Supplementary Materials:

Article

(*S*)-3-(3-((7-Ethynyl-9*H*-pyrimido[4,5-*b*]indol-4-yl)amino)piperidin-1-yl)propanenitrile

Stanislav Andreev [1], Nicole Plank [1], Dieter Schollmeyer [2] and Pierre Koch [1]*

[1] Department of Pharmaceutical/Medicinal Chemistry II, Institute of Pharmacy, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany
[2] Department of Chemistry, Johannes Gutenberg-Universität Mainz, Duesbergweg 10-14, 55128 Mainz, Germany
* Correspondence: pierre.koch@chemie.uni-regensburg.de; Tel.: +49-941-943-4827

Table of Contents

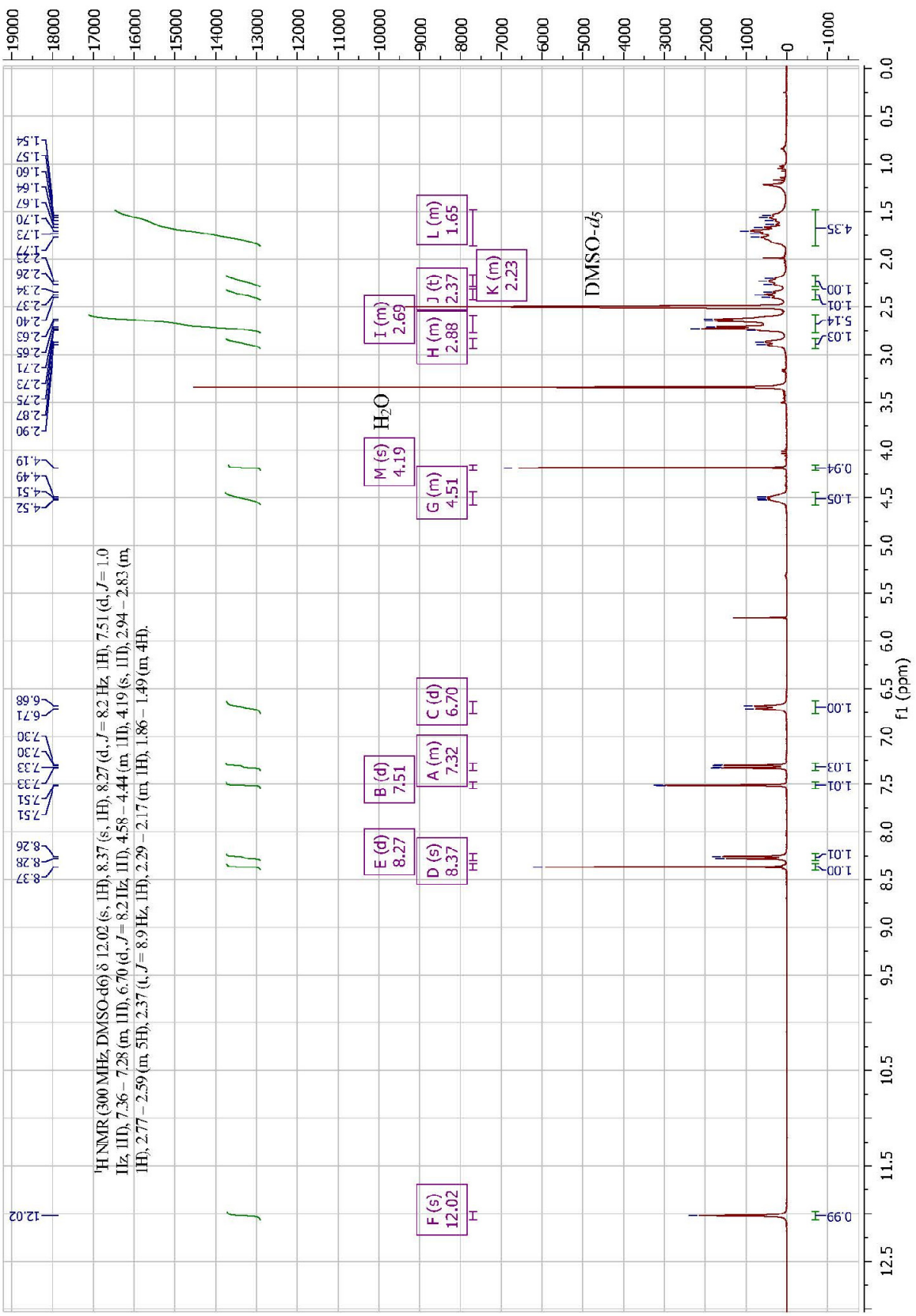


Figure S1. [1]H-NMR spectrum of title compound **2**.

