SUPPLEMENTARY MATERIAL: Ecological and Pharmacological Activities of Polybrominated Diphenyl Ethers (PBDEs) From the Indonesian Marine Sponge *Lamellodysidea herbacea*

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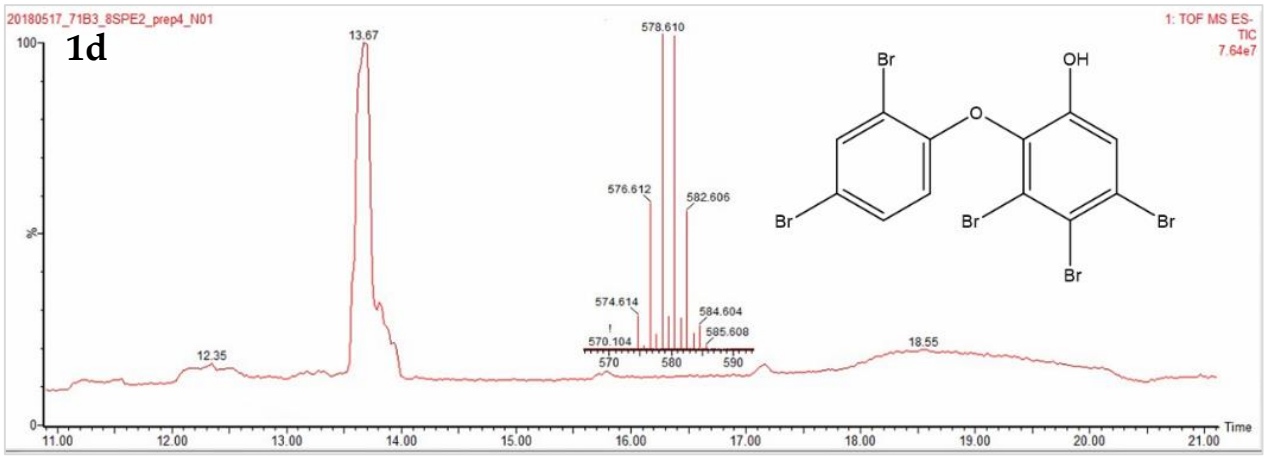
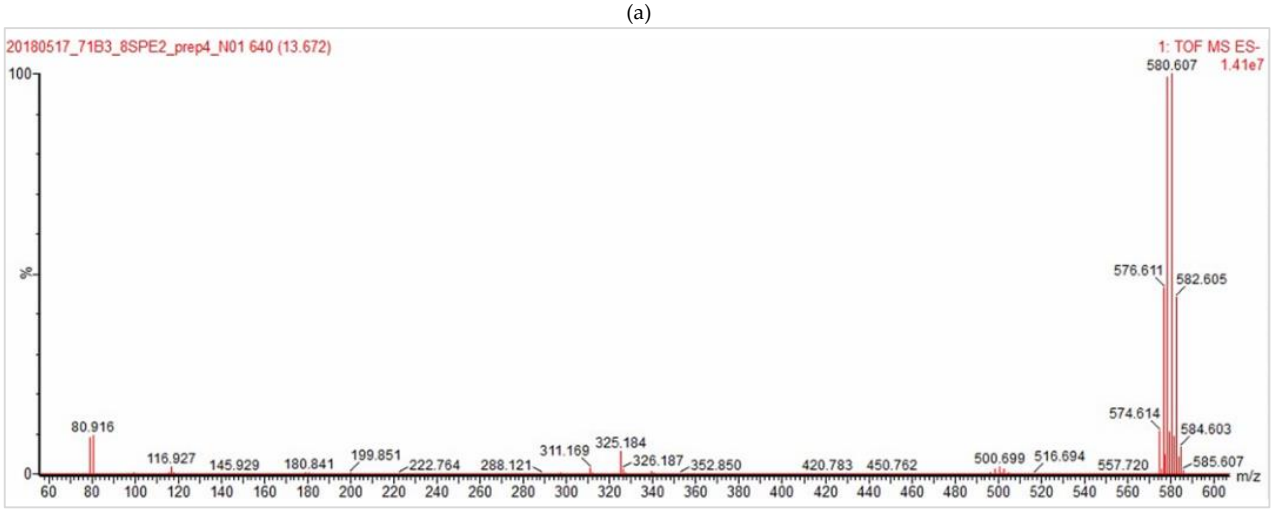
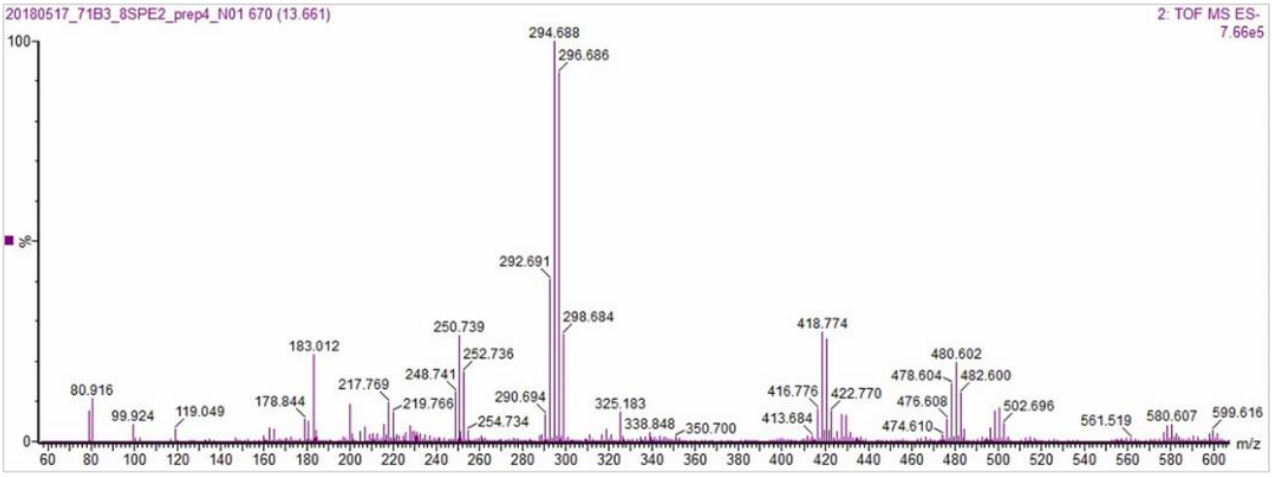


