

Supporting Info

## A Substrate Scope Driven Optimization of an Encapsulated Hydroformylation Catalyst

Pim R. Linnebank,<sup>a</sup> Alexander M. Kluwer<sup>b</sup> and Joost N. H. Reek<sup>\*a,b</sup>

### General comments

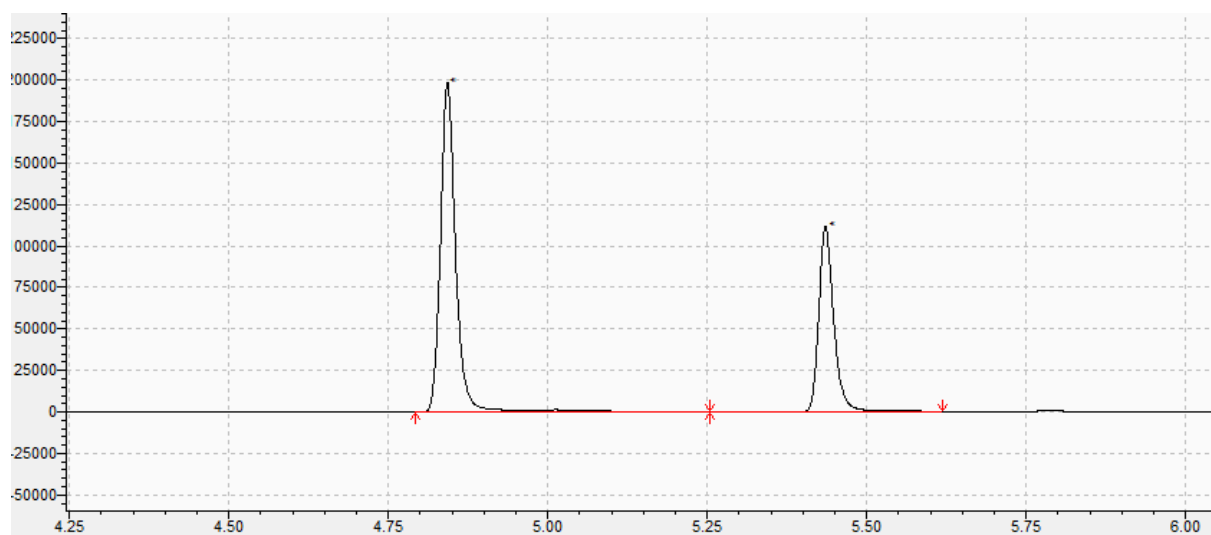
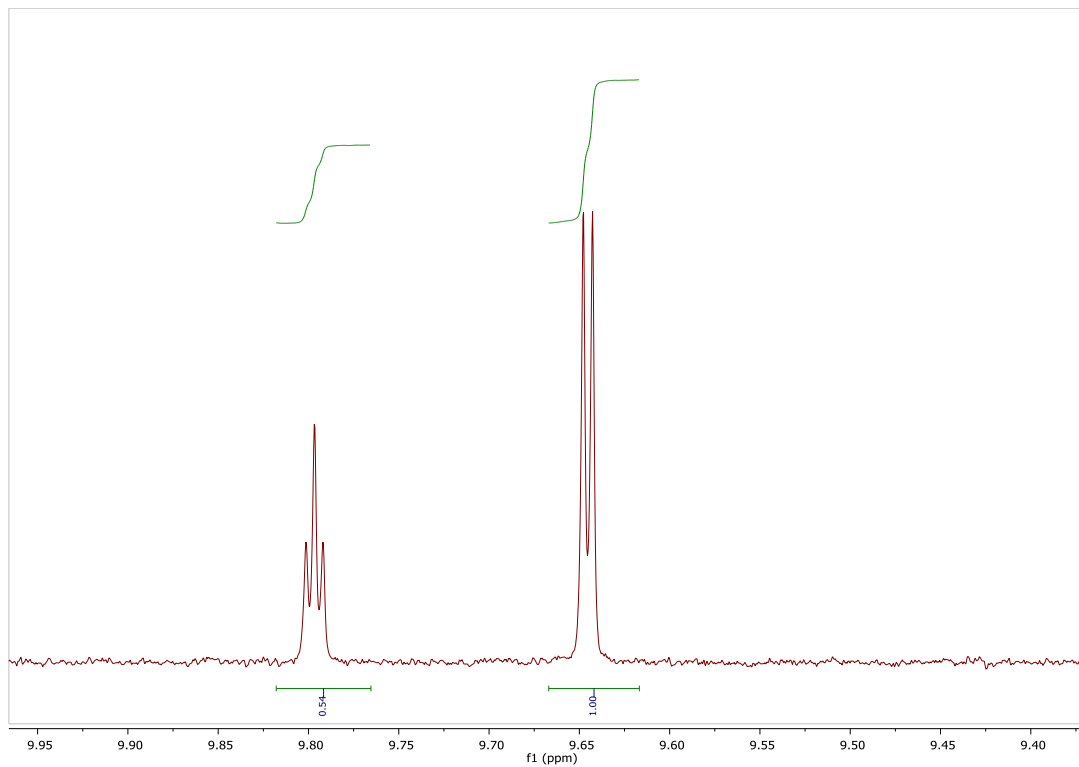
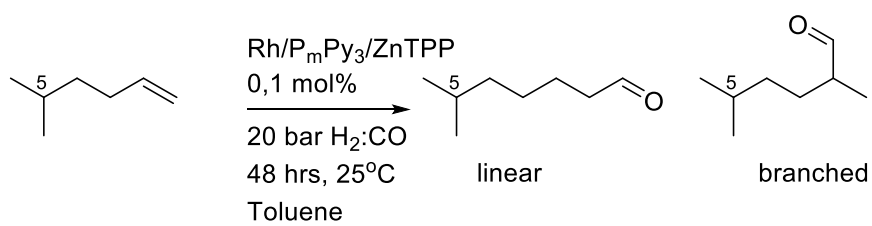
Reactions were carried out under N<sub>2</sub> atmosphere using standard Schlenk techniques. THF, pentane, hexane and diethyl ether were distilled from sodium benzophenone ketyl under nitrogen; CH<sub>2</sub>Cl<sub>2</sub>, methanol and Et<sub>3</sub>N were distilled from CaH<sub>2</sub> under nitrogen and toluene was distilled from sodium under nitrogen. NMR spectra were measured on a Bruker DRX 300 or a Bruker AMX 400. Measurements were done at room temperature (rt) unless otherwise stated. High resolution mass spectrometry was carried out using the AccuTOF GC v 4g, JMS-T100GCV mass spectrometer (JEOL, Japan).

### Experimental details

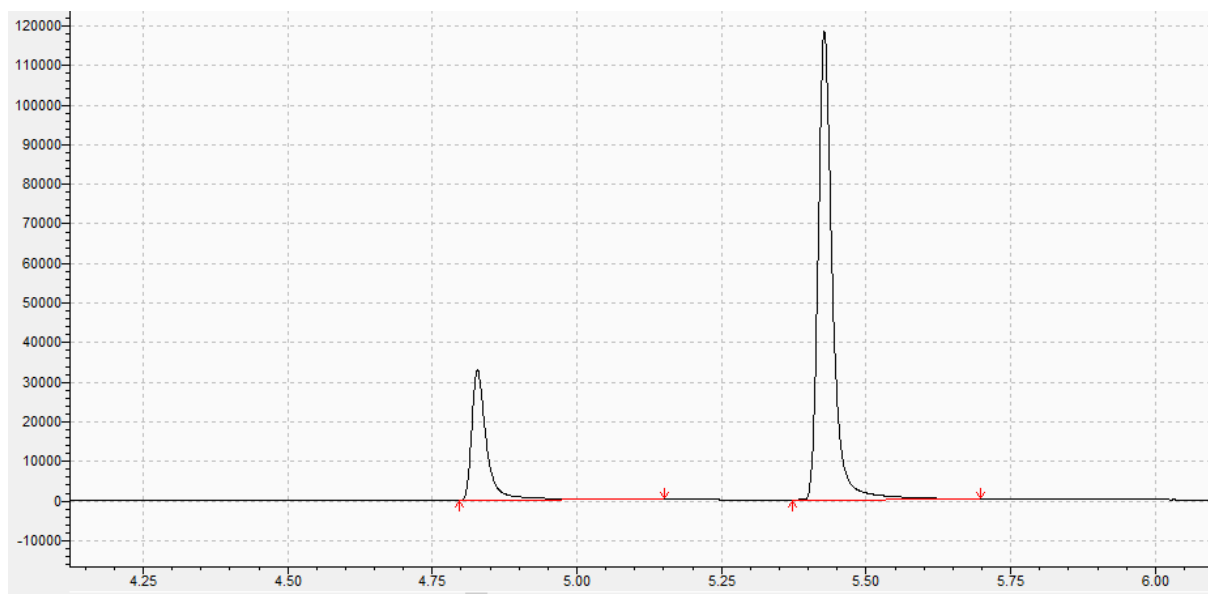
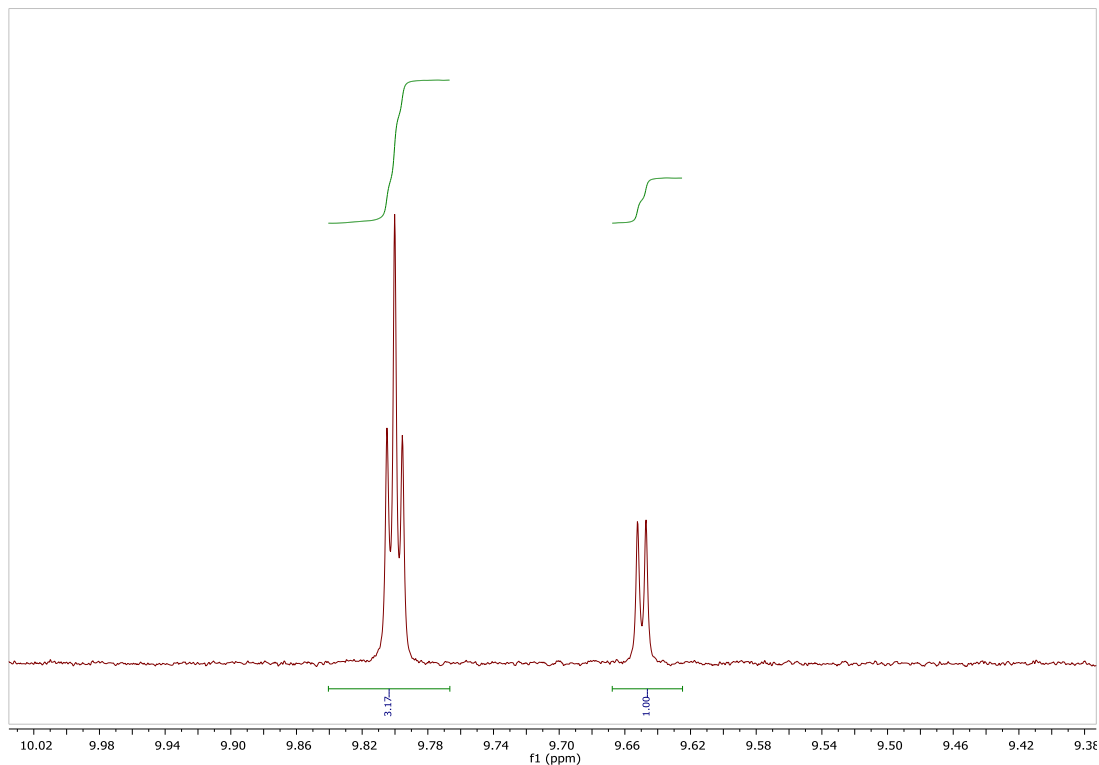
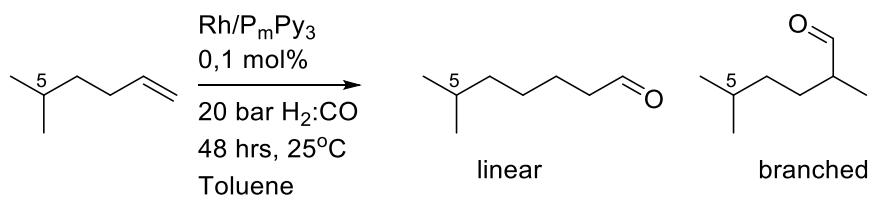
The hydroformylation experiments were carried out in a stainless steel autoclave (volume 150 ml) charged with an insert suitable for 15 reaction vessels (including Teflon mini stirring bars) for conducting parallel reactions. The substrates were filtered over basic alumina to remove possible peroxide impurities. The solvent toluene was distilled from sodium prior to use. GC vials were charged with 0.35 μmol of [Rh(acac)(CO)<sub>2</sub>], 3.2 μmol of phosphine, (if necessary) 9.6 μmol of zinc(II) tetraphenylporphyrin or the analog, 368 μmol of substrate and a known amount of 1,3,5 trimethoxybenzene in 0.50 ml of toluene. The autoclave was charged purged three times with 20 bar syngas (H<sub>2</sub>:CO, 1:1) after which the autoclave was pressurized to 20 bar of syngas and the Teflon stirring bars were stirred vigorously for 48 hrs at 25°C. After 48 hrs the pressure was carefully released and ~0,05 ml of the reaction mixture was taken and diluted with 0,4 ml CDCl<sub>3</sub> for NMR analysis. Simultaneously ~0,03 ml of the reaction mixtures were diluted with dichloromethane for GC-analysis. GC-MS and GC-FID measurements were conducted on a Shimadzu GC-2010 Plus Capillary GC-MS containing a splitter to an MS detector and an FID detector with a SH-Rtx-5 Amine column of 30 m x 0,25 mm, df 0.25. All reaction mixtures were separated by diluting the reaction mixture and injecting reaction mixtures at 50°C after which the temperature was increased at 10°C/min up to 300°C. The oven was kept at 300°C for 5 minutes. This method was applied to all reaction mixtures tested and gave successful separation for all the reaction mixtures.

**Note:** for the branched products of 4- and 3- methyl hexene two different diastereoisomers are possible, which are also observed in the GC and <sup>1</sup>H-NMR spectra in nearly equal amounts. The integrals of the two peaks were combined and reported together as the branched product.

## Catalytic results

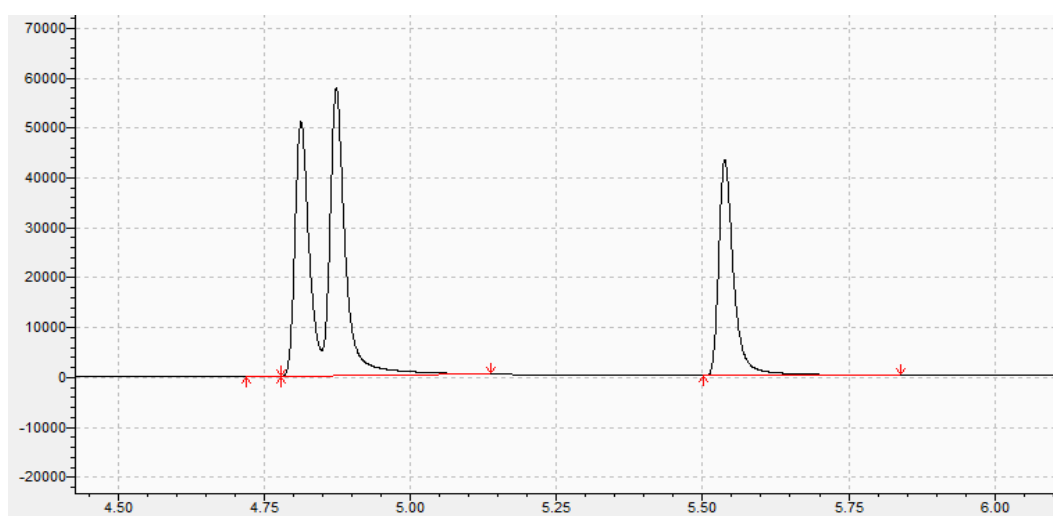
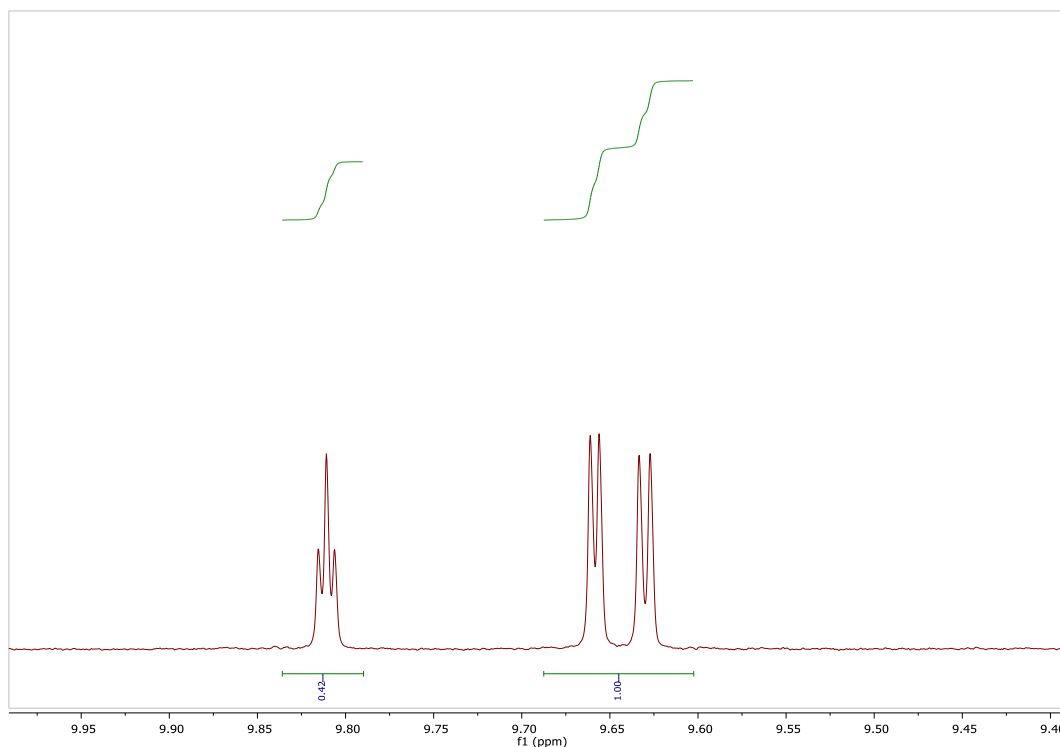
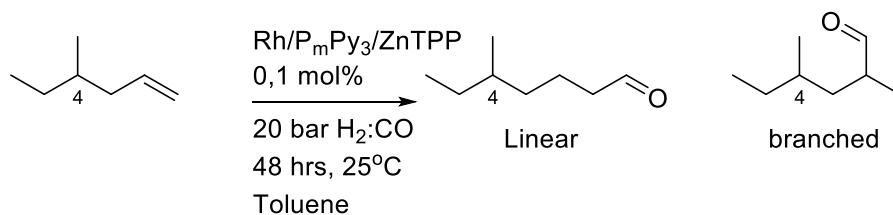


Retention time	Area		I/b ratio
4,843	327033	Branched	0.55
5,436	180465	Linear	



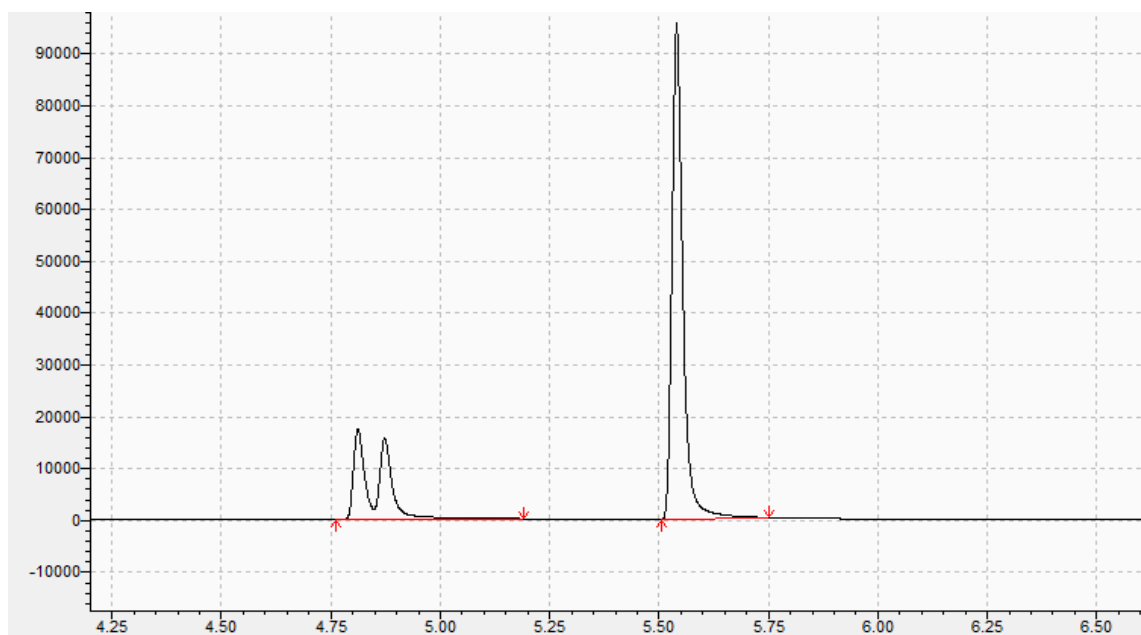
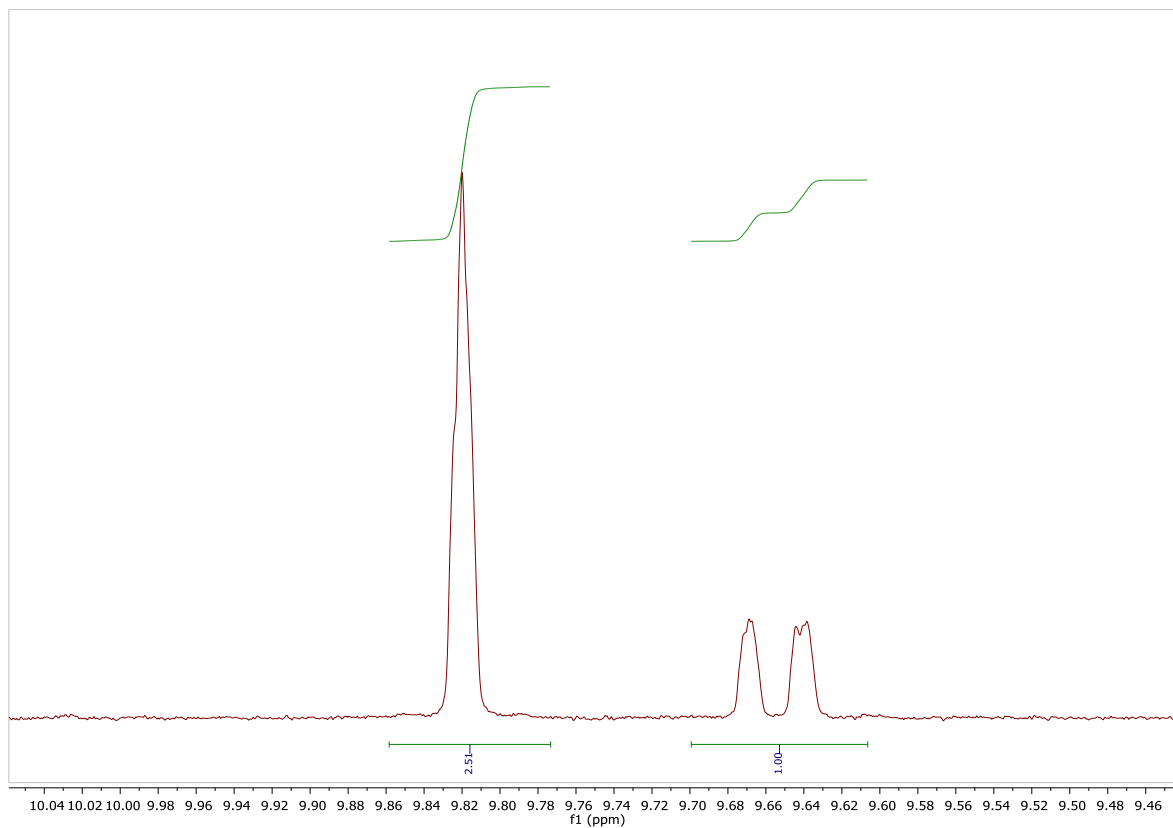
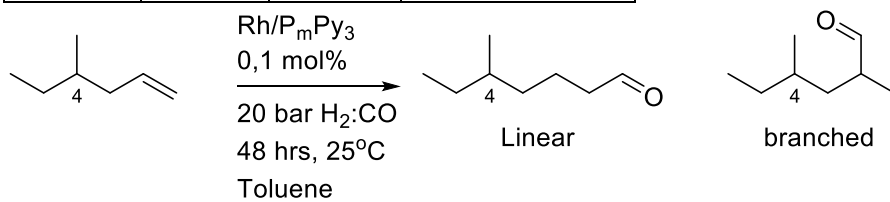
Retention time	Area		l/b ratio
4,828	60055	Branched	3.44
5,428	207017	Linear	

**Note:** For the branched products of 4-methyl hexene two different branched diastereoisomers are possible, which are also observed in the GC and <sup>1</sup>H-NMR spectra in nearly equal amounts. No alkene isomerization was observed, which excludes an isomerization/hydroformylation sequence. The integrals of the two peaks were combined and reported together as the branched product.



Retention time	Area		I/b ratio
4,874	190671	branched	0,41

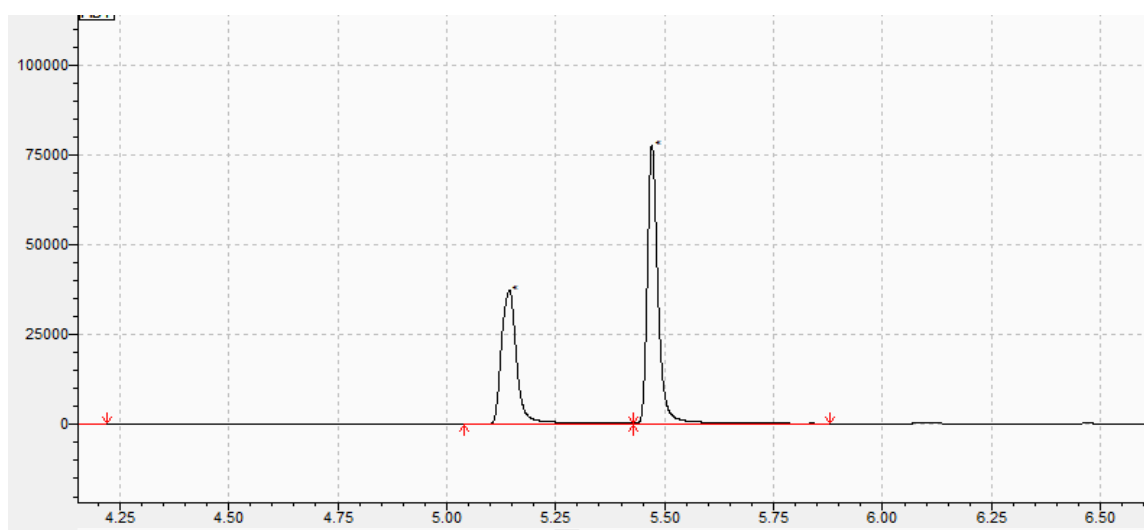
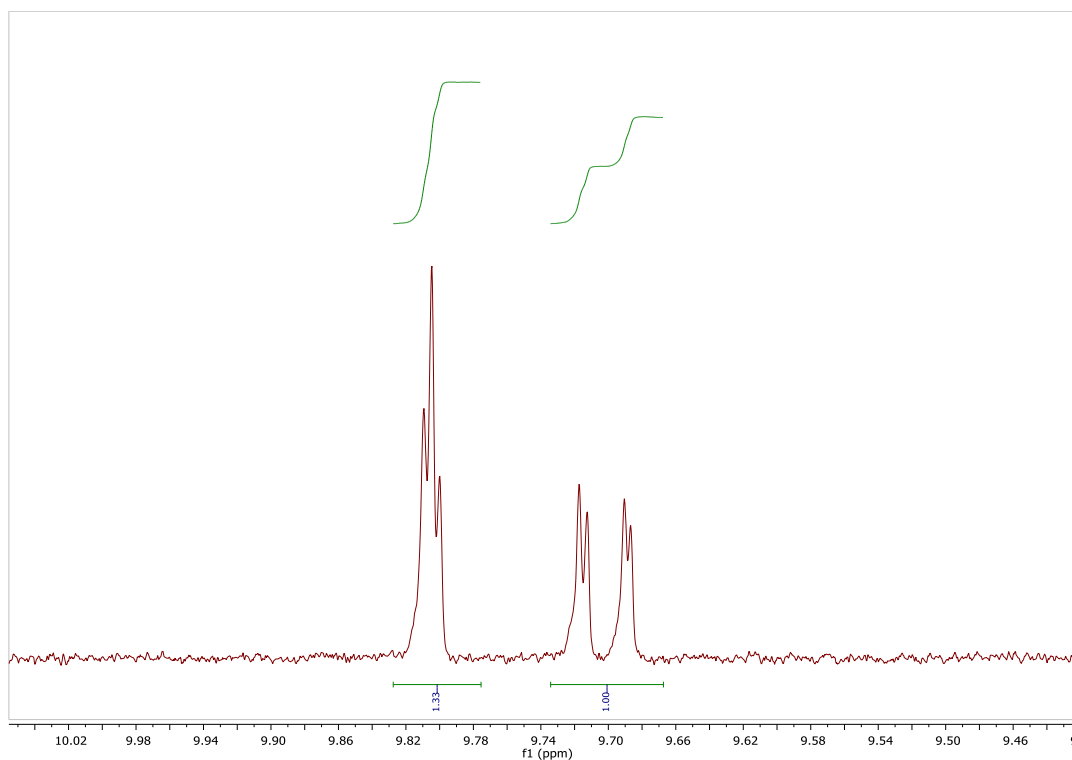
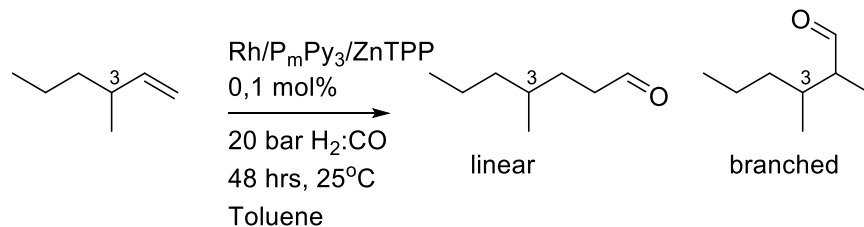
5,538	78073	linear	
-------	-------	--------	--



Retention time	Area		I/b ratio
4,812	61821	Branched	2,68

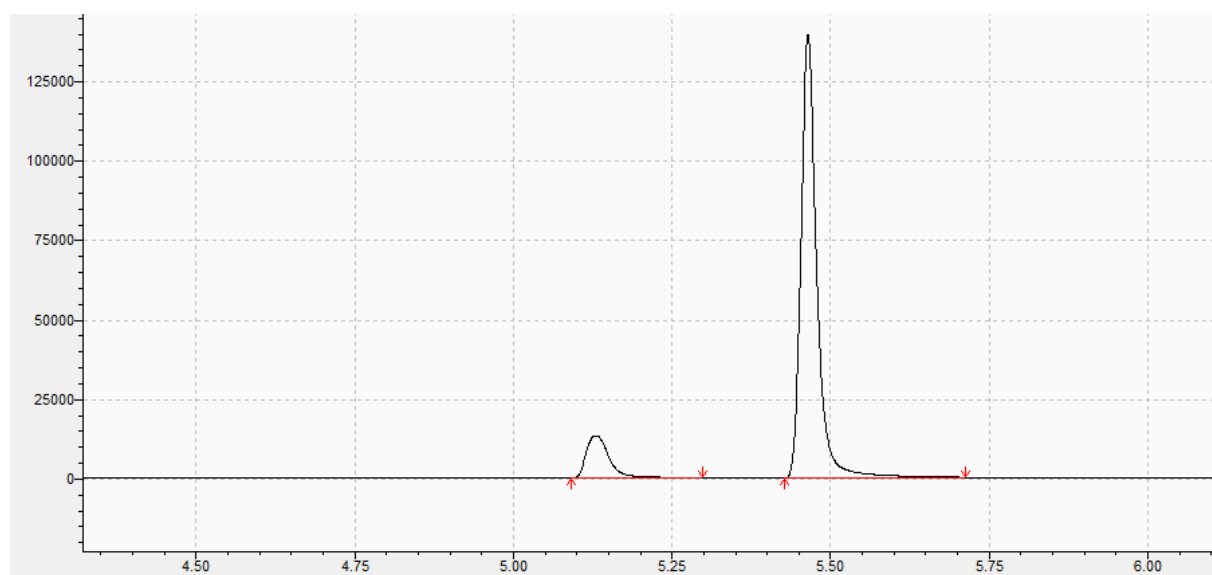
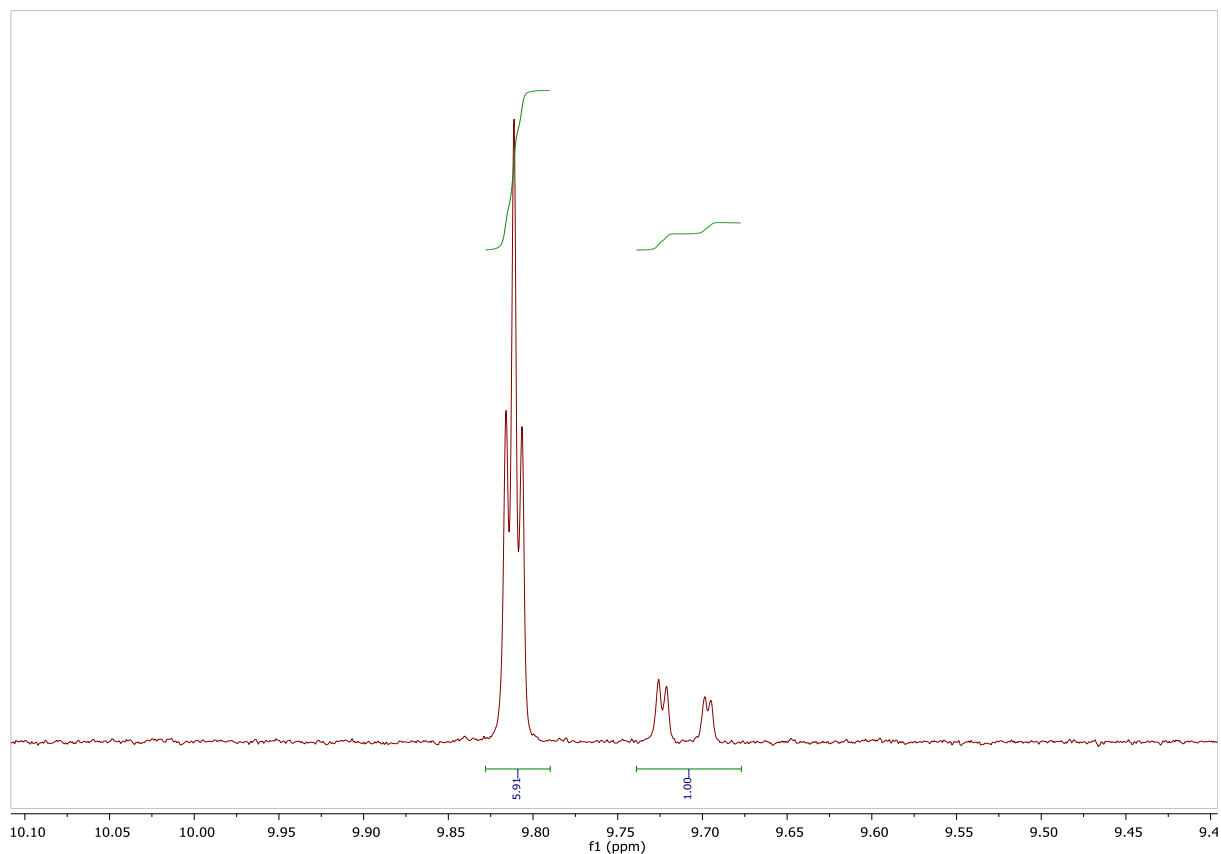
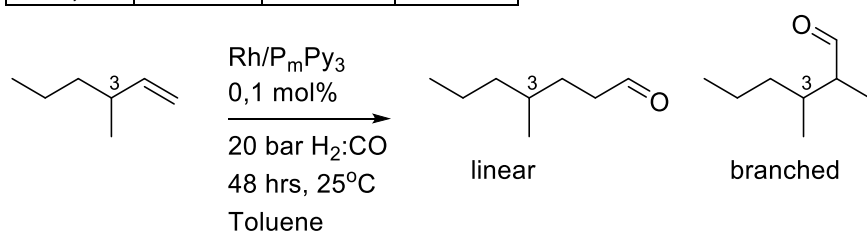
5,54	165445	Linear	
------	--------	--------	--

**Note:** For the branched products of 3- methyl hexene two different branched diastereoisomers are possible, which are also observed in the GC and <sup>1</sup>H-NMR spectra in nearly equal amounts. No alkene isomerization was observed, which excludes an isomerization/hydroformylation sequence. The integrals of the two peaks were combined and reported together as the branched product.



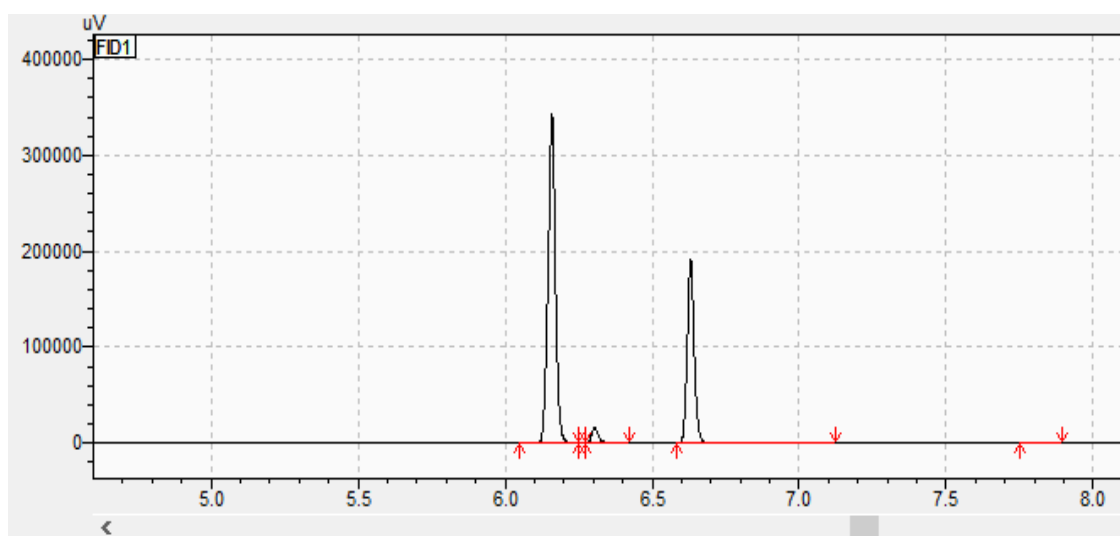
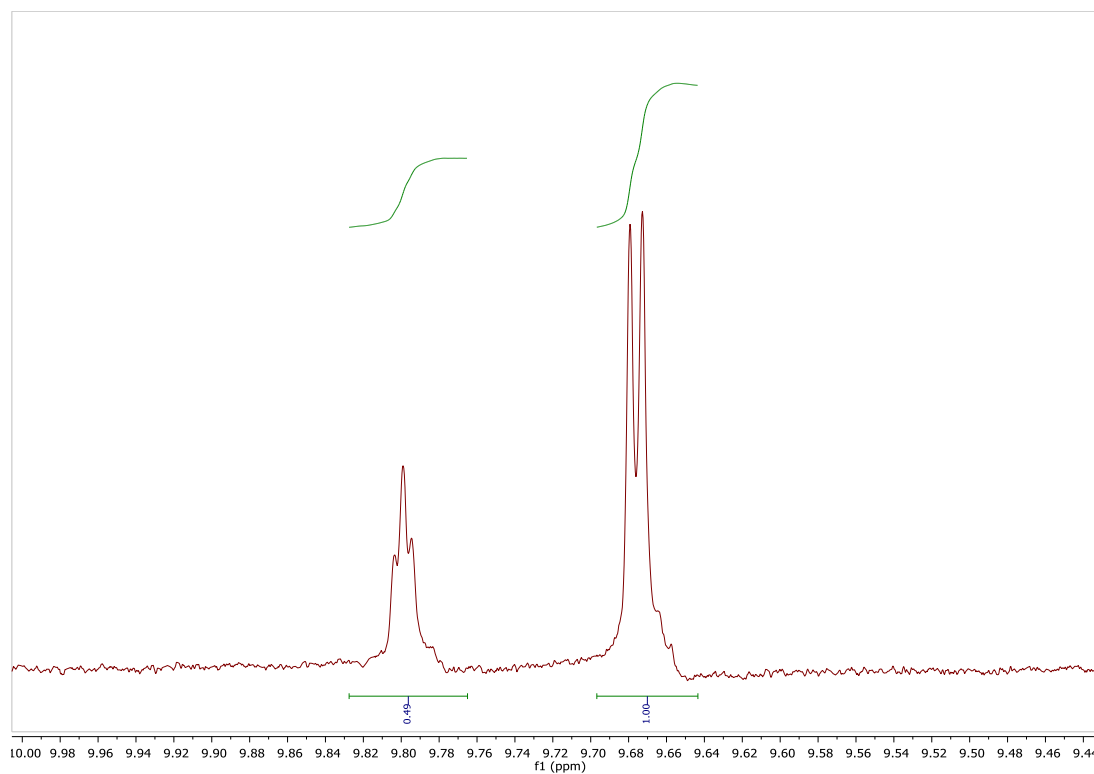
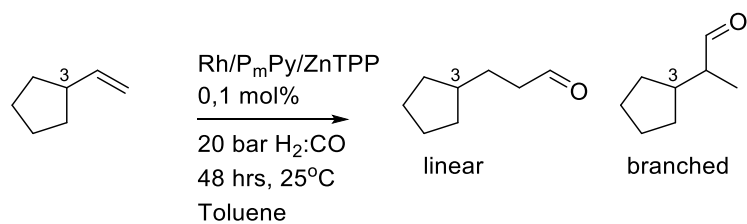
Time	Area	I/b ratio
------	------	-----------

8,317	760155	Branched	0.408
9,185	310593	Linear	



Time	Area	I/b ratio
------	------	-----------

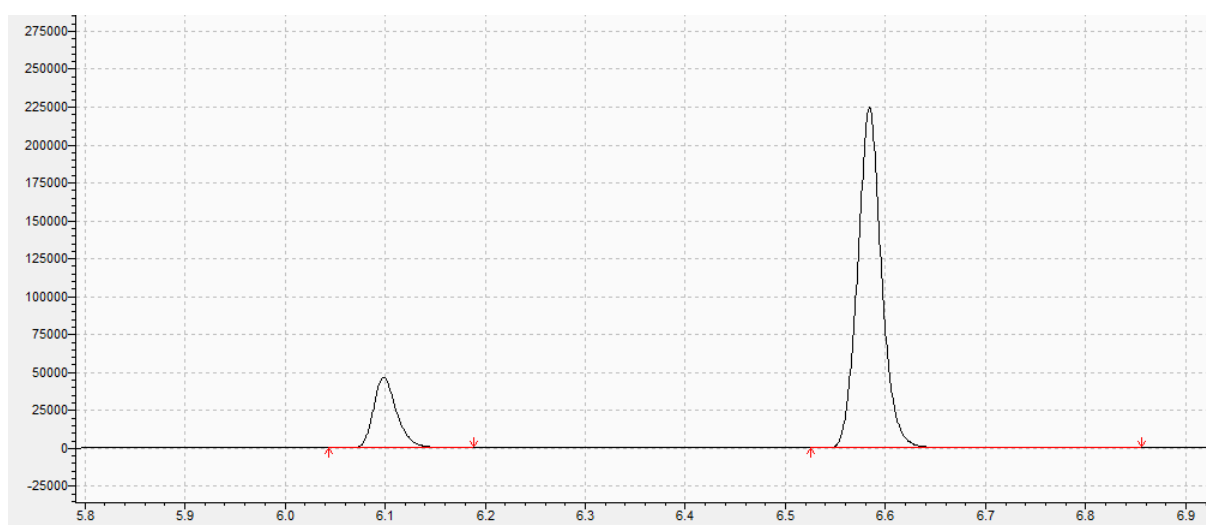
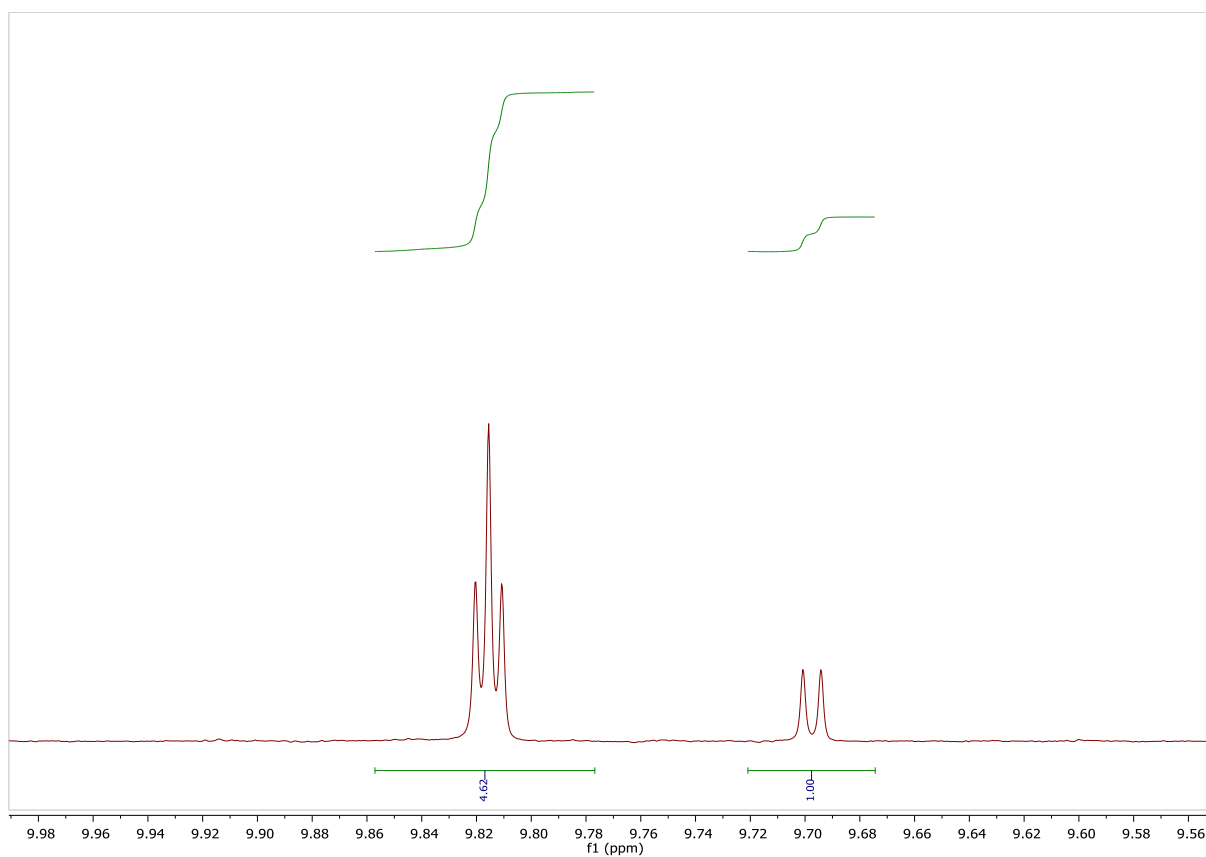
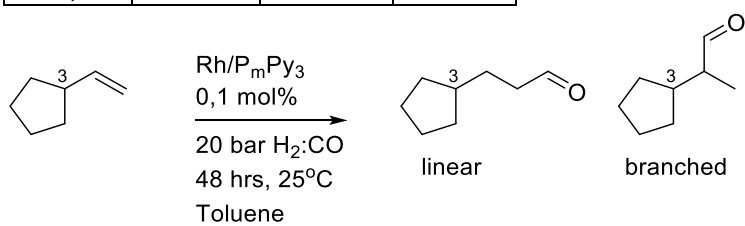
5,13	33902	Branched	7,10
5,464	240696	Linear	



Time	Area	I/b ratio
------	------	-----------

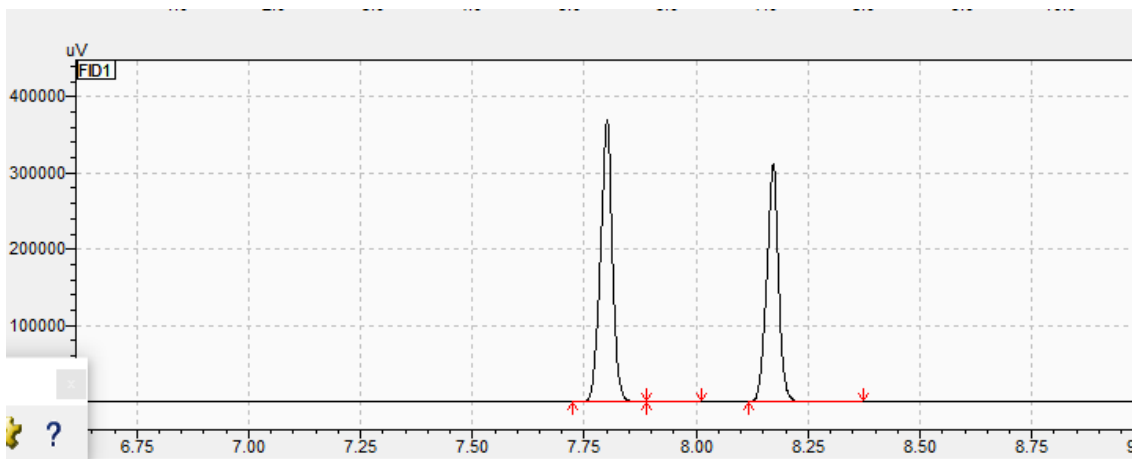
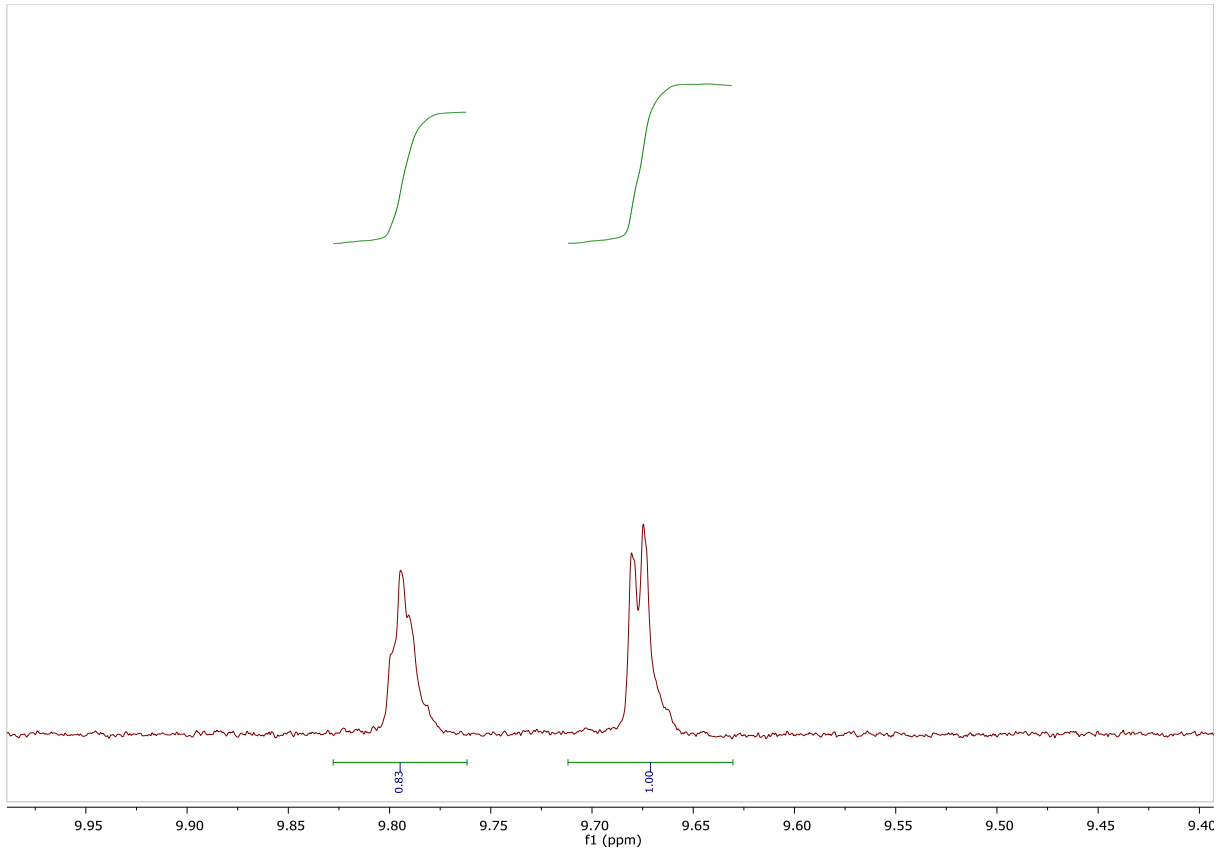
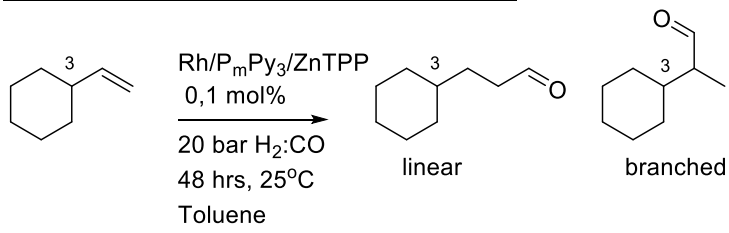


6,159	594020	Branched	0,50
6,631	311345	Linear	

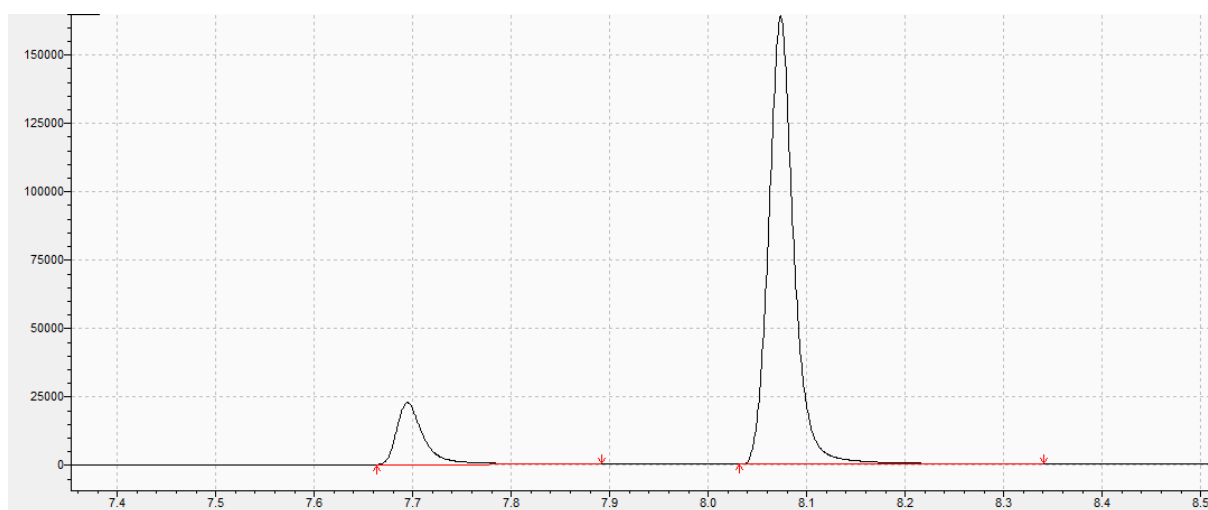
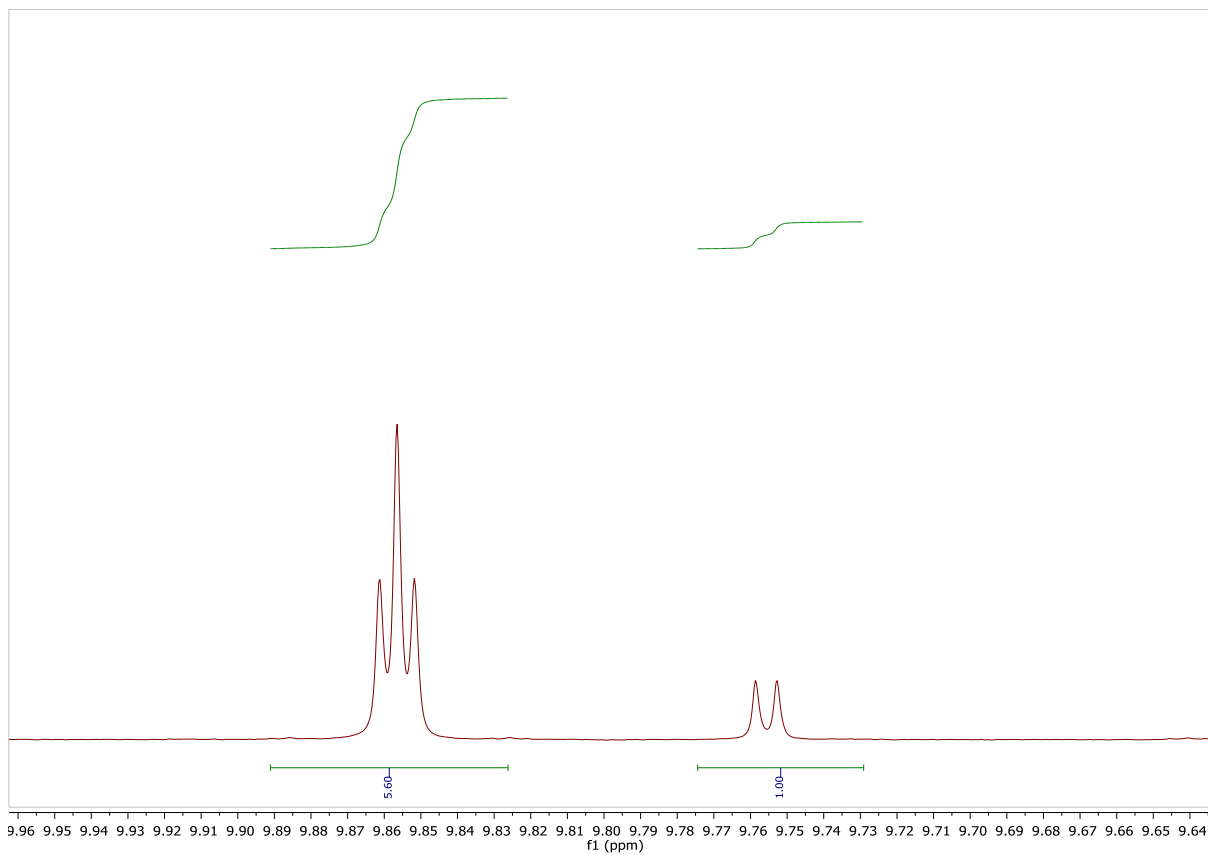
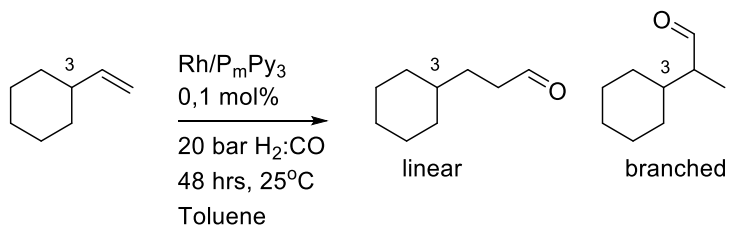


Time	Area		l/b ratio
6,159	32421	Branched	5.31

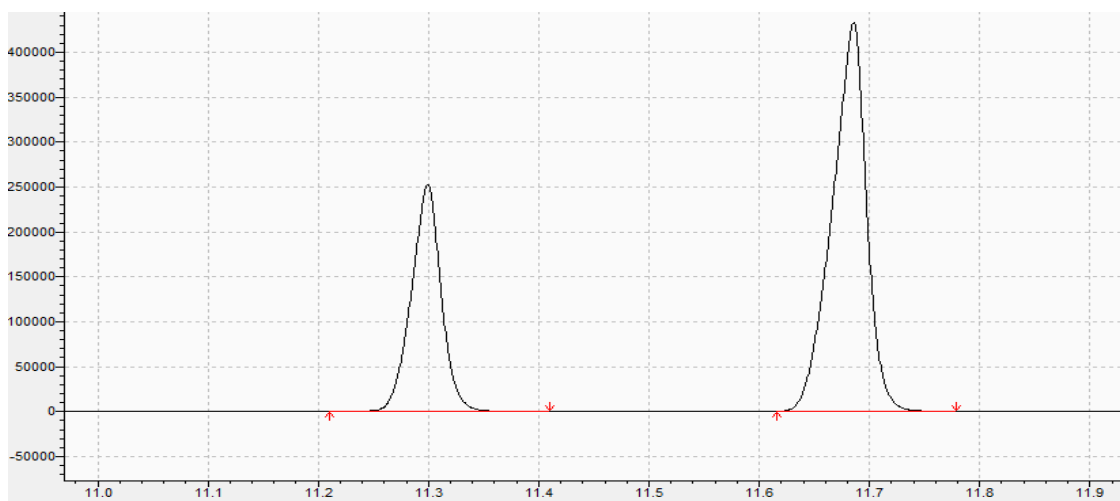
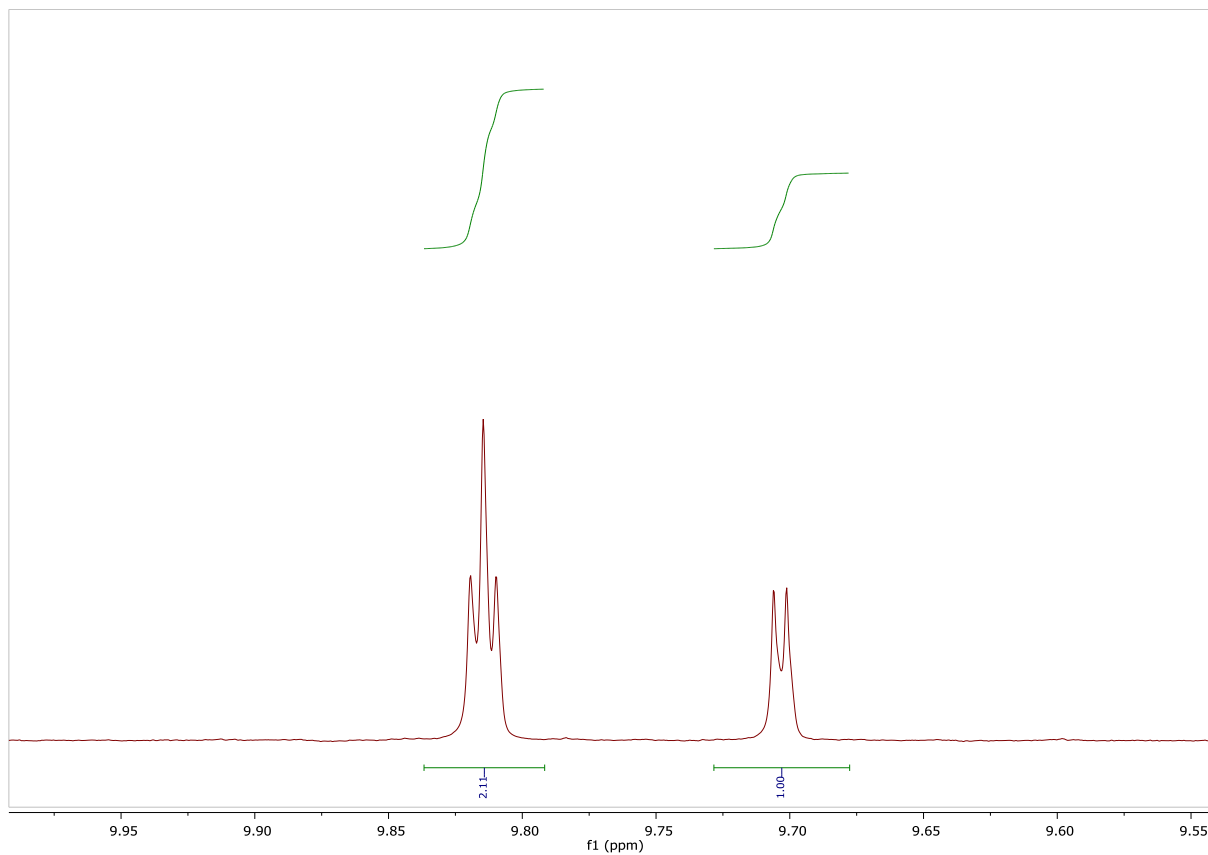
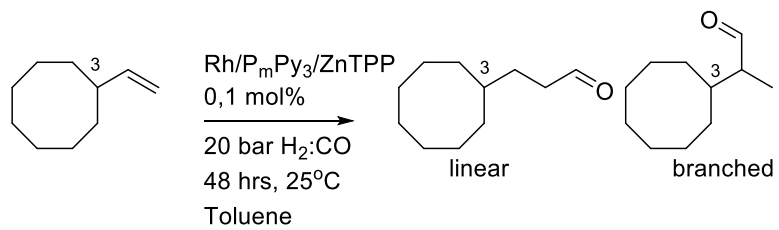
6,631	172425	Linear	
-------	--------	--------	--



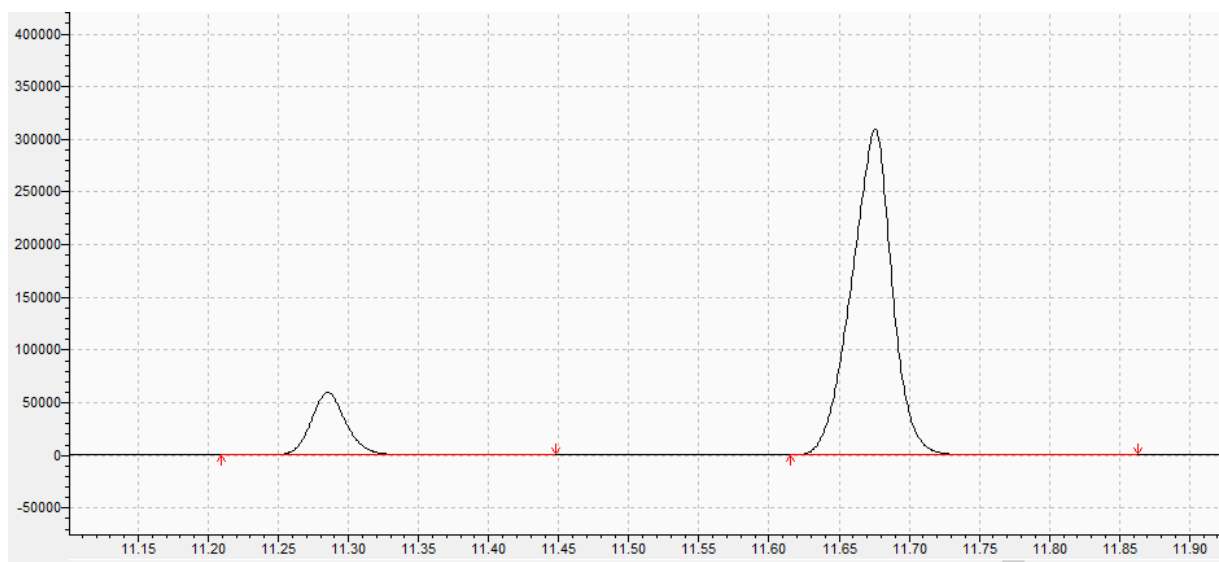
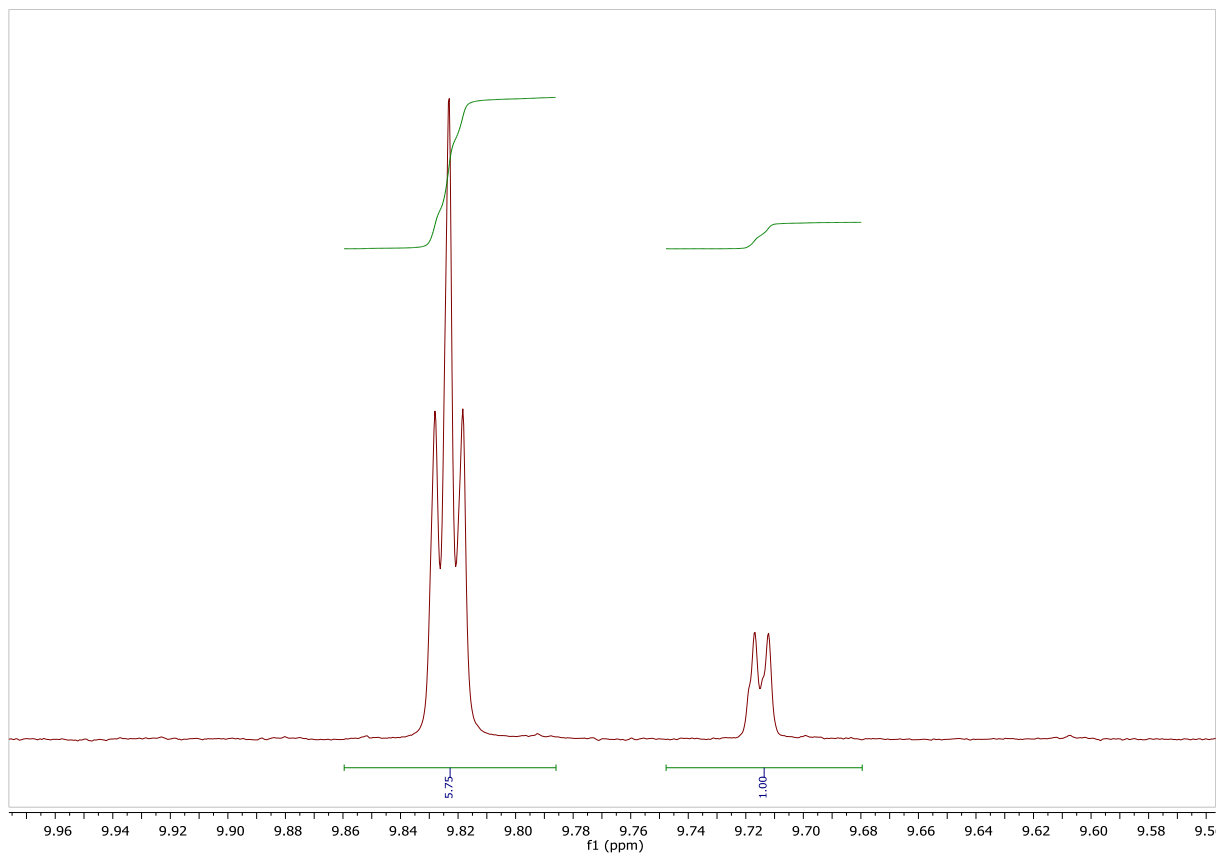
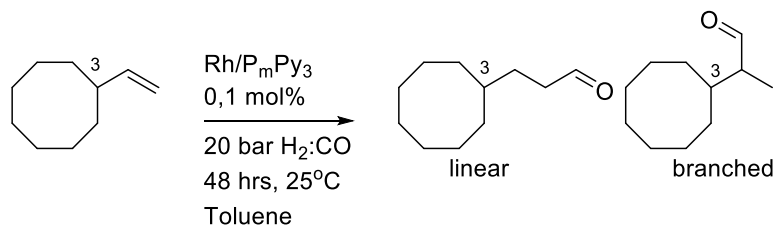
Retention time	Area		I/b ratio
7,869	682471	branched	0,84
8,172	570411		



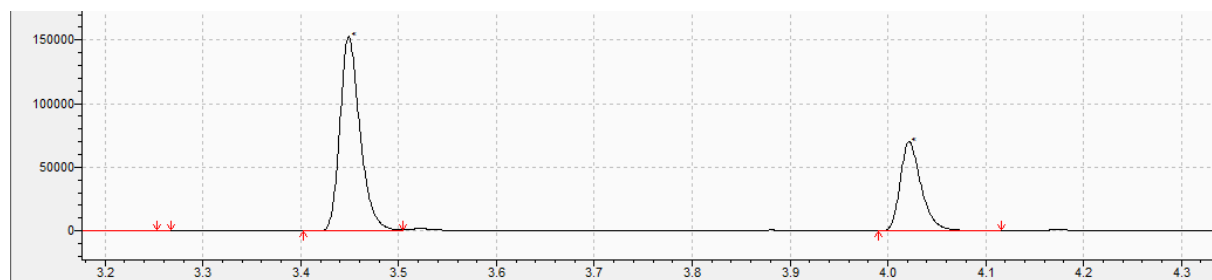
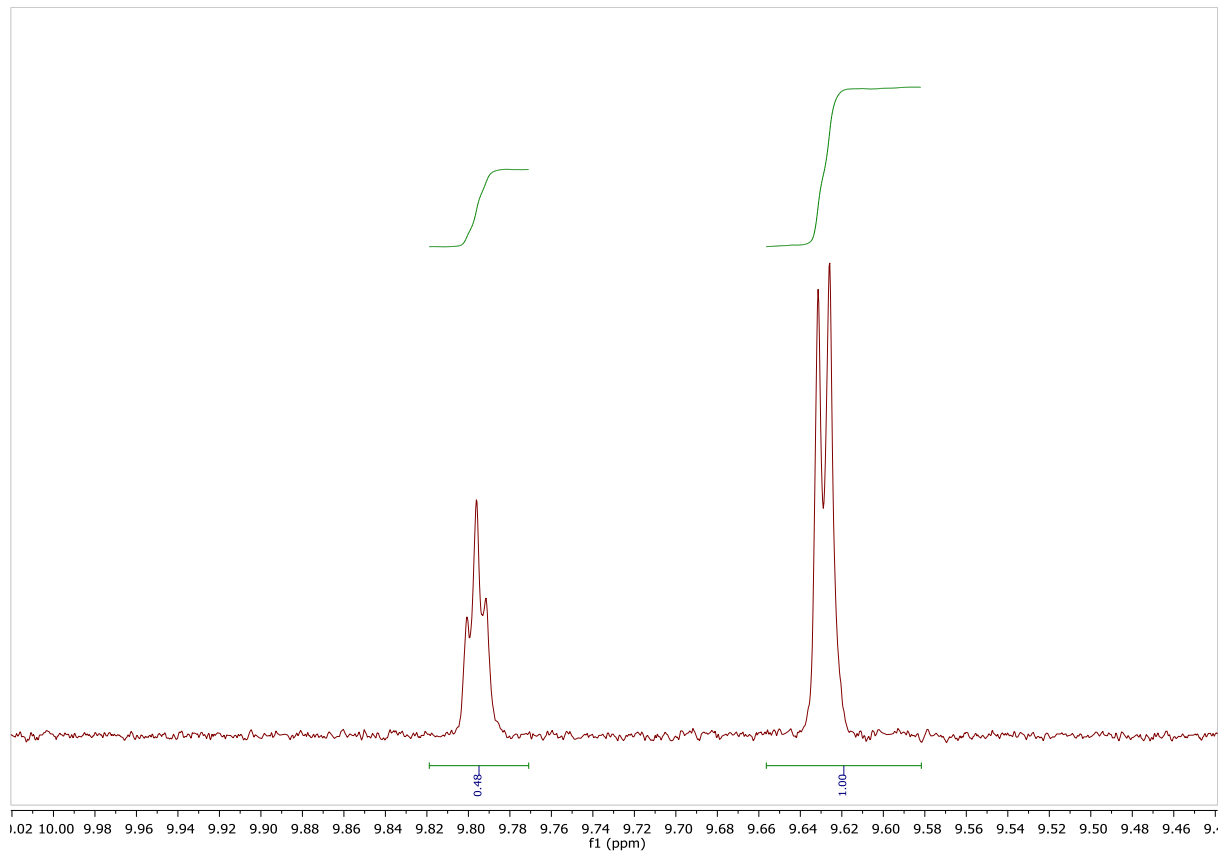
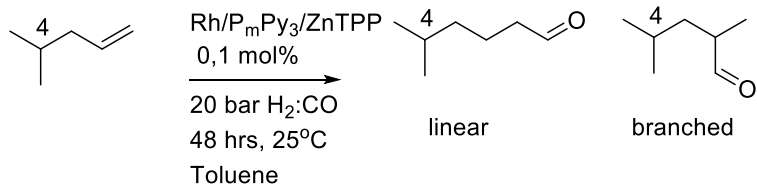
Retention time	Area		l/b ratio
7.695	43449	branched	6.7
8.073	292083	Linear	



