ELECTRONIC SUPPLEMENTARY INFORMATION

Synthesis, Self-Assembly, Bacterial and Fungal Toxicity, and Preliminary Biodegradation Studies of a Series of L-Phenylalanine-Derived Surface Active Ionic Liquids

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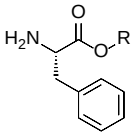
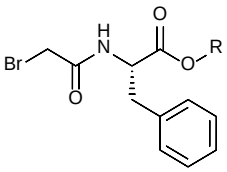
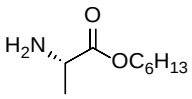
CONTENT

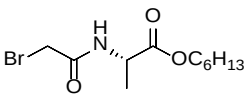
1. Surface active ILs with pyridinium, imidazolium, and cholinium headgroup

R		
C_2H_5-	**1**	**9**
C_4H_9-	**2**	**10**
C_6H_{13}-	**3**	**11**
C_8H_{17}-	**4**	**12**
$C_{10}H_{21}$-	**5**	**13**
$C_{12}H_{25}$-	**6**	**14**
$C_{14}H_{29}$-	**7**	**15**
$C_{16}H_{33}$-	**8**	**16**

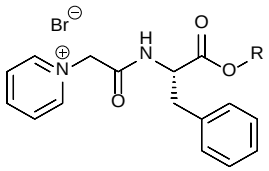
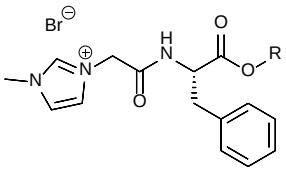
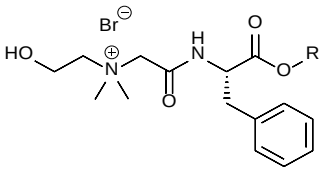
L-Ala derived precursors of ILs



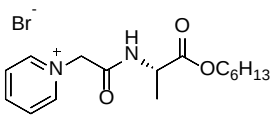
3Ala



11Ala

R			
C_2H_5-	**17**	**25**	**33**
C_4H_9-	**18**	**26**	**34**
C_6H_{13}-	**19**	**27**	**35**
C_8H_{17}-	**20**	**28**	**36**
$C_{10}H_{21}$-	**21**	**29**	**37**
$C_{12}H_{25}$-	**22**	**30**	**38**
$C_{14}H_{29}$-	**23**	**31**	**39**
$C_{16}H_{33}$-	**24**	**32**	**40**

L-Ala derived ILs



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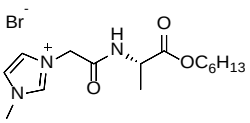

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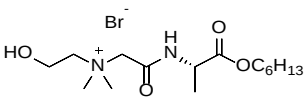
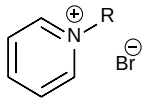
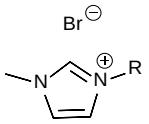


35Ala



C_8PB, R = C_8H_{17}
C_{10}PB, R = $C_{10}H_{21}$
C_{11}PB, R = $C_{11}H_{23}$
C_{12}PB, R = $C_{12}H_{25}$

C_{13}PB, R = $C_{13}H_{27}$
C_{14}PB, R = $C_{14}H_{29}$
C_{15}PB, R = $C_{15}H_{31}$
C_{16}PB, R = $C_{16}H_{33}$



C_{10}MIM, R = $C_{10}H_{21}$
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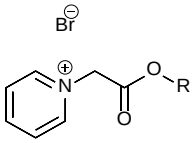
C_{16}MIM, R = $C_{16}H_{33}$



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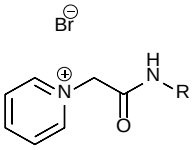
43, R = $C_{10}H_{21}$
44, R = $C_{12}H_{25}$
45, R = $C_{14}H_{29}$



46, R = C_6H_{13}
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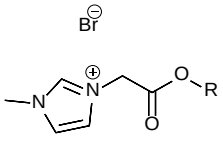
48, R = $C_{10}H_{21}$
49, R = $C_{12}H_{25}$
50, R = $C_{14}H_{29}$



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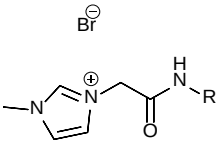
54, R = $C_{12}H_{25}$
55, R = $C_{14}H_{29}$



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58, R = $C_{10}H_{21}$
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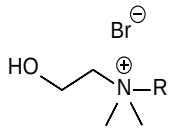
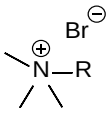
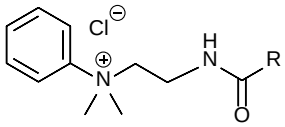
60, R = $C_{14}H_{29}$



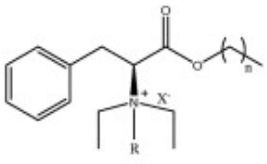
DHDABr, R = $C_{12}H_{25}$
THDABr, R = $C_{14}H_{29}$
CHDABr, R = $C_{16}H_{33}$