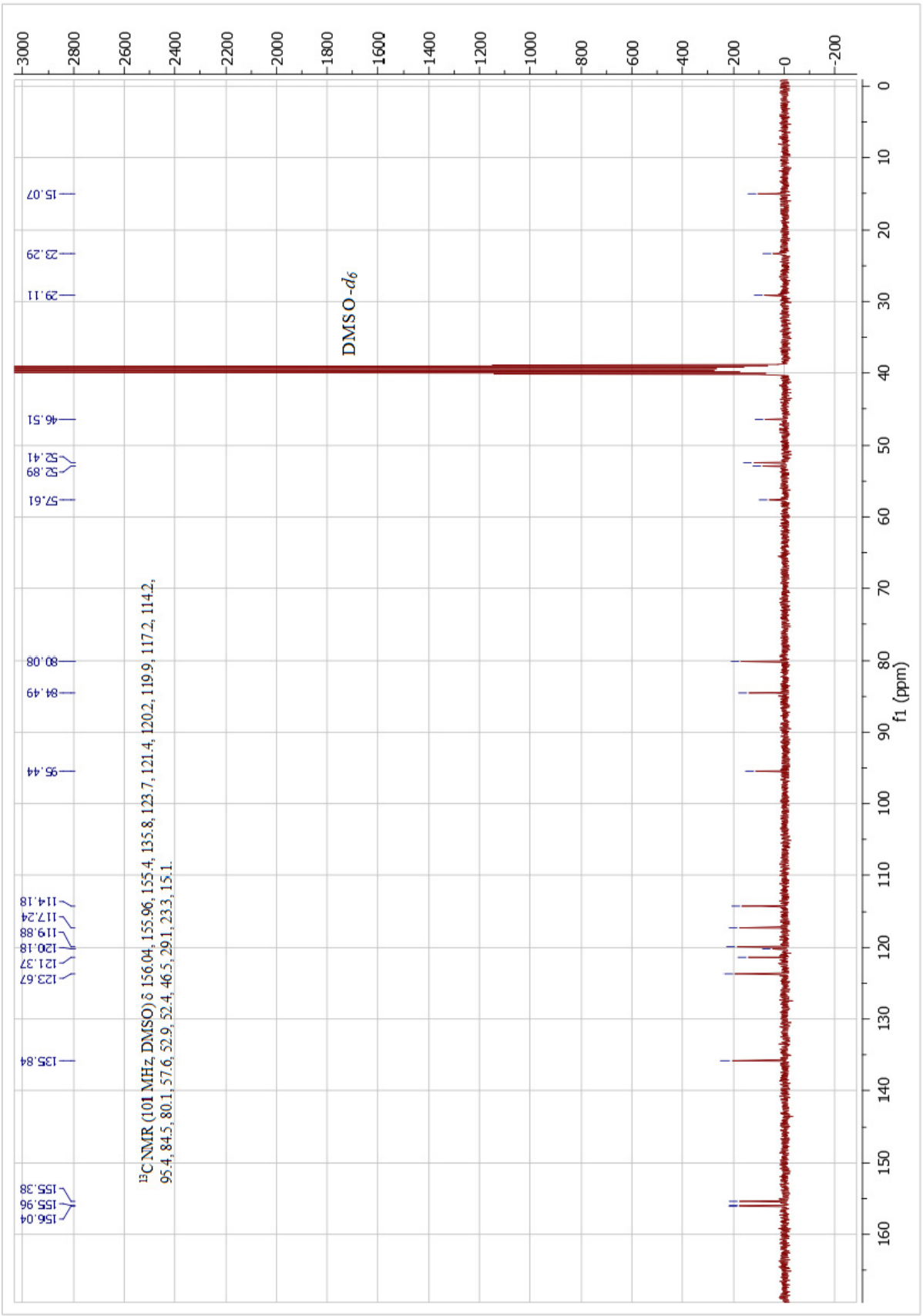
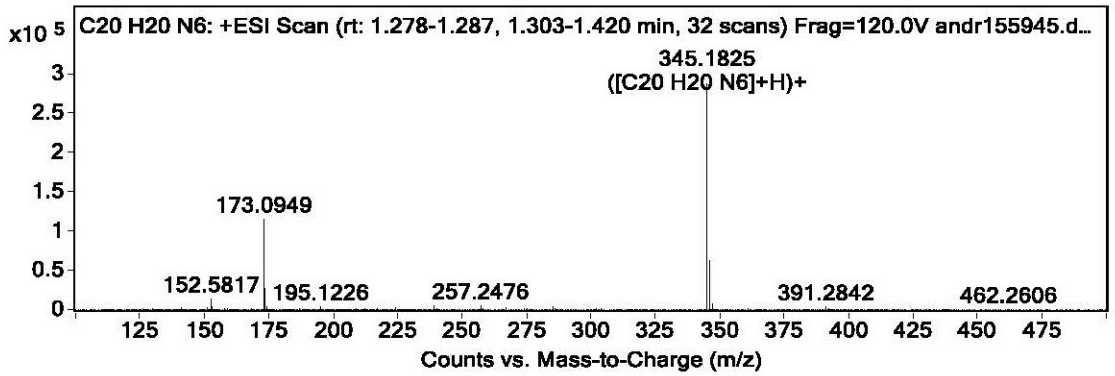


