

Kinetic and dynamic kinetic resolution of secondary alcohols with ionic-surfactant-coated *Burkholderia cepacia* lipase: substrate scope and enantioselectivity

Cheolwoo Kim[‡], Jusuk Lee[‡], Jeonghun Cho[‡], Yeonock Oh[‡], Yoon Kyung Choi, Eunjeong Choi,

Jaiwook Park* and Mahn-Joo Kim*

Department of Chemistry, Pohang University of Science and Technology

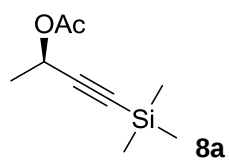
San-31 Hyojadong, Pohang 790-784, Republic of Korea

mjkim@postech.ac.kr (MJK); pjw@postech.ac.kr (JP)

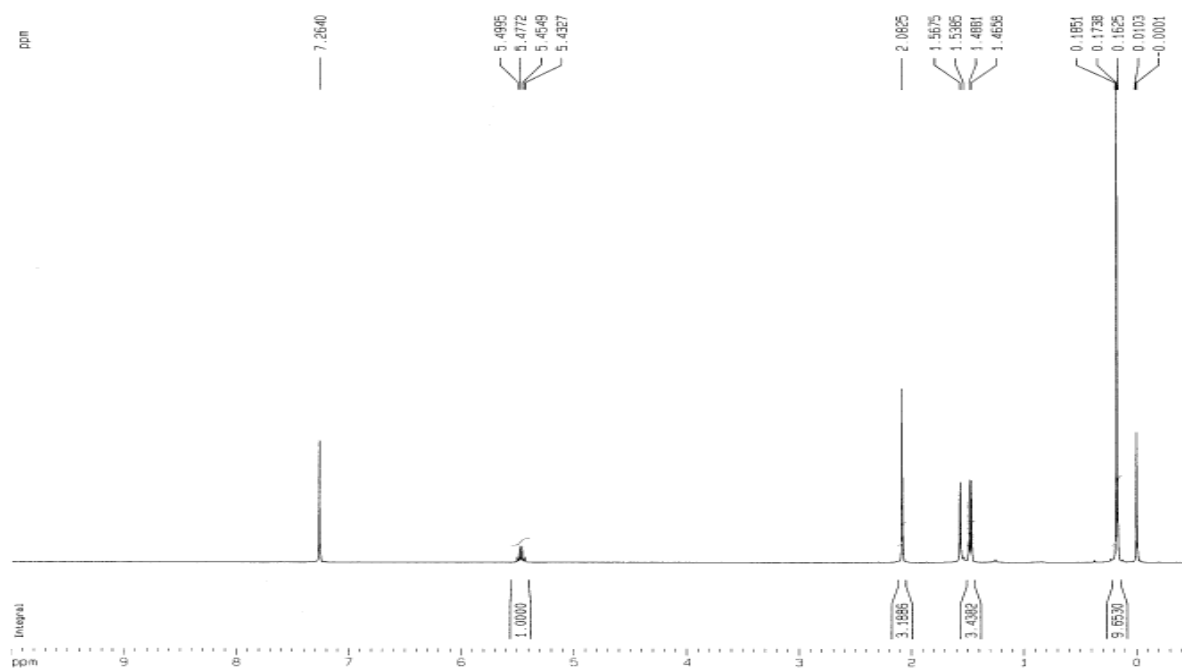
Supporting Information

Table of Contents

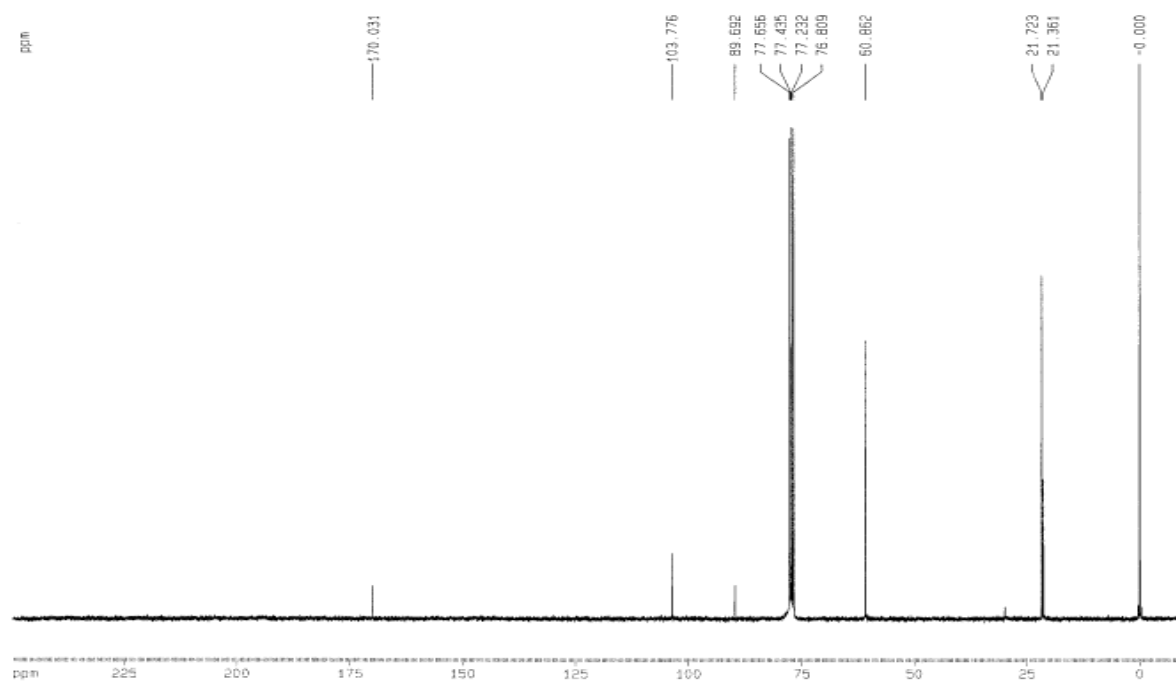
1. NMR Spectra and GC Chromatograms of 8a-g	S2-S15
2. NMR Spectra and HPLC Chromatograms of 9a-f	S16-S27
3. NMR Spectra and HPLC Chromatograms of 10a, b, d, g-q	S28-S55
4. NMR Spectra and HPLC Chromatograms of 11a, b, h, i	S56-S63



¹H-NMR

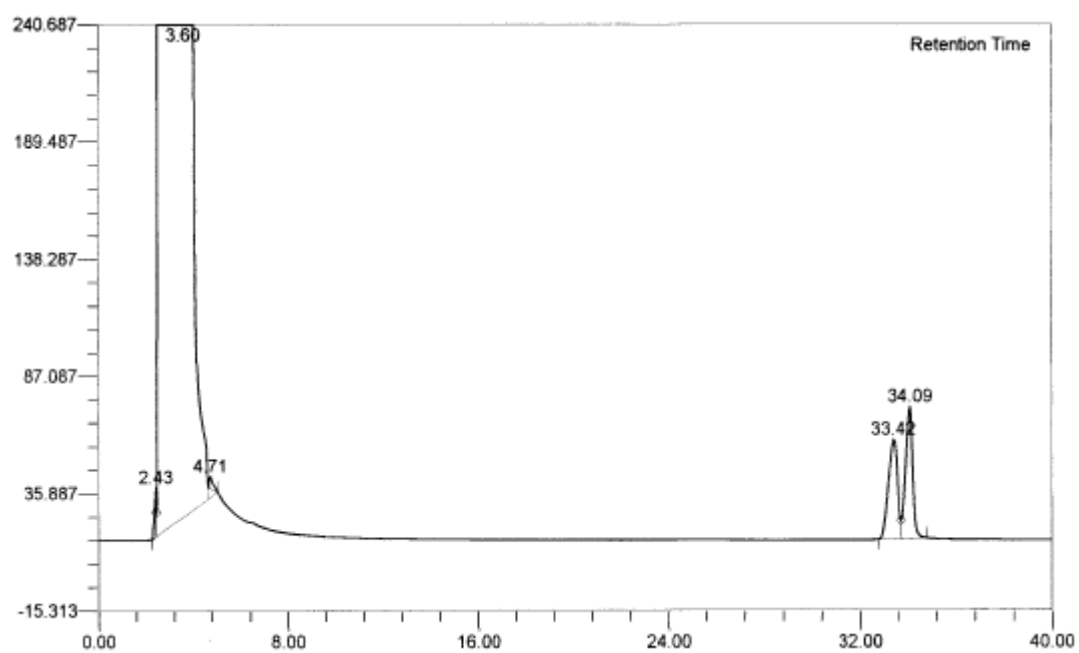


¹³C-NMR

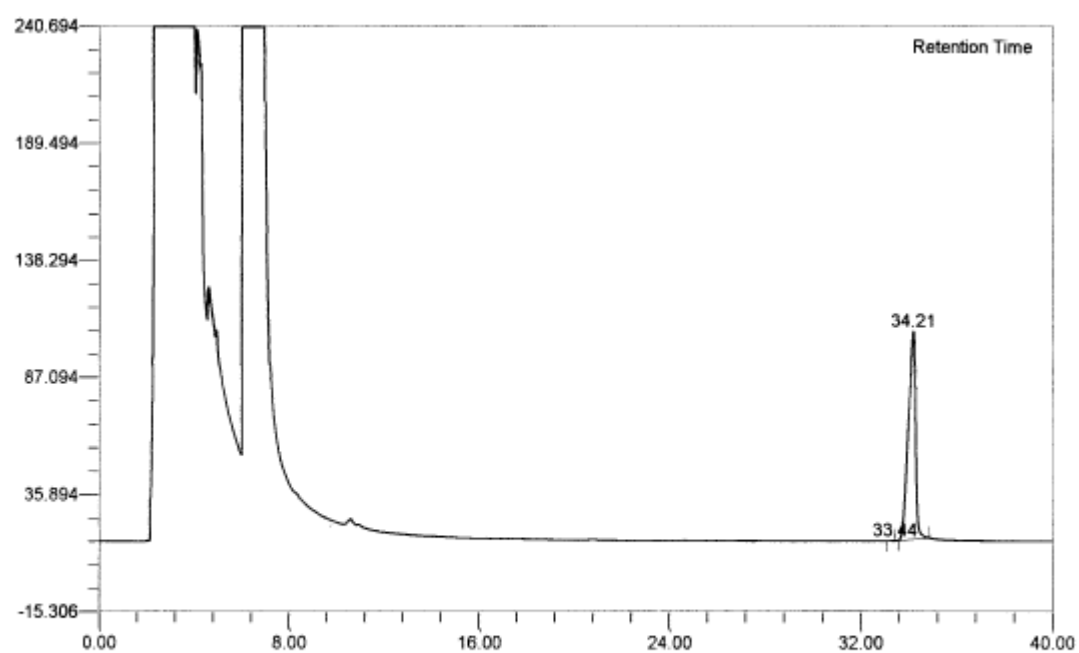


GC

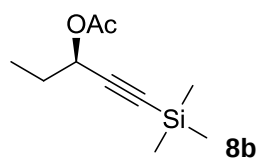
(±)-8a



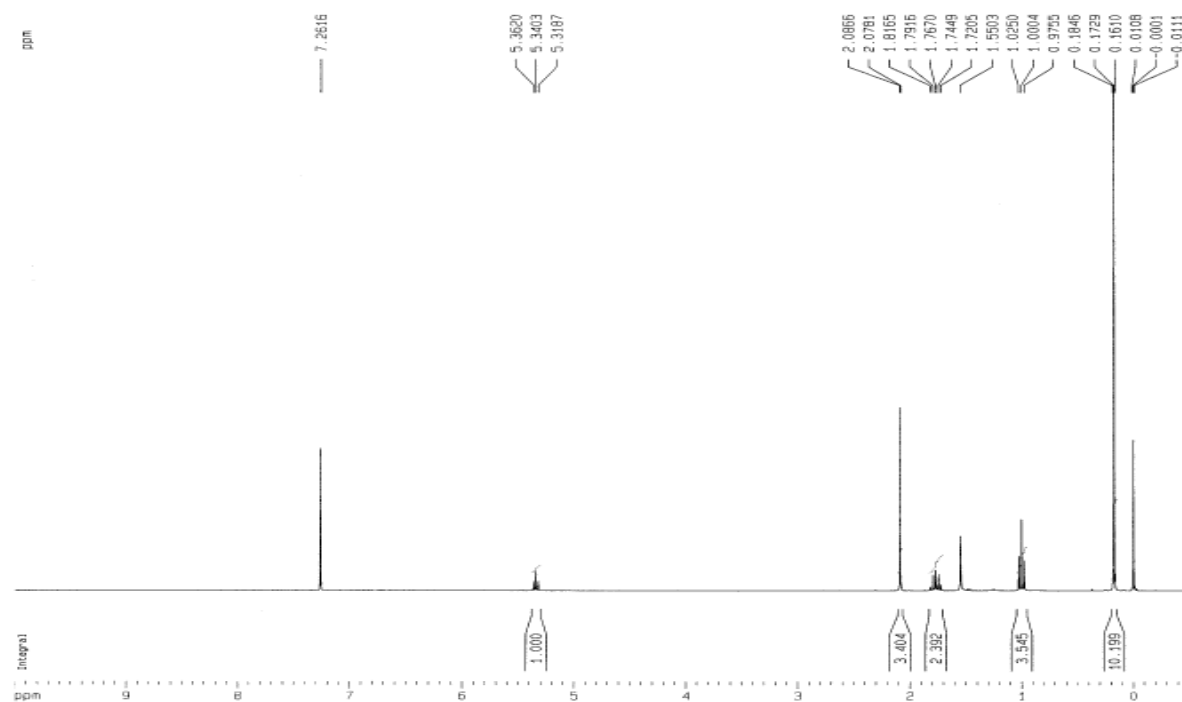
(+)-8a



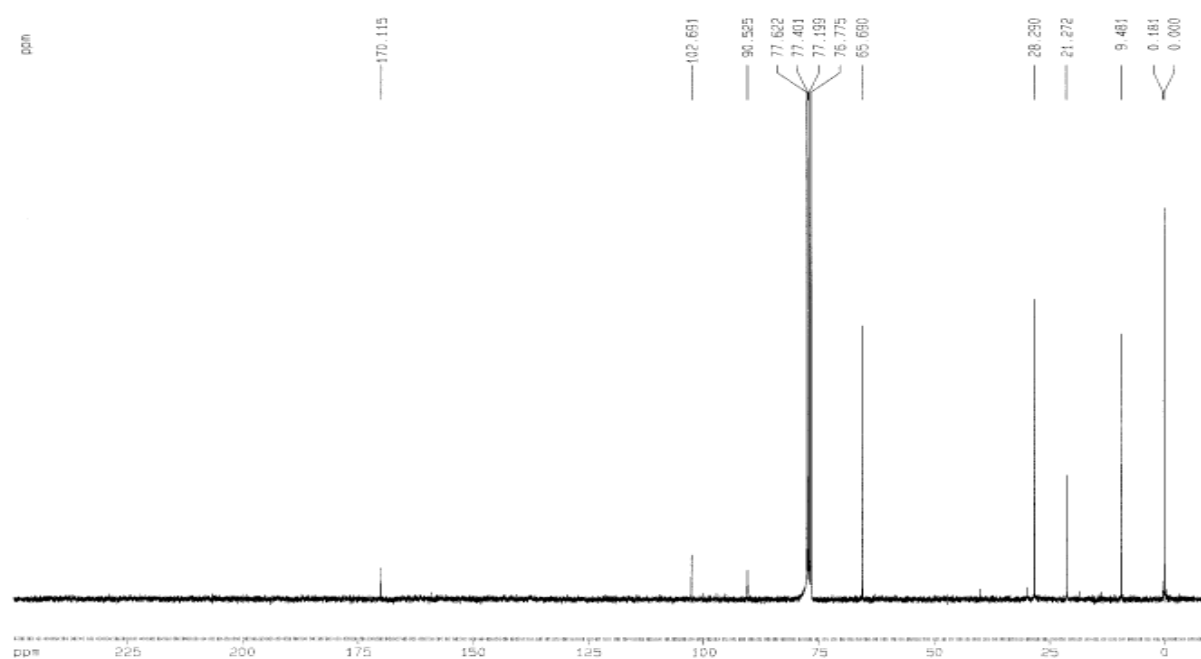
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	33.440	0.003	4972	12	0.01302	0.01318	tep-BB
2	34.206	0.328	38178695	91009	99.98698	99.98682	BB



¹H-NMR

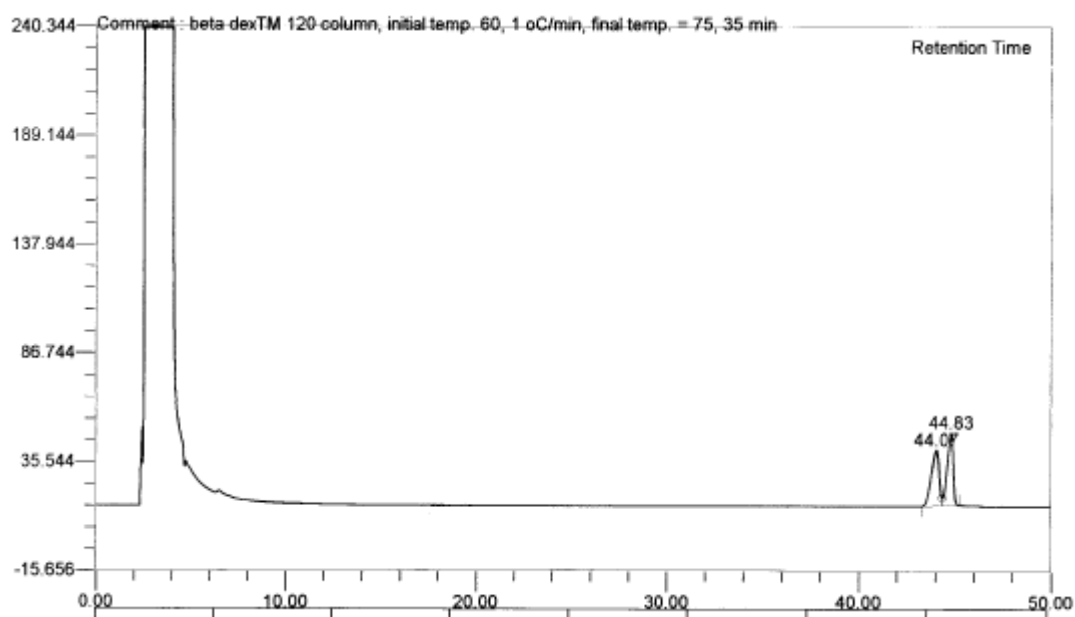


¹³C-NMR

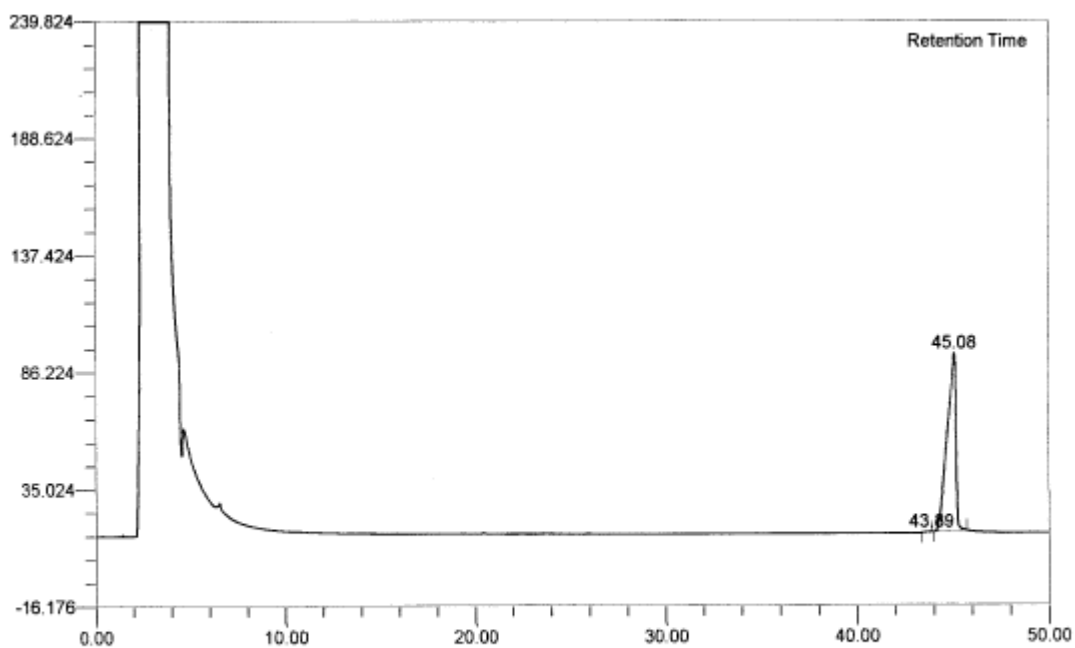


GC

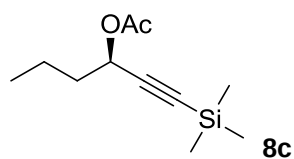
(±)-8b



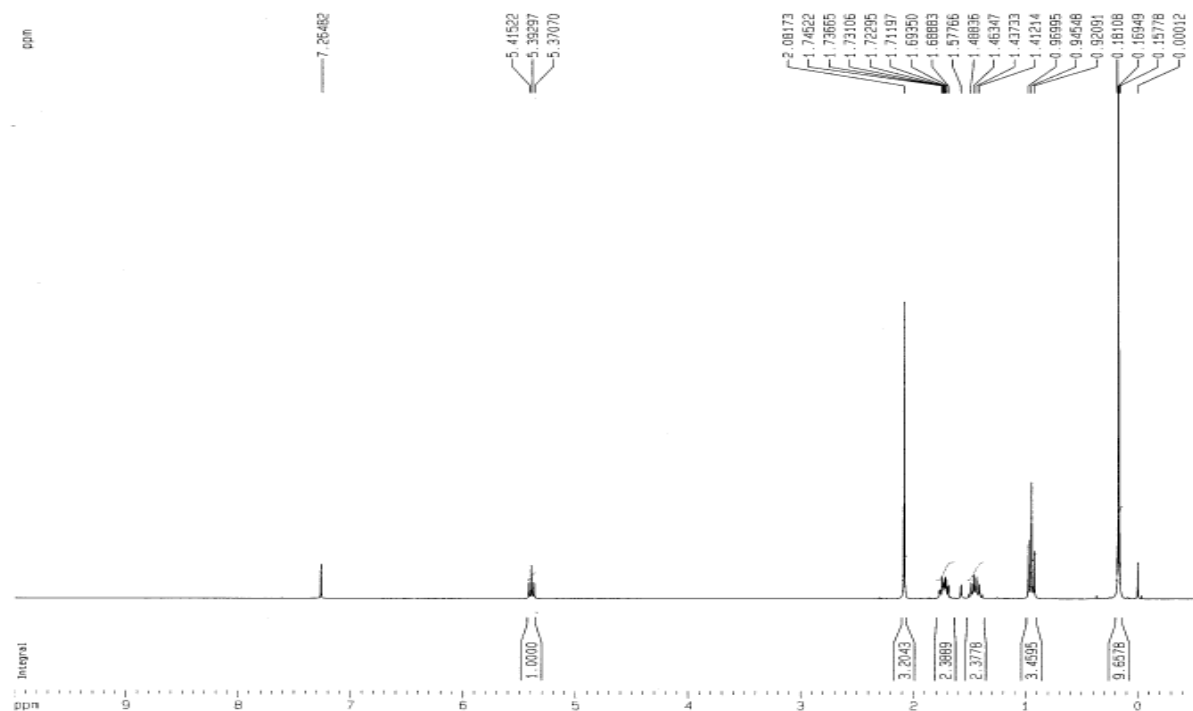
(+)-8b



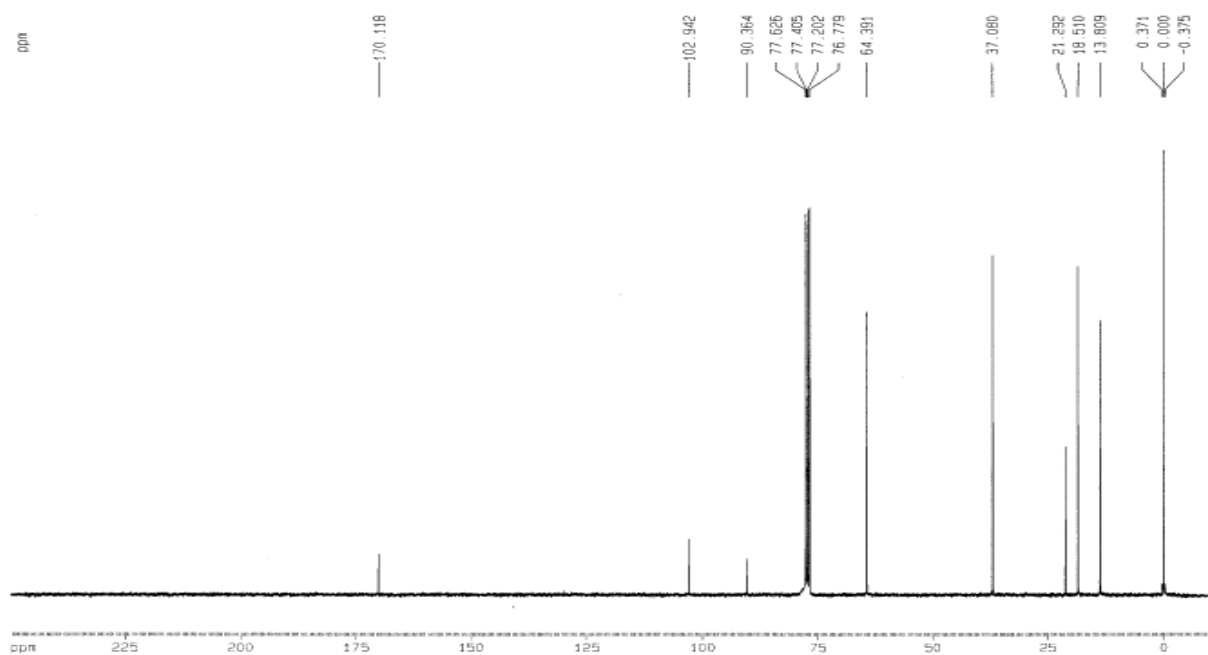
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	43.886	0.000	33263	20	0.06594	0.02561	tep-BB
2	45.079	0.517	50412840	78068	99.93406	99.97439	BB



¹H-NMR

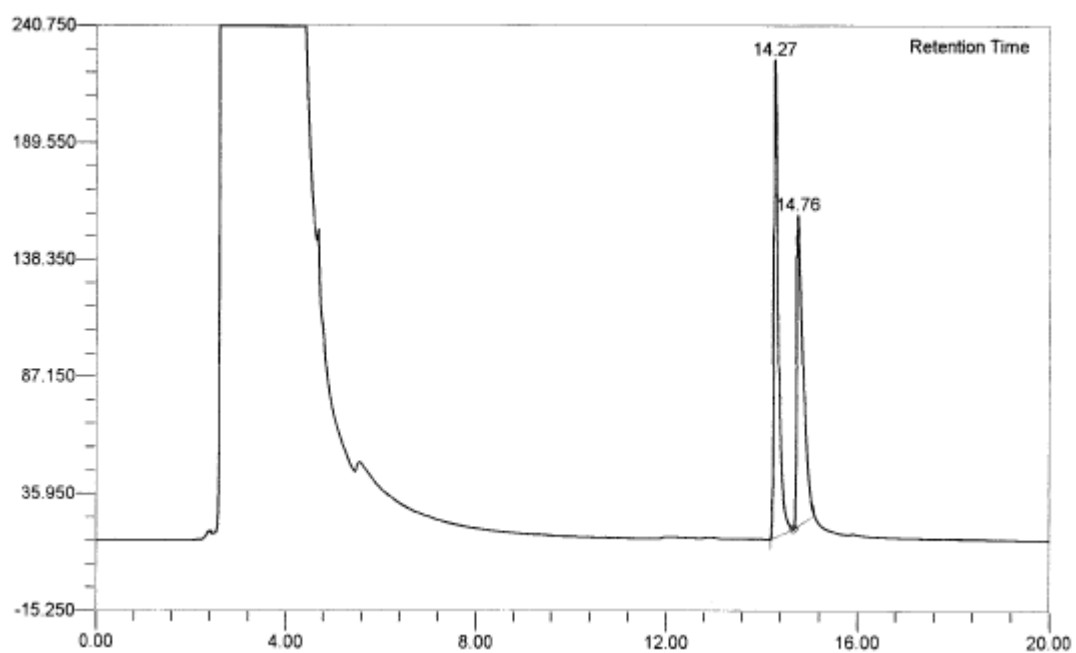


¹³C-NMR

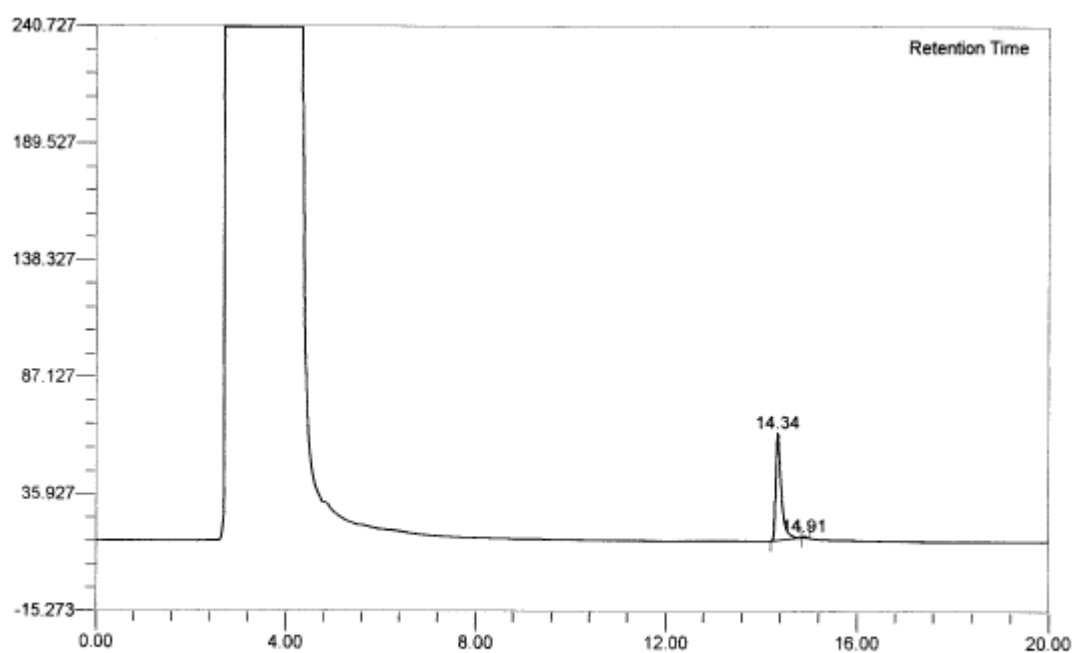


GC (Enantiomeric excess (ee) was determined after deprotection of TMS group.)

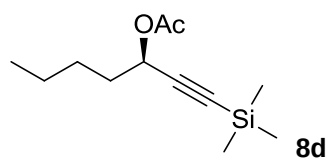
(±)-8c



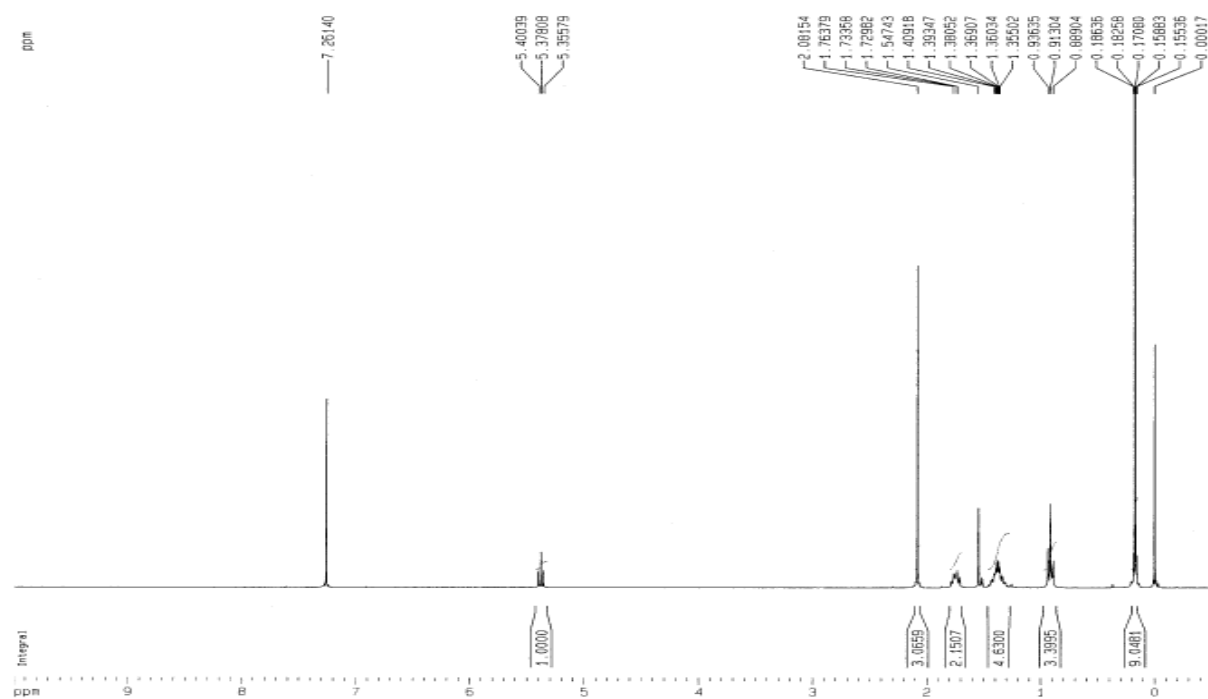
(+)-8c



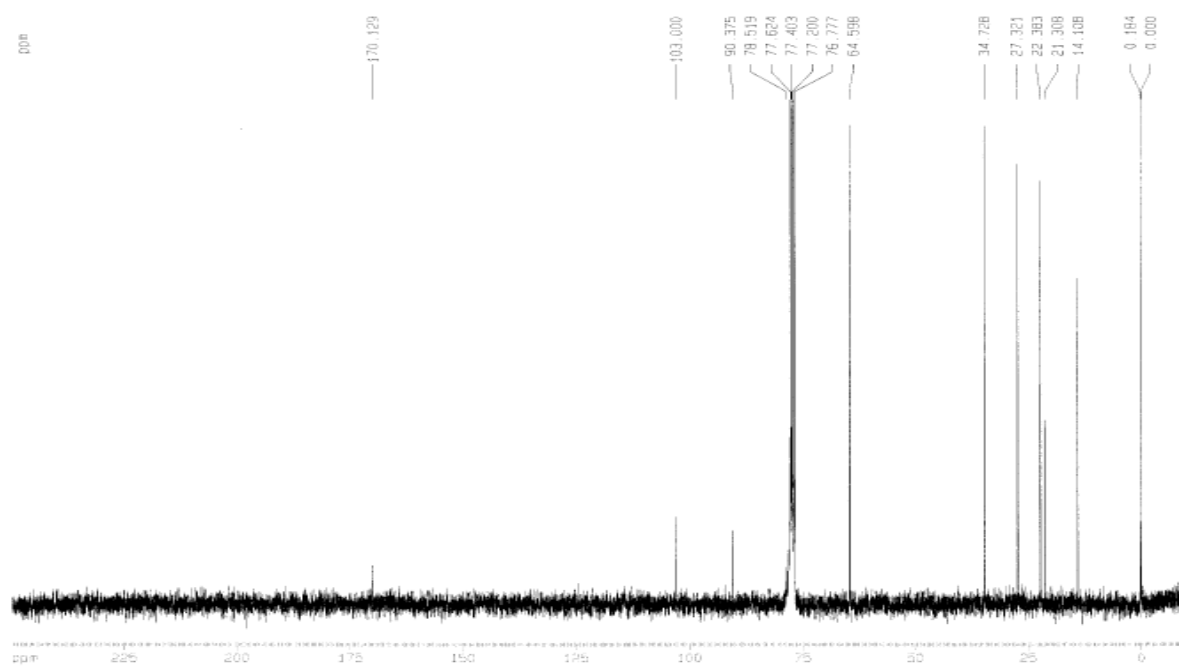
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	14.337	0.108	7638424	47242	99.13265	98.58103	tep-mBB
2	14.915	0.076	66814	680	0.86735	1.41897	tep-tBB



¹H-NMR

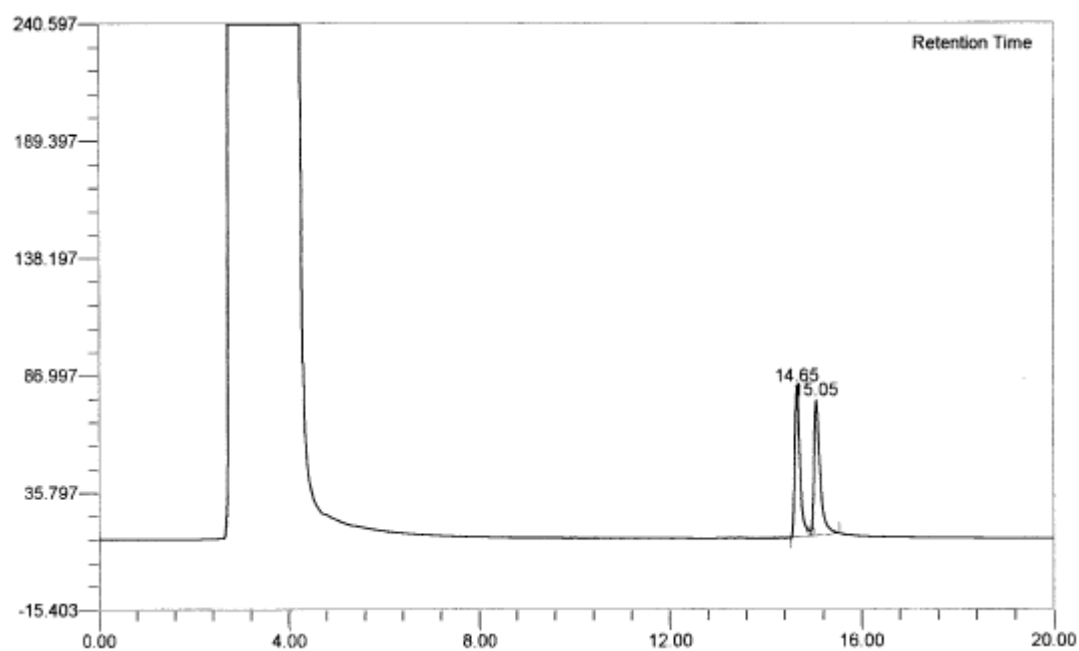


¹³C-NMR

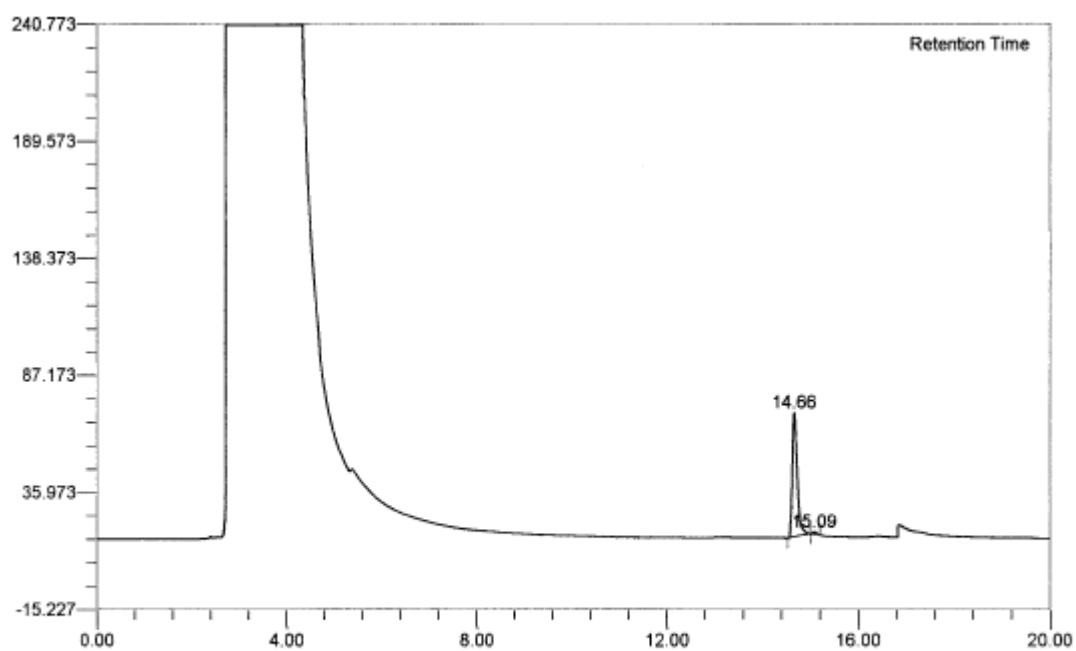


GC (Enantiomeric excess (ee) was determined after deprotection of TMS group.)

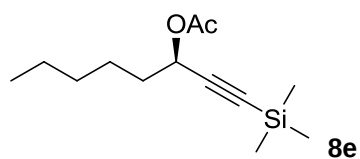
(±)-8d



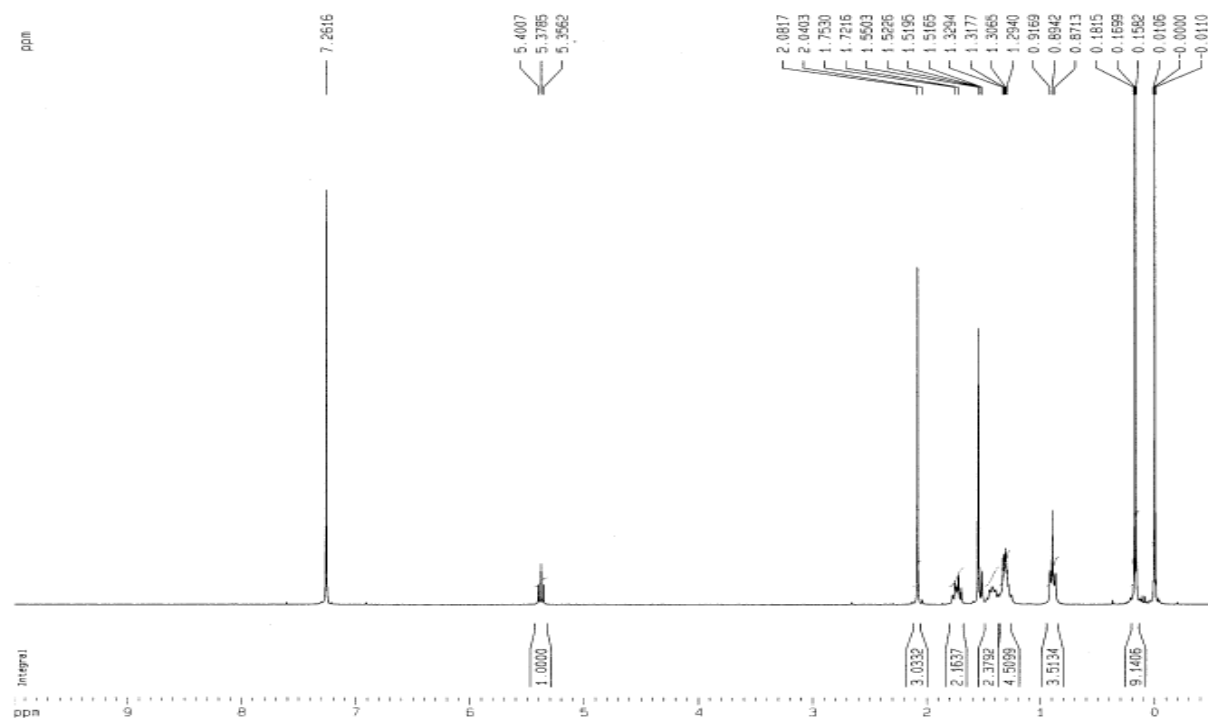
(+)-8d



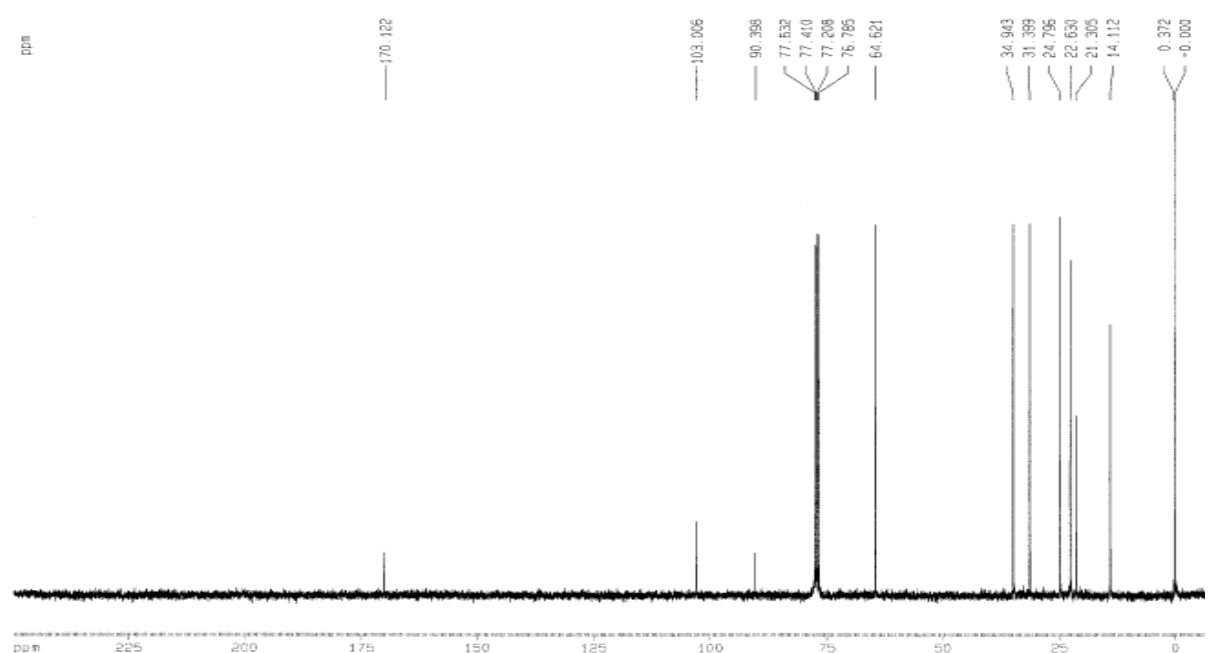
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	14.665	0.104	7731508	54462	98.33867	97.95676	tep-mBB
2	15.088	0.081	130616	1136	1.66133	2.04324	tep-tBB



¹H-NMR

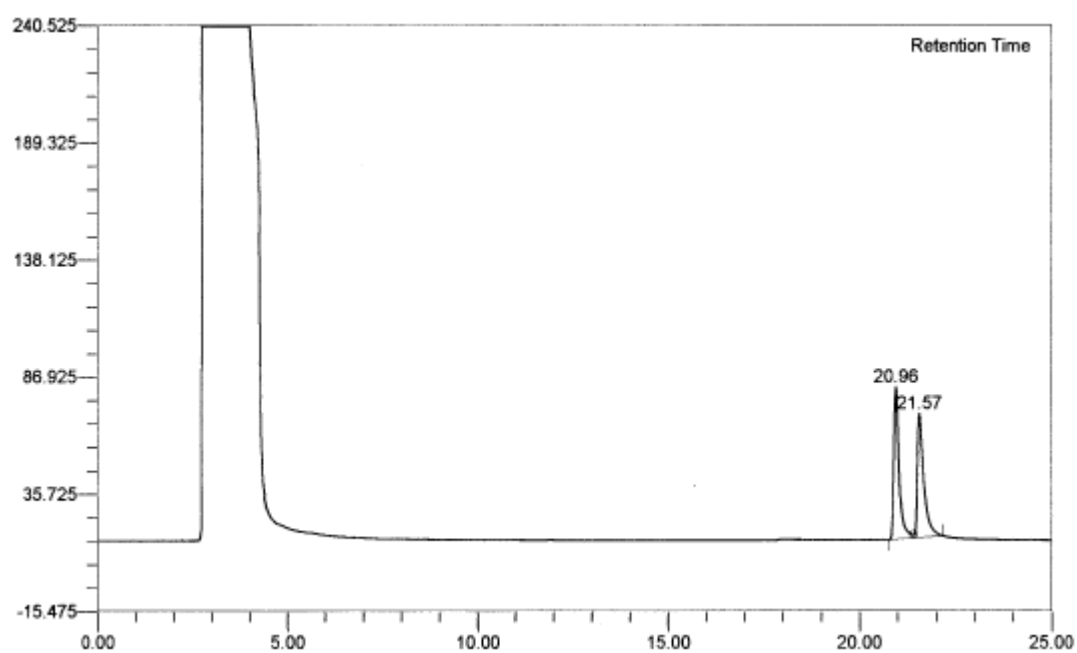


¹³C-NMR

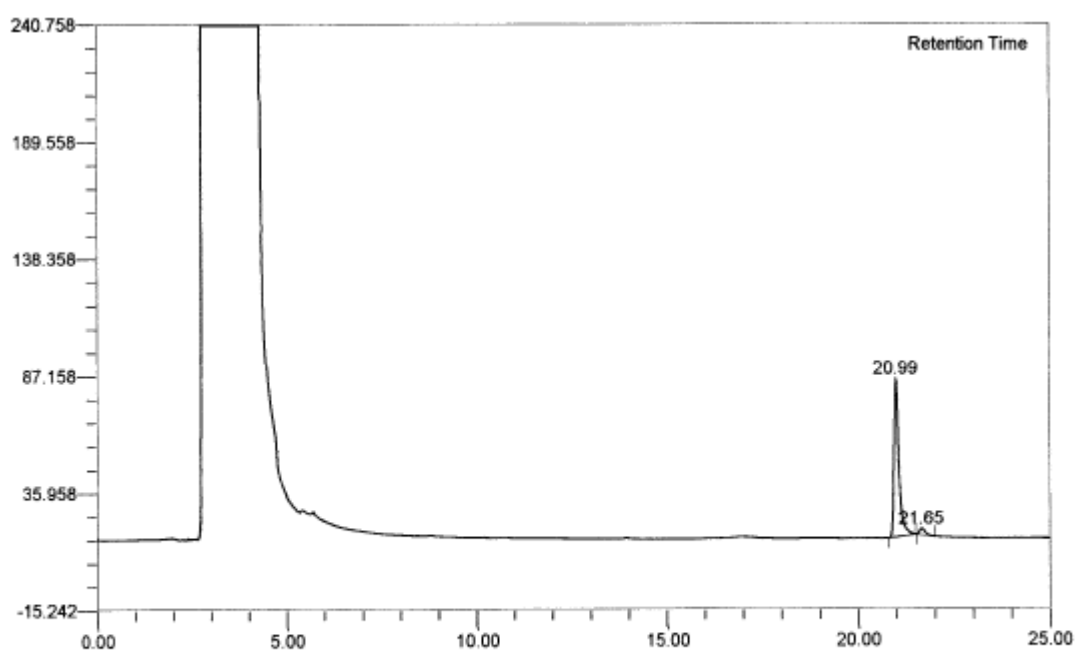


GC (Enantiomeric excess (ee) was determined after deprotection of TMS group.)

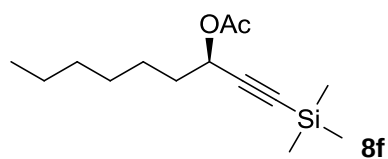
(±)-**8e**



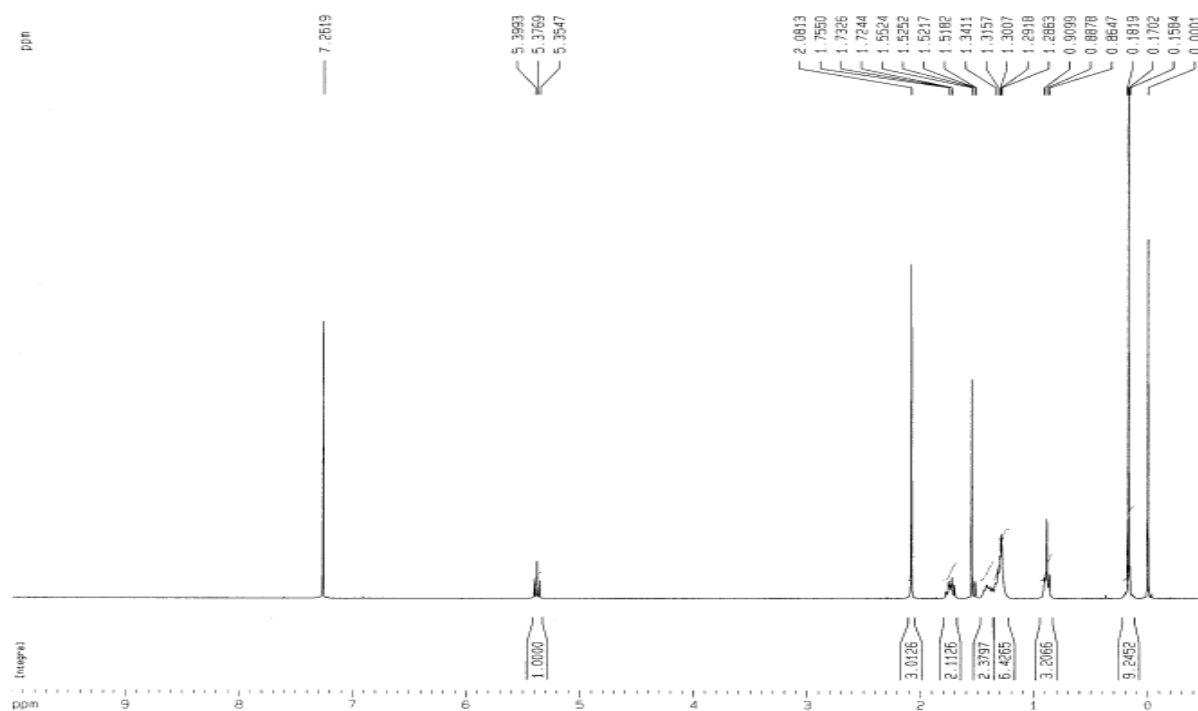
(+)-**8e**



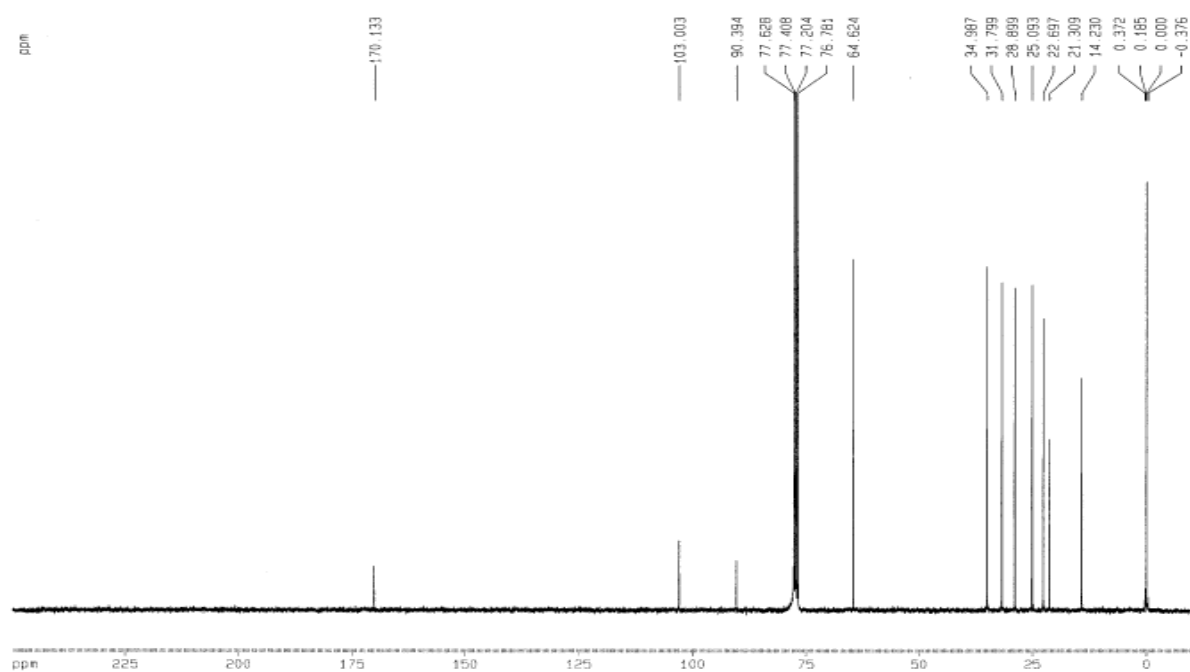
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	20.988	0.133	13044582	69620	96.05887	96.13765	tep-mBB
2	21.653	0.134	535197	2797	3.94113	3.86235	tBB



$^1\text{H-NMR}$

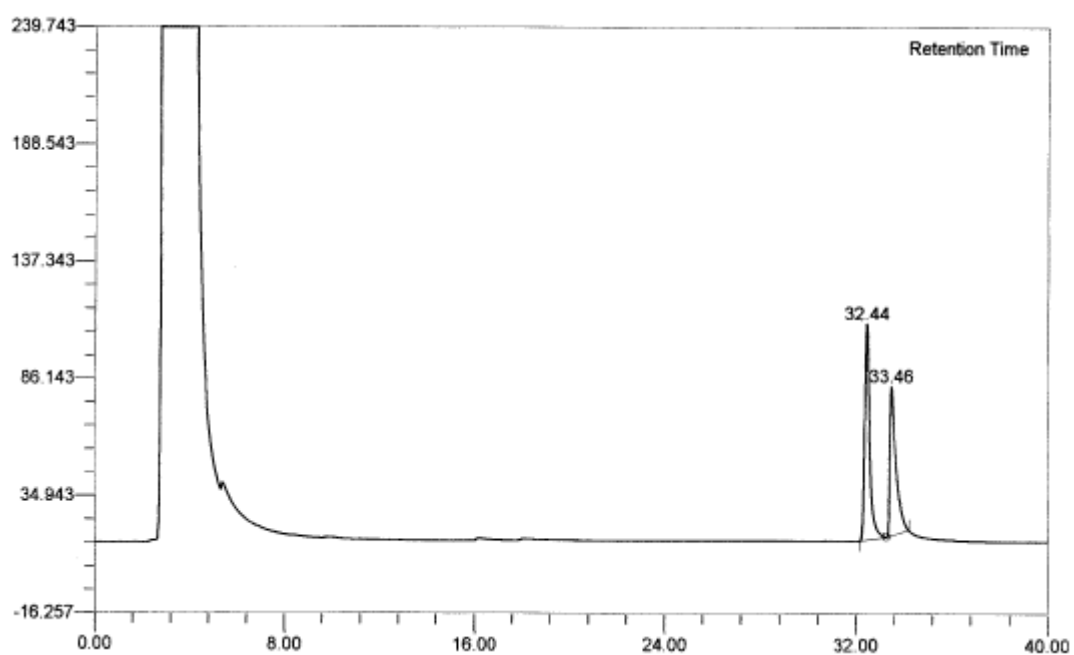


$^{13}\text{C-NMR}$

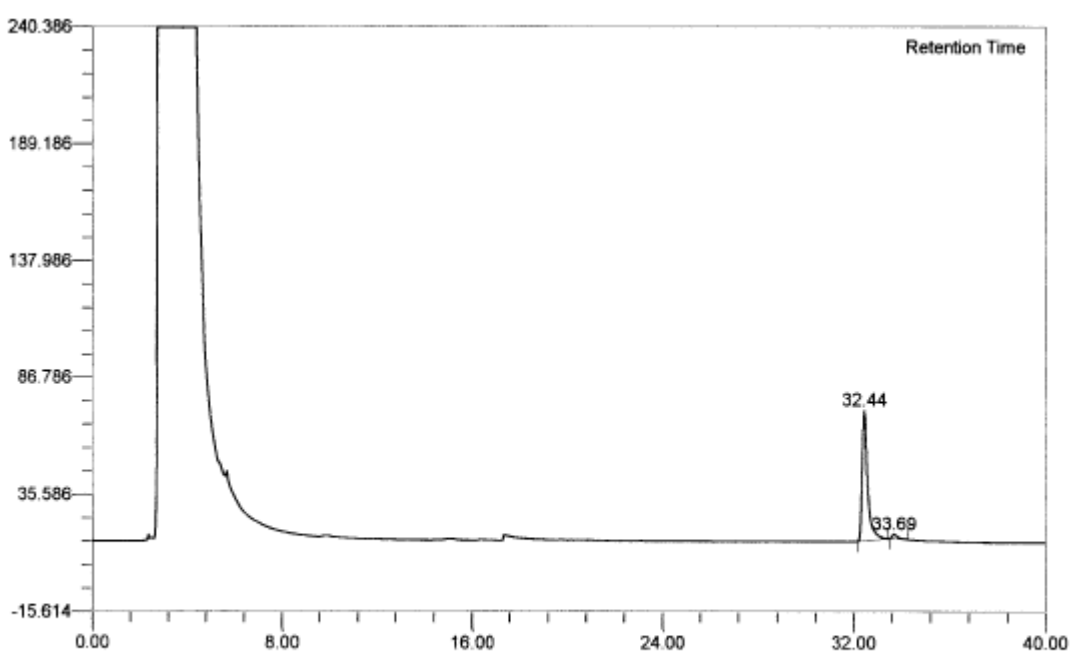


GC (Enantiomeric excess (ee) was determined after deprotection of TMS group.)

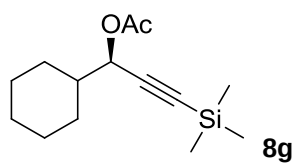
(±)-**8f**



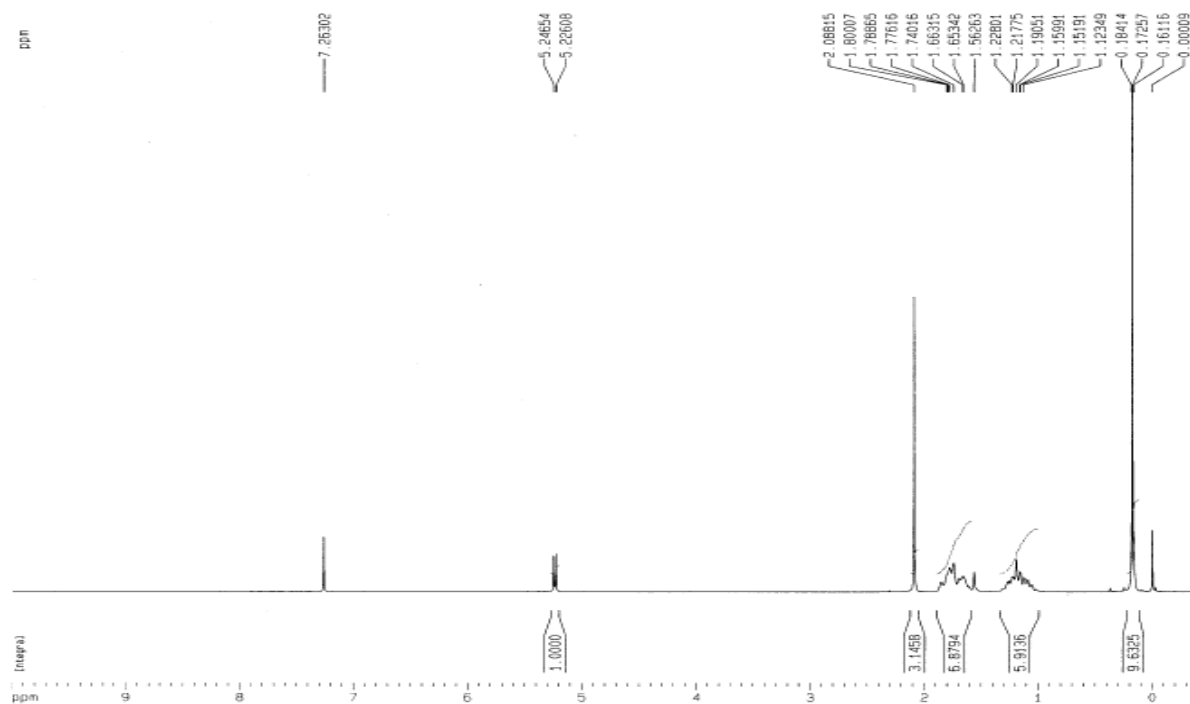
(+)-**8f**



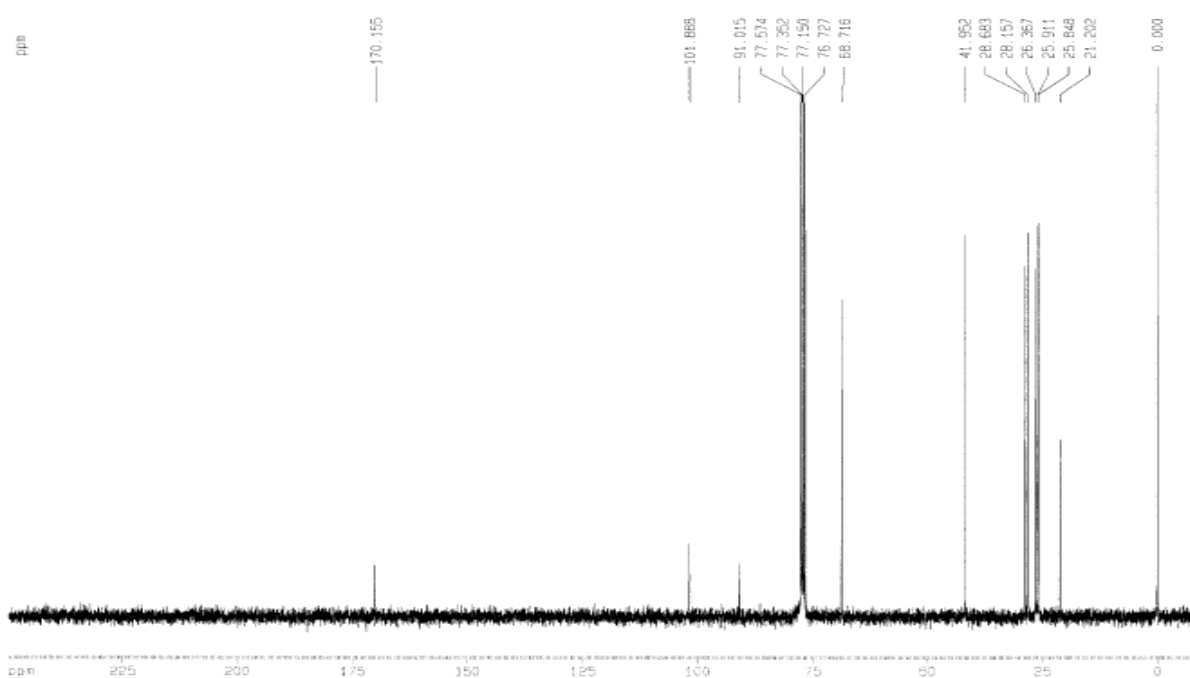
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	32.443	0.212	17931747	57181	96.11688	96.49499	BB
2	33.688	0.236	724442	2077	3.88312	3.50501	BB



¹H-NMR

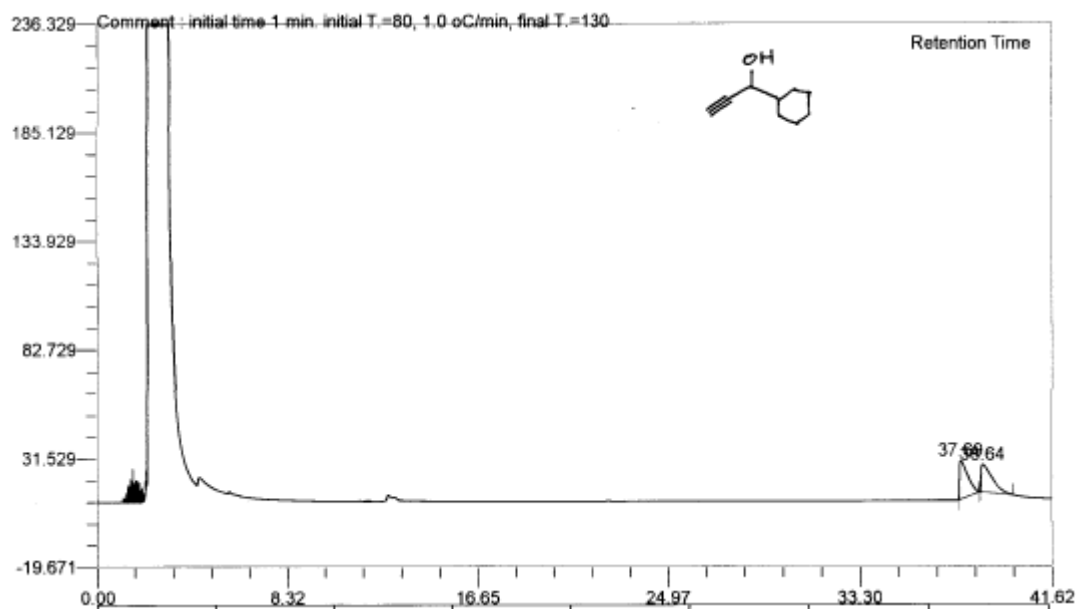


¹³C-NMR

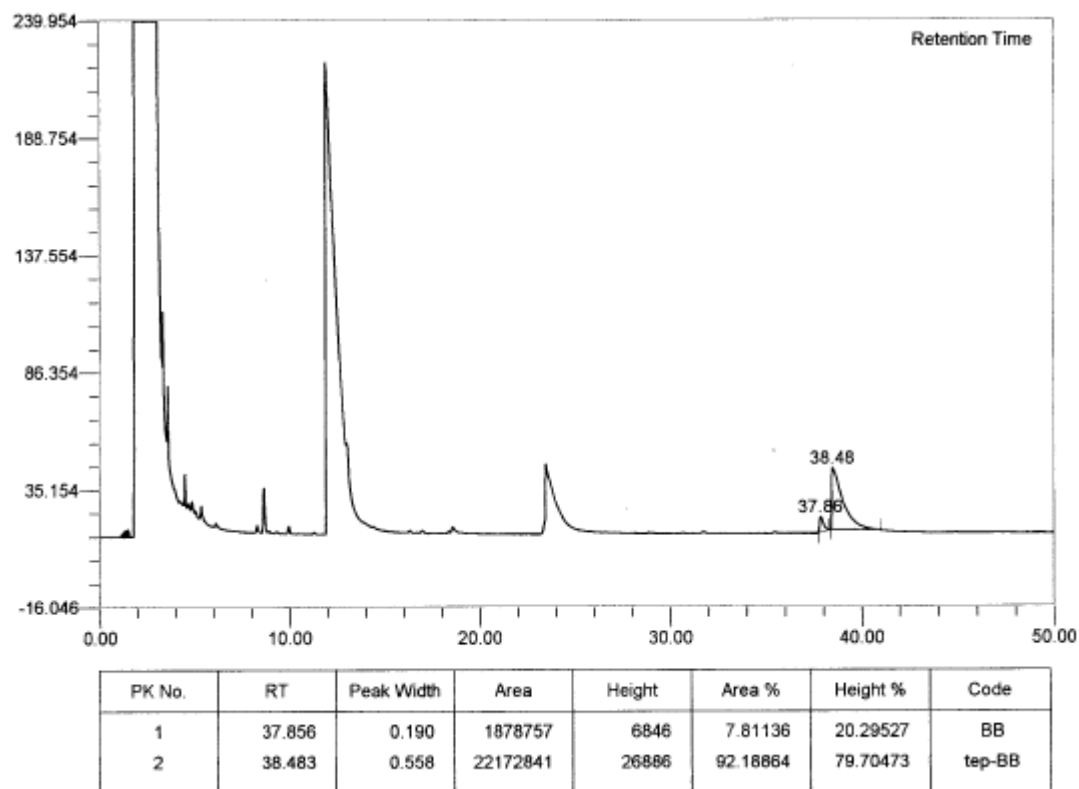


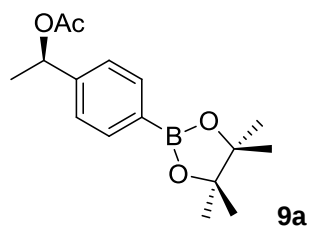
GC (Enantiomeric excess (ee) was determined after deprotection of acetyl and TMS group.)

(±)-8g

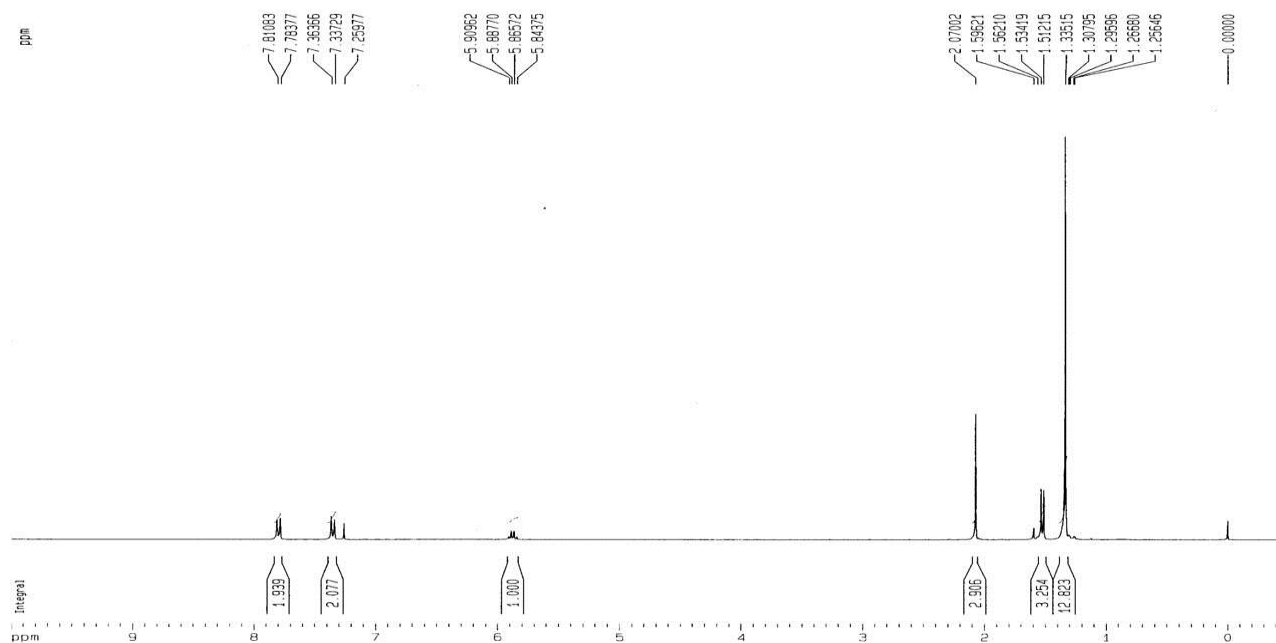


(+)-8g

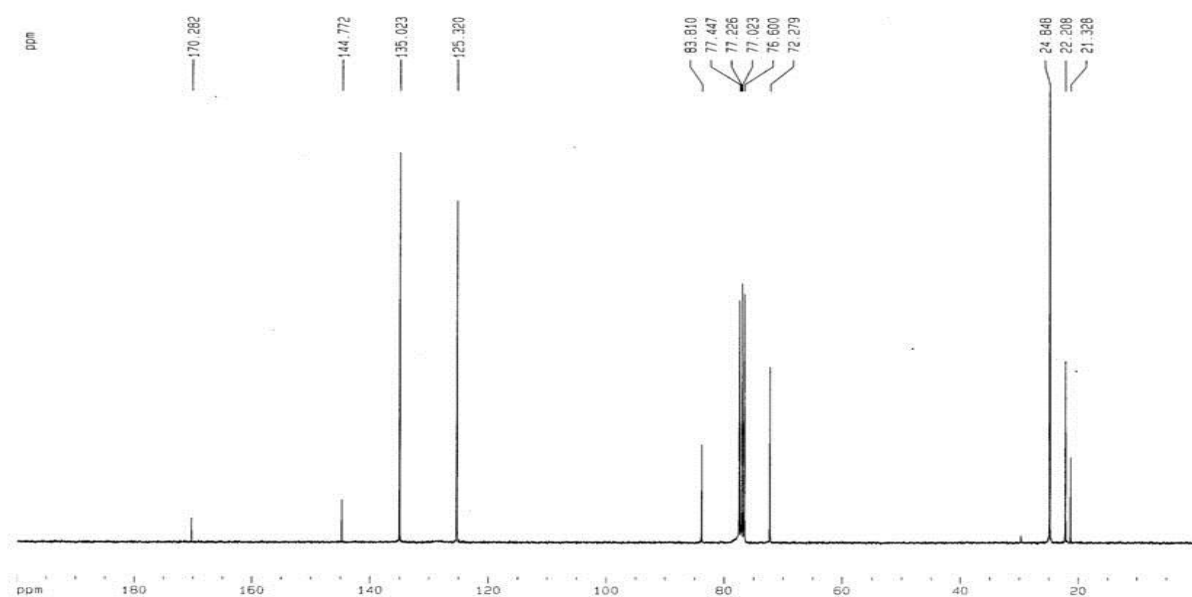




¹H-NMR

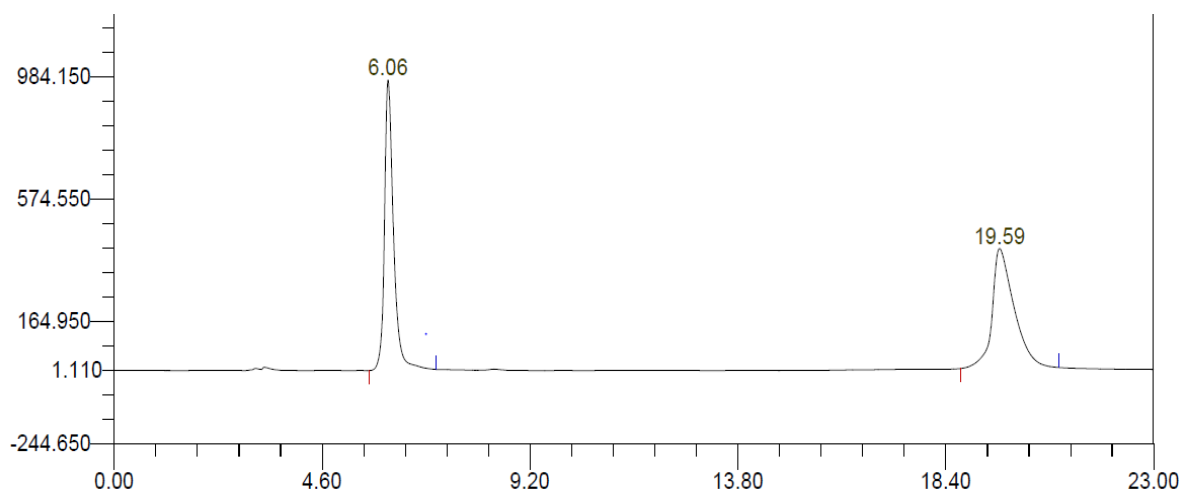


¹³C-NMR

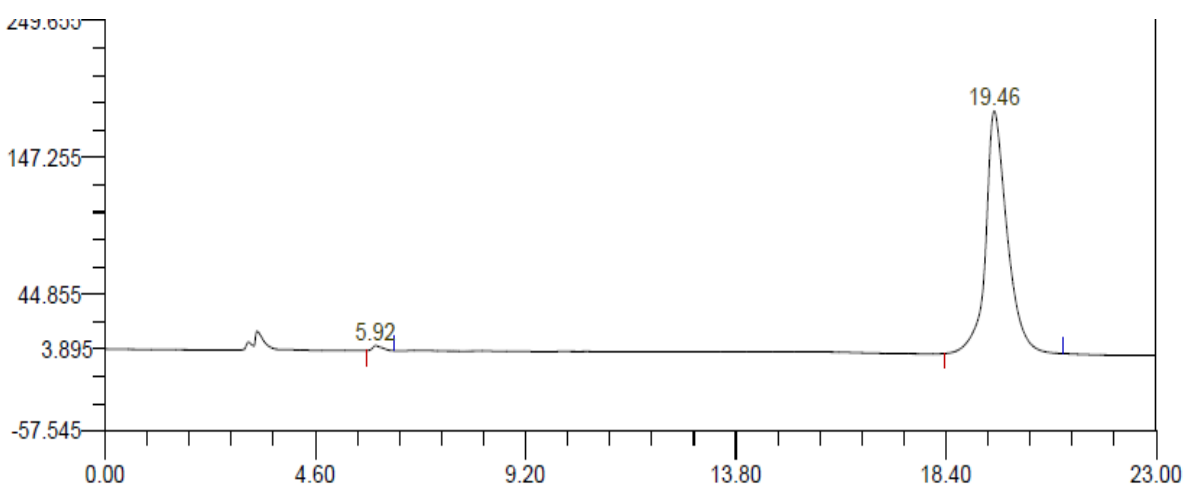


HPLC

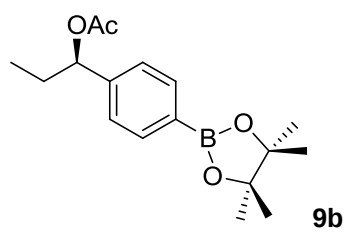
(±)-9a



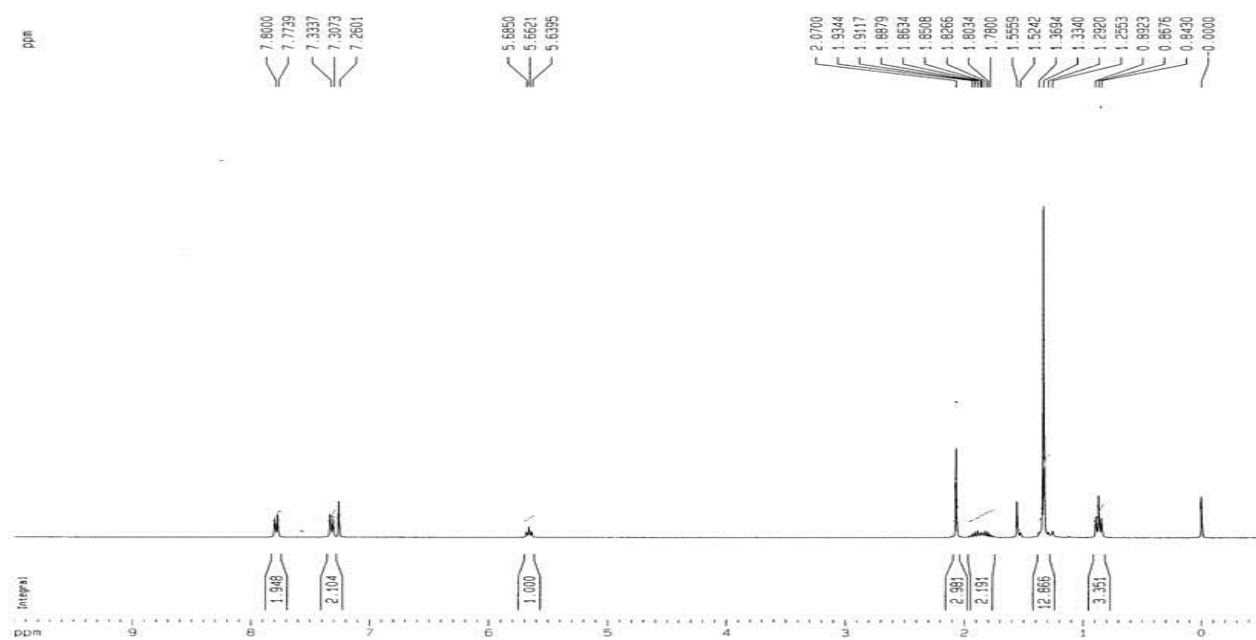
(+)-9a



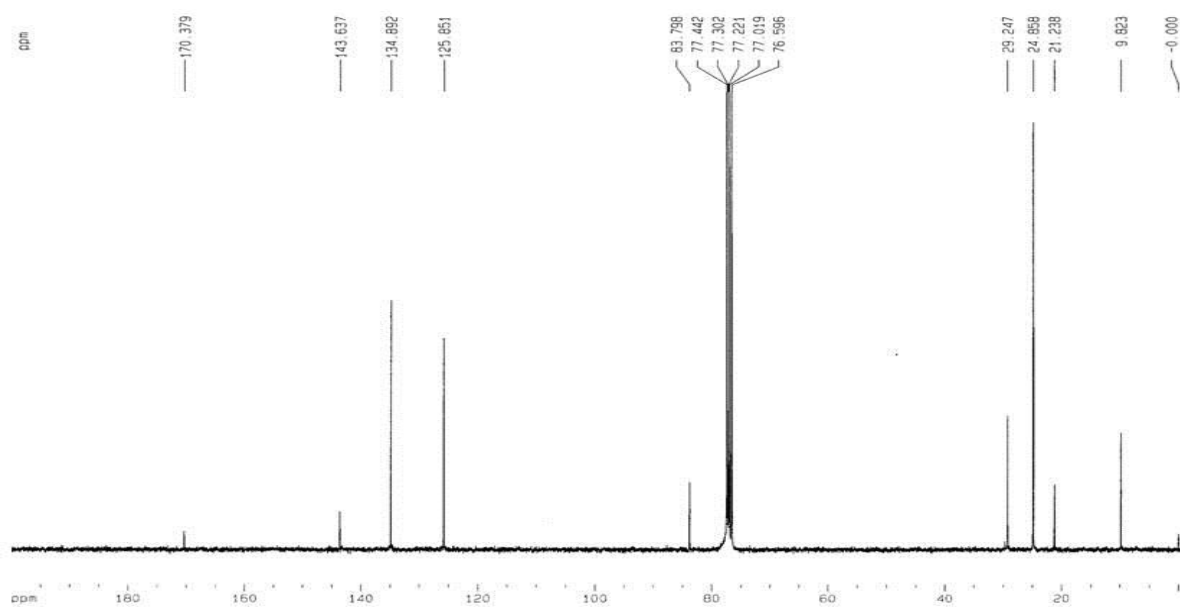
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.915	0.229	1097414	3859	0.91453	2.08187	BB
2	19.457	0.456	118900183	181503	99.08547	97.91813	BB



$^1\text{H-NMR}$

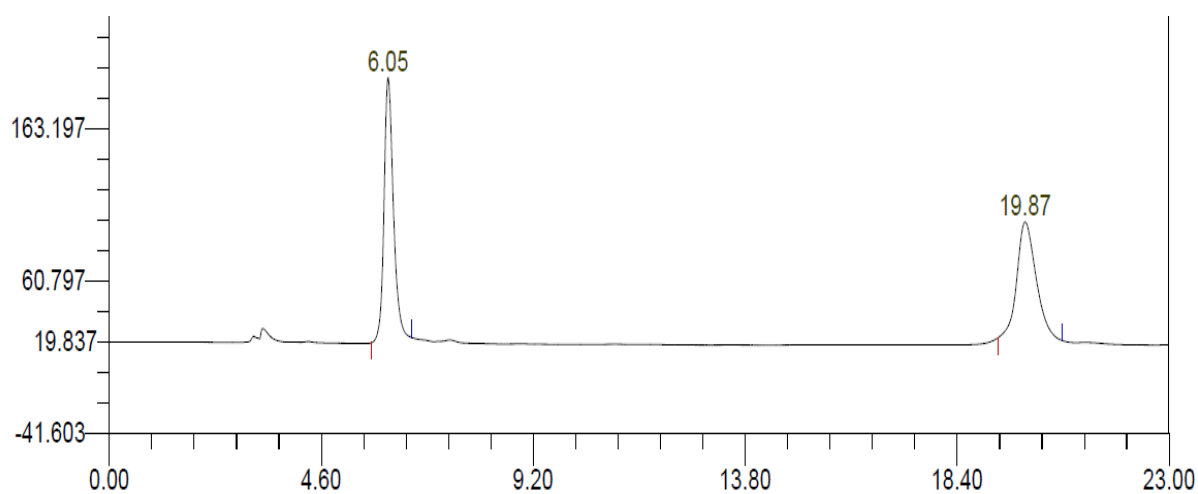


$^{13}\text{C-NMR}$

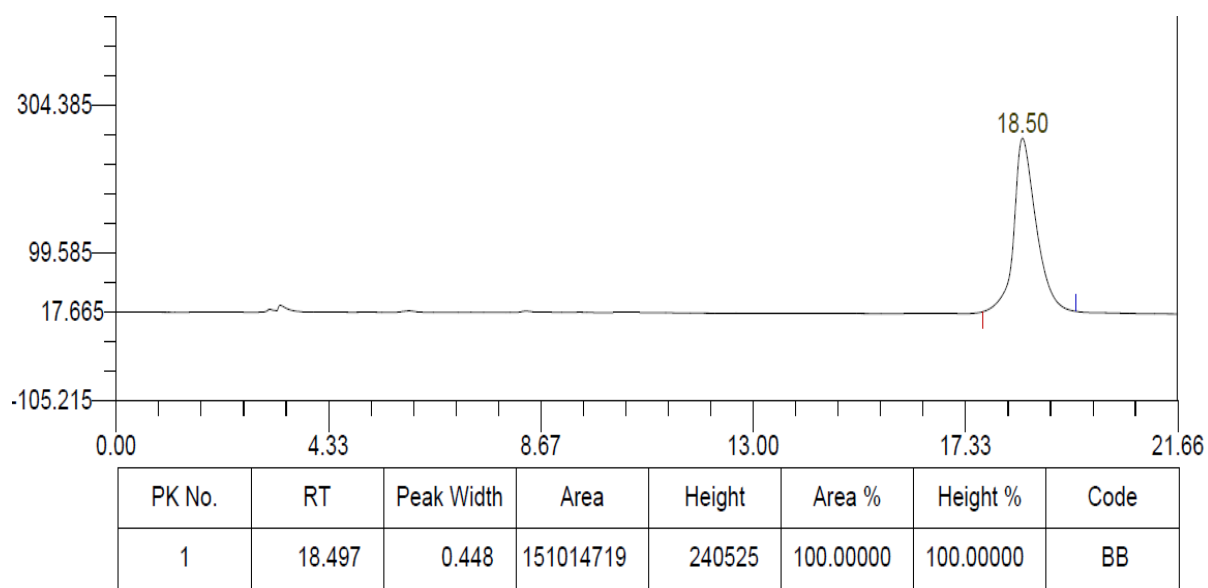


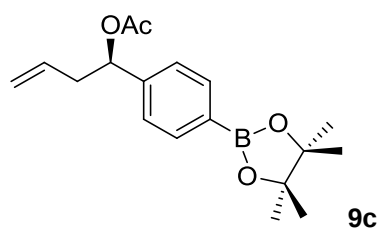
HPLC

(±)-**9b**

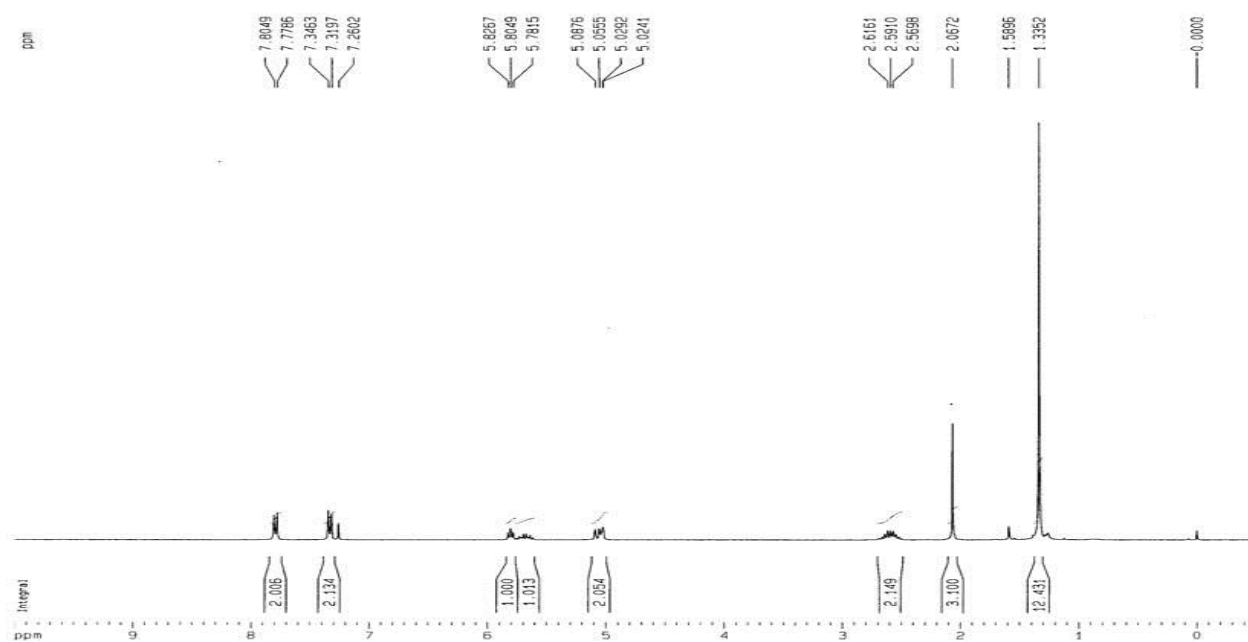


(+)-**9b**

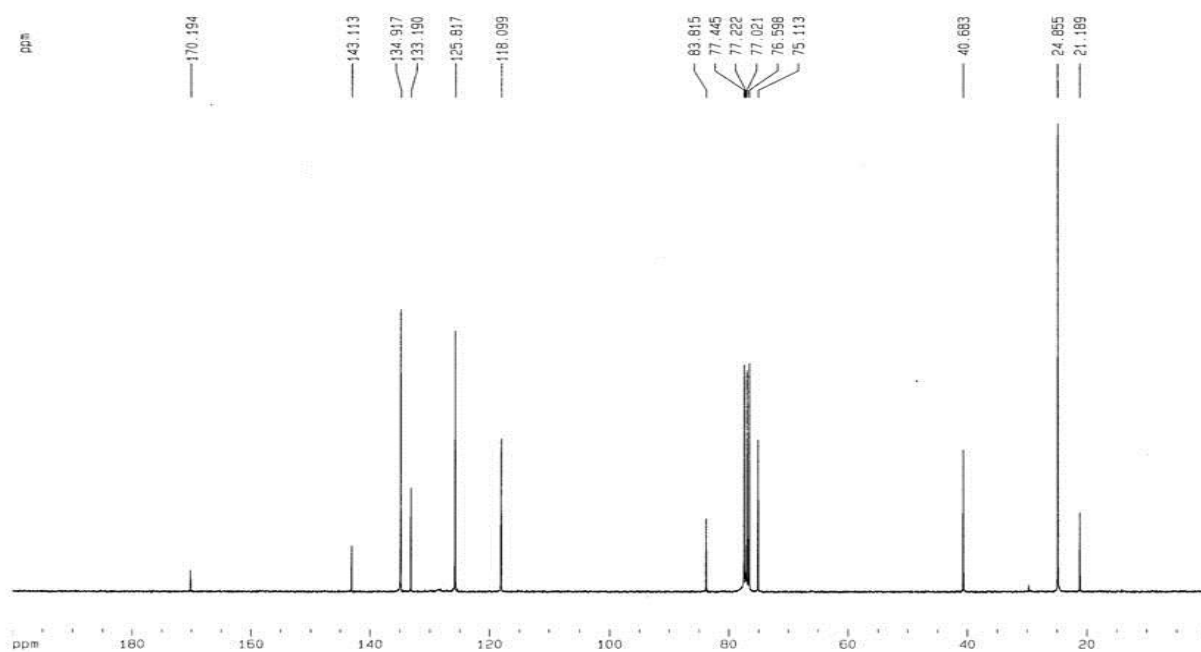




¹H-NMR

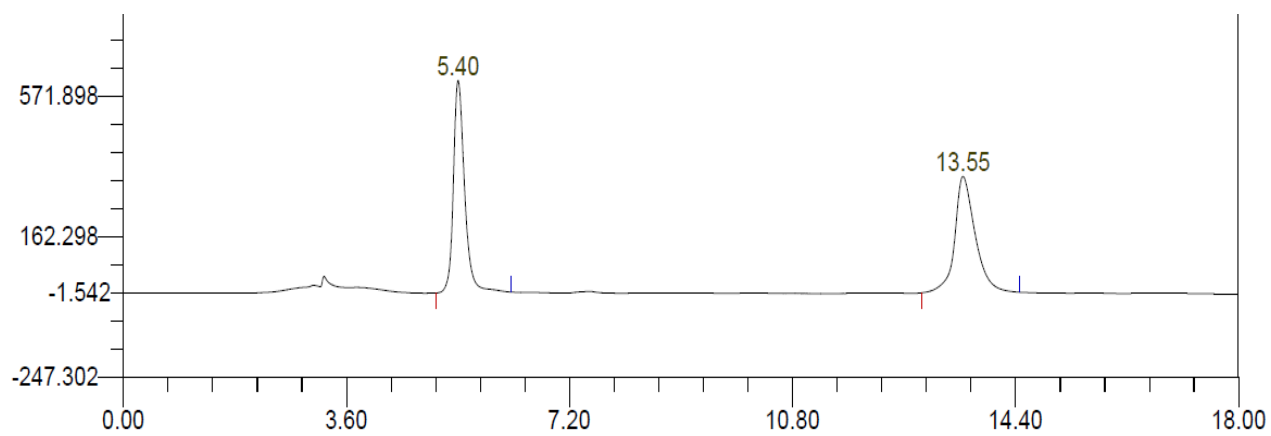


¹³C-NMR

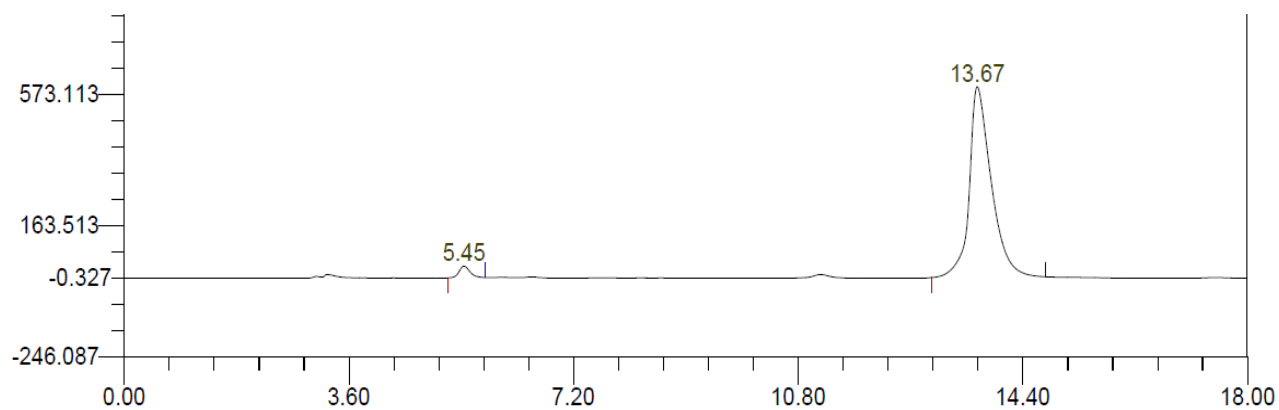


HPLC

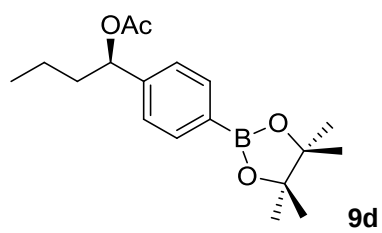
(±)-9c



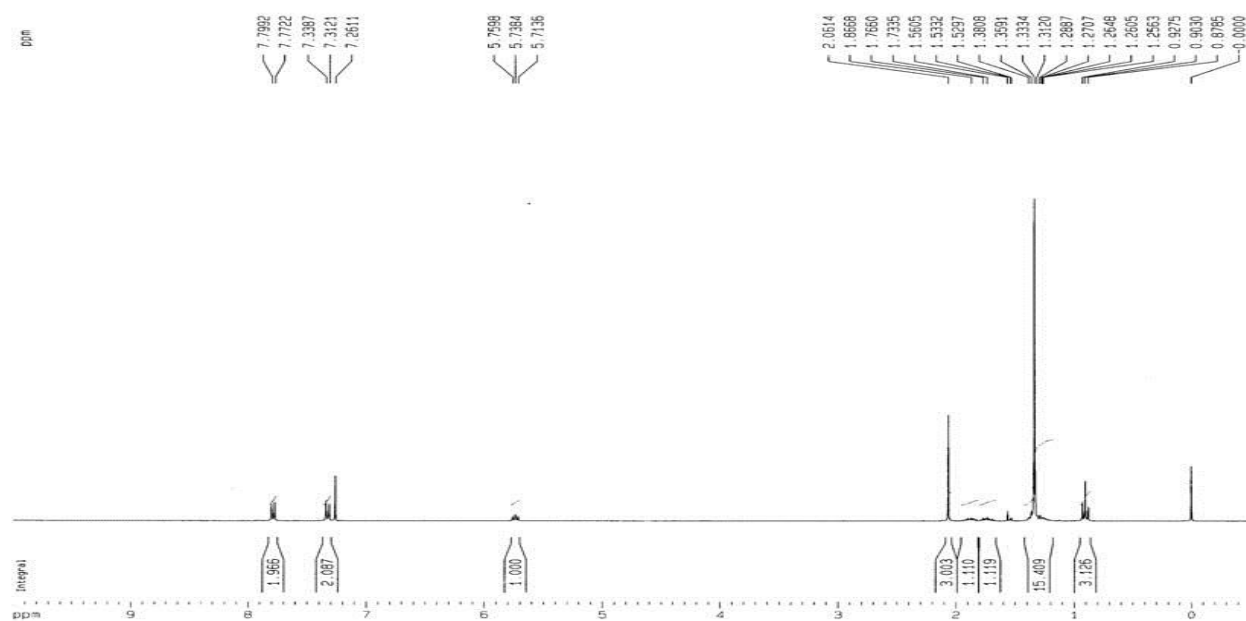
(+)-9c



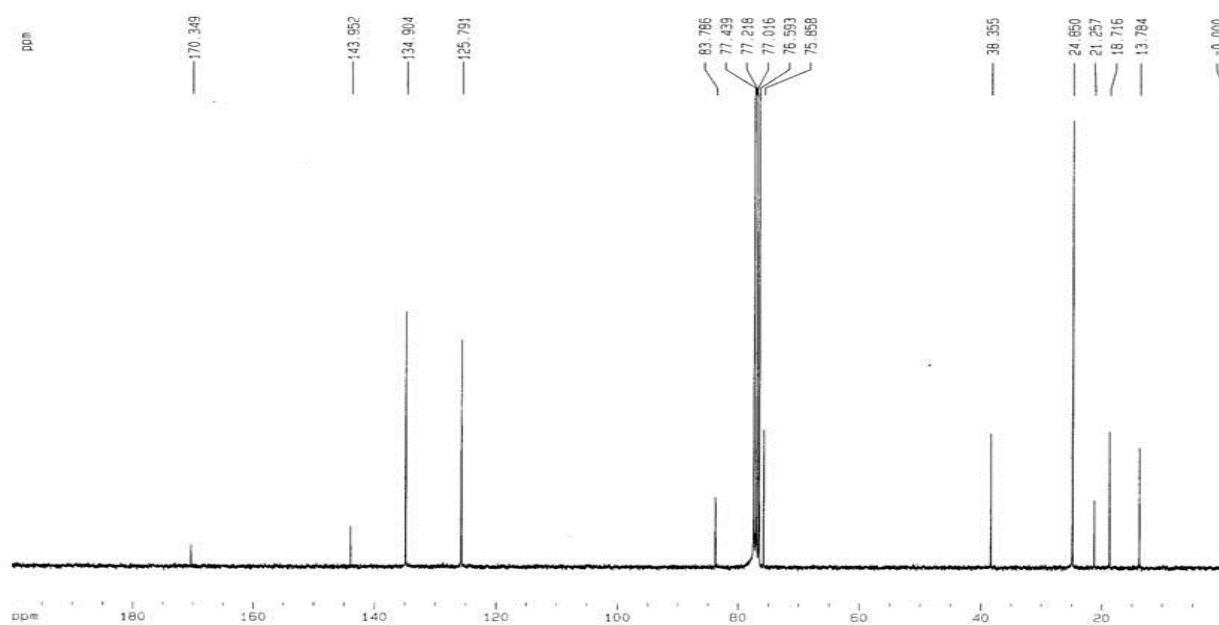
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.445	0.180	8778315	36285	2.91851	5.74423	BB
2	13.671	0.344	292002533	595392	97.08149	94.25577	BB



¹H-NMR

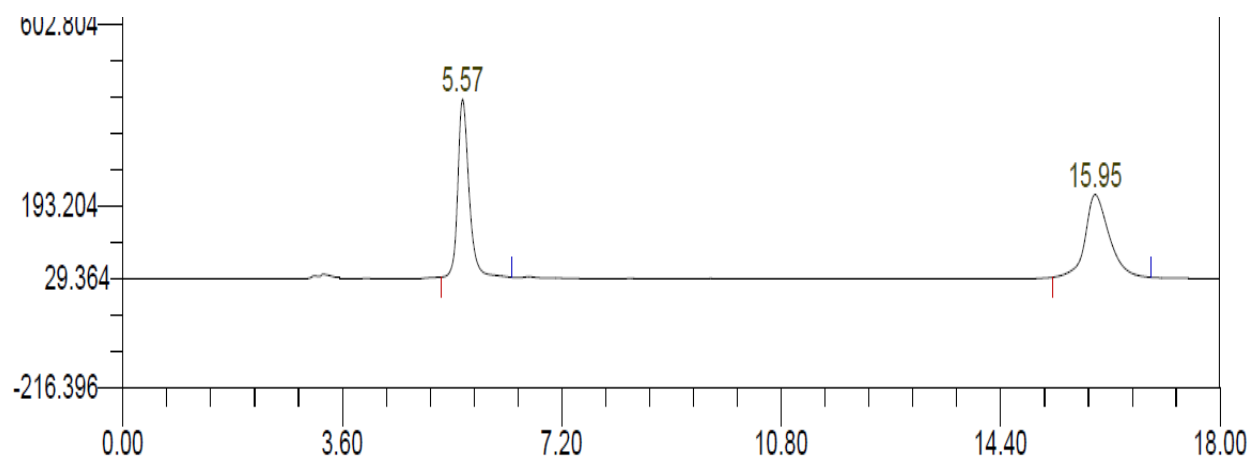


¹³C-NMR

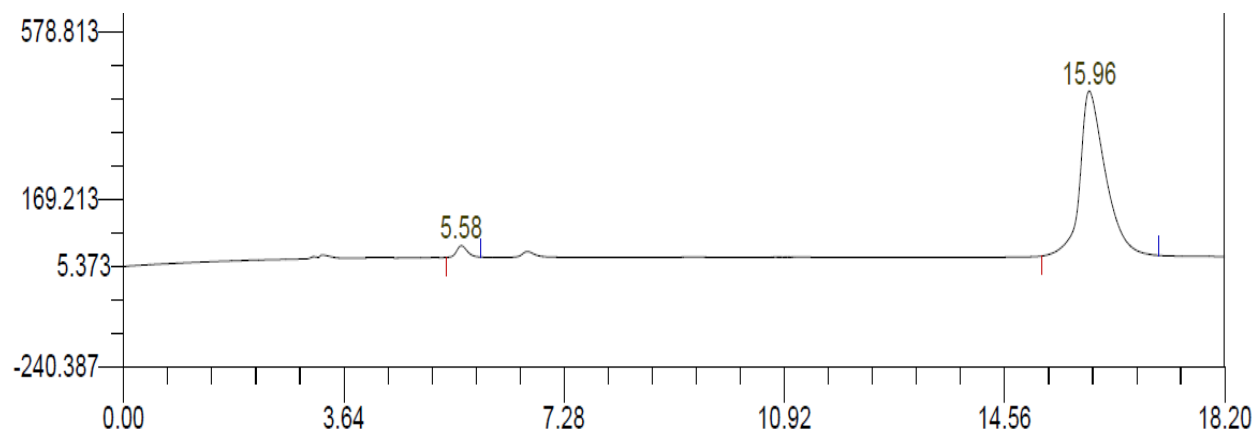


HPLC

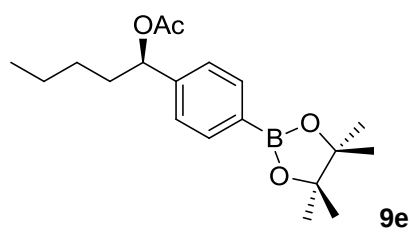
(±)-9d



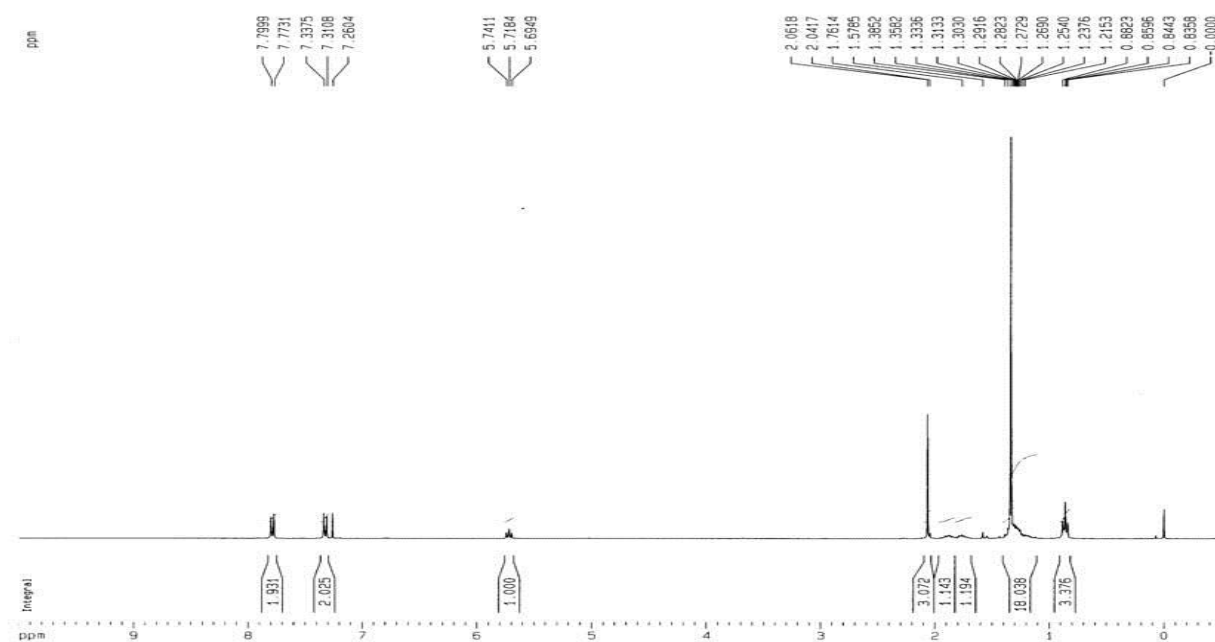
(+)-9d



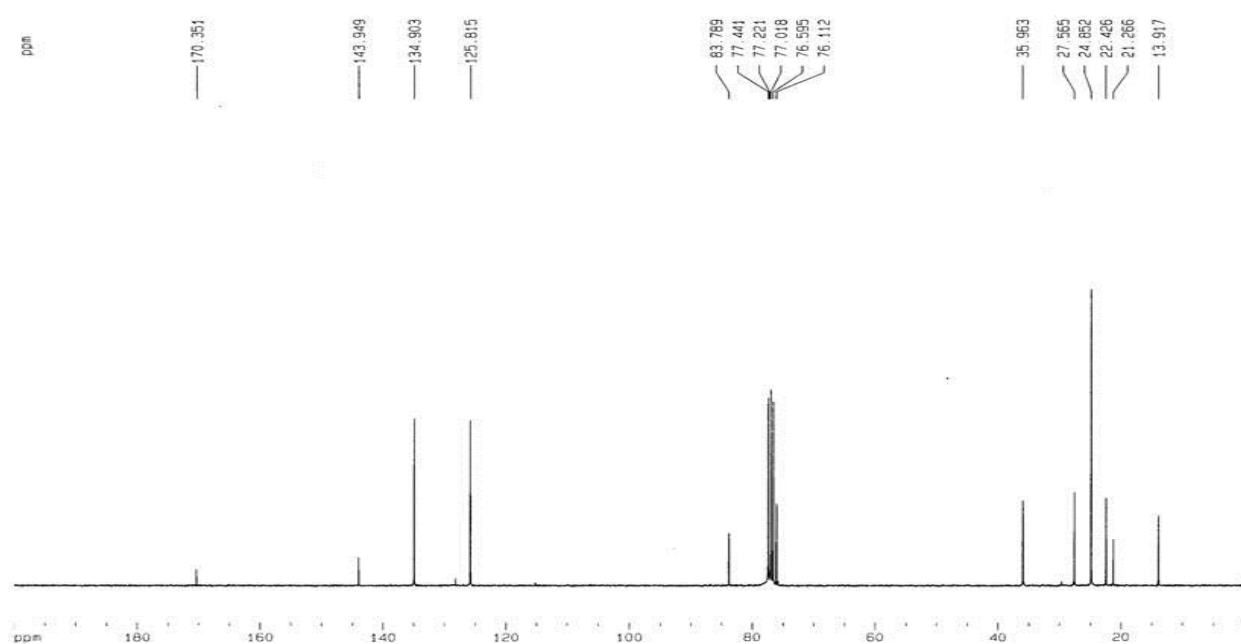
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.582	0.183	6871964	28206	2.83325	6.54246	BB
2	15.961	0.416	235674774	402916	97.16675	93.45754	BB



¹H-NMR

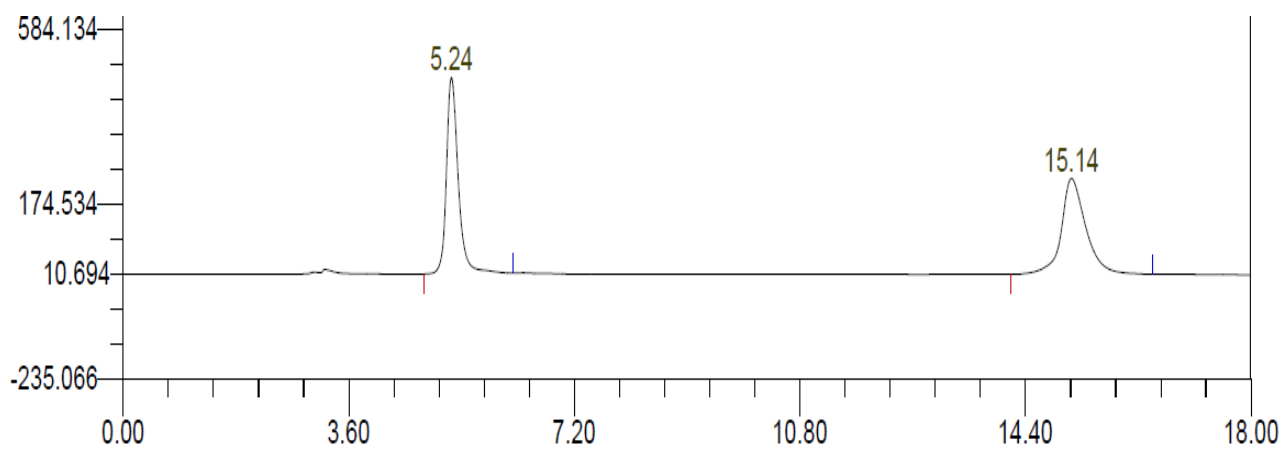


¹³C-NMR

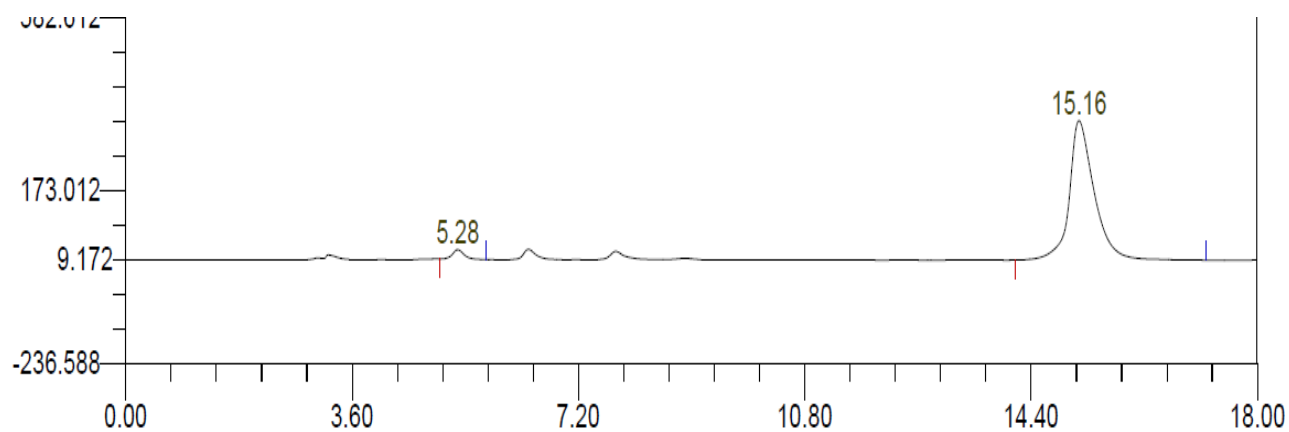


HPLC

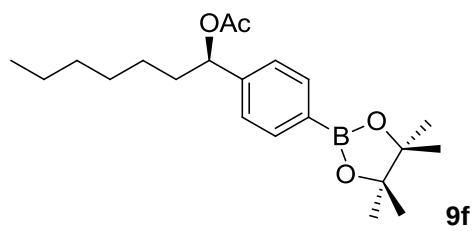
(±)-9e



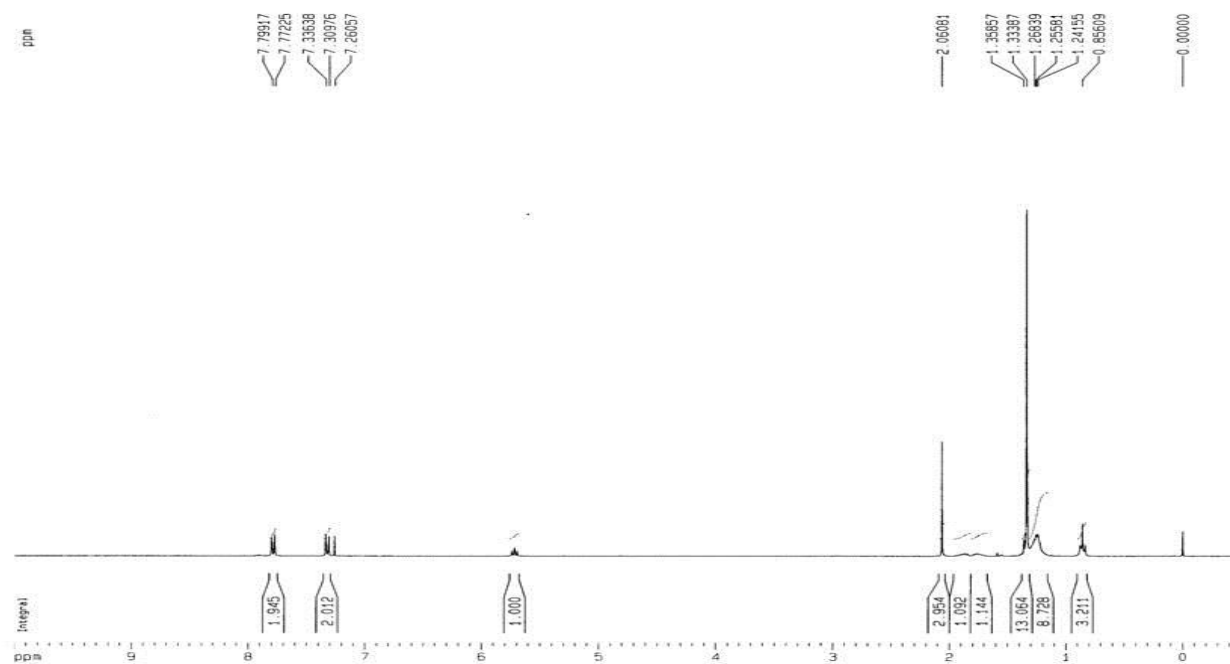
(+)-9e



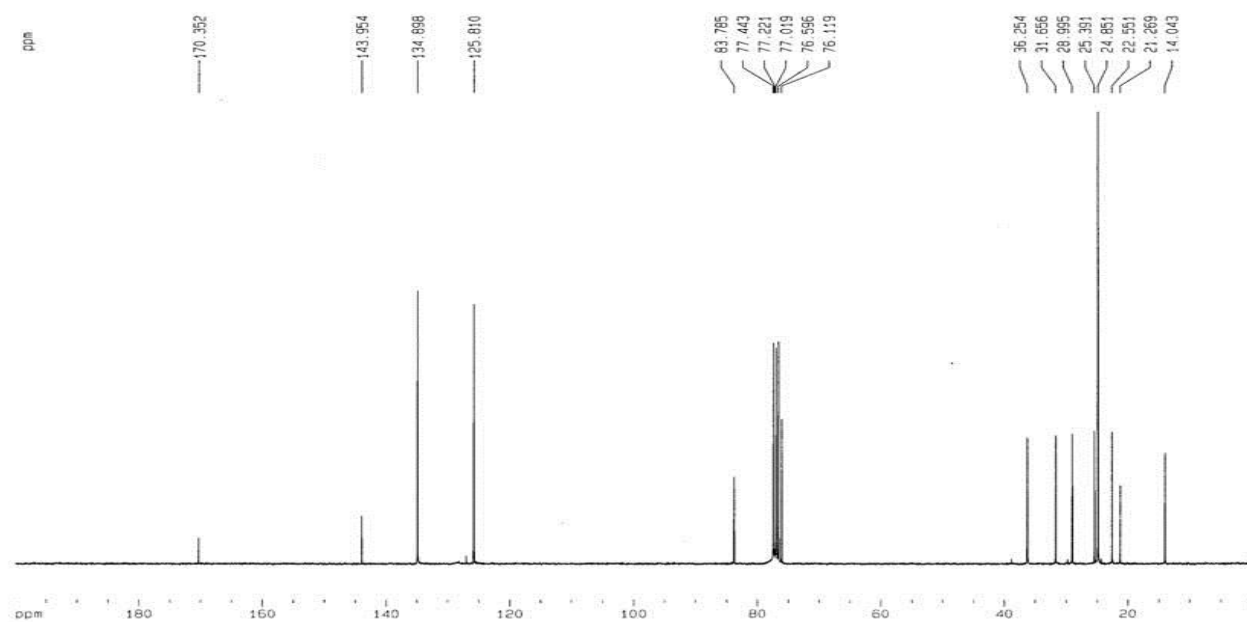
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.282	0.185	5801771	22598	3.09077	6.40667	BB
2	15.164	0.382	181910841	330128	96.90923	93.59333	BB



$^1\text{H-NMR}$

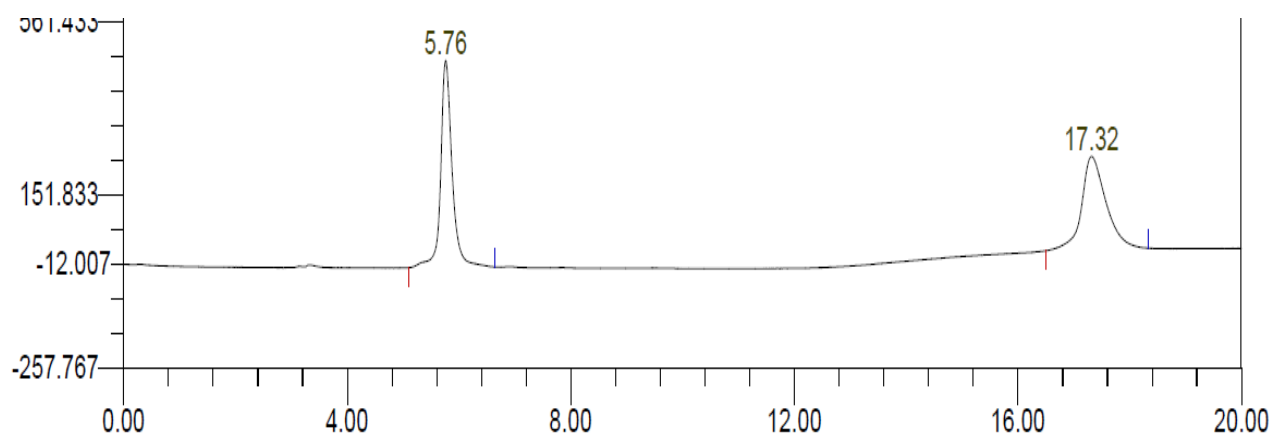


$^{13}\text{C-NMR}$

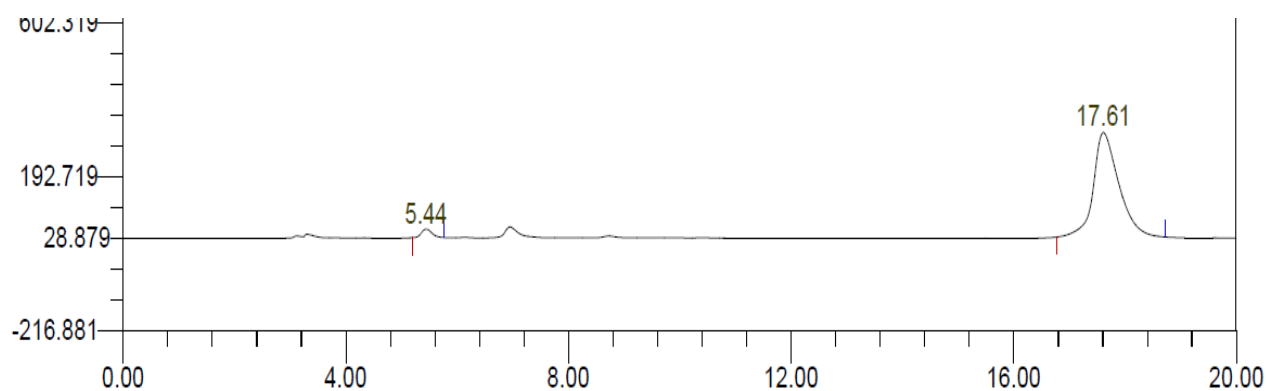


HPLC

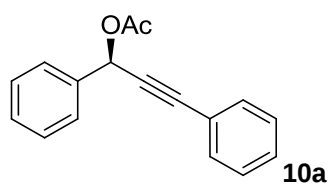
(±)-9f



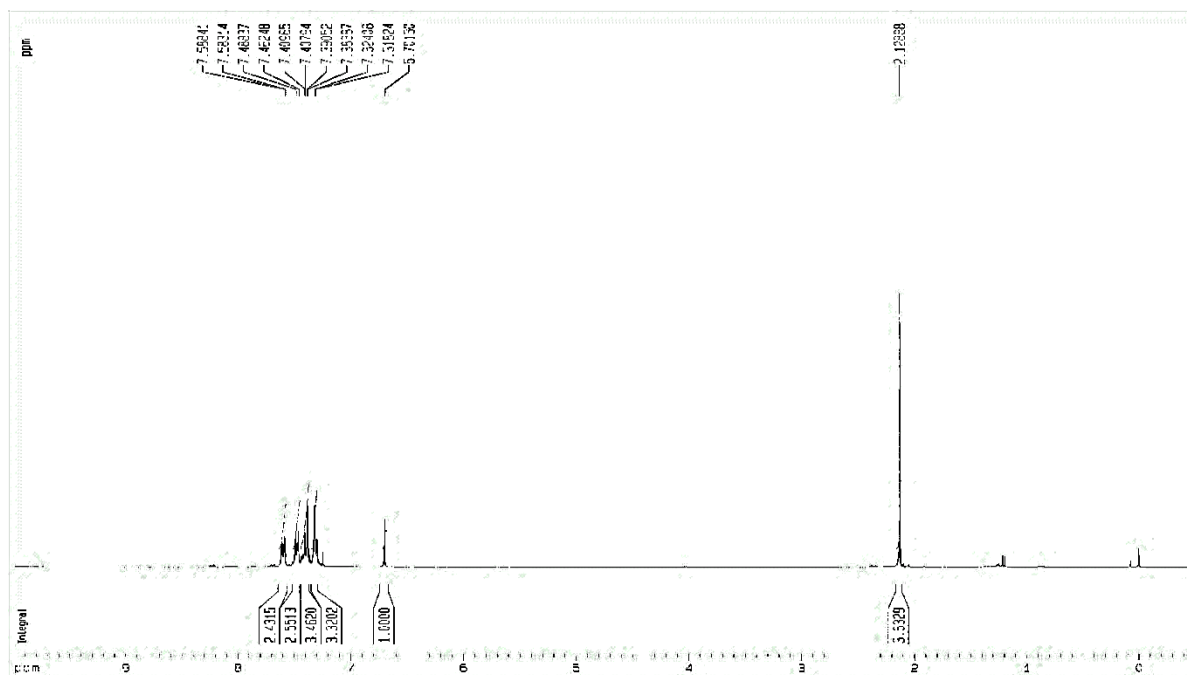
(+)-9f



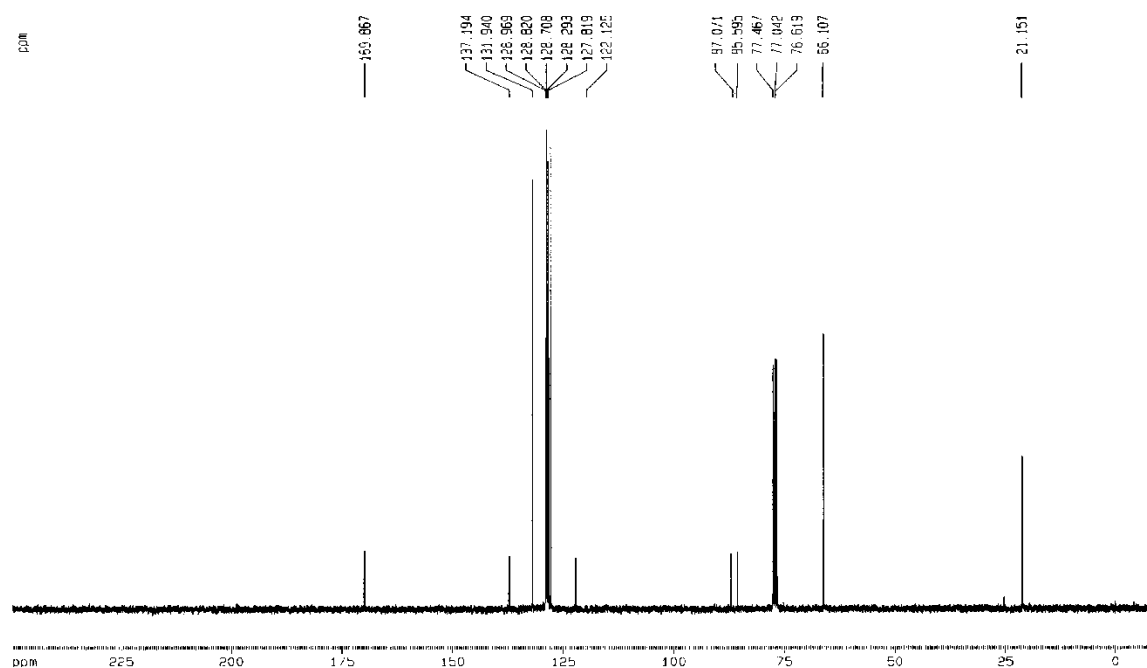
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.443	0.203	6040835	22998	3.29604	7.63683	BB
2	17.609	0.458	177234594	278148	96.70396	92.36317	BB



¹H-NMR

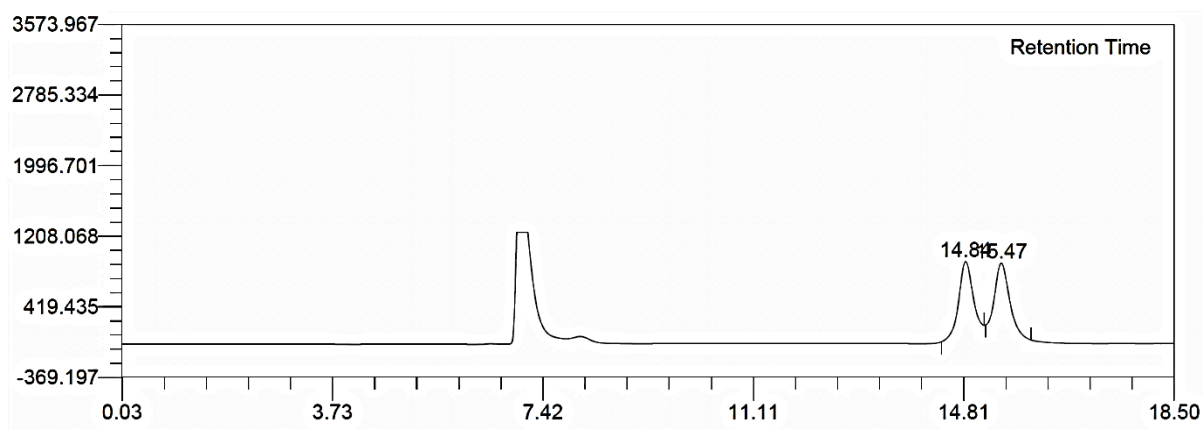


¹³C-NMR

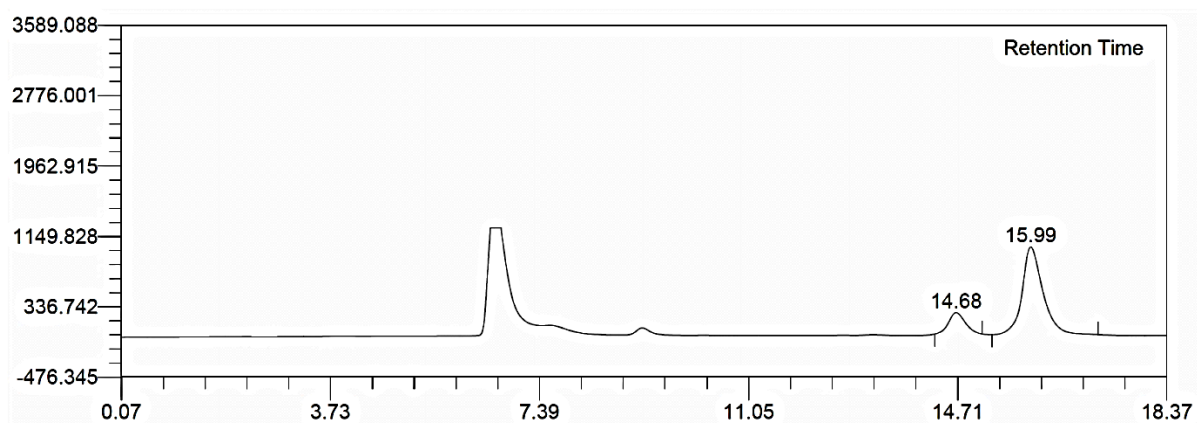


HPLC

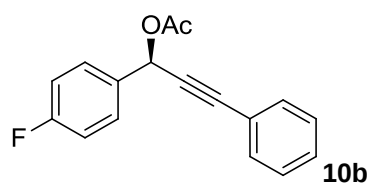
(±)-10a



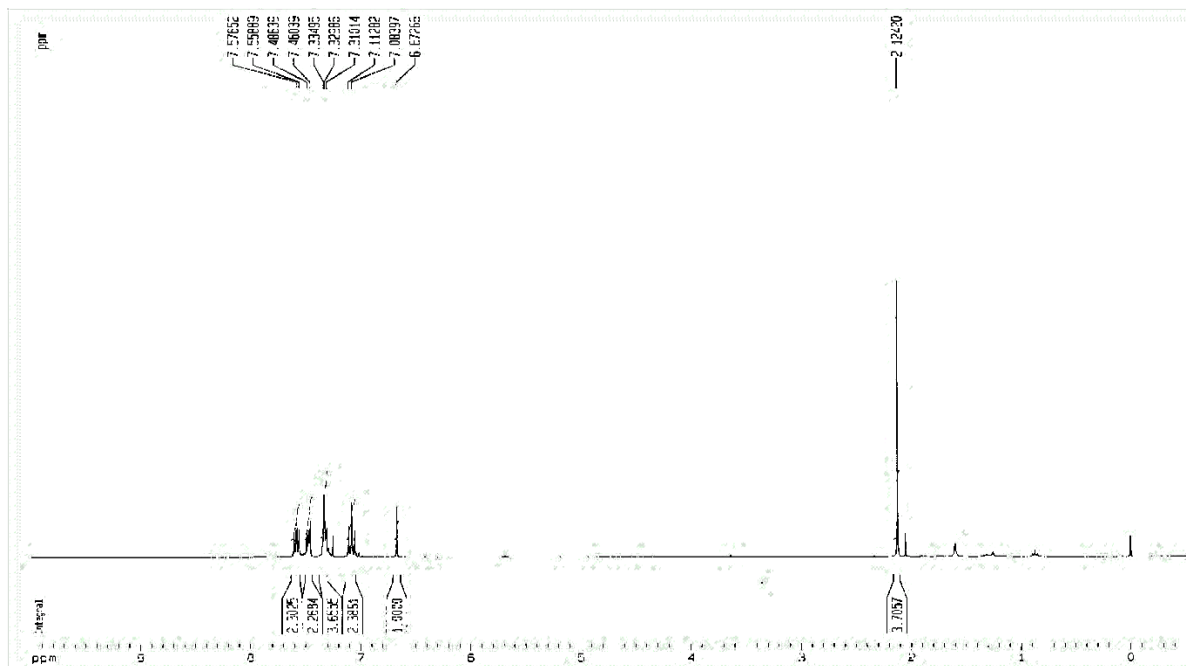
(+)-10a



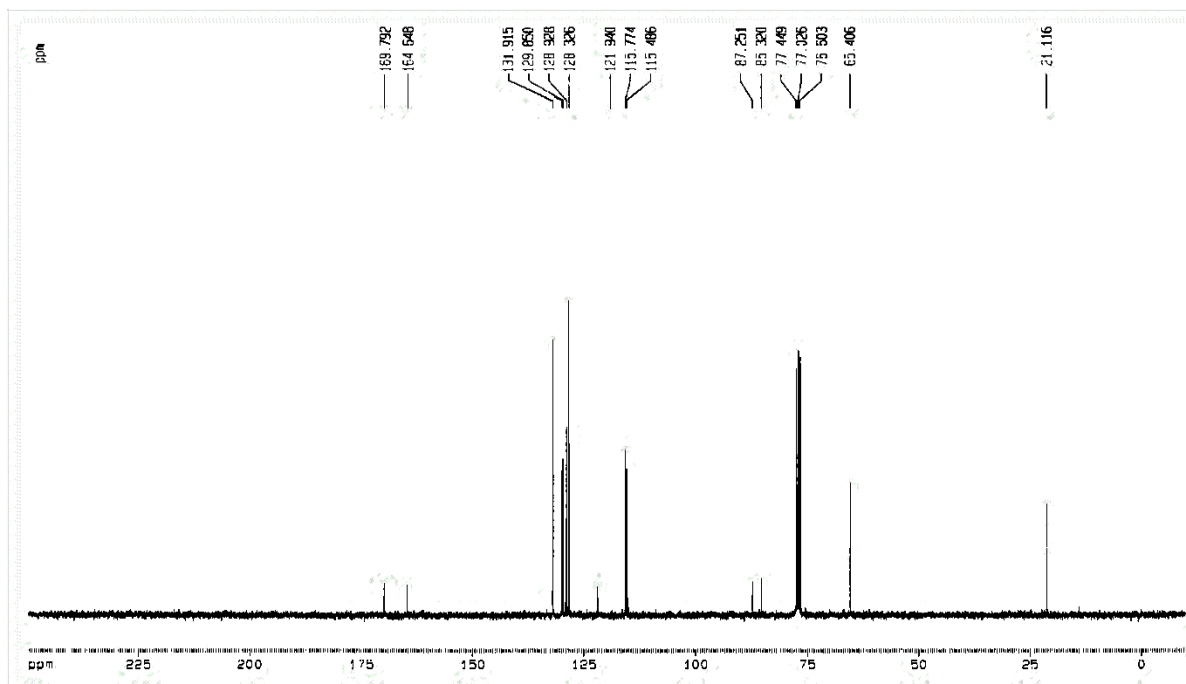
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	14.682	0.310	99209112	245758	16.25298	19.51977	tep-BB
2	15.988	0.357	511196457	1013263	83.74702	80.48023	tep-BB



¹H-NMR

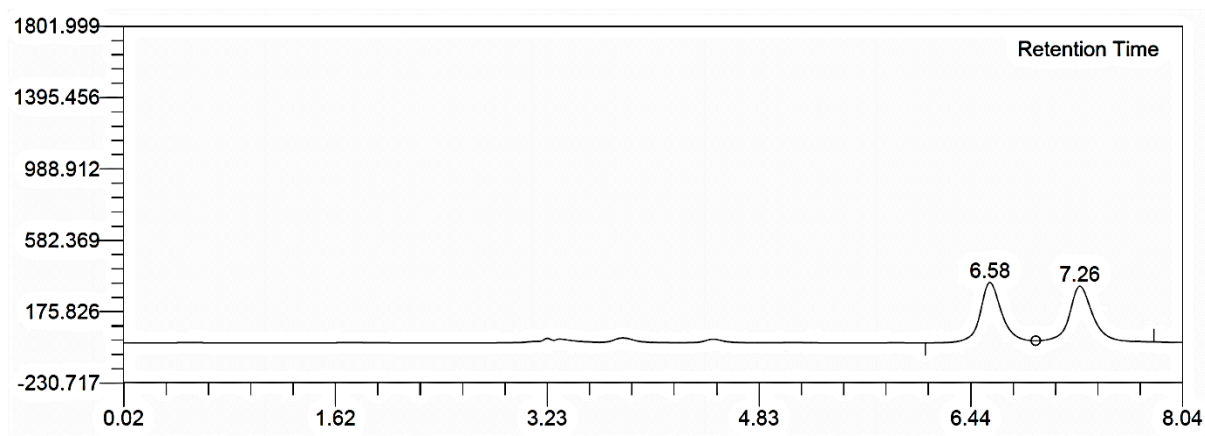


¹³C-NMR

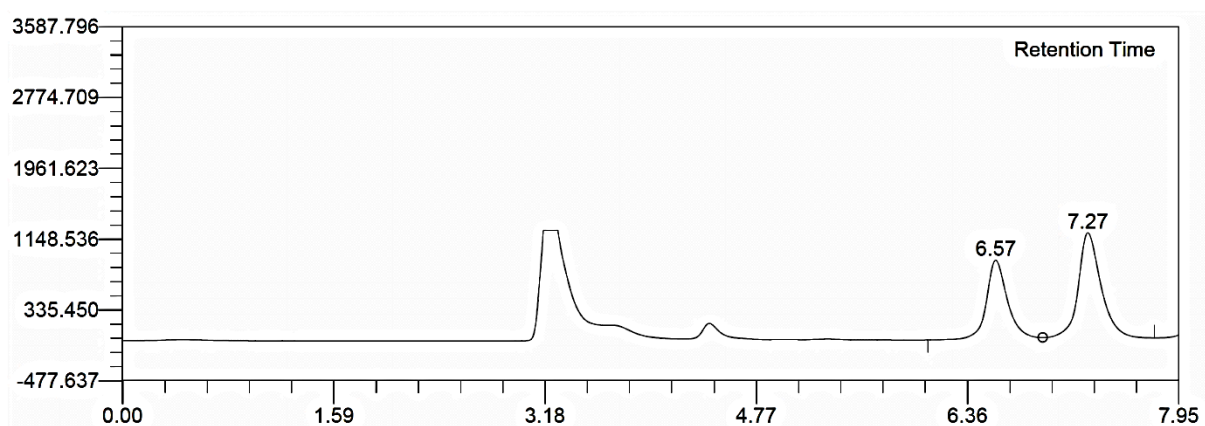


HPLC

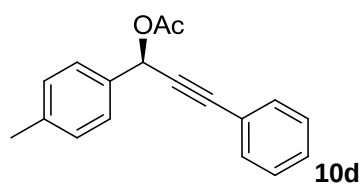
(±)- 10b



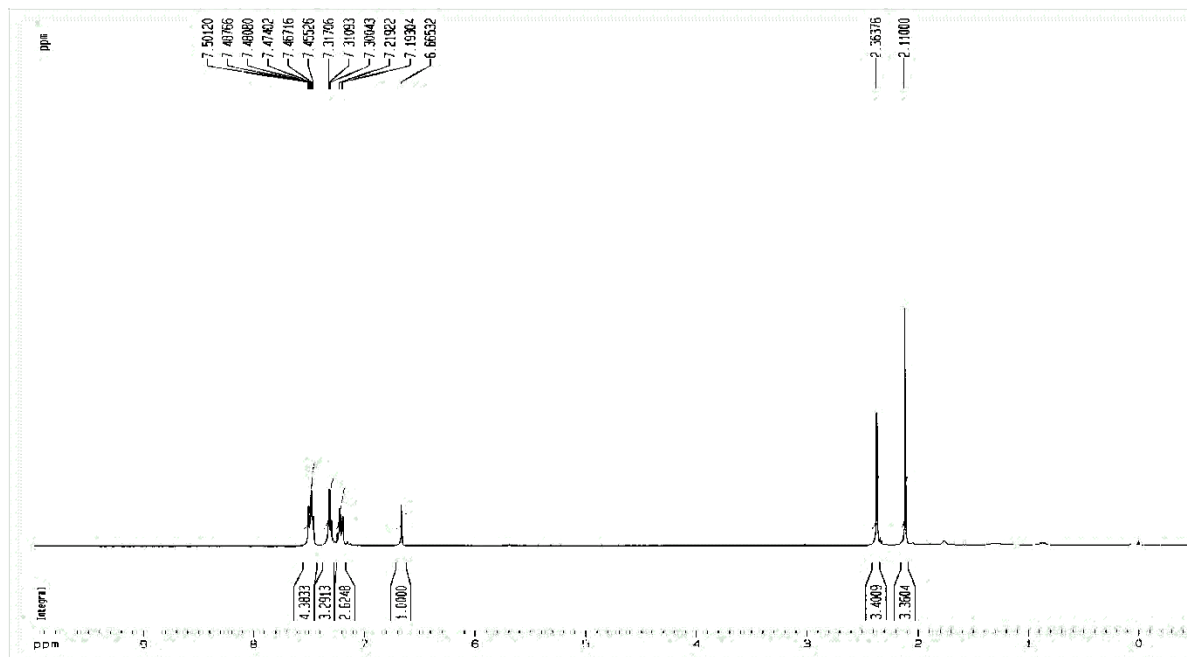
(+)-10b



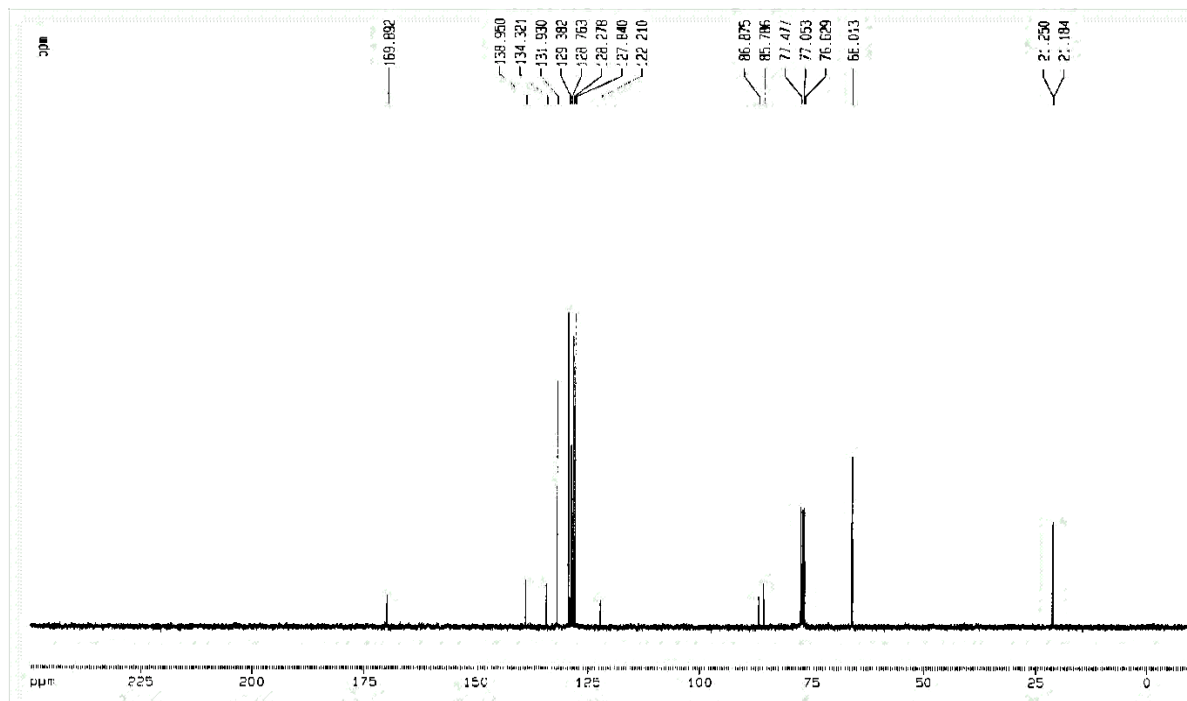
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.572	0.153	201293646	909185	40.72491	42.81433	BV
2	7.266	0.169	292982804	1214368	59.27509	57.18567	VB



¹H-NMR

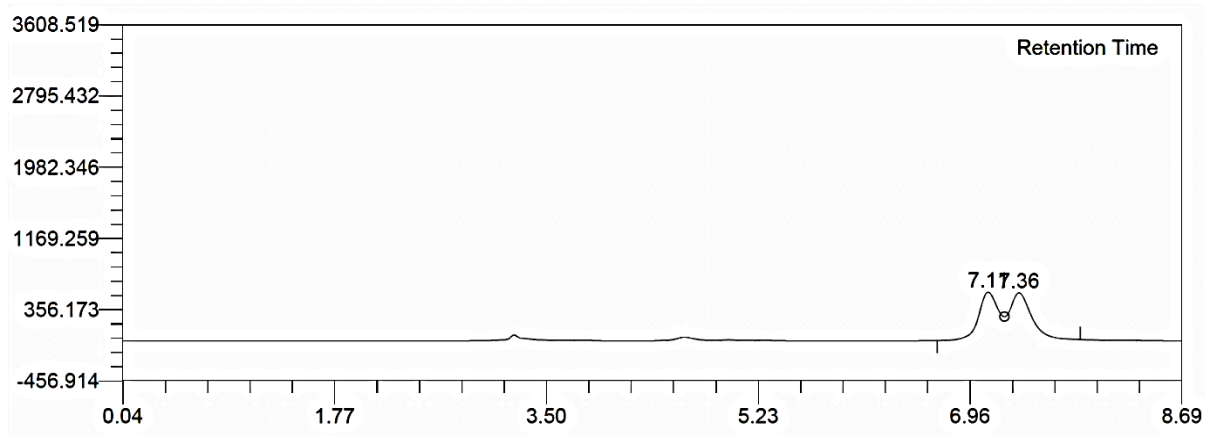


¹³C-NMR

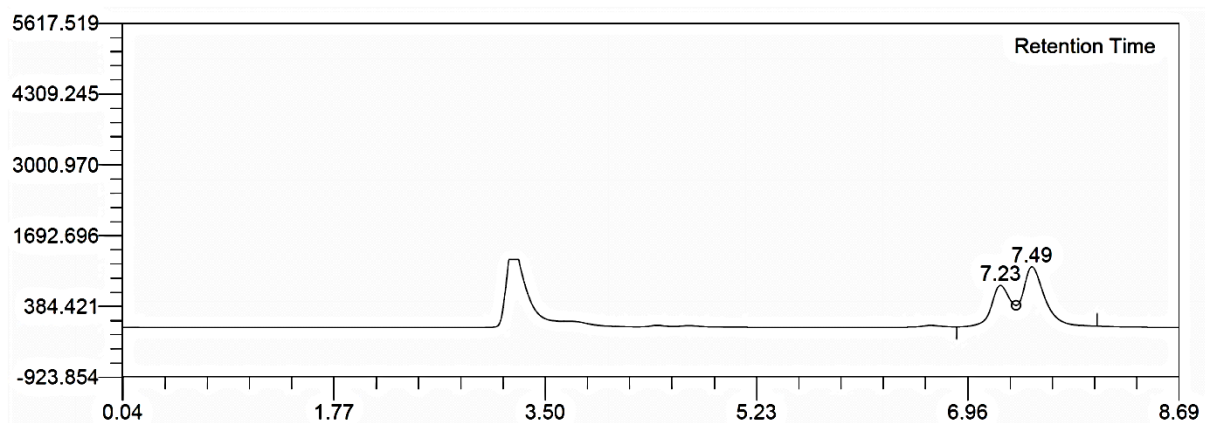


HPLC

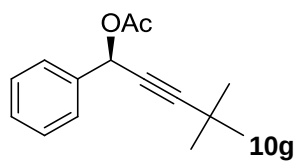
(±)- 10d



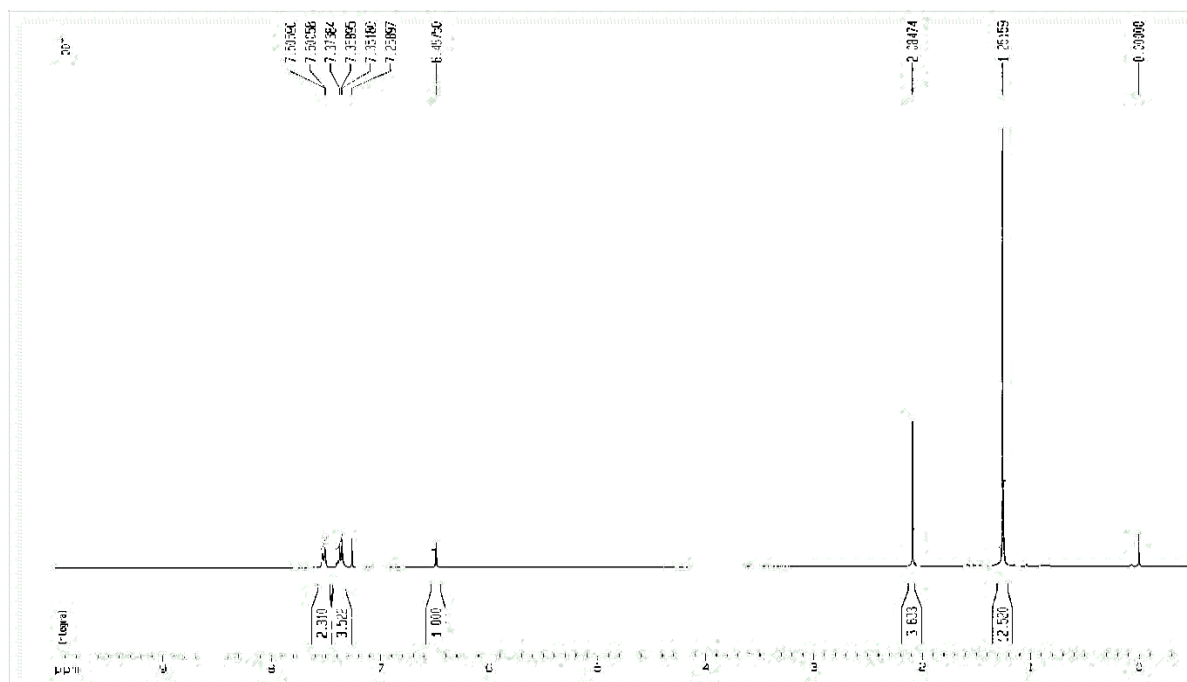
(+)-10d



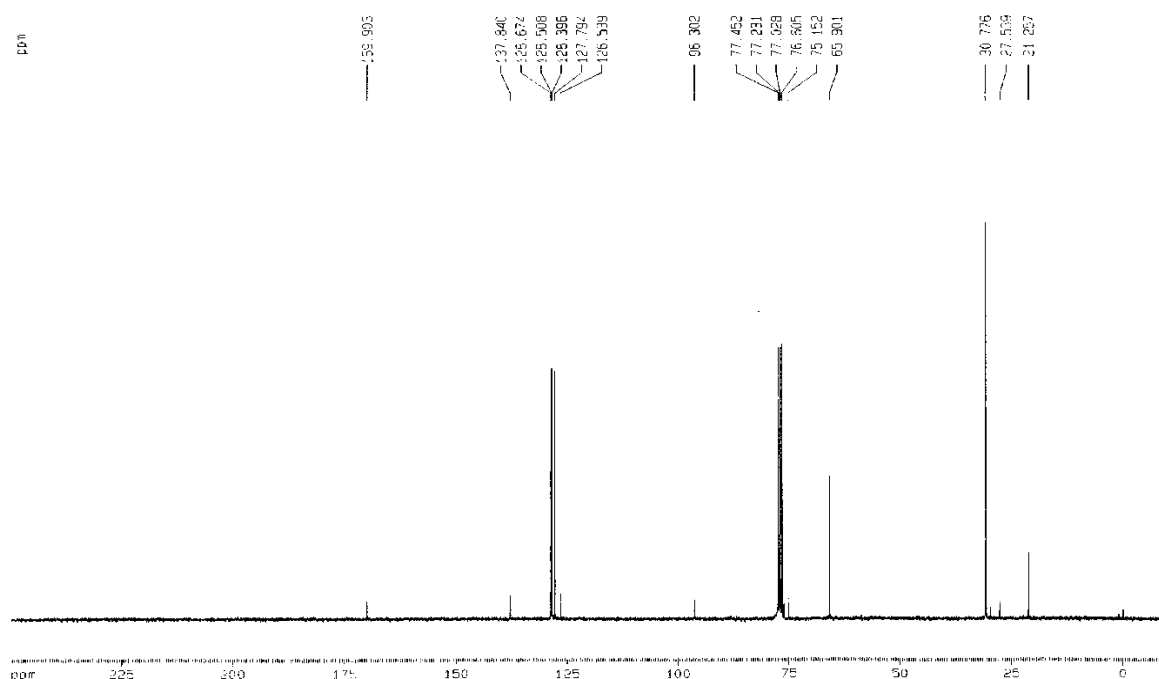
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	7.229	0.110	166921260	762709	37.86619	40.88792	BV
2	7.488	0.134	273897465	1102656	62.13381	59.11208	VB



$^1\text{H-NMR}$

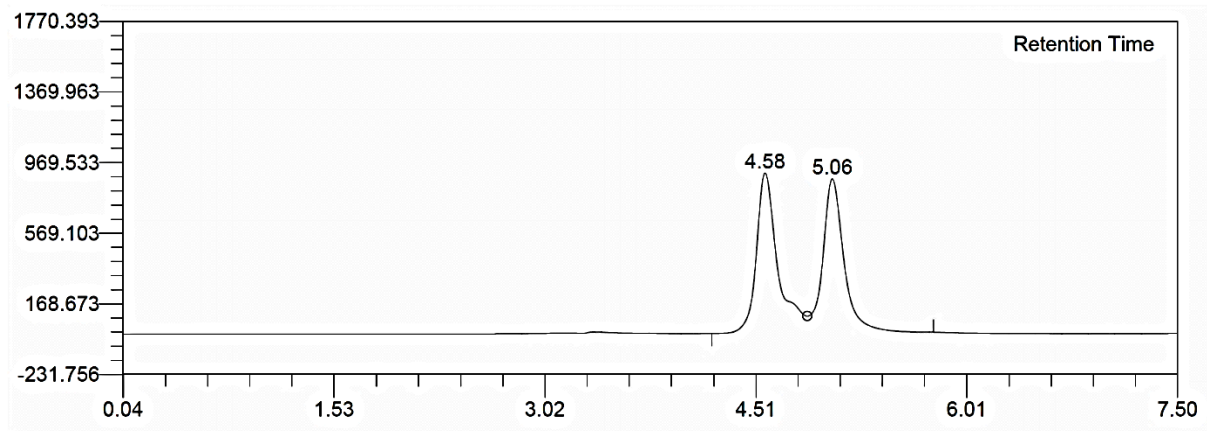


$^{13}\text{C-NMR}$

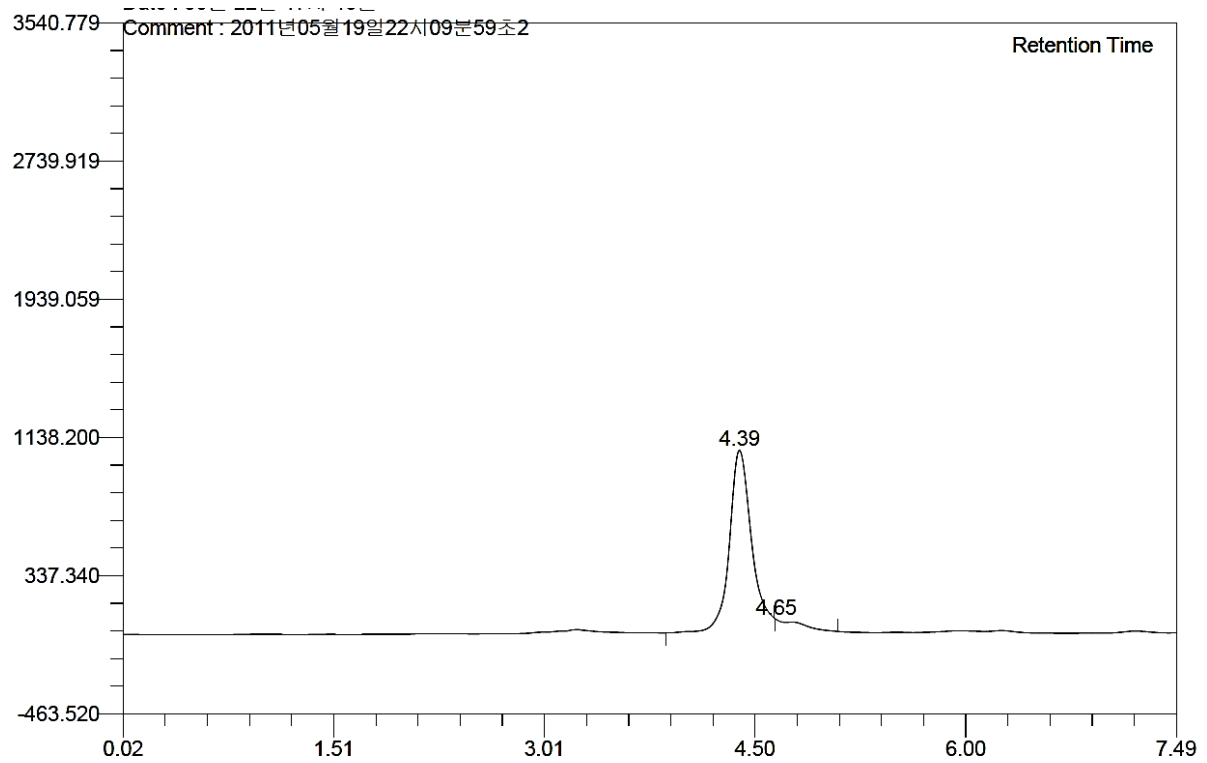


HPLC

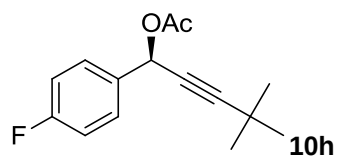
(±)- 10g



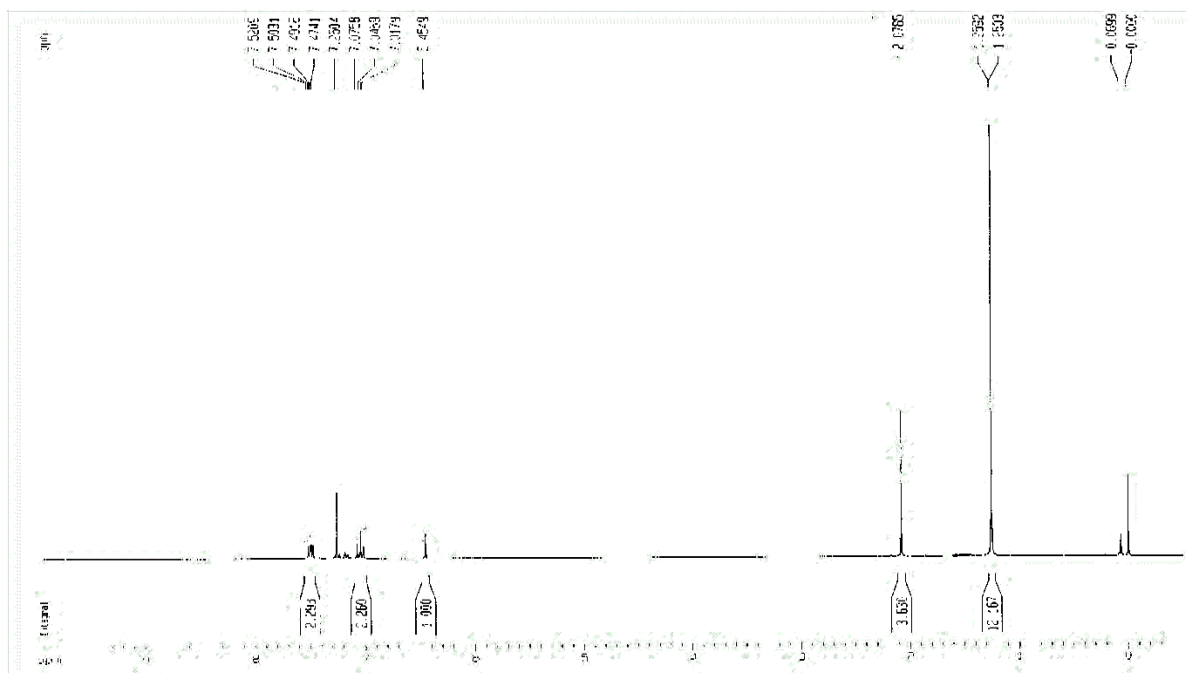
(+)-10g



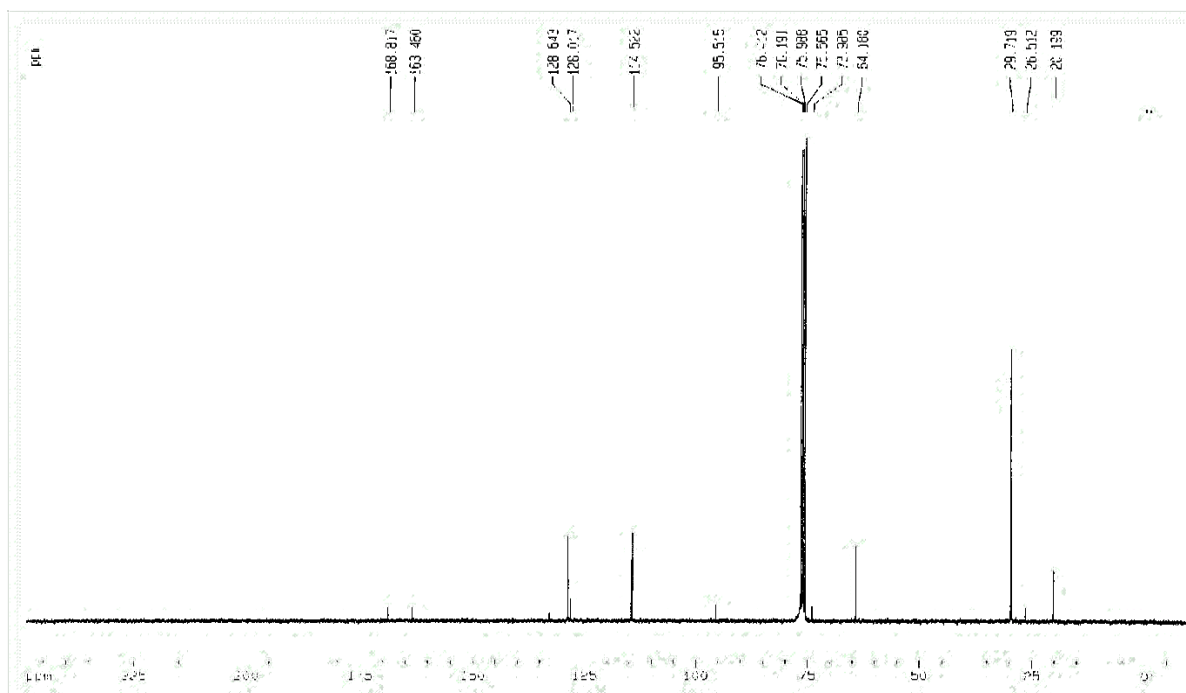
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	4.391	0.147	198683679	999704	99.87531	99.83393	tep-BB
2	4.651	0.000	248049	1663	0.12469	0.16607	tep-BB



¹H-NMR

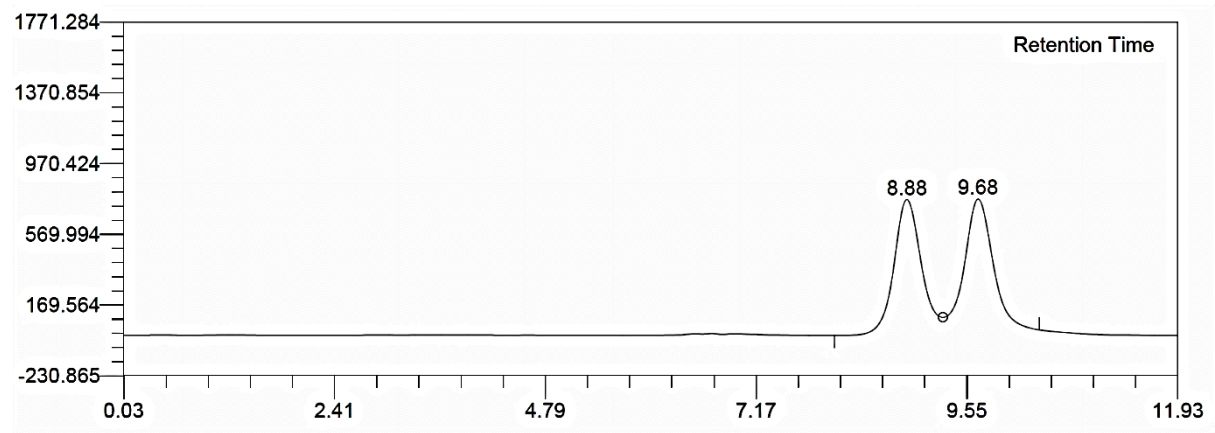


¹³C-NMR

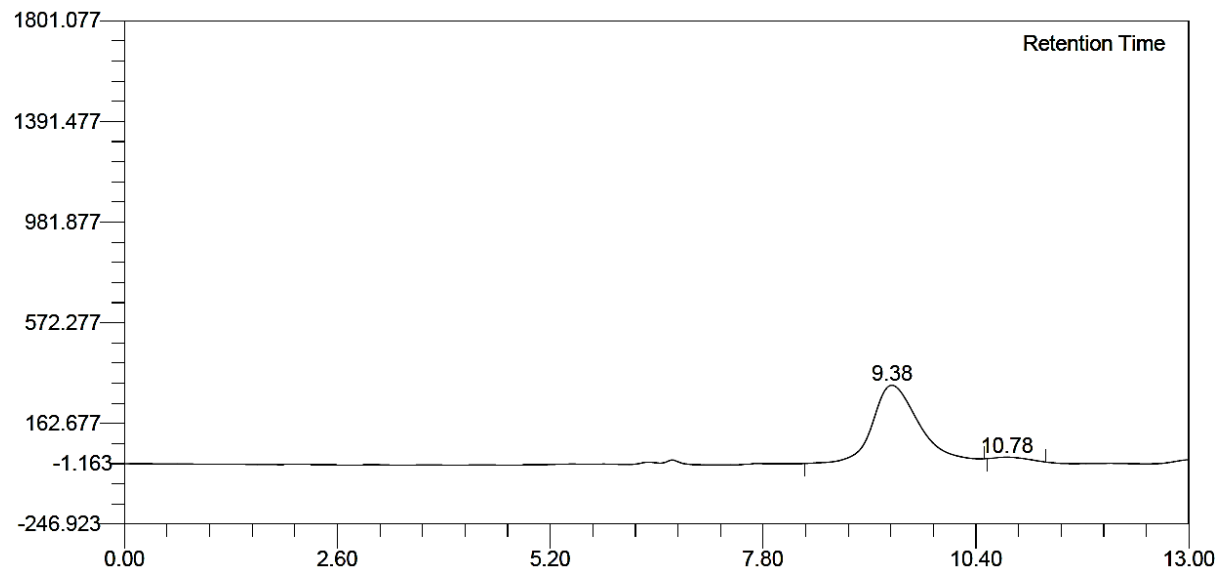


HPLC

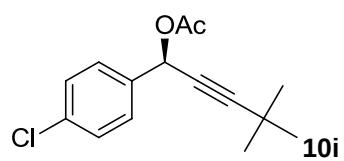
(±)- 10h



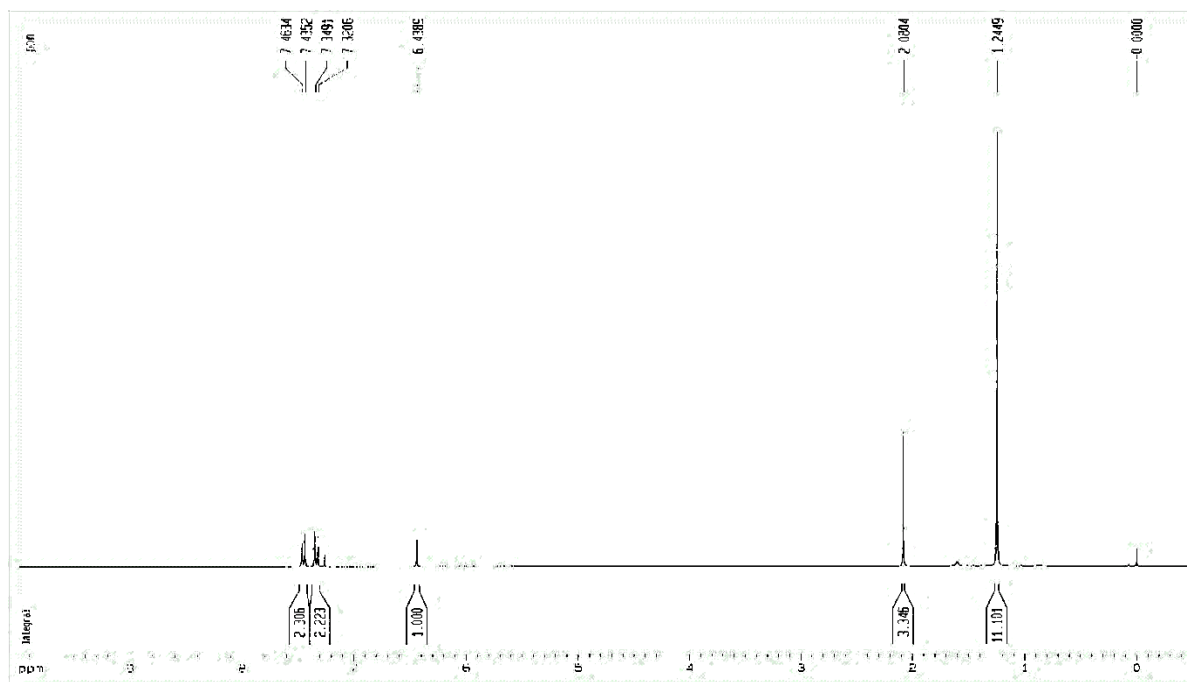
(+)-10h



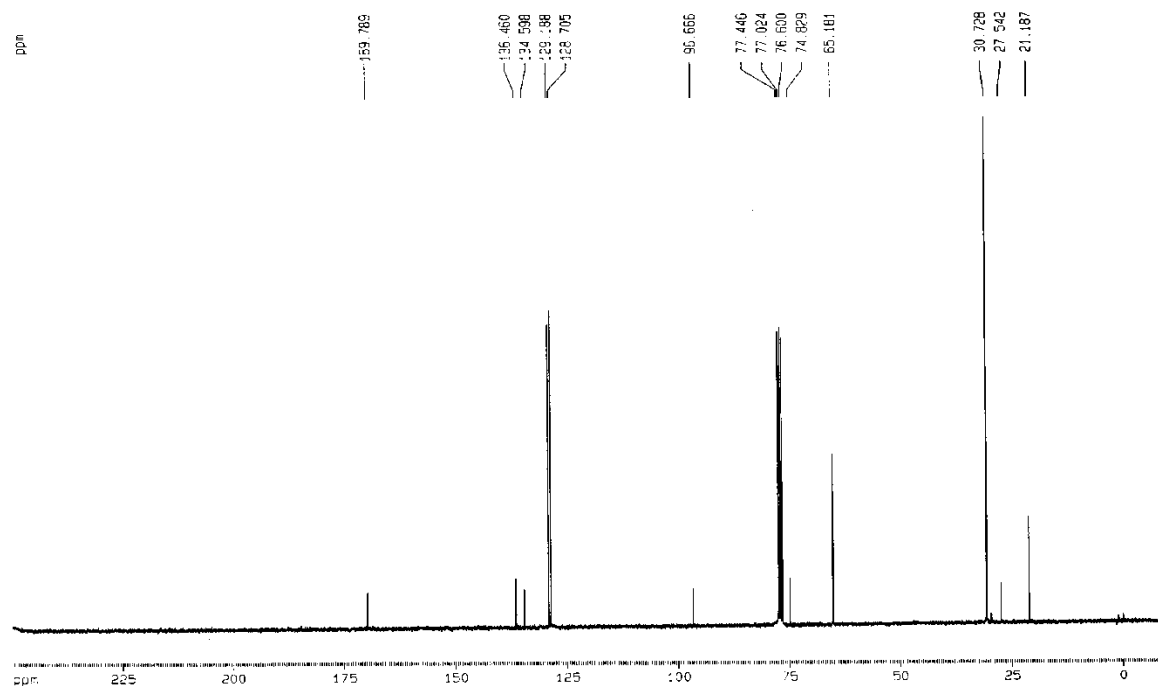
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	9.375	0.553	232114422	309206	97.58406	96.67914	tep-BB
2	10.779	0.292	5746585	10621	2.41594	3.32086	tep-BB



¹H-NMR

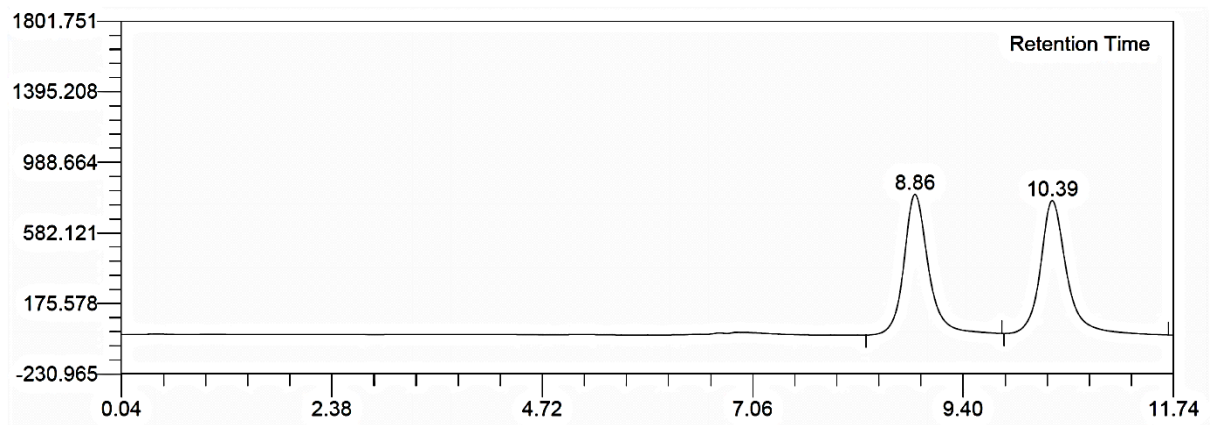


¹³C-NMR

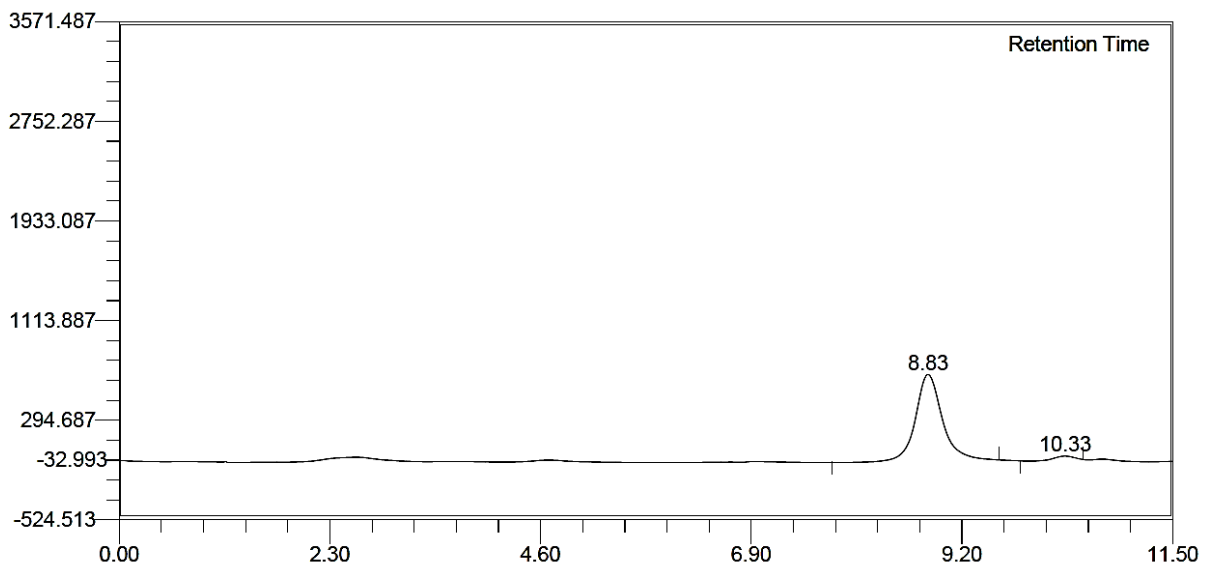


HPLC

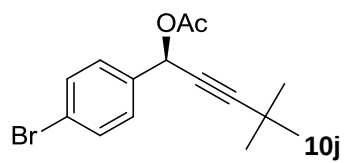
(±)- 10i



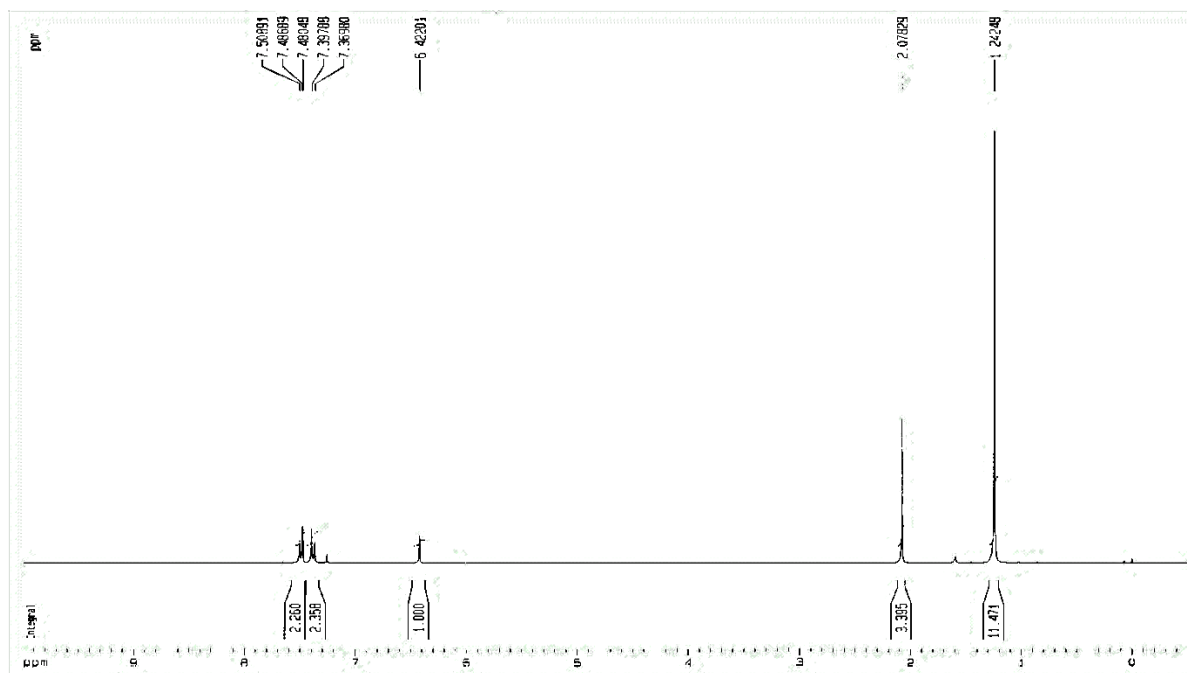
(+)-10i



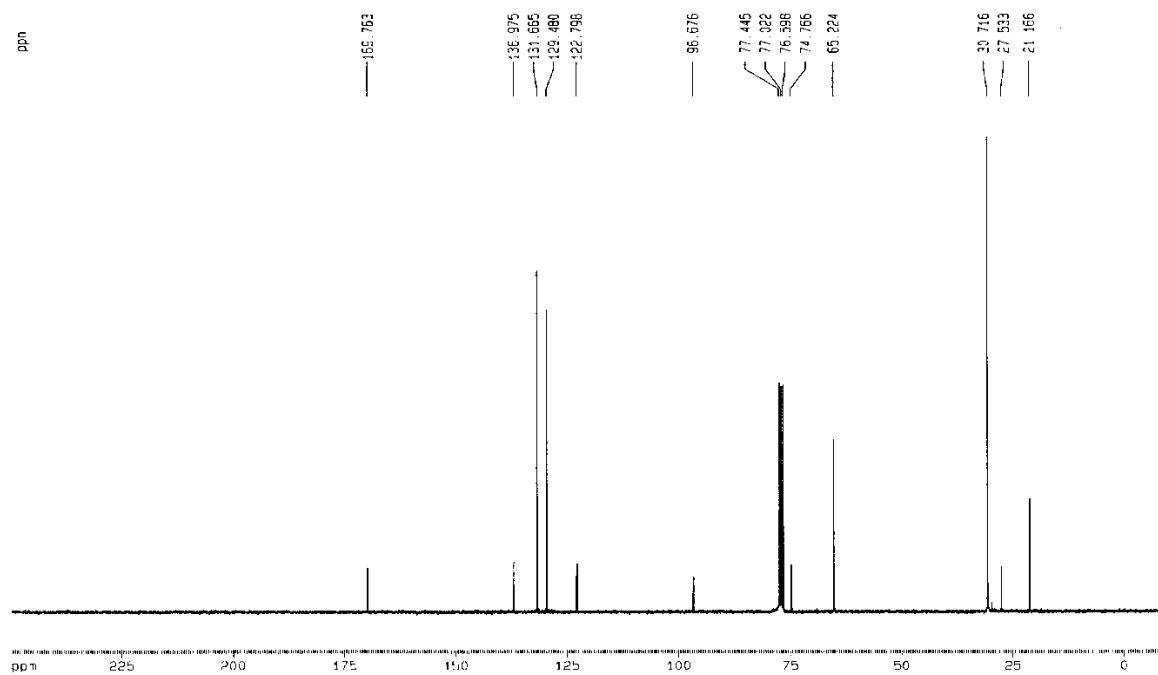
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	8.833	0.287	286970685	709836	97.15321	95.82821	tep-BB
2	10.329	0.212	8408829	30902	2.84679	4.17179	tep-BB



¹H-NMR

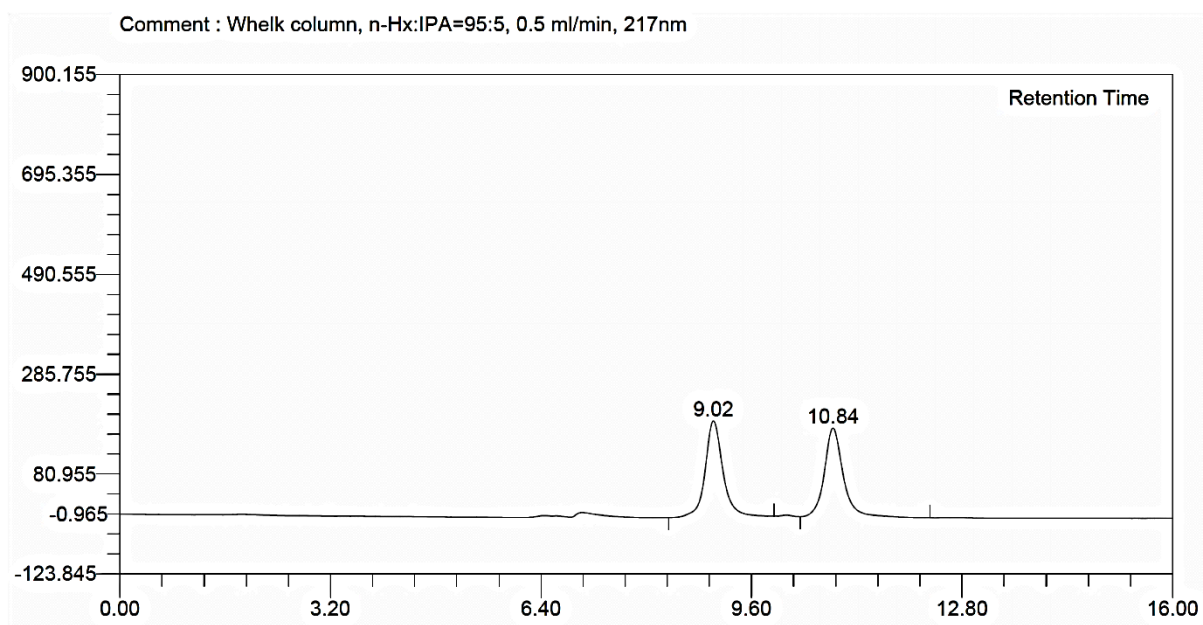


¹³C-NMR

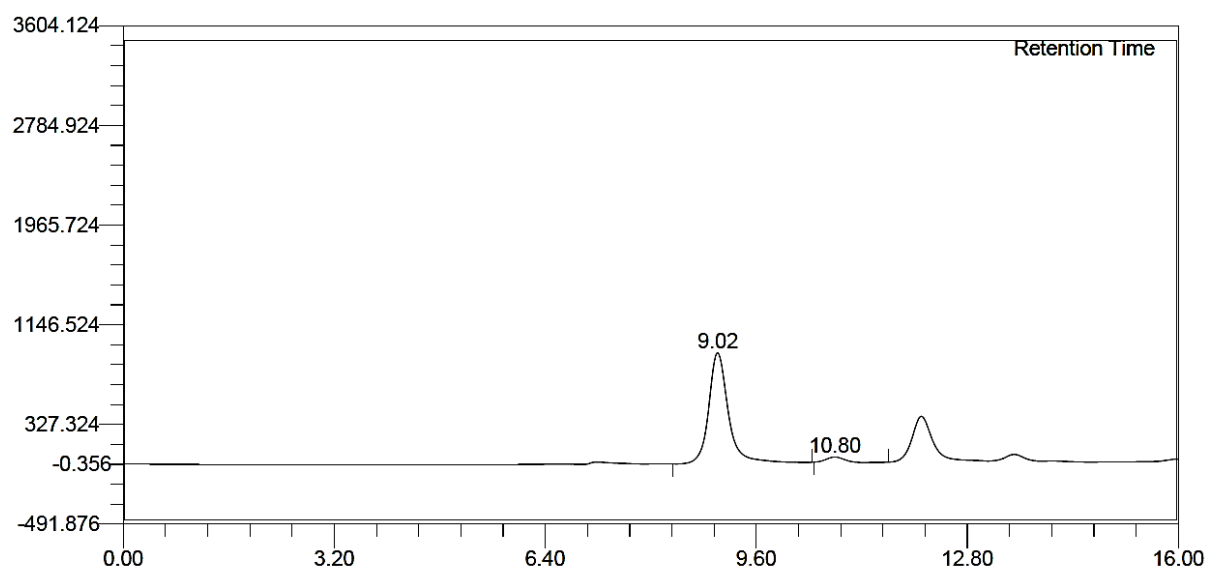


HPLC

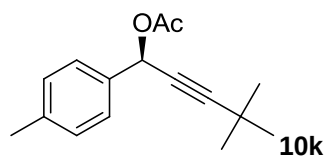
(±)- 10j



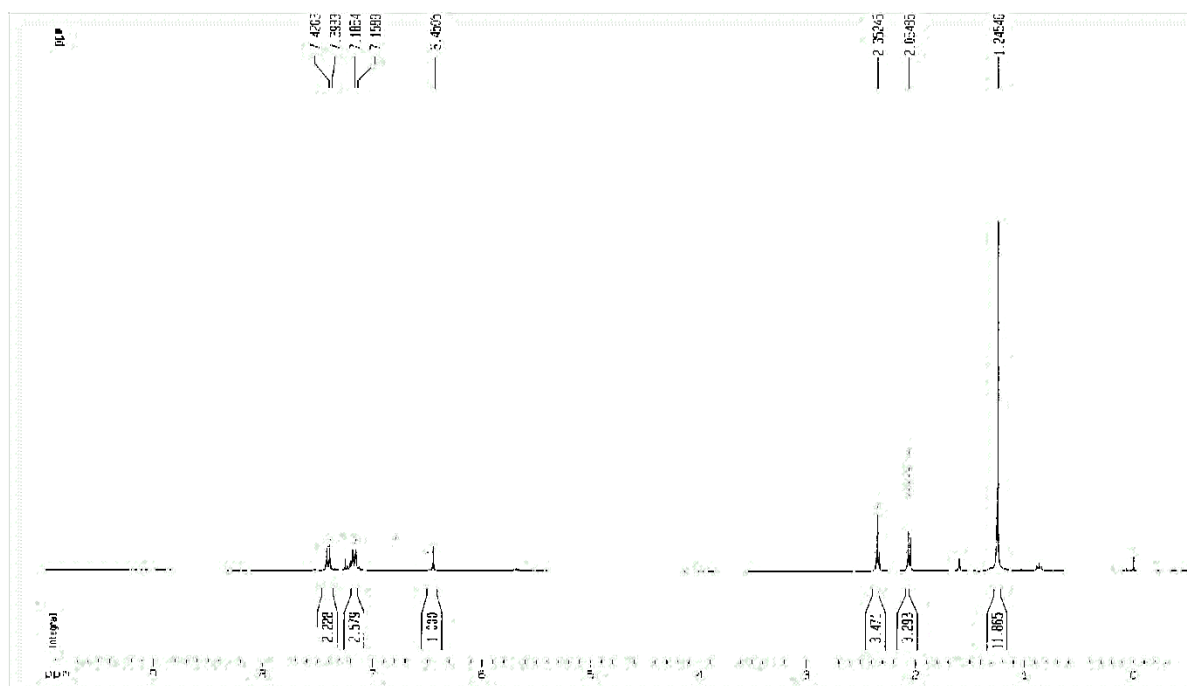
(+)-10j



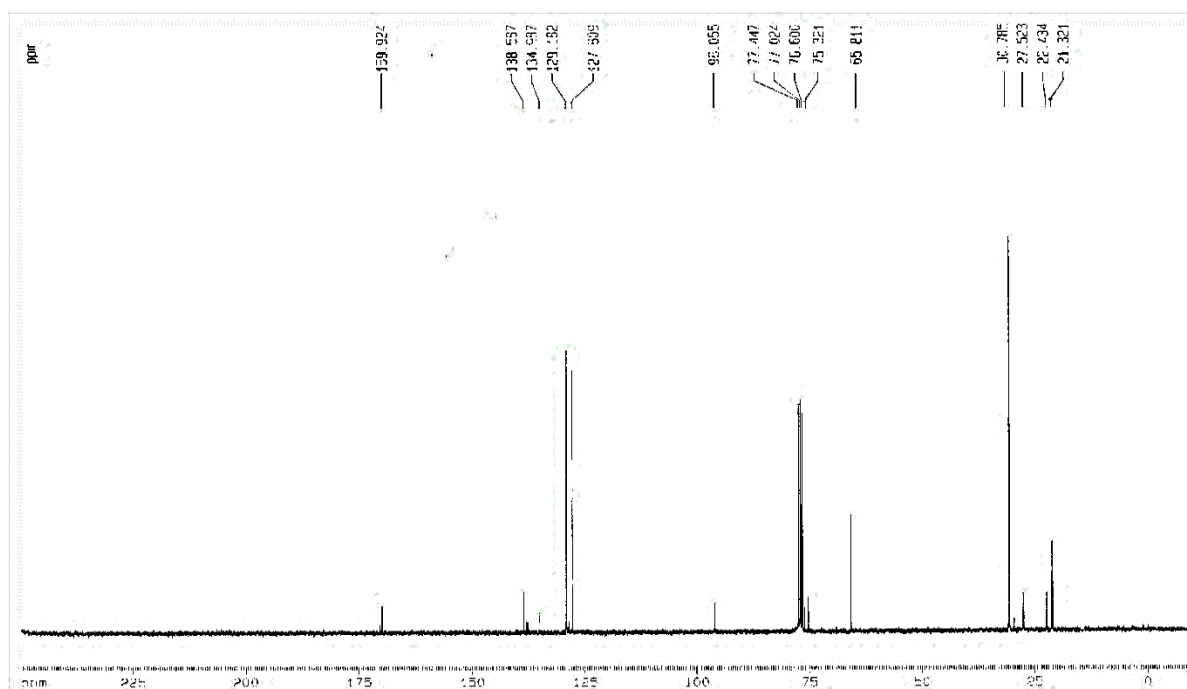
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	9.015	0.287	374124122	909154	96.12971	95.58632	tep-BB
2	10.795	0.288	15062651	41980	3.87029	4.41368	tep-BB



¹H-NMR

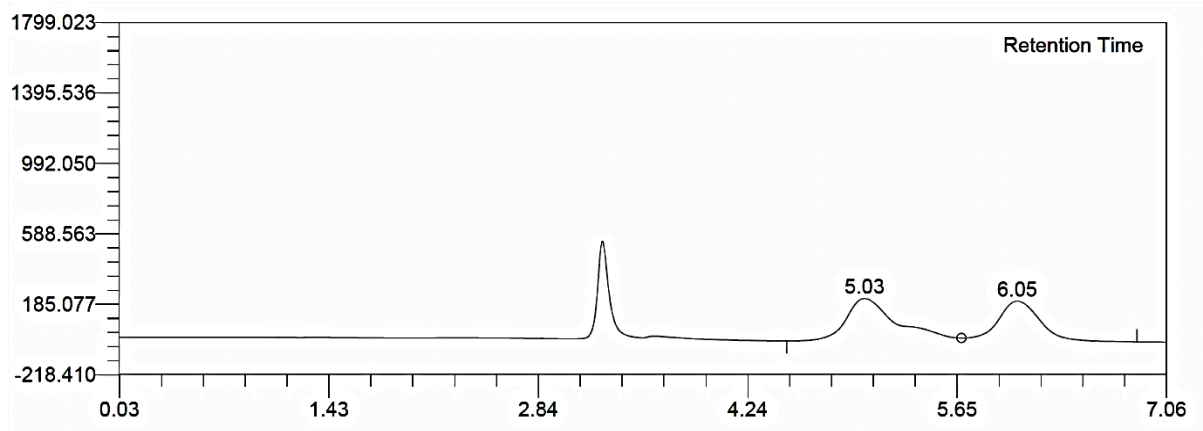


¹³C-NMR

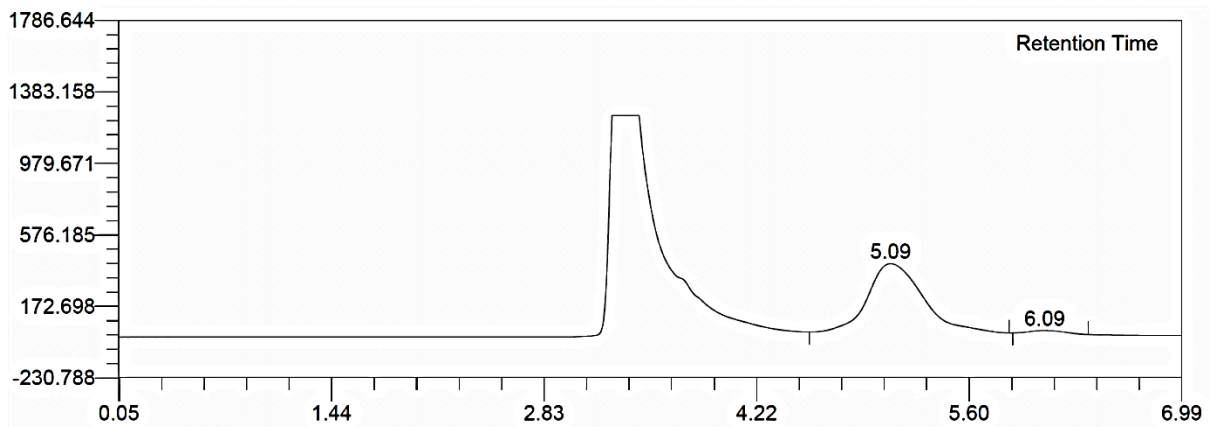


HPLC

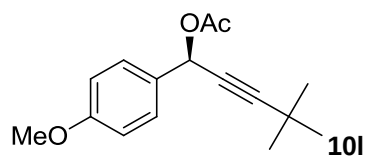
(±)- 10k



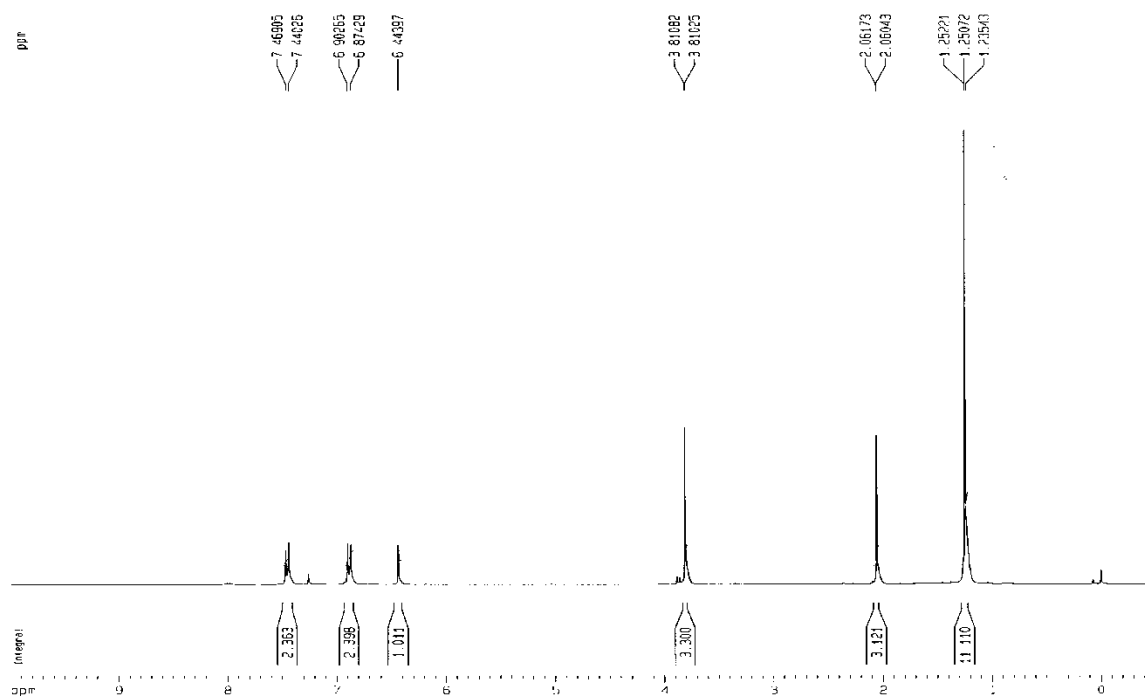
(+)-10k



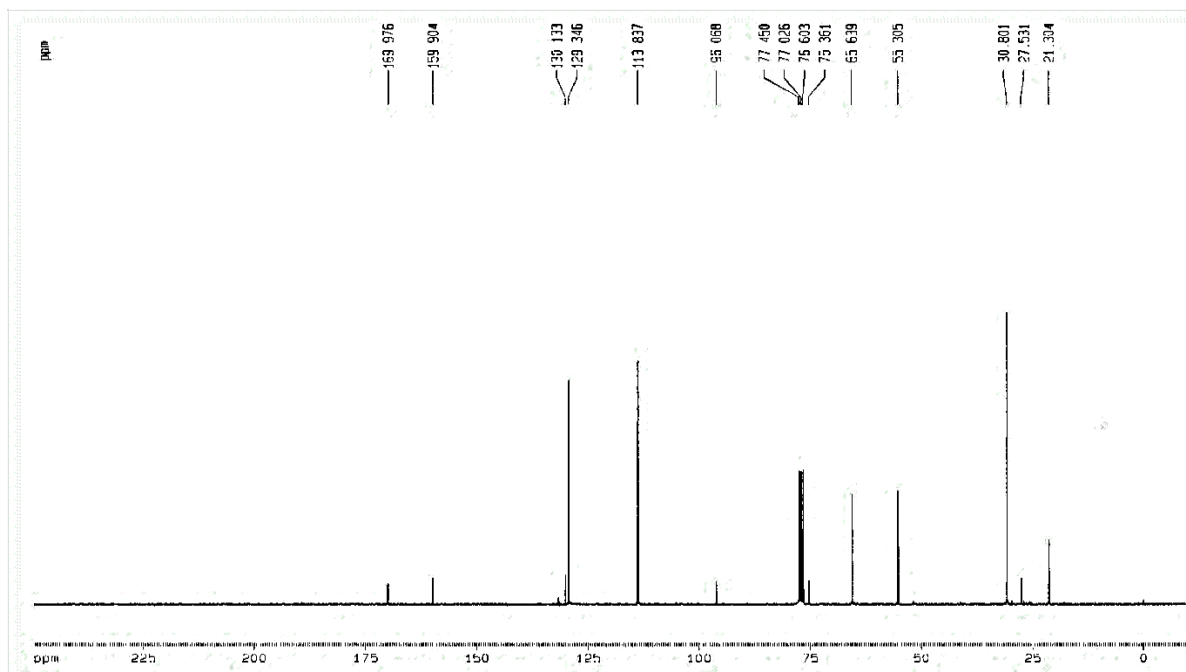
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.088	0.368	192339952	387520	97.37922	95.89682	tep-mBB
2	6.094	0.214	5176463	16581	2.62078	4.10318	tep-tBB



¹H-NMR

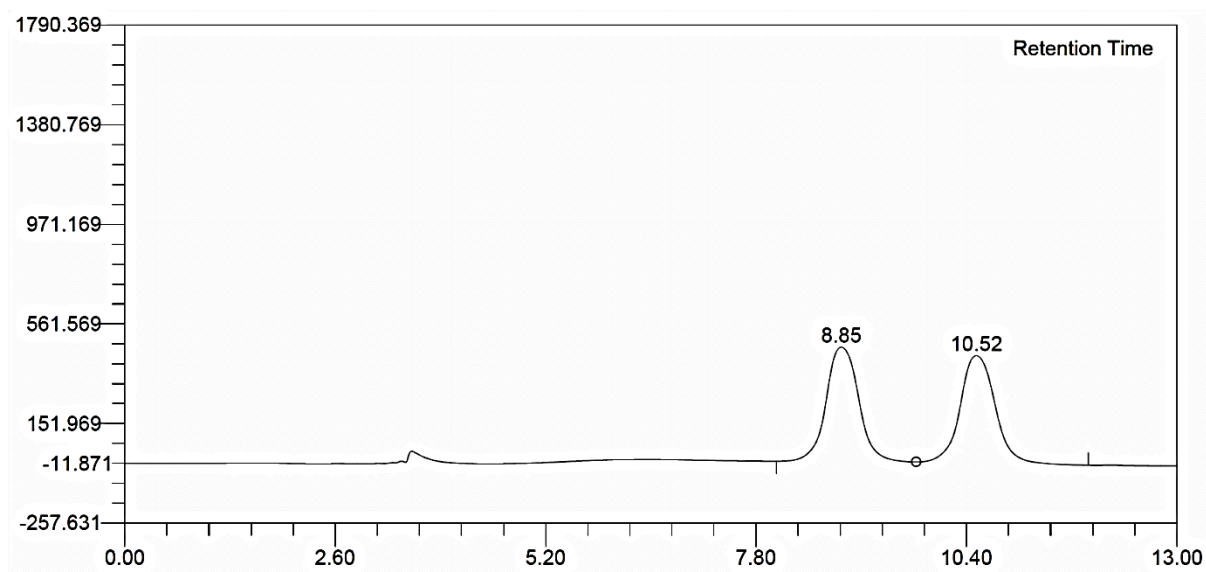


¹³C-NMR

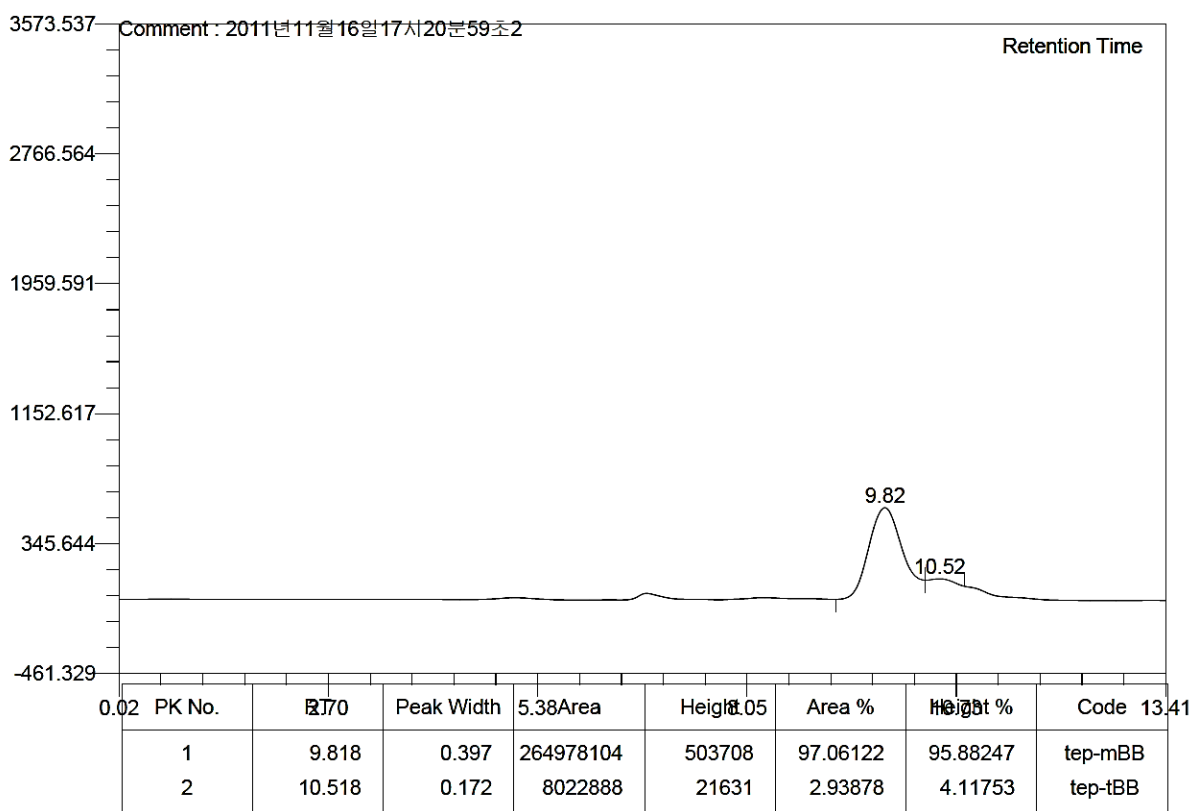


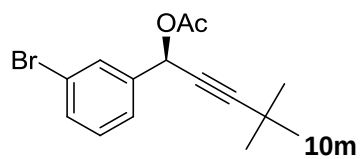
HPLC (Enantiomeric excess (ee) was determined after hydrolysis of acetate)

(±)- **10I**

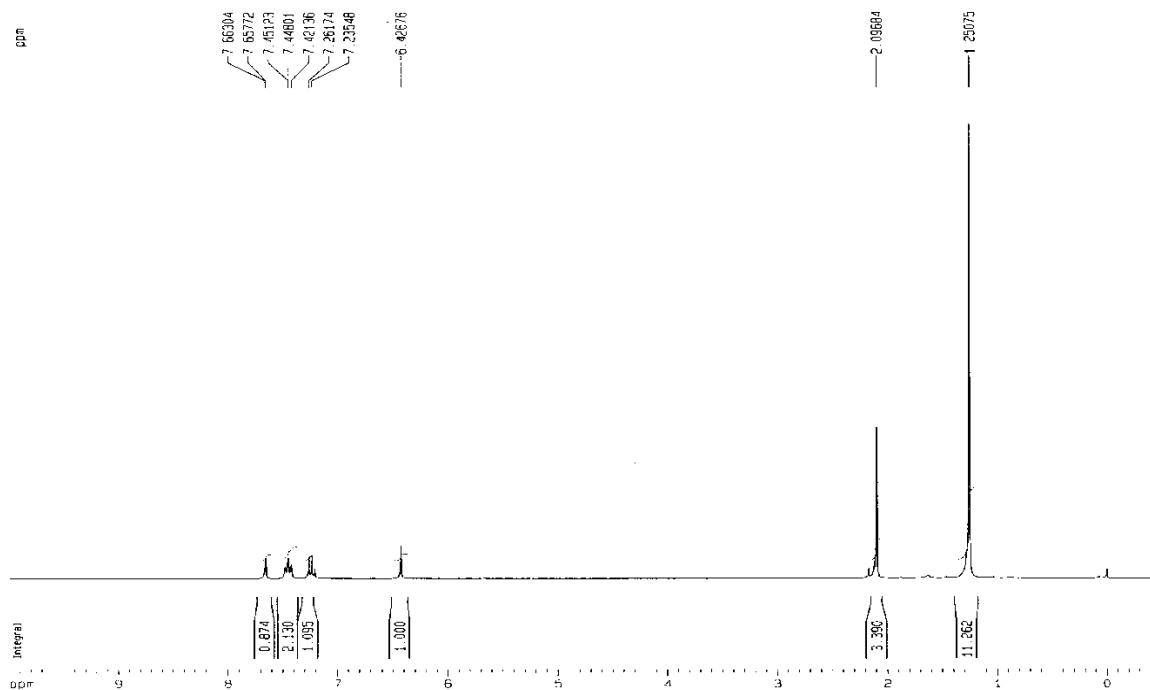


(+)-**10I**

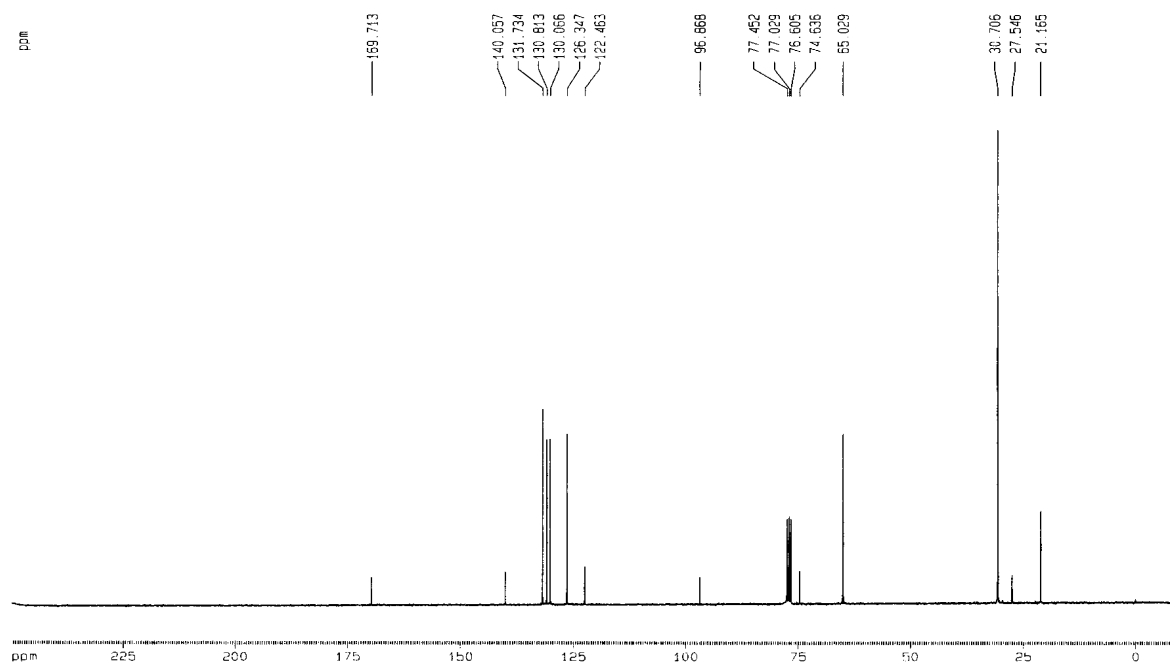




¹H-NMR

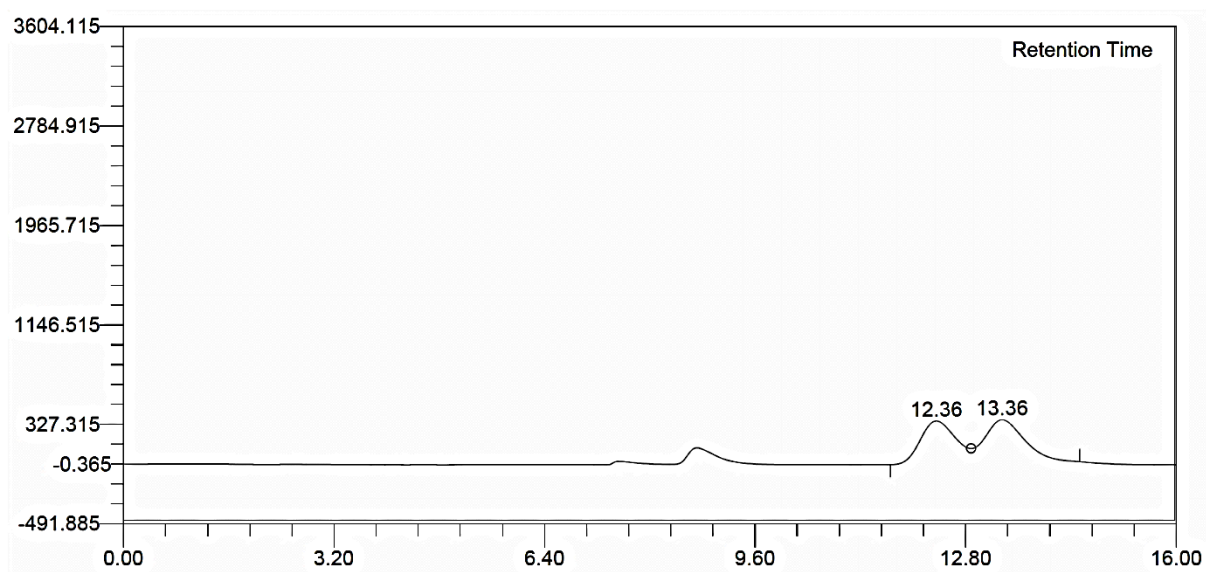


¹³C-NMR

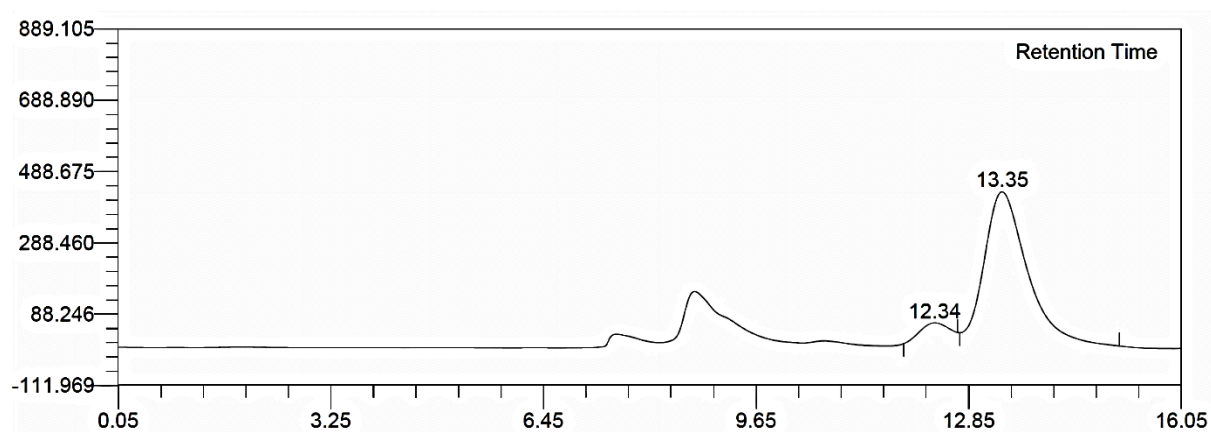


HPLC (Enantiomeric excess (ee) was determined after hydrolysis of acetate)

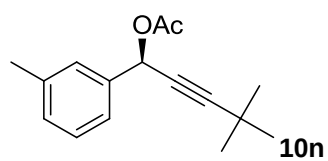
(±)- 10m



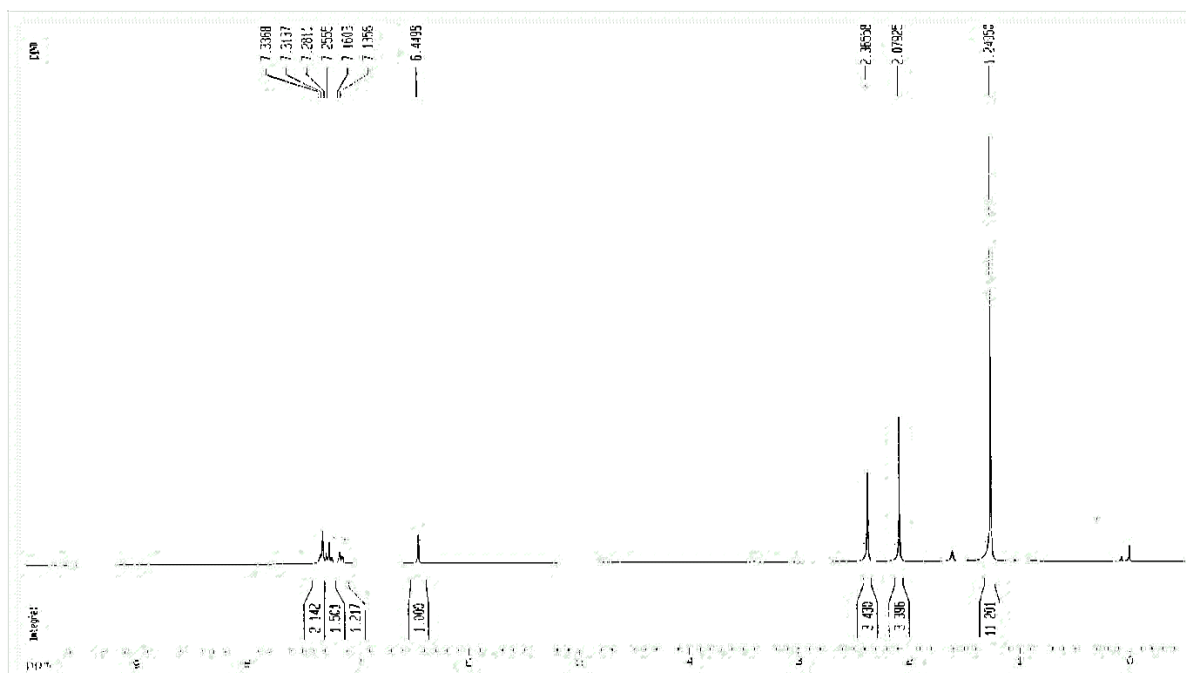
(+)-10m



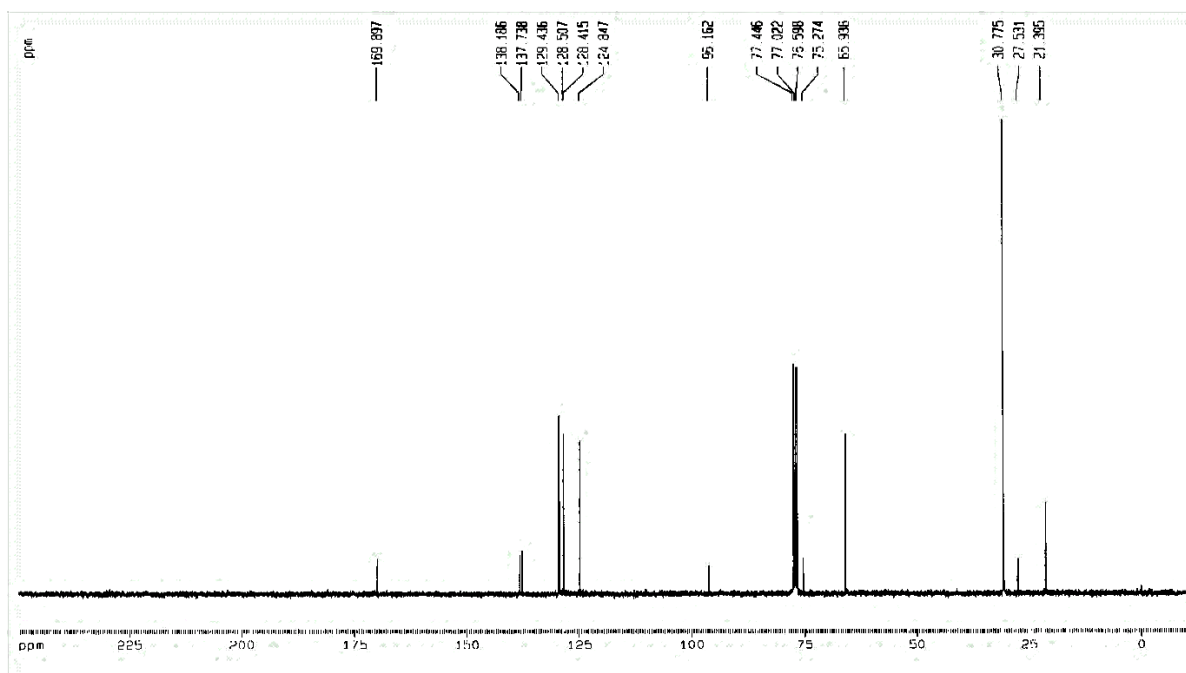
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	12.338	0.354	21513418	40229	5.93460	9.02663	tep-BB
2	13.353	0.621	340995071	405441	94.06540	90.97337	tep-BB



¹H-NMR

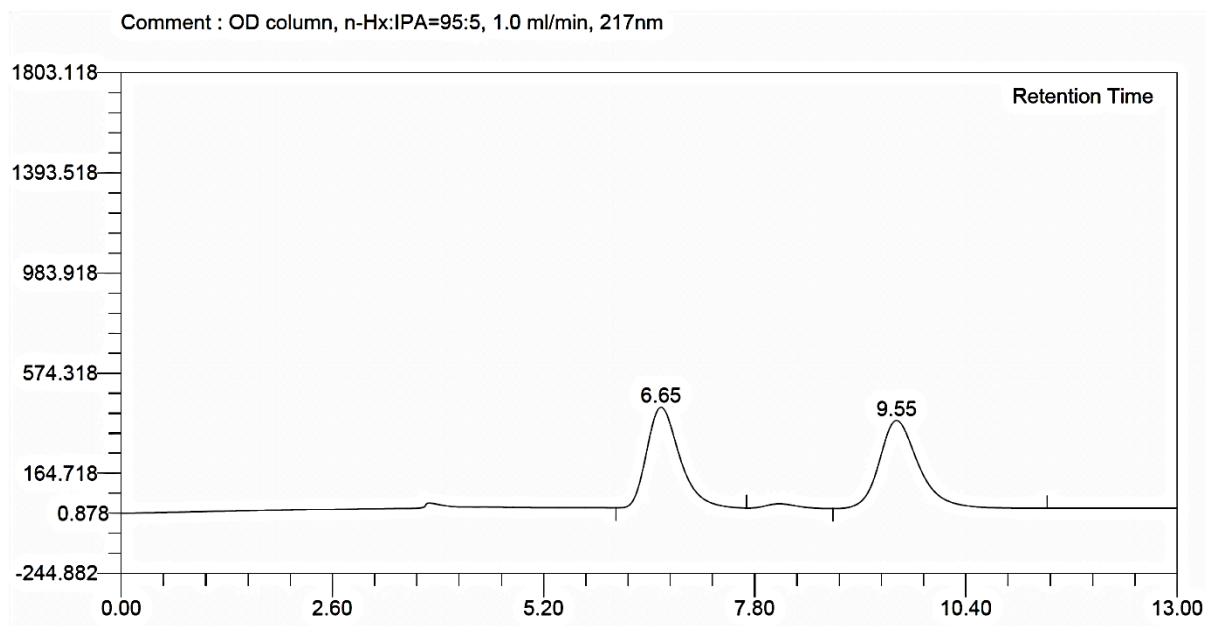


¹³C-NMR

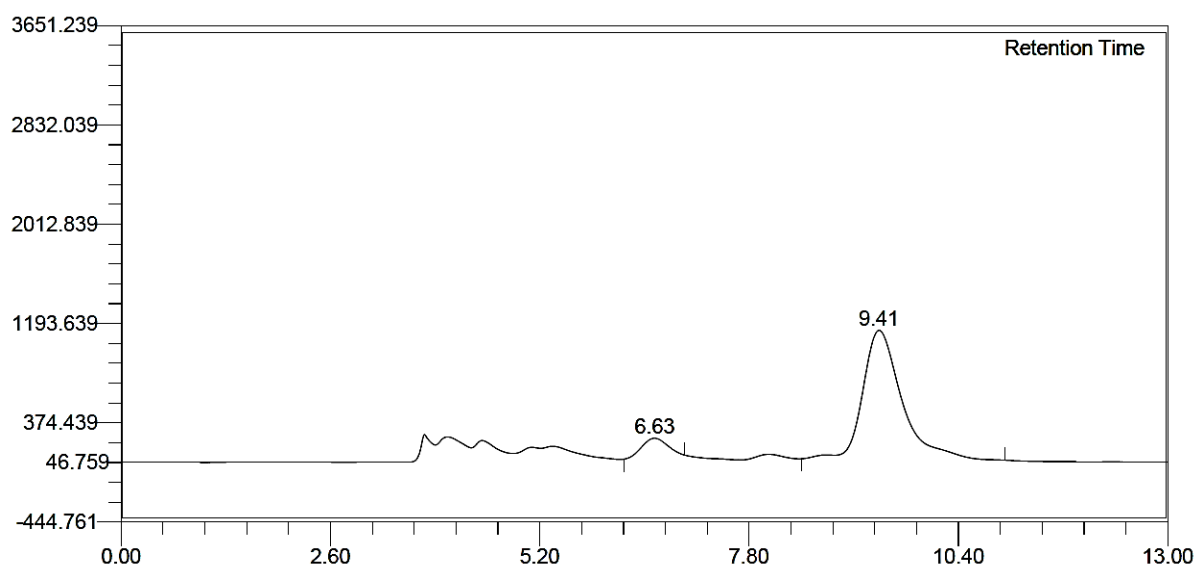


HPLC (Enantiomeric excess (ee) was determined after hydrolysis of acetate)

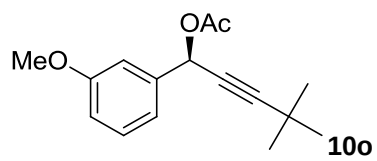
(±)- **10n**



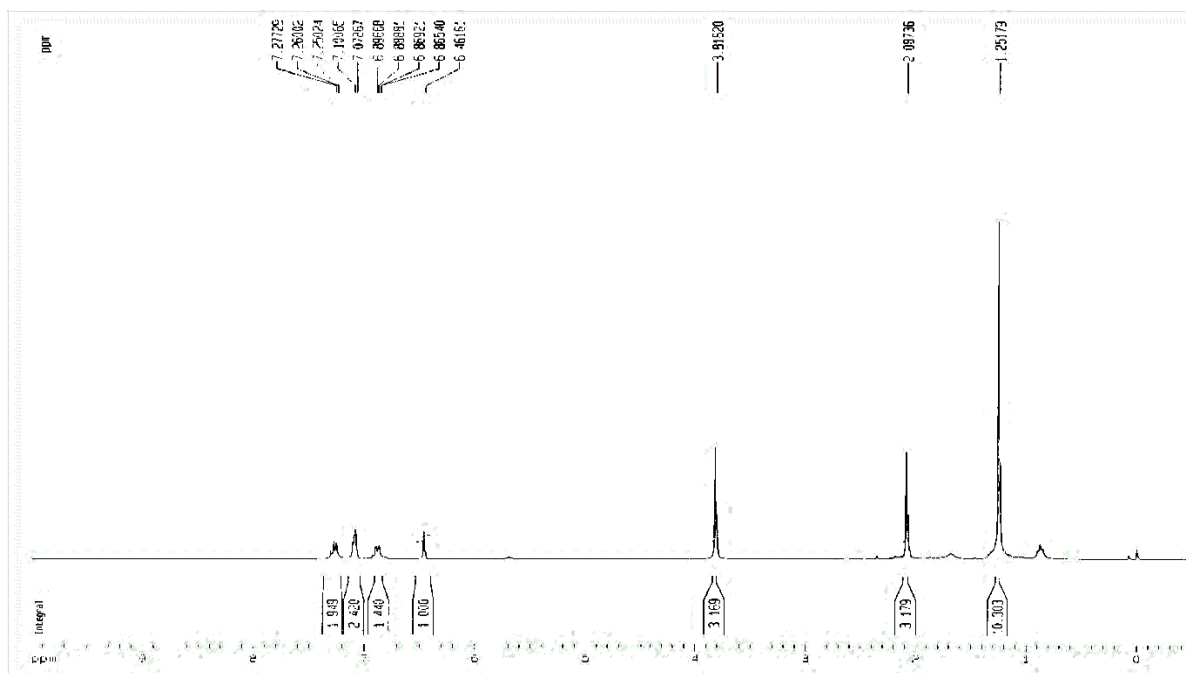
(+)-**10n**



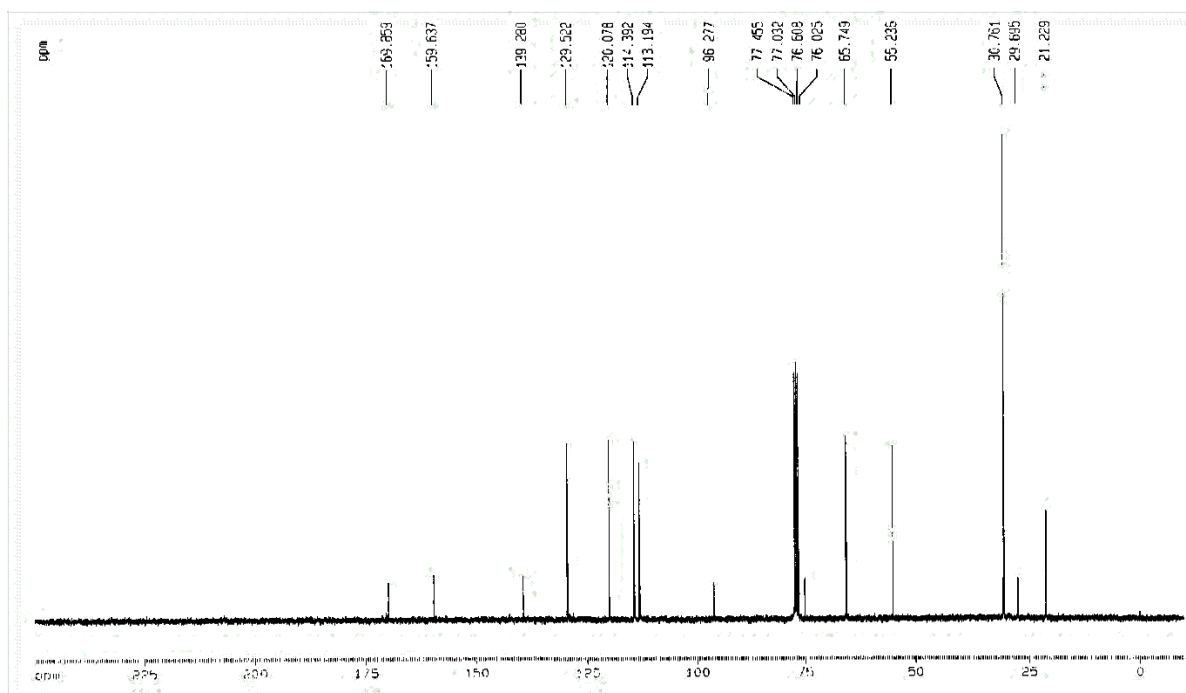
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.628	0.337	68635038	155649	8.71951	12.75890	tep-BB
2	9.413	0.474	718507990	1064276	91.28049	87.24110	tep-BB



¹H-NMR

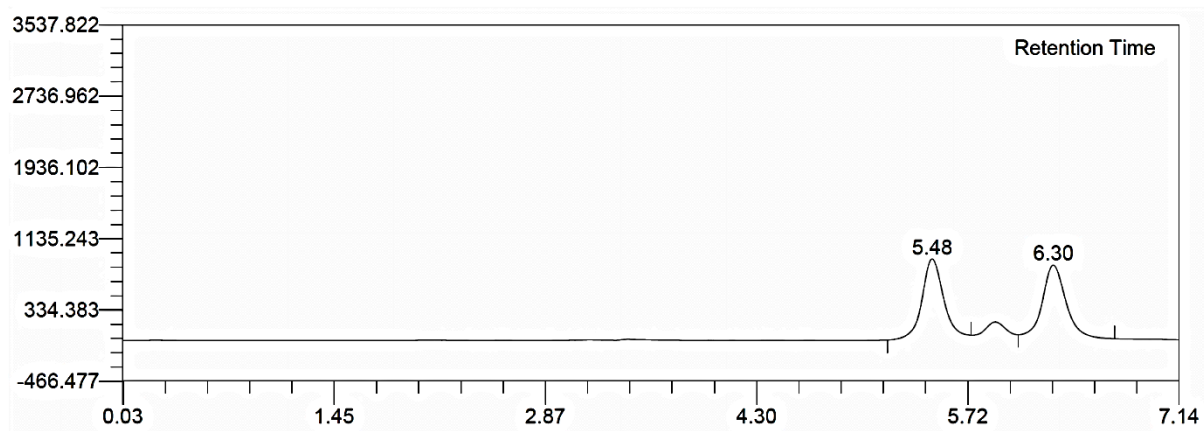


¹³C-NMR

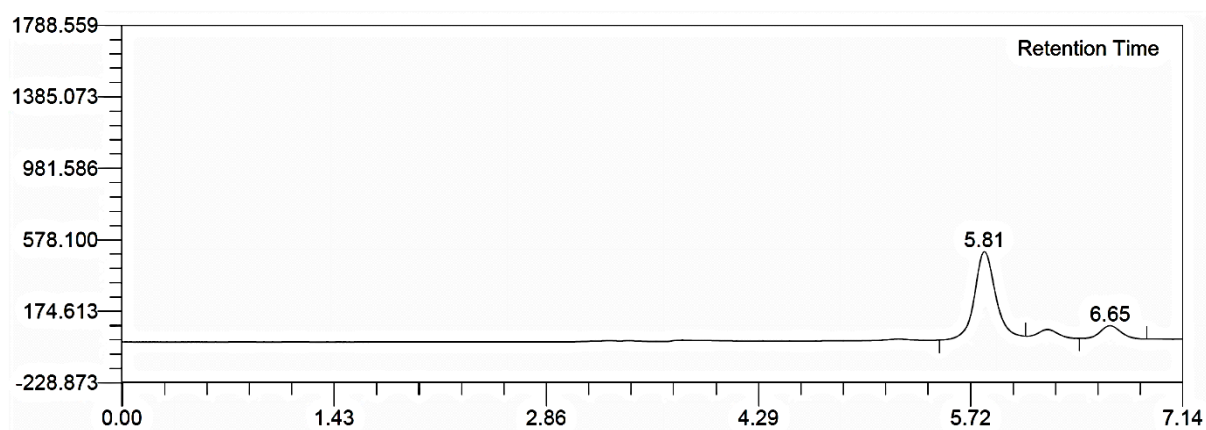


HPLC

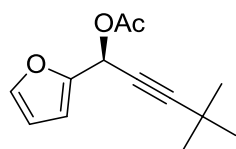
(±)- **10o**



(+)-**10o**

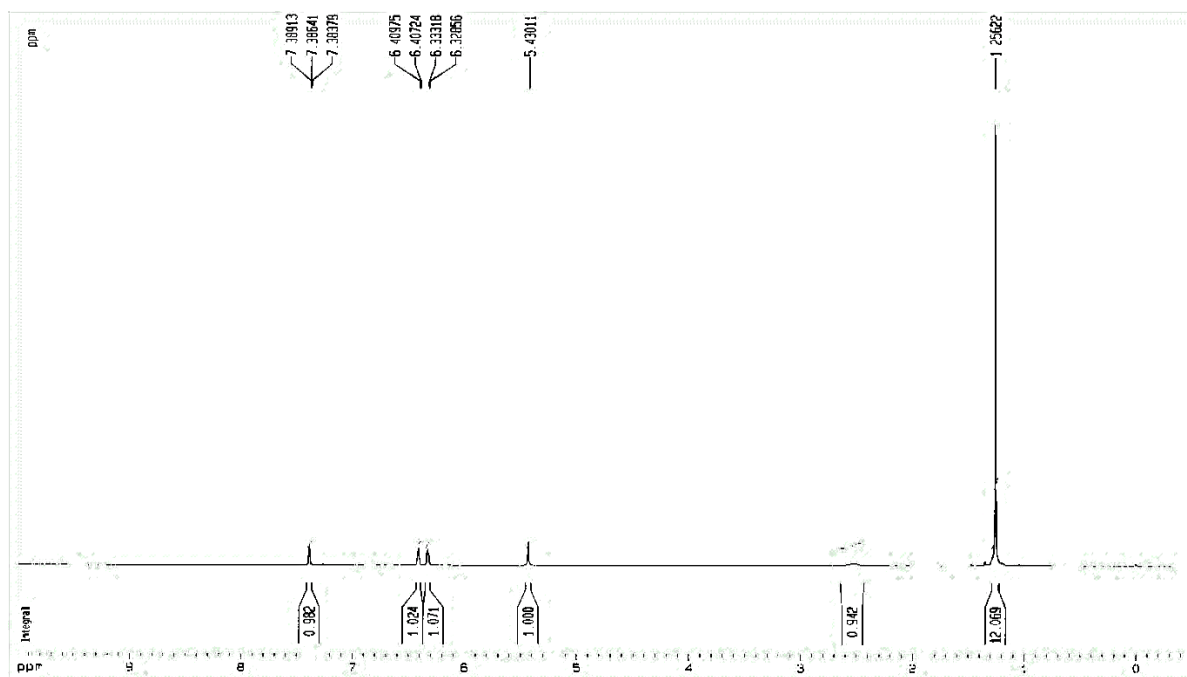


PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	5.808	0.140	93392324	488244	87.03760	86.90445	BB
2	6.654	0.143	13908798	73573	12.96240	13.09555	BB

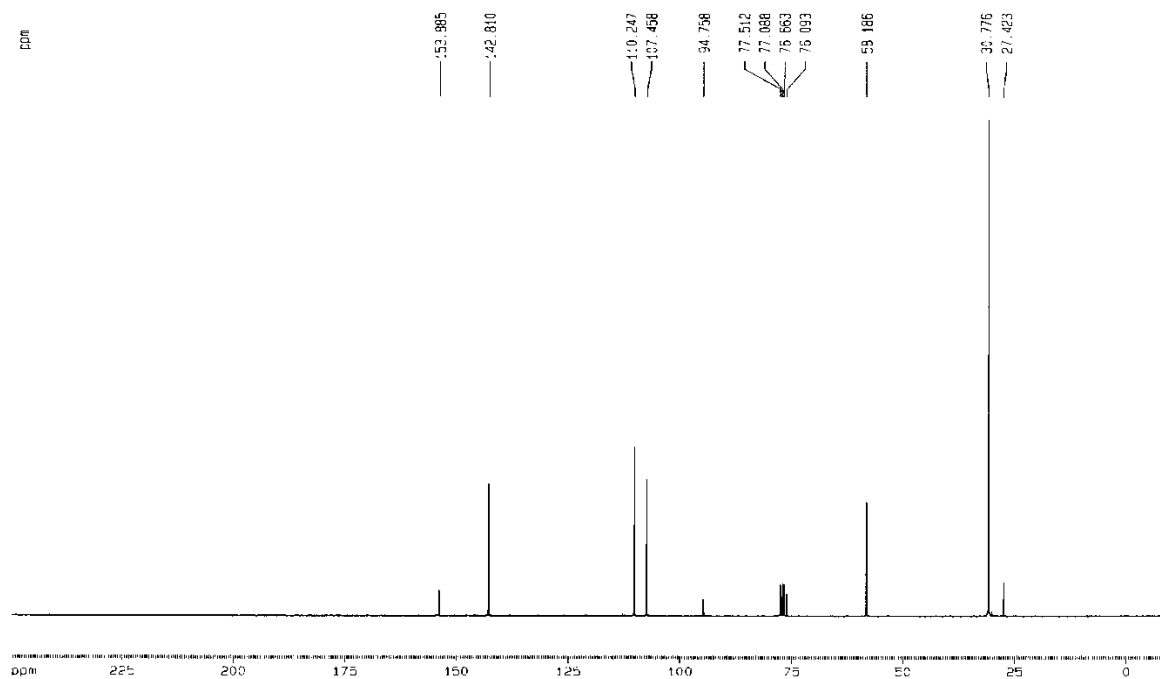


10p (Material analysis was carried out after hydrolysis of acetate.)

¹H-NMR

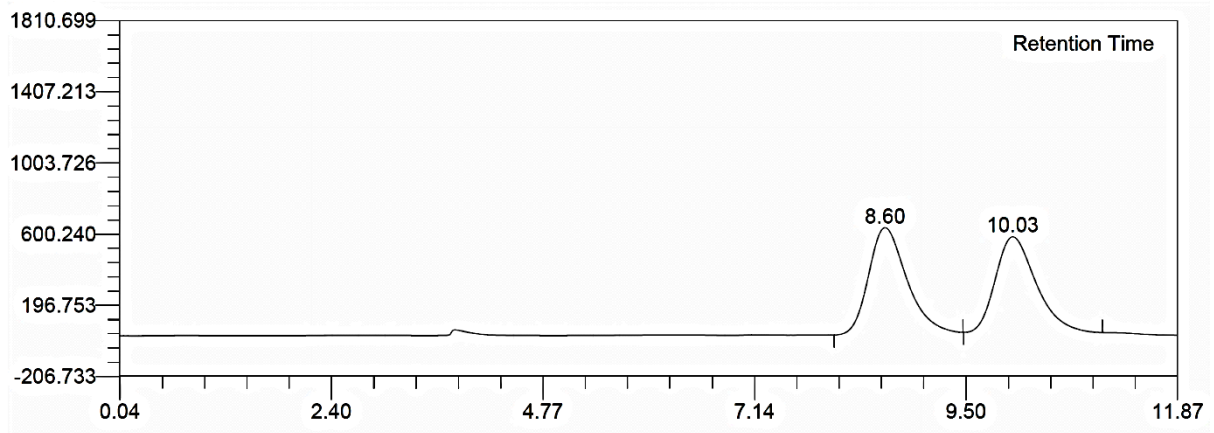


¹³C-NMR

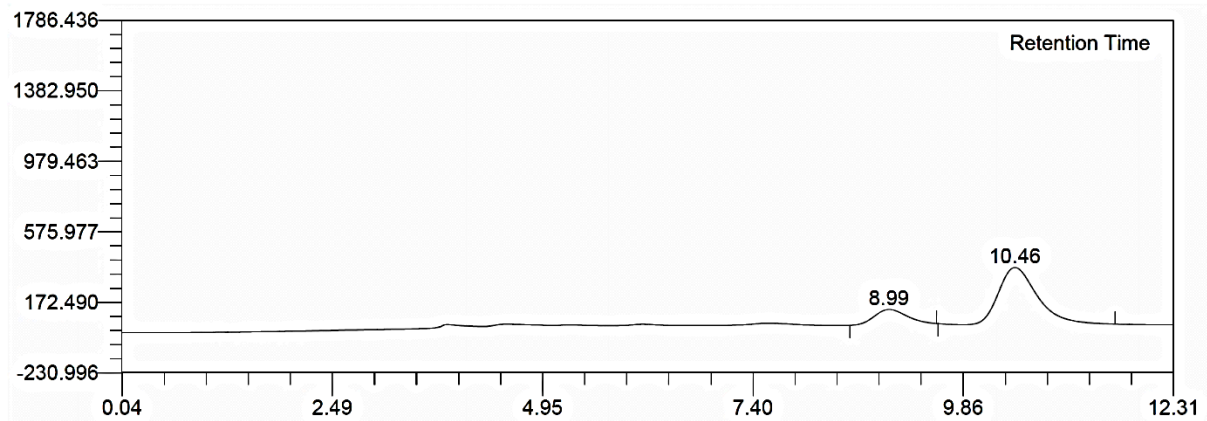


HPLC

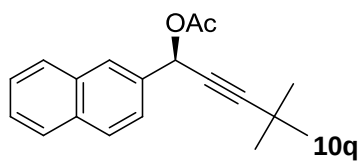
(±)- 10p



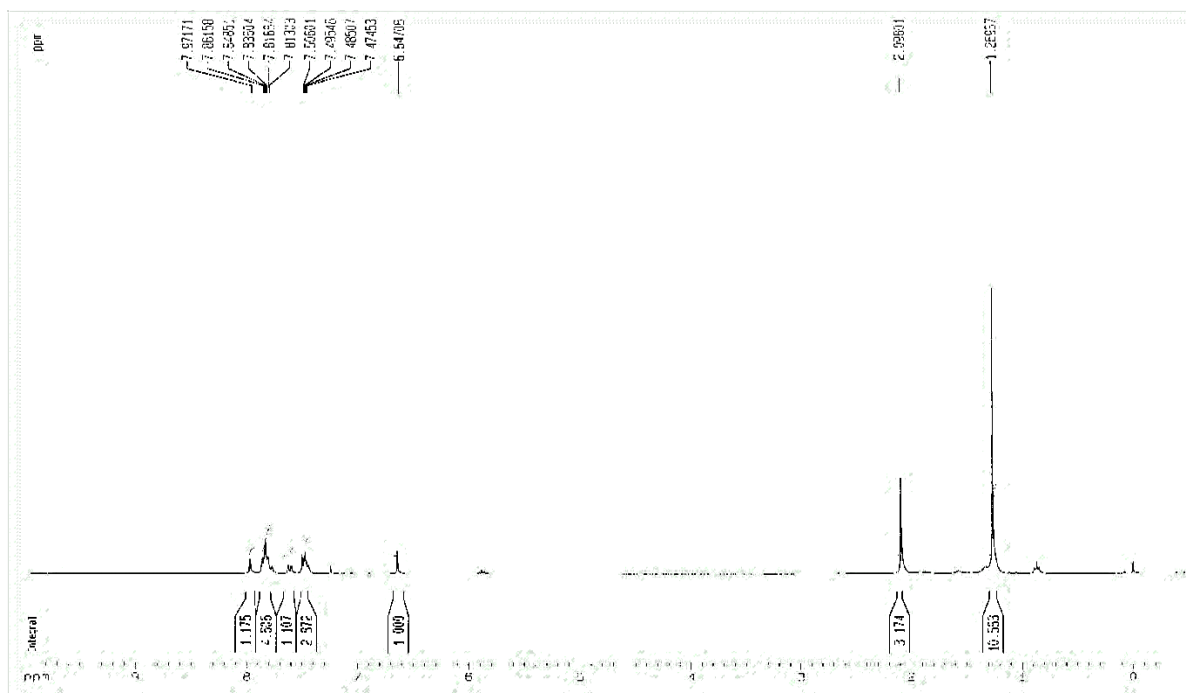
(+)-10p



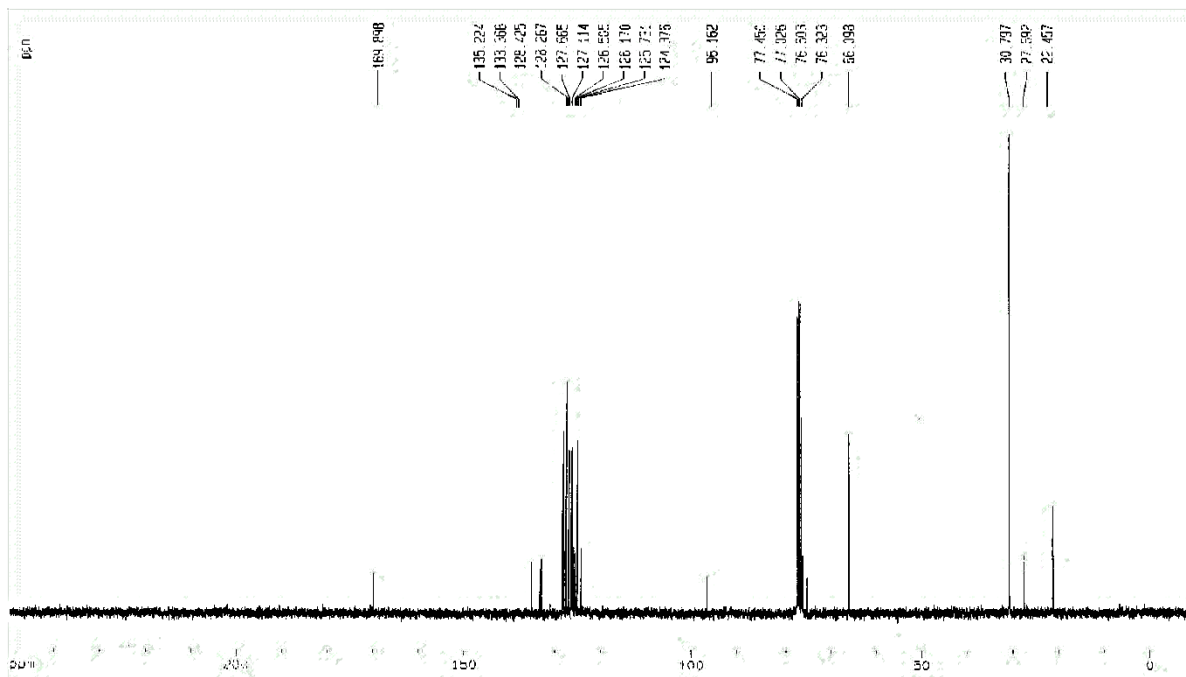
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	8.988	0.396	45011657	86481	18.31162	21.10894	tep-BB
2	10.458	0.467	200797636	323208	81.68838	78.89106	tep-BB



¹H-NMR

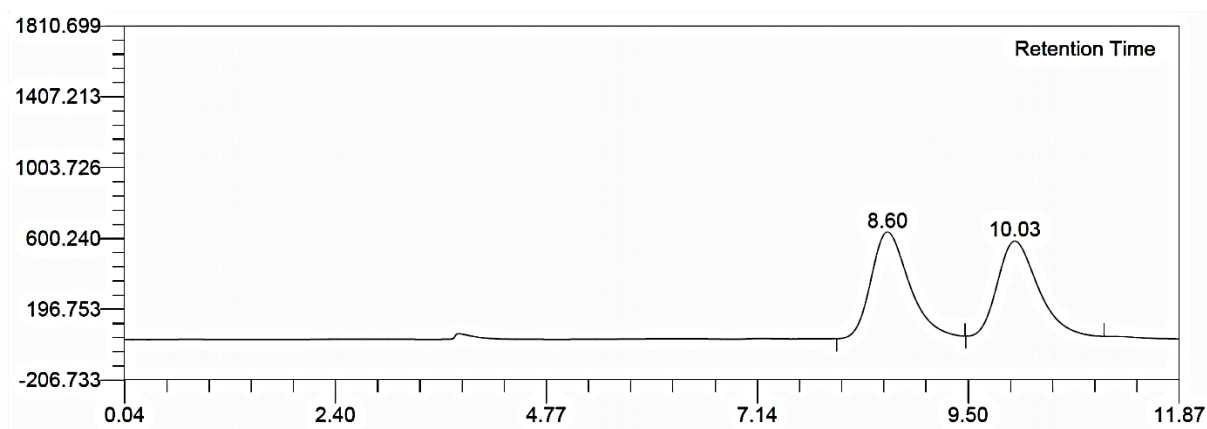


¹³C-NMR

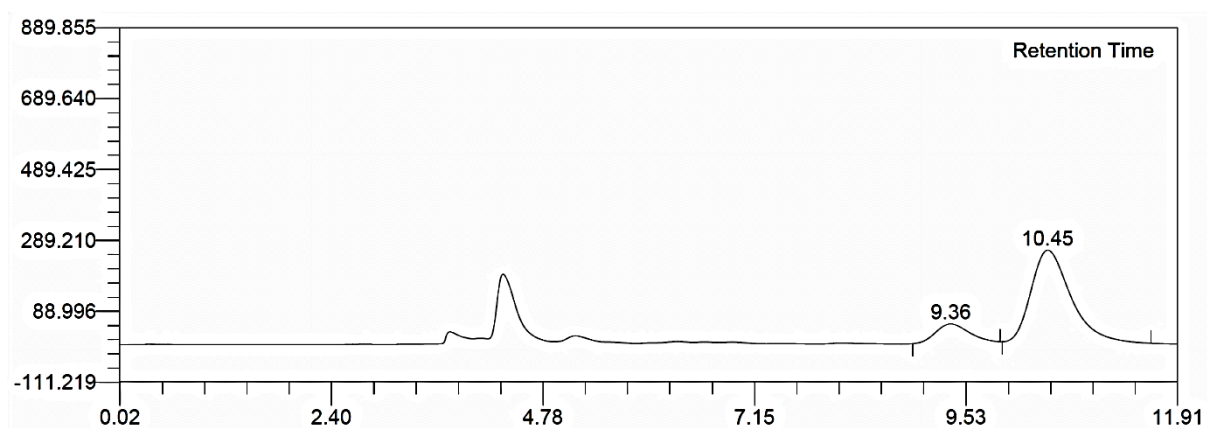


HPLC (Enantiomeric excess (ee) was determined after hydrolysis of acetate)

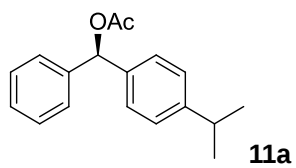
(±)- **10q**



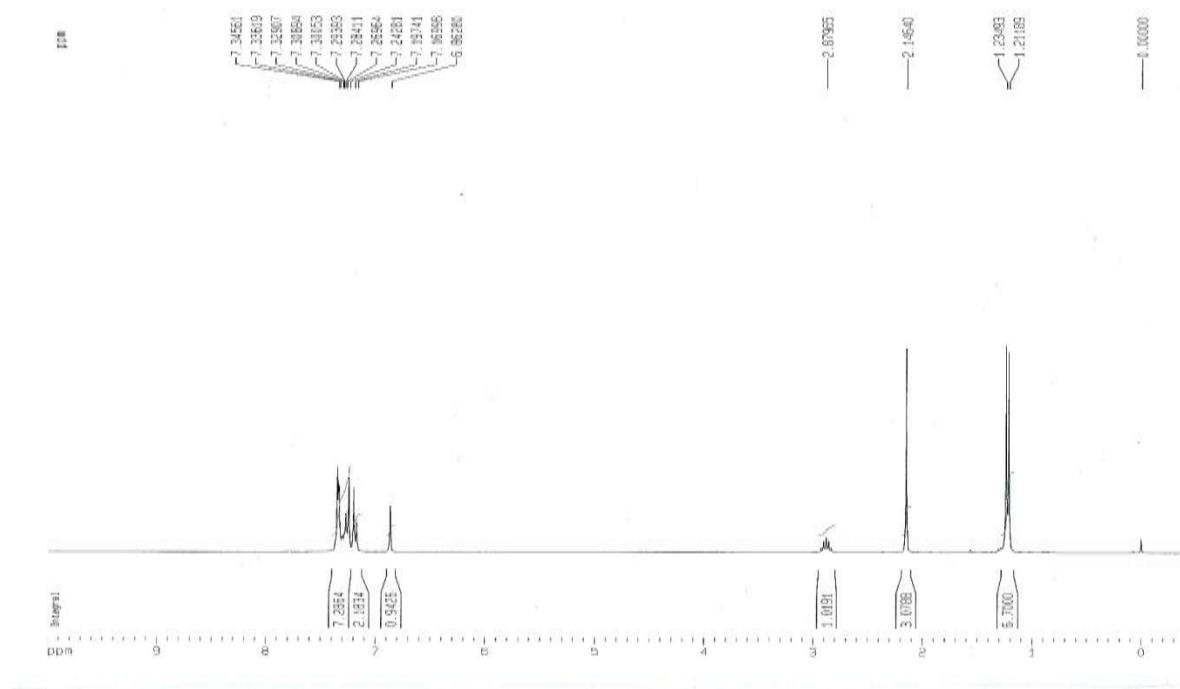
(+)-**10q**



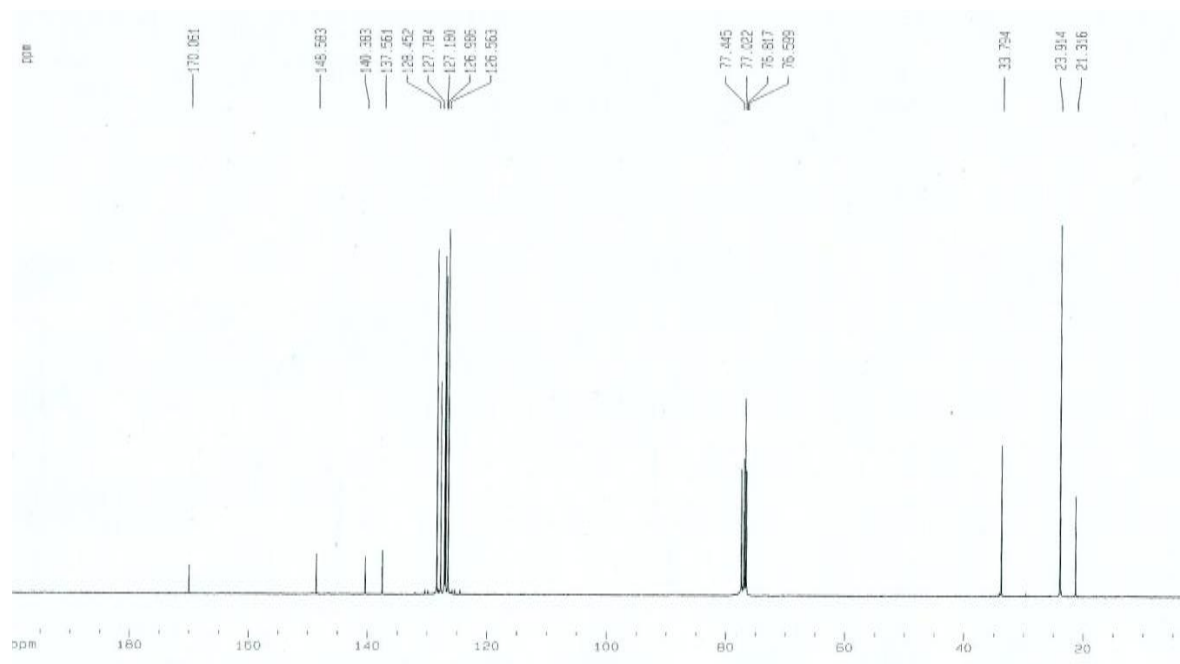
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	9.358	0.393	27327232	53205	14.52477	16.99400	BB
2	10.446	0.463	160815075	259876	85.47523	83.00600	BB



¹H-NMR

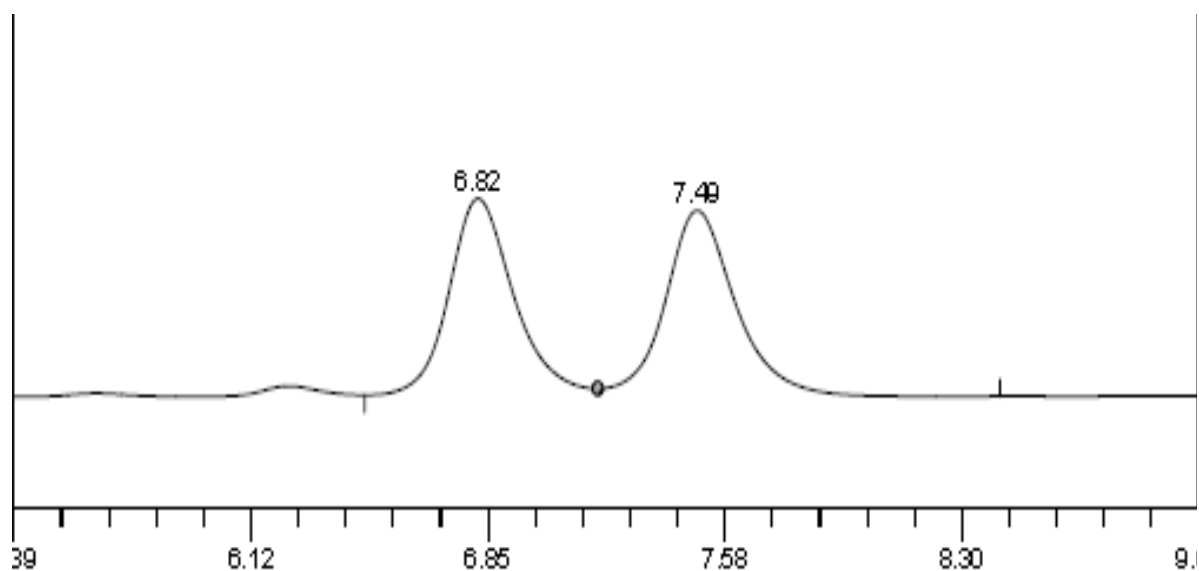


¹³C-NMR

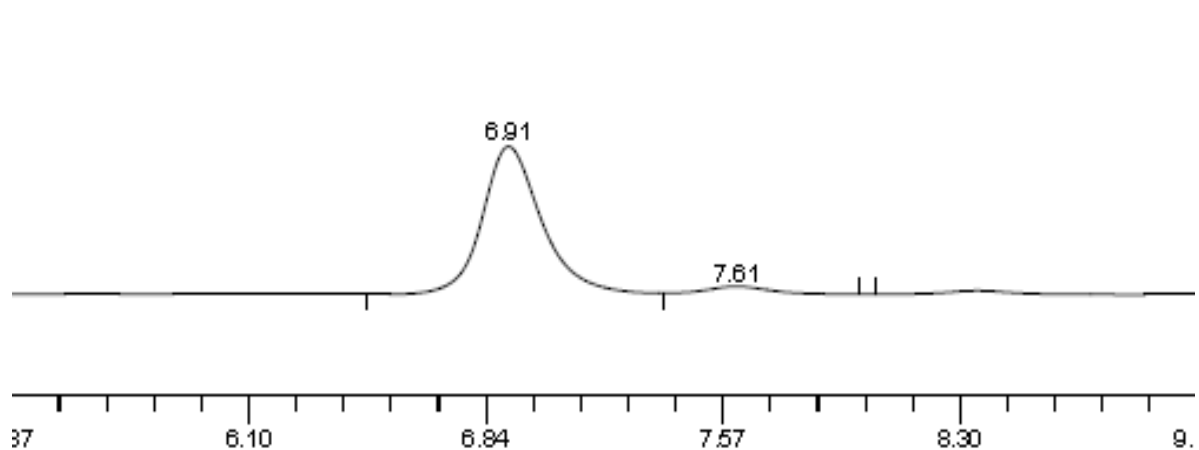


HPLC

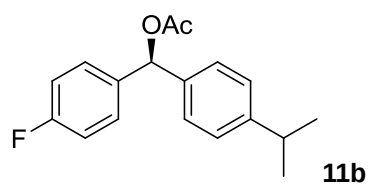
(±)-**11a**



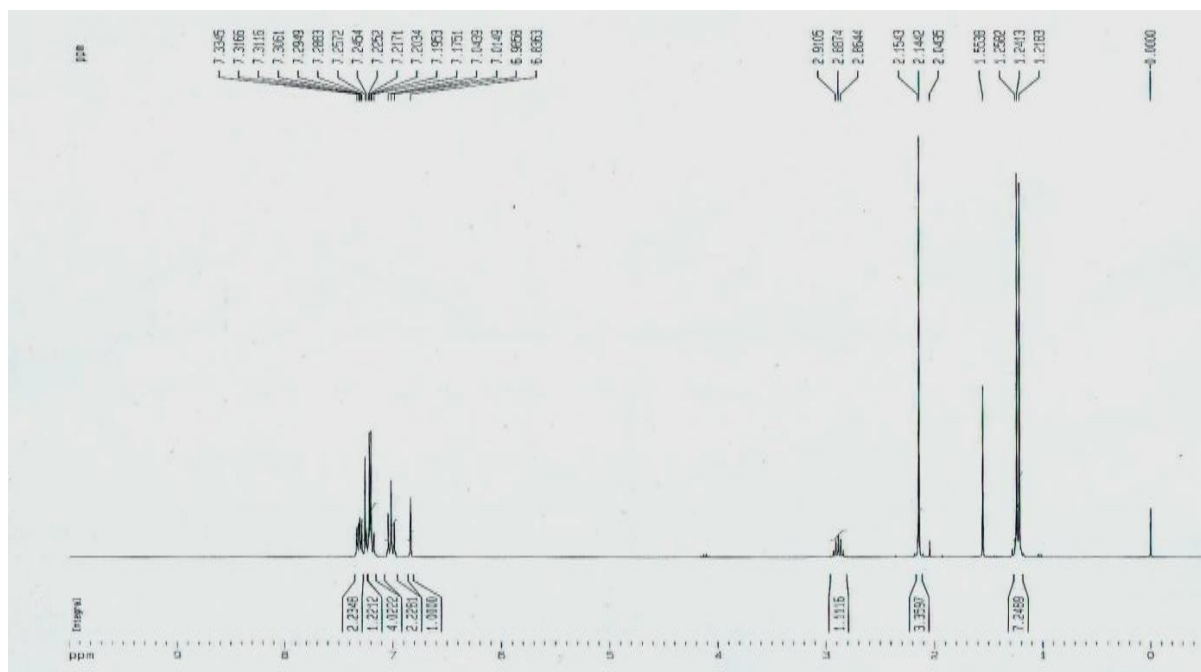
(+)-**11a**



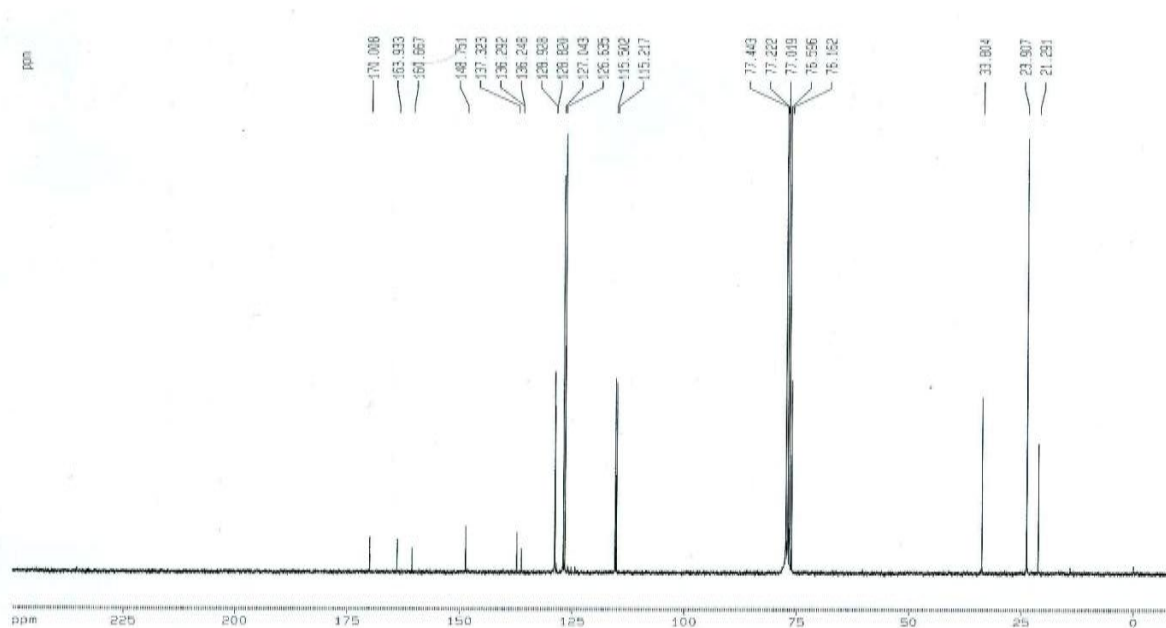
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.905	0.187	177691383	679080	95.67965	95.45403	mBB
2	7.609	0.180	8023530	32341	4.32035	4.54597	tBB



¹H-NMR

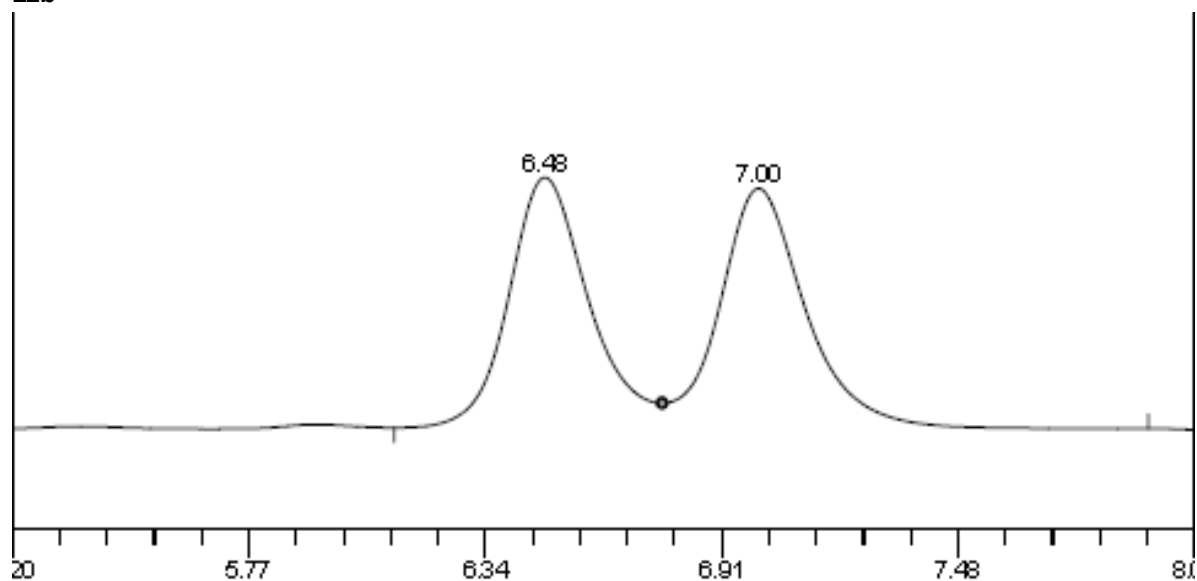


¹³C-NMR

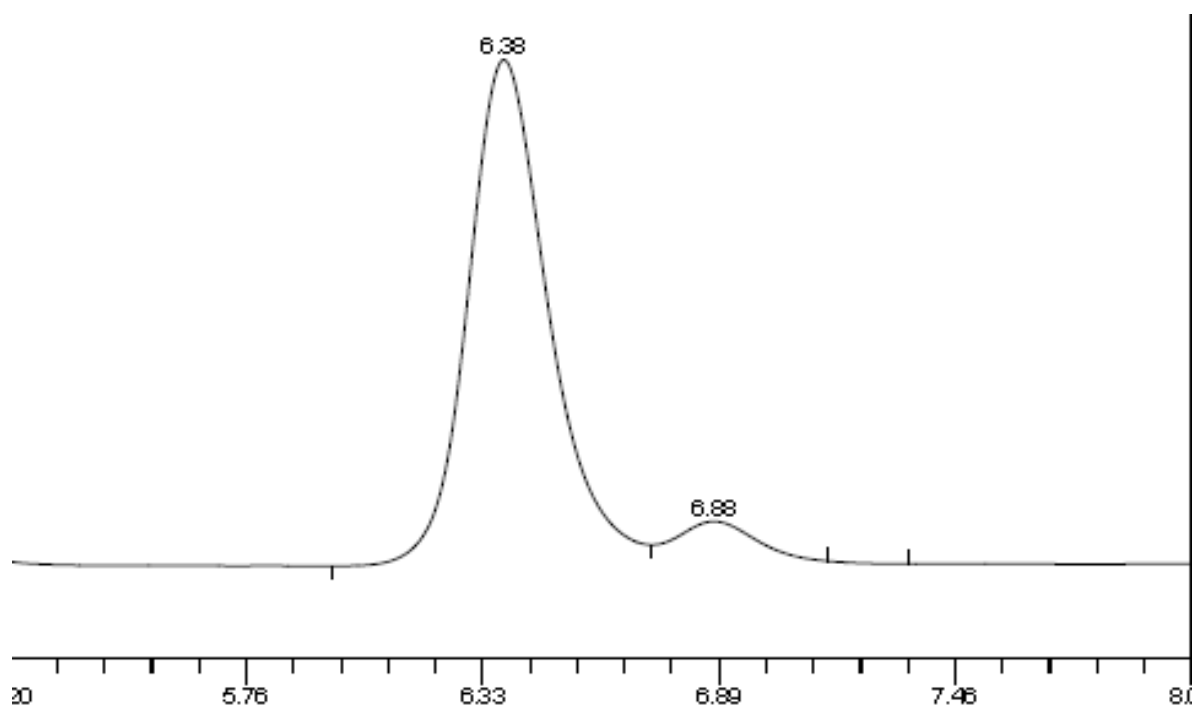


HPLC

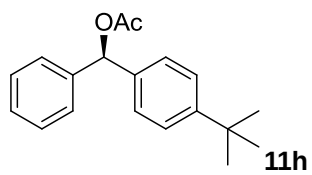
(±)-**11b**



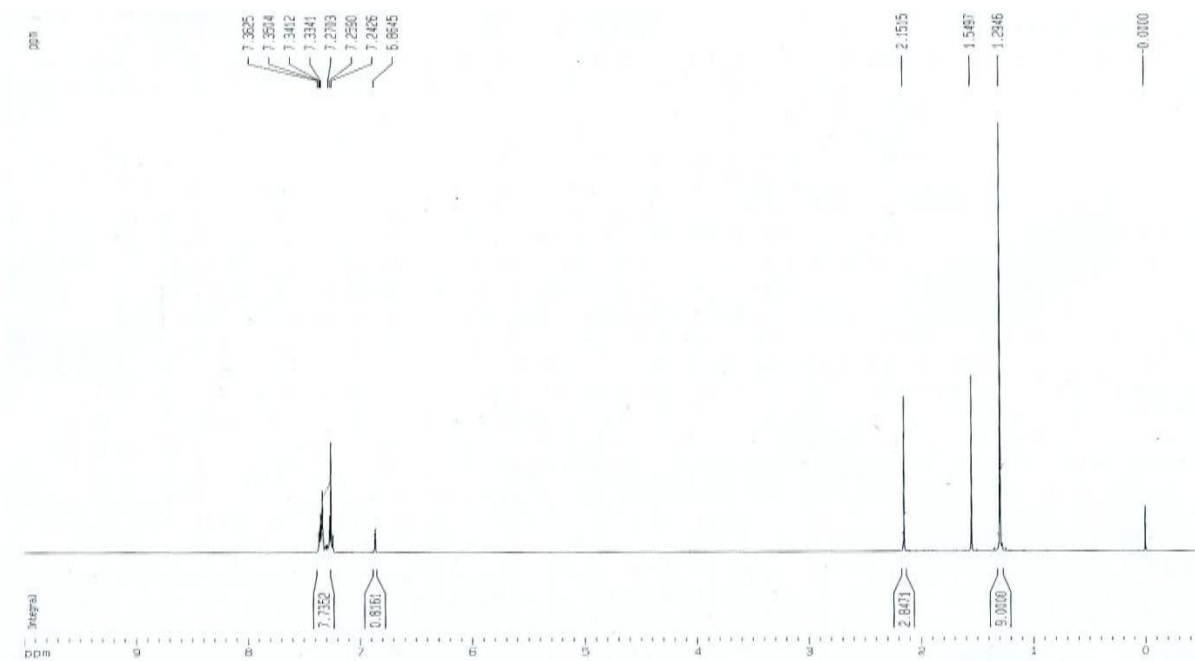
(+)-**11b**



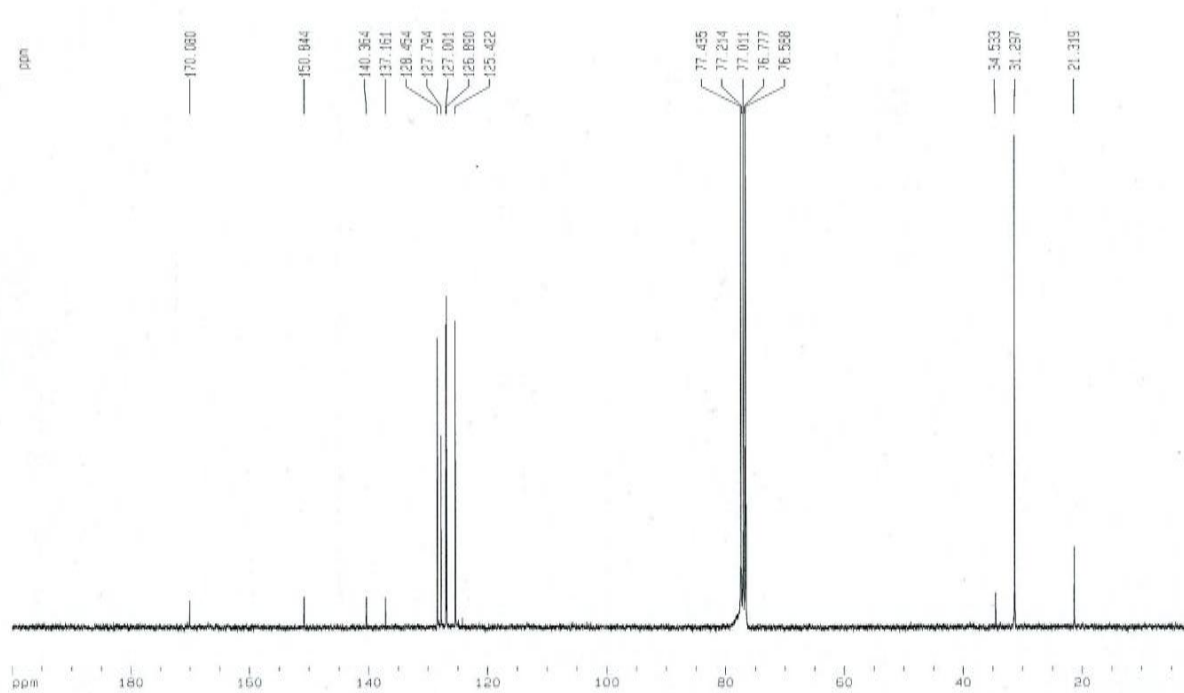
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.380	0.198	306419681	1091655	95.76436	94.55234	mBB
2	6.883	0.147	13552884	62896	4.23564	5.44766	tBB



¹H-NMR

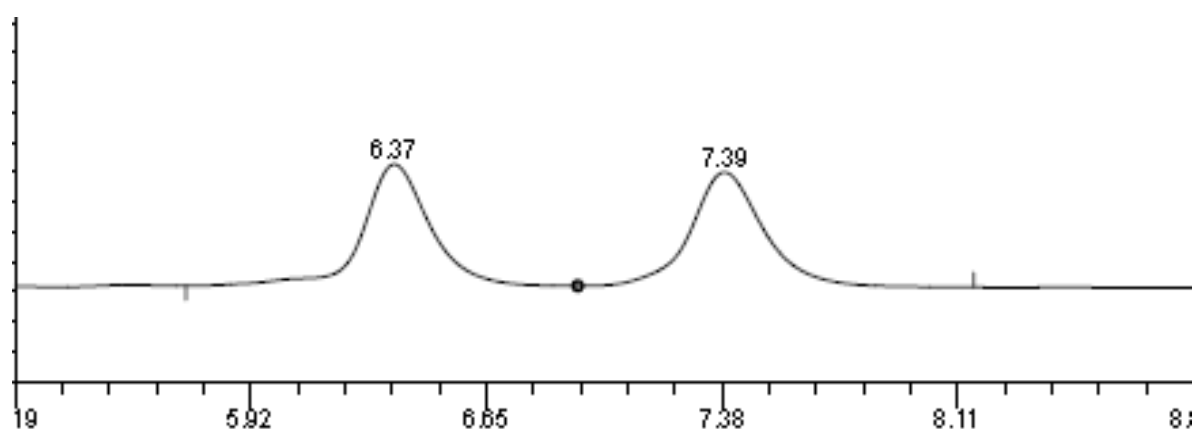


¹³C-NMR

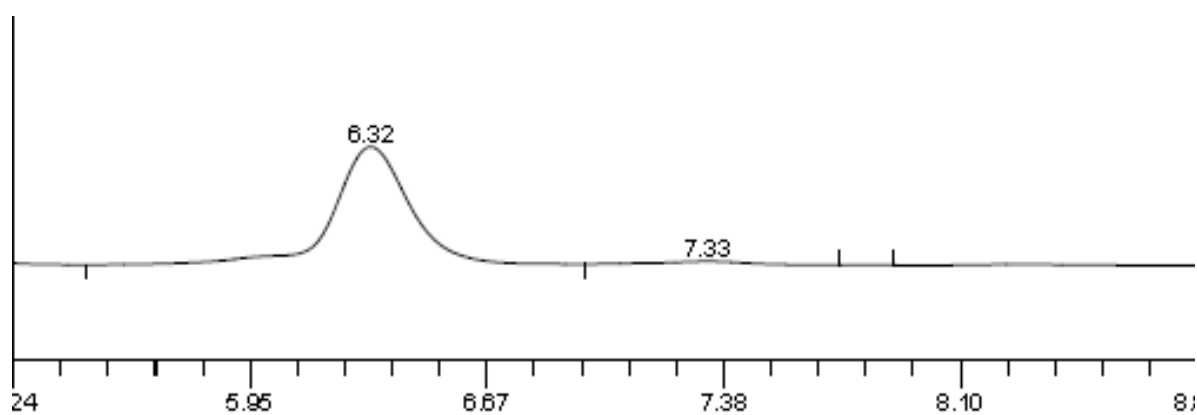


HPLC

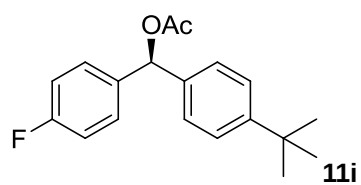
(±)-11h



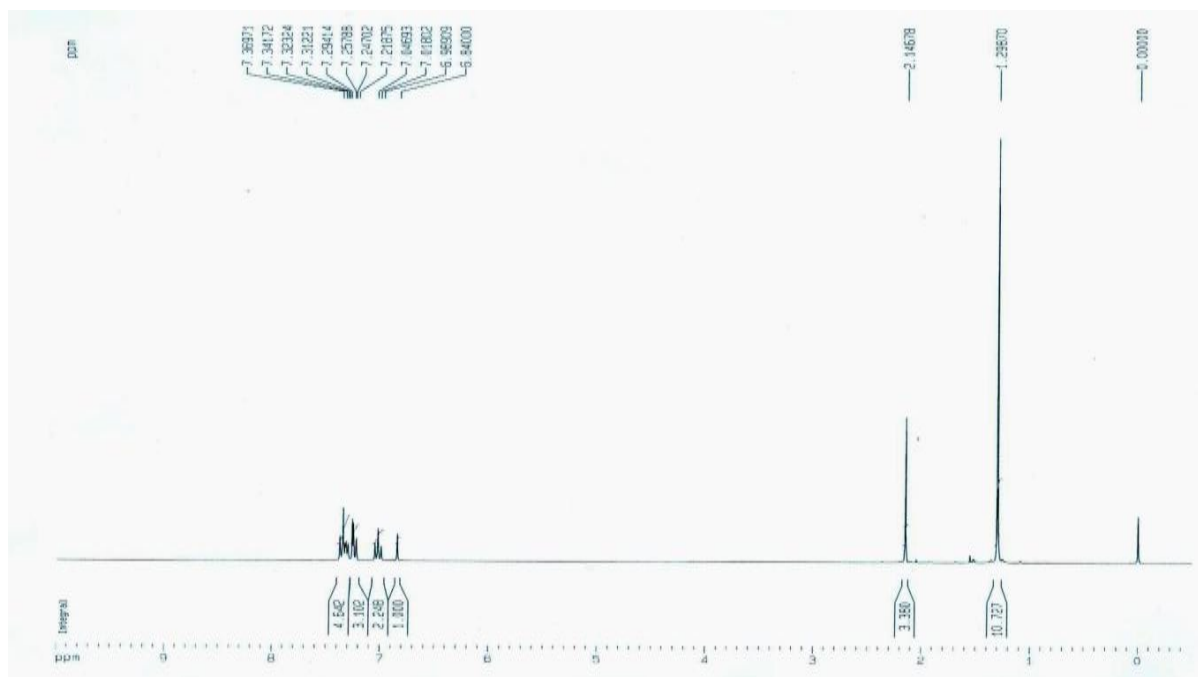
(+)-11h



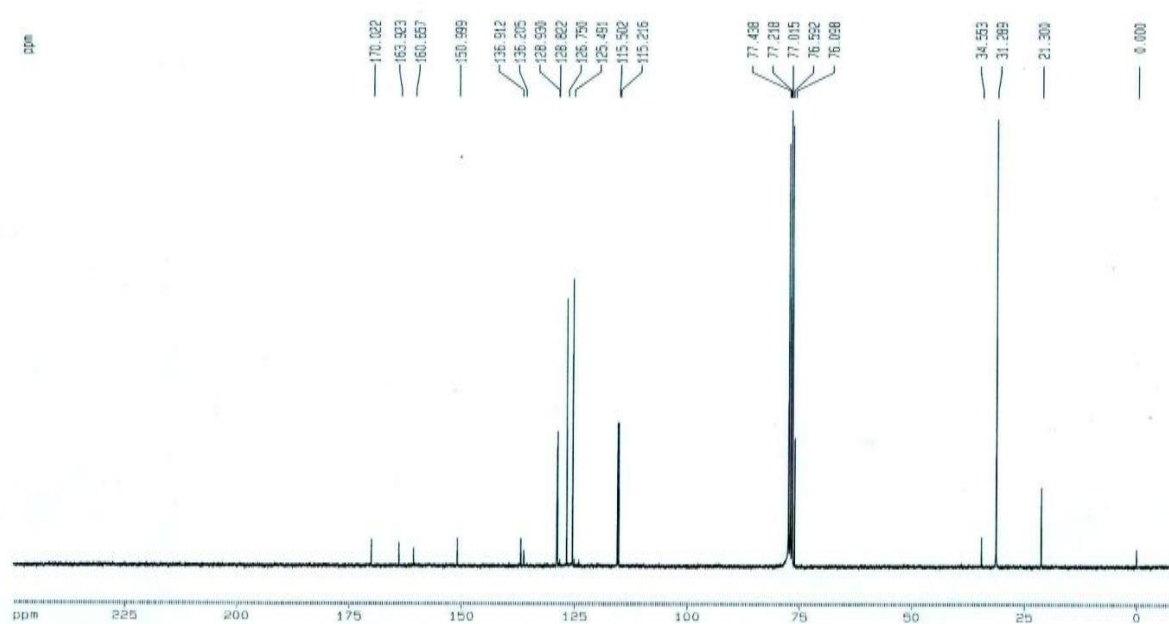
PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.316	0.223	376221723	1146206	97.27774	97.38195	mBB
2	7.332	0.227	10528341	30815	2.72226	2.61805	tBB
Total		0.2(+/-)0.000	386750064	1177021	100.00000	100.00000	



¹H-NMR

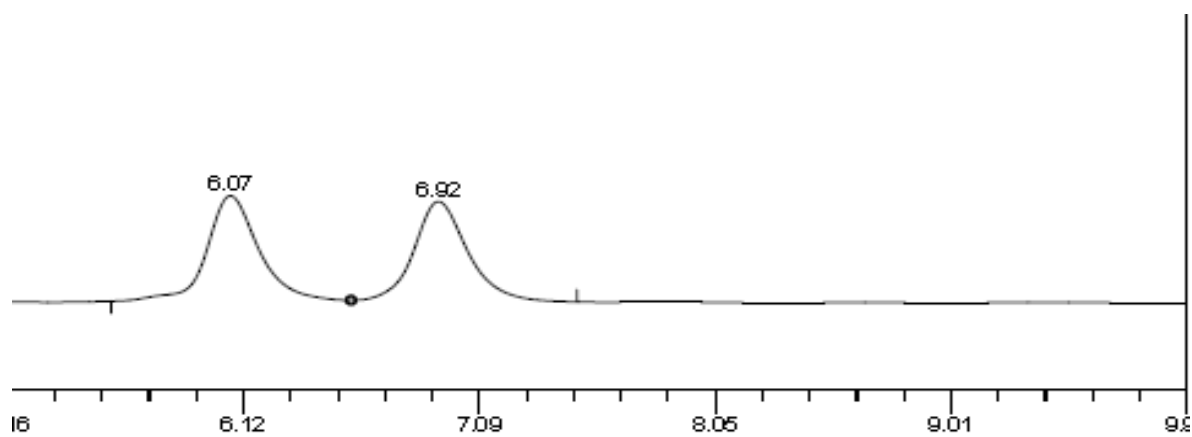


¹³C-NMR

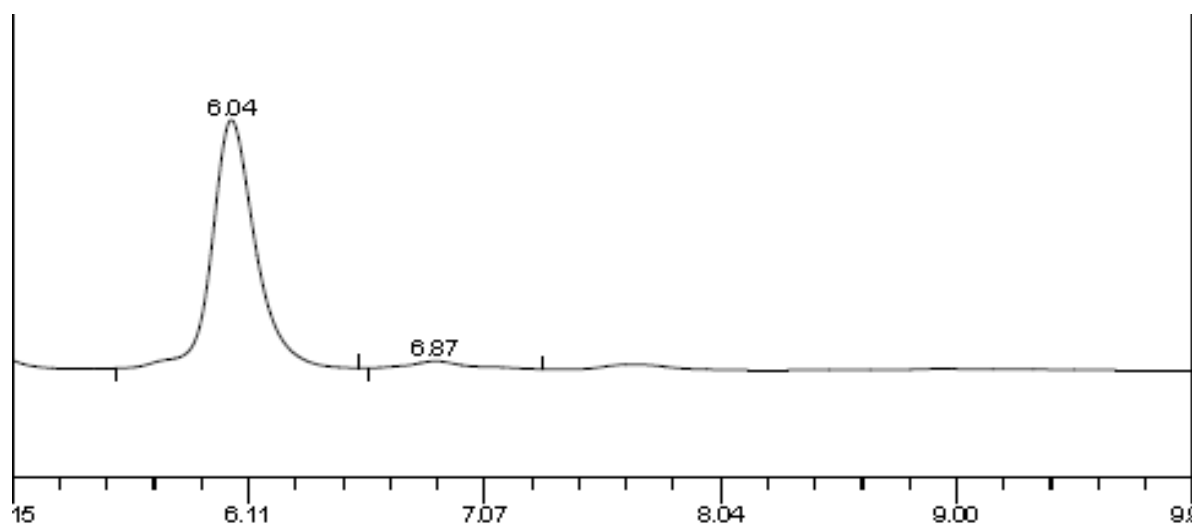


HPLC

(±)-**11i**



(+)-**11i**



PK No.	RT	Peak Width	Area	Height	Area %	Height %	Code
1	6.039	0.177	132104967	533406	96.42283	97.13338	BB
2	6.871	0.191	4900936	15742	3.57717	2.86662	BB