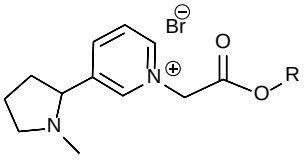
DTABr, R = $C_{12}H_{25}$
TTABr, R = $C_{14}H_{29}$
CTABr, R = $C_{16}H_{33}$



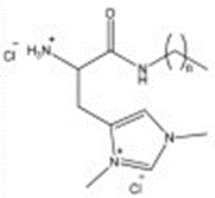
DecABzDACl, R = $C_{10}H_{21}$
DABzDACl, R = $C_{12}H_{25}$
TABzDACl, R = $C_{14}H_{29}$
CABzDACl, R = $C_{16}H_{33}$



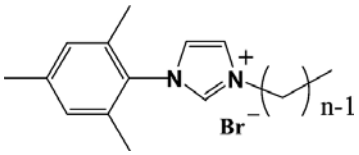
MeEtEtPhe-ODec, R = $C_{12}H_{25}$
MeEtEtPhe-ODod, R = $C_{12}H_{25}$
MeEtEtPhe-OTetr, R = $C_{14}H_{29}$
MeEtEtPhe-OCet, R = $C_{16}H_{33}$



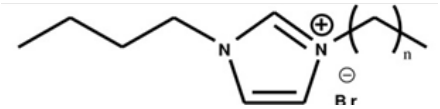
C_8-ENic, R = C_8H_{17},
C_{10}-ENic, R = $C_{10}H_{21}$
C_{12}-ENic, R = $C_{12}H_{25}$



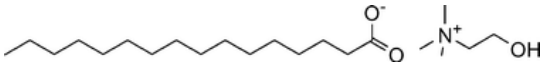
C_{10}-His, R = $C_{10}H_{21}$
C_{12}-His, R = $C_{12}H_{25}$
C_{14}-His, R = $C_{14}H_{29}$
C_{16}-His, R = $C_{16}H_{33}$



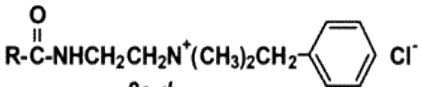
Dod-PIM, R = $C_{12}H_{25}$
Tetr-PIM, R = $C_{14}H_{29}$
Cet-PIM, R = $C_{16}H_{33}$



C_4-BIm, R = C_4
C_8-BIm, R = C_8
C_{12}-BIm, R = C_{12}



Chol-C_{12}
Chol-C_{14}
Chol-C_{16}



C_{10}-BzDACl, R = $C_{10}H_{21}$
C_{12}-BzDACl, R = $C_{12}H_{25}$
C_{14}-BzDACl, R = $C_{14}H_{29}$
C_{16}-BzDACl, R = $C_{16}H_{33}$

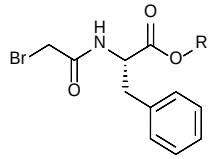
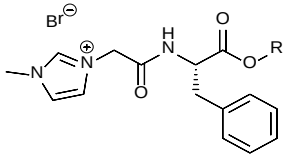
2. Table S1. CMC values for pyridinium, imidazolium, and cholinium surface active ILs (literature)

IL	Chain Length	CMC (mM)	Refs
		Pyridinium head group	
C_8PB	8	180 (C); 190 (ST)	1
C_{10}PB	10	44 (C); 30 (C); 48 (ST)	1; 2
C_{11}PB	11	21 (C)	2
C_{12}PB	12	10; 9.3 (C); 12 (ST); 10 (F)	1; 2
C_{13}PB	13	5.3 (C)	
C_{14}PB	14	2.2; 1.9 (C); 2.8 (ST); 2.4 (F)	2
C_{15}PB	15	1.3 (C)	1; 2
C_{16}PB	16	0.64 (C)	2
41	6	200 (C); 190 (ST);	2
42	8	73 (C); 60 (ST); 70 (F)	3
43	10	17 (C); 14 (ST); 14 (F)	3
44	12	4.1 (C); 3.4 (ST); 3.4 (F)	3
45	14	0.94 (C); 0.90 (ST); 1.0 (F)	3
46	6	262 (C)	3
47	8	73 (C); 70 (ST);	4
48	10	18 (C); 12 (ST); 18 (F)	4
49	12	4.6 (C); 4.8 (ST); 3.6 (F)	4
50	14	1.2 (C); 1.0 (ST); 1.1 (F)	4
C_8-ENic	8	55.0	4
C_8-ENic	10	16.6	5
C_8-ENic	12	8.70	5
			5
		Imidazolium head group	
C_{10}MIM	10	41 (C)	6
C_{12}MIM	12	9.8 (C); 9.53 (C)	6; 7
C_{14}MIM	14	2.5 (C); 2.61 (C)	6; 7
C_{16}MIM	16	0.61 (C); 0.653 (C)	6; 7
51	6	195 (C); 90 (ST)	3
52	8	73 (C); 43 (ST); 74 (F)	3
53	10	17 (C); 12 (ST); 16 (F)	3
54	12	3.8 (C); 2.5 (ST); 3.8 (F)	3
55	14	0.94 (C); 0.90 (ST); 1.0 (F)	3
56	6	278 (C)	4
57	8	77 (C); 65 (ST); 80 (F)	4
58	10	19 (C); 16 (ST); 15 (F)	4
59	12	5.2 (C); 5.5 (ST); 6.0 (F)	4
60	10	1.2 (C); 0.95 (ST); 1.2 (F)	4
C_{10}-His	10	15.5	8
C_{12}-His	12	6.20	8
C_{14}-His	14	1.50	8
C_{14}-His	16	0.40	8

