SUPPORTING INFORMATION

Harnessing the role of HDAC6 in Idiopathic Pulmonary Fibrosis: Design, Synthesis, Structural Analysis, and Biological Evaluation of Potent Inhibitors

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HPLC separation of racemic mixture (±)-25b

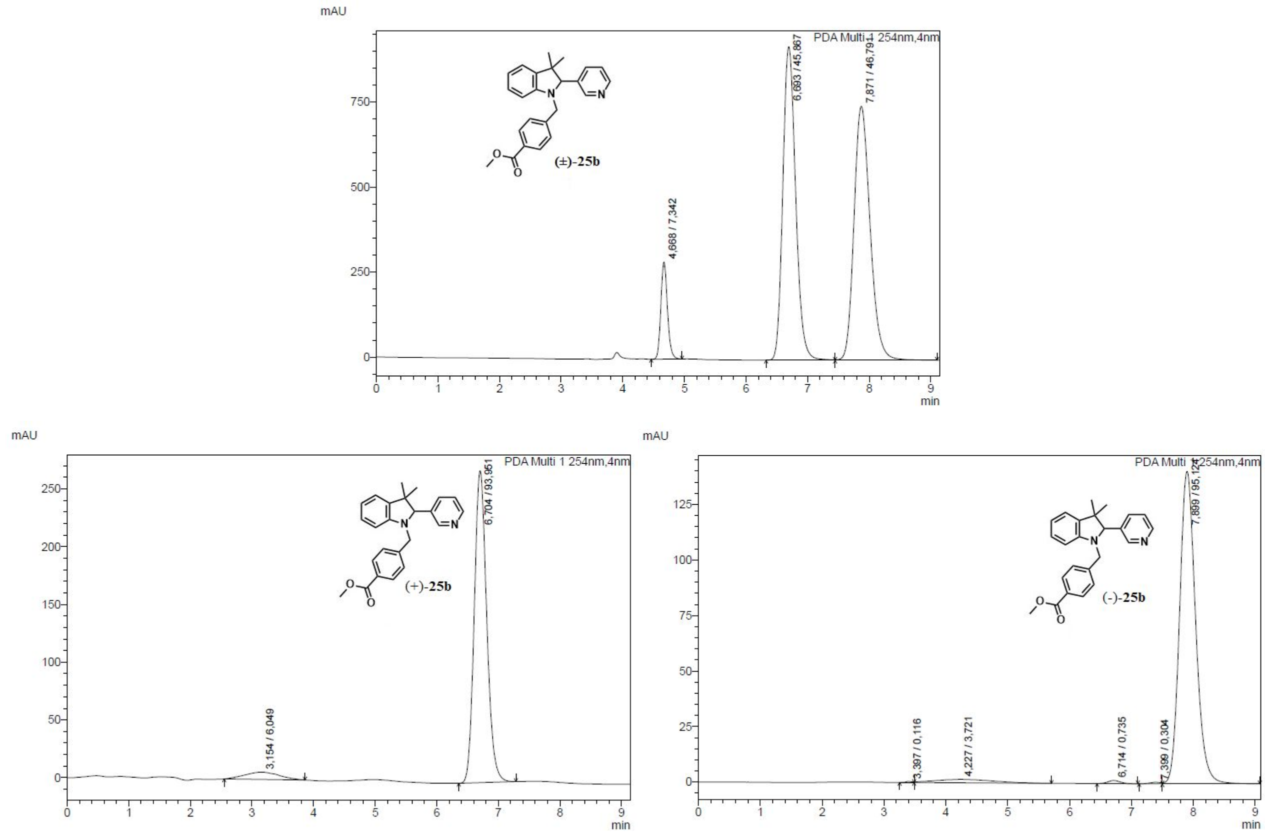


Figure S1. HPLC separation of racemic mixture (±)-**25b**. and analytical control of enantiomeric excess for compounds (+)-**25b** and (−)-**25b**.

Table S1. Relative MM energies (ΔE_{MM}), electronic energies (E_{QM} and ΔE_{QM}), free energies (G and ΔG) and corresponding Boltzmann populations (χ) for the conformers of **(*S*)-25b**, as obtained after B97D/def2-TZVP/IEFPCM(2-PrOH) optimization.

Conf.	ΔE_{MM} (kcal/mol)	E_{QM} (Ha)	ΔE_{QM} (kcal/mol)	χ_{QM} (%)	G (Ha)	ΔG (kcal/mol)	χ_G (%)	Clustering
(*S*)-**25b.01**	0.000	−1188.569884	0.034	13.57	−1188.209626	0.000	15.67	
(*S*)-**25b.02**	0.037	−1188.569938	0.000	14.36	−1188.209168	0.287	9.65	
(*S*)-**25b.03**	0.074	−1188.568378	0.979	2.75	−1188.209267	0.225	10.72	
(*S*)-**25b.04**	0.247	−1188.568313	1.020	2.57	−1188.208413	0.761	4.34	
(*S*)-**25b.05**	0.247	—	—	—	—	—	—	(*S*)-**25b.04** (RMSD = 0.00000 Å)
(*S*)-**25b.06**	0.417	−1188.569636	0.189	10.43	−1188.208489	0.713	4.70	
(*S*)-**25b.07**	0.462	−1188.567746	1.376	1.41	−1188.208138	0.934	3.24	
(*S*)-**25b.08**	0.584	−1188.567809	1.336	1.51	−1188.208551	0.675	5.02	
(*S*)-**25b.09**	0.600	−1188.569576	0.227	9.79	−1188.208736	0.558	6.11	
(*S*)-**25b.10**	1.243	−1188.569012	0.581	5.39	−1188.207657	1.236	1.95	
(*S*)-**25b.11**	1.297	−1188.569111	0.519	5.99	−1188.207410	1.391	1.50	
(*S*)-**25b.12**	1.470	−1188.566094	2.412	0.25	−1188.205622	2.513	0.23	
(*S*)-**25b.13**	1.536	−1188.568879	0.664	4.68	−1188.208720	0.569	6.00	
(*S*)-**25b.14**	1.604	−1188.567294	1.659	0.87	−1188.207620	1.259	1.87	
(*S*)-**25b.15**	1.684	−1188.568828	0.696	4.43	−1188.209397	0.144	12.30	
(*S*)-**25b.16**	1.734	−1188.567326	1.639	0.90	−1188.207327	1.443	1.37	
(*S*)-**25b.17**	1.756	−1188.566078	2.423	0.24	−1188.205927	2.321	0.31	
(*S*)-**25b.18**	1.756	—	—	—	—	—	—	(*S*)-**25b.17** (RMSD = 0.00001 Å)
(*S*)-**25b.19**	1.805	—	—	—	—	—	—	(*S*)-**25b.11** (RMSD = 0.00002 Å)
(*S*)-**25b.20**	1.848	−1188.566096	2.411	0.25	−1188.205816	2.391	0.28	
(*S*)-**25b.21**	1.848	—	—	—	—	—	—	(*S*)-**25b.20** (RMSD = 0.00001 Å)
(*S*)-**25b.22**	1.980	−1188.566752	1.999	0.49	−1188.207056	1.613	1.03	
(*S*)-**25b.23**	2.038	−1188.566825	1.953	0.53	−1188.206705	1.833	0.71	
(*S*)-**25b.24**	2.042	−1188.565996	2.474	0.22	−1188.205630	2.508	0.23	
(*S*)-**25b.25**	2.243	−1188.568508	0.897	3.16	−1188.208212	0.887	3.51	
(*S*)-**25b.26**	2.243	—	—	—	—	—	—	(*S*)-**25b.25** (RMSD = 0.00000 Å)
(*S*)-**25b.27**	2.360	−1188.568236	1.068	2.37	−1188.206233	2.129	0.43	
(*S*)-**25b.28**	2.452	−1188.568119	1.142	2.09	−1188.206818	1.762	0.80	
(*S*)-**25b.29**	2.615	−1188.568437	0.942	2.93	−1188.208454	0.735	4.53	
(*S*)-**25b.30**	2.615	—	—	—	—	—	—	(*S*)-**25b.29** (RMSD = 0.00000 Å)
(*S*)-**25b.31**	3.174	−1188.568737	0.753	4.03	−1188.207086	1.594	1.06	
(*S*)-**25b.32**	3.240	—	—	—	—	—	—	(*S*)-**25b.25** (RMSD = 0.00003 Å)
(*S*)-**25b.33**	3.331	−1188.568639	0.815	3.63	−1188.207604	1.269	1.84	
(*S*)-**25b.34**	3.331	—	—	—	—	—	—	(*S*)-**25b.33** (RMSD = 0.00001 Å)
(*S*)-**25b.35**	3.678	−1188.567565	1.489	1.16	−1188.206568	1.919	0.61	

Table S2. Oscillator strengths (f_j), rotational strengths in dipole length formalism (R_j) and excitation wavelengths (λ_j) for the conformers of (*S*)-**25b**, as obtained by PBE0/def2-TZVP/IEFPCM(2-PrOH)//B97D/def2-TZVP/IEFPCM(2-PrOH) calculations.

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	(*S*)-**25b.01**	(*S*)-**25b.02**	(*S*)-**25b.03**	(*S*)-**25b.04**	(*S*)-**25b.06**
1	0.0571; 5.9968 (362.15)	0.0572; 7.7275 (359.88)	0.0027; 5.3268 (368.44)	0.0025; 4.2300 (368.37)	0.0574; 7.2756 (361.40)
2	0.0021; −3.8026 (315.90)	0.0030; −11.8980 (314.29)	0.0083; 26.9966 (333.10)	0.0083; 27.0680 (334.15)	0.0007; −0.4345 (310.40)
3	0.0015; −1.1374 (288.43)	0.0012; −1.0538 (285.90)	0.0464; 19.4049 (294.06)	0.0489; 18.1884 (294.39)	0.0054; −23.8405 (294.54)
4	0.0380; 21.6121 (282.54)	0.0165; 1.4111 (284.96)	0.0295; −2.7633 (284.33)	0.0358; −0.6986 (284.51)	0.0214; 20.5234 (282.33)
5	0.0295; 5.5128 (278.95)	0.0517; 31.2297 (276.16)	0.0492; −5.3731 (278.92)	0.0451; −5.2580 (278.85)	0.0451; 23.9081 (276.58)
6	0.0063; 2.2309 (252.75)	0.0190; −6.8924 (253.21)	0.0228; −21.8880 (255.35)	0.0213; −15.2334 (255.16)	0.0201; −6.5819 (253.26)
7	0.0021; −3.6965 (250.92)	0.0021; −4.5022 (251.15)	0.0196; −9.2408 (251.66)	0.0170; −9.0631 (251.42)	0.0017; −11.7861 (251.35)
8	0.0178; 22.3064 (249.56)	0.0014; 9.5698 (249.60)	0.0368; −37.9815 (248.45)	0.0322; −46.6066 (248.23)	0.0020; 4.4294 (249.94)
9	0.0165; 17.6588 (247.54)	0.0049; −16.4844 (247.17)	0.0022; −14.2641 (247.73)	0.0071; 10.2123 (247.77)	0.0059; −20.8772 (247.25)
10	0.3389; −82.0299 (244.92)	0.3232; −52.1725 (245.19)	0.6021; −60.2169 (243.15)	0.5843; −48.7815 (243.01)	0.3274; −39.5092 (245.35)
11	0.1308; −46.0227 (237.28)	0.0981; −3.2457 (236.54)	0.0705; 56.8521 (240.24)	0.0680; 36.9523 (239.81)	0.1430; −48.6926 (237.42)
12	0.1596; 6.0384 (234.62)	0.2279; −36.2013 (234.15)	0.0937; 51.0961 (235.83)	0.0983; 40.9349 (236.10)	0.0043; 4.0624 (234.67)
13	0.0546; −3.0528 (233.08)	0.0632; −16.8386 (232.98)	0.0408; 23.6750 (233.62)	0.0428; 22.2915 (233.89)	0.2127; 3.2442 (234.30)
14	0.0950; 13.8739 (232.17)	0.0645; 45.9828 (231.70)	0.0373; −20.3820 (231.19)	0.0514; −16.7268 (231.35)	0.0534; 32.4725 (230.52)
15	0.0035; 3.1015 (225.12)	0.0047; 4.0106 (224.72)	0.0702; 7.1193 (227.75)	0.0746; 7.0133 (228.05)	0.0073; −2.2259 (225.58)
16	0.0011; 0.8030 (224.61)	0.0020; 0.7298 (224.38)	0.0040; 5.7832 (224.13)	0.0037; 5.5278 (224.34)	0.0013; −1.8668 (222.29)
17	0.0183; −10.6760 (212.40)	0.0141; −0.1381 (211.61)	0.0198; −14.3790 (215.90)	0.0198; −13.2451 (215.76)	0.0594; 30.9135 (214.65)
18	0.0233; −7.4320 (211.38)	0.0427; 6.4009 (210.46)	0.0544; −63.2154 (213.05)	0.0605; −72.0290 (213.02)	0.0073; 6.5013 (210.42)
19	0.0458; 9.4055 (209.13)	0.0377; 20.0388 (209.78)	0.0279; 15.9308 (211.50)	0.0266; 10.9801 (211.14)	0.0141; 7.9997 (208.19)
20	0.0282; −5.4507 (207.22)	0.0345; 11.2264 (209.26)	0.0006; −1.9980 (210.78)	0.0045; 10.4999 (210.91)	0.0215; −38.9496 (207.87)
21	0.0744; −19.3640 (206.37)	0.0063; −10.2419 (206.34)	0.0281; 18.2091 (207.46)	0.0318; 16.3381 (207.28)	0.0933; 38.0606 (206.62)
22	0.0283; −24.0595 (205.90)	0.1116; −28.4955 (205.14)	0.0518; 28.9810 (206.72)	0.0483; 27.6446 (206.54)	0.0342; 7.6949 (206.05)
23	0.0219; 3.9732 (204.55)	0.0095; 4.4255 (204.37)	0.0116; −3.4275 (205.13)	0.0088; −0.8225 (205.26)	0.0380; 9.4878 (204.59)
24	0.0032; 4.6573 (203.80)	0.0193; −3.7811 (202.83)	0.0089; −1.2825 (204.53)	0.0080; −1.1246 (204.55)	0.0051; 2.8601 (202.54)
25	0.0328; 78.3542 (201.11)	0.0251; 5.5216 (200.33)	0.0505; 35.1777 (201.78)	0.0395; 25.2496 (201.63)	0.0745; −17.0133 (201.18)
26	0.0541; 16.3245 (200.14)	0.1119; 14.3698 (199.71)	0.0003; 1.2165 (201.21)	0.0004; 1.5272 (201.16)	0.0421; 52.3192 (199.86)
27	0.0918; −3.7364 (199.80)	0.0065; −5.9431 (198.95)	0.0621; −24.0802 (200.68)	0.0928; −10.0150 (200.62)	0.0588; −34.3729 (199.51)
28	0.0673; −64.3893 (198.44)	0.0453; 48.0465 (198.65)	0.2154; 83.2843 (198.50)	0.2165; 81.7942 (198.40)	0.0687; 13.6497 (198.64)
29	0.2267; 96.8525 (197.59)	0.0992; 43.0448 (197.70)	0.1222; −50.7324 (196.67)	0.1361; −31.6325 (196.74)	0.1138; 4.7045 (198.37)
30	0.2510; −25.5813 (196.04)	0.1440; 6.0671 (196.67)	0.0301; −29.2203 (195.64)	0.0220; −26.3305 (195.50)	0.3261; 12.5997 (196.35)
31	0.0843; 4.5304 (195.84)	0.1870; −42.5027 (196.07)	0.3566; 17.5196 (194.94)	0.3016; 1.5558 (194.89)	0.0230; −36.6618 (195.95)
32	0.0017; 2.4047 (192.35)	0.1189; 7.6245 (191.87)	0.0131; −2.0521 (193.39)	0.0274; −0.7260 (193.51)	0.0967; −35.4357 (193.08)
33	0.1025; 2.5517 (192.14)	0.0401; 118.1174 (191.63)	0.0587; −21.9013 (192.96)	0.0729; −29.4588 (193.09)	0.0360; −54.0862 (191.67)
34	0.1841; 15.3192 (191.39)	0.1876; −137.0198 (191.54)	0.0921; 67.1108 (191.47)	0.0156; −22.7956 (191.01)	0.0657; 35.8897 (190.79)
35	0.0545; 12.5003 (190.18)	0.0992; 52.8467 (190.65)	0.0597; 2.4589 (190.83)	0.0671; 24.1915 (190.54)	0.1341; 115.2071 (190.66)
36	0.0651; 12.5290 (189.61)	0.3489; −120.8026 (189.81)	0.0150; −17.3526 (190.19)	0.0788; 89.3619 (190.16)	0.2149; −23.7902 (189.91)
37	0.2739; 1.0822 (188.70)	0.1541; −124.8121 (189.20)	0.0290; −17.7743 (189.58)	0.0385; −32.2708 (189.42)	0.2956; −267.2801 (188.76)
38	0.0629; 10.9315 (188.47)	0.0493; −23.3730 (188.23)	0.0022; −2.8765 (188.35)	0.0005; 0.4444 (188.75)	0.0469; 60.7848 (187.51)
39	0.0102; 6.5482 (187.98)	0.0434; 24.9748 (187.46)	0.1156; −144.0896 (187.29)	0.0488; −73.0907 (187.42)	0.1366; 102.6110 (187.17)
40	0.0216; 14.9054 (187.33)	0.0744; 80.8361 (187.25)	0.2565; −46.4429 (186.88)	0.2815; −90.4169 (187.00)	0.0084; 0.5480 (185.86)
41	0.1471; −165.5014 (186.32)	0.0028; −1.5790 (185.90)	0.0801; 32.7000 (186.30)	0.0955; 11.7498 (186.24)	0.0109; 12.5921 (185.41)
42	0.0087; 3.1162 (185.43)	0.0012; −2.4322 (185.61)	0.0017; 2.0430 (184.43)	0.0011; 1.5162 (184.56)	0.0075; −4.0741 (184.80)
43	0.0109; −18.7813 (184.40)	0.0091; −10.9924 (183.53)	0.0043; 0.6242 (183.95)	0.0034; 1.3198 (184.10)	0.0421; −15.2020 (183.73)
44	0.0357; −0.7590 (182.57)	0.0675; −2.9056 (182.13)	0.0589; −37.9798 (182.56)	0.0672; −39.7666 (182.67)	0.1405; −50.2964 (183.35)
45	0.1025; −31.7294 (181.87)	0.0975; −32.6899 (181.75)	0.0013; 0.6500 (182.28)	0.0576; −31.7221 (182.28)	0.1529; 47.2200 (182.02)
46	0.0325; −9.1734 (181.24)	0.0120; 4.6378 (180.93)	0.0737; −22.0937 (182.08)	0.0178; −0.0320 (182.08)	0.0114; −0.1651 (181.26)
47	0.0710; −1.9485 (180.35)	0.0253; 5.7369 (180.80)	0.0225; 24.3151 (181.59)	0.0302; 22.3721 (181.53)	0.0495; 22.5414 (180.75)
48	0.0668; 4.9007 (180.29)	0.1874; 14.0297 (179.85)	0.0017; −9.5081 (180.54)	0.0021; −3.8516 (180.49)	0.0556; 6.9237 (180.42)
49	0.0811; −11.8452 (179.67)	0.0886; 11.7503 (179.60)	0.0115; −3.1726 (180.29)	0.0019; −12.5603 (180.31)	0.0332; −77.8597 (179.59)
50	0.0115; −9.8022 (179.01)	0.0426; −31.1240 (178.95)	0.1312; 45.5751 (179.58)	0.1236; 43.5793 (179.59)	0.0048; 20.7228 (179.38)

Table S2. *(continued)*

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	(*S*)-**25b.07**	(*S*)-**25b.08**	(*S*)-**25b.09**	(*S*)-**25b.10**	(*S*)-**25b.11**
1	0.0023; 1.5417 (368.72)	0.0028; 2.1272 (368.25)	0.0562; 6.3763 (363.34)	0.0037; 0.8114 (345.77)	0.0038; 0.7074 (346.05)
2	0.0105; 8.2723 (319.59)	0.0131; 6.9519 (319.92)	0.0001; 0.6440 (310.94)	0.0084; −14.8602 (302.52)	0.0080; −14.4611 (302.43)
3	0.0364; 48.6230 (307.68)	0.0317; 47.1358 (306.86)	0.0014; −7.2381 (296.29)	0.0843; −15.1077 (275.23)	0.0852; −14.6237 (275.30)
4	0.0410; −0.6480 (284.73)	0.0299; −0.3665 (284.46)	0.0523; 16.8586 (282.58)	0.0062; −1.6069 (272.31)	0.0062; −1.4839 (272.51)
5	0.0486; −14.2650 (276.59)	0.0548; −15.5690 (277.02)	0.0174; 11.5572 (277.62)	0.0326; 5.7742 (266.99)	0.0339; 4.4528 (267.45)
6	0.0210; 0.8872 (254.02)	0.0209; −0.1822 (253.82)	0.0052; 1.9511 (252.54)	0.2023; 18.3959 (261.20)	0.1993; 22.7441 (261.49)
7	0.0033; −0.3597 (250.76)	0.0035; 1.1400 (250.84)	0.0011; −1.8091 (250.85)	0.0539; −6.6744 (254.33)	0.0534; −5.2793 (254.23)
8	0.0110; −24.9973 (248.41)	0.0099; −16.8559 (248.23)	0.0208; 6.5223 (249.93)	0.0052; −4.5478 (249.93)	0.0051; −4.8895 (249.77)
9	0.0024; 3.8395 (247.71)	0.0014; −10.6162 (247.73)	0.0134; 13.0910 (247.57)	0.0002; −3.7349 (247.42)	0.0026; 10.8186 (247.40)
10	0.6666; −24.1317 (242.69)	0.6883; −16.3215 (242.66)	0.3535; −67.1358 (245.00)	0.0100; 0.4511 (243.86)	0.0093; 1.4844 (243.93)
11	0.0080; −0.2282 (240.52)	0.0075; −2.4004 (240.23)	0.1103; −46.3866 (237.40)	0.2961; 19.2307 (240.05)	0.0935; 157.3454 (240.24)
12	0.0444; 17.6765 (239.34)	0.0480; 7.5109 (239.06)	0.1564; −15.6321 (235.67)	0.0136; 30.1321 (239.97)	0.2246; −116.8494 (240.02)
13	0.0710; 18.8851 (234.78)	0.0609; 19.3065 (235.01)	0.0673; 14.0538 (234.56)	0.0301; 1.6183 (239.07)	0.0202; 3.3679 (238.69)
14	0.0186; 4.0371 (231.67)	0.0248; 5.1543 (231.83)	0.0601; 36.4556 (230.75)	0.1025; −20.2437 (230.55)	0.1042; −23.0096 (230.22)
15	0.0009; −1.2091 (226.14)	0.0006; −0.7099 (225.72)	0.0067; −3.8148 (225.87)	0.0048; 0.8272 (226.19)	0.0048; 0.5373 (226.16)
16	0.0200; 3.8544 (224.38)	0.0157; 4.9486 (224.70)	0.0012; −3.0841 (221.80)	0.0437; 5.4566 (222.30)	0.0417; 4.5957 (222.13)
17	0.1529; −40.2521 (218.87)	0.1537; −38.3345 (218.42)	0.0215; −15.8010 (215.13)	0.0471; 34.9869 (219.65)	0.0476; 33.9736 (219.47)
18	0.0023; 0.2518 (213.08)	0.0027; 2.7028 (213.41)	0.0042; 1.5831 (211.18)	0.0243; −14.2454 (216.19)	0.0199; −10.3887 (216.54)
19	0.0189; −27.3847 (211.14)	0.0163; −27.8856 (210.94)	0.0162; −30.8897 (208.73)	0.0117; 43.0150 (215.71)	0.0103; 36.1582 (215.93)
20	0.0065; −14.7730 (210.11)	0.0121; −18.6766 (209.88)	0.1214; 6.3163 (207.11)	0.0881; −32.9264 (212.06)	0.0986; −41.7667 (212.35)
21	0.1207; 42.8240 (208.07)	0.1108; 28.6494 (207.71)	0.0430; 35.3635 (206.28)	0.1858; −113.6796 (209.52)	0.1828; −111.5415 (209.69)
22	0.0156; −2.0613 (207.00)	0.0077; 13.6706 (206.71)	0.0183; −18.7670 (206.13)	0.0006; 3.0664 (205.08)	0.0016; 3.5258 (205.15)
23	0.0587; 30.1251 (205.81)	0.0440; 27.1216 (205.93)	0.0220; −14.4535 (205.39)	0.0497; 5.1486 (203.82)	0.0452; 5.1956 (203.96)
24	0.0412; −43.7383 (204.75)	0.0337; −45.6863 (204.59)	0.0081; 12.7172 (203.02)	0.0303; −33.0566 (202.75)	0.0281; −29.6419 (202.92)
25	0.0268; −10.8891 (203.98)	0.0255; −11.3829 (203.92)	0.1166; −23.2999 (201.93)	0.0045; 4.8471 (202.12)	0.0045; 4.5770 (202.22)
26	0.0223; 28.1857 (201.25)	0.0097; 15.7147 (200.86)	0.0305; −12.2448 (199.80)	0.0027; −9.1000 (201.20)	0.0033; −6.2643 (201.16)
27	0.0126; 12.7223 (200.49)	0.0363; 35.4072 (200.27)	0.0857; 76.8585 (199.18)	0.0641; −2.3613 (200.63)	0.0669; 1.8868 (200.71)
28	0.0761; 27.2101 (199.95)	0.0939; 37.9858 (199.93)	0.1866; 23.5612 (198.68)	0.0792; 4.5826 (197.68)	0.0743; 1.3418 (197.67)
29	0.0534; −33.7887 (197.44)	0.0453; −57.6653 (197.42)	0.0506; 6.9104 (198.38)	0.0140; 10.4237 (197.07)	0.0142; 10.7555 (197.04)
30	0.1386; −21.4188 (196.95)	0.1142; 8.9119 (197.11)	0.3643; −13.0002 (196.17)	0.0827; −0.3890 (196.61)	0.0300; 3.0164 (196.62)
31	0.3043; 11.6489 (194.87)	0.3681; 0.6209 (194.85)	0.0141; −6.9530 (195.74)	0.1261; −17.3163 (196.41)	0.1604; −12.1189 (196.29)
32	0.2159; 6.6931 (193.96)	0.1990; −15.0488 (194.12)	0.0048; −7.5902 (192.73)	0.4672; −63.7676 (195.09)	0.4952; −50.0334 (195.06)
33	0.0402; −35.8958 (192.39)	0.0398; −26.2320 (192.44)	0.0835; 25.7465 (191.92)	0.0097; 36.1265 (193.93)	0.0052; −7.4710 (193.37)
34	0.1404; 59.2293 (191.04)	0.0965; 90.0005 (191.28)	0.1591; 11.6883 (191.36)	0.0066; −23.7700 (190.97)	0.0564; −49.3656 (191.72)
35	0.0384; −39.1243 (190.69)	0.0276; −16.3867 (190.73)	0.0969; 43.8719 (190.17)	0.0277; −59.9778 (190.38)	0.0085; 10.7354 (190.99)
36	0.0511; 66.4145 (188.89)	0.0110; 29.1118 (189.27)	0.0535; −13.0873 (189.50)	0.0074; −5.2600 (190.07)	0.0006; −1.9795 (189.67)
37	0.2704; −81.7632 (188.36)	0.3722; −120.2752 (188.21)	0.2887; 29.8653 (188.50)	0.0710; 6.9621 (189.63)	0.0489; 5.4554 (189.48)
38	0.0133; −3.1047 (187.31)	0.0091; −13.6023 (187.40)	0.0021; 1.7118 (187.56)	0.1370; 193.9821 (188.74)	0.1203; 179.4962 (188.31)
39	0.0043; 0.2828 (187.26)	0.0007; 1.3316 (187.26)	0.0040; −7.2327 (186.75)	0.0017; 11.2223 (186.92)	0.0026; 13.4972 (186.97)
40	0.0051; −11.1796 (186.42)	0.0096; −24.2837 (186.33)	0.1909; −207.3680 (186.40)	0.0202; −8.4801 (186.44)	0.0324; 21.2174 (186.43)
41	0.0154; −29.3387 (186.21)	0.0157; −17.0154 (185.90)	0.0071; 5.8346 (185.52)	0.0397; −14.1816 (186.22)	0.0328; −35.3141 (185.98)
42	0.1057; −51.6806 (184.98)	0.1035; −53.3260 (185.00)	0.0456; −7.7490 (185.24)	0.0001; −0.6783 (185.52)	0.0005; −1.1121 (185.48)
43	0.0042; −5.1847 (184.58)	0.0045; −3.7089 (184.41)	0.0125; 14.9766 (184.21)	0.0008; 0.2495 (184.77)	0.0010; 0.1876 (184.60)
44	0.0020; −4.5702 (183.98)	0.0049; −5.1572 (183.69)	0.0922; 33.8446 (183.81)	0.0946; −3.0409 (184.09)	0.0799; 7.0269 (184.31)
45	0.0435; −8.8419 (182.10)	0.0541; −16.5371 (182.05)	0.2139; 44.0311 (182.23)	0.0662; −44.7774 (182.59)	0.0526; −26.1935 (182.88)
46	0.0695; 18.0532 (181.91)	0.0667; 9.7786 (181.86)	0.0040; −0.5375 (181.14)	0.0448; 31.6253 (181.69)	0.0500; 45.3027 (181.76)
47	0.0058; 1.1391 (181.56)	0.0388; 3.6918 (181.35)	0.0232; 7.8727 (181.02)	0.0016; −1.7290 (181.21)	0.0035; −1.1494 (181.10)
48	0.0330; 0.4026 (181.42)	0.0003; −0.8118 (181.05)	0.0233; 4.3591 (180.47)	0.0323; −8.4471 (179.94)	0.0327; −15.6785 (180.58)
49	0.0229; 19.9801 (180.82)	0.0367; 22.8260 (180.70)	0.0250; −57.9467 (179.84)	0.1093; −3.5154 (178.83)	0.1829; −10.1161 (178.84)
50	0.0184; −5.9831 (180.51)	0.0151; 1.3531 (180.31)	0.0101; 29.2102 (179.24)	0.2376; 56.9349 (178.57)	0.1711; 46.4183 (178.65)

Table S2. *(continued)*

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	(*S*)-**25b.12**	(*S*)-**25b.13**	(*S*)-**25b.14**	(*S*)-**25b.15**	(*S*)-**25b.16**
1	0.0256; 8.7217 (388.24)	0.0005; −1.9462 (347.52)	0.0032; 10.4353 (367.41)	0.0006; −1.6281 (347.01)	0.0031; 9.9387 (367.25)
2	0.0423; −17.0446 (329.55)	0.0028; −7.3573 (309.72)	0.0044; 10.1405 (332.19)	0.0029; −7.6461 (309.03)	0.0043; 10.9268 (332.19)
3	0.0051; 23.2269 (313.54)	0.0343; 14.4309 (282.93)	0.0334; 19.8504 (296.97)	0.0363; 14.2793 (282.80)	0.0333; 20.4343 (296.83)
4	0.0318; −6.9210 (291.47)	0.0078; 3.5089 (282.55)	0.0179; −13.4278 (291.96)	0.0035; 1.3439 (281.82)	0.0194; −14.4286 (291.89)
5	0.0535; −15.7095 (287.22)	0.0474; −17.5903 (266.55)	0.0451; −7.6930 (274.41)	0.0470; −14.6728 (265.93)	0.0449; −6.4777 (274.21)
6	0.0866; −14.8838 (264.02)	0.0177; −20.4451 (252.87)	0.0187; 17.9377 (252.99)	0.0170; −18.3630 (252.96)	0.0175; 18.6322 (253.05)
7	0.0929; −13.6860 (253.95)	0.0032; 9.3367 (250.89)	0.0107; −3.8331 (250.61)	0.0030; 7.2253 (250.81)	0.0108; −5.6637 (250.79)
8	0.0260; −87.0971 (249.27)	0.1061; −58.4541 (246.69)	0.0097; 0.2533 (249.48)	0.0959; −0.9213 (246.74)	0.0102; 1.7975 (249.47)
9	0.0463; 39.7047 (248.44)	0.0138; 30.6934 (246.04)	0.0039; −17.6587 (246.50)	0.0046; −11.7029 (246.18)	0.0012; −7.7099 (246.53)
10	0.1590; −33.9667 (247.65)	0.3706; 15.5245 (243.60)	0.4808; −52.1960 (244.43)	0.3998; −10.2789 (243.70)	0.4971; −51.1900 (244.40)
11	0.1120; 125.2722 (247.30)	0.2783; 10.5313 (238.72)	0.3134; 61.8024 (239.22)	0.2714; 18.9645 (238.89)	0.3028; 57.1147 (239.23)
12	0.0002; −0.9592 (242.54)	0.0082; 4.8423 (233.22)	0.0310; 34.2305 (234.91)	0.0079; 4.3449 (233.24)	0.0319; 35.2588 (234.97)
13	0.0227; −40.5630 (238.35)	0.0902; −6.7290 (232.42)	0.0065; 5.3781 (230.07)	0.0911; −9.9705 (232.32)	0.0076; 5.5645 (230.10)
14	0.0017; 5.3397 (231.37)	0.0069; −1.1394 (228.37)	0.0572; −27.9700 (228.91)	0.0054; −0.3044 (228.65)	0.0561; −29.8984 (229.01)
15	0.1674; −21.0388 (229.11)	0.0070; 3.2010 (224.93)	0.0168; −5.3559 (225.03)	0.0079; 3.1249 (224.87)	0.0159; −5.2163 (224.97)
16	0.0106; 0.9524 (223.41)	0.0005; 0.7468 (218.34)	0.0007; 0.1920 (216.90)	0.0005; 0.7809 (218.35)	0.0007; −0.0529 (216.90)
17	0.1399; 220.4103 (220.94)	0.0055; −1.6308 (217.02)	0.0048; 8.5383 (214.92)	0.0055; −1.0580 (216.90)	0.0044; 9.1146 (215.06)
18	0.0108; 13.3972 (216.90)	0.0188; −2.1612 (210.81)	0.0628; −55.5443 (214.25)	0.0326; 0.3777 (210.78)	0.0651; −55.8382 (214.26)
19	0.0839; −118.0954 (216.20)	0.1407; 42.8217 (209.99)	0.0277; −12.4622 (211.57)	0.1227; 39.7779 (210.16)	0.0327; −14.7206 (211.51)
20	0.0326; 3.5696 (214.45)	0.0301; 2.2968 (207.70)	0.0359; −11.1403 (210.85)	0.0309; 1.9569 (207.42)	0.0320; −9.3816 (210.83)
21	0.0183; 24.1570 (213.84)	0.1434; 40.4562 (205.16)	0.0142; −7.6287 (206.70)	0.1503; 51.8012 (205.19)	0.0168; −8.0436 (206.92)
22	0.0908; −66.8286 (210.58)	0.0272; −44.3244 (203.19)	0.0596; 64.3549 (205.78)	0.0700; −54.2718 (203.30)	0.0525; 65.1625 (205.79)
23	0.0165; −4.7145 (209.89)	0.0486; 29.3073 (202.96)	0.0040; 2.5459 (204.99)	0.0390; 48.6851 (202.79)	0.0035; 1.8512 (204.89)
24	0.0057; 3.1545 (209.70)	0.0626; 21.9478 (202.41)	0.1263; −48.2393 (202.56)	0.0199; 5.5534 (202.37)	0.1216; −47.7041 (202.58)
25	0.0228; −18.2402 (204.57)	0.0258; −14.5809 (201.65)	0.0097; −4.4584 (200.40)	0.0272; −13.1615 (201.52)	0.0096; −7.5802 (200.43)
26	0.0344; 73.3312 (204.03)	0.0273; −51.6185 (199.64)	0.0054; −4.6978 (199.68)	0.0260; −48.7224 (199.78)	0.0064; −4.9130 (199.67)
27	0.0216; 6.2556 (202.61)	0.0071; 4.2625 (199.14)	0.0207; −12.5545 (198.22)	0.0035; 6.0643 (199.16)	0.0238; −10.8977 (198.21)
28	0.0037; 1.5032 (201.78)	0.0320; −31.0216 (197.18)	0.1957; −8.0078 (196.48)	0.0466; −62.3706 (197.11)	0.1578; −16.4978 (196.42)
29	0.0012; −4.5038 (199.80)	0.1102; −106.9708 (196.05)	0.1951; 170.6541 (195.97)	0.0830; −99.4071 (196.02)	0.2442; 155.2055 (196.09)
30	0.0505; 8.7468 (199.05)	0.4067; 11.1420 (195.42)	0.0395; −29.8598 (195.17)	0.4362; 52.6980 (195.33)	0.0466; −31.2336 (195.17)
31	0.0346; −24.2542 (198.33)	0.0007; 2.0796 (194.18)	0.1171; 45.4193 (194.01)	0.0013; 2.4426 (193.93)	0.1334; 5.2047 (194.14)
32	0.1707; 20.1862 (197.33)	0.0546; −126.9380 (191.98)	0.0683; −25.3471 (192.70)	0.1945; 34.1264 (192.17)	0.0472; 2.8589 (192.72)
33	0.0293; −0.7392 (196.36)	0.2131; 133.2870 (191.77)	0.2242; 83.6506 (191.13)	0.2161; −39.9685 (191.57)	0.4507; 67.8755 (190.99)
34	0.1156; −2.8719 (195.62)	0.2772; 233.1723 (190.92)	0.2225; −288.9027 (190.88)	0.1544; −48.9129 (190.51)	0.0075; 36.6924 (190.83)
35	0.2597; −23.3716 (194.19)	0.0263; −9.2110 (189.90)	0.0367; 42.2287 (189.92)	0.0383; 3.6638 (190.01)	0.0040; −13.6594 (189.78)
36	0.0069; −15.4474 (192.51)	0.2221; −80.2649 (189.34)	0.3108; 82.9911 (189.42)	0.1723; 175.8544 (189.30)	0.2855; −107.7795 (189.54)
37	0.0700; −9.9140 (191.58)	0.0022; −4.1164 (187.84)	0.0265; −28.3392 (188.15)	0.0015; −1.1151 (187.87)	0.0196; −27.9159 (188.23)
38	0.0159; 22.3420 (191.21)	0.0047; −4.6534 (187.65)	0.1030; −84.3249 (187.83)	0.0099; −7.4667 (187.49)	0.0843; −36.3867 (187.78)
39	0.0005; −2.5050 (189.55)	0.0510; 19.1460 (187.27)	0.0031; −11.4127 (187.59)	0.0943; 55.4551 (187.13)	0.0732; −129.8307 (187.63)
40	0.0734; −163.5475 (188.24)	0.0895; 16.3715 (187.05)	0.0147; −52.2845 (187.50)	0.0586; 4.7598 (186.84)	0.0089; −17.7720 (187.47)
41	0.0981; 33.0637 (187.51)	0.0379; 2.9505 (185.39)	0.0014; −3.6842 (187.16)	0.0409; 7.0591 (185.20)	0.0039; −7.5872 (187.16)
42	0.0168; 10.8472 (187.14)	0.2467; 147.6305 (183.74)	0.0005; 0.5004 (183.77)	0.0062; 12.5775 (183.80)	0.0018; −0.0834 (183.64)
43	0.0017; −1.8274 (185.27)	0.0145; −5.5397 (183.50)	0.1116; 17.6316 (183.57)	0.2391; 136.6992 (183.63)	0.1105; 31.1956 (183.53)
44	0.0338; 8.7813 (184.06)	0.0014; 2.4405 (183.41)	0.0111; 6.3677 (182.70)	0.0073; 1.1996 (183.42)	0.0149; 6.9708 (182.47)
45	0.0241; −0.4323 (183.86)	0.2760; −62.0928 (181.01)	0.0466; 22.2410 (181.39)	0.2734; −86.6188 (181.08)	0.0255; 14.5022 (181.65)
46	0.2925; 27.5135 (183.41)	0.0048; −0.8857 (180.64)	0.0268; 10.8082 (181.29)	0.0034; −4.1649 (180.79)	0.0540; 18.4563 (181.21)
47	0.0262; −0.3325 (182.97)	0.0070; −29.5501 (179.49)	0.0818; −63.8872 (180.89)	0.0072; −27.0957 (179.45)	0.0745; −59.8179 (180.83)
48	0.0532; −25.4408 (180.93)	0.0963; 70.4107 (178.96)	0.1163; −11.1695 (180.02)	0.0822; 82.5981 (178.98)	0.1134; −8.1317 (179.96)
49	0.0012; −3.6124 (180.56)	0.0870; −59.0035 (178.73)	0.0091; −39.6933 (179.32)	0.0736; −70.1576 (178.79)	0.0105; −32.2831 (179.34)
50	0.0089; 1.6678 (180.14)	0.0964; −31.4548 (178.15)	0.2148; 144.5152 (178.74)	0.1337; −45.7941 (178.27)	0.2057; 136.2163 (178.73)

Table S2. *(continued)*

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)			
	(*S*)-**25b.17**	(*S*)-**25b.20**	(*S*)-**25b.22**	(*S*)-**25b.23**
1	0.0222; 13.1219 (387.11)	0.0201; 11.7848 (386.55)	0.0032; 7.5956 (366.06)	0.0030; 6.9136 (365.43)
2	0.0184; −23.2325 (343.49)	0.0184; −22.5277 (342.13)	0.0266; −2.0491 (322.30)	0.0259; −1.3300 (321.74)
3	0.0432; 21.2784 (303.23)	0.0466; 20.5871 (302.89)	0.0160; 36.9273 (306.52)	0.0169; 38.4891 (306.57)
4	0.0673; −18.4765 (290.75)	0.0665; −16.4974 (290.36)	0.0074; −9.4043 (290.61)	0.0088; −10.8303 (290.30)
5	0.0053; −5.1699 (285.19)	0.0054; −5.3162 (285.19)	0.0494; −5.9398 (273.55)	0.0491; −4.9013 (273.17)
6	0.1343; −25.7045 (258.37)	0.1368; −12.6872 (258.18)	0.0223; 11.8371 (252.91)	0.0211; 12.2077 (252.97)
7	0.0242; 8.8951 (256.28)	0.0190; 7.3899 (256.06)	0.0044; 3.8037 (251.33)	0.0043; 3.3109 (251.23)
8	0.0244; −19.2182 (252.34)	0.0230; −16.6345 (251.97)	0.0210; 2.4538 (249.27)	0.0218; 5.2380 (249.21)
9	0.2564; −56.7929 (248.40)	0.3226; 14.0626 (248.28)	0.0034; −16.1739 (246.48)	0.0010; −6.5958 (246.49)
10	0.0922; 86.4279 (247.79)	0.0345; 25.2760 (247.78)	0.4462; −20.0445 (244.17)	0.4650; −19.7648 (244.07)
11	0.0108; 17.6564 (247.20)	0.0095; 8.0794 (247.49)	0.3291; 27.1779 (238.37)	0.3142; 22.0599 (238.34)
12	0.0028; 8.4573 (240.91)	0.0027; 9.0528 (240.91)	0.0080; 3.3470 (237.09)	0.0087; 3.7066 (237.28)
13	0.0325; 61.6544 (239.89)	0.0332; 56.2141 (239.46)	0.0358; −0.9121 (231.70)	0.0360; −0.0546 (231.70)
14	0.1461; −63.1168 (232.03)	0.1566; −62.4713 (232.09)	0.0019; −0.1867 (228.38)	0.0020; −0.7504 (228.37)
15	0.0121; 7.4560 (228.50)	0.0145; 3.8362 (228.13)	0.0207; 16.7781 (226.21)	0.0209; 16.3772 (226.15)
16	0.0031; 0.2407 (224.94)	0.0044; 1.0370 (225.30)	0.0038; 0.9568 (220.69)	0.0040; 0.4387 (220.55)
17	0.0980; 22.5171 (222.50)	0.0869; 24.0427 (221.82)	0.1454; −25.4145 (218.08)	0.1467; −26.9546 (218.31)
18	0.0084; 21.6875 (217.10)	0.0060; 24.8843 (217.04)	0.0011; −2.4199 (212.21)	0.0012; −2.2454 (212.27)
19	0.0111; 6.6162 (216.45)	0.0124; −5.1806 (216.41)	0.0291; −17.3405 (211.45)	0.0404; −24.7598 (211.31)
20	0.0459; −64.7384 (214.40)	0.0446; −59.0578 (214.43)	0.0258; −0.6890 (210.98)	0.0169; 7.1875 (210.86)
21	0.0831; −73.1174 (211.25)	0.0860; −85.9699 (211.36)	0.0575; −15.3646 (207.32)	0.0485; −15.9008 (207.45)
22	0.0336; 34.9298 (209.35)	0.0391; 47.6354 (209.43)	0.0000; −0.1843 (204.88)	0.0005; 0.5051 (204.63)
23	0.0512; −16.6795 (208.68)	0.0328; −9.2211 (208.69)	0.1005; 56.9653 (203.76)	0.0959; 53.3360 (203.96)
24	0.0267; 35.5372 (208.17)	0.0444; 22.5925 (208.04)	0.0009; 0.2049 (203.40)	0.0017; 0.2184 (203.47)
25	0.0122; −17.2554 (202.29)	0.0097; −14.7691 (202.29)	0.0537; −68.4135 (201.38)	0.0642; −72.9509 (201.49)
26	0.0081; −10.3550 (201.82)	0.0047; −8.1469 (201.85)	0.0040; 2.9104 (199.58)	0.0033; 3.1915 (199.55)
27	0.1250; −87.1248 (200.67)	0.0973; −84.2241 (200.61)	0.0396; 41.2230 (197.59)	0.0290; 63.4366 (197.59)
28	0.0797; 0.2234 (200.37)	0.1142; −3.2857 (200.14)	0.0304; 1.8053 (196.76)	0.0703; 21.2910 (196.82)
29	0.0008; −2.2479 (199.90)	0.0162; −7.4317 (199.35)	0.2896; 43.6476 (196.56)	0.2415; −37.0140 (196.63)
30	0.0037; −5.7224 (198.66)	0.0067; −14.6551 (198.85)	0.1265; −29.6924 (195.37)	0.1806; 5.5498 (195.44)
31	0.0497; 20.1240 (197.64)	0.0306; 7.7430 (197.77)	0.0765; −3.5059 (195.29)	0.0544; −7.8435 (195.31)
32	0.2632; 33.6794 (196.60)	0.2899; 40.0667 (196.43)	0.0808; 54.3482 (193.59)	0.0824; 19.5986 (193.63)
33	0.0404; −3.6739 (195.85)	0.0297; 30.7987 (195.80)	0.0185; 11.3039 (191.66)	0.0522; 34.7918 (191.74)
34	0.0408; 5.0585 (195.27)	0.0369; 3.3667 (195.08)	0.2735; −33.4796 (190.82)	0.3289; 131.6901 (190.72)
35	0.2203; −80.9233 (194.59)	0.2066; −54.2708 (194.50)	0.1192; −76.3915 (190.00)	0.0048; −0.7745 (189.75)
36	0.0407; 132.0181 (193.62)	0.0295; 67.9025 (192.99)	0.0649; −53.0059 (189.87)	0.0263; −48.3388 (189.70)
37	0.0081; 7.2898 (192.16)	0.0699; 3.2778 (192.69)	0.3780; 160.7371 (189.07)	0.2887; 35.5523 (189.24)
38	0.0438; −10.3966 (191.27)	0.0002; −0.0557 (192.11)	0.0582; −128.5026 (188.43)	0.1971; −233.8417 (188.39)
39	0.0075; −7.6345 (190.35)	0.0110; −9.0517 (189.82)	0.0004; −1.4114 (187.06)	0.0004; −0.1054 (187.09)
40	0.0418; −74.0857 (189.05)	0.0345; −25.2413 (188.98)	0.0301; −31.1537 (186.56)	0.0337; −33.9586 (186.23)
41	0.1256; 103.3745 (187.67)	0.1333; 174.8062 (187.56)	0.0607; −93.5502 (185.24)	0.0604; −95.9399 (185.21)
42	0.0299; 45.6536 (187.23)	0.0124; 0.5198 (186.85)	0.0132; 33.7926 (184.00)	0.0147; 51.7363 (183.91)
43	0.0050; 11.6765 (185.25)	0.0146; −8.9298 (185.39)	0.0014; −2.6864 (183.85)	0.0013; −1.2317 (183.72)
44	0.0631; −3.7526 (185.24)	0.0526; 9.8761 (185.18)	0.1142; −39.7252 (183.22)	0.1162; −39.6560 (183.16)
45	0.0008; −2.8853 (185.10)	0.0024; 0.4005 (185.10)	0.0302; −3.0239 (182.02)	0.0525; −8.9415 (181.85)
46	0.0103; 1.2174 (182.18)	0.0116; −3.2288 (181.95)	0.1292; −38.5223 (181.30)	0.1055; −43.4715 (181.25)
47	0.0562; −12.1963 (181.55)	0.0097; 0.9160 (181.55)	0.1519; −5.2797 (180.36)	0.1457; −3.8550 (180.38)
48	0.0359; −76.4390 (181.05)	0.0705; −110.9627 (181.29)	0.2025; −31.4726 (179.33)	0.1478; −5.4241 (179.50)
49	0.3779; −29.3448 (180.57)	0.3757; −28.7345 (180.74)	0.0057; −1.3984 (179.20)	0.0027; −2.1863 (179.19)
50	0.0439; −8.0751 (180.15)	0.0373; −7.2697 (180.14)	0.0006; −0.2338 (179.02)	0.0463; 0.4245 (178.99)

Table S2. *(continued)*

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)			
	(*S*)-**25b.24**	(*S*)-**25b.25**	(*S*)-**25b.27**	(*S*)-**25b.28**
1	0.0213; 7.9652 (387.33)	0.0006; −1.5967 (346.54)	0.0046; −0.0542 (345.16)	0.0048; −0.2728 (344.85)
2	0.0474; −17.4309 (328.36)	0.0015; −3.2777 (306.80)	0.0087; −8.1895 (295.93)	0.0065; −6.1890 (295.50)
3	0.0046; 22.0305 (312.34)	0.0199; −11.5031 (288.84)	0.0151; −19.1479 (284.16)	0.0159; −20.0321 (284.08)
4	0.0300; −7.5497 (290.98)	0.0250; 17.5026 (279.88)	0.0864; −13.9863 (275.09)	0.0880; −14.3578 (274.94)
5	0.0534; −12.1903 (286.89)	0.0449; −14.2519 (266.11)	0.0138; 6.2225 (263.85)	0.0178; 6.2968 (264.51)
6	0.0872; −13.8505 (263.50)	0.0178; −13.9492 (252.88)	0.2234; 24.9488 (261.69)	0.2255; 33.7731 (261.26)
7	0.1001; −10.7541 (253.61)	0.0024; 5.1993 (251.35)	0.0175; −16.4329 (254.86)	0.0153; −15.3478 (254.65)
8	0.0167; −71.0569 (249.13)	0.1038; −63.7359 (246.53)	0.0031; 6.3899 (251.27)	0.0034; 7.6243 (251.24)
9	0.0552; 46.8657 (248.39)	0.0257; 38.6580 (245.96)	0.0001; 0.4136 (247.24)	0.0013; 8.5883 (247.31)
10	0.1019; 55.5163 (247.78)	0.3663; 28.4270 (243.85)	0.0125; −21.9775 (243.71)	0.0135; −19.7310 (243.69)
11	0.1717; 19.1090 (247.46)	0.2988; 14.1892 (239.31)	0.0126; −27.4715 (241.21)	0.0152; −31.6787 (240.97)
12	0.0001; −0.7619 (242.53)	0.0057; −4.8515 (235.19)	0.3311; −23.0540 (240.47)	0.3260; −24.0251 (240.40)
13	0.0237; −38.1785 (237.95)	0.0527; −23.6410 (231.51)	0.0126; 1.9358 (237.58)	0.0143; 2.5030 (237.38)
14	0.0023; 6.2404 (231.58)	0.0193; 15.2783 (229.22)	0.0026; −0.2688 (232.05)	0.0023; −0.7085 (232.43)
15	0.1808; −21.7342 (229.43)	0.0042; 2.5919 (223.56)	0.1642; 22.8601 (228.60)	0.1718; 19.2623 (228.35)
16	0.0092; 0.9583 (223.16)	0.0082; 3.0861 (222.57)	0.1991; 195.2108 (220.54)	0.1849; 182.0919 (220.53)
17	0.1278; 209.9249 (220.07)	0.0021; 5.4849 (215.44)	0.0005; 0.8234 (217.61)	0.0007; 1.1116 (217.53)
18	0.0121; 14.7742 (216.58)	0.0939; 28.2799 (213.30)	0.0253; −19.4068 (214.43)	0.0215; −15.4576 (214.40)
19	0.0840; −105.6646 (216.00)	0.0693; −3.4529 (208.59)	0.0105; −45.4821 (213.51)	0.0122; −50.3874 (213.13)
20	0.0323; −20.7213 (214.06)	0.0756; −110.7770 (206.57)	0.0093; −17.8807 (210.70)	0.0106; −24.0521 (210.78)
21	0.0193; 33.5544 (213.63)	0.0493; −30.1909 (206.15)	0.0268; 3.0542 (209.53)	0.0262; 0.4763 (209.63)
22	0.0799; −59.4734 (210.60)	0.0933; 213.0988 (204.48)	0.0192; 3.3548 (208.94)	0.0174; 7.1035 (208.97)
23	0.0328; −8.0494 (209.77)	0.0278; 7.1579 (202.62)	0.0631; 6.9795 (204.67)	0.0851; 25.9439 (204.64)
24	0.0054; −0.8836 (209.62)	0.0399; −10.7920 (202.05)	0.0468; 38.7242 (204.33)	0.0303; 15.0341 (204.29)
25	0.0323; −1.3077 (204.49)	0.0057; −17.9824 (201.35)	0.0177; −6.7064 (201.52)	0.0144; −9.1117 (201.85)
26	0.0218; 61.6900 (203.92)	0.0179; −46.4222 (199.91)	0.0034; 0.0878 (200.91)	0.0034; −1.0959 (200.93)
27	0.0231; 2.2647 (202.28)	0.0346; −6.8603 (198.18)	0.0746; 10.9537 (200.49)	0.0708; 6.0077 (200.44)
28	0.0011; 3.0223 (201.76)	0.1436; −56.9932 (196.87)	0.0216; −15.8880 (199.92)	0.0218; −5.5743 (200.13)
29	0.0014; −4.7831 (199.91)	0.2245; 48.6935 (196.47)	0.0284; −77.3649 (198.12)	0.0360; −76.4375 (198.23)
30	0.0622; 46.4446 (198.74)	0.0353; −25.8144 (195.73)	0.0651; 31.8817 (197.12)	0.0892; 28.4361 (197.18)
31	0.0824; −81.8776 (197.96)	0.2398; −37.3949 (194.94)	0.0120; 5.4797 (195.63)	0.0067; 7.2437 (195.66)
32	0.1263; 26.2562 (196.80)	0.0420; 22.7286 (193.55)	0.6532; −87.1356 (195.17)	0.6472; −68.0853 (195.09)
33	0.0484; −0.1379 (196.22)	0.0926; 5.2428 (192.40)	0.0181; 27.9749 (192.64)	0.0201; −6.9820 (192.79)
34	0.1327; −23.4630 (195.23)	0.3011; 178.2169 (190.90)	0.0061; −3.3879 (191.52)	0.0060; −4.3060 (191.42)
35	0.1971; −8.6438 (194.21)	0.0222; 35.4690 (190.19)	0.1609; 160.2055 (190.40)	0.1040; −0.0403 (190.24)
36	0.0645; −22.6358 (193.20)	0.2234; −139.8668 (189.09)	0.0335; −13.9735 (189.30)	0.1384; 129.3356 (189.13)
37	0.0054; −8.0672 (191.44)	0.0043; −3.1161 (187.51)	0.0414; −120.8931 (188.28)	0.0099; −37.8900 (188.68)
38	0.0377; 42.5539 (190.51)	0.0119; −0.9580 (187.41)	0.0138; −28.8825 (188.00)	0.0022; 3.7280 (187.57)
39	0.0004; −0.6415 (189.58)	0.1118; 13.9890 (187.06)	0.0077; −8.0255 (187.28)	0.0092; 7.7285 (187.30)
40	0.1004; −77.1785 (188.75)	0.0394; 54.8622 (185.58)	0.0054; 1.0529 (186.04)	0.0043; 3.0280 (185.91)
41	0.0704; −35.3941 (187.60)	0.0424; −12.1017 (185.48)	0.0033; −3.6904 (185.38)	0.0016; −1.3333 (185.21)
42	0.0198; 56.9509 (187.06)	0.0845; 58.9410 (184.22)	0.0322; 0.6973 (185.32)	0.0278; −15.1748 (185.14)
43	0.0016; 0.9381 (185.16)	0.1059; 2.8409 (183.86)	0.0180; −8.9893 (183.40)	0.0218; −9.4547 (183.41)
44	0.0370; 0.8952 (184.04)	0.0013; 1.3709 (183.16)	0.0106; −14.7676 (183.24)	0.0031; −2.6177 (183.14)
45	0.0054; 3.4690 (183.79)	0.3446; −26.6561 (181.71)	0.1674; 65.6287 (182.30)	0.1494; 61.3233 (182.23)
46	0.3121; 8.4893 (183.44)	0.1212; 102.0818 (180.63)	0.1179; −42.6114 (182.07)	0.1281; −75.6379 (182.02)
47	0.0023; 2.2617 (182.47)	0.0189; 8.4123 (180.55)	0.3750; 29.4981 (181.33)	0.3496; 9.8179 (181.24)
48	0.0023; −4.1615 (181.09)	0.0370; −24.6808 (179.47)	0.0271; −7.5782 (178.57)	0.0146; −10.9430 (178.79)
49	0.0481; −15.7460 (180.96)	0.1650; −173.6329 (178.15)	0.0245; −22.9524 (178.28)	0.0381; −13.0282 (178.53)
50	0.0089; 0.4241 (180.04)	0.0049; −2.1266 (177.76)	0.1181; −65.4649 (177.34)	0.0957; −24.5571 (177.47)

Table S2. *(continued)*

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)			
	(*S*)-**25b.29**	(*S*)-**25b.31**	(*S*)-**25b.33**	(*S*)-**25b.35**
1	0.0007; −1.3559 (346.63)	0.0523; 4.2589 (381.84)	0.0511; 2.9578 (381.75)	0.0525; 1.8554 (380.07)
2	0.0010; −2.6929 (306.39)	0.0019; −2.0840 (340.08)	0.0020; −1.2705 (340.26)	0.0179; −3.6579 (327.79)
3	0.0206; −11.5052 (288.55)	0.0263; 10.6695 (298.56)	0.0263; 11.3463 (298.62)	0.0054; 26.0114 (312.45)
4	0.0214; 14.8718 (279.68)	0.0110; 2.1882 (292.28)	0.0119; 1.0867 (292.11)	0.0154; −11.3507 (287.57)
5	0.0452; −11.3527 (265.76)	0.0458; −39.7747 (284.93)	0.0451; −39.5921 (285.27)	0.0435; −37.7085 (284.75)
6	0.0171; −13.8898 (252.98)	0.1306; 24.2432 (262.56)	0.1358; 23.4017 (261.91)	0.1675; 17.5655 (262.16)
7	0.0024; 6.9031 (251.47)	0.0394; 17.1768 (255.07)	0.0400; 17.6094 (254.96)	0.0145; −7.7584 (255.46)
8	0.0932; 9.2287 (246.68)	0.0325; −9.2970 (249.93)	0.0254; −12.7281 (250.08)	0.0026; −5.8790 (251.56)
9	0.0095; −16.3035 (246.17)	0.1196; −0.8917 (248.21)	0.0924; −67.7225 (248.30)	0.0279; −47.6199 (248.06)
10	0.4015; −0.1763 (244.02)	0.0252; −6.0547 (247.03)	0.0930; 76.1557 (246.88)	0.1710; 87.1952 (246.79)
11	0.2954; 23.6753 (239.51)	0.1176; 6.6382 (245.84)	0.0790; −14.9219 (245.68)	0.0789; −23.3382 (246.32)
12	0.0041; −4.7707 (235.00)	0.0397; 112.5782 (242.77)	0.0414; 114.2299 (242.30)	0.0145; 11.9272 (244.24)
13	0.0501; −30.1044 (231.79)	0.0056; 7.8266 (236.69)	0.0055; 7.7325 (237.08)	0.0145; −18.0971 (239.43)
14	0.0217; 15.7490 (229.15)	0.1179; −59.7116 (229.19)	0.1136; −46.3700 (229.53)	0.0083; −7.9648 (233.33)
15	0.0050; 2.9292 (223.55)	0.0520; 20.0964 (228.24)	0.0545; 5.4400 (228.06)	0.1490; 30.4176 (228.14)
16	0.0075; 2.2653 (222.74)	0.0052; −0.4208 (225.39)	0.0044; 0.2344 (225.55)	0.0469; 5.2233 (223.50)
17	0.0023; 5.8133 (215.29)	0.0741; 34.5581 (221.08)	0.0726; 31.9756 (221.35)	0.1772; 132.4098 (222.12)
18	0.0979; 29.8806 (213.32)	0.0218; −32.8565 (218.64)	0.0245; −25.4960 (218.16)	0.0212; 39.3107 (216.10)
19	0.0577; −8.2231 (208.67)	0.0079; 23.6962 (216.59)	0.0078; 33.2670 (216.24)	0.0262; −81.2074 (215.60)
20	0.0930; −138.3122 (206.67)	0.0036; 5.0949 (214.98)	0.0039; 4.8685 (215.01)	0.0074; −14.8626 (215.03)
21	0.0388; −0.6440 (206.04)	0.0856; −110.0455 (213.55)	0.0767; −113.2972 (213.22)	0.0303; −32.7555 (214.24)
22	0.0907; 230.3022 (204.43)	0.1232; −71.1590 (210.58)	0.1247; −66.9521 (210.43)	0.0167; −17.7070 (210.70)
23	0.0212; −9.8725 (202.39)	0.0378; −0.1175 (209.07)	0.0342; −13.3293 (208.93)	0.0335; 8.0576 (208.97)
24	0.0389; 8.7184 (202.10)	0.0126; 7.6518 (208.50)	0.0178; 17.9836 (208.45)	0.0141; −4.8645 (207.45)
25	0.0096; −27.7595 (201.37)	0.0163; −19.2044 (205.25)	0.0124; −16.5523 (205.00)	0.0338; 26.3361 (206.15)
26	0.0119; −35.2246 (200.02)	0.0340; 1.8867 (203.60)	0.0348; −0.0300 (203.40)	0.0100; 3.8343 (203.97)
27	0.0301; −10.1209 (198.18)	0.0032; −8.4849 (201.54)	0.0033; −10.6278 (201.56)	0.0375; 33.7261 (203.74)
28	0.1255; −93.3192 (196.88)	0.0067; −4.6512 (201.35)	0.0060; −6.4584 (201.22)	0.0007; 2.8288 (201.67)
29	0.2908; 62.0258 (196.33)	0.0152; 1.4637 (198.47)	0.0117; 2.0564 (198.66)	0.0004; −0.9870 (200.58)
30	0.0310; −14.7084 (195.70)	0.0367; 12.7568 (197.52)	0.0442; 15.1066 (197.61)	0.0459; 32.5401 (198.50)
31	0.2373; −32.9992 (194.78)	0.0536; 37.4764 (197.03)	0.0594; 41.6792 (197.10)	0.0057; −13.8104 (197.73)
32	0.0525; 23.0230 (193.79)	0.1448; 44.8427 (195.76)	0.1375; 49.5957 (195.72)	0.2075; 16.2846 (196.03)
33	0.1208; 30.7833 (192.59)	0.3045; −100.0070 (195.06)	0.3221; −153.7425 (195.14)	0.2985; −109.6702 (195.28)
34	0.2343; −60.2772 (190.70)	0.0203; −2.6653 (194.34)	0.0352; 22.3614 (194.03)	0.1218; −83.5352 (193.43)
35	0.1245; 92.1092 (189.41)	0.0901; −67.5313 (193.36)	0.0223; 18.2408 (193.84)	0.0787; 18.9356 (192.43)
36	0.1188; 34.8231 (189.29)	0.0268; −2.8730 (192.71)	0.0832; −8.2102 (192.85)	0.1128; 120.7656 (191.66)
37	0.0061; −7.3936 (187.61)	0.0835; 74.2224 (191.92)	0.0017; −1.4556 (191.40)	0.0014; 0.5580 (190.31)
38	0.0292; 20.4171 (187.10)	0.0009; −0.9755 (191.04)	0.0278; −31.3240 (190.55)	0.0007; 0.0345 (189.45)
39	0.1036; −8.2666 (186.95)	0.0681; 99.1003 (189.02)	0.1933; 162.4254 (189.29)	0.0364; −47.7309 (189.23)
40	0.0489; 50.7570 (185.51)	0.1070; 53.9395 (188.24)	0.0349; 2.8599 (188.22)	0.0946; −59.9943 (188.30)
41	0.0426; −0.2963 (185.38)	0.0274; 1.9924 (187.99)	0.0461; −26.3563 (187.76)	0.0318; 26.9208 (187.63)
42	0.0250; 27.0765 (184.33)	0.0375; −6.9751 (187.66)	0.0227; 16.6724 (187.06)	0.0052; 18.3199 (187.16)
43	0.1525; 33.1982 (183.90)	0.0263; −41.9277 (186.33)	0.0106; −34.8948 (186.54)	0.0295; −42.2952 (186.64)
44	0.0018; 0.7544 (183.17)	0.0057; −4.1514 (185.86)	0.0017; 2.8511 (185.88)	0.0013; −0.6022 (185.75)
45	0.3483; −32.1379 (181.69)	0.1501; −20.0946 (184.57)	0.1681; −59.0485 (184.20)	0.0155; −25.6234 (183.80)
46	0.0002; 0.1175 (180.78)	0.0109; −31.8625 (183.37)	0.0082; −32.7303 (183.60)	0.0015; 0.2169 (183.05)
47	0.1375; 95.3615 (180.61)	0.0034; −1.7179 (182.15)	0.0015; 0.9663 (182.36)	0.1605; −149.5012 (181.84)
48	0.0360; −35.0554 (179.46)	0.0591; −49.3650 (181.12)	0.0441; −42.7860 (181.20)	0.2571; −1.5988 (181.52)
49	0.1414; −156.0378 (178.15)	0.1053; 60.8966 (180.18)	0.1160; 79.0890 (180.10)	0.2198; 33.6652 (181.07)
50	0.0276; −29.1457 (178.00)	0.0033; 0.2950 (180.07)	0.0034; 0.0192 (179.95)	0.0070; 12.7839 (179.54)

Table S3. X-ray Crystallographic Data Collection and Refinement Statistics, *zf*HDAC6–6h Complex

Data collection[a]	
Space group	$P2_1$
a,b,c (Å)	48.3, 108.1, 74.4
α, β, γ (°)	90.00, 90.01, 90.00
R_{merge}[b]	0.174 (0.767)
R_{pim}[c]	0.112 (0.498)
$CC_{1/2}$[d]	0.982 (0.662)
Redundancy	3.4 (3.2)
Completeness (%)	96.2 (95.8)
I/σ	5.6 (1.3)
Refinement[a]	
Resolution (Å)	64.3-2.04 (2.11-2.04)
No. reflections	46680 (4751)
R_{work}/R_{free}[e]	0.195/0.235 (0.258/0.314)
No. atoms[f]	
Protein	5481
Ligand	66
Solvent	224
Average B factors (Å²)	
Protein	24
Ligand	36
Solvent	25
R.m.s. deviations	
Bond lengths (Å)	0.007
Bond angles (°)	0.9
Ramachandran plot[g]	
Favored	95.63
Allowed	4.08
Outliers	0.28
PDB code	6V79

[a]Values in parentheses refer to the highest-resolution shell indicated. [b]$R_{merge} = \sum_{hkl}\sum_i|I_{i,hkl} - \langle I\rangle_{hkl}|/\sum_{hkl}\sum_i I_{i,hkl}$, where $\langle I\rangle_{hkl}$ is the average intensity calculated for reflection *hkl* from replicate measurements. [c]$R_{p.i.m.} = (\sum_{hkl}(1/(N-1))^{1/2}\sum_i|I_{i,hkl} - \langle I\rangle_{hkl}|)/\sum_{hkl}\sum_i I_{i,hkl}$, where $\langle I\rangle_{hkl}$ is the average intensity calculated for reflection *hkl* from replicate measurements and N is the number of reflections. [d]Pearson correlation coefficient between random half-datasets. [e]$R_{work} = \sum||F_o| - |F_c||/\sum|F_o|$ for reflections contained in the working set. $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes, respectively. R_{free} is calculated using the same expression for reflections contained in the test set held aside during refinement. [f]Per asymmetric unit. [g]Calculated with MolProbity.

Description of the interaction retrieved by docking studies of compounds 6a-m.

For both enantiomers of compound **6a** (**Figure S3**) in HDAC1, in addition to the metal coordination bond, the hydroxamate moiety targets G149 and Y303. The benzyl linker establishes a π-π stacking with H141 and F205 for one enantiomer, (*S*)-**6a**, while only with H141 for the (*R*)-enantiomer. The cap-group of the (*R*)-**6a** stacks with Y204 and forms hydrophobic contacts mainly with L271. Compound **6b** presented a *p*-Cl on the phenyl of the corresponding **6a**. As reported in Figure S4, the *S*-enantiomer docked into HDAC6, interacts in a similar fashion of (*S*)-**6a** with the exclusion of the interaction with F679. The *R*-enantiomer, in addition to the mentioned contacts, established a π-π stacking with F620. The analysis of docking output of **6b** into HDAC1 did not reveal any difference with that described for **6a** (IC_{50} values: HDAC1 = 3650 nM; HDAC6 = 164.8 nM). The introduction of *m*-Cl on the phenyl substituent of **6a** led to compound **6c**. This compound establishes similar contacts into HDAC1 and HDAC6 (Figure S5) to those observed for the previously described derivatives. Accordingly, the activity reported for compound **6c** against HDACs maintained the same trends with a micromolar activity against HDAC1 and a nanomolar potency on HDAC6 (IC_{50} values: HDAC1 = 8100 nM; HDAC6 = 110.6 nM). Introduction of a *p*-F-phenyl at C2 (**6e**) or a pyridin-3-yl (**6f**) confirmed the binding mode and potency at HDAC1 and HDAC6 as for other analogues (Figure S7 and S8; **6e**: IC_{50} values: HDAC1 = 6160 nM and HDAC6 = 141.9 nM; **6f**: IC_{50} values: HDAC1 = 7600 nM and HDAC6 = 111.7 nM). Computational investigations were performed using the crystal structure of *zf*HDAC6 in comparison with *h*HDAC6. Generally, for the selected compounds we observed a common trend in their binding mode with the HDAC6 enzyme, establishing higher number of contacts compared to HDAC1. In particular, as refers to the crystallized compound, (*S*)-(−)-**6h**, when docked into *h*HDAC6 and *zf*HDAC6 (**Figure S2**) it similarly accommodated in both enzymes. We only noted slight differences due to the different aminoacidic composition of the binding sites (residues D567, T678 and M682 in *h*HDAC6 are replaced by N530, A641, and N645 in *zf*HDAC6, respectively). The presence of M682 in *h*HDAC6 determines only a slightly different orientation of the cap-group with respect to the crystal structure of **6h** in complex with *zf*HDAC6 and the docked pose of (*S*)-(−)-**6h** into *zf*HDAC6. In both enzymes we found a similar orientation of the hydroxamate moiety of the ligand, indeed the carbonyl function chelates the zinc ion, as found in previous docking calculations.[28–30] When the docking output was compared to the X-ray structure of **6h** with *zf*HDAC6 an alternate mechanism of metal coordination was observed *via* the oxygen of the *N*-hydroxyl group responsible for metal coordination/interaction.

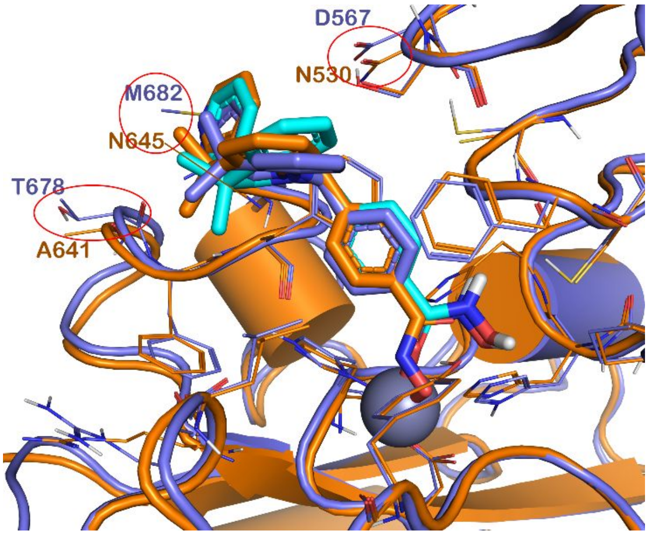


Figure S2. Comparison among **(S)-(-)-6h-***zf*HDAC6 crystal structure (orange sticks and cartoon, respectively), **(S)-(-)-6h** docked into *zf*HDAC6 in cyan sticks and **(S)-(-)-6h** docked into *h*HDAC6 (PDB ID 5EDU) as already reported in Figure 3 (purple sticks and cartoon, respectively). Binding site residues are represented by lines and the different residues between *zf*HDAC6 (orange lines) and *h*HDAC6 (purple lines) are rounded by red circles and labelled. Zn^{2+} is represented by a gray sphere.

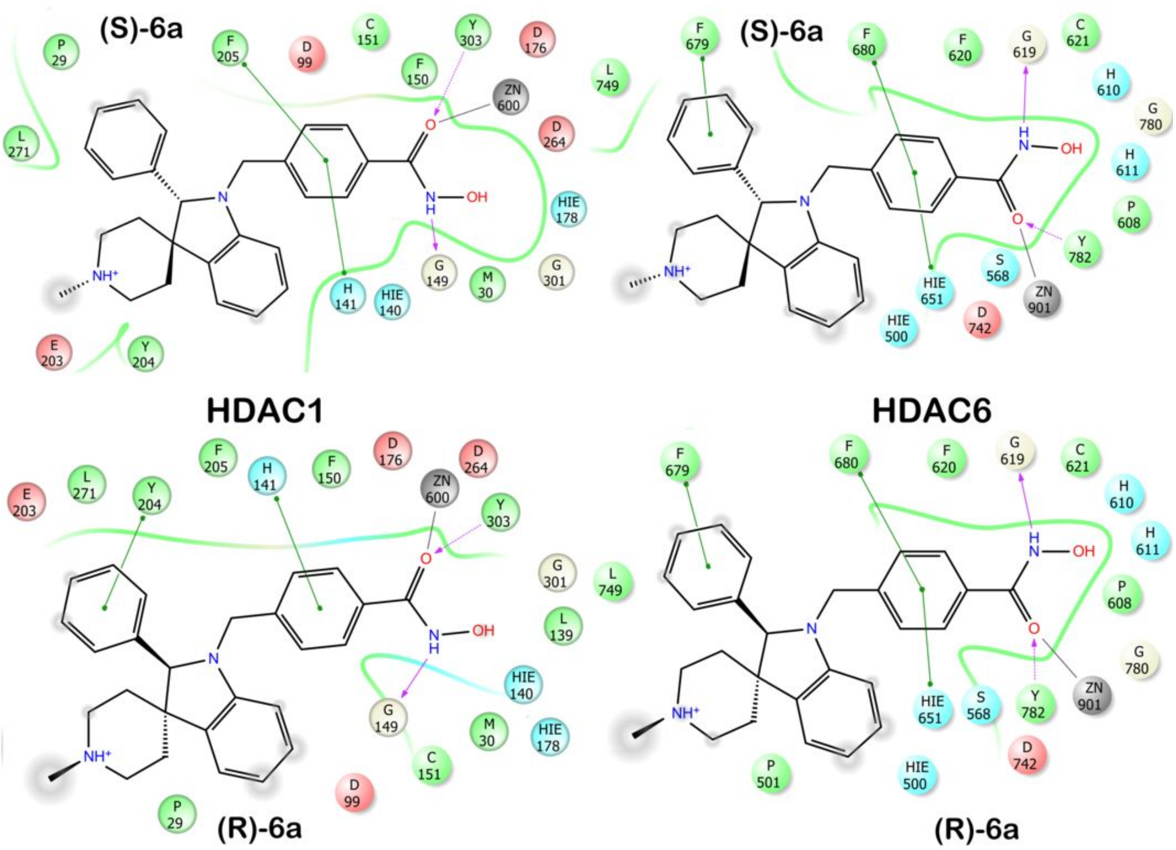


Figure S3. Ligand-interaction diagram of both enantiomers of compound **6a** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

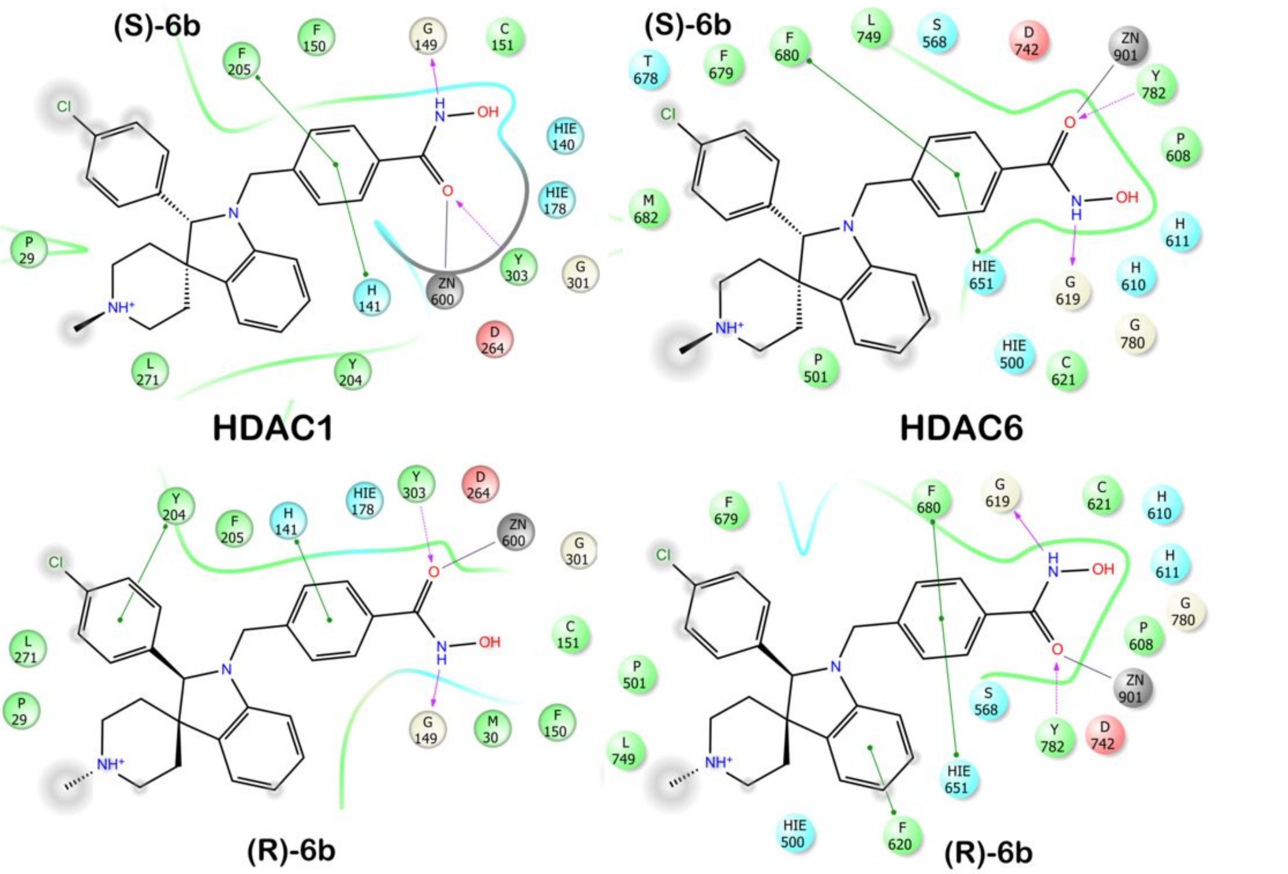


Figure S4. Ligand-interaction diagram of both enantiomers of compound **6b** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

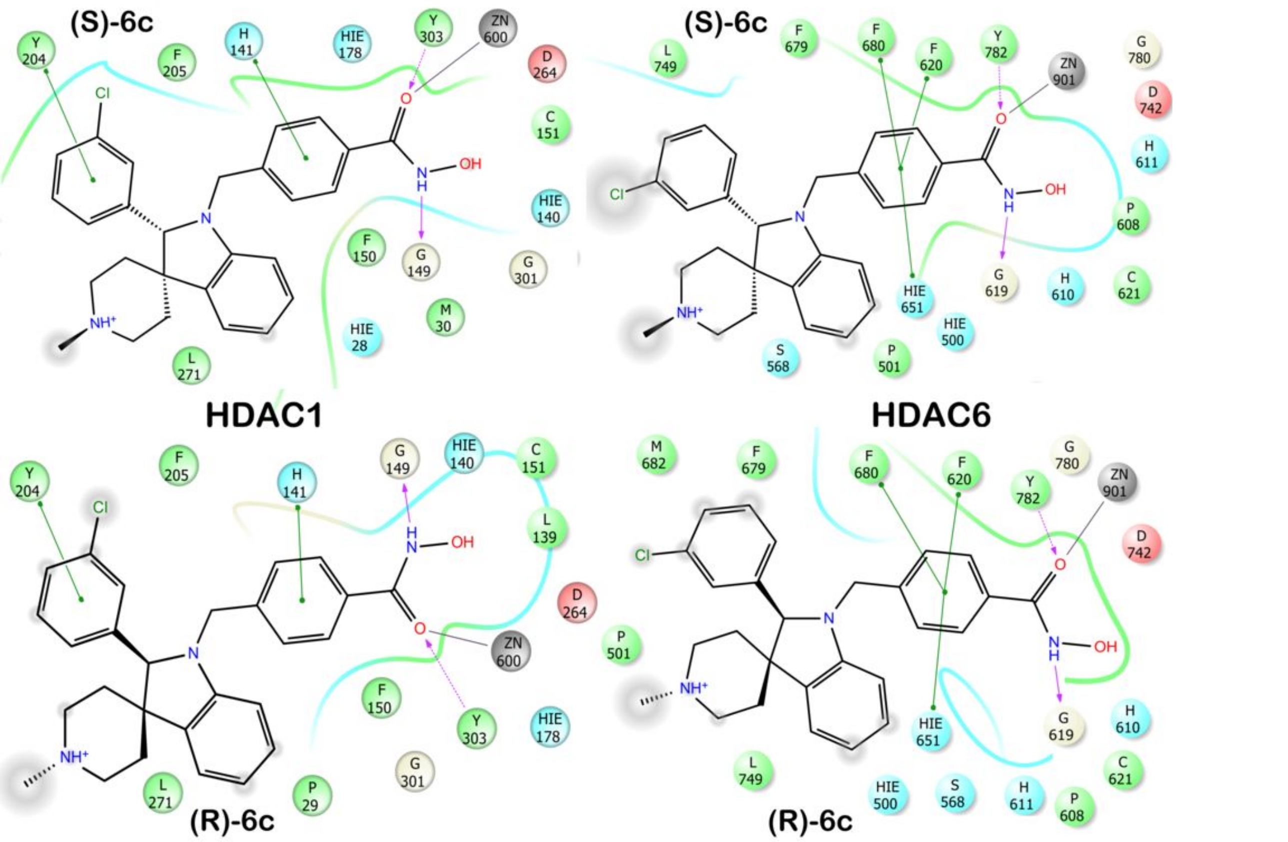


Figure S5. Ligand-interaction diagram of both enantiomers of compound **6c** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

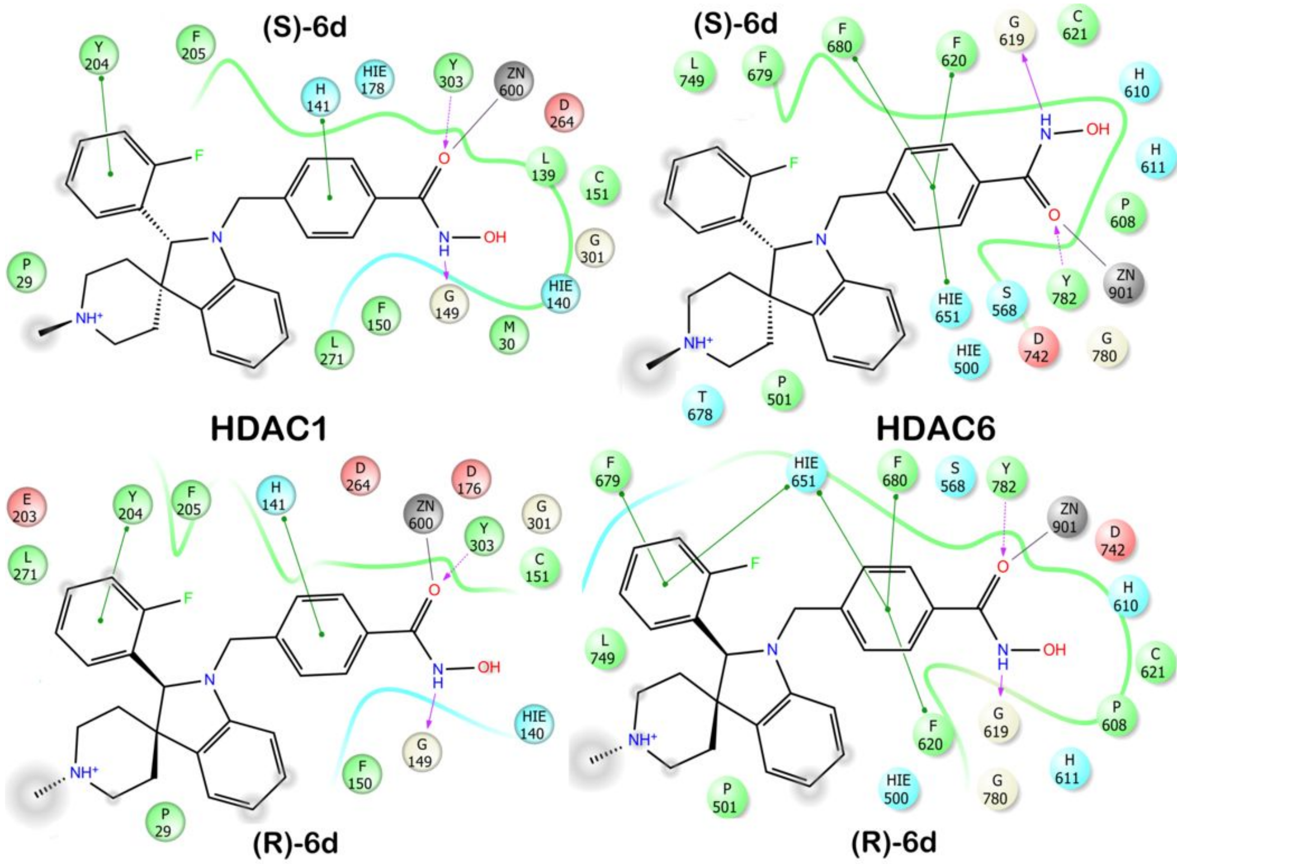


Figure S6. Ligand-interaction diagram of both enantiomers of compound **6d** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

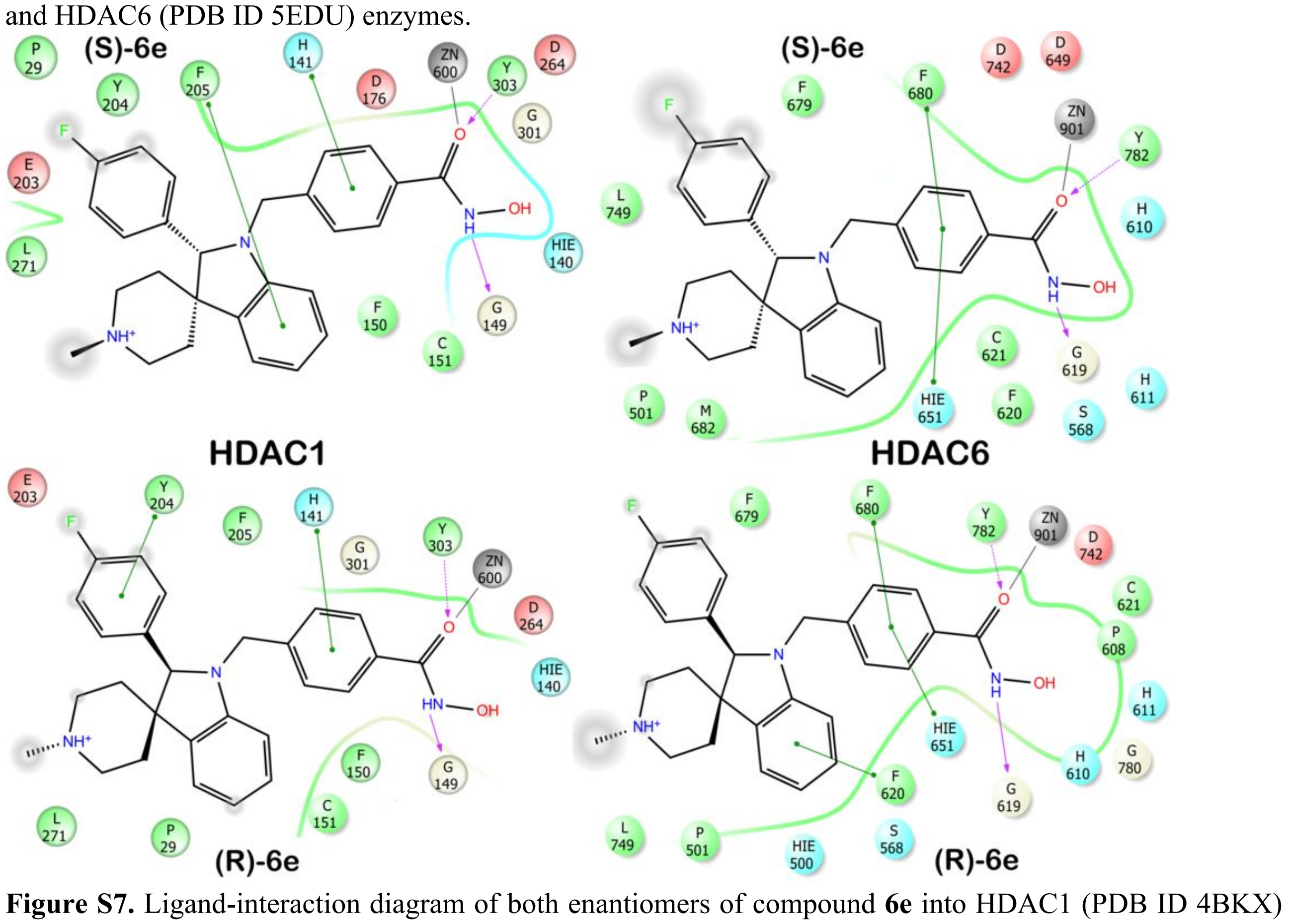


Figure S7. Ligand-interaction diagram of both enantiomers of compound **6e** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

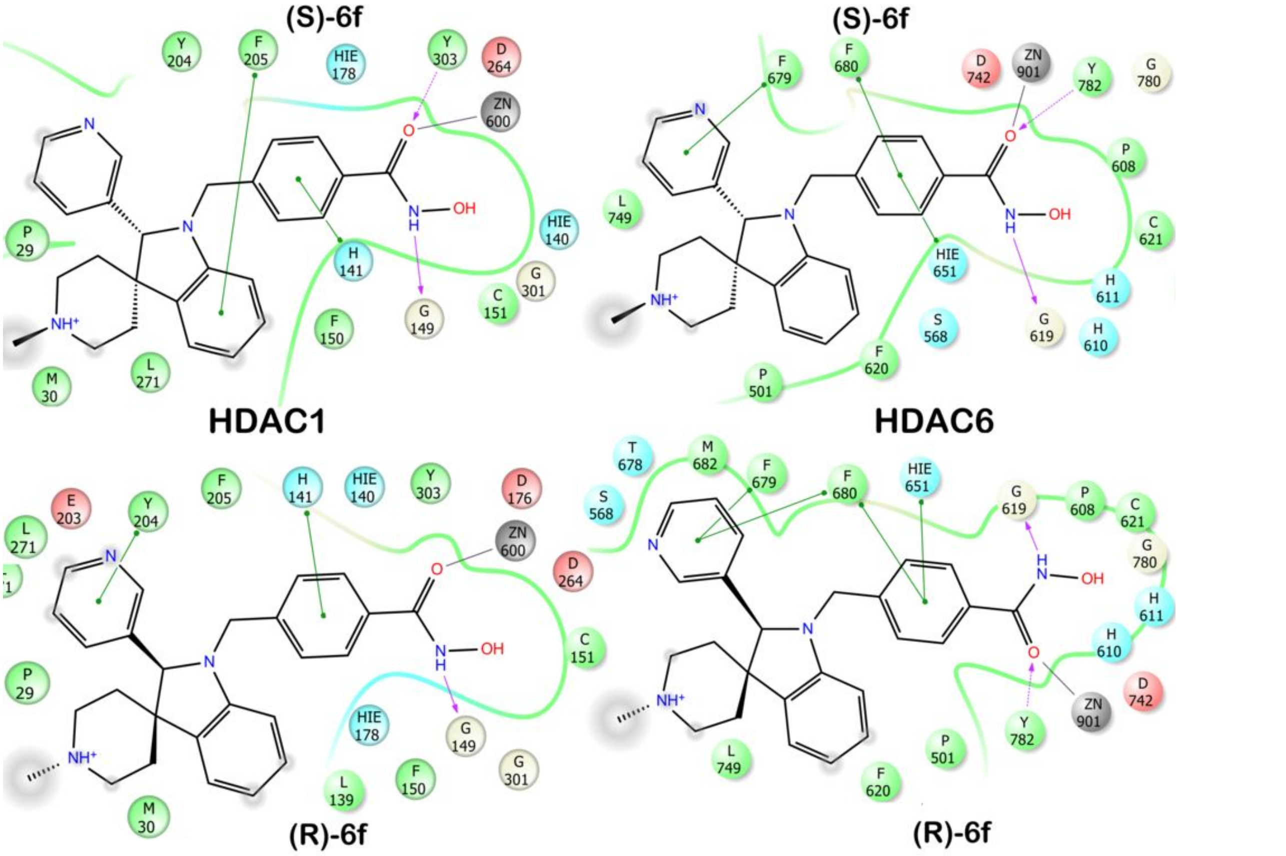


Figure S8. Ligand-interaction diagram of both enantiomers of compound **6f** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

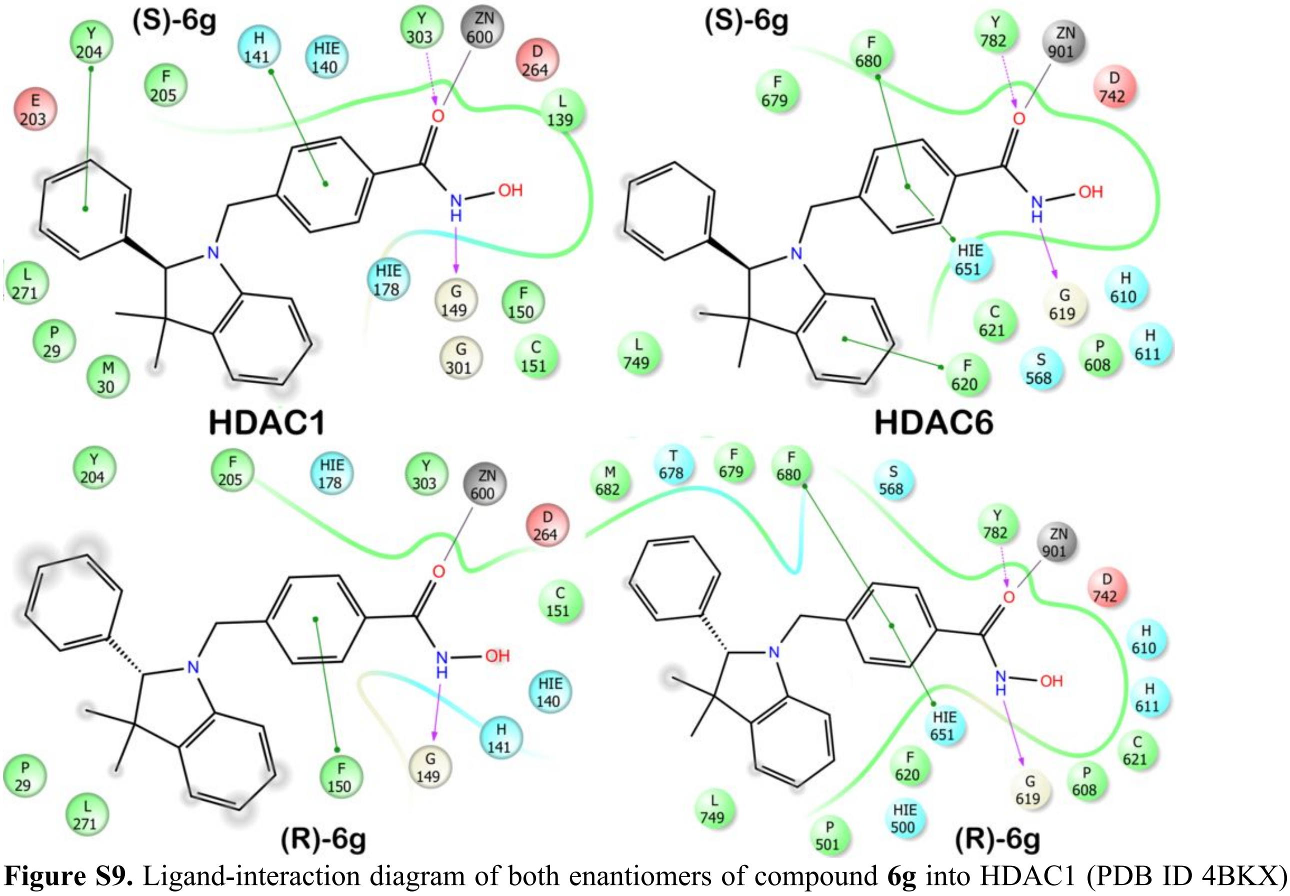


Figure S9. Ligand-interaction diagram of both enantiomers of compound **6g** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

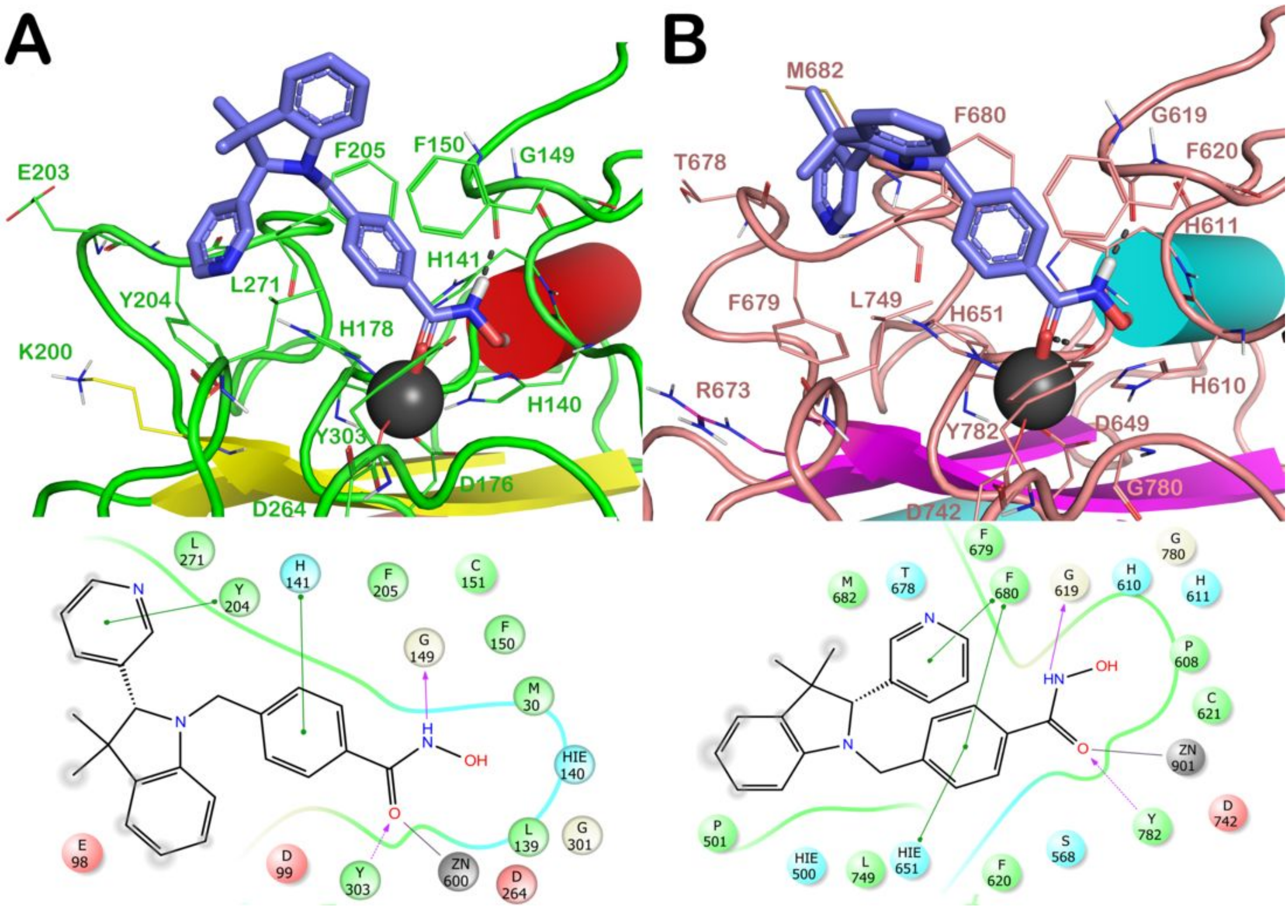


Figure S10. Docked poses of **(R)-(-)-6h** (light blue sticks) into HDAC1 (PDB ID 4BKX; panel A) and HDAC6 (PDB ID 5EDU; panel B). The residues in the active sites are represented as line and the proteins are represented as cartoon. Zn^{2+} is represented as a gray sphere. H-bonds are represented as black dotted lines, while red stick represents the metal coordination bond.

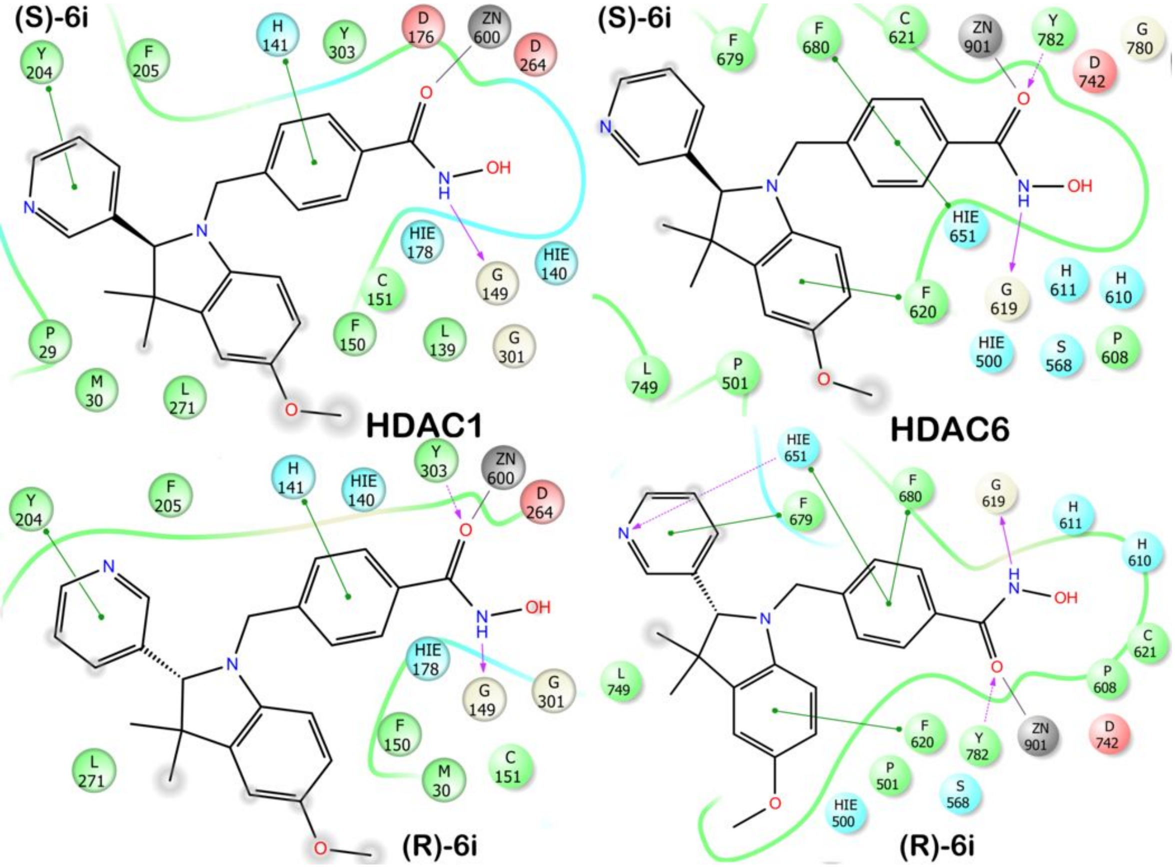


Figure S11. Ligand-interaction diagram of both enantiomers of compound **6i** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

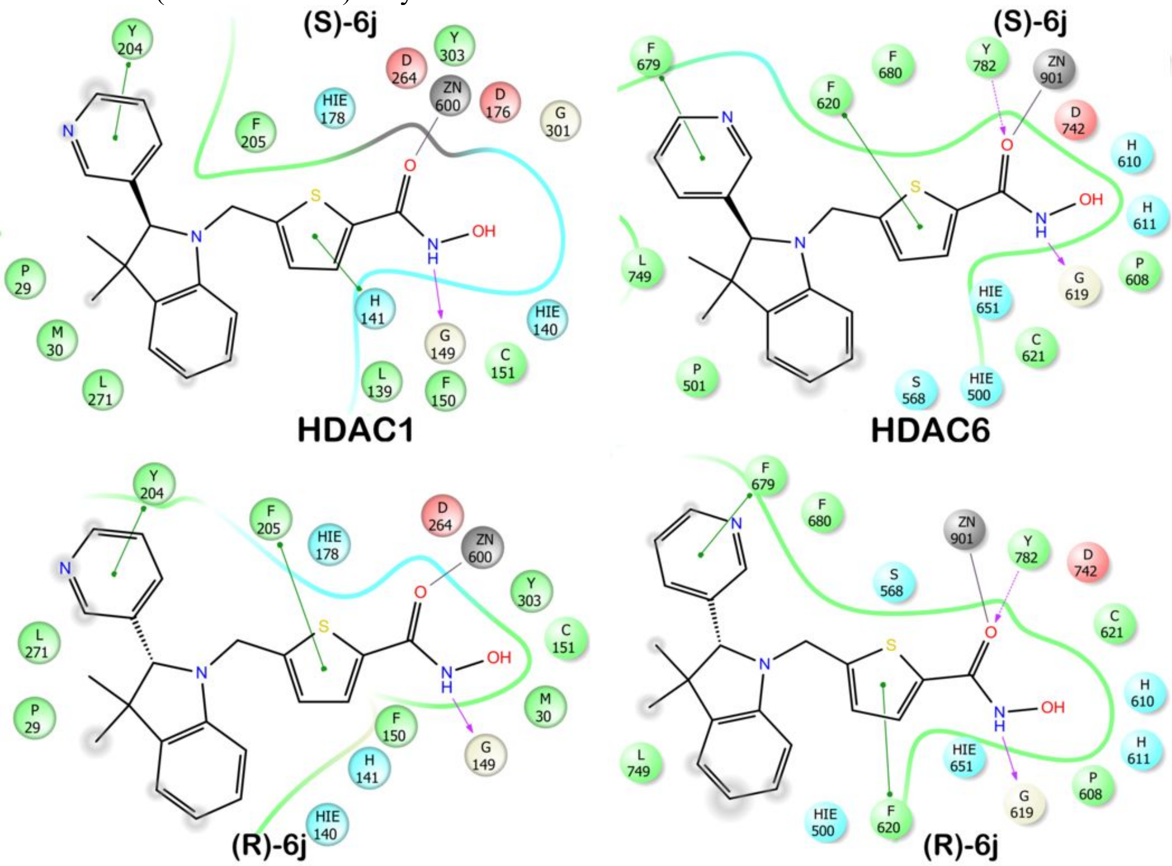


Figure S12. Ligand-interaction diagram of both enantiomers of compound **6j** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

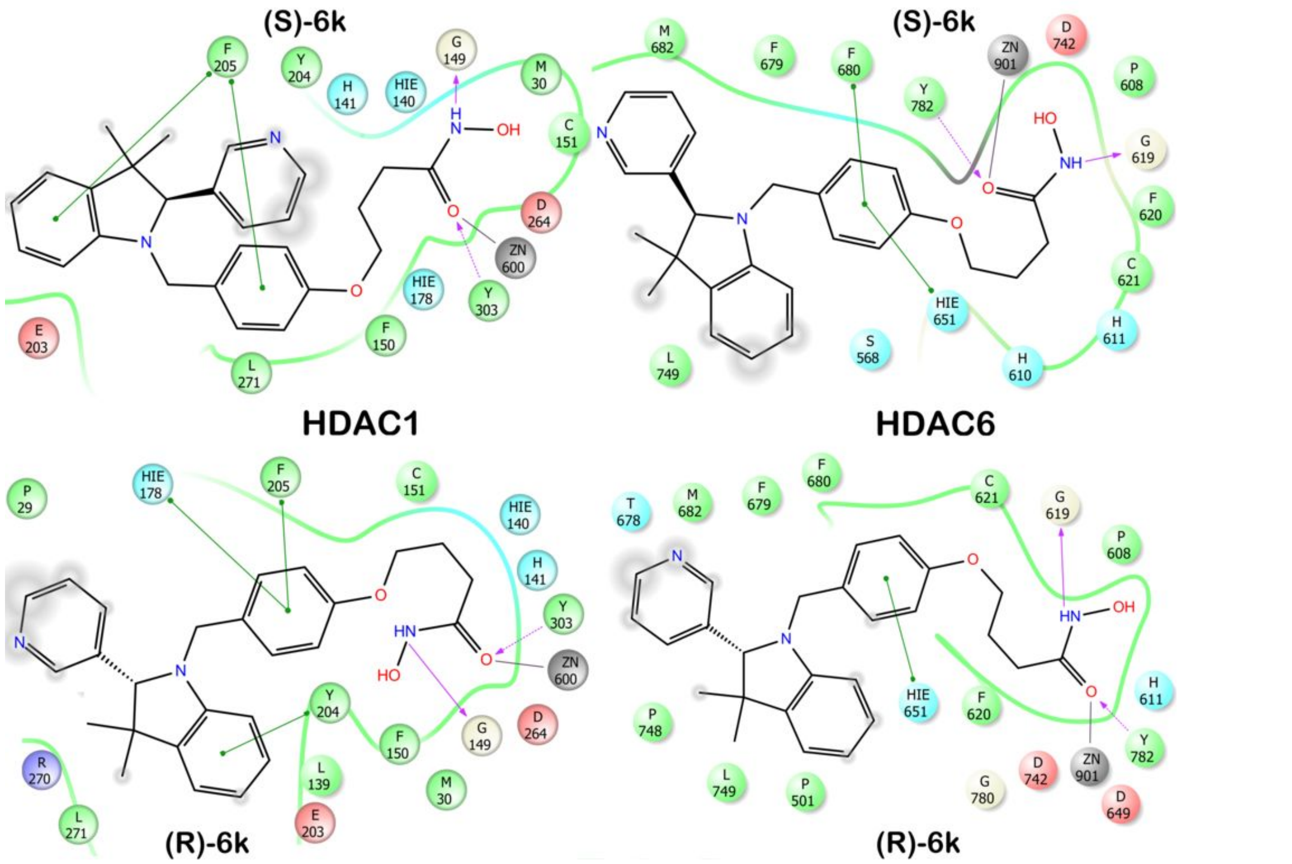


Figure S13. Ligand-interaction diagram of both enantiomers of compound **6k** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU enzymes.

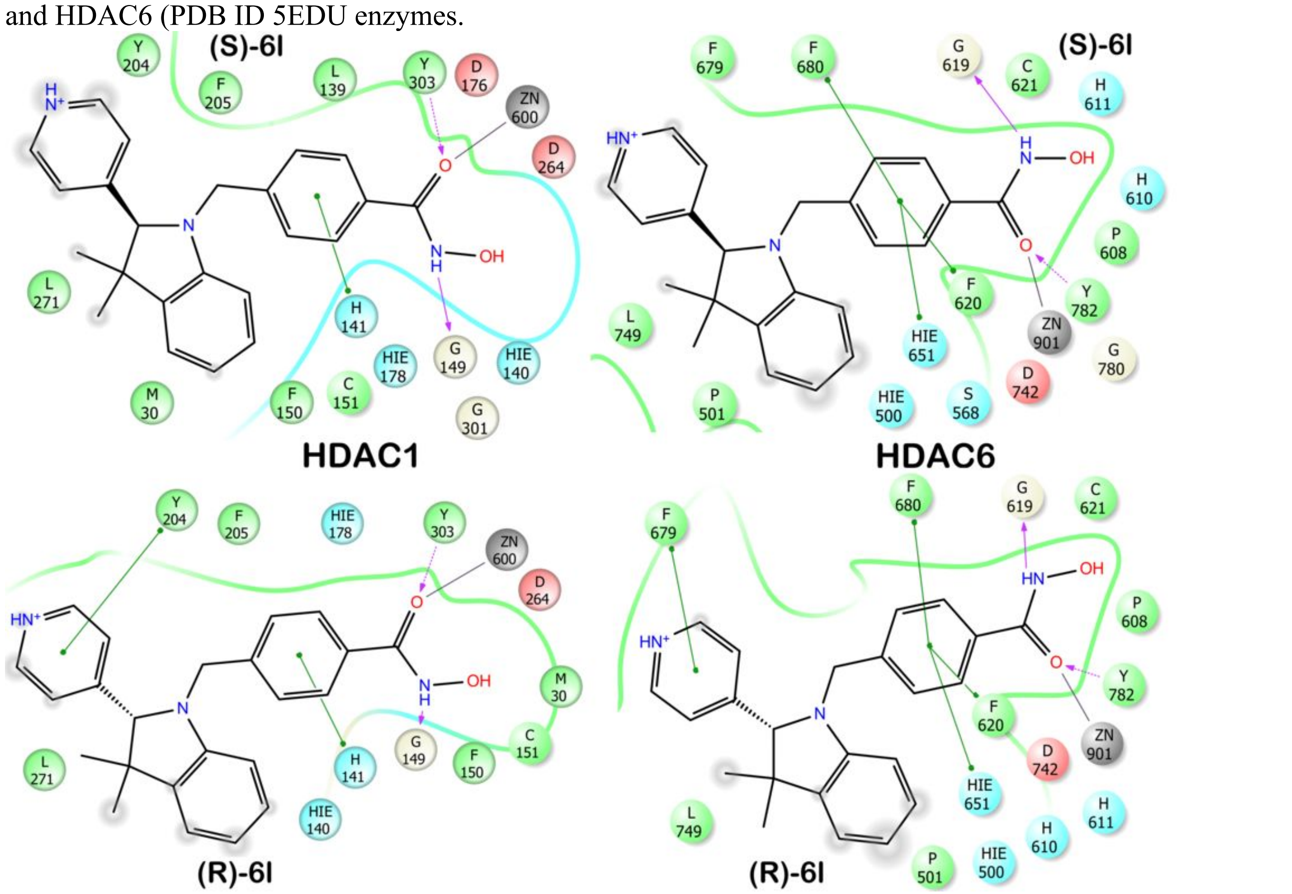


Figure S14. Ligand-interaction diagram of both enantiomers of compound **6l** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

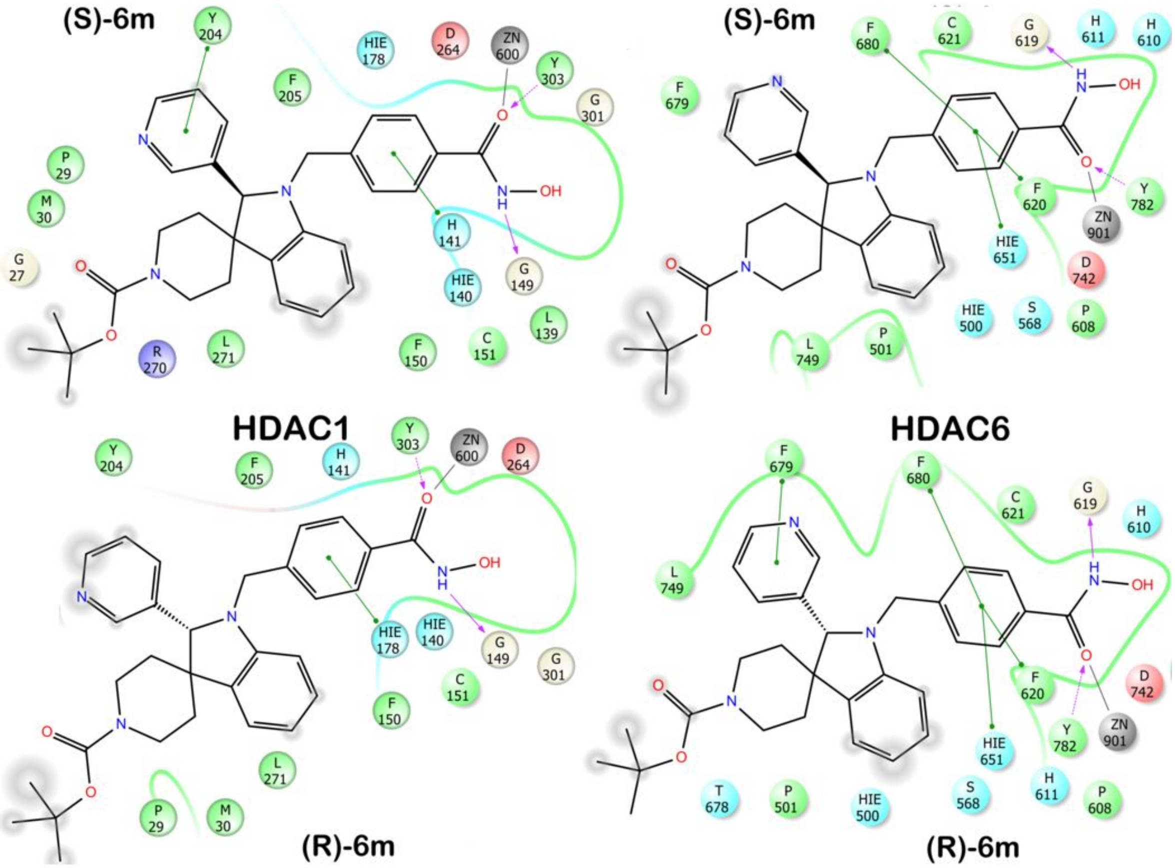


Figure S15. Ligand-interaction diagram of both enantiomers of compound **6m** into HDAC1 (PDB ID 4BKX) and HDAC6 (PDB ID 5EDU) enzymes.

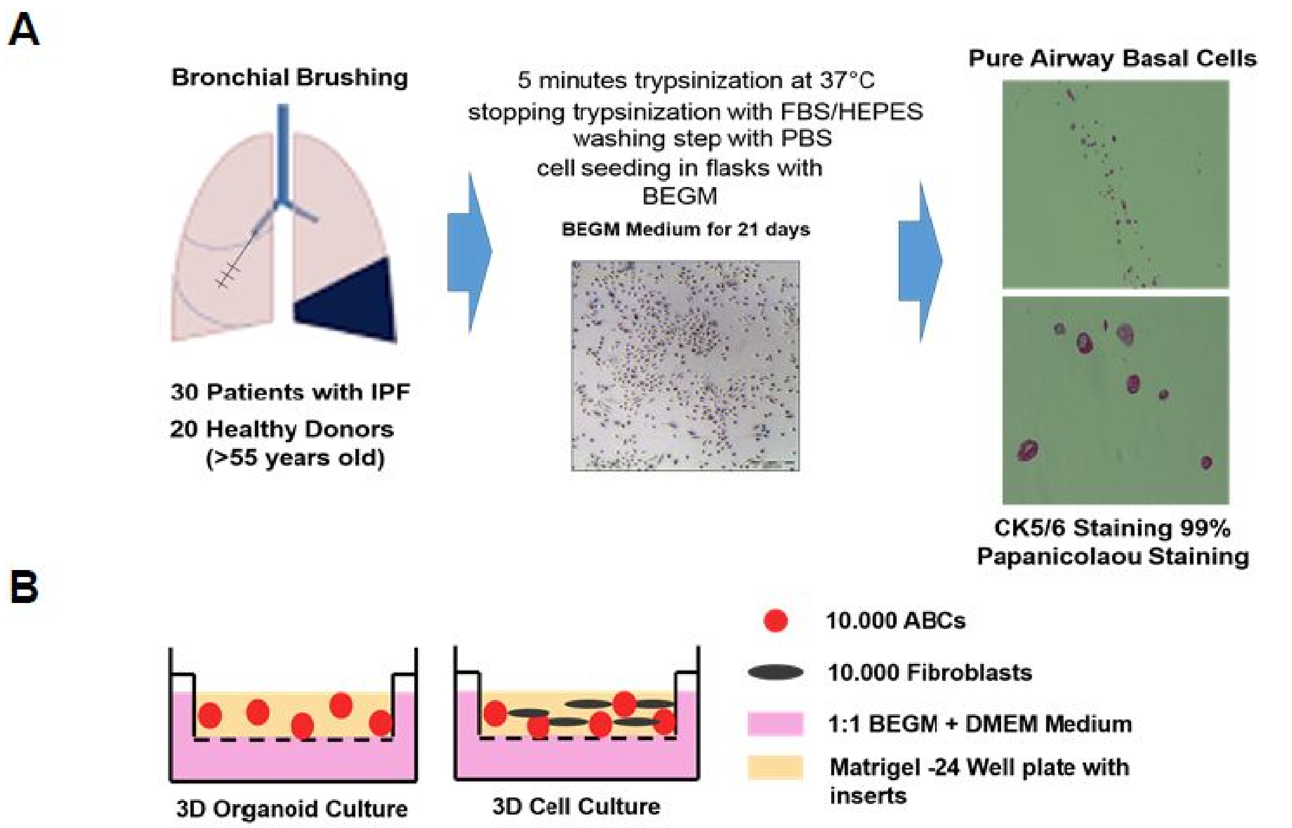


Figure S16. Isolation of human airway basal cells (ABCs). **Panel A**: During routine diagnostic work-up of IPF patients a bronchoscopy with brushing of the distal bronchi of the lower lobe was performed. Thereby bronchial epithelial cells are harvested from the small airways and immediately placed in lukewarm BEGM medium. Harvested cells were centrifuged and the cell pellet trypsinized for 5 minutes at 37 °C. Next, trypsinization was stopped by FBS/HEPES and cells centrifuged again. After washing the cells with PBS, the cells were incubated in BEGM medium for 21 days at 37 °C. This procedure resulted in a pure outgrowth of airway basal cells as tested by CK5/6 immunocytology and papanicolaou staining. **Panel B**: The isolated ABCs were used for multiple experiments including a 3D organoid model. This model is widely used in cancer and developmental biology. Therefor 10.000 ABCs were placed in 50 µl Corning® Matrigel® and pipetted in an insert of a 24 well plate. Next, Corning® Matrigel® was stiffened through incubation for 30 min. 700 µl of BEGM and DMEM (1:1) were then added to the wells.

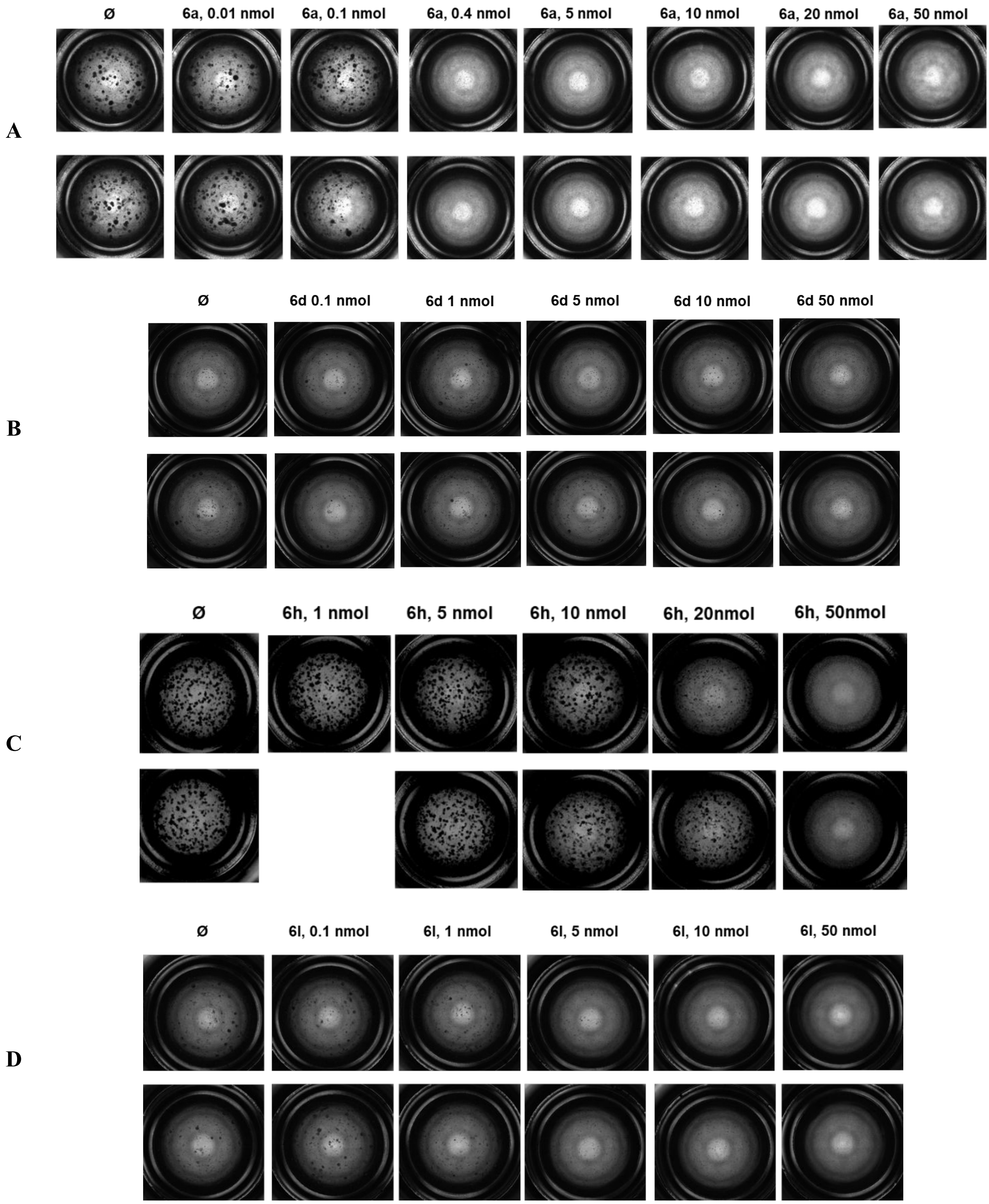
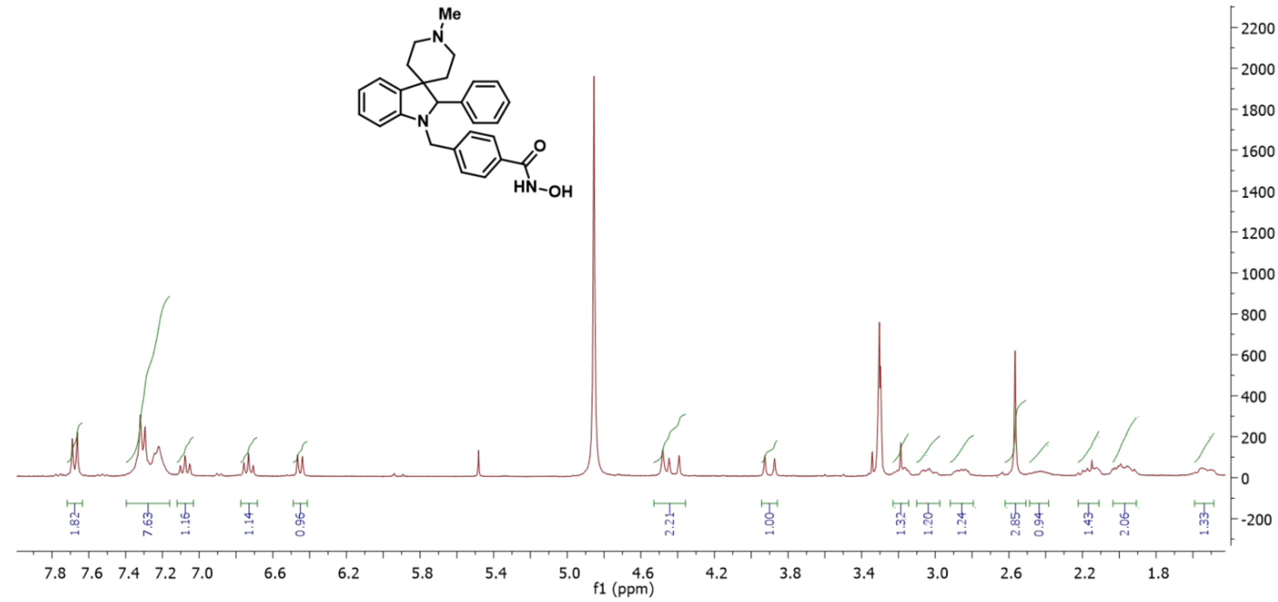
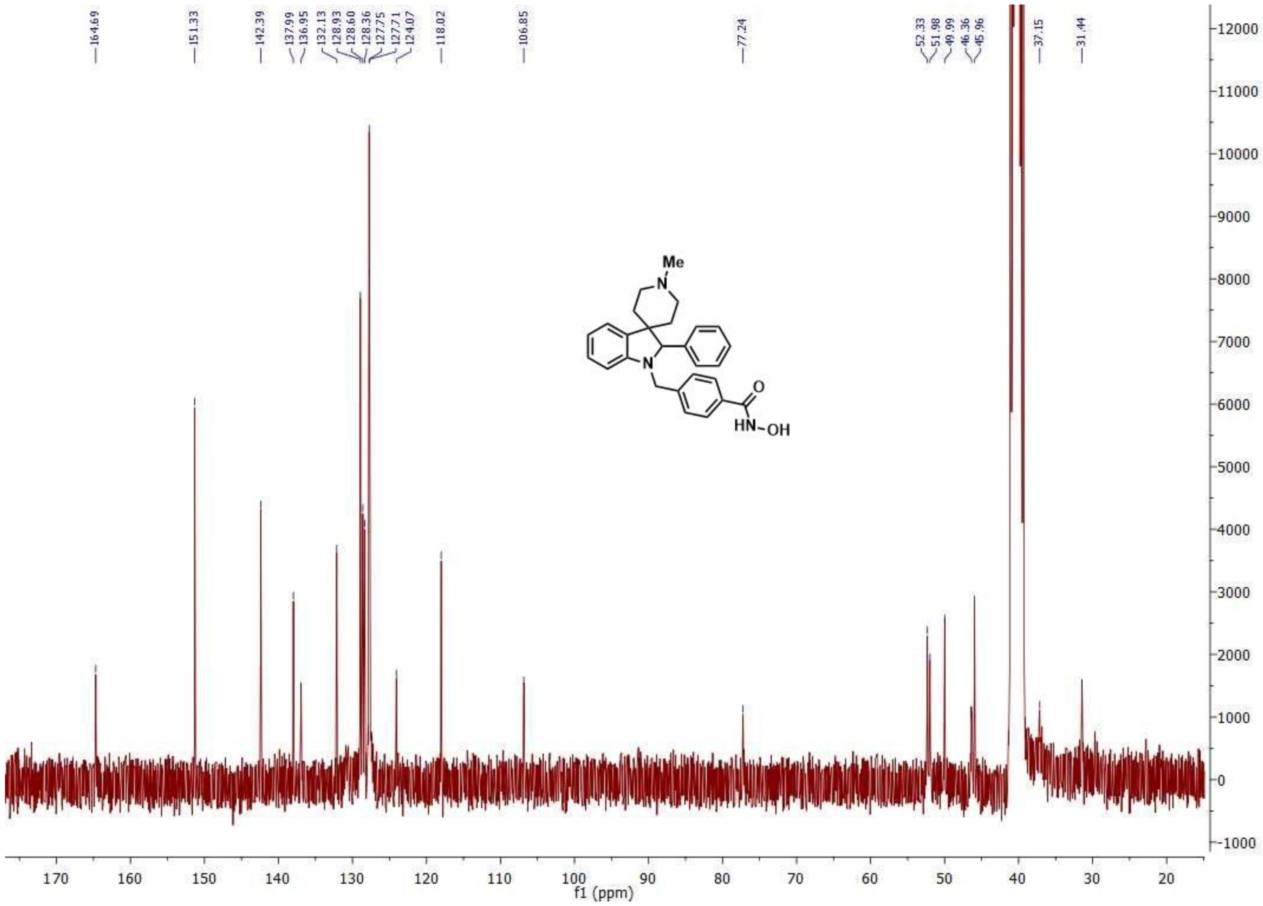


Figure S17. Bronchosphere generation blocked by compounds 6a, 6d, 6h and 6l. Bright field microscopy mosaic images were taken with an Observer.Z1 Zeiss microscope and exemplary registrations of the experiments of 4 different HDAC6 inhibitors are depicted.

^{1}H , ^{13}C NMR spectra and HPLC purity of final compounds (±)-6a-m

6a





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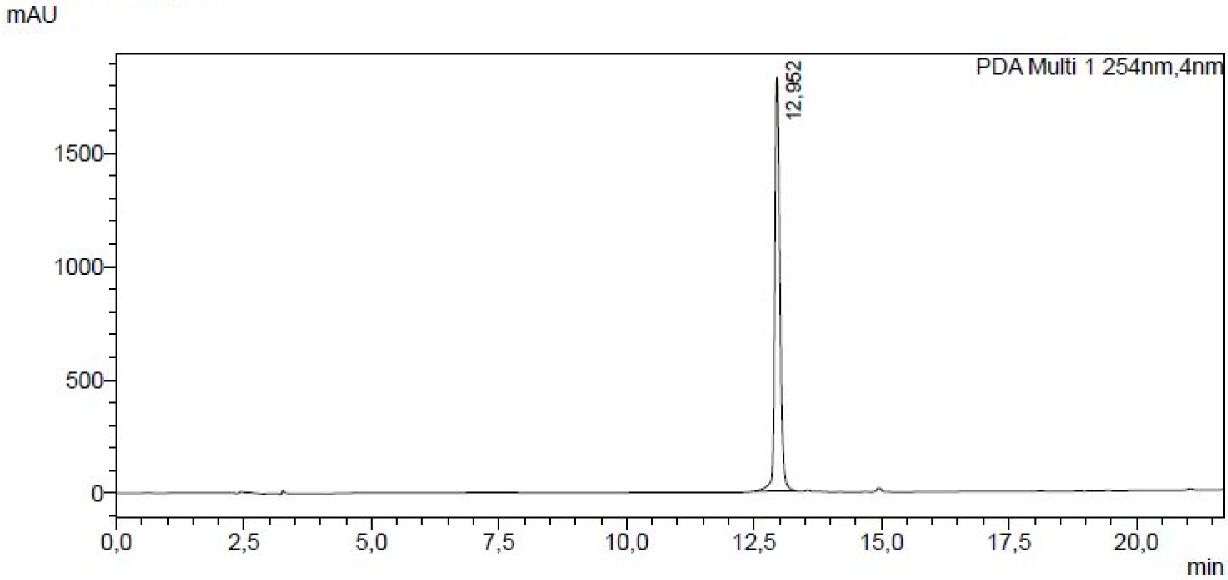

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PDA Ch1 254nm

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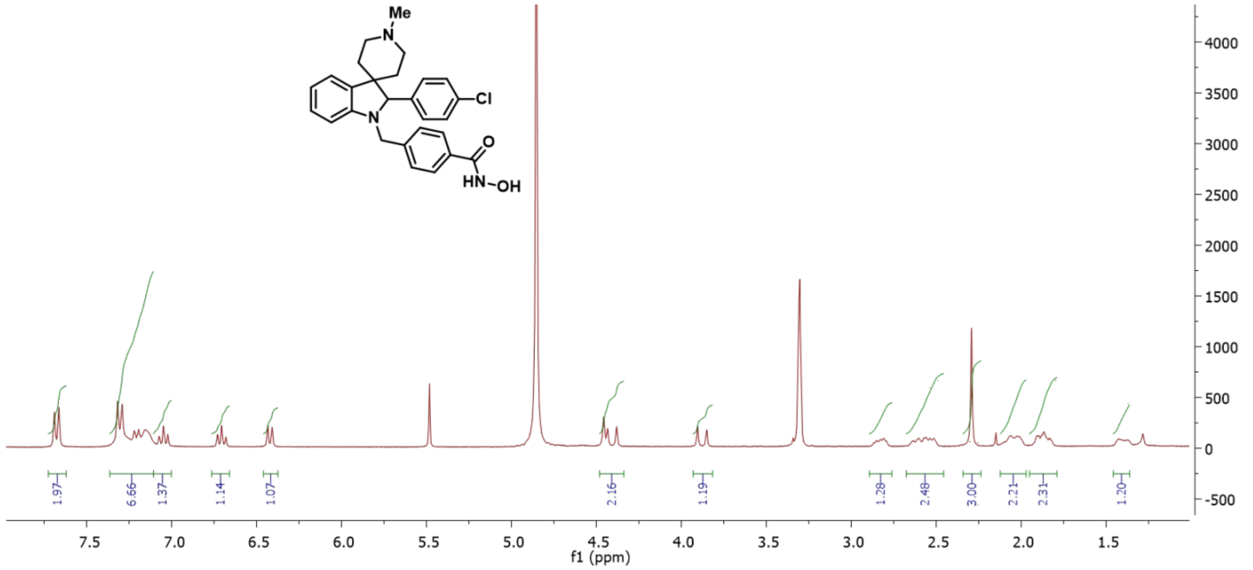
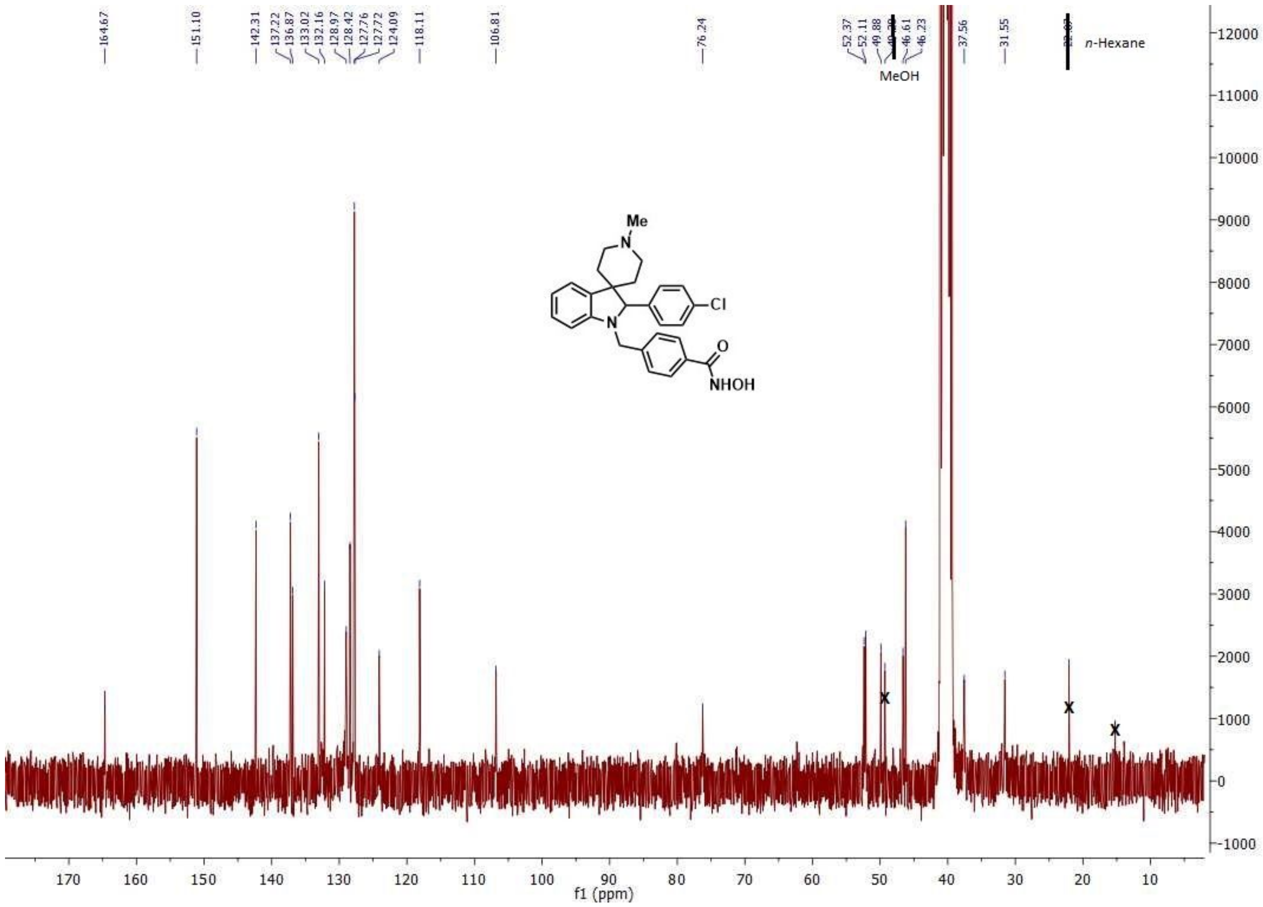
Total		12827040	100,000

6b





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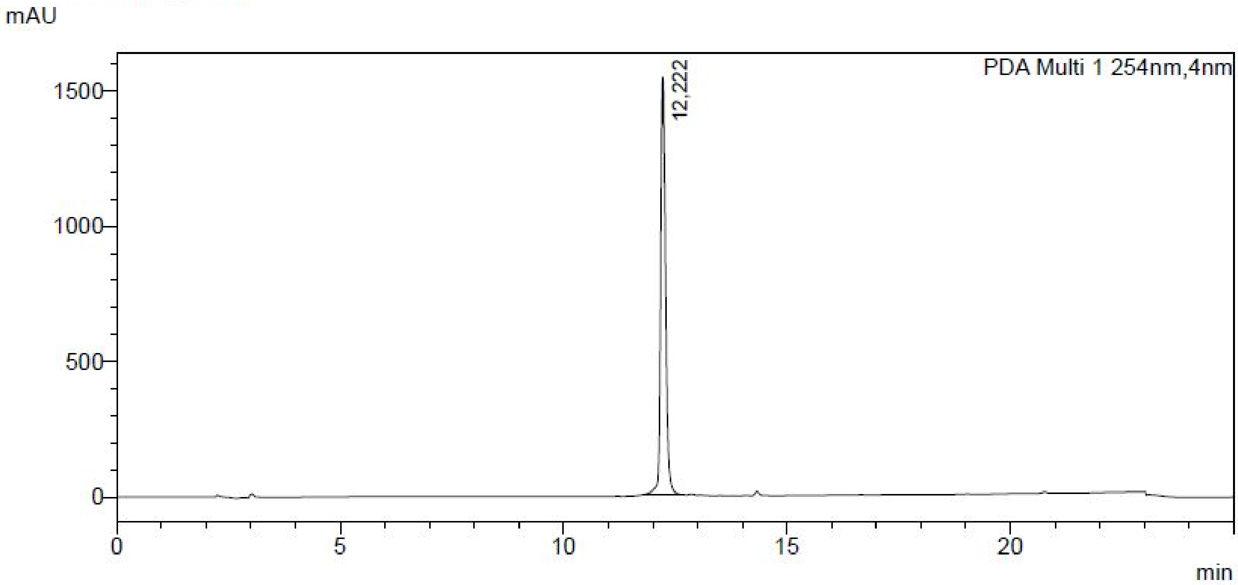

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PDA Ch1 254nm

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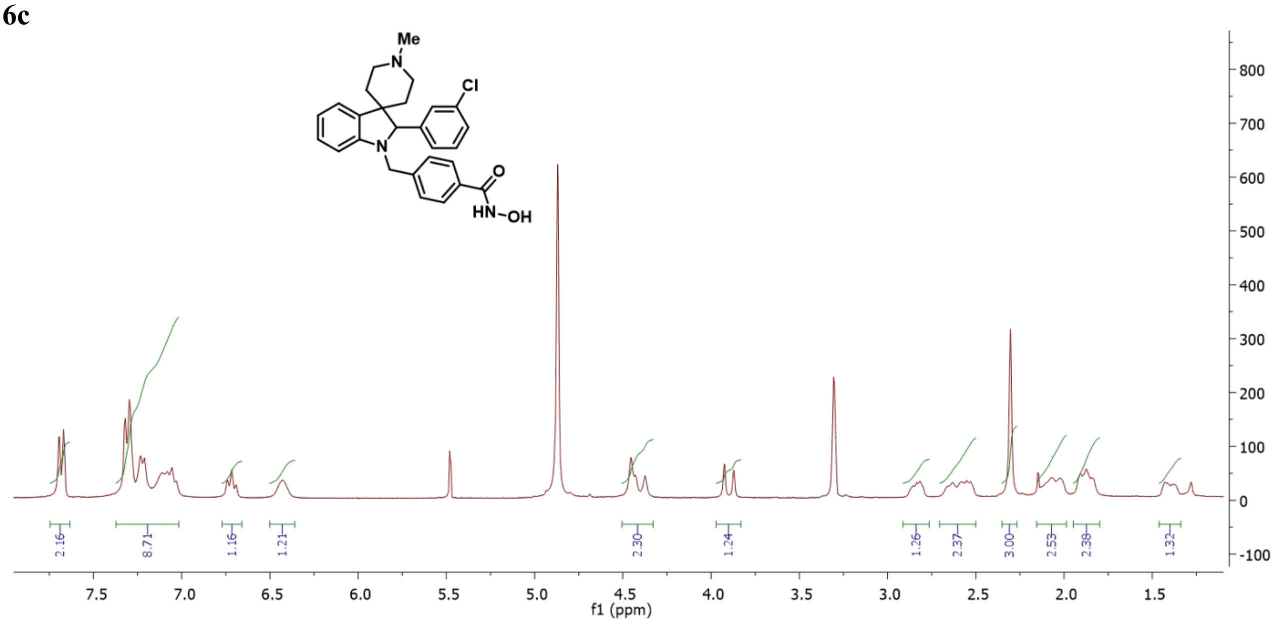
6c



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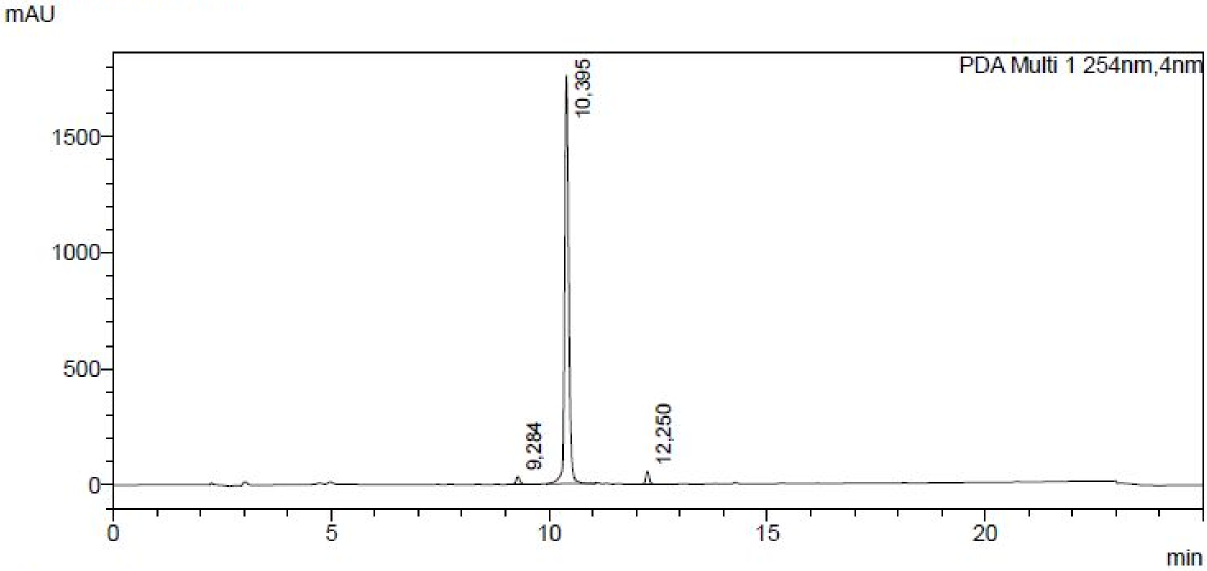

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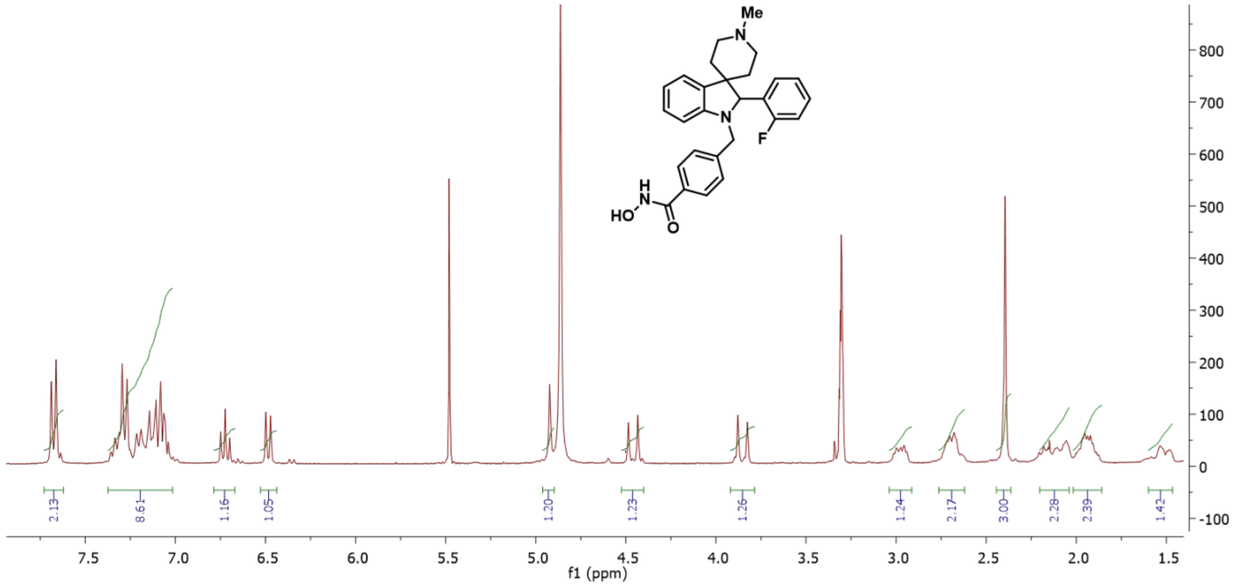
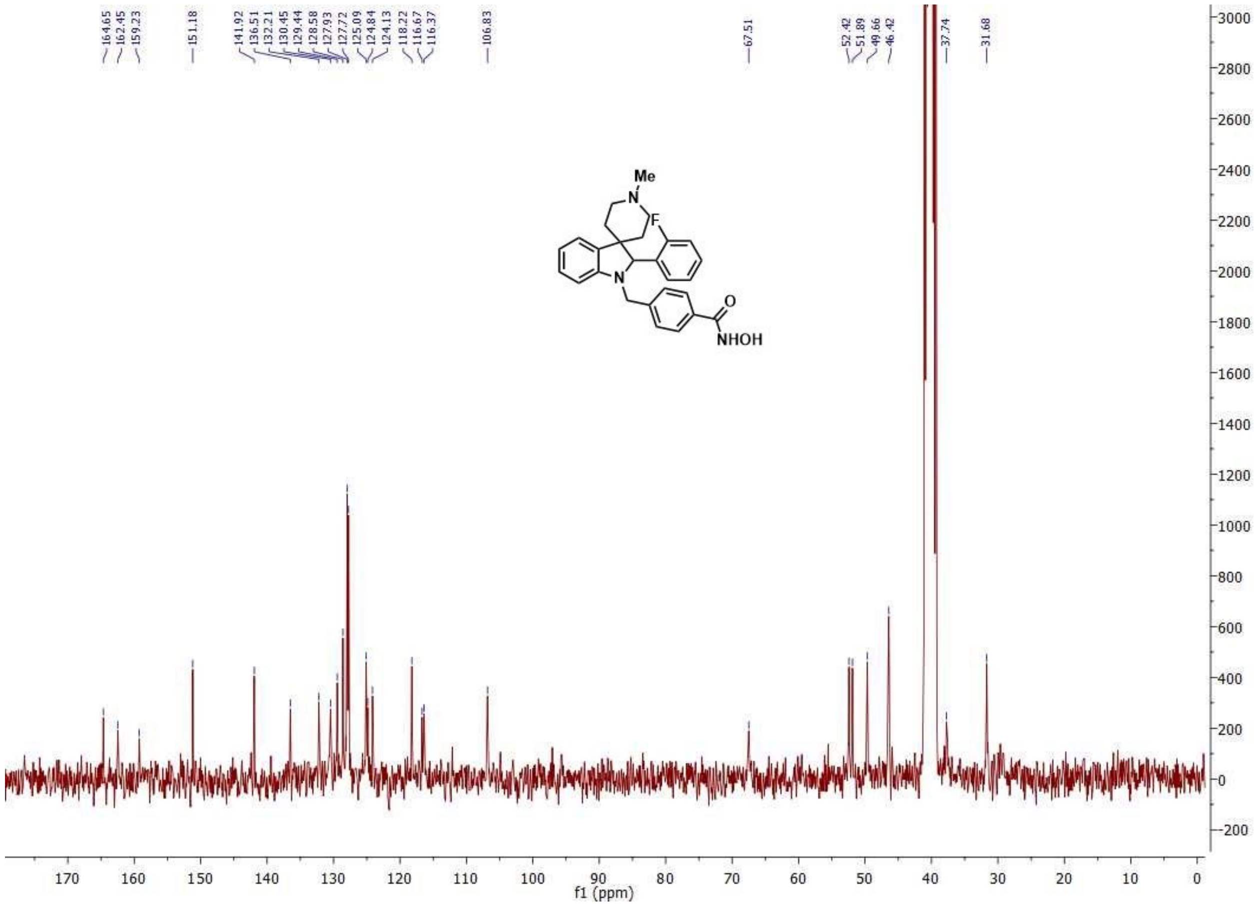
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	9,284	187511	1,533
2	10,395	11738361	95,997
3	12,250	301946	2,469
Total		12227817	100,000

6d





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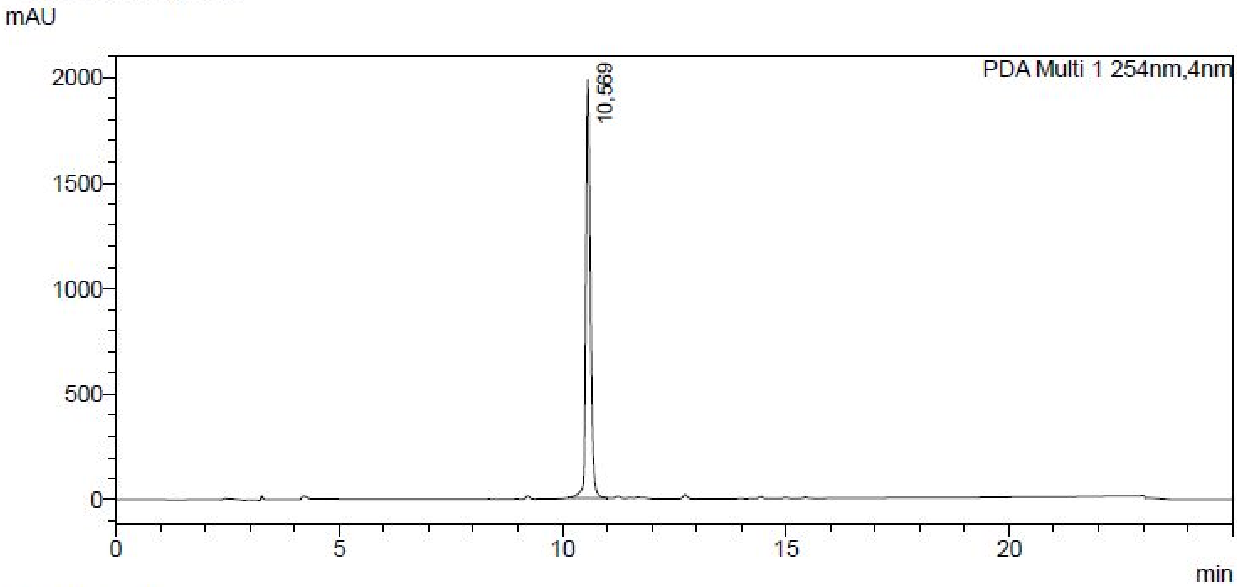

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
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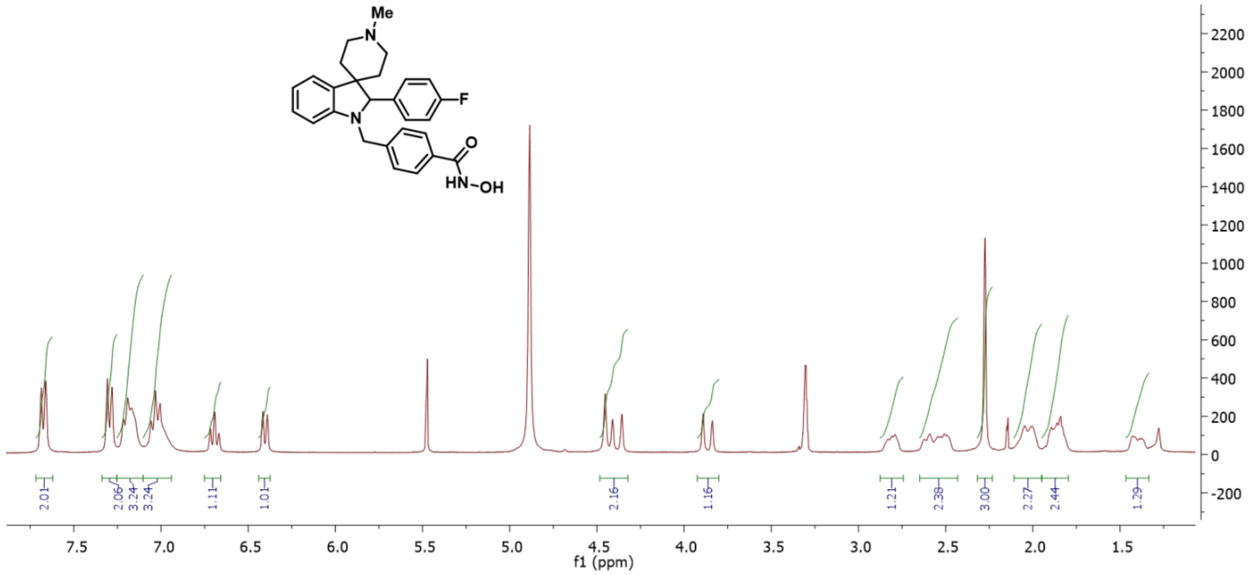
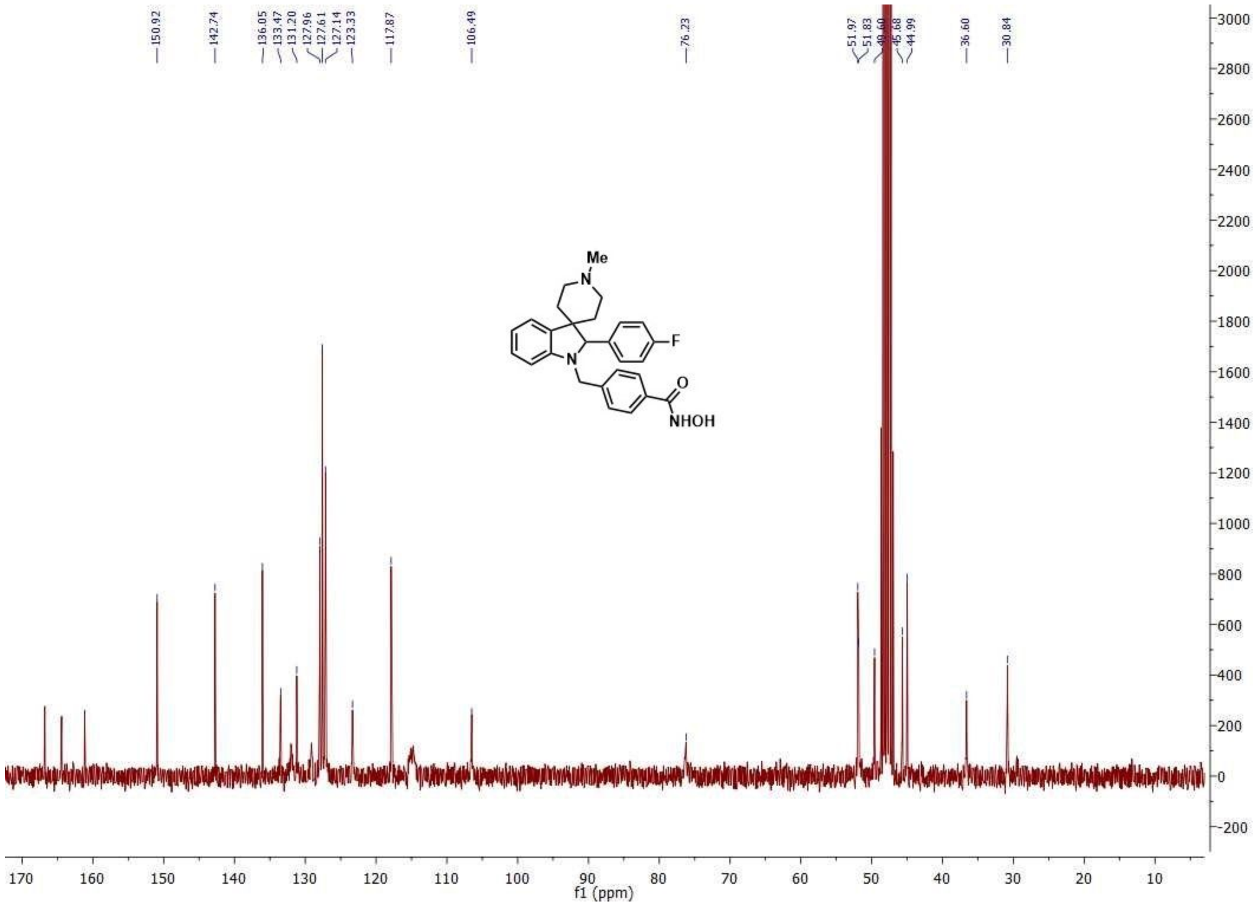
Total		14220350	100,000

6e





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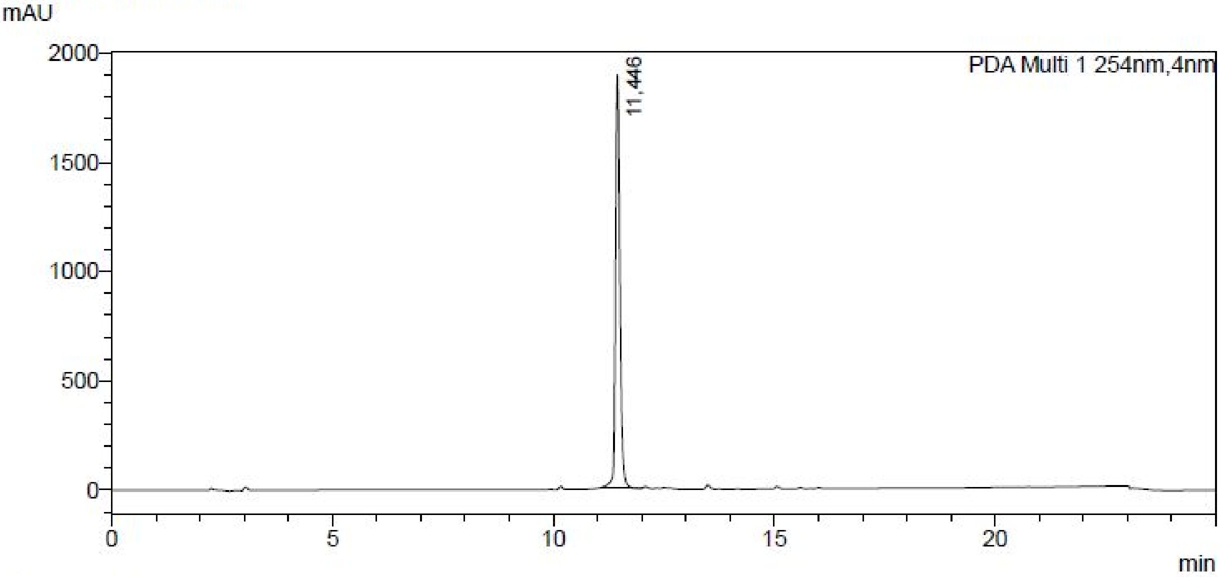

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
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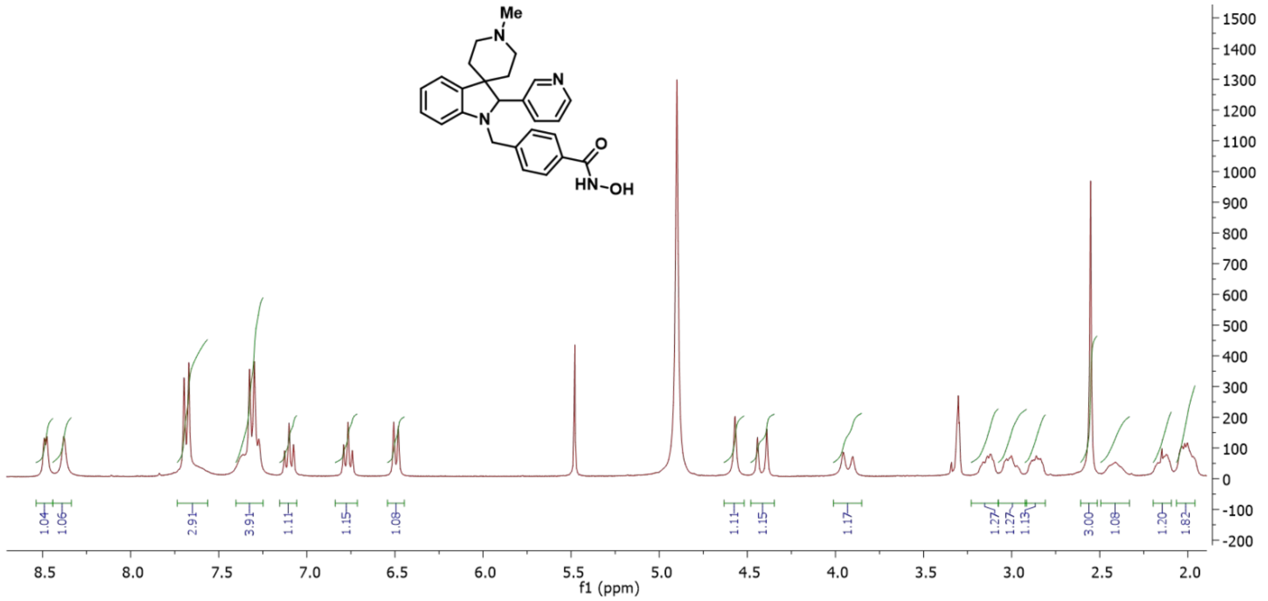
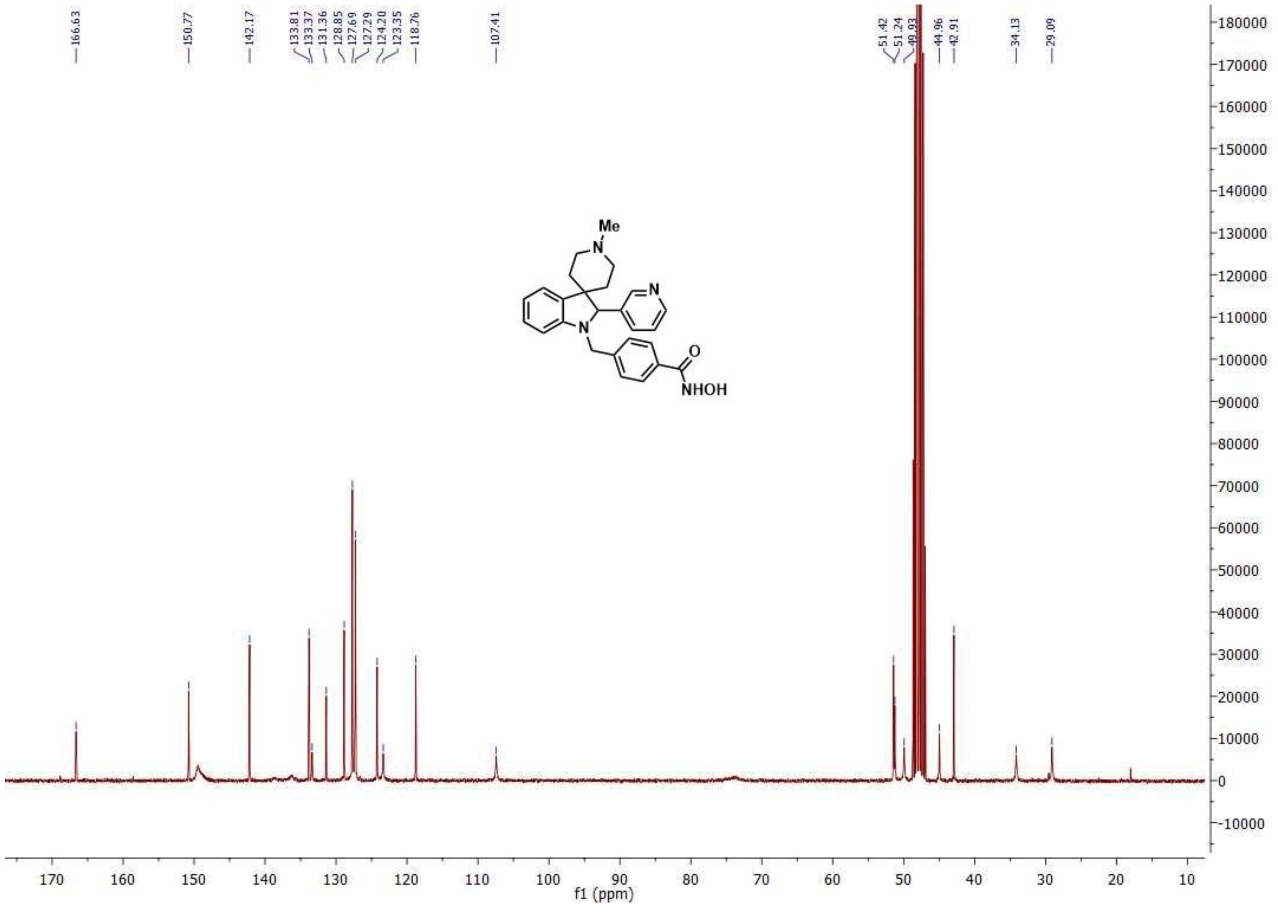
Total		13170953	100,000

6f





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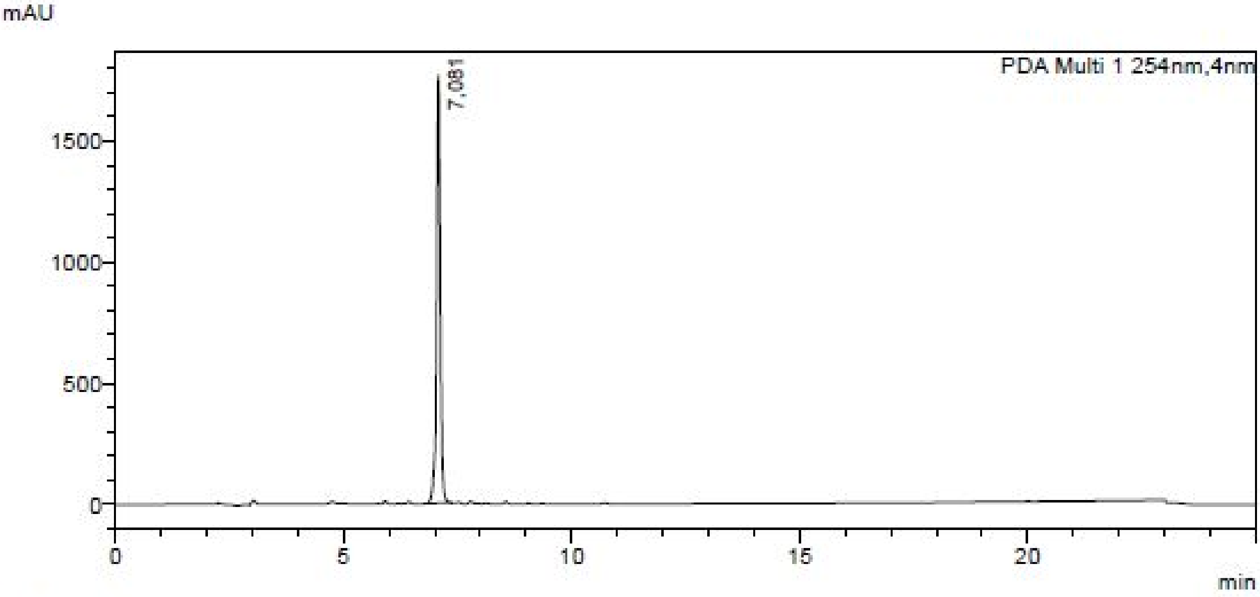

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
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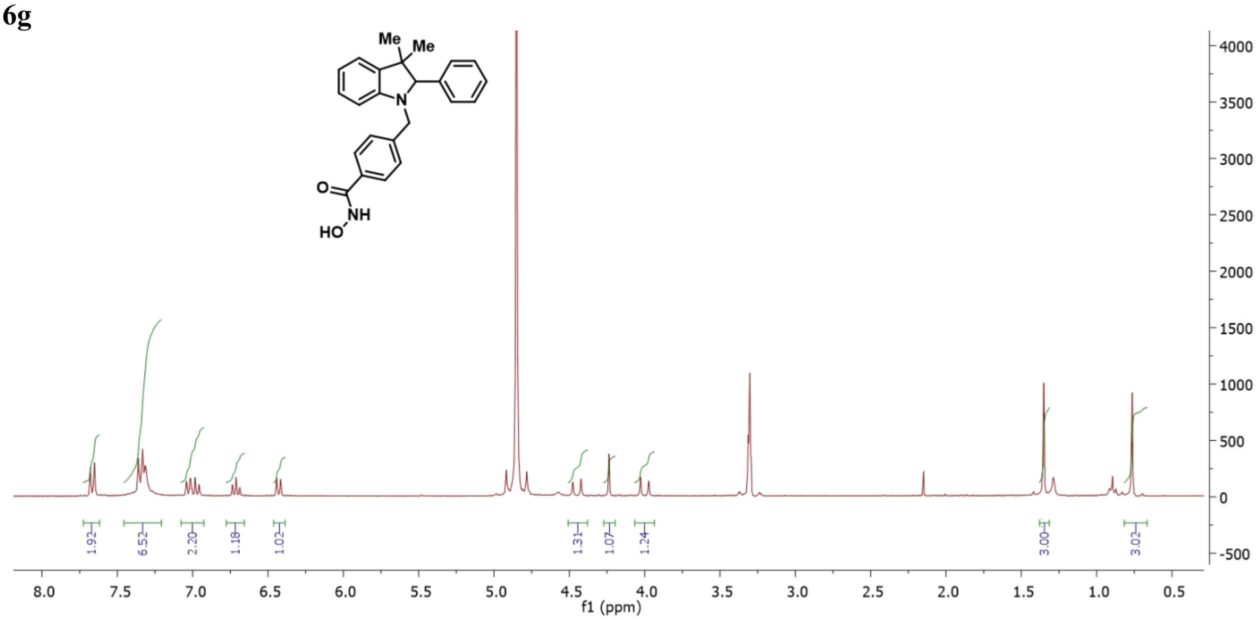
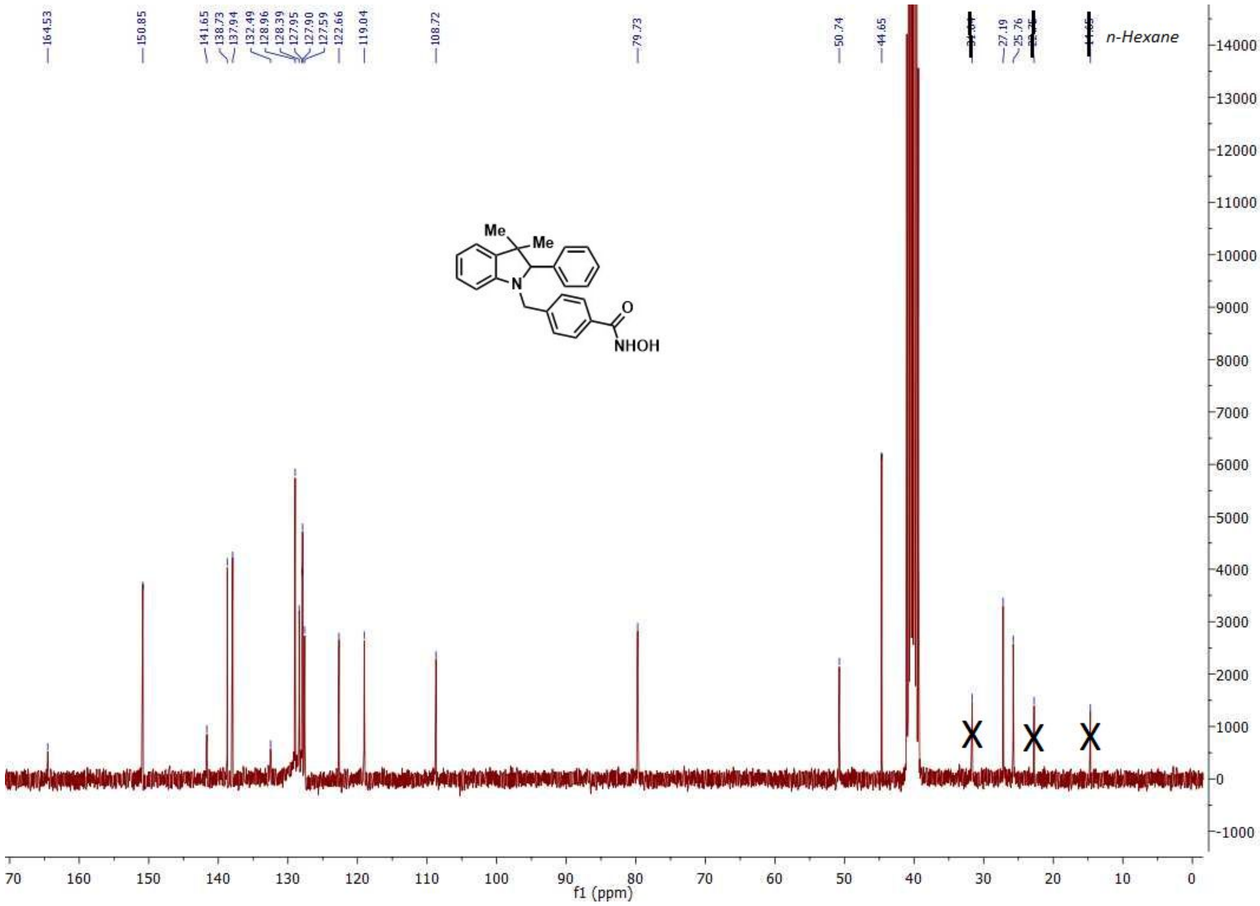
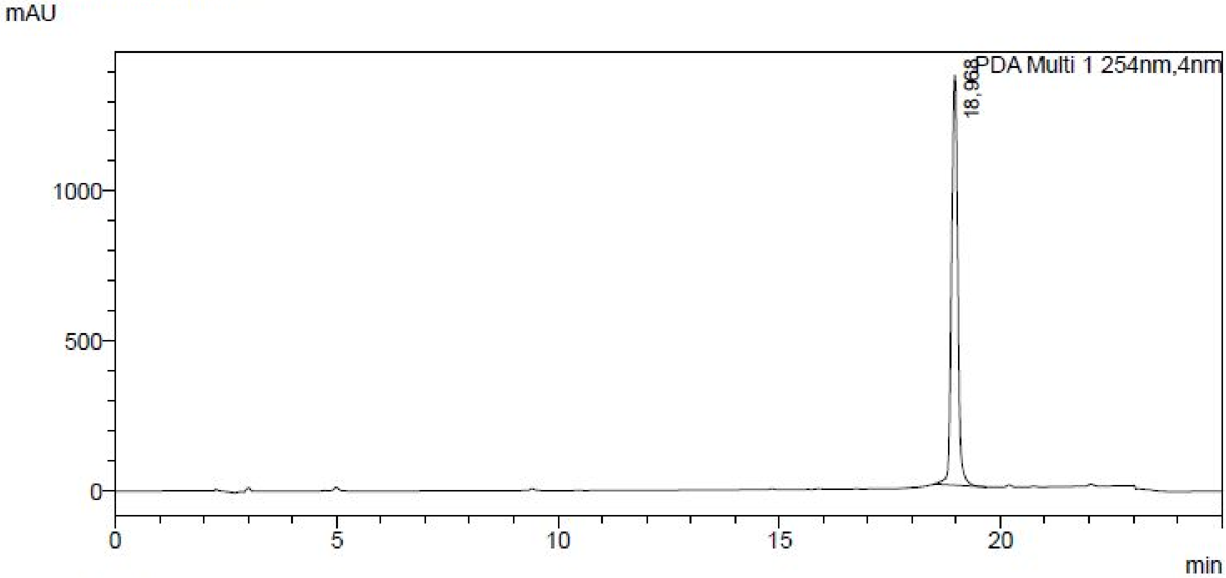
Total		10191709	100,000

6g


Me
Me
N
O
NH
HO
1.92
6.52
2.20
1.18
1.02
1.31
1.07
1.24
3.00
3.02
f1 (ppm)


164.53
150.85
141.65
138.73
137.94
132.49
128.96
128.39
127.95
127.90
127.59
122.66
119.04
108.72
79.73
50.74
44.65
27.19
25.76
n-Hexane
Me
Me
N
O
NHOH
f1 (ppm)

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

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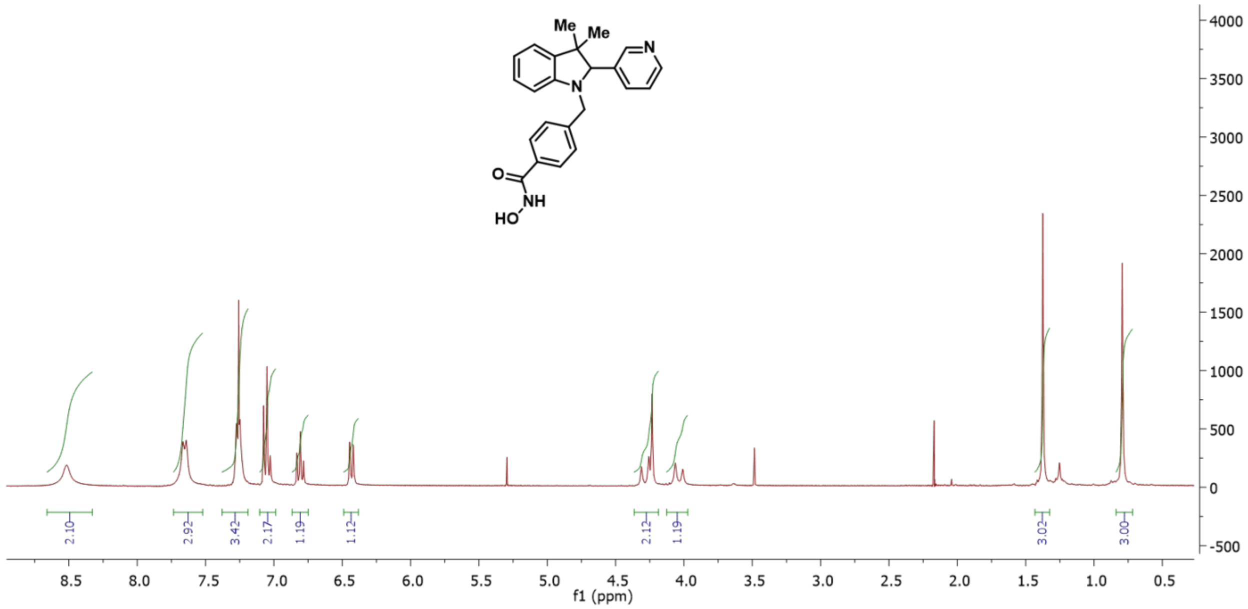
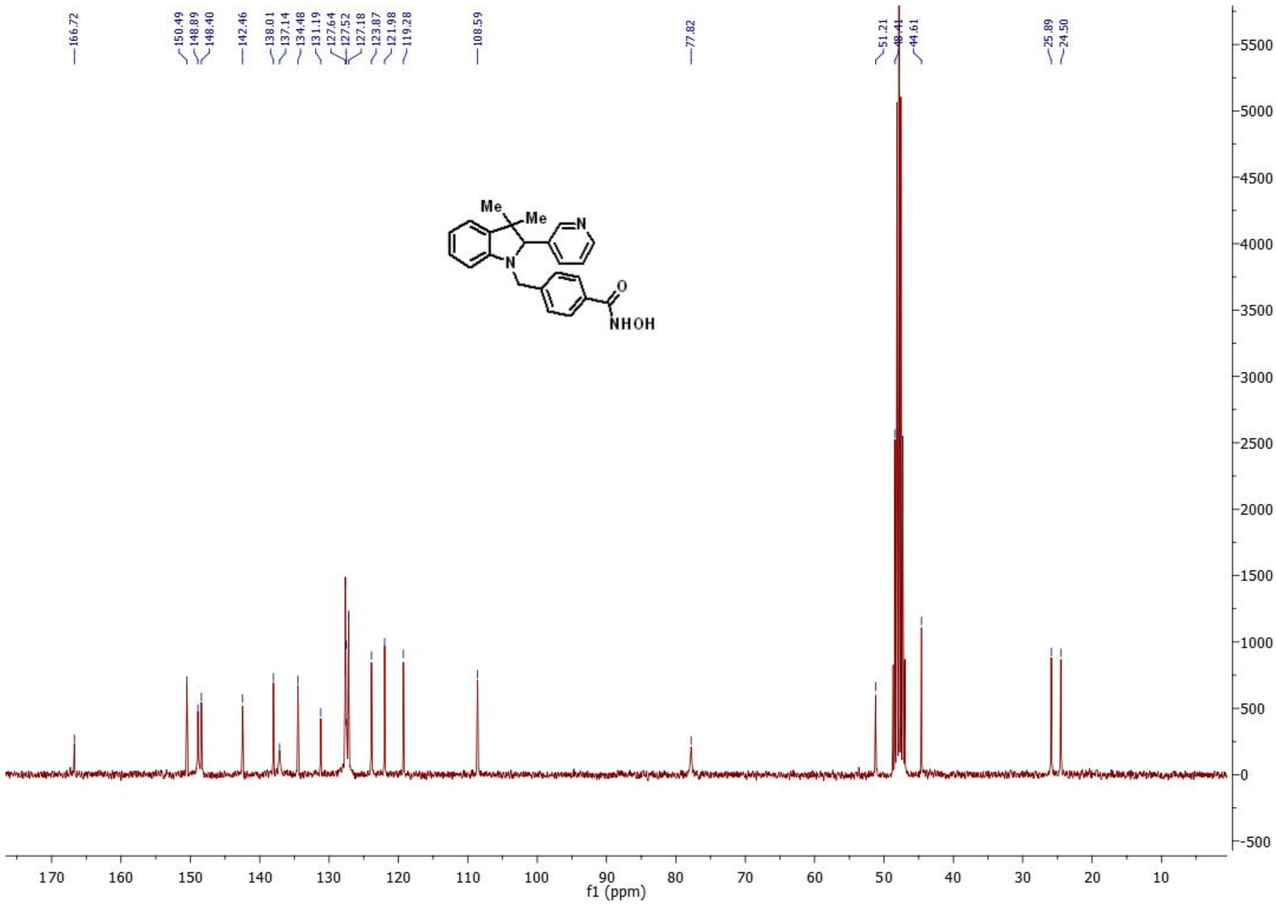
Total		13372848	100,000

6h





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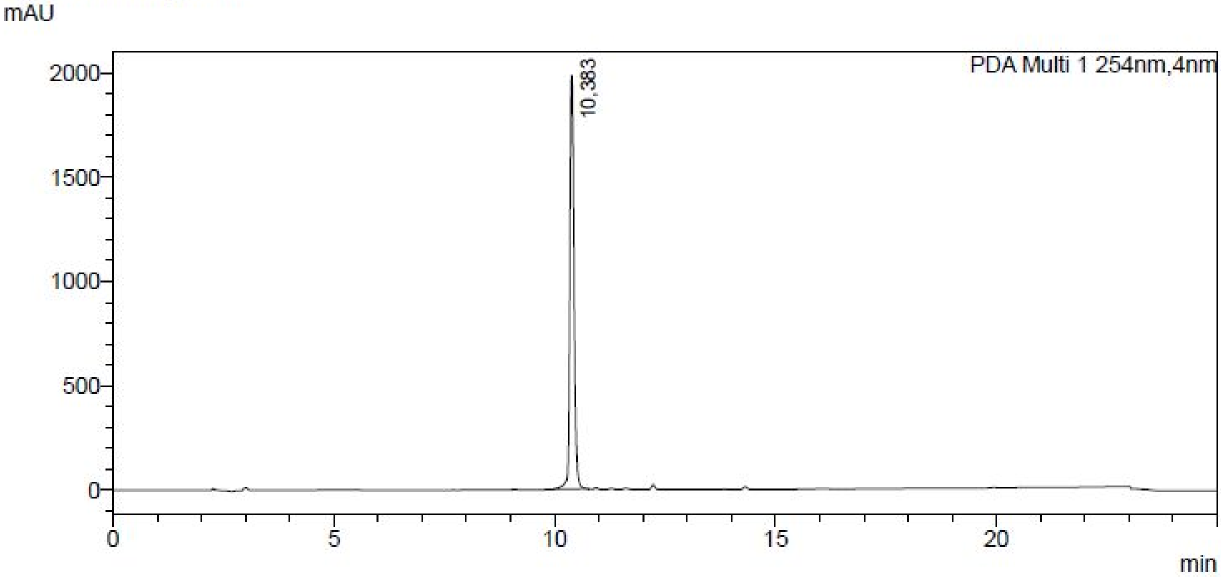

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
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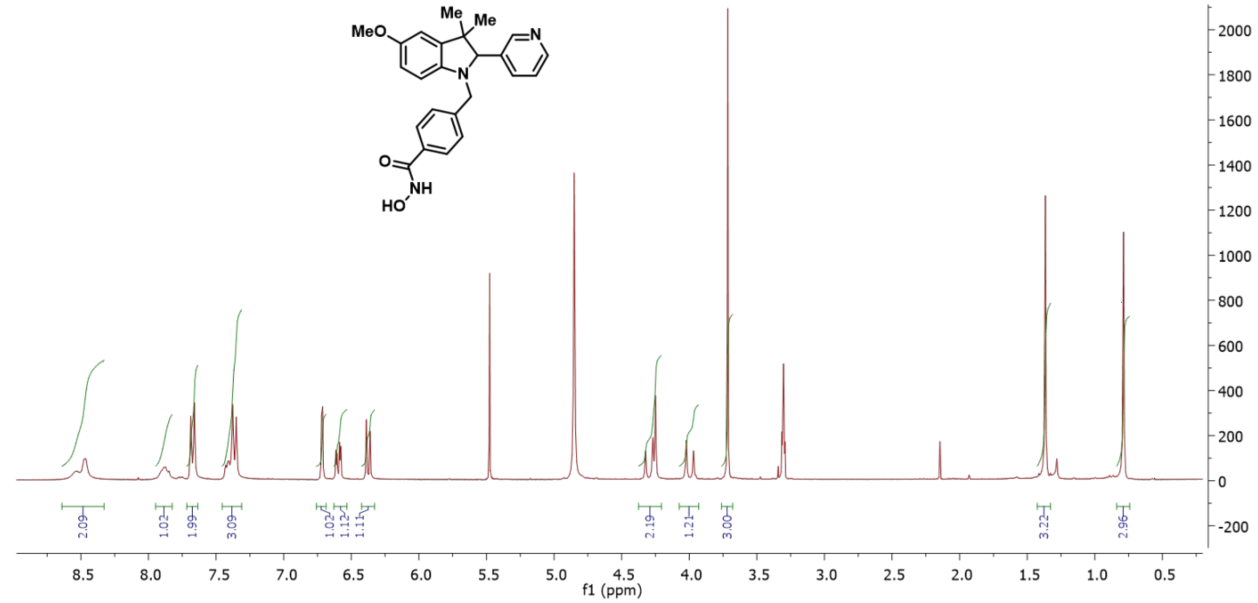
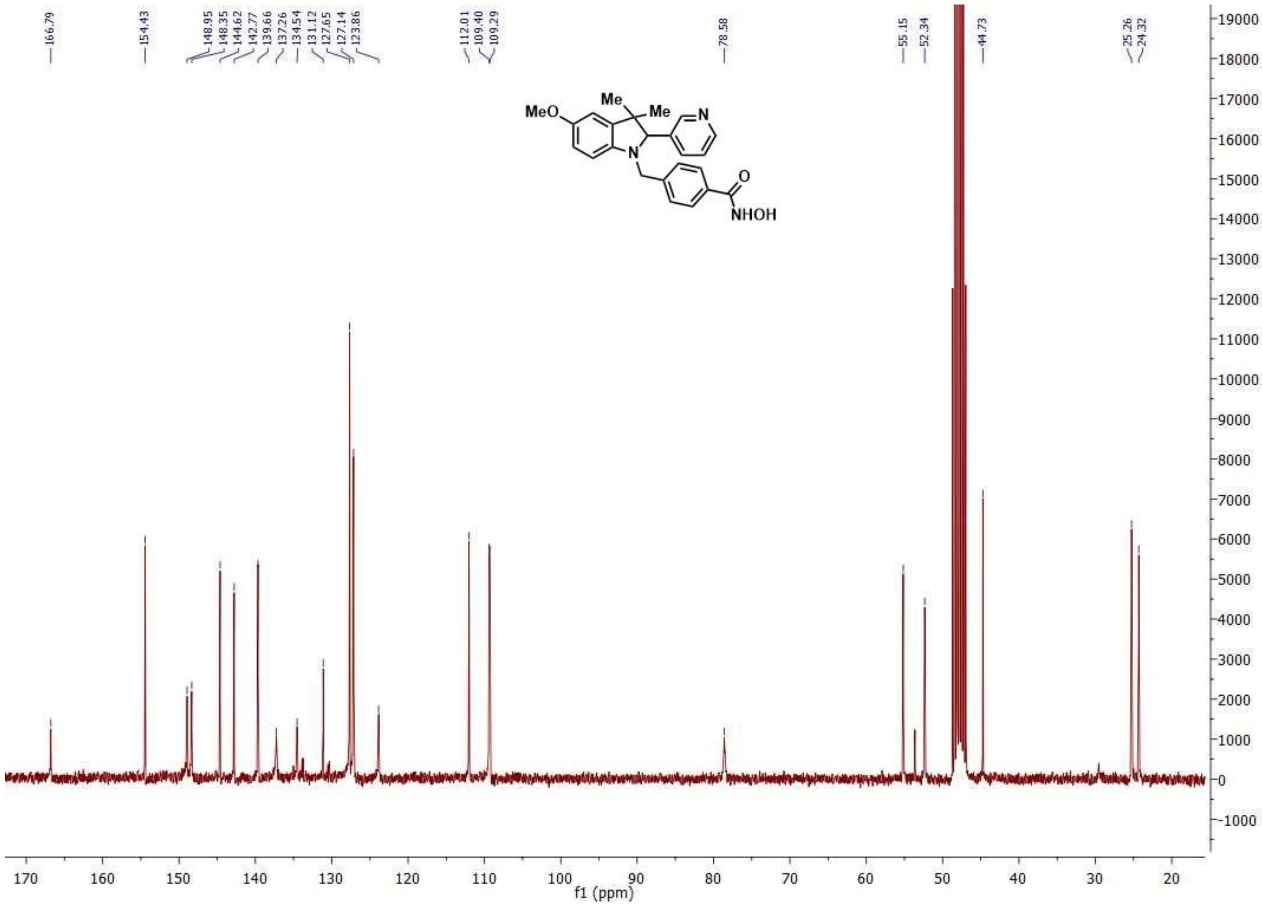
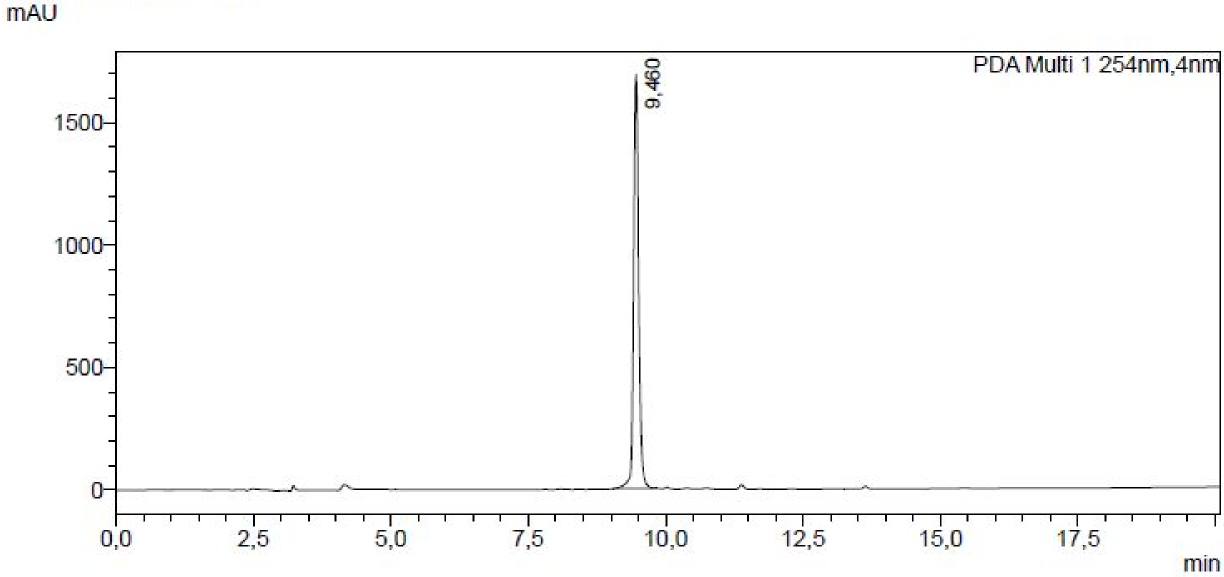
Total		13014410	100,000

6i


MeO
Me
Me
N
N
O
NH
HO
2.09
1.02
1.99
3.09
1.02
1.12
1.11
2.19
1.21
3.00
3.22
2.96
f1 (ppm)


166.79
154.43
148.95
148.35
144.62
142.77
139.66
137.26
134.54
131.12
127.65
127.14
123.86
112.01
109.40
109.29
78.58
55.15
52.34
44.73
25.26
24.32
MeO
Me
Me
N
N
O
NHOH
f1 (ppm)

<Chromatogram>

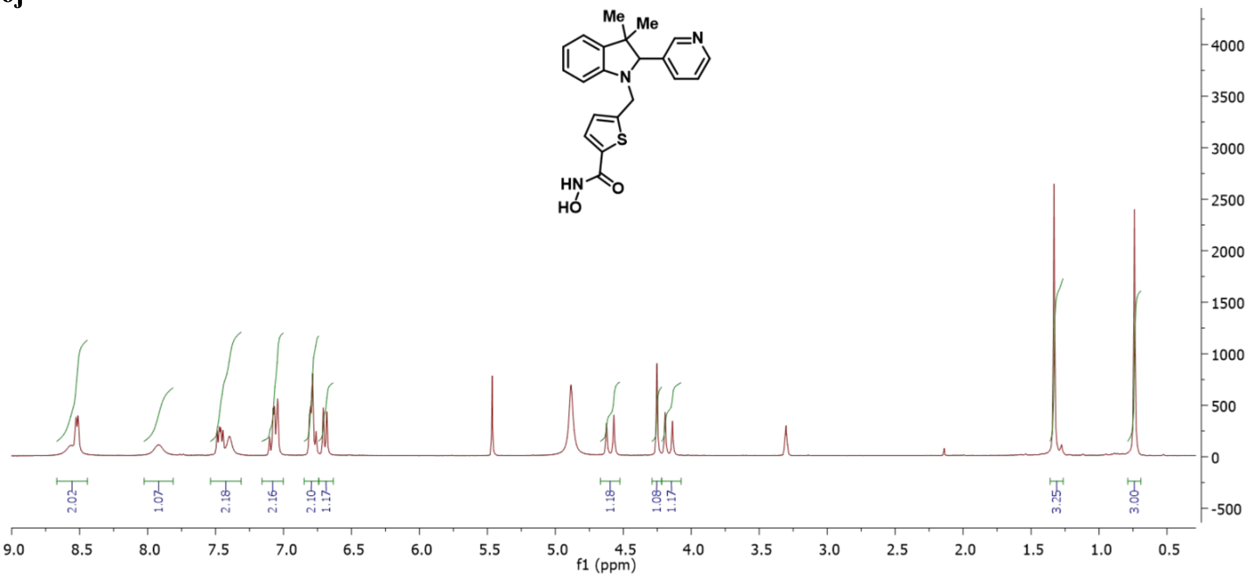


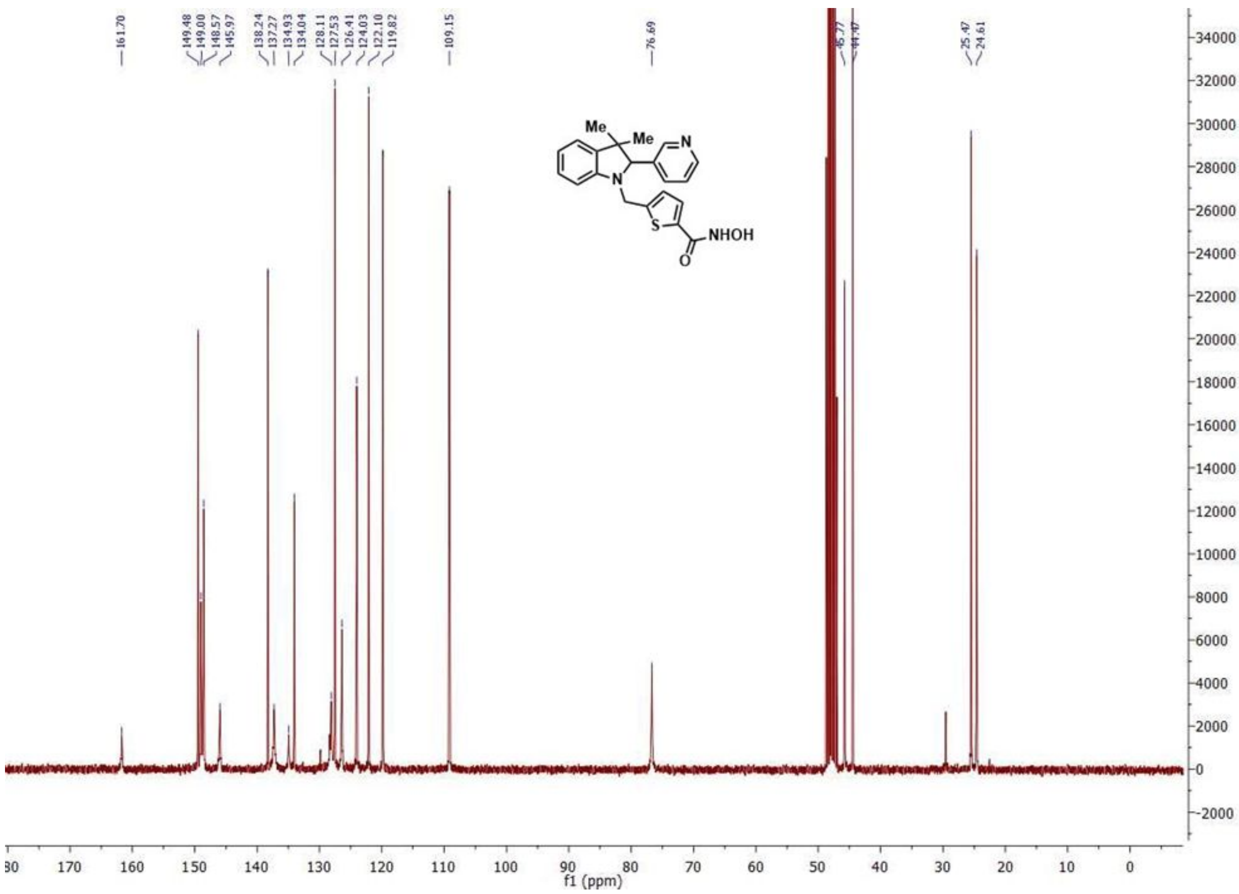
<Peak Table>

PDA Ch1 254nm

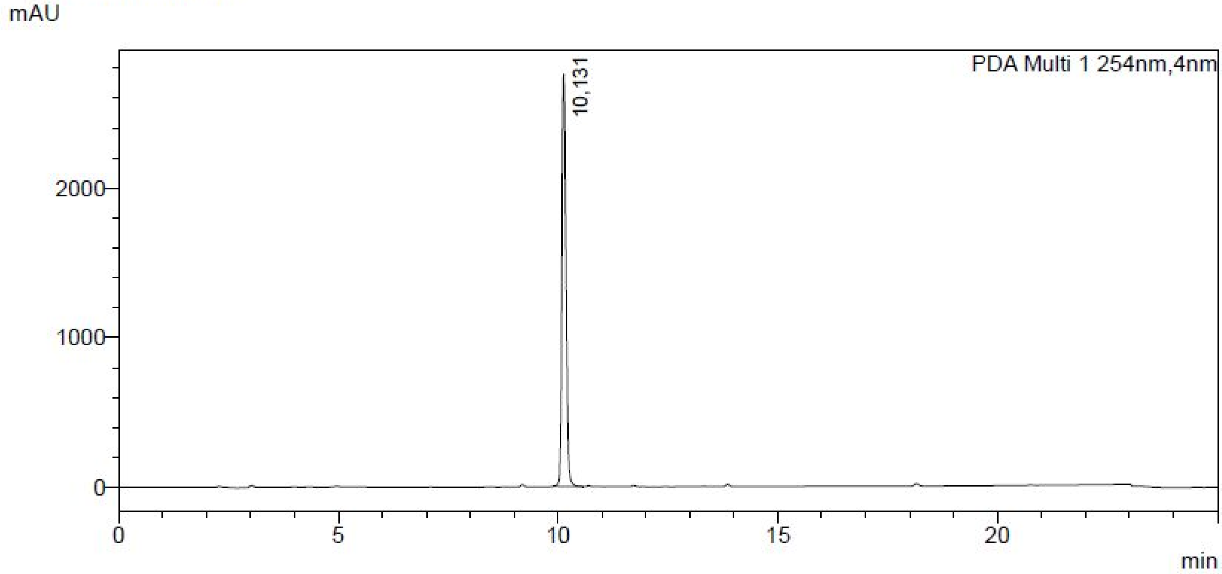
Peak#	Ret. Time	Area	Area%
1	9,460	10804418	100,000
Total		10804418	100,000

6j





<Chromatogram>

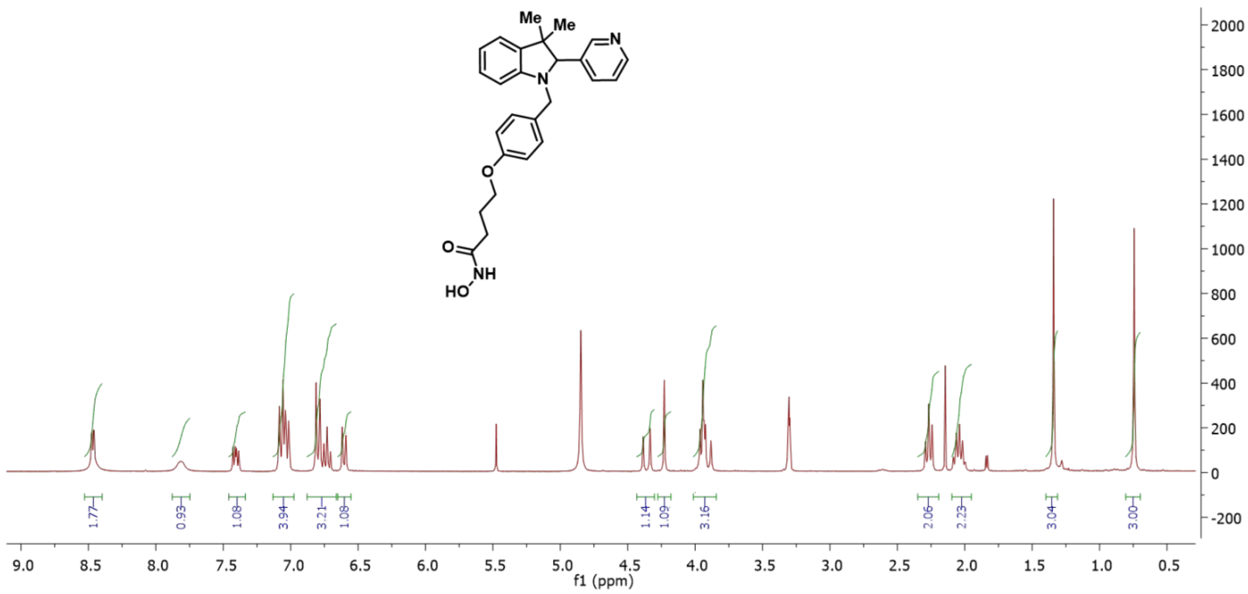


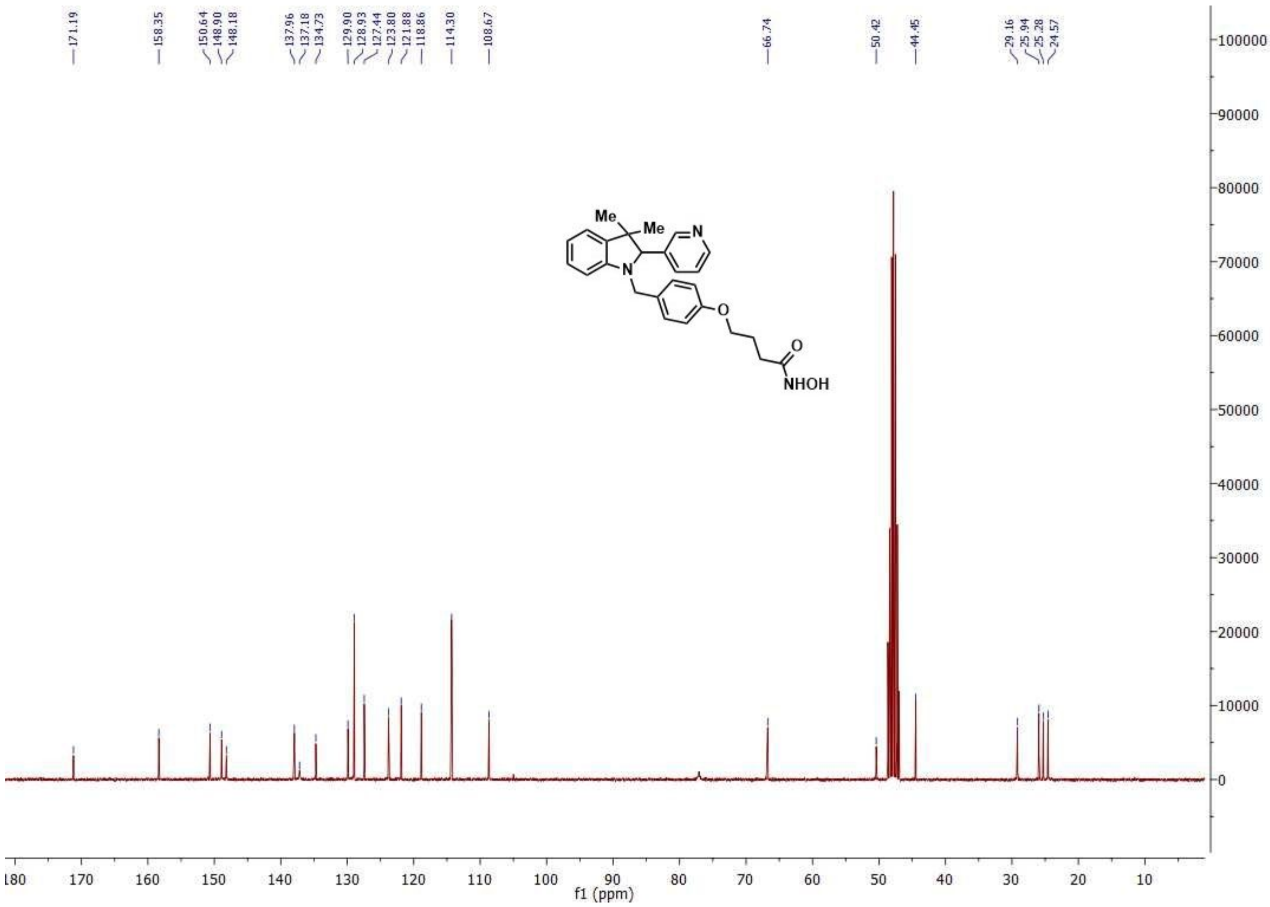
<Peak Table>

PDA Ch1 254nm

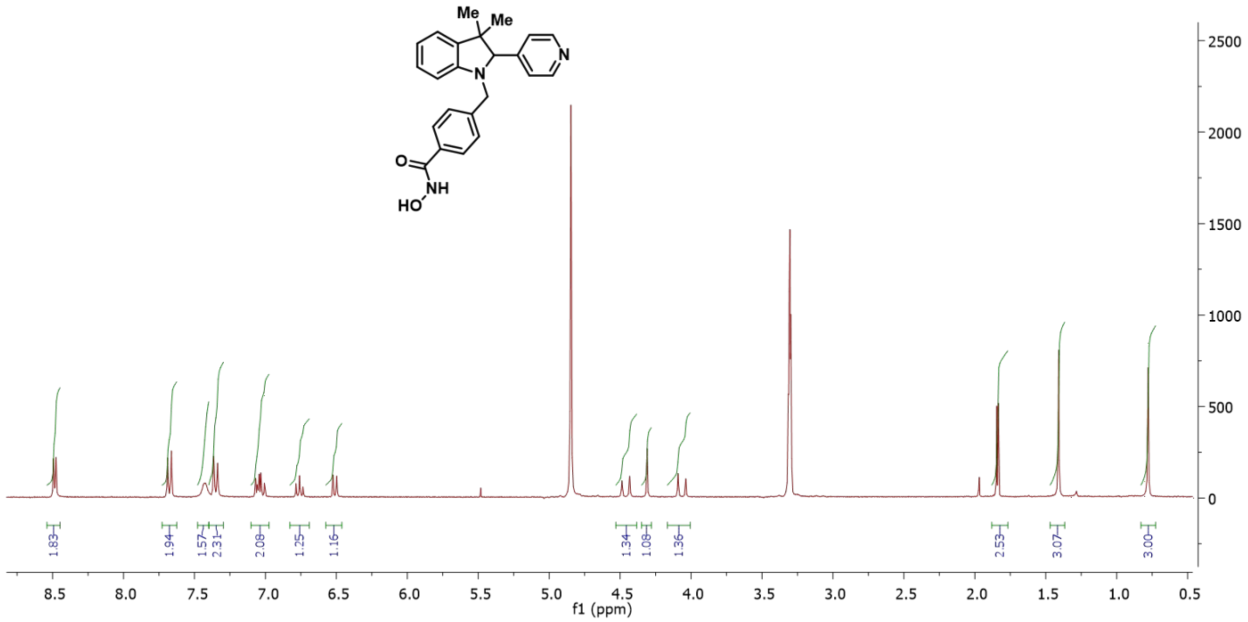
Peak#	Ret. Time	Area	Area%
1	10,131	18080318	100,000
Total		18080318	100,000

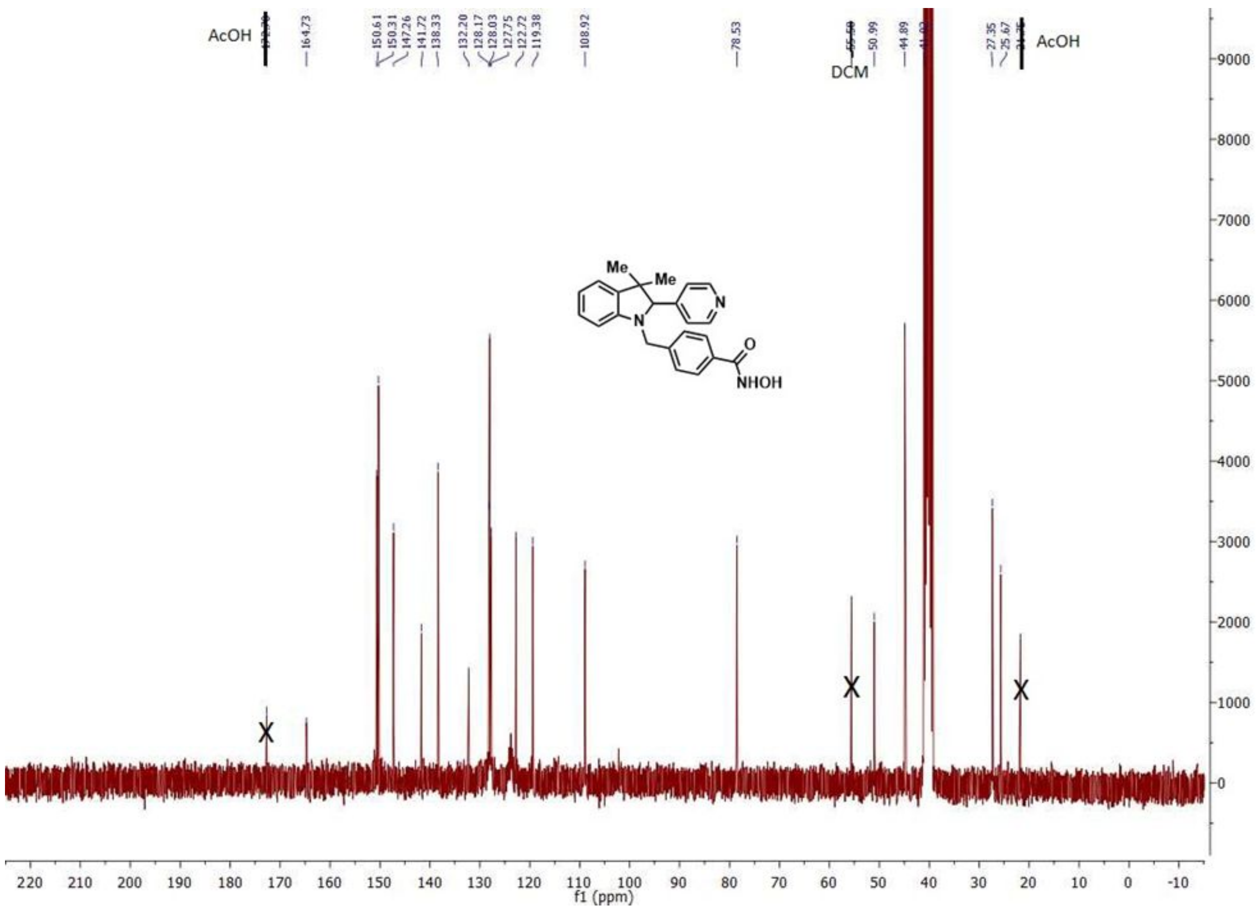
6k


Me
Me
N
N
O
O
NH
HO
1.77
0.93
1.08
3.94
3.21
1.08
1.14
1.09
3.16
2.06
2.23
3.04
3.00
f1 (ppm)

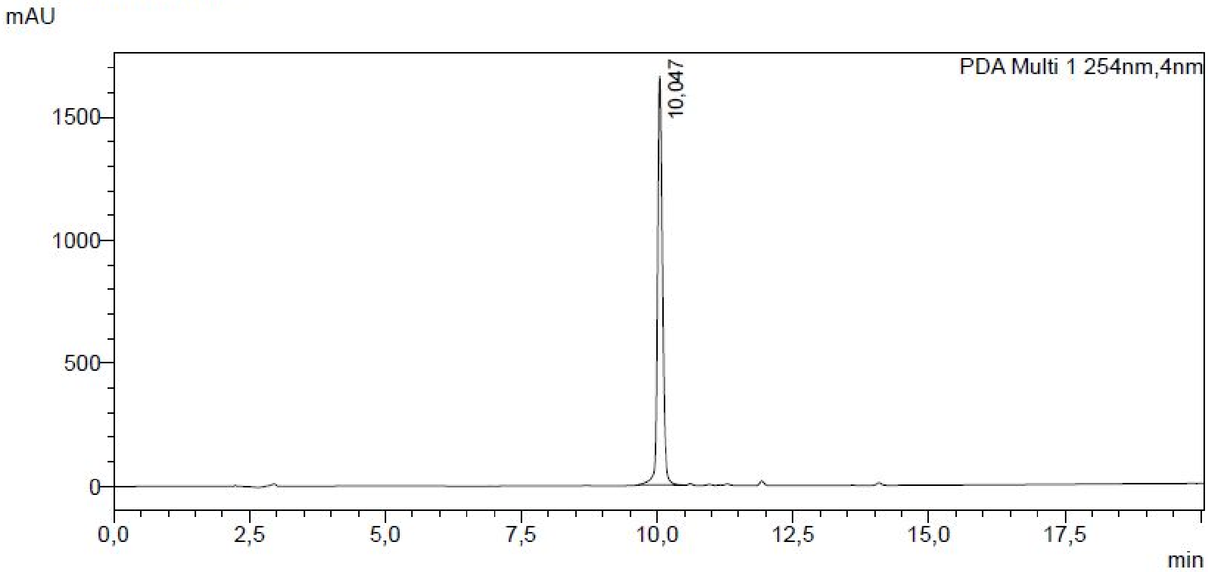

171.19
158.35
150.64
148.90
148.18
137.96
137.18
134.73
129.90
128.93
127.44
123.80
121.88
118.86
114.30
108.67
66.74
50.42
44.45
29.16
25.94
25.28
24.57
Me
Me
N
N
O
O
NHOH
f1 (ppm)

6l





<Chromatogram>

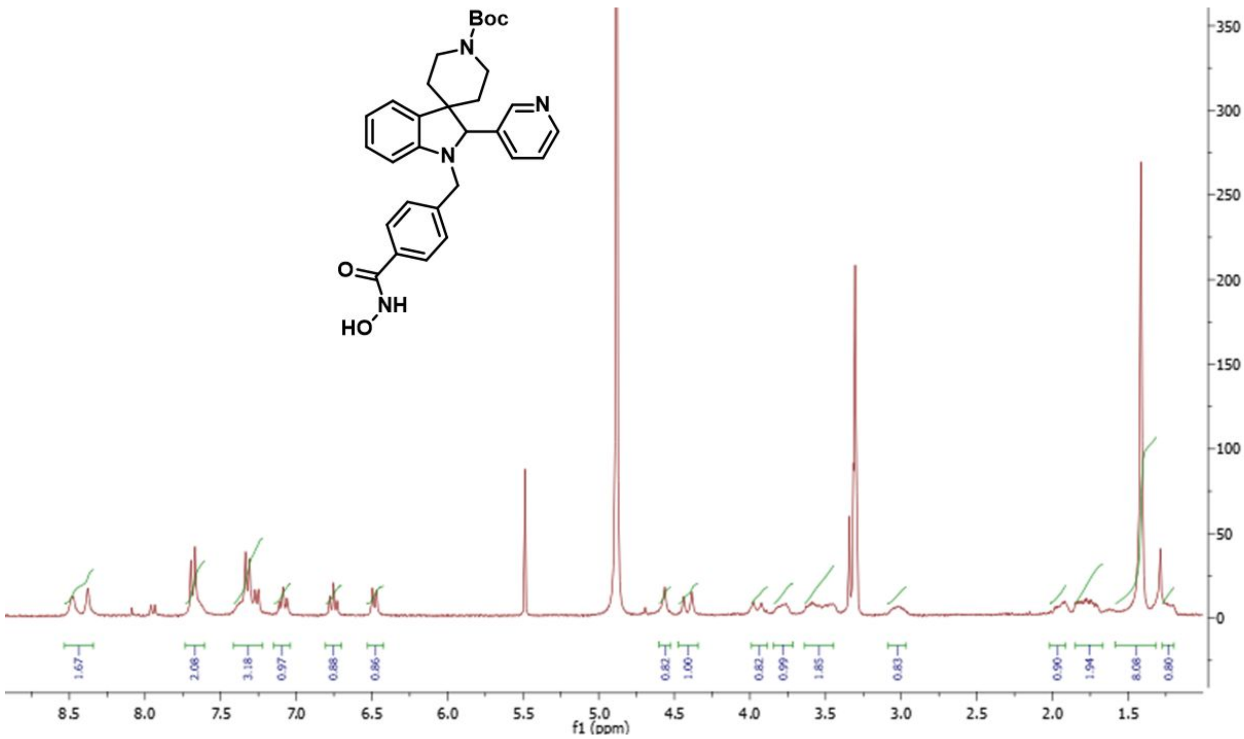


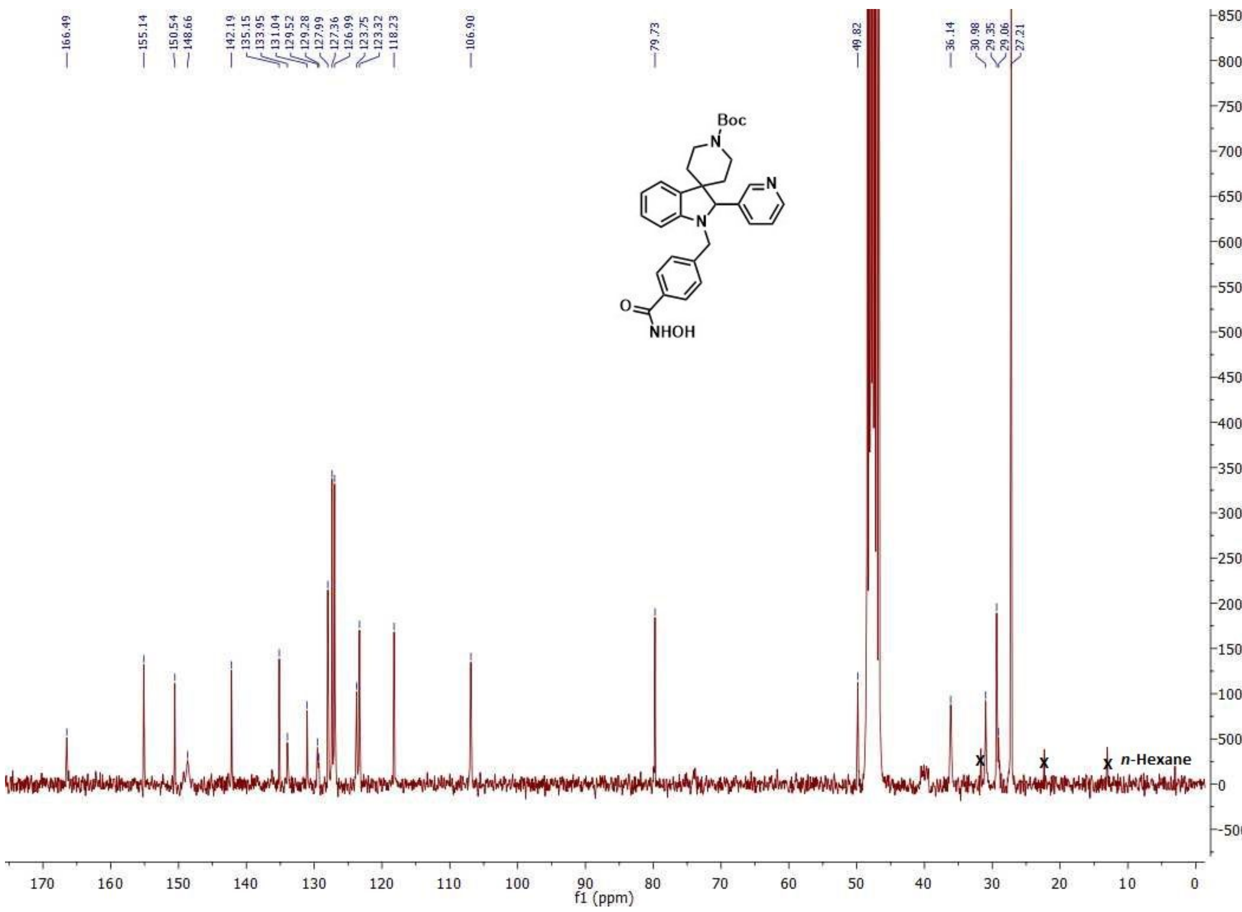
<Peak Table>

PDA Ch1 254nm

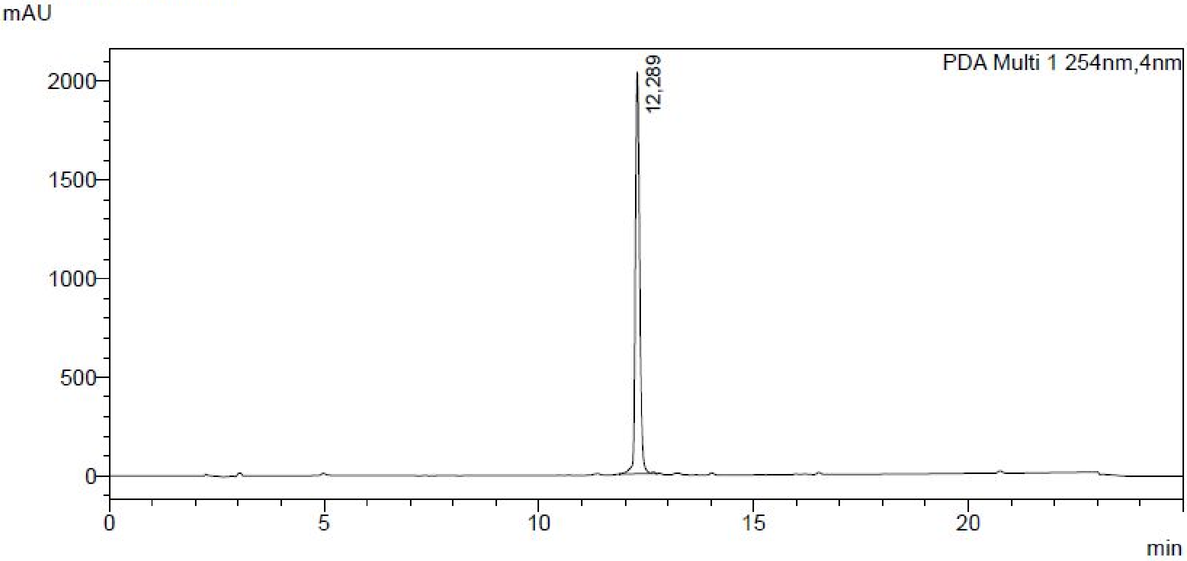
Peak#	Ret. Time	Area	Area%
1	10,047	10599576	100,000
Total		10599576	100,000

6m


Boc
N
N
N
O
NH
HO
1.67
2.08
3.18
0.97
0.88
0.86
0.82
1.00
0.82
0.99
1.85
0.83
0.90
1.94
8.08
0.80
f1 (ppm)


166.49
155.14
150.54
148.66
142.19
135.15
133.95
131.04
129.52
129.28
127.99
127.36
126.99
123.75
123.32
118.23
106.90
79.73
49.82
36.14
30.98
29.35
29.06
27.21
Boc
N
N
N
O
NHOH
x
x
x
n-Hexane
f1 (ppm)

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12,289	14100554	100,000
Total		14100554	100,000