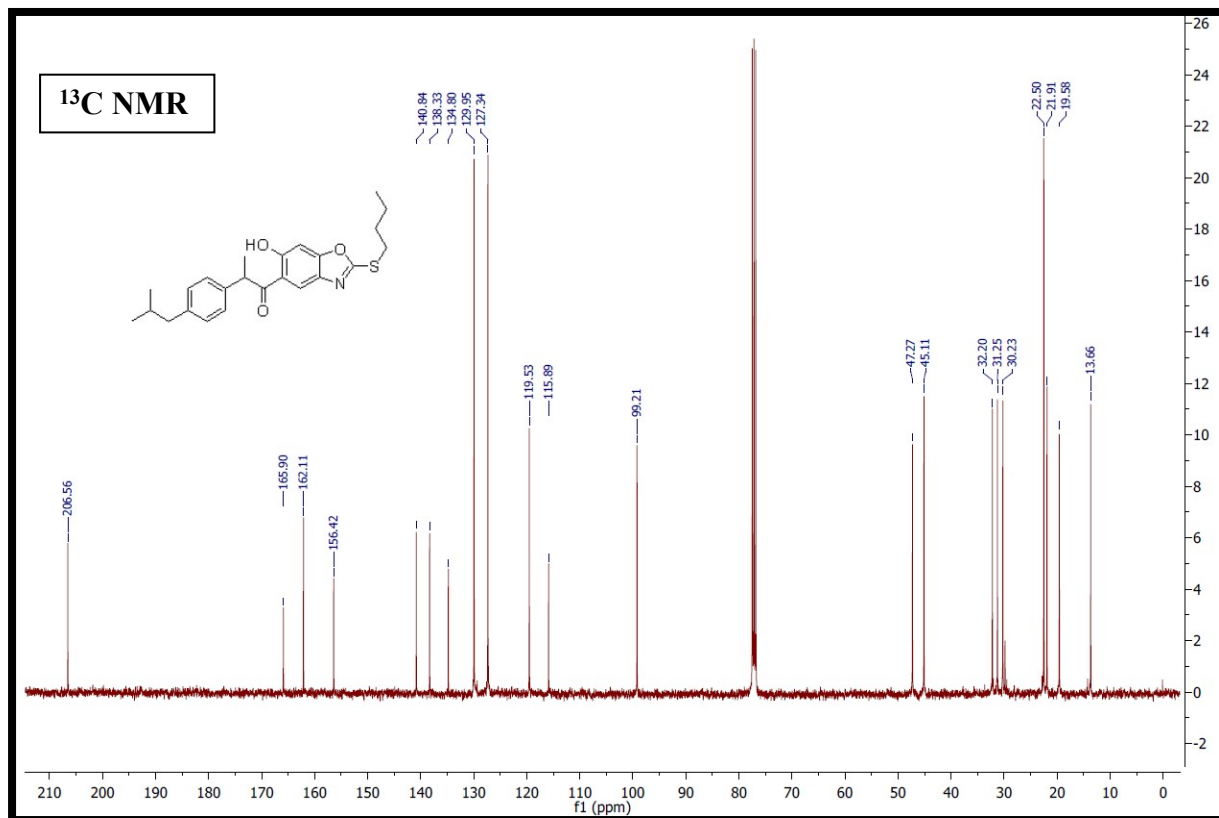
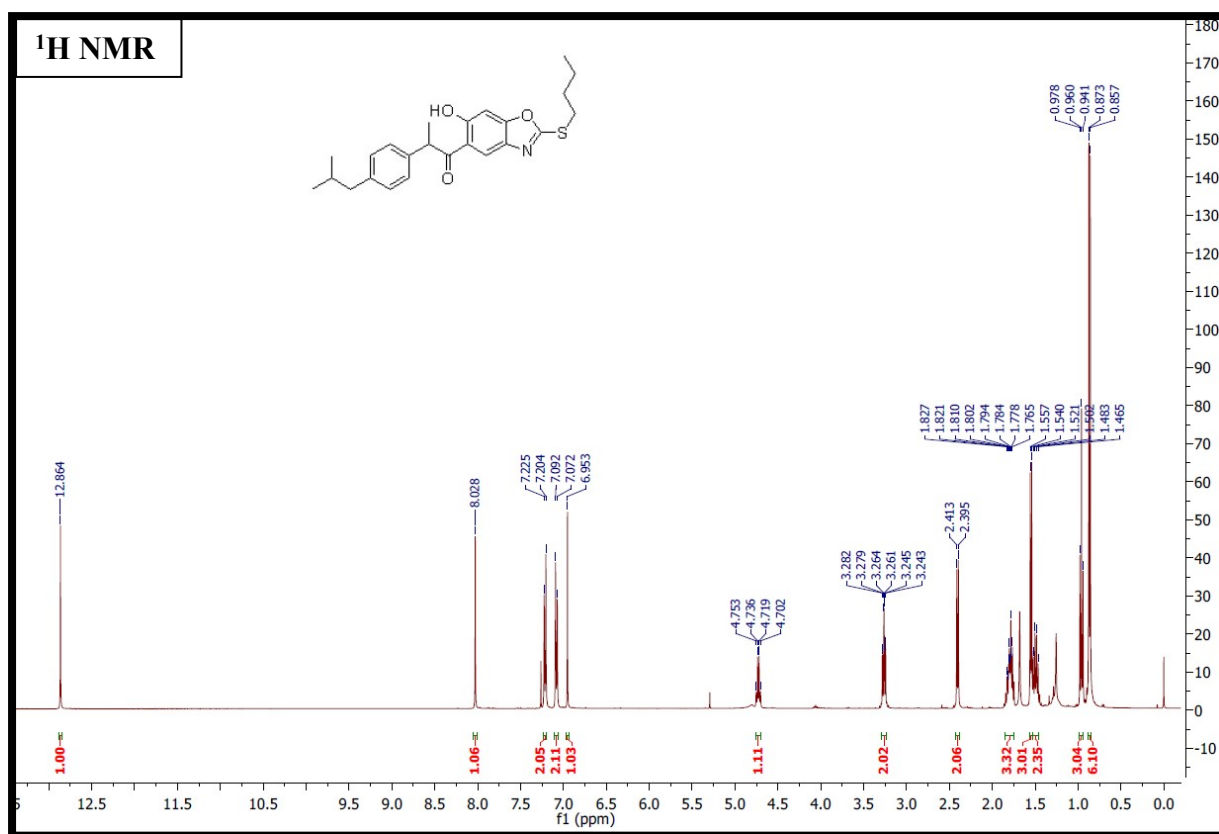
1-(2,4-dihydroxy-5-nitrophenyl)-2-(4-isobutylphenyl) propan-1-one (4):



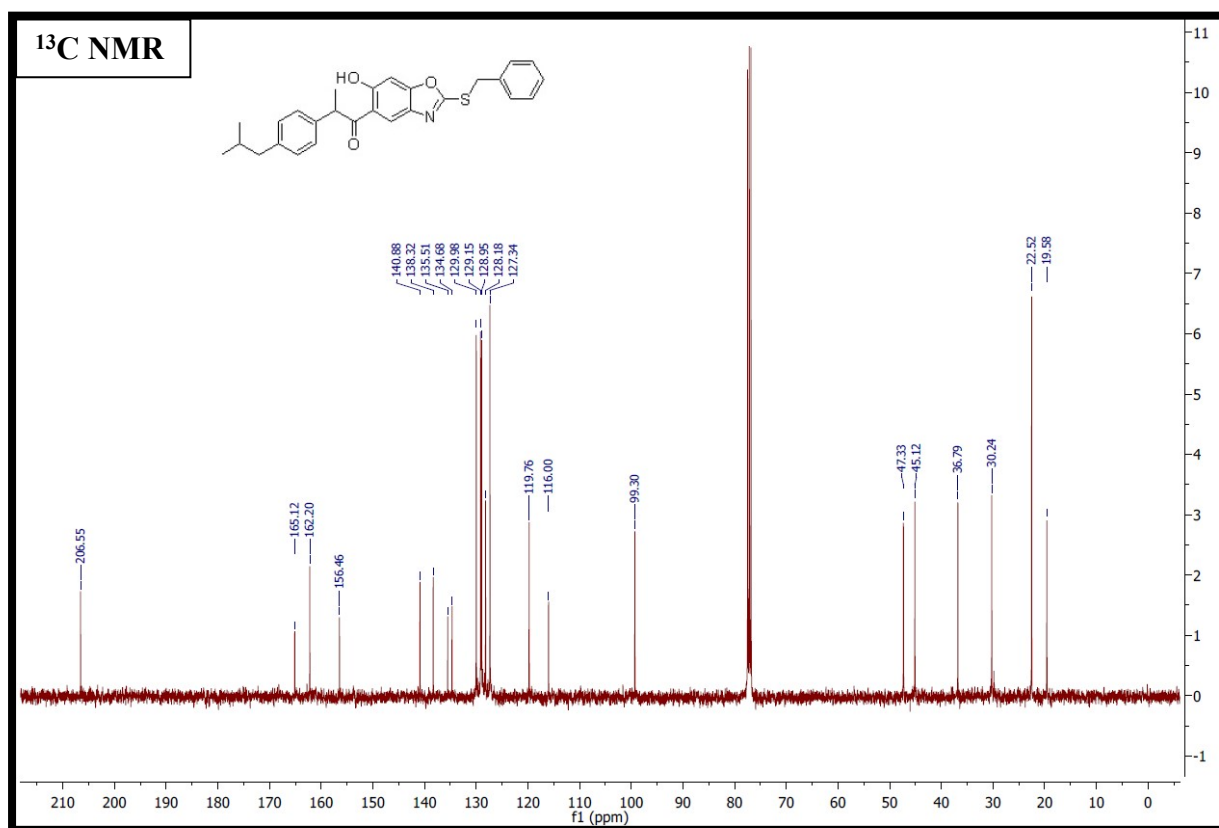
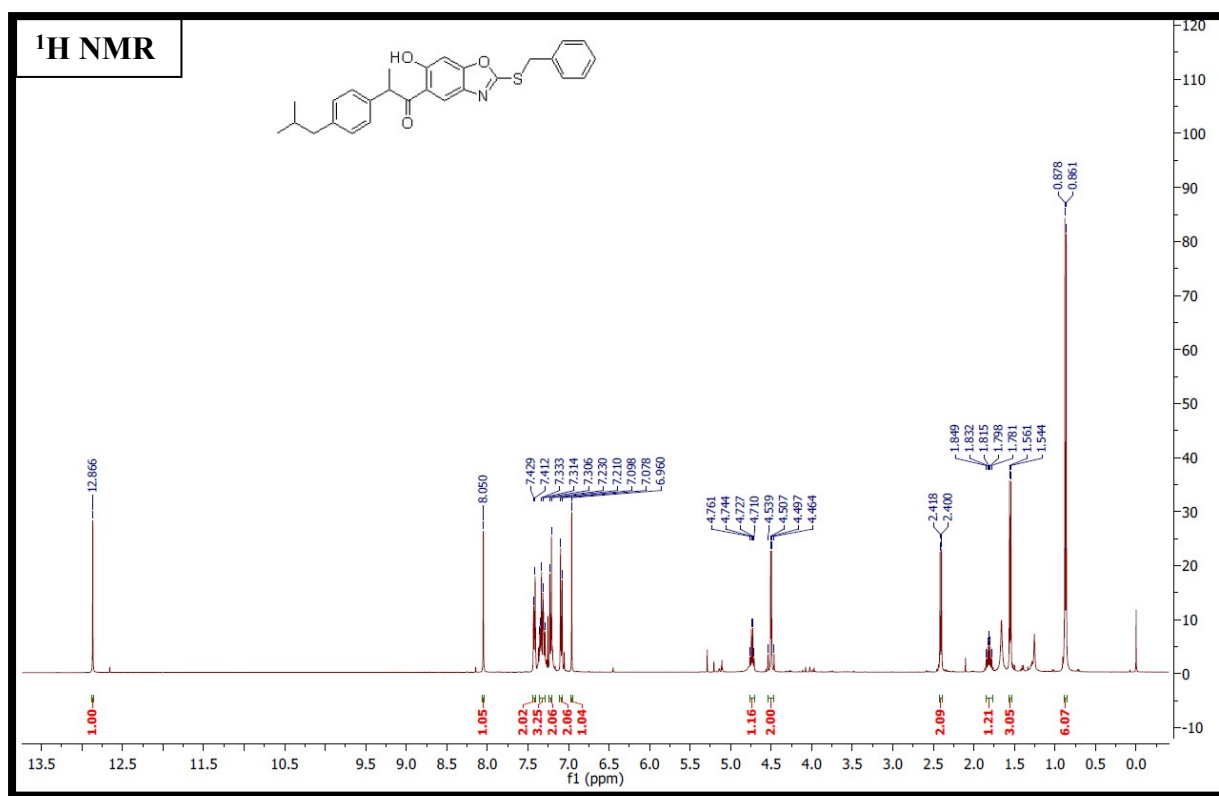
1-(6-hydroxy-2-mercaptobenzo[d]oxazol-5-yl)-2-(4-isobutyl phenyl)propan-1-one (5)