Figure S2. ^{13}C-NMR spectrum of title compound **2**.



Peak List

m/z	z	Abund	Formula	Ion
125.9858	1	882.38		
130.0076		1129.89		
141.0658	1	1982.34		
151.0963	1	2416.87		
152.5817	2	13503.78		
153.0838	2	3149.04		
158.0026	1	749.18		
158.9612	1	1096.12		
168.1228	2	725.62		
173.0949	2	114970.66		
173.5967	2	27164.54		
174.0982	2	3417.82		
186.9561	1	1323.76		
195.1226	1	3543.26		
209.082	1	1016.56		
217.1046	1	1303.92		
224.1283	1	2197.21		
239.2368	1	4676.81		
240.2404	1	805.24		
257.2476	1	4799.97		
258.2509	1	876.77		
267.2681	1	2466.97		
285.279	1	3138.71		
302.305	1	845.17		
304.1557	1	691.31		
345.1825	1	287502.34	C20 H20 N6	(M+H)+
346.1855	1	62789.1	C20 H20 N6	(M+H)+
347.1882	1	6822.94	C20 H20 N6	(M+H)+
361.2371	1	738.98		
391.2842	1	3121.61		
392.2874	1	924.33		
735.459	1	2317.61		
736.4634	1	1083.25		
922.0098	1	3582.59		
923.0128	1	772.77		

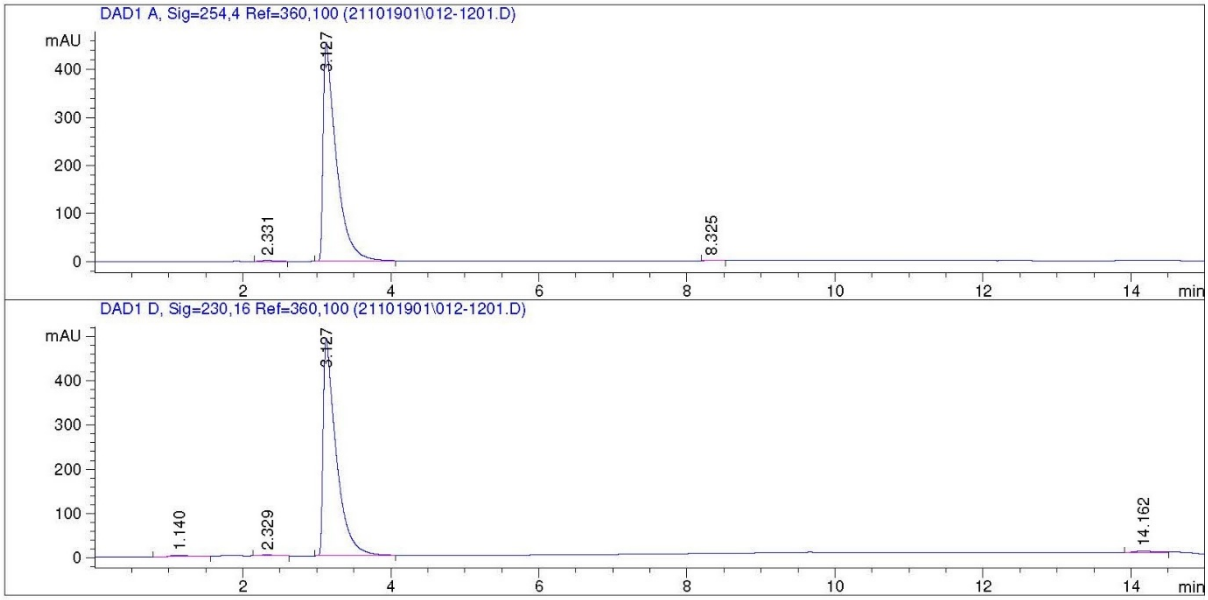
Figure S3. Mass spectrum of title compound **2**.