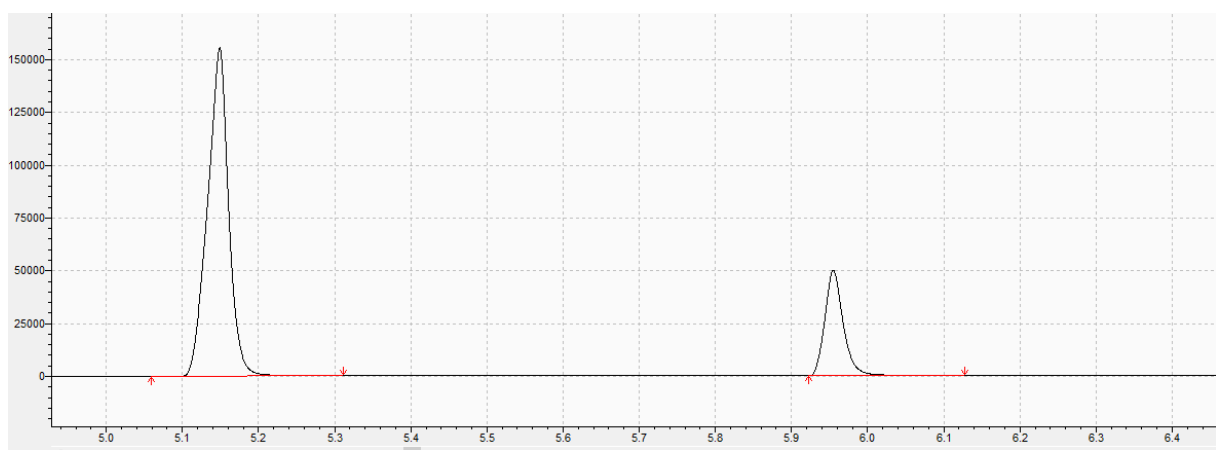
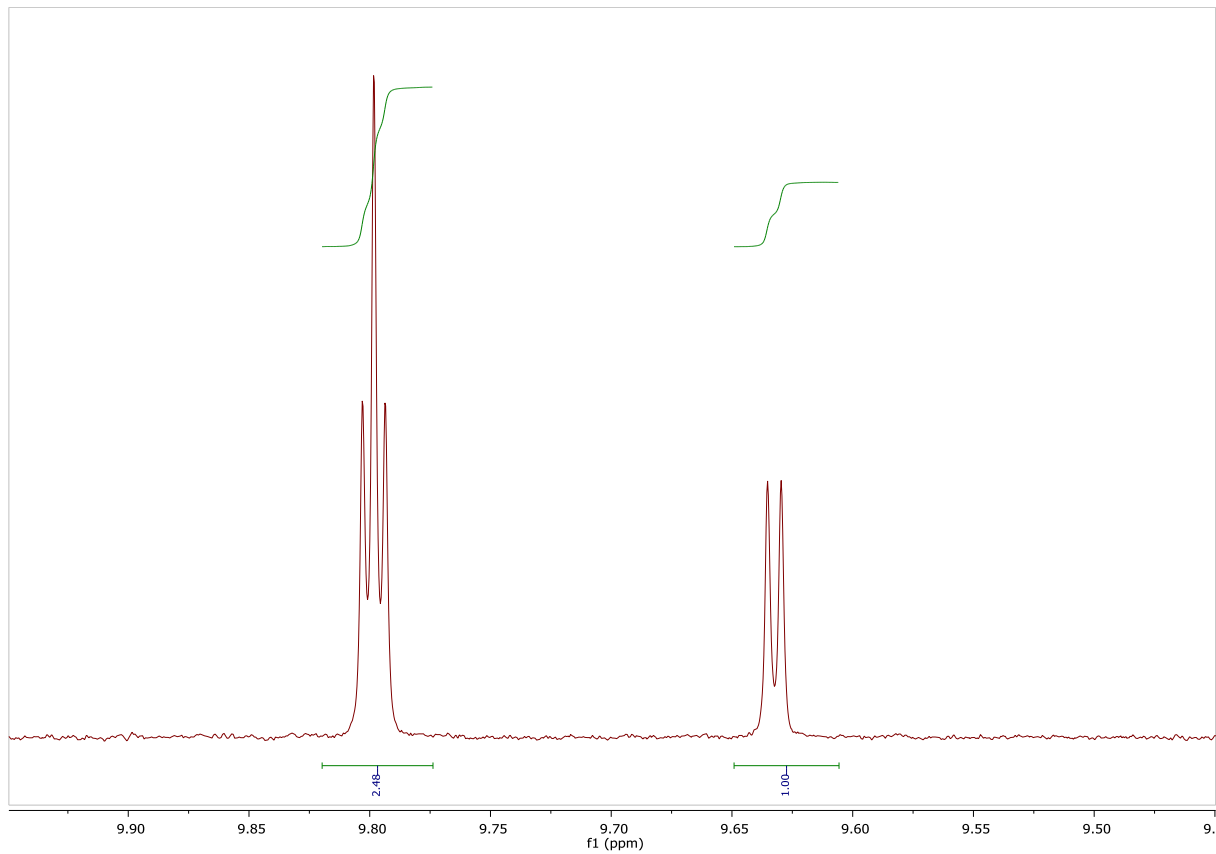
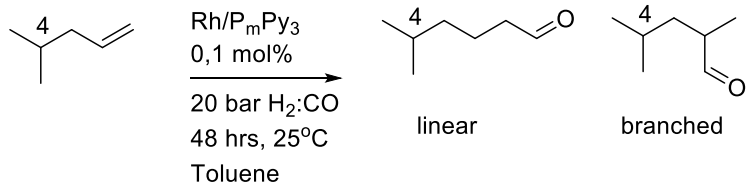
Retention time	Area		l/b ratio
11,299	473573	Branched	
11,685	939316	Linear	1.98



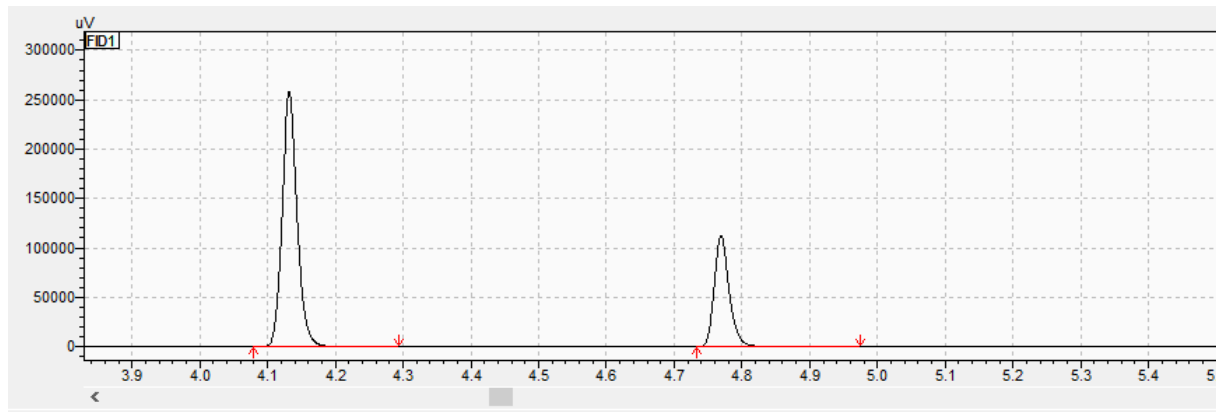
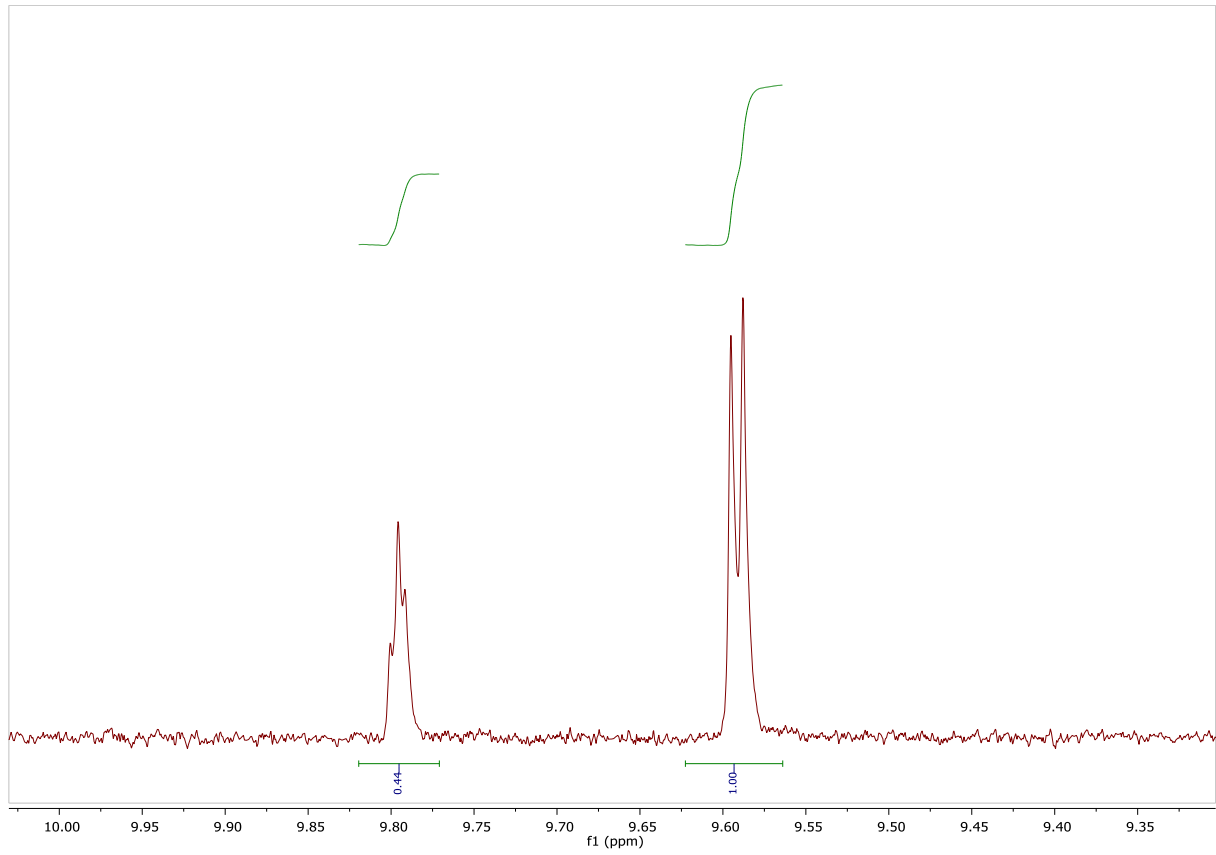
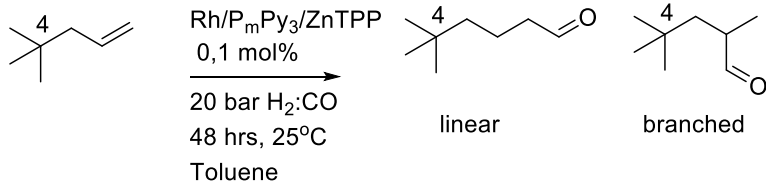
Retention time	Area		I/b ratio
11,378	103245	Branched	
11,675	621022	Linear	6,015032



Retention time	Area		l/b ratio
3,449	217641	Branched	0,47
4,022	102969	Linear	

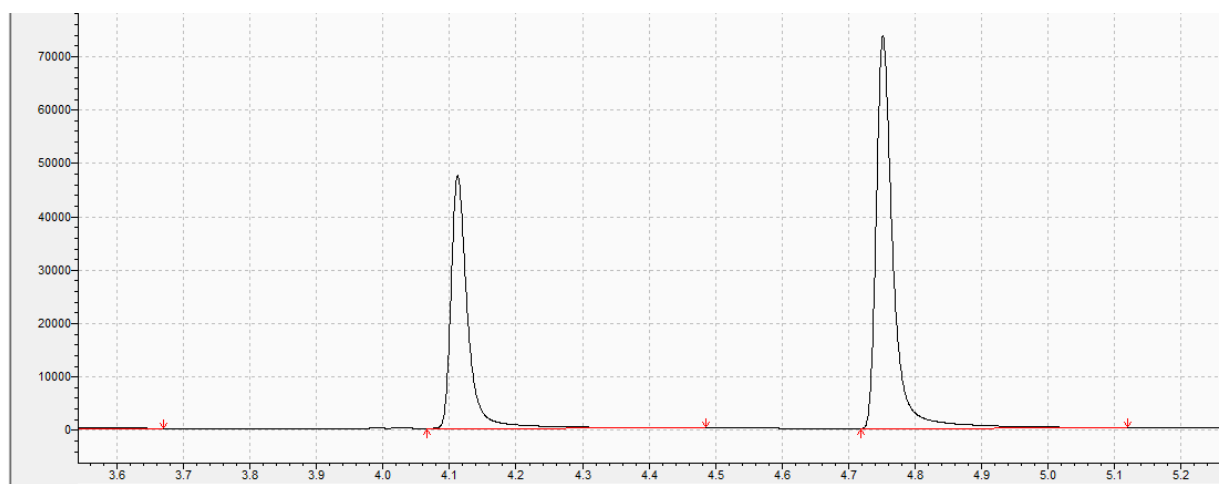
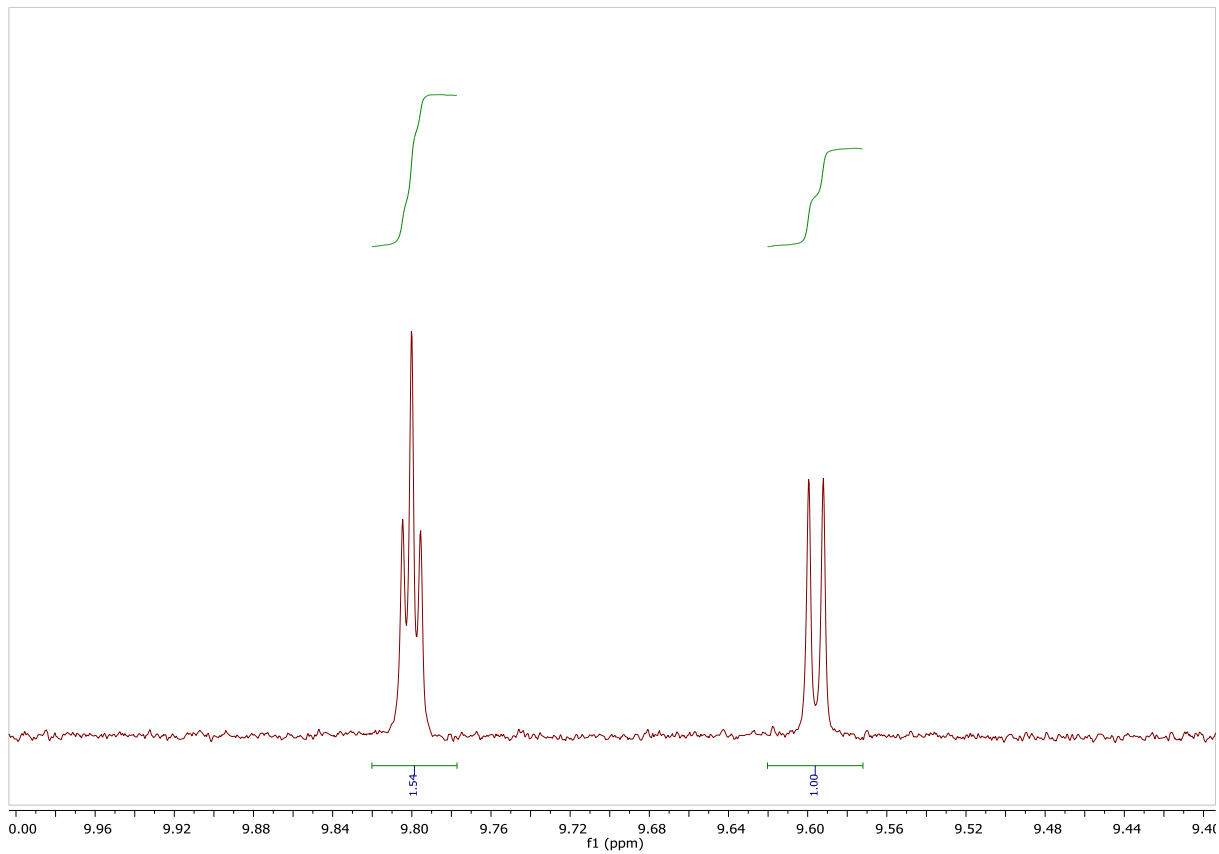
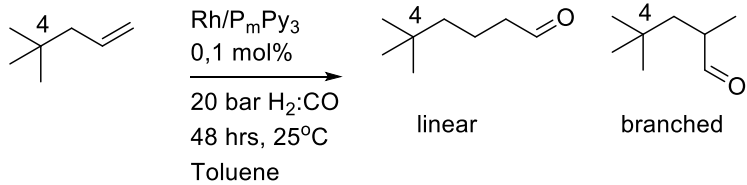


Retention time	area		l/b ratio
3,44	59918	Branched	2.72
4,013	163327	Linear	

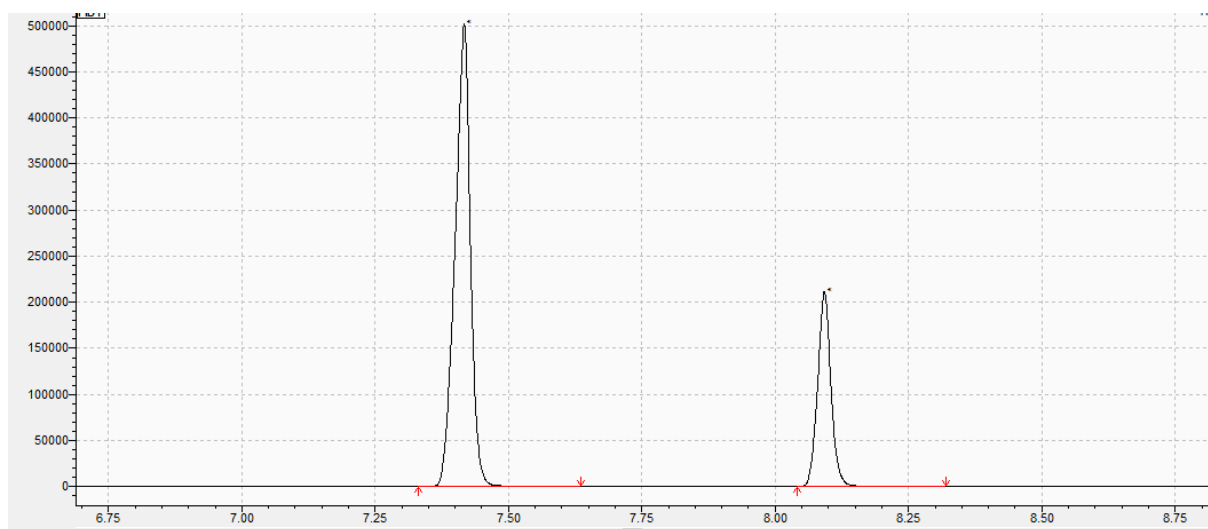
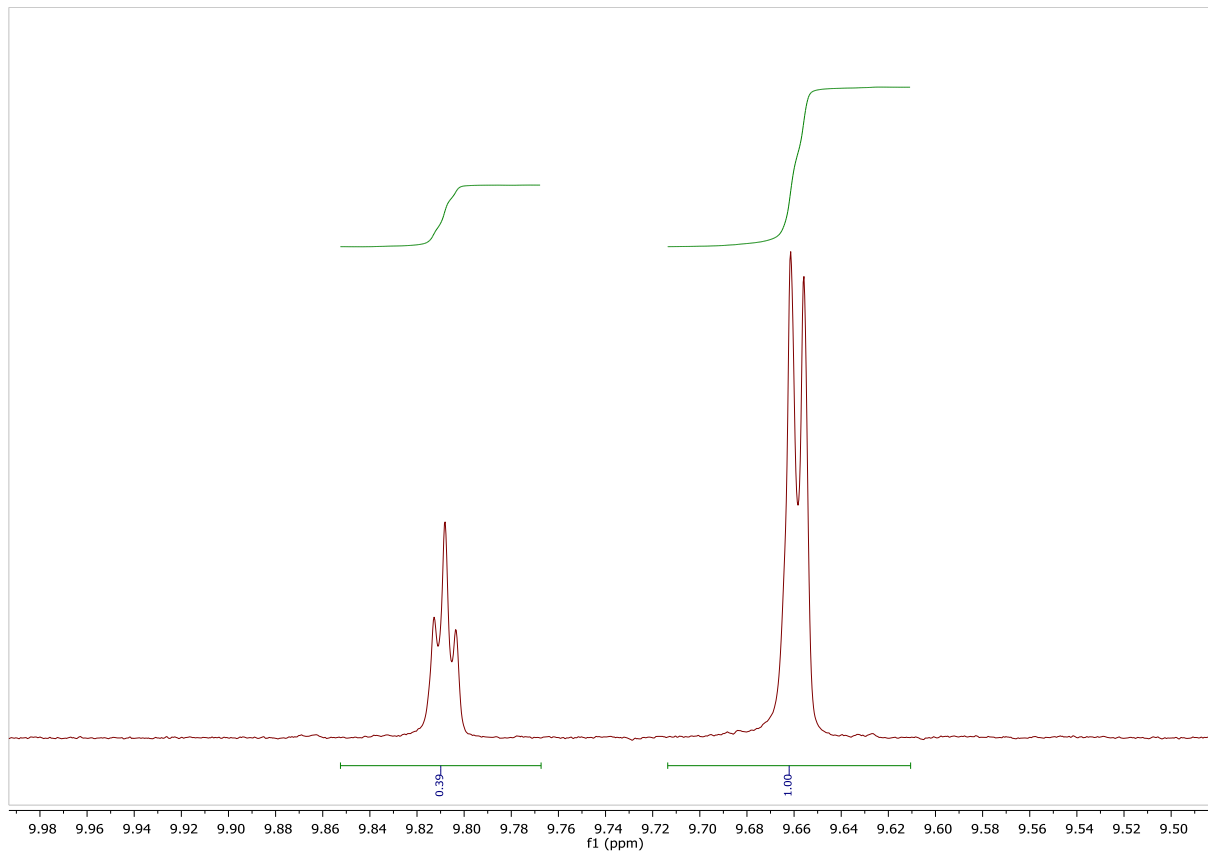
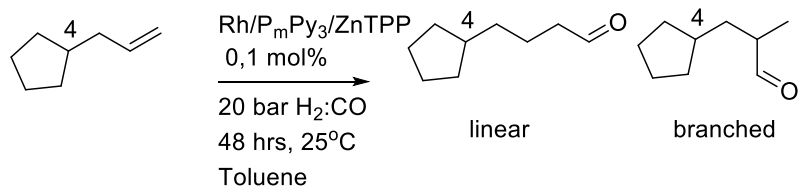


Retention time	Area		l/b ratio
4,132	391595	Branched	0,44
4,769	171142	Linear	

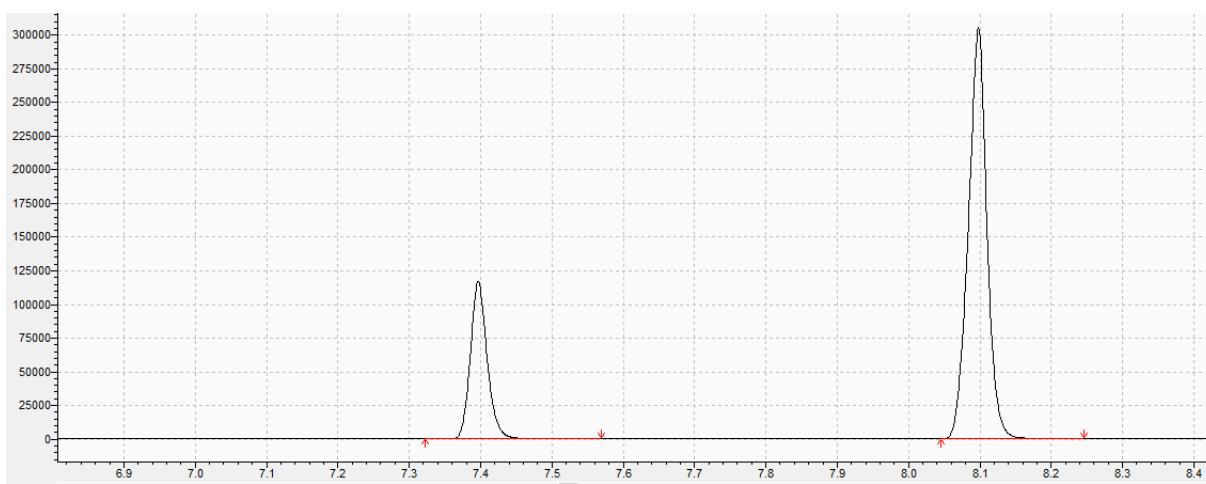
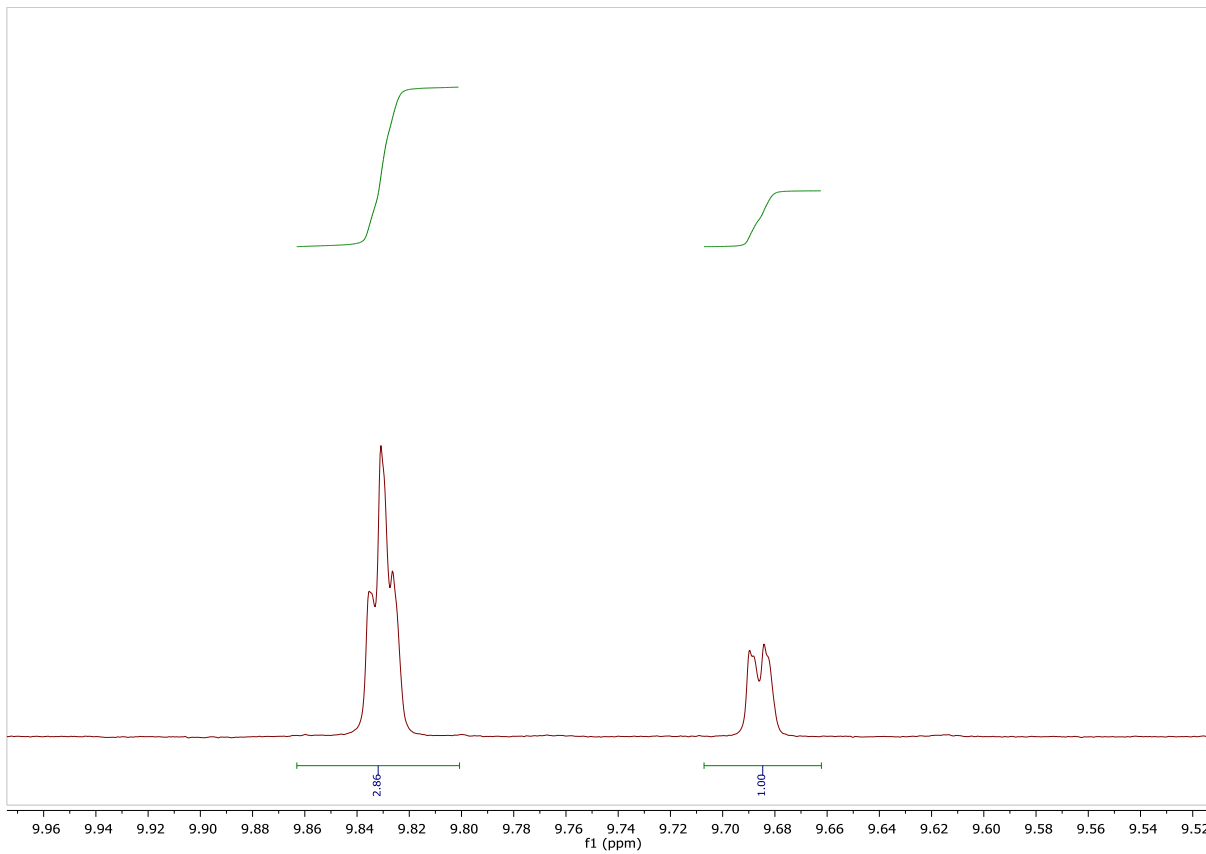
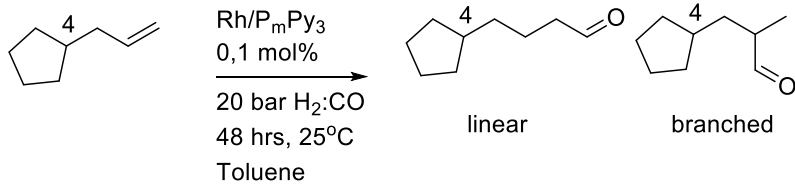




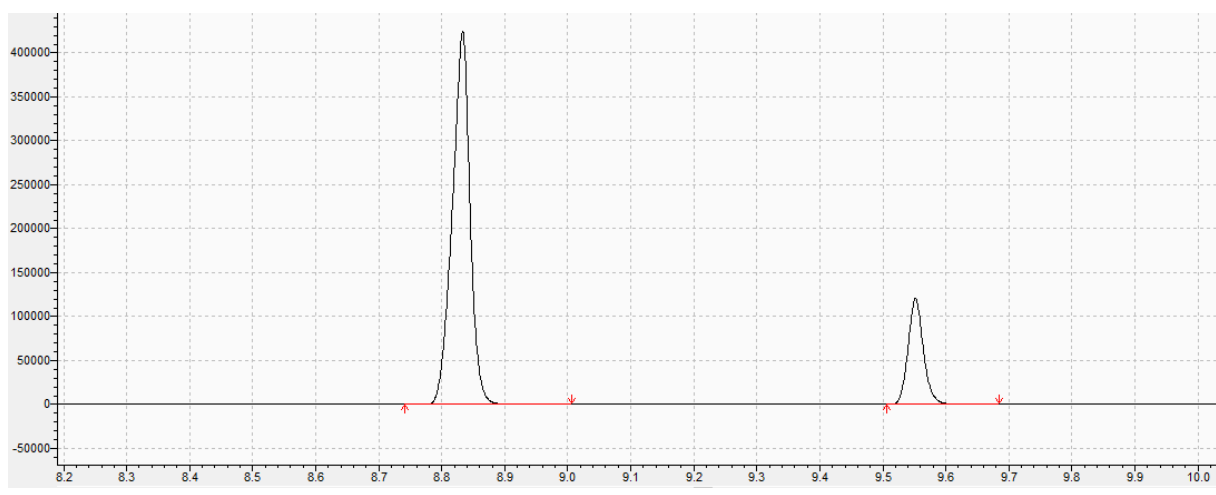
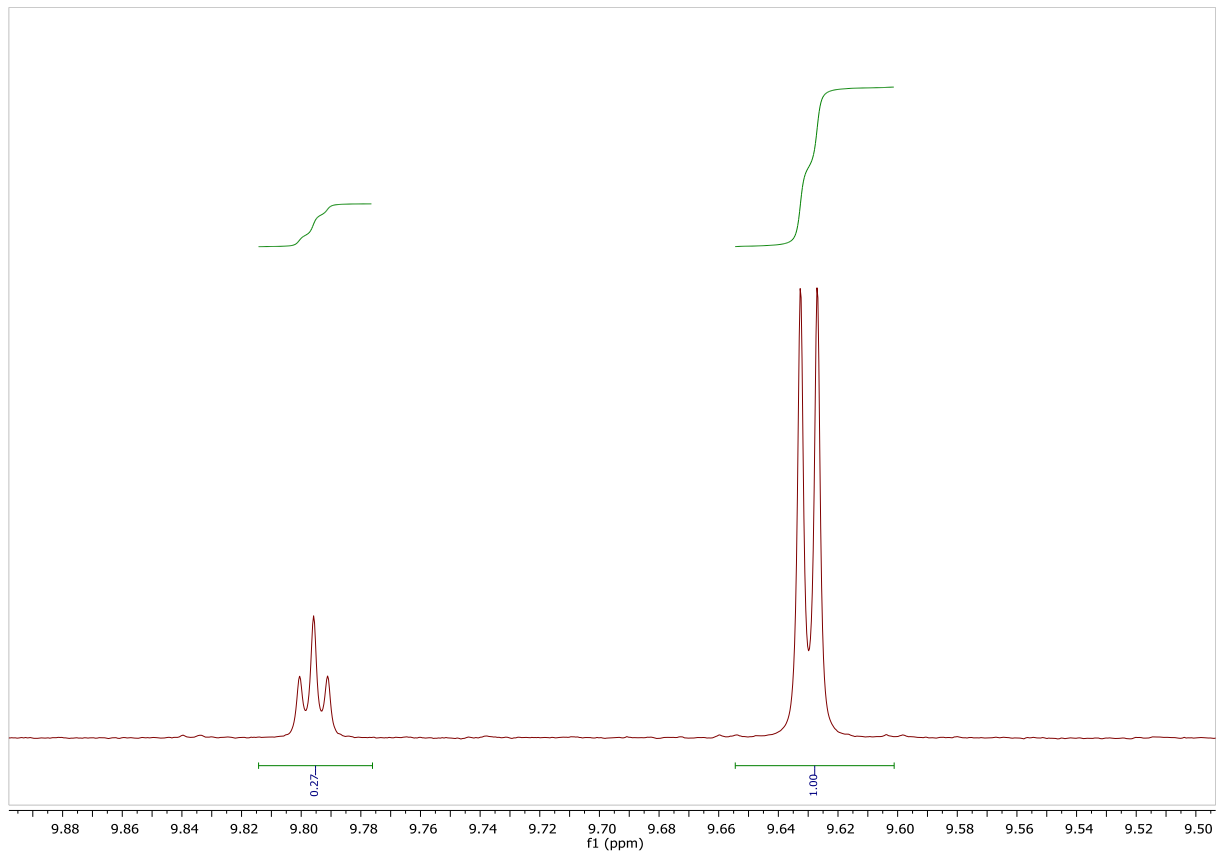
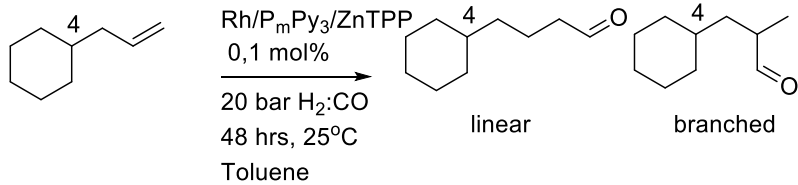
Retention time	area		l/b ratio
4,112	83980	branched	1.56
4,752	131076	Linear	



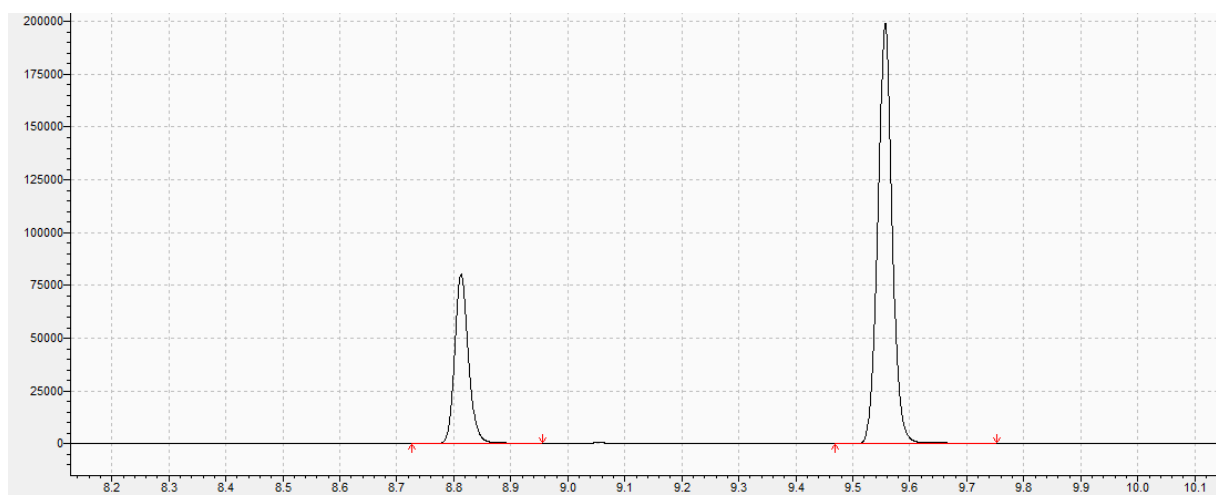
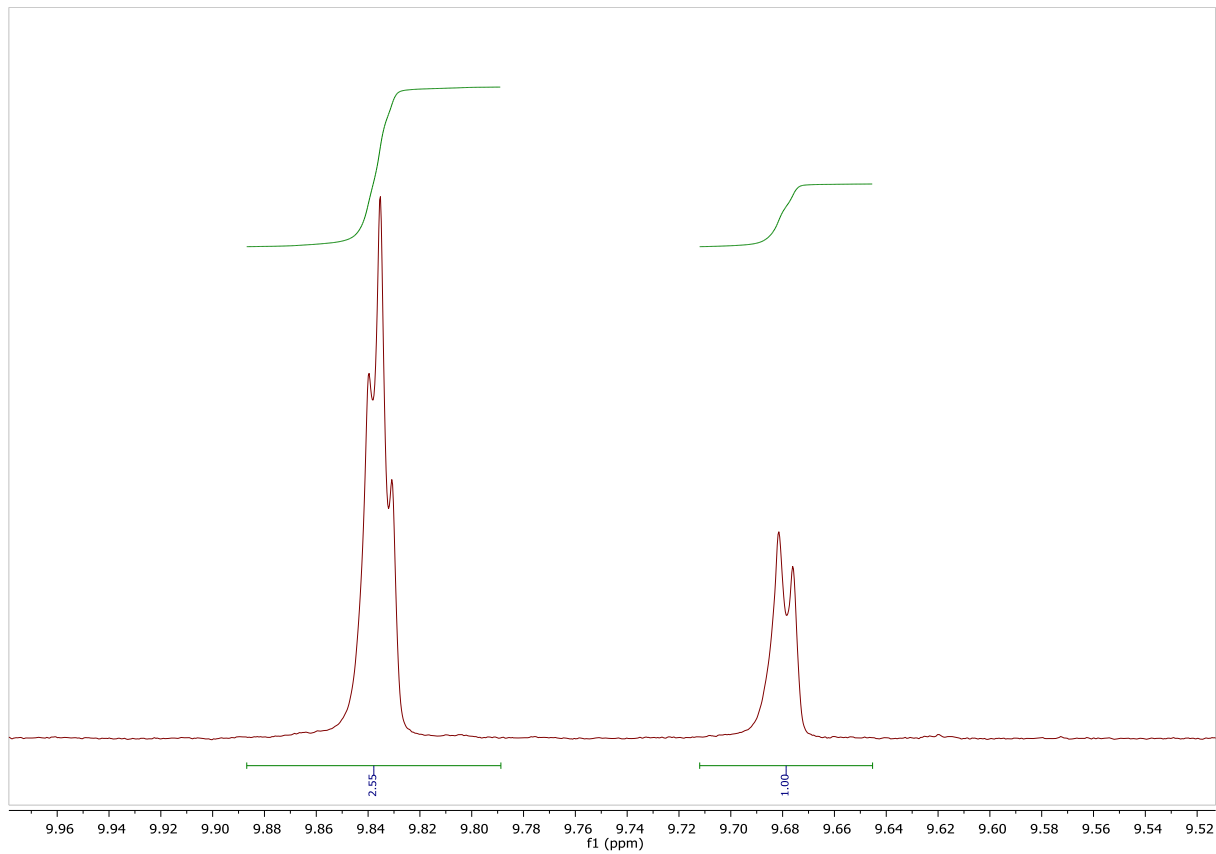
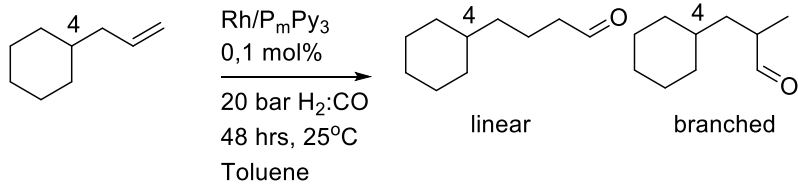
Retention time	Area		l/b ratio
7,417	1001993	Branched	0.36
8,092	366610	Linear	



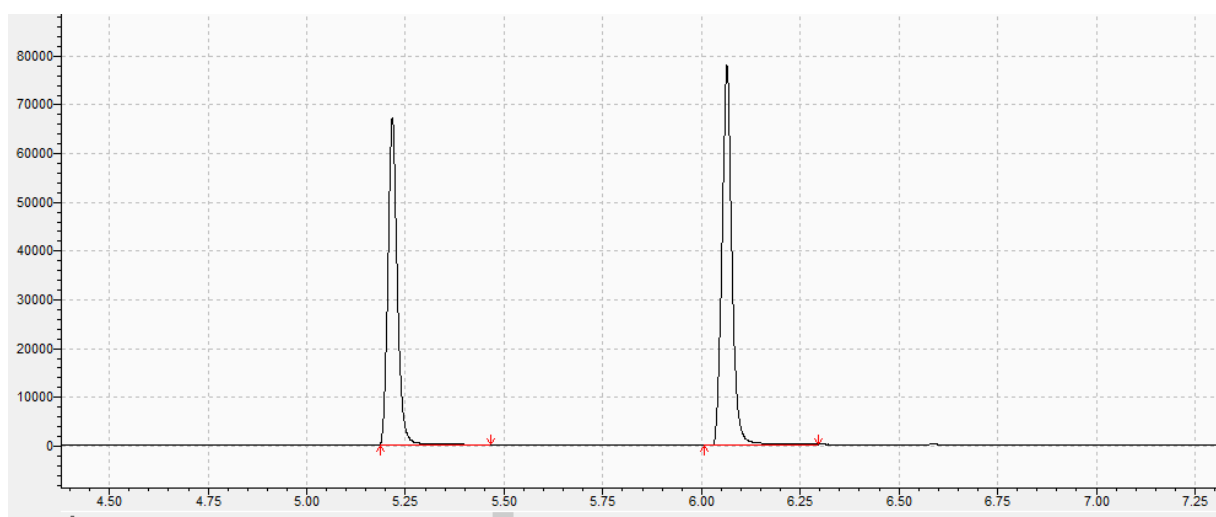
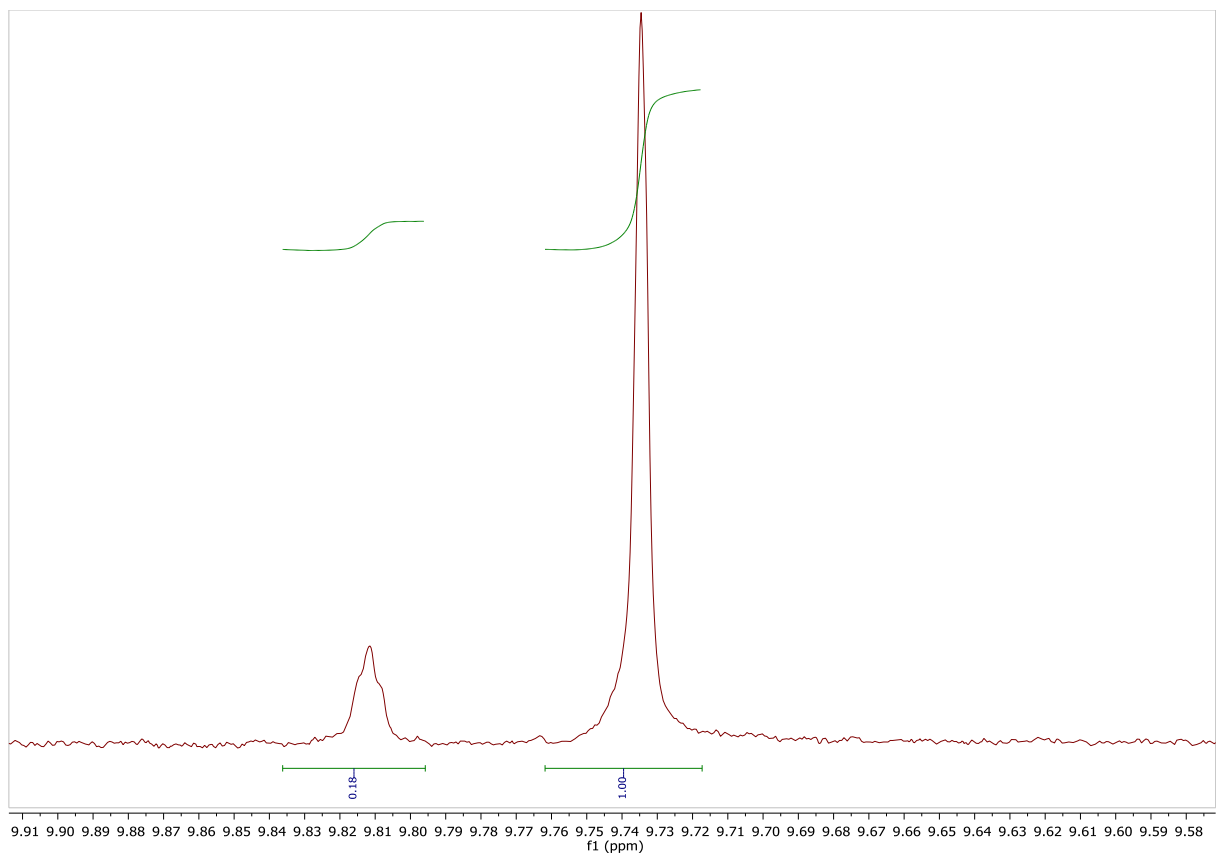
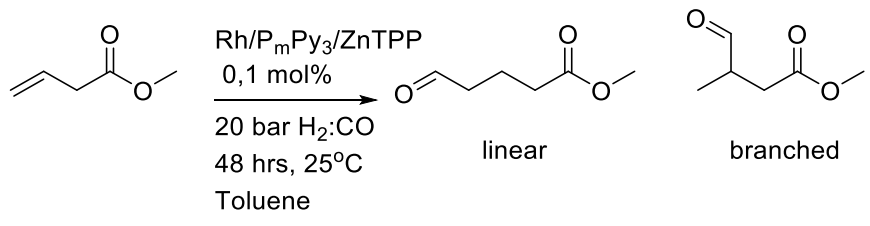
Retention time	Area		I/b ratio
7,397	189808	Branched	2.91
8,098	551937	Linear	



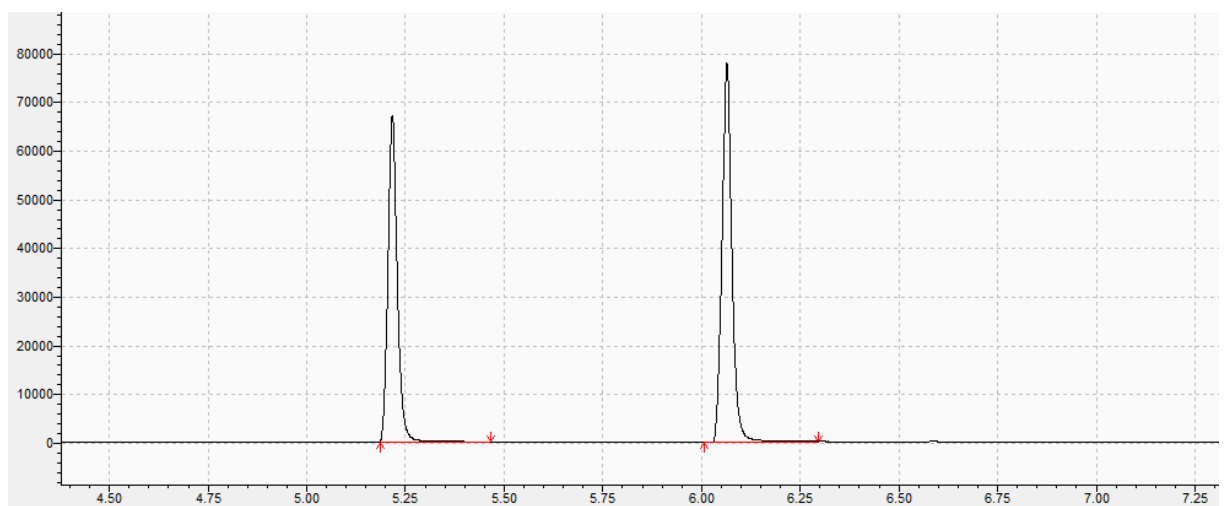
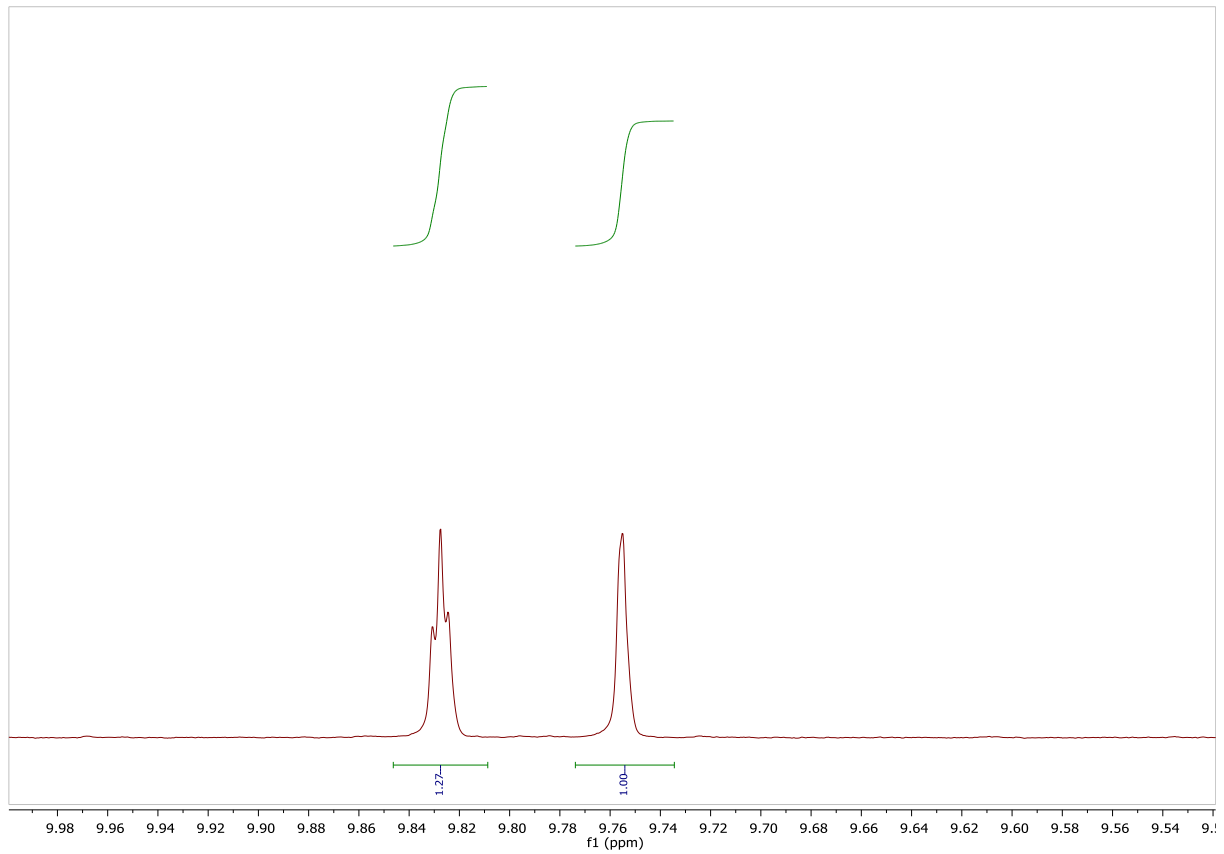
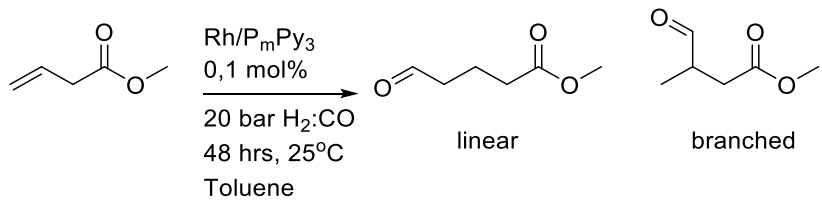
Retention time	area		l/b ratio
8,833	831630	Branched	0.244
9,552	202663	Linear	



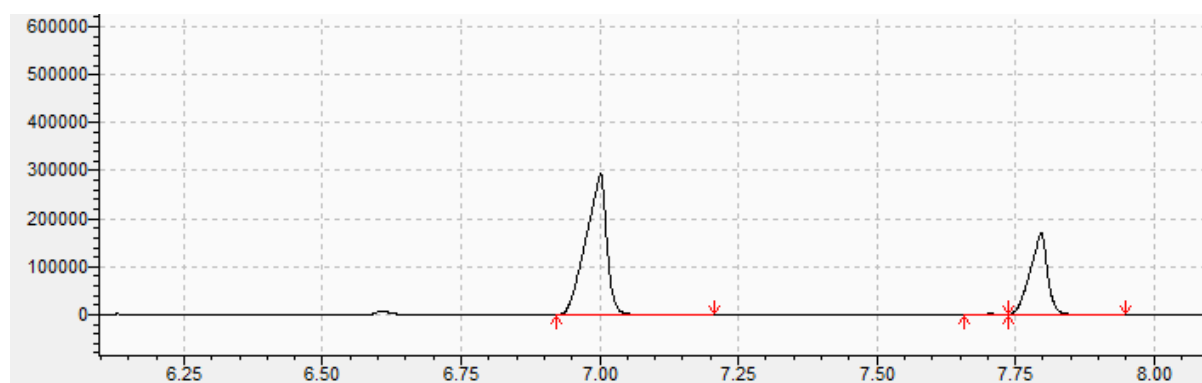
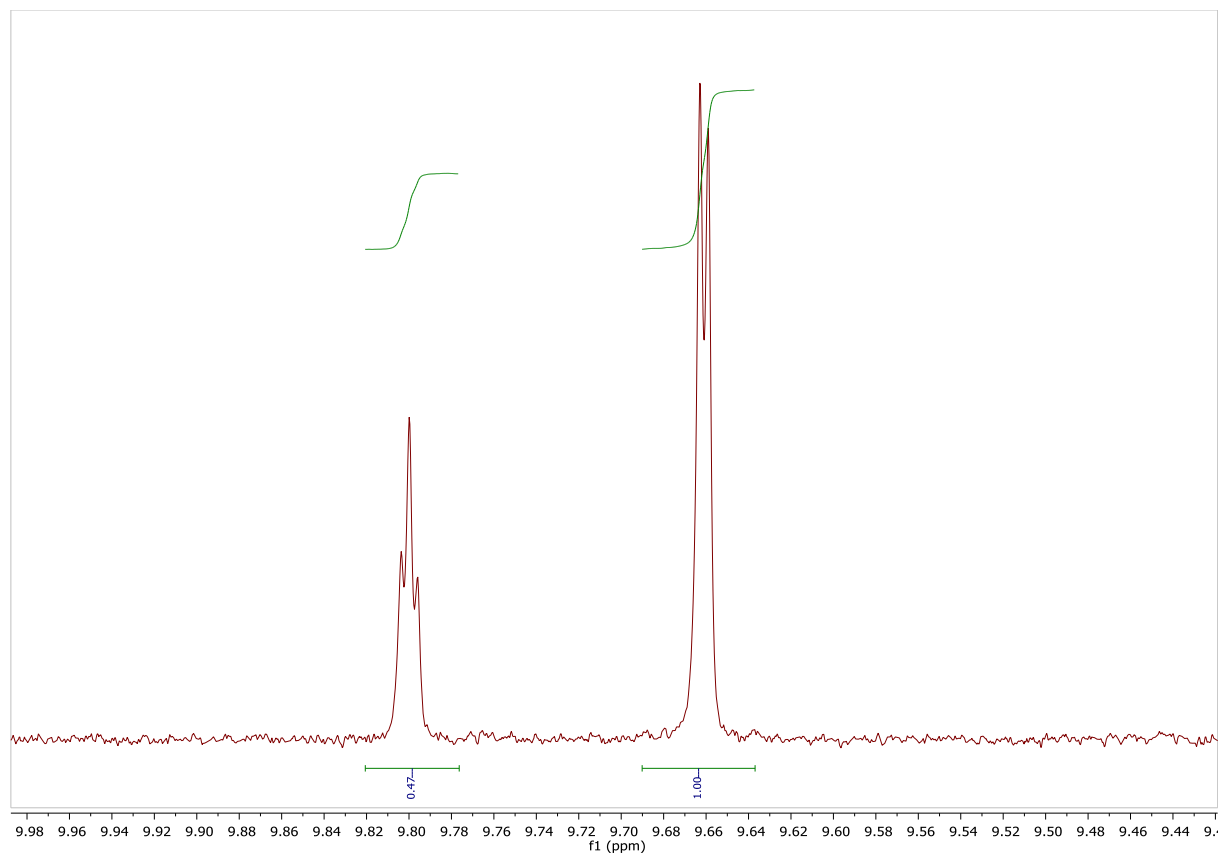
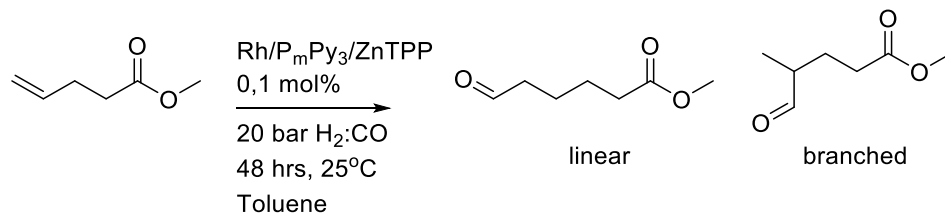
Retention time	area		l/b ratio
8,813	133295	Branched	2.62
9,557	348725	Linear	



Retention time	Area		l/b ratio
5,271	456918	branched	0.18
6,093	83979	Linear	

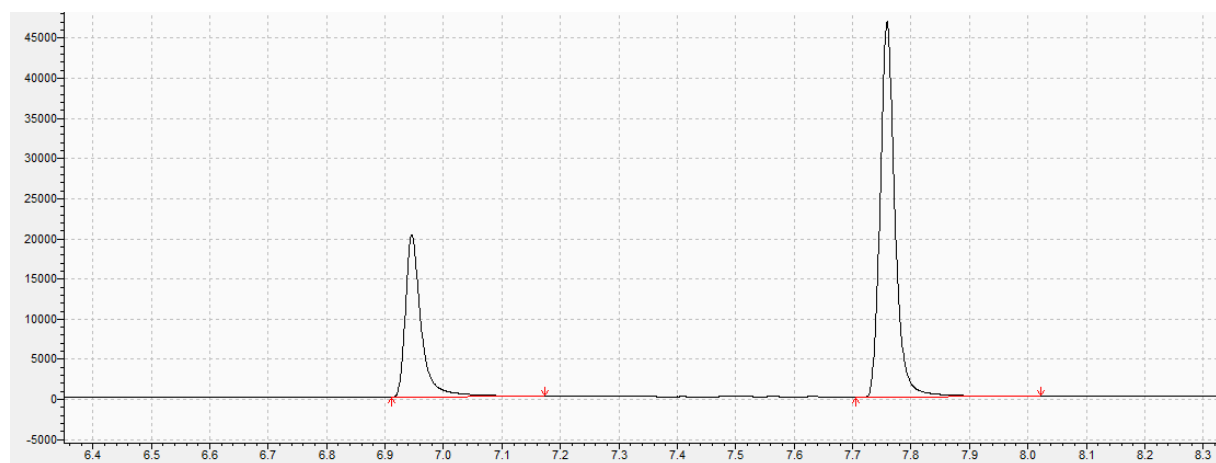
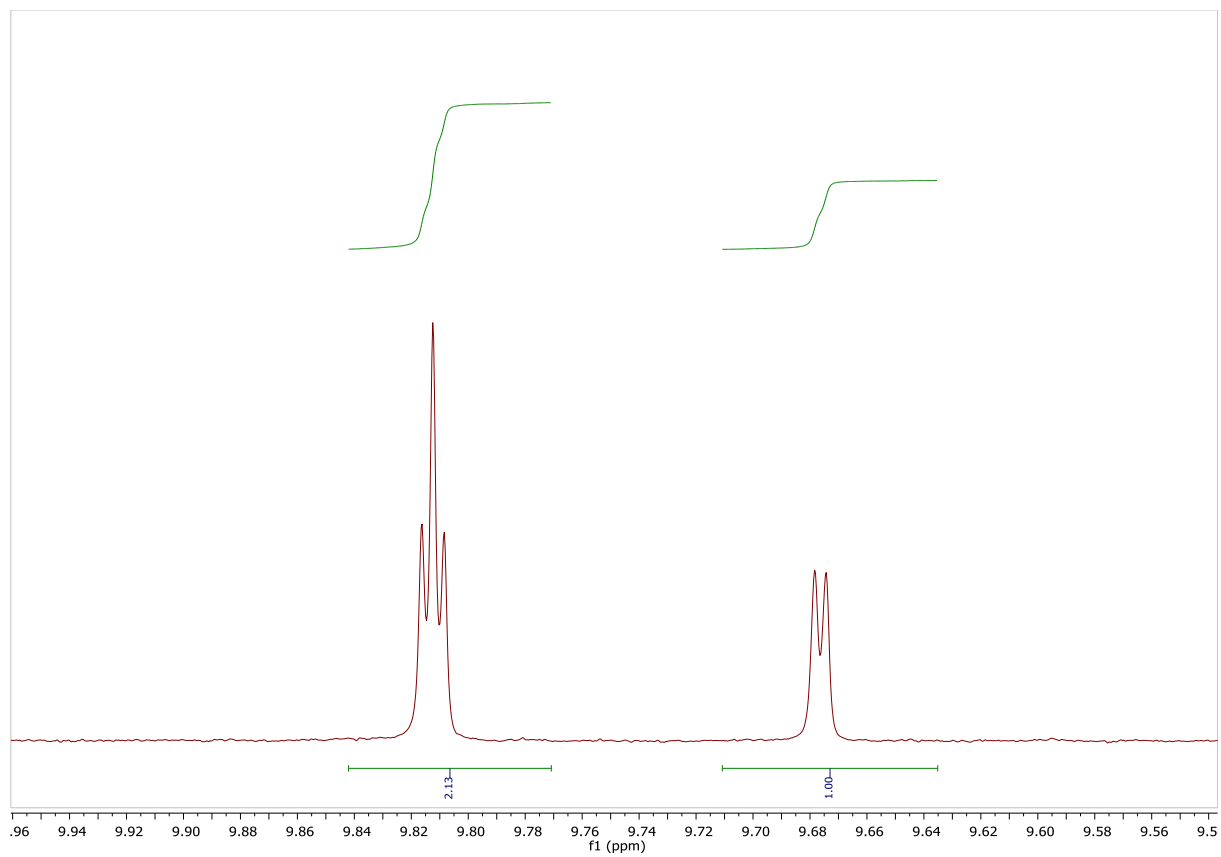
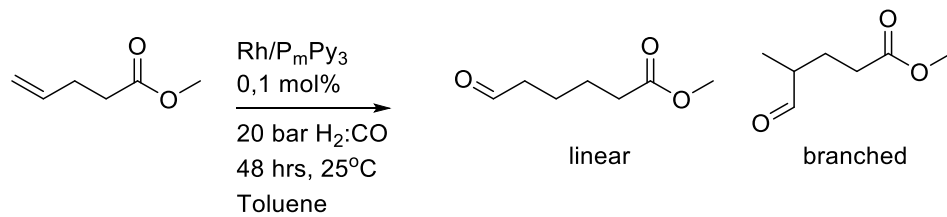


Retention time	Area		I/b ratio
5,217	109812	Branched	1.23
6,064	135468	Linear	

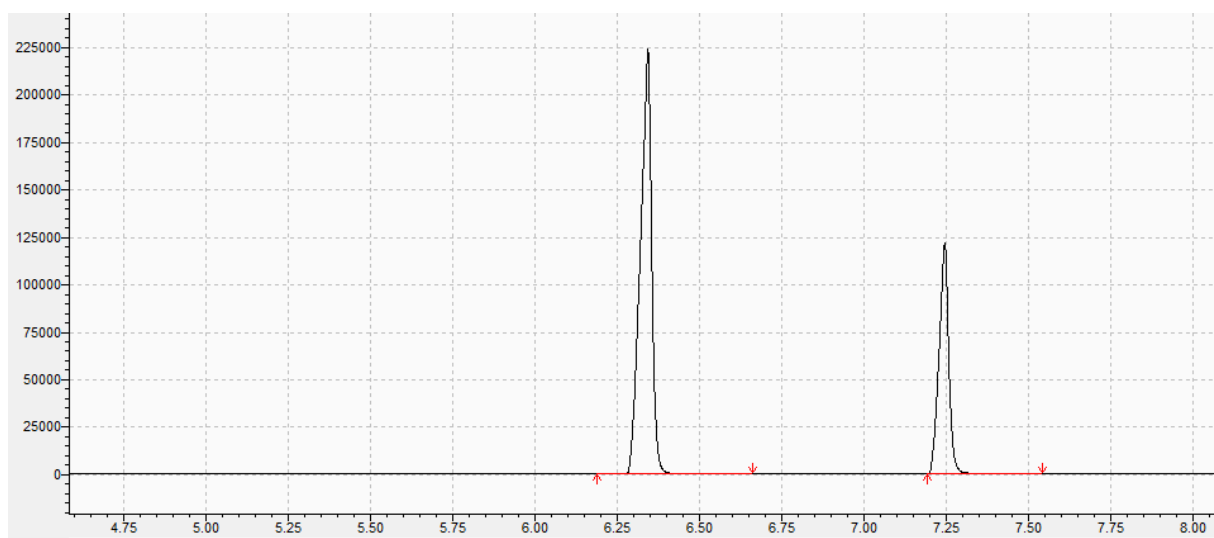
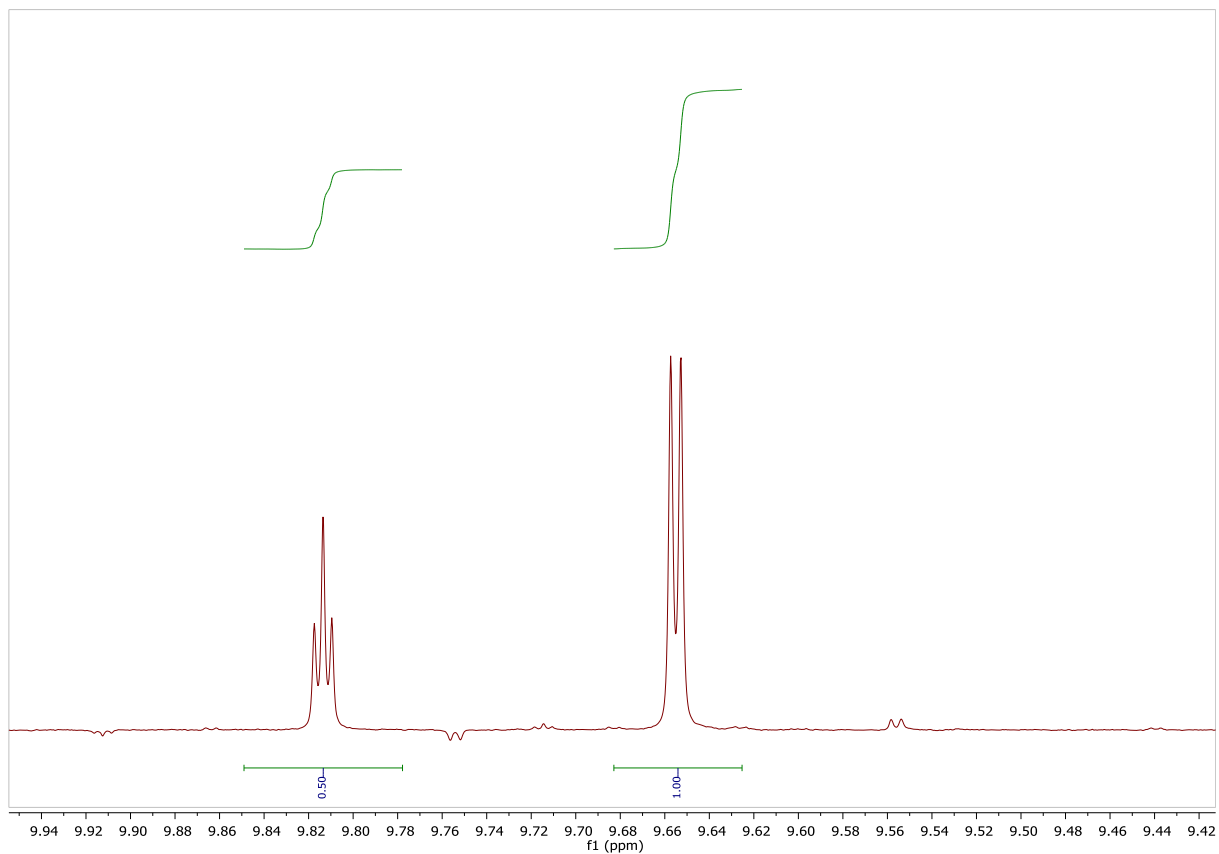
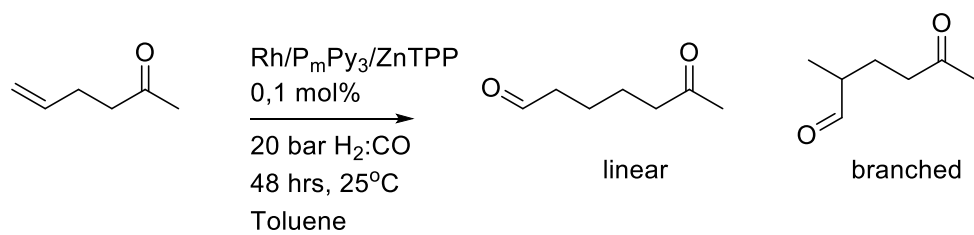


Retention time	Area		l/b ratio
7,001	764538	Branched	0.48
7,796	370191	Linear	

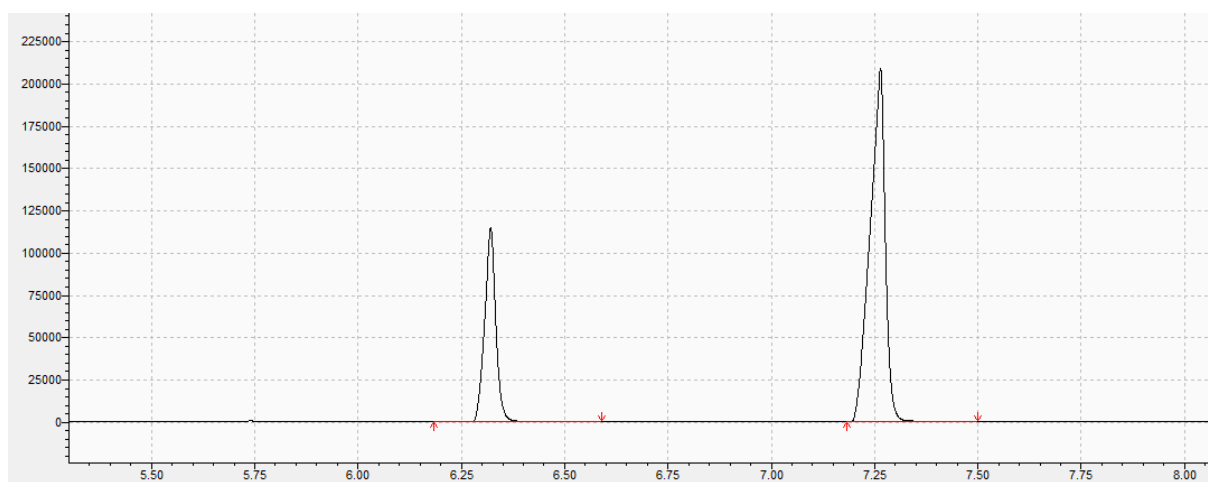
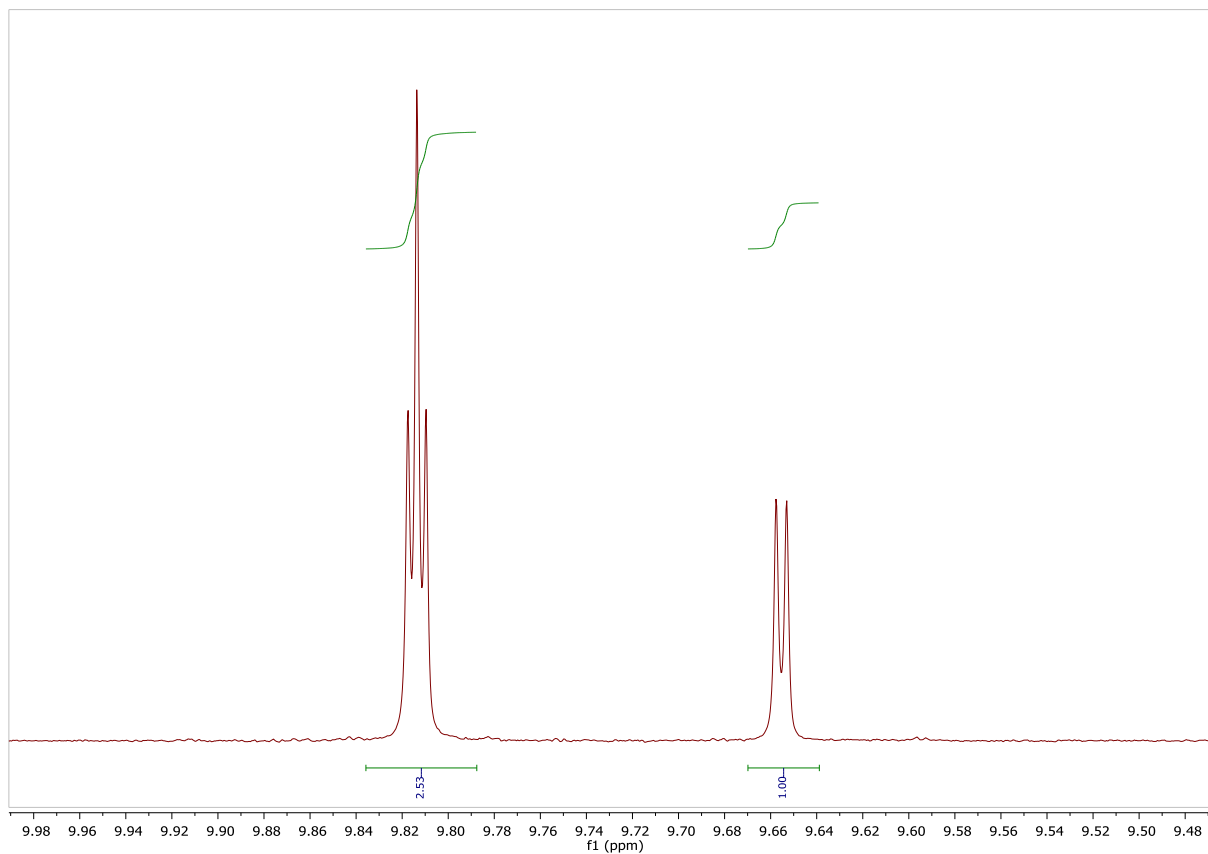
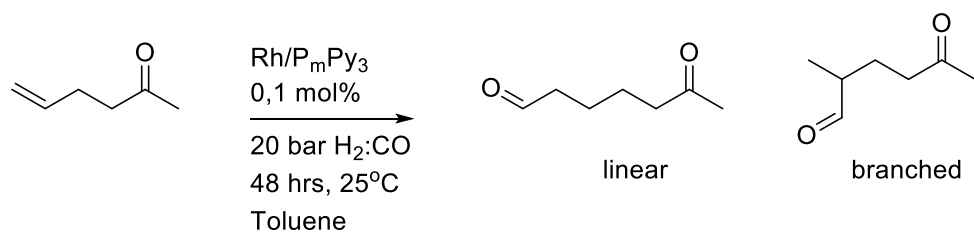




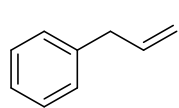
Retention time	Area		I/b ratio
6,946	37795	Branched	2,18
7,759	82380	Linear	



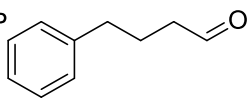
Retention time	Area		
6,341	534134	Branched	0.47
7,244	250453	Linear	



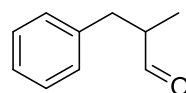
Retention time	Area		l/b ratio
6,321	214852	Branched	2.50
7,264	538596	Linear	



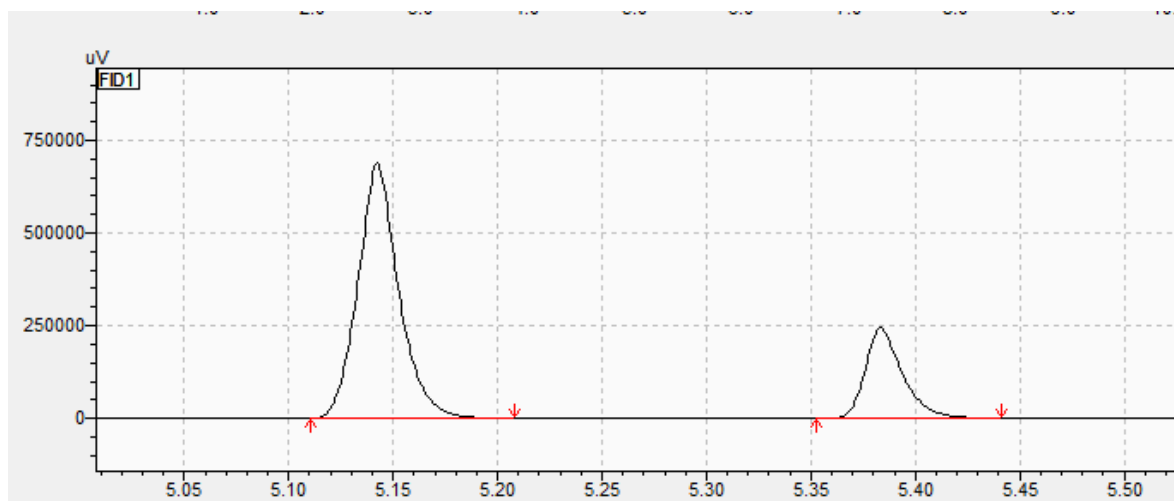
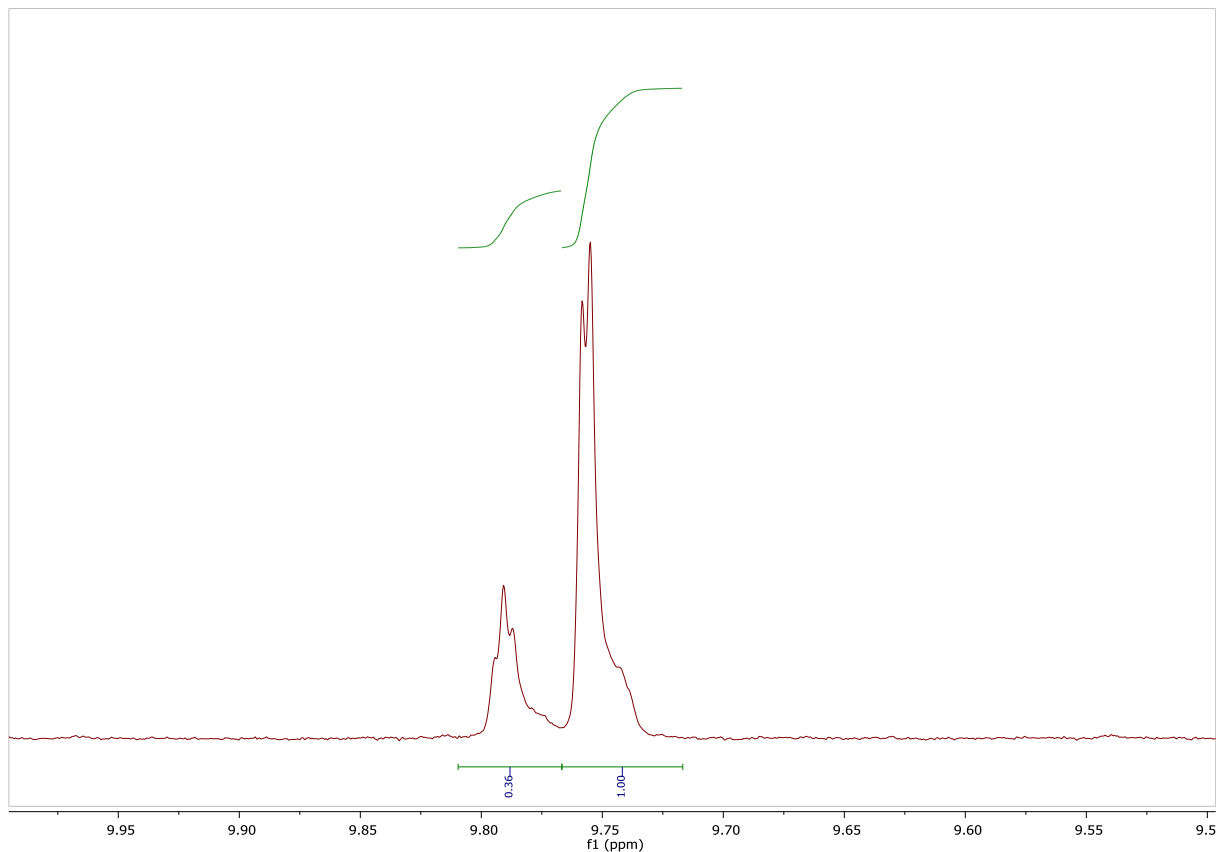
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



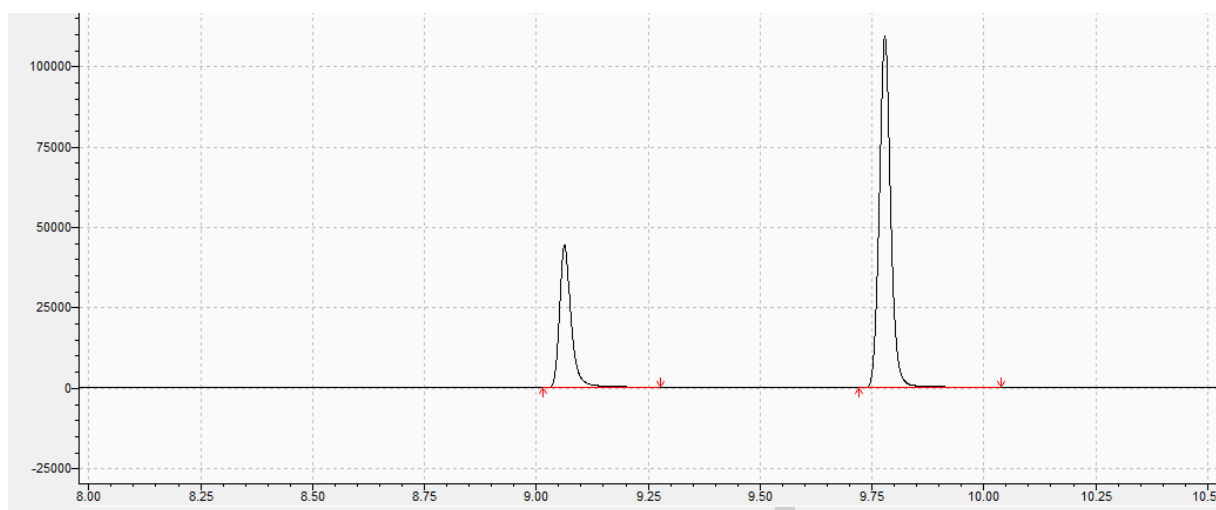
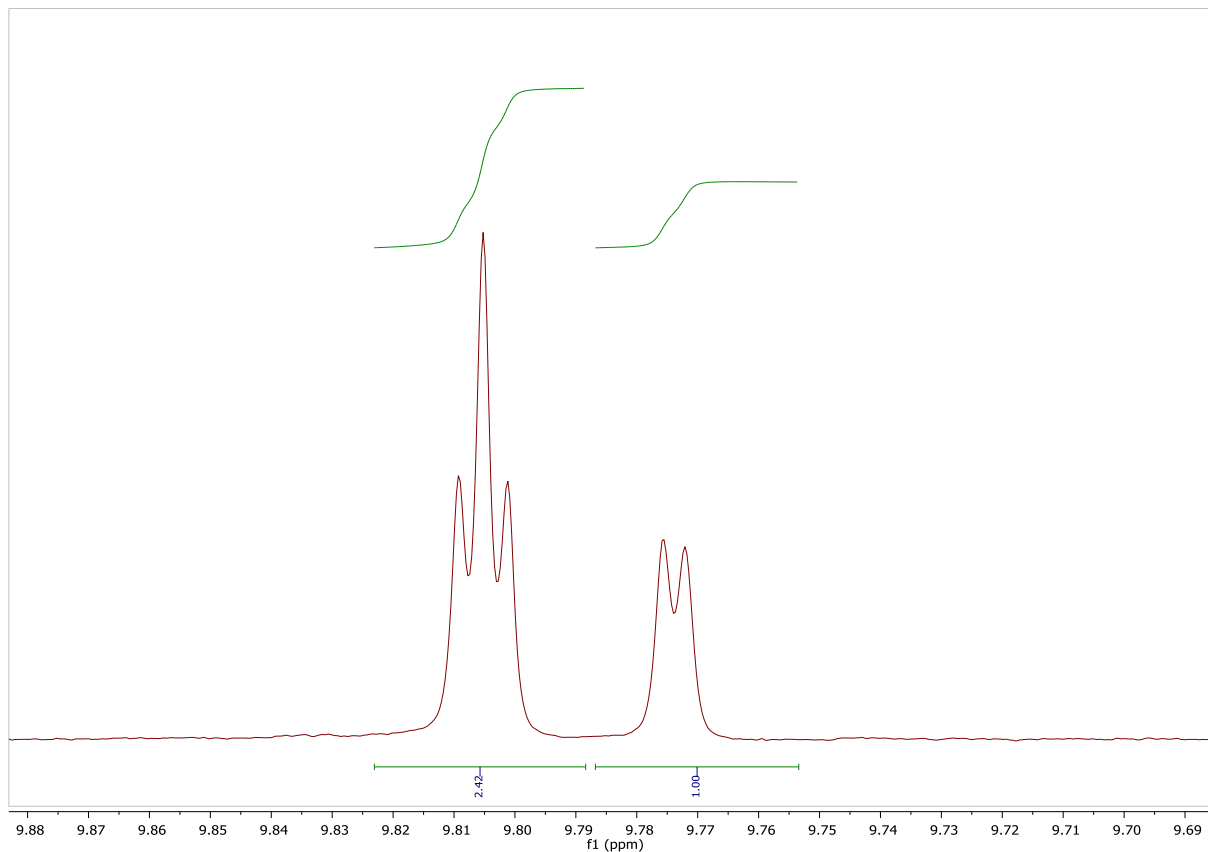
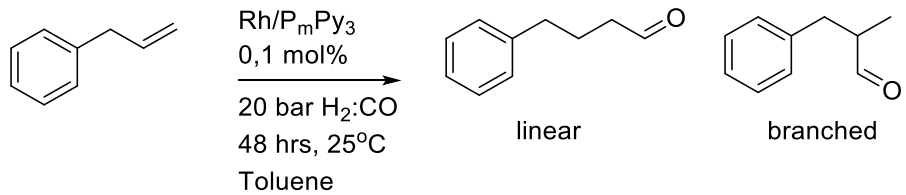
linear



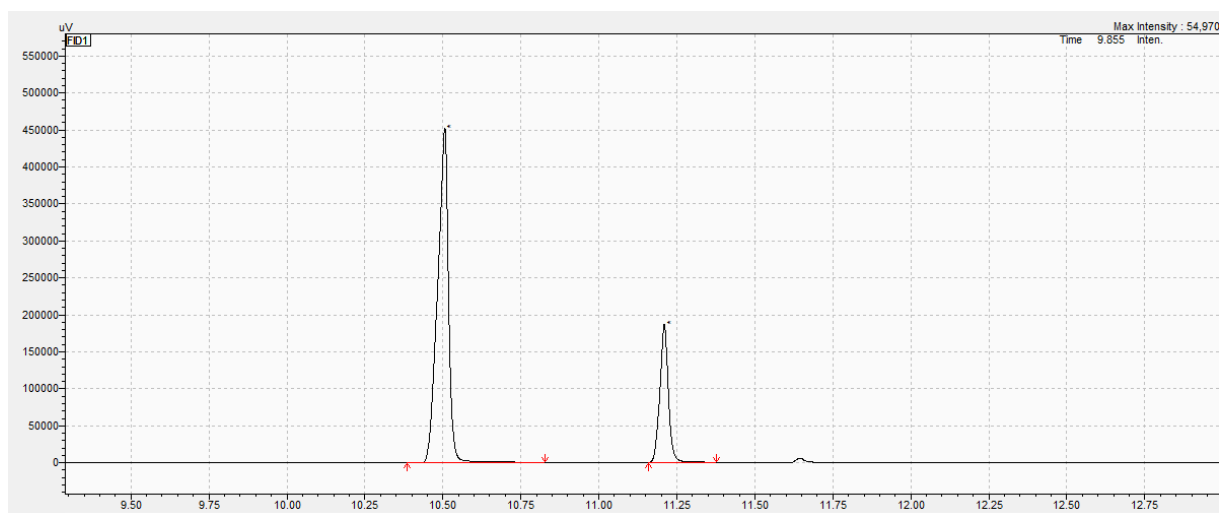
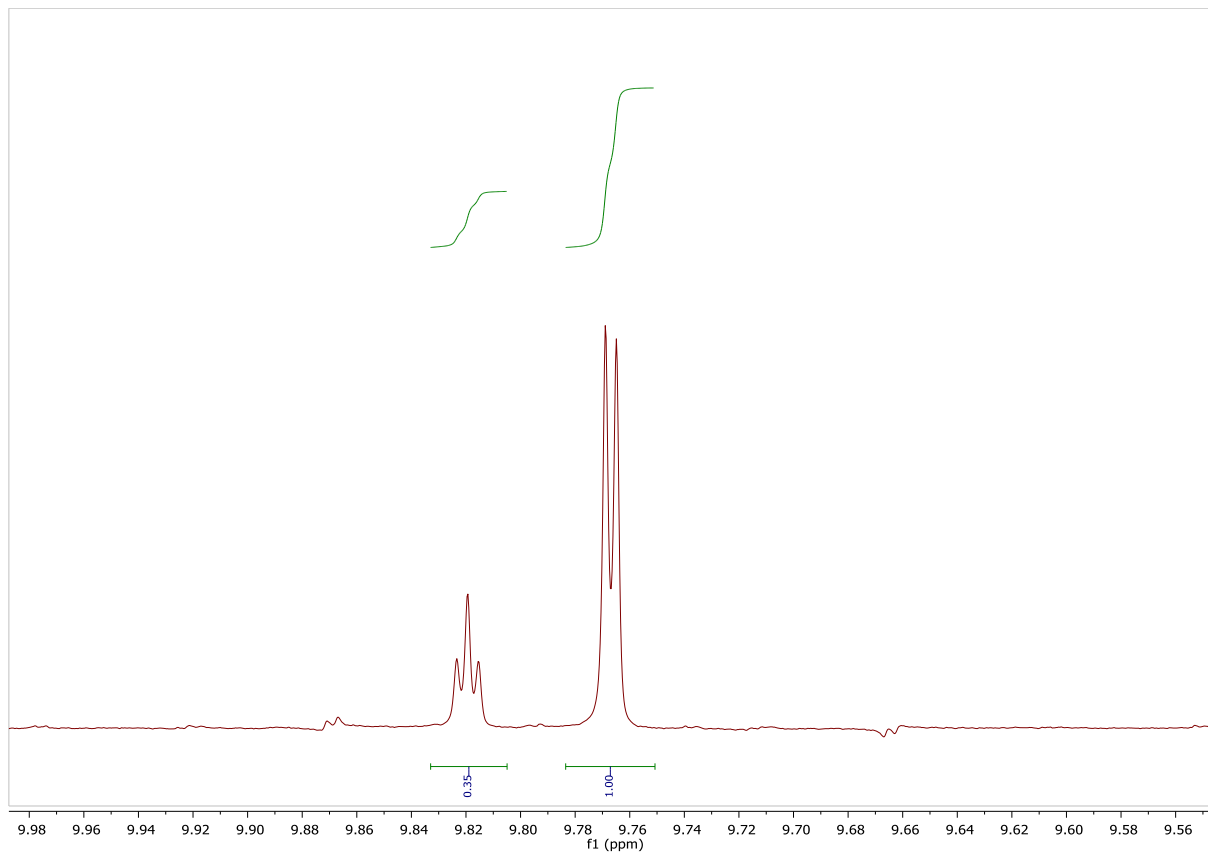
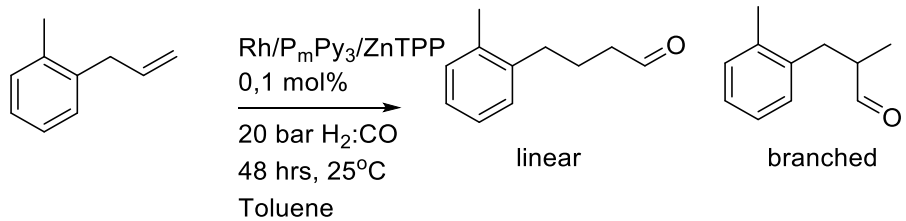
branched



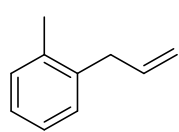
Retention time	Area		l/b ratio
5,142	933705	Branched	0,32
5,384	301168	Linear	



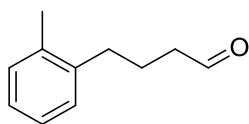
Retention time	area		I/b ratio
9,063	80319	Branched	2,39
9,779	192015	linear	



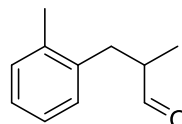
Retention time	area		l/b ratio
10.506	1090548	Branched	0.32
11.210	353117	linear	



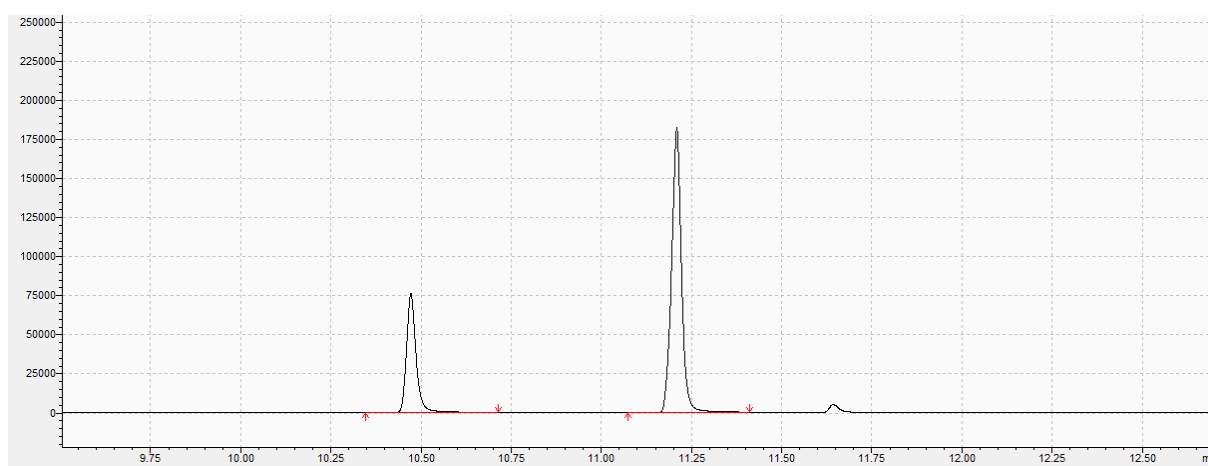
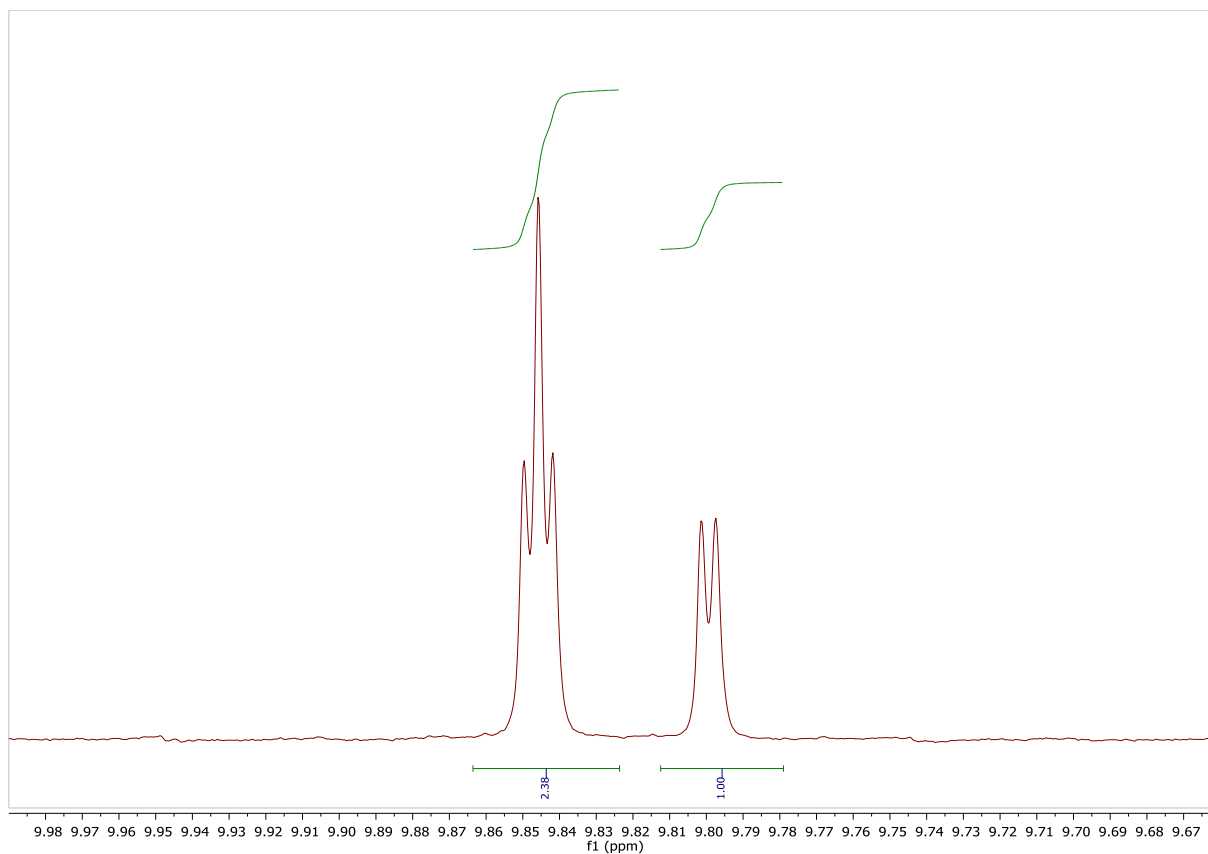
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



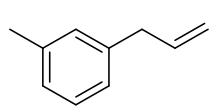
linear



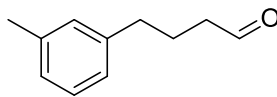
branched



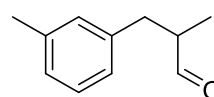
Retention time	area		l/b ratio
10.472	140662	Branched	2.46
11.209	346380	linear	



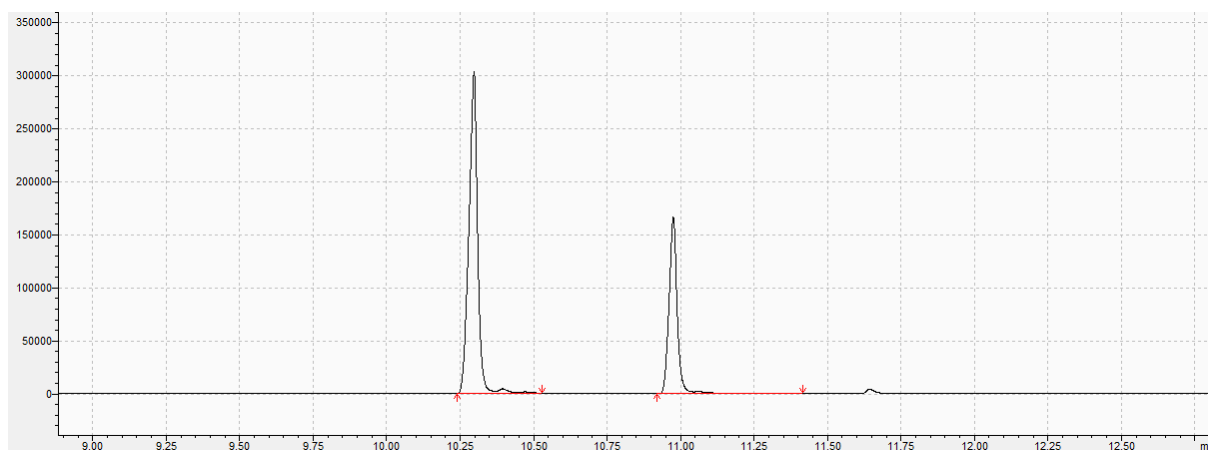
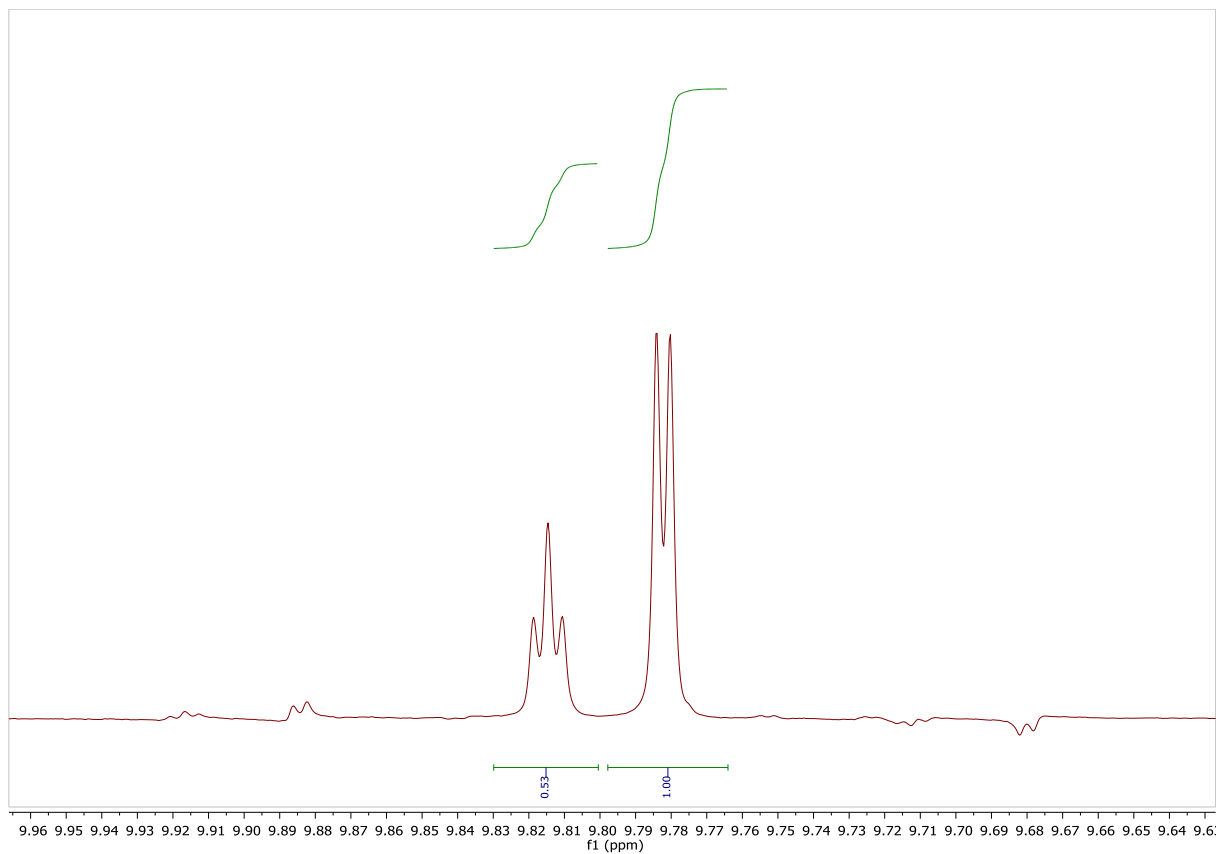
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



linear

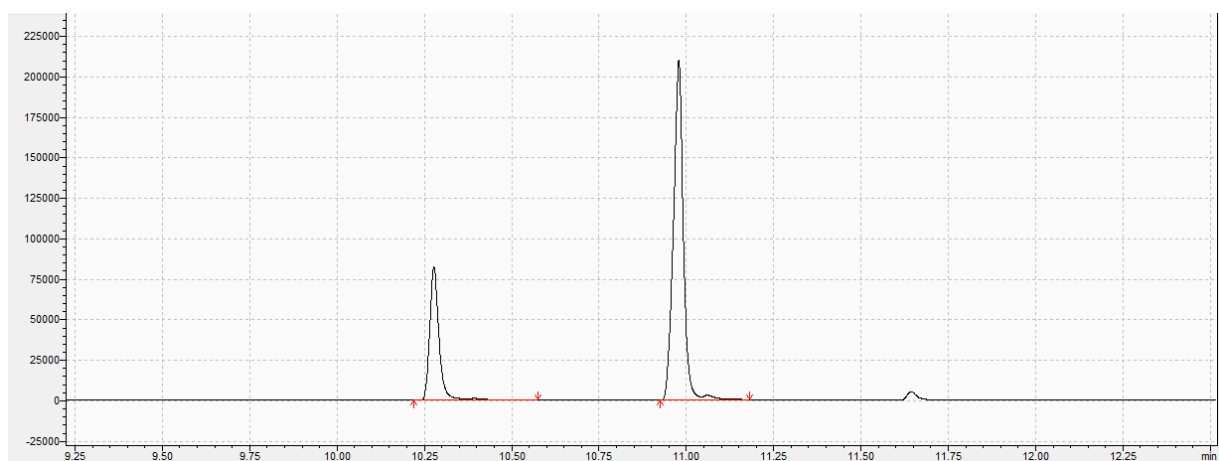
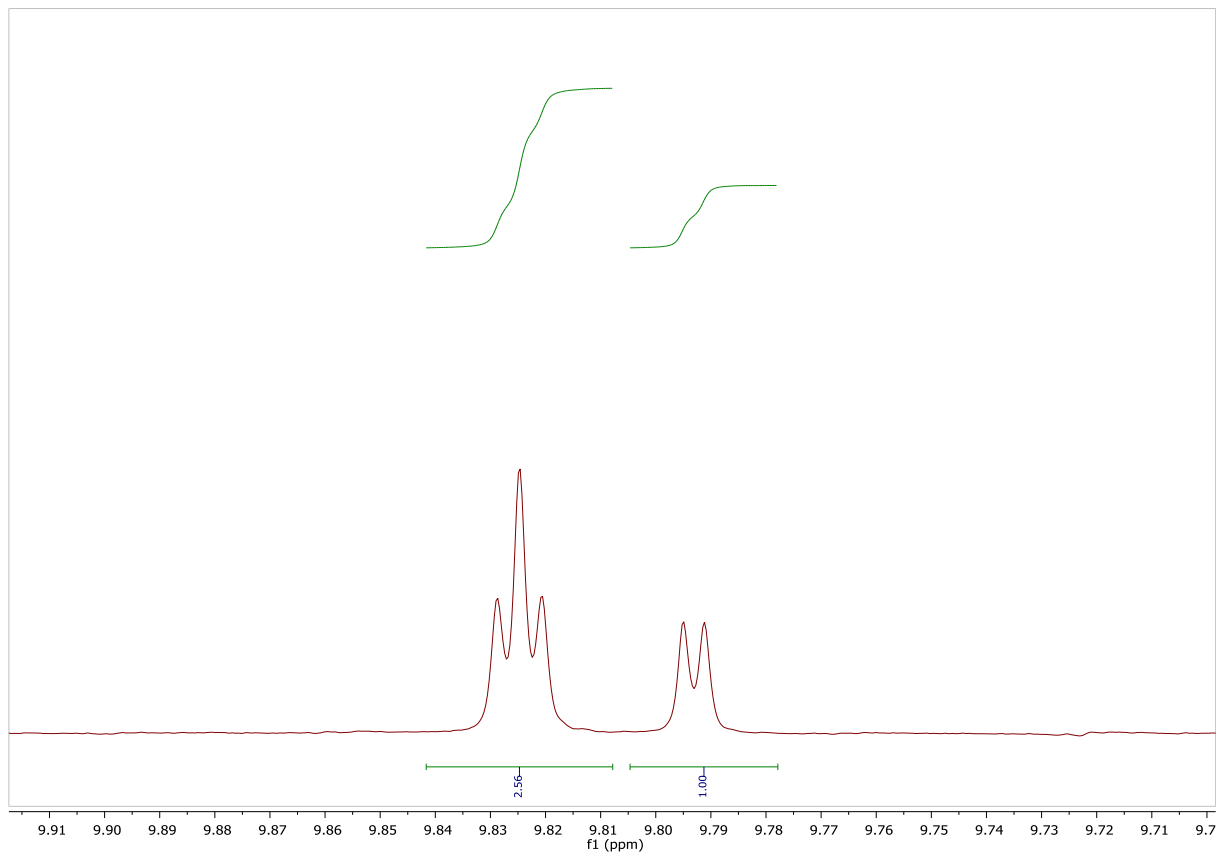
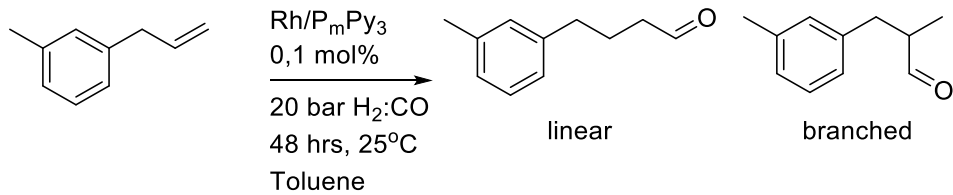


branched

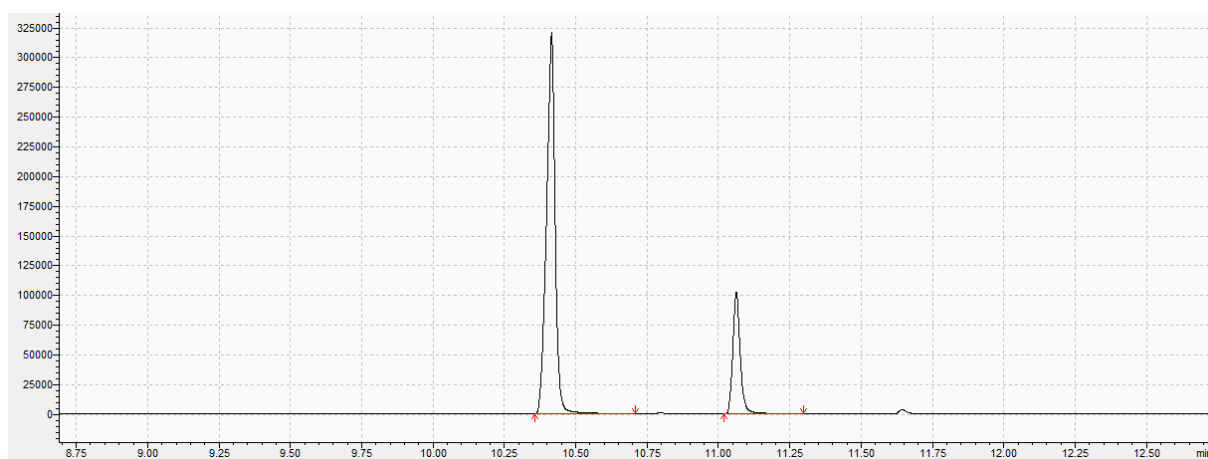
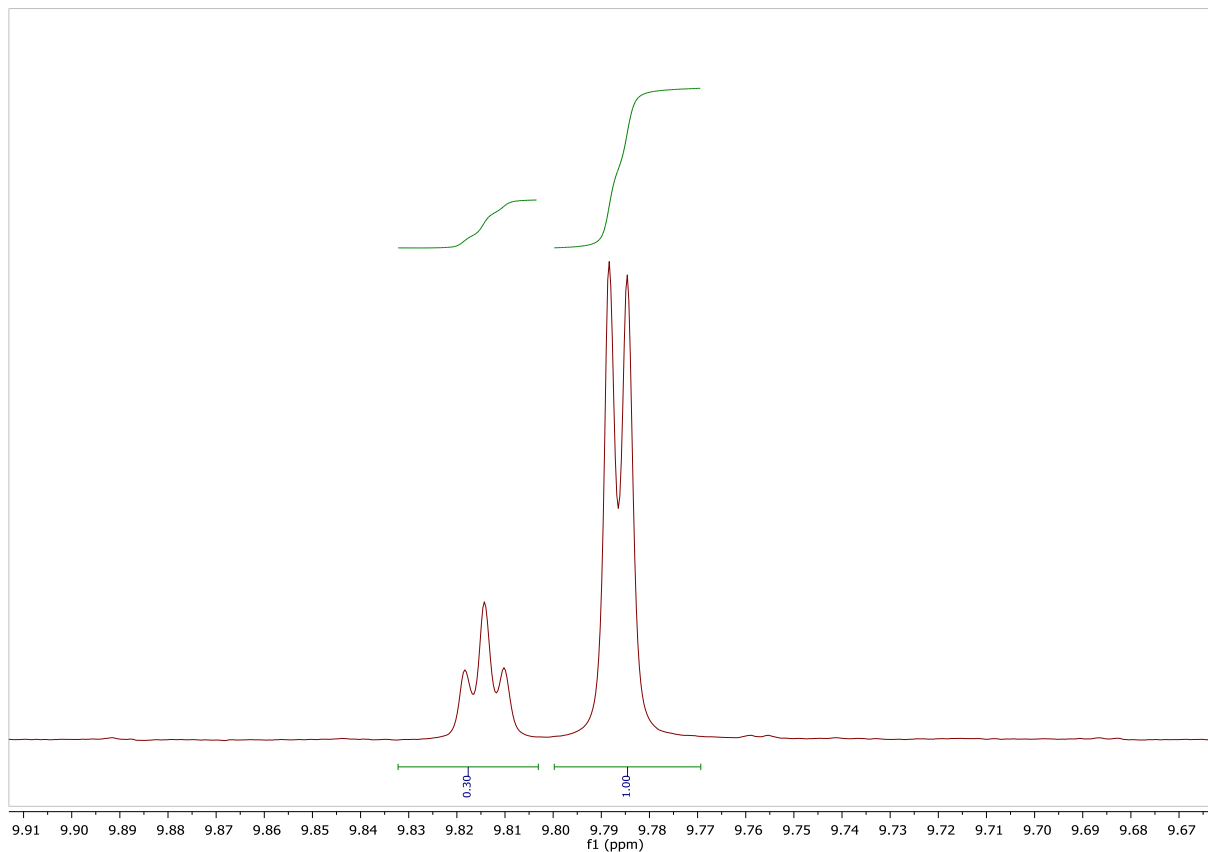
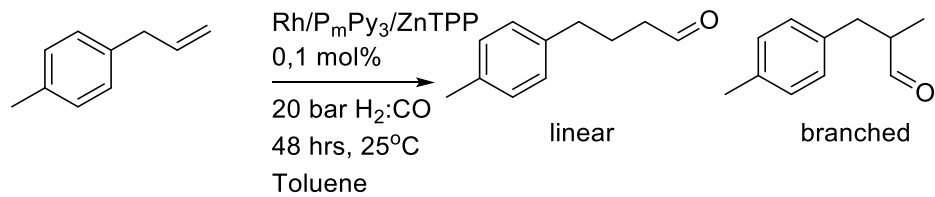


Retention time	area		l/b ratio
10.297	631686	Branched	0.50
10.975	318492	linear	

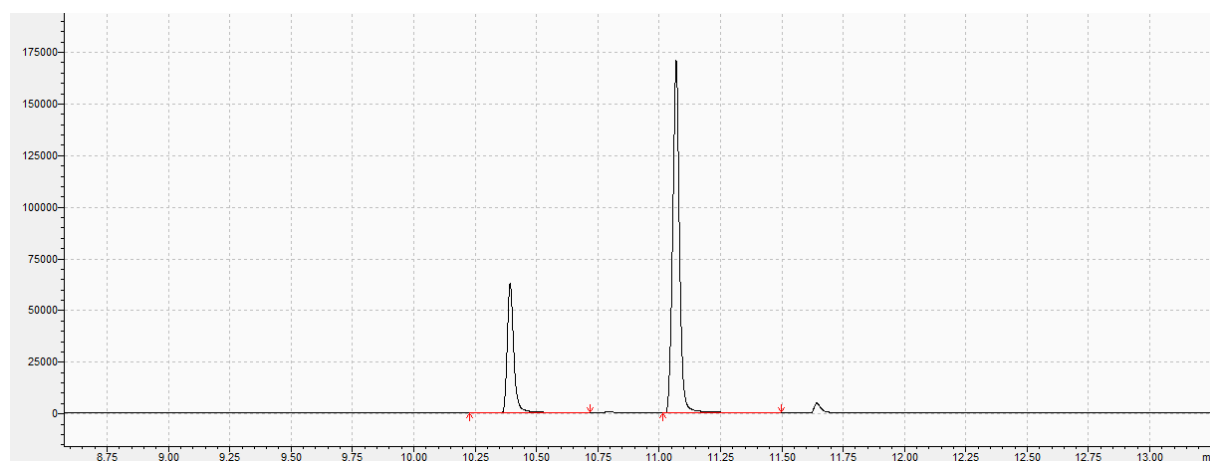
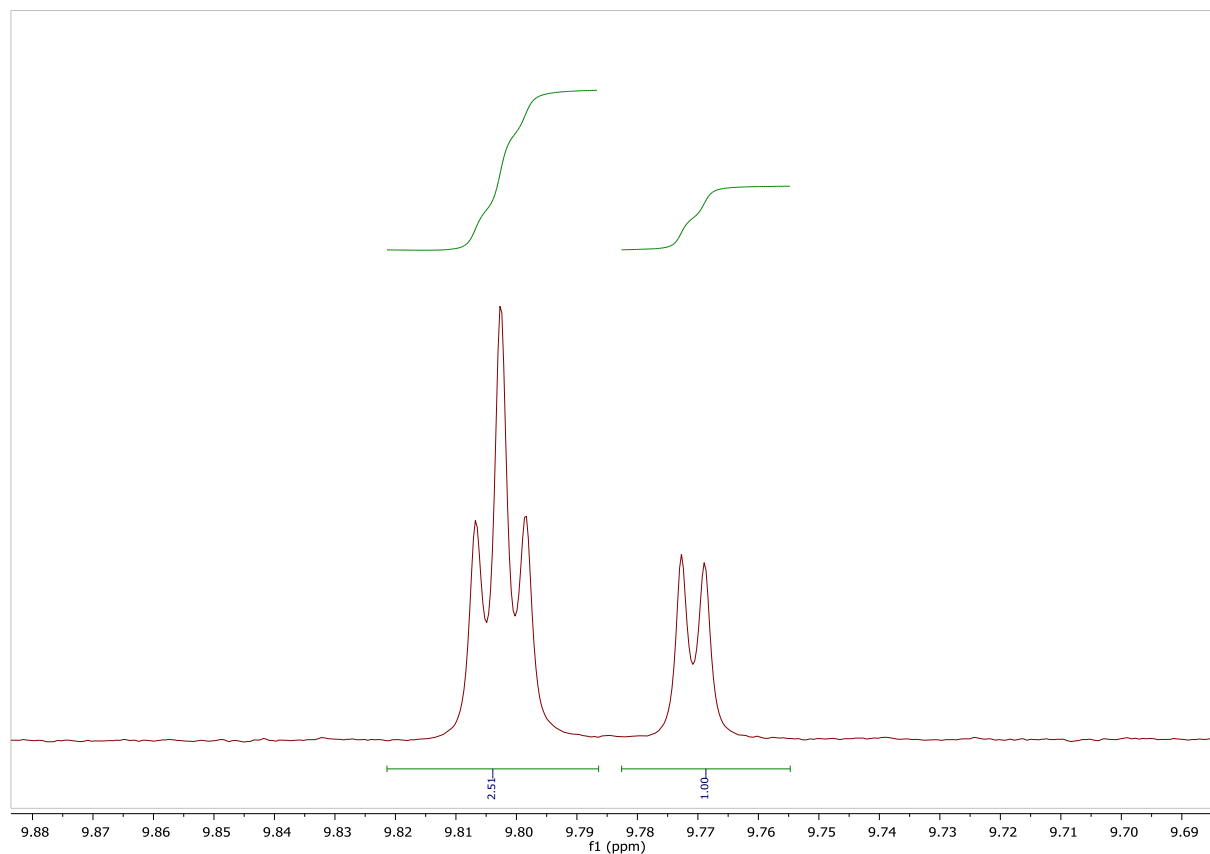
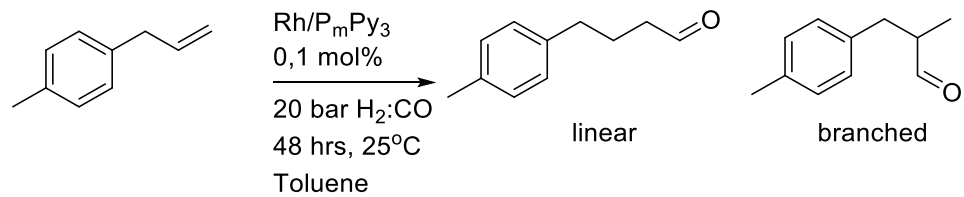




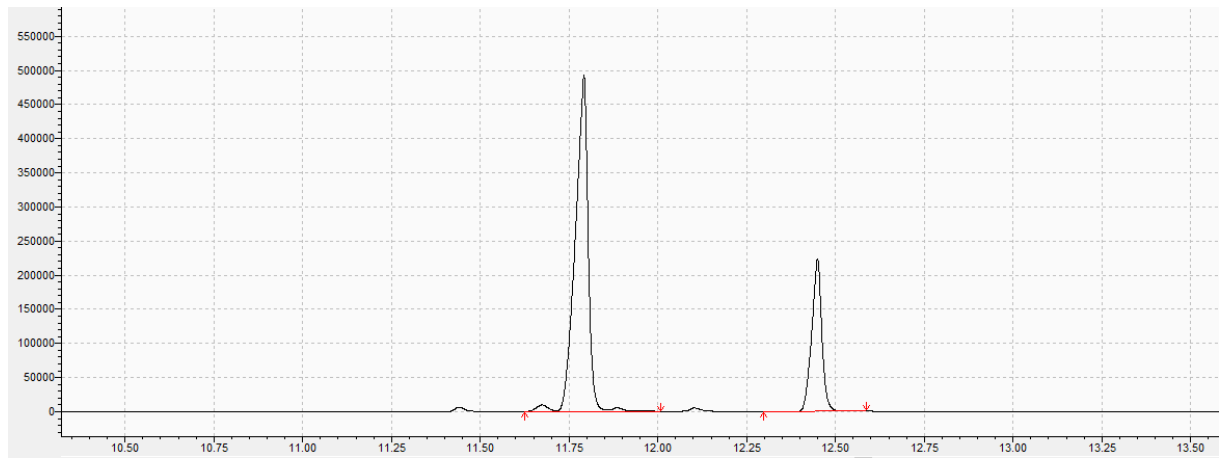
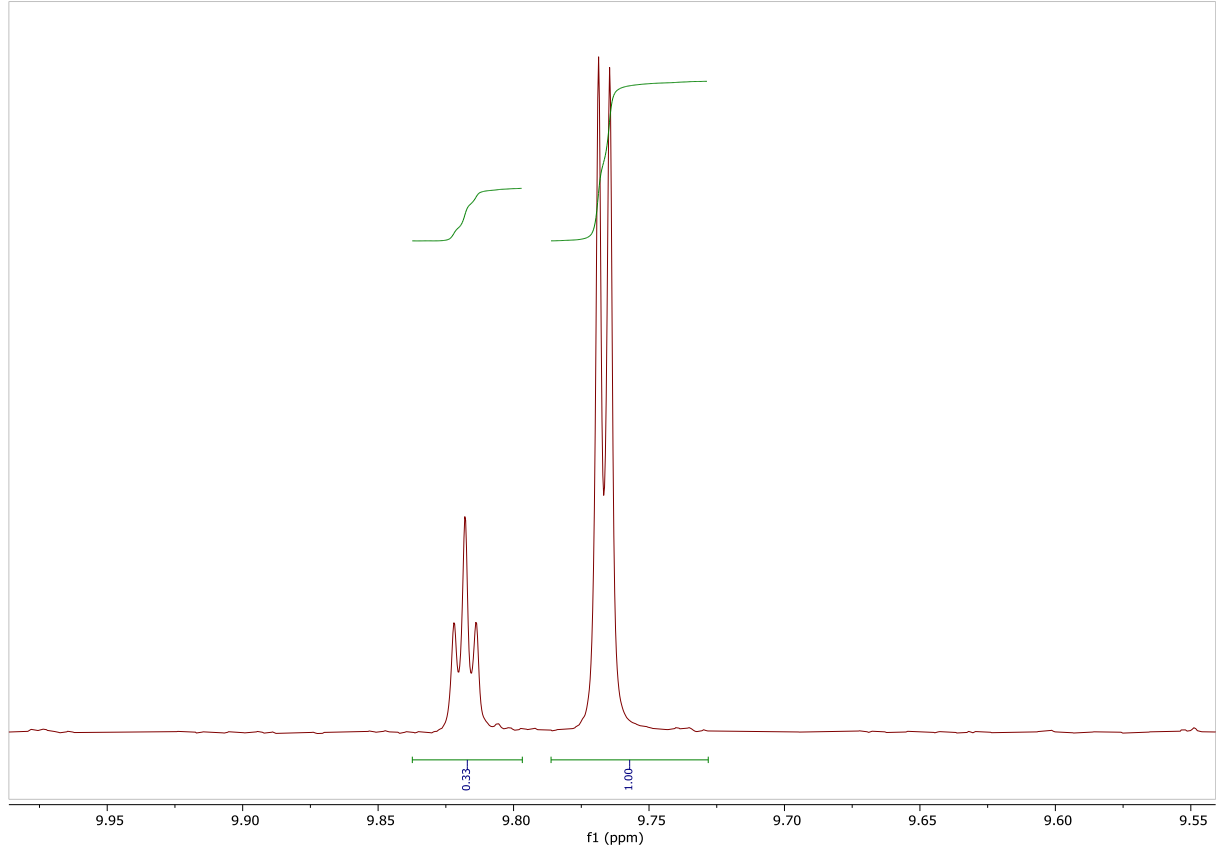
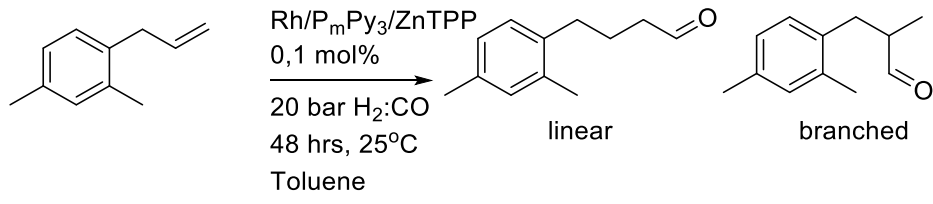
Retention time	area		l/b ratio
10.278	153913	Branched	2.72
10.978	419454	linear	



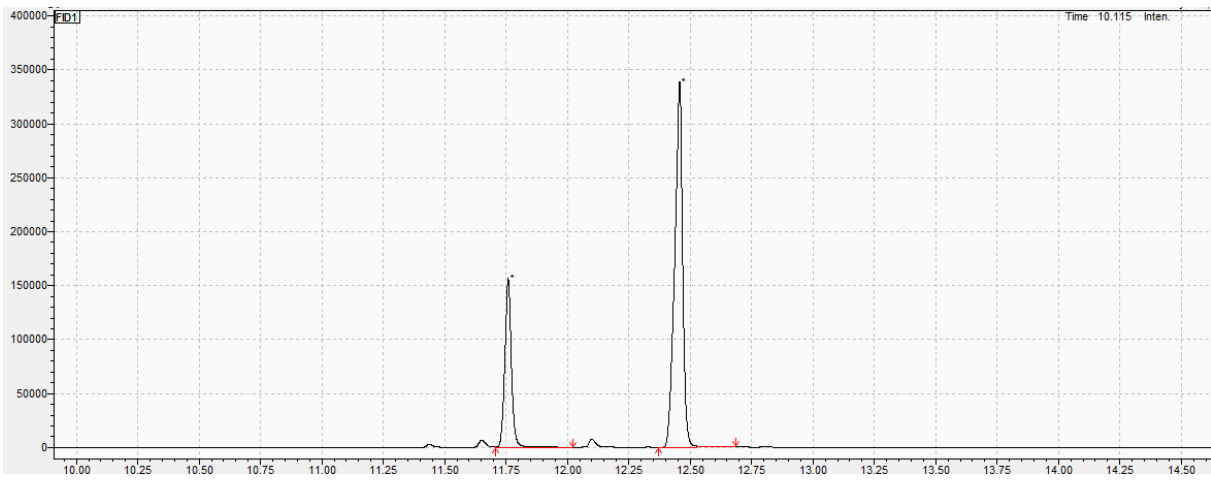
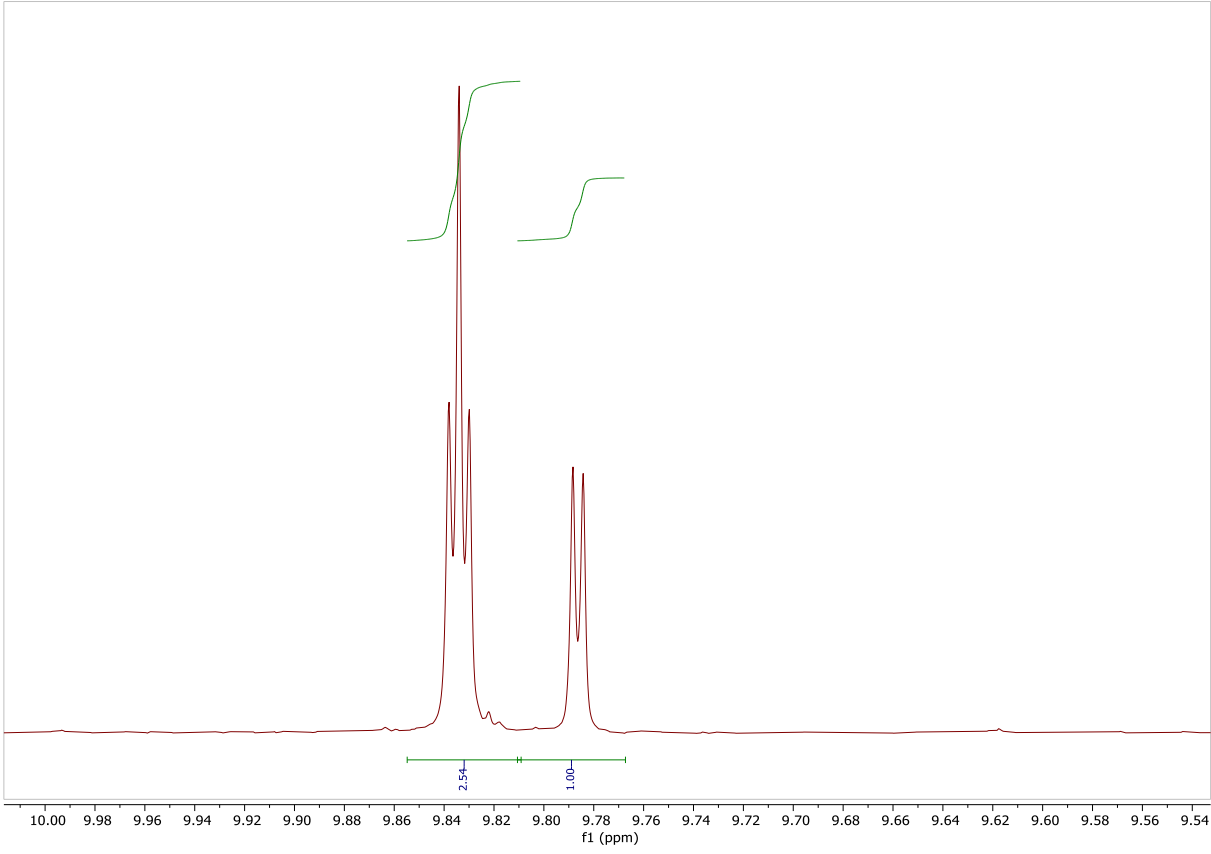
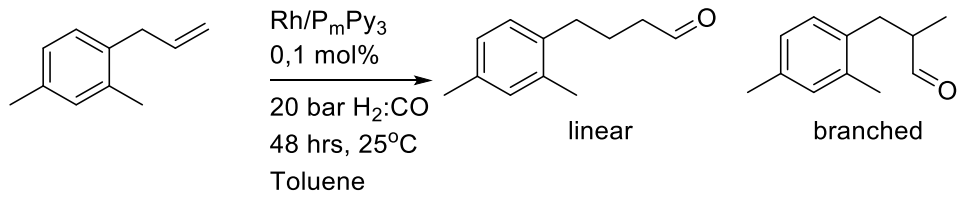
Retention time	area		l/b ratio
10.415	673871	Branched	0.27
11.063	184421	linear	



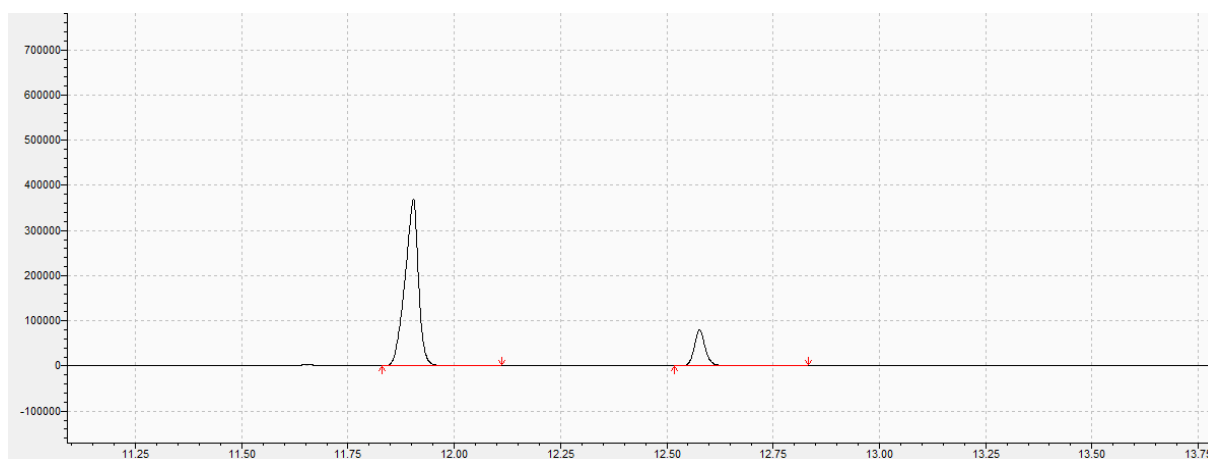
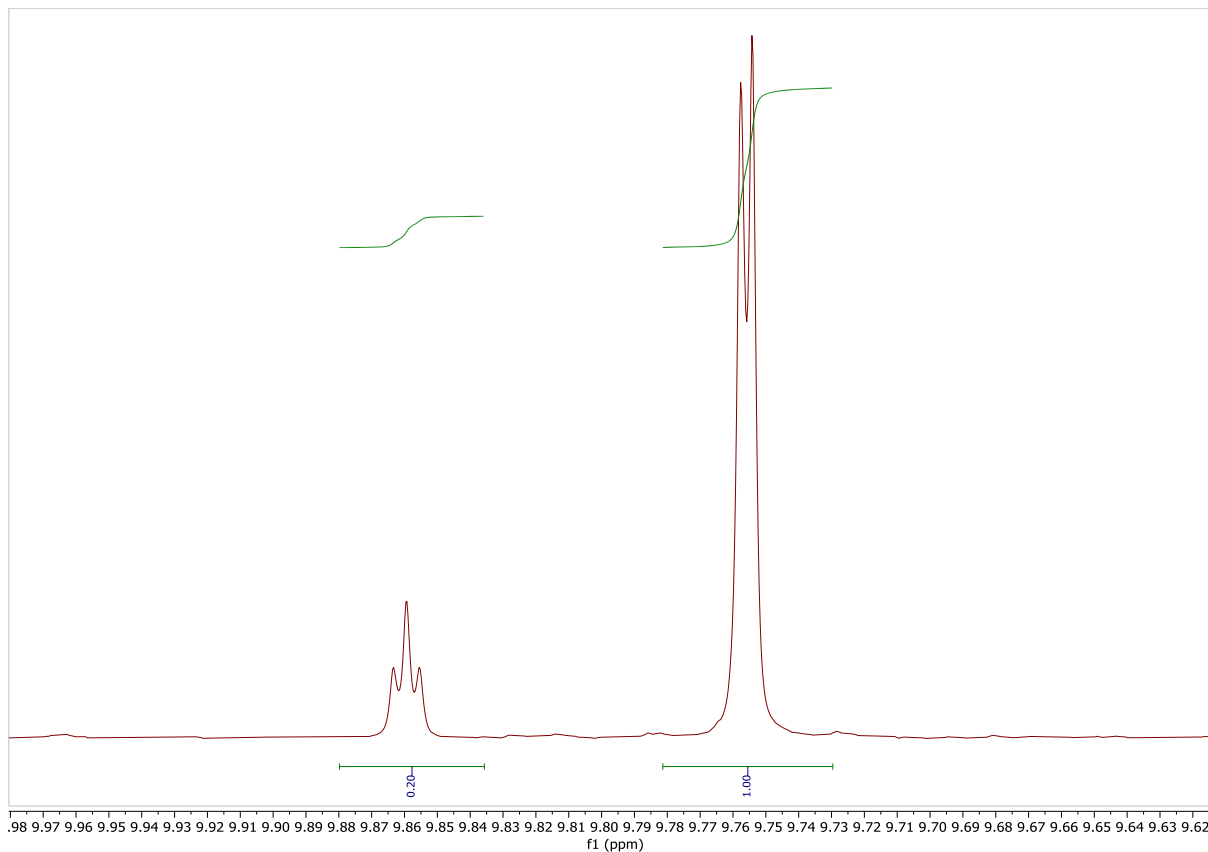
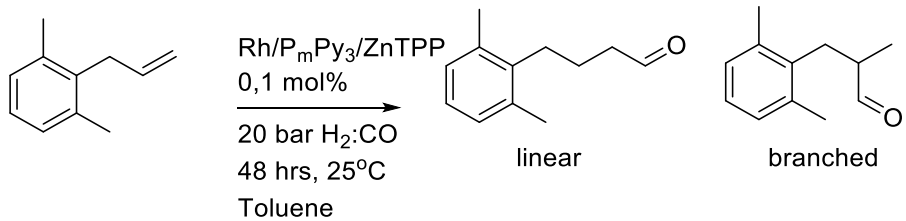
Retention time	area		l/b ratio
10.393	117082	Branched	2.79
11.069	327655	linear	



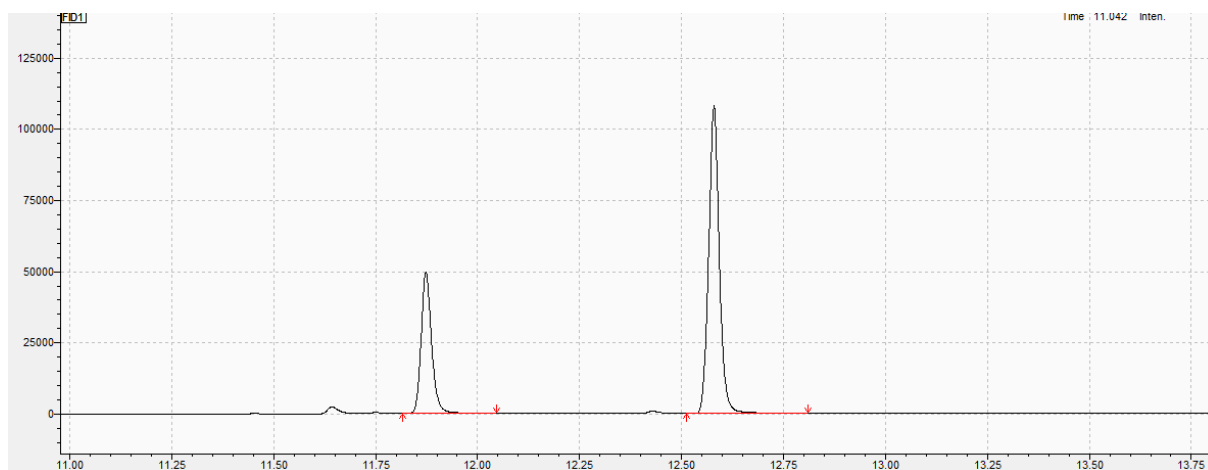
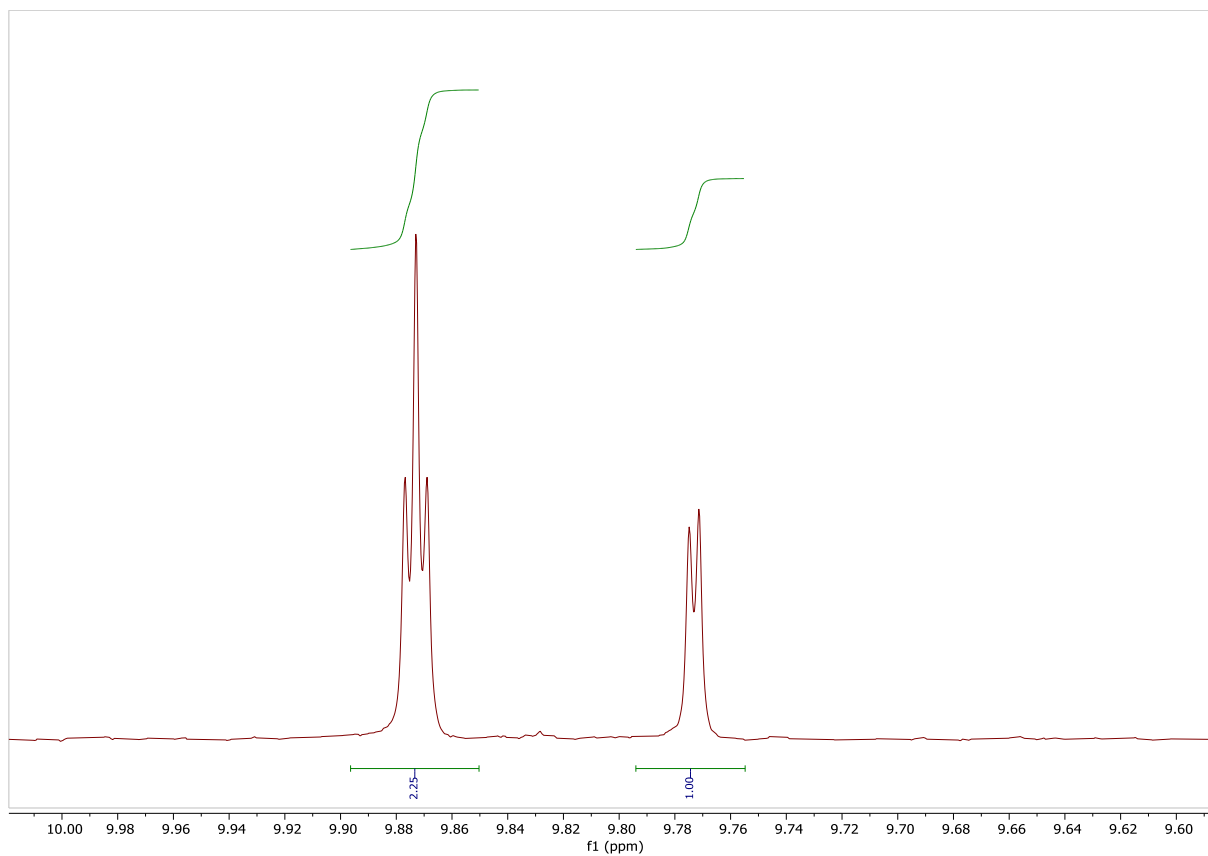
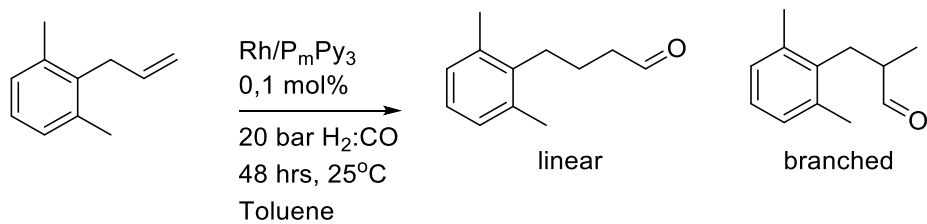
Retention time	area		l/b ratio
11.791	1254642	Branched	0.34
12.449	437058	linear	



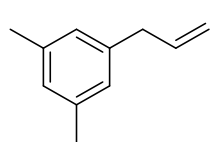
Retention time	area		I/b ratio
11.759	289522	Branched	2.61
12.457	757073	linear	



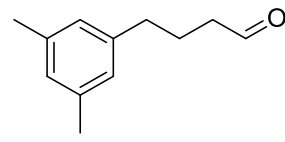
Retention time	area		I/b ratio
11.903	815456	Branched	0.18
12.577	143108	linear	



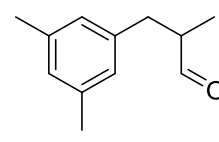
Retention time	area		I/b ratio
11.873	88791	Branched	2.20
12.580	195099	linear	



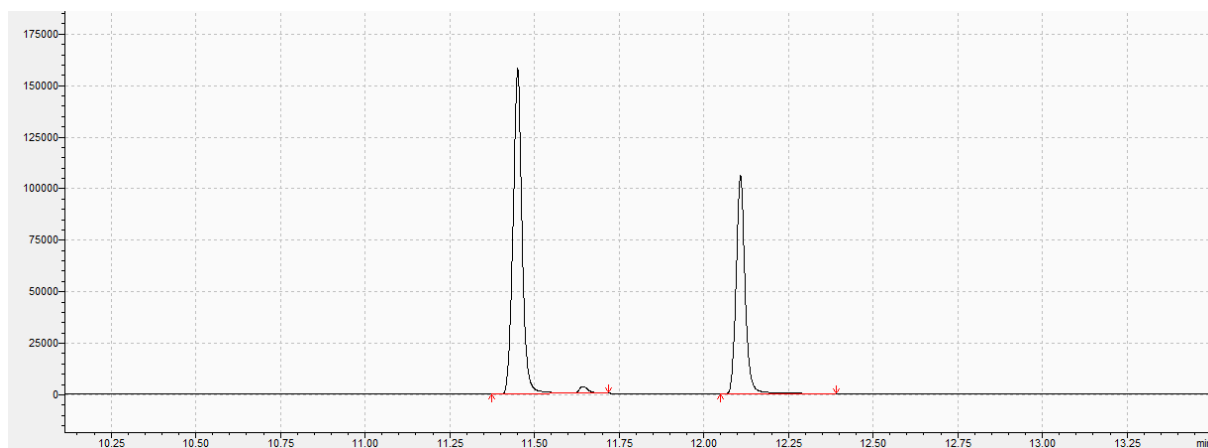
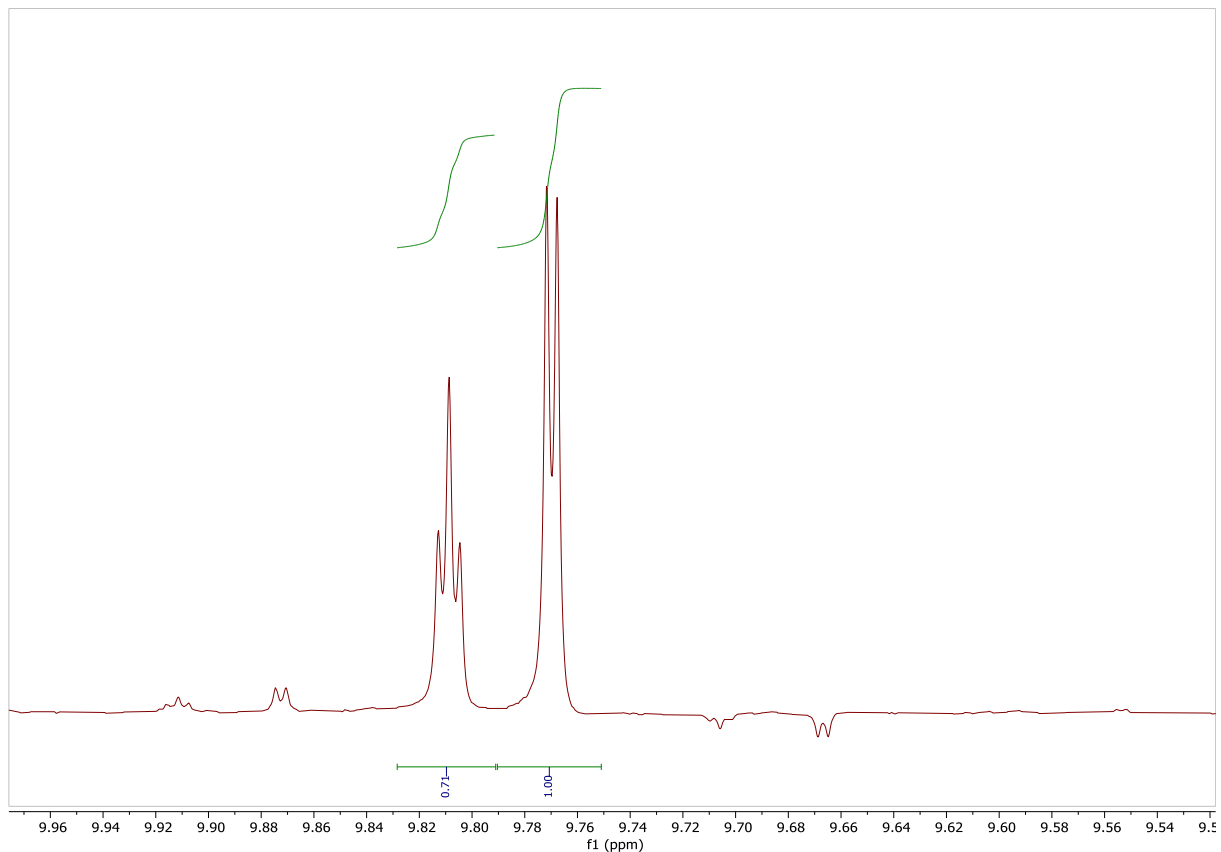
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



linear

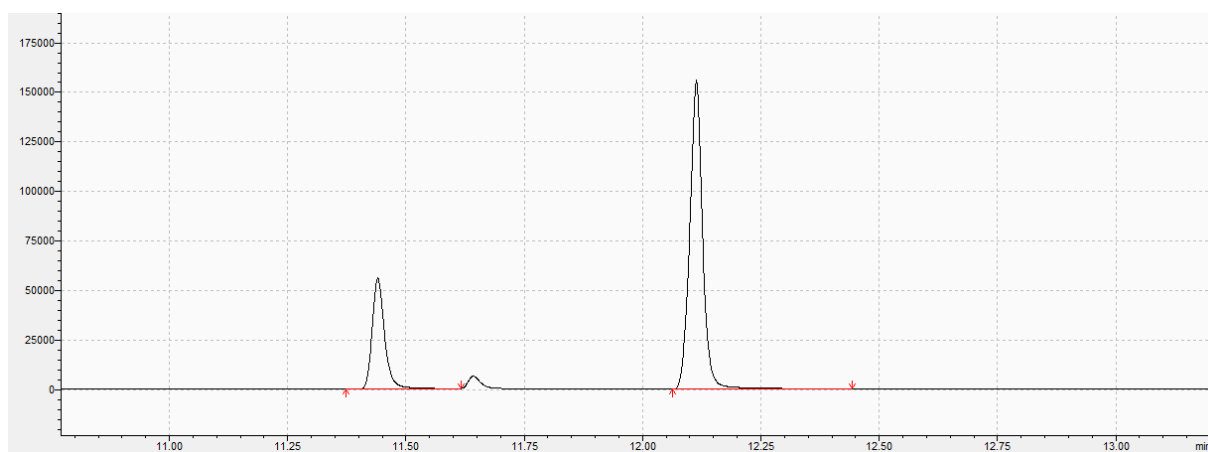
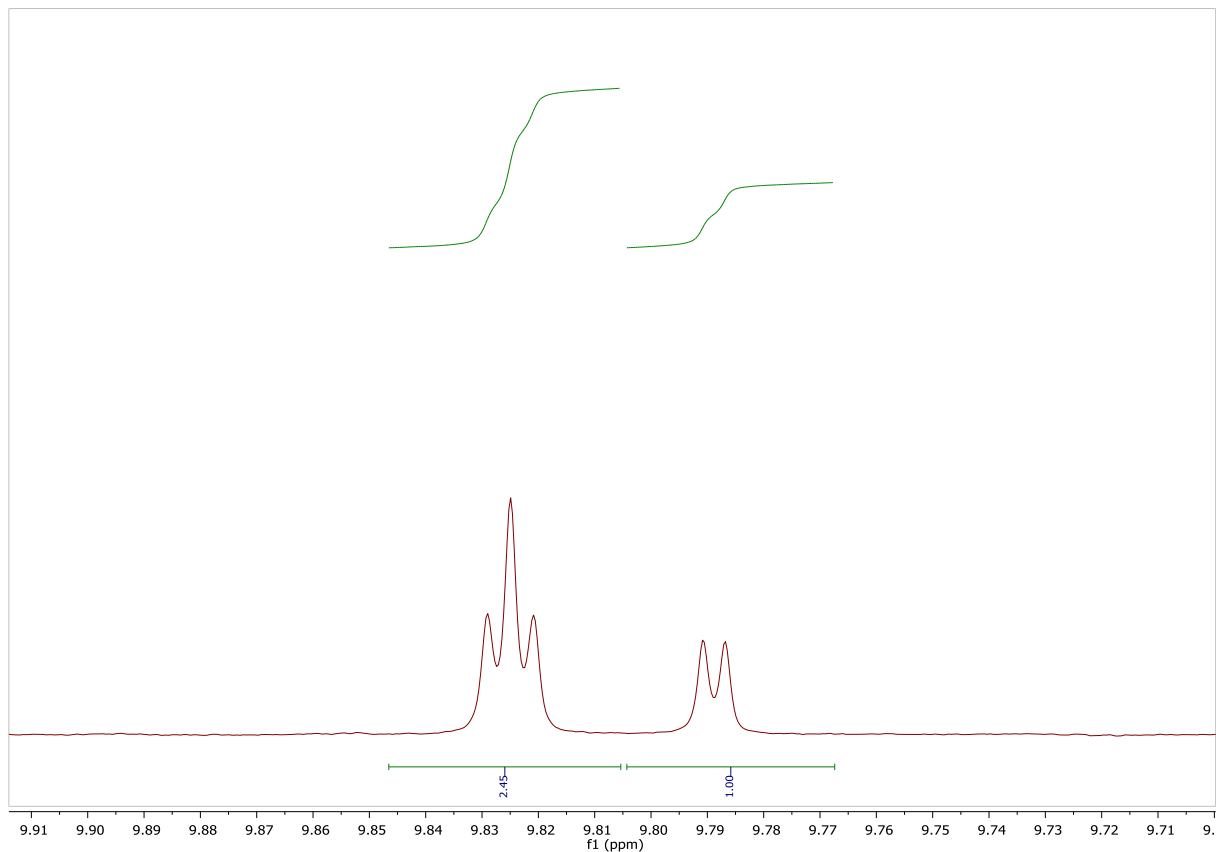
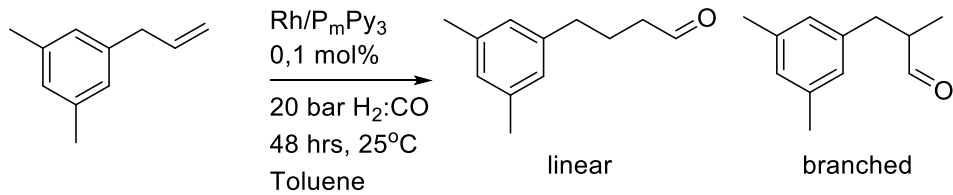


branched

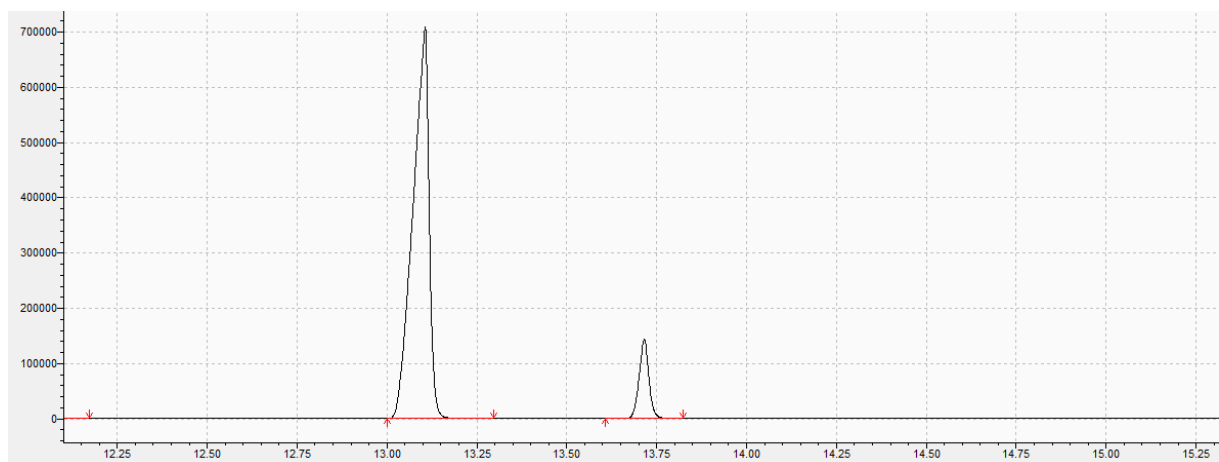
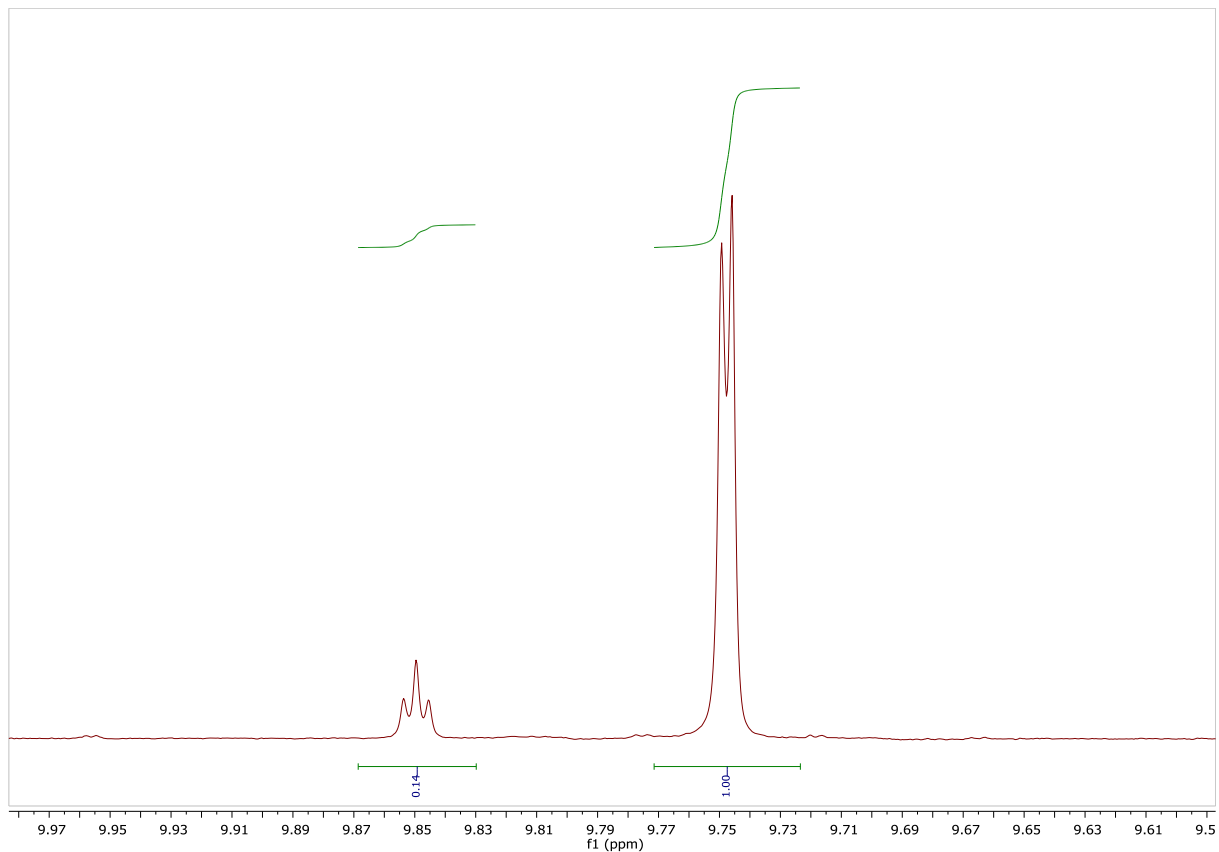
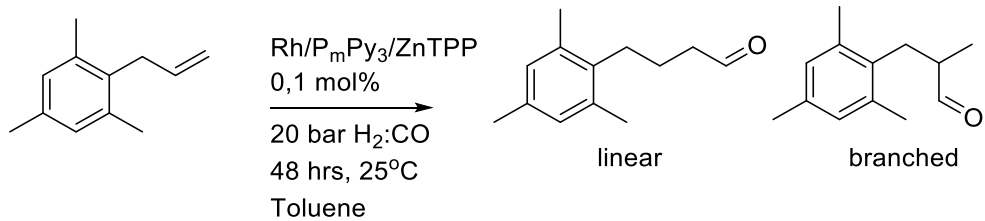


Retention time	area		I/b ratio
11.450	299423	Branched	0.64
12.108	193961	linear	

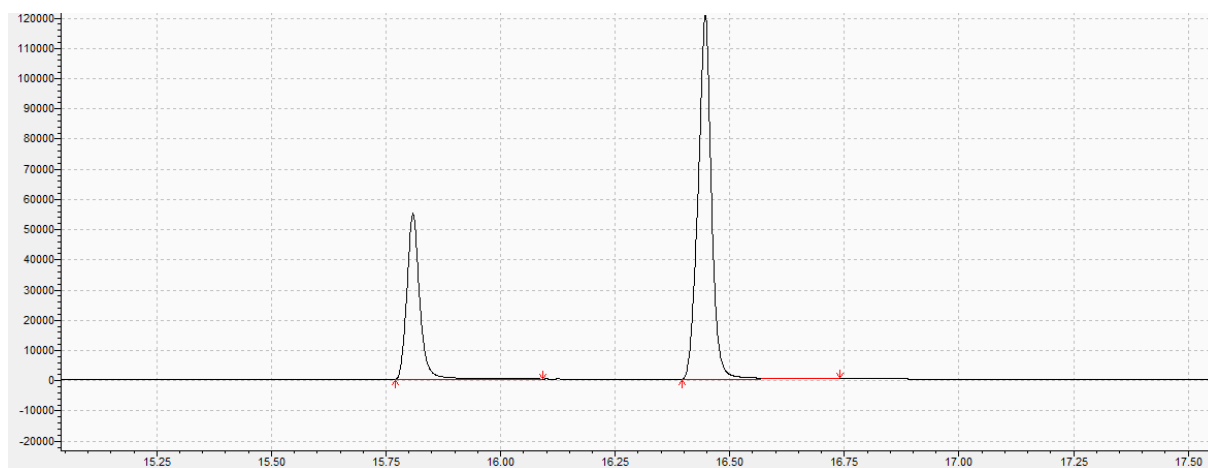
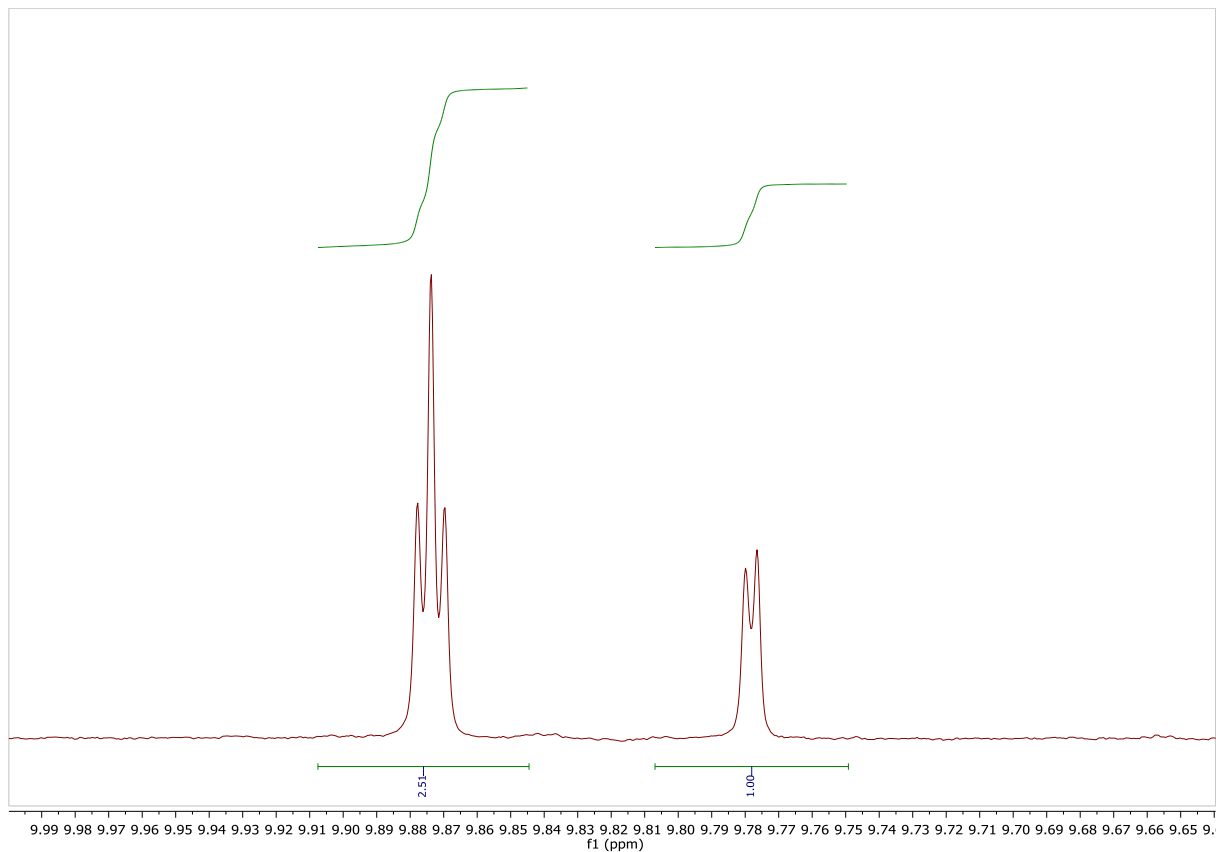
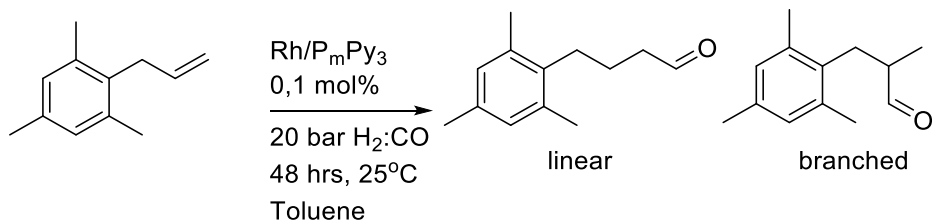




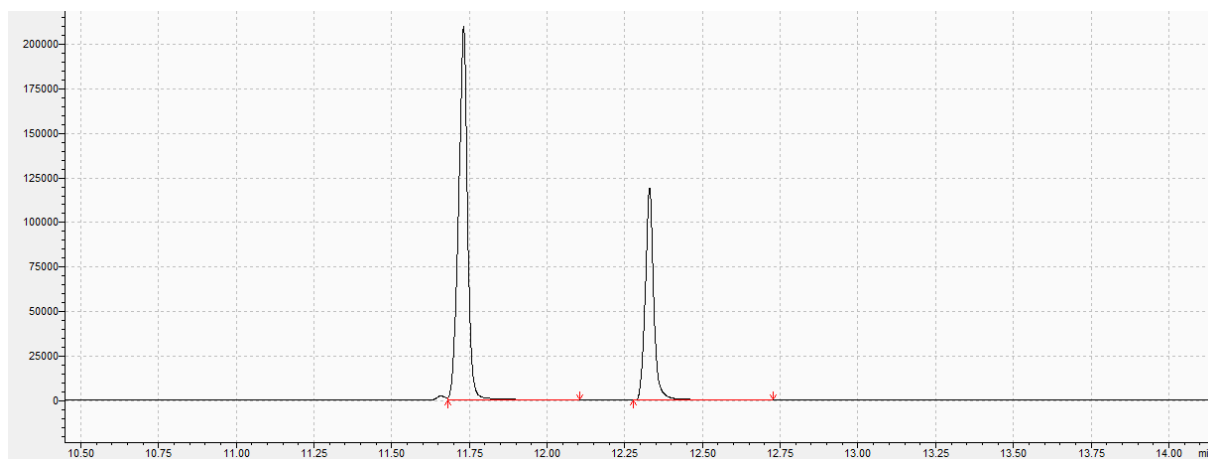
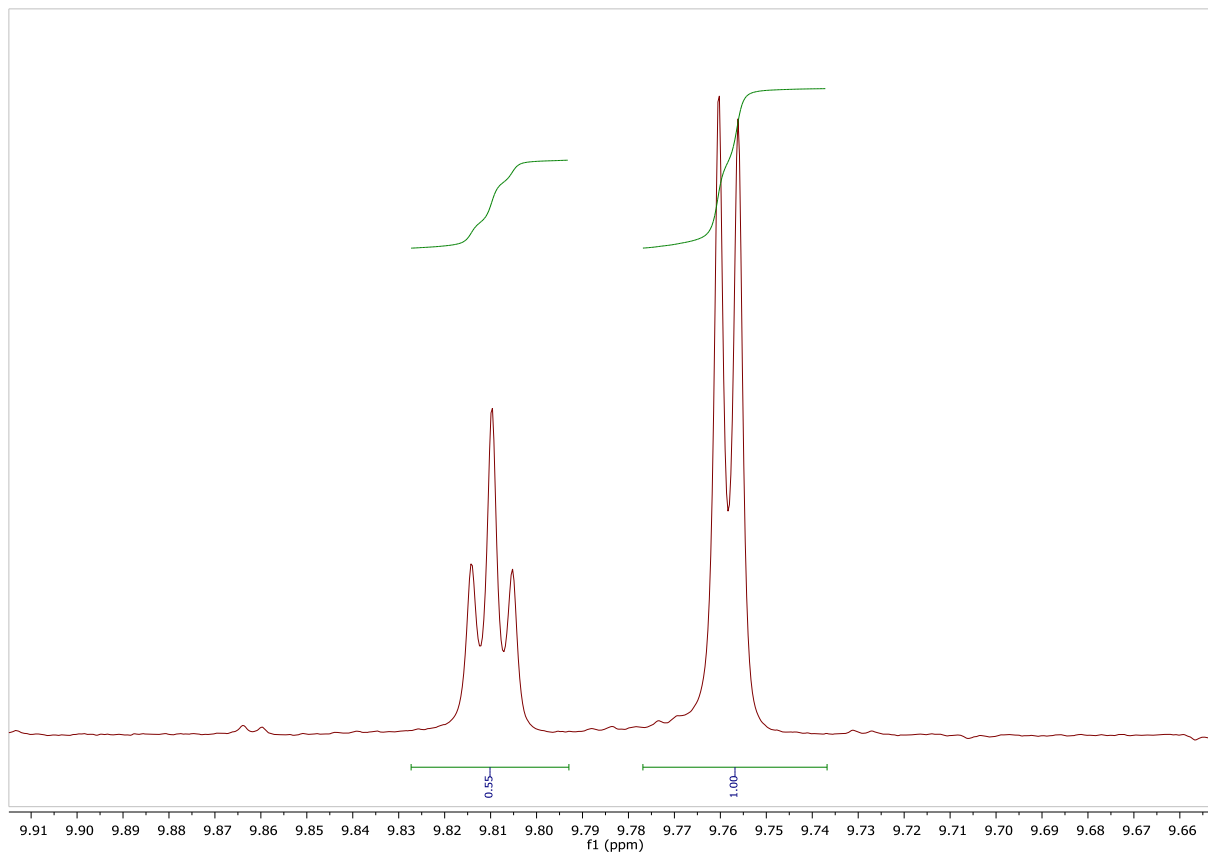
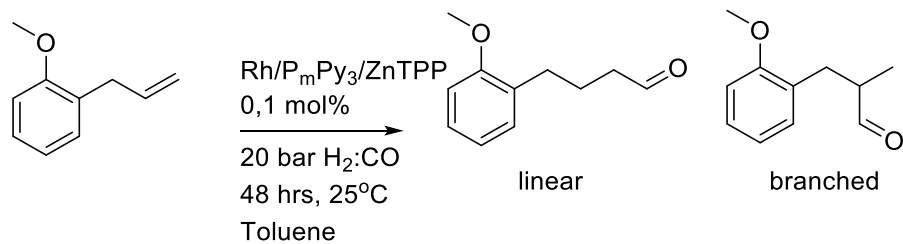
Retention time	area		l/b ratio
11.441	102230	Branched	2.87
12.114	293548	linear	



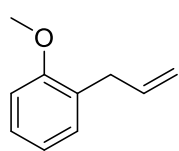
Retention time	Area		l/b ratio
13.105	2202113	Branched	0.12
13.716	268013	Linear	



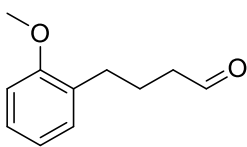
Retention time	Area		l/b ratio
13.045	132974	Branched	2.77
13.717	336991	Linear	



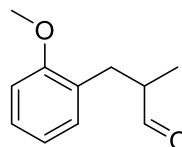
Retention time	area		l/b ratio
11.731	424279	Branched	0.53
12.329	225839	linear	



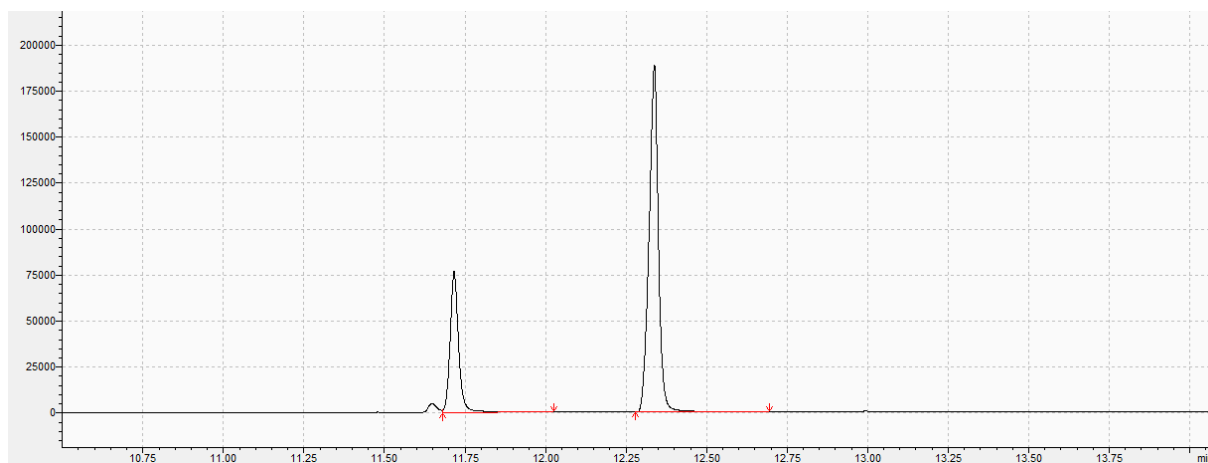
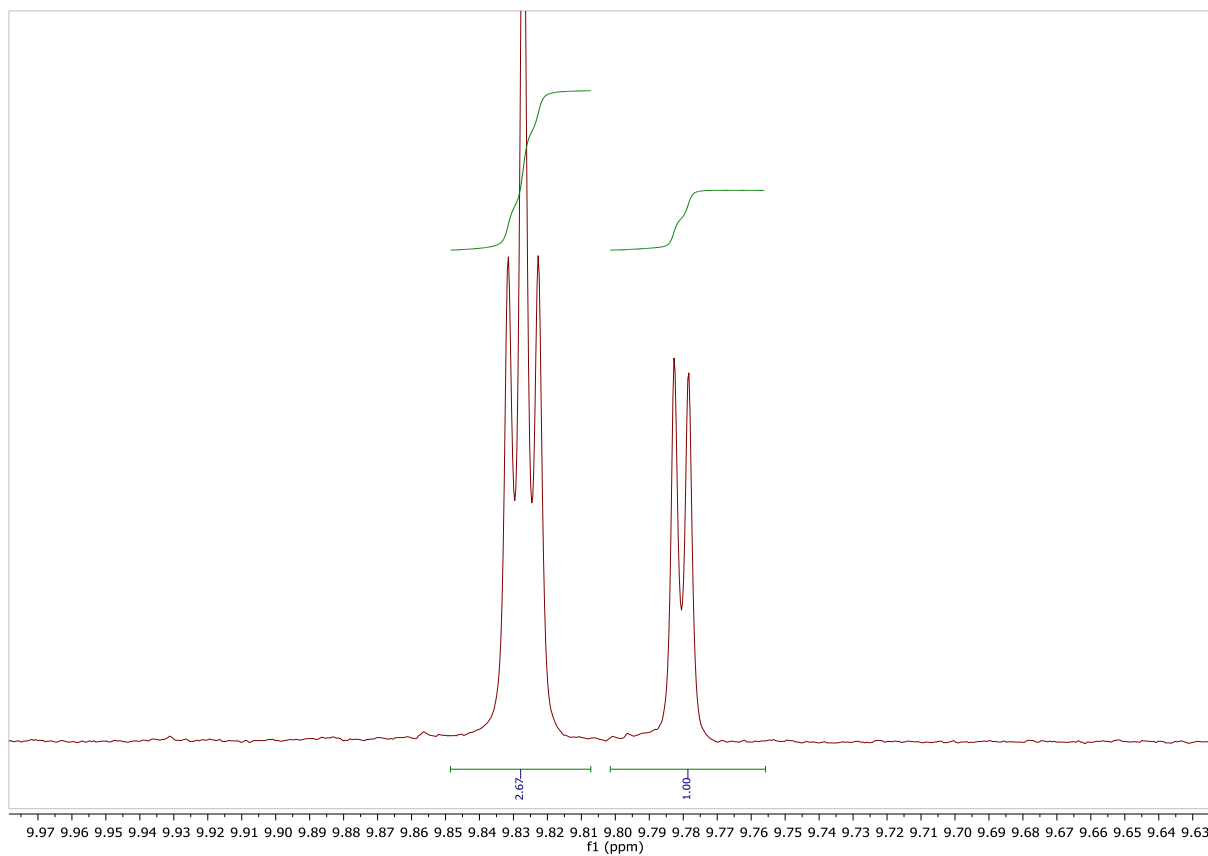
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



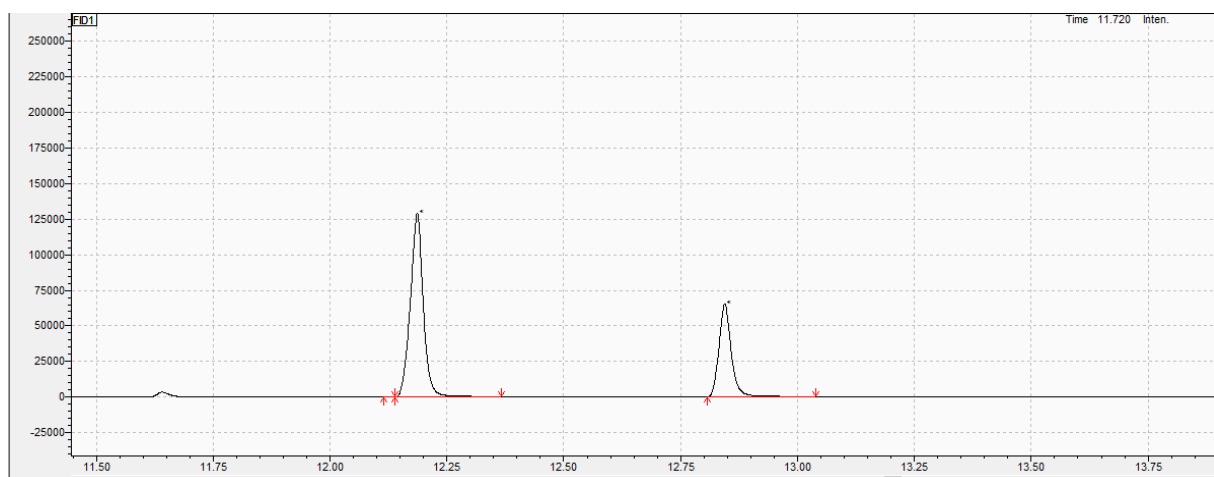
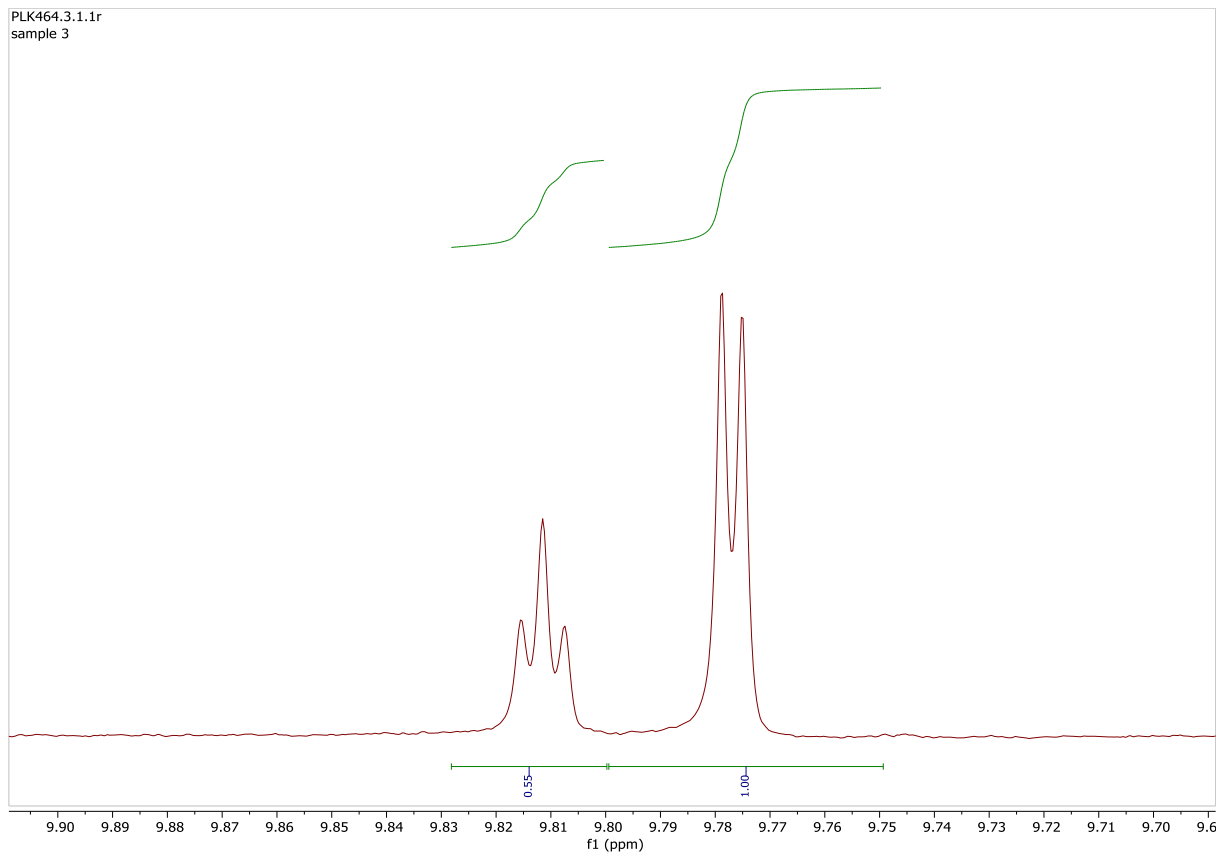
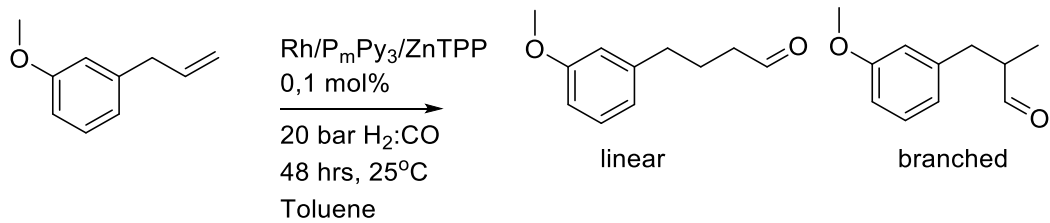
linear



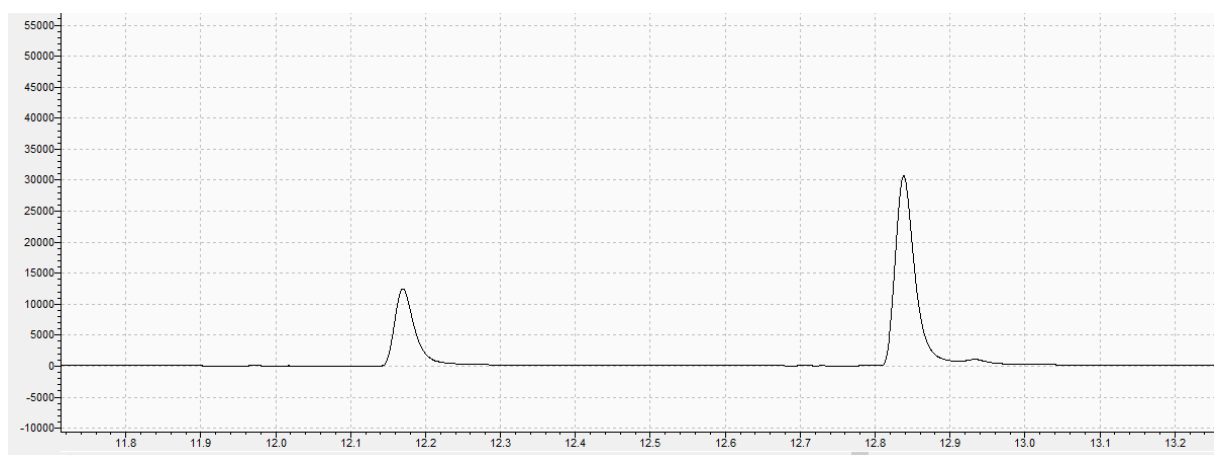
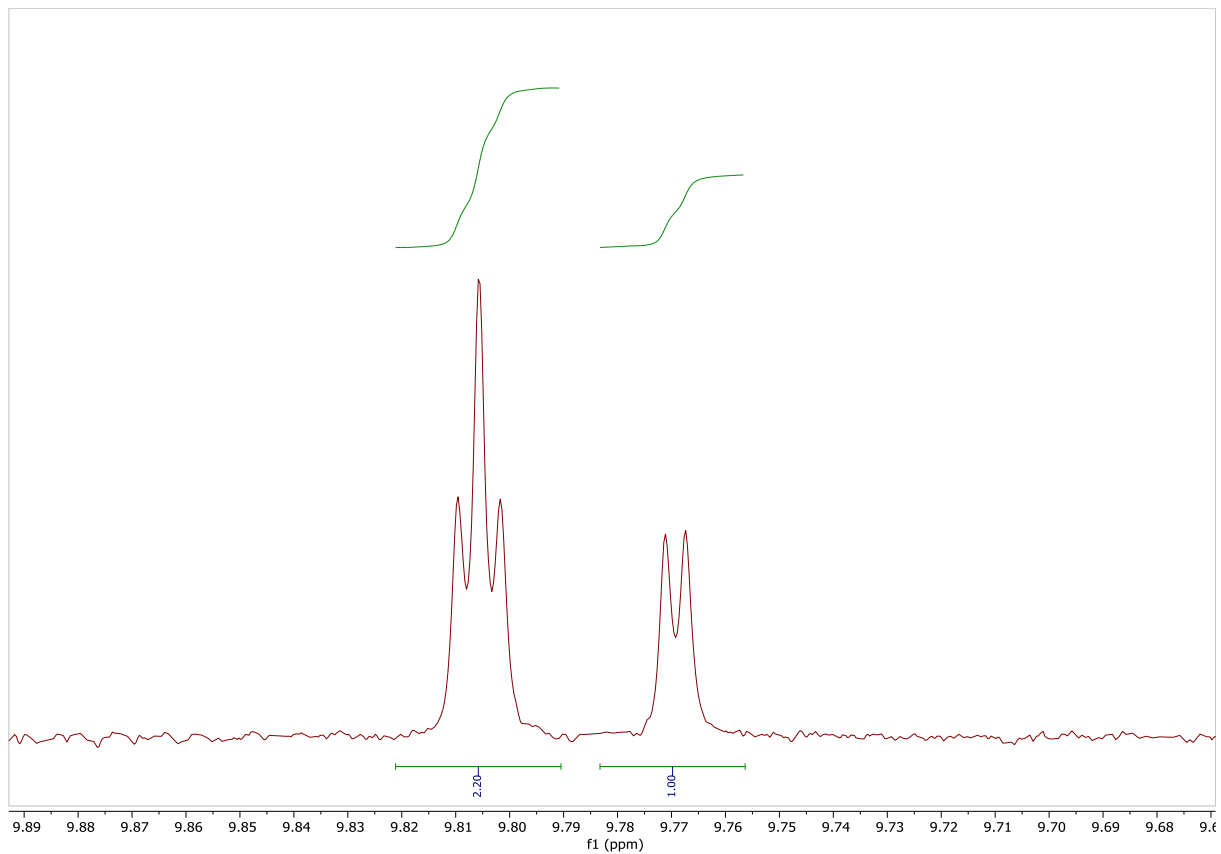
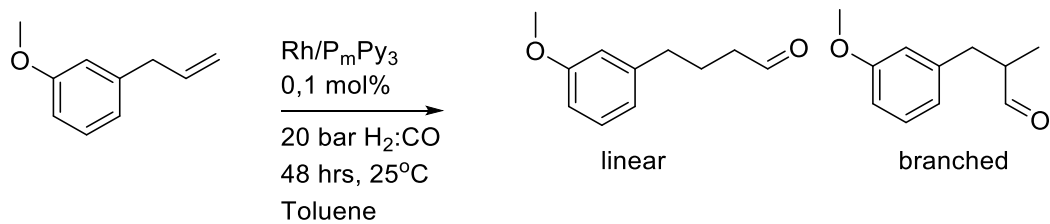
branched



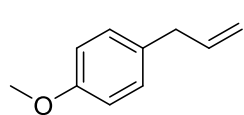
Retention time	area		l/b ratio
11.716	139763	Branched	2.73
12.338	382820	linear	



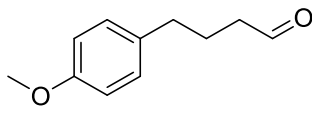
Retention time	area		l/b ratio
12.187	247202	Branched	0.49
12.845	121414	linear	



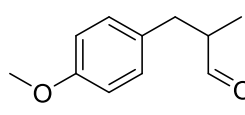
Retention time	area		l/b ratio
12.170	23922	Branched	2.39
12.838	57327	linear	



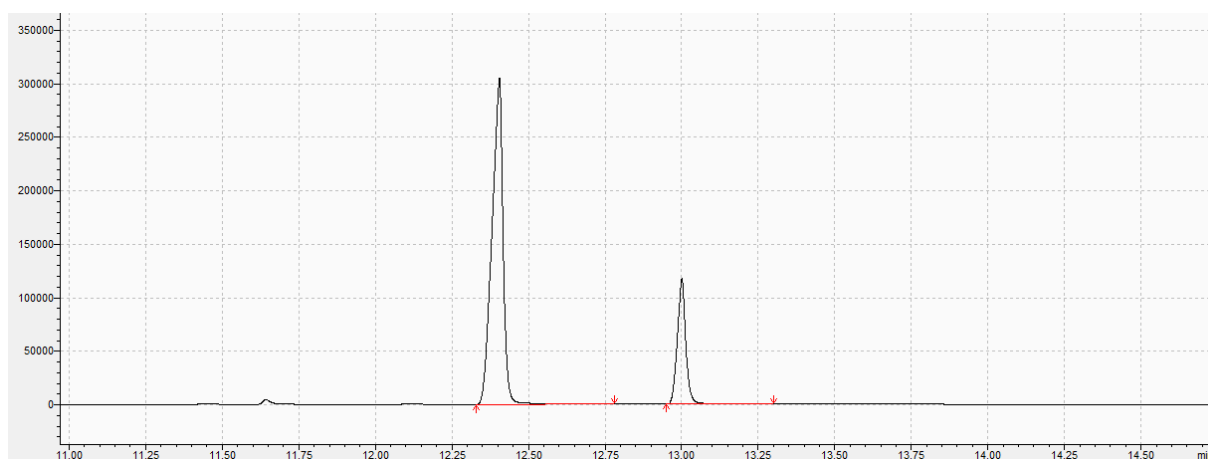
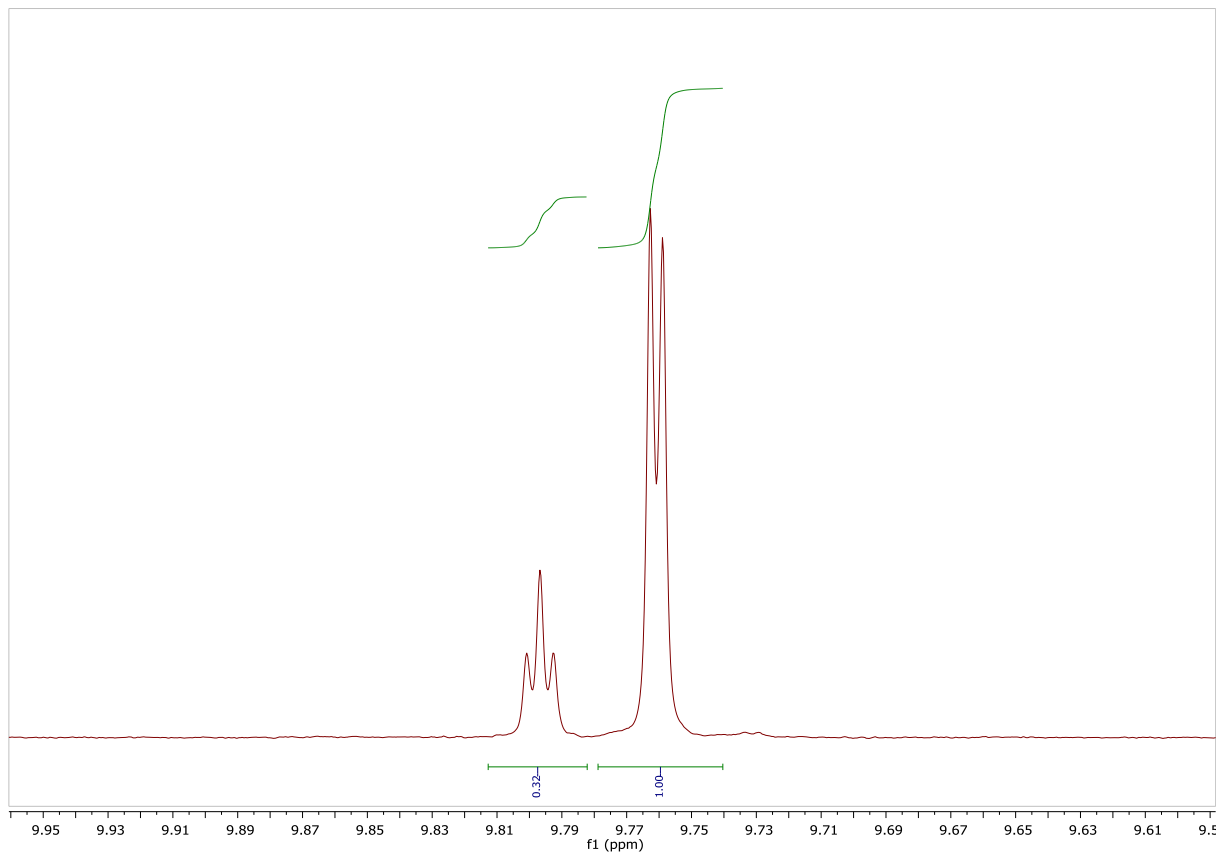
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



linear

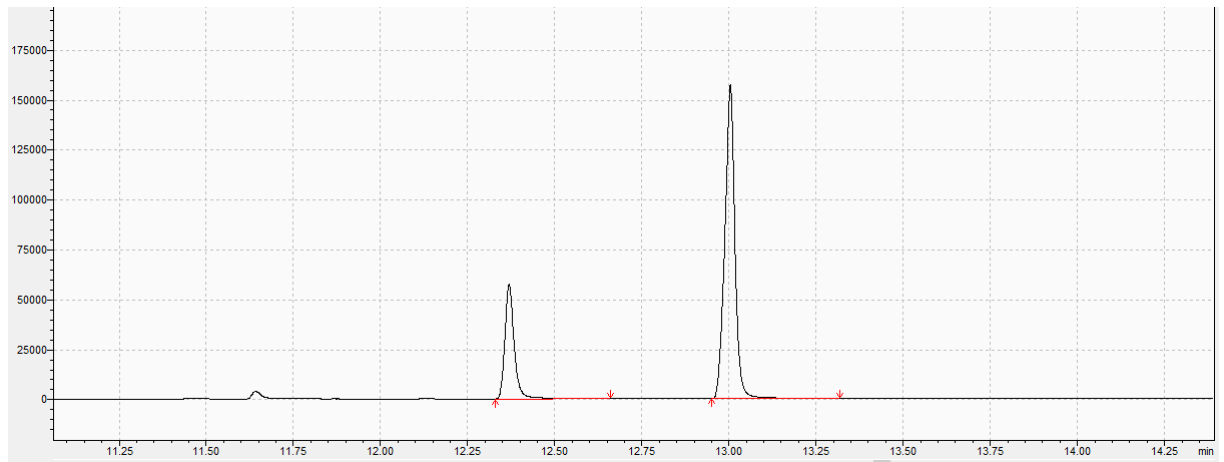
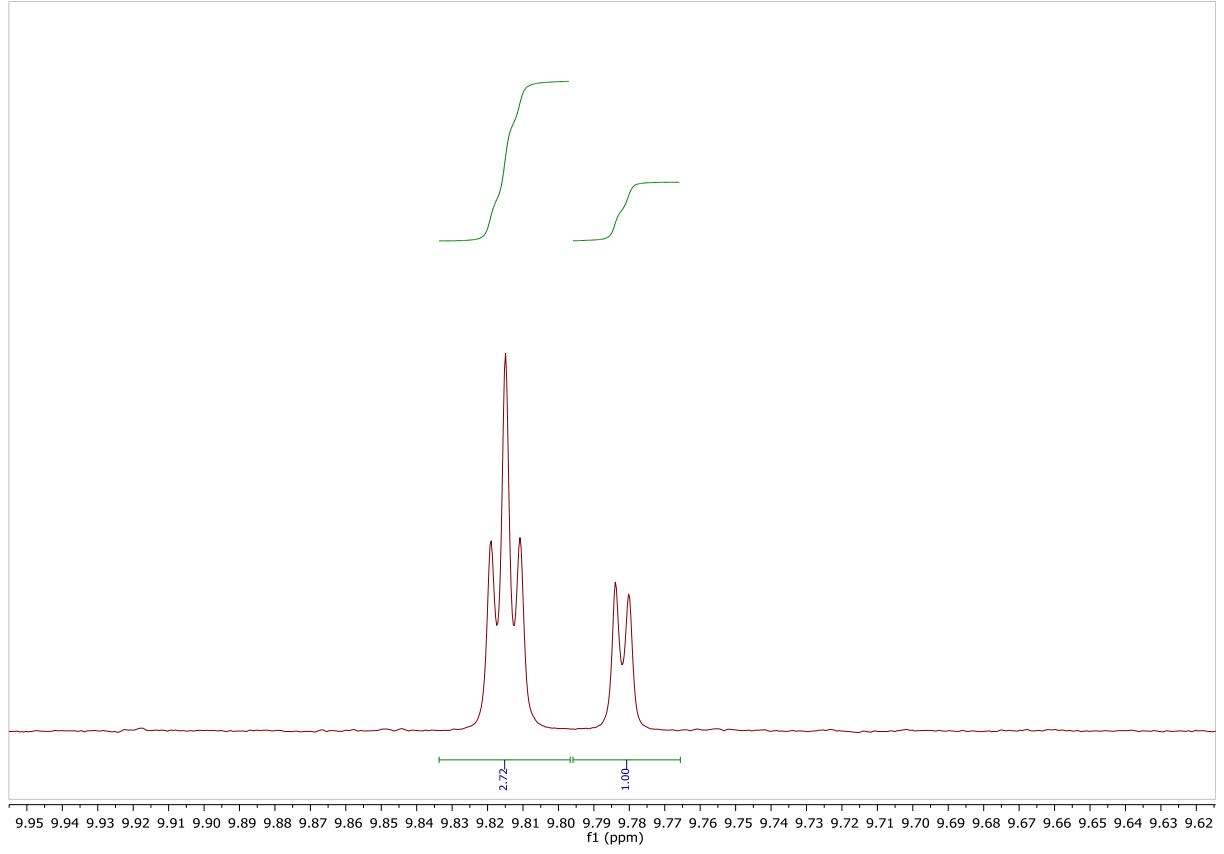
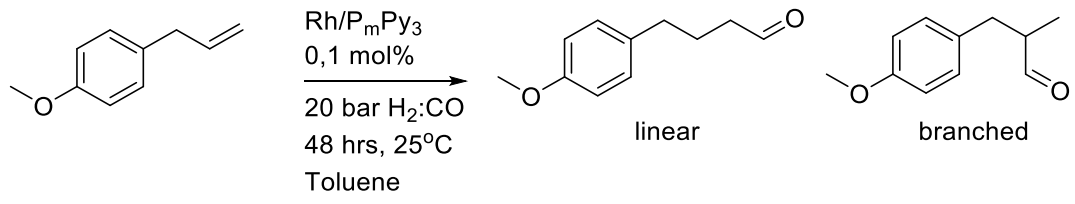


branched

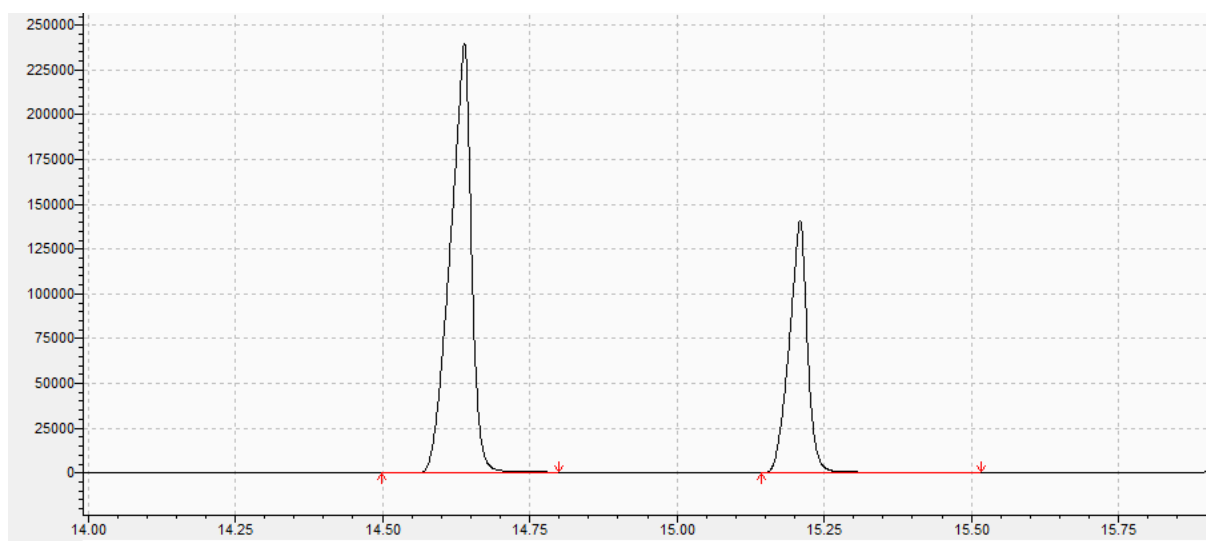
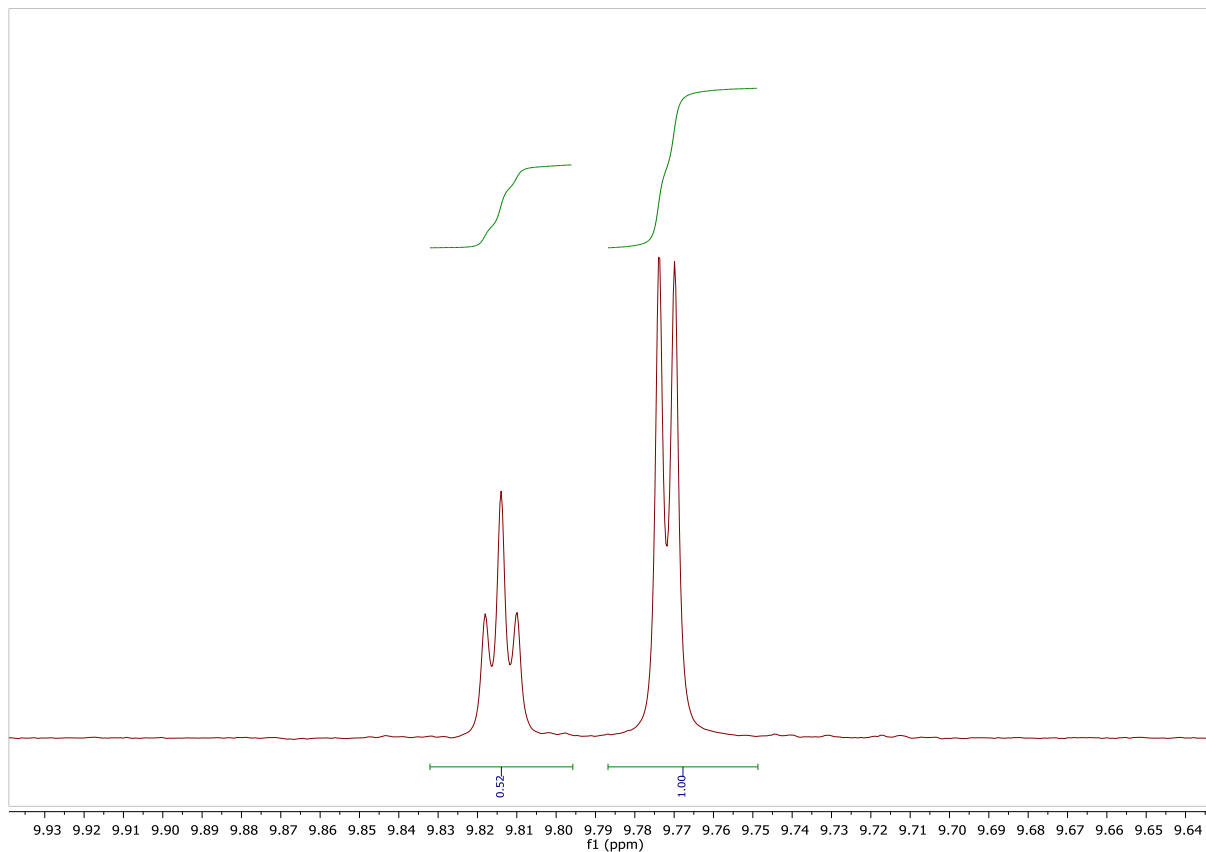
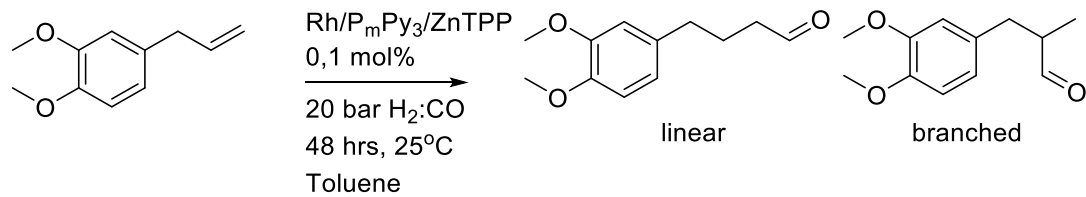


Retention time	area		l/b ratio
12.405	762404	Branched	0.29
13.001	225848	linear	

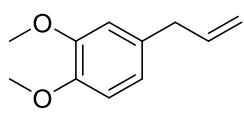




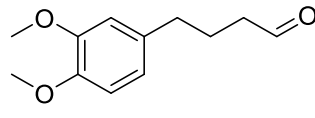
Retention time	area		I/b ratio
12.369	106661	Branched	2.96
13.004	316684	linear	



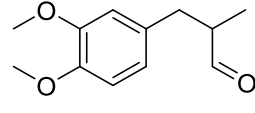
Retention time	area		l/b ratio
14.639	597052	Branched	0.50
15.209	300990	linear	



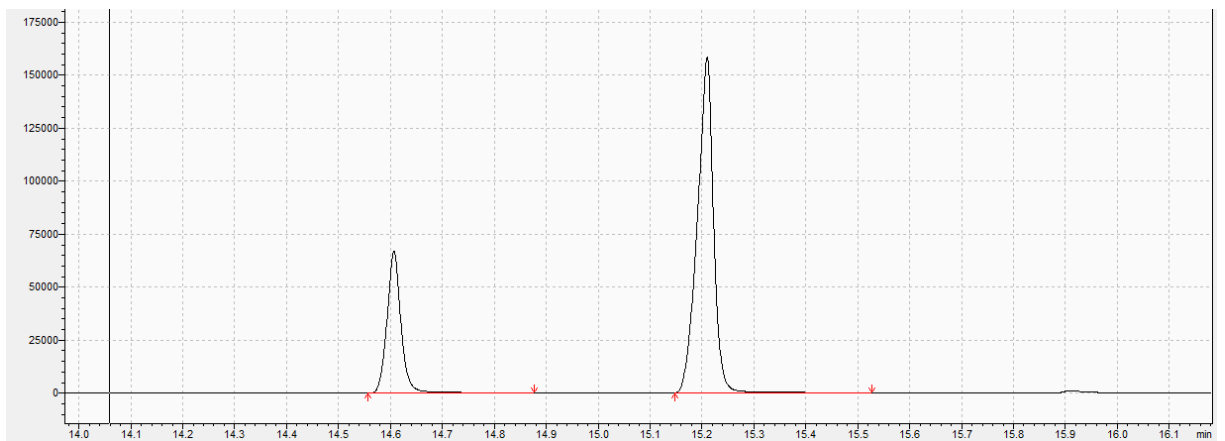
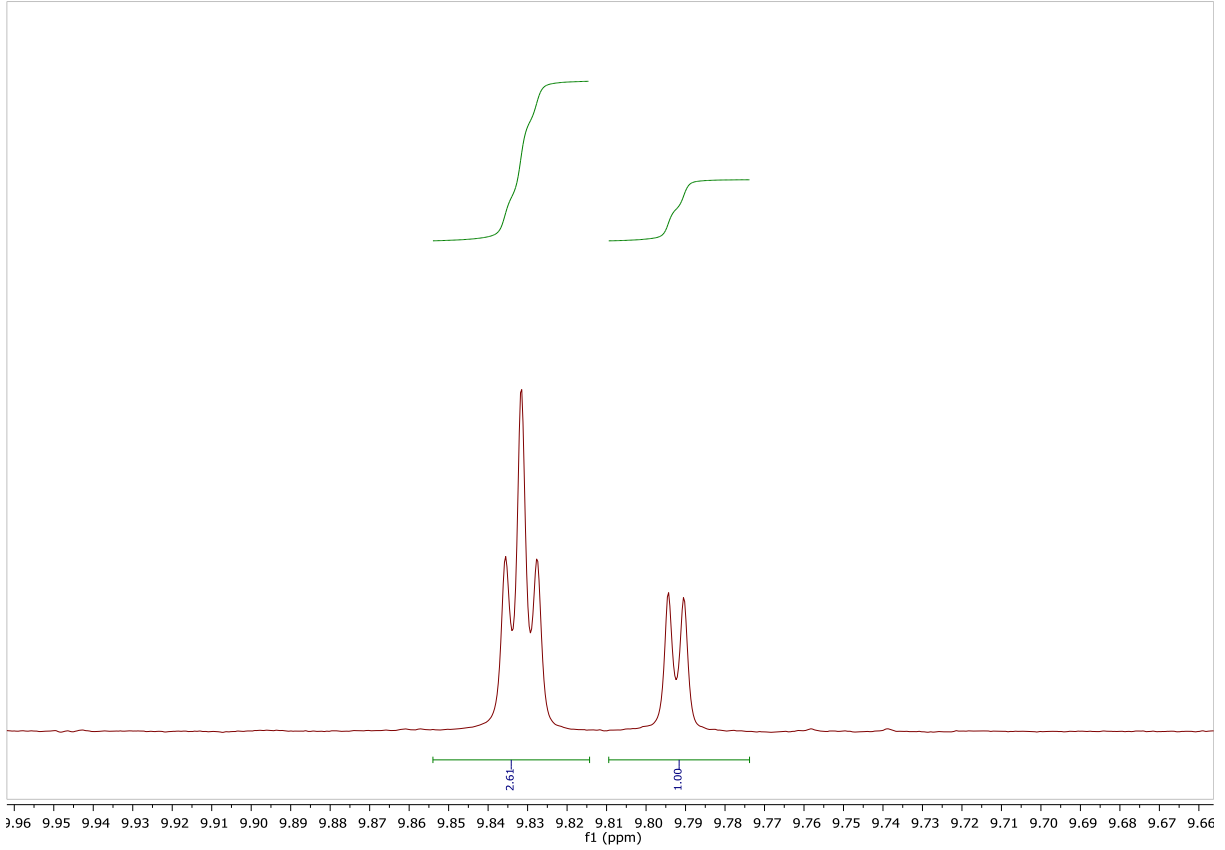
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



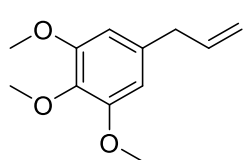
linear



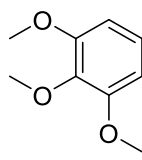
branched



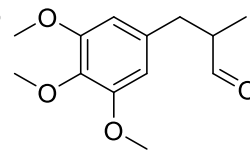
Retention time	area		l/b ratio
14.607	123895	Branched	2.76
15.210	342959	linear	



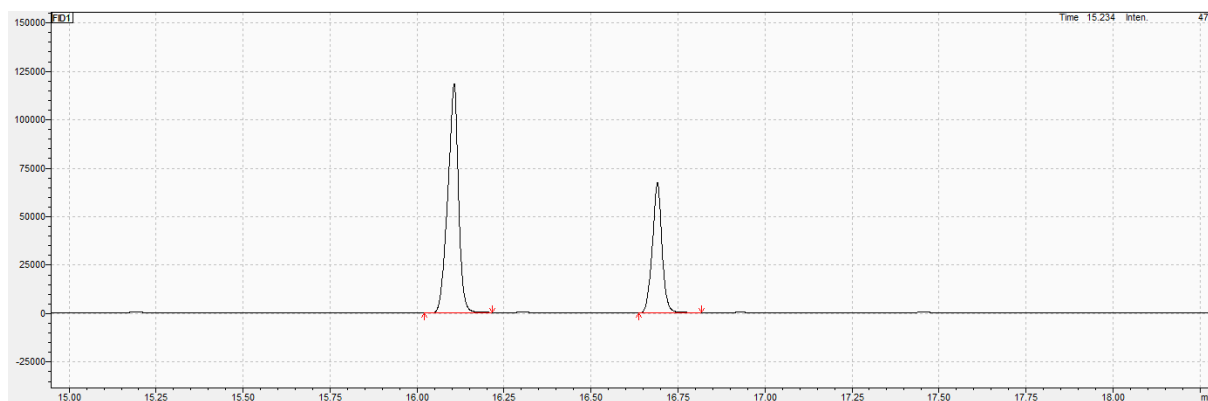
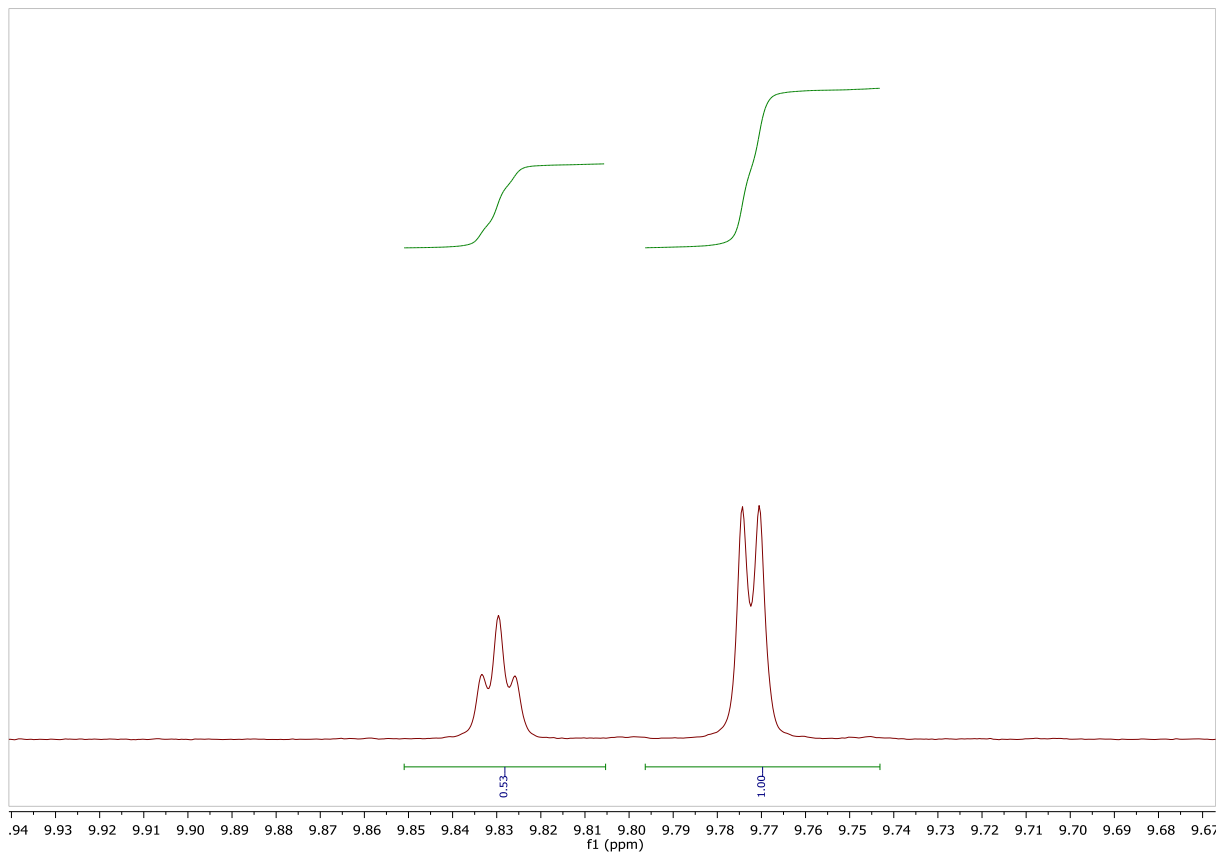
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



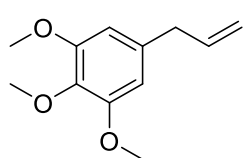
linear



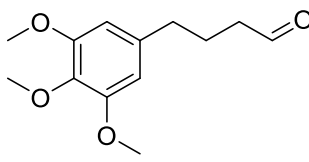
branched



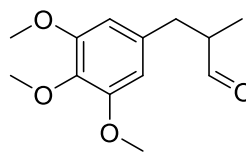
Retention time	area		I/b ratio
16.106	251444	Branched	0.51
16.691	128919	linear	



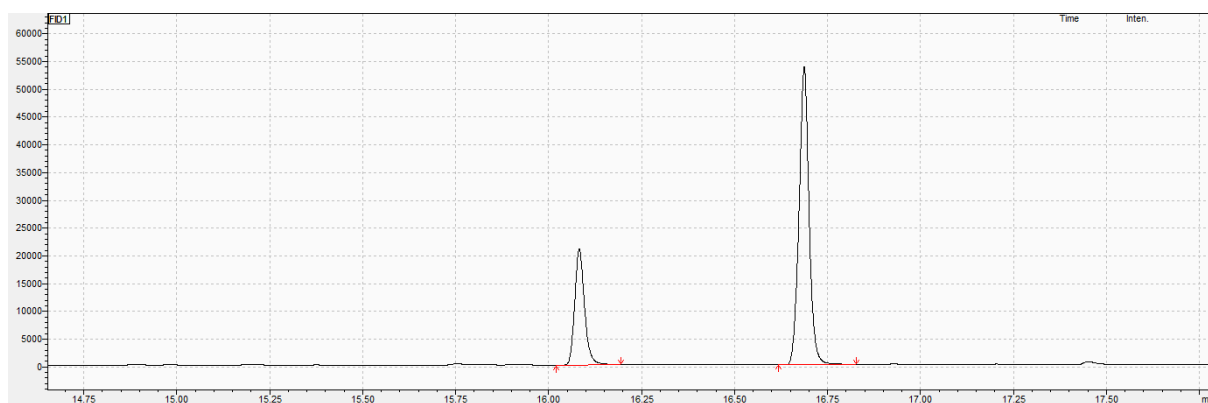
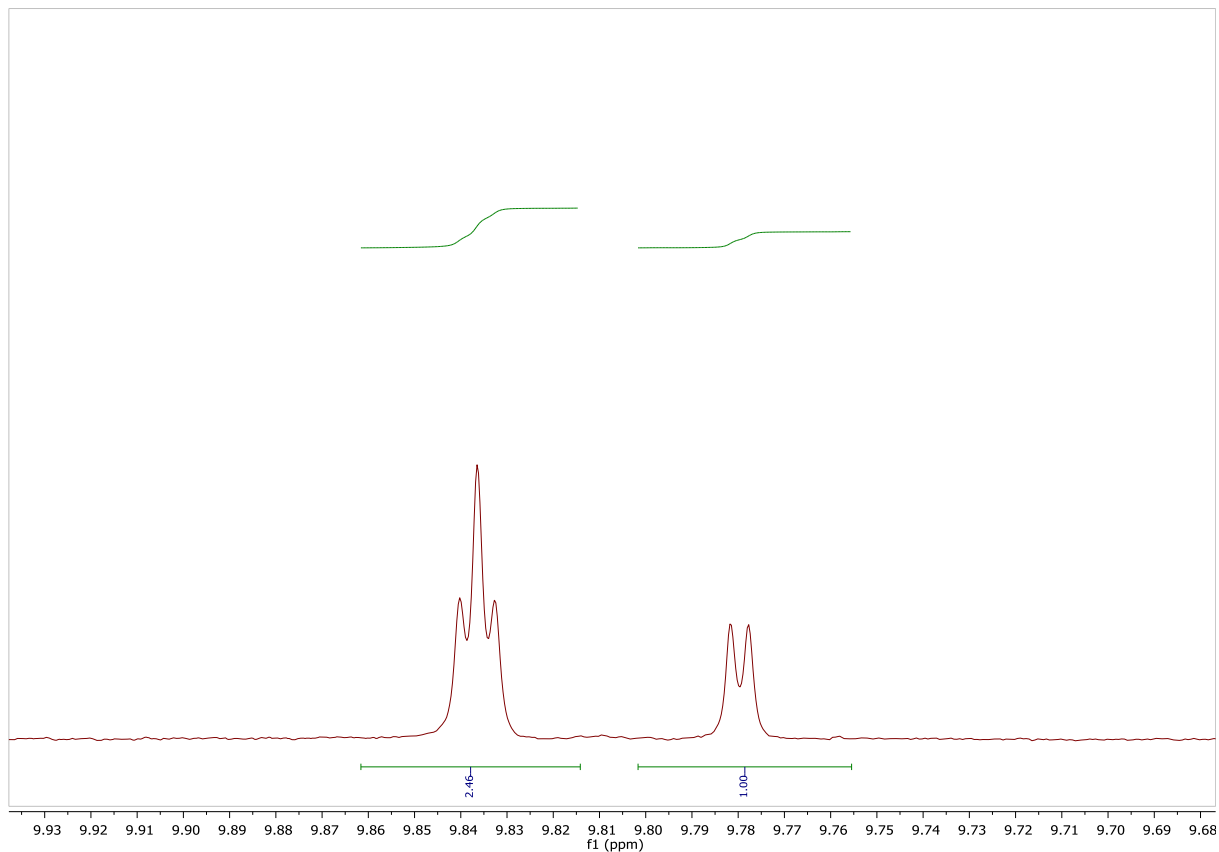
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



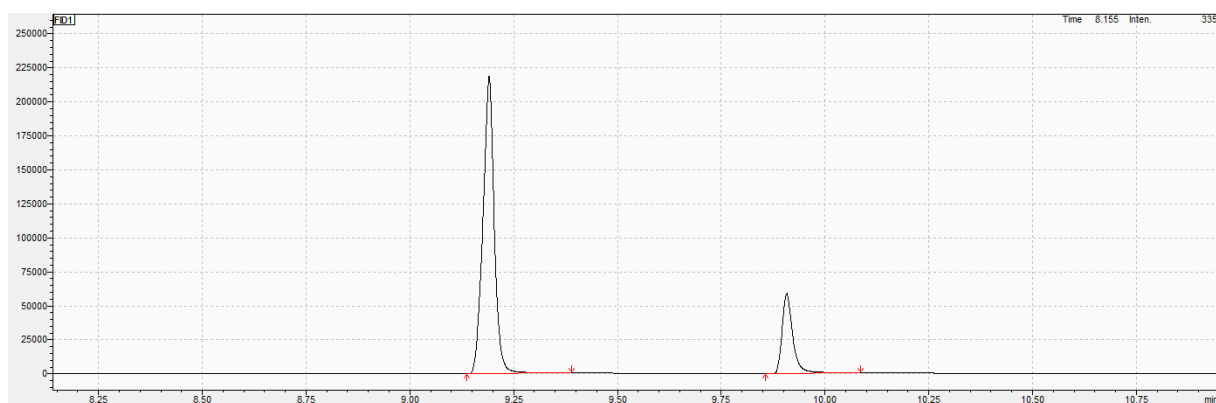
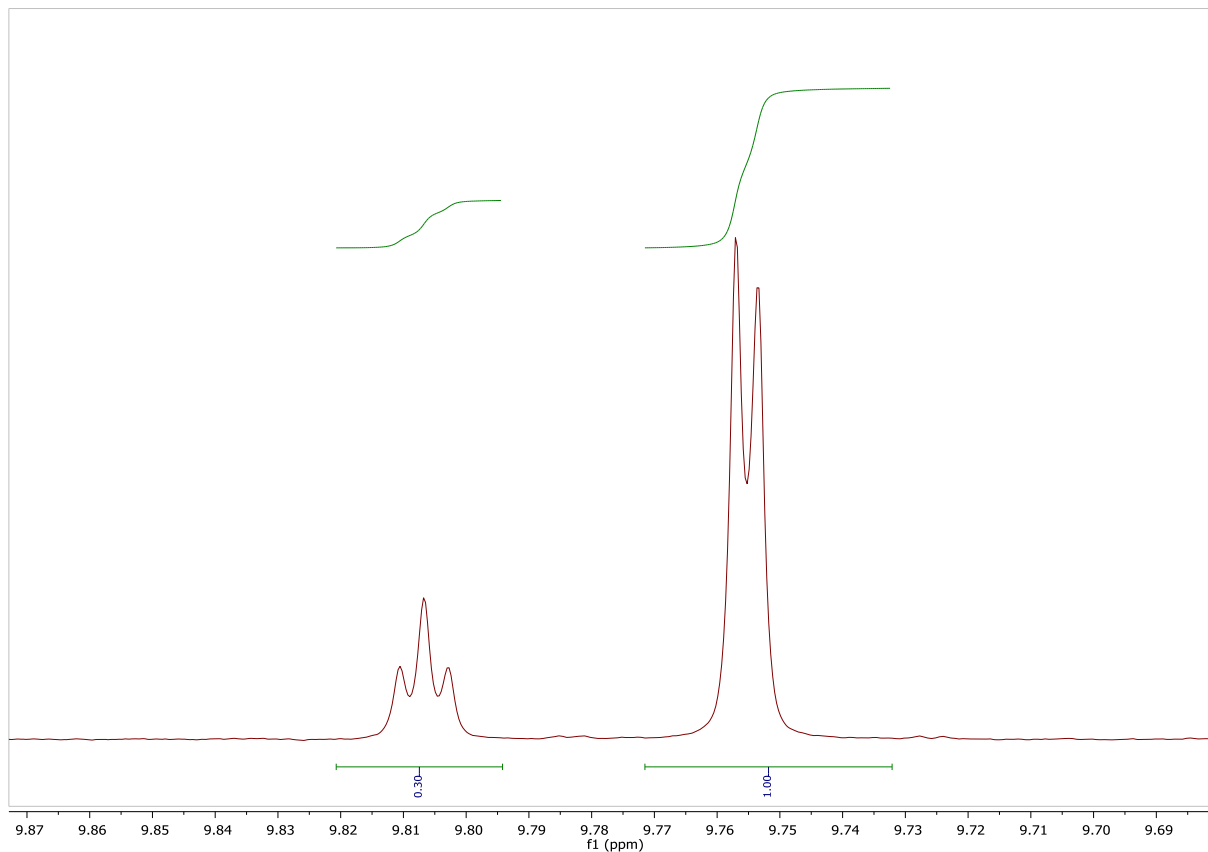
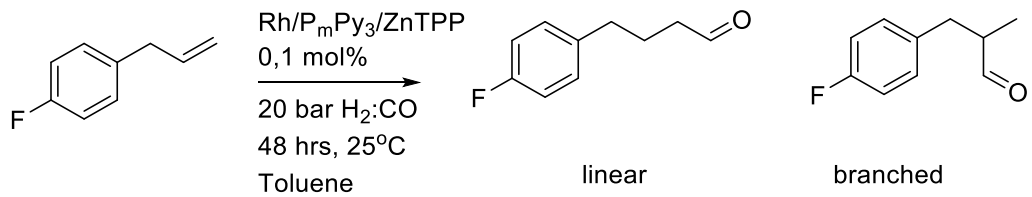
linear



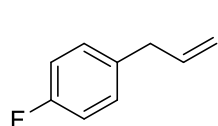
branched



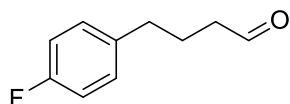
Retention time	area		I/b ratio
16.185	38125	Branched	2.64
16.687	100914	linear	



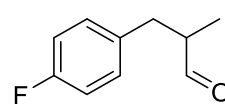
Retention time	area		l/b ratio
9.191	411500	Branched	0.25
9.908	104325	linear	



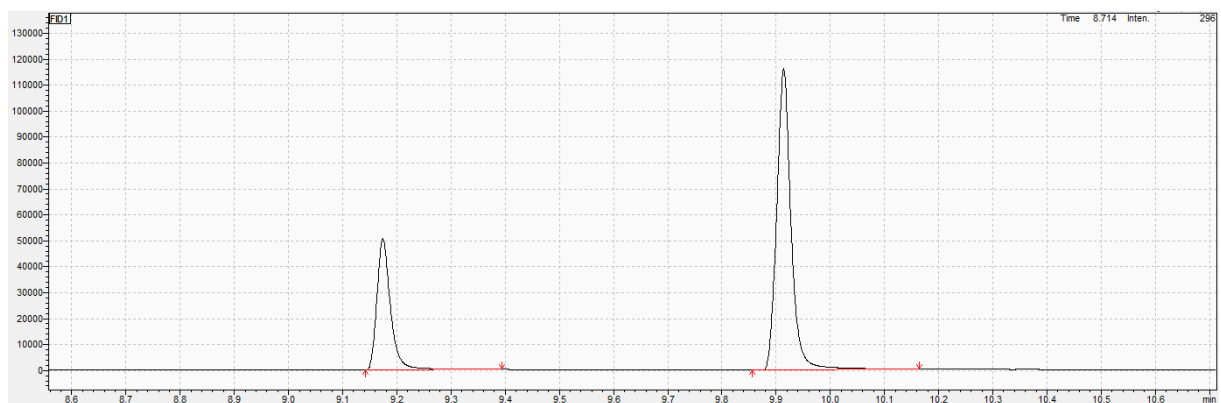
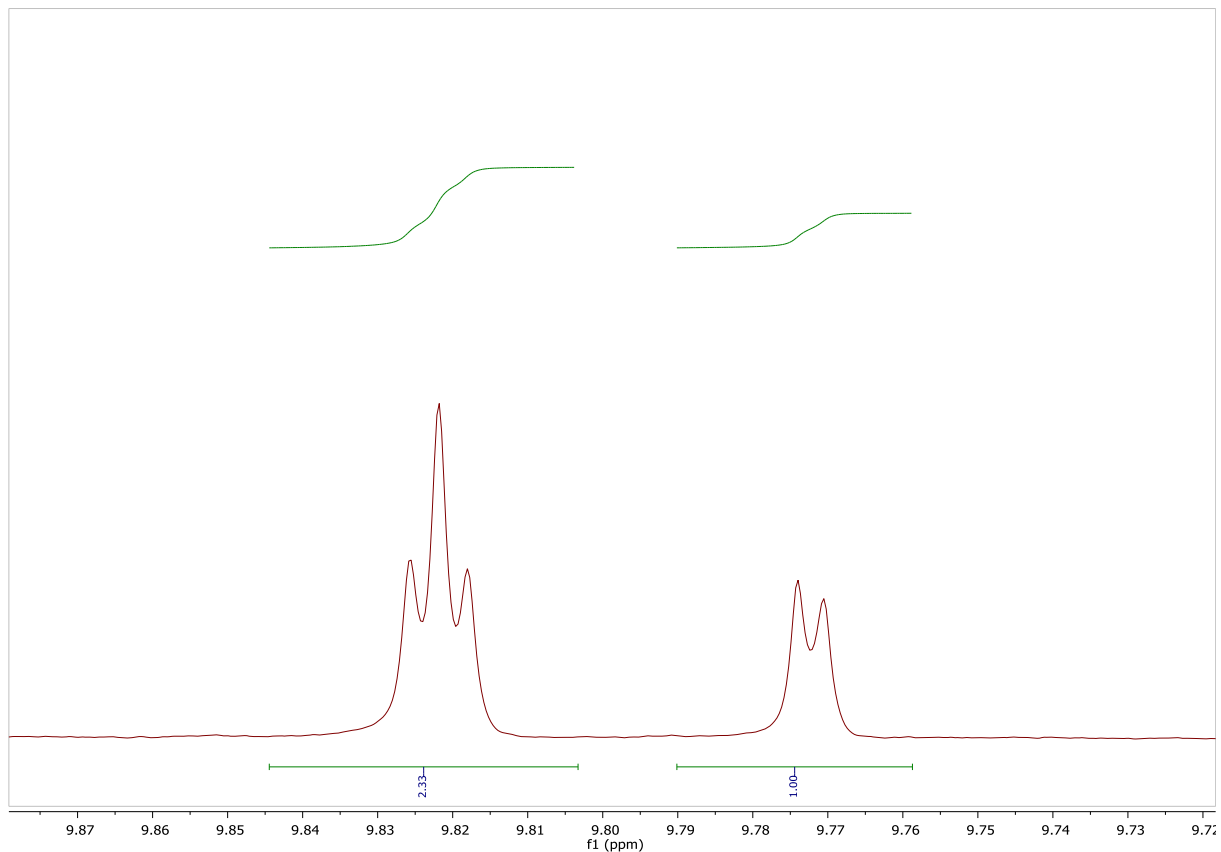
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



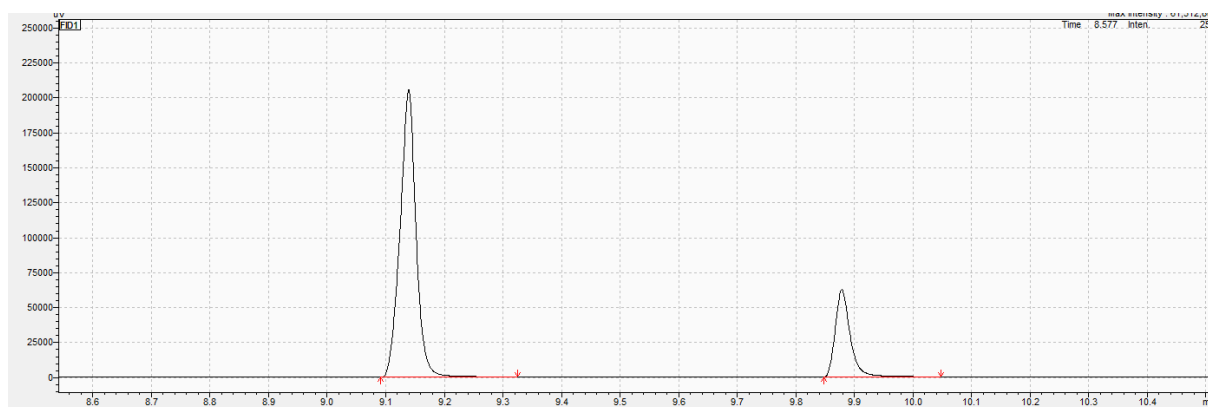
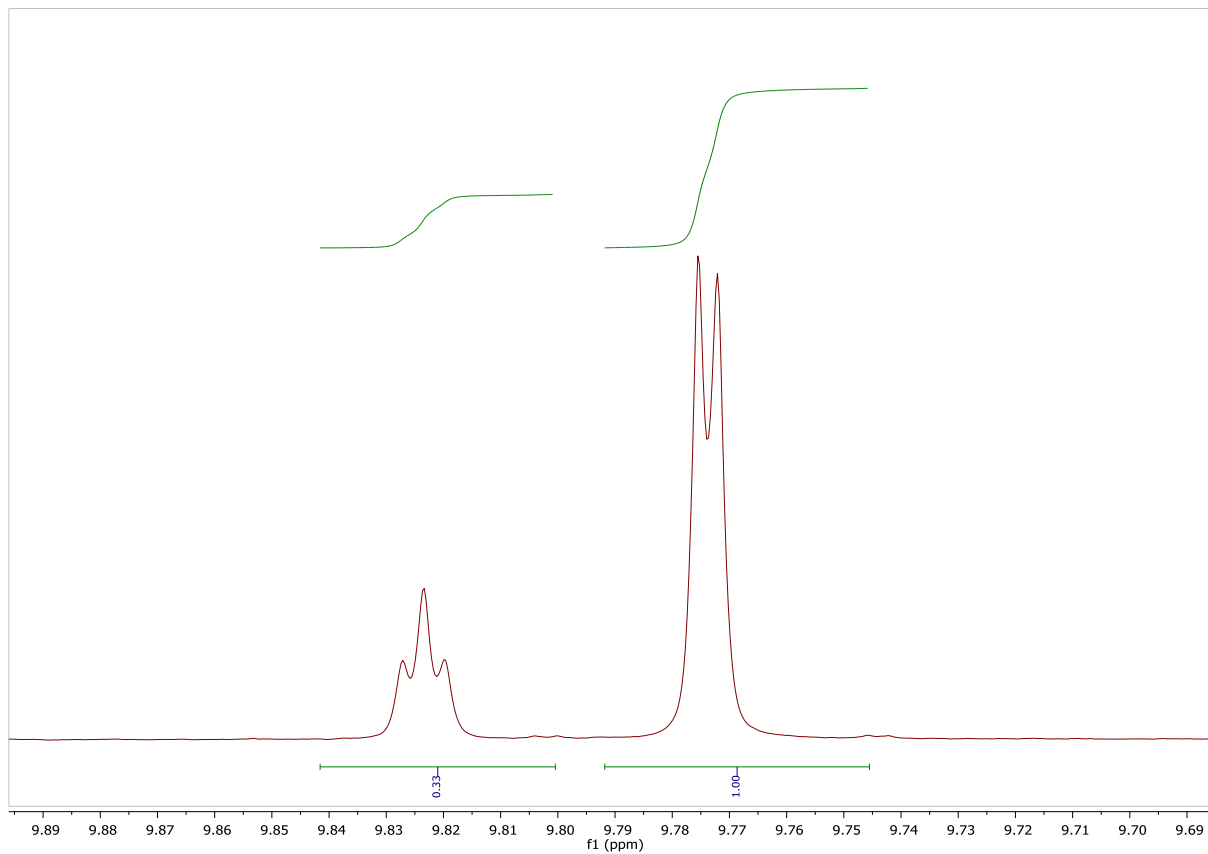
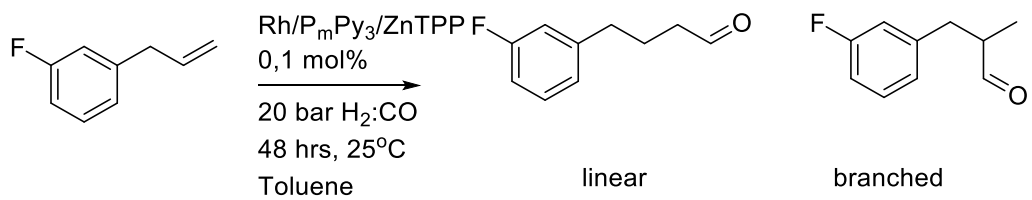
linear



branched

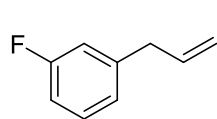


Retention time	area		l/b ratio
9.174	88218	Branched	2.40
9.914	212334	linear	

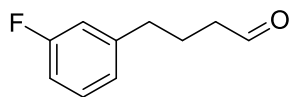


Retention time	area		l/b ratio
9.139	389583	Branched	0.28
9.879	111635	linear	

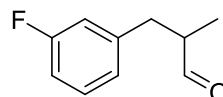




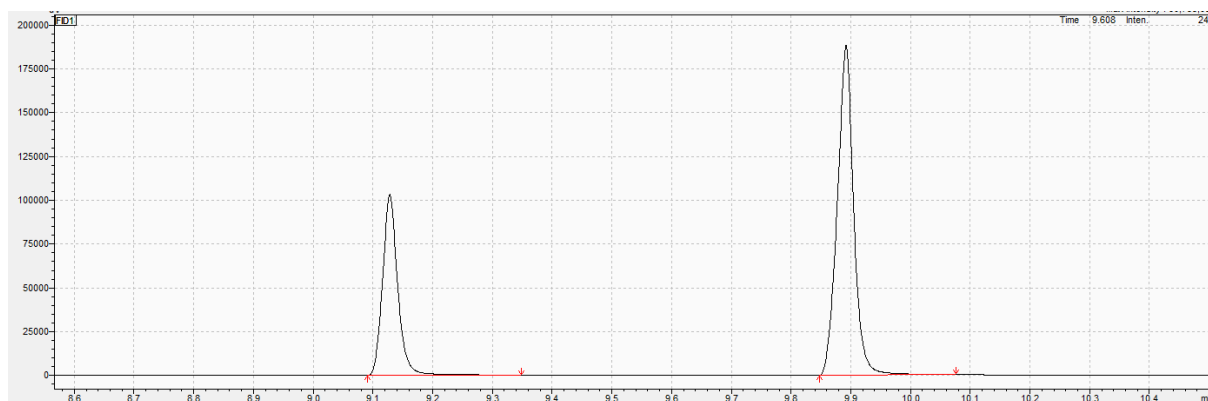
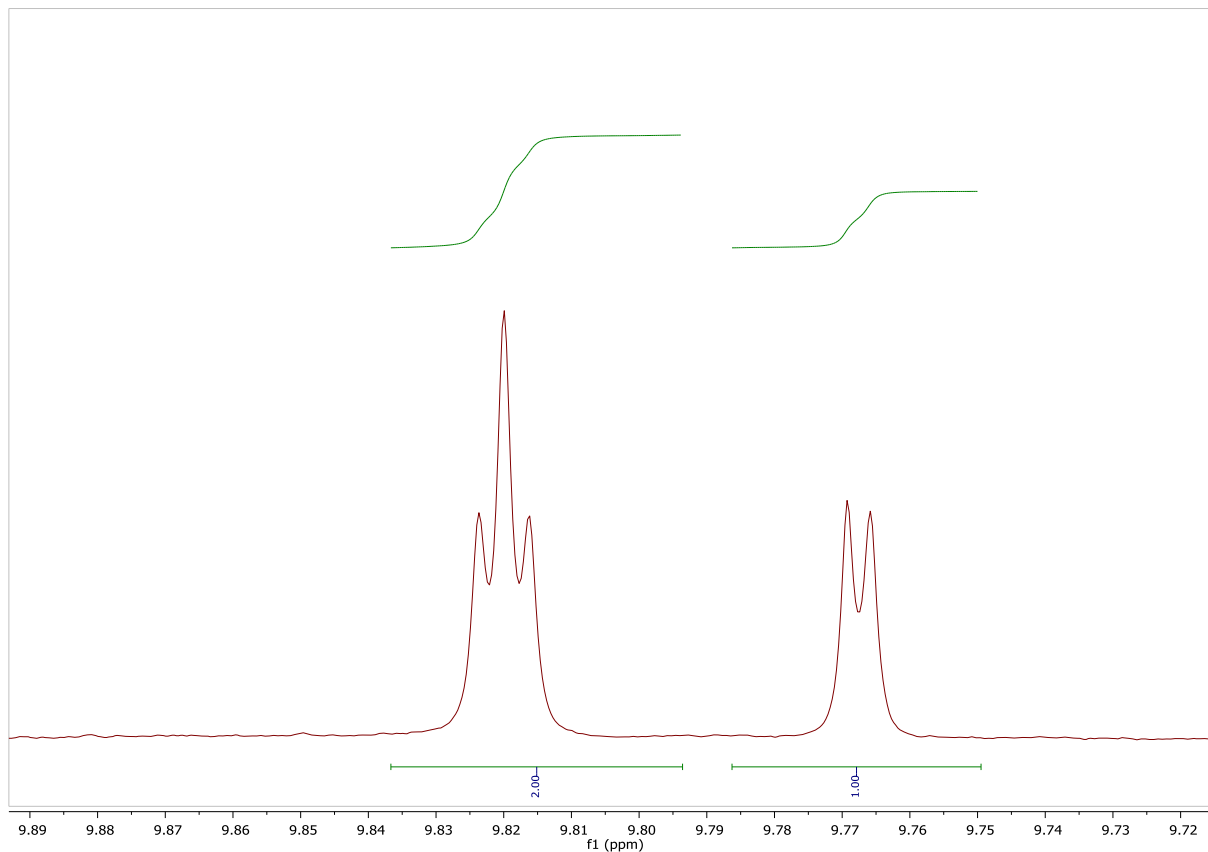
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



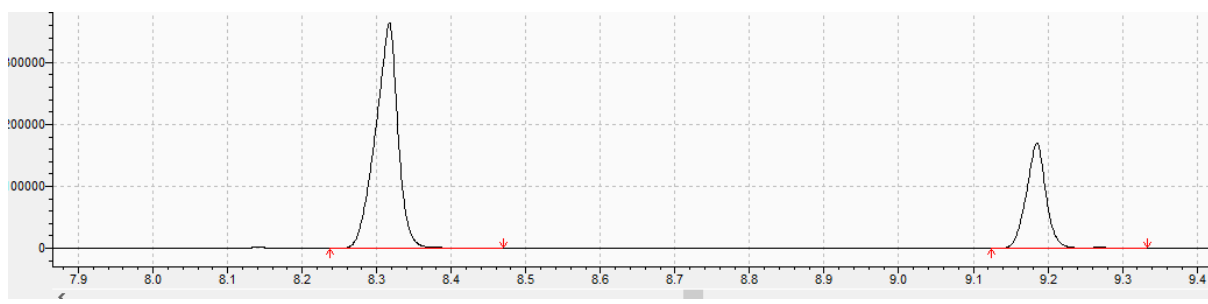
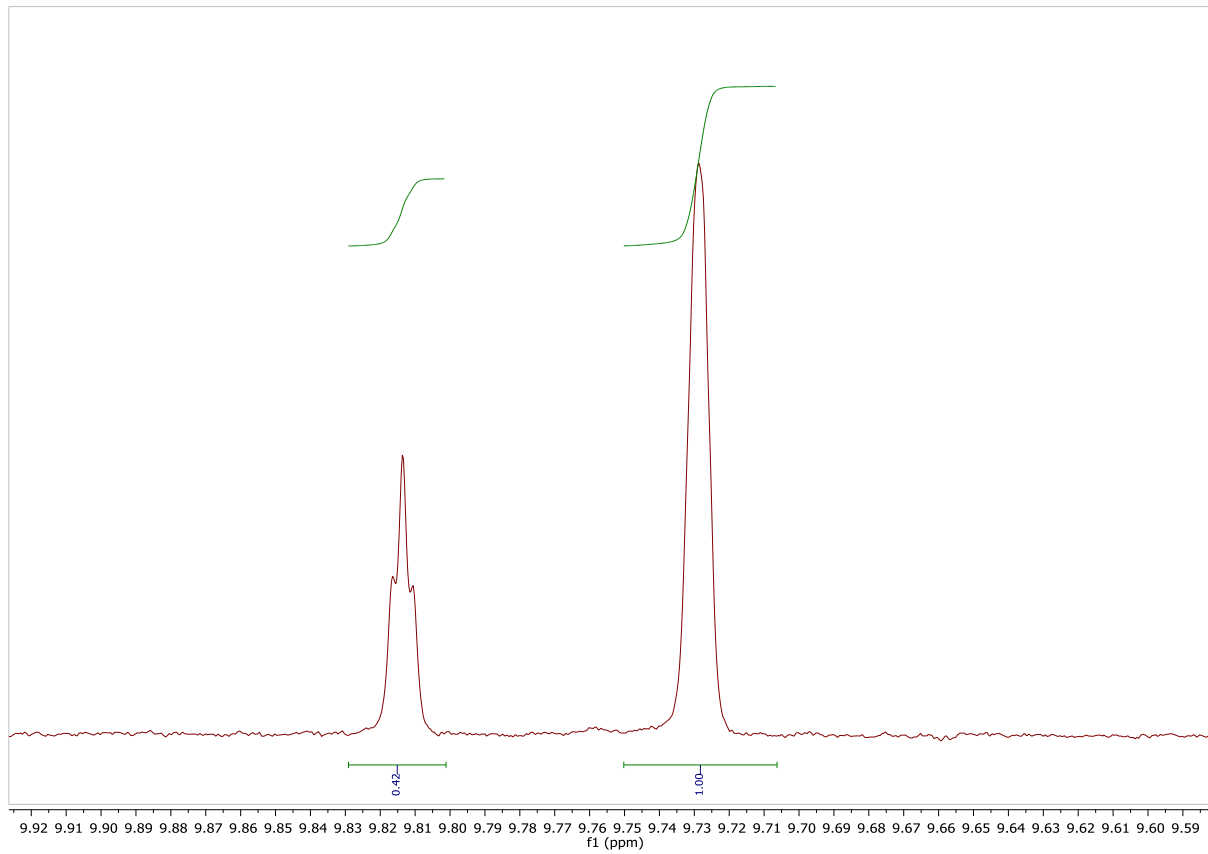
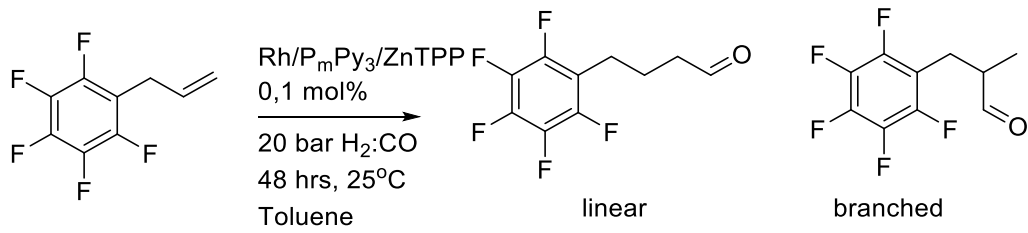
linear



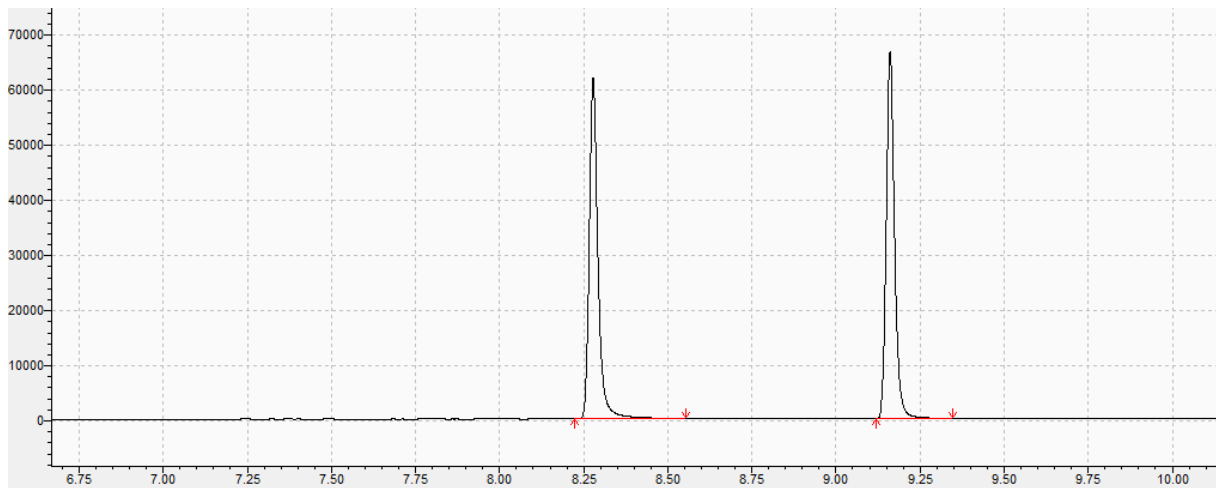
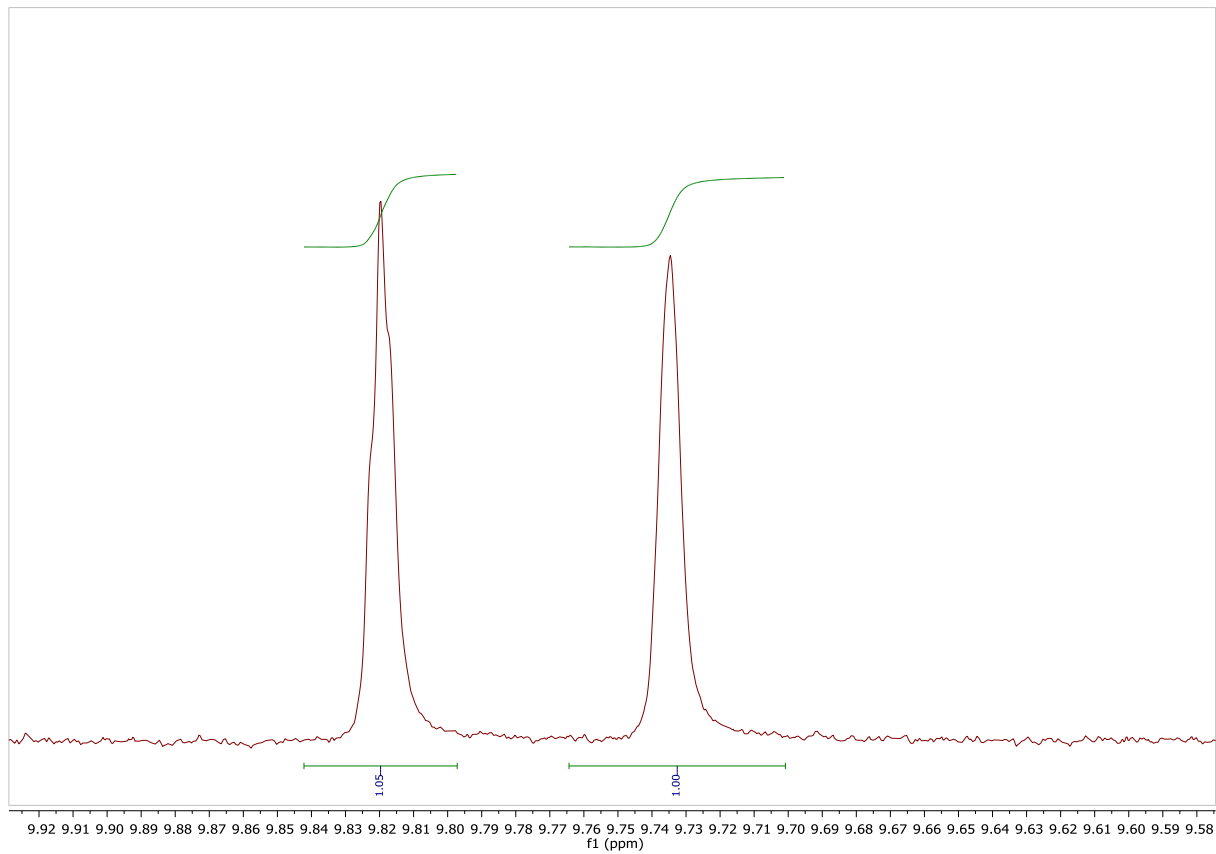
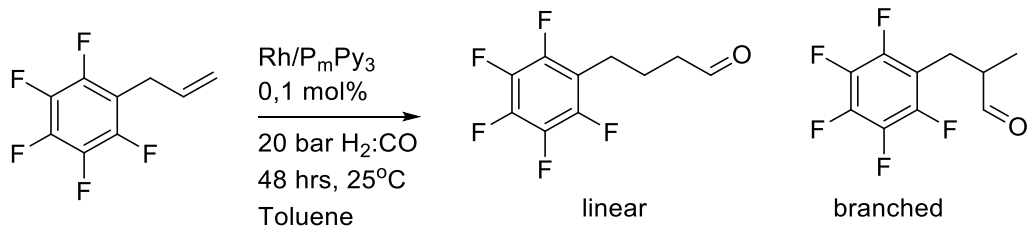
branched



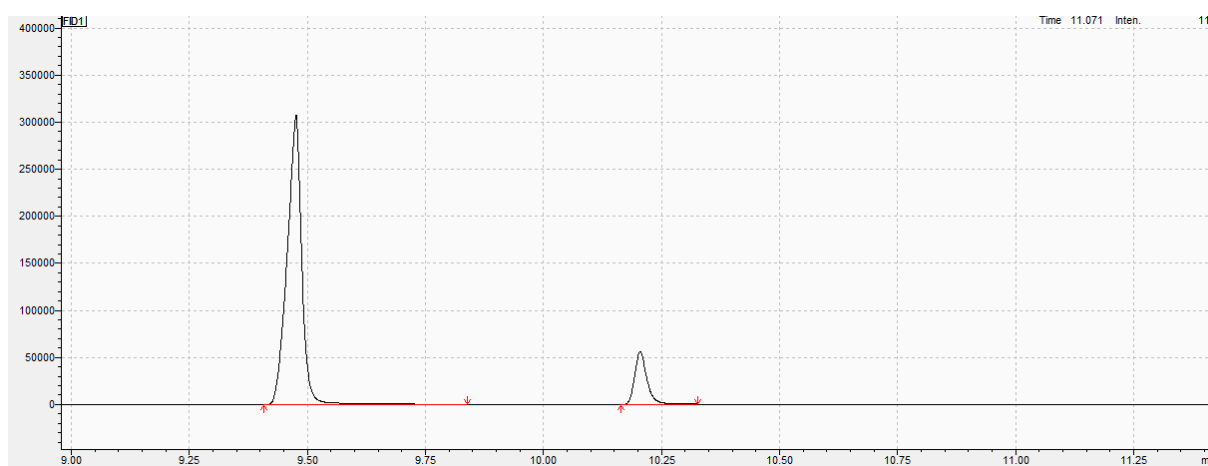
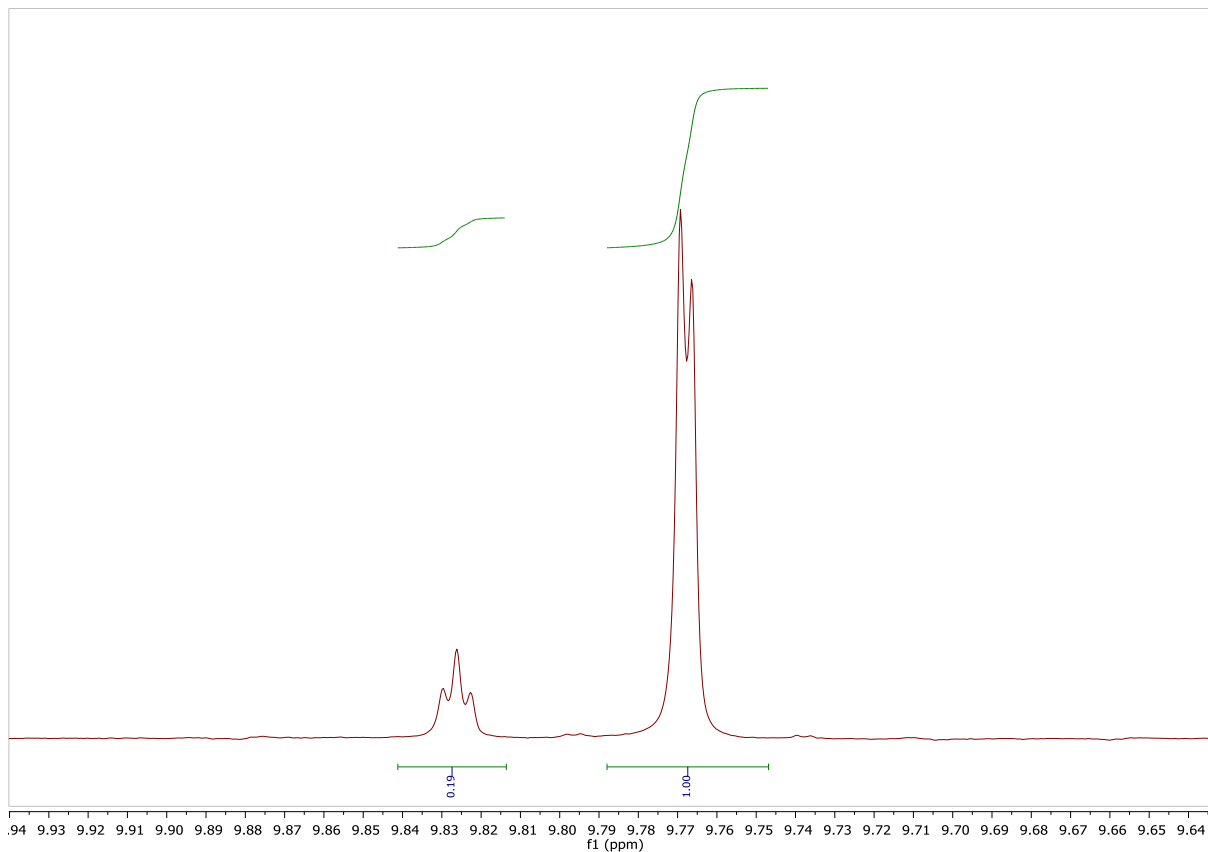
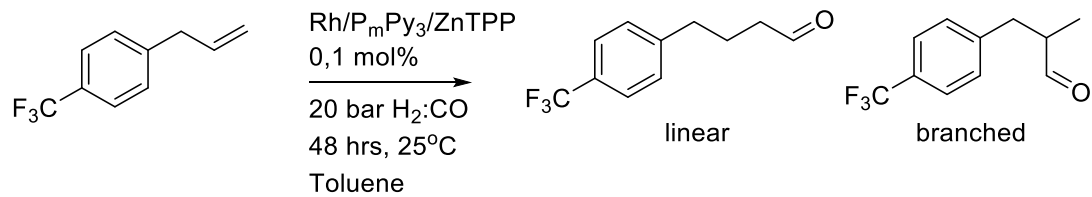
Retention time	area		l/b ratio
9.128	181077	Branched	1.97
9.892	358046	linear	



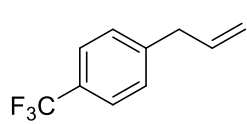
Time	Area		I/b ratio
8,317	760155	Branched	0.41
9,185	310593	Linear	



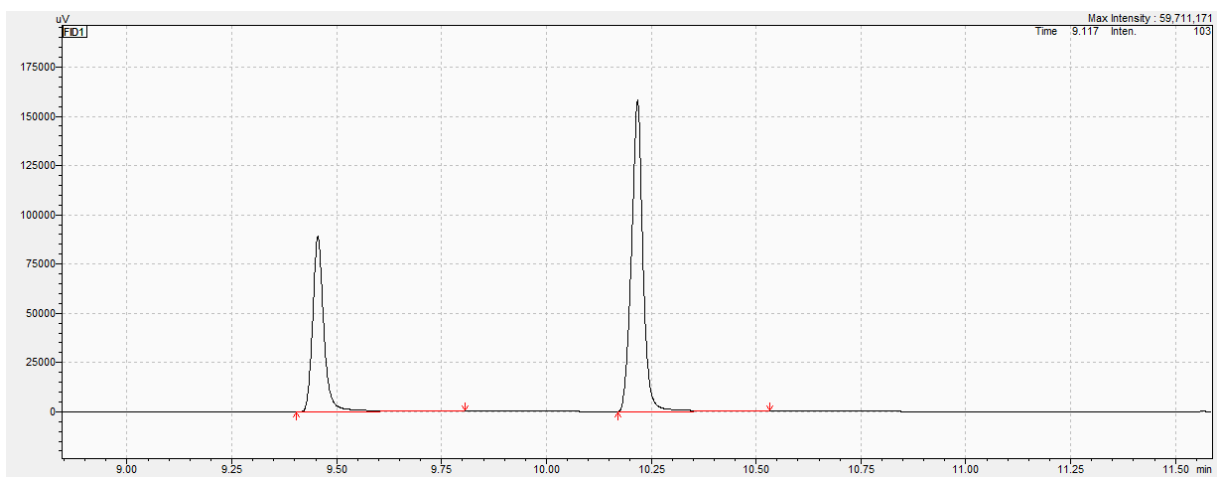
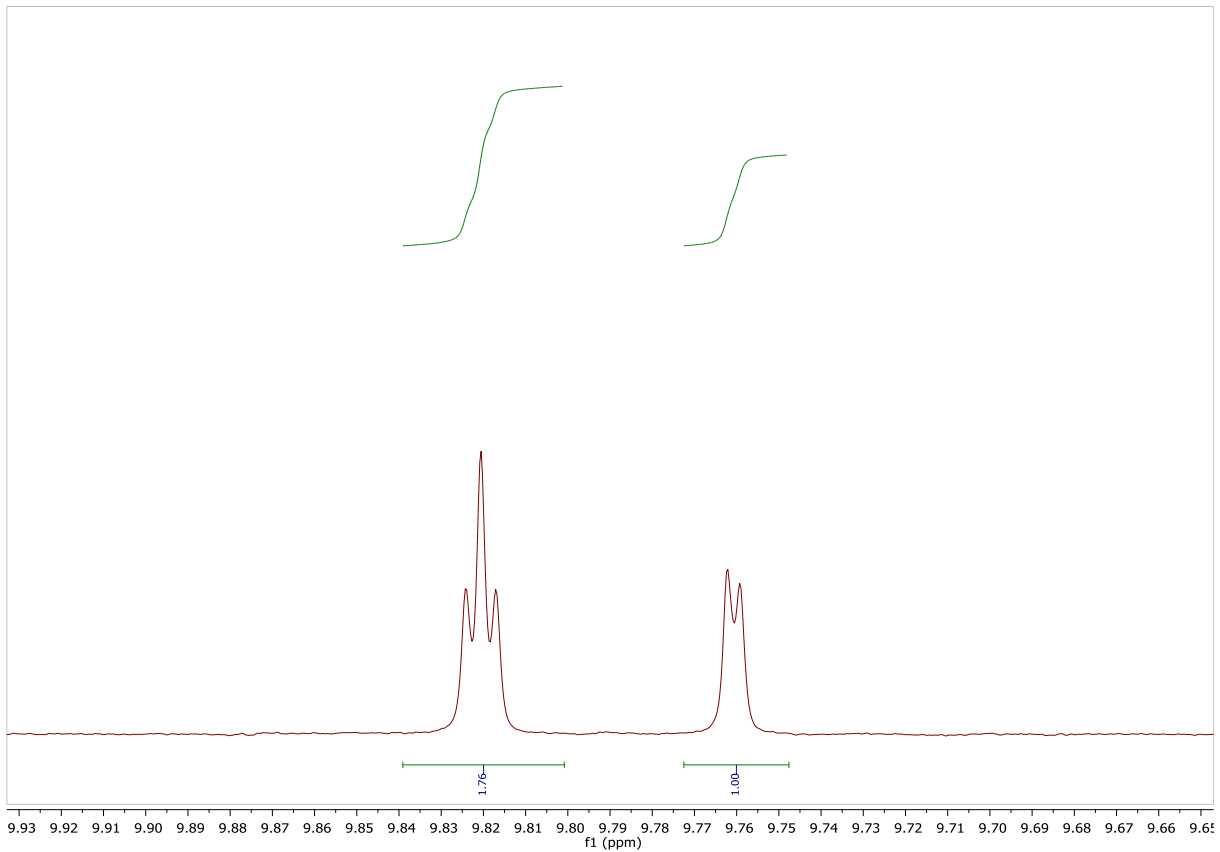
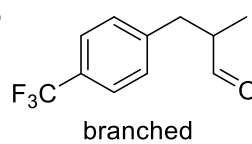
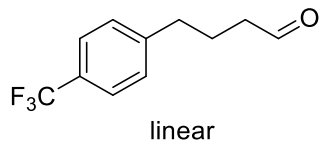
Retention time	area		l/b ratio
8,278	111900	Branched	1,02
9,161	114574	Linear	



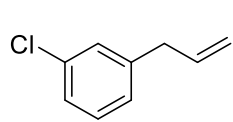
Retention time	area		I/b ratio
9.475	657809	Branched	0.15
10.205	99756	Linear	



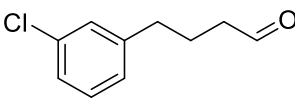
Rh/P<sub>m</sub>Py<sub>3</sub>  
0,1 mol%  
20 bar H<sub>2</sub>:CO  
48 hrs, 25°C  
Toluene



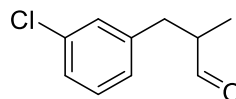
Retention time	area		l/b ratio
9.455	164989	Branched	1.82
10.217	300997	Linear	



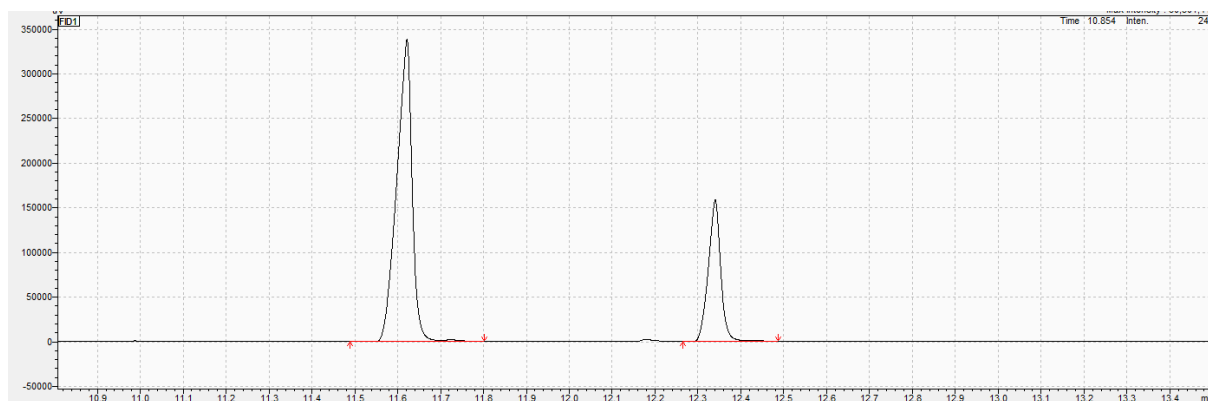
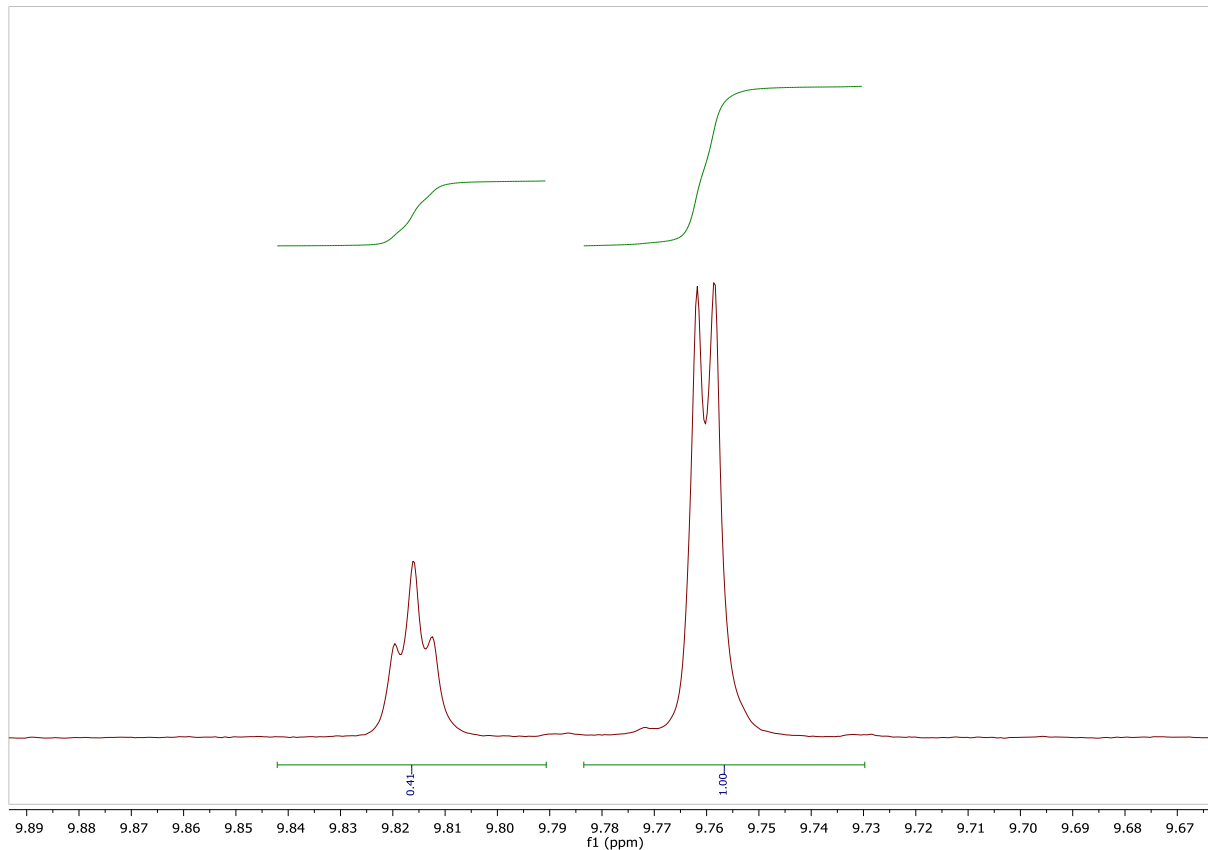
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



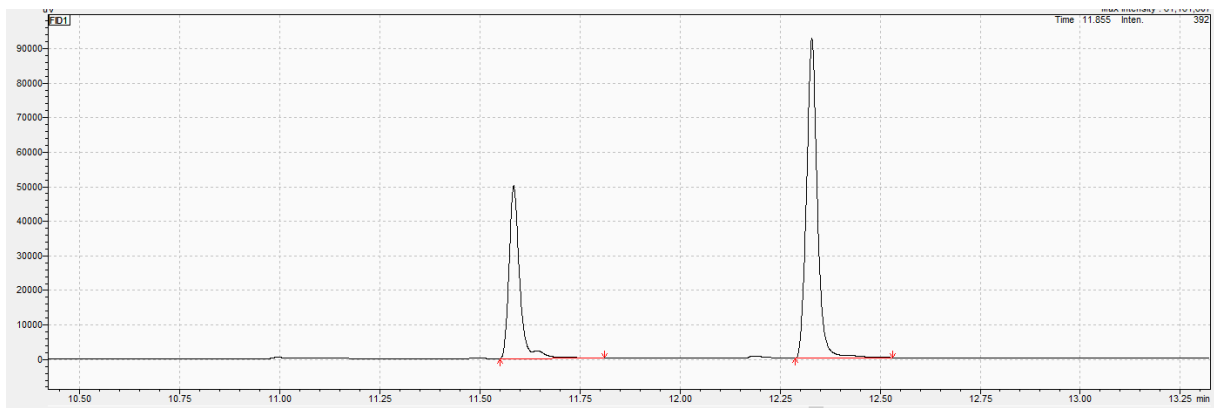
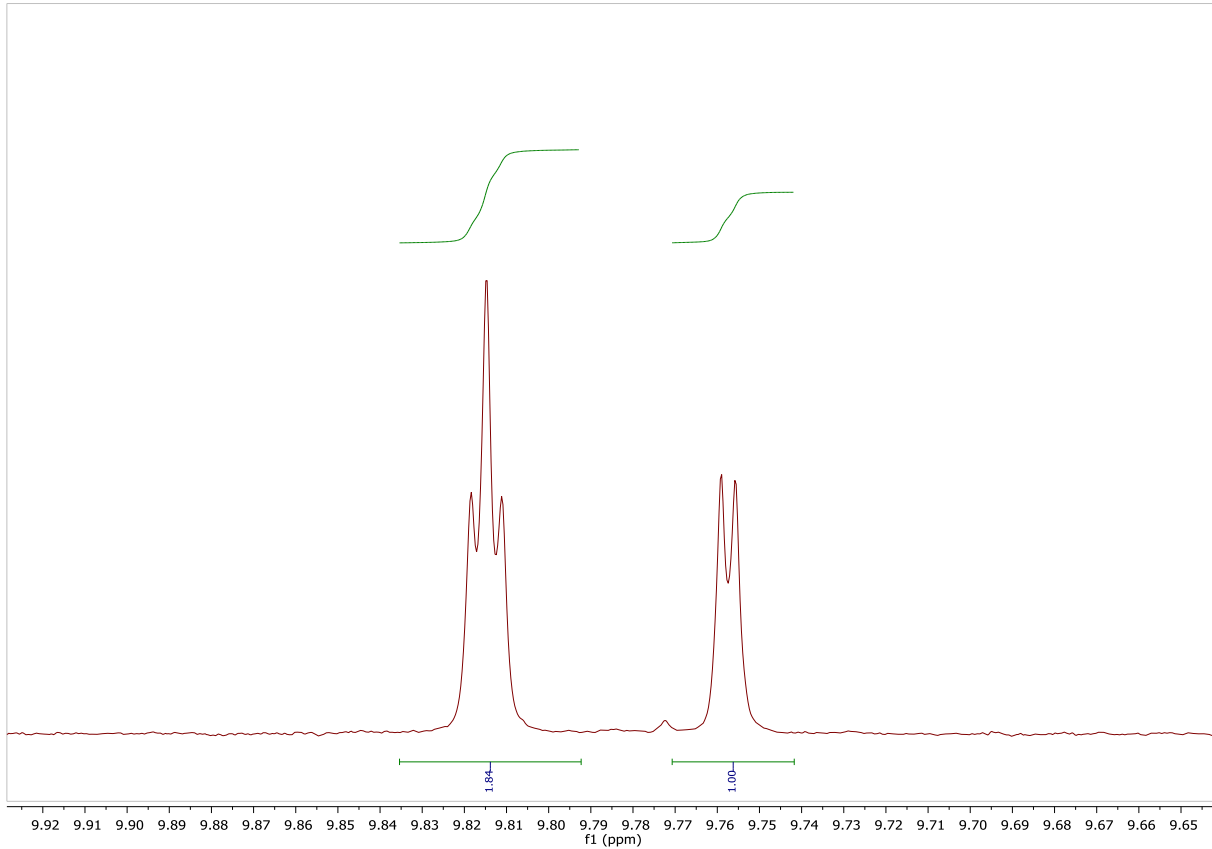
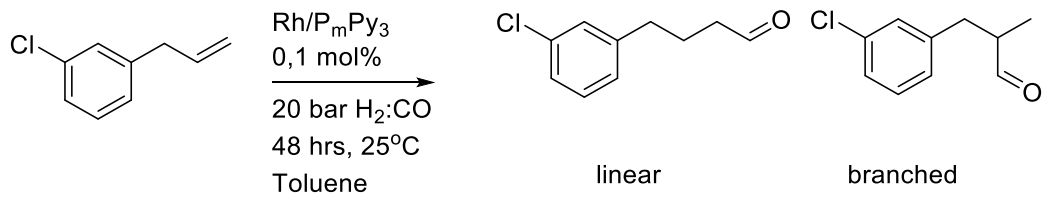
linear



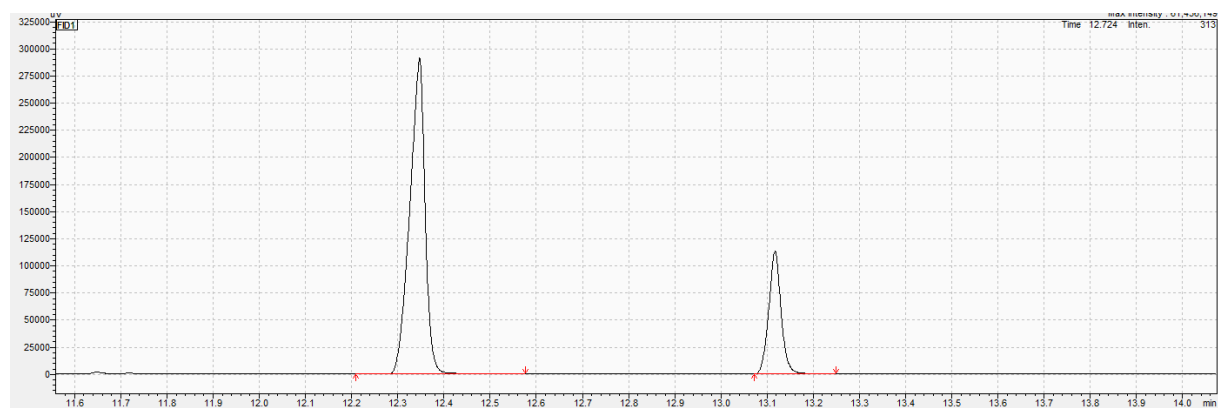
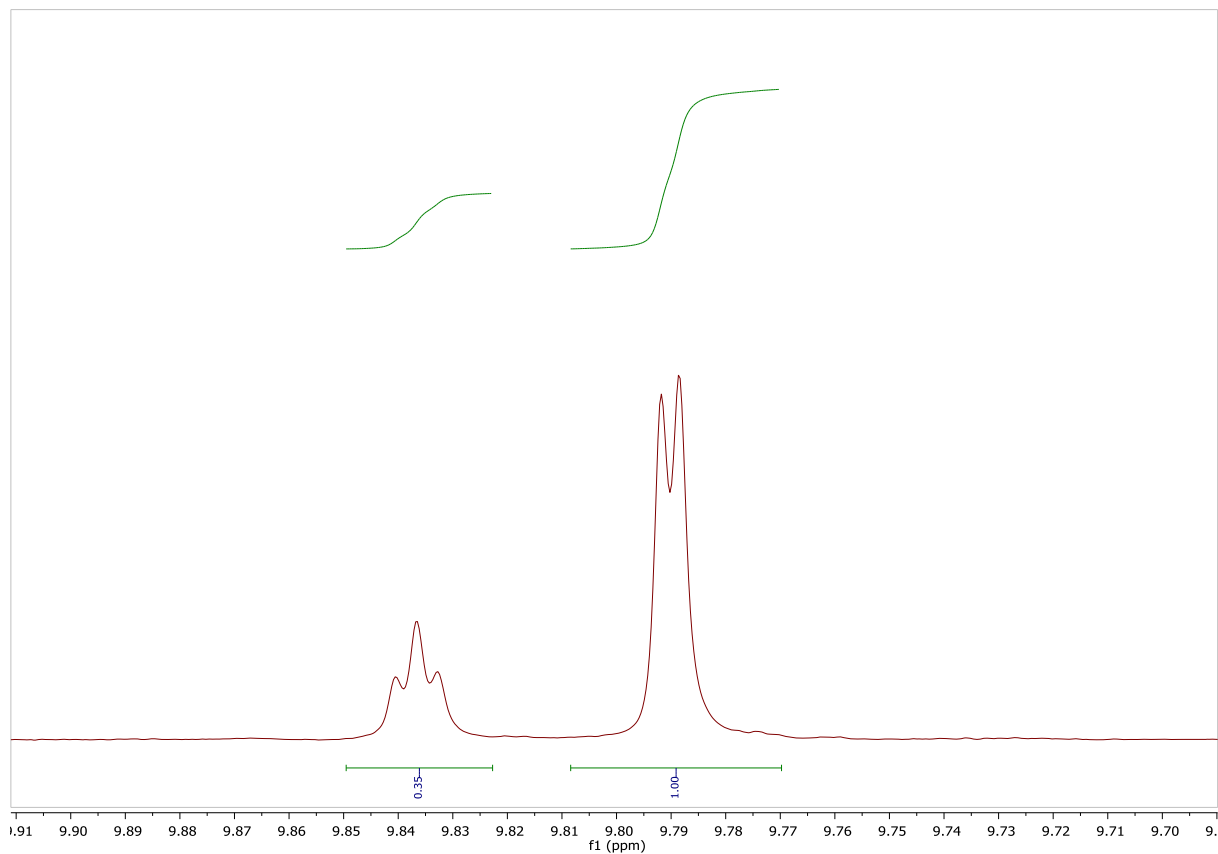
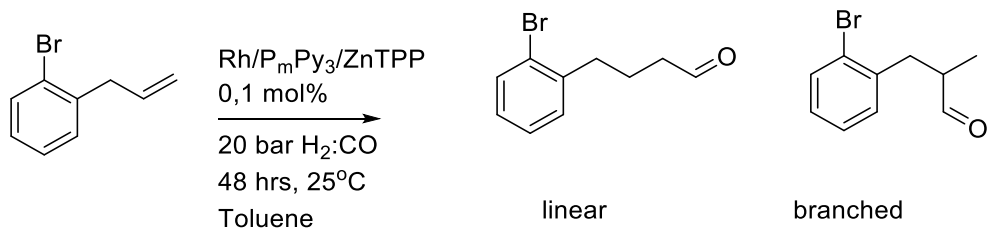
branched



Retention time	area		l/b ratio
11.621	837114	Branched	0.37
12.340	313939	Linear	

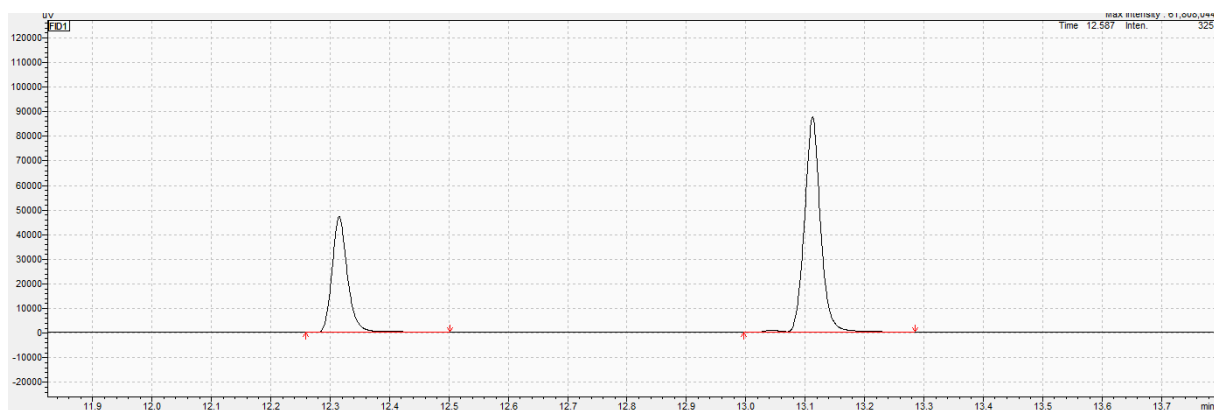
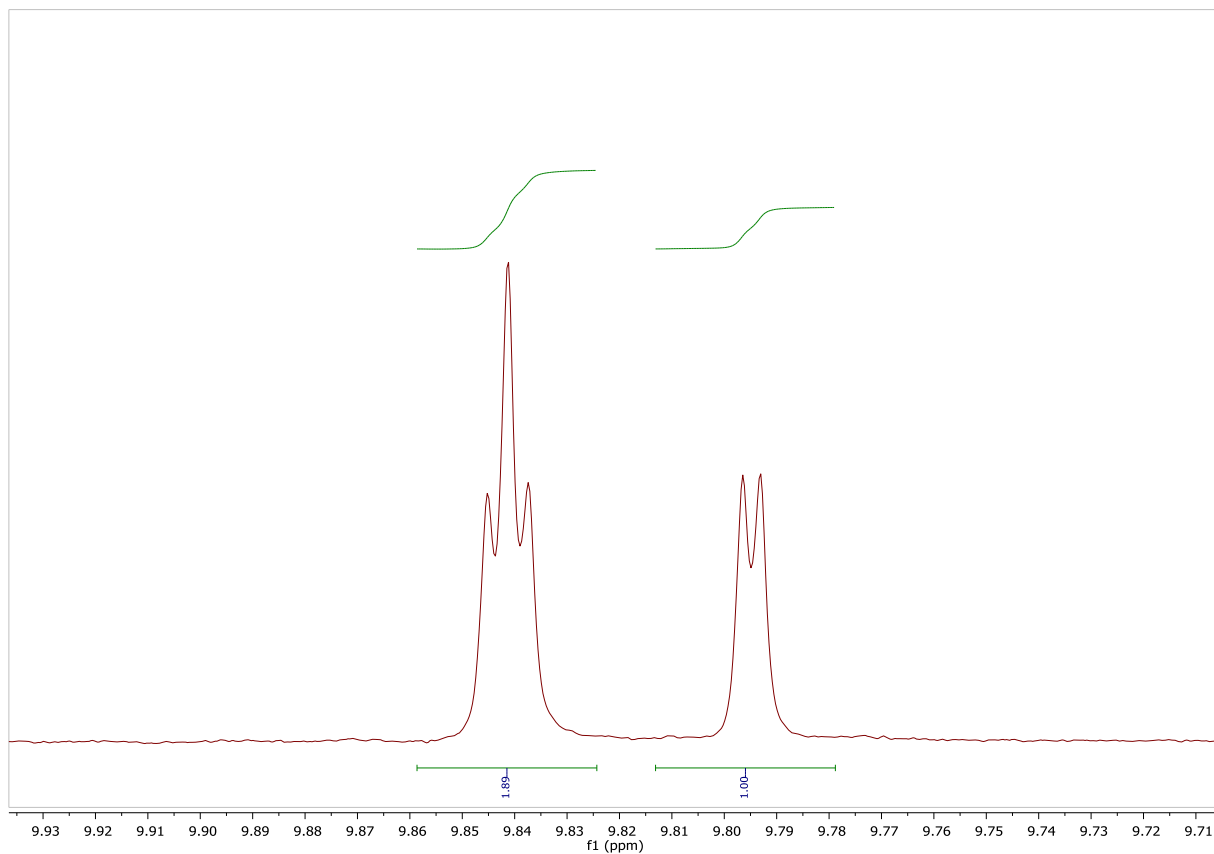
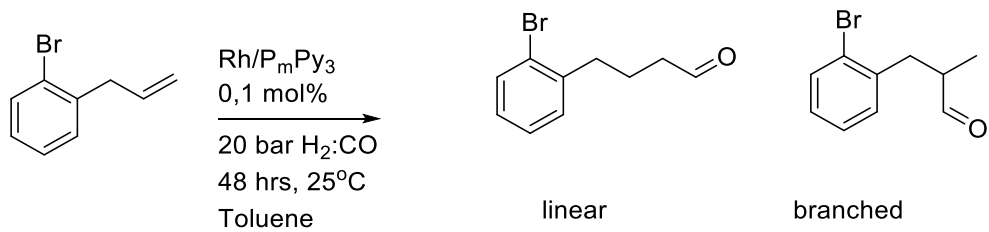


Retention time	area		l/b ratio
11.584	92942	Branched	1.88
12.329	175077	Linear	

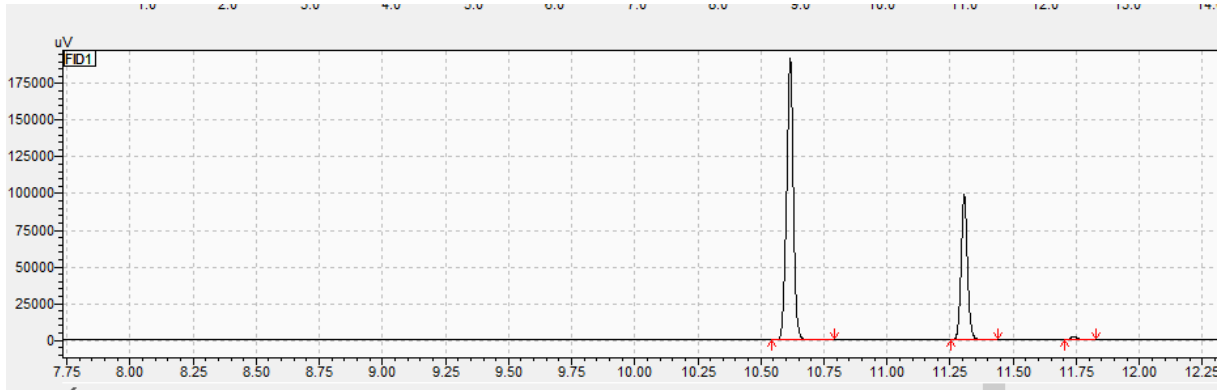
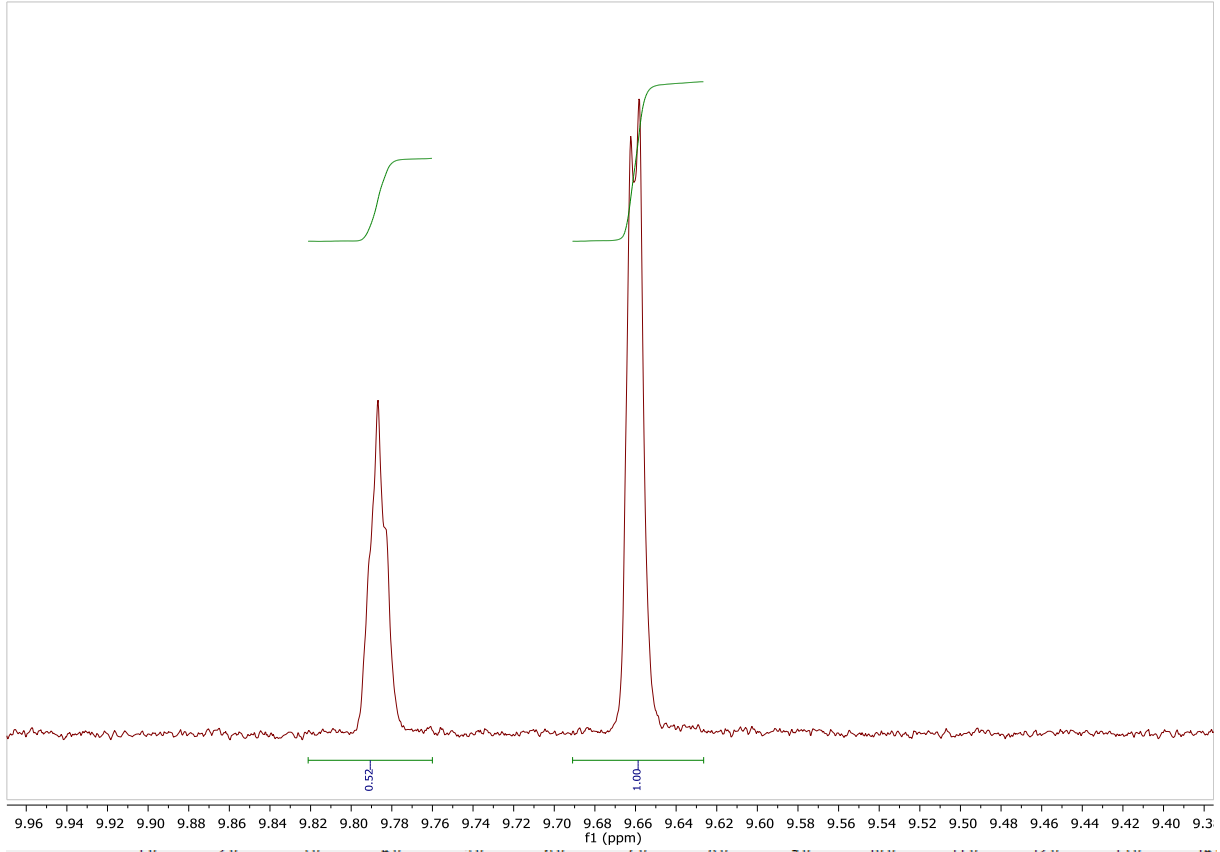
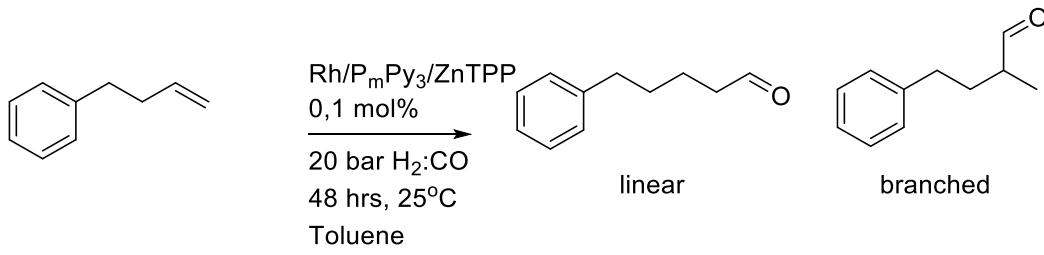


Retention time	area		l/b ratio
12.522	669865	Branched	0.31
13.117	210584	Linear	

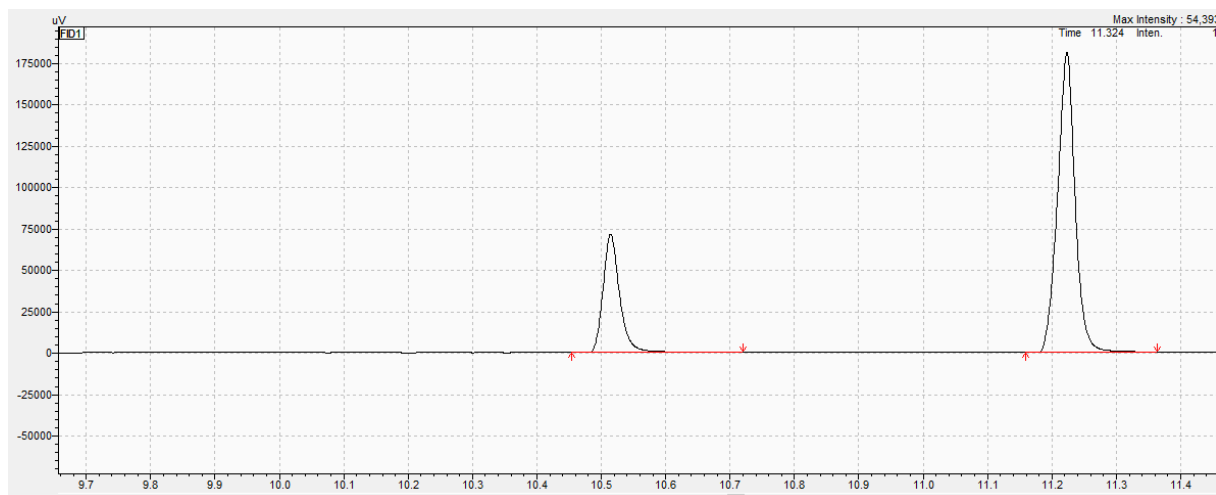
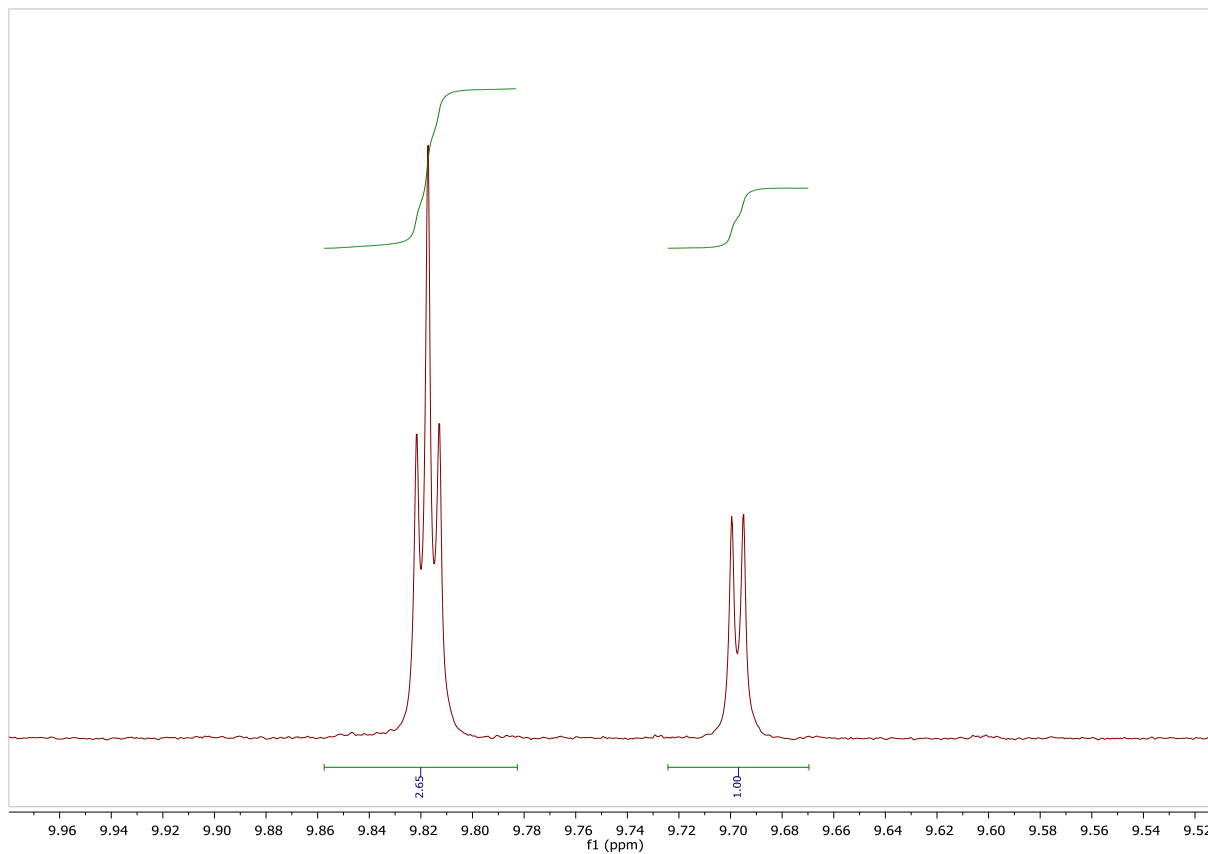
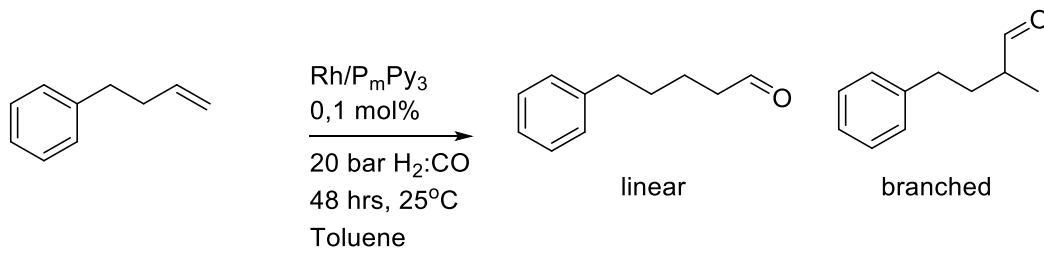




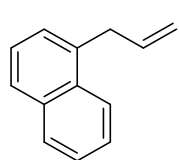
Retention time	area		l/b ratio
12.315	85273	Branched	1.93
13.113	164803	Linear	



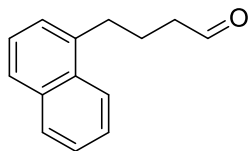
Retention time	area		l/b ratio
10,616	353443	Branched	0.49
11,306	172529	Linear	



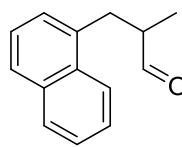
Retention time	area		l/b ratio
10.514	128428	Branhced	2.67
11.223	343725	linear	



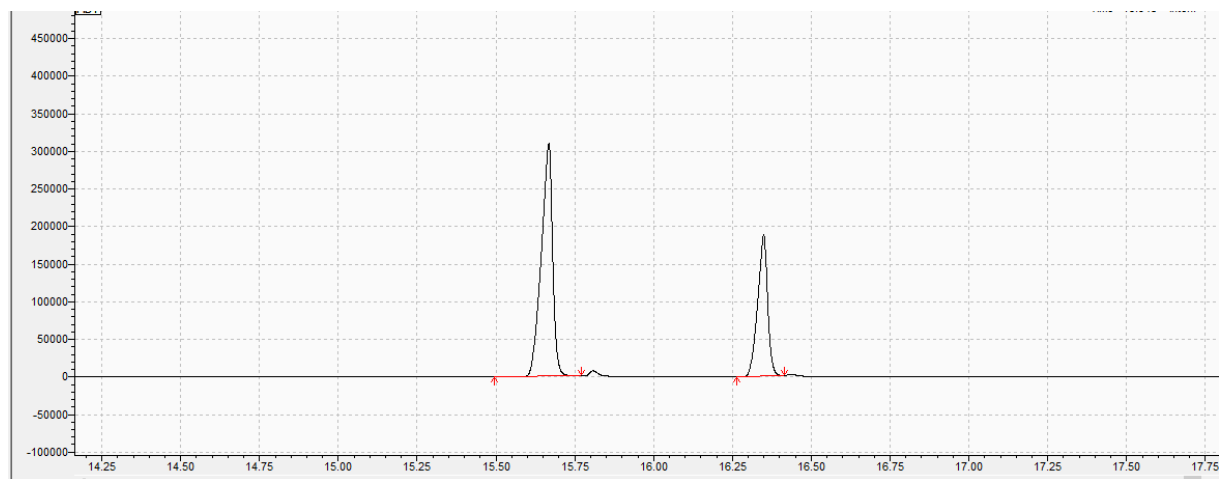
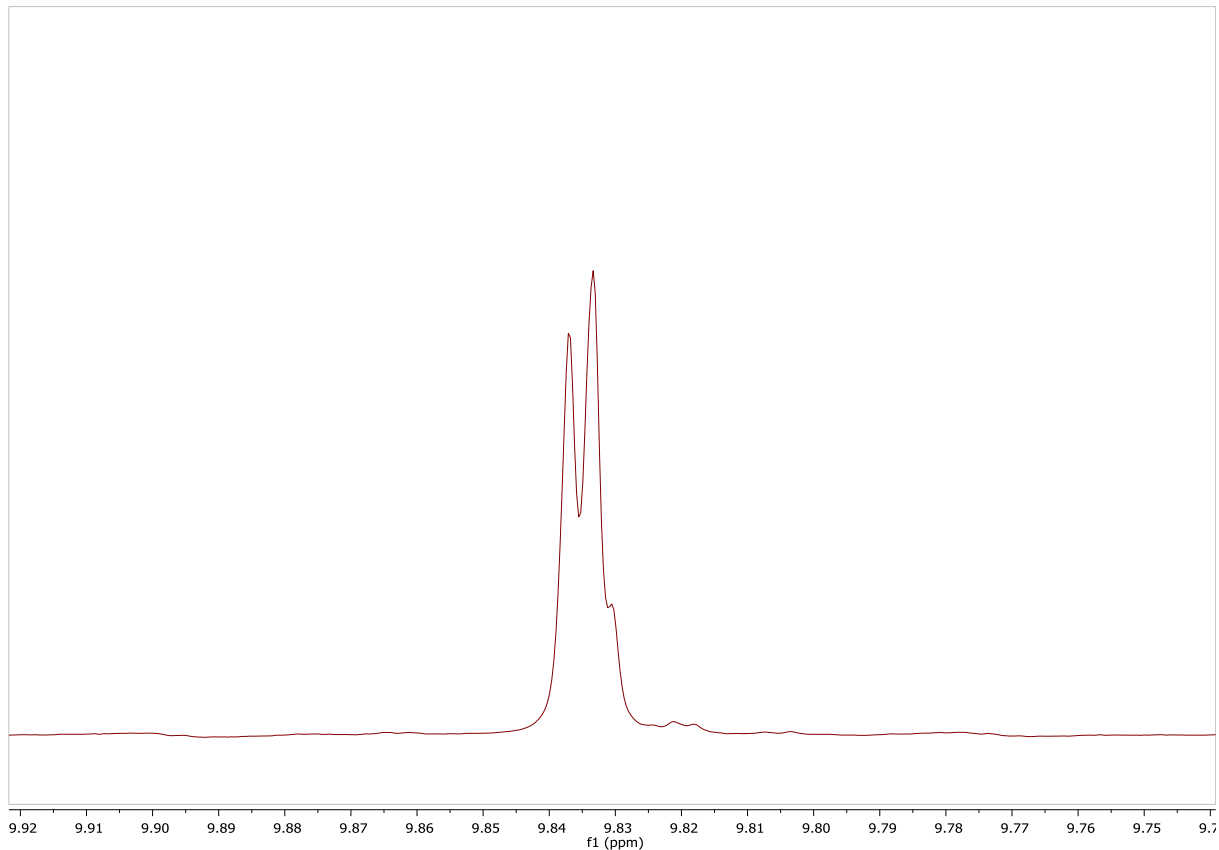
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



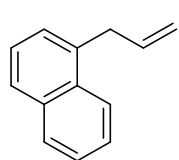
linear



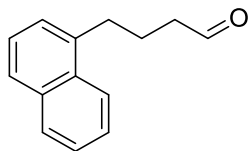
branched



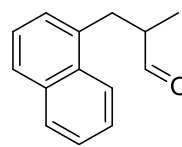
Retention time	Area		l/b ratio
15.667	768927	Branched	0.53
16.349	410501	Linear	



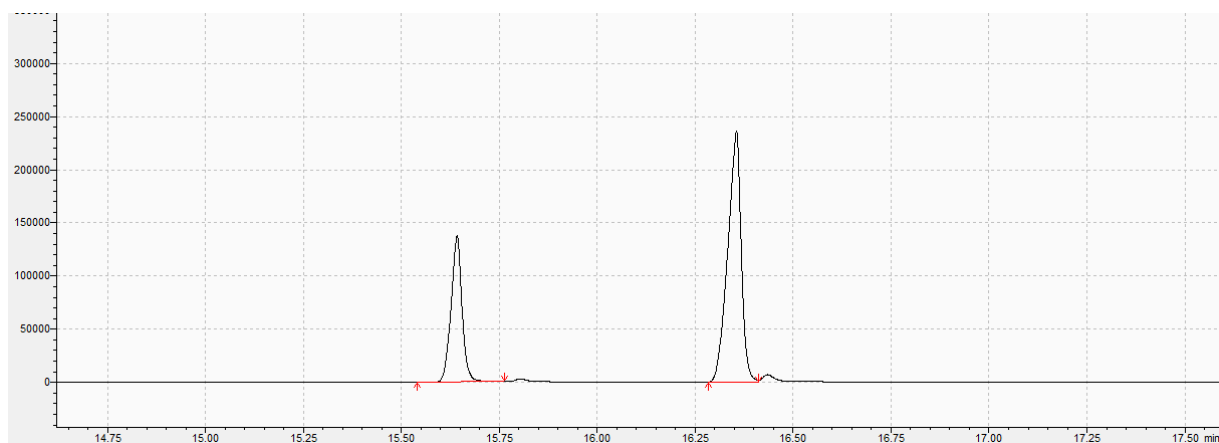
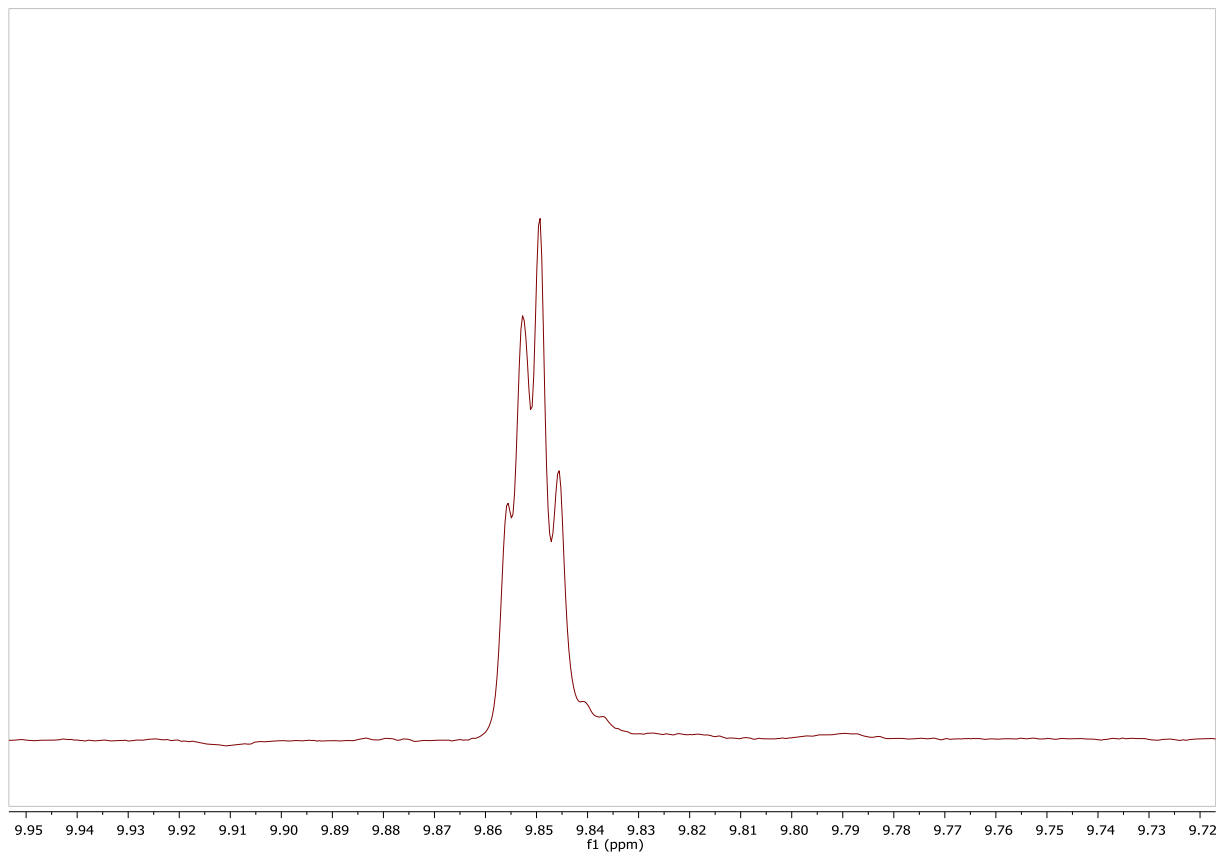
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



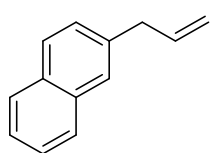
linear



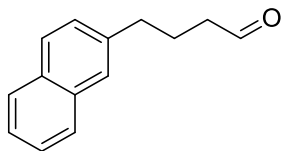
branched



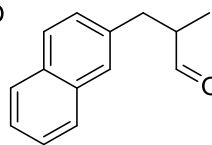
Retention time	Area		I/b ratio
15.642	266118	Branched	2.11
16.355	562816	Linear	



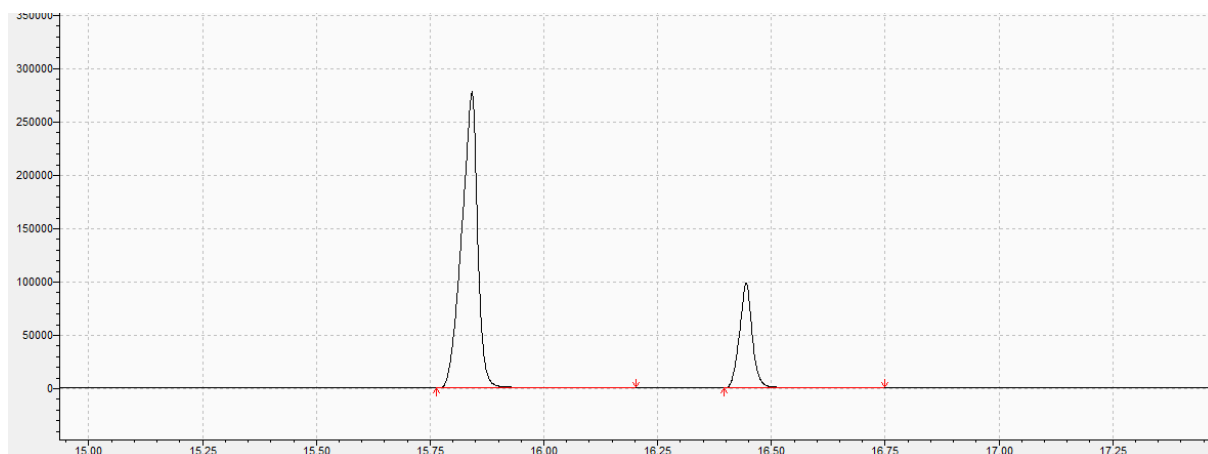
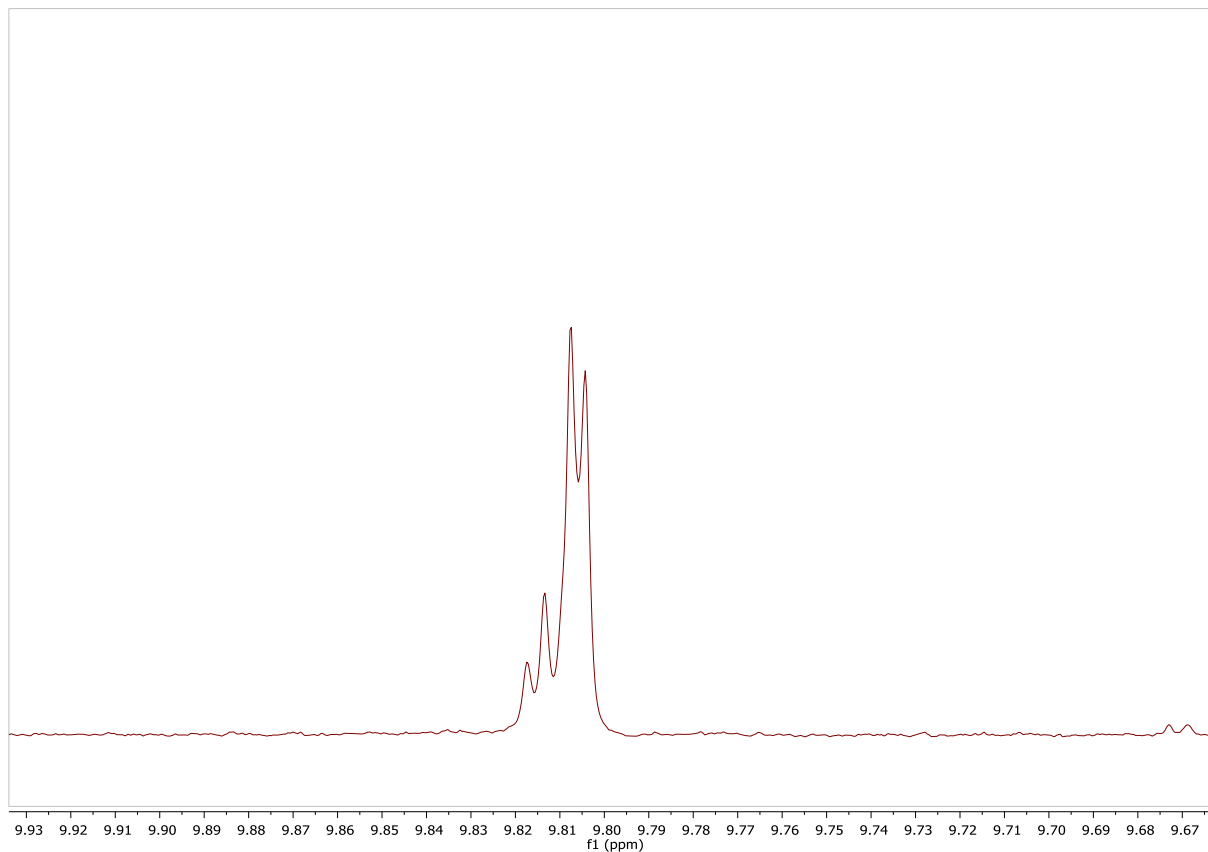
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



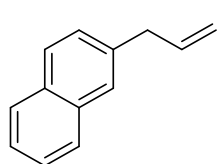
linear



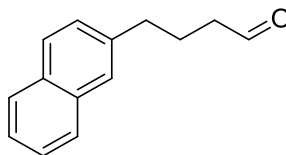
branched



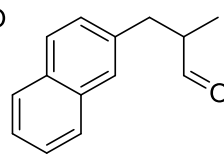
Retention time	Area		l/b ratio
15.842	675010	Branched	0.29
16.444	194156	Linear	



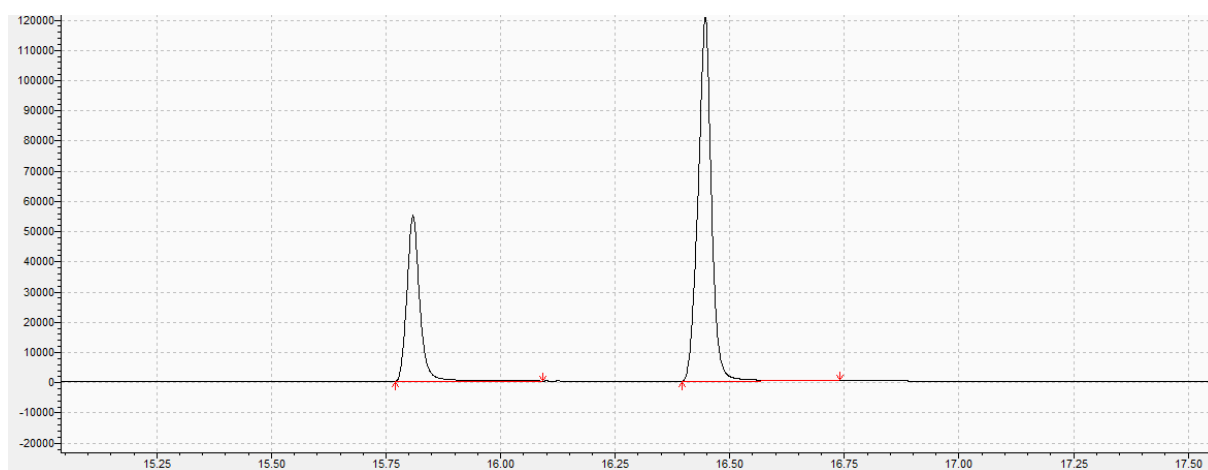
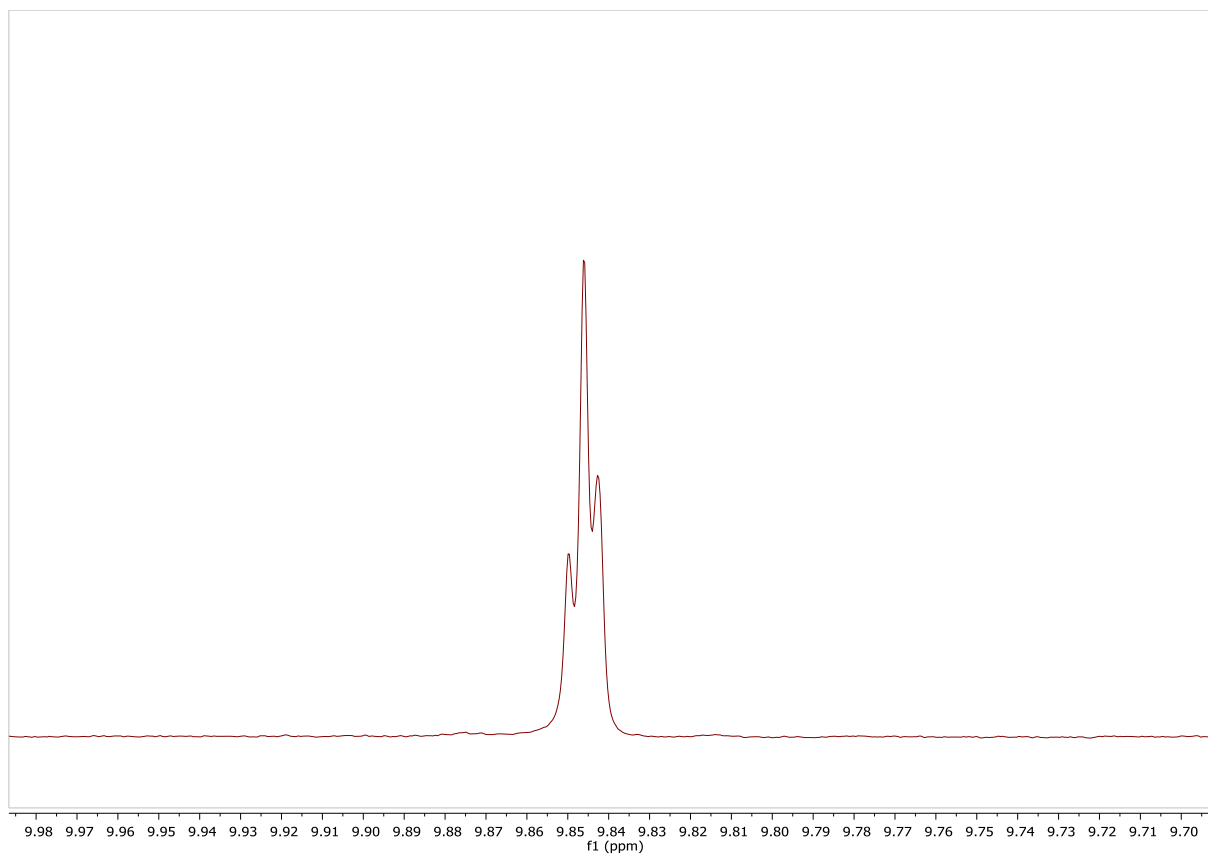
Rh/P<sub>m</sub>Py<sub>3</sub>  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



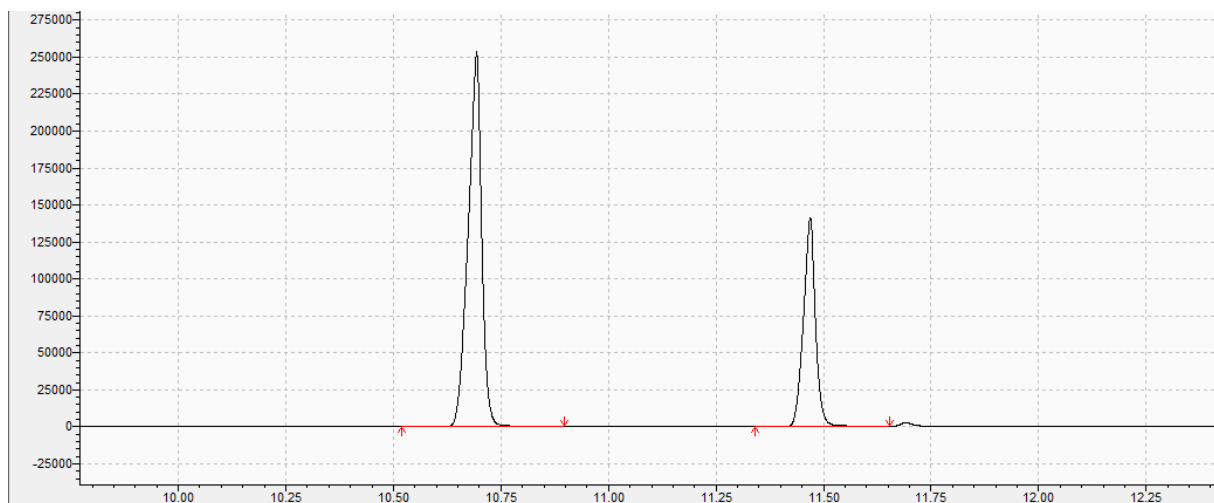
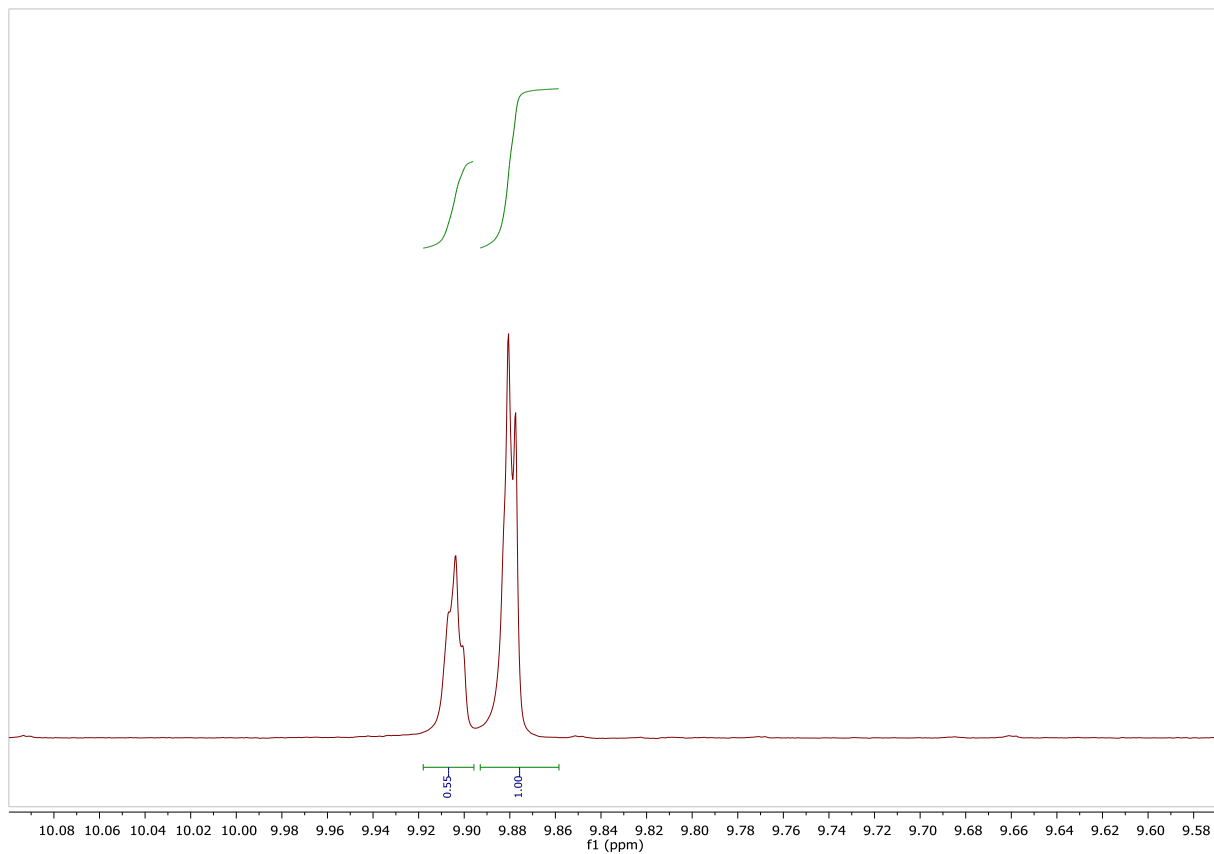
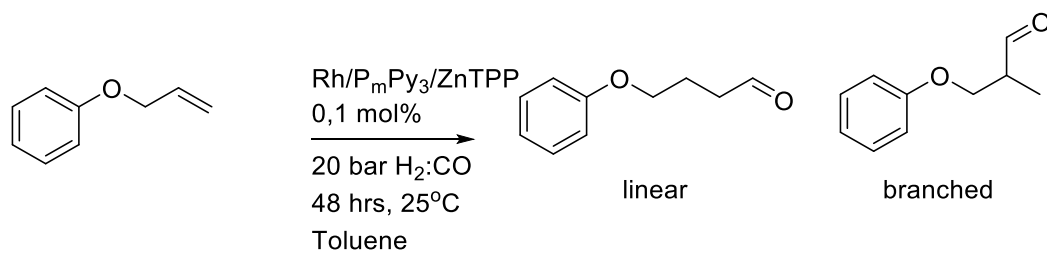
linear



branched

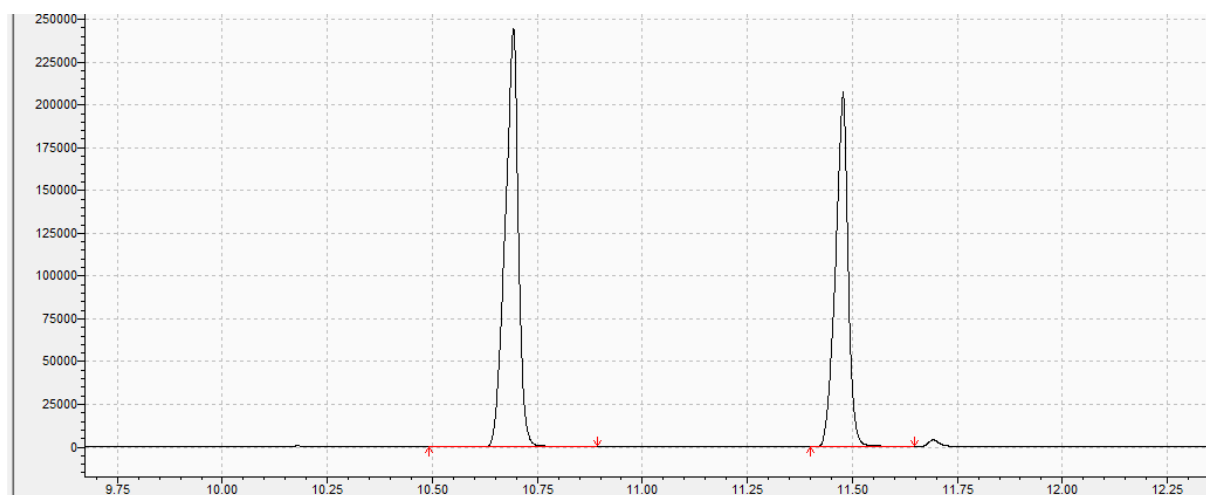
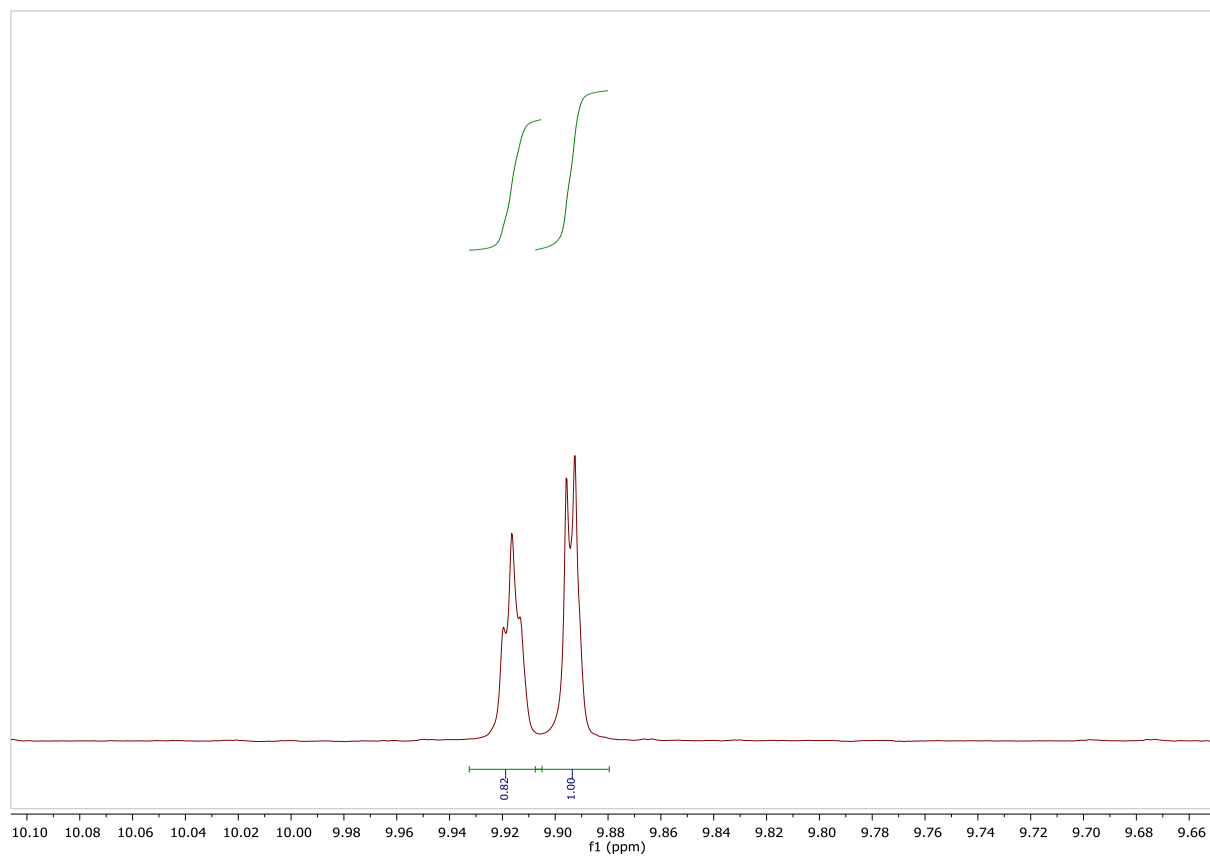
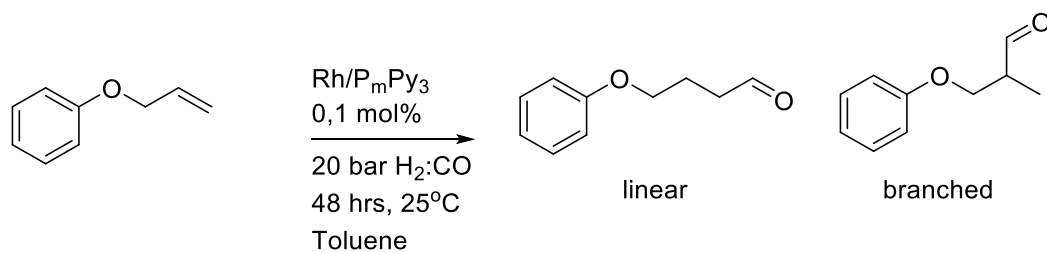


Retention time	Area		l/b ratio
15.809	106270	Branched	2.3
16.447	245019	Linear	

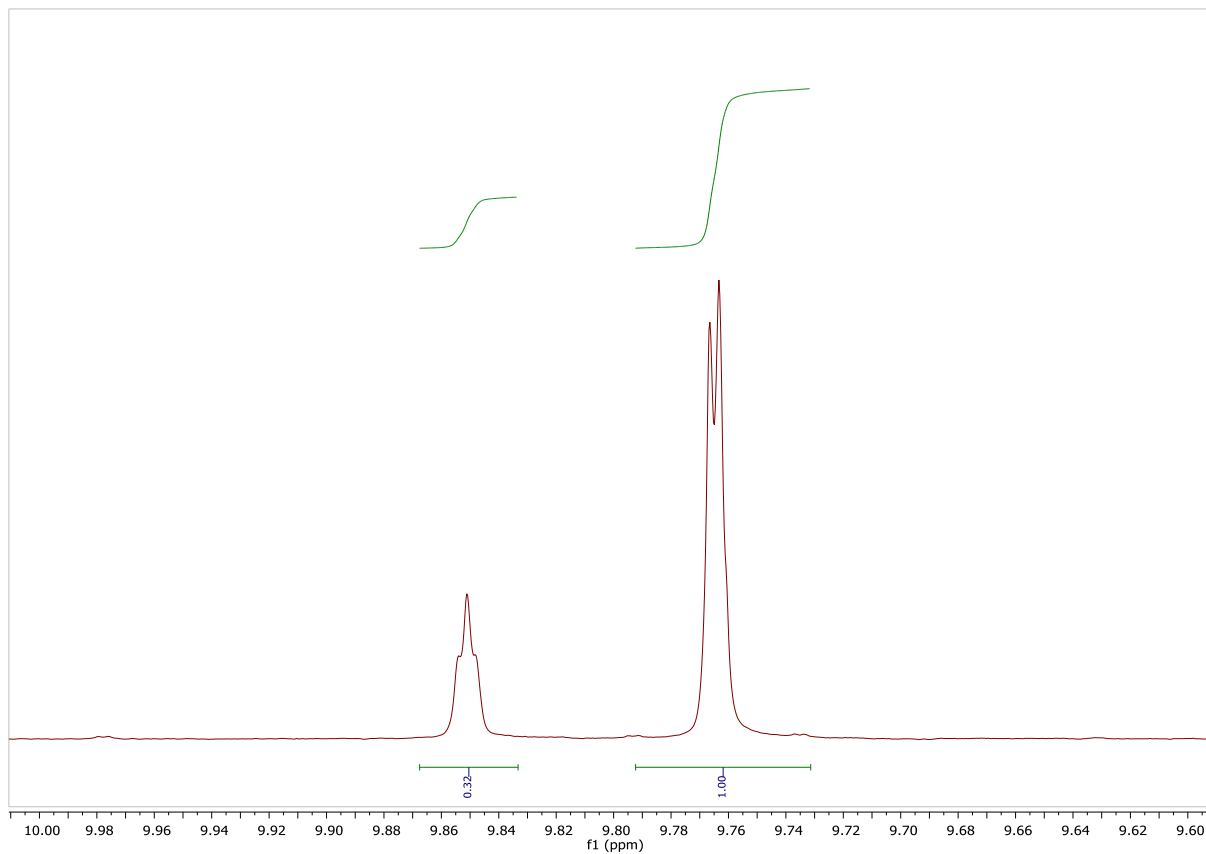
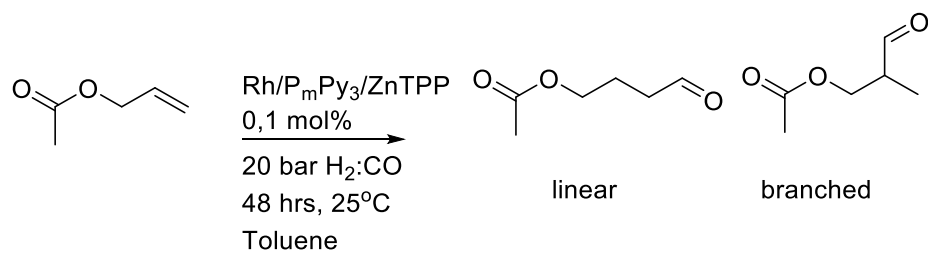


Retention time	area		l/b ratio
10,693	551755	Branhced	0.49
11,469	271895	linear	

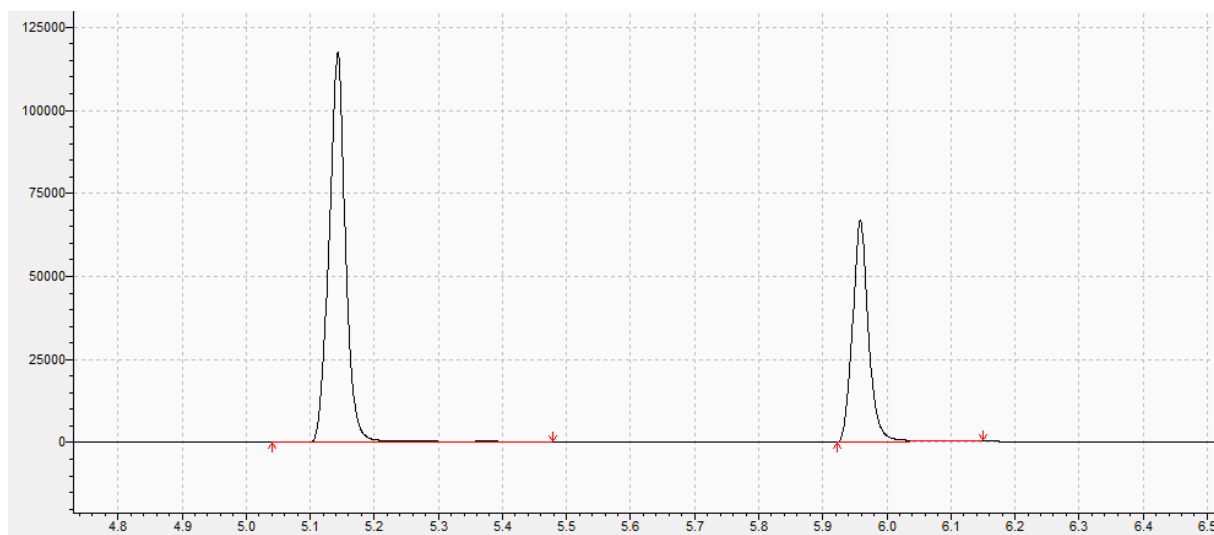
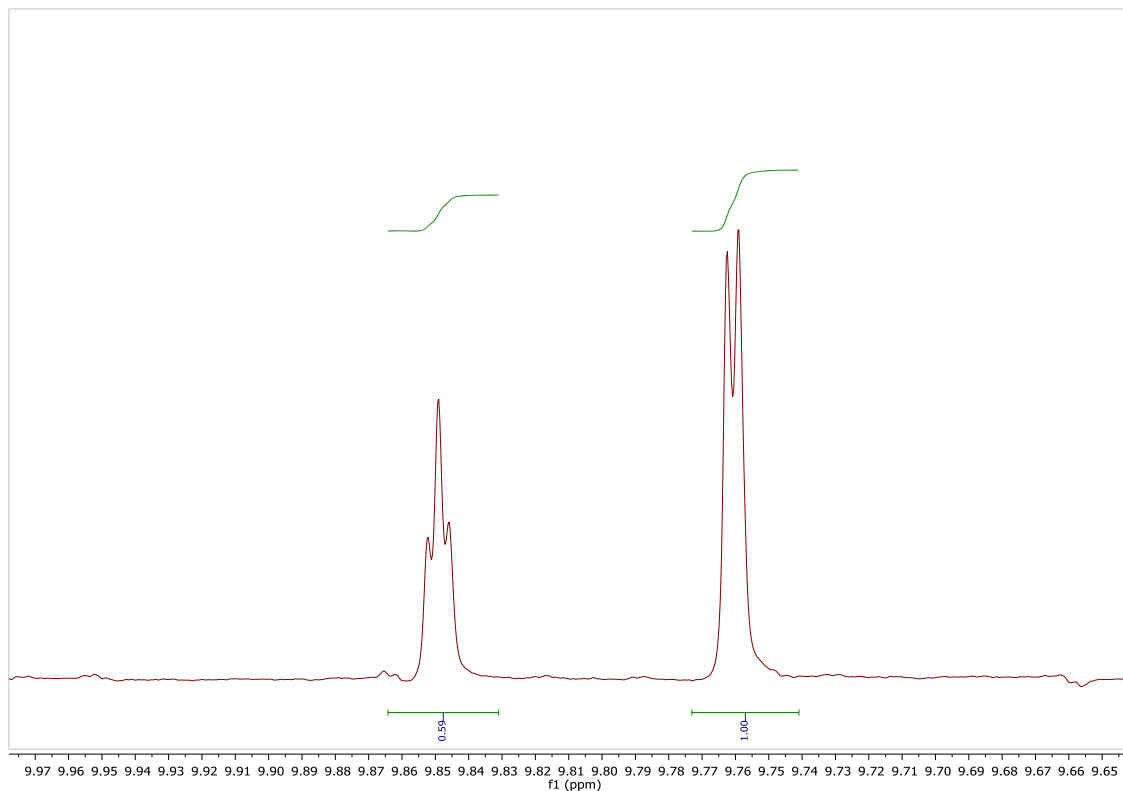
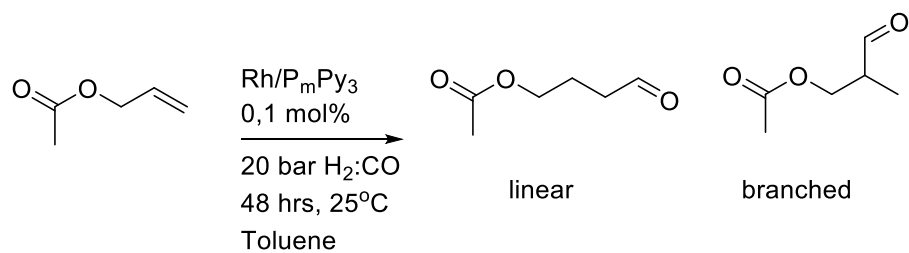




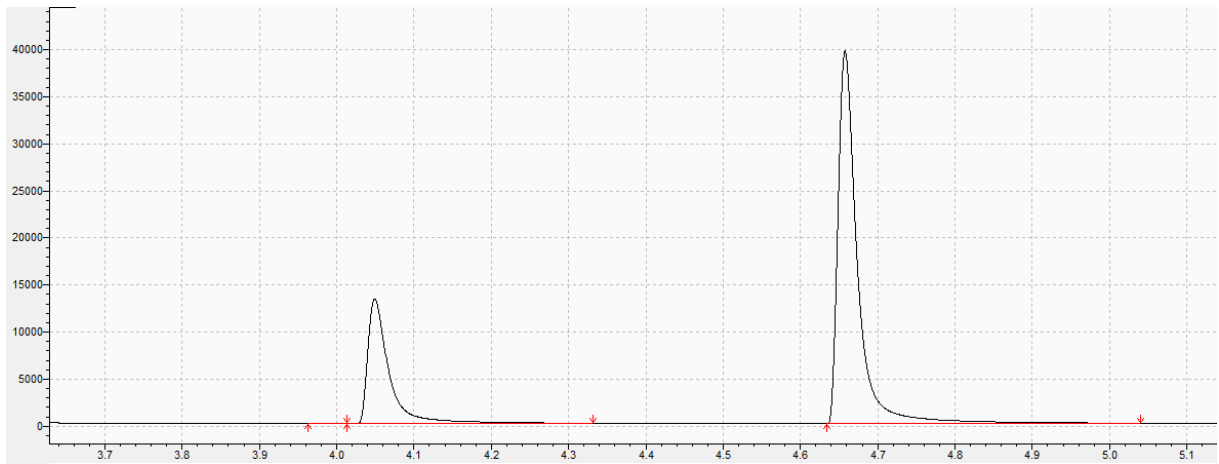
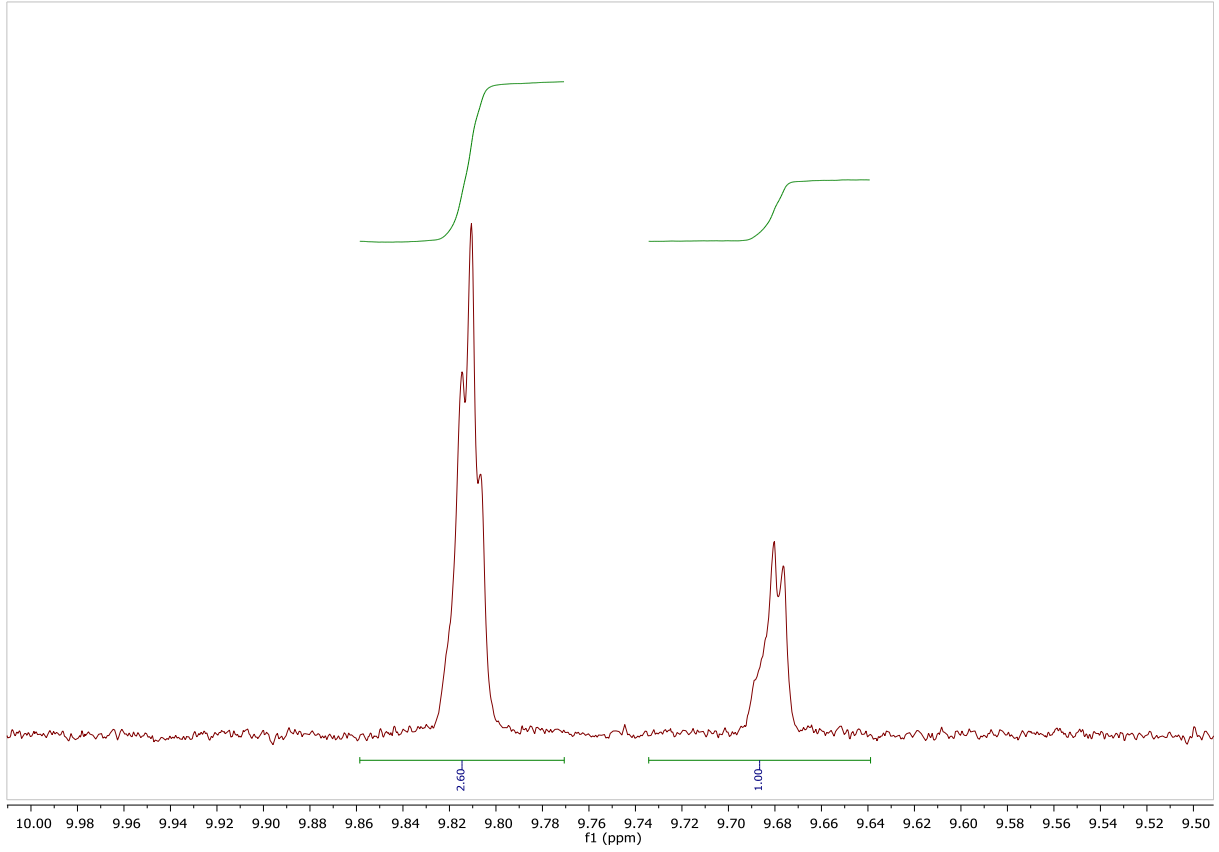
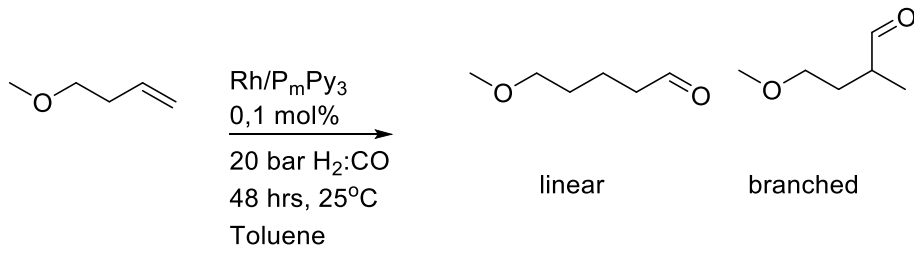
Retention time	area		l/b ratio
10,693	534301	Branched	0.81
11,478	430359	Linear	



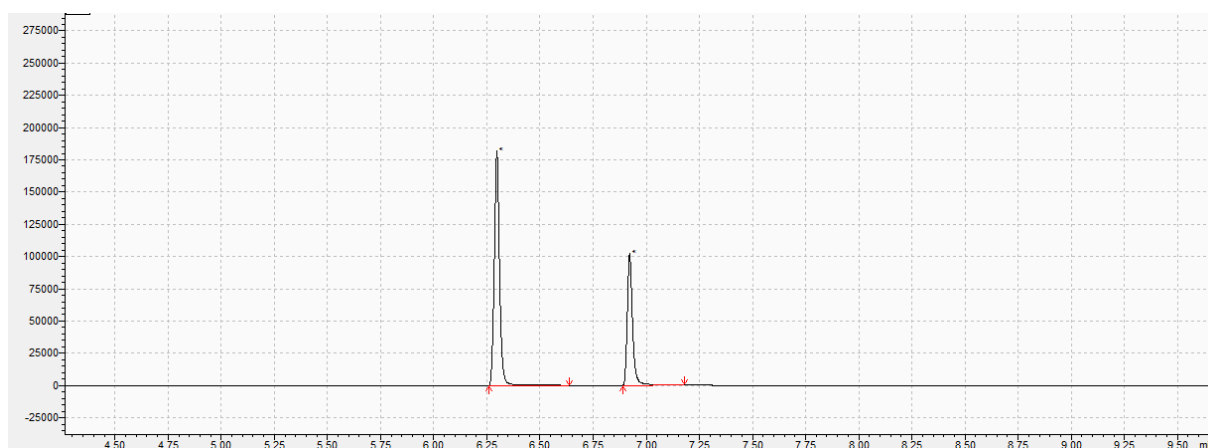
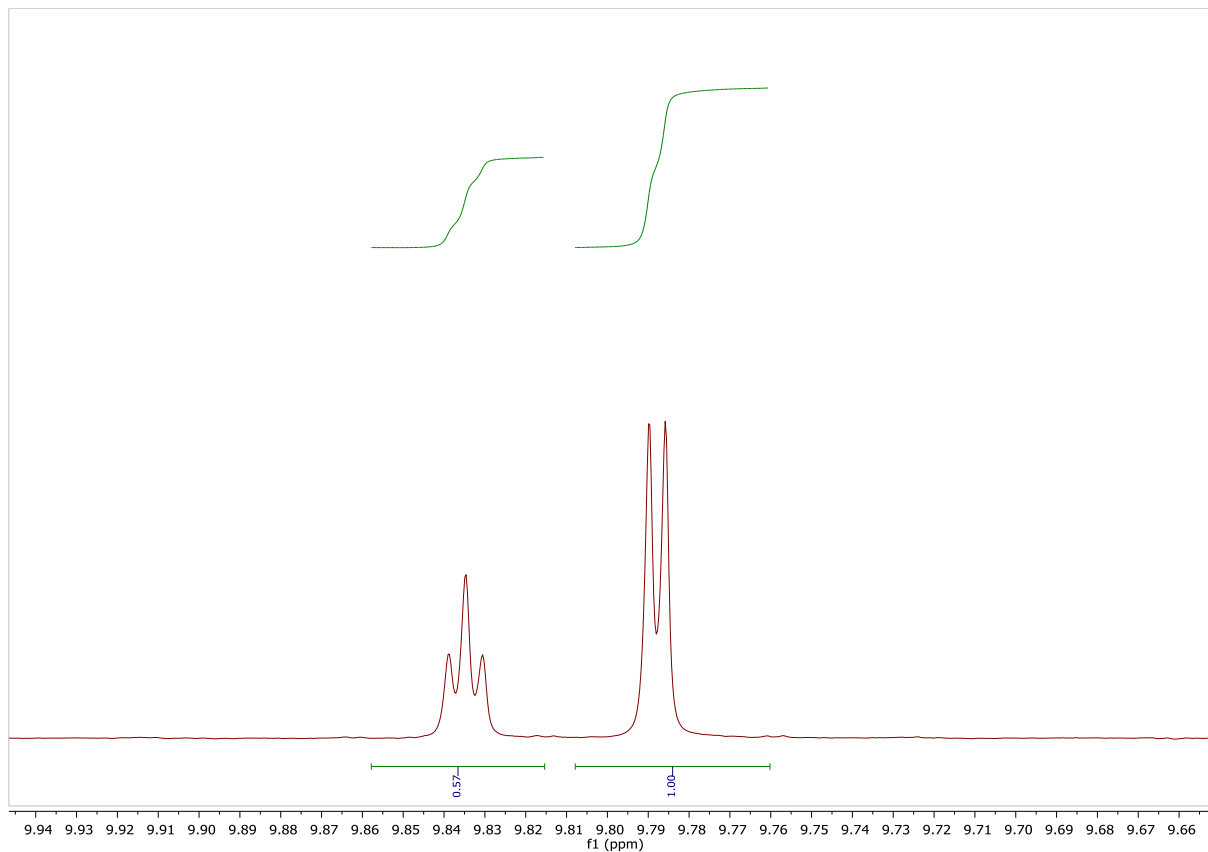
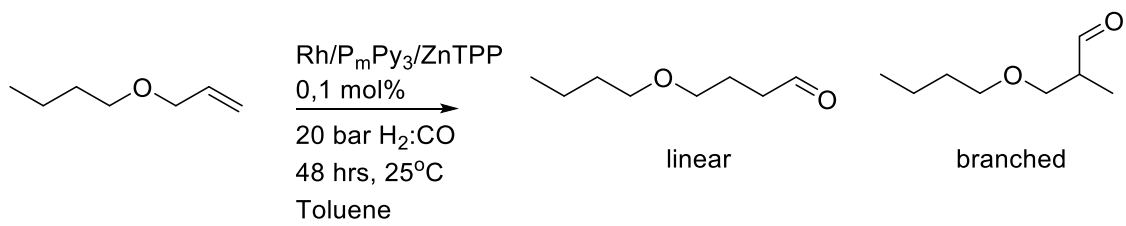
Retention time	Area		l/b ratio
5,149	296142	Branched	0.28
5,955	83859	linear	



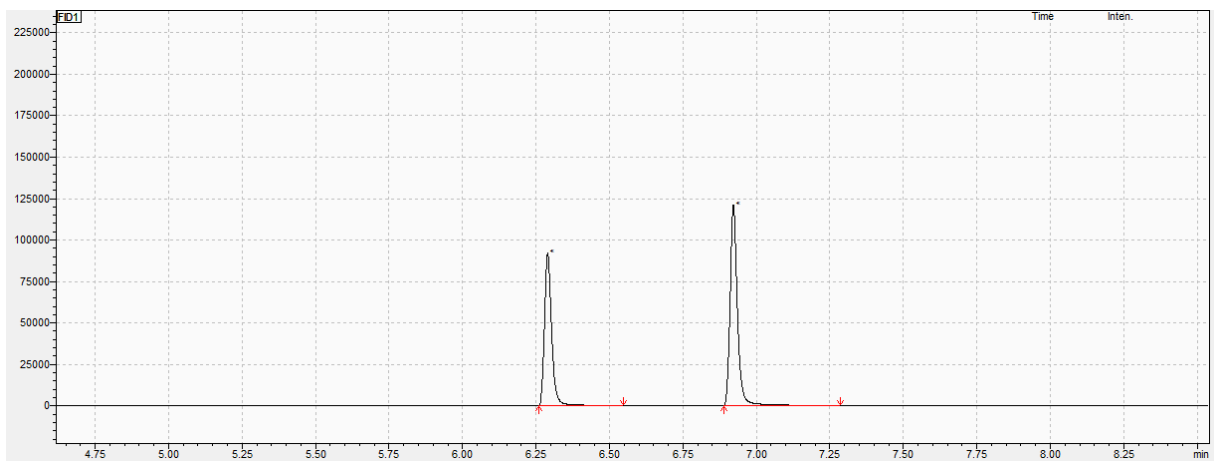
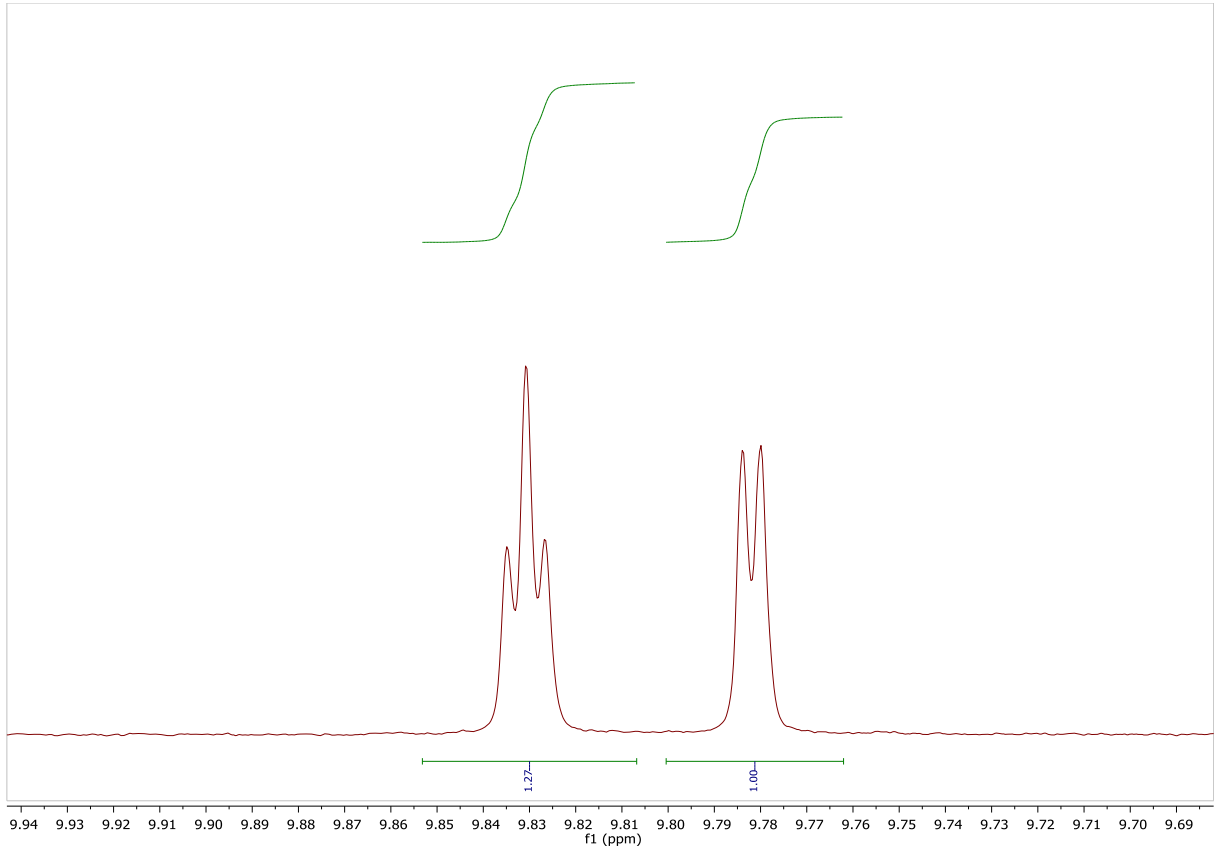
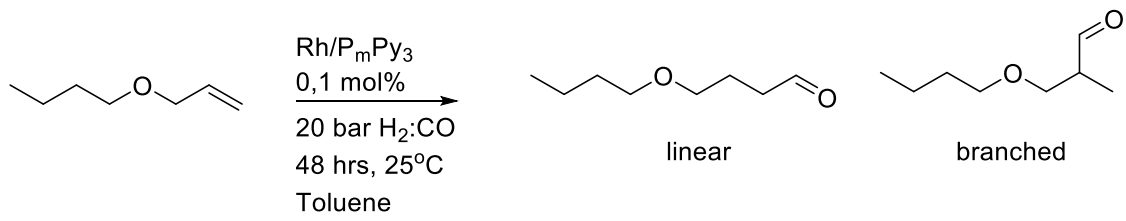
Retention time	Area		I/b ratio
		Branched	0,55
5,143	208037		
5,959	115130	Linear	



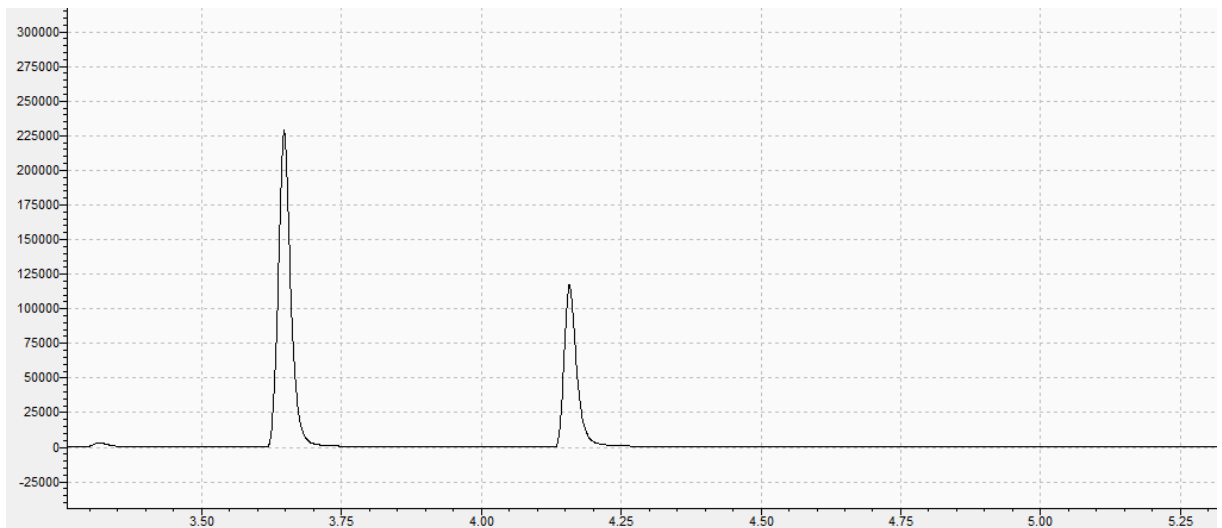
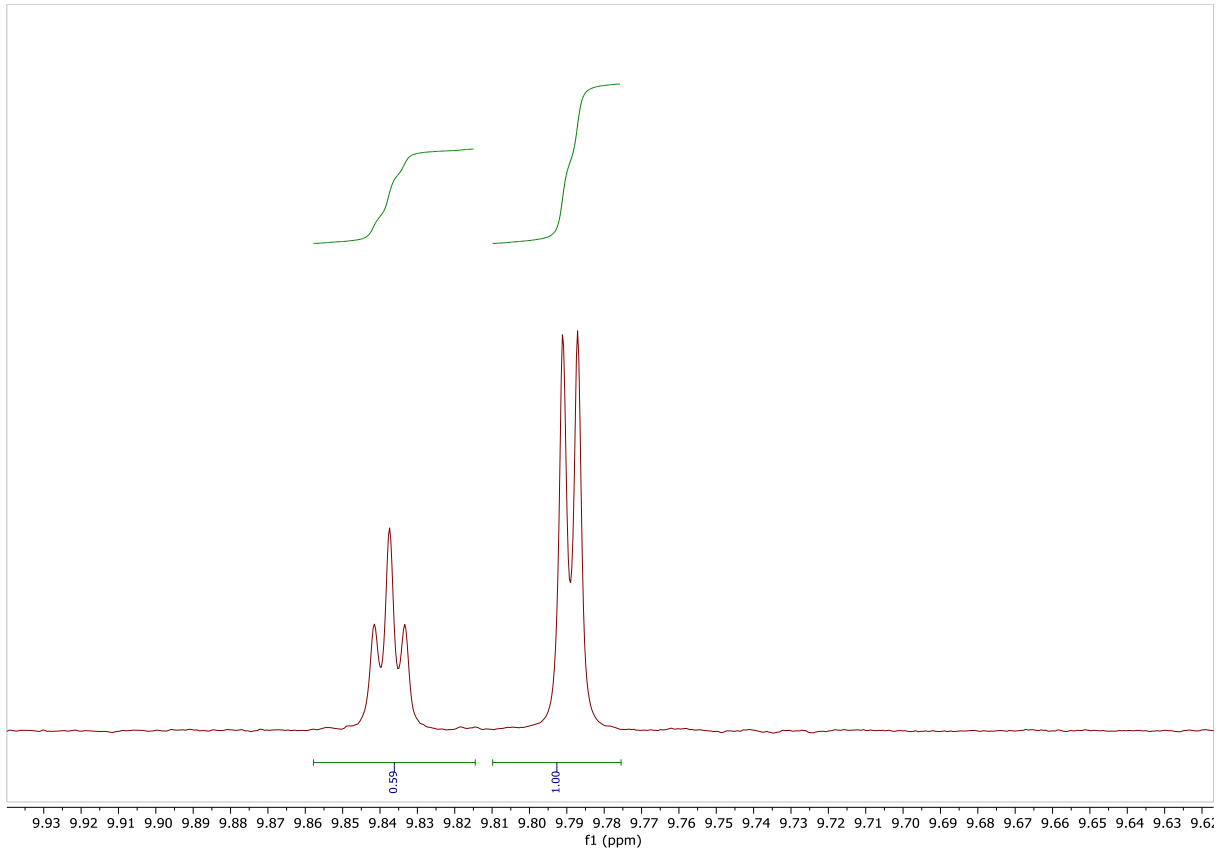
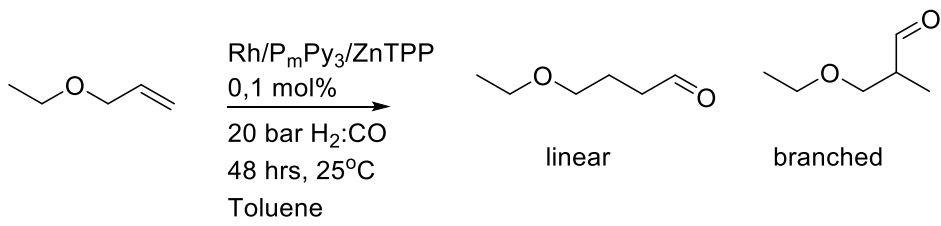
Retention time	Area		l/b ratio
4.050	25122	Branched	2.77
4.658	69836	Linear	



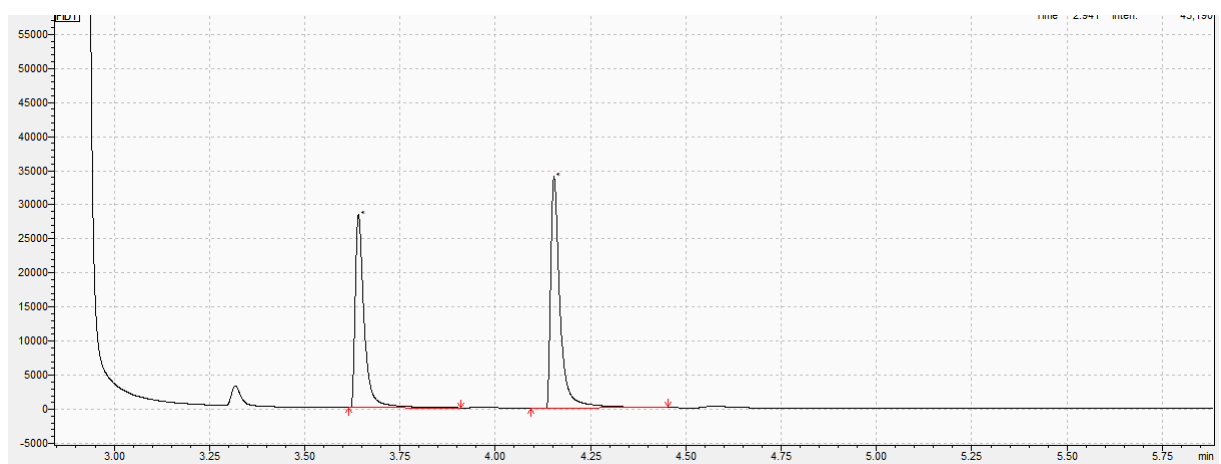
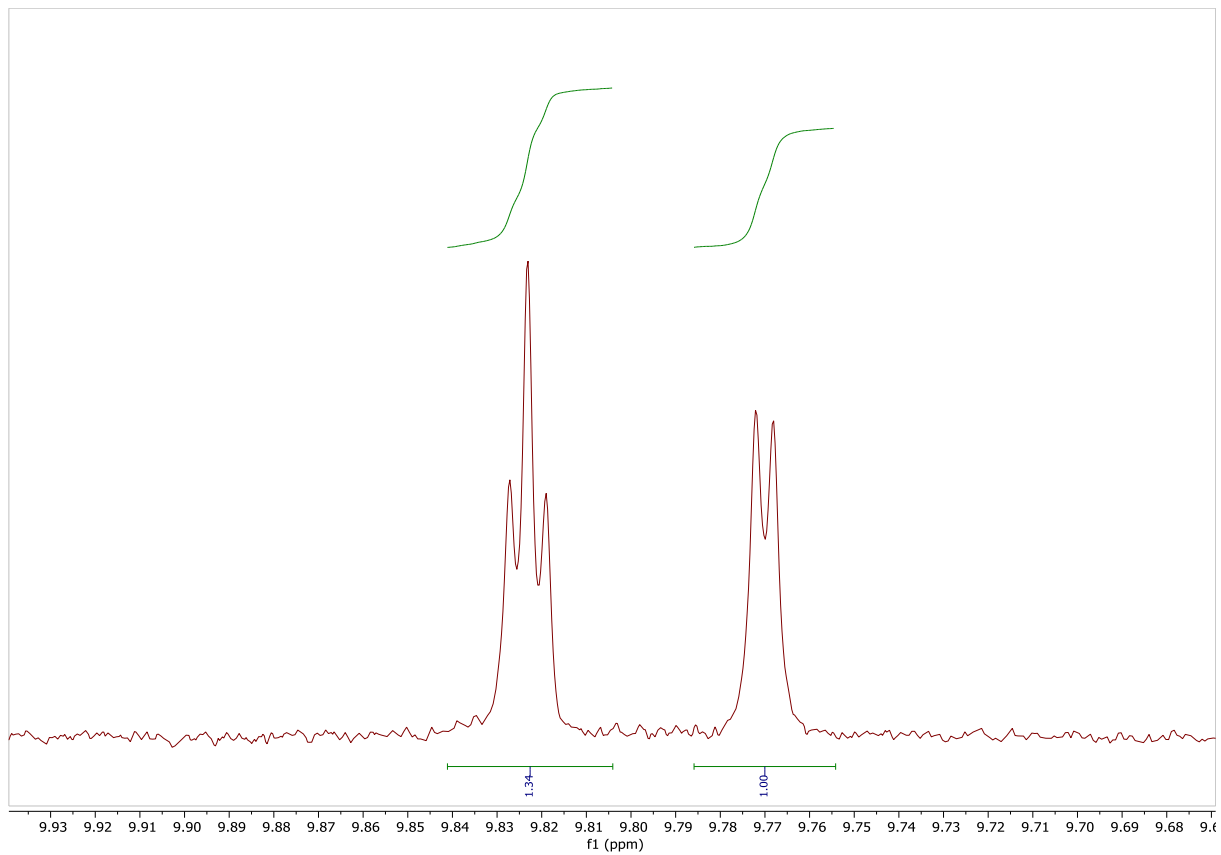
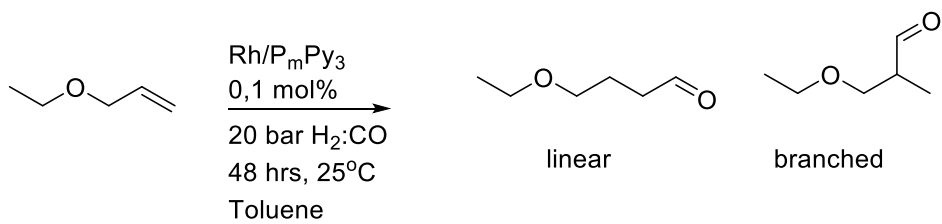
Retention time	Area		I/b ratio
6.297	309236	Branched	0.56
6.922	175534	Linear	



Retention time	Area		I/b ratio
6.290	153685	Branched	1.37
6.922	210656	Linear	

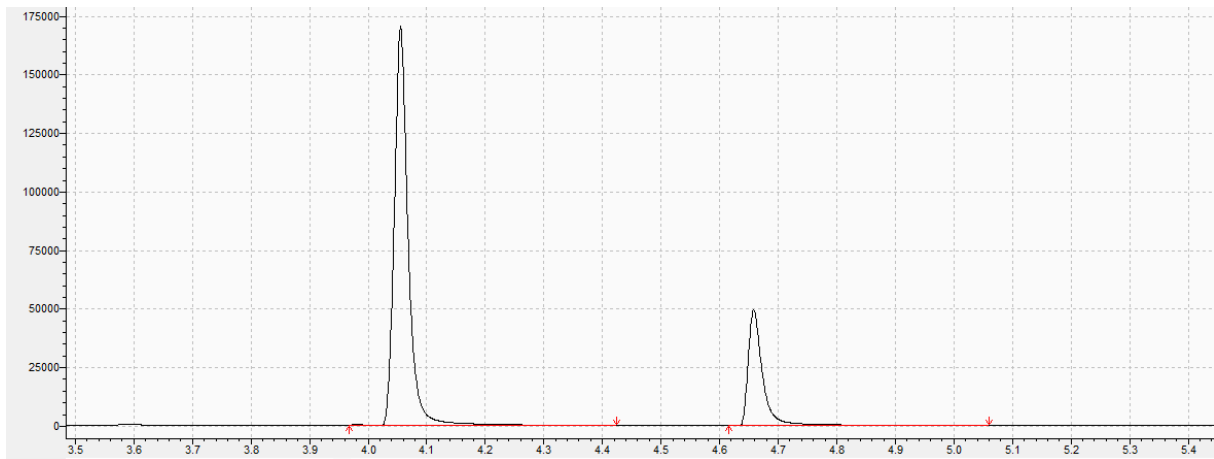
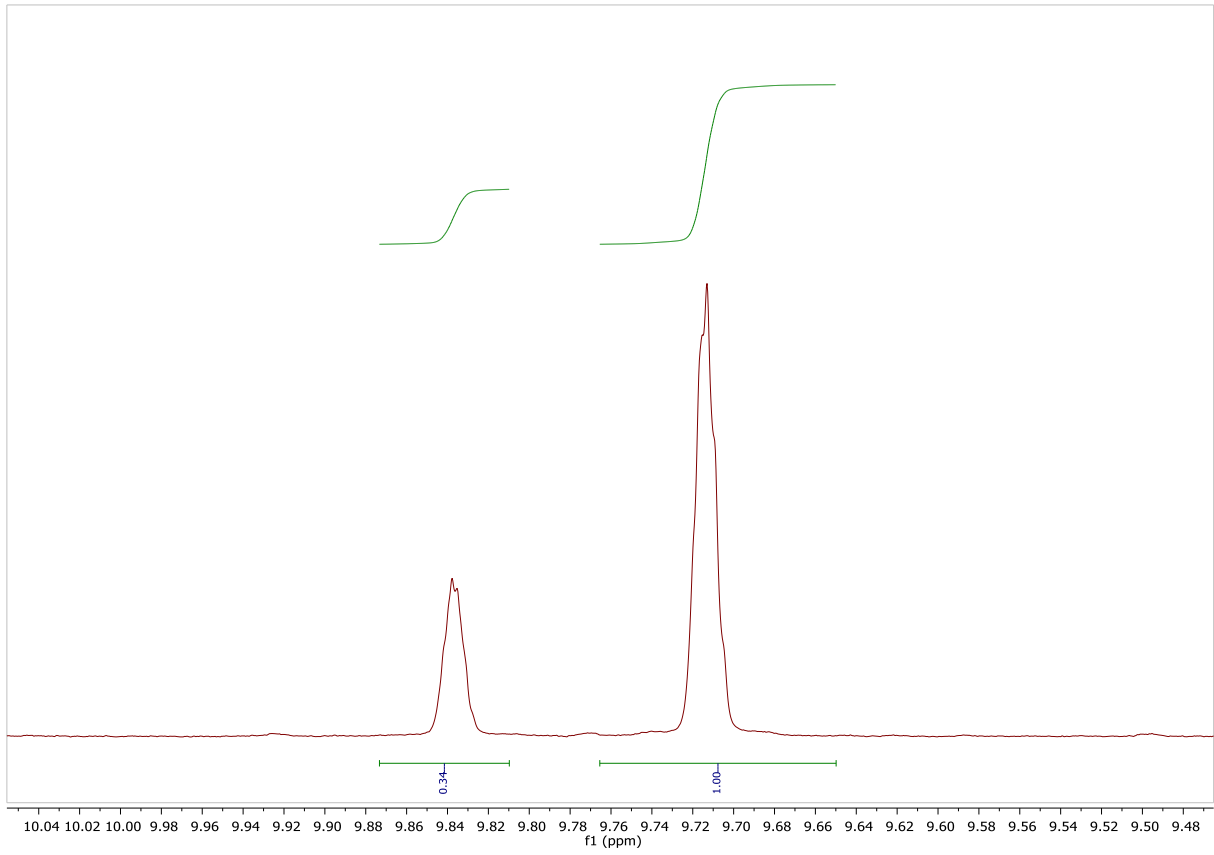
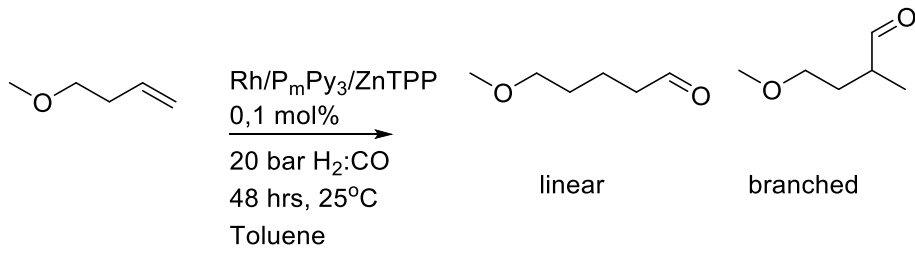


Retention time	Area		l/b ratio
3.648	357585	Branched	0.52
4.158	188152	Linear	

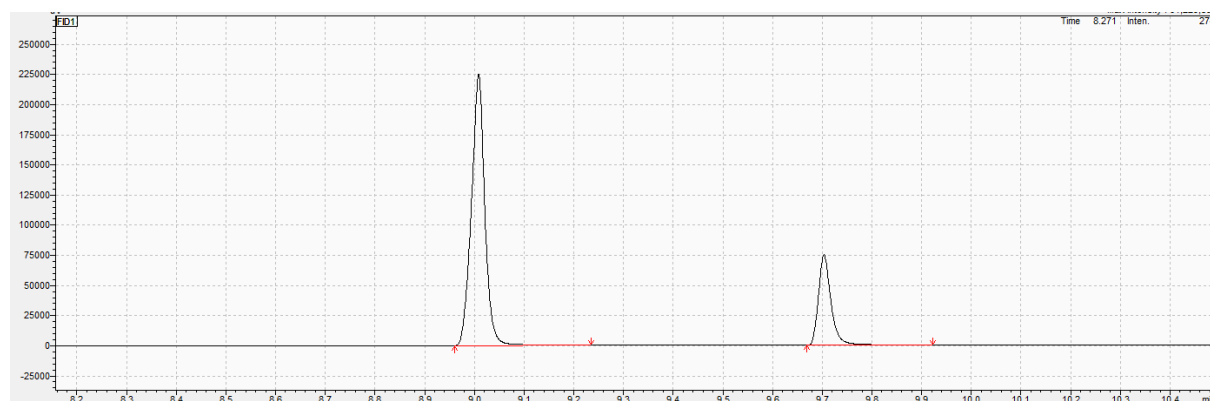
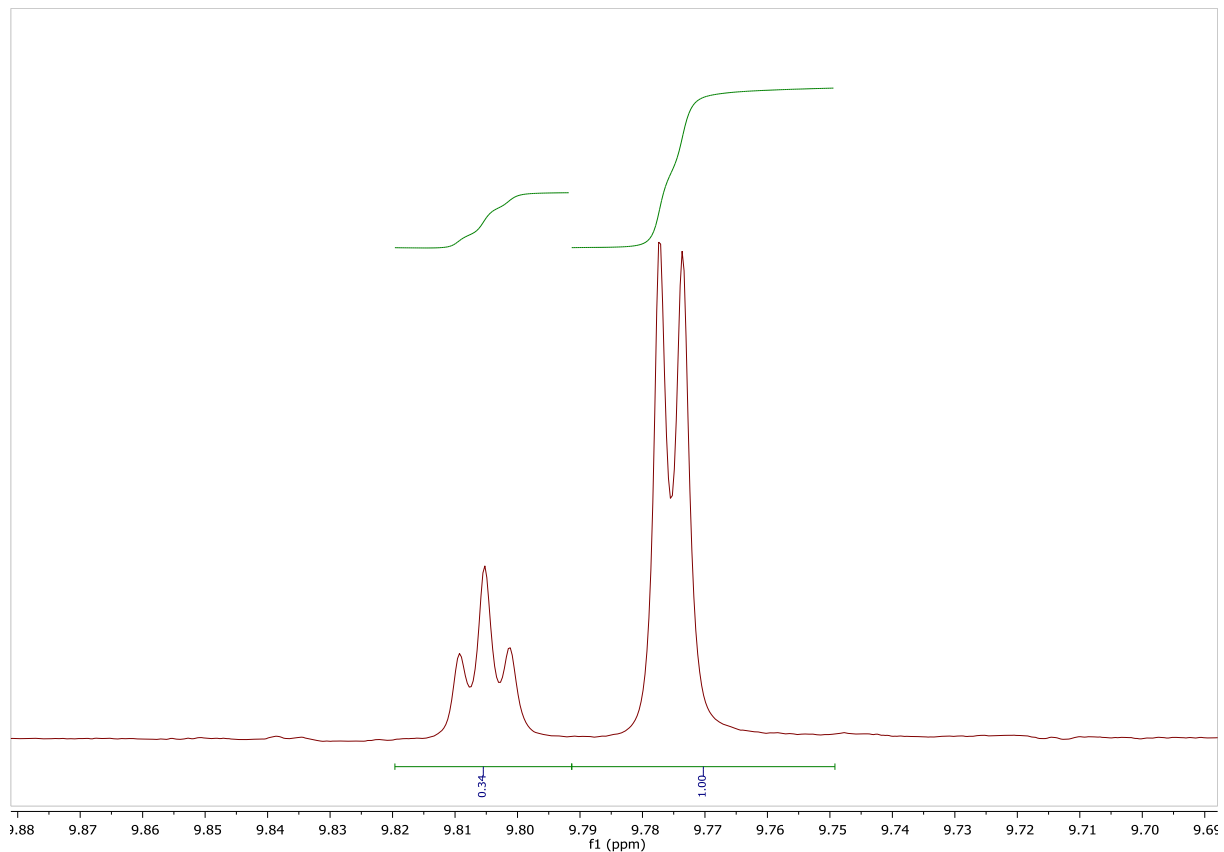
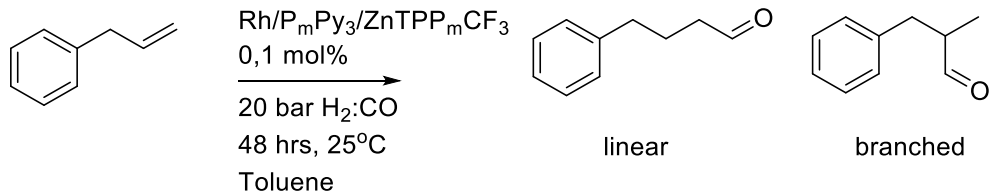


Retention time	Area		I/b ratio
3.641	47225	Branched	1.24
4.154	58604	Linear	

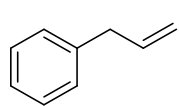




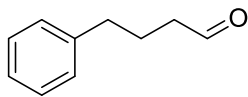
Retention time	Area		l/b ratio
4.055	278529	Branched	0.30
4.658	84464	Linear	



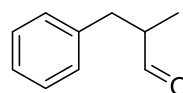
Retention time	Area		I/b ratio
9.008	420479	Branched	0.31
9.704	133089	Linear	



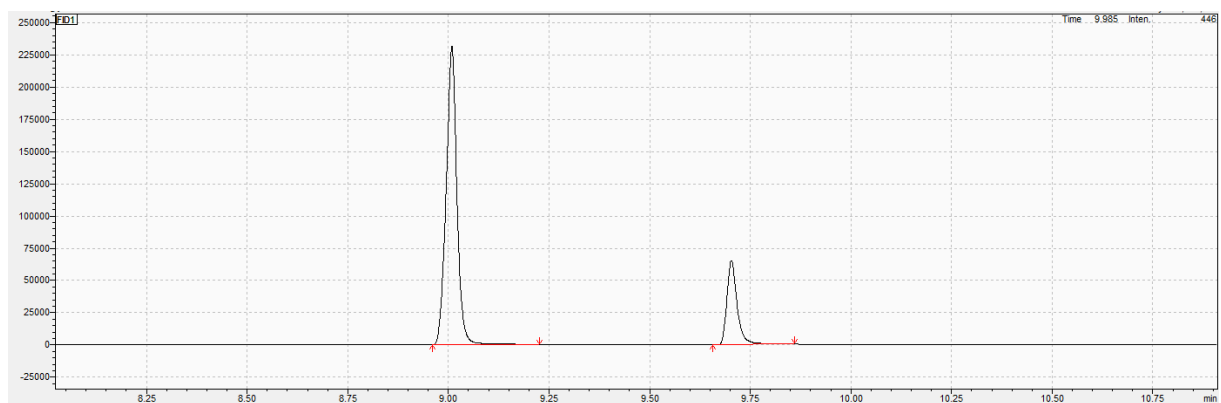
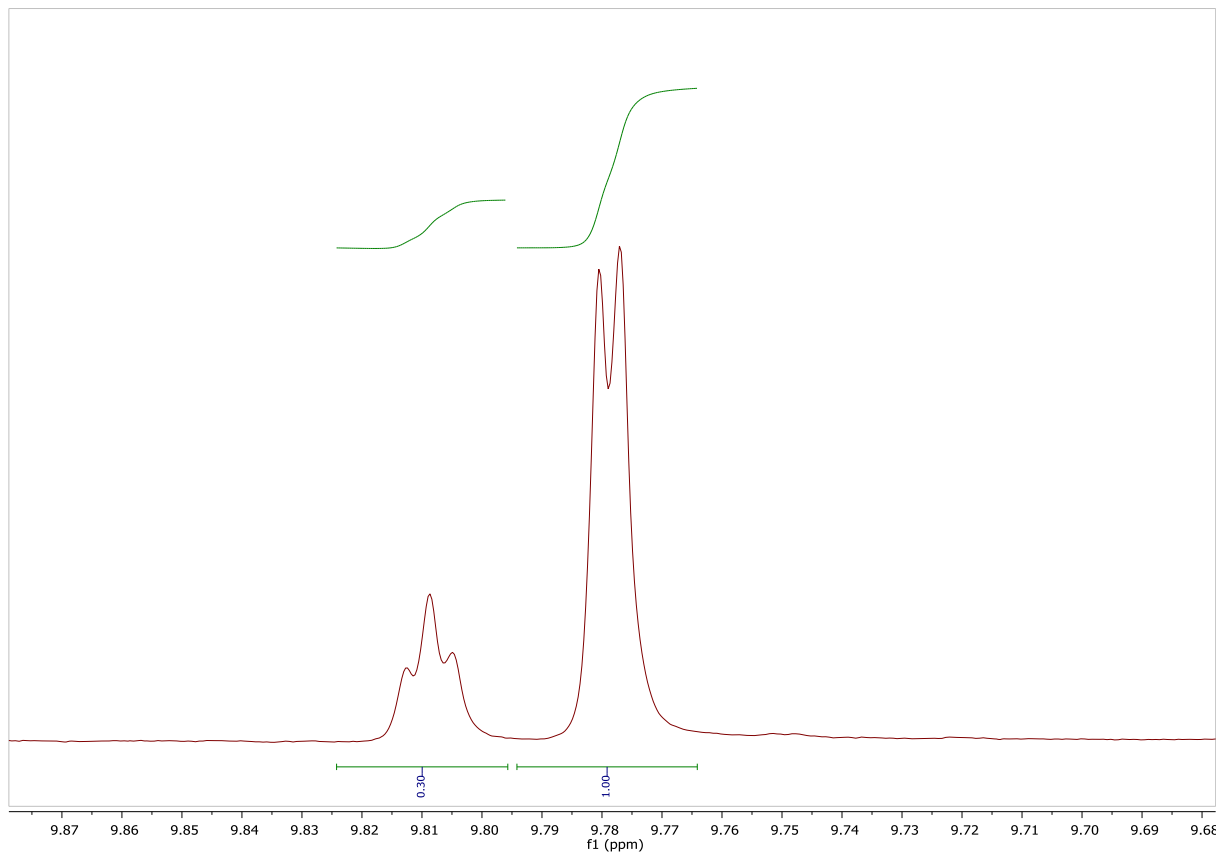
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP<sub>m</sub>O<sub>i</sub>Pr  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



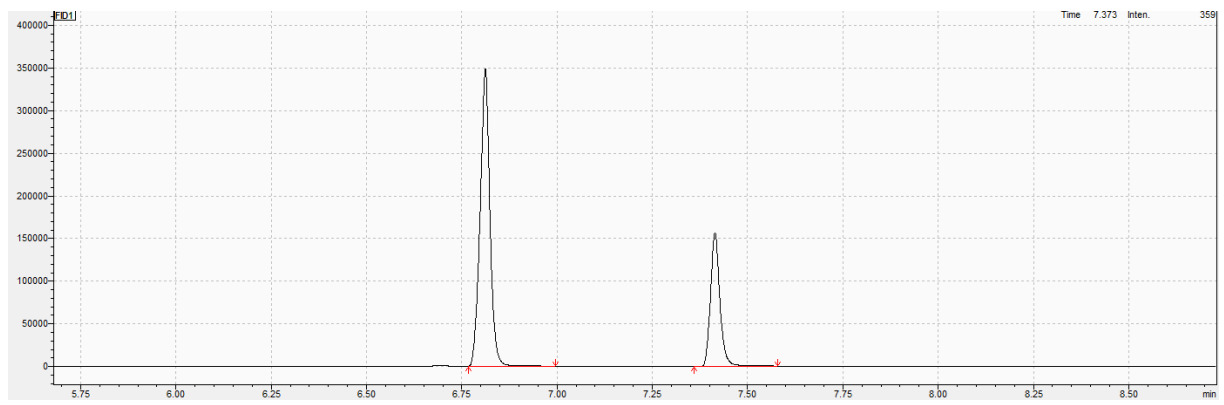
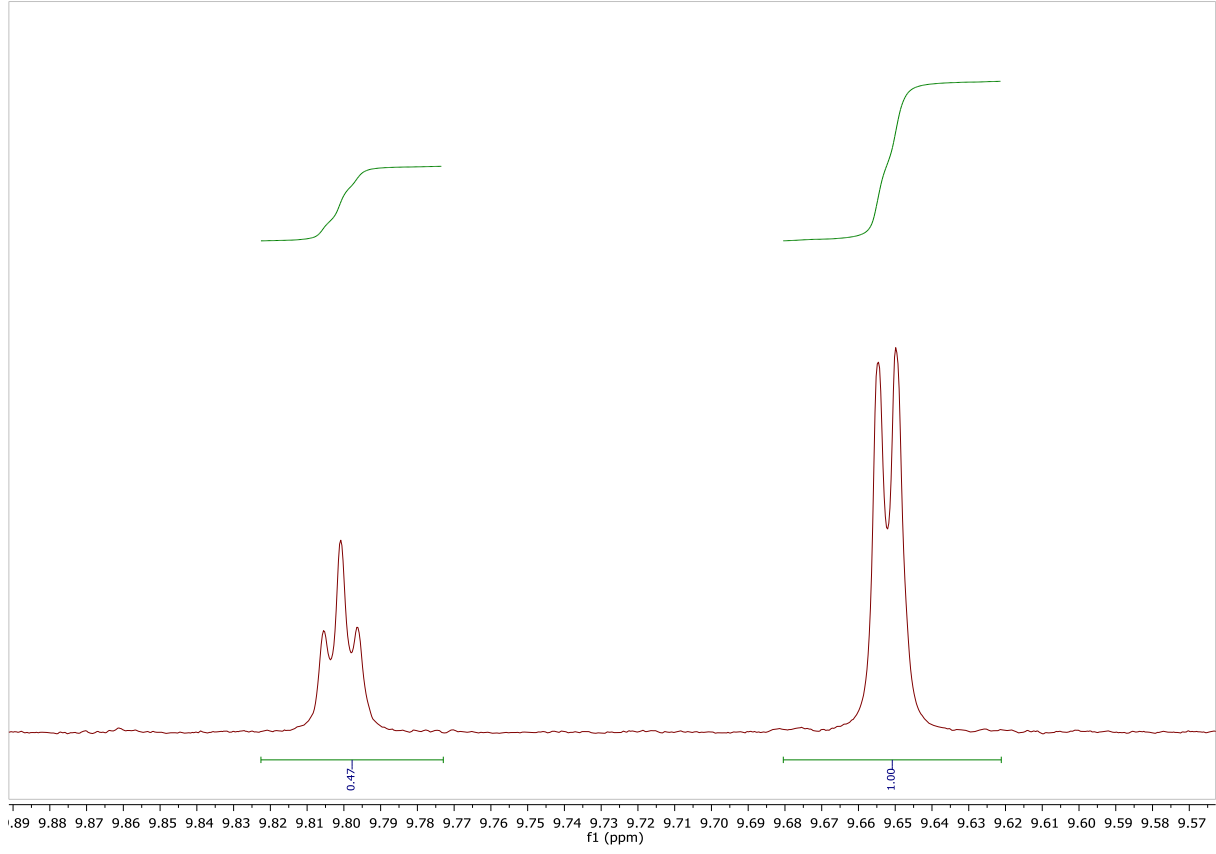
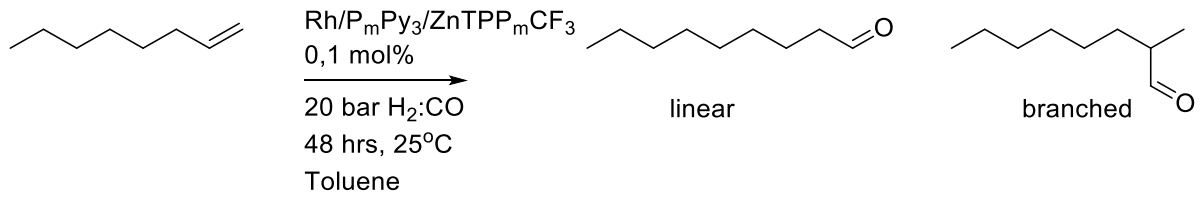
linear



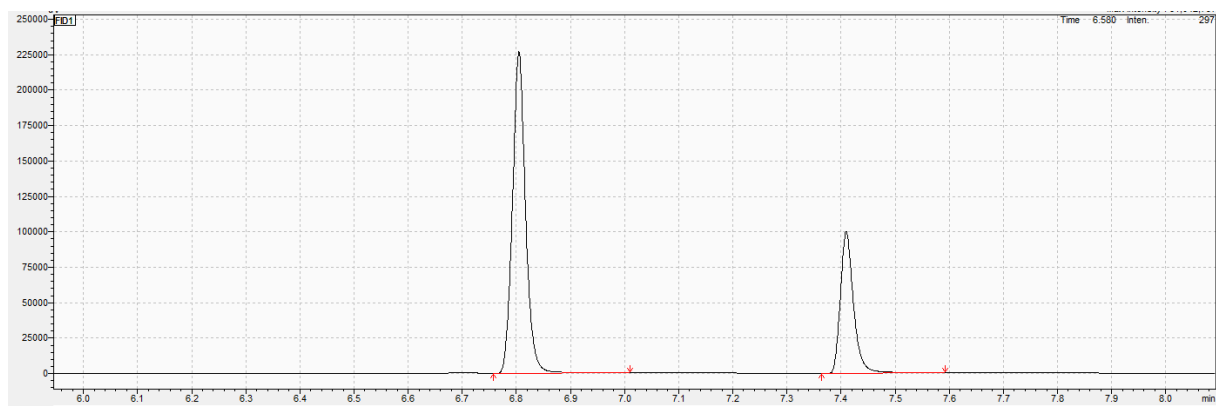
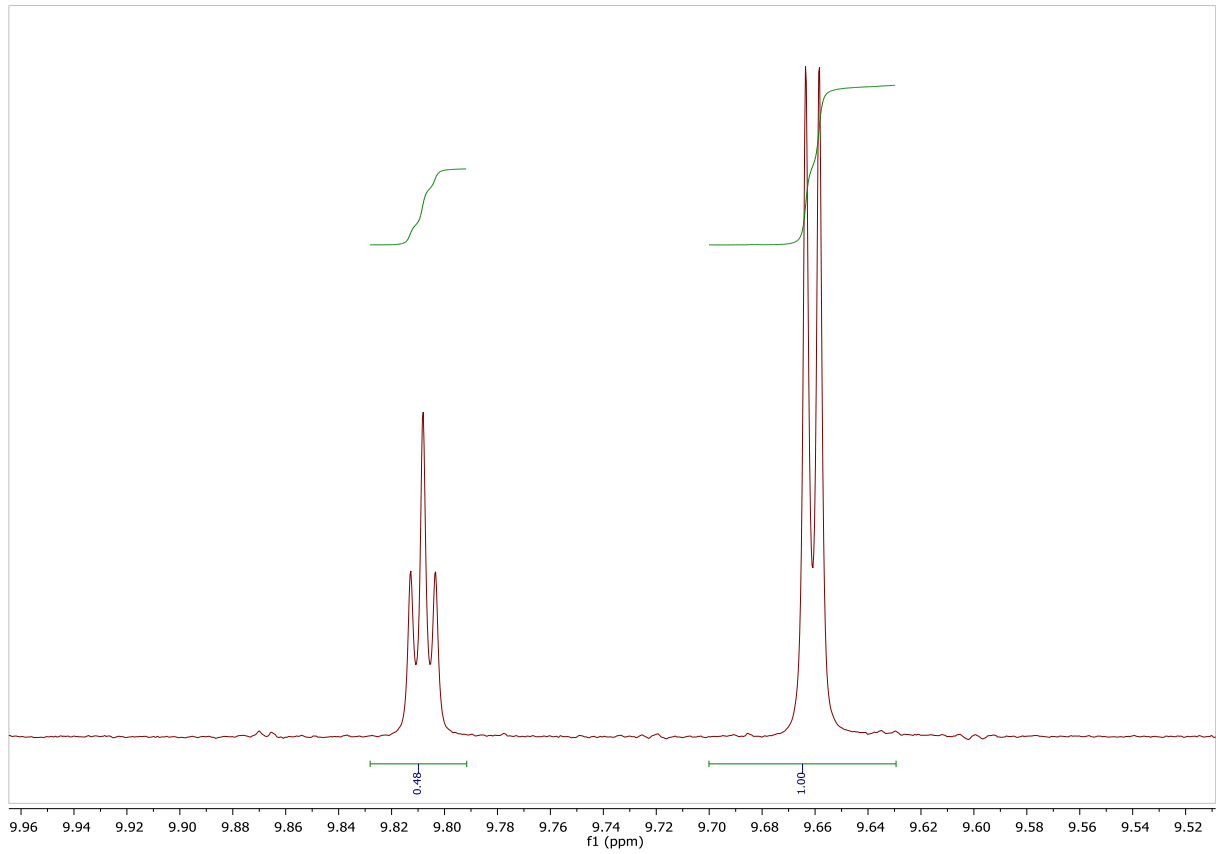
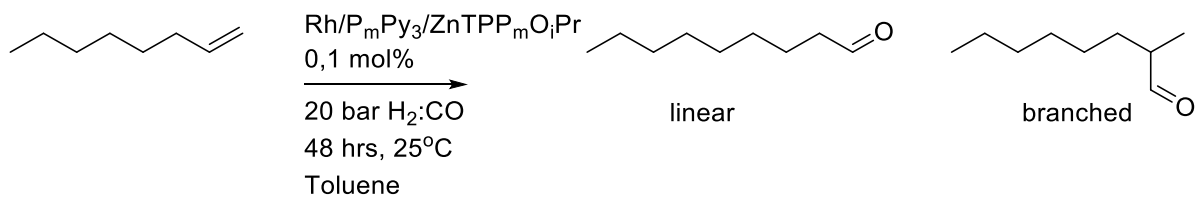
branched



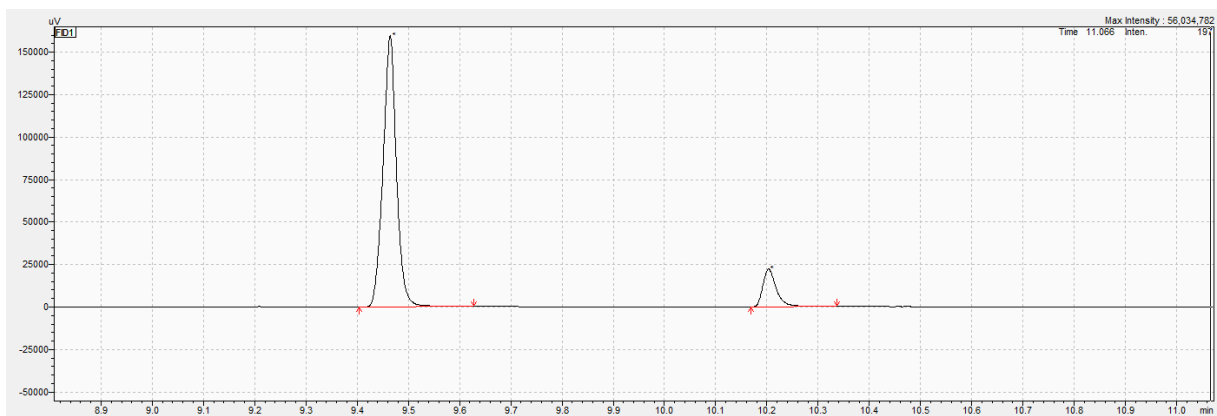
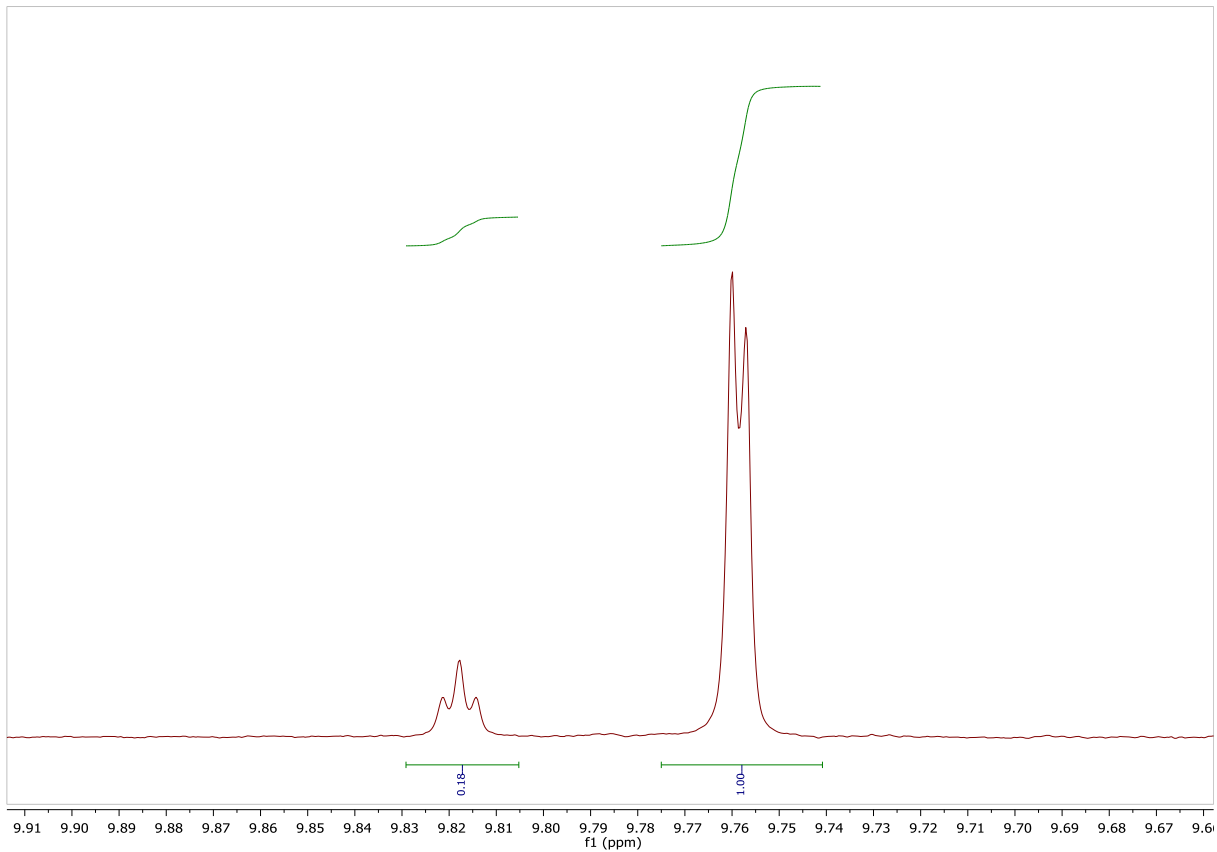
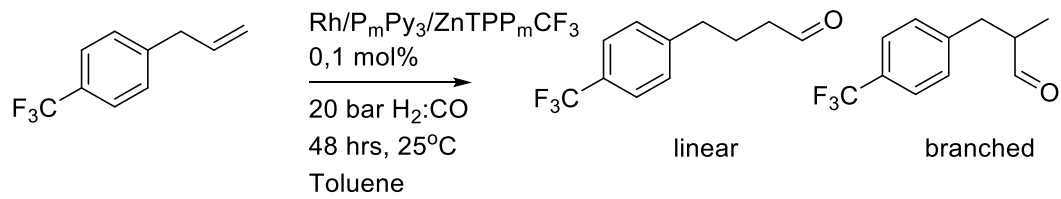
Retention time	Area		I/b ratio
9.009	430000	Branched	0.26
9.703	114749	Linear	



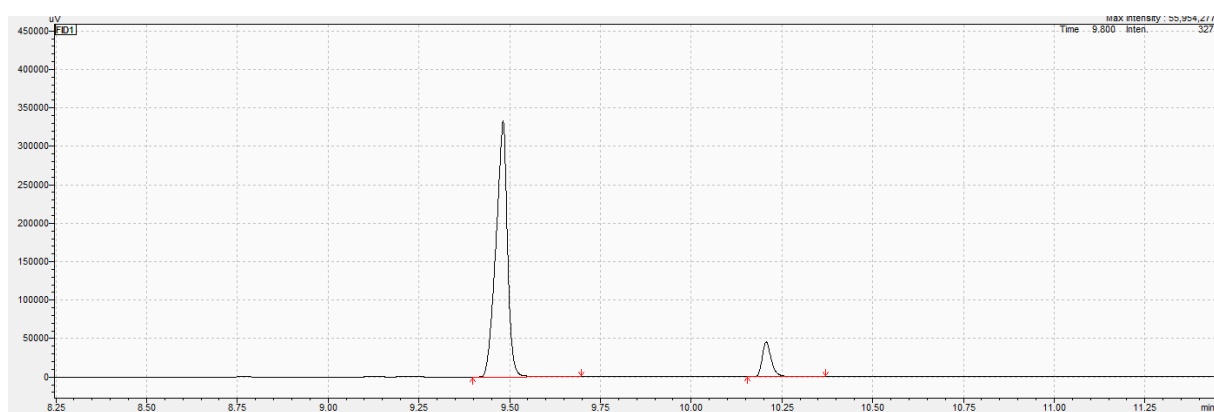
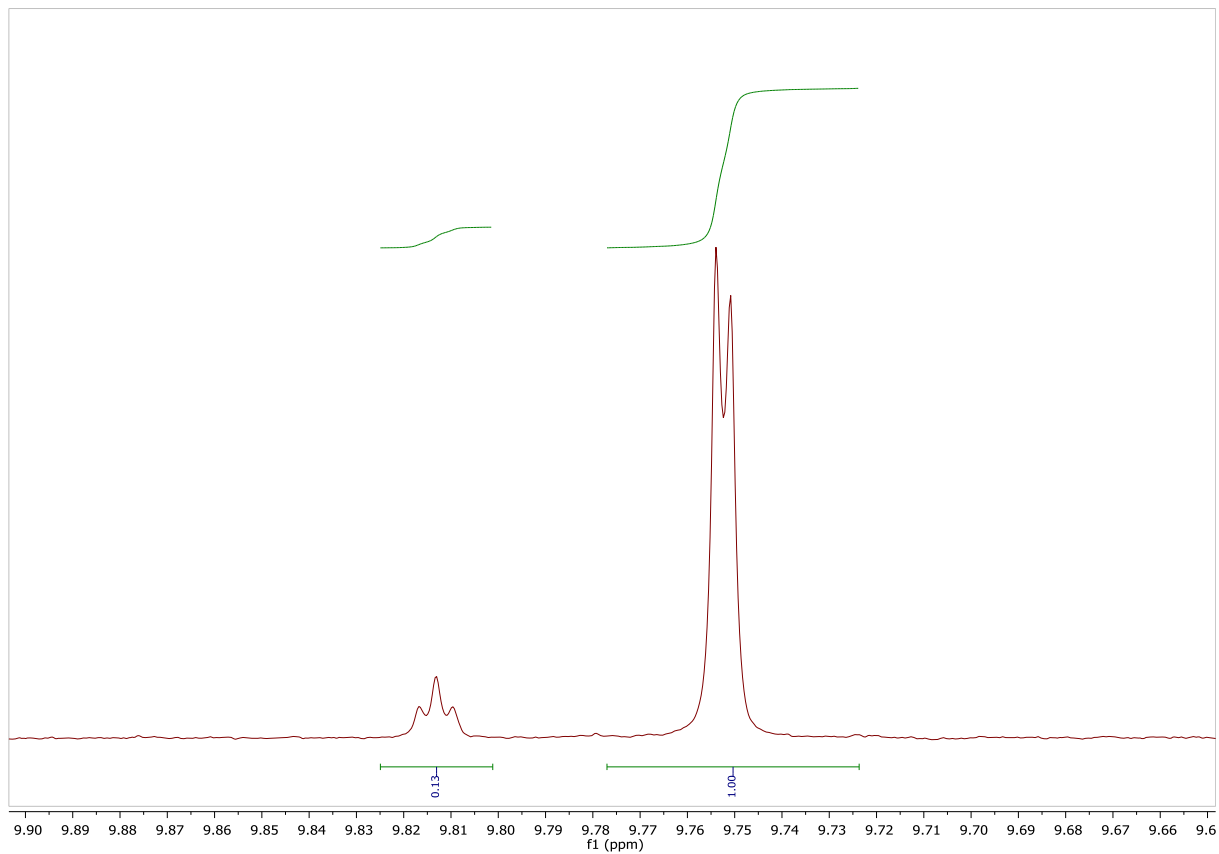
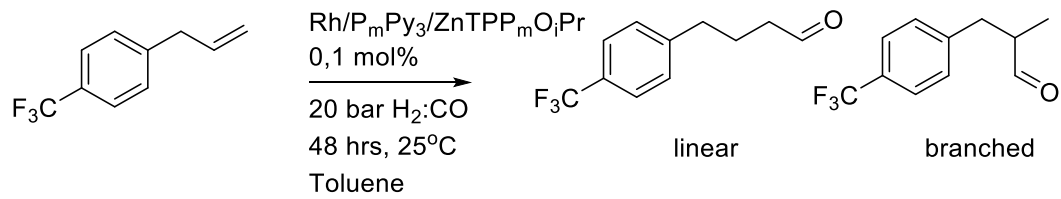
Retention time	Area		l/b ratio
6.805	381259	Branched	0.44
7.410	168008	Linear	



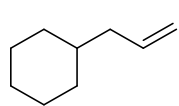
Retention time	Area		I/b ratio
6.812	620366	Branched	0.42
7.414	266142	Linear	



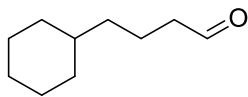
Retention time	Area		l/b ratio
9.464	290015	Branched	0.14
10.203	40255	Linear	



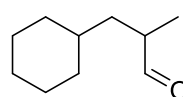
Retention time	Area		I/b ratio
9.482	727369	Branched	0.11
10.207	79417	Linear	



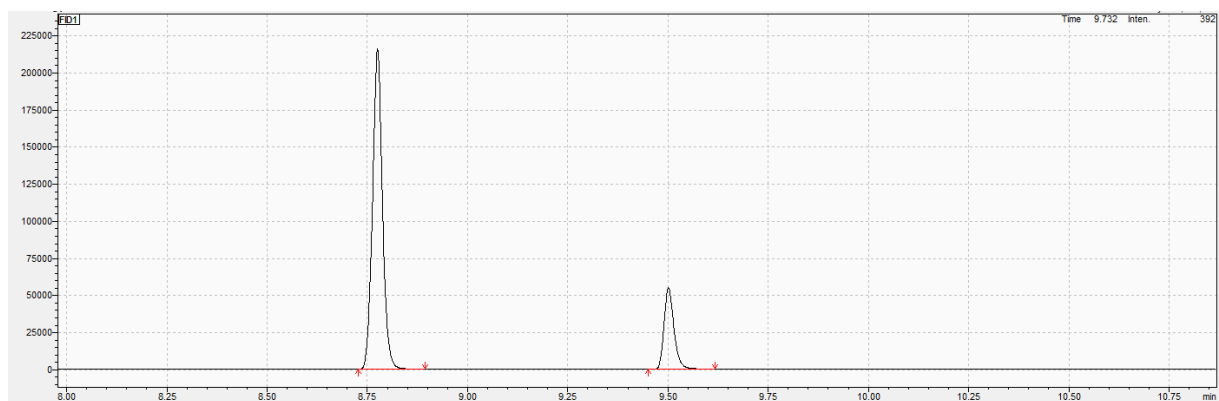
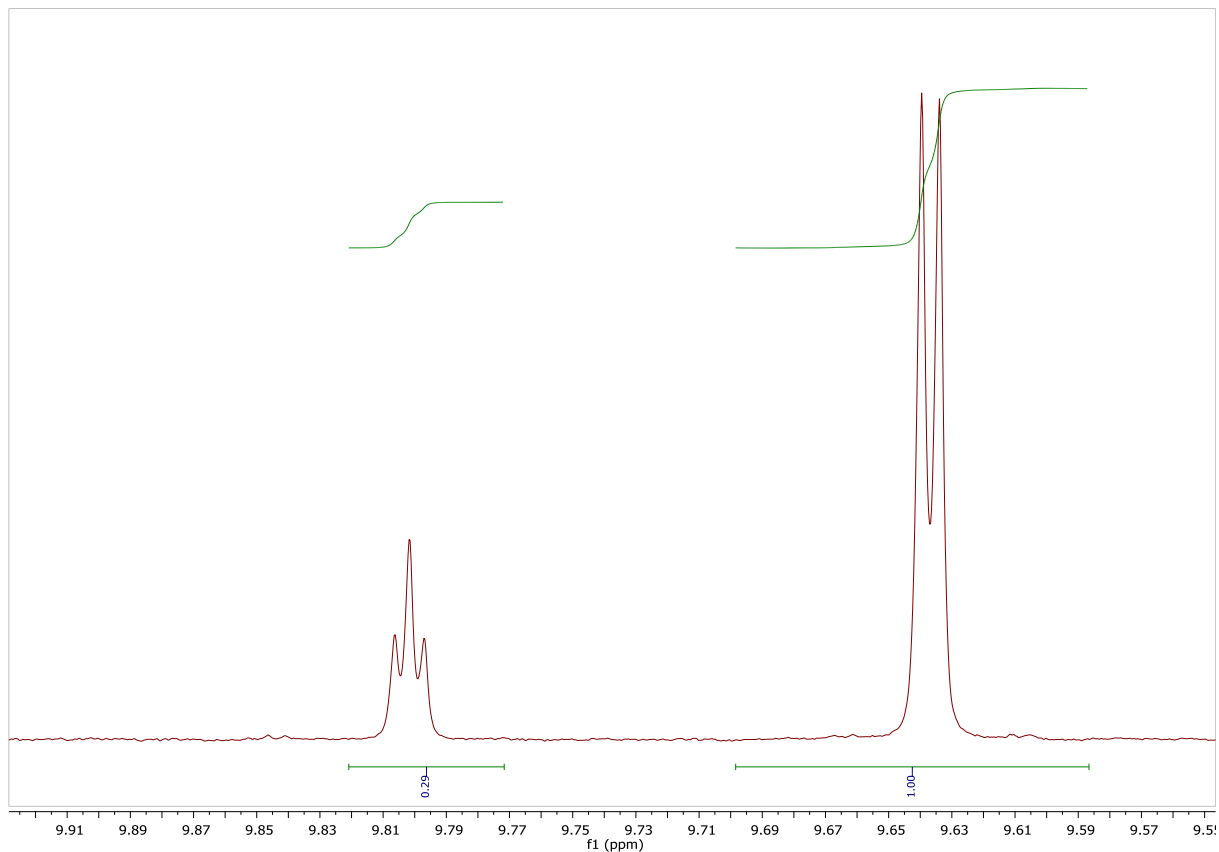
$\text{Rh}/\text{P}_m\text{Py}_3/\text{ZnTPP}_m\text{CF}_3$   
 0,1 mol%  
 20 bar  $\text{H}_2:\text{CO}$   
 48 hrs, 25°C  
 Toluene



linear

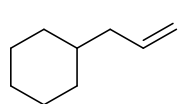


branched

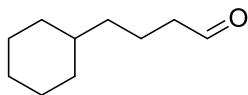


Retention time	Area		I/b ratio
8.776	371792	Branched	0.25
9.501	94446	Linear	

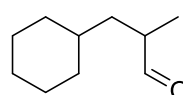




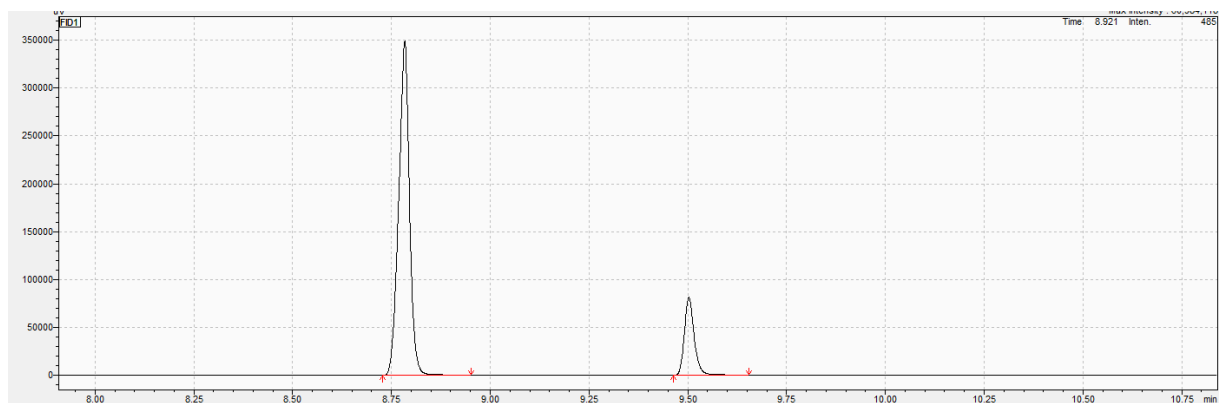
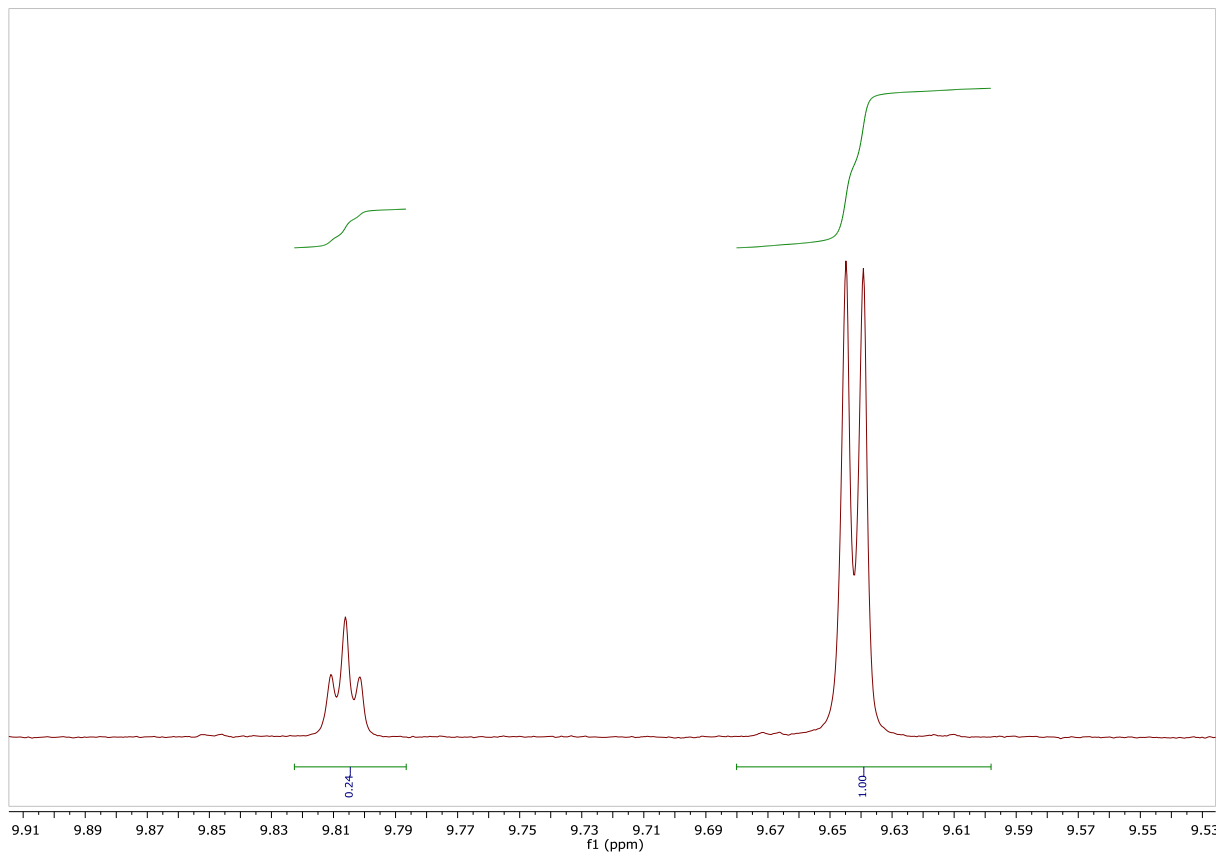
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP<sub>m</sub>O<sub>i</sub>Pr  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



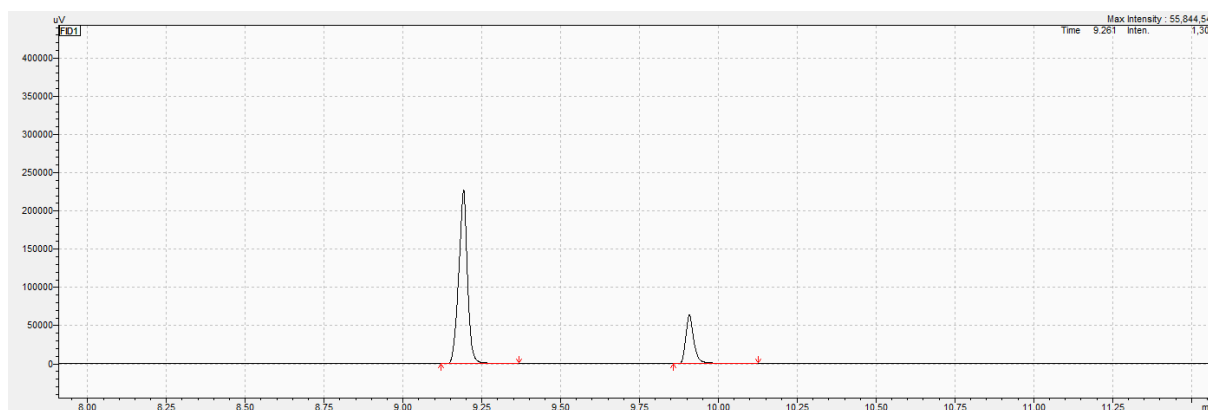
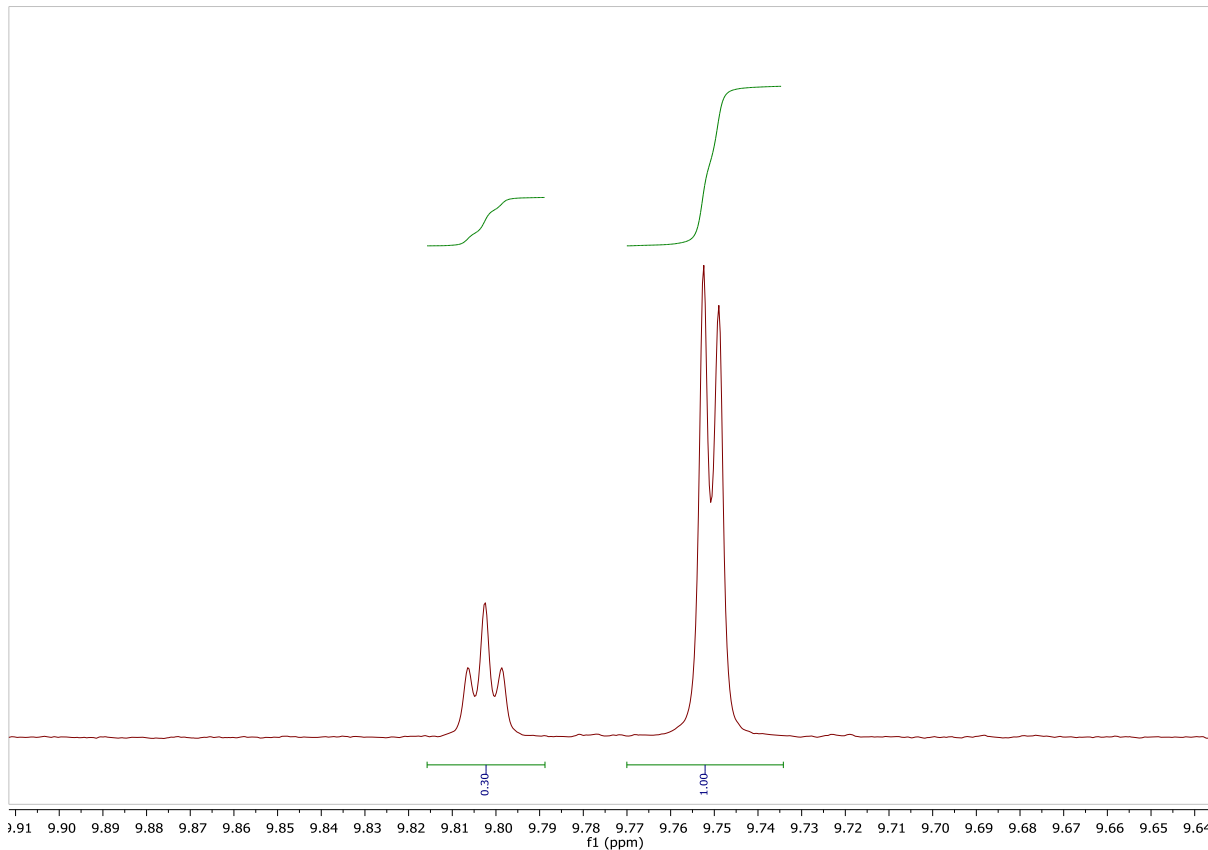
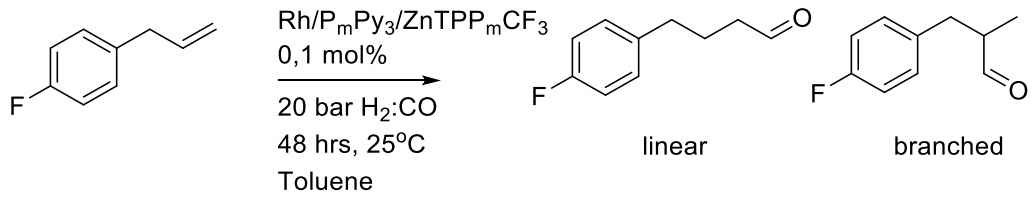
linear



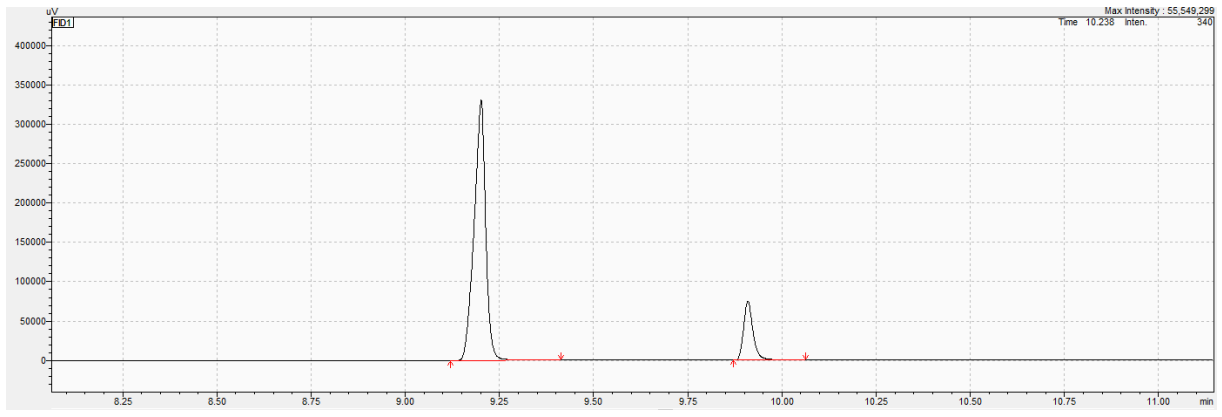
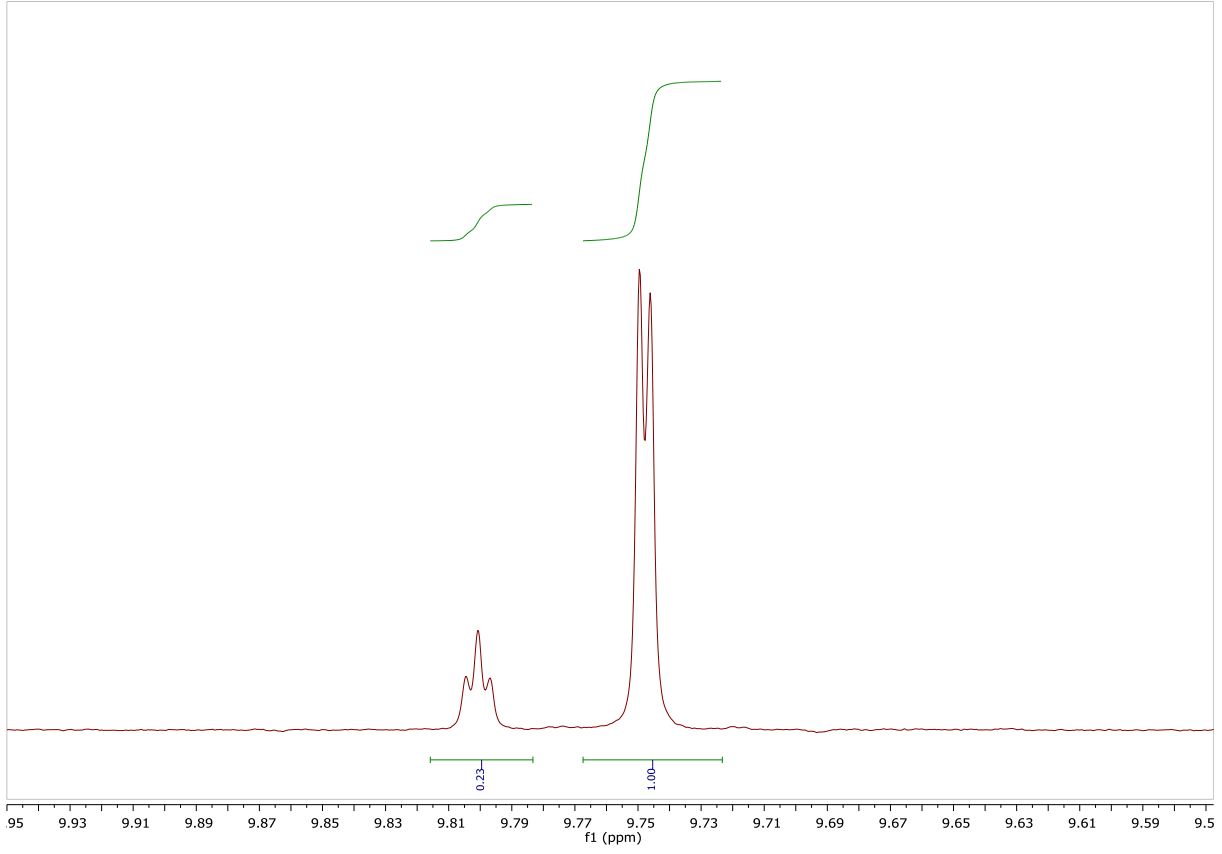
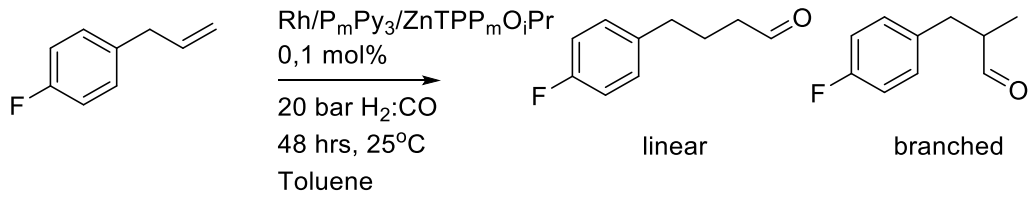
branched



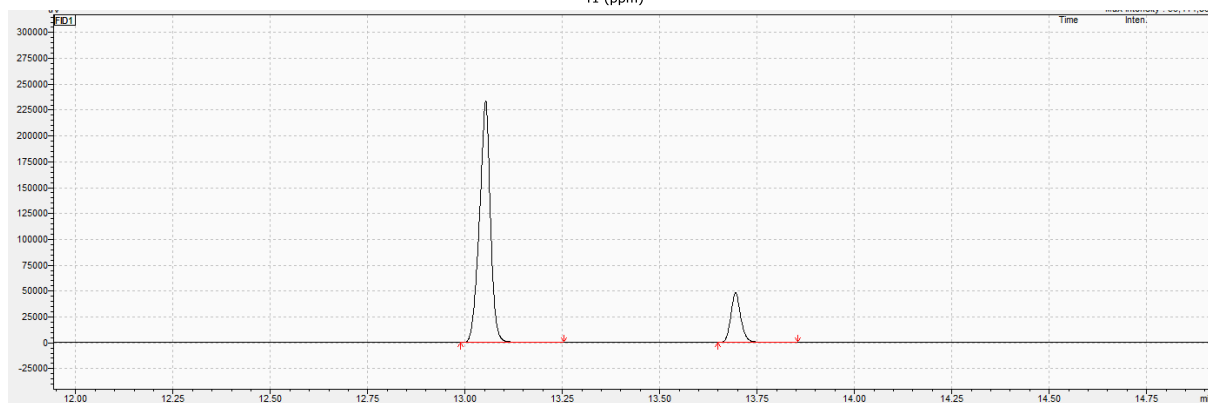
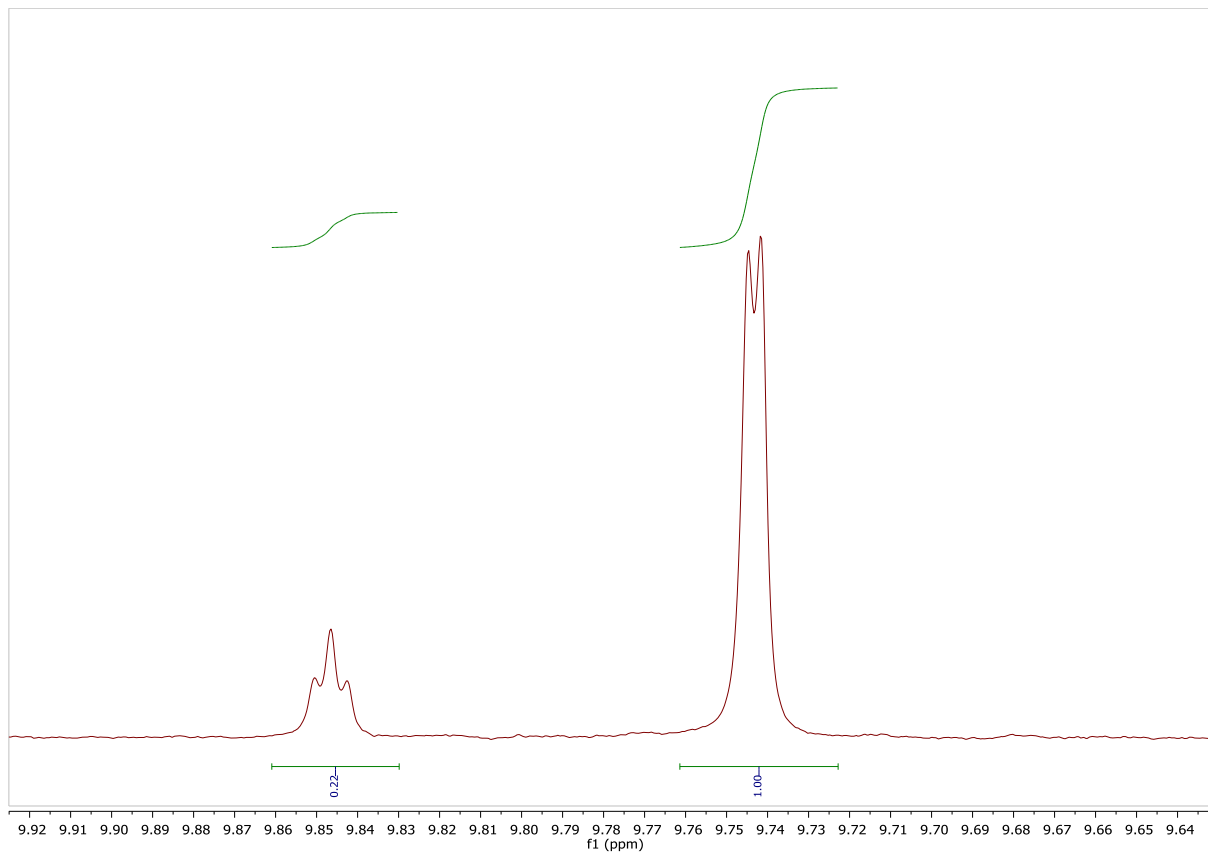
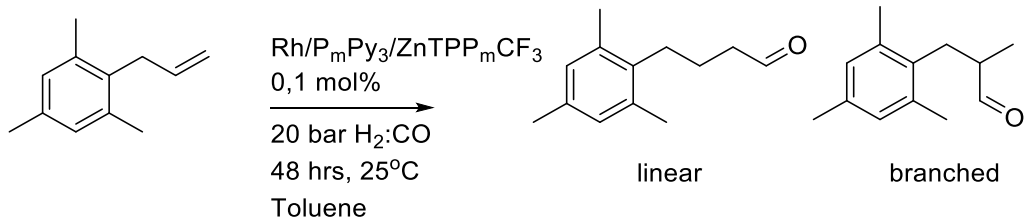
Retention time	Area		I/b ratio
8.784	659584	Branched	0.21
9.503	138535	Linear	



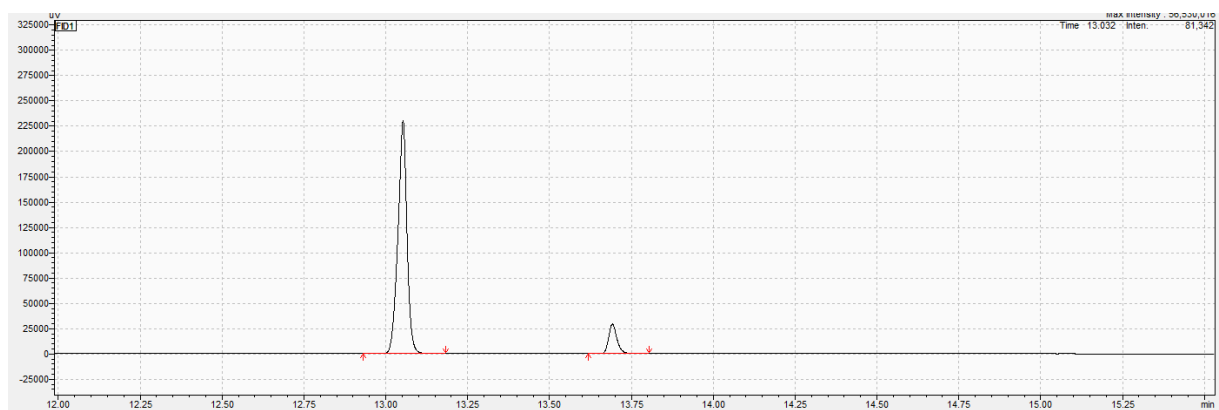
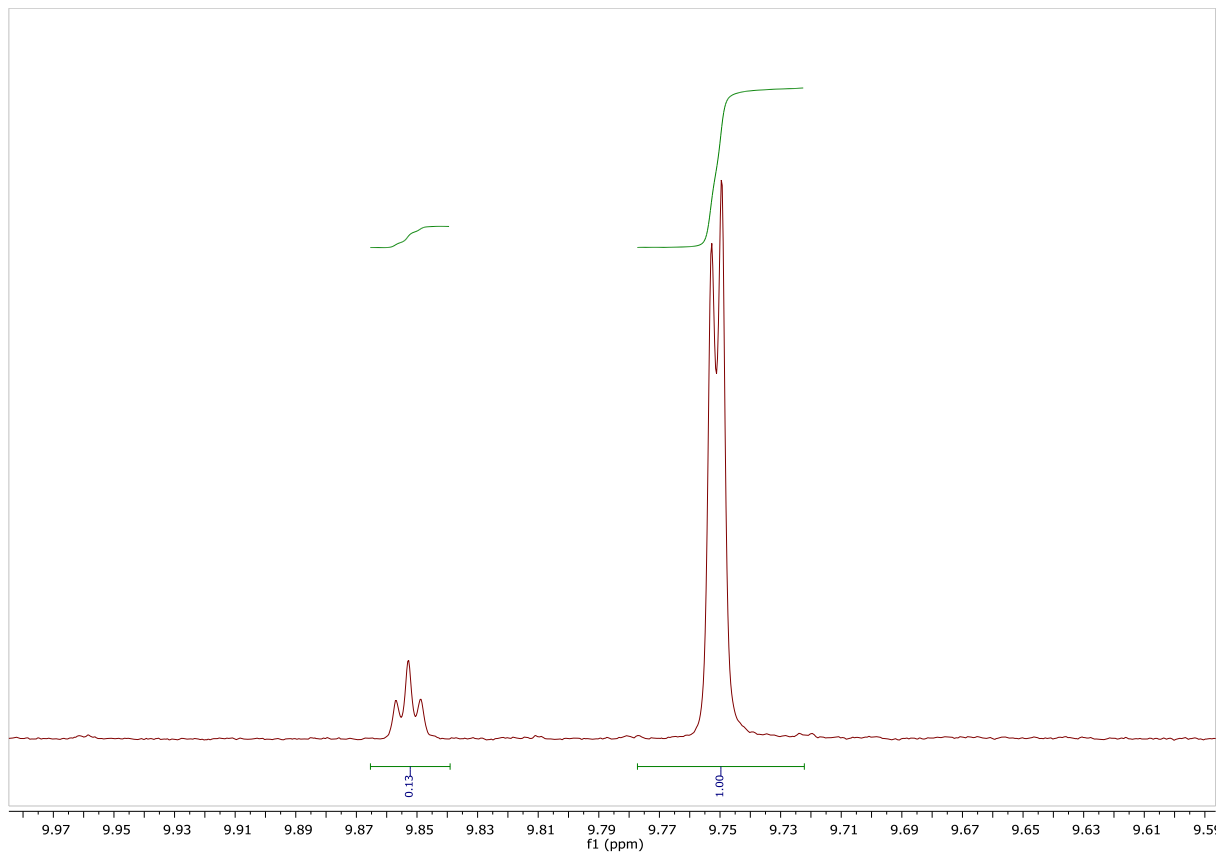
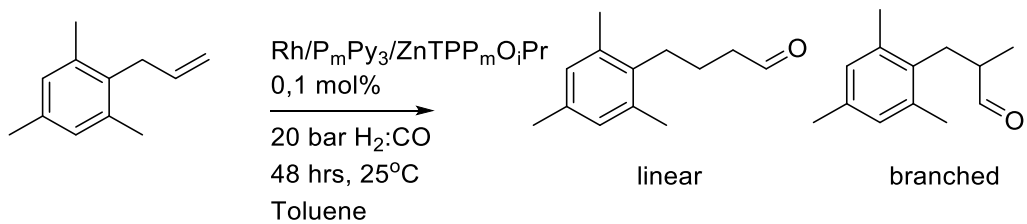
Retention time	Area		l/b ratio
9.192	435578	Branched	0.26
9.908	113801	Linear	



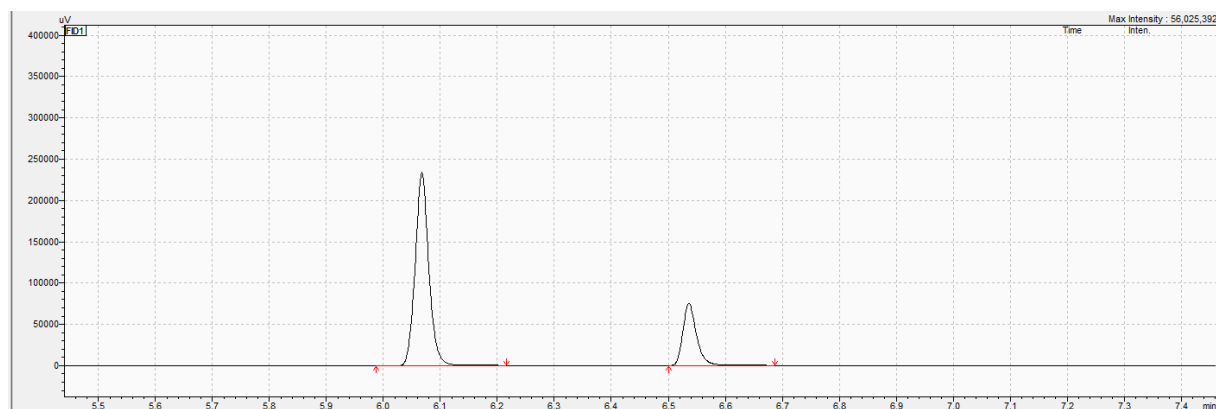
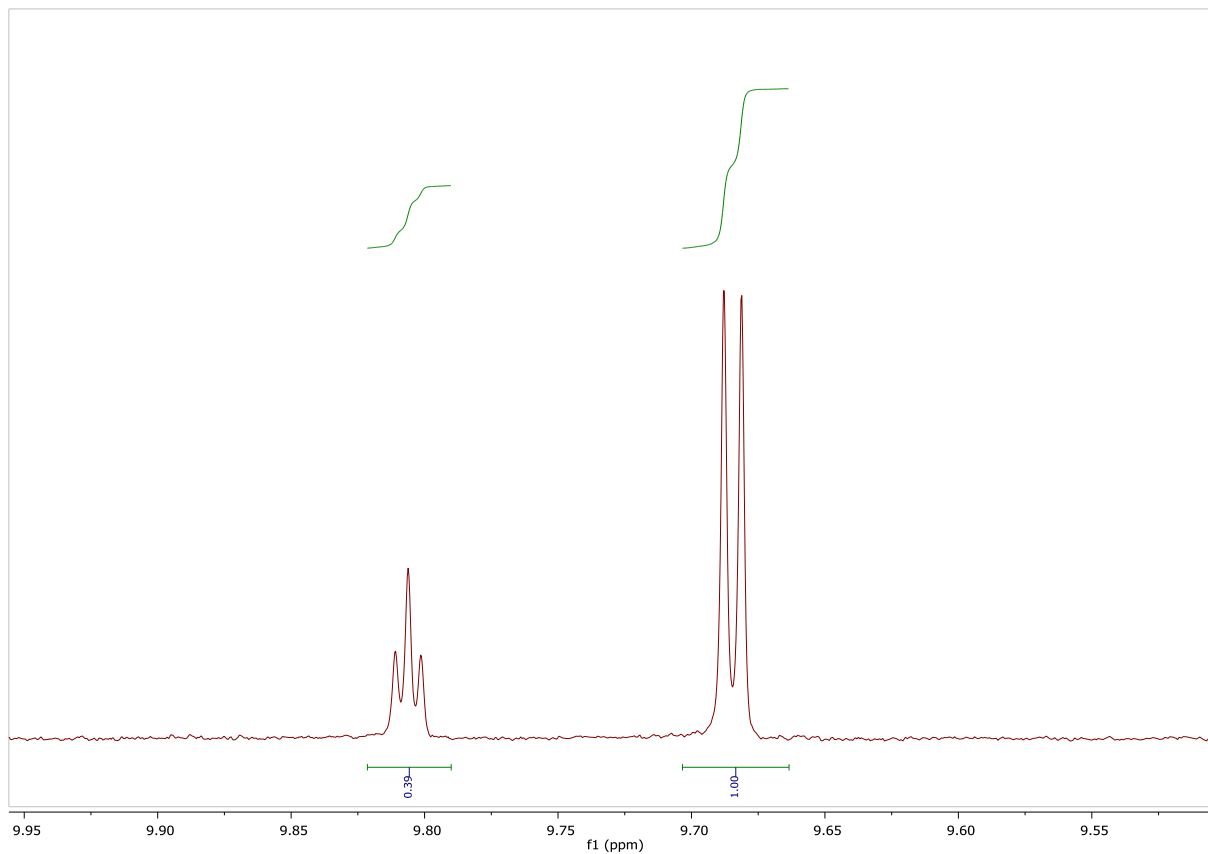
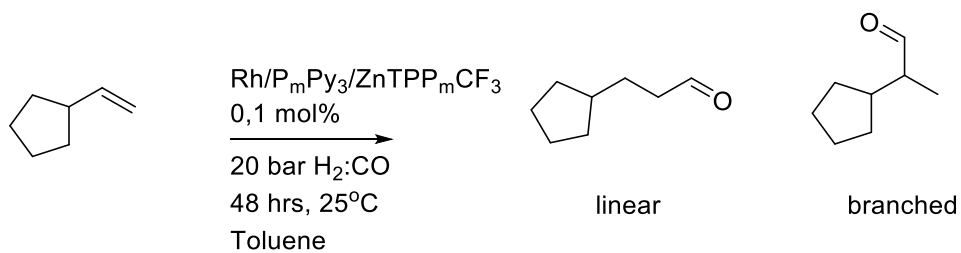
Retention time	Area		I/b ratio
9.201	701901	Branched	0.18
9.910	131047	Linear	



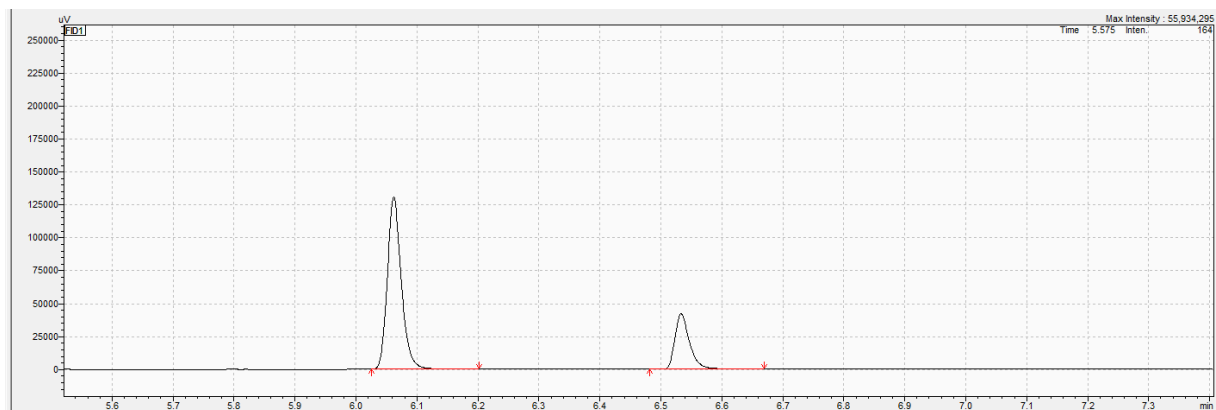
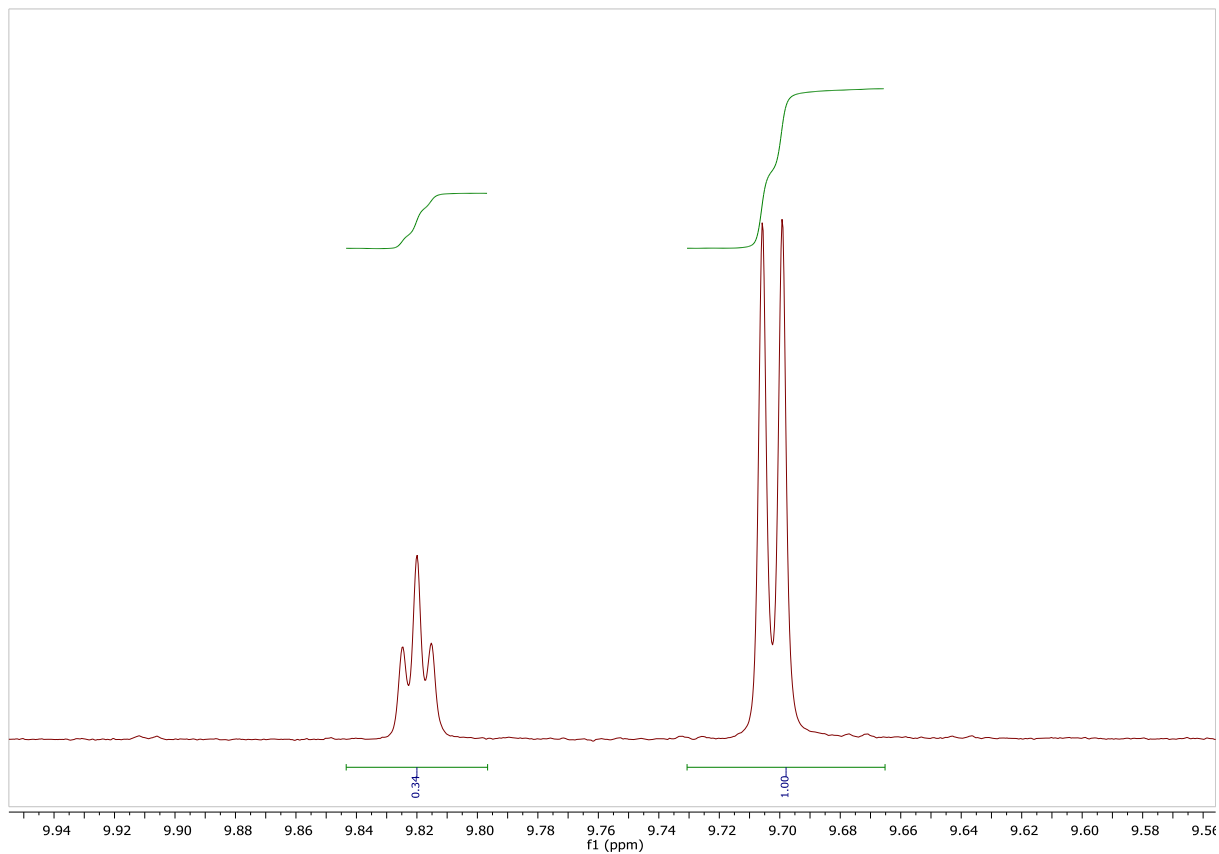
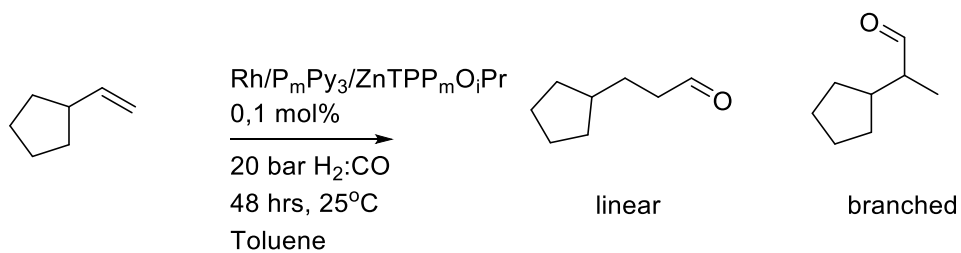
Retention time	Area		I/b ratio
13.053	455483	Branched	0.19
13.695	86167	Linear	



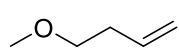
Retention time	Area		l/b ratio
13.052	443075	Branched	0.11
13.692	50236	Linear	



Retention time	Area		I/b ratio
6.068	386748	Branched	0.32
6.536	124379	Linear	



Retention time	Area		I/b ratio
6.062	208145	Branched	0.33
6.533	69799	Linear	



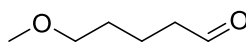
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP<sub>m</sub>CF<sub>3</sub>

0,1 mol%

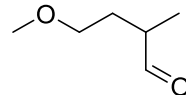
20 bar H<sub>2</sub>:CO

48 hrs, 25°C

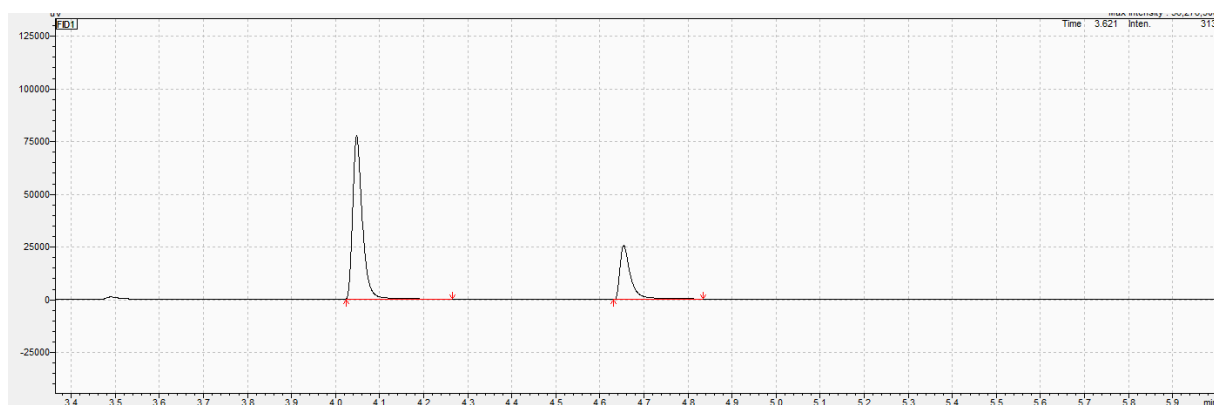
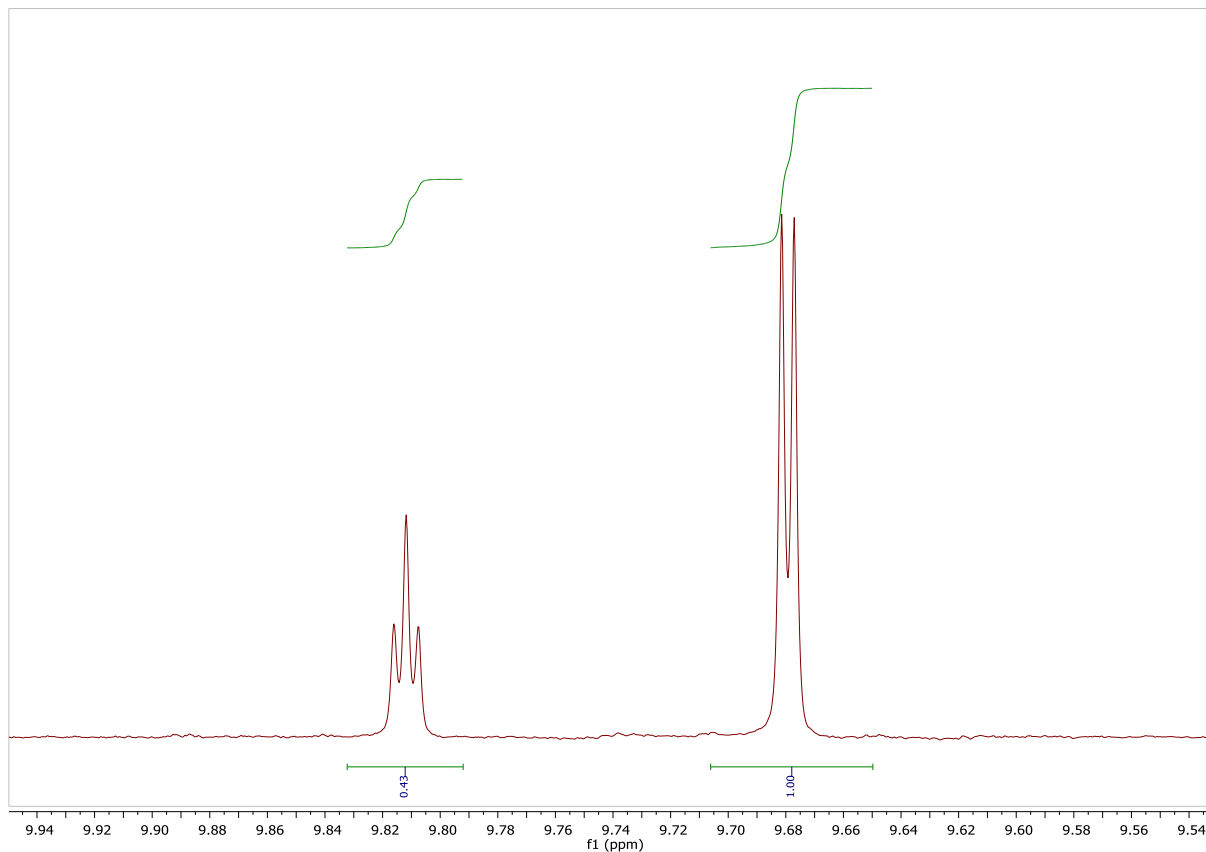
Toluene



linear

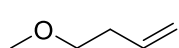


branched

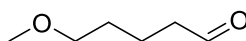


Retention time	Area		I/b ratio
4.048	118624	Branched	0.35
4.654	42487	Linear	

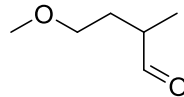




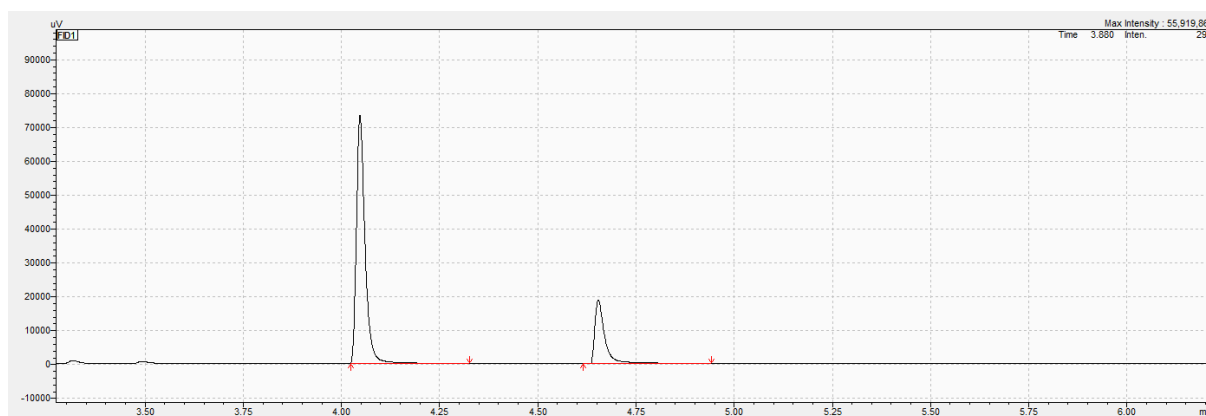
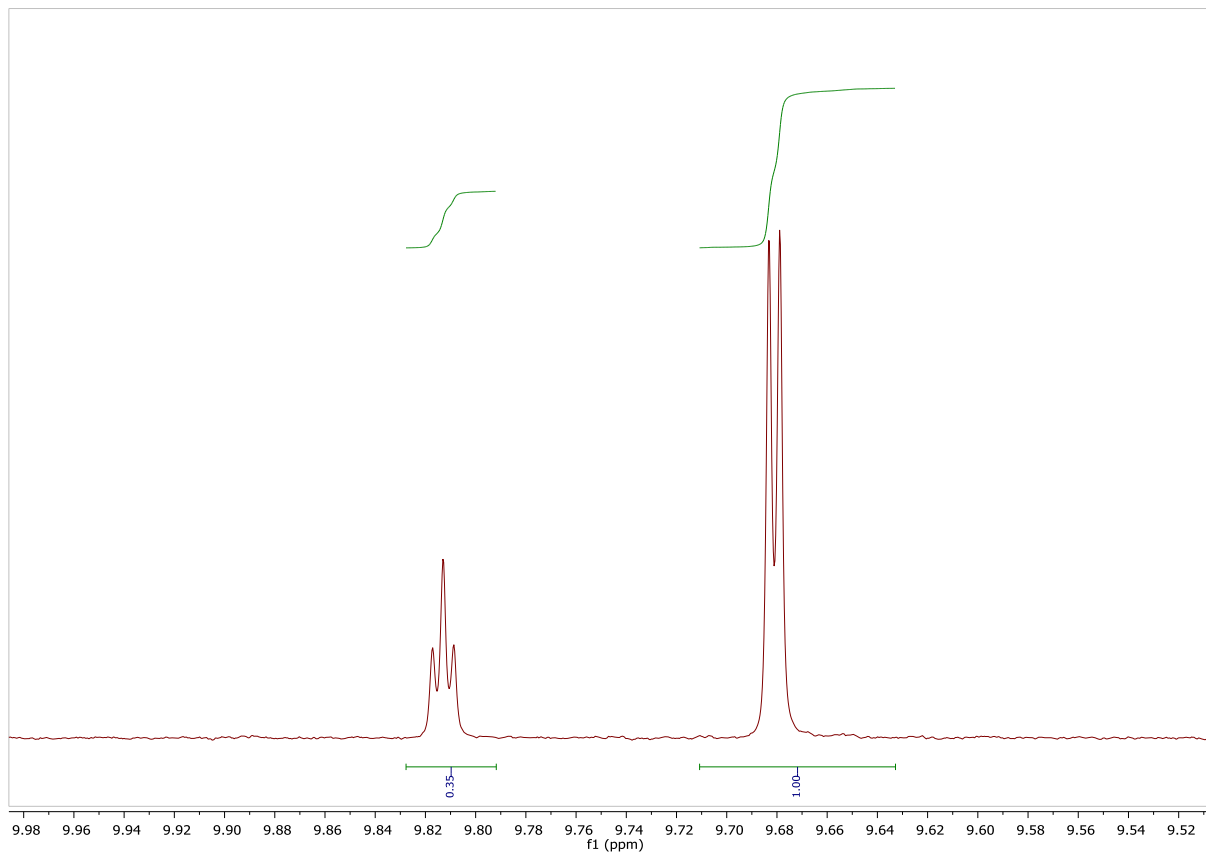
Rh/P<sub>m</sub>Py<sub>3</sub>/ZnTPP<sub>m</sub>O<sub>i</sub>Pr  
 0,1 mol%  
 20 bar H<sub>2</sub>:CO  
 48 hrs, 25°C  
 Toluene



linear



branched



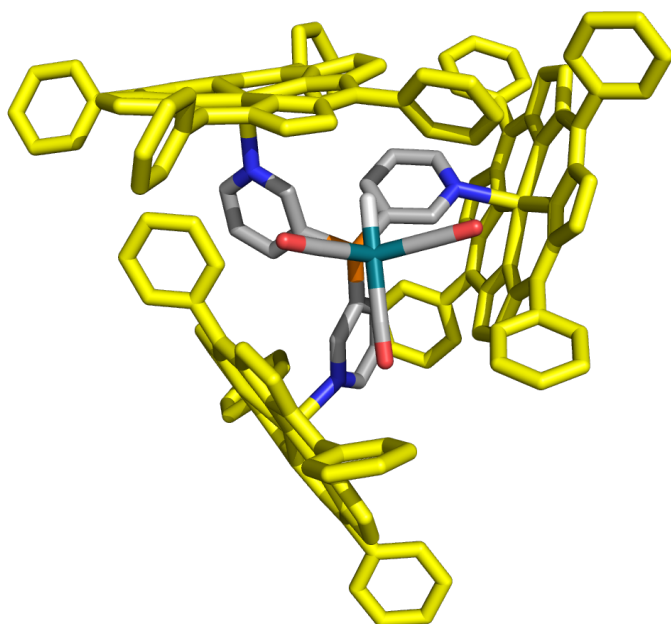
Retention time	Area		l/b ratio
4.047	112187	Branched	0.29
4.654	33000	Linear	

## DFT calculations

All DFT calculations were performed with the Amsterdam Density Functional<sup>1,2</sup> (ADF) program. The BLYP-D3BJ<sup>3,4</sup> functional was used together with a small core and a DZP basis set for all atoms apart from rhodium, for which a TZP basis set was used. Relativistic effects were accounted for by running calculations with zeroth-order regular approximation (ZORA).<sup>5-7</sup>

### XYZ coordinates:

#### CAT1



Energy: -41002.68 kcal/mol

Rh	-0.28099407	-0.41538670	2.83657412
C	0.44467885	-1.97193646	3.84378523
C	-2.19349210	-0.99865171	2.80829011
P	0.05230499	-0.43235954	0.46833882
O	-3.27835521	-1.37640478	2.71888701
O	0.87048277	-2.85873977	4.44603488
H	7.77477252	-6.01957431	1.84452678
H	8.08346663	-5.63151079	-0.80133166
C	1.51969977	-1.36401037	-0.16764564
C	2.49746875	-0.79372420	-1.00028903
C	1.71905794	-2.68095990	0.26922031
C	3.64674338	-1.52253847	-1.29965084
N	2.82285364	-3.38193043	-0.03294056

C	3.78673221	-2.80035846	-0.77440609
C	0.42598730	1.20611118	-0.28452337
C	-0.13021376	1.69172001	-1.47401432
C	1.45068904	1.94683428	0.31848939
C	0.38189201	2.87129757	-2.01973911
N	1.96618970	3.05317663	-0.23242907
C	1.44431687	3.51111328	-1.38822180
C	-1.32375076	-1.05109091	-0.58503302
C	-1.18116037	-1.97858067	-1.62616960
C	-2.60998668	-0.57376798	-0.30054569
C	-2.32041860	-2.39530825	-2.31762026
N	-3.70158311	-0.97935838	-0.96343205
C	-3.56215745	-1.88688835	-1.95257347
H	1.26983219	0.02056209	2.81288911
H	-2.41929673	-5.52757317	0.72704355
H	-2.12475418	-5.16868700	-1.90134660
H	1.89479644	1.62706998	1.25920102
H	1.90468433	4.40641219	-1.80030702
H	-0.02700802	3.27539469	-2.94252613
H	-0.94254012	1.16702407	-1.97248000
H	-0.20553992	-2.37748263	-1.88830073
H	-2.24714250	-3.10696568	-3.13224189
H	-4.47627641	-2.19014585	-2.45769682
H	-2.77947956	0.17333004	0.47077982
H	0.98125735	-3.18993208	0.88773833
H	2.38999132	0.21573715	-1.38497745
H	4.43344876	-1.09339678	-1.90983388
H	4.68230248	-3.39101537	-0.94110155
N	3.53213125	3.28300702	2.63593643
N	4.84843213	1.99654080	0.38118357
N	4.56673076	4.45494846	-1.20981730

N	3.25741007	5.75022767	1.06609558
C	2.92495625	1.95504364	4.42607757
C	3.64499616	2.00952459	3.16471906
C	2.42147871	3.20520644	4.65899489
C	2.81088332	4.04106970	3.53853201
C	4.34481472	0.93723976	2.56828949
C	4.98283667	0.98504945	1.30781656
C	5.84411599	-0.04936629	0.76092139
C	6.18321600	0.33740012	-0.50797552
C	5.53505741	1.61320081	-0.75262833
C	4.35928029	-0.37112629	3.27961617
C	4.25320438	-2.86321402	4.58055021
C	4.86507960	-0.51486503	4.58176055
C	3.82812659	-1.50191907	2.63572556
C	3.77299501	-2.73808742	3.27448649
C	4.80938247	-1.75419143	5.22595143
C	5.55889506	2.31728100	-1.97220230
C	5.07923004	3.62318635	-2.18420238
C	5.04806641	4.30918080	-3.46291629
C	4.51348305	5.55132465	-3.24064449
C	4.21818448	5.64206736	-1.81983890
C	3.63334470	6.75087835	-1.17235348
C	6.12275493	1.57966754	-3.14725894
C	7.17645594	0.10682608	-5.29793425
C	7.44791714	1.77446764	-3.55847313
C	5.32796937	0.64794077	-3.83259473
C	5.85032040	-0.08947847	-4.89857664
C	7.97235528	1.04188190	-4.62846322
C	3.33162460	7.95087808	-2.00662117
C	2.72933872	10.19173067	-3.59475698
C	4.36050355	8.72965570	-2.55700851

C	1.99664054	8.30938324	-2.25702915
C	1.69699963	9.42121410	-3.04837699
C	4.06146574	9.84396076	-3.34580857
C	3.26525632	6.81237052	0.18800540
C	2.79623150	8.00189348	0.87801830
C	2.48937225	7.62974346	2.16006141
C	2.76002362	6.20646684	2.26824725
C	2.48838918	5.40647872	3.39596530
C	1.77022776	6.05656658	4.53382856
C	0.42229254	7.26766912	6.68212656
C	2.42858837	6.27736538	5.75310731
C	0.42894865	6.44818163	4.40071992
C	-0.24119409	7.04804891	5.47035957
C	1.75973844	6.88135583	6.82089220
Zn	3.85021607	3.81473375	0.64091830
H	5.30376752	0.34828231	5.08086833
H	3.43783218	-1.38473663	1.63296133
H	3.34225195	-3.59385685	2.76302128
H	5.20562729	-1.85624825	6.23635597
H	4.20153682	-3.82209448	5.08852931
H	8.06521236	2.49765750	-3.02638686
H	4.29083201	0.51405458	-3.52864497
H	5.22461342	-0.81567774	-5.41738187
H	9.00574964	1.19974641	-4.93721279
H	7.58514310	-0.46329096	-6.13172729
H	5.39570374	8.45674282	-2.35479032
H	1.19722534	7.70367761	-1.83194733
H	0.65724170	9.68524165	-3.24191584
H	4.86943354	10.44475337	-3.76323525
H	2.49671838	11.05992220	-4.21094272
H	3.47060196	5.97525612	5.85263566

H	-0.09146202	6.27084804	3.46207427
H	-1.28502068	7.34088829	5.35702962
H	2.28406731	7.05342855	7.76080186
H	-0.10061180	7.73755509	7.51490851
H	2.11931467	8.25589134	2.96294386
H	2.72644015	8.99013398	0.43929280
H	6.82218146	-0.18359544	-1.21186485
H	6.15126427	-0.94642675	1.28396924
H	2.79879444	1.07108961	5.03773739
H	1.81281472	3.52775988	5.49444536
H	5.38774587	3.89004270	-4.40324663
H	4.33032480	6.33260500	-3.96867037
N	-4.92234581	1.38863784	0.92391197
N	-4.50095181	1.71354830	-1.94675373
N	-6.38870887	-0.49583449	-2.47432083
N	-6.78777062	-0.82484245	0.40642308
C	-3.77805499	2.79558171	2.35146897
C	-4.02464893	2.44093806	0.96414316
C	-4.50848823	1.93754955	3.12681703
C	-5.24436260	1.06722461	2.22968107
C	-3.41362027	3.05155179	-0.15523081
C	-3.64216291	2.69898235	-1.50648500
C	-2.90793871	3.22675258	-2.64654873
C	-3.30444452	2.52132495	-3.74976467
C	-4.29861417	1.56220261	-3.30412829
C	-2.38019639	4.09490336	0.11163430
C	-0.35488361	6.00528221	0.56220990
C	-2.47799745	5.38496467	-0.43813824
C	-1.26355486	3.79209469	0.90822740
C	-0.26571132	4.73566681	1.14000053
C	-1.46814193	6.32713778	-0.22185317

C	-4.90937155	0.60289085	-4.13193245
C	-5.88697091	-0.33325601	-3.74973202
C	-6.45540473	-1.34492905	-4.62167945
C	-7.29360457	-2.11094028	-3.85529705
C	-7.23735522	-1.58299931	-2.50256605
C	-7.87379956	-2.15818105	-1.38313625
C	-4.41447074	0.51417205	-5.54263694
C	-3.47136622	0.29677884	-8.17947558
C	-5.10804412	1.12514885	-6.59524922
C	-3.24414252	-0.20873916	-5.82011543
C	-2.77496836	-0.31596560	-7.13177984
C	-4.63924764	1.01736579	-7.90848549
C	-8.79078473	-3.30738235	-1.64354540
C	-10.49569997	-5.48226585	-2.16345446
C	-9.99530943	-3.11746766	-2.33829607
C	-8.45126345	-4.59861475	-1.20977926
C	-9.29721139	-5.67986414	-1.46899160
C	-10.84320561	-4.19796264	-2.59605764
C	-7.68404789	-1.77408110	-0.04145908
C	-8.39185669	-2.33542793	1.09659260
C	-7.89738662	-1.72770198	2.21796448
C	-6.88240598	-0.78325126	1.78057785
C	-6.13632655	0.05347248	2.63449440
C	-6.30106293	-0.17015274	4.10229678
C	-6.58900517	-0.61348290	6.86569949
C	-6.89511133	0.80179053	4.92172296
C	-5.86372806	-1.37227169	4.68256025
C	-6.00360771	-1.59162229	6.05443075
C	-7.03781854	0.58227917	6.29430433
Zn	-5.50664287	0.30412733	-0.76050097
H	-3.35289089	5.64280786	-1.03372126

H	-1.17546339	2.79772906	1.33020580
H	0.59184676	4.47384899	1.75205034
H	-1.55782996	7.32256510	-0.65765535
H	0.43076183	6.73731271	0.72825271
H	-6.01764571	1.68339110	-6.37536044
H	-2.71470176	-0.69215126	-5.00051185
H	-1.86759452	-0.87937705	-7.34403414
H	-5.18579370	1.49656487	-8.72072053
H	-3.10532633	0.21206090	-9.20249742
H	-10.26121846	-2.11459304	-2.67066053
H	-7.51528261	-4.74701106	-0.67219331
H	-9.01927597	-6.67835789	-1.13151465
H	-11.77820966	-4.03677175	-3.13254618
H	-11.15588381	-6.32539258	-2.36581400
H	-7.25023945	1.72807465	4.47156844
H	-5.41471343	-2.13132694	4.04672907
H	-5.65248005	-2.52585131	6.49223575
H	-7.50551559	1.34397597	6.91811513
H	-6.69814003	-0.78378304	7.93652573
H	-8.20429597	-1.88242986	3.24504309
H	-9.17769028	-3.07849436	1.03702065
H	-2.96513197	2.63772450	-4.77251579
H	-2.17905491	4.02312466	-2.60283509
H	-3.13230041	3.59398941	2.69155361
H	-4.54519779	1.90125335	4.20831157
H	-6.23235060	-1.45649187	-5.67625969
H	-7.87572437	-2.97030752	-4.16611817
N	4.88750911	-5.87487528	0.16240613
N	2.58717439	-6.05797045	1.98094751
N	0.76280982	-5.66454019	-0.29183248
N	3.06748892	-5.55286352	-2.10579886

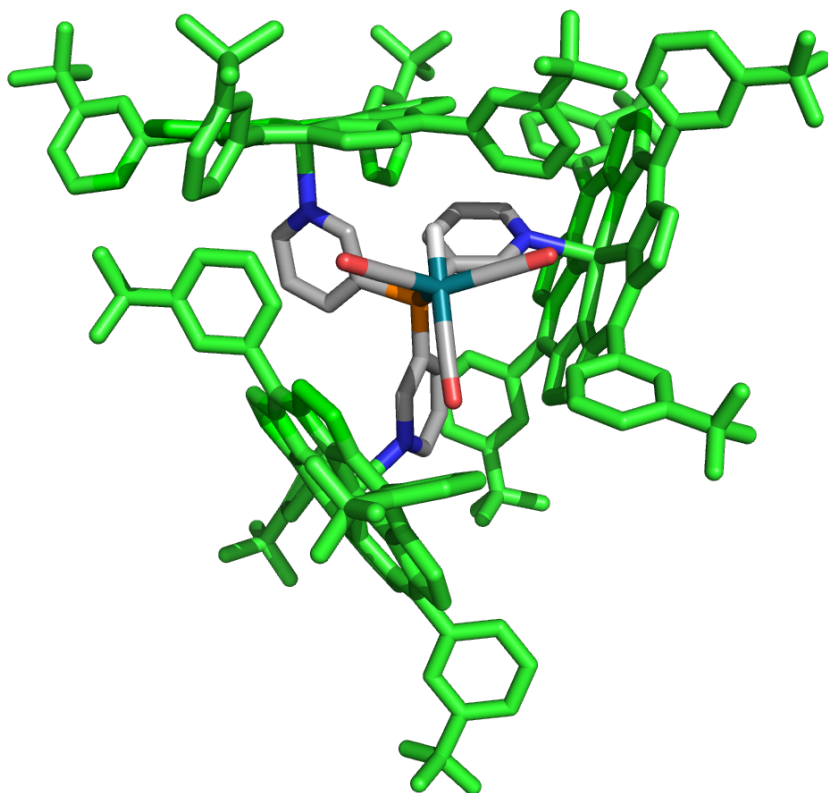


C	6.99888477	-5.92855574	1.09474338
C	5.57087290	-5.99261949	1.35525866
C	7.15651803	-5.73964607	-0.25133529
C	5.82835107	-5.71664762	-0.83694357
C	4.98654874	-6.12625317	2.63086138
C	3.60454355	-6.16314318	2.91091441
C	3.02670729	-6.17739467	4.24269446
C	1.67251124	-6.05530680	4.09970727
C	1.39527391	-5.98705595	2.67673696
C	5.91541099	-6.15670272	3.80082383
C	7.63216997	-6.17618604	6.02732911
C	6.03390668	-7.30584371	4.59761582
C	6.67152041	-5.01967742	4.12810832
C	7.52221697	-5.02820995	5.23518288
C	6.88741339	-7.31595783	5.70422830
C	0.11597435	-5.81701878	2.10522923
C	-0.16764315	-5.69576468	0.72872954
C	-1.49312421	-5.51644044	0.16645246
C	-1.33840456	-5.33681240	-1.18018185
C	0.08283487	-5.42469917	-1.47056587
C	0.68467725	-5.22684312	-2.73500413
C	-1.04069037	-5.71811665	3.04710647
C	-3.18262545	-5.50590794	4.85941818
C	-1.41285861	-6.81283642	3.84314795
C	-1.76636739	-4.52142600	3.16081174
C	-2.82730079	-4.41311997	4.06177104
C	-2.47617432	-6.70792783	4.74340163
C	-0.18275760	-4.74528167	-3.85168453
C	-1.84117183	-3.71097545	-5.88774637
C	-1.27104721	-5.48924877	-4.33620357
C	0.07780516	-3.48770519	-4.42769920

C	-0.74144904	-2.97555052	-5.43449996
C	-2.09654971	-4.97357137	-5.33993580
C	2.06248051	-5.34012961	-3.02338722
C	2.64914935	-5.19810647	-4.34806230
C	4.00630457	-5.27901773	-4.19854691
C	4.26674248	-5.48060391	-2.78516813
C	5.54642673	-5.51040713	-2.20149505
C	6.70104524	-5.17025643	-3.09083087
C	8.88068743	-4.46225670	-4.71762969
C	7.60451489	-6.14741459	-3.52891177
C	6.89629407	-3.83525019	-3.48162237
C	7.98104930	-3.48060777	-4.28679987
C	8.68812962	-5.79555323	-4.34011533
Zn	2.83190841	-5.60907189	-0.02571362
H	5.45355327	-8.19109645	4.33988374
H	6.57011034	-4.12219079	3.52199859
H	8.09391741	-4.13397125	5.48302402
H	6.97426271	-8.21604994	6.31271582
H	8.29594569	-6.18351788	6.89178024
H	-0.86135444	-7.74739474	3.74760965
H	-1.48760385	-3.67381578	2.54035094
H	-3.37027609	-3.47518732	4.14758132
H	-2.75467942	-7.56690450	5.35384217
H	-4.00878909	-5.42275106	5.56512101
H	-1.46478093	-6.47698489	-3.92029524
H	0.92343132	-2.90557345	-4.06360385
H	-0.52863316	-1.99141766	-5.84927263
H	-2.94181437	-5.56114914	-5.69834850
H	-2.49758828	-3.30313302	-6.65461849
H	7.44989144	-7.18360119	-3.22946879
H	6.19287018	-3.07219446	-3.15094587

H	8.12319027	-2.43843351	-4.56764860
H	9.38338253	-6.56409055	-4.67780396
H	9.72929069	-4.18943706	-5.34476220
H	4.76522188	-5.22501063	-4.96992326
H	2.09305459	-5.07348282	-5.26886768
H	0.93115558	-5.98531830	4.88517153
H	3.58692027	-6.24108992	5.16704672
C	-0.52965253	1.42028327	3.55164989
O	-0.62902780	2.50391523	3.93866373

### CAT3



Energy: -45663.28 kcal/mol

Rh	-0.28125335	-0.37804533	2.84525355
C	0.43381596	-1.94632764	3.84103644
C	-2.19626567	-0.94998438	2.88013011
P	0.04168004	-0.35850386	0.46781770
O	-3.28663998	-1.32281573	2.87389059

O	0.83840576	-2.83895542	4.44893768
H	7.78938403	-5.91001998	1.73341434
H	8.11419104	-5.59194106	-0.91554697
C	1.51701896	-1.25158291	-0.21052233
C	2.45450376	-0.66112501	-1.07576737
C	1.74690280	-2.57111979	0.19886524
C	3.59333144	-1.37612393	-1.44057507
N	2.84370877	-3.25731389	-0.15894208
C	3.76594847	-2.66120350	-0.94043047
C	0.40043272	1.29872899	-0.25015539
C	-0.18062395	1.82167670	-1.41112301
C	1.44586469	2.01367787	0.34766507
C	0.32474865	3.01526154	-1.93423490
N	1.95817986	3.12912299	-0.18531957
C	1.40989403	3.62670035	-1.31270504
C	-1.31766530	-0.97042071	-0.61032368
C	-1.12886134	-1.76650898	-1.74936887
C	-2.62686983	-0.61635492	-0.26478658
C	-2.24835601	-2.19106449	-2.46461766
N	-3.70167257	-1.03191882	-0.95075416
C	-3.51629085	-1.82658810	-2.02548618
H	1.27049848	0.05465123	2.81644922
H	-2.39408274	-5.34013353	0.56845832
H	-2.08334270	-4.89228973	-2.03489167
H	1.91066892	1.66418121	1.26776587
H	1.86769015	4.53011064	-1.71016521
H	-0.10671298	3.45281313	-2.83132158
H	-1.00889597	1.31661562	-1.90333080
H	-0.13210439	-2.06194153	-2.06456193
H	-2.14606651	-2.80525823	-3.35063773
H	-4.41257111	-2.15894422	-2.54236920

H	-2.83345180	0.04494861	0.57217962
H	1.03911170	-3.09505801	0.83967129
H	2.32116153	0.35121230	-1.44373775
H	4.34030456	-0.93357197	-2.09168769
H	4.65288562	-3.24753658	-1.16317178
N	3.52153711	3.30835571	2.67337349
N	4.85908506	2.03085648	0.42416642
N	4.55749984	4.47530531	-1.17496116
N	3.24952188	5.77757874	1.10083437
C	2.93631652	1.98419940	4.47459592
C	3.64832418	2.03936386	3.20888857
C	2.41827772	3.22920216	4.70094191
C	2.79209992	4.06266725	3.57243986
C	4.34649586	0.97008625	2.60766681
C	4.98235003	1.01508113	1.34762478
C	5.80919067	-0.03955005	0.78789502
C	6.12827934	0.33334172	-0.48902609
C	5.51168856	1.62760646	-0.72256342
C	4.33877105	-0.35039945	3.29753886
C	4.18028245	-2.86927670	4.54381402
C	4.85198809	-0.53152119	4.58610897
C	3.77768510	-1.45608243	2.63276371
C	3.69709771	-2.70130582	3.24448390
C	4.76867934	-1.78752953	5.20303818
C	5.50083658	2.32227343	-1.94870750
C	5.04489495	3.63691783	-2.15564087
C	5.04656722	4.33793290	-3.42708275
C	4.55745875	5.59608925	-3.19338057
C	4.25132156	5.67893389	-1.77376568
C	3.68129071	6.79279032	-1.12140635
C	5.94668478	1.53544085	-3.14153672

C	6.71788963	-0.12409341	-5.28070076
C	7.29995723	1.31433663	-3.40964838
C	4.98166383	0.93910024	-3.97040659
C	5.36329209	0.11490554	-5.02965660
C	7.68182608	0.48341231	-4.47180734
C	3.44029472	8.01309722	-1.94671198
C	2.95757325	10.29079185	-3.52295433
C	4.50996964	8.76219971	-2.44834404
C	2.12694588	8.41580617	-2.23648161
C	1.88774510	9.54619326	-3.01814069
C	4.26763221	9.89547428	-3.23357185
C	3.27418191	6.84503826	0.22822530
C	2.77603962	8.02723737	0.91110201
C	2.43777041	7.64644300	2.18196918
C	2.72170638	6.22536135	2.29259483
C	2.44861176	5.42194764	3.41816075
C	1.71517937	6.06560627	4.54993078
C	0.34017932	7.24801286	6.69894376
C	2.36188106	6.27286783	5.77461719
C	0.37543226	6.45865159	4.40897761
C	-0.30582945	7.04462260	5.47812429
C	1.67651882	6.85821301	6.84327511
Zn	3.86267947	3.84970368	0.68477547
H	5.31745993	0.30426407	5.10466556
H	3.38776447	-1.31003896	1.63349051
H	3.24487961	-3.53714678	2.72023162
C	5.35163445	-1.94908953	6.58118940
H	4.10652379	-3.83155259	5.03634234
H	8.05410610	1.78082802	-2.77854690
H	3.92731653	1.12518306	-3.76813081
H	4.60744359	-0.34980676	-5.66180985

C	9.15196877	0.24527911	-4.70005667
H	7.02031882	-0.76765183	-6.10257109
H	5.53025765	8.46237868	-2.21777562
H	1.29299290	7.83645744	-1.85040805
H	0.86360066	9.84620737	-3.23598733
C	5.44419097	10.65453768	-3.78986054
H	2.77843205	11.17345651	-4.13209853
H	3.40078373	5.97214182	5.88835789
H	-0.13791454	6.29349067	3.46508528
H	-1.34820823	7.33897625	5.36112720
H	-0.18767951	7.70068204	7.53531927
C	2.40381347	7.12289321	8.13613507
H	2.04569494	8.26974141	2.97650128
H	2.70842559	9.01795636	0.47836991
H	6.73601182	-0.21469415	-1.19877722
H	6.10964153	-0.94221342	1.30469000
H	2.82801097	1.10702927	5.09961923
H	1.81390437	3.54681564	5.54123219
H	5.39155295	3.92603823	-4.36866207
H	4.41752564	6.39326947	-3.91367029
N	-4.95909305	1.31809320	0.97285039
N	-4.52549781	1.65290877	-1.89366962
N	-6.39625043	-0.56994612	-2.44213941
N	-6.79802653	-0.91224775	0.44436890
C	-3.85554987	2.74957787	2.40875675
C	-4.07268961	2.37855489	1.02045372
C	-4.59817053	1.89765205	3.17846433
C	-5.30790691	1.01151055	2.27547464
C	-3.46464106	2.99913181	-0.09468645
C	-3.69440429	2.66106253	-1.44964699
C	-3.00512453	3.23859989	-2.59382613

C	-3.40509868	2.54633027	-3.70363857
C	-4.34769042	1.53634437	-3.25731920
C	-2.43884573	4.04680724	0.18471313
C	-0.40372927	5.95188735	0.63978776
C	-2.53093412	5.33178012	-0.36780549
C	-1.33058485	3.74864845	0.99623532
C	-0.33287397	4.68955053	1.23179797
C	-1.51217952	6.26806265	-0.15340148
C	-4.93941681	0.56869351	-4.09240743
C	-5.88787551	-0.40164793	-3.71404803
C	-6.38976482	-1.45825037	-4.57625785
C	-7.19761519	-2.25275291	-3.80915646
C	-7.18968050	-1.69955656	-2.46610597
C	-7.81797324	-2.28702463	-1.34915045
C	-4.45738792	0.50859814	-5.50541243
C	-3.55311602	0.31665076	-8.16242201
C	-5.30410483	0.84603407	-6.56622765
C	-3.15071673	0.07491729	-5.78504222
C	-2.70244792	-0.01168827	-7.10340506
C	-4.85600519	0.74388493	-7.88795976
C	-8.68229938	-3.47571661	-1.60867786
C	-10.28333650	-5.72854529	-2.13116872
C	-9.86609918	-3.34591394	-2.34277773
C	-8.30714738	-4.74394782	-1.13535500
C	-9.10176147	-5.86062242	-1.39606211
C	-10.66074952	-4.46828320	-2.60389798
C	-7.66627563	-1.88368345	-0.00886267
C	-8.38776038	-2.44493227	1.12055139
C	-7.92999762	-1.81332439	2.24378228
C	-6.92214722	-0.85719465	1.81538666
C	-6.20227636	-0.00221021	2.67204559



C	-6.39733041	-0.20305162	4.13894830
C	-6.72595263	-0.58653965	6.90805331
C	-7.01347892	0.77927849	4.92093338
C	-5.96042953	-1.38841831	4.75436890
C	-6.12391941	-1.57720846	6.12642323
C	-7.17227408	0.58961692	6.29853199
Zn	-5.53252438	0.23341383	-0.71938265
H	-3.39966860	5.59946921	-0.96482315
H	-1.24969856	2.75709282	1.42489983
H	0.51766857	4.43301978	1.85578298
C	-1.60106290	7.60558521	-0.83524842
H	0.38309043	6.68219214	0.80005574
H	-6.31608435	1.18540515	-6.35473731
H	-2.49982730	-0.20504920	-4.95847079
H	-1.68761489	-0.34304151	-7.31769525
C	-5.81685641	1.05766354	-9.00685498
H	-3.20974774	0.24357440	-9.19153933
H	-10.16352960	-2.36620591	-2.71111625
H	-7.38204356	-4.84562813	-0.56950234
H	-8.79869478	-6.84162894	-1.03198792
C	-11.94168775	-4.28188649	-3.37548199
H	-10.90417509	-6.59624452	-2.34002093
H	-7.37319353	1.69153652	4.44945134
H	-5.49400427	-2.15764431	4.14374623
H	-5.77885102	-2.49809862	6.59507657
C	-7.80799650	1.69096928	7.10666045
H	-6.85330422	-0.72743240	7.97857156
H	-8.26161788	-1.95861221	3.26454067
H	-9.16179849	-3.19975534	1.05515425
H	-3.10658346	2.71473277	-4.73147072
H	-2.31024390	4.06509747	-2.55872978

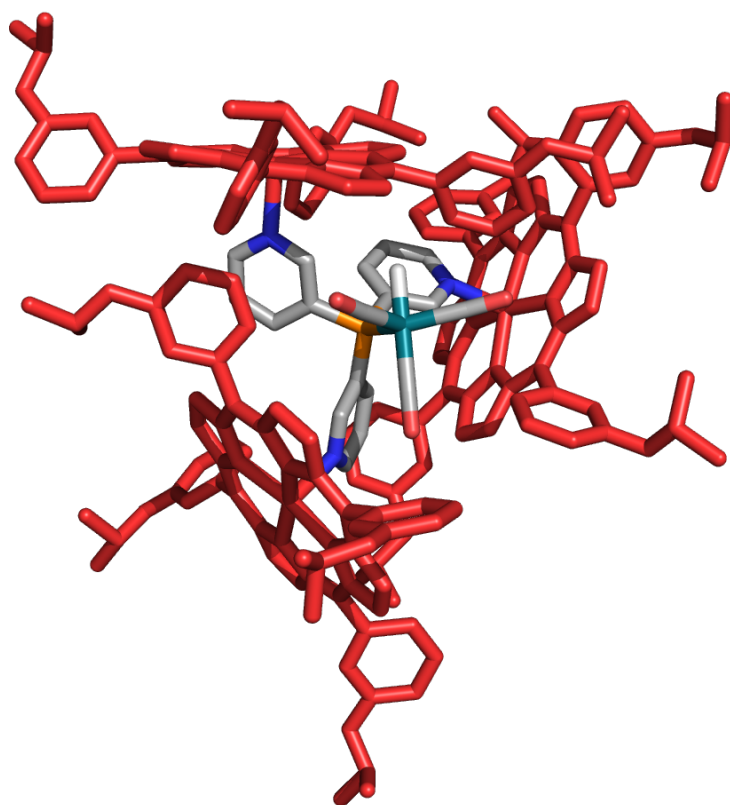
H	-3.22920408	3.56057275	2.75577508
H	-4.66152384	1.88130604	4.25924900
H	-6.14234261	-1.59256976	-5.62198042
H	-7.72210469	-3.14916933	-4.11692664
N	4.90909971	-5.75236053	0.03912682
N	2.60210620	-5.94621180	1.84066199
N	0.78939327	-5.51928087	-0.44220694
N	3.10382740	-5.42216228	-2.23971654
C	7.01639171	-5.81806853	0.98064838
C	5.58619715	-5.85968796	1.23578368
C	7.18197497	-5.66465170	-0.36852774
C	5.85558296	-5.63129288	-0.95902592
C	4.99480325	-5.99110466	2.50865273
C	3.61161194	-6.06129293	2.77872709
C	3.01875257	-6.12951073	4.10314334
C	1.66387560	-6.03191750	3.94801765
C	1.40251481	-5.91767248	2.52508581
C	5.91665009	-5.97644457	3.68380439
C	7.58999212	-5.87764062	5.94160341
C	6.04245106	-7.09288227	4.51776079
C	6.64985271	-4.81517064	3.98200808
C	7.47628902	-4.76640385	5.10363442
C	6.87354175	-7.04117554	5.64266970
C	0.13001365	-5.73416414	1.94497789
C	-0.14537841	-5.56175038	0.57346368
C	-1.46400081	-5.33006658	0.01454541
C	-1.29977828	-5.10658166	-1.32380775
C	0.11986562	-5.22696847	-1.61474781
C	0.73381764	-5.02727291	-2.87380952
C	-1.03870286	-5.68379752	2.87636545
C	-3.22868568	-5.58820209	4.64002865

C	-1.43654787	-6.83124857	3.57293198
C	-1.75549579	-4.49187132	3.06377916
C	-2.83980861	-4.44388582	3.94058993
C	-2.52641808	-6.78314508	4.44819756
C	-0.10791627	-4.48984056	-3.98230312
C	-1.72606395	-3.32556392	-5.98471356
C	-1.26231605	-5.14485283	-4.43699270
C	0.23775133	-3.25845820	-4.57075287
C	-0.55596611	-2.68984639	-5.56711456
C	-2.07290186	-4.55567042	-5.41261225
C	2.10826628	-5.18873977	-3.16067369
C	2.70002886	-5.08965154	-4.48736871
C	4.05306324	-5.22040234	-4.33628382
C	4.30550468	-5.40399206	-2.91911572
C	5.58074721	-5.45966289	-2.32959633
C	6.75358646	-5.22296605	-3.22809198
C	8.99230651	-4.73995132	-4.85780510
C	7.58301735	-6.27905385	-3.61503404
C	7.04601654	-3.92295913	-3.67236071
C	8.15968631	-3.68378752	-4.47853742
C	8.69628770	-6.03748931	-4.42877047
Zn	2.85901830	-5.48869388	-0.16223883
H	5.48631955	-7.99950734	4.28963199
H	6.54495903	-3.94235568	3.34161783
H	8.01623265	-3.85153972	5.34085070
C	7.02219618	-8.27129169	6.50006766
H	8.22308539	-5.84024329	6.82484747
H	-0.89667576	-7.76322535	3.42133940
H	-1.45520182	-3.60364009	2.51469143
H	-3.38144028	-3.51255619	4.08309876
C	-2.90825348	-8.01884624	5.22172696

H	-4.07448634	-5.55911763	5.32308271
H	-1.52922795	-6.11287550	-4.02112448
H	1.13271162	-2.74310064	-4.22516819
H	-0.27179159	-1.73340923	-6.00265479
C	-3.38130516	-5.19992946	-5.79103465
H	-2.36973040	-2.87182593	-6.73362210
H	7.35596698	-7.28893890	-3.27971994
H	6.39786223	-3.09781128	-3.38014027
H	8.39273984	-2.67434848	-4.80543661
C	9.60134651	-7.18752545	-4.78806246
H	9.86317718	-4.55744898	-5.48299093
H	4.81143831	-5.21422925	-5.11008689
H	2.15063472	-4.96743973	-5.41262365
H	0.91403640	-6.01313548	4.72882509
H	3.56411254	-6.21975872	5.03408916
C	-0.51747116	1.44494504	3.59365497
O	-0.61758204	2.51764954	4.00906250
F	-8.98920195	2.11606973	6.54730447
F	-8.07813906	1.31375997	8.39451763
F	-6.98642032	2.79785166	7.17389471
F	-12.88708315	-3.61452461	-2.62812555
F	-12.50107248	-5.47029468	-3.76316379
F	-11.74242993	-3.53391717	-4.51304092
F	-6.53006771	2.20466801	-8.76078631
F	-5.18484295	1.21847316	-10.21158378
F	-6.73922920	0.04596224	-9.16709336
F	-1.20374321	7.51407319	-2.16378255
F	-0.79428916	8.54963332	-0.25698516
F	-2.87660274	8.10472913	-0.84955135
F	-4.41481318	-4.67444039	-5.03463357
F	-3.38325324	-6.55140138	-5.57915021

F	-3.70721696	-4.98376822	-7.10357844
F	10.37460827	-6.92153330	-5.88744964
F	10.46287093	-7.48638424	-3.75346256
F	8.89258029	-8.33339444	-5.05286939
F	-2.16494988	-8.13413248	6.37772430
F	-4.22769218	-8.00951608	5.59778622
F	-2.69664092	-9.16573301	4.49983298
F	3.02710180	8.35256279	8.11914921
F	3.37898870	6.18819020	8.38055084
F	1.55790390	7.12255597	9.21626788
F	5.82970473	-8.94027123	6.64538119
F	7.91111138	-9.16740852	5.94605402
F	7.48146244	-7.98002765	7.75783435
F	6.71728474	-1.73866379	6.57757239
F	5.14078992	-3.19451536	7.10484155
F	4.82432269	-1.03697779	7.46746620
F	6.04844998	9.95611850	-4.81610897
F	5.09238680	11.87847350	-4.29355359
F	6.41289447	10.86553428	-2.83860707
F	9.84449719	1.42019503	-4.84079878
F	9.39537645	-0.51074974	-5.81930505
F	9.71862134	-0.42404679	-3.63581326.

# CAT4



Energy: -55801.234 kcal/mol

Rh	-0.32317551	-0.24703920	2.87032977
C	0.43062733	-1.68067812	4.03115401
C	-2.19307730	-0.95261360	2.72162428
P	0.14243500	-0.23372843	0.51039970
O	-3.24838189	-1.39305803	2.57623468
O	0.86217168	-2.44838553	4.77701861
H	7.90075767	-5.15446688	1.17883741
H	7.97974854	-5.03419314	-1.50385579
C	1.64020476	-1.10470149	-0.14708185
C	2.62374060	-0.47907947	-0.93110345
C	1.81528037	-2.45953849	0.16471074
C	3.74113193	-1.20751878	-1.33667679
N	2.88405872	-3.16127831	-0.24368218
C	3.84143859	-2.54287873	-0.96555334

C	0.49913964	1.43884079	-0.16736738
C	-0.02079873	1.95618498	-1.35914820
C	1.47761340	2.17971926	0.50592017
C	0.47448498	3.17420558	-1.83113386
N	1.98085226	3.32220427	0.02431238
C	1.48765352	3.81826981	-1.12807778
C	-1.17704829	-0.85168936	-0.61974756
C	-0.96936428	-1.74824882	-1.67829308
C	-2.48644903	-0.41380122	-0.37810549
C	-2.07013497	-2.18399015	-2.41667302
N	-3.53955468	-0.83435676	-1.09350854
C	-3.33721278	-1.72111282	-2.08945444
H	1.19272160	0.28525336	2.93119564
H	-2.29635562	-5.20646509	0.95172072
H	-2.24257996	-4.88575330	-1.68937775
H	1.89345759	1.83260041	1.44964353
H	1.93030951	4.74716748	-1.47952436
H	0.09319138	3.60598221	-2.75296199
H	-0.79304434	1.42773082	-1.91412896
H	0.02513429	-2.11500207	-1.92081721
H	-1.94661321	-2.87643540	-3.23764764
H	-4.22013905	-2.04700888	-2.63262612
H	-2.70787423	0.31102303	0.40163373
H	1.07823396	-3.00417676	0.75380954
H	2.54410926	0.56647023	-1.21095132
H	4.51446934	-0.73880752	-1.93727311
H	4.69511187	-3.15382304	-1.24736973
N	3.38896131	3.52234926	2.98161701
N	4.85942871	2.30269625	0.77746922
N	4.56126147	4.73631876	-0.82911473
N	3.15951258	5.99996041	1.41883366

C	2.70868503	2.15995911	4.72003923
C	3.48921426	2.24284367	3.49809721
C	2.17251576	3.39947101	4.94113655
C	2.60535134	4.25606214	3.85150191
C	4.21872416	1.18995825	2.90875979
C	4.92931628	1.27194091	1.69113378
C	5.76222821	0.21417607	1.15068551
C	6.12387827	0.59057395	-0.11170351
C	5.53691852	1.89861849	-0.35602739
C	4.16495191	-0.16812153	3.52246281
C	4.06242784	-2.78003725	4.54143975
C	4.64115764	-0.43617832	4.80724706
C	3.64122568	-1.22147920	2.74585838
C	3.59092377	-2.51078644	3.25600222
C	4.60025149	-1.74645741	5.31617689
C	5.54013370	2.58898934	-1.58976490
C	5.06945770	3.89931036	-1.80243144
C	5.05280010	4.58939098	-3.07903711
C	4.52199161	5.83373410	-2.85870674
C	4.21310599	5.92305931	-1.44008018
C	3.59060802	7.02010541	-0.80262440
C	5.95956484	1.76395997	-2.76693415
C	6.60780581	-0.19701336	-4.68082932
C	7.27180563	1.29780756	-2.88930942
C	4.97643212	1.28888850	-3.65481290
C	5.31008378	0.32180435	-4.60512366
C	7.59832821	0.30040570	-3.82033930
C	3.29339877	8.21637511	-1.64563354
C	2.75660634	10.42389693	-3.28479845
C	4.35114570	8.96807283	-2.18199334
C	1.96545960	8.57699241	-1.91863826



C	1.71215380	9.67762810	-2.74506314
C	4.08909773	10.07413924	-3.00080844
C	3.17359977	7.06643293	0.54473316
C	2.62975767	8.23473120	1.21624082
C	2.26751518	7.84369820	2.47795553
C	2.58009617	6.42989038	2.59430846
C	2.25869259	5.61377849	3.69764038
C	1.43486261	6.23812732	4.77966151
C	-0.09782755	7.41586717	6.81898365
C	2.00447976	6.51088115	6.02406393
C	0.08291942	6.54937632	4.55016178
C	-0.66661523	7.12901818	5.57214562
C	1.25031855	7.10349528	7.05310824
Zn	3.80849528	4.08816683	1.00866334
H	5.07830788	0.35525164	5.41381713
H	3.28008157	-1.00554402	1.74947688
H	3.17966864	-3.32084367	2.65999833
O	5.14330973	-1.91335608	6.57099697
H	4.01020203	-3.79249640	4.91150373
H	8.04508545	1.65108233	-2.20986272
H	3.95238747	1.64813177	-3.56172849
H	4.54407140	-0.05934690	-5.28107963
O	8.90884665	-0.12516438	-3.81382356
H	6.83697935	-0.97564077	-5.40239434
H	5.36522421	8.66770943	-1.93855969
H	1.14450252	8.00864265	-1.48668975
H	0.68594149	9.96071295	-2.97418052
O	5.04704996	10.86769892	-3.58645781
H	2.56777189	11.28389209	-3.92558117
H	3.05044334	6.27349573	6.21232740
H	-0.37154671	6.33214644	3.58788401

H	-1.71661457	7.36944594	5.40210905
H	-0.70925322	7.87970243	7.58140565
O	1.96079604	7.34296482	8.20701371
H	1.82502346	8.44784584	3.26083952
H	2.53892803	9.21993865	0.77515012
H	6.73277870	0.02812860	-0.80551135
H	6.02430402	-0.70054428	1.66527741
H	2.57618248	1.26573681	5.31608362
H	1.52021870	3.70564852	5.74943933
H	5.40865601	4.17470887	-4.01534046
H	4.34937789	6.61770440	-3.58629434
N	-4.96035087	1.44171917	0.74827592
N	-4.40297767	1.84641230	-2.08454146
N	-6.15240695	-0.46216781	-2.75602796
N	-6.67116184	-0.86805399	0.09193968
C	-3.98849138	2.88597800	2.26434120
C	-4.11136487	2.52796303	0.86019905
C	-4.74140394	1.99490028	2.97866861
C	-5.36143765	1.09557017	2.02521449
C	-3.43357765	3.16408342	-0.20752177
C	-3.58154970	2.83352991	-1.57634290
C	-2.78933873	3.38893790	-2.66286430
C	-3.11444283	2.70341926	-3.80058864
C	-4.11657764	1.72181009	-3.43001830
C	-2.40156633	4.18110014	0.15429706
C	-0.37162419	6.01608899	0.79645572
C	-2.41141994	5.47192046	-0.40817962
C	-1.37764252	3.83196478	1.04597949
C	-0.38221657	4.75187706	1.37416197
C	-1.38961160	6.38061523	-0.10025946
C	-4.63951454	0.75372592	-4.30583233

C	-5.58750723	-0.23802250	-3.99639991
C	-6.01294558	-1.27861888	-4.91326328
C	-6.81323490	-2.13385868	-4.20584370
C	-6.88726846	-1.62902276	-2.84433585
C	-7.50861948	-2.29364258	-1.76305202
C	-4.04300502	0.69001108	-5.67918625
C	-2.93969068	0.51378797	-8.24329228
C	-4.72500488	1.24362074	-6.77127917
C	-2.81334505	0.04778072	-5.86519535
C	-2.26879490	-0.03085355	-7.15213792
C	-4.17972313	1.15247324	-8.06077124
C	-8.20566471	-3.57851602	-2.05988428
C	-9.44789766	-6.03115843	-2.66966684
C	-9.25807423	-3.63493415	-2.98399209
C	-7.78829543	-4.76433619	-1.42714274
C	-8.41332133	-5.97328382	-1.73050443
C	-9.86916562	-4.85284075	-3.30198644
C	-7.45055404	-1.88831218	-0.41175041
C	-8.19074584	-2.50226240	0.67839008
C	-7.82505518	-1.85824927	1.82865830
C	-6.85873873	-0.83962888	1.45827772
C	-6.22325905	0.03377899	2.36093098
C	-6.49427428	-0.19198206	3.81484884
C	-7.02883121	-0.60247249	6.53272840
C	-7.29096676	0.72335287	4.51969335
C	-5.96988105	-1.31409661	4.46725260
C	-6.23963994	-1.50746540	5.82702976
C	-7.56246187	0.52289303	5.87966418
Zn	-5.39501557	0.35739864	-0.97973107
H	-3.22230665	5.73720624	-1.07847434
H	-1.35308649	2.83073880	1.45755872

H	0.40804059	4.47155377	2.06482802
O	-1.28972281	7.66258434	-0.59847057
H	0.40437606	6.73925487	1.02572967
H	-5.67607781	1.73236835	-6.58545058
H	-2.30137588	-0.39004816	-5.01099445
H	-1.30866873	-0.52081570	-7.31075462
O	-4.76892858	1.62983380	-9.20573213
H	-2.52765912	0.45509713	-9.24956546
H	-9.61639186	-2.72822966	-3.46809074
H	-6.96575958	-4.73043779	-0.71406813
H	-8.07566315	-6.89090471	-1.24816814
O	-10.84620759	-4.81367023	-4.28035256
H	-9.90688663	-6.98589496	-2.91271086
H	-7.69045548	1.57494005	3.97904264
H	-5.36294347	-2.02352775	3.91131151
H	-5.83166481	-2.37729562	6.34186370
O	-8.32015117	1.36013146	6.66492076
H	-7.24931135	-0.74415166	7.58964911
H	-8.18243914	-2.04045942	2.83481181
H	-8.90982190	-3.30453513	0.56914660
H	-2.71293779	2.83778656	-4.79820643
H	-2.06555371	4.18163664	-2.55868876
H	-3.40301923	3.70879017	2.65251851
H	-4.86793504	1.95023926	4.05328981
H	-5.72021762	-1.34910052	-5.95407717
H	-7.29193547	-3.03315252	-4.56494813
N	4.92295681	-5.59586992	-0.27580400
N	2.79166510	-5.80318718	1.74339959
N	0.76676821	-5.48681952	-0.36135526
N	2.89810612	-5.43559695	-2.36939097
C	7.07473979	-5.26299913	0.48691239

C	5.69329536	-5.49914710	0.86463363
C	7.11593037	-5.21671009	-0.88109477
C	5.76322941	-5.44076192	-1.36028705
C	5.22829326	-5.63720017	2.18794597
C	3.89091488	-5.85553423	2.58005126
C	3.43076914	-5.99114599	3.95104835
C	2.06349449	-5.95946745	3.92670086
C	1.66143418	-5.83048929	2.53661496
C	6.23232579	-5.44414863	3.28011879
C	8.08176072	-5.03877245	5.35942206
C	6.64150167	-6.51436438	4.08384004
C	6.75065602	-4.16181141	3.52906213
C	7.67132565	-3.96663302	4.55988127
C	7.55264901	-6.31534563	5.12722659
C	0.33678960	-5.64568780	2.08398824
C	-0.06337309	-5.47723584	0.74244239
C	-1.42779284	-5.24397736	0.30700777
C	-1.39728877	-5.09018307	-1.05022359
C	-0.01741437	-5.26434223	-1.47806377
C	0.45814963	-5.22924168	-2.81142075
C	-0.73755639	-5.56394374	3.12029456
C	-2.72463376	-5.37605121	5.10219105
C	-1.04658960	-6.67151505	3.92152393
C	-1.43855407	-4.36415615	3.31565221
C	-2.42584245	-4.27340698	4.29811373
C	-2.02858157	-6.57601161	4.91101457
C	-0.50772299	-4.87676111	-3.89231546
C	-2.45411086	-3.94602232	-5.71868508
C	-1.73238457	-5.53532711	-4.03024688
C	-0.23166356	-3.77736628	-4.73465855
C	-1.19557186	-3.33715337	-5.63827529

C	-2.72420048	-5.05953647	-4.90672128
C	1.80245950	-5.42322859	-3.20401850
C	2.24685891	-5.60282778	-4.57510012
C	3.61201809	-5.68217560	-4.54917497
C	4.02211734	-5.54417665	-3.16297394
C	5.35754286	-5.46075169	-2.71417077
C	6.41331503	-5.34106615	-3.76030433
C	8.38640656	-5.13463332	-5.75390486
C	7.45726825	-6.27609100	-3.82864795
C	6.36832943	-4.29967928	-4.70273970
C	7.33902465	-4.21300291	-5.70136982
C	8.45286474	-6.16436545	-4.80562935
Zn	2.84778761	-5.37175114	-0.28399265
H	6.25771424	-7.51703989	3.90177865
H	6.41333227	-3.32342460	2.92466173
H	8.06197541	-2.96655769	4.75017087
O	7.94737004	-7.42263878	5.86968439
H	8.81734710	-4.89573894	6.14687732
H	-0.52367000	-7.61582337	3.78386526
H	-1.20046471	-3.50663777	2.69480687
H	-2.96699257	-3.33998332	4.43873454
O	-2.31559657	-7.70523377	5.66574412
H	-3.50358900	-5.31843167	5.86066694
H	-1.96087852	-6.40565238	-3.42023005
H	0.71649852	-3.25241418	-4.63790906
H	-0.98903188	-2.47763414	-6.27095618
O	-3.91051192	-5.74405694	-4.85822294
H	-3.19675582	-3.54304913	-6.39989971
H	7.47379681	-7.11153130	-3.13427938
H	5.56984106	-3.56442095	-4.64458875
H	7.28643687	-3.41716894	-6.44284895

O	9.46420313	-7.11116441	-4.91286516
H	9.15152595	-5.08095911	-6.52646000
H	4.28079930	-5.84403736	-5.38367631
H	1.59464561	-5.68453578	-5.43507924
H	1.38981578	-5.98936544	4.77226986
H	4.06975998	-6.07383721	4.82011159
C	-0.71442190	1.54410580	3.62683857
O	-0.88319590	2.57856068	4.11064147
C	-9.05296633	2.45673192	6.02287096
C	-12.82501876	-5.56943791	-5.37337099
C	-12.82010689	-5.10211350	-2.86174478
C	-1.77765835	7.50321666	-2.99836836
C	-2.16476682	9.61813422	-1.62485547
C	-12.04565537	-5.63837086	-4.06422911
C	-3.89886167	-7.89901039	-3.85043008
C	-6.01604294	2.39431198	-9.09883912
C	-4.15183054	-9.25457601	5.27578636
C	-6.64140639	2.33954819	-10.48922358
C	-5.71541449	3.81912331	-8.63229970
C	-2.20777203	8.09311277	-1.65339327
C	-3.60093904	-7.26444068	-6.30011051
C	-4.37046788	-7.02024773	-5.00355310
C	-1.83064146	-9.40207045	4.22627418
C	8.81639087	-9.27584706	-3.74120701
C	10.37306689	-7.46806279	-2.85176751
C	9.88231509	0.37328152	-2.87944583
C	-2.64815880	-9.13622380	5.49158954
C	8.08951227	-6.70807065	8.24672869
C	5.84118452	-7.31350381	7.20797823
C	6.44547491	10.69966189	-3.17554574
C	9.86849022	-8.21982208	-4.08239817

C	1.31169273	7.71391986	9.47290548
C	4.38656532	-0.62056661	8.13840292
C	6.73537242	0.25466466	7.69281480
C	7.35023622	-7.56452353	7.21666051
C	6.65921651	11.30624978	-1.78851748
C	5.82665972	-0.96788724	7.75294377
C	7.26977579	11.38524192	-4.26093721
C	9.47335643	0.44191181	-1.40839386
C	10.09895908	1.74336274	-3.51063450
C	0.29463580	6.67048506	9.94230293
C	0.80167338	9.15866518	9.46765018
C	-9.41704681	3.41452829	7.15262587
C	-10.27613483	1.91052206	5.28537164
H	-9.99228206	1.18099464	4.51667166
H	-10.82092502	2.73121801	4.79696276
H	-10.95036593	1.41760496	6.00025894
H	-8.37217541	2.96753089	5.32365890
H	-8.51084966	3.77060303	7.66013692
H	-10.05643113	2.90708074	7.88860750
H	-9.96234231	4.27979980	6.75161026
H	-13.10264103	-4.05431926	-3.03785047
H	-12.21171010	-5.15298143	-1.94980820
H	-13.73292955	-5.69021677	-2.70005371
H	-13.09263691	-4.52842195	-5.59908412
H	-13.74810835	-6.16212356	-5.29579979
H	-12.22117425	-5.96421789	-6.20212642
H	-11.73537406	-6.67954601	-3.88283618
H	-3.97821140	-8.96184792	-4.11224722
H	-4.50429822	-7.72143244	-2.95407918
H	-2.84857163	-7.68154042	-3.61193042
H	-5.44990651	-7.16674766	-5.15698383

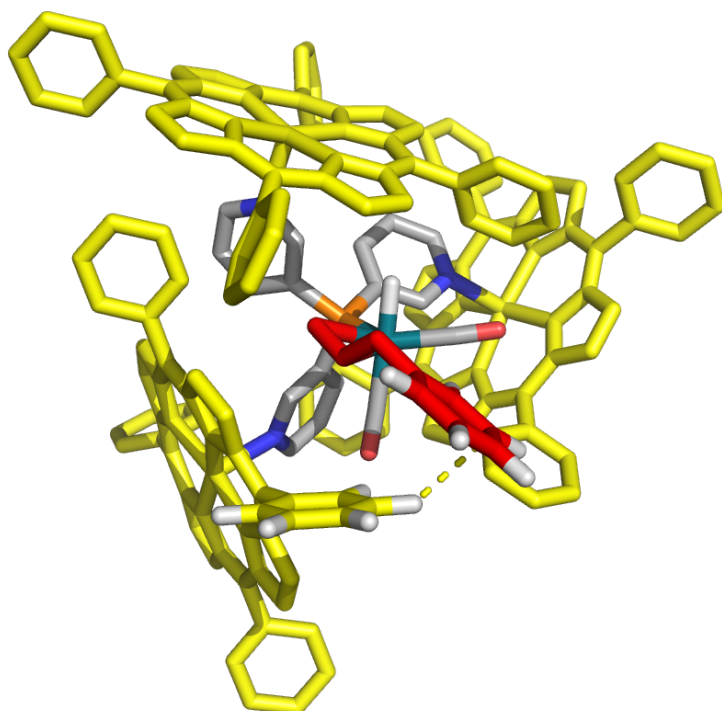


H	-3.91643682	-6.57864400	-7.09641840
H	-3.76975843	-8.29531468	-6.64184832
H	-2.52384746	-7.12365074	-6.12931296
H	-0.75707184	-9.27831750	4.42151470
H	-2.12667835	-8.69938363	3.43203414
H	-1.99811521	-10.43104050	3.87279474
H	-2.32908197	-9.82795554	6.29037154
H	-4.40654779	-10.26212749	4.91883423
H	-4.48429956	-8.52227303	4.52604434
H	-4.69015100	-9.06271200	6.21382757
H	-5.07443079	4.32034355	-9.37096603
H	-5.20140821	3.82580377	-7.66286135
H	-6.64903910	4.38942728	-8.53145919
H	-6.67767379	1.88035420	-8.38330418
H	-7.60579308	2.86463676	-10.48954853
H	-6.80527011	1.29750918	-10.79446830
H	-5.97912798	2.82079121	-11.22357362
H	9.19024698	2.35528677	-3.41726518
H	10.34534460	1.63988832	-4.57646189
H	10.92321623	2.26046494	-3.00485384
H	10.27751305	0.89897357	-0.81885196
H	9.29577453	-0.55973608	-0.99533969
H	8.55782868	1.04074345	-1.29754391
H	10.80197363	-0.21754185	-2.98712580
H	7.70617562	11.17911188	-1.47692845
H	6.01665893	10.83161393	-1.03606154
H	6.42786017	12.38029764	-1.81663339
H	6.68177997	9.62374323	-3.17024647
H	8.34094528	11.28640270	-4.03811496
H	7.01779051	12.45401188	-4.31197539
H	7.06912952	10.93091845	-5.24027986

H	-2.49913092	9.99109930	-0.64808963
H	-2.81772682	10.03129958	-2.40562278
H	-1.14077300	9.97202418	-1.79736473
H	-3.22480029	7.75900118	-1.39367413
H	-0.76357301	7.84037604	-3.25322169
H	-2.46671470	7.82627189	-3.79242486
H	-1.78337616	6.40702545	-2.97223317
H	0.62146002	9.48144514	10.50422412
H	-0.13361263	9.28023516	8.90993382
H	1.55930885	9.81936528	9.02485717
H	2.17597544	7.66963125	10.15339620
H	0.72896523	5.66399093	9.86848616
H	-0.63607357	6.68930004	9.36296015
H	0.04354253	6.86488269	10.99605211
H	9.17212532	-6.88230324	8.17867548
H	7.75558726	-6.97159480	9.26253495
H	7.88986939	-5.64138891	8.09299315
H	5.42251044	-7.55319429	8.19692488
H	5.34014393	-7.93828733	6.45550636
H	5.61892964	-6.26086895	6.99168841
H	4.35912006	-0.21914966	9.16252828
H	3.73219717	-1.49968867	8.09443482
H	3.98822619	0.14156017	7.45218355
H	7.76492045	-0.04584643	7.45670168
H	6.73072678	0.77568884	8.65916976
H	6.38355937	0.95125095	6.91743813
H	7.54084002	-8.62663768	7.43006750
H	6.25505703	-1.69759907	8.45601384
H	10.84189573	-8.17212487	-2.14917908
H	9.54535305	-6.97293514	-2.32935833
H	11.11527711	-6.70917900	-3.13463743

H	9.26946322	-10.05360777	-3.10888542
H	8.43470839	-9.75095047	-4.65485490
H	7.97246885	-8.84655603	-3.18761720
H	10.71531064	-8.70622694	-4.58838264

### CAT1 with allylbenzene



Energy: -43255.17 kcal/mol

Rh	-0.64617531	-0.35747327	2.52840583
C	0.17456065	-1.66525223	3.72443930
C	-2.47336014	-1.08317972	2.25398497
P	-0.09872108	-0.26550565	0.26019921
O	-3.54196151	-1.47782355	2.05258930
O	0.72615460	-2.46459978	4.35443373
H	7.61069665	-5.92710153	1.95553808
H	7.85005637	-5.58336778	-0.70407270
C	1.38592692	-1.24910411	-0.24533551
C	2.44887121	-0.71713671	-0.99382254

C	1.52300861	-2.55513612	0.24977918
C	3.60829621	-1.47239526	-1.16275668
N	2.63599453	-3.28369160	0.06997876
C	3.67489763	-2.73835531	-0.59568391
C	0.34586102	1.33724195	-0.53475188
C	-0.01504226	1.72321345	-1.83481085
C	1.26487821	2.13268849	0.15864311
C	0.59771856	2.84406690	-2.39594562
N	1.87714604	3.18940351	-0.39762668
C	1.56299557	3.53199375	-1.66225400
C	-1.45057295	-0.86203996	-0.82991734
C	-1.41395489	-2.00267522	-1.63910023
C	-2.65879441	-0.15648108	-0.73729186
C	-2.58338384	-2.39743038	-2.29671911
N	-3.77304828	-0.53549690	-1.36979921
C	-3.74411615	-1.65003567	-2.13238224
H	0.83157772	0.27392418	2.70960237
H	-2.60367100	-5.38780469	1.09851978
H	-2.38539510	-5.18541339	-1.55150951
H	1.55965692	1.88729731	1.17700576
H	2.10371641	4.38096956	-2.07521411
H	0.34054391	3.17041000	-3.40121496
H	-0.74646242	1.15548000	-2.40721845
H	-0.50161698	-2.58252729	-1.74616735
H	-2.59313586	-3.27493901	-2.93400399
H	-4.67839666	-1.92558652	-2.61550428
H	-2.74720231	0.74435011	-0.13139113
H	0.72635480	-3.02747849	0.82240787
H	2.39874708	0.28513413	-1.40811065
H	4.46077914	-1.06806089	-1.69776194
H	4.57189932	-3.34678708	-0.65991339

N	3.11574206	3.31306878	2.60492337
N	4.71497944	2.18013793	0.45691044
N	4.52561870	4.70516753	-1.03251748
N	2.95237870	5.85827264	1.15787617
C	2.51239506	1.91334478	4.34066367
C	3.32791726	2.05956361	3.14785904
C	1.81496432	3.08044471	4.49626876
C	2.19365149	3.95687339	3.40465627
C	4.14130257	1.05265934	2.59047181
C	4.83089505	1.14707451	1.36423767
C	5.73762222	0.14586592	0.83295957
C	6.12664900	0.57338767	-0.40830920
C	5.46766933	1.84615279	-0.64726564
C	4.19799798	-0.25255523	3.30737269
C	4.15314641	-2.72179779	4.64082504
C	4.74524289	-0.37052435	4.59409926
C	3.65094937	-1.38960542	2.69401852
C	3.62543649	-2.61722704	3.35133051
C	4.72216637	-1.60195540	5.25507018
C	5.58323793	2.61040285	-1.82833048
C	5.15026099	3.93971498	-1.99756321
C	5.29625690	4.72918473	-3.20720301
C	4.77296854	5.96855102	-2.94652222
C	4.27211447	5.94449729	-1.58216688
C	3.58986139	7.00364068	-0.94686302
C	6.21252278	1.91352721	-2.99128537
C	7.39086342	0.48963891	-5.11218938
C	7.49561458	2.24947231	-3.44571924
C	5.52381666	0.86213758	-3.61935784
C	6.10744680	0.15091436	-4.67029469
C	8.08063102	1.54201439	-4.50060816

C	3.38463641	8.25330190	-1.74358913
C	2.95210886	10.60373644	-3.22447792
C	4.10377430	9.42032385	-1.44931116
C	2.45057322	8.27407049	-2.79078918
C	2.23291283	9.44199585	-3.52569391
C	3.88874588	10.58941386	-2.18547720
C	2.99861610	6.96374713	0.33297843
C	2.18528936	8.02120488	0.91297719
C	1.61267062	7.51515834	2.04876775
C	2.08758679	6.15101792	2.19422732
C	1.67005510	5.24724614	3.18739488
C	0.48327745	5.61930044	4.02324711
C	-1.80641408	6.09734255	5.57956859
C	0.60799083	6.06110493	5.34650981
C	-0.79919779	5.43584779	3.48079633
C	-1.93782779	5.66761787	4.25478710
C	-0.53213689	6.30089619	6.12095555
Zn	3.65115369	3.96155003	0.69467940
H	5.18306356	0.50683543	5.06940482
H	3.21622045	-1.28271003	1.70823399
H	3.17608148	-3.47972936	2.86918649
H	5.14827736	-1.68829039	6.25470080
H	4.12293619	-3.67310649	5.16366033
H	8.03597328	3.05818917	-2.95482438
H	4.52004425	0.61310475	-3.27944038
H	5.56208422	-0.66500582	-5.14455329
H	9.08181649	1.80759210	-4.83990328
H	7.85036657	-0.06093488	-5.93272851
H	4.83275769	9.40269078	-0.63974545
H	1.88605404	7.37107939	-3.01694971
H	1.49922512	9.44617055	-4.33190015

H	4.45601665	11.48973862	-1.94962000
H	2.78399728	11.51553962	-3.79716716
H	1.60322367	6.20240039	5.76724108
H	-0.89784396	5.09433472	2.45386046
H	-2.92557610	5.50721985	3.82605405
H	-0.42488049	6.64280666	7.15041859
H	-2.69371565	6.27637880	6.18671171
H	0.92140063	8.00679001	2.72363639
H	2.04887794	9.00832014	0.48769535
H	6.81291777	0.08763356	-1.09229504
H	6.03682687	-0.75859613	1.34814756
H	2.46633261	1.02701823	4.96048082
H	1.11052714	3.33143641	5.27701917
H	5.74556945	4.38182565	-4.13012187
H	4.73045338	6.82249153	-3.61205188
N	-4.71925204	2.26257609	0.11033460
N	-4.39739840	2.04953245	-2.78536116
N	-6.43303300	-0.08579550	-2.85418475
N	-6.68154978	0.08166983	0.06386477
C	-3.70898686	4.05099564	1.16418956
C	-3.88551069	3.34737134	-0.09345232
C	-4.40217172	3.35722289	2.11782204
C	-5.05232606	2.24381391	1.45222190
C	-3.26046828	3.68964878	-1.31134170
C	-3.47023811	3.04054537	-2.54786706
C	-2.69147381	3.26256781	-3.75529696
C	-3.14908005	2.38245422	-4.69988764
C	-4.22426840	1.62274099	-4.08626734
C	-2.28449458	4.81450658	-1.27810673
C	-0.45718707	6.95531012	-1.18299669
C	-2.47894822	5.95714701	-2.07388870

C	-1.15788040	4.76241216	-0.44198629
C	-0.25222087	5.82054093	-0.39430836
C	-1.57074700	7.01812378	-2.02786271
C	-4.95161471	0.59916458	-4.72179313
C	-5.98678776	-0.16882517	-4.15799363
C	-6.67093920	-1.25996894	-4.82860117
C	-7.50681107	-1.83654576	-3.90915936
C	-7.33873337	-1.10759099	-2.66211062
C	-7.91364111	-1.47518865	-1.42701010
C	-4.52879526	0.23359698	-6.11154107
C	-3.71865502	-0.49281023	-8.70006688
C	-5.11163658	0.84020319	-7.23101293
C	-3.53639124	-0.74034739	-6.29668460
C	-3.13265747	-1.10142795	-7.58439004
C	-4.70918451	0.47855287	-8.52069050
C	-8.88277354	-2.61184286	-1.44639638
C	-10.69192590	-4.76309472	-1.50012812
C	-10.14117457	-2.46777789	-2.04986311
C	-8.54018119	-3.84504214	-0.87031601
C	-9.43832580	-4.91478813	-0.89728676
C	-11.04116703	-3.53658473	-2.07552115
C	-7.61391358	-0.90683802	-0.17252826
C	-8.23717289	-1.28314597	1.08634267
C	-7.65685420	-0.52510326	2.06591111
C	-6.67752471	0.33231867	1.41944347
C	-5.90191696	1.30682454	2.07631054
C	-6.00037746	1.36598410	3.56662928
C	-6.09732723	1.48074002	6.37308809
C	-6.62479370	2.44403301	4.21250409
C	-5.44451131	0.33700289	4.34348343
C	-5.48990022	0.39540223	5.73705922



C	-6.67179356	2.50172074	5.60842161
Zn	-5.42636347	0.92711534	-1.34252798
H	-3.35795913	6.01026478	-2.71520455
H	-0.98386563	3.87197979	0.15685527
H	0.62094977	5.74767843	0.24222497
H	-1.74051328	7.90276517	-2.64199921
H	0.24684547	7.78203467	-1.13812008
H	-5.88352283	1.59482866	-7.08223440
H	-3.09228623	-1.21218507	-5.42217485
H	-2.36214578	-1.85823846	-7.72490167
H	-5.16996940	0.95460390	-9.38615097
H	-3.40496864	-0.77580639	-9.70473186
H	-10.40829877	-1.50907876	-2.49323108
H	-7.56191422	-3.95735578	-0.40399071
H	-9.15850555	-5.86871680	-0.45024629
H	-12.01820817	-3.41068526	-2.54184566
H	-11.39394971	-5.59652347	-1.52041464
H	-7.07430743	3.23377849	3.61138766
H	-4.96823036	-0.50310329	3.84404542
H	-5.03158149	-0.39399053	6.32658353
H	-7.16050484	3.34413813	6.09845490
H	-6.11769205	1.53023357	7.46092521
H	-7.88260452	-0.52262453	3.12533623
H	-9.02870833	-2.01439689	1.19551154
H	-2.80280260	2.25988973	-5.71967588
H	-1.90030263	3.99355492	-3.85996054
H	-3.13412386	4.95784354	1.29495963
H	-4.46575838	3.57700962	3.17504927
H	-6.51710391	-1.55101318	-5.86116707
H	-8.15534942	-2.69311015	-4.04909846
N	4.67980613	-5.79345424	0.34975117

N	2.42944615	-5.92002323	2.23103959
N	0.54742209	-5.59667838	-0.00078498
N	2.79918423	-5.55419285	-1.88013782
C	6.81549963	-5.84310690	1.22529994
C	5.39505039	-5.89556430	1.52509510
C	6.93761730	-5.67673082	-0.12763142
C	5.59422213	-5.65938930	-0.67728279
C	4.84475154	-6.00744984	2.81749287
C	3.47080979	-6.02349300	3.13465393
C	2.93134330	-5.99925182	4.48214402
C	1.57679668	-5.84963631	4.37474701
C	1.25946558	-5.81186865	2.95896314
C	5.80432710	-6.03532974	3.96263110
C	7.57704475	-6.05204781	6.14510010
C	5.93340954	-7.17897064	4.76562331
C	6.57839549	-4.90248086	4.26108695
C	7.45663507	-4.90956995	5.34643103
C	6.81454417	-7.18776932	5.85029068
C	-0.03336654	-5.63972193	2.41951501
C	-0.35348240	-5.57044503	1.04642534
C	-1.69360984	-5.41509296	0.51277048
C	-1.57776931	-5.31657922	-0.84625360
C	-0.16595490	-5.42957620	-1.17270985
C	0.39620714	-5.31825774	-2.46682702
C	-1.15924137	-5.46176180	3.38665827
C	-3.23847942	-5.04740201	5.23860919
C	-1.52968873	-6.47865599	4.28043440
C	-1.85936605	-4.24609710	3.42216265
C	-2.88694811	-4.03401026	4.34099520
C	-2.56147604	-6.27161727	5.20064358
C	-0.51895994	-4.97183733	-3.59502079

C	-2.27050530	-4.21653801	-5.67440895
C	-1.60840648	-5.78671042	-3.94664732
C	-0.30872627	-3.78576638	-4.32269120
C	-1.17157524	-3.41363045	-5.35430172
C	-2.48136718	-5.40754479	-4.97002919
C	1.76909302	-5.42156454	-2.78466625
C	2.32398438	-5.34699289	-4.12922674
C	3.68579261	-5.37600932	-4.00526264
C	3.98090348	-5.49282865	-2.58938446
C	5.27484508	-5.48643467	-2.03769120
C	6.40308807	-5.15034392	-2.96206997
C	8.54231996	-4.43737038	-4.63971914
C	7.30474297	-6.12361444	-3.41184441
C	6.57867725	-3.81715093	-3.36816518
C	7.64377292	-3.45940039	-4.19802841
C	8.36801910	-5.76916277	-4.24852172
Zn	2.61949251	-5.51252199	0.20569877
H	5.33853059	-8.06086481	4.53035873
H	6.46914451	-4.00907703	3.65021877
H	8.04241429	-4.01855841	5.57227510
H	6.90892759	-8.08364965	6.46387780
H	8.26242754	-6.05806976	6.99255758
H	-1.00470366	-7.43260582	4.24703939
H	-1.57818593	-3.46368731	2.72643020
H	-3.40990161	-3.07962102	4.35900590
H	-2.84038666	-7.07058087	5.88763609
H	-4.04074014	-4.88774216	5.95879816
H	-1.76446603	-6.72189247	-3.41094174
H	0.53135006	-3.14516981	-4.05845289
H	-0.99356302	-2.48346683	-5.89161717
H	-3.32677355	-6.04728004	-5.22327652

H	-2.96125020	-3.91754721	-6.46104345
H	7.16599838	-7.15832209	-3.09975367
H	5.87573351	-3.05934511	-3.02542176
H	7.77601985	-2.41792146	-4.48742722
H	9.06286778	-6.53445507	-4.59433996
H	9.37644632	-4.16241370	-5.28500382
H	4.42727554	-5.34530806	-4.79486534
H	1.74705016	-5.29780343	-5.04398644
H	0.86117176	-5.74363415	5.17970151
H	3.51645228	-6.05456521	5.39157568
C	-1.36900861	1.71087592	5.20094093
C	-1.22821724	2.03057366	2.67509915
C	-2.63541867	-1.34766587	7.14323634
C	-3.18464272	-0.74813112	8.28271523
C	-3.17217974	0.64475689	8.39852985
C	-2.60521144	1.42855720	7.38872511
H	-1.65342019	-1.03198651	5.25826176
H	-2.63758566	-2.43208645	7.03455412
H	-3.62172540	-1.36122315	9.07101360
H	-3.60607620	1.12394643	9.27640235
H	-2.60359693	2.51492458	7.48383121
H	-2.92577571	1.26515983	3.69033508
H	-0.25779803	2.51413374	2.76565624
H	-1.77613114	2.18825239	1.75103031
C	-1.87570978	1.55026811	3.78355247
H	-1.52820633	2.76849471	5.47846755
H	-0.28419963	1.54672805	5.22282538
C	-2.03895872	0.83994127	6.24977019
C	-2.07356100	-0.55845840	6.13765486

## References

- 1 G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *Journal of Computational Chemistry*, 2001, **22**, 931–967.
- 2 C. F. Guerra, J. G. Snijders, G. Velde and E. J. Baerends, *Theor. Chem. Accounts Theory, Comput Model*, 1998, 391–403.
- 3 A. D. Becke, *Physical Review A*, 1988, **38**, 3098–3100.
- 4 C. Lee, W. Yang and R. Parr G., *Phys. Rev. B*, 1988, **37**, 785–789.
- 5 E. Van Lenthe, E. J. Baerends, J. G. Snijders, E. Van Lenthe, E. J. Baerends and J. G. Snijders, *Chem. Phys.*, 1993, **99**, 4597–4610.
- 6 E. Van Lenthe, E. J. Baerends, J. G. Snijders, E. Van Lenthe, E. J. Baerends and J. G. Snijders, *Chem. Phys.*, 1994, **101**, 9783–9792.
- 7 E. Van Lenthe, A. Ehlers, E. Baerends, E. Van Lenthe, A. Ehlers and E. Baerends, *Chem. Phys.*, 1999, **110**, 8943–8953.