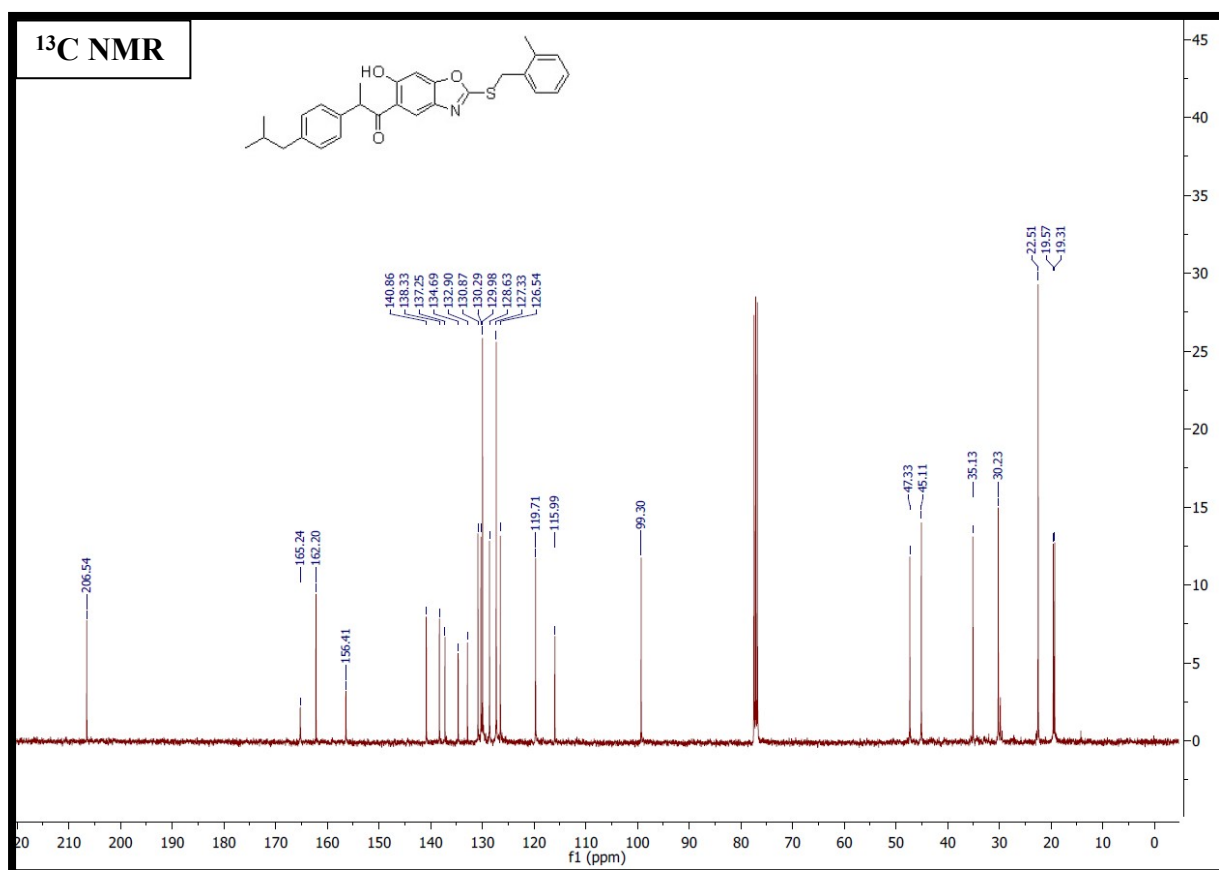
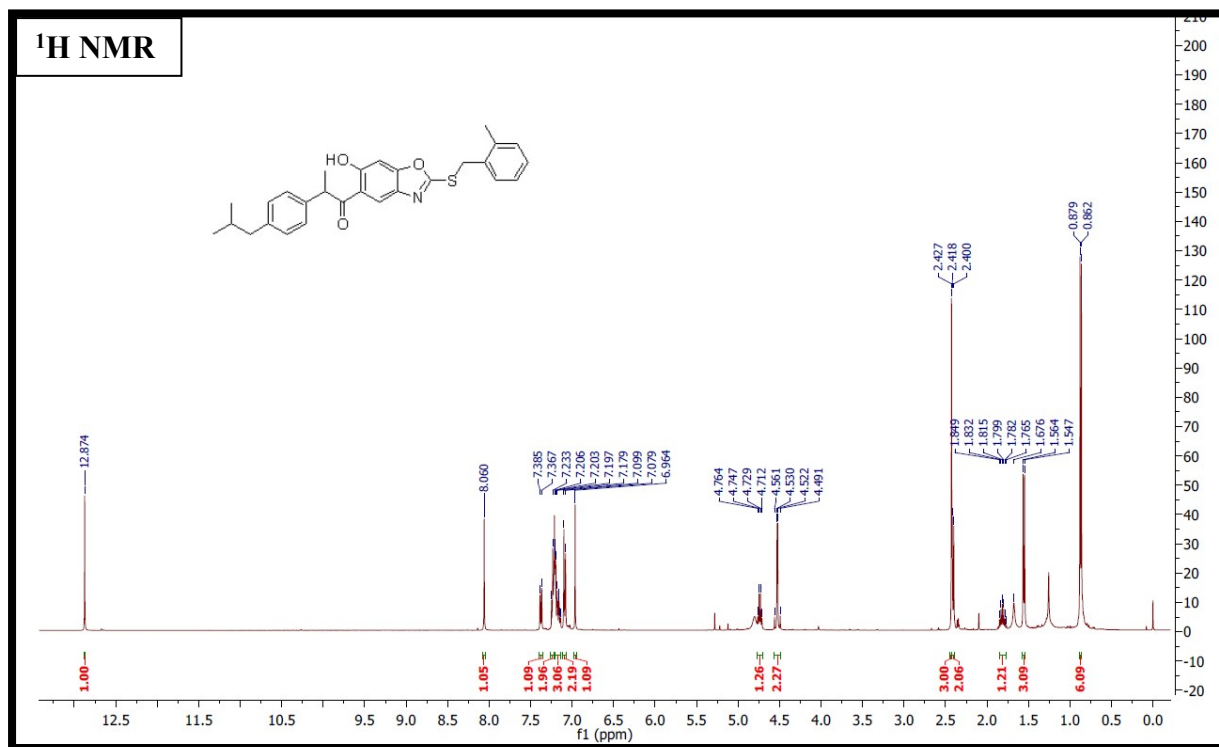
1-(2-(butylthio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7a)



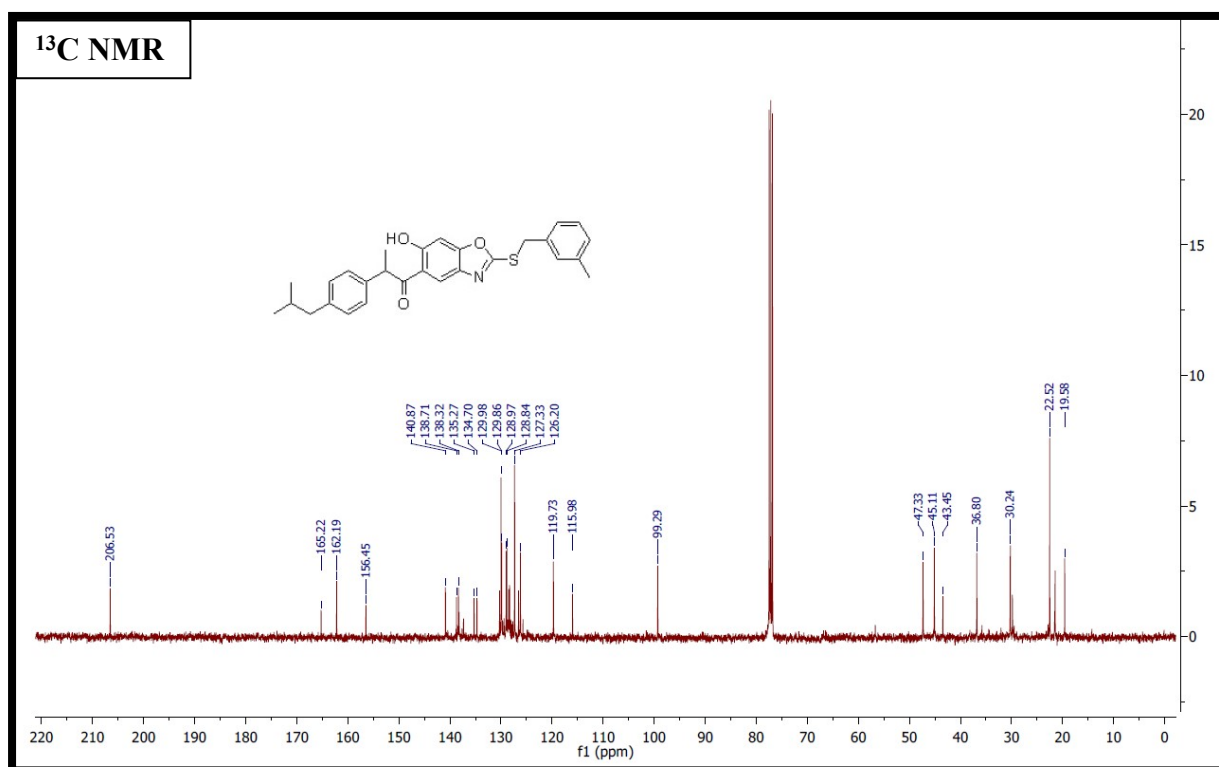
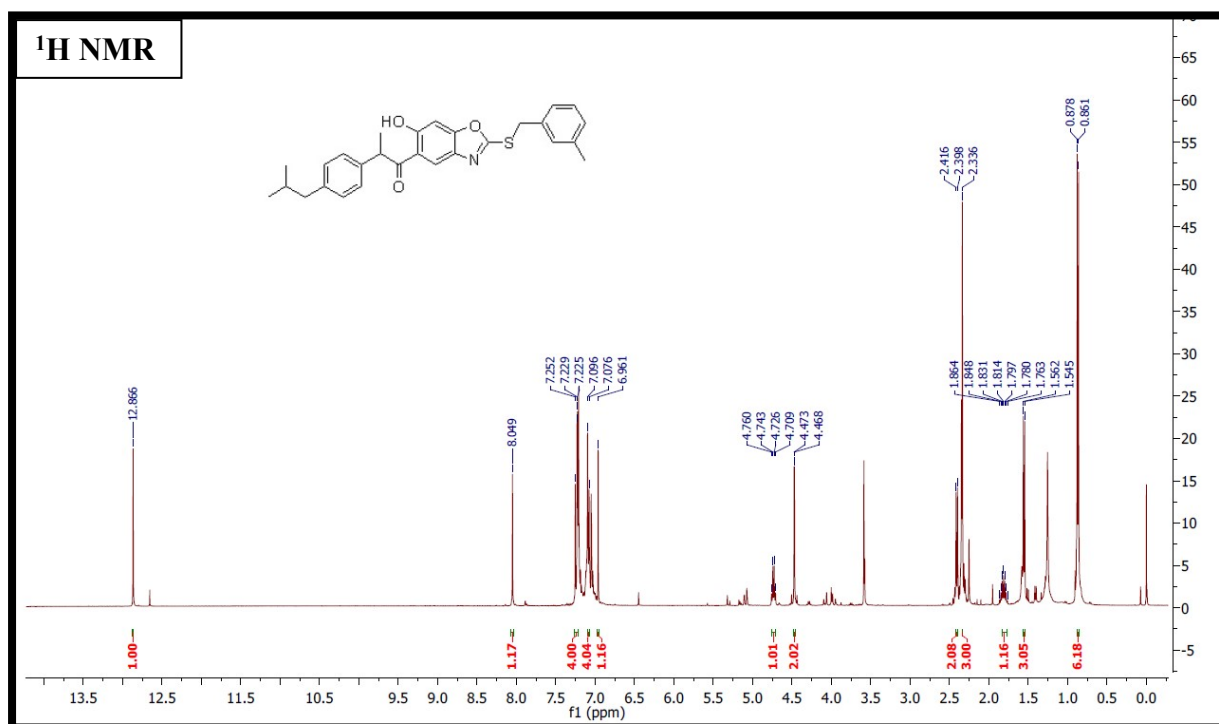
1-(2-(benzylthio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7b)



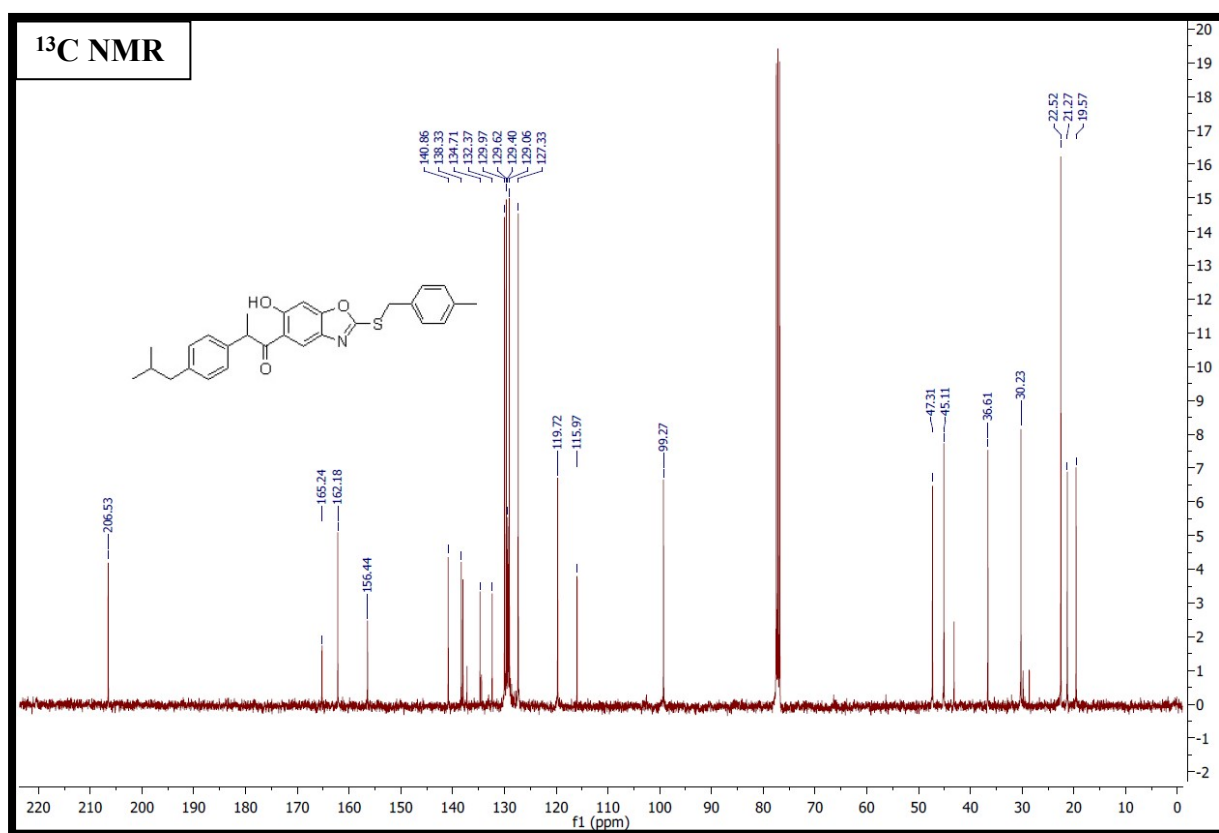
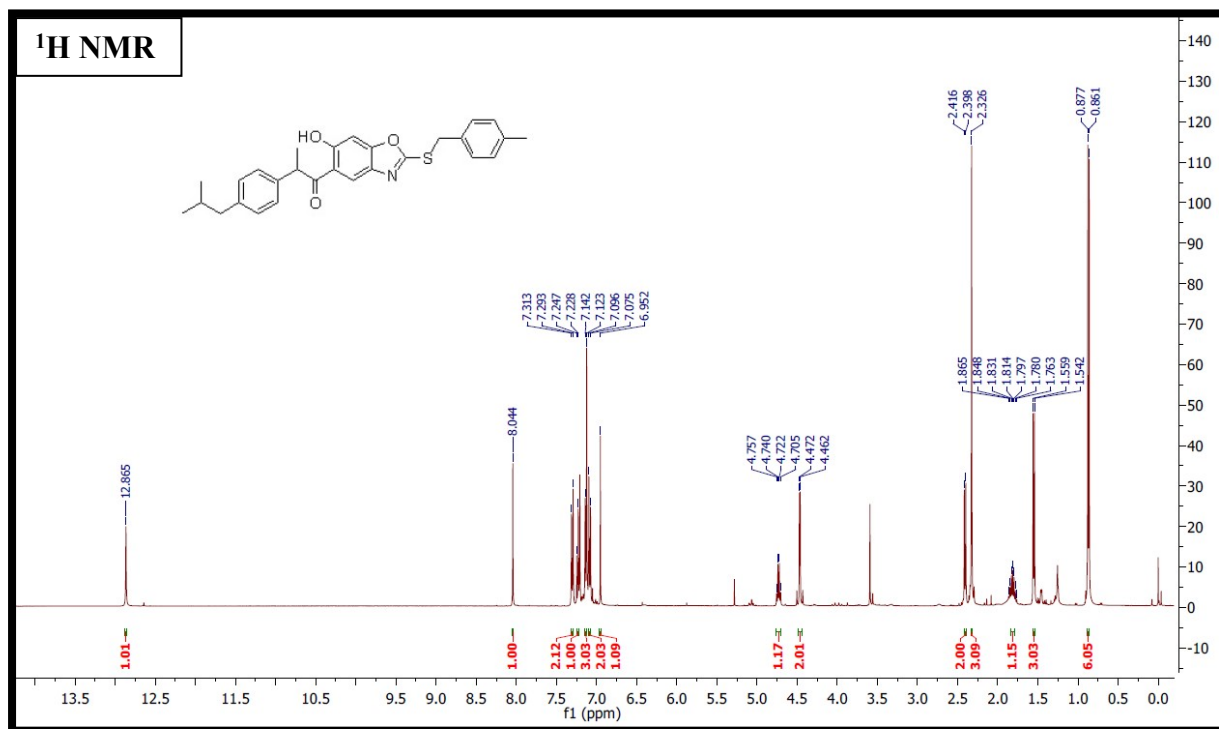
1-(6-hydroxy-2-((2-methylbenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7c)



