

Supplementary Information

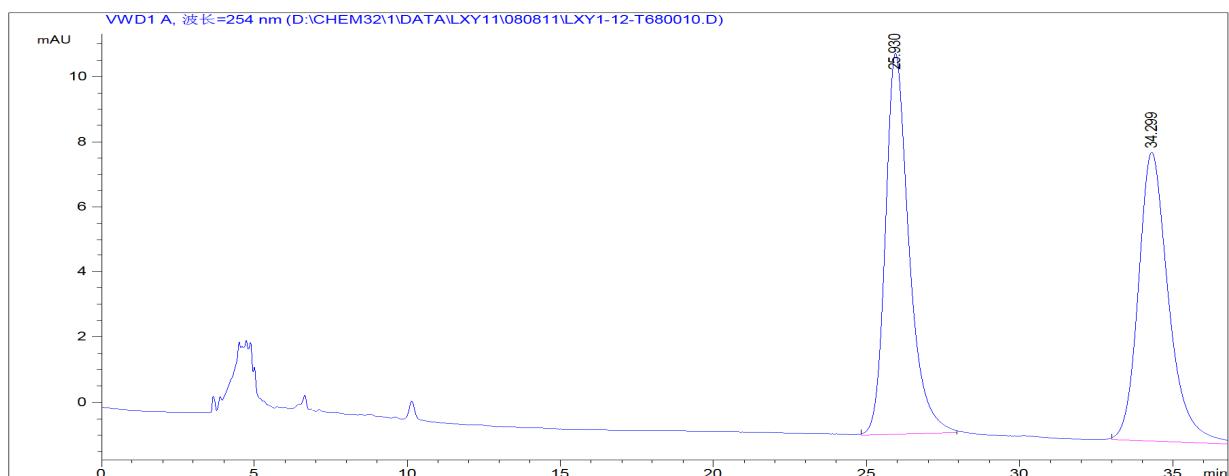
Catalytic Asymmetric Michael Addition of α , β -Unsaturated Aldehydes with Ni(II) Complexes of the Schiff Base of Glycine

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Xinmiao Liang, Jinxing Ye*

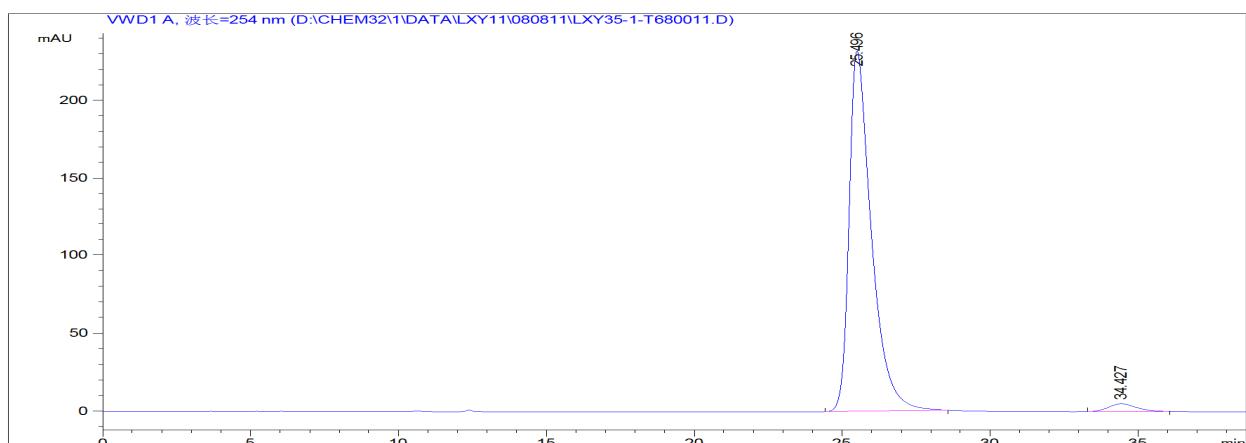
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A: HPLC Analysis of Products

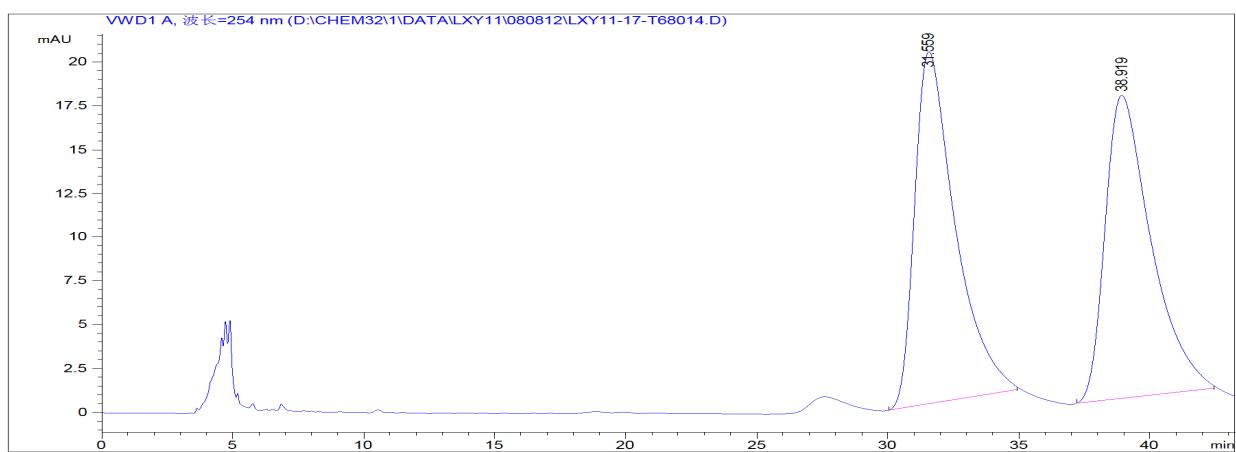


峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	*s	峰面积 [mAU]	峰高 [mAU]	峰面积 %
1	25.930	MM R	0.8935	627.18622		11.69965	50.9207	
2	34.299	MM R	1.1371	604.50586		8.86067	49.0793	
总量 :							1231.69208	20.56032

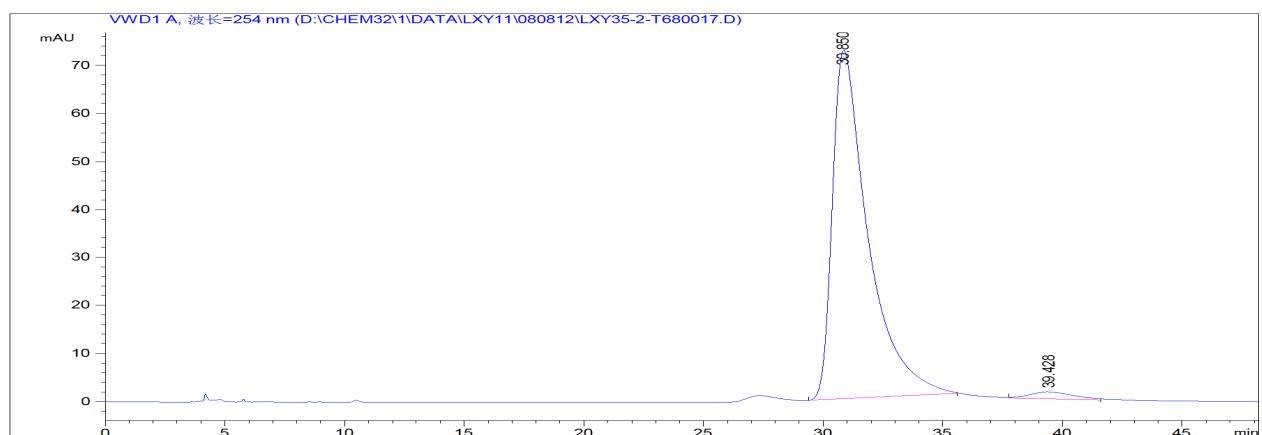


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	25.496	BB	0.7805	1.21470e4		231.72899	97.4051
2	34.427	BB	0.9614	323.59479		4.96462	2.5949
总量 :						1.24706e4	236.69361

Figure S-1. Racemic and optically enriched HPLC chromatogram of compound **7aa-major**.

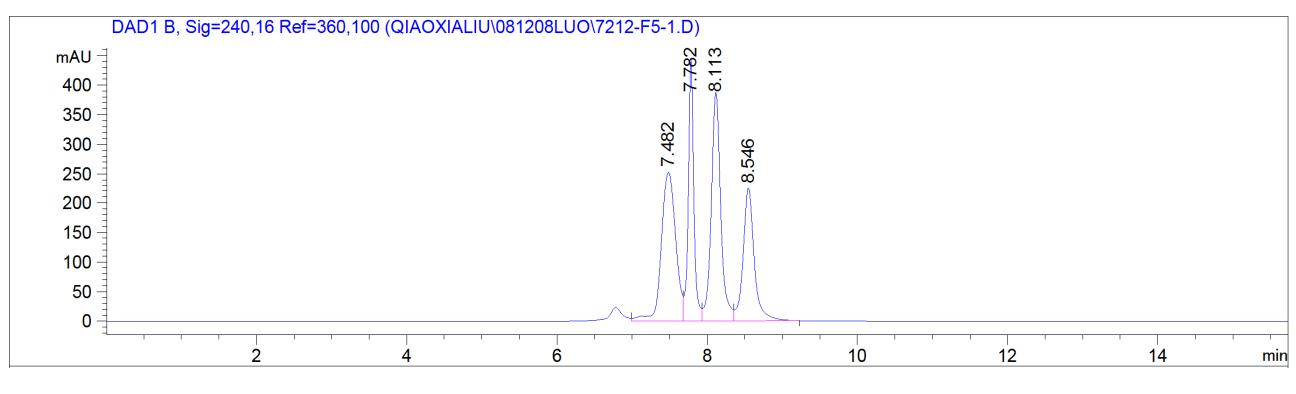


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	31.559	BB	1.5374	2163.62378		20.09137	50.6166
2	38.919	BB	1.7126	2110.90625		17.30837	49.3834
总量 :				4274.53003		37.39974	

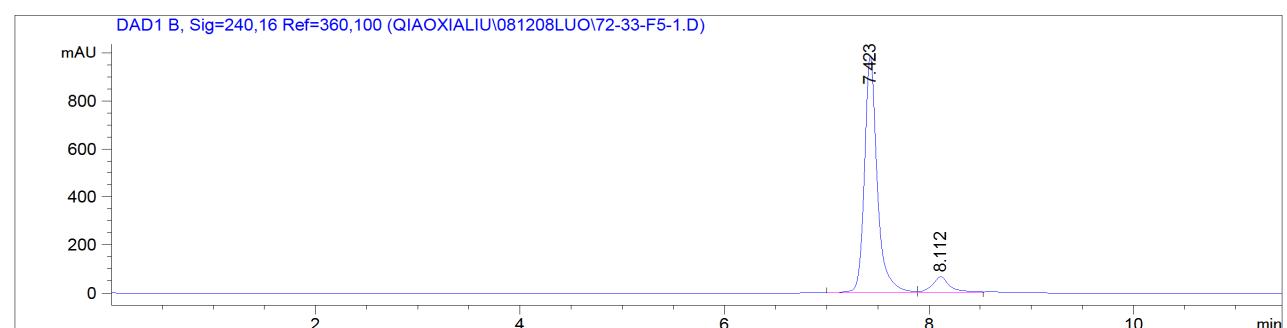


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	30.850	BB	1.4967	7519.68604		72.59675	97.6336
2	39.428	MM R	2.1006	182.26198		1.44611	2.3664
总量 :				7701.94801		74.04286	

Figure S-2. Racemic and optically enriched HPLC chromatogram of compound **7aa-minor**.



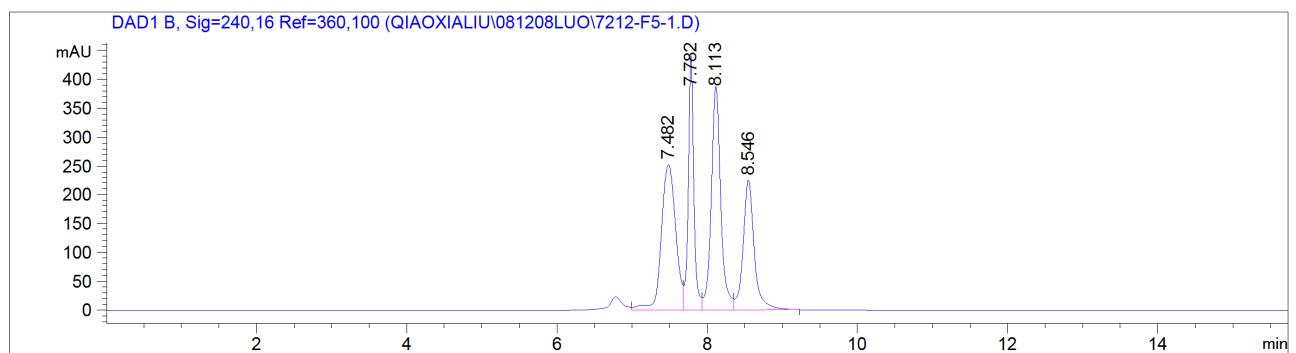
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.482	VV	0.2070	3360.41479	252.95384	29.5266
2	7.782	VV	0.0759	2270.90332	442.56232	19.9535
3	8.113	VV	0.1330	3420.32373	387.57928	30.0530
4	8.546	VB	0.1528	2329.33984	224.95746	20.4670
总量 :				1.13810e4	1308.05290	



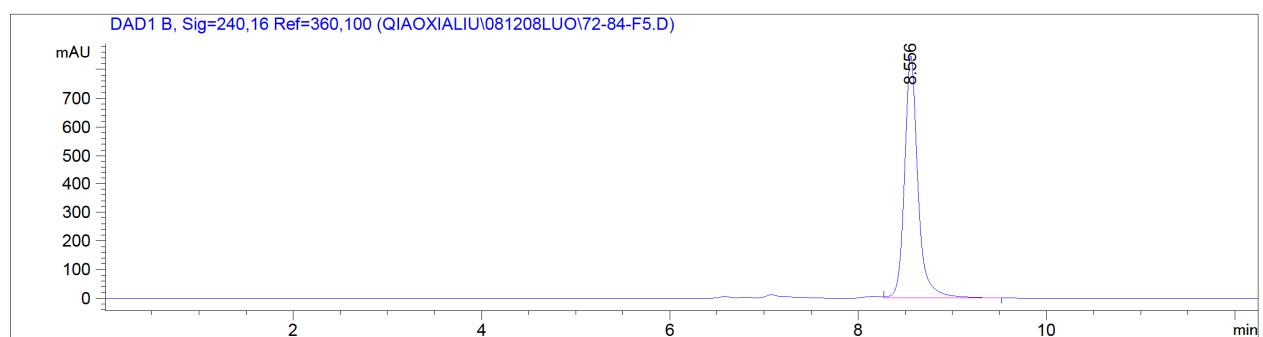
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.423	VV	0.1324	8673.05957	987.84760	90.6399
2	8.112	VV	0.1857	895.64331	68.00128	9.3601

总量 : 9568.70288 1055.84888

Figure S-3. Racemic and optically enriched HPLC chromatogram of compound **7ba-major**.



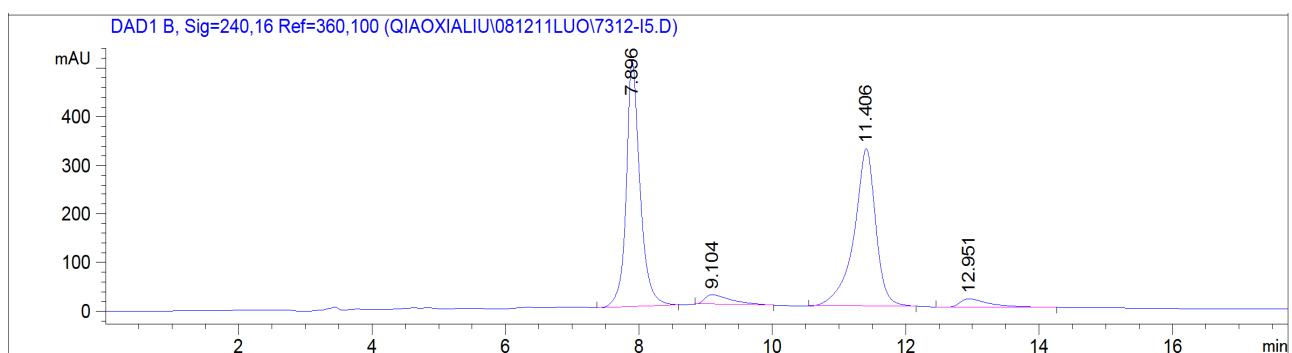
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.482	VV	0.2070	3360.41479	252.95384	29.5266
2	7.782	VV	0.0759	2270.90332	442.56232	19.9535
3	8.113	VV	0.1330	3420.32373	387.57928	30.0530
4	8.546	VB	0.1528	2329.33984	224.95746	20.4670
总量 :				1.13810e4	1308.05290	



信号 1: DAD1 B, Sig=240,16 Ref=360,100

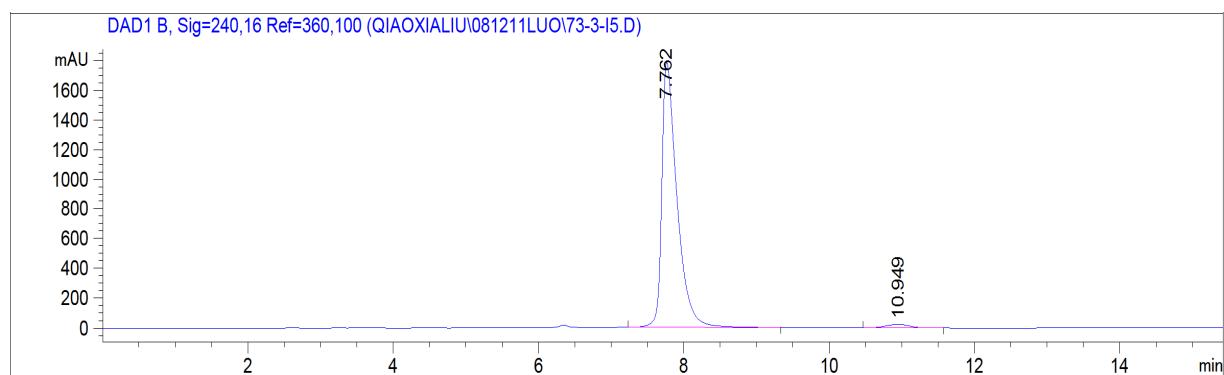
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.556	VB	0.1502	8443.38672	847.67200	100.0000
总量 :						8443.38672 847.67200

Figure S-4. Racemic and optically enriched HPLC chromatogram of compound **7ba-minor**.



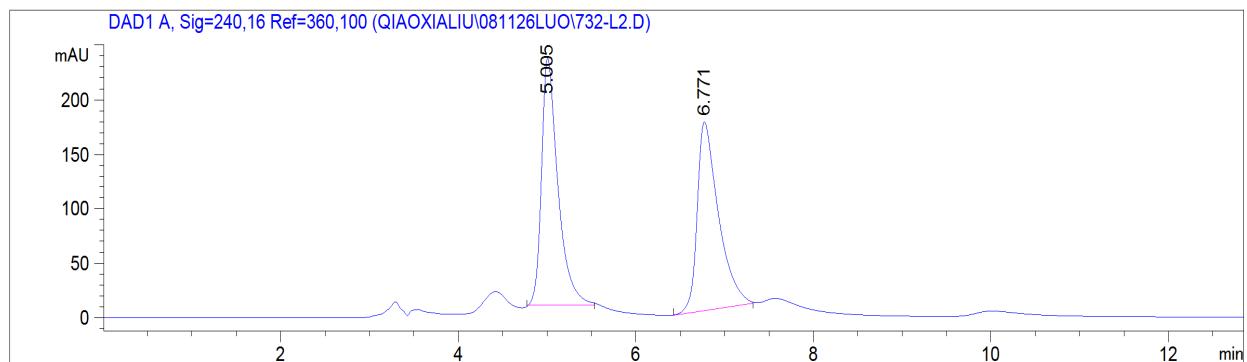
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.896	MM R	0.2205	7258.92236	505.13535	46.2437
2	9.104	MM R	0.4664	546.55261	19.53179	3.4819
3	11.406	MM R	0.3407	7330.60156	323.98285	46.7004
4	12.951	MM R	0.5393	561.02063	17.33781	3.5740

总量 : 1.56971e4 865.98779

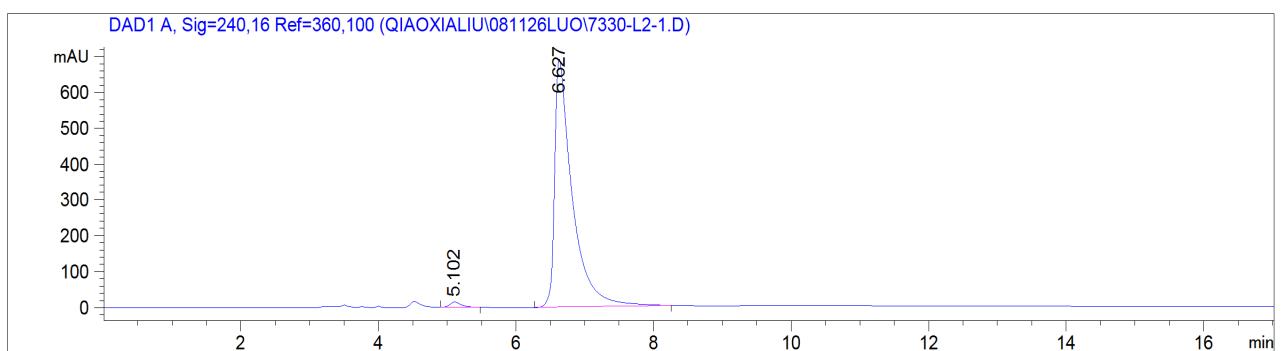


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.762	BB	0.2139	2.60252e4	1786.74341	97.8440
2	10.949	BB	0.3591	573.47766	24.67860	2.1560
总量 :						2.65987e4 1811.42201

Figure S-5. Racemic and optically enriched HPLC chromatogram of compound **7ca-major**.



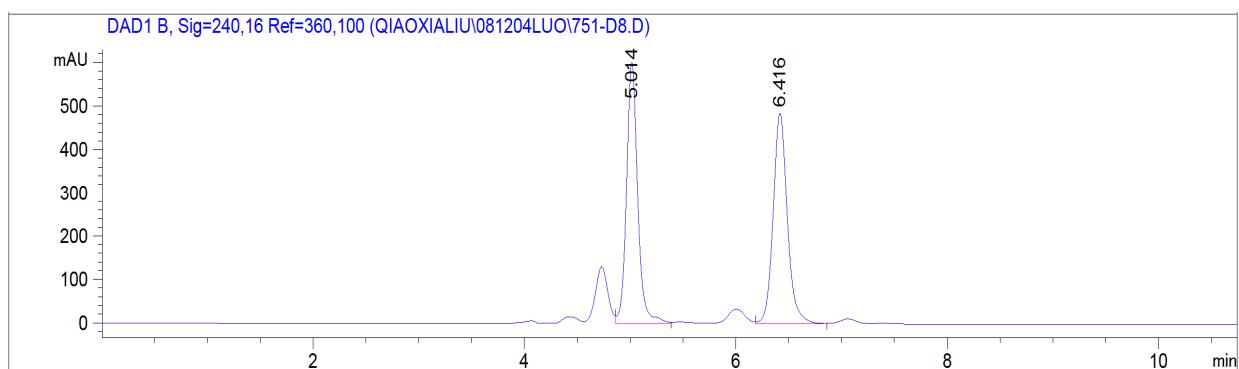
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.005	MM R	0.2141	2914.47998	226.82774	50.1482
2	6.771	MM R	0.2777	2897.25830	173.89793	49.8518
总量 :						5811.73828 400.72568



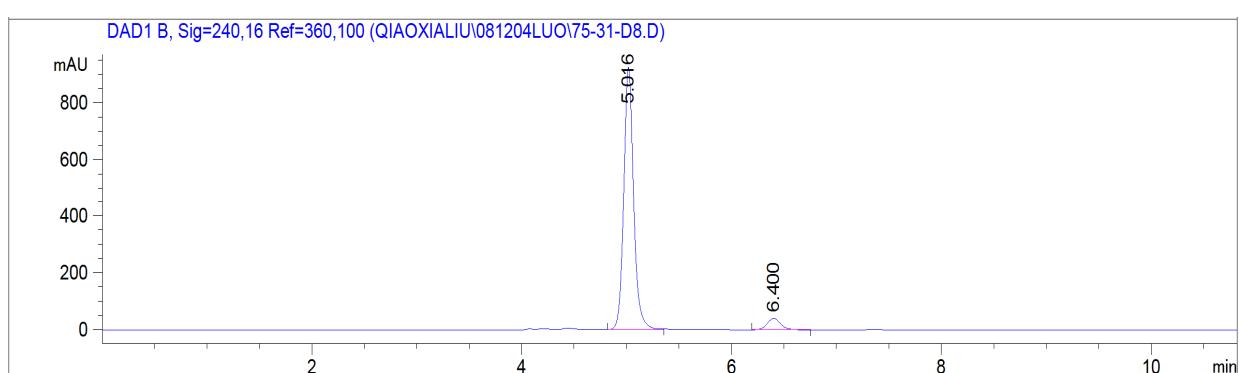
信号 1: DAD1 A, Sig=240,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.102	BB	0.1866	194.78331	15.29746	1.5472
2	6.627	BB	0.2530	1.23947e4	692.01996	98.4528
总量 :					1.25895e4	707.31742

Figure S-6. Racemic and optically enriched HPLC chromatogram of compound **7ca-minor**.

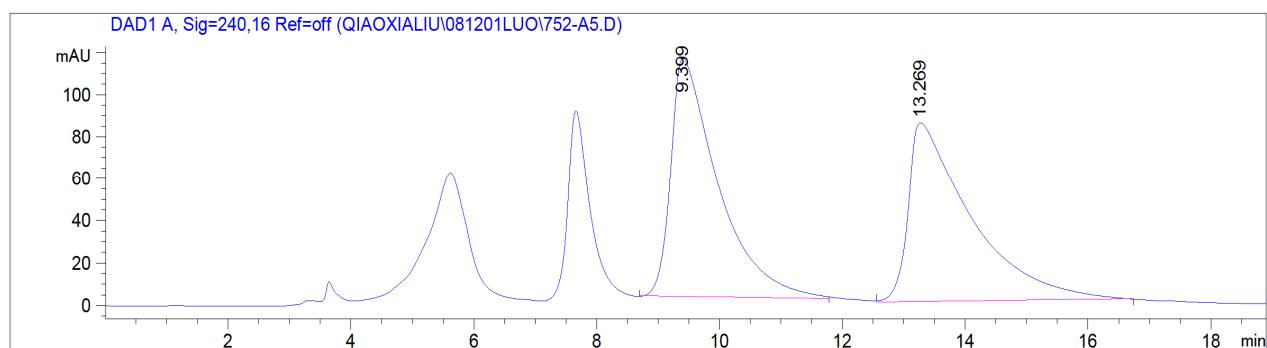


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.014	VV	0.1121	4448.48535	603.01459	49.4125
2	6.416	VB	0.1412	4554.26416	486.55774	50.5875
总量 :					9002.74951	1089.57233

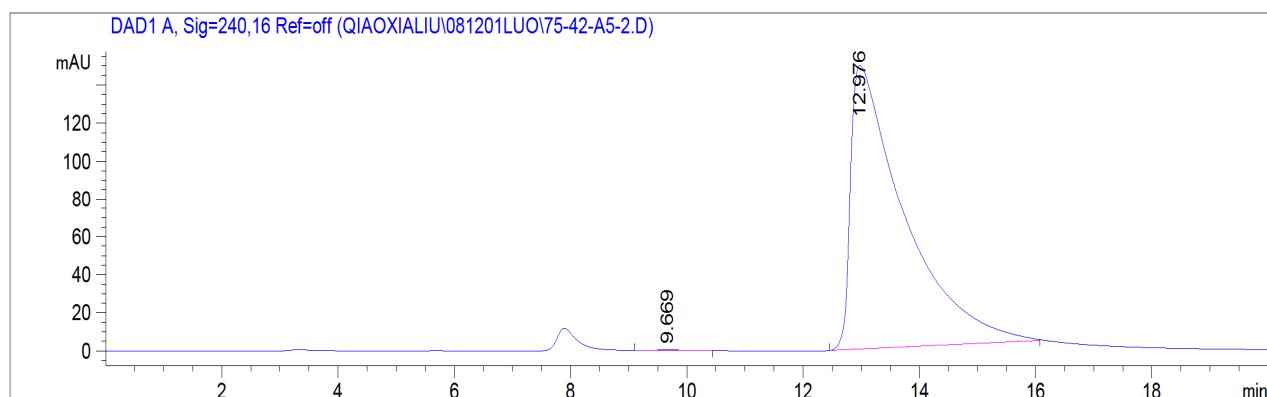


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.016	VB	0.0982	6047.23291	925.65747	94.2731
2	6.400	BB	0.1373	367.35898	40.71919	5.7269
总量 :						6414.59189 966.37666

Figure S-7. Racemic and optically enriched HPLC chromatogram of compound **7da-major**.

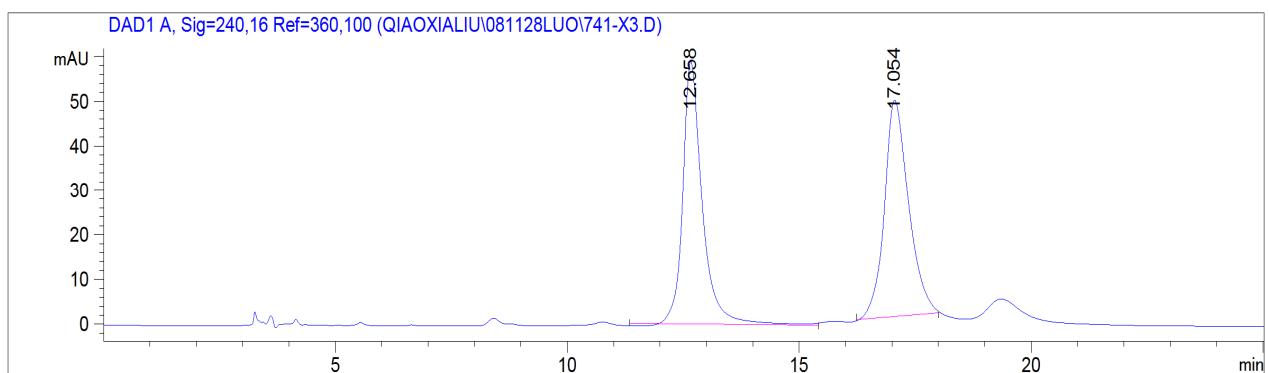


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.399	MM R	0.8887	6022.75830	112.94743	50.1598
2	13.269	MM R	1.1754	5984.38867	84.85582	49.8402
总量 :						1.20071e4 197.80325

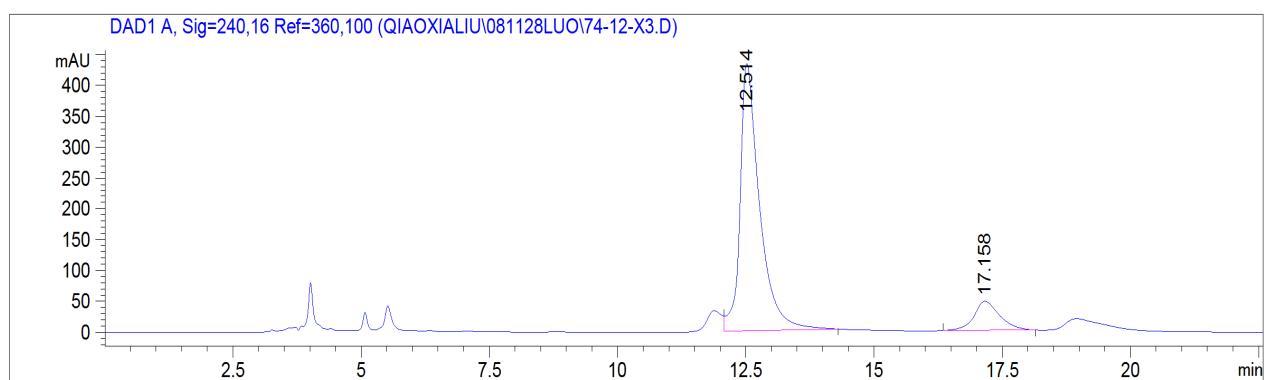


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.669	MM R	0.6743	13.64056	3.37154e-1	0.1417
2	12.976	BB	0.8948	9610.56836	149.34262	99.8583
总量 :						9624.20892 149.67977

Figure S-8. Racemic and optically enriched HPLC chromatogram of compound **7da-minor**.

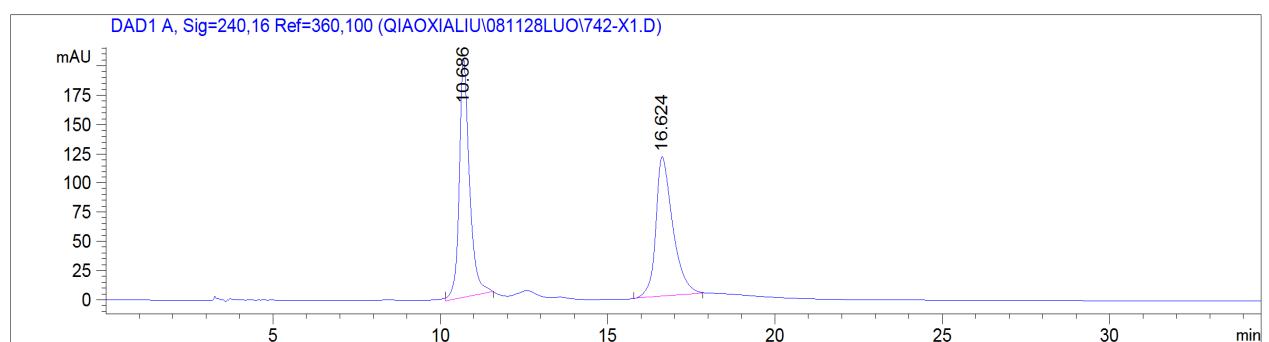


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.658	MM R	0.4914	1735.30737	58.85978	49.5812
2	17.054	MM R	0.6051	1764.61975	48.60346	50.4188
总量 :						3499.92712 107.46324

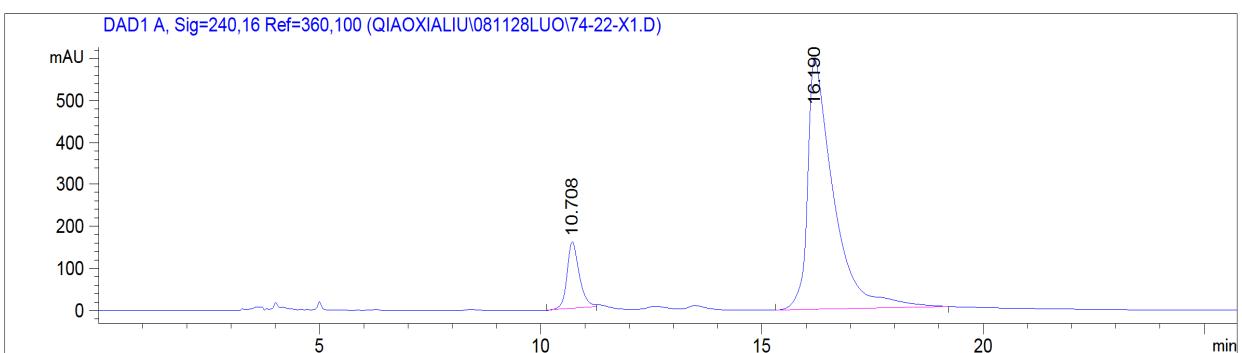


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.514	VB	0.3845	1.15409e4	433.66553	87.3575
2	17.158	BB	0.5178	1670.21484	47.31310	12.6425
总量 :					1.32111e4	480.97863

Figure S-9. Racemic and optically enriched HPLC chromatogram of compound 7ea-major.

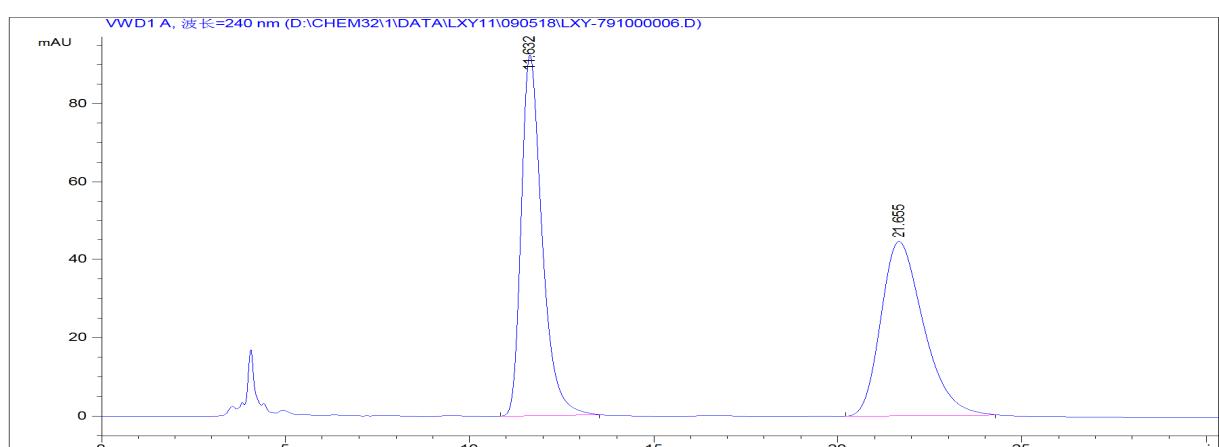


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.686	MM R	0.3554	4339.10400	203.50629	50.6651
2	16.624	BB	0.5168	4225.18652	120.00403	49.3349
总量 :					8564.29053	323.51031

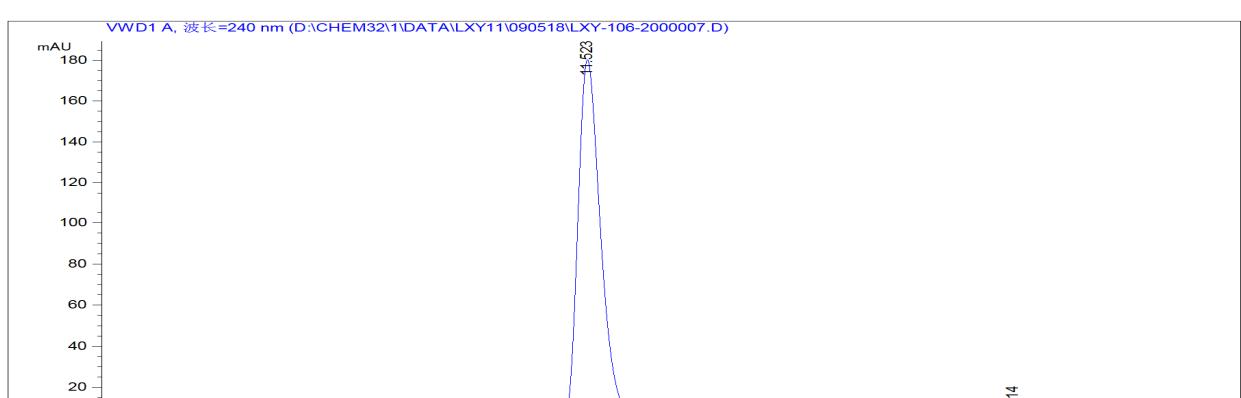


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.708	BB	0.2873	3044.76587	157.68771	11.1085
2	16.190	BB	0.5817	2.43645e4	595.07269	88.8915
总量 :				2.74093e4	752.76041	

Figure S-10. Racemic and optically enriched HPLC chromatogram of compound **7ea-minor**.

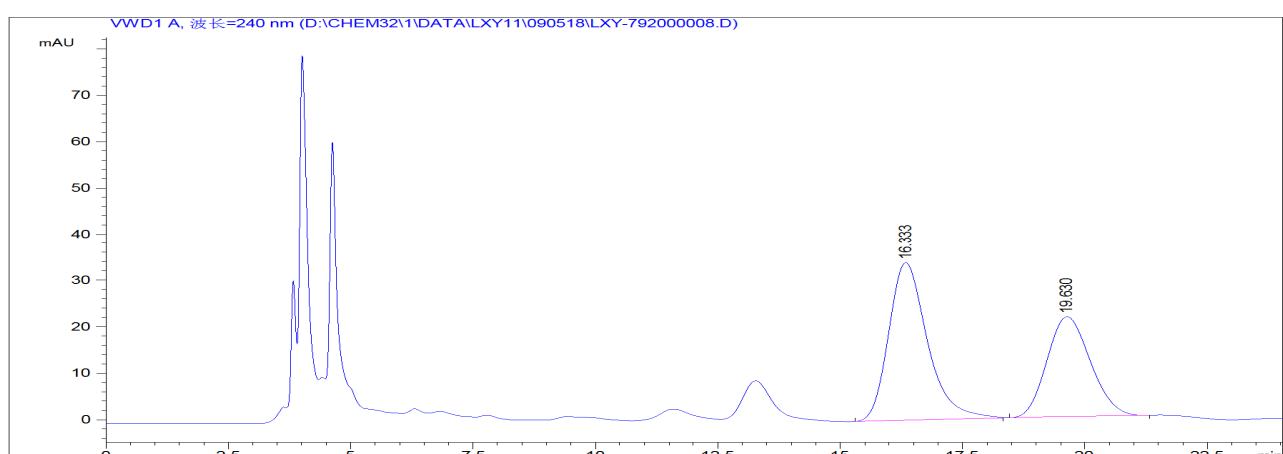


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU * s	峰高 [mAU]	峰面积 %
1	11.632	BB	0.5993	3641.56104	92.46124	50.3907
2	21.655	BB	1.2235	3585.09424	44.51663	49.6093
总量 :				7226.65527	136.97787	



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	11.523	BB	0.5869	7014.01514		180.67999	97.2953
2	21.614	BB	0.9416	194.98051		2.44621	2.7047
总量 :						7208.99565	183.12621

Figure S-11. Racemic and optically enriched HPLC chromatogram of compound **7ab-major**.

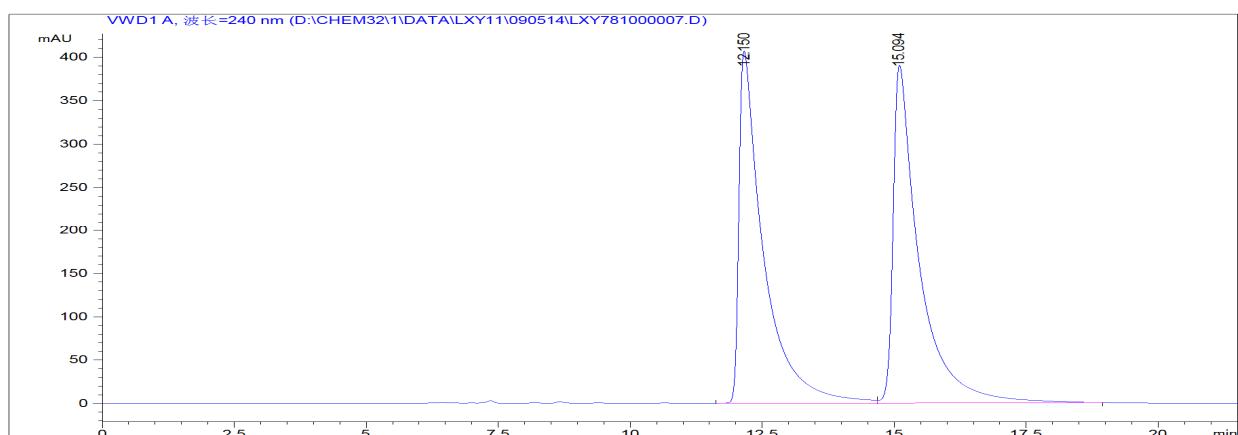


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	16.333	BB	0.8325	1856.97034		33.83324	58.5005
2	19.630	BB	0.9594	1317.30994		21.45834	41.4995
总量 :						3174.28027	55.29158

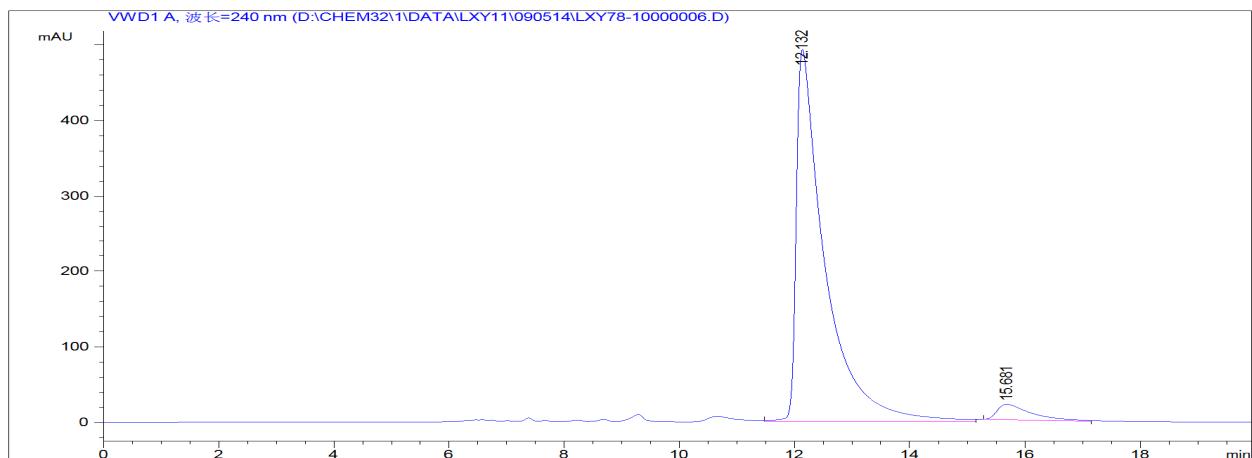


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	16.329	BB	0.8035	221.35989	3.71210	4.1094
2	19.506	BB	0.9776	5165.24756	81.40826	95.8906
总量 :					5386.60745	85.12035

Figure S-12. Racemic and optically enriched HPLC chromatogram of compound **7ab-minor**.

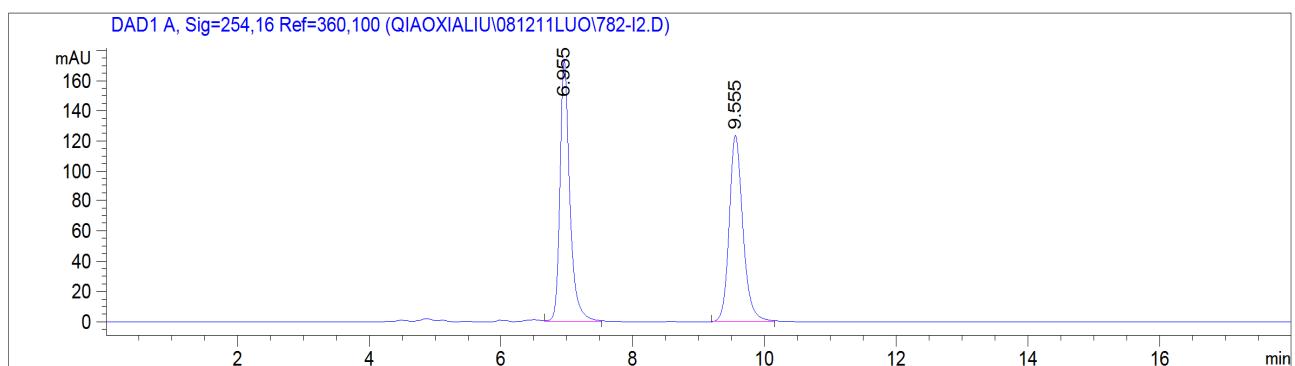


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	12.150	BV	0.4472	1.31642e4	407.09341	49.5974
2	15.094	VB	0.4784	1.33779e4	390.38611	50.4026
总量 :					2.65422e4	797.47952

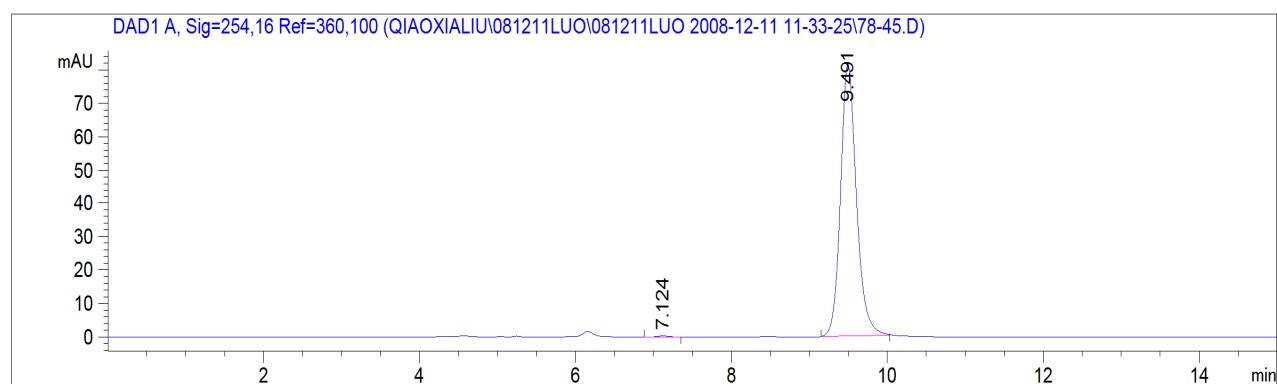


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	12.132	VB	0.4796	1.69914e4	492.55096	95.2877
2	15.681	MM R	0.6881	840.28003	20.35279	4.7123
总量 :					1.78317e4	512.90375

Figure S-13. Racemic and optically enriched HPLC chromatogram of compound **7ac-major**.

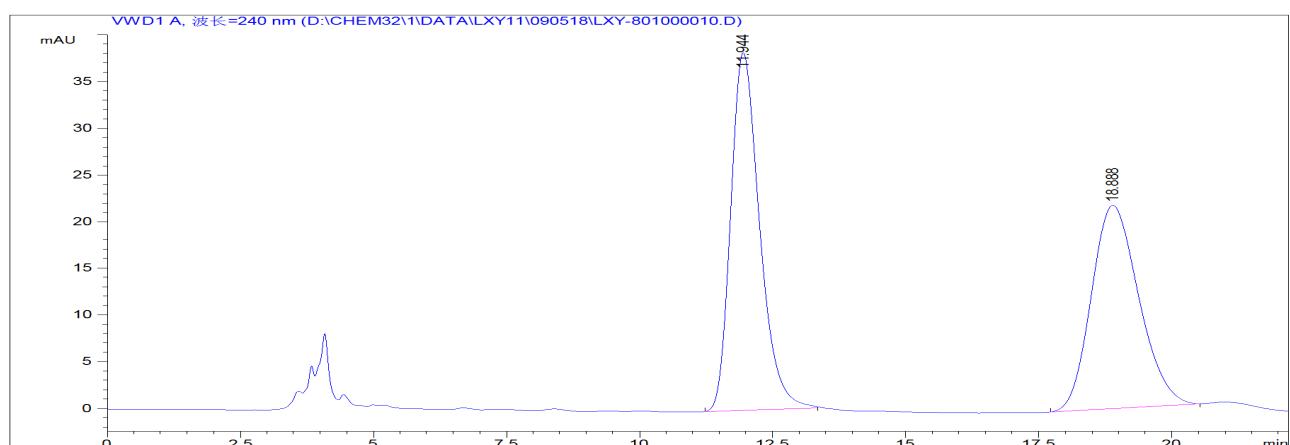


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.955	VB	0.1531	1798.81421	173.32510	50.2388
2	9.555	BB	0.2181	1781.71082	123.65146	49.7612
总量 :					3580.52502	296.97656

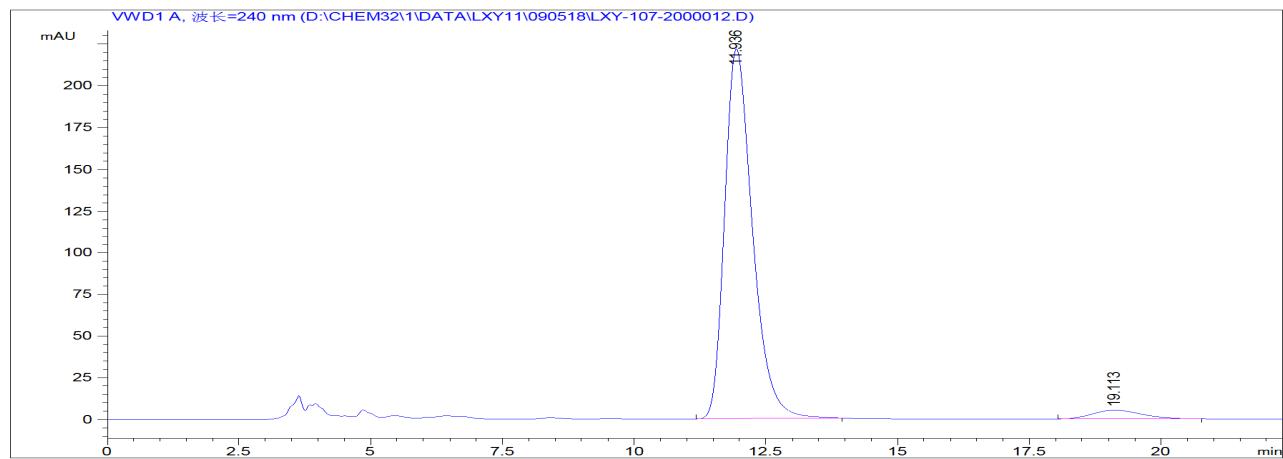


峰	保留时间	类型	峰宽	峰面积	峰高	峰面积
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.124	MM R	0.2324	5.42792	3.89243e-1	0.4661
2	9.491	BB	0.2158	1159.18140	81.58594	99.5339
总量 :					1164.60932	81.97518

Figure S-14. Racemic and optically enriched HPLC chromatogram of compound **7ac-minor**.

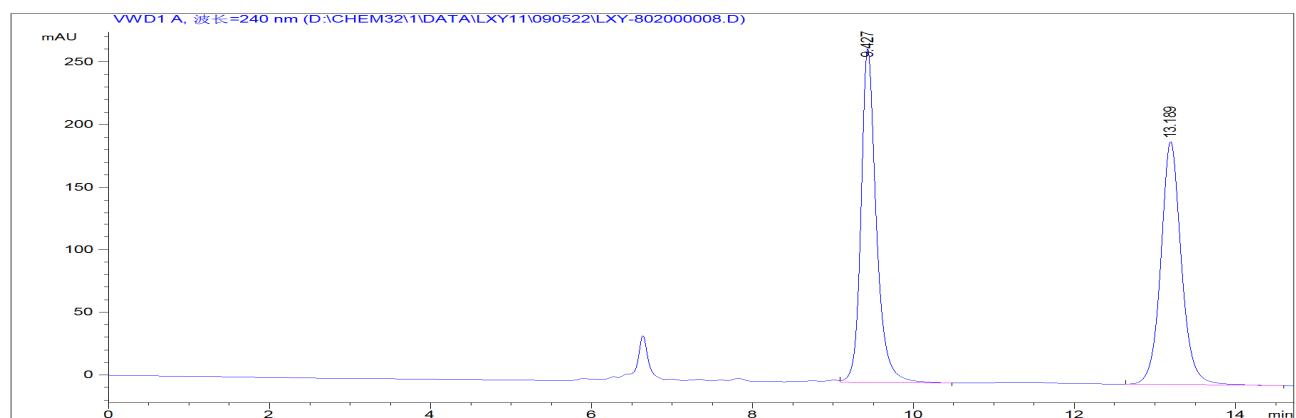


峰	保留时间	类型	峰宽	峰面积	峰高	峰面积
#	[min]		[min]	mAU * s	[mAU]	%
1	11.944	BB	0.5786	1445.01611	38.28611	51.7842
2	18.888	BB	0.9462	1345.44226	21.82915	48.2158
总量 :					2790.45837	60.11526

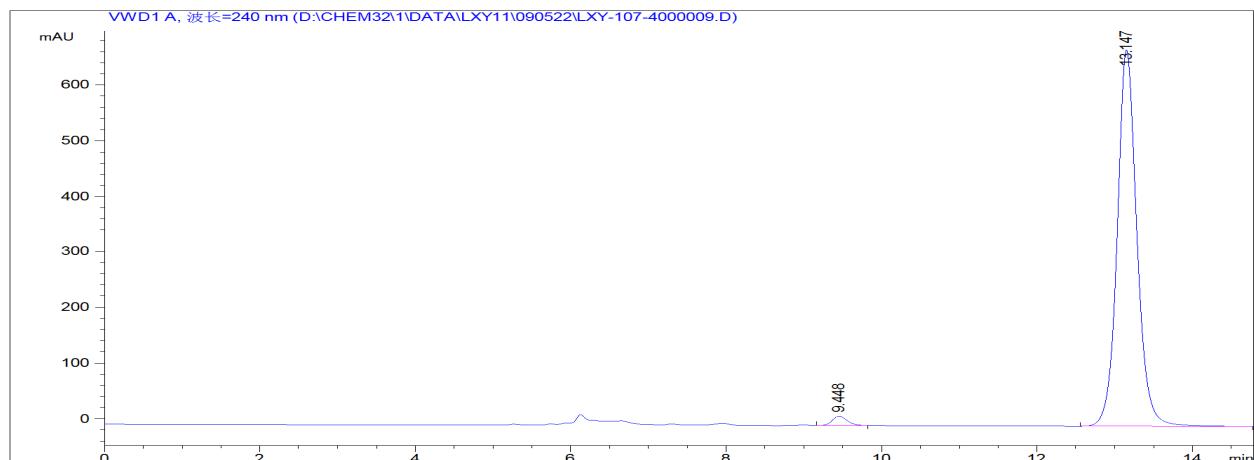


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	11.936	BB	0.5647	8151.35303	221.52138	95.9772
2	19.113	BB	0.9206	341.65982	5.26161	4.0228
总量 :						8493.01285 226.78299

Figure S-15. Racemic and optically enriched HPLC chromatogram of compound **7ad-major**.

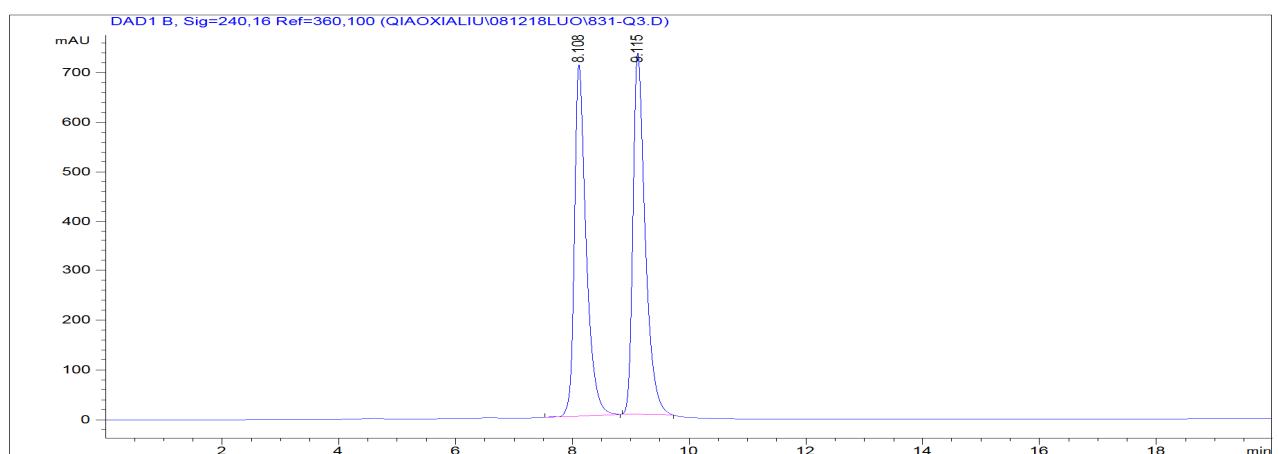


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	9.427	VB	0.1963	3518.21729	266.42493	50.5501
2	13.189	BB	0.2678	3441.64624	194.27721	49.4499
总量 :						6959.86353 460.70213

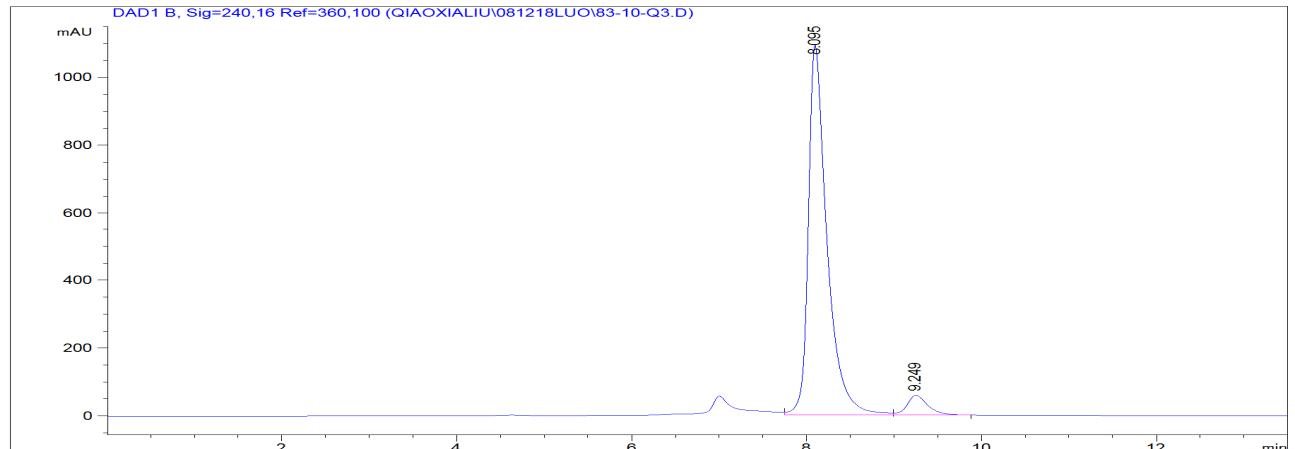


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 [mAU]	峰面积 %
1	9.448	VV	0.2103	241.85493	17.23767	1.9950
2	13.147	BB	0.2661	1.18813e4	676.40424	98.0050
总量 :					1.21232e4	693.64191

Figure S-16. Racemic and optically enriched HPLC chromatogram of compound **7ad-minor**.

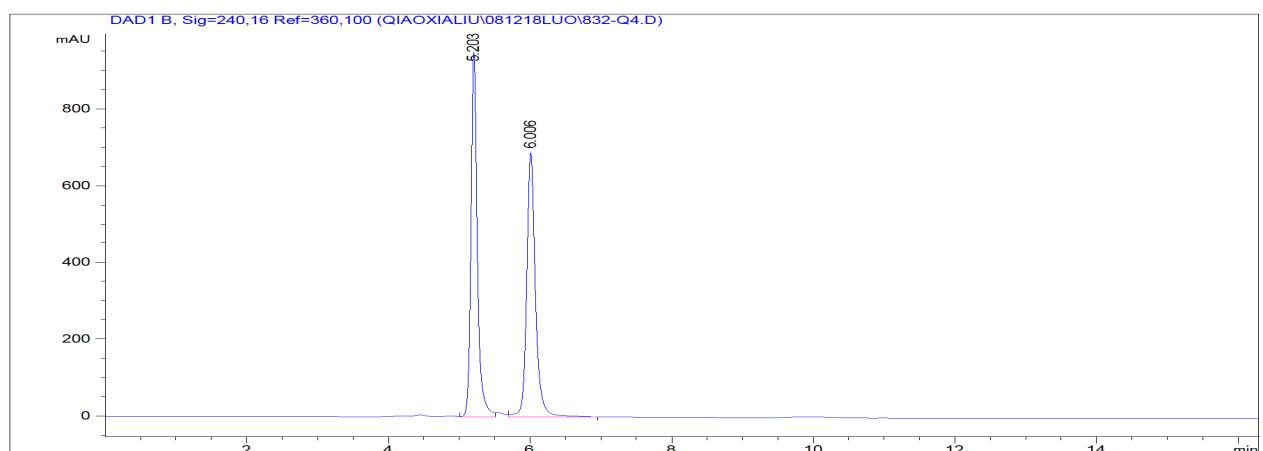


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.108	MM R	0.2323	9887.60840	709.44495	48.3234
2	9.115	MM R	0.2417	1.05737e4	729.17169	51.6766
总量 :					2.04613e4	1438.61664

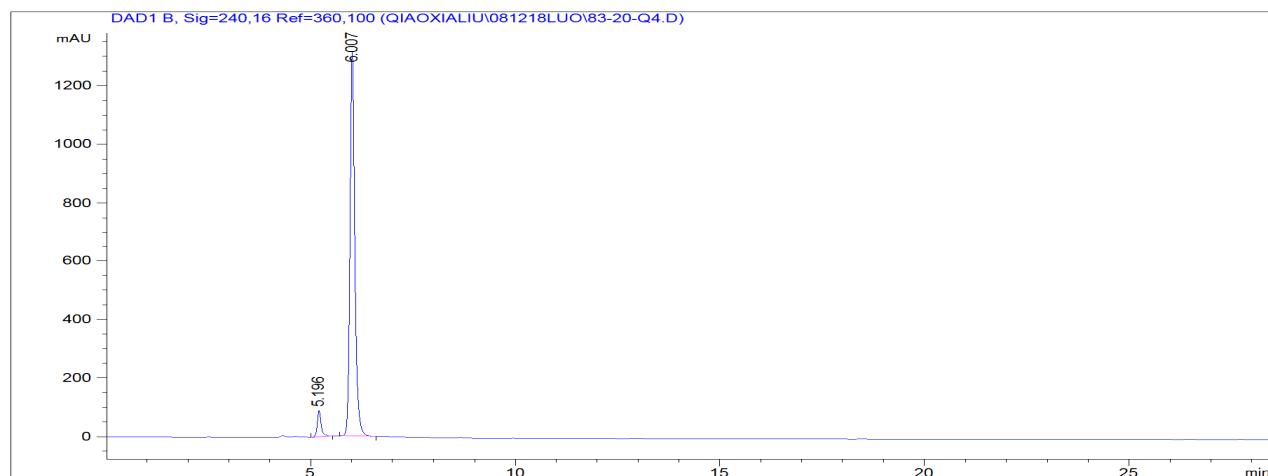


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.095	BV	0.2177	1.62811e4	1093.46899	94.2626
2	9.249	VB	0.2488	990.96753	58.75582	5.7374
总量 :				1.72721e4	1152.22481	

Figure S-17. Racemic and optically enriched HPLC chromatogram of compound **7ae-major**.

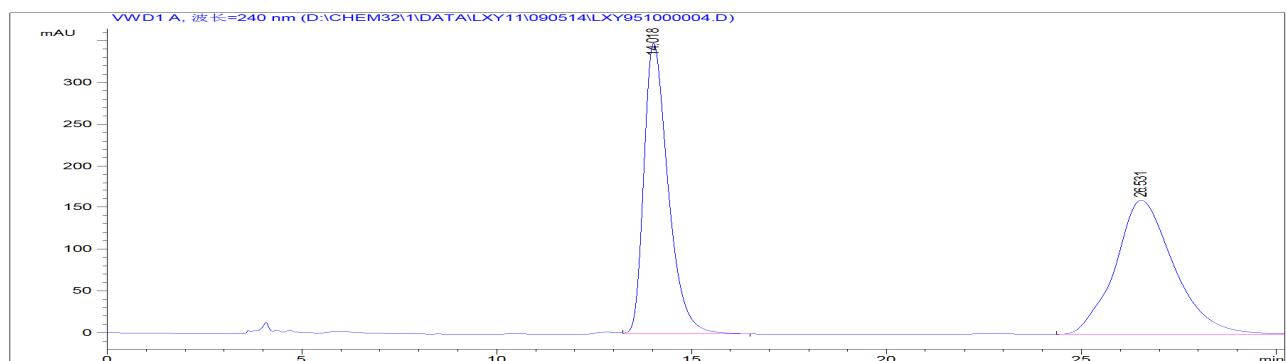


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.203	VV	0.0925	5910.17139	950.47656	49.9464
2	6.006	VB	0.1282	5922.86182	689.64862	50.0536
总量 :						1.18330e4 1640.12518

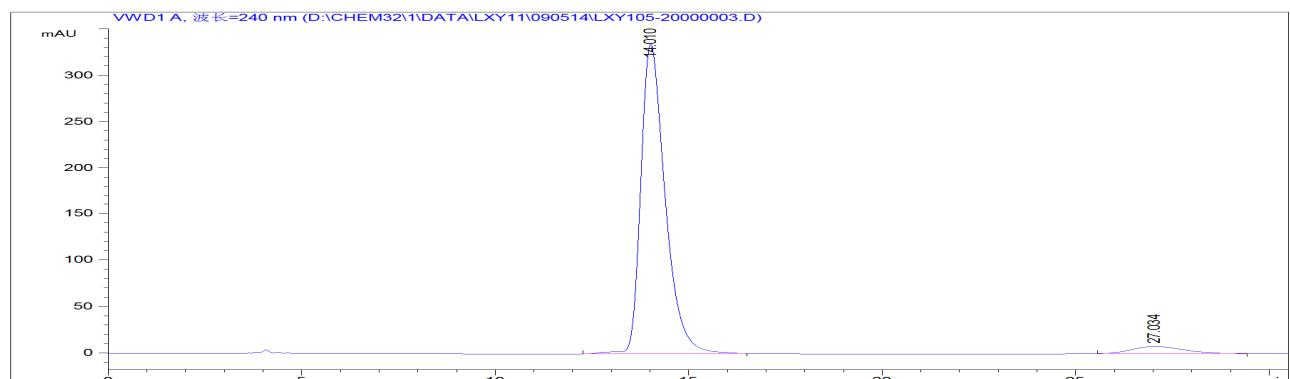


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.196	VB	0.0993	615.97278	90.61393	5.3933
2	6.007	BB	0.1240	1.08052e4	1313.02502	94.6067
总量 :						1.14211e4 1403.63895

Figure S-18. Racemic and optically enriched HPLC chromatogram of compound **7ae-minor**.

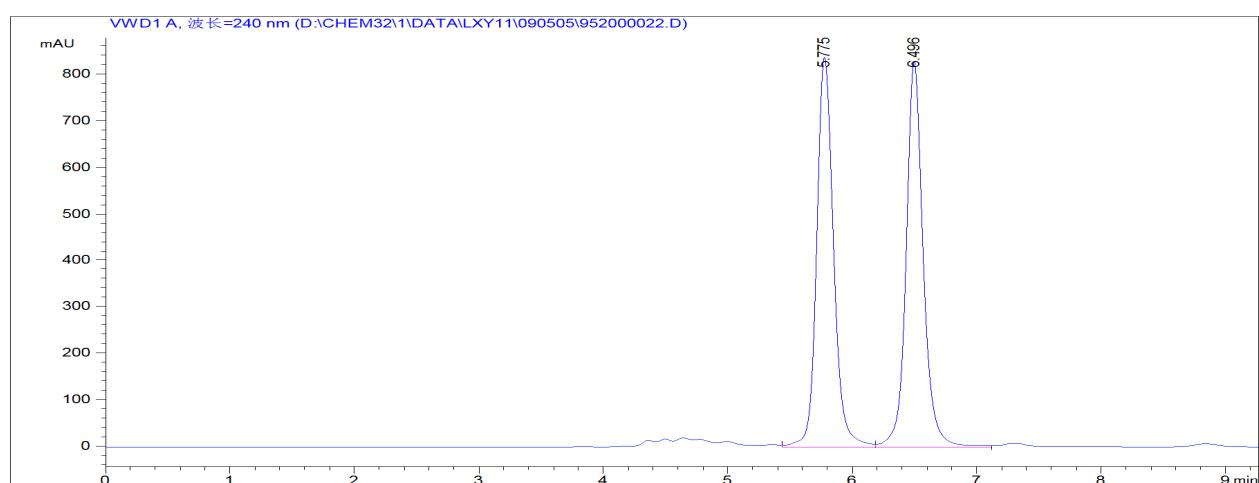


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	14.018	VB	0.6640	1.51049e4		348.75403	47.3120
2	26.531	BBA	1.5528	1.68212e4		160.17230	52.6880
总量 :				3.19261e4		508.92633	

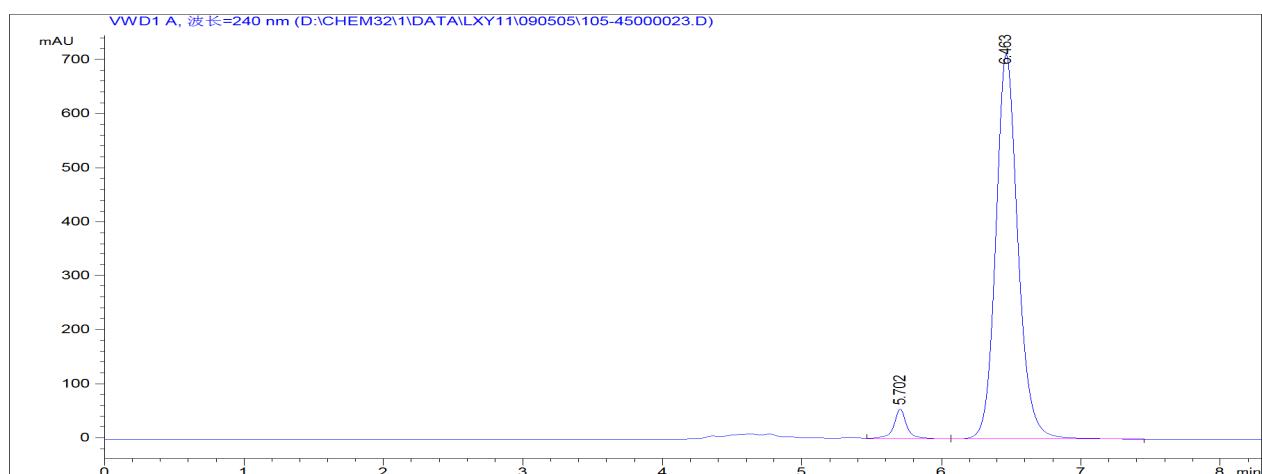


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	*s	峰高 [mAU]	峰面积 %
1	14.010	BB	0.6682	1.45924e4		334.12091	95.3558
2	27.034	BB	1.3105	710.71002		7.72656	4.6442
总量 :				1.53031e4		341.84747	

Figure S-19. Racemic and optically enriched HPLC chromatogram of compound 7af-major.

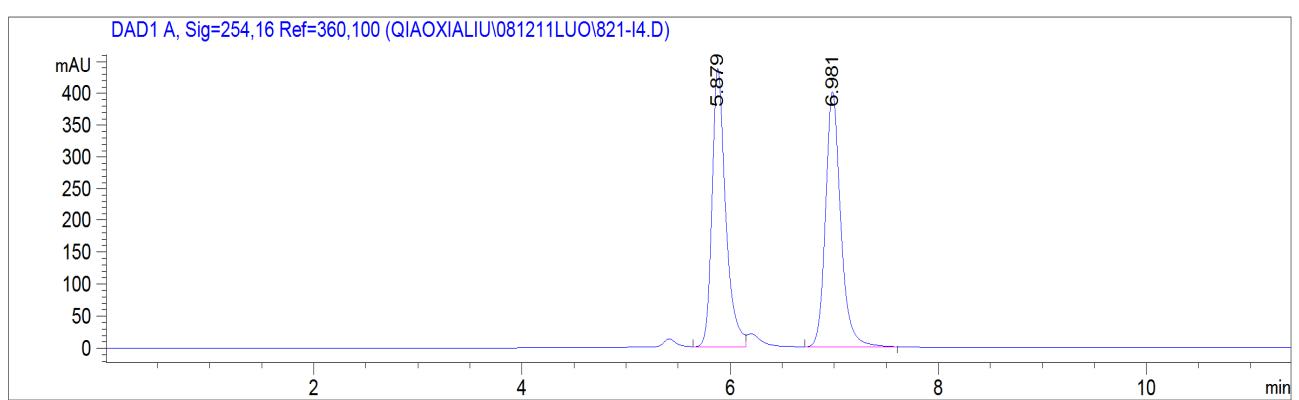


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	5.775	VV	0.1453	7928.59766	838.29089	49.9412
2	6.496	VV	0.1438	7947.27686	829.29688	50.0588
总量 :				1.58759e4	1667.58777	

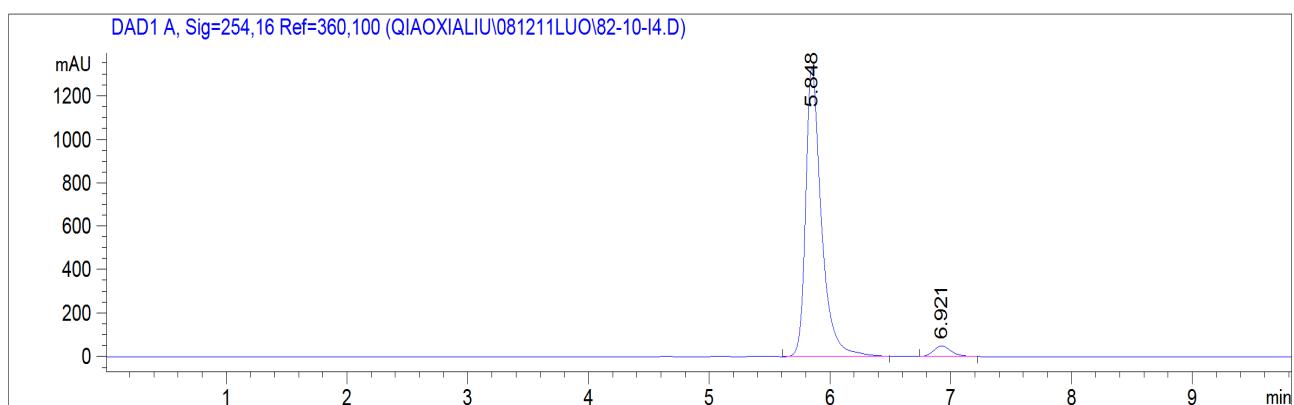


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	5.702	VV	0.1002	389.40747	55.88429	4.7114
2	6.463	VB	0.1670	7875.88867	711.58185	95.2886
总量 :				8265.29614	767.46614	

Figure S-20. Racemic and optically enriched HPLC chromatogram of compound **7af-minor**.

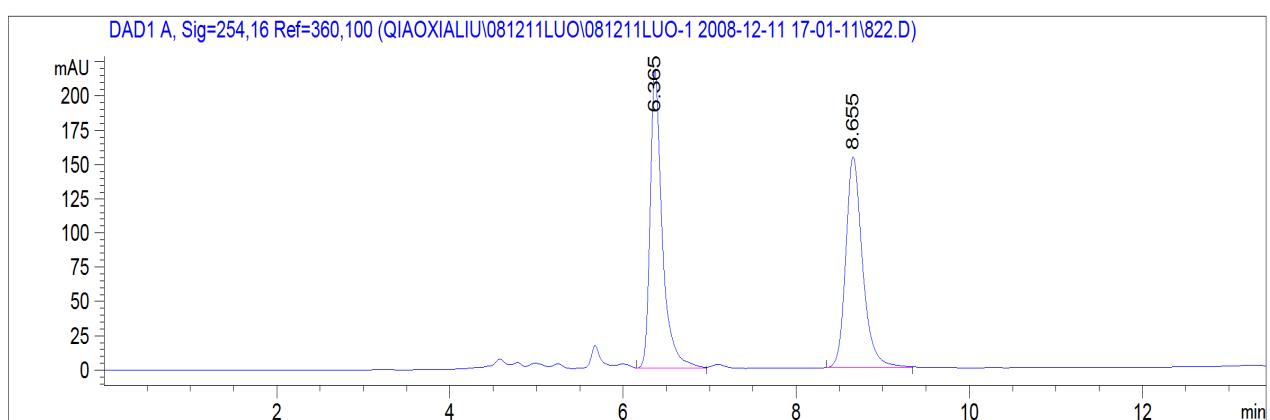


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.879	VV	0.1363	3993.96899	438.34521	49.5141
2	6.981	BB	0.1525	4072.35937	401.05209	50.4859
总量 :						8066.32837 839.39731

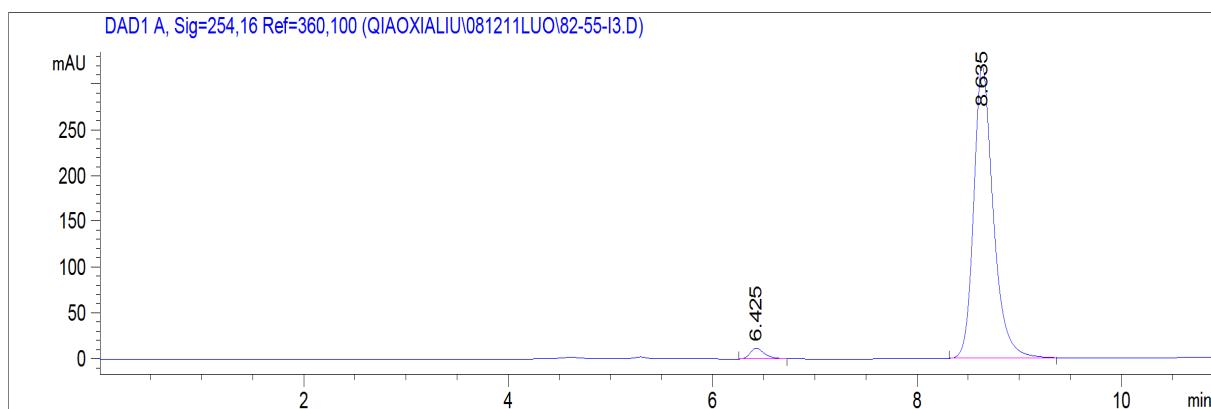


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.848	MM R	0.1505	1.20413e4	1333.20789	96.0684
2	6.921	MM R	0.1673	492.79077	49.09856	3.9316
总量 :						1.25341e4 1382.30644

Figure S-21. Racemic and optically enriched HPLC chromatogram of compound **7ag-major**.

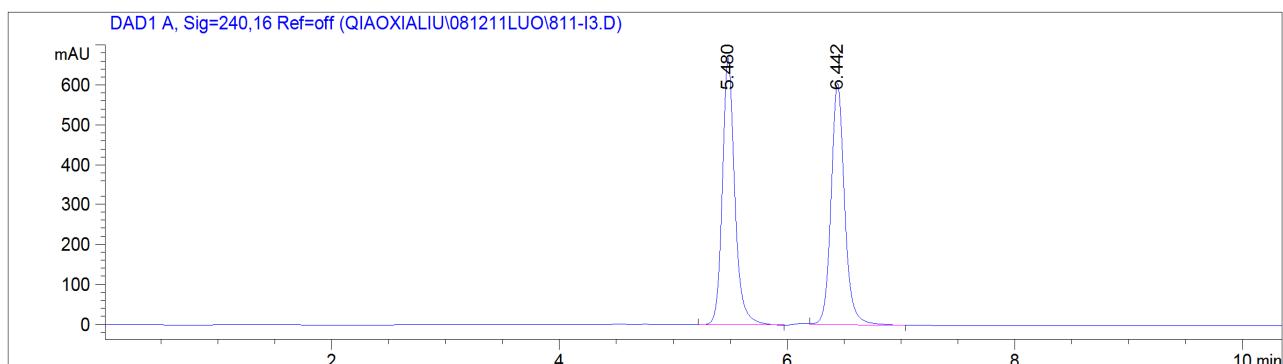


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.365	VB	0.1442	2124.52734	217.07884	50.5540
2	8.655	BB	0.2033	2077.96533	154.07631	49.4460
总量 :					4202.49268	371.15515

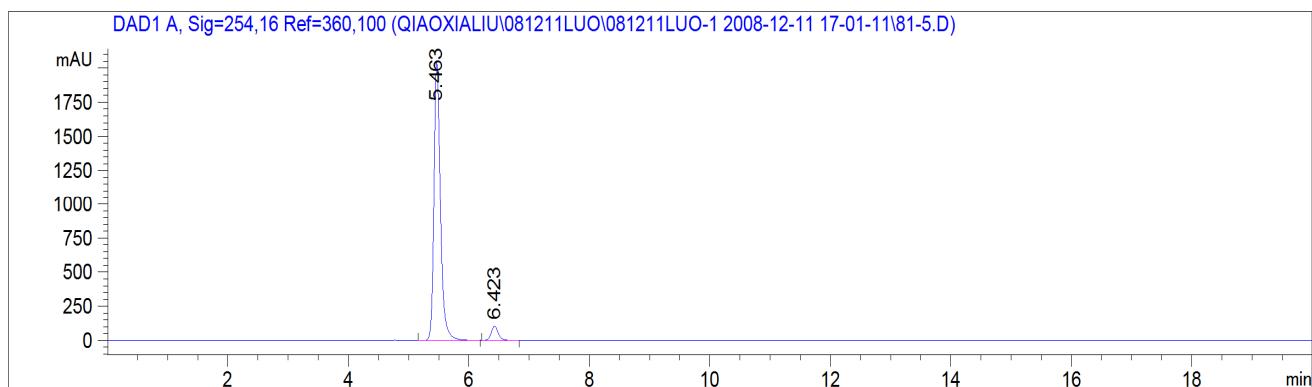


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.425	BB	0.1482	116.64379	11.70767	2.6738
2	8.635	BB	0.1993	4245.89844	318.97534	97.3262
总量 :					4362.54223	330.68302

Figure S-22. Racemic and optically enriched HPLC chromatogram of compound **7ag-minor**.

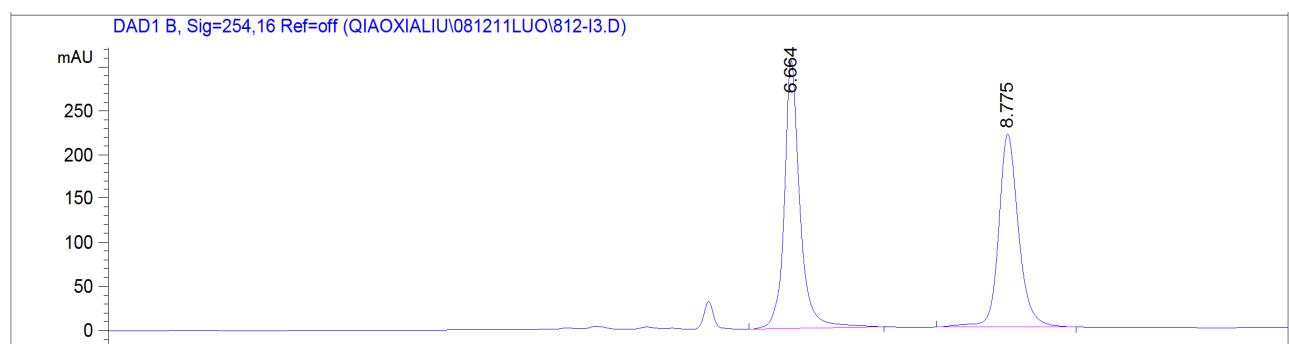


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.480	VB	0.1144	5073.22168	669.30927	50.1419
2	6.442	VB	0.1250	5044.51172	606.47723	49.8581
总量 :					1.01177e4	1275.78650

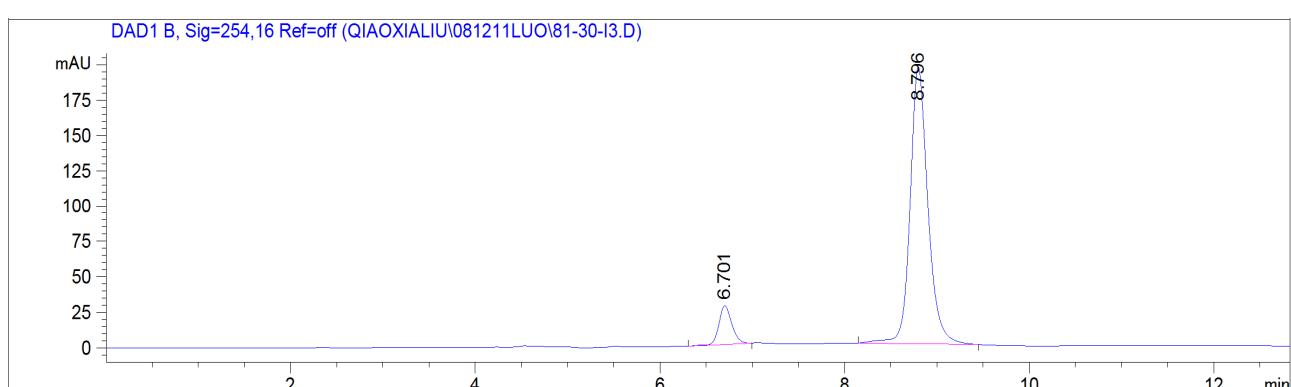


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.463	VB	0.1133	1.52991e4	2043.82532	94.4522
2	6.423	BB	0.1261	898.60724	106.87696	5.5478
总量 :					1.61977e4	2150.70228

Figure S-23. Racemic and optically enriched HPLC chromatogram of compound 7ah-major.

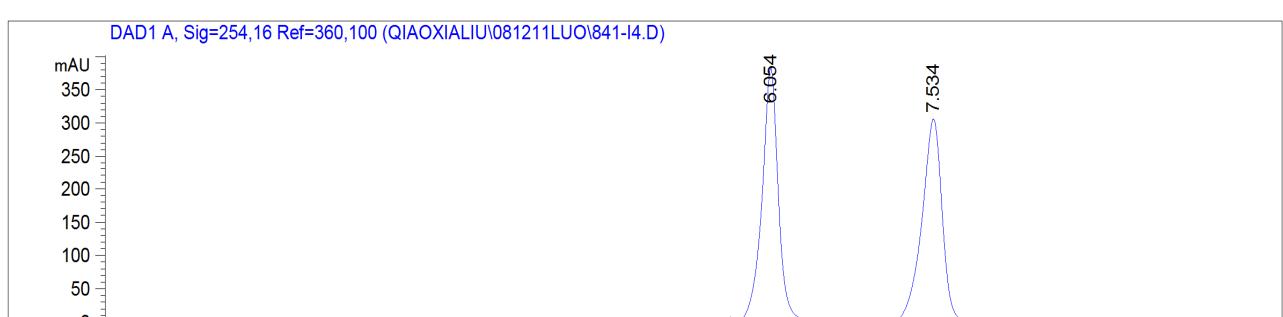


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.664	BB	0.1562	3248.57568	305.26599	52.1528
2	8.775	BB	0.2020	2980.37744	220.01924	47.8472
总量 :						6228.95313 525.28523

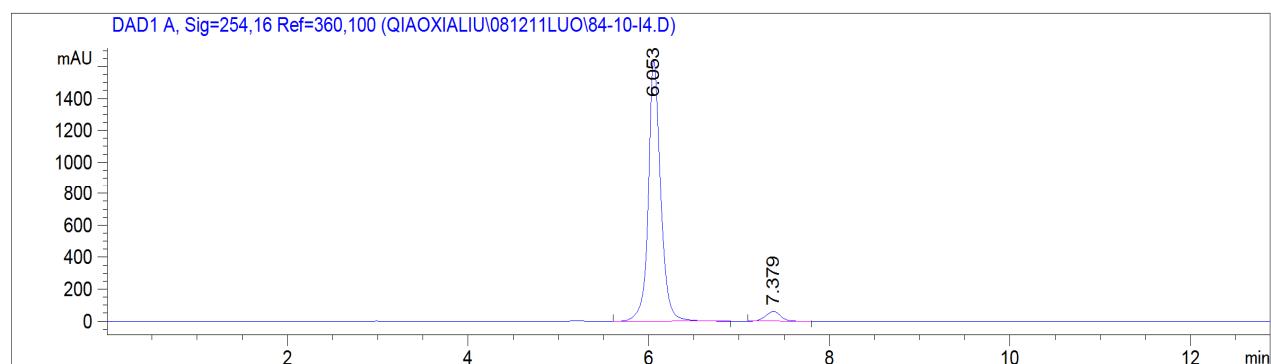


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.701	BB	0.1498	270.76654	27.28201	9.2857
2	8.796	BB	0.2036	2645.18604	195.85548	90.7143
总量 :						2915.95258 223.13750

Figure S-24. Racemic and optically enriched HPLC chromatogram of compound **7ah-minor**.

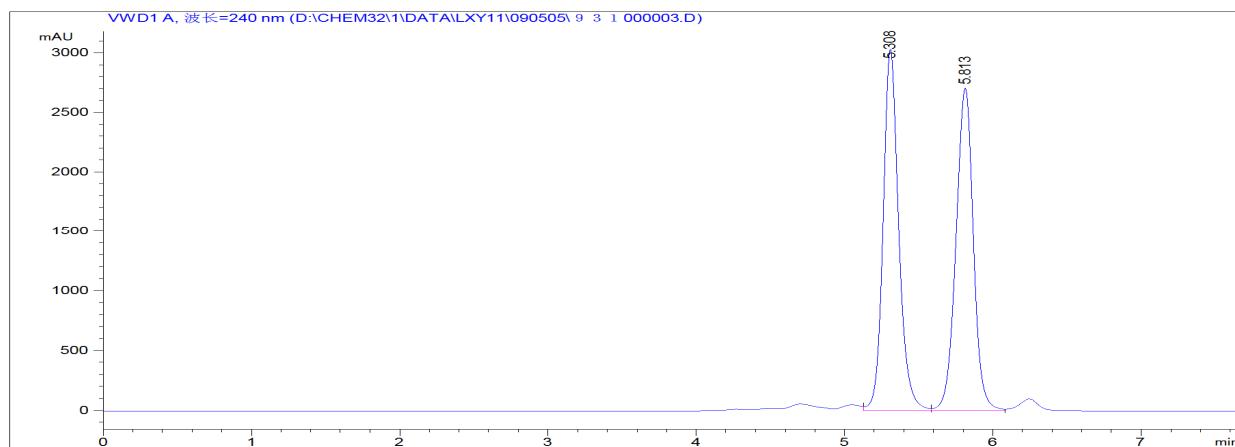


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.054	BB	0.1529	4052.04932	384.55136	50.0972
2	7.534	BB	0.1945	4036.32324	308.82632	49.9028
总量 :				8088.37256	693.37769	

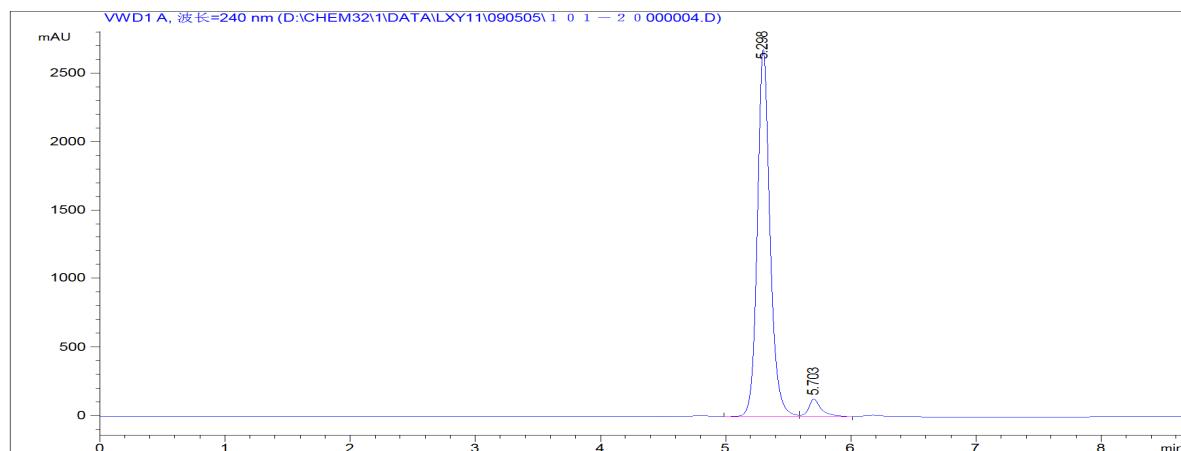


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.053	VB	0.1412	1.56305e4	1640.30603	95.4948
2	7.379	BB	0.1811	737.41473	61.82762	4.5052
总量 :				1.63680e4	1702.13365	

Figure S-25. Racemic and optically enriched HPLC chromatogram of compound **7ai-major**.

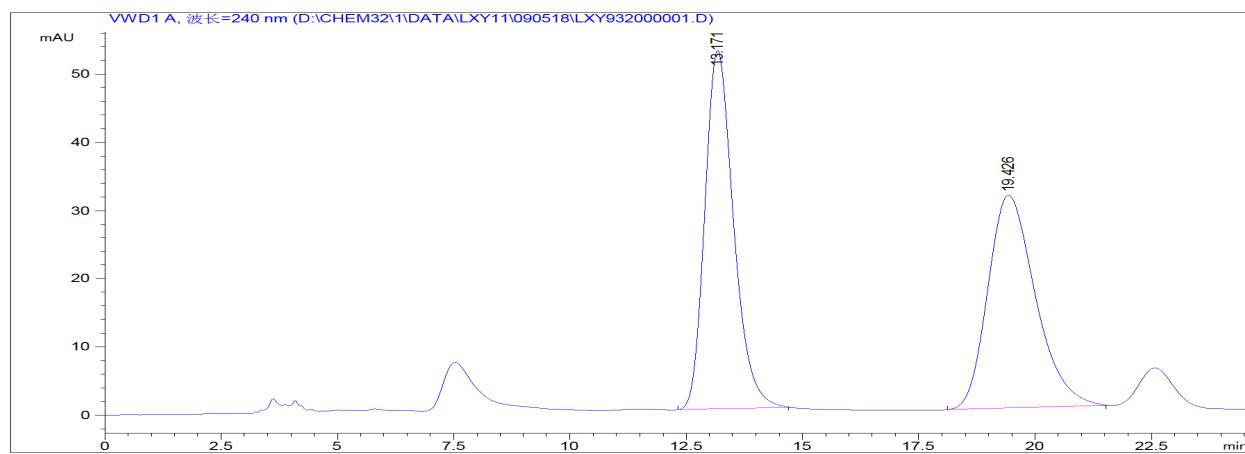


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	5.308	VV	0.1116	2.22413e4	3038.85864	50.0729
2	5.813	VV	0.1260	2.21766e4	2712.54492	49.9271
总量 :					4.44179e4	5751.40356

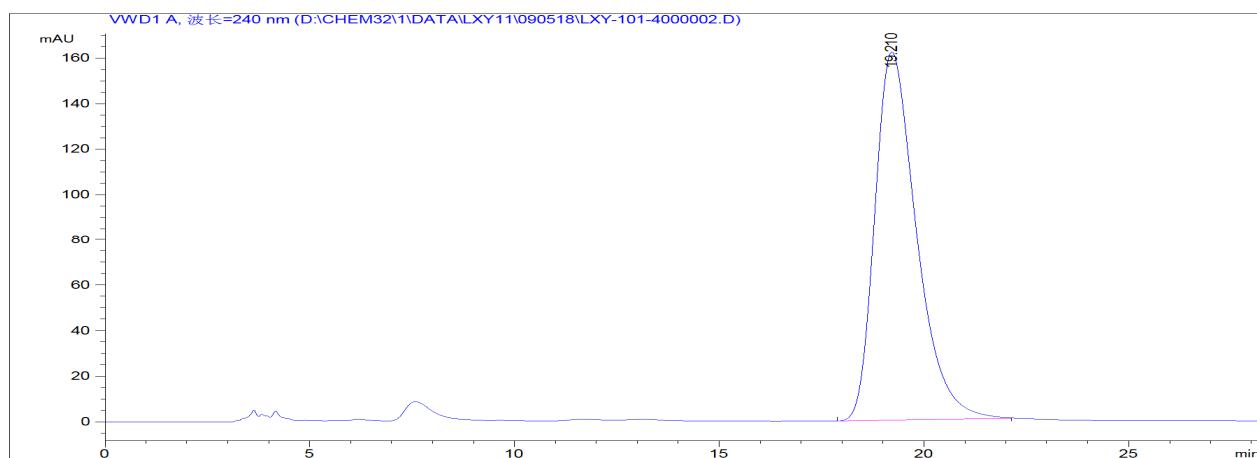


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	5.298	VV	0.1057	1.89485e4	2681.42822	95.1739
2	5.703	VV	0.1046	960.84381	130.81091	4.8261
总量 :					1.99093e4	2812.23914

Figure S-26. Racemic and optically enriched HPLC chromatogram of compound **7aj-major**.

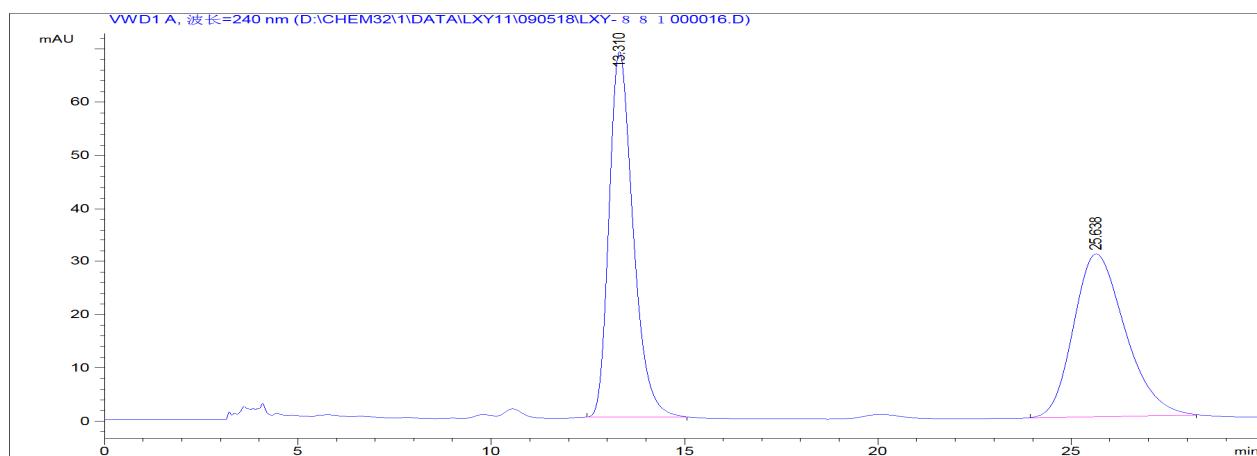


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	13.171	BB	0.6627	2257.11206	52.54758	50.4809
2	19.426	BB	1.0764	2214.10498	31.27304	49.5191
总量 :				4471.21704	83.82062	

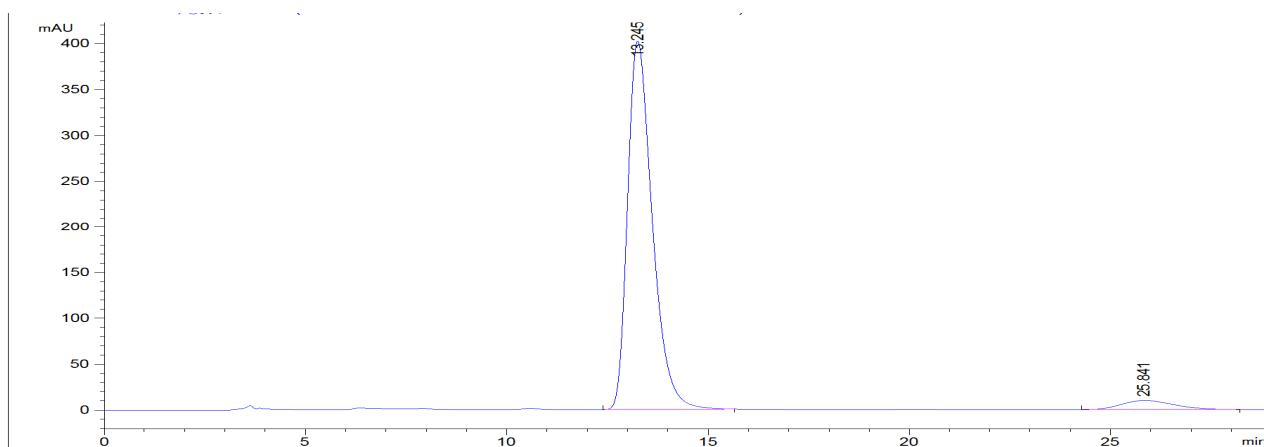


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s [mAU]	峰面积 %
1	19.210	BB	1.0686	1.14315e4	161.84758	100.0000
总量 :				1.14315e4	161.84758	

Figure S-27. Racemic and optically enriched HPLC chromatogram of compound **7aj-minor**.

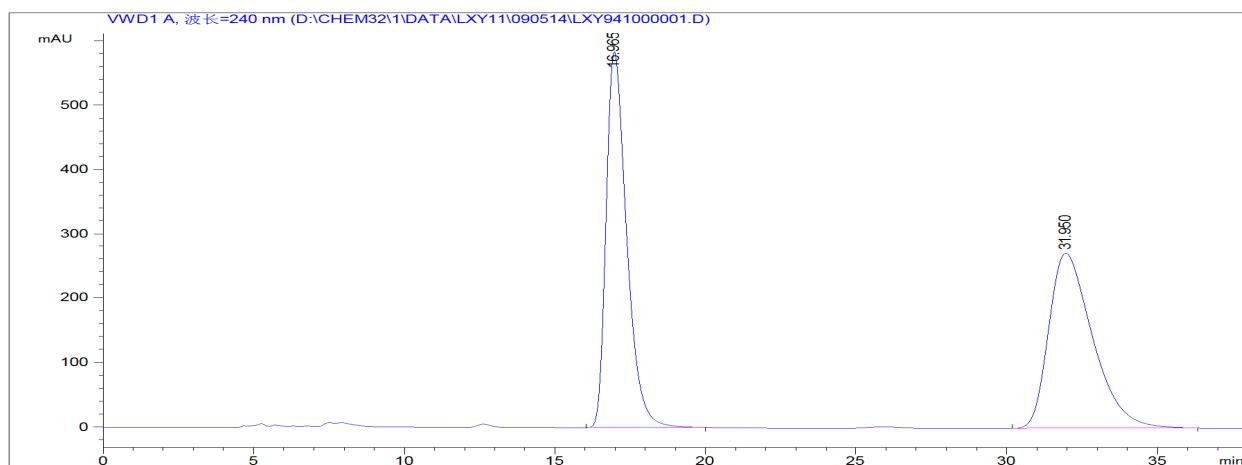


峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	峰面积 *s	峰高 [mAU]	峰面积 %
1	13.310	BB	0.6653	2977.11060	68.76101	51.2435	
2	25.638	BB	1.3922	2832.62427	30.54127	48.7565	
总量 :						5809.73486	99.30228

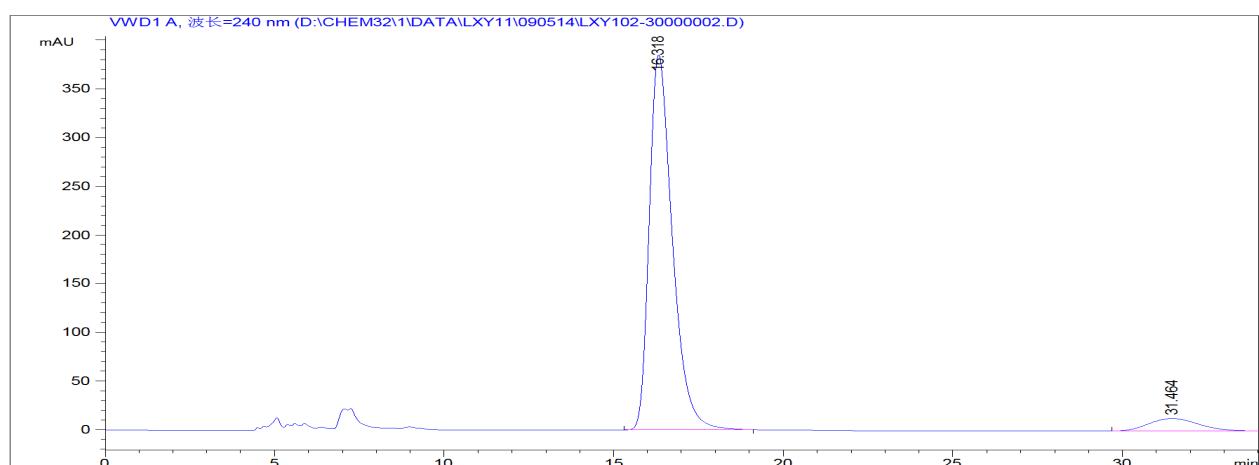


峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	峰面积 *s	峰高 [mAU]	峰面积 %
1	13.245	BB	0.6588	1.71879e4	402.11801	94.8773	
2	25.841	BB	1.3232	928.01971	10.10661	5.1227	
总量 :						1.81160e4	412.22462

Figure S-28. Racemic and optically enriched HPLC chromatogram of compound **7ak-minor**.



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s	峰面积 [mAU]	峰面积 %
1	16.965	BB	0.7240	2.77022e4	583.75024	50.2782	
2	31.950	BB	1.5316	2.73956e4	270.36716	49.7218	
总量 :						5.50978e4	854.11740



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU	峰高 *s	峰面积 [mAU]	峰面积 %
1	16.318	BB	0.7165	1.82546e4	384.83643	93.2652	
2	31.464	BBA	1.4604	1318.17957	12.74100	6.7348	
总量 :						1.95728e4	397.57743

Figure S-29. Racemic and optically enriched HPLC chromatogram of compound **7al-major**.

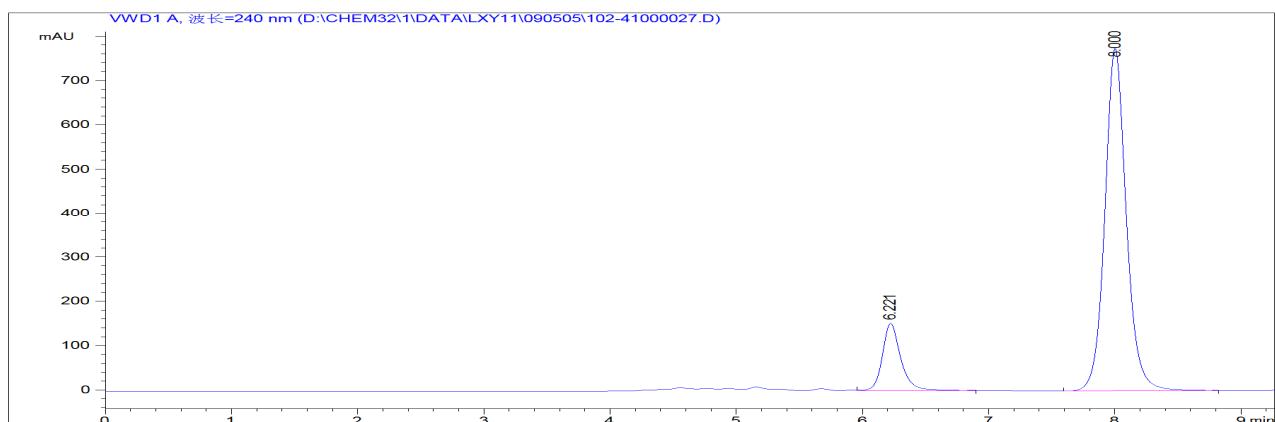
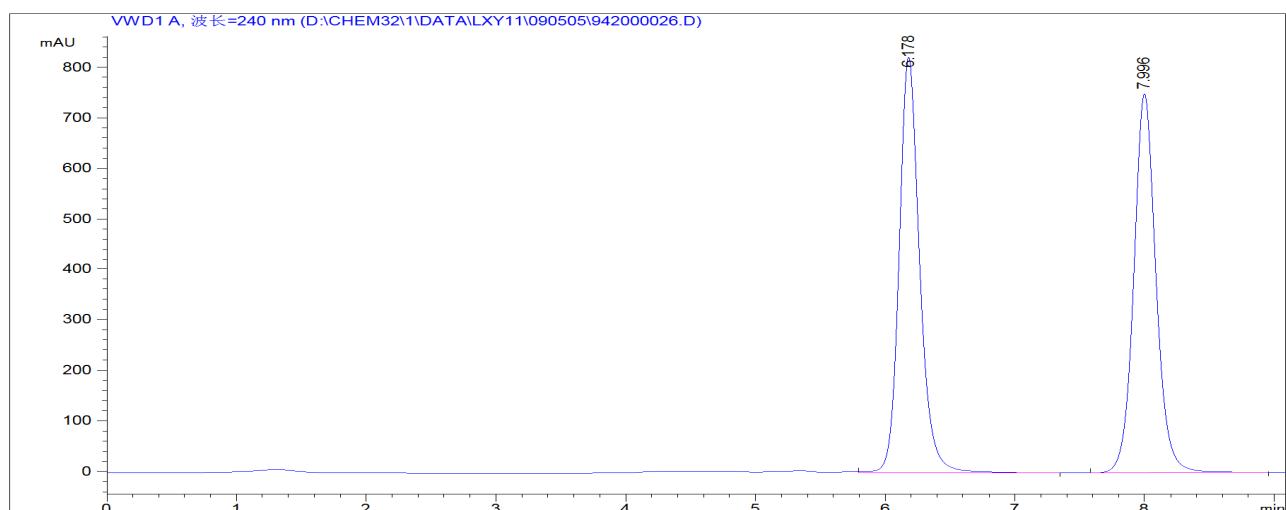
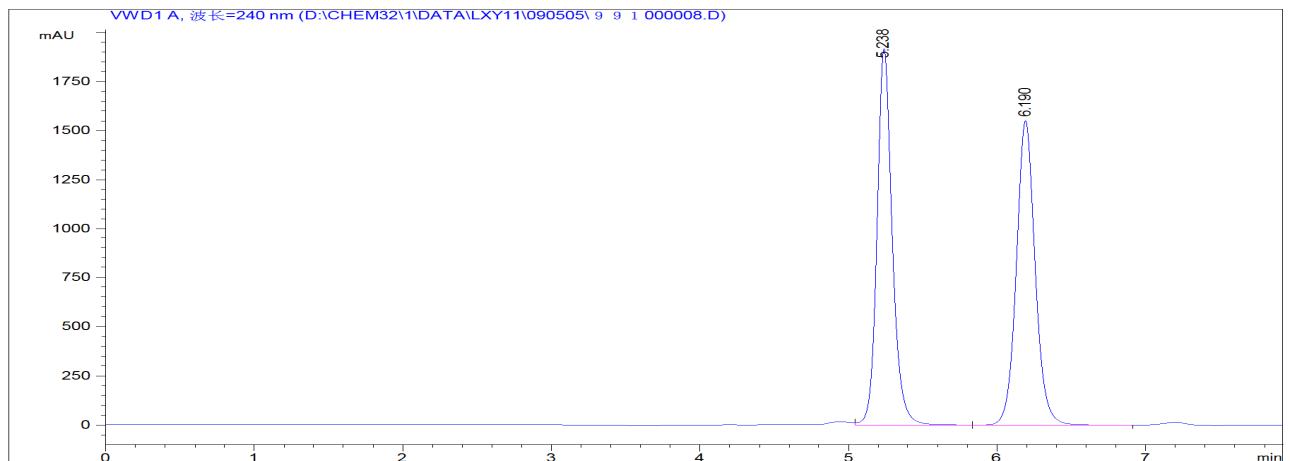
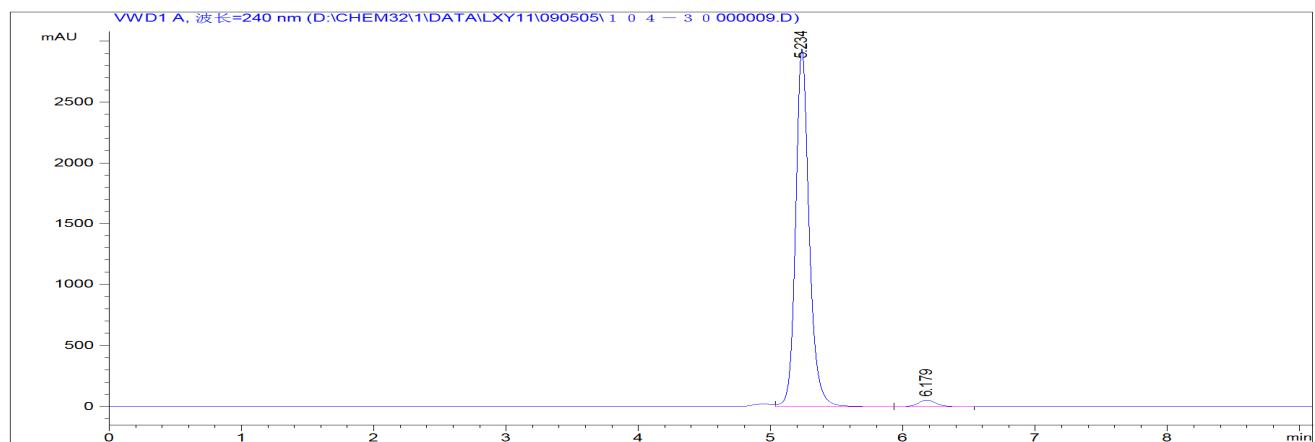


Figure S-30. Racemic and optically enriched HPLC chromatogram of compound **7al-minor**.

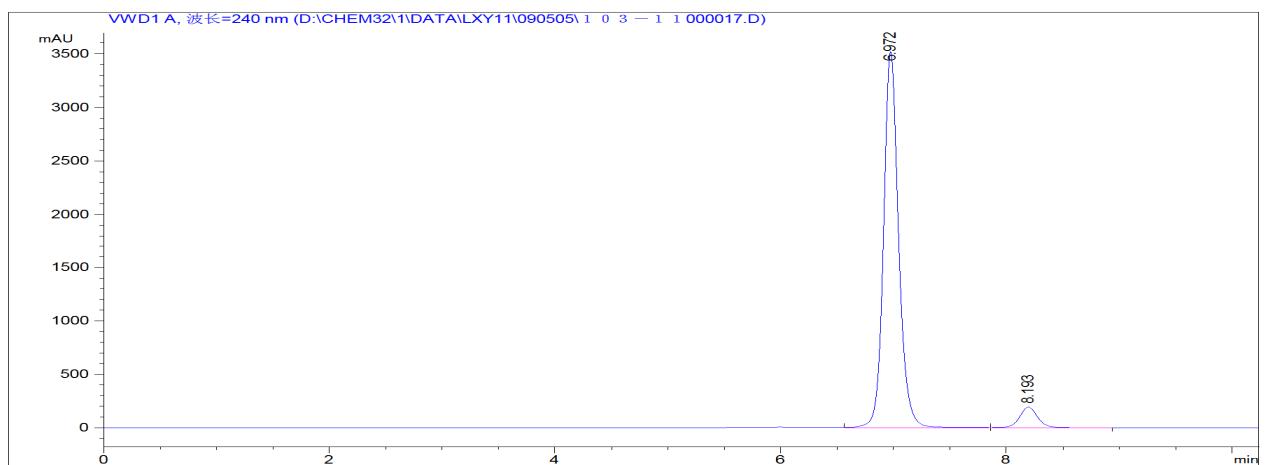
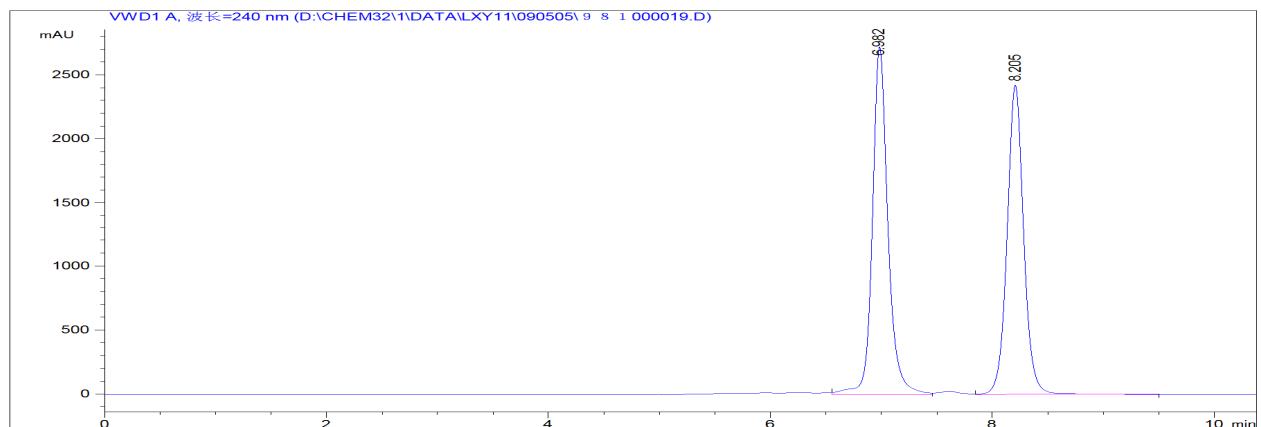


峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	*s	峰高 [mAU]	峰面积 %
1	5.238	VV	0.1080	1.37003e4	1.37003e4	1920.33276	49.9945
2	6.190	VV	0.1350	1.37033e4	1.37033e4	1552.01843	50.0055
总量 :							2.74036e4 3472.35120



峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	*s	峰高 [mAU]	峰面积 %
1	5.234	VV	0.1065	2.09666e4	2.09666e4	2938.50977	97.4029
2	6.179	VV	0.1526	559.05212	559.05212	54.73634	2.5971
总量 :							2.15256e4 2993.24610

Figure S-31. Racemic and optically enriched HPLC chromatogram of compound **7am-major**.

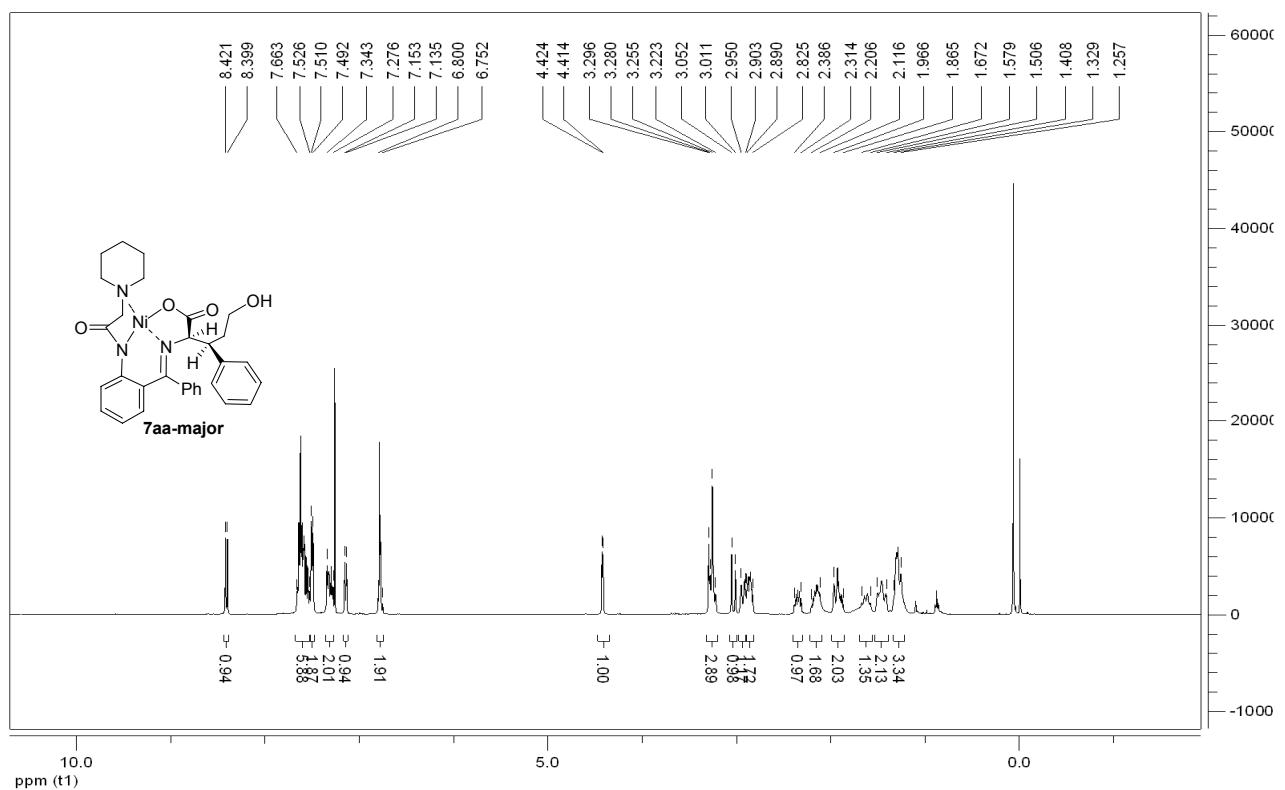


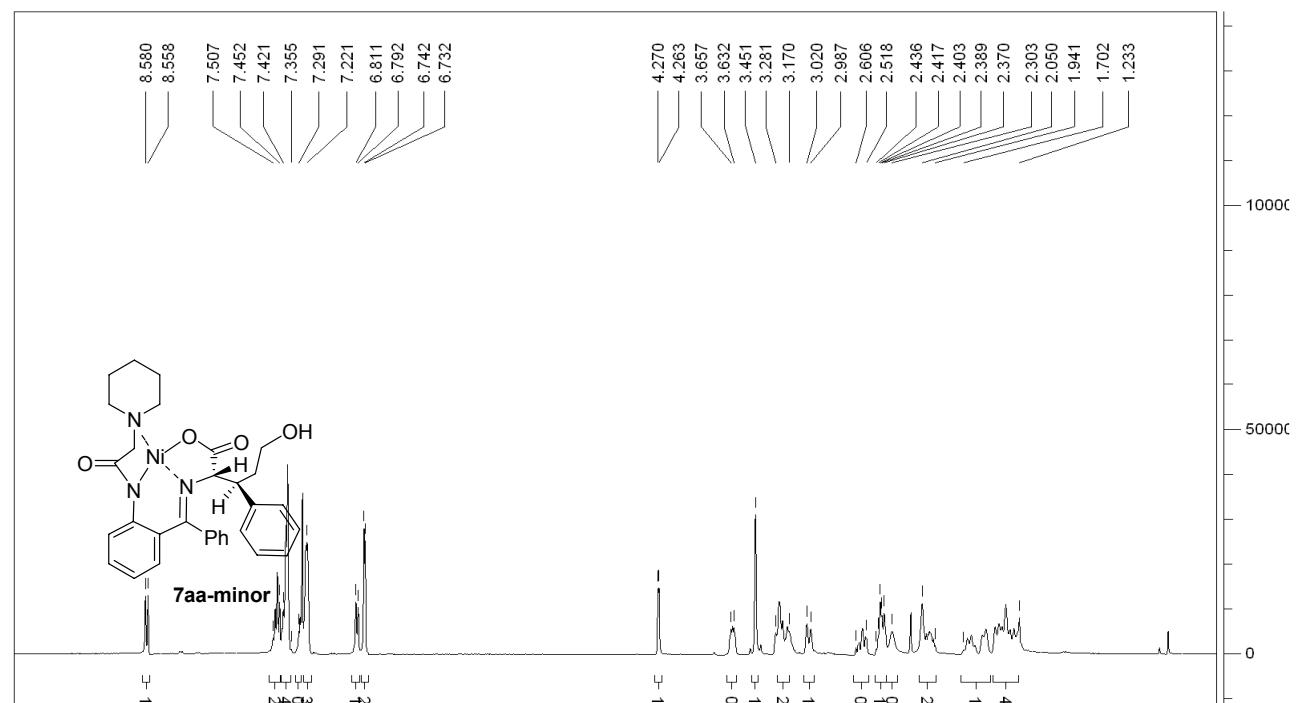
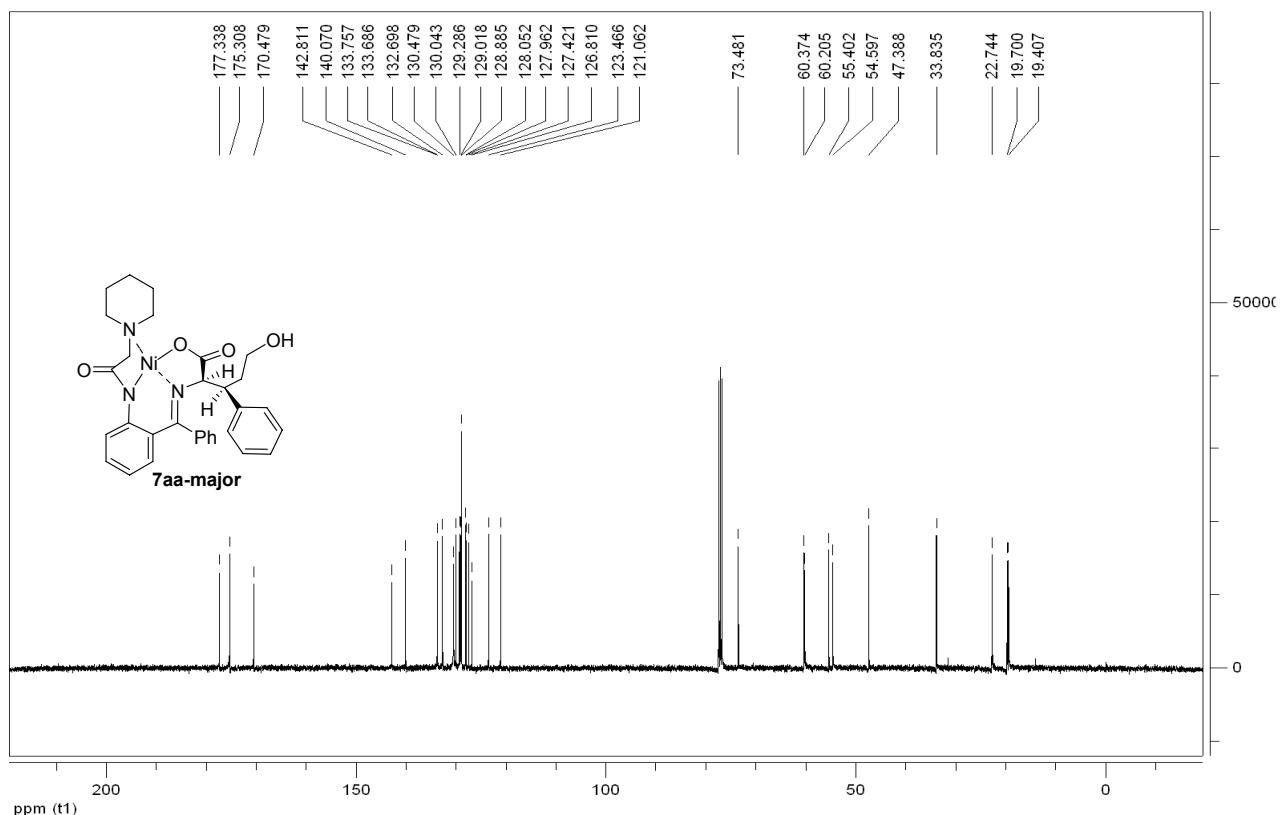
峰 #	保留时间 [min]	类型	峰宽 [min]	mAU	*s	峰高 [mAU]	峰面积 %
1	6.972	VV	0.1404	3.27243e4		3523.19702	93.8160
2	8.193	VB	0.1697	2157.07251		192.93533	6.1840

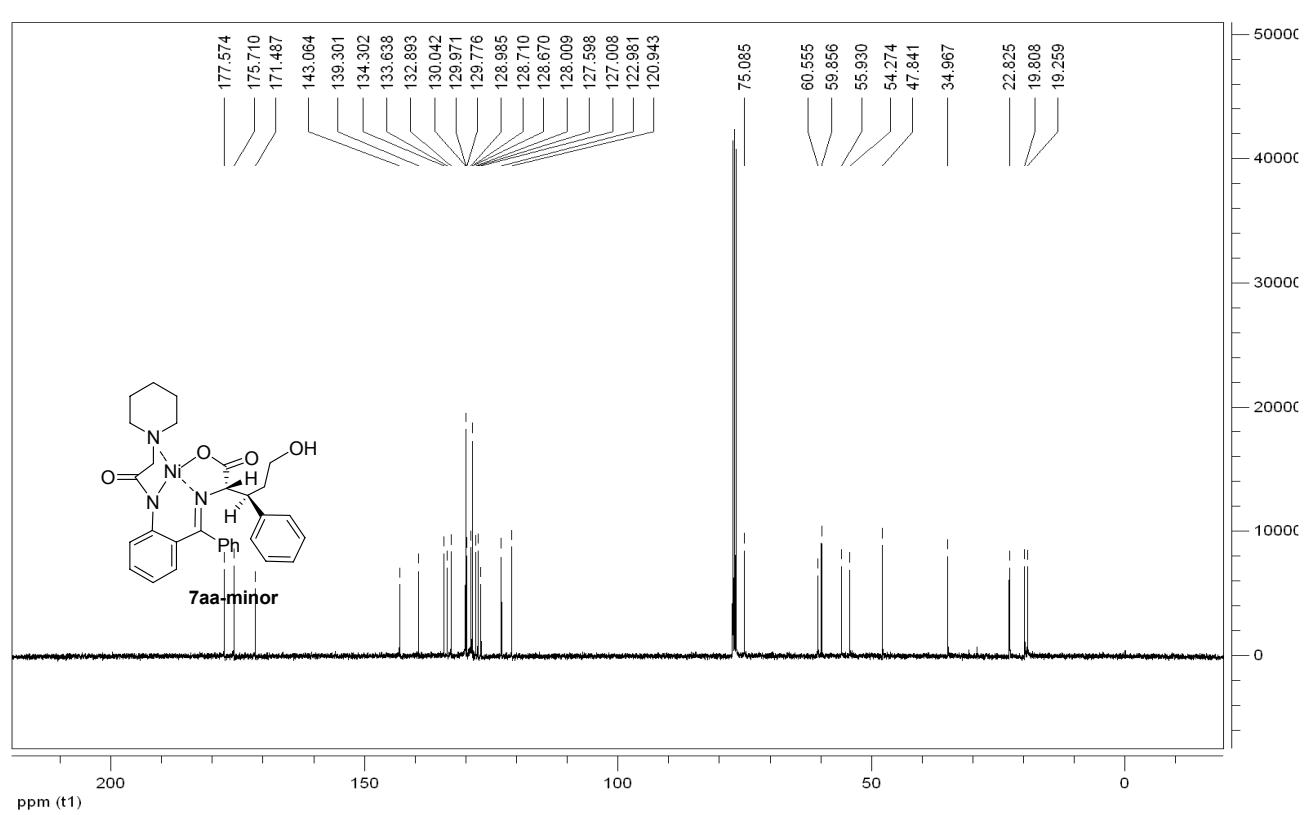
总量 : 3.48814e4 3716.13235

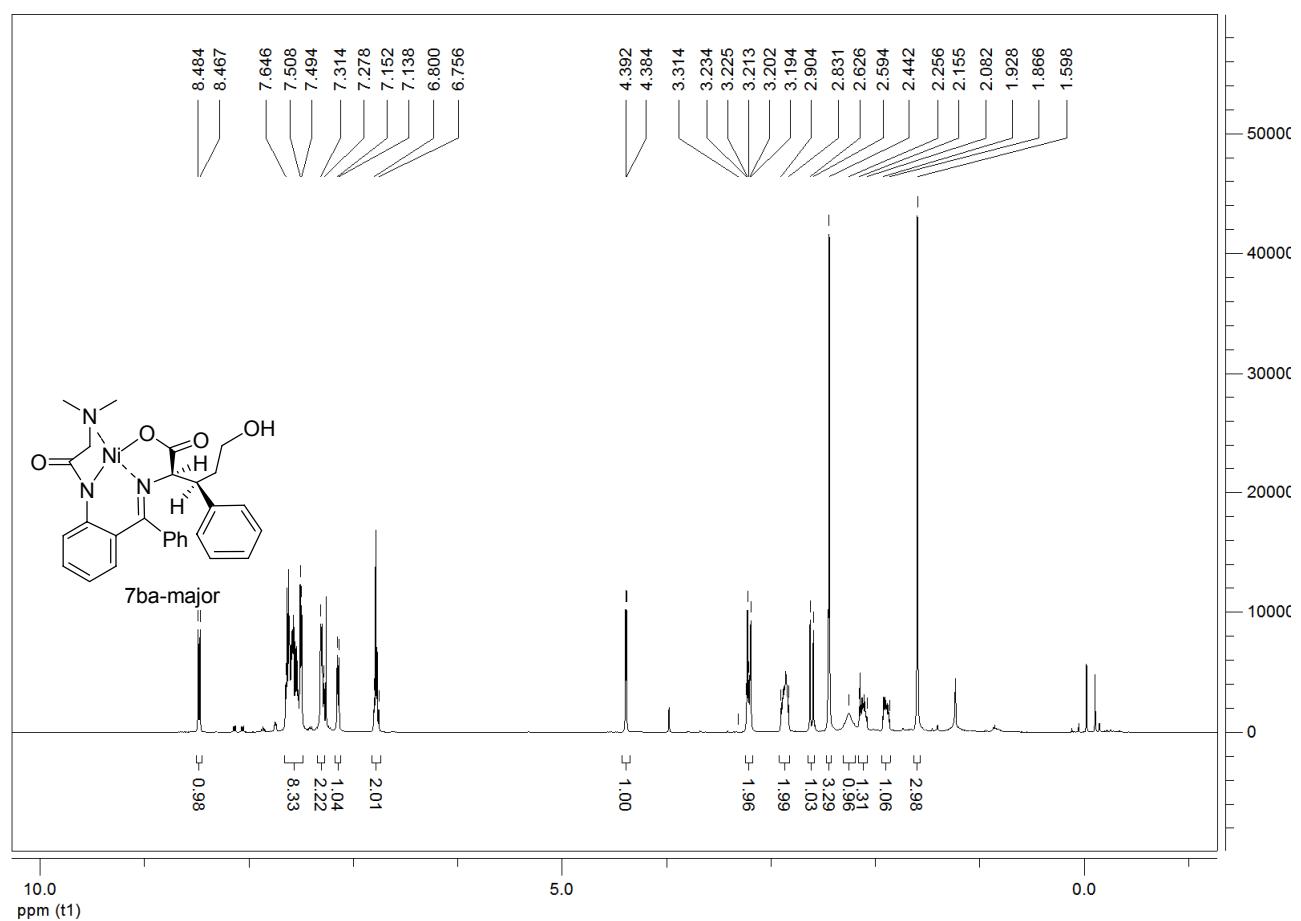
Figure S-32. Racemic and optically enriched HPLC chromatogram of compound **7an-major**.

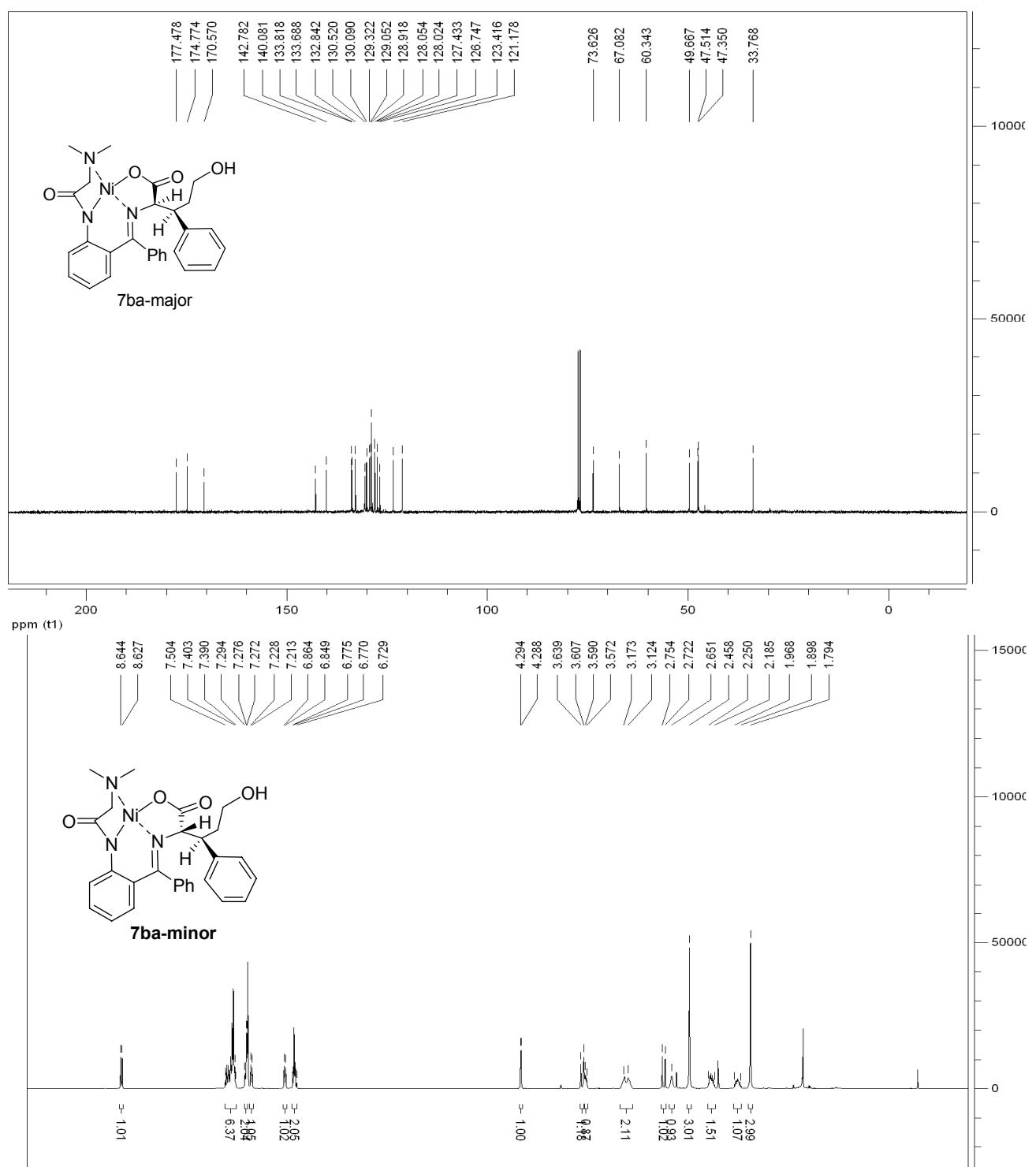
B: NMR Analysis of Products

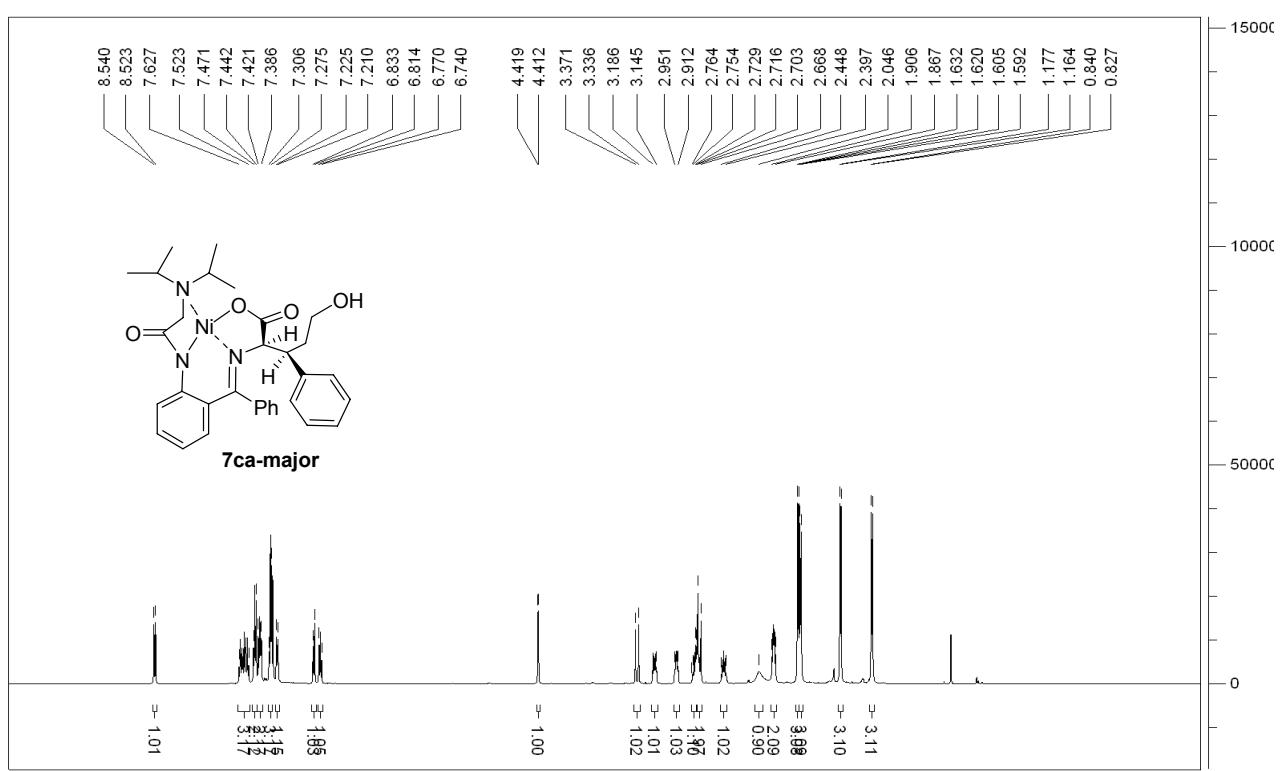
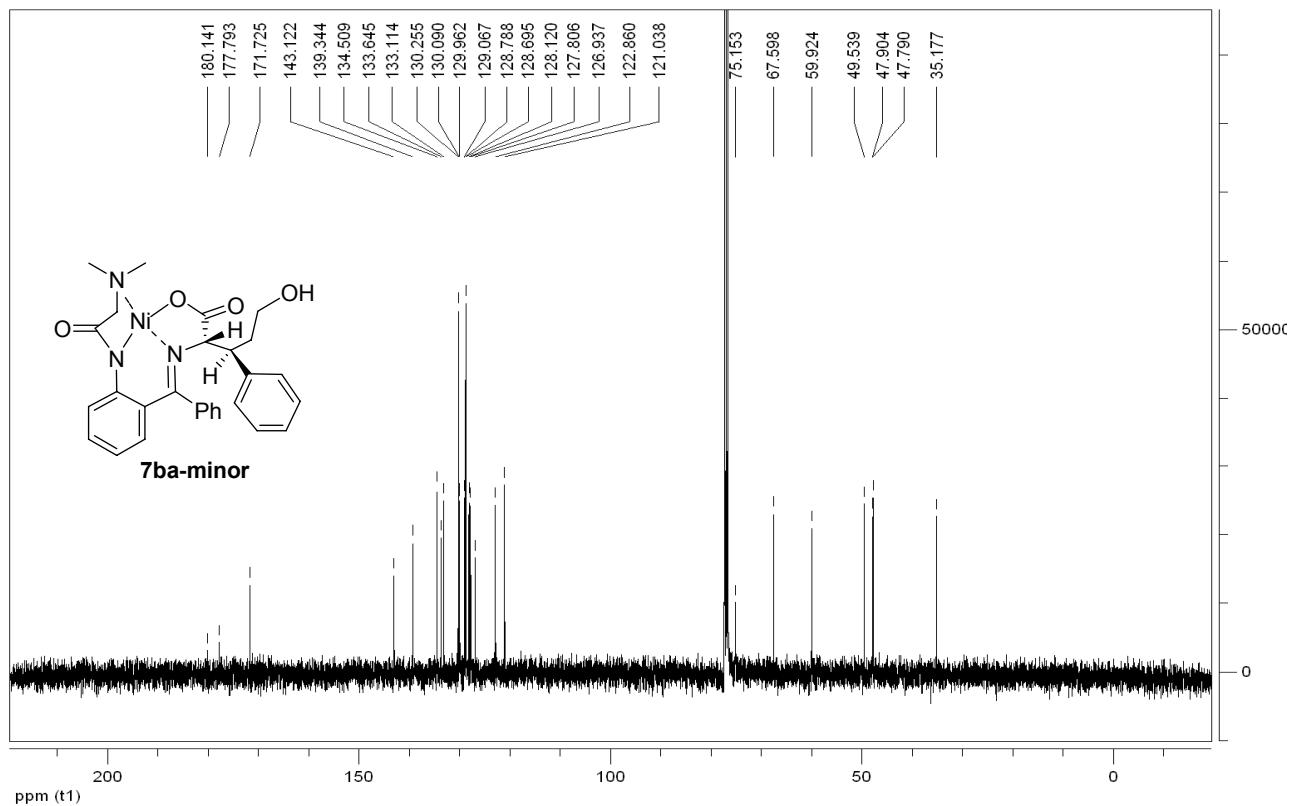


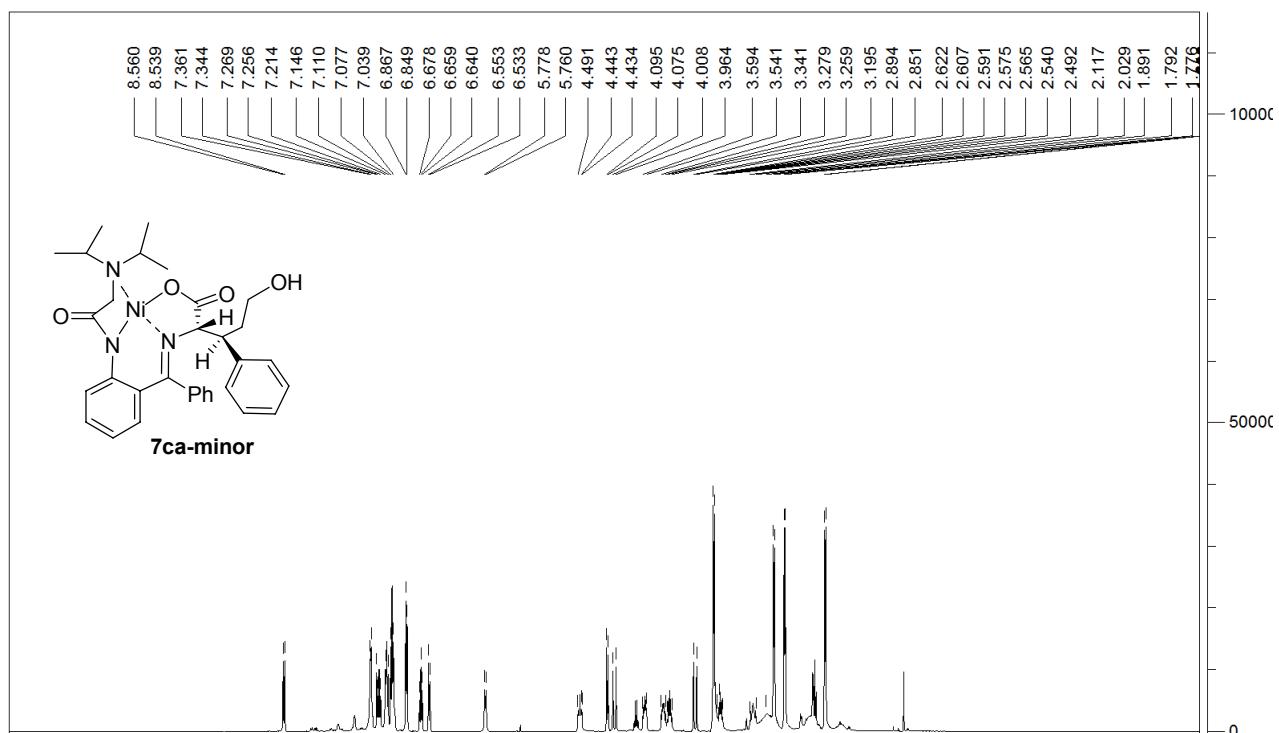
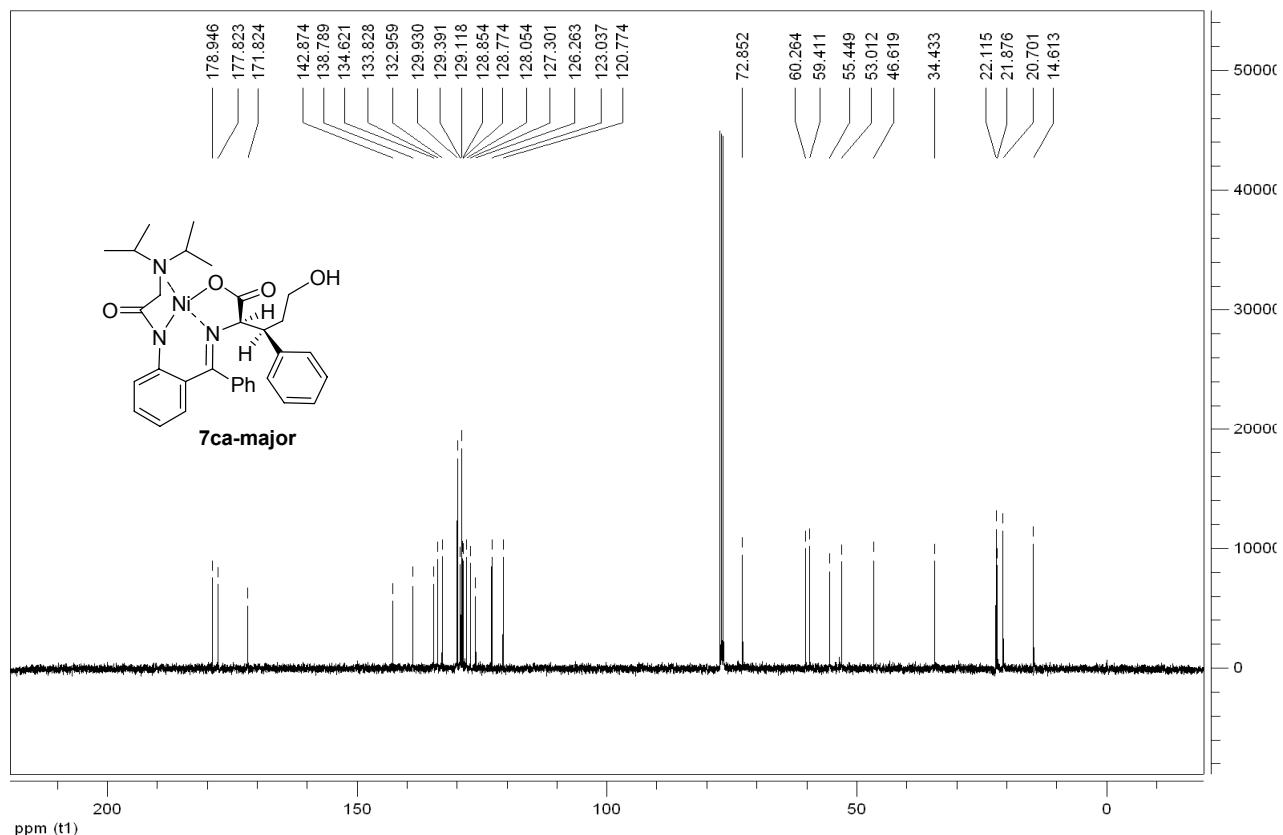


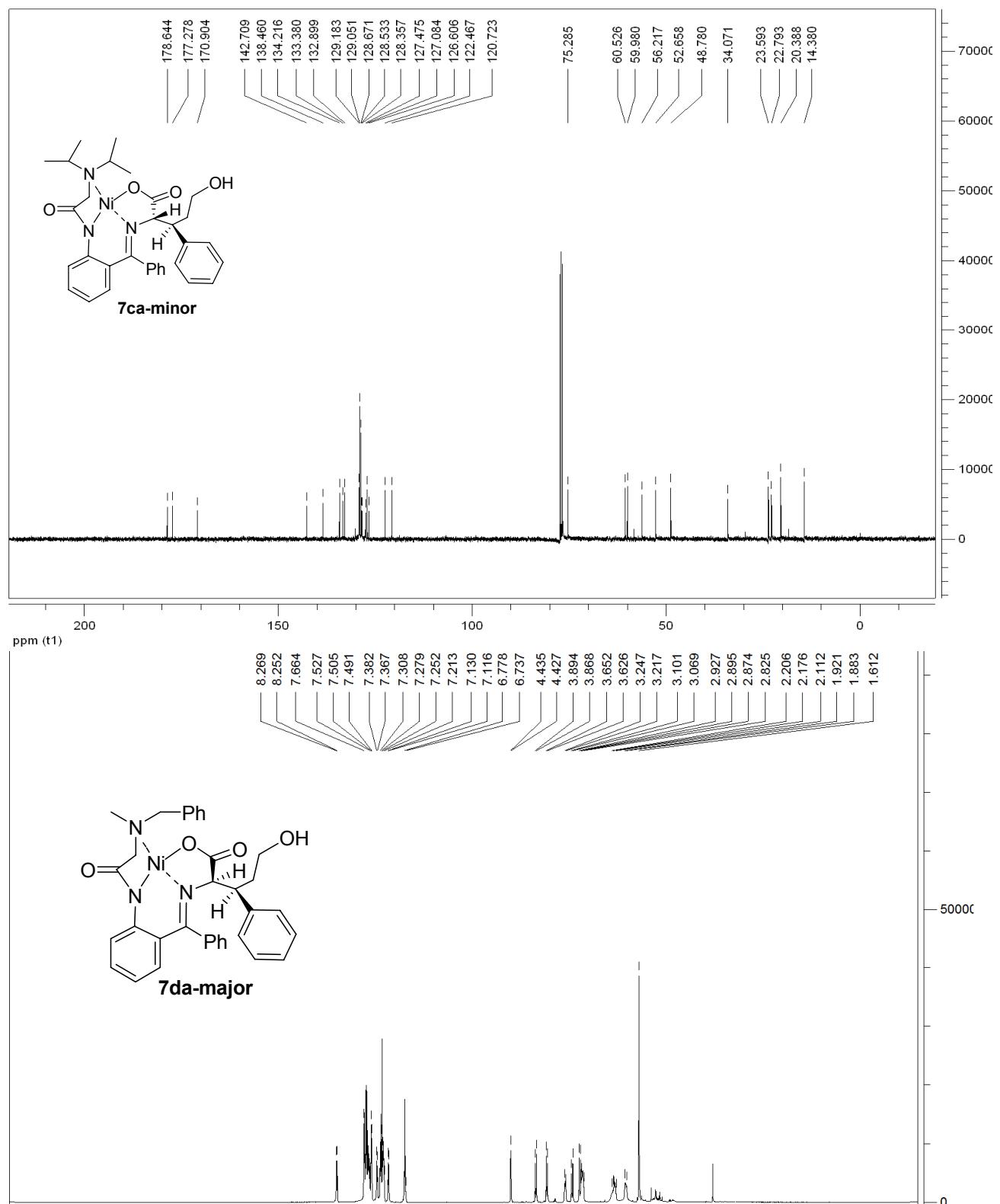


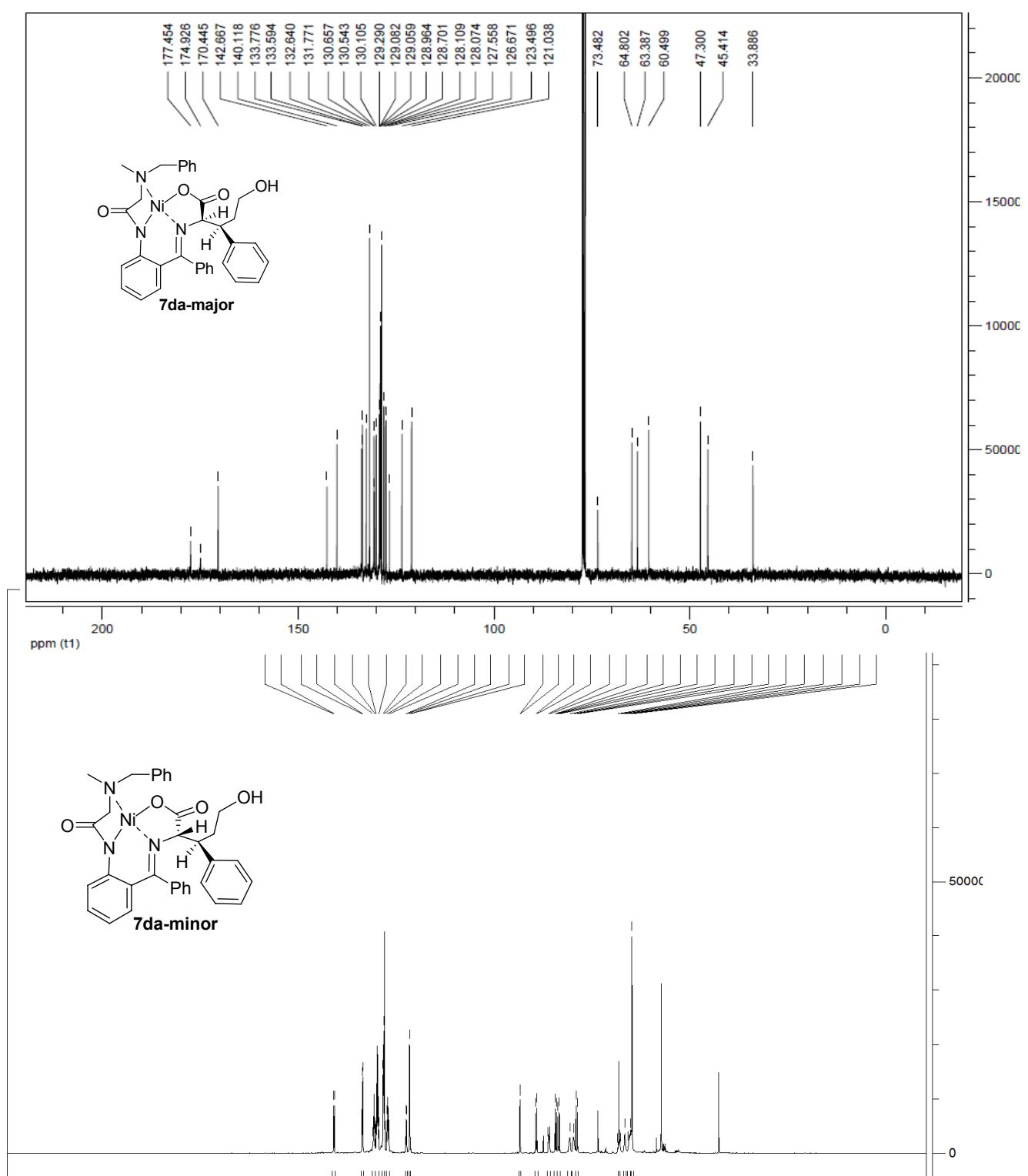


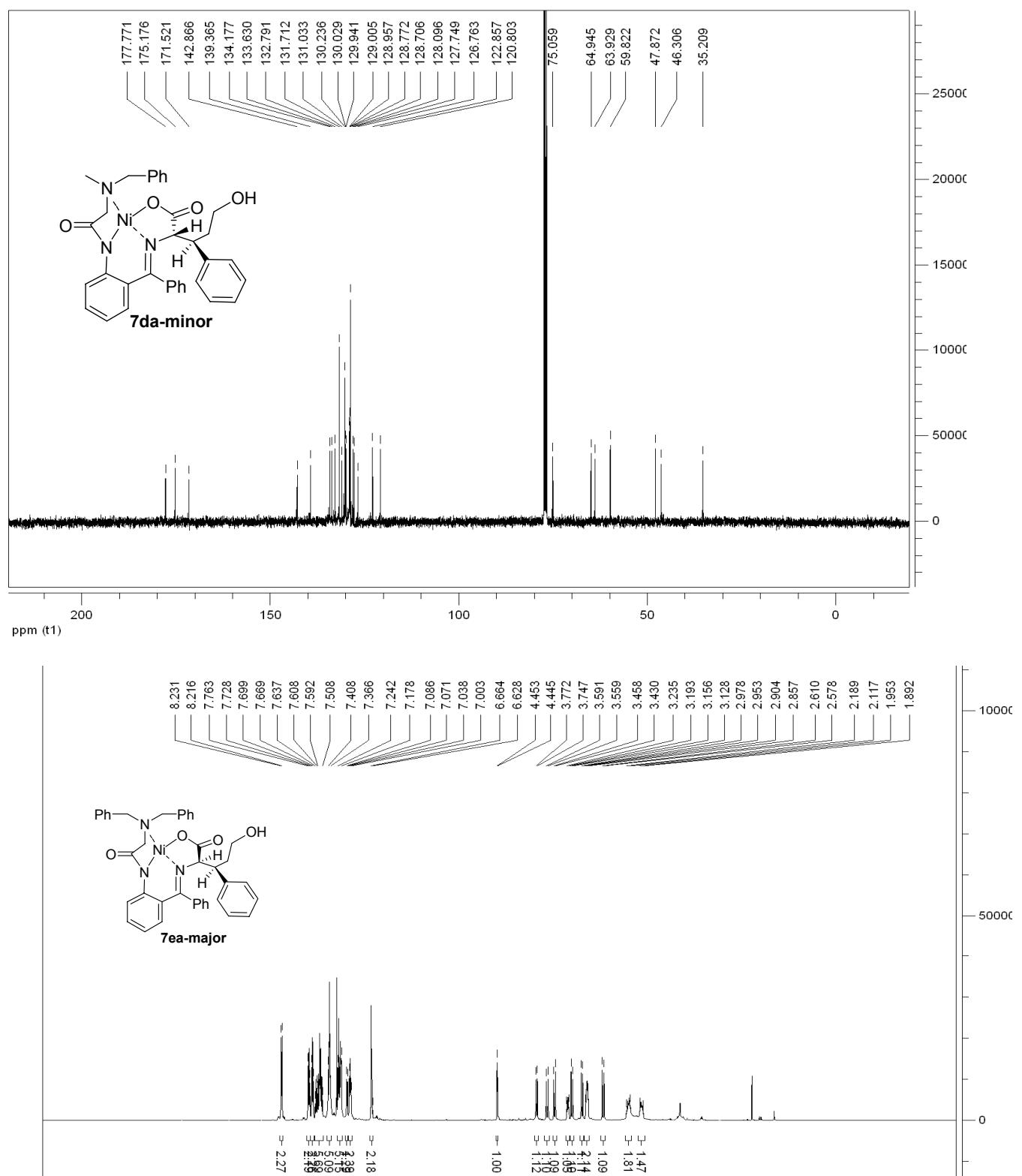


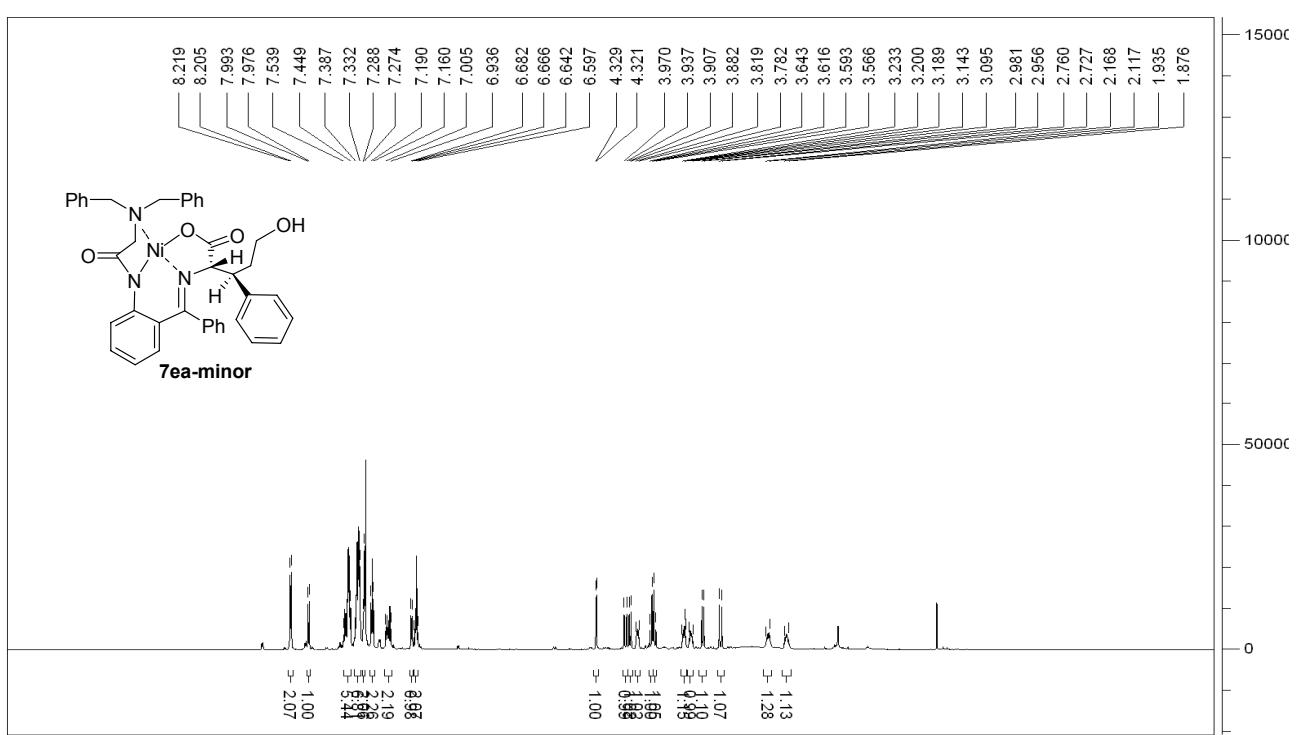
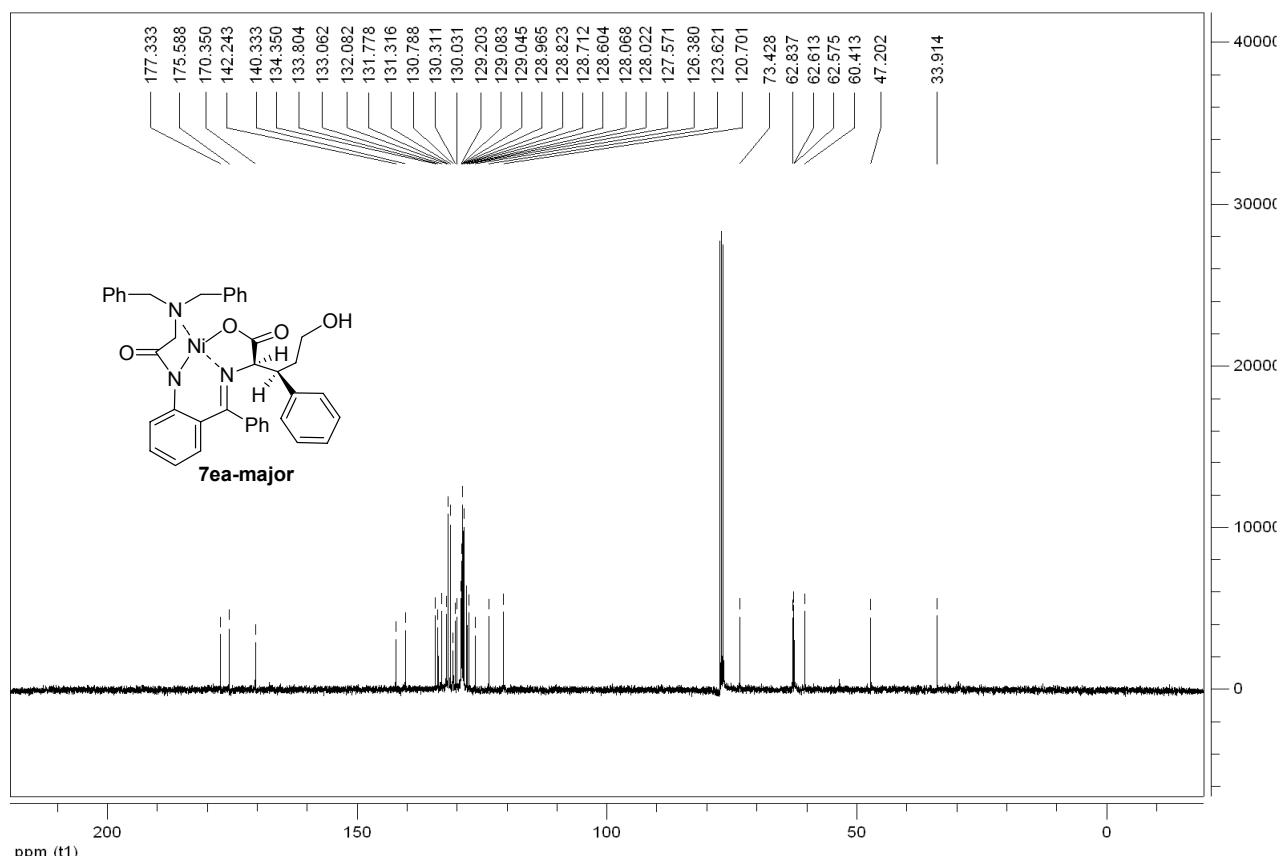


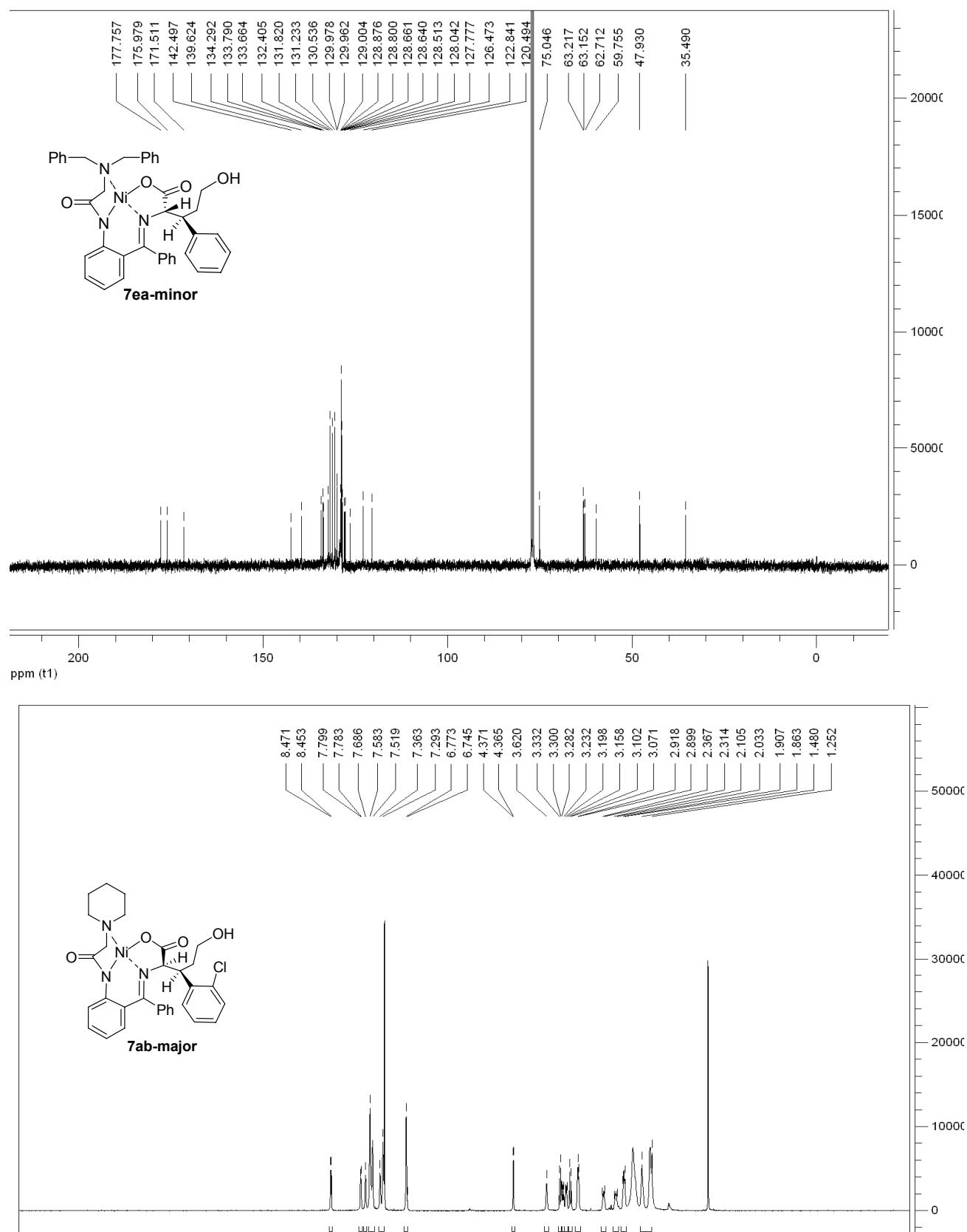


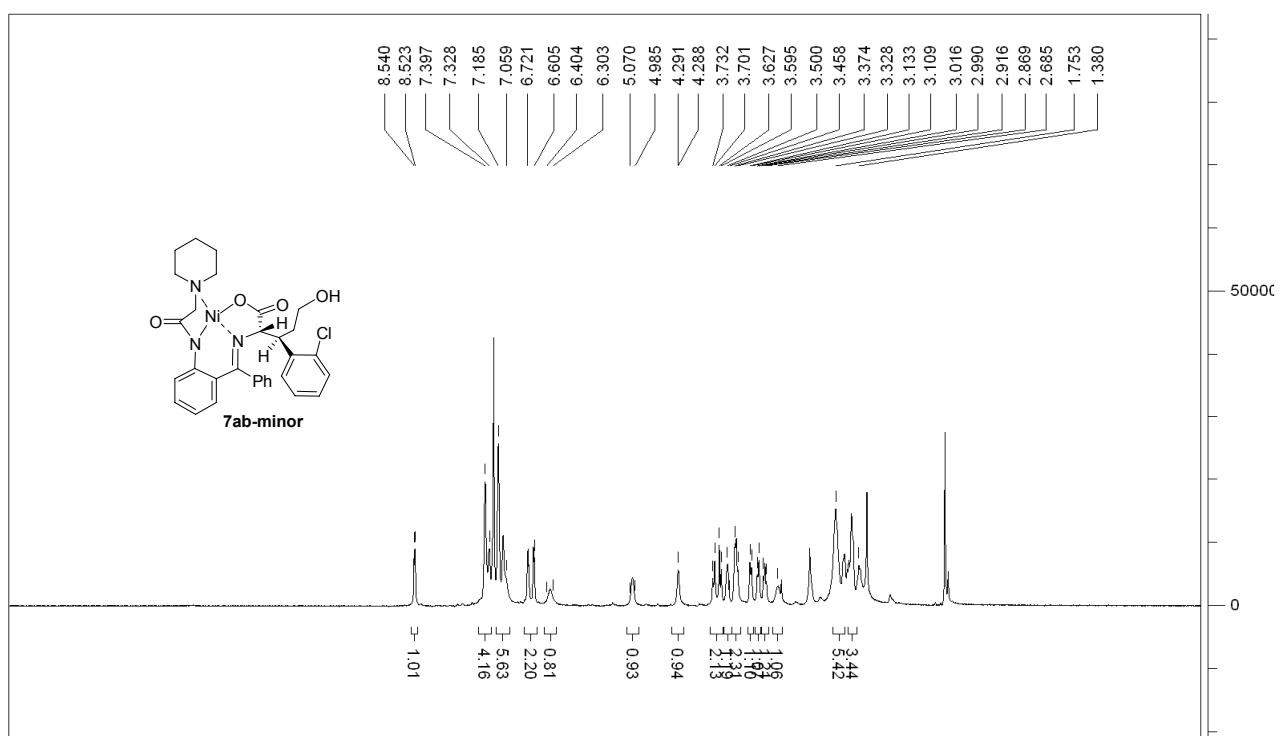
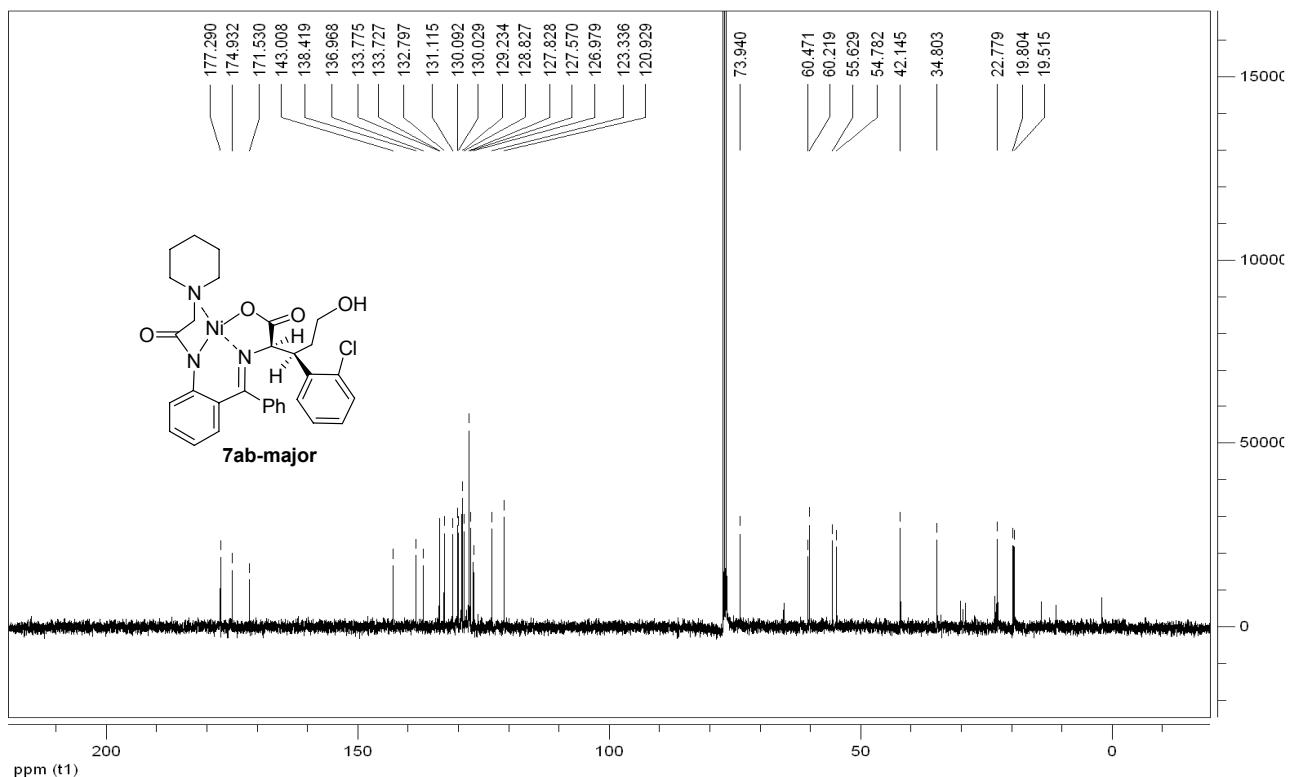


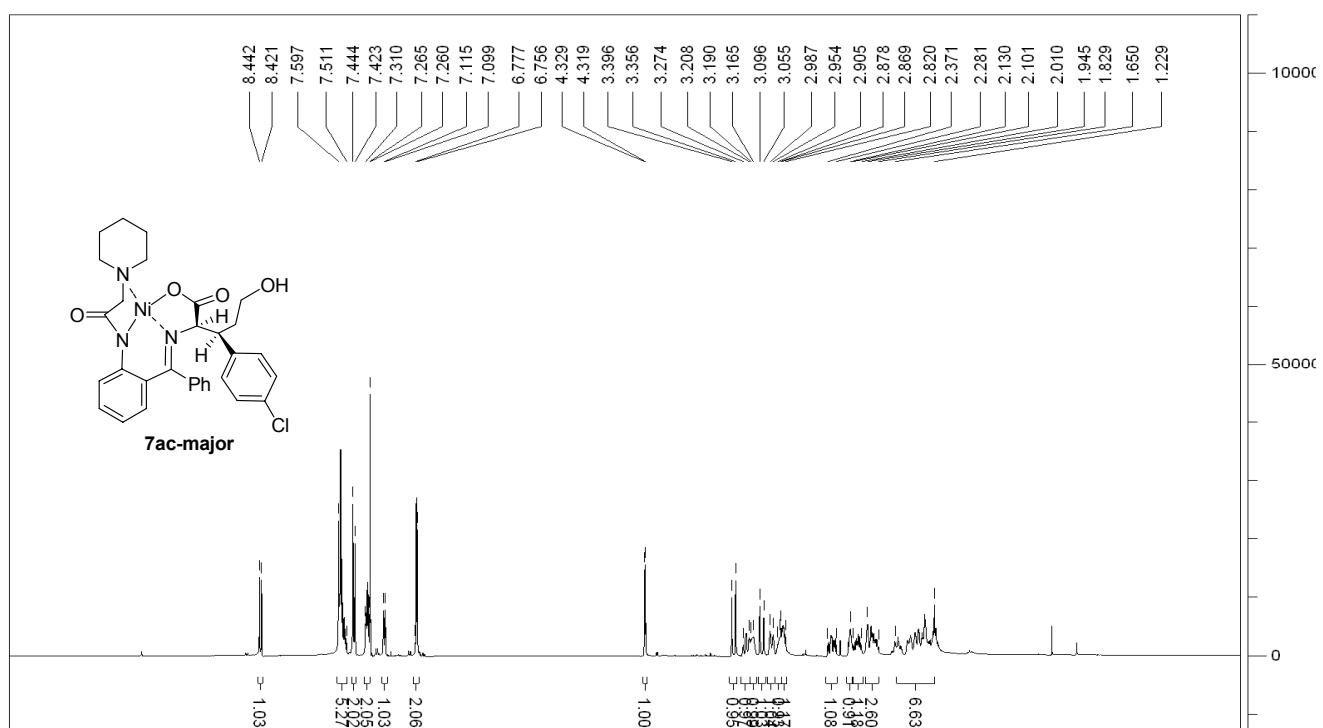
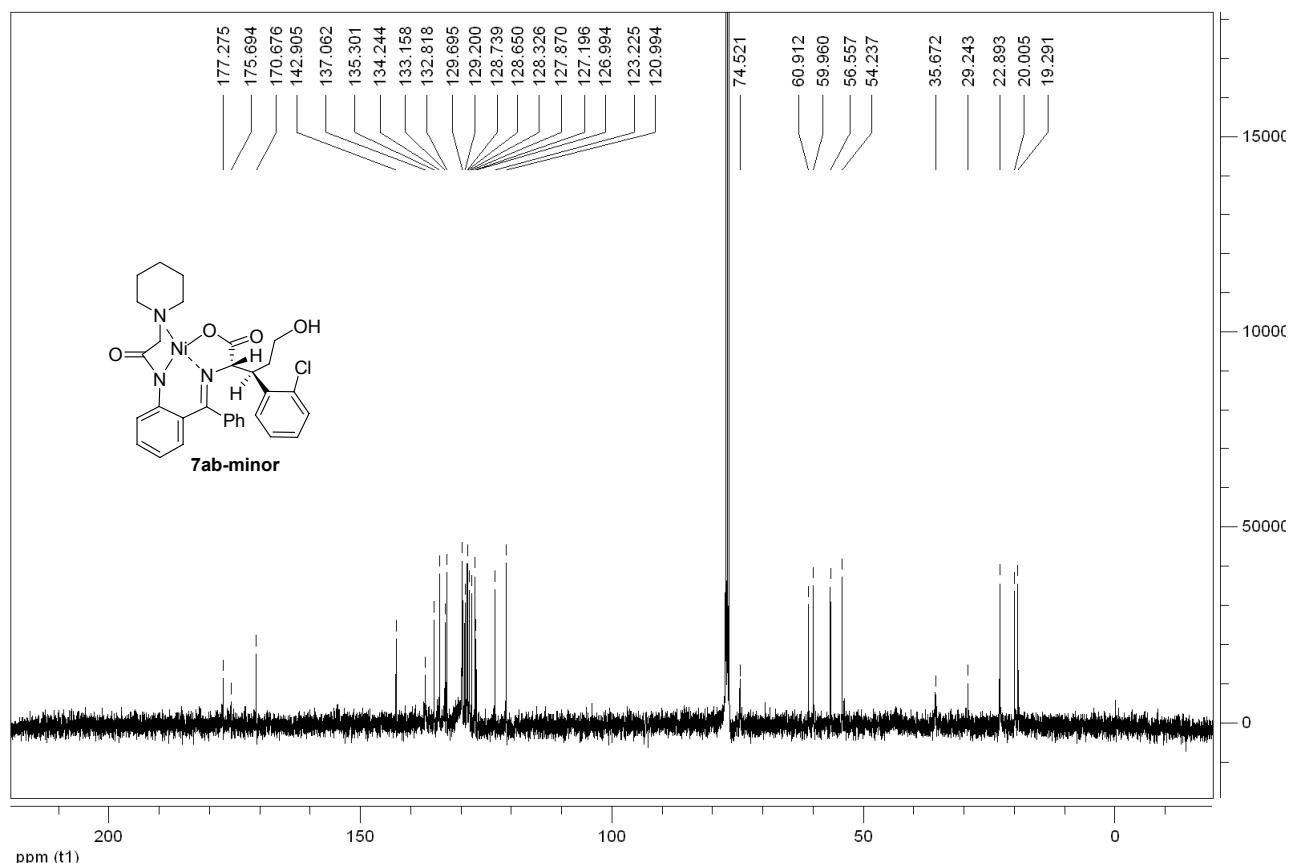


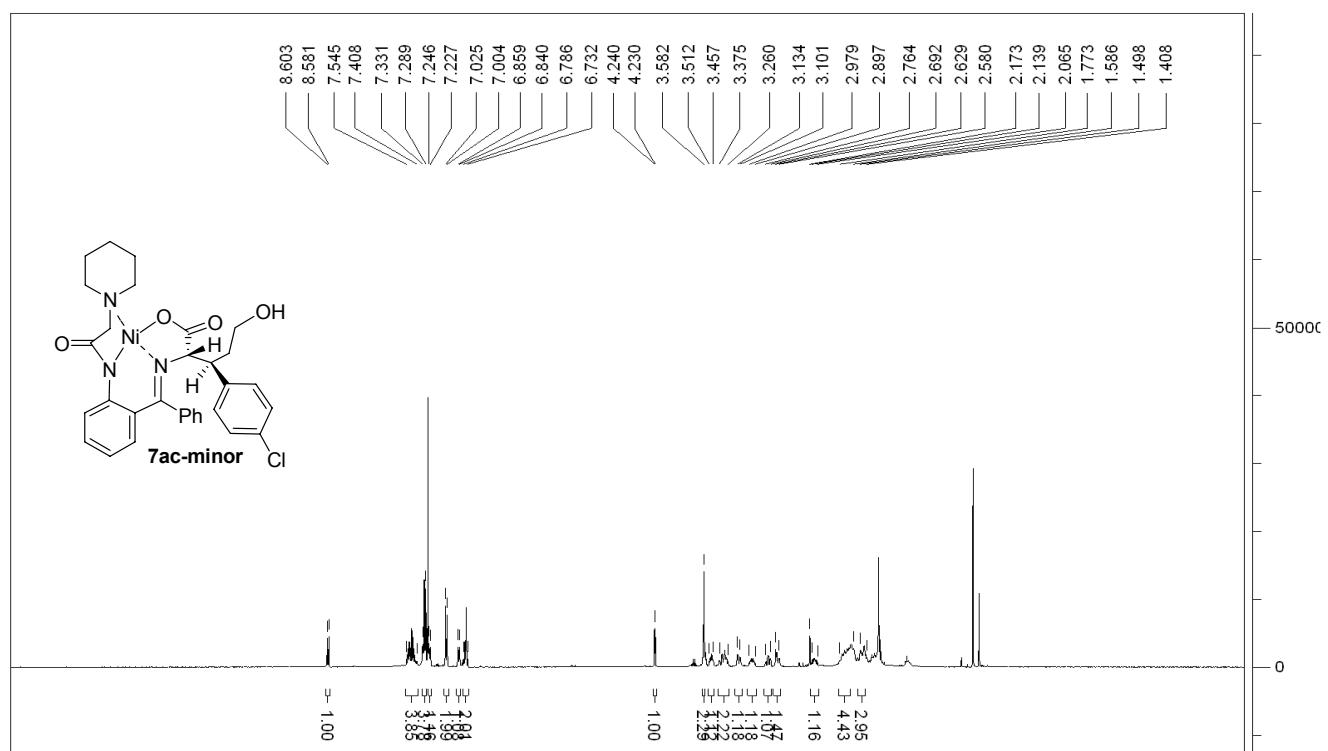
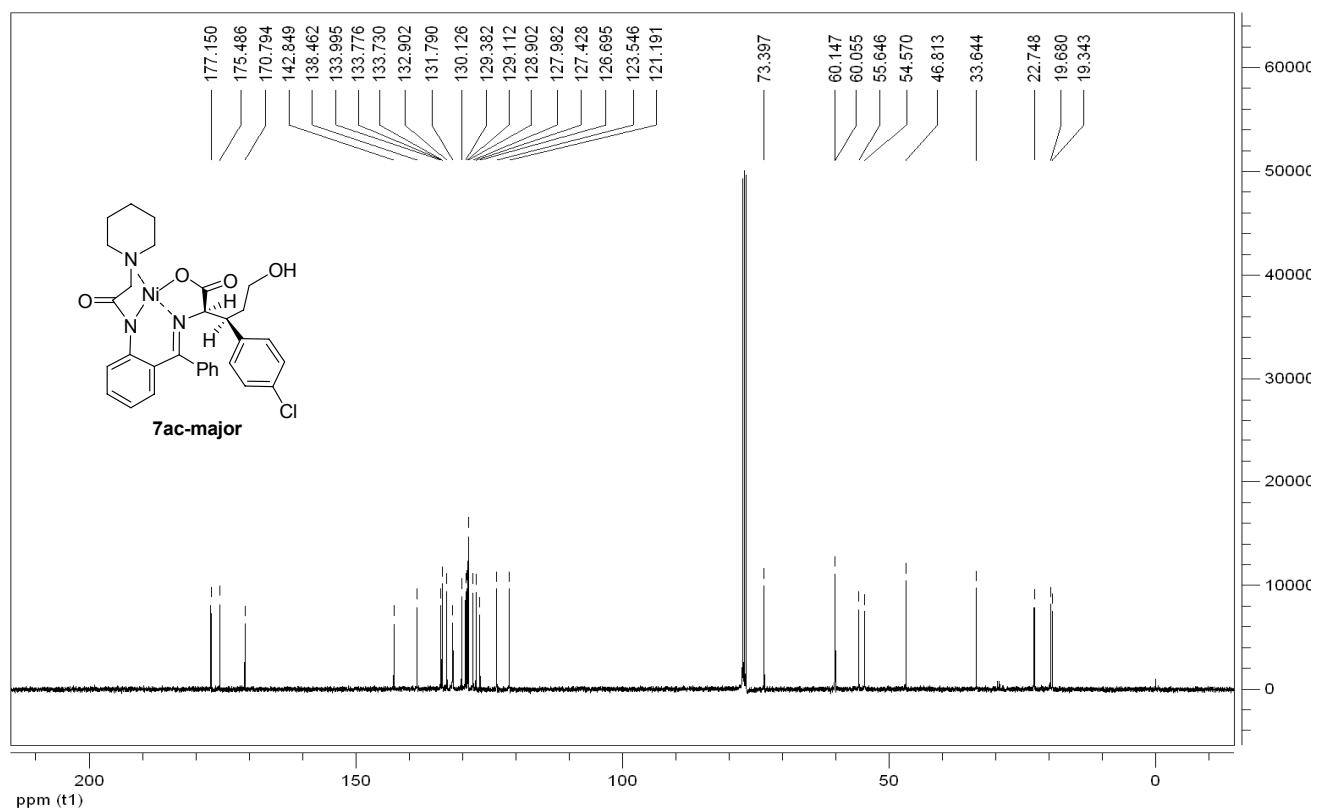


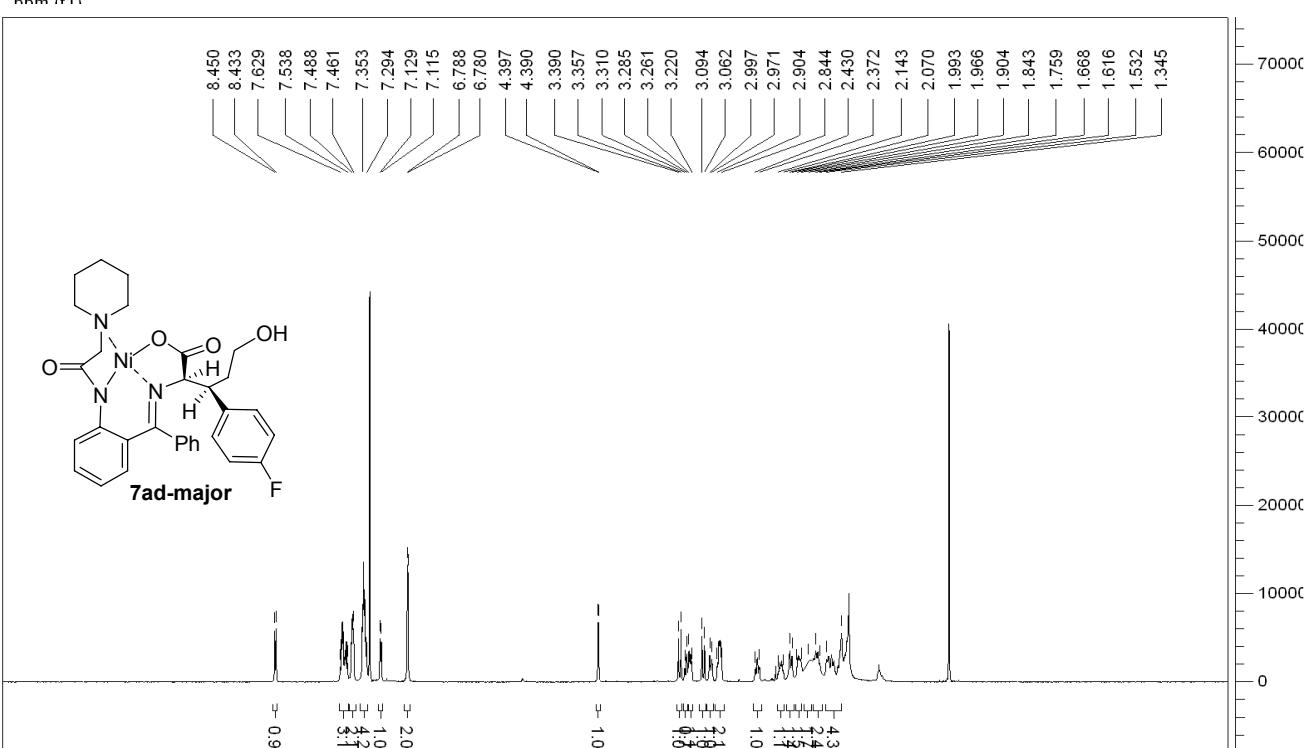
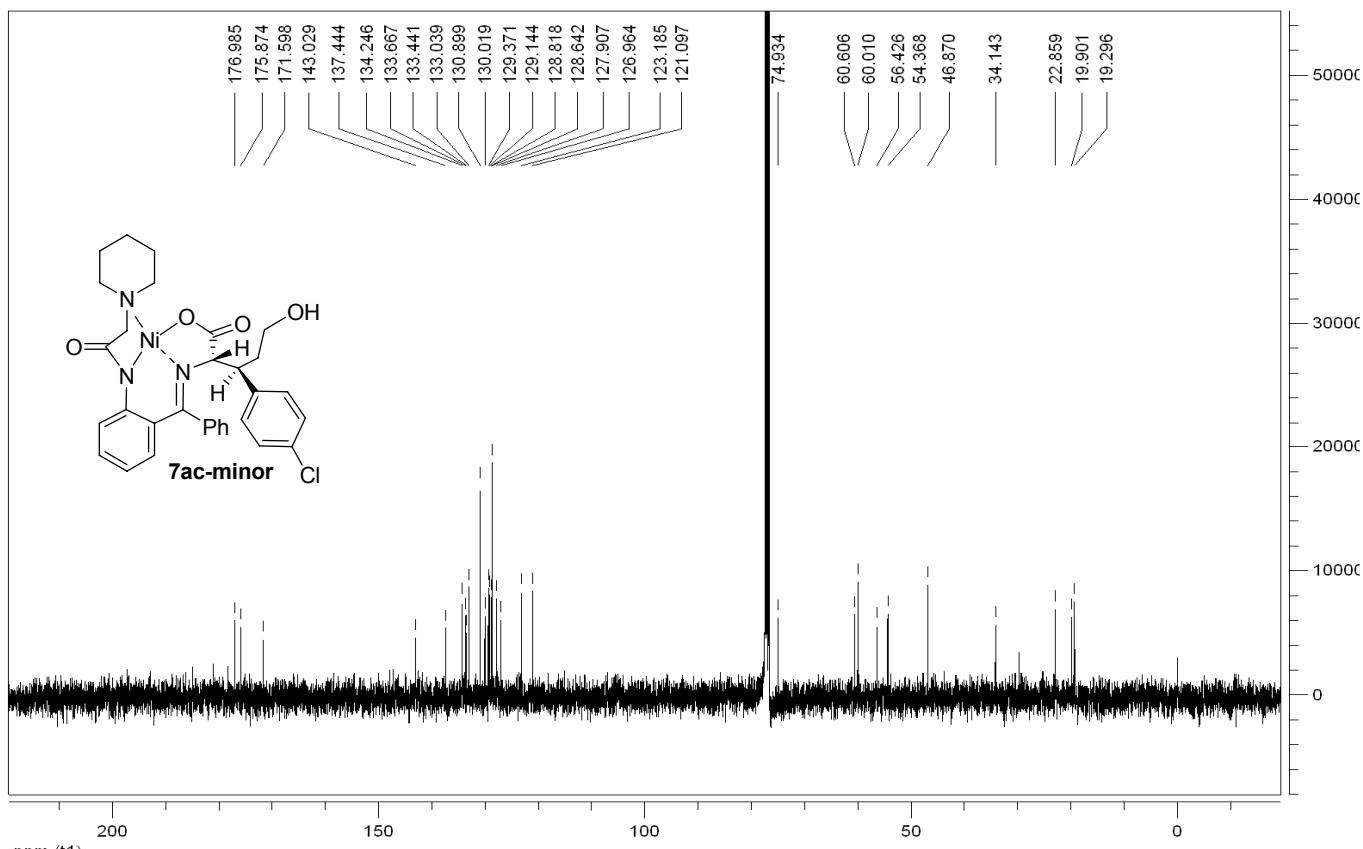


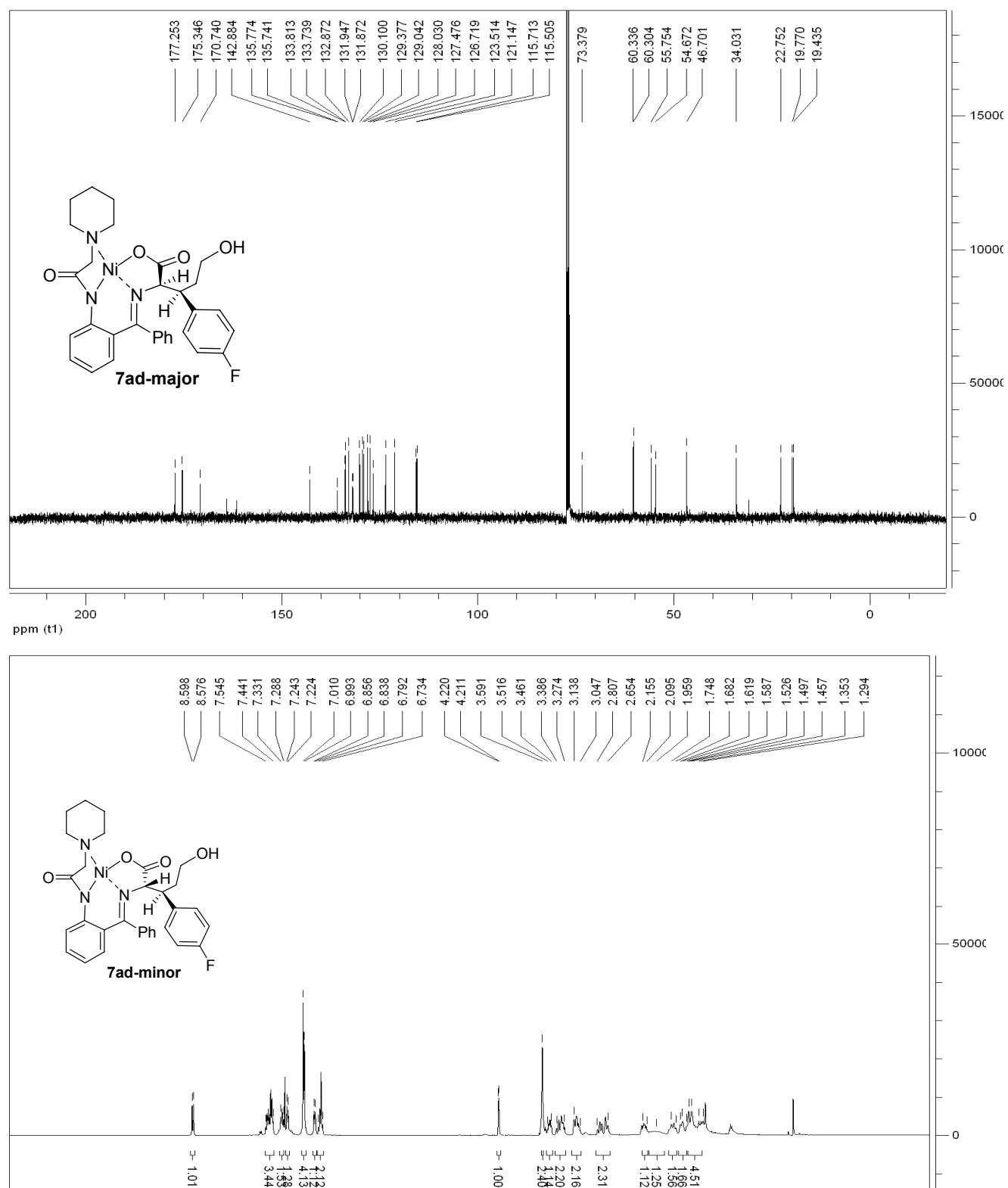


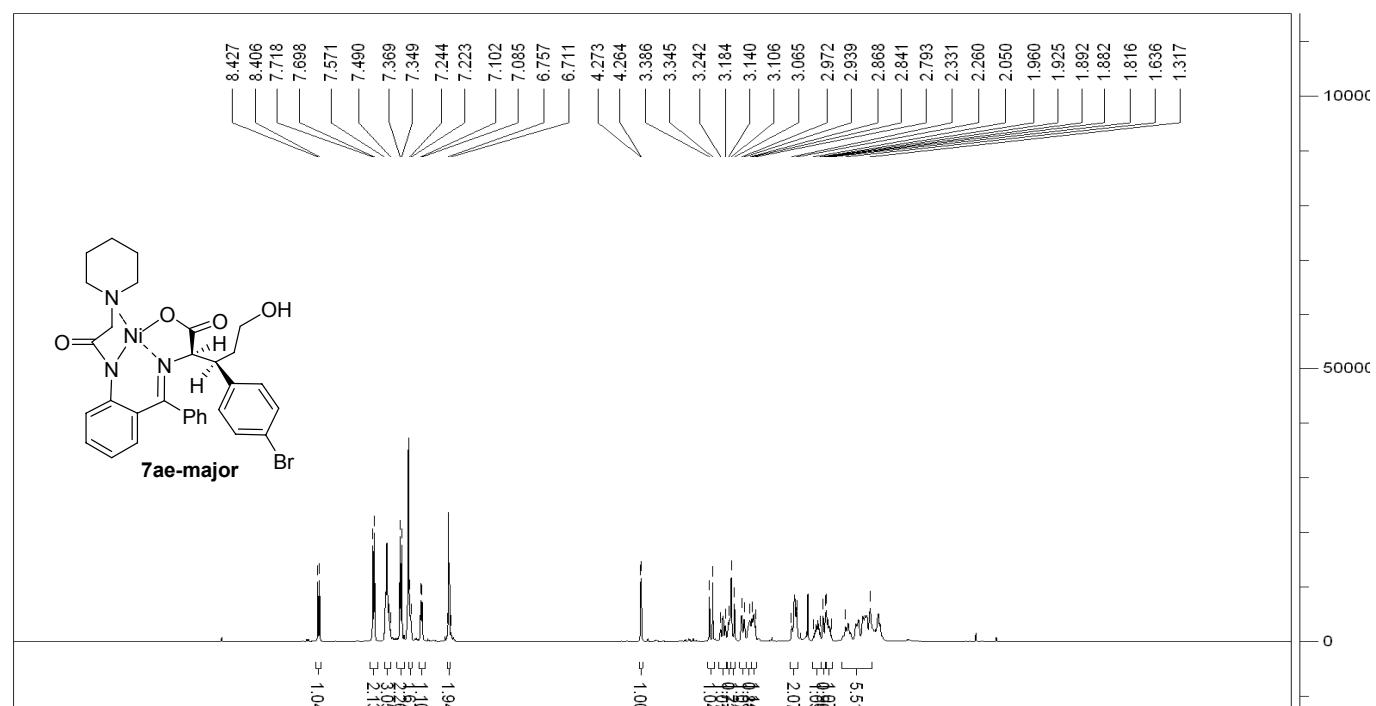
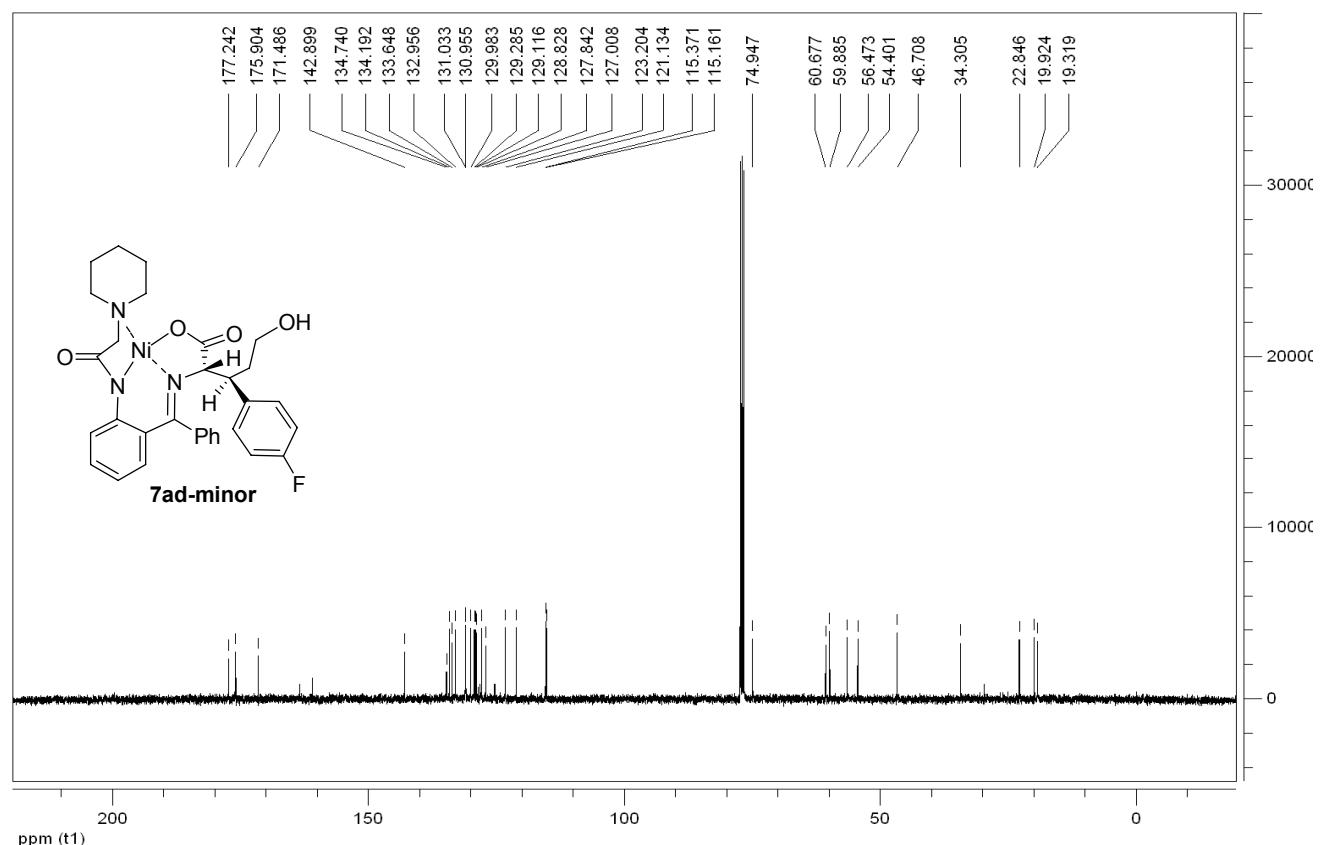


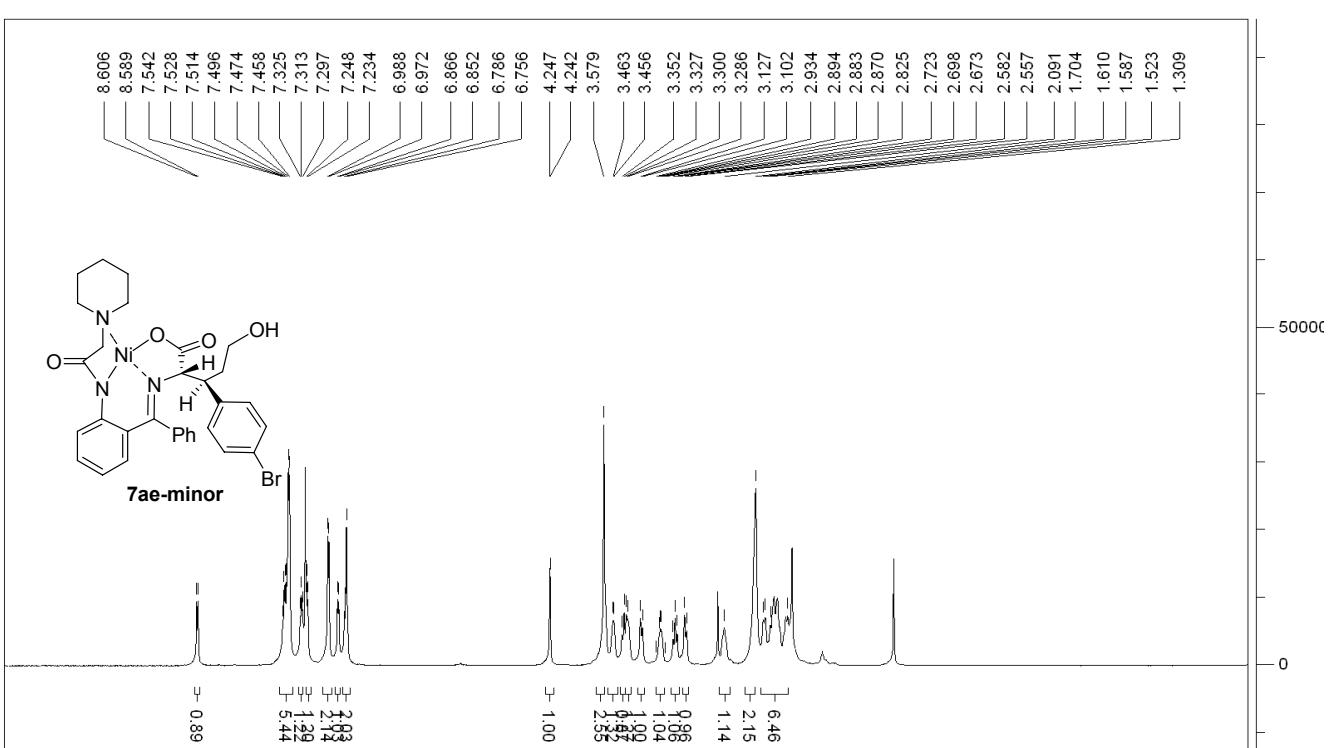
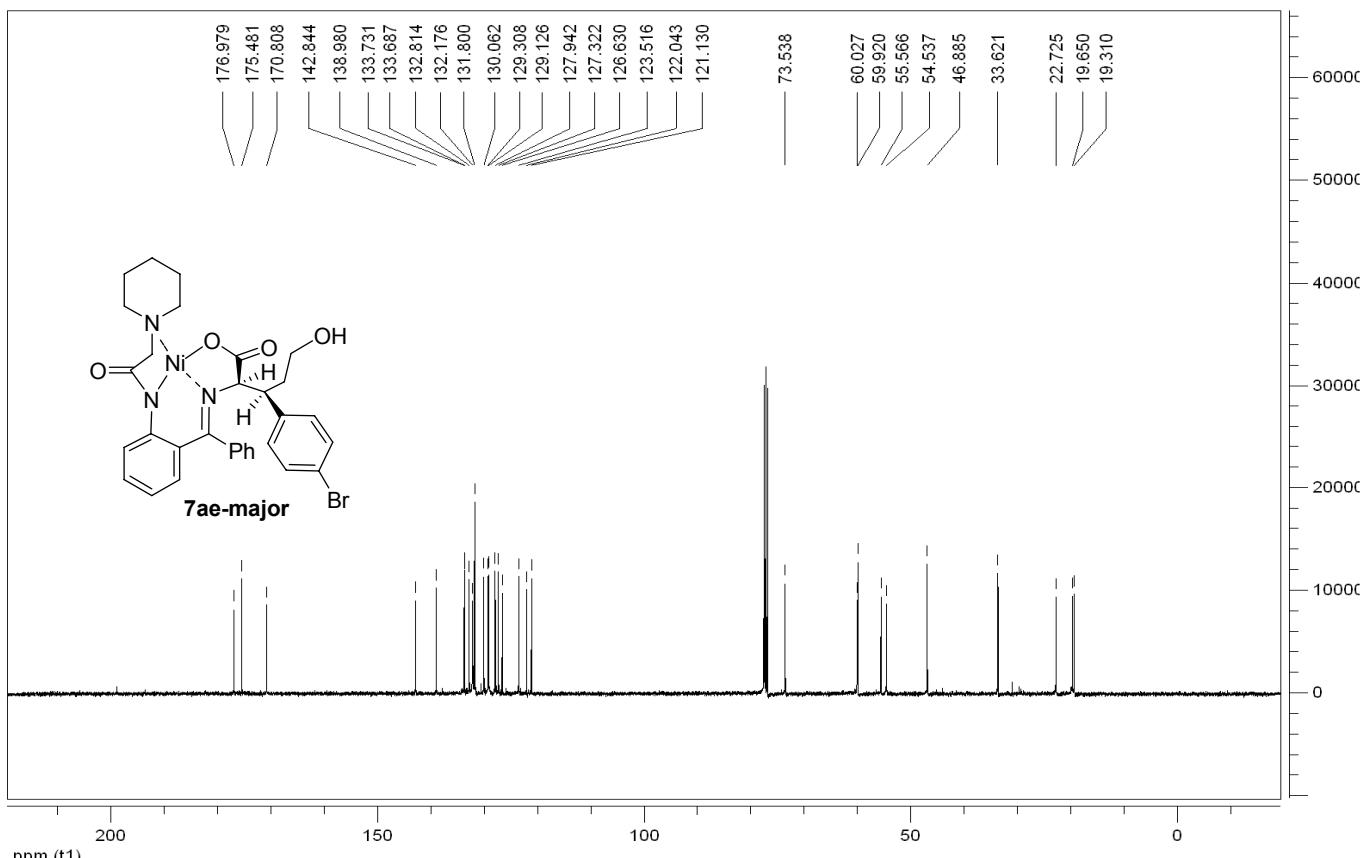


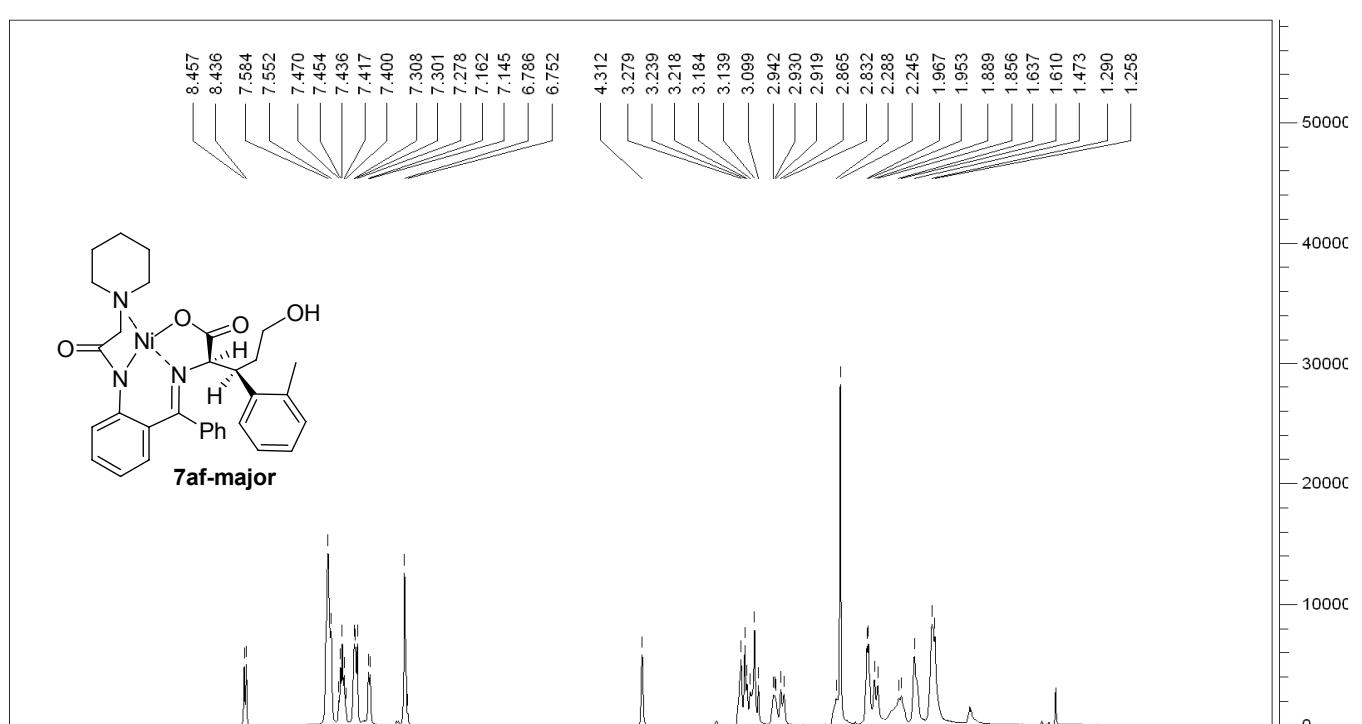
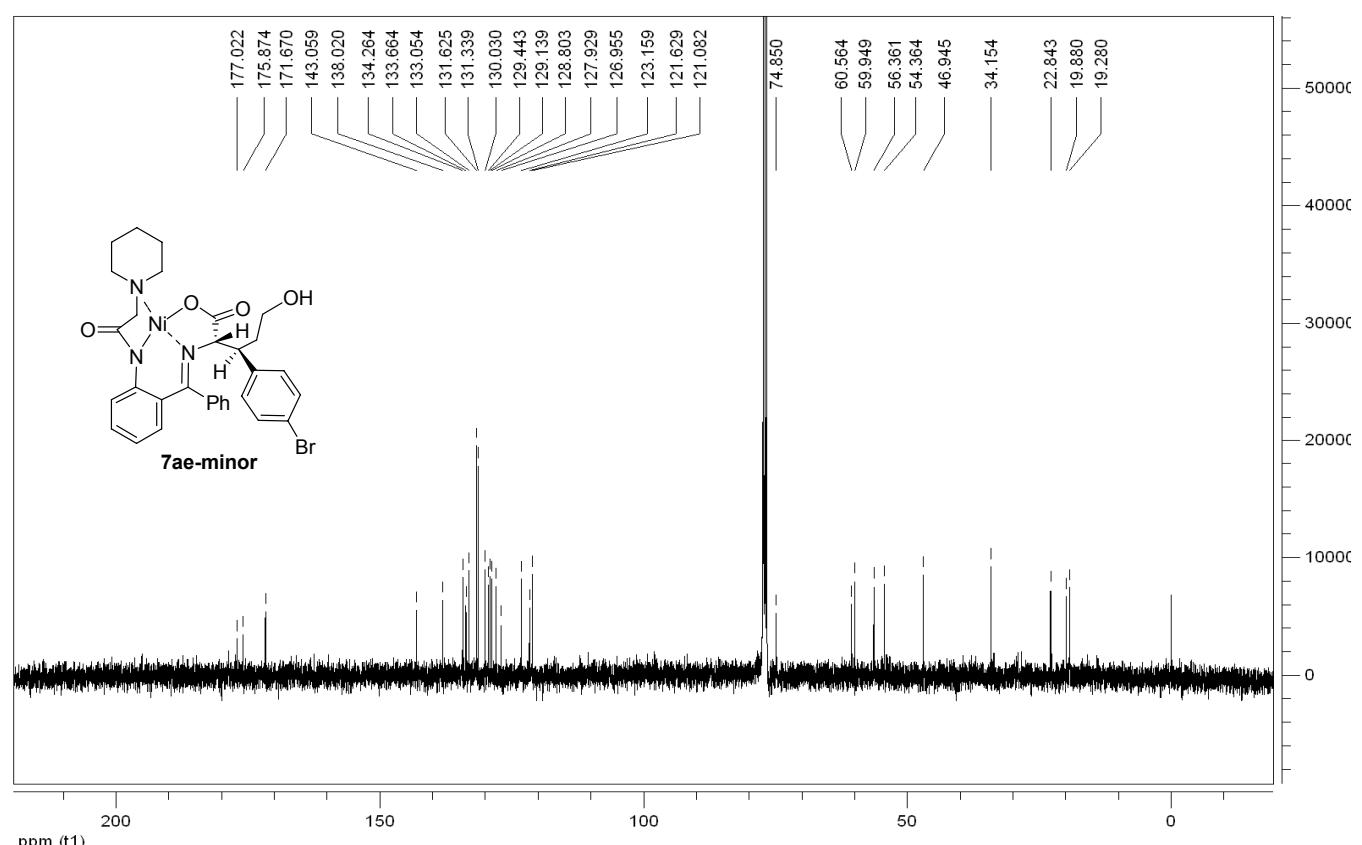


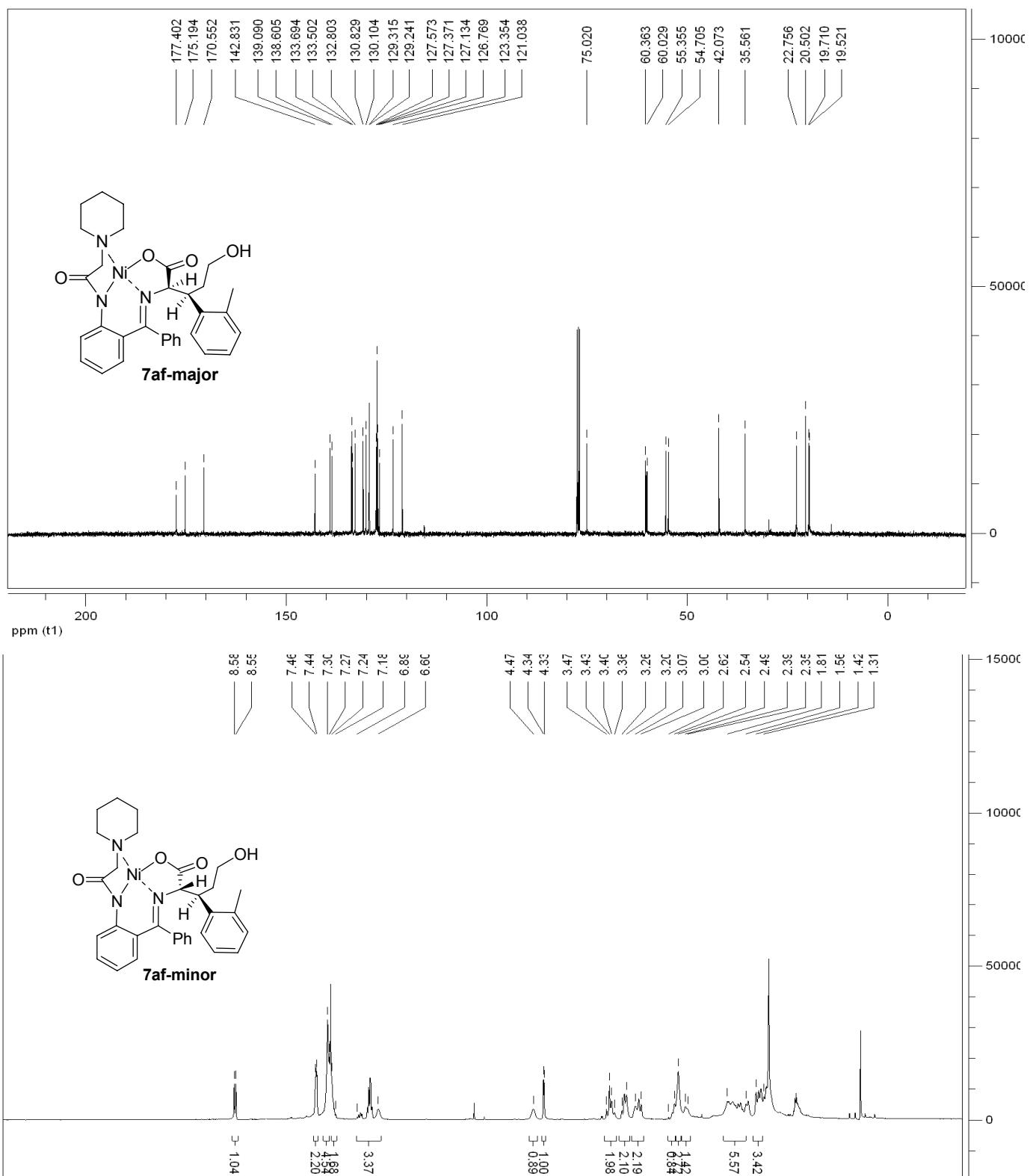


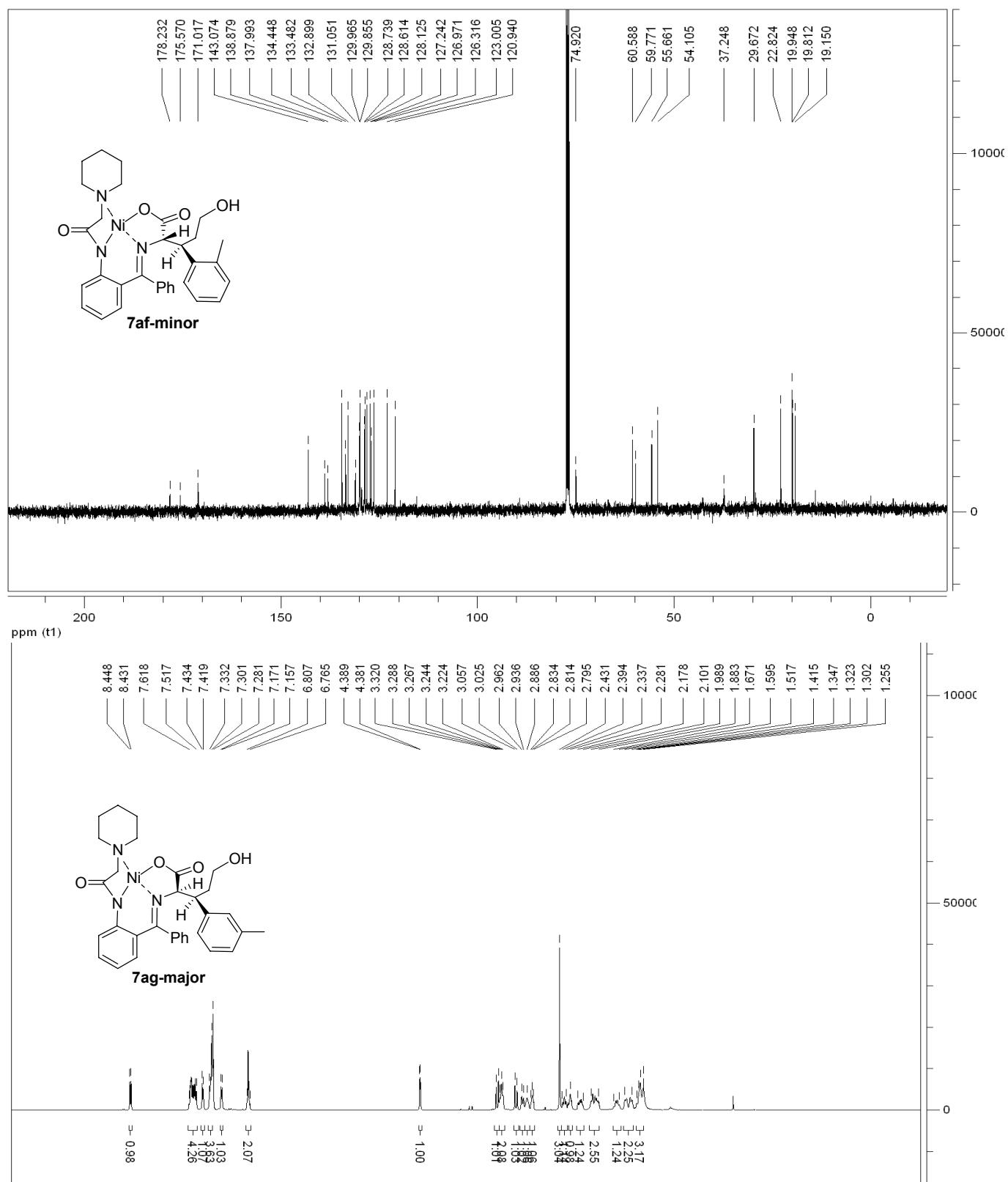


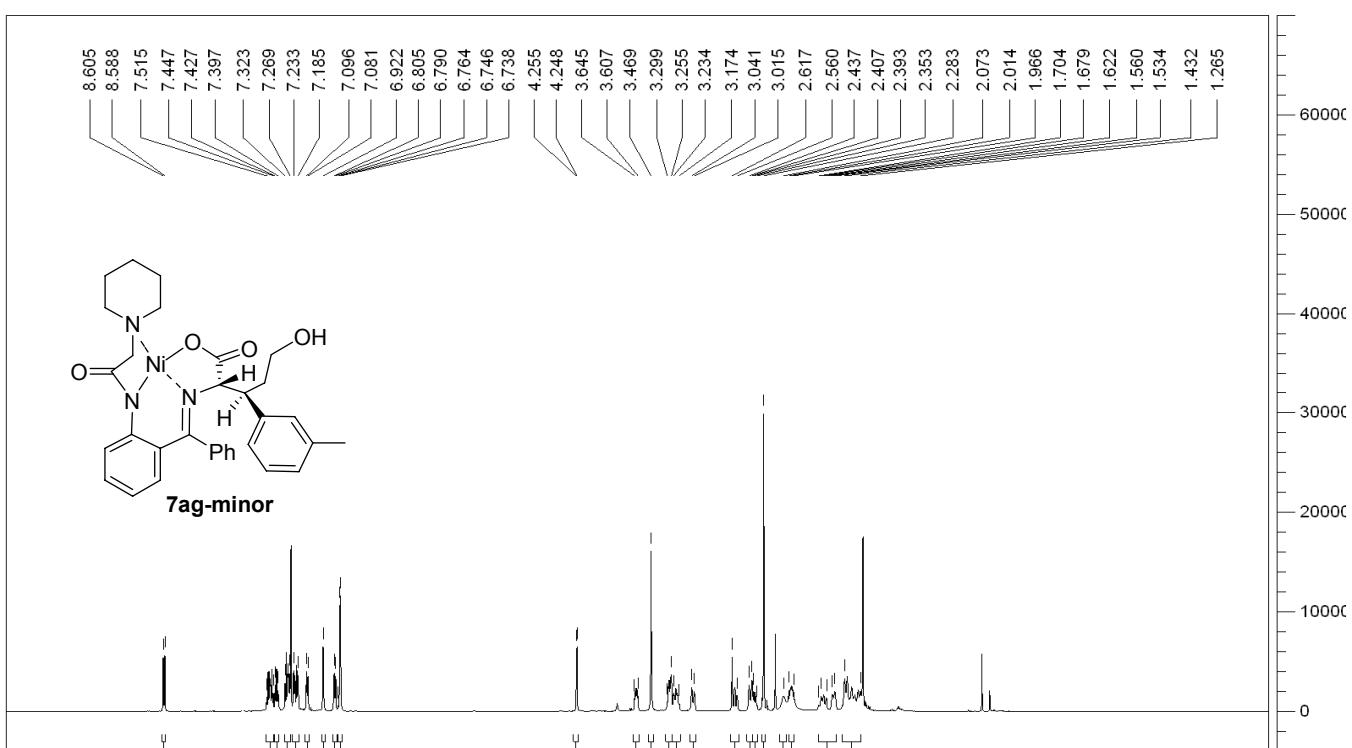
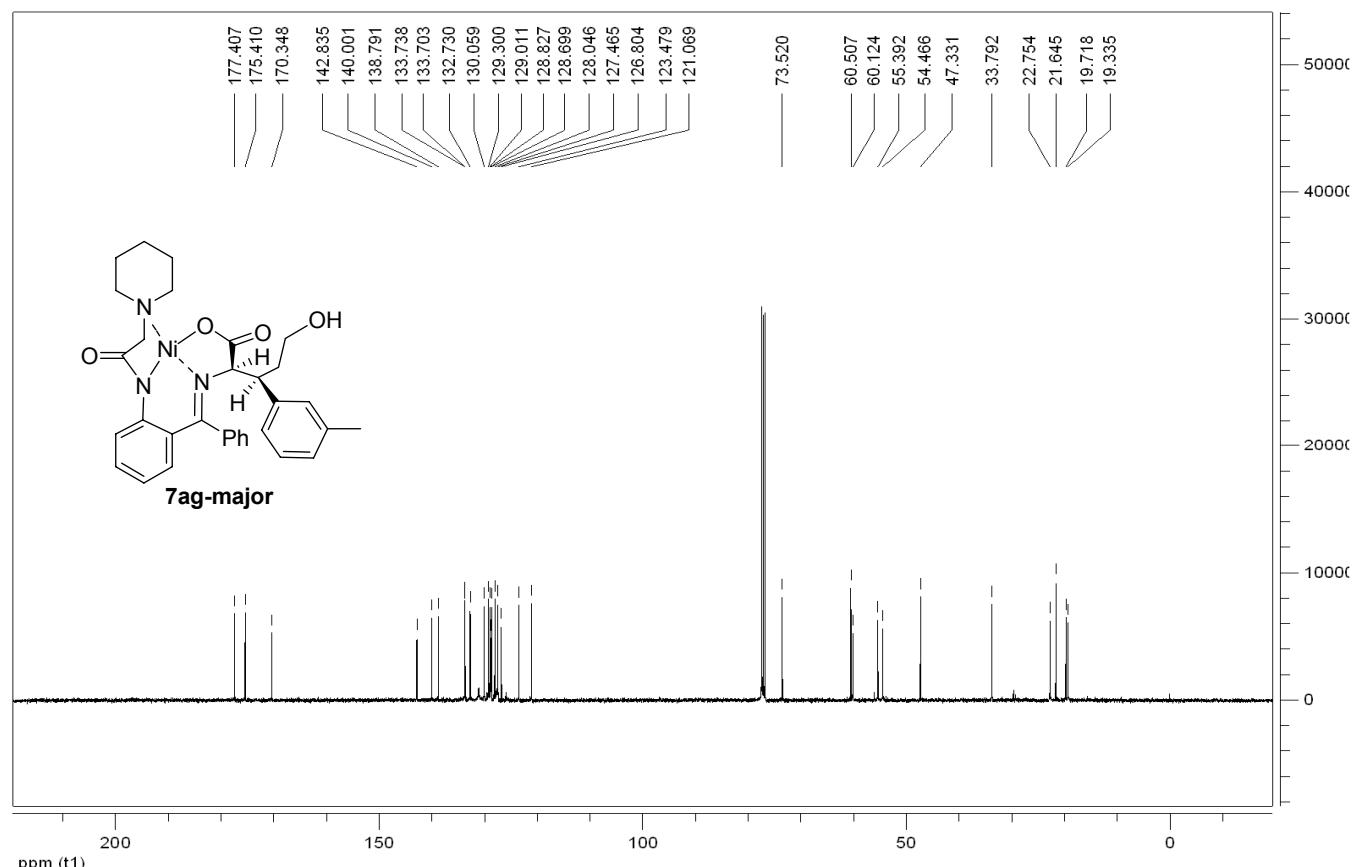


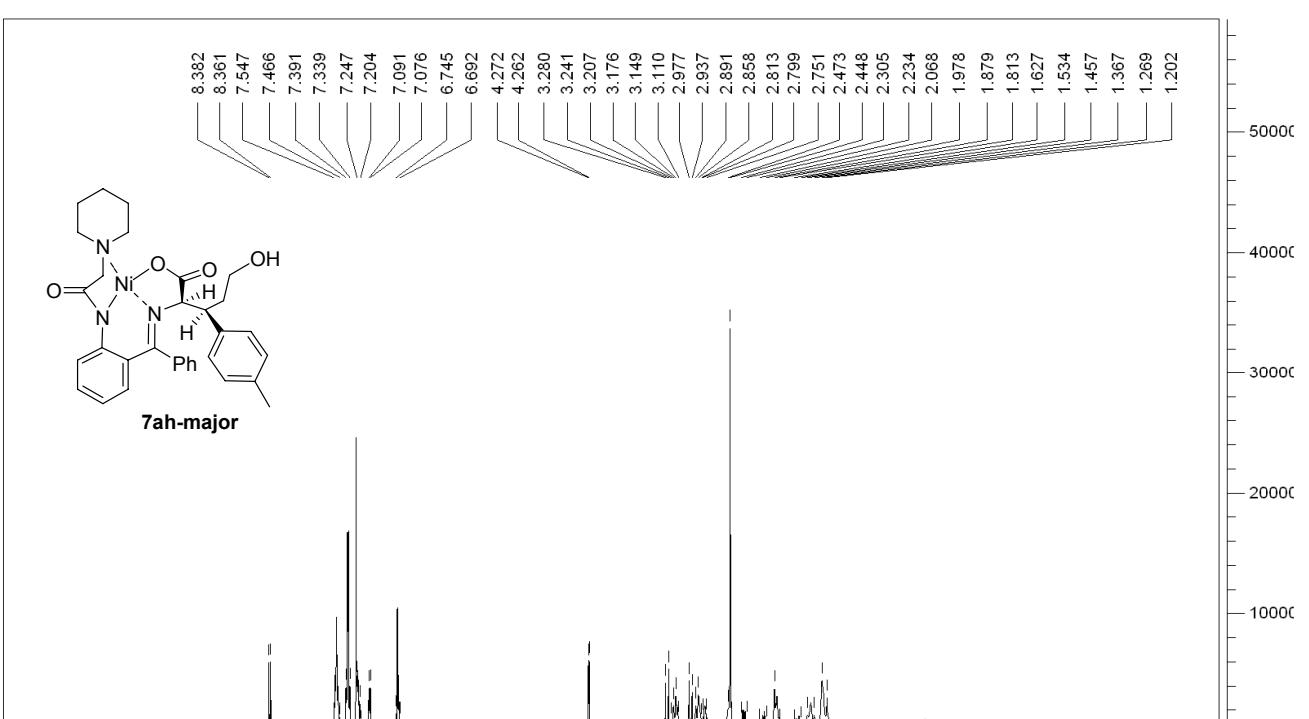
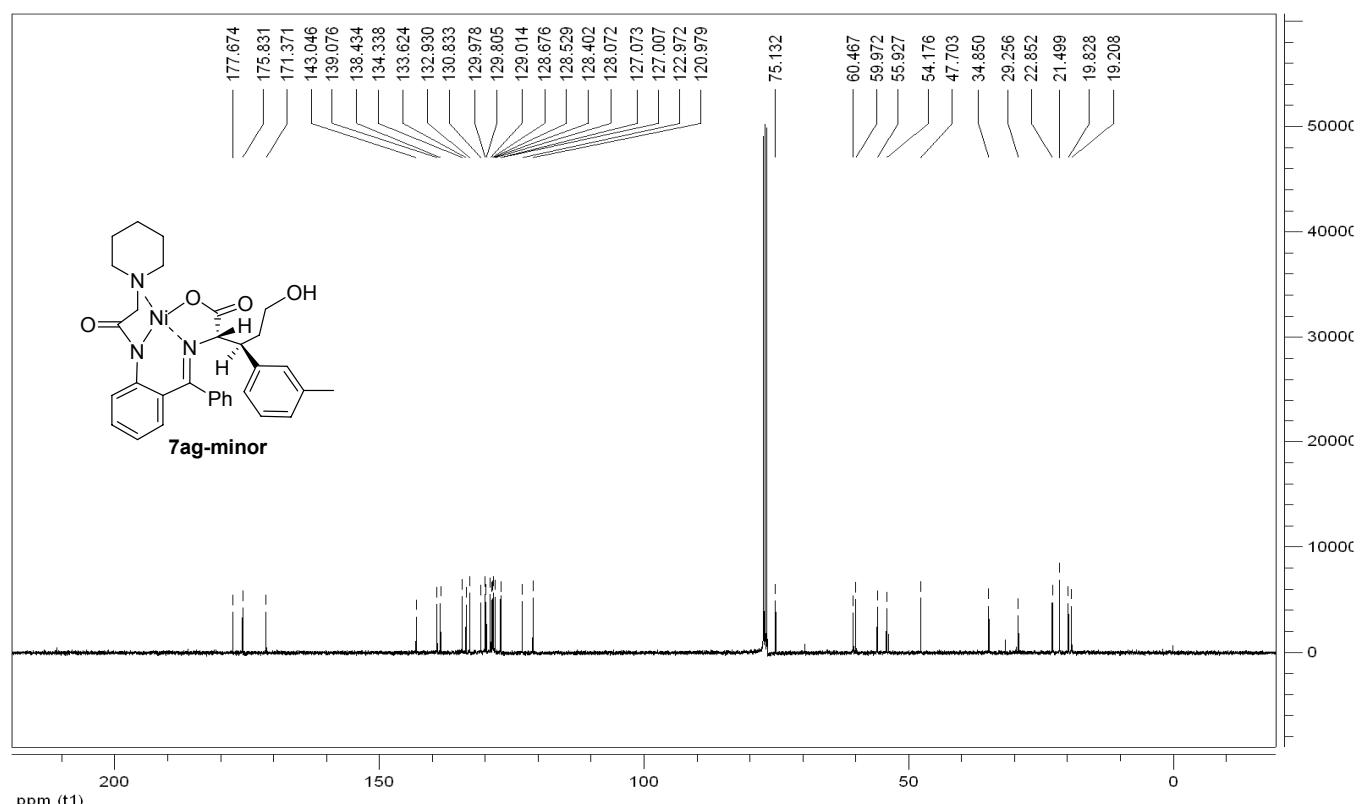


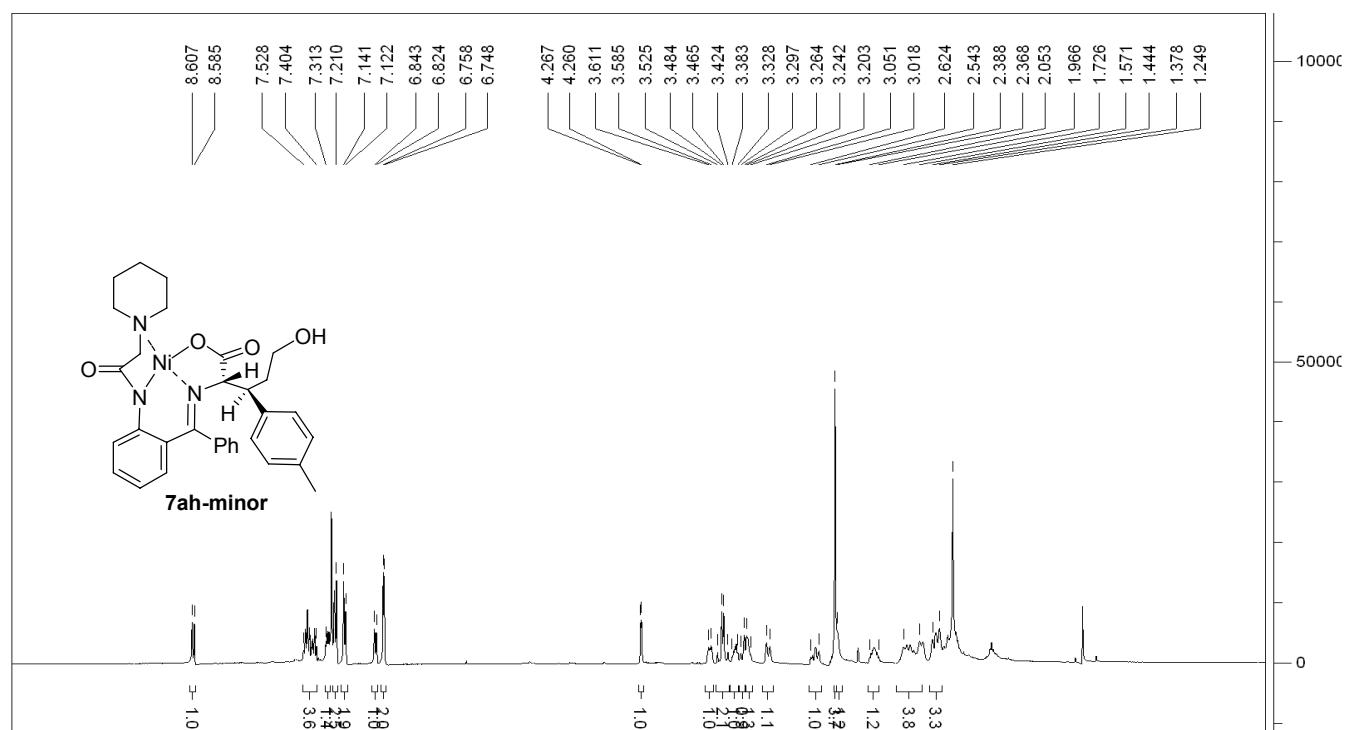
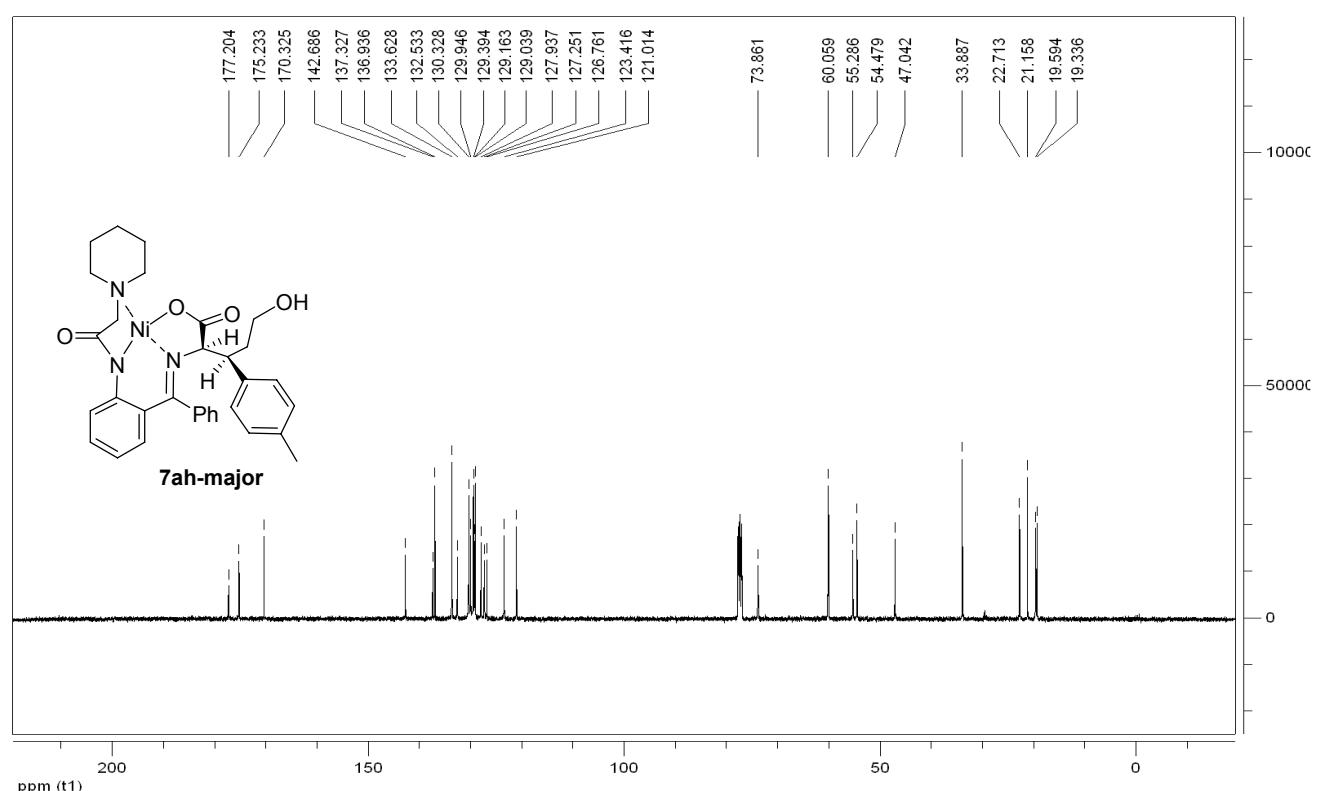


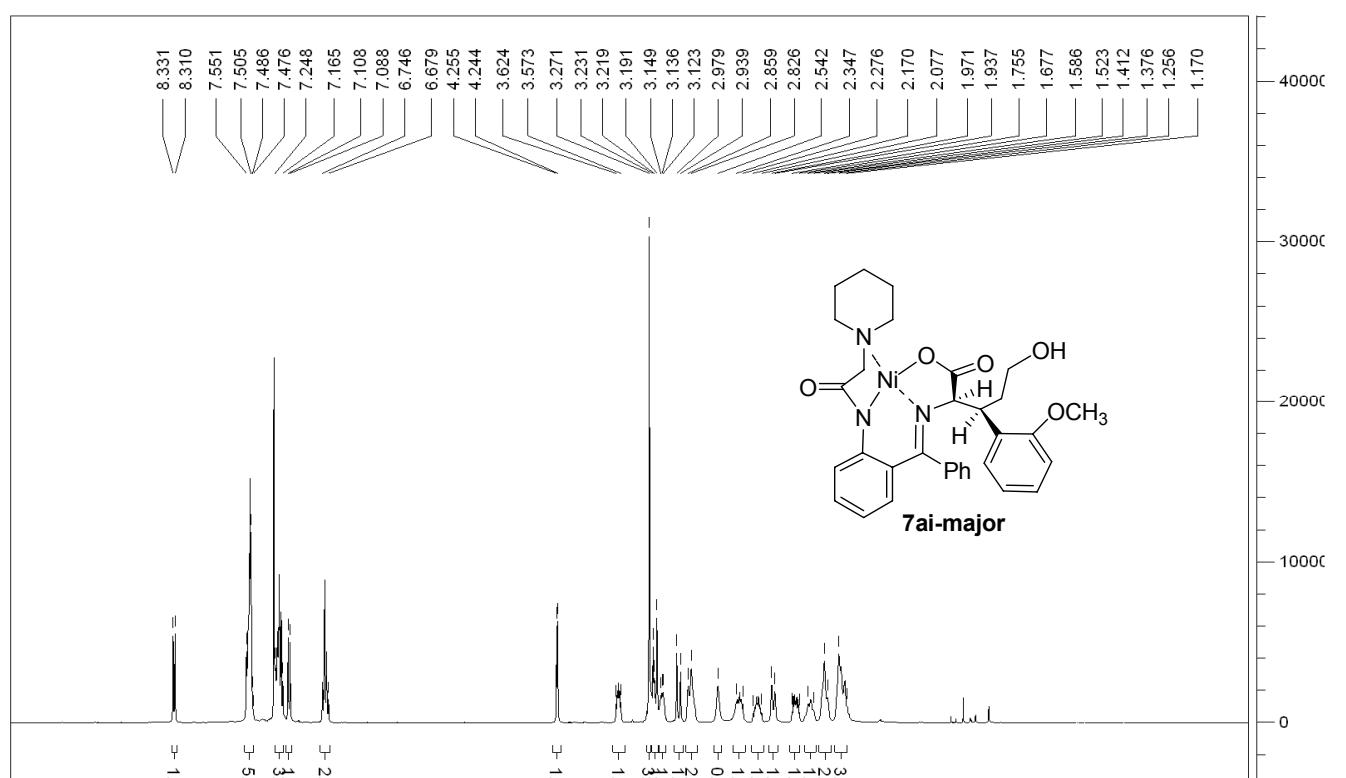
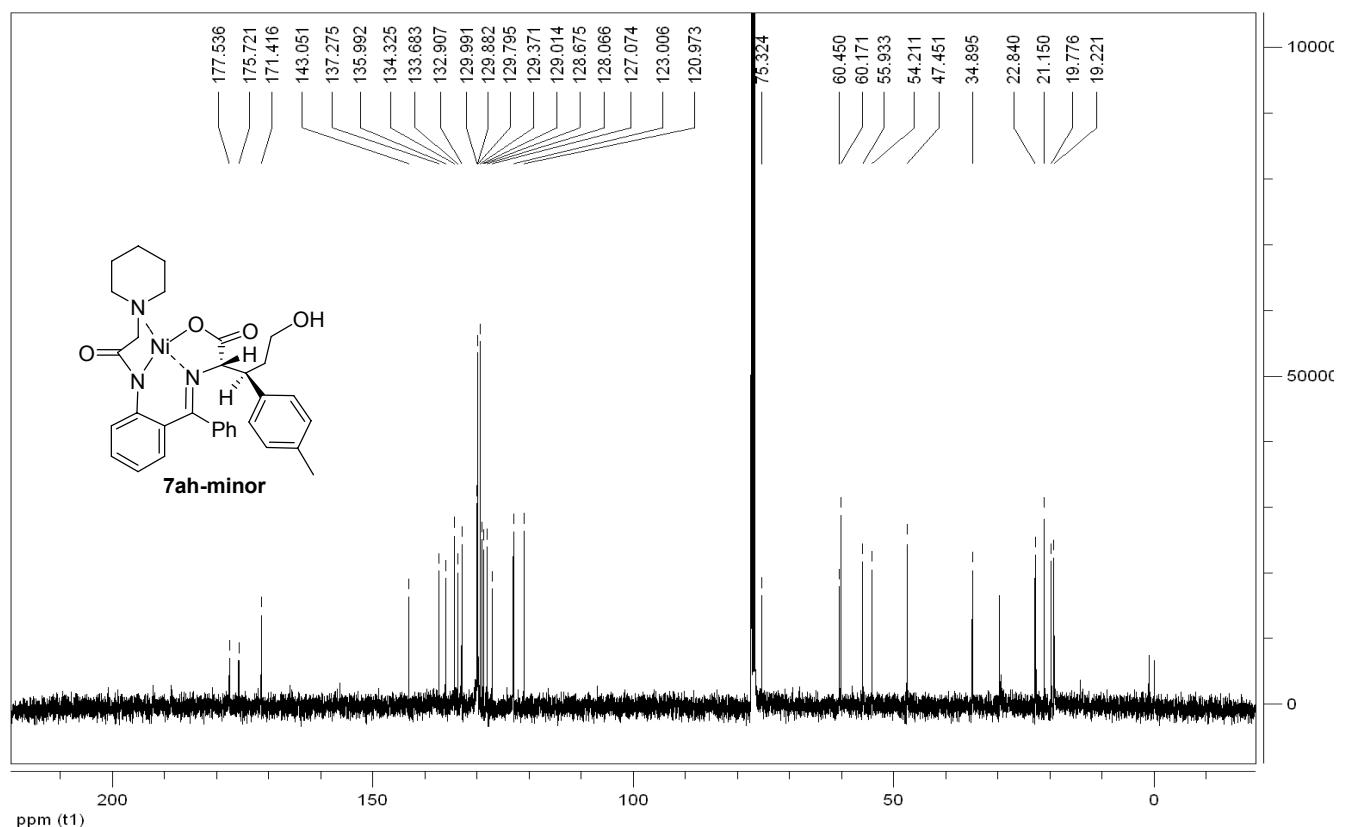


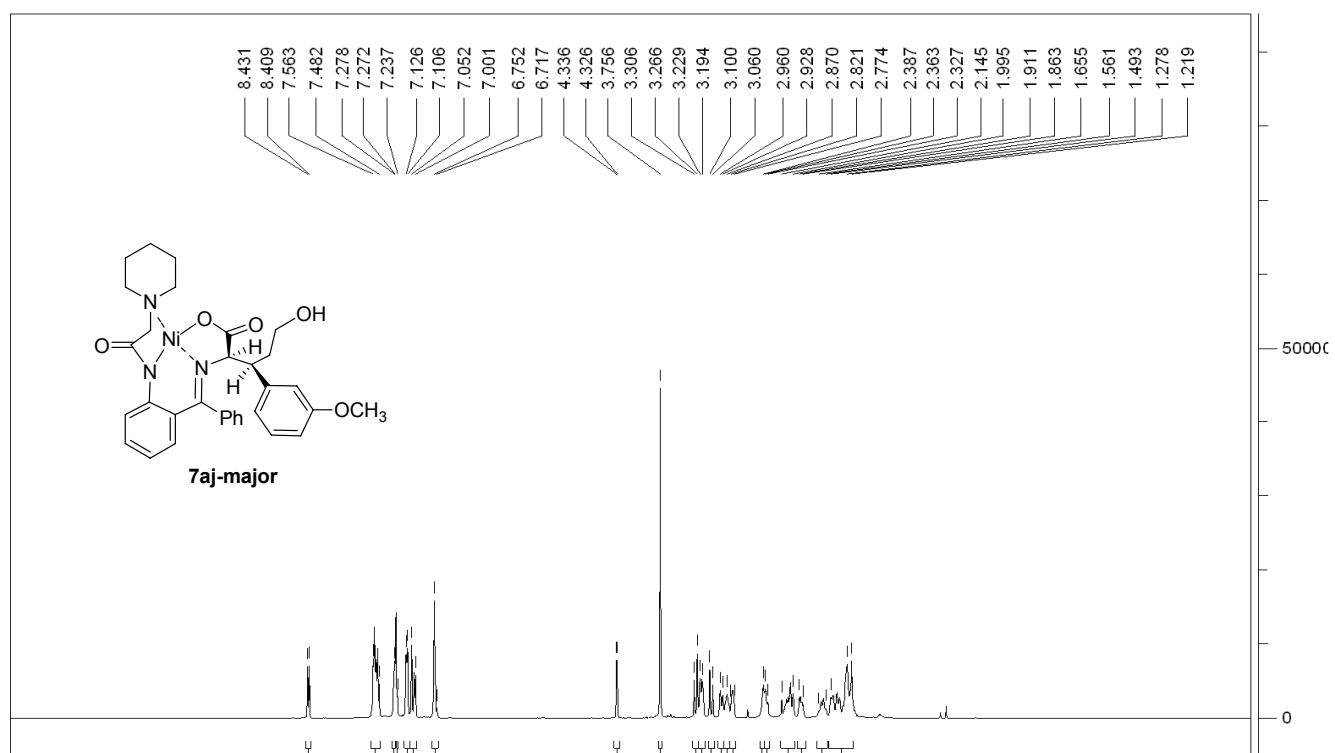
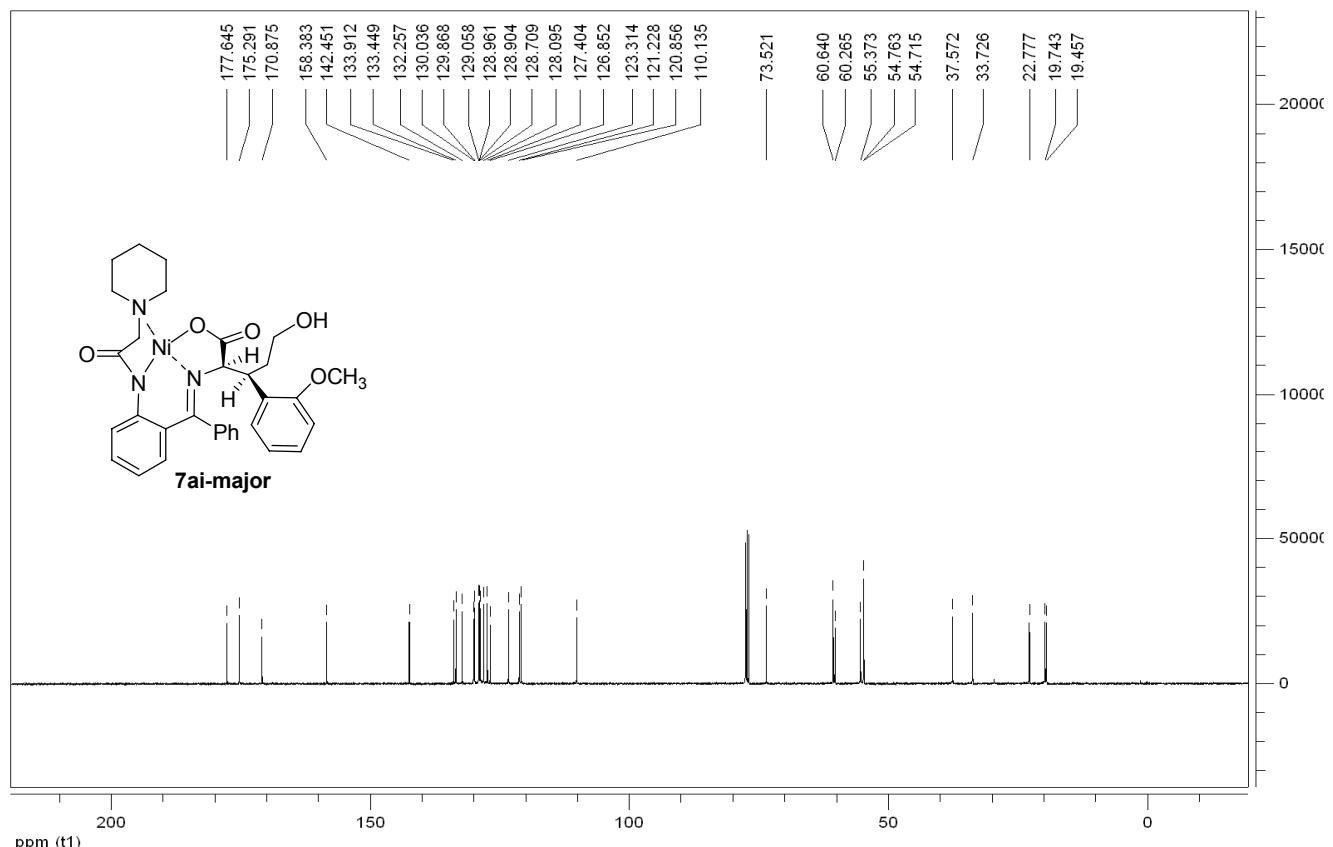


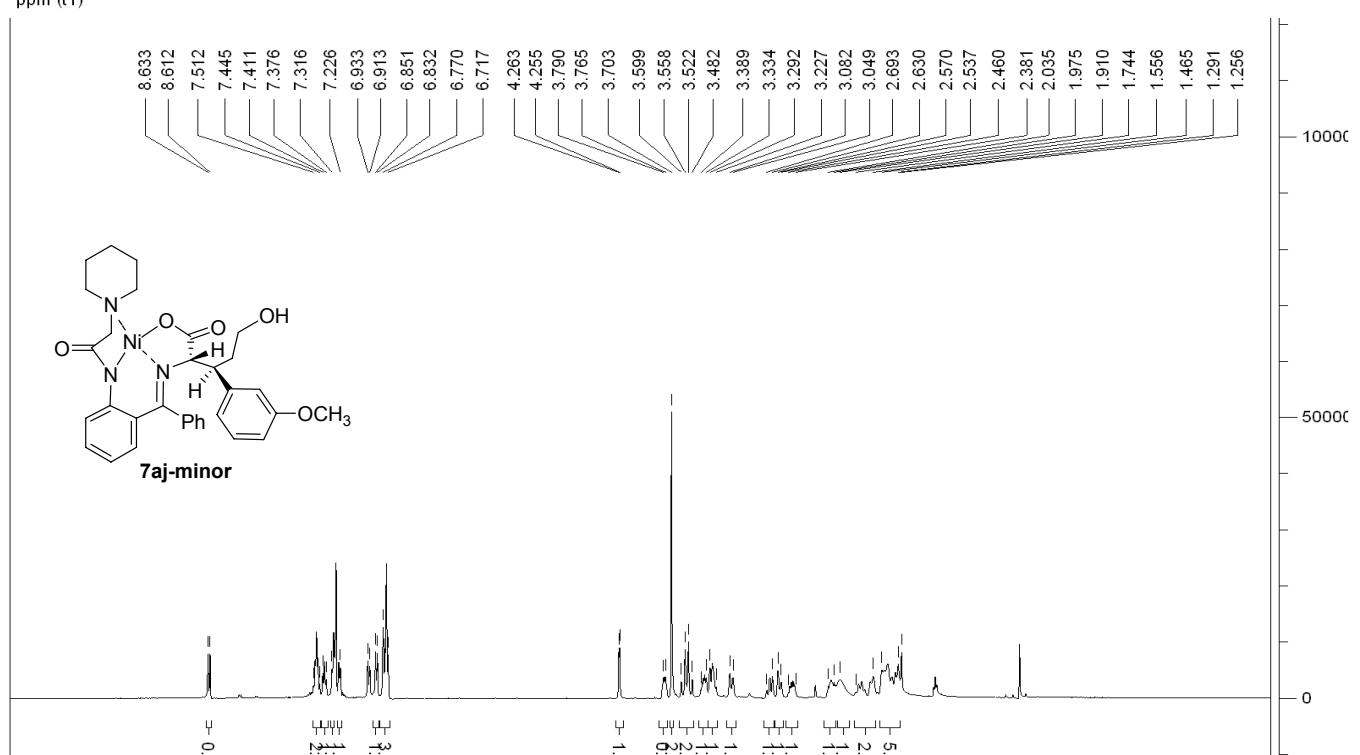
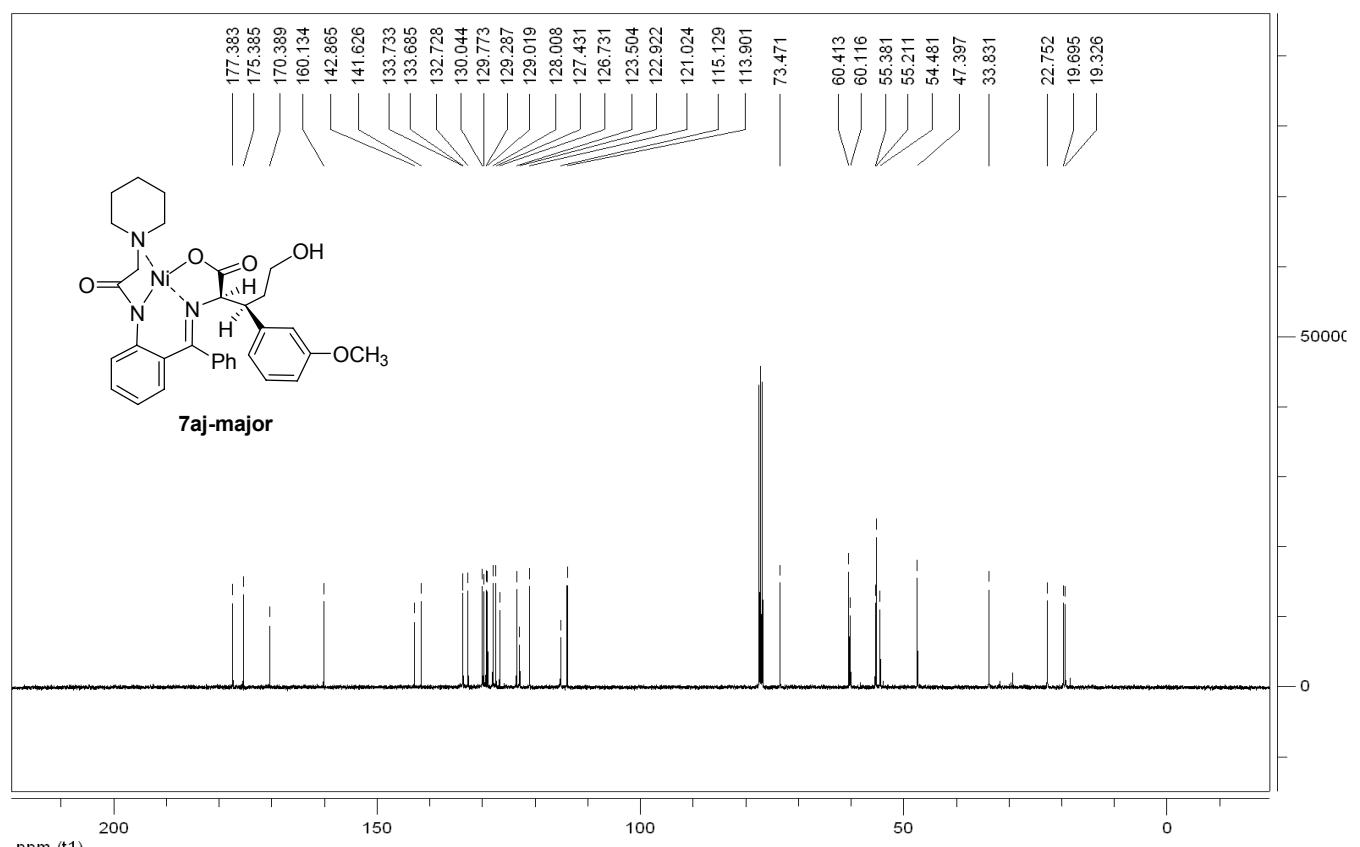


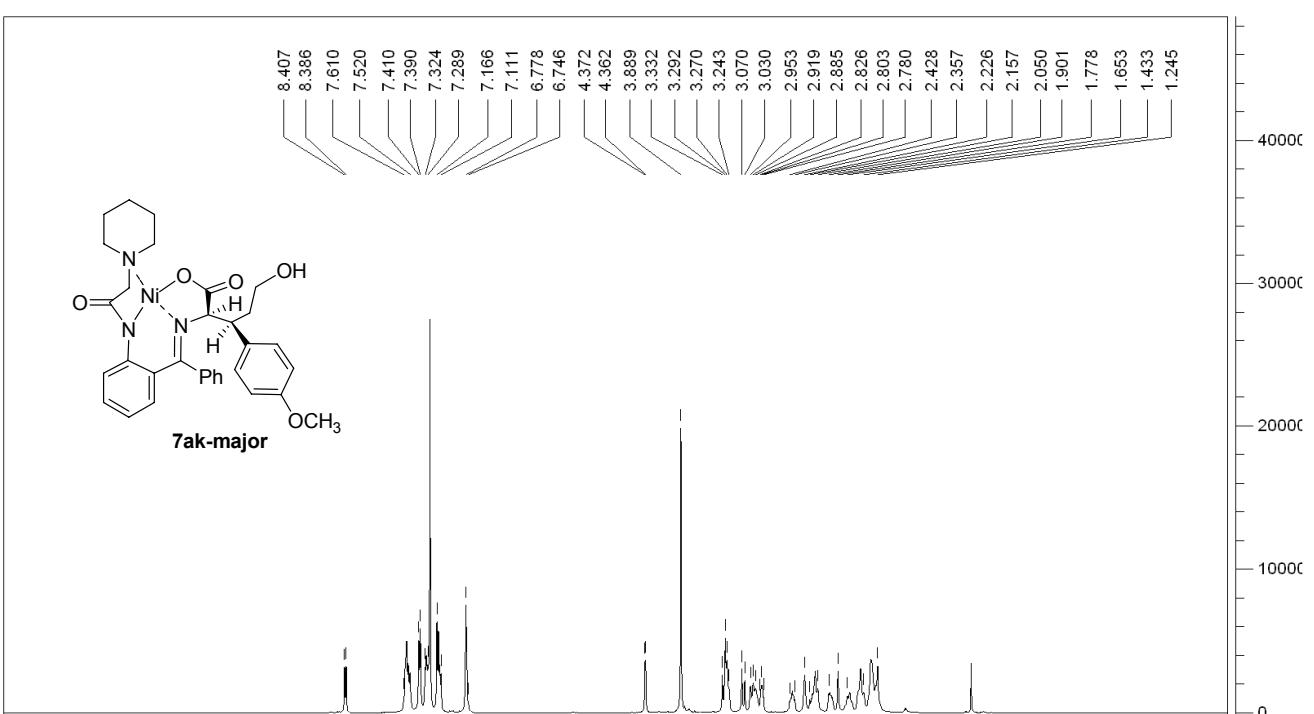
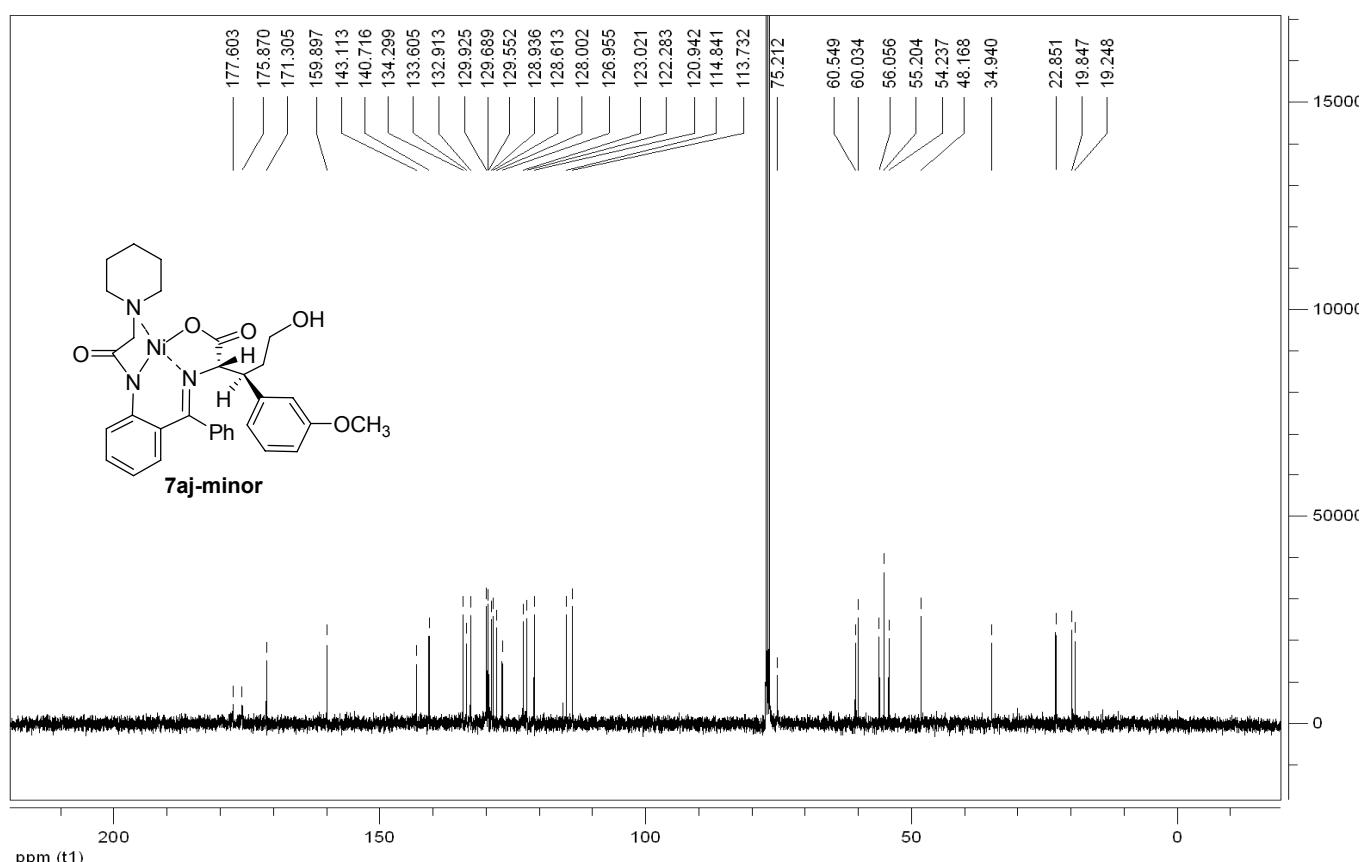


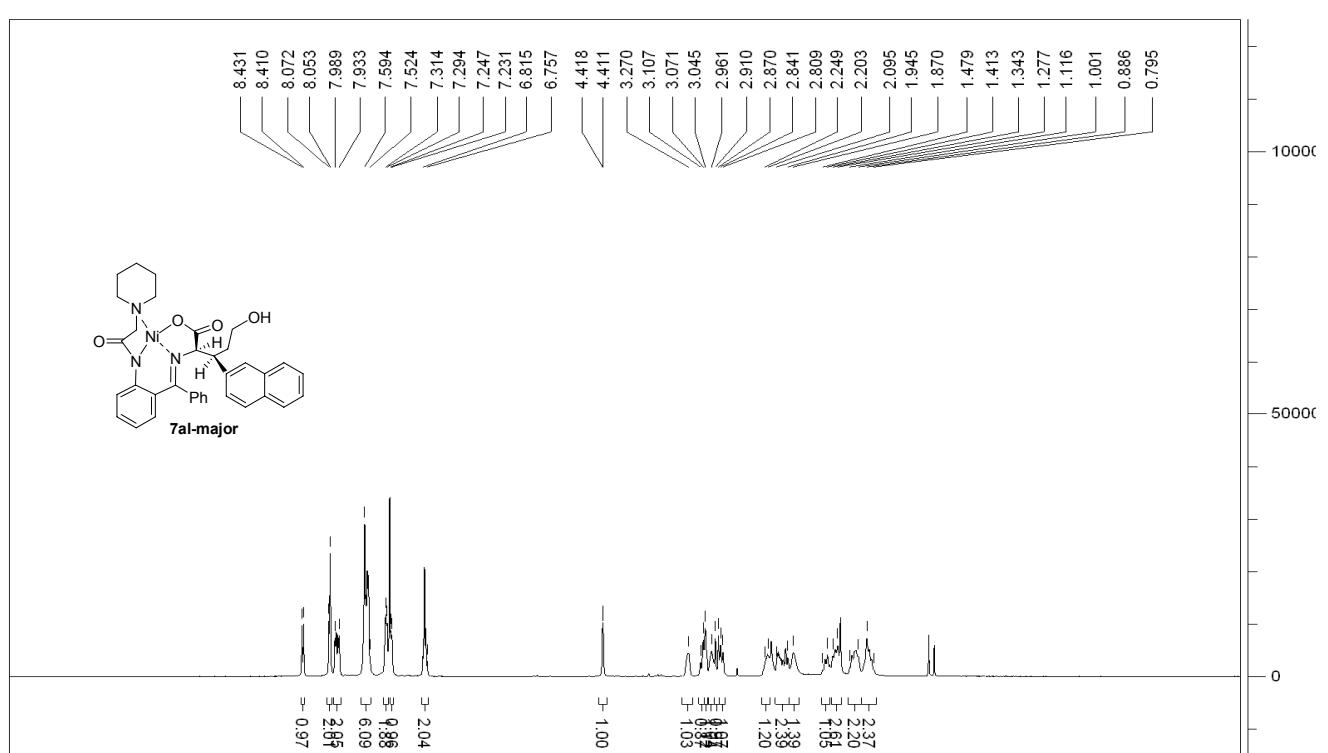
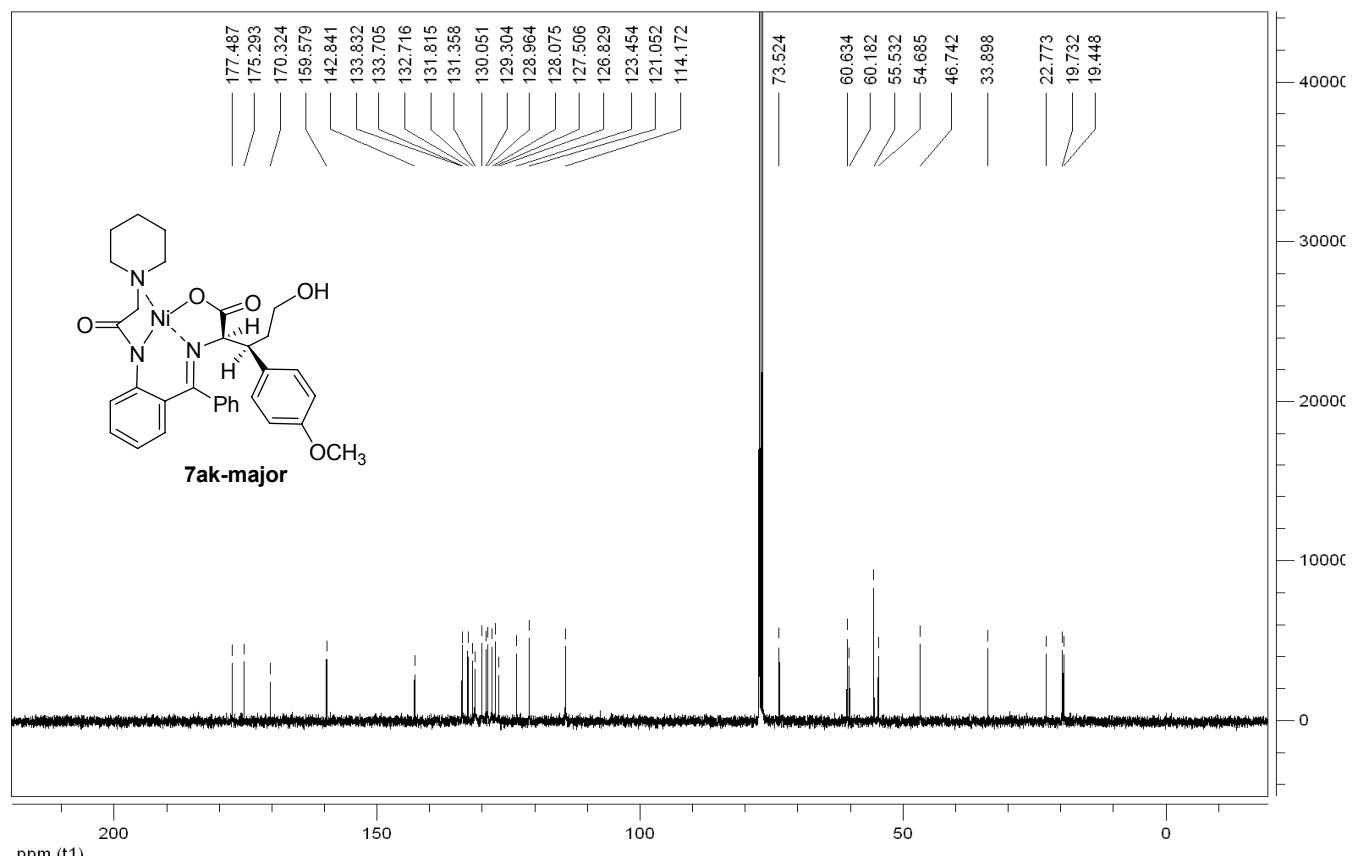


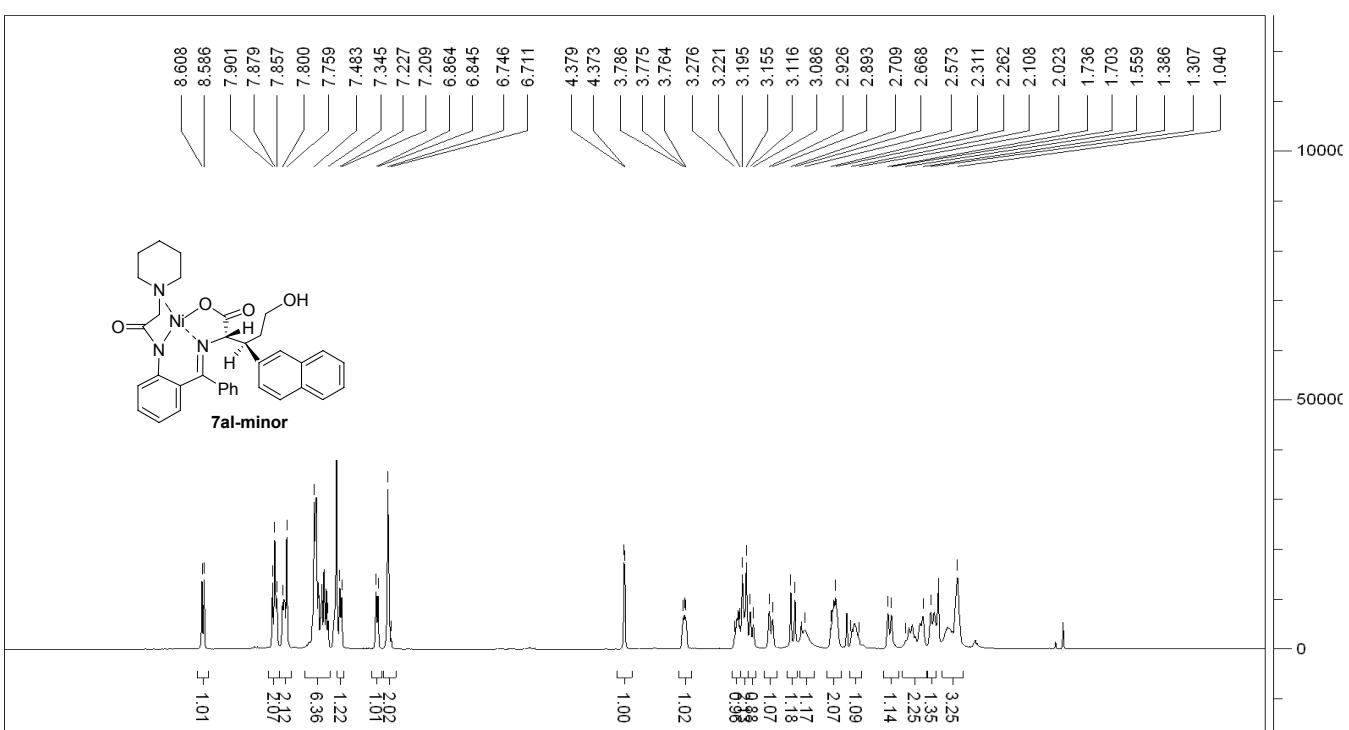
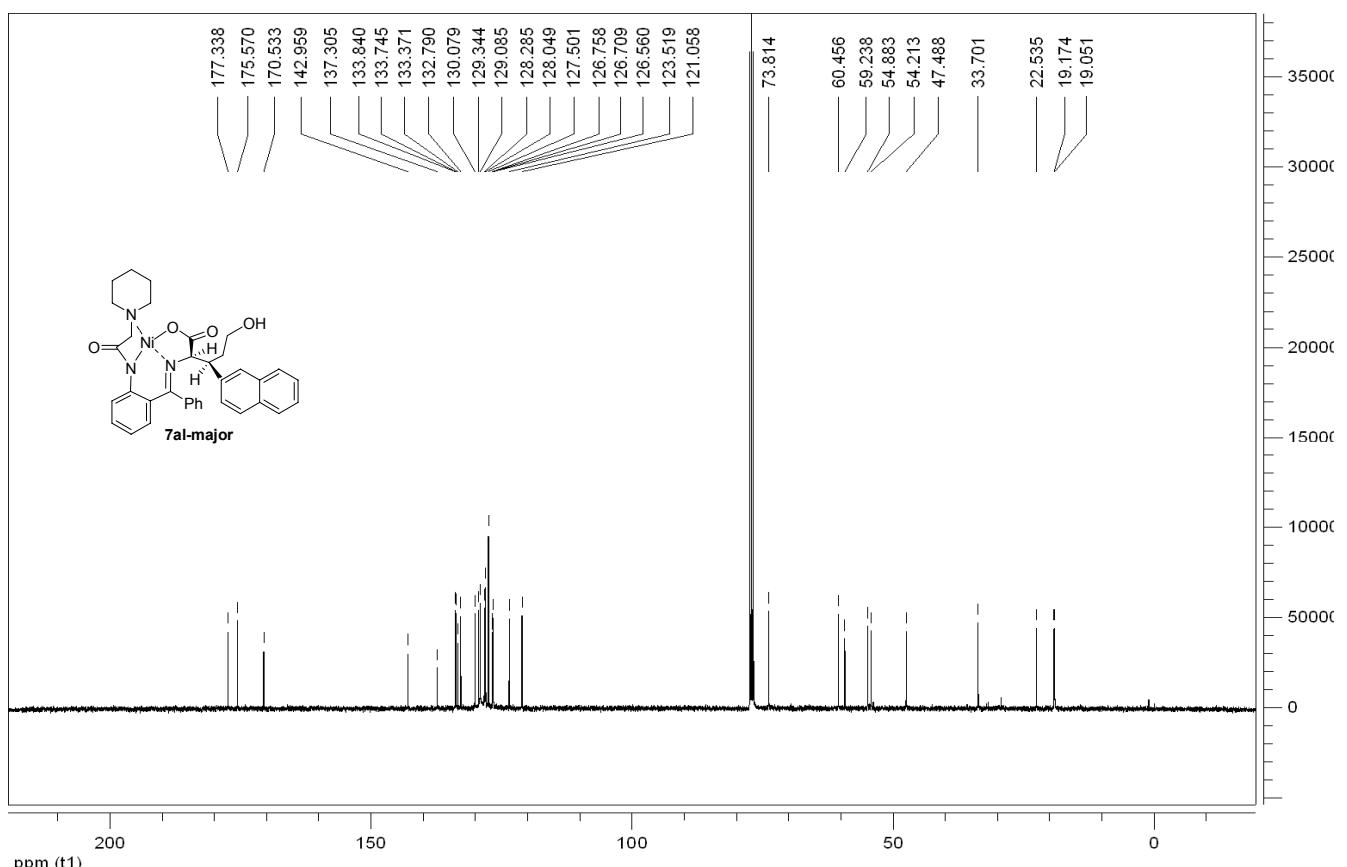


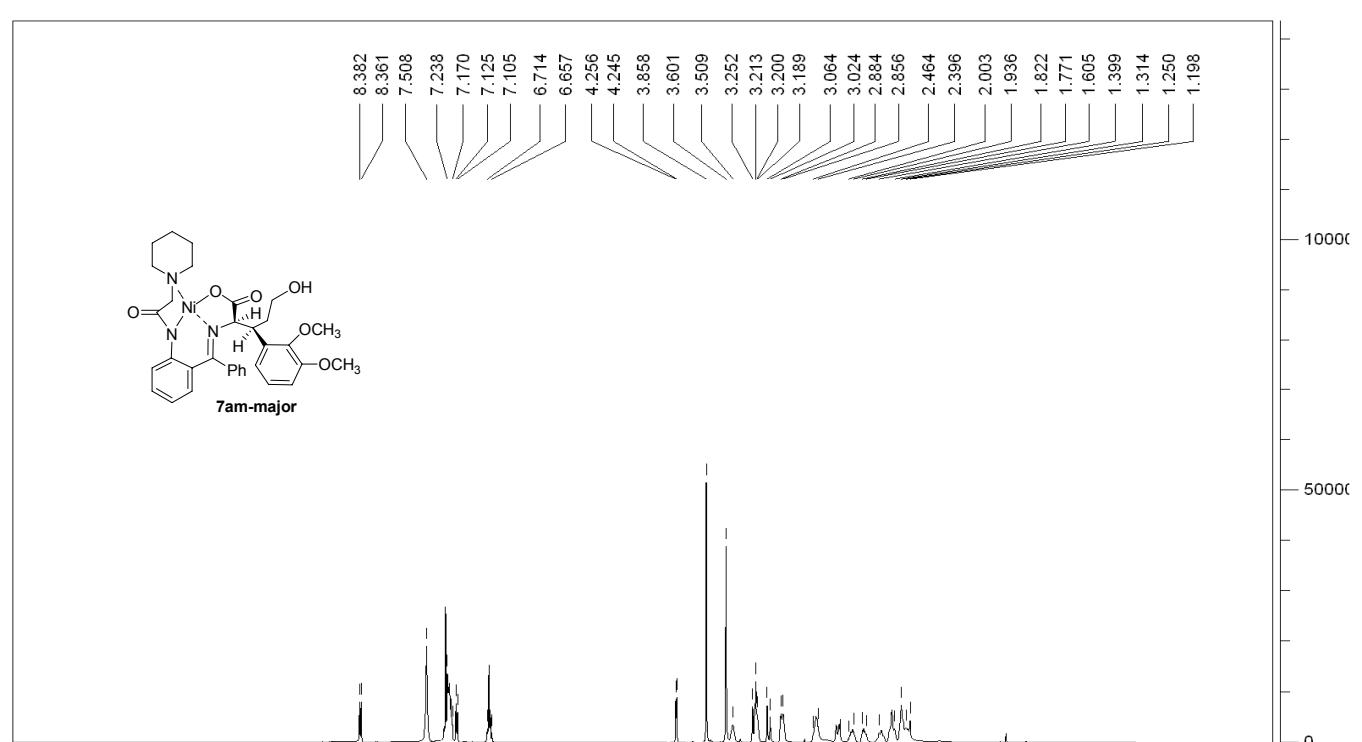
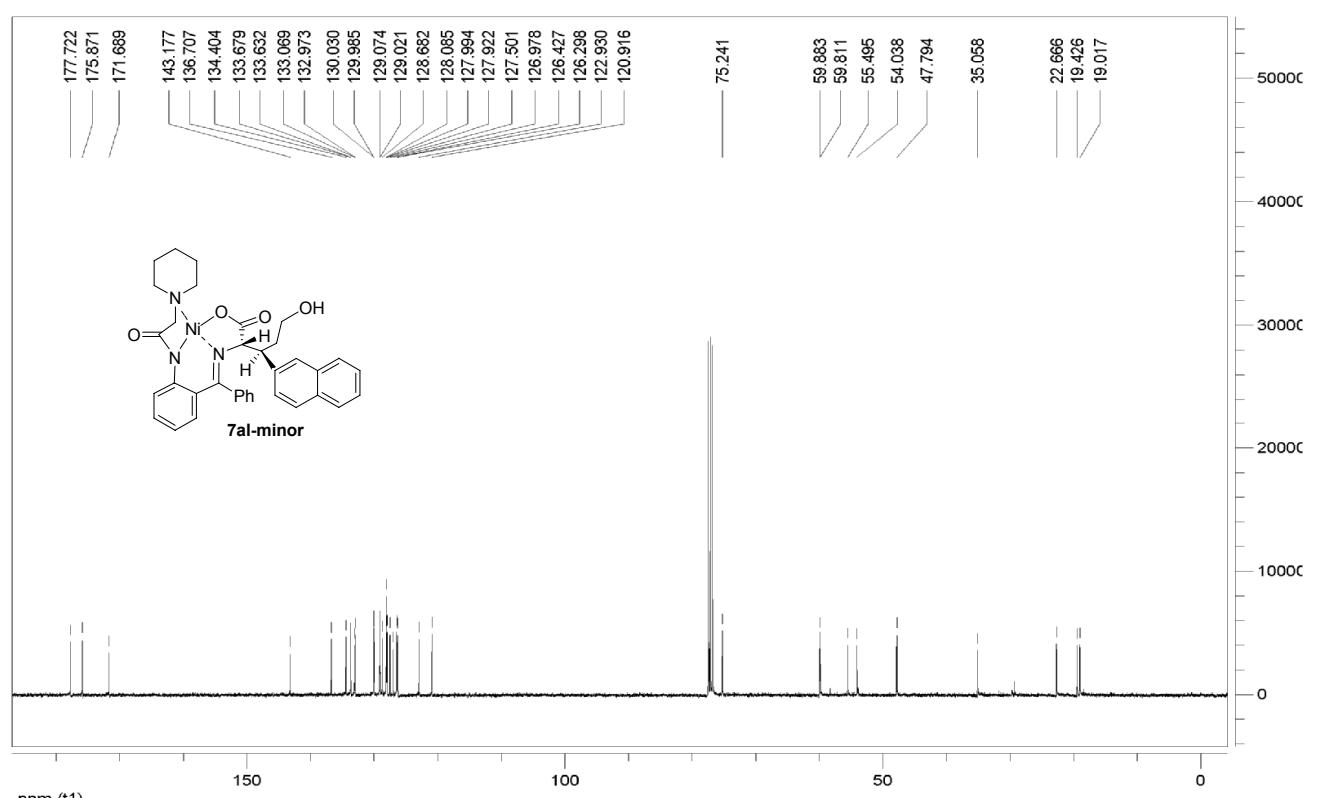


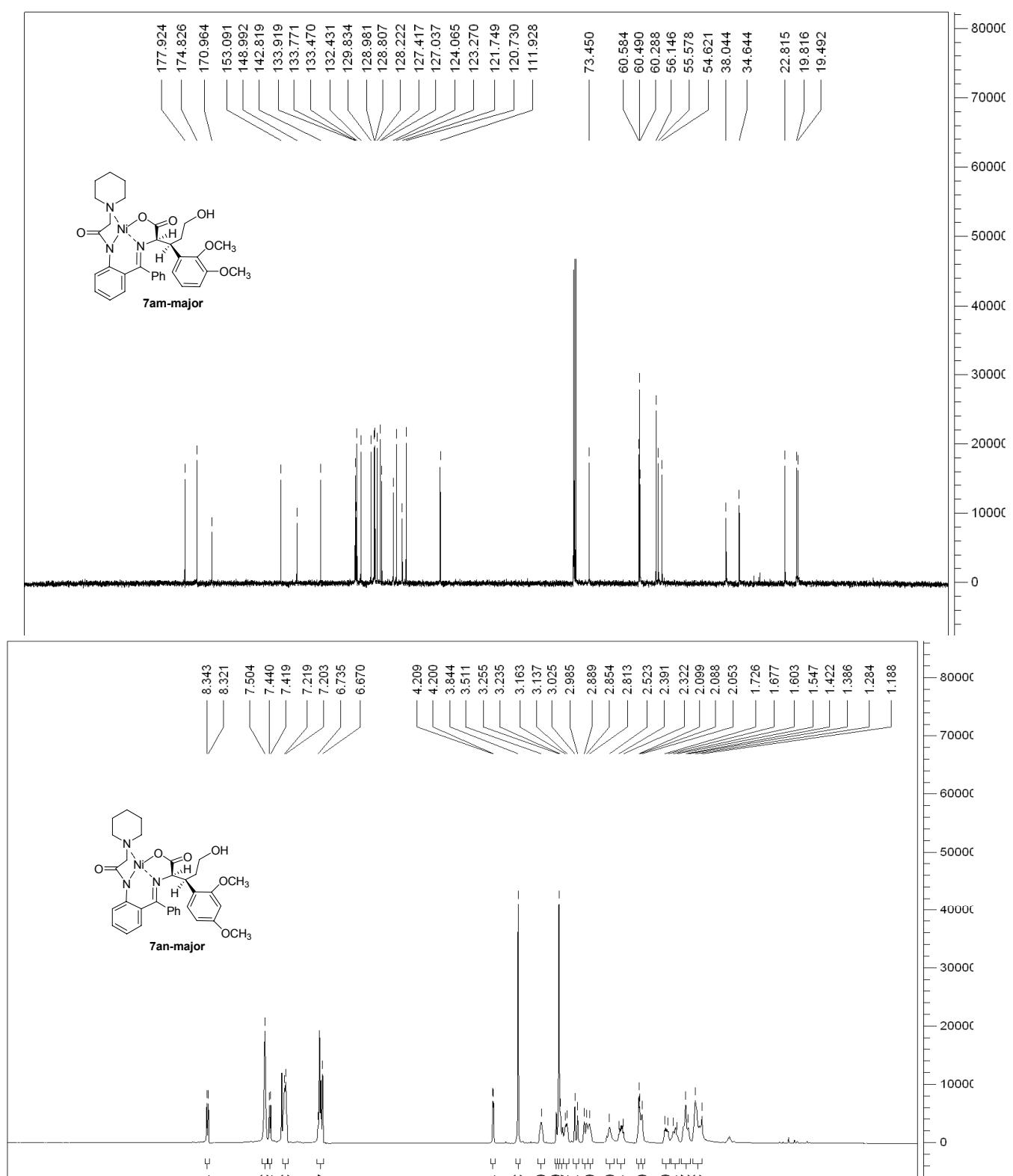


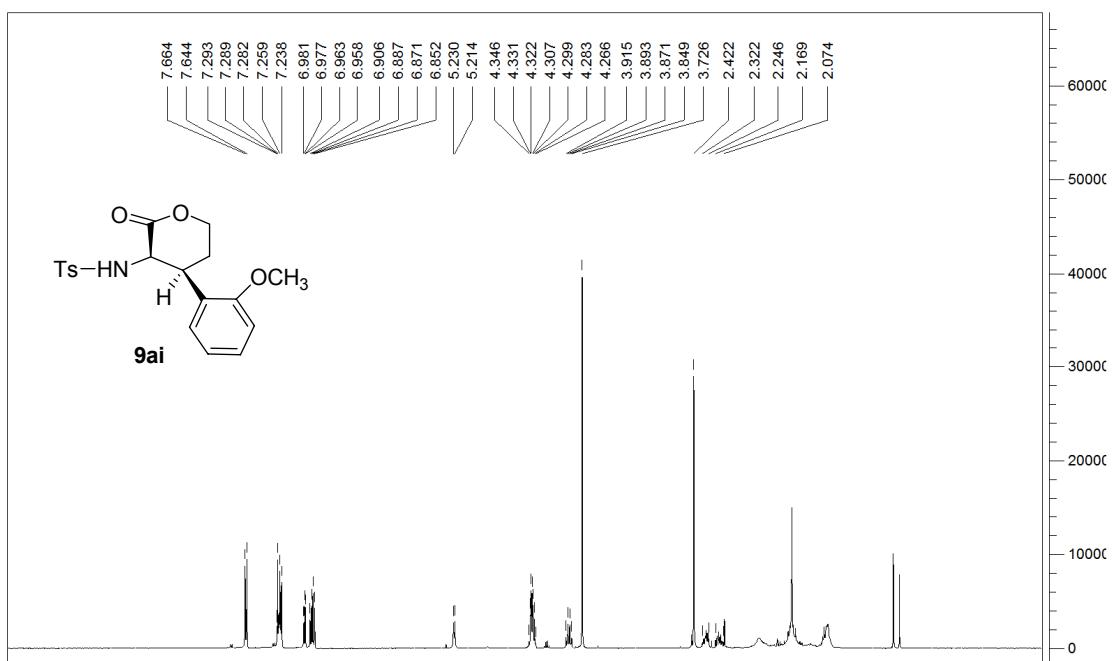
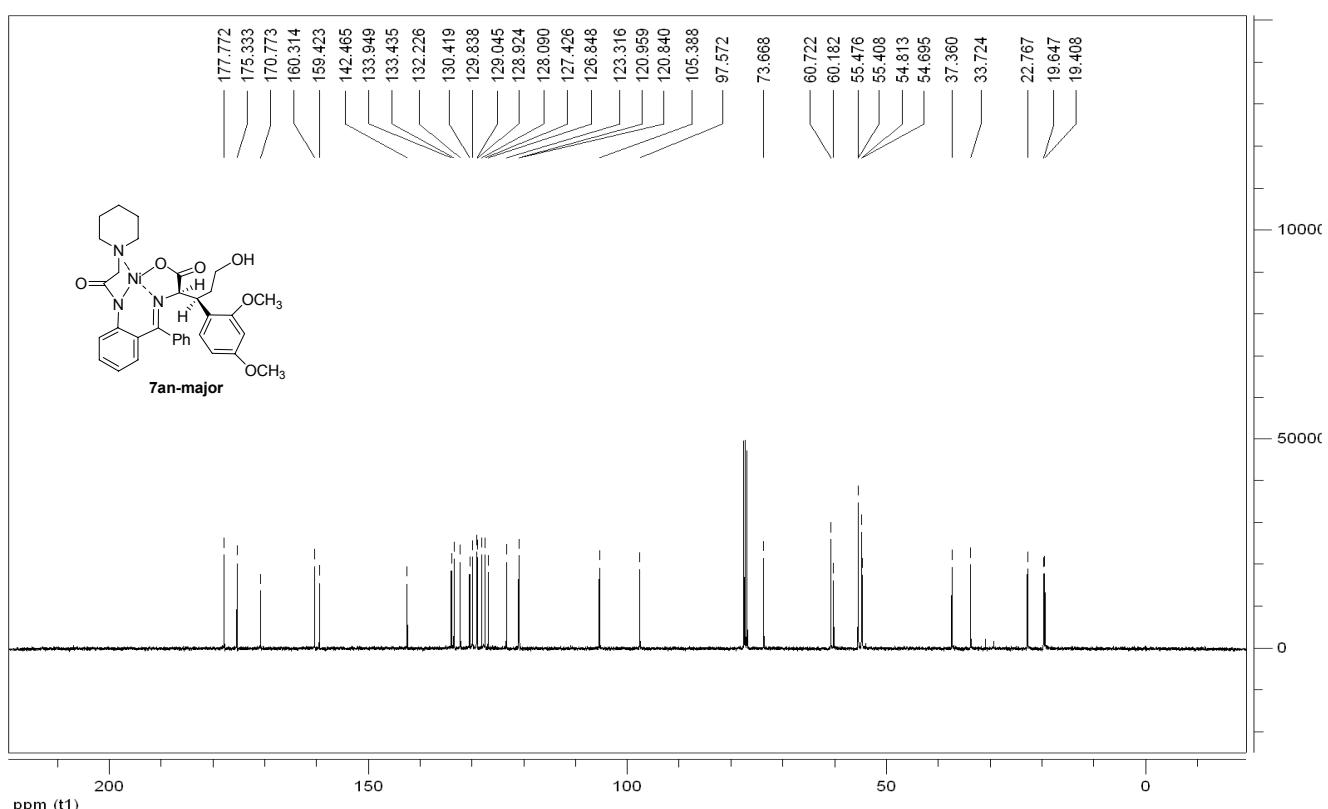


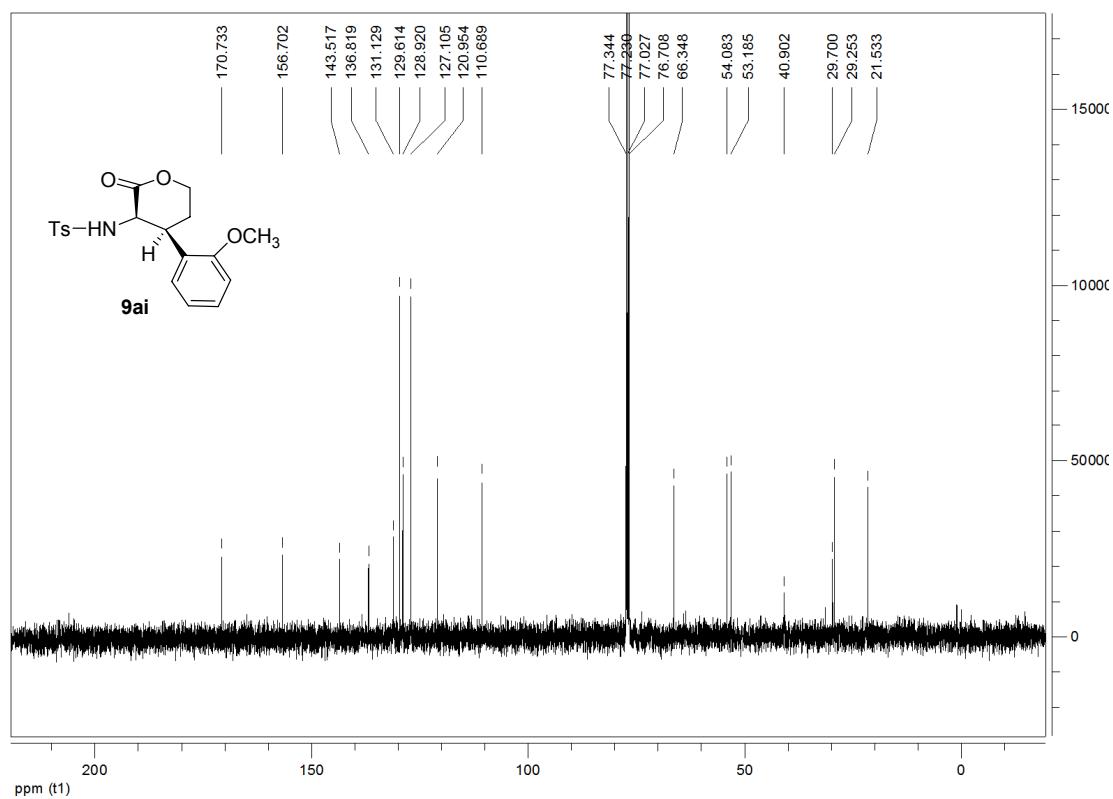












C: X-ray Crystal Data

Table 1. Crystal data and structure refinement for 7ai.

Identification code	7ai
Empirical formula	C33 H36 Cl3 N3 Ni O5
Formula weight	719.71
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	$a = 8.565(4)$ Å $\alpha = 90$ deg. $b = 12.029(6)$ Å $\beta = 91.239(10)$ deg. $c = 16.760(8)$ Å $\gamma = 90$ deg.
Volume	1726.3(15) Å ³
Z, Calculated density	2, 1.385 Mg/m ³
Absorption coefficient	0.837 mm ⁻¹

F(000)	748
Crystal size	0.15 x 0.10 x 0.05 mm
Theta range for data collection	1.22 to 26.00 deg.
Limiting indices	-10<=h<=10, -14<=k<=14, -20<=l<=15
Reflections collected / unique	9261 / 6621 [R(int) = 0.0409]
Completeness to theta = 26.00	99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.9593 and 0.8847
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6621 / 10 / 410

Goodness-of-fit on F² 1.016

Final R indices [$I > 2\sigma(I)$] R1 = 0.0793, wR2 = 0.2011

R indices (all data) R1 = 0.1231, wR2 = 0.2399

Absolute structure parameter 0.06(3)

Largest diff. peak and hole 0.823 and -0.555 e. \AA^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 7ai.

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Ni	3629(1)	8497(1)	7523(1)	44(1)
N(1)	4920(8)	7149(6)	7465(4)	51(2)
N(2)	5279(8)	9211(6)	7041(4)	47(2)
N(3)	2469(7)	9781(5)	7636(4)	41(2)
O(1)	8004(7)	9120(6)	7077(5)	73(2)
O(2)	1950(7)	7758(5)	7977(4)	55(2)
O(3)	-108(7)	8062(5)	8735(4)	63(2)
O(4)	316(12)	10768(8)	11094(5)	102(3)
O(5)	4950(6)	10998(5)	8658(4)	57(2)
C(1)	4525(13)	6298(8)	8087(6)	67(3)

C(2)	5439(14)	5197(8)	7981(7)	80(3)
C(3)	5100(15)	4708(8)	7151(8)	89(4)
C(4)	5536(16)	5565(10)	6514(8)	94(4)
C(5)	4659(13)	6665(8)	6649(6)	60(3)
C(6)	6525(10)	7593(8)	7572(6)	58(2)
C(7)	6690(10)	8731(7)	7197(6)	53(2)
C(8)	5132(10)	10187(8)	6598(5)	46(2)
C(9)	6237(11)	10479(9)	6016(6)	63(2)
C(10)	6067(13)	11420(9)	5557(6)	72(3)
C(11)	4873(13)	12149(9)	5664(6)	72(3)
C(12)	3734(12)	11905(8)	6225(5)	60(2)
C(13)	3836(10)	10918(7)	6701(5)	50(2)
C(14)	2605(8)	10725(6)	7265(5)	39(2)
C(15)	1511(10)	11678(7)	7429(5)	50(2)
C(16)	1982(11)	12581(7)	7916(6)	58(2)
C(17)	994(12)	13464(11)	8047(6)	75(2)
C(18)	-477(11)	13475(12)	7644(7)	82(3)
C(19)	-920(12)	12621(9)	7165(7)	71(3)
C(20)	36(10)	11693(8)	7052(6)	58(2)
C(21)	1326(8)	9662(6)	8295(5)	40(2)
C(22)	988(8)	8426(9)	8344(5)	49(2)

C(23)	2066(8)	10107(6)	9091(4)	40(2)
C(24)	879(10)	10127(8)	9765(5)	56(2)
C(25)	1433(15)	10766(13)	10449(8)	102(4)
C(26)	3610(9)	9562(7)	9313(5)	46(2)
C(27)	3697(11)	8599(9)	9747(5)	61(2)
C(28)	5141(13)	8085(8)	9995(6)	67(3)
C(29)	6467(12)	8599(12)	9783(5)	74(3)
C(30)	6446(11)	9561(9)	9341(6)	69(3)
C(31)	5045(9)	10037(7)	9105(5)	50(2)
C(32)	6415(13)	11473(10)	8366(8)	83(3)
Cl(1)	438(17)	6207(13)	6329(9)	193(5)
Cl(2)	-200(500)	6030(60)	4860(70)	210(20)
Cl(3)	1620(12)	8419(12)	5745(6)	174(3)
C(33)	290(40)	7260(30)	5590(30)	200(20)

Table 3. Bond lengths [Å] and angles [deg] for 7ai.

Ni-N(3)	1.848(6)
Ni-N(2)	1.855(7)
Ni-O(2)	1.866(6)
Ni-N(1)	1.967(7)
N(1)-C(6)	1.482(11)
N(1)-C(1)	1.503(12)
N(1)-C(5)	1.499(12)
N(2)-C(7)	1.360(10)
N(2)-C(8)	1.393(12)
N(3)-C(14)	1.301(10)
N(3)-C(21)	1.499(10)
O(1)-C(7)	1.239(10)
O(2)-C(22)	1.313(11)
O(3)-C(22)	1.236(9)
O(4)-C(25)	1.459(12)
O(4)-H(4)	0.8396
O(5)-C(31)	1.379(11)

O(5)-C(32)	1.472(11)
C(1)-C(2)	1.551(13)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.532(17)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.537(17)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.541(14)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.514(13)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(8)-C(9)	1.418(12)
C(8)-C(13)	1.430(12)
C(9)-C(10)	1.374(15)

C(9)-H(9)	0.9300
C(10)-C(11)	1.362(14)
C(10)-H(10)	0.9300
C(11)-C(12)	1.401(13)
C(11)-H(11)	0.9300
C(12)-C(13)	1.432(12)
C(12)-H(12)	0.9300
C(13)-C(14)	1.450(11)
C(14)-C(15)	1.510(11)
C(15)-C(20)	1.400(12)
C(15)-C(16)	1.412(12)
C(16)-C(17)	1.379(13)
C(16)-H(16)	0.9300
C(17)-C(18)	1.417(14)
C(17)-H(17)	0.9300
C(18)-C(19)	1.352(17)
C(18)-H(18)	0.9300
C(19)-C(20)	1.400(13)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(21)-C(22)	1.518(13)

C(21)-C(23)	1.560(11)
C(21)-H(21)	0.9800
C(23)-C(26)	1.515(10)
C(23)-C(24)	1.536(10)
C(23)-H(23)	0.9800
C(24)-C(25)	1.452(15)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(27)	1.371(13)
C(26)-C(31)	1.406(11)
C(27)-C(28)	1.436(13)
C(27)-H(27)	0.9300
C(28)-C(29)	1.347(15)
C(28)-H(28)	0.9300
C(29)-C(30)	1.374(17)
C(29)-H(29)	0.9300
C(30)-C(31)	1.380(12)
C(30)-H(30)	0.9300
C(32)-H(32A)	0.9600

C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
Cl(1)-C(33)	1.78(2)
Cl(2)-C(33)	1.96(3)
Cl(3)-C(33)	1.82(2)
C(33)-H(33)	1.0(5)
N(3)-Ni-N(2)	94.2(3)
N(3)-Ni-O(2)	86.3(3)
N(2)-Ni-O(2)	178.1(3)
N(3)-Ni-N(1)	176.6(3)
N(2)-Ni-N(1)	85.7(3)
O(2)-Ni-N(1)	93.8(3)
C(6)-N(1)-C(1)	112.6(8)
C(6)-N(1)-C(5)	111.7(7)
C(1)-N(1)-C(5)	109.7(7)
C(6)-N(1)-Ni	102.6(5)
C(1)-N(1)-Ni	113.0(5)
C(5)-N(1)-Ni	107.0(5)
C(7)-N(2)-C(8)	122.0(7)
C(7)-N(2)-Ni	113.7(6)

C(8)-N(2)-Ni	124.2(6)
C(14)-N(3)-C(21)	120.1(6)
C(14)-N(3)-Ni	128.9(5)
C(21)-N(3)-Ni	110.9(5)
C(22)-O(2)-Ni	113.4(5)
C(25)-O(4)-H(4)	110.5
C(31)-O(5)-C(32)	117.7(7)
N(1)-C(1)-C(2)	112.4(8)
N(1)-C(1)-H(1A)	109.2
C(2)-C(1)-H(1A)	109.1
N(1)-C(1)-H(1B)	109.0
C(2)-C(1)-H(1B)	109.2
H(1A)-C(1)-H(1B)	107.9
C(3)-C(2)-C(1)	110.2(9)
C(3)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	109.2(9)
C(4)-C(3)-H(3A)	109.8

C(2)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3B)	109.8
C(2)-C(3)-H(3B)	109.9
H(3A)-C(3)-H(3B)	108.3
C(3)-C(4)-C(5)	110.3(10)
C(3)-C(4)-H(4A)	109.7
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1
N(1)-C(5)-C(4)	113.8(8)
N(1)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5A)	108.8
N(1)-C(5)-H(5B)	108.8
C(4)-C(5)-H(5B)	108.8
H(5A)-C(5)-H(5B)	107.7
N(1)-C(6)-C(7)	111.8(7)
N(1)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6A)	109.4
N(1)-C(6)-H(6B)	109.2
C(7)-C(6)-H(6B)	109.0

H(6A)-C(6)-H(6B)	107.9
O(1)-C(7)-N(2)	127.9(8)
O(1)-C(7)-C(6)	120.2(8)
N(2)-C(7)-C(6)	111.9(7)
N(2)-C(8)-C(9)	121.4(8)
N(2)-C(8)-C(13)	121.0(7)
C(9)-C(8)-C(13)	117.5(8)
C(10)-C(9)-C(8)	121.6(9)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.1
C(11)-C(10)-C(9)	121.9(9)
C(11)-C(10)-H(10)	119.1
C(9)-C(10)-H(10)	119.0
C(10)-C(11)-C(12)	119.3(10)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.5
C(11)-C(12)-C(13)	120.8(9)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(8)-C(13)-C(12)	118.8(8)
C(8)-C(13)-C(14)	123.9(7)

C(12)-C(13)-C(14)	117.4(8)
N(3)-C(14)-C(13)	121.7(7)
N(3)-C(14)-C(15)	120.9(7)
C(13)-C(14)-C(15)	117.4(7)
C(20)-C(15)-C(16)	119.7(8)
C(20)-C(15)-C(14)	119.0(8)
C(16)-C(15)-C(14)	121.2(8)
C(17)-C(16)-C(15)	121.0(9)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	118.3(11)
C(16)-C(17)-H(17)	120.8
C(18)-C(17)-H(17)	120.9
C(19)-C(18)-C(17)	120.7(11)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	121.9(10)
C(18)-C(19)-H(19)	119.1
C(20)-C(19)-H(19)	119.0
C(19)-C(20)-C(15)	118.3(9)
C(19)-C(20)-H(20)	120.8

C(15)-C(20)-H(20)	120.9
N(3)-C(21)-C(22)	105.2(6)
N(3)-C(21)-C(23)	109.8(6)
C(22)-C(21)-C(23)	111.4(6)
N(3)-C(21)-H(21)	110.1
C(22)-C(21)-H(21)	110.1
C(23)-C(21)-H(21)	110.2
O(3)-C(22)-O(2)	121.5(9)
O(3)-C(22)-C(21)	121.6(8)
O(2)-C(22)-C(21)	116.8(7)
C(26)-C(23)-C(24)	114.5(7)
C(26)-C(23)-C(21)	113.4(6)
C(24)-C(23)-C(21)	111.8(6)
C(26)-C(23)-H(23)	105.3
C(24)-C(23)-H(23)	105.4
C(21)-C(23)-H(23)	105.4
C(25)-C(24)-C(23)	112.3(8)
C(25)-C(24)-H(24A)	109.0
C(23)-C(24)-H(24A)	109.1
C(25)-C(24)-H(24B)	109.2
C(23)-C(24)-H(24B)	109.2

H(24A)-C(24)-H(24B)	107.9
C(24)-C(25)-O(4)	112.2(10)
C(24)-C(25)-H(25A)	109.2
O(4)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.0
O(4)-C(25)-H(25B)	109.1
H(25A)-C(25)-H(25B)	107.8
C(27)-C(26)-C(31)	115.9(8)
C(27)-C(26)-C(23)	122.2(8)
C(31)-C(26)-C(23)	121.8(7)
C(26)-C(27)-C(28)	123.6(9)
C(26)-C(27)-H(27)	118.3
C(28)-C(27)-H(27)	118.0
C(29)-C(28)-C(27)	116.9(10)
C(29)-C(28)-H(28)	121.6
C(27)-C(28)-H(28)	121.5
C(28)-C(29)-C(30)	121.8(10)
C(28)-C(29)-H(29)	119.0
C(30)-C(29)-H(29)	119.1
C(29)-C(30)-C(31)	120.3(10)
C(29)-C(30)-H(30)	119.9

C(31)-C(30)-H(30)	119.8
C(30)-C(31)-O(5)	123.0(8)
C(30)-C(31)-C(26)	121.4(9)
O(5)-C(31)-C(26)	115.7(7)
O(5)-C(32)-H(32A)	109.2
O(5)-C(32)-H(32B)	109.6
H(32A)-C(32)-H(32B)	109.5
O(5)-C(32)-H(32C)	109.6
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Cl(1)-C(33)-Cl(3)	114.0(18)
Cl(1)-C(33)-Cl(2)	84.6(19)
Cl(3)-C(33)-Cl(2)	143(10)
Cl(1)-C(33)-H(33)	103(8)
Cl(3)-C(33)-H(33)	102(7)
Cl(2)-C(33)-H(33)	104(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 7ai.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ni	39(1)	37(1)	55(1)	-1(1)	9(1)	4(1)
N(1)	50(4)	46(4)	58(4)	-9(3)	5(3)	6(3)
N(2)	34(3)	47(4)	62(4)	-5(3)	11(3)	4(3)
N(3)	31(3)	40(4)	52(4)	0(3)	4(3)	0(3)
O(1)	38(3)	71(4)	109(5)	-4(4)	9(3)	3(3)
O(2)	43(3)	35(3)	87(5)	-5(3)	10(3)	-2(3)
O(3)	52(4)	53(4)	84(4)	6(3)	13(3)	-12(3)
O(4)	148(8)	68(5)	93(6)	0(5)	66(5)	-3(6)
O(5)	39(3)	55(4)	79(4)	0(3)	14(3)	-7(3)
C(1)	80(7)	46(5)	74(7)	12(5)	12(5)	14(5)
C(2)	78(8)	50(6)	111(9)	6(6)	14(7)	25(6)

C(3)	89(8)	37(5)	142(11)	-7(6)	19(7)	21(5)
C(4)	105(9)	81(8)	94(8)	-38(7)	-15(7)	42(7)
C(5)	74(7)	49(6)	56(6)	0(5)	-5(5)	16(5)
C(6)	47(5)	49(5)	79(7)	-7(5)	4(5)	6(4)
C(7)	40(4)	50(7)	70(5)	-5(4)	5(4)	5(4)
C(8)	40(5)	55(5)	43(5)	-4(4)	7(4)	-2(4)
C(9)	47(5)	70(6)	71(6)	-2(5)	23(5)	-5(4)
C(10)	78(7)	82(7)	58(6)	-2(5)	24(5)	-15(6)
C(11)	82(7)	74(7)	61(6)	16(5)	15(5)	-8(6)
C(12)	73(6)	58(5)	49(5)	9(4)	11(4)	3(5)
C(13)	55(5)	41(5)	53(5)	4(4)	7(4)	-2(4)
C(14)	27(4)	42(4)	50(4)	2(4)	0(3)	-3(3)
C(15)	57(5)	39(4)	55(5)	6(4)	3(4)	9(4)
C(16)	56(5)	45(5)	73(6)	-1(4)	6(4)	3(4)
C(17)	81(7)	44(4)	100(7)	-9(7)	16(5)	9(7)
C(18)	64(6)	62(6)	122(8)	8(9)	36(6)	25(7)
C(19)	50(5)	68(6)	96(8)	13(6)	3(5)	15(5)
C(20)	51(5)	55(5)	67(6)	1(4)	-2(4)	5(4)
C(21)	27(4)	40(4)	53(5)	2(3)	9(3)	5(3)
C(22)	39(4)	47(4)	62(4)	10(6)	2(3)	-6(5)
C(23)	36(4)	33(4)	52(4)	1(3)	11(3)	4(3)

C(24)	53(5)	55(5)	61(5)	-5(4)	22(4)	4(4)
C(25)	91(9)	125(11)	92(9)	-34(8)	41(7)	-6(8)
C(26)	43(4)	50(5)	46(4)	-7(4)	1(3)	6(4)
C(27)	70(5)	52(5)	61(5)	1(5)	8(4)	18(6)
C(28)	78(7)	58(6)	65(6)	6(4)	0(5)	22(5)
C(29)	65(6)	86(8)	70(6)	-5(7)	-12(5)	25(7)
C(30)	42(5)	80(7)	85(7)	-15(6)	-3(5)	8(5)
C(31)	38(4)	51(5)	61(5)	-11(4)	1(4)	-2(4)
C(32)	56(6)	77(7)	116(9)	-8(7)	34(6)	-17(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 7ai.

	x	y	z	U(eq)
H(4)	-489	11080	10943	153
H(1A)	3414	6144	8055	80
H(1B)	4762	6600	8612	80
H(2A)	6550	5336	8046	96
H(2B)	5135	4669	8386	96
H(3A)	5704	4034	7081	107
H(3B)	4001	4521	7096	107
H(4A)	5270	5277	5988	112
H(4B)	6653	5699	6539	112
H(5A)	4988	7203	6256	72
H(5B)	3549	6538	6564	72
H(6A)	7258	7085	7332	70

H(6B)	6782	7642	8137	70
H(9)	7099	10023	5943	75
H(10)	6788	11563	5163	87
H(11)	4814	12802	5367	87
H(12)	2900	12390	6289	72
H(16)	2975	12580	8152	69
H(17)	1285	14037	8391	90
H(18)	-1146	14076	7709	98
H(19)	-1888	12651	6903	86
H(20)	-300	11101	6735	69
H(21)	365	10072	8163	48
H(23)	2316	10889	8989	48
H(24A)	-93	10446	9564	67
H(24B)	668	9371	9932	67
H(25A)	1626	11526	10284	122
H(25B)	2414	10456	10644	122
H(27)	2769	8258	9890	73
H(28)	5160	7429	10289	80
H(29)	7423	8293	9939	89
H(30)	7381	9894	9201	83
H(32A)	7104	11631	8810	124

H(32B)	6193	12147	8079	124
H(32C)	6903	10950	8018	124
H(33)	-700(600)	7600(500)	5700(300)	243

Table 6. Torsion angles [deg] for 7ai.

N(3)-Ni-N(1)-C(6)	-56(5)
N(2)-Ni-N(1)-C(6)	33.5(6)
O(2)-Ni-N(1)-C(6)	-148.3(5)
N(3)-Ni-N(1)-C(1)	66(5)
N(2)-Ni-N(1)-C(1)	155.0(7)
O(2)-Ni-N(1)-C(1)	-26.8(7)
N(3)-Ni-N(1)-C(5)	-173(5)
N(2)-Ni-N(1)-C(5)	-84.2(6)
O(2)-Ni-N(1)-C(5)	94.0(6)
N(3)-Ni-N(2)-C(7)	149.1(6)
O(2)-Ni-N(2)-C(7)	-104(10)
N(1)-Ni-N(2)-C(7)	-27.6(6)
N(3)-Ni-N(2)-C(8)	-27.2(7)
O(2)-Ni-N(2)-C(8)	80(10)
N(1)-Ni-N(2)-C(8)	156.1(7)
N(2)-Ni-N(3)-C(14)	18.7(7)
O(2)-Ni-N(3)-C(14)	-159.5(7)

N(1)-Ni-N(3)-C(14)	108(5)
N(2)-Ni-N(3)-C(21)	-156.7(5)
O(2)-Ni-N(3)-C(21)	25.1(5)
N(1)-Ni-N(3)-C(21)	-68(5)
N(3)-Ni-O(2)-C(22)	-16.7(5)
N(2)-Ni-O(2)-C(22)	-124(10)
N(1)-Ni-O(2)-C(22)	159.9(6)
C(6)-N(1)-C(1)-C(2)	-69.9(11)
C(5)-N(1)-C(1)-C(2)	55.1(11)
Ni-N(1)-C(1)-C(2)	174.4(7)
N(1)-C(1)-C(2)-C(3)	-58.2(12)
C(1)-C(2)-C(3)-C(4)	57.4(12)
C(2)-C(3)-C(4)-C(5)	-56.1(13)
C(6)-N(1)-C(5)-C(4)	71.1(12)
C(1)-N(1)-C(5)-C(4)	-54.5(12)
Ni-N(1)-C(5)-C(4)	-177.4(9)
C(3)-C(4)-C(5)-N(1)	56.0(14)
C(1)-N(1)-C(6)-C(7)	-156.2(7)
C(5)-N(1)-C(6)-C(7)	79.9(9)
Ni-N(1)-C(6)-C(7)	-34.4(8)
C(8)-N(2)-C(7)-O(1)	10.0(15)

Ni-N(2)-C(7)-O(1)	-166.4(8)
C(8)-N(2)-C(7)-C(6)	-170.9(8)
Ni-N(2)-C(7)-C(6)	12.7(9)
N(1)-C(6)-C(7)-O(1)	-164.4(8)
N(1)-C(6)-C(7)-N(2)	16.4(11)
C(7)-N(2)-C(8)-C(9)	27.3(13)
Ni-N(2)-C(8)-C(9)	-156.7(7)
C(7)-N(2)-C(8)-C(13)	-154.2(8)
Ni-N(2)-C(8)-C(13)	21.8(12)
N(2)-C(8)-C(9)-C(10)	177.6(9)
C(13)-C(8)-C(9)-C(10)	-0.9(14)
C(8)-C(9)-C(10)-C(11)	3.3(16)
C(9)-C(10)-C(11)-C(12)	-3.7(16)
C(10)-C(11)-C(12)-C(13)	1.8(15)
N(2)-C(8)-C(13)-C(12)	-179.4(8)
C(9)-C(8)-C(13)-C(12)	-1.0(13)
N(2)-C(8)-C(13)-C(14)	0.9(14)
C(9)-C(8)-C(13)-C(14)	179.3(8)
C(11)-C(12)-C(13)-C(8)	0.5(14)
C(11)-C(12)-C(13)-C(14)	-179.8(9)
C(21)-N(3)-C(14)-C(13)	171.6(7)

Ni-N(3)-C(14)-C(13)	-3.4(11)
C(21)-N(3)-C(14)-C(15)	-6.3(11)
Ni-N(3)-C(14)-C(15)	178.6(6)
C(8)-C(13)-C(14)-N(3)	-10.7(13)
C(12)-C(13)-C(14)-N(3)	169.6(8)
C(8)-C(13)-C(14)-C(15)	167.4(8)
C(12)-C(13)-C(14)-C(15)	-12.3(11)
N(3)-C(14)-C(15)-C(20)	-81.4(10)
C(13)-C(14)-C(15)-C(20)	100.6(9)
N(3)-C(14)-C(15)-C(16)	102.3(10)
C(13)-C(14)-C(15)-C(16)	-75.7(11)
C(20)-C(15)-C(16)-C(17)	2.0(14)
C(14)-C(15)-C(16)-C(17)	178.3(8)
C(15)-C(16)-C(17)-C(18)	-3.6(15)
C(16)-C(17)-C(18)-C(19)	2.3(16)
C(17)-C(18)-C(19)-C(20)	0.6(17)
C(18)-C(19)-C(20)-C(15)	-2.2(15)
C(16)-C(15)-C(20)-C(19)	0.9(13)
C(14)-C(15)-C(20)-C(19)	-175.4(8)
C(14)-N(3)-C(21)-C(22)	157.1(6)
Ni-N(3)-C(21)-C(22)	-27.0(7)

C(14)-N(3)-C(21)-C(23)	-83.0(8)
Ni-N(3)-C(21)-C(23)	92.9(6)
Ni-O(2)-C(22)-O(3)	-173.6(6)
Ni-O(2)-C(22)-C(21)	3.8(8)
N(3)-C(21)-C(22)-O(3)	-167.6(7)
C(23)-C(21)-C(22)-O(3)	73.6(9)
N(3)-C(21)-C(22)-O(2)	15.0(9)
C(23)-C(21)-C(22)-O(2)	-103.8(8)
N(3)-C(21)-C(23)-C(26)	-55.1(8)
C(22)-C(21)-C(23)-C(26)	60.9(8)
N(3)-C(21)-C(23)-C(24)	173.5(7)
C(22)-C(21)-C(23)-C(24)	-70.4(8)
C(26)-C(23)-C(24)-C(25)	62.4(11)
C(21)-C(23)-C(24)-C(25)	-166.8(9)
C(23)-C(24)-C(25)-O(4)	-179.0(10)
C(24)-C(23)-C(26)-C(27)	42.2(11)
C(21)-C(23)-C(26)-C(27)	-87.7(9)
C(24)-C(23)-C(26)-C(31)	-135.7(8)
C(21)-C(23)-C(26)-C(31)	94.4(9)
C(31)-C(26)-C(27)-C(28)	0.7(13)
C(23)-C(26)-C(27)-C(28)	-177.3(8)

C(26)-C(27)-C(28)-C(29)	0.2(15)
C(27)-C(28)-C(29)-C(30)	-0.8(15)
C(28)-C(29)-C(30)-C(31)	0.4(16)
C(29)-C(30)-C(31)-O(5)	-179.6(8)
C(29)-C(30)-C(31)-C(26)	0.6(14)
C(32)-O(5)-C(31)-C(30)	5.4(12)
C(32)-O(5)-C(31)-C(26)	-174.8(8)
C(27)-C(26)-C(31)-C(30)	-1.1(12)
C(23)-C(26)-C(31)-C(30)	177.0(8)
C(27)-C(26)-C(31)-O(5)	179.1(7)
C(23)-C(26)-C(31)-O(5)	-2.9(11)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 7ai [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
O(4)-H(4)...O(3)#1	0.84	2.49	2.781(11)	101.2

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+2

D: References

1. Trevor K. Ellis, Hisanori Ueki, Takeshi Yamada, and Vadim A. Soloshonok.
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