Best	Formula		Species		m/z	Mass	Diff (ppm)	Diff (mDa)	Score	DBE
	C20 H20 N6		(M+H)+		345.1825	344.1752	0.84	0.29	98.72	14

Species	m/z	Score (iso. abund)	Score (mass)	Score (MS)	Score (MFG)	Score (iso. spacing)	Height	Ion Formula
(M+H)+	345.1825	96.59	99.46	98.72	98.72	99.78	287502.3	C20 H21 N6

m/z	m/z (Calc)	Diff (mDa)	Diff (ppm)	Height	Height (Calc)	Height %	Height % (Calc)
345.1825	345.1822	0.2	0.72	287502.3	281548.1	100	100
346.1855	346.185	0.5	1.31	62789.1	67754.4	21.84	24.06
347.1882	347.1878	0.4	1.16	6822.9	7811.9	2.37	2.77

Figure S4. High resolution mass spectrometry report of title compound **2**.




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   2.331 BB    0.1478   24.94723    2.39001   0.4466
   2   3.127 BB    0.1660 5552.47412  456.27173  99.3969
   3   8.325 BB    0.1092    8.74256    1.19776   0.1565

Totals :                  5586.16392  459.85950


Signal 2: DAD1 D, Sig=230,16 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   1.140 BB    0.2404   46.83119    2.57193   0.7680
   2   2.329 BB    0.1684   27.09175    2.42310   0.4443
   3   3.127 BB    0.1650 5978.08936  494.61877  98.0318
   4  14.162 BB    0.2078   46.10008    3.40875   0.7560

Totals :                  6098.11238  503.02255


=====================================================================
                        *** End of Report ***
```

Figure S5. HPLC chromatogram of title compound **2**.

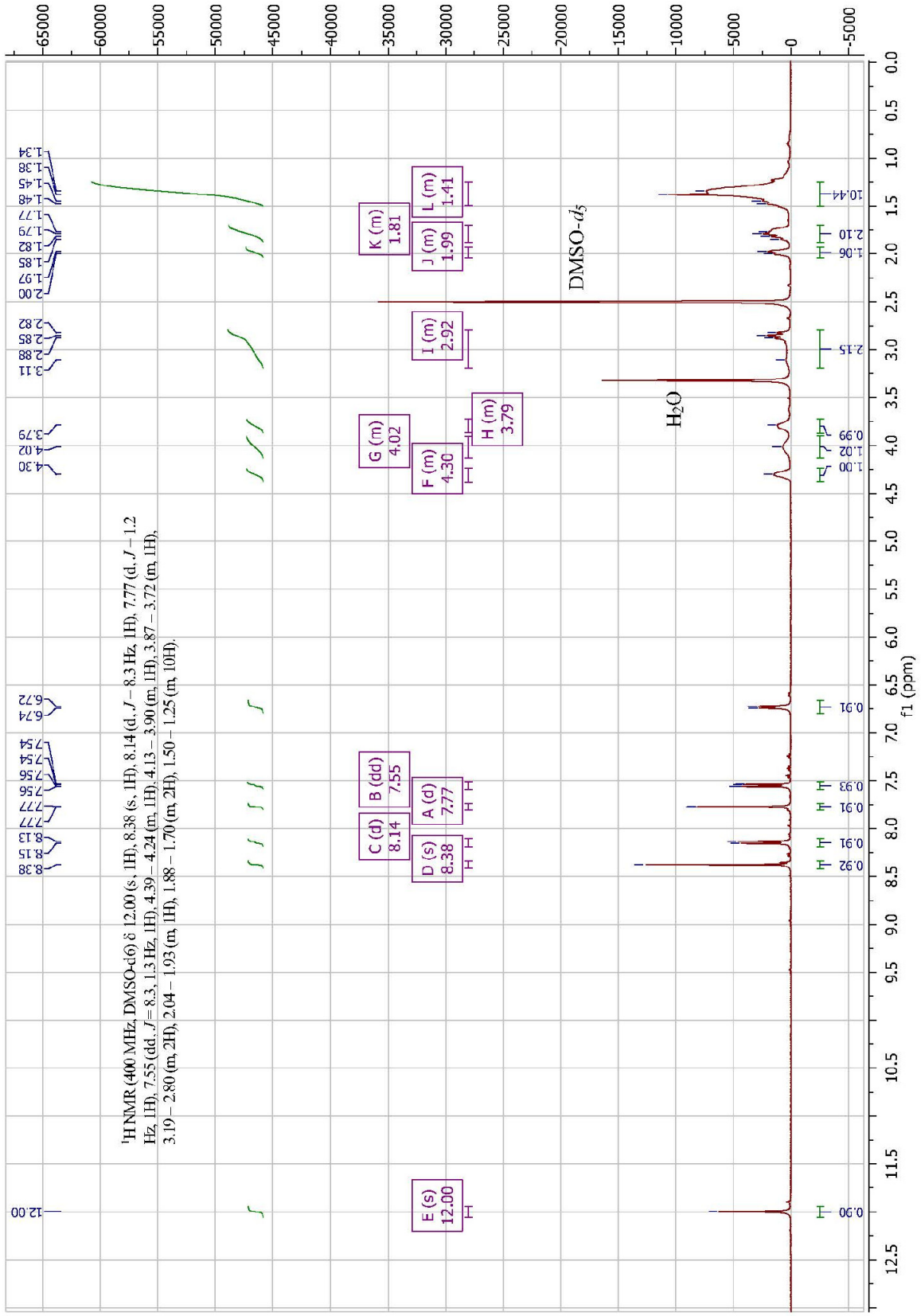


Figure S6. ^{1}H-NMR spectrum of intermediate **4**.

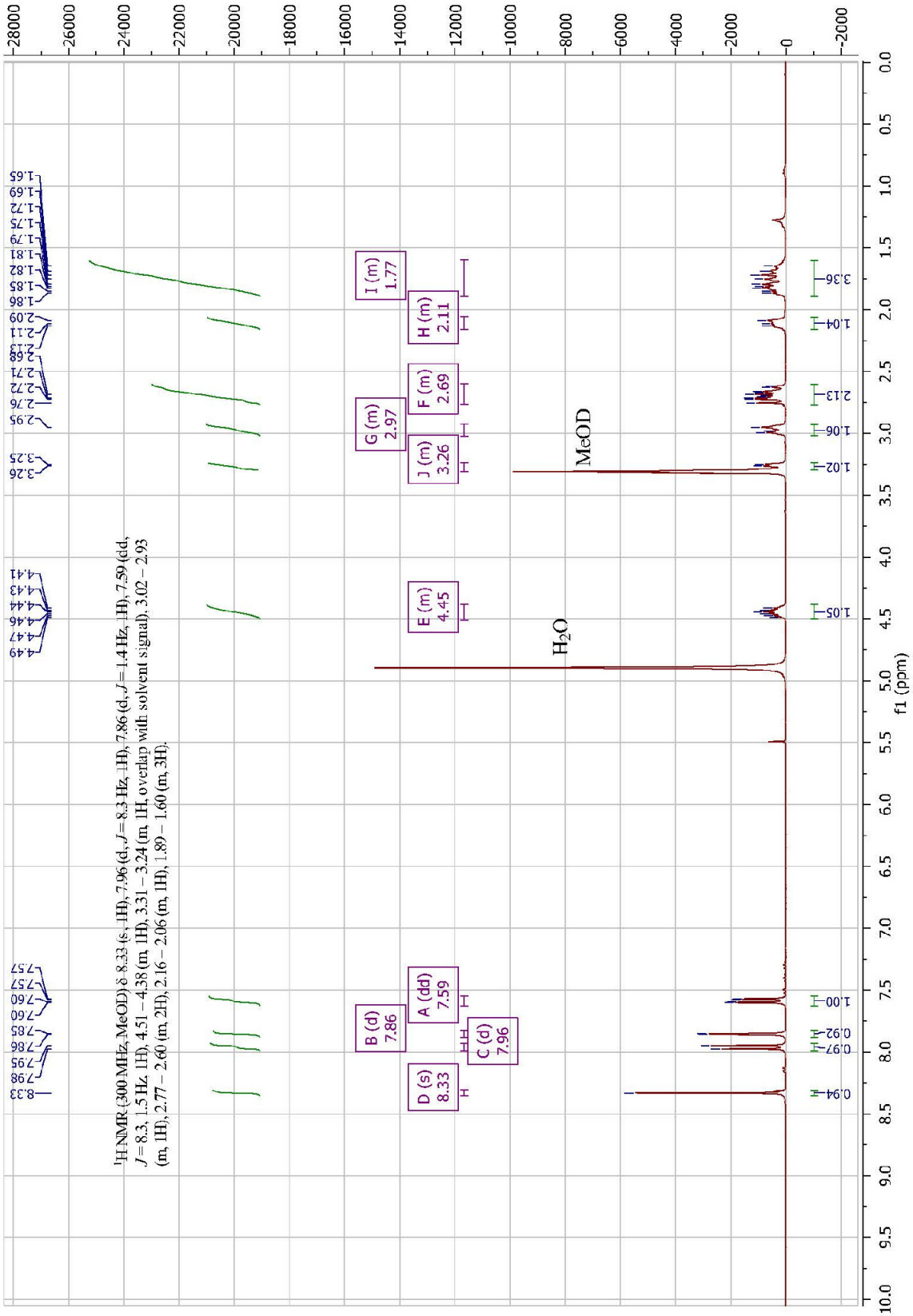


Figure S7. [1]H-NMR spectrum of intermediate **5**.

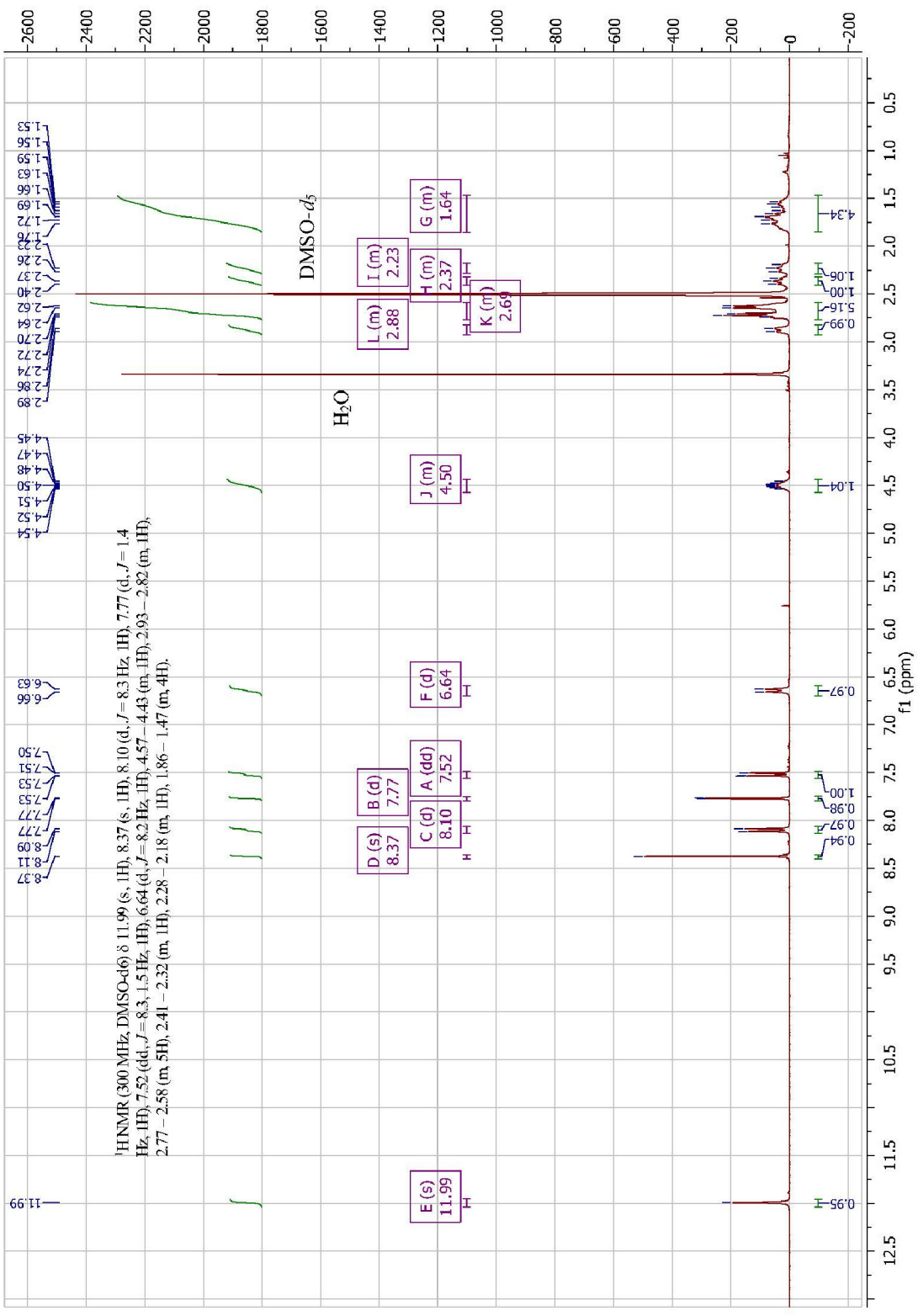
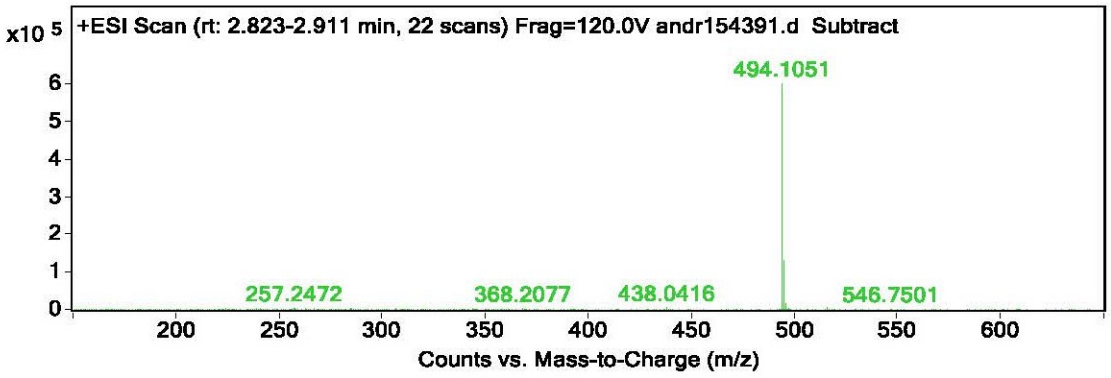


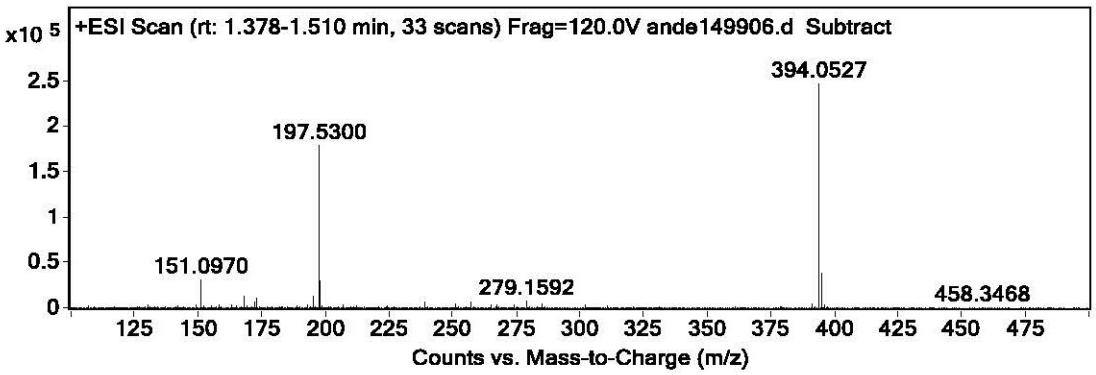
Figure S8. ^{1}H-NMR spectrum of intermediate **6**.



Peak List

m/z	z	Abund
224.1279	1	2606.55
239.2364	1	2906.53
257.2472	1	3186.21
262.8876		2694.11
284.8699		2643.12
285.2786	1	2006.45
368.2077	1	1850.99
438.0416	1	3931.29
494.1051	1	601025.38
495.108	1	129750.55
496.1103	1	14920.21
516.0862	1	3833.79
922.0098	1	1800.38
1009.1839	1	7709.52
1010.1866	1	3628.59

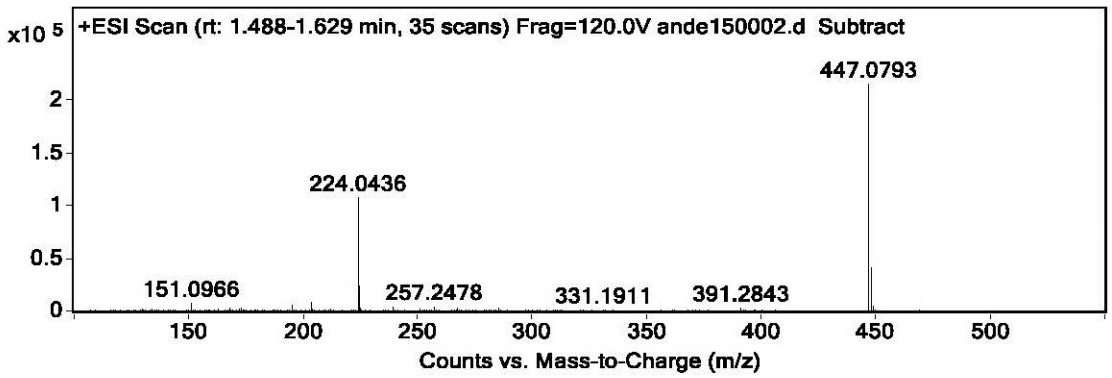
Figure S9. Mass spectrum of intermediate **4**.



Peak List

m/z	z	Abund
89.0604	1	3582.71
107.0703	1	2003
129.0525		1647.48
130.1588	1	3643.3
141.9583	1	2013.26
149.0232	1	3159.04
151.097	1	30956.61
152.1009	1	2144.55
155.1062	1	2352.16
158.1536	1	3500.4
163.1324	1	3540.68
165.112		2090.23
168.1228	1	12526.56
169.1238	1	1830.12
172.1329	1	6333.95
173.0782	1	10355.63
173.1152	1	1685.3
189.0166	2	1895.02
193.1432	1	3802.81
195.1226	1	12710.7
197.53	2	178643.58
198.0317	2	29788.06
198.5328	2	2607.27
207.1588	1	3339.96
212.1492		2485.66
224.1854	1	1974.38
239.2367	1	6339.85
251.1851	1	4566.17
257.2474	1	6688.45
265.1038		3899.7
267.2682	1	3389.5
274.2739	1	3253.18
279.1592	1	7215.59
285.2791	1	4545.89
302.3052	1	3166.62
310.9783	1	2637.5
391.2843	1	4242.23
394.0527	1	246889.47
395.0555	1	37862.16
396.0582	1	3186

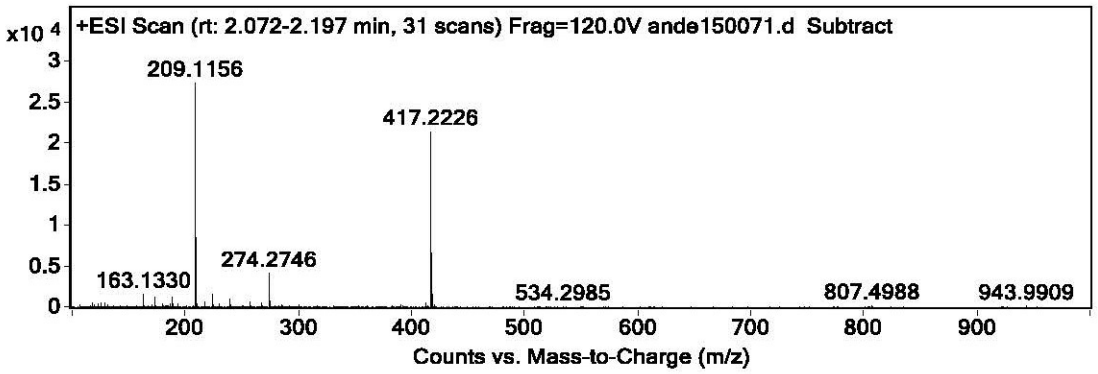
Figure S10. Mass spectrum of intermediate **5**.



Peak List

m/z	z	Abund
89.0602	1	913.58
130.0077		1071.45
134.0634	1	1108.6
151.0966	1	6823.38
158.0027		923.62
163.1327	1	1561.06
168.1231	2	2303.77
172.133		1278.8
173.0786	1	2356.54
186.9562	1	997.71
195.1228	1	5468.87
203.5302	2	7502.79
204.0315	2	1425.95
212.1493	1	1147.02
224.0436	2	107105.57
224.1277	2	1030.83
224.5451	2	23178.67
225.0465	2	2475.59
239.2371	1	3634.52
251.1856	1	1083.14
257.2478	1	3735.28
267.2683	1	2066.24
279.1592	1	929.51
285.2796	1	2041.57
391.2843	1	2459.33
447.0793	1	214960.52
448.0822	1	40278.11
449.0845	1	4022.36
837.3559	1	1714.35
922.0098	1	2077.62

Figure S11. Mass spectrum of intermediate **6**.



Peak List

m/z	z	Abund
107.0706		220.89
118.0865	1	529.43
120.0112		293.88
122.9641		354.92
125.9862		512.92
129.0525	1	444.36
131.9296		218.15
163.133	1	1528.23
171.0626		240.93
173.079	1	1182.3
180.1595	1	406.68
186.9567		406.12
188.6021	2	1181.7
189.1039	2	385.57
194.1174		356.4
209.1156	2	27320.22
209.6166	2	8481.56
210.1174	2	2114.8
210.6166	2	388.14
217.1054	1	569.8
224.1284	1	1554.94
225.1325	1	267.08
230.2475	1	406.71
239.2374	1	937.15
257.2482	1	587.34
267.2685	1	481.84
274.2746	1	4072.26
275.2778	1	673.85
285.2797	1	280.91
301.1412		310.85
391.2847	1	308.3
413.2664	1	490.8
417.2226	1	21383.16
418.2249	1	6630.94
419.2244	1	1597.71
420.2241	1	268.22

Figure S12. Mass spectrum of intermediate **7**.