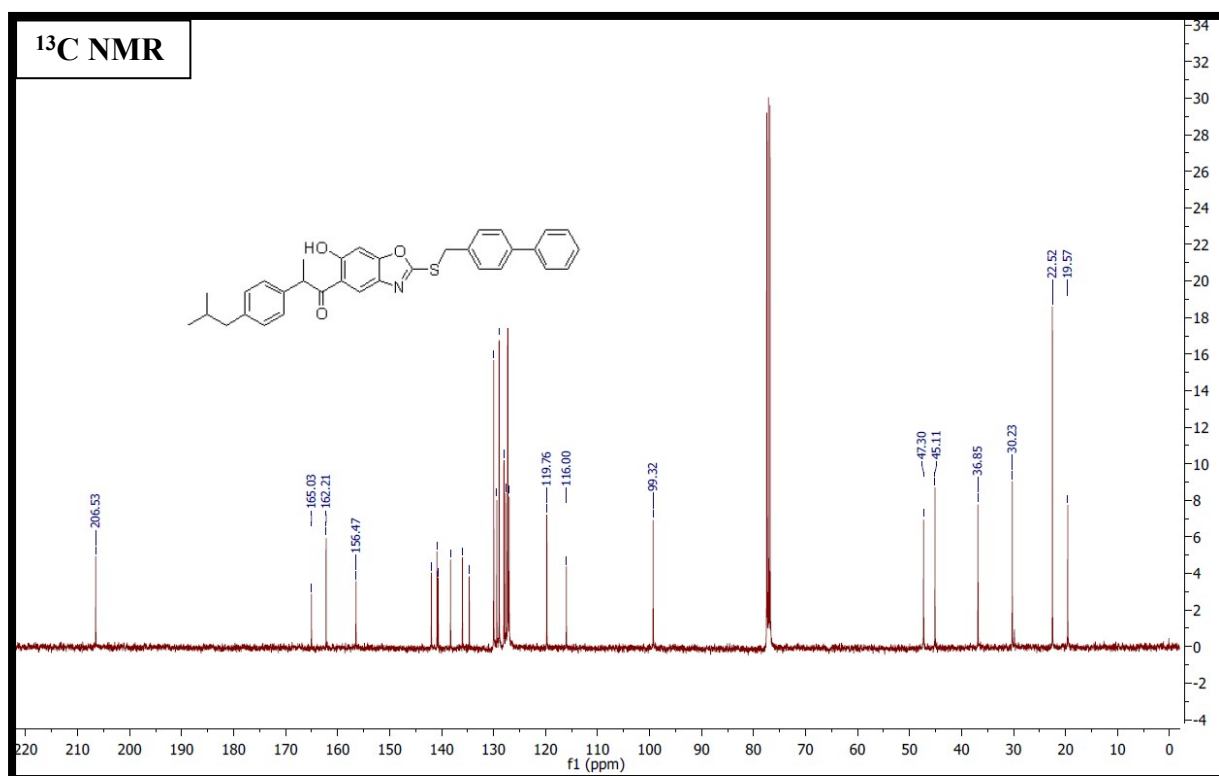
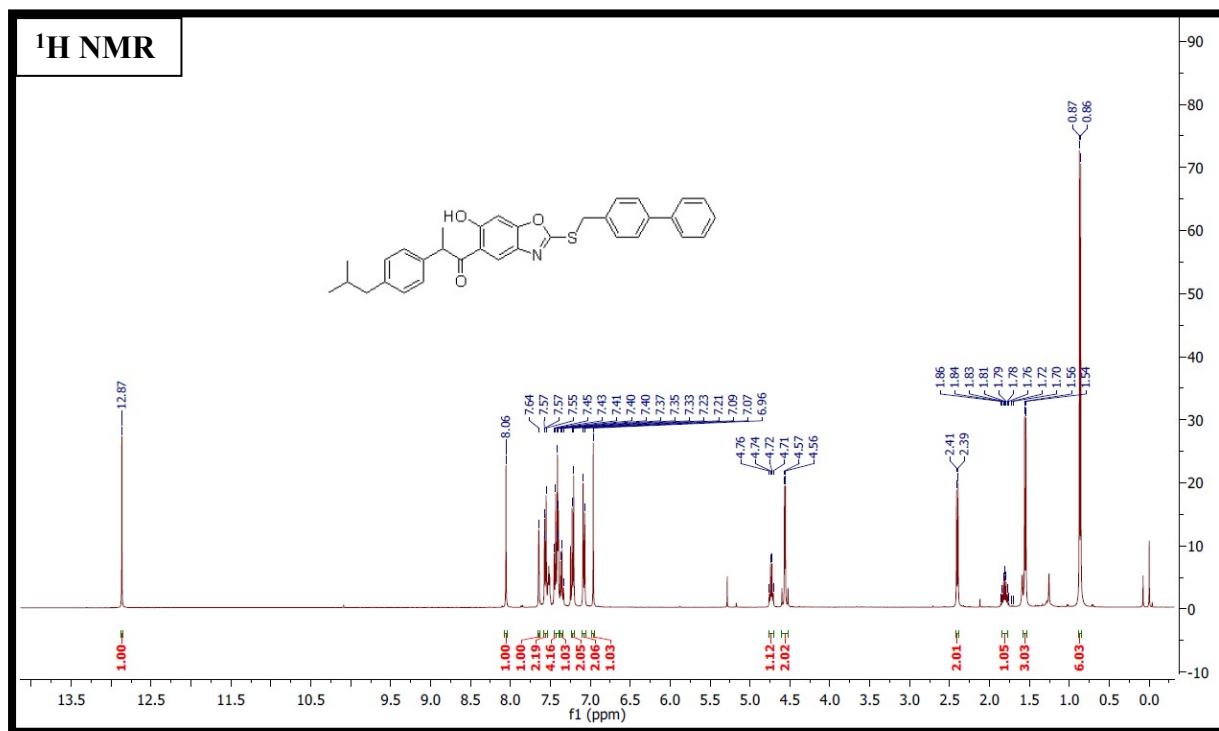
1-(6-hydroxy-2-((3-methylbenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7d)



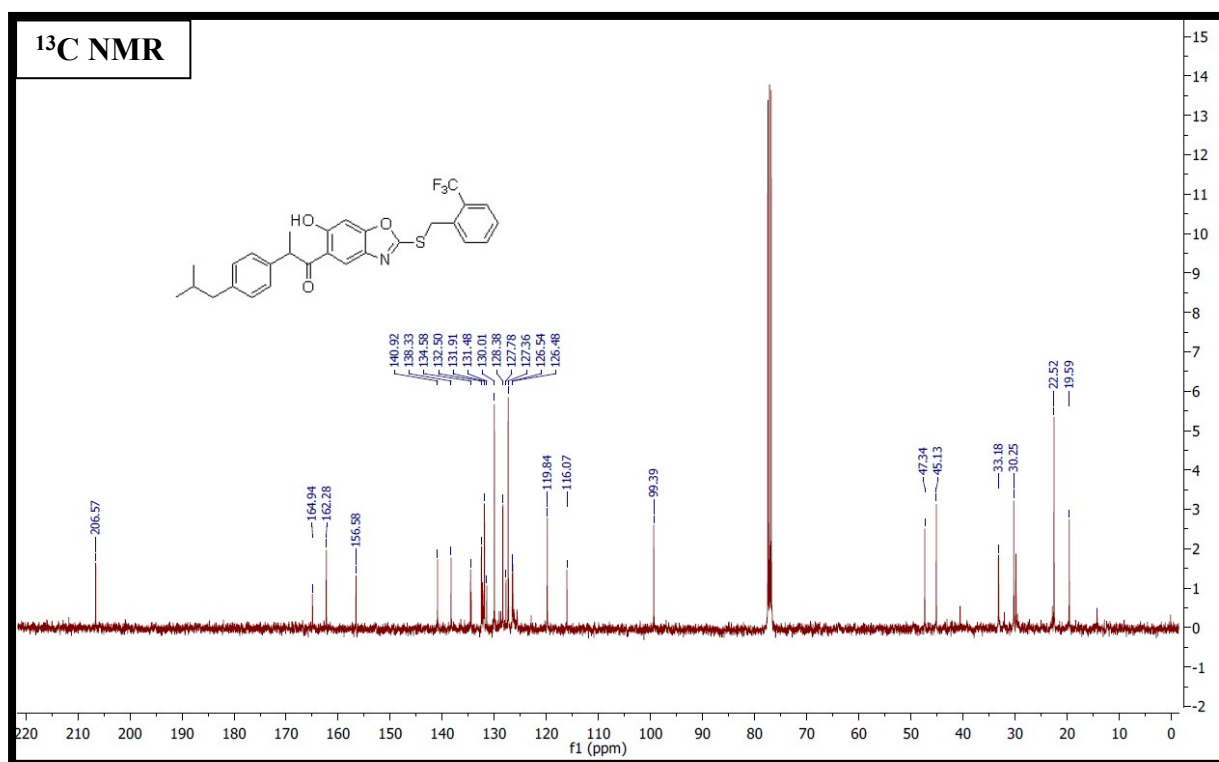
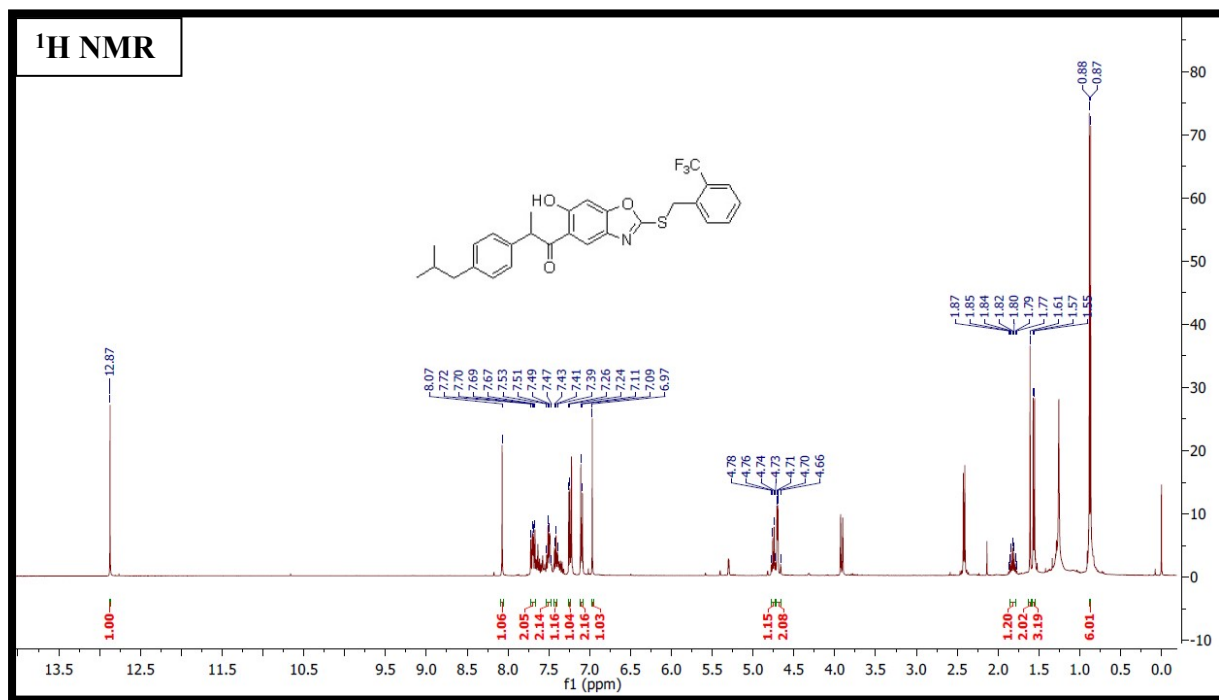
1-(6-hydroxy-2-((4-methylbenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7e):



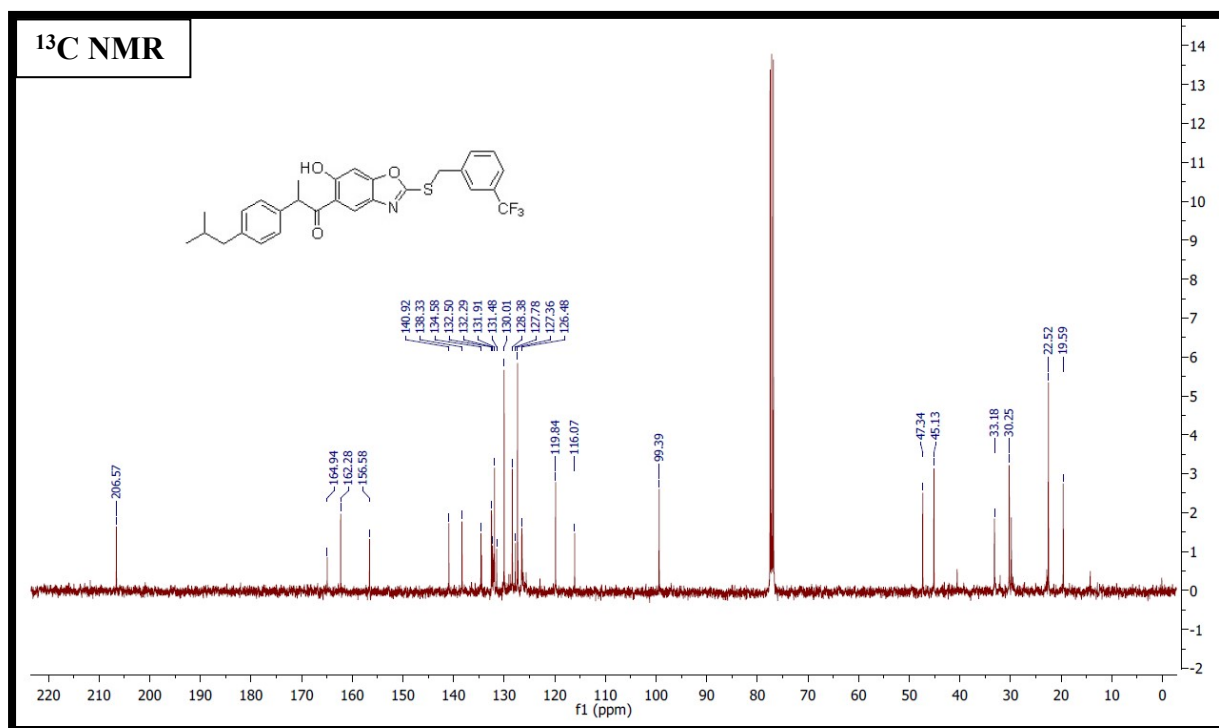
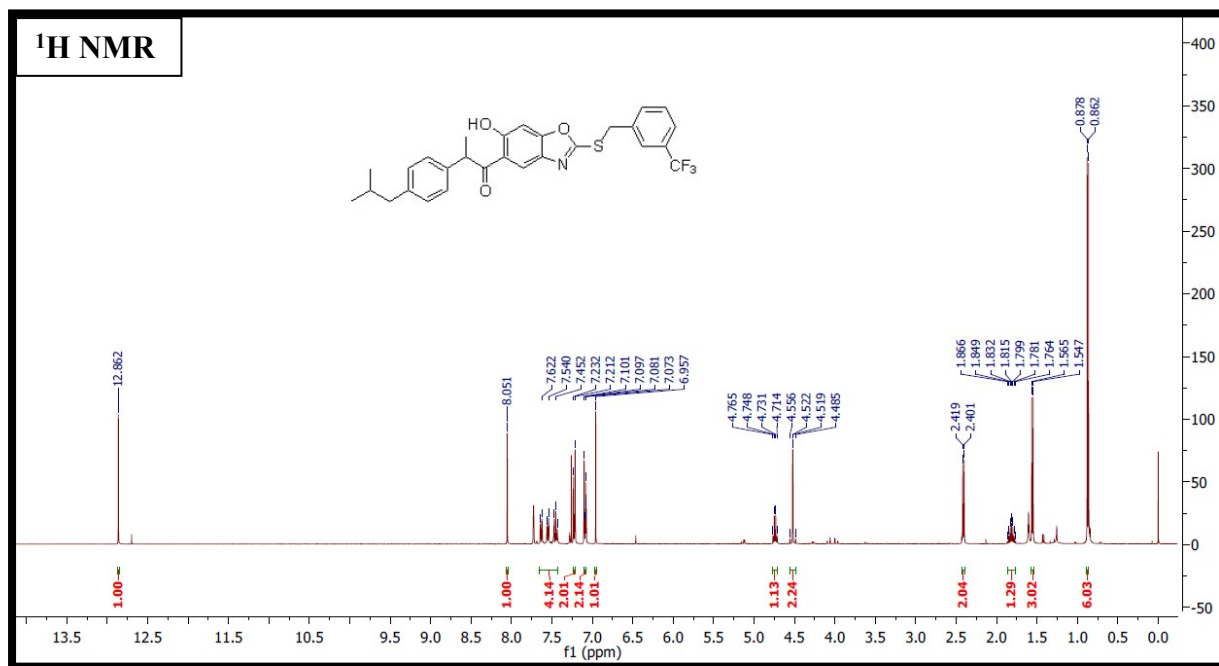
1-(2-((1,1'-biphenyl)-4-ylmethylthio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7f)



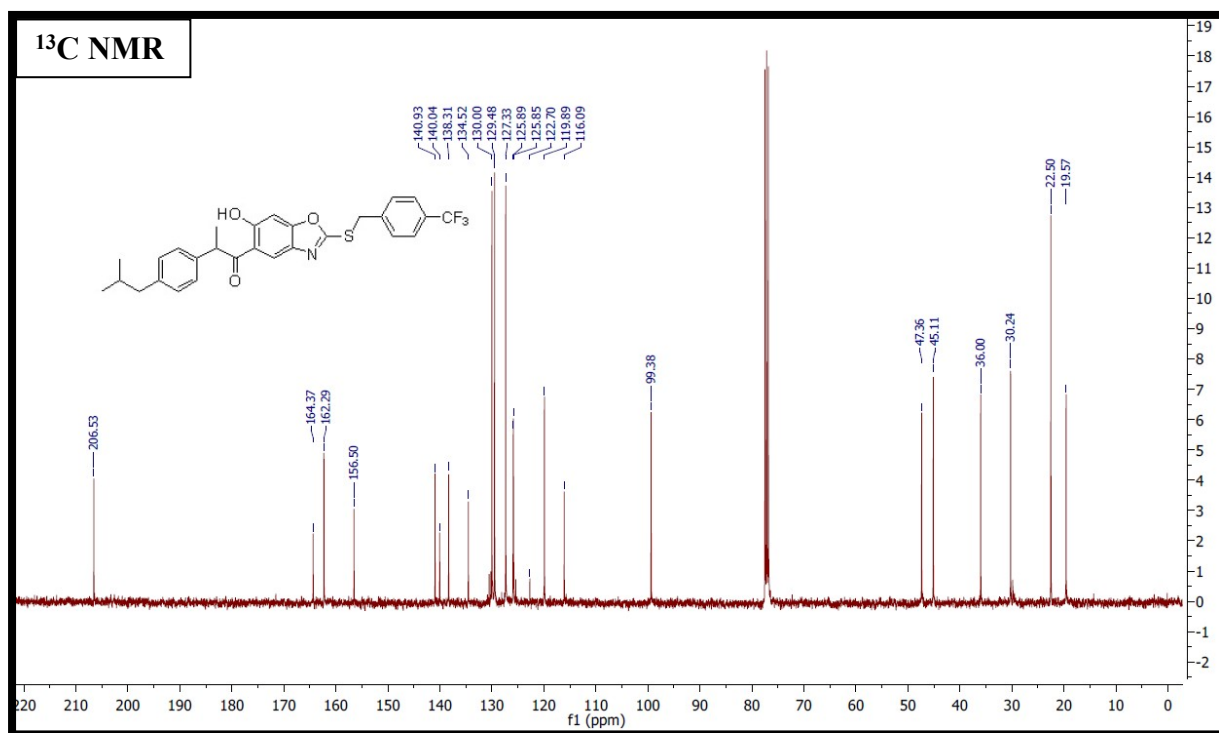
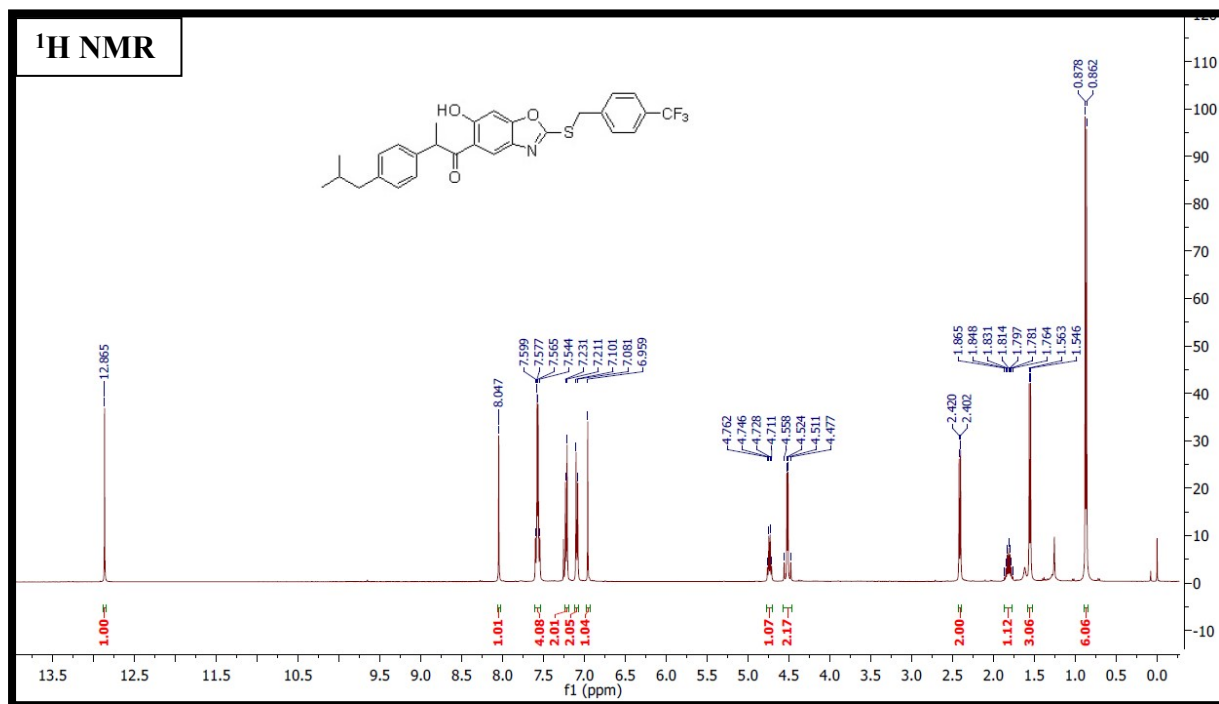
1-(6-hydroxy-2-((2-(trifluoromethyl)benzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7g):



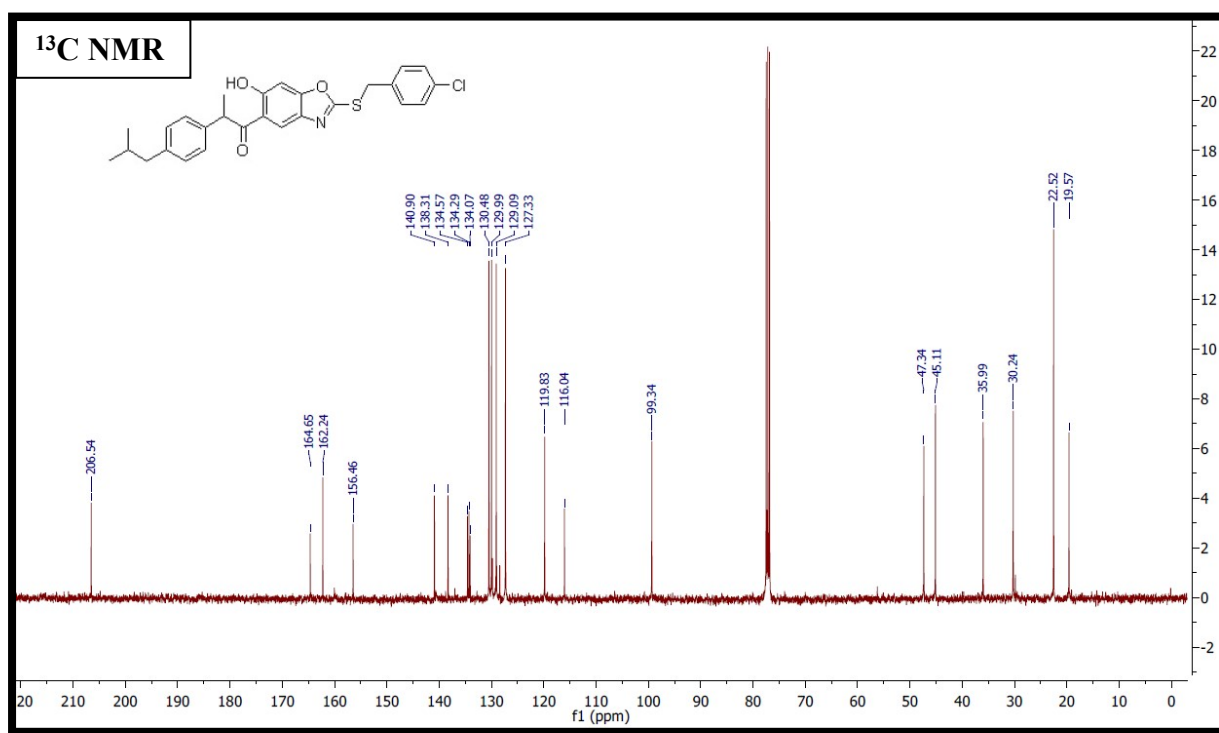
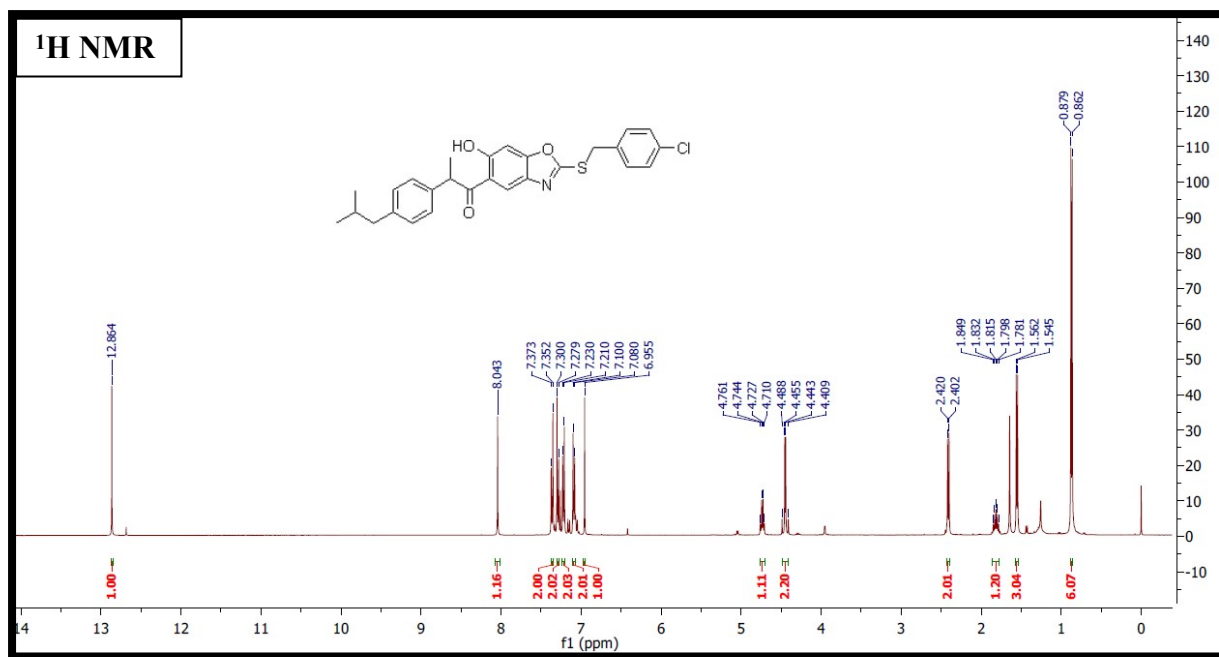
1-(6-hydroxy-2-((3-(trifluoromethyl)benzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutyl phenyl)propan-1-one (7h):



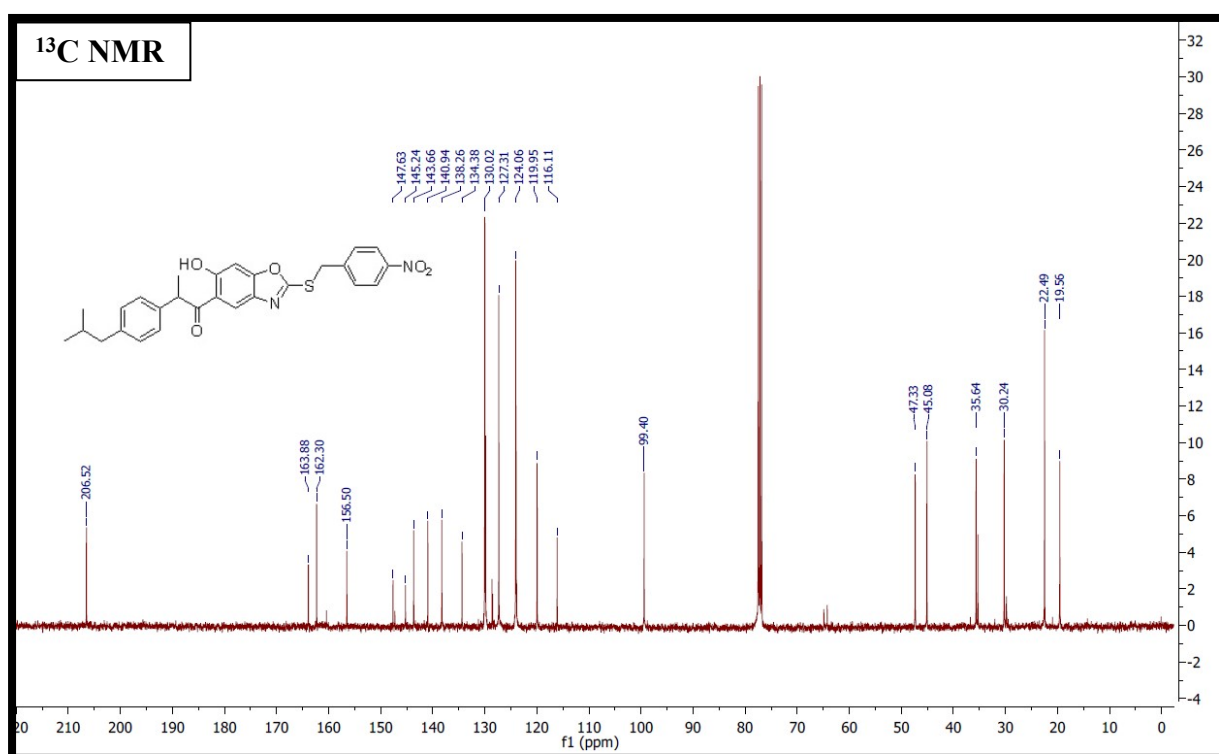
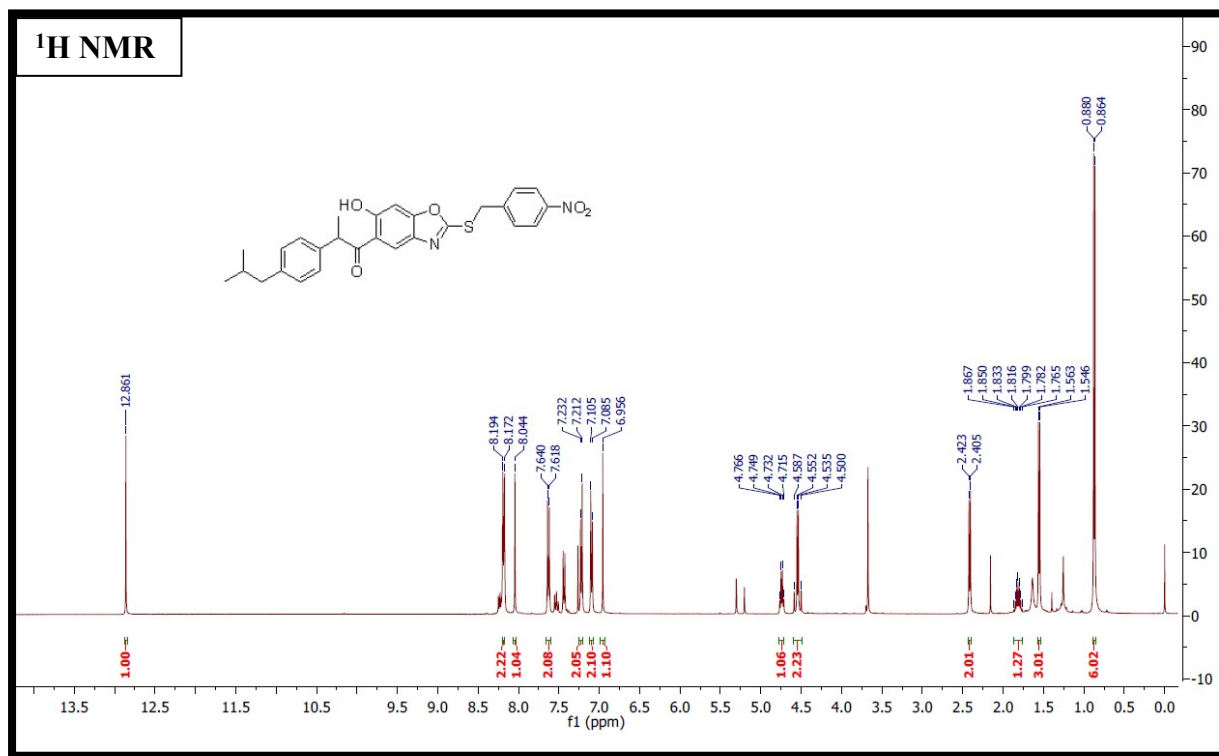
1-(6-hydroxy-2-((4-(trifluoromethyl)benzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7i):



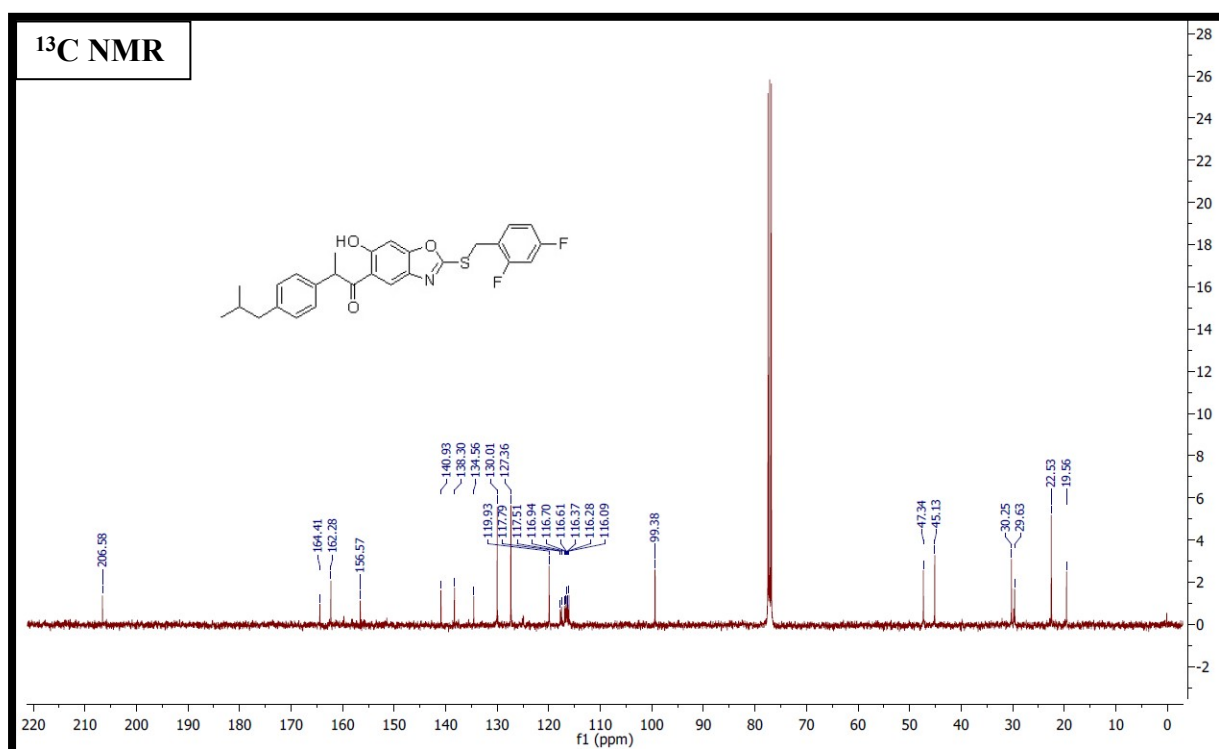
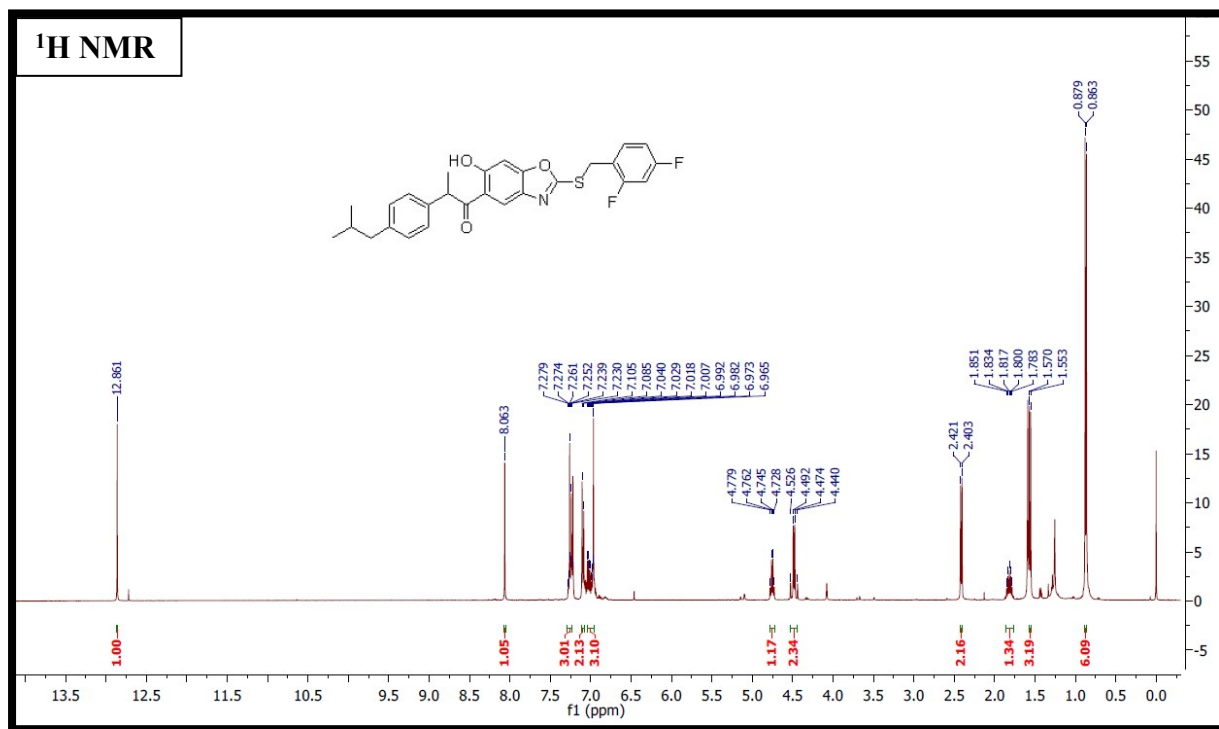
1-(2-((4-chlorobenzyl)thio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7j):



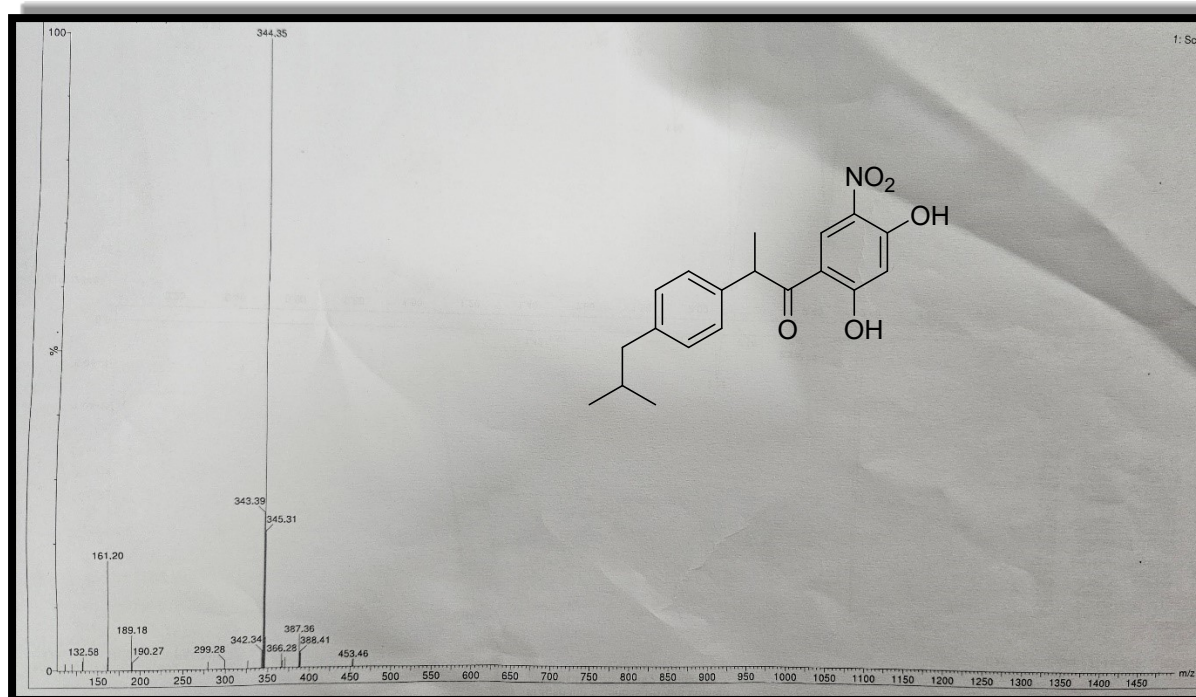
1-(6-hydroxy-2-((4-nitrobenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl) propan-1-one (7k):



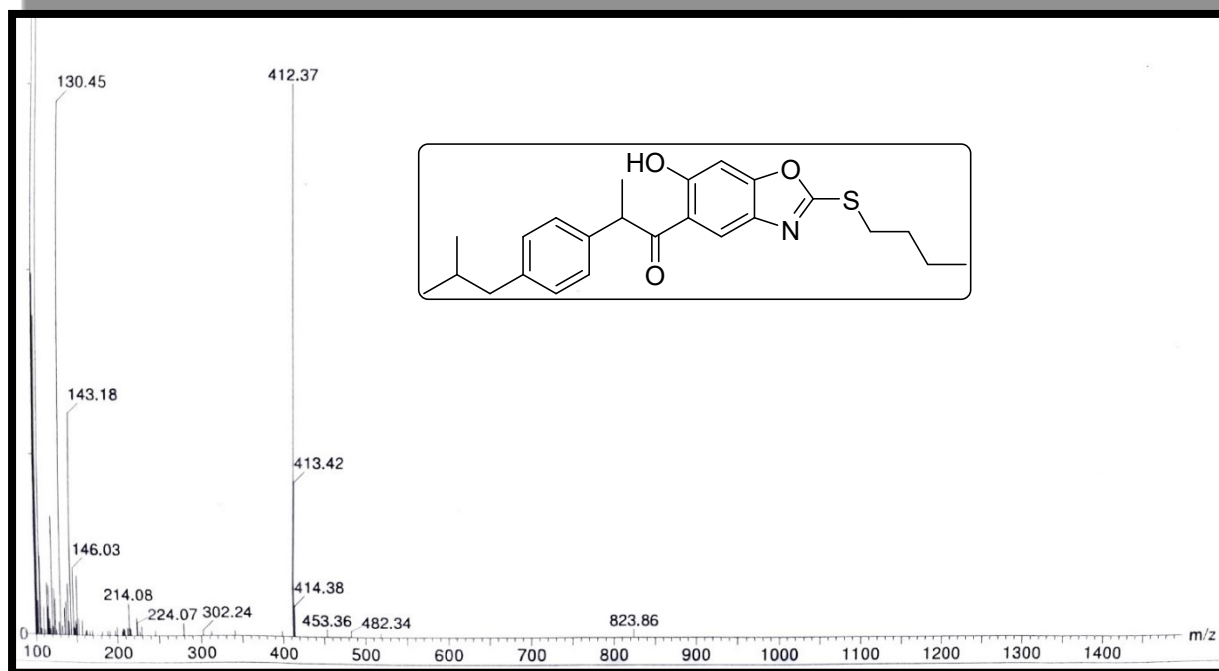
1-(2-((2,4-difluorobenzyl)thio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl) propan-1-one (7l):



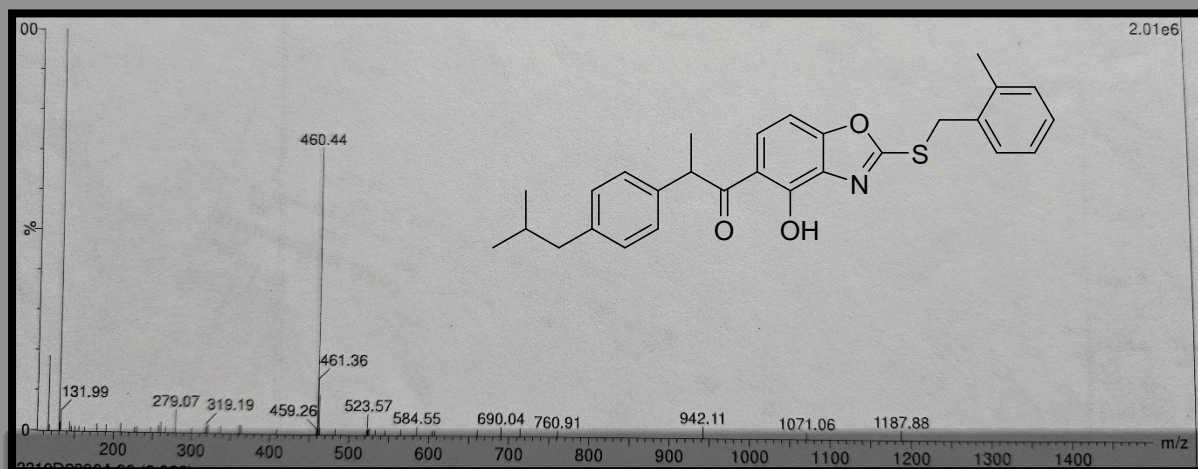
Mass spectrum of 1-(2,4-dihydroxy-5-nitrophenyl)-2-(4-isobutylphenyl) propan-1-one (4):



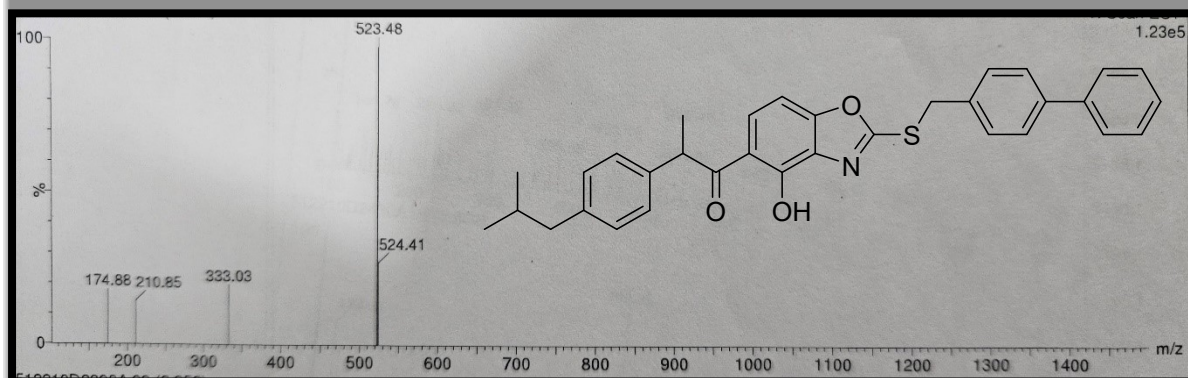
Mass spectrum of 1-(2-(butylthio)-4-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl) propan-1-one (7a):



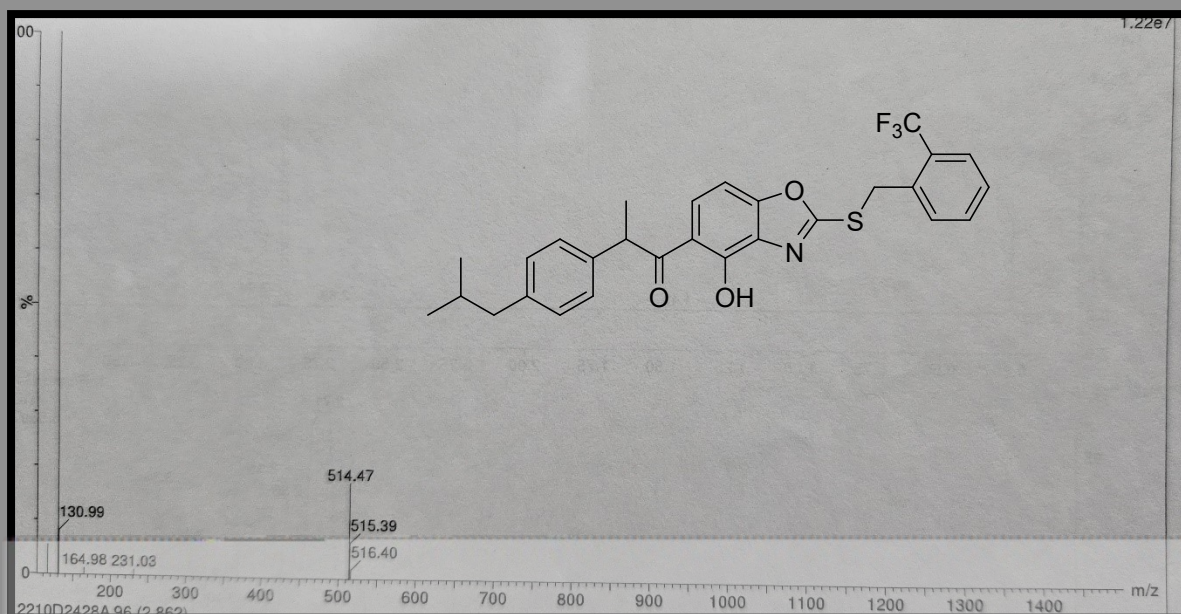
Mass spectrum of 1-(4-hydroxy-2-((2-methylbenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutyl phenyl)propan-1-one (7c):



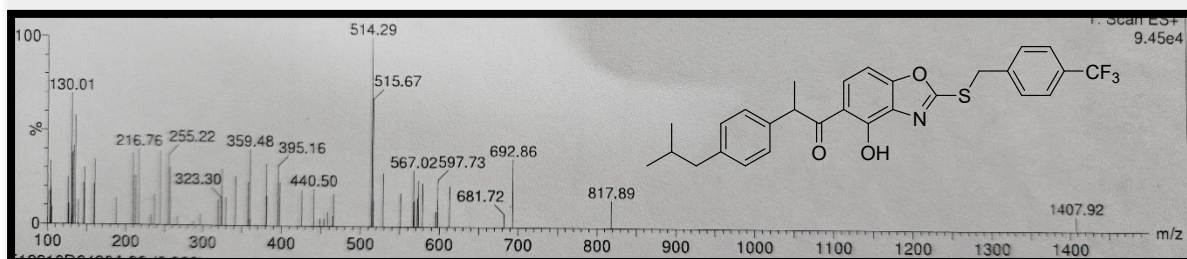
Mass spectrum of 1-(2-((1,1'-biphenyl)-4-ylmethyl)thio)-4-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutyl phenyl)propan-1-one (7f):



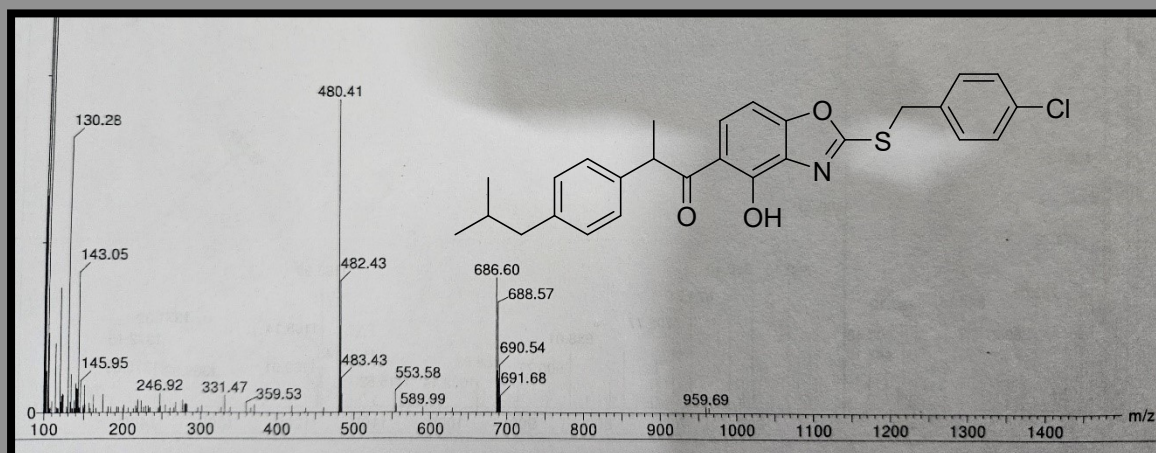
Mass spectrum of 1-(6-hydroxy-2-((2-(trifluoromethyl)benzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7g):



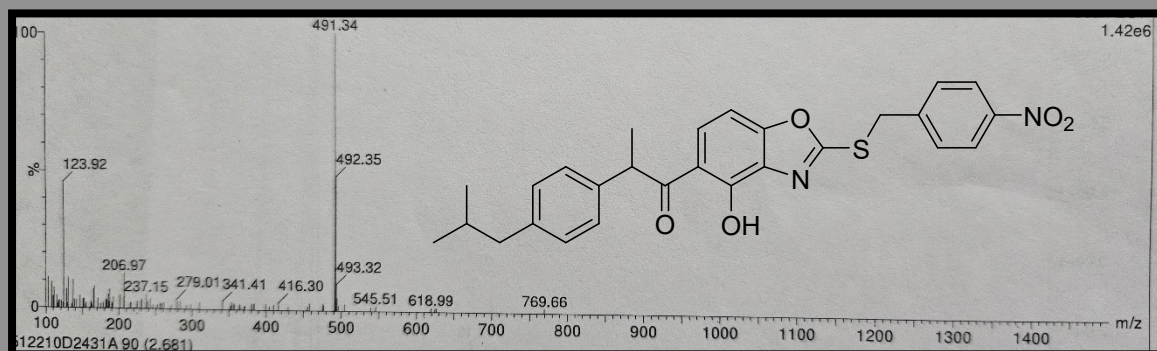
Mass spectrum of 1-(6-hydroxy-2-((4-(trifluoromethyl)benzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutyl phenyl)propan-1-one (7i):



1-(2-((4-chlorobenzyl)thio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl)propan-1-one (7j):



Mass spectrum of 1-(6-hydroxy-2-((4-nitrobenzyl)thio)benzo[d]oxazol-5-yl)-2-(4-isobutylphenyl) propan-1-one (7k):



Mass spectrum of 1-(2-((2,4-difluorobenzyl)thio)-6-hydroxybenzo[d]oxazol-5-yl)-2-(4-isobutylphenyl) propan-1-one (7l):