(a)

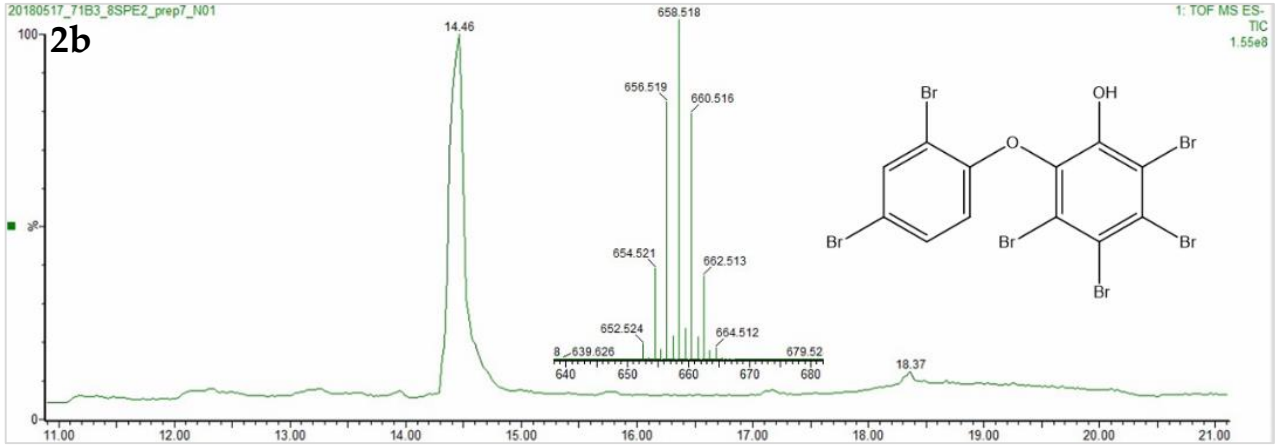


(b)

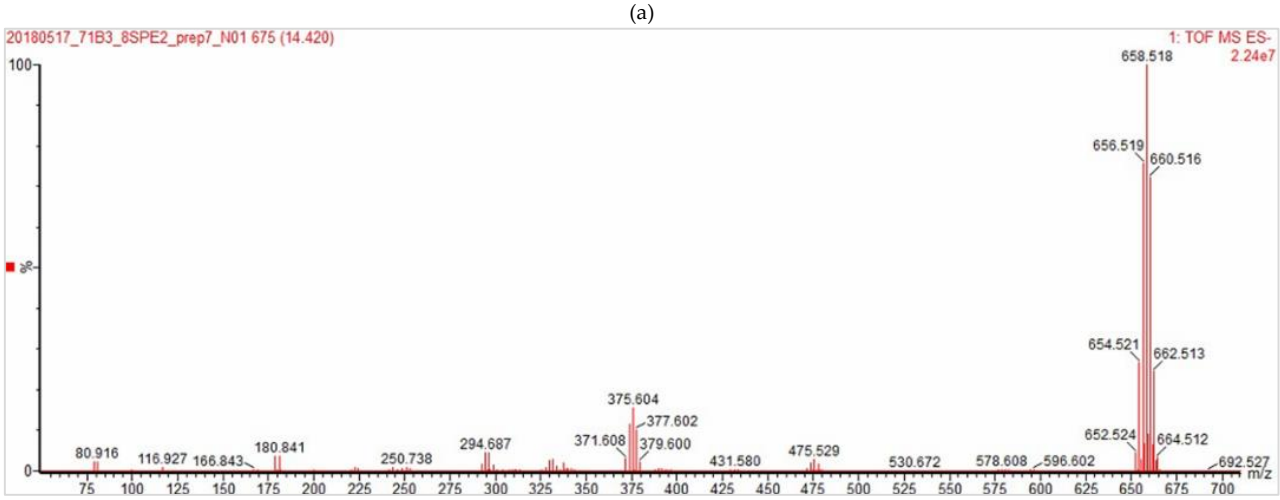


(c)

Figure S1a. The HRMS (a,b) and MS/MS spectra (c) of the compound **1d.**



(a)



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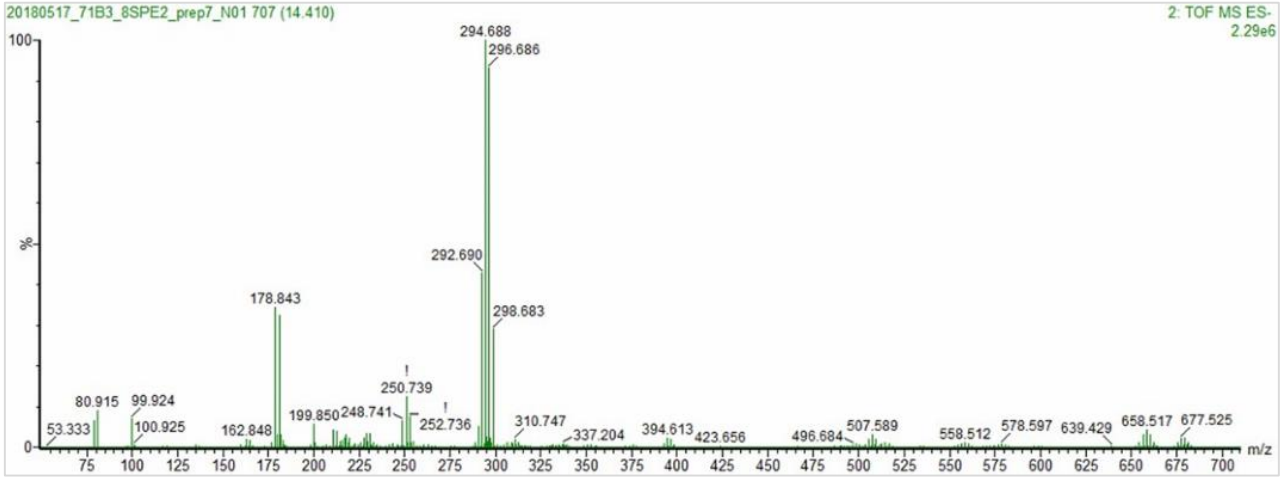
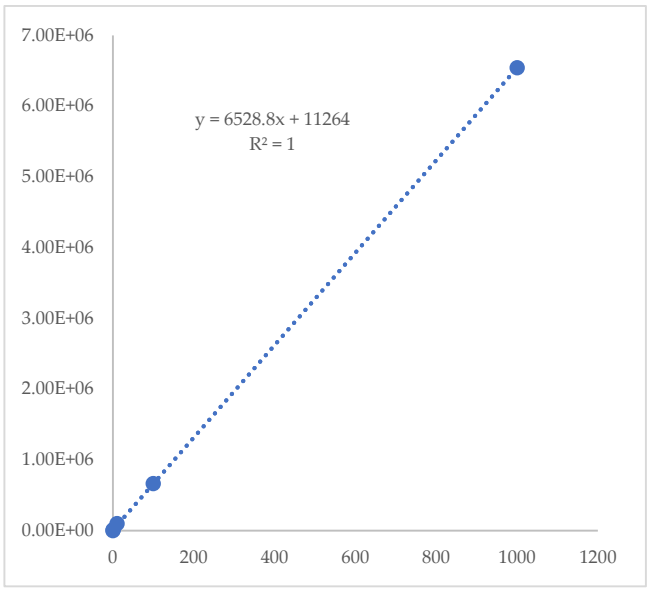
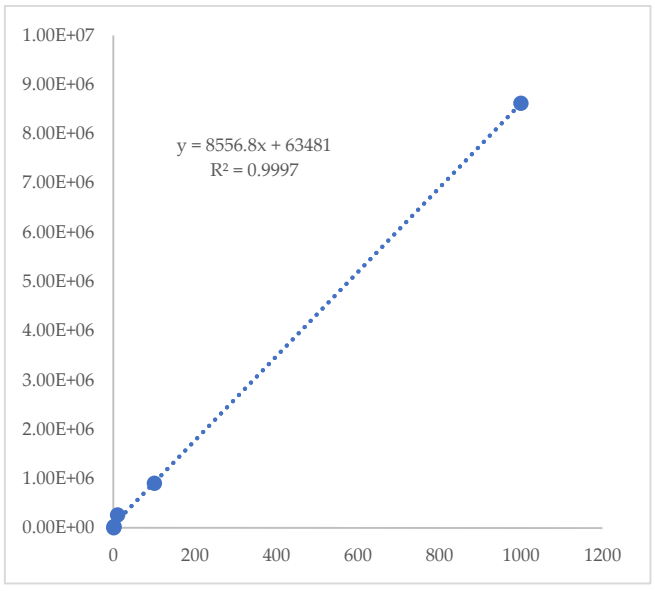


(c)

Figure S1b. The HRMS (a,b) and MS/MS spectra (c) of the compound **2b.**



(a)



(b)

Figure S2. Calibration curves of compounds **1d** (a) and **2b** (b) showing correlation between observed peak areas and injected compound concentrations (0.1 µg/mL, 1 µg/mL, 10 µg/mL, 100 µg/mL, 1 mg/mL).

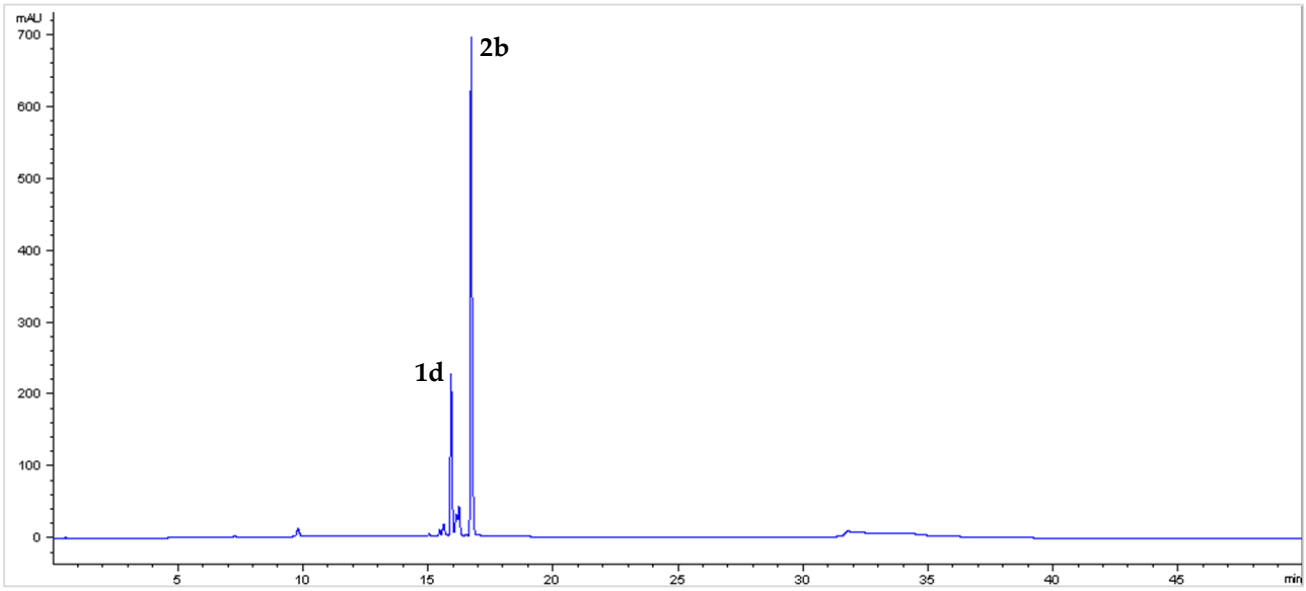
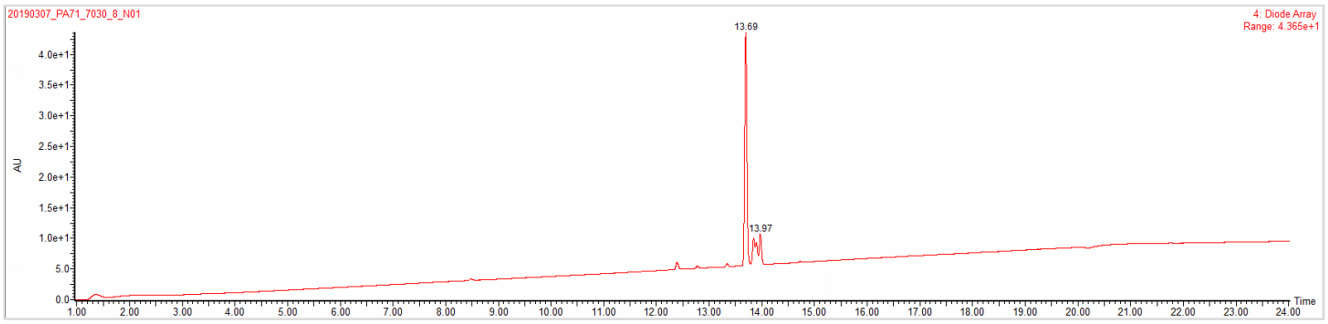
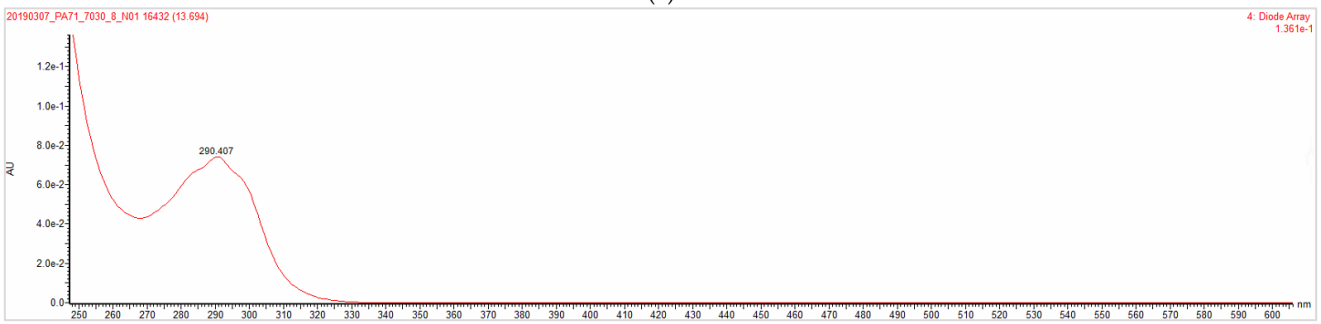


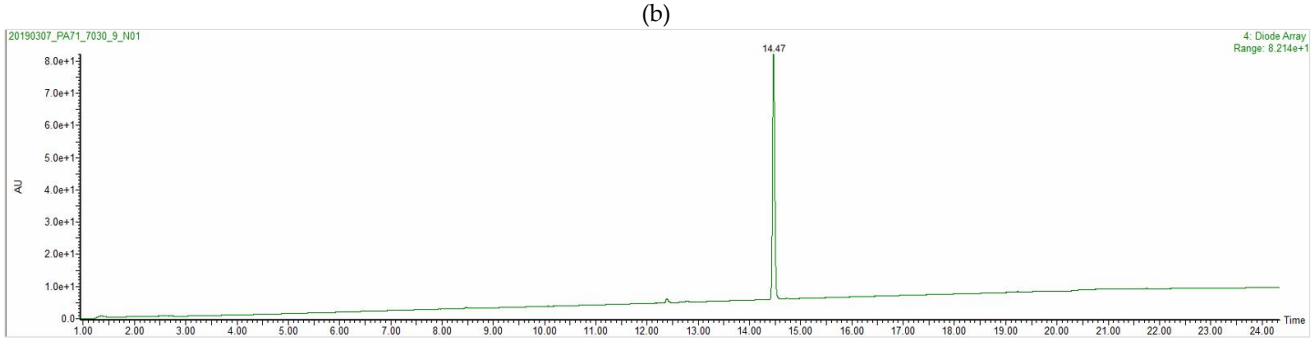
Figure S3. HPLC chromatogram of the crude extract of *Lamellodysidea herbacea*. It shows that compounds **1d** and **2b** are the major metabolites of the extract.



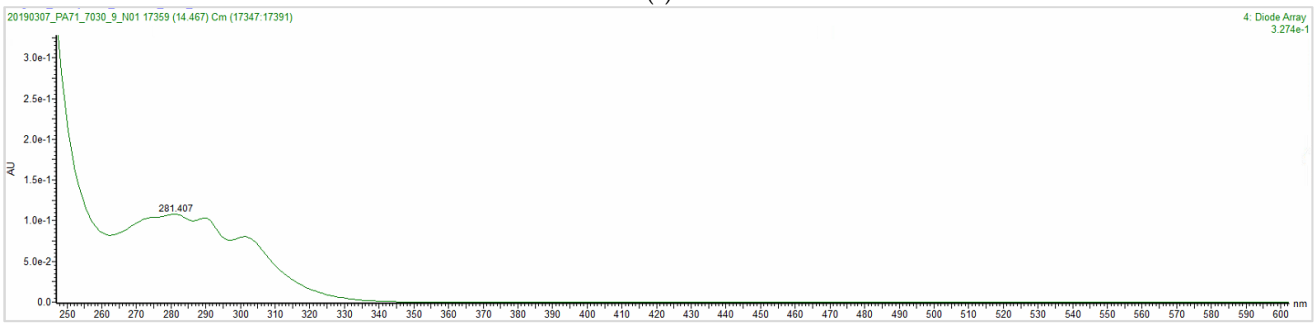
(a)



(b)



(c)



(d)

Figure S4. UV chromatogram of compounds **1d** and **2b** (a,c), including their UV spectra and λmax [nm] (b,d).

Table S1. ^{13}C NMR data for compound **1d** in $CDCl_3$ compared to their chemical shift calculations by two NMR prediction programs NMRShiftDB and CSEARCH.

Position	$\delta^{13}C$ [ppm]								
	1d – $CDCl_3$	**NMRShiftDB**				**CSEARCH**			
		1a	**1b**	**1c**	**1d**	**1a**	**1b**	**1c**	**1d**
1	148.9	144.37	144.37	144.37	146.74	147.4	148.3	146,6	150.1
2	139.5	148.95	145.52	145.52	145.52	143.5	138.3	140.5	139.7
3	121.1	113.60	110.20	114.70	120.40	121.4	116.8	120.2	119.1
4	119.2	120.40	135.01	124.93	127.88	117.3	127.7	114.7	118.1
5	122.9	127.88	127.88	135.01	123.46	122.6	122.5	133.0	122.5
6	120.7	114.70	114.70	111.12	119.00	122.1	114.0	111.3	120.9
1'	151.7	152.90	152.90	152.90	152.90	151.7	152.3	151.9	152.0
2'	112.7	114.90	114.90	114.90	114.90	115.6	112.8	112.8	112.8
3'	136.3	136.20	136.20	136.20	136.20	136.0	136.1	136.1	136.1
4'	116.2	116.40	116.40	116.40	116.40	116.2	116.2	116.2	116.2
5'	131.6	116.40	131.60	131.60	131.60	132.6	131.7	131.7	131.7
6'	115.7	120.10	120.10	120.10	120.10	121.6	115.9	116.3	116.3

The chemical shift of ^{13}C for compound **1d** (this work) measured in $CDCl_3$ was compared with the publicly accessible NMRShiftDB database (https://nmrshiftdb.nmr.uni-koeln.de/) and CSEARCH (https://nmrpredict.orc.univie.ac.at/c13robot/robot.php).