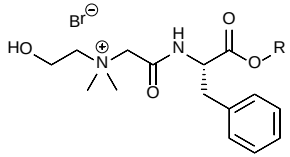
Dod-PIM	12	9.30	[9]
Tetr-PIM	14	2.60	[9]
Cet-PIM	16	0.560	[9]
C_4-Bim	4	280	[10]
C_8-BIm	8	75.80	[10]
C_{12}-BIm	12	5.30	[10]
		Cholinium head group	
DHDAB	12	13.20 (ITC)	[11]
THDABr	14	3.32 (ITC)	[11]
CHDABr	16	0.797 (ITC)	[11]
Chol-C_{12}	12	25.5	[12]
Chol-C_{14}	14	6.40	[12]
Chol-C_{16}	16	1.80	[12]
		Tetraalkylammonium head group	
DecTABr	10	66.3 (ST)	[13]
DTABr	12	14.8 (ST)	[13]
TTABr	14	4.08 (ST)	[13]
CTABr	16	0.93 (ST)	[13]
DecABzDACl	10	24 (C)	[14]
DecABzDACl	12	5.9 (C)	[14]
DecABzDACl	14	1.41 (C)	[14]
DecABzDACl	16	0.35 (C)	[14]
MeEtEtPhe-ODec	10	0.455	[15]
MeEtEtPhe-ODec	12	0.0741	[15]
MeEtEtPhe-ODec	14	0.00566	[15]
MeEtEtPhe-ODec	16	0.00196	[15]
C_{10}-BzDACl	10	21.80	[14]
C_{10}-BzDACl	12	5.85	[14]
C_{10}-BzDACl	14	1.41	[14]
C_{10}-BzDACl	16	0.35	[14]

[a] Obtained from conductivity (C), surface tension (ST), fluorescence (F), and isothermal titration calorimetry (ISC) measurements;

3. Table S2. Green Chemistry metrics calculated for imidazolium (**25 - 32**) and cholinium (**33 - 40**) L-Phe derived SAILs and their precursors (**9-16**).

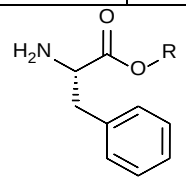
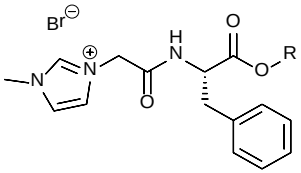
Compounds (chain length)	Yield	Conversion	Selectivity	AE	RME	OE	PMI total	PMI Reaction	PMI reactants, reagents, catalyst	PMI reaction solvents	PMI Workup	PMI Workup chemical	PMI workup solvents
													
9 (C2)	92.8	100.0	92.8	79.5	64.0	80.5	17.4	5.9	2.1	3.8	11.5	0.1	11.4
10 (C4)	95.0	100.0	95.0	80.9	67.2	83.1	15.7	5.4	2.0	3.4	10.4	0.1	10.3
11 (C6)	97.0	100.0	97.0	82.1	70.2	85.5	14.3	4.9	1.9	3.1	9.4	0.1	9.3
12 (C8)	95.0	100.0	95.0	83.1	70.1	84.3	13.7	4.8	1.8	2.9	8.9	0.1	8.8
13 (C10)	98.1	100.0	98.1	84.0	73.7	87.6	12.4	4.4	1.7	2.6	8.0	0.1	8.0
14 (C12)	97.0	100.0	97.0	84.9	74.0	87.1	11.9	4.2	1.7	2.5	7.6	0.1	7.6
15 (C14)	98.1	100.0	98.1	85.6	75.9	88.6	11.1	4.0	1.7	2.3	7.1	0.1	7.0
16 (C16)	96.0	100.0	96.0	86.3	75.1	87.0	10.8	3.9	1.7	2.3	6.9	0.1	6.8
													
25 (C2)	90.8	100.0	90.8	100.0	90.8	90.8	11.0	5.1	1.1	4.0	5.9	0.0	5.9
26 (C4)	96.2	100.0	96.2	100.0	96.2	96.2	9.8	4.5	1.0	3.5	5.2	0.0	5.2
27 (C6)	94.2	100.0	94.2	100.0	94.2	94.2	9.4	4.4	1.1	3.3	5.0	0.0	5.0
28 (C8)	97.0	100.0	97.0	100.0	97.0	97.0	8.7	4.1	1.0	3.1	4.6	0.0	4.6

29 (C10)	96.0	100.0	96.0	100.0	96.0	96.0	8.3	4.0	1.0	2.9	4.4	0.0	4.4
30 (C12)	95.1	100.0	95.1	100.0	95.1	95.1	10.8	5.2	1.1	4.1	5.6	0.0	5.6
31 (C14)	97.0	100.0	97.0	100.0	97.0	97.0	10.1	4.9	1.0	3.9	5.2	0.0	5.2
32 (C16)	96.0	100.0	96.0	100.0	96.0	96.0	9.8	4.8	1.0	3.7	5.0	0.0	5.0

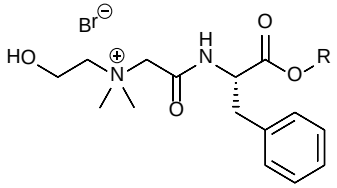


33 (C2)	95.0	100.0	95.0	100.0	94.9	94.9	10.4	4.8	1.1	3.7	5.6	0.0	5.6
34 (C4)	96.9	100.0	96.9	100.0	96.9	96.9	9.6	4.4	1.0	3.4	5.1	0.0	5.1
35 (C6)	97.8	100.0	97.8	100.0	97.7	97.7	9.0	4.2	1.0	3.2	4.8	0.0	4.8
36 (C8)	96.0	100.0	96.0	100.0	96.0	96.0	8.7	4.1	1.0	3.0	4.6	0.0	4.6
37 (C10)	97.0	100.0	97.0	100.0	97.0	97.0	8.2	3.9	1.0	2.9	4.3	0.0	4.3
38 (C12)	96.0	100.0	96.0	100.0	96.0	96.0	10.5	5.1	1.0	4.0	5.5	0.0	5.5
39 (C14)	97.9	100.0	97.9	100.0	97.9	97.9	9.9	4.8	1.0	3.8	5.1	0.0	5.1
40 (C16)	97.0	100.0	97.0	100.0	97.0	97.0	9.6	4.7	1.0	3.6	4.9	0.0	4.9

4. Table S3. Antibacterial activity obtained for the *n*-alkyl-L-phenylalaninates (**2-8**) and SAILs (**25-40**).

IL	Side chain length	Time	MIC_{95}, µM							
			Gram Positive				Gram Negative			
			SA	MRSA	SE	EF	EC	KP	KP-E	PA
										
2	C4	24h	1000	1000	500	>1000	1000	>1000	>1000	1000
		48h	1000	1000	500	>1000	1000	>1000	>1000	1000
3	C6	24h	500	500	125	1000	500	1000	2000	1000
		48h	500	1000	125	2000	500	2000	2000	1000
4	C8	24h	62.5	250	62.5	250	1000	>2000	>2000	>2000
		48h	250	250	250	250	1000	>2000	>2000	>2000
5	C10	24h	125	125	125	1000	>2000	>2000	>2000	>2000
		48h	125	500	1000	1000	>2000	>2000	>2000	>2000
6	C12	24h	7.81	7.81	3.9	500	>2000	>2000	>2000	>2000
		48h	7.81	7.81	3.9	500	>2000	>2000	>2000	>2000
7	C14	24h	125	>500	>500	>500	>500	>500	>500	>500
		48h	125	>500	>500	>500	>500	>500	>500	>500
8	C16	24h	>500	>500	>500	>500	>500	>500	>500	>500
		48h	>500	>500	>500	>500	>500	>500	>500	>500
										
25	$C2^{20, 21}$	24h	2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000

26	C4	24h	500	1000	250	2000	>2000	>2000	>2000	>2000
		48h	1000	1000	250	2000	>2000	>2000	>2000	>2000
27	C6	24h	125	125	125	500	500	2000	2000	2000
		48h	500	1000	1000	2000	2000	2000	2000	2000
28	C8	24h	7.81	31.25	15.62	31.25	62.5	62.5	125	125
		48h	7.81	31.25	31.25	31.25	62.5	62.5	250	125
29	C10	24h	1.95	3.9	3.9	3.9	31.25	31.25	31.25	31.25
		48h	1.95	3.9	3.9	3.9	31.25	31.25	31.25	31.25
30	C12	24h	1.95	3.9	1.95	1.95	31.25	62.5	62.5	125
		48h	1.95	3.9	1.95	1.95	31.25	62.5	62.5	125
31	C14	24h	1.95	1.95	1.95	1.95	>500	>500	>500	>500
		48h	31.25	62.5	62.5	62.5	>500	>500	>500	>500
32	C16	24h	3.9	7.81	7.81	7.81	>500	>500	>500	>500
		48h	62.5	250	250	125	>500	>500	>500	>500

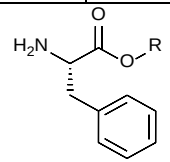
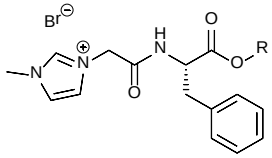


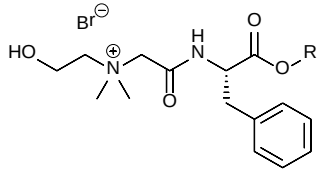
33	C2[20, 21]	24h	2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
34	C4	24h	500	12000	250	2000	>2000	>2000	>2000	>2000
		48h	1000	1000	250	>2000	>2000	>2000	>2000	>2000
35	C6	24h	125	125	125	500	500	2000	2000	2000
		48h	500	1000	1000	2000	2000	2000	2000	2000
36	C8	24h	3.9	31.25	7.81	31.25	62.5	62.5	250	125
		48h	3.9	31.25	7.81	31.25	62.5	62.5	250	125
37	C10	24h	1.95	1.95	1.95	1.95	15.62	7.81	15.62	31.25
		48h	1.95	1.95	1.95	1.95	15.62	7.81	15.62	31.25
38	C12	24h	1.95	1.95	1.95	1.95	7.81	7.81	15.62	62.5
		48h	1.95	1.95	1.95	1.95	7.81	7.81	15.62	62.5

39	C14	24h	1.95	1.95	1.95	3.9	>500	>500	>500	>500
		48h	31.25	125	250	250	>500	>500	>500	>500
40	C16	24h	1.95	7.81	7.81	7.81	>500	>500	>500	>500
		48h	62.5	125	250	250	>500	>500	>500	>500

Notes**. SA**: *Staphylococcus aureus* subsp. *Aureus* (ATCC 29213), **MRSA**: *Staphylococcus aureus* subsp. *aureus* methicillin resistant (ATCC 43300), **SE**: *Staphylococcus epidermidis* (HK6966, 112-2016, dialysis tube, University Hospital Hradec Králové, Institute of Clinical Microbiology), **EF**: *Enterococcus faecalis* (ATCC 29212), **EC**: *Escherichia coli* (ATCC 25922), **KP**: *Klebsiella pneumoniae* (HK 11750, 64-2016, urine catheter tube, University Hospital Hradec Králové, Institute of Clinical Microbiology), **KP-E**: *Klebsiella pneumoniae* (ESBL positive, HK 14368, University Hospital Hradec Králové, Institute of Clinical Microbiology), **PA**: *Pseudomonas aeruginosa* (ATCC 27853)

5. Table S4. Antifungal results obtained for the *n*-alkyl-L-phenylalaninates (**2**-**8**) and SAILs (**25**-**40**).

IL	Side chain length	Time (h)	MIC_{95}, µM											
			CA1	CA2	CP	CK1	CK2	CT	CG	CL	TA	AF	AC	TM[a]
1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*
														
2	C4	24h	1000	1000	500	125	125	1000	1000	500	500	500	1000	500
		48h	1000	1000	1000	125	125	1000	>1000	1000	500	1000	>1000	1000
3	C6	24h	500	500	500	125	125	500	500	250	250	500	2000	250
		48h	500	500	500	125	125	500	1000	250	250	1000	>2000	250
4	C8	24h	62.5	62.5	62.5	31.25	62.5	250	250	31.25	62.5	125	2000	31.25
		48h	62.5	62.5	125	31.25	62.5	250	250	31.25	62.5	500	>2000	31.25
5	C10	24h	62.5	62.5	1000	15.62	15.62	15.62	7.81	125	15.26	1000	>2000	62.5
		48h	62.5	62.5	>2000	15.62	15.62	15.62	7.81	500	62.5	>2000	>2000	62.5
6	C12	24h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
7	C14	24h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
8	C16	24h	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500
		48h	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500	>500
														
25	C2[20, 21]	24h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
26	C4	24h	>2000	>2000	>2000	2000	2000	2000	>2000	>2000	2000	>2000	>2000	2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	2000	>2000	>2000	2000

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
27	C6	24h	2000	2000	500	250	500	500	2000	2000	1000	>2000	>2000	1000
		48h	2000	2000	500	250	500	500	2000	2000	1000	>2000	>2000	1000
28	C8	24h	500	500	250	250	250	250	500	250	1000	500	500	1000
		48h	500	1000	500	500	500	250	500	250	1000	1000	500	1000
29	C10	24h	31.25	31.25	31.25	31.25	15.62	62.5	62.5	62.5	250	15.62	62.5	62.5
		48h	31.25	62.5	31.25	31.25	31.25	62.5	62.5	62.5	250	15.62	62.5	62.5
30	C12	24h	7.81	7.81	7.81	7.81	7.81	7.81	7.81	31.25	125	7.81	15.62	7.81
		48h	7.81	7.81	7.81	7.81	7.81	15.62	15.62	31.25	125	7.81	15.62	7.81
31	C14	24h	3.9	7.81	3.9	7.81	7.81	7.81	3.9	15.62	15.62	7.81	31.25	15.62
		48h	7.81	7.81	7.81	3.9	7.81	15.62	3.9	15.62	15.62	7.81	31.25	15.62
32	C16	24h	7.81	7.81	3.9	7.81	7.81	3.9	3.9	>500	7.81	16.62	15.62	15.62
		48h	15.62	15.62	3.9	7.81	7.81	7.81	3.9	>500	7.81	31.25	15.62	15.62
														
33	C2[20, 21]	24h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
		48h	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000	>2000
34	C4	24h	>2000	>2000	>2000	>2000	>2000	2000	>2000	>2000	2000	>2000	>2000	2000
		48h	>2000	>2000	>2000	>2000	2000	>2000	>2000	>2000	2000	>2000	>2000	2000
35	C6	24h	1000	1000	1000	1000	1000	1000	2000	2000	500	1000	>2000	500
		48h	1000	2000	1000	1000	2000	2000	2000	2000	500	1000	>2000	500
36	C8	24h	500	500	500	125	62.5	250	1000	250	500	250	500	500
		48h	500	500	500	125	125	250	1000	500	500	500	500	500
37	C10	24h	15.62	15.62	31.25	15.62	15.62	31.25	62.5,	125	250	31.25	31.25	31.25
		48h	31.25	31.25	31.25	15.62	15.62	31.25	62.5	125	250	31.25	31.25	31.25

1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*
38	C12	24h	1.95	3.9	7.81	3.9	3.9	7.81	3.9	3.9	125	3.9	7.81	15.62
		48h	3.9	3.9	7.81	3.9	3.9	7.81	3.9	3.9	125	3.9	7.81	15.62
39	C14	24h	7.81	7.81	3.9	3.9	7.81	7.81	3.9	7.81	7.81	7.81	31.25	7.81
		48h	7.81	7.81	7.81	7.81	7.81	7.81	3.9	7.81	7.81	7.81	31.25	7.81
40	C16	24h	>500	>500	3.9	15.62	3.9	7.81	1.95	>500	3.9	31.25	7.81	7.81
		48h	>500	>500	7.81	31.25	3.9	15.62	1.95	>500	3.9	62.5	15.62	7.81

Notes: [a] evaluation after 72 h and 120 h, respectively.

CA1*: Candida albicans* (ATCC 24433), CA2: *Candida albicans* (ATCC 90028), CP: *Candida parapsilosis* (ATCC 22019), CK1: *Candida krusei* (ATCC 6258), CK2: *Candida krusei* (E28, University Hospital Hradec Králové, Institute of Clinical Microbiology), CT: *Candida tropicalis* (ATCC 750), CG: *Candida glabrata* (ATCC 90030), CL: *Candida lusitaniae* (2446/I, University Hospital Hradec Králové, Institute of Clinical Microbiology), TA: *Trichosporon asahii* (1188, University Hospital Hradec Králové, Institute of Clinical Microbiology), AF: *Aspergillus fumigatus* (ATCC 204305), AC*: Absidia corymbifera* (CCM 8077), TM: *Trichophyton mentagrophytes* (445, University Hospital Hradec Králové, Institute of Clinical Microbiology)

6. Figure S1.

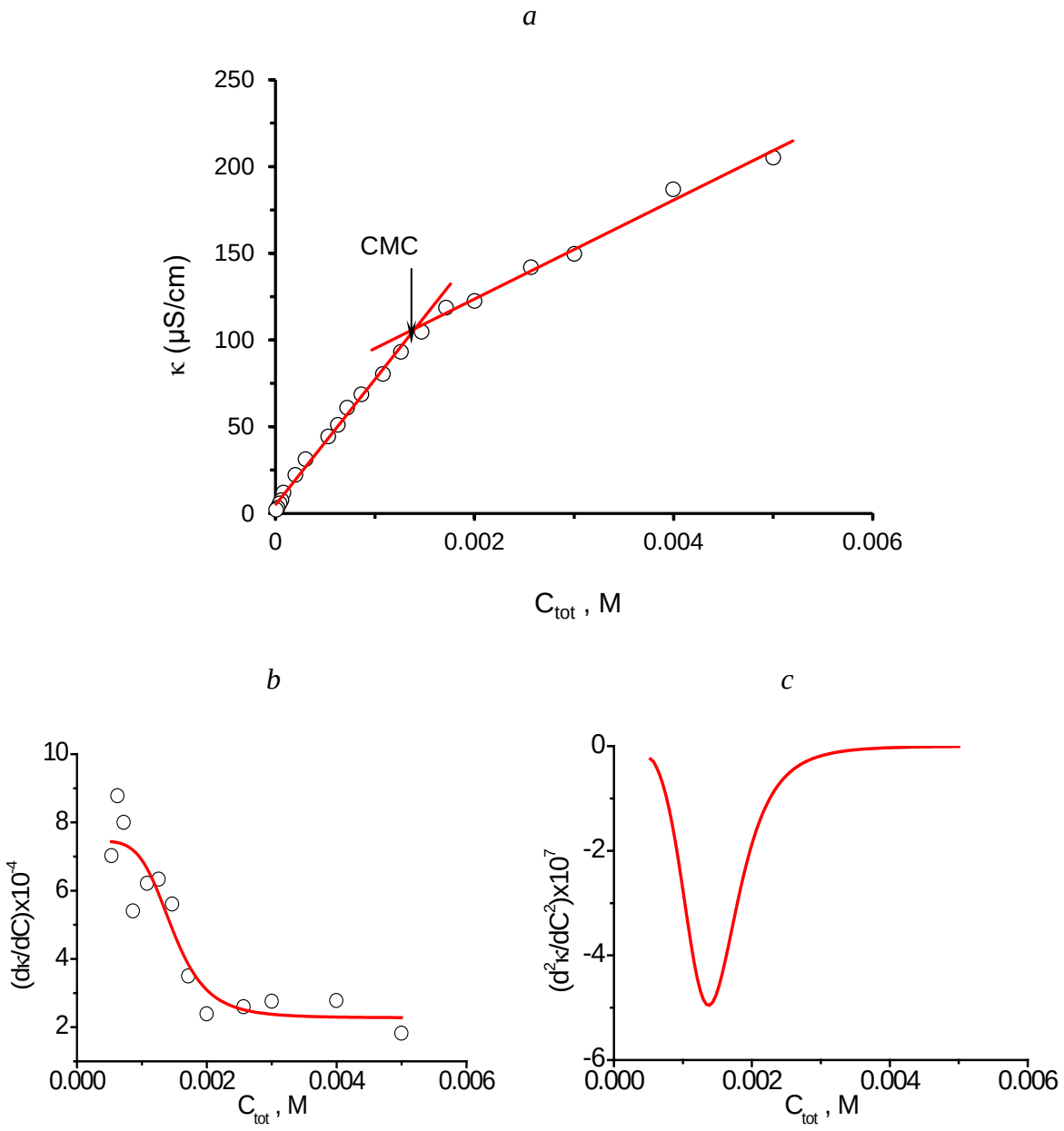


Fig. S1. Determination of the CMC value from specific conductivity *vs.* total concentration plot for SAIL (**21**). *a* – concentration profile; *b* – first derivative plot; c – second derivative plot; water, 25 ^{0}C.

7. Figure S2

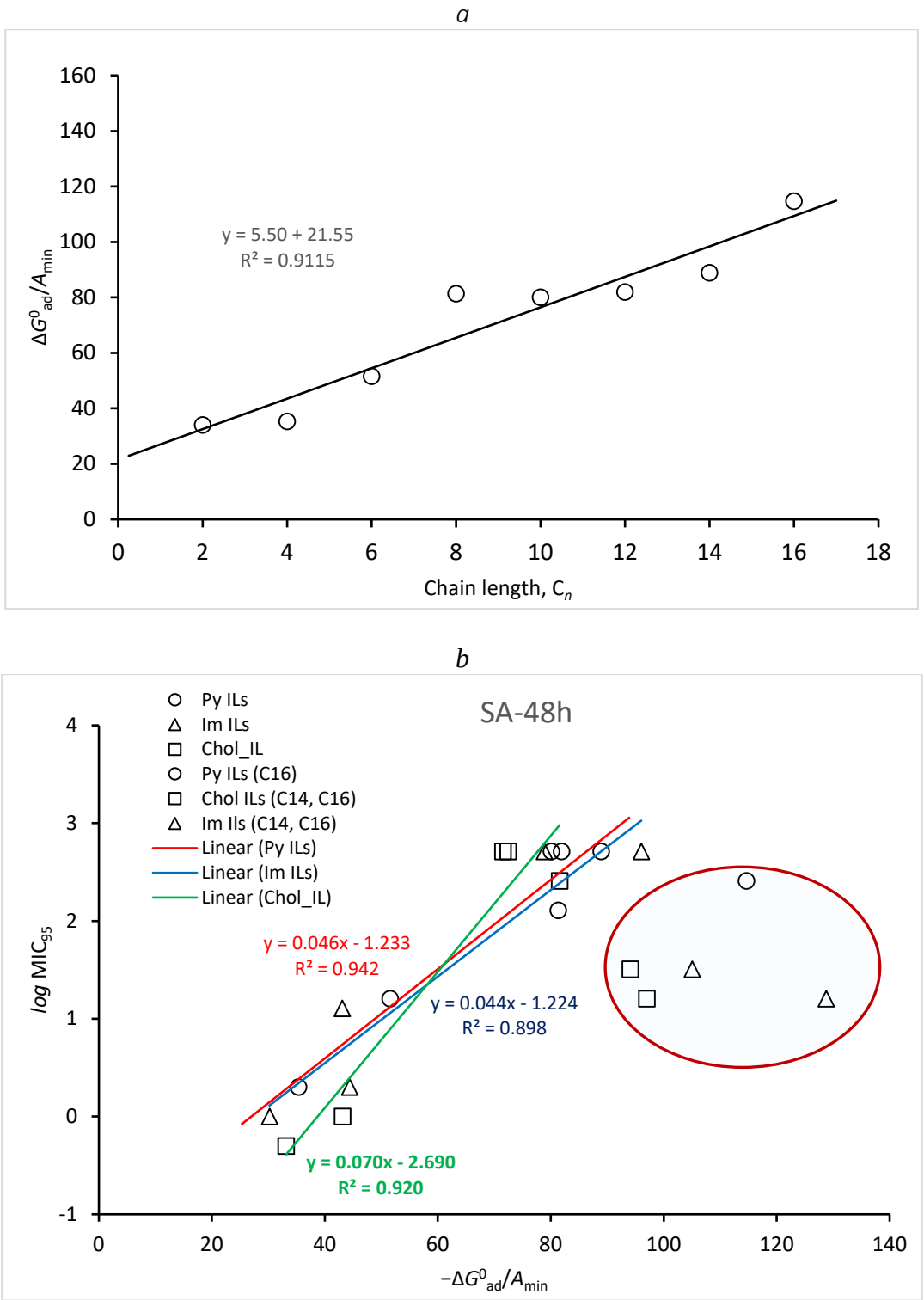


Fig. S2. Plot of $-\Delta G^0_{ad}/A_{min}$ (Table 8) *vs* chainlength for the SAILs (**17 - 24**) (*a)* and *vs log* MIC_{95} (*S. aureus*, screening for 48 h, see Table 4) vs $-\Delta G^0_{ad}/A_{min}$ for the SAILs (**17 - 40**) (*b*) presented as the separate series of pyridinium (circles), imidazolium (triangles), and cholinium (rectangles) ILs. The C_2 and C_{16} for pyridinium and C_{14} and C_{16} for imidazolium and cholinium ILs (circled at Fig.S1 *b*) have not been taken into account for calculation of the linear correlations.

8. Screening for bacterial and fungal toxicity.

The bacterial toxicity (determination of MIC in μM) was evaluated by microdilution broth method according to EUCAST (The European Committee on Antimicrobial Susceptibility Testing) instructions.[16] A panel of reference strains from American Type Culture Collection (ATCC, five strains) and clinical isolates (three strains) with declared identification (Vitek, MALDI-TOF MS) and susceptibility profiles were employed for antibacterial activity screening part. The cultivation was carried out in Cation-adjusted Mueller-Hinton broth (CAMHB, M-H 2 Broth, Sigma-Aldrich) at 35±2°C. Tested compounds were dissolved in DMSO (Sigma-Aldrich) to produce stock solutions, which were diluted with CAMHB to final concentrations (with respect to their solubility limit) of 2000 – 1000 – 500 – 250 – 125 – 62.5 – 31.25 – 15.62 – 7.81 – 3.9 – 1.953 – 0.977 – 0.488 μM. Positive controls (cultivation medium inoculated by bacteria), negative controls (sterility media testing) and internal quality standards (gentamycin, ciprofloxacin – both from Sigma-Aldrich) were involved in each assay. The final concentration of DMSO in the test medium did not exceed 1% (v/v) of the total solution composition and did not affect the growth of bacteria. Antibacterial activity was expressed as minimum inhibitory concentration (MIC) after 24 and 48 h of static incubation in humidified atmosphere, at 35±2 °C. MIC was defined as the concentration, which the measured absorbance is equal or lower than that of the control. Visual inspection and metabolic activity indicator (AlamarBlue™ Cell Viability reagent[17] from ThermoFisher Scientific) were used for MIC endpoint evaluation for both antibacterial and antifungal screenings.

The fungal toxicity (determination of MIC in μM) was evaluated by microdilution broth method according to the EUCAST instructions.[18, 19] A panel of reference strains from American Type Culture Collection (ATCC, 7 strains), Czech Collection of Microorganisms (CCM, Brno, Czech Republic, 1 strain) and clinical isolates (4 strains) with declared identification (Vitek, MALDI-TOF MS) and susceptibility profiles were employed for antifungal activity screening part. Tested compounds are dissolved in DMSO and diluted in a twofold manner with RPMI 1640 medium with glutamine, supplemented with 2% w/v glucose and buffered to pH 7.0 with 3-morpholinopropane-1-sulfonic acid (all are from Sigma-Aldrich). The final concentration of DMSO in the tested medium did not exceed 1% (v/v) of the total solution composition, and it was confirmed that this concentration did not inhibit the growth of tested fungi. Static incubation was performed in the dark and humidified atmosphere, at 35±2 °C for 24 and 48 h (72 and 120 h for Trichophyton mentagrophytes, respectively). Positive, negative controls and internal quality controls and standards (fluconazole and amphotericin B, both are from Sigma-Aldrich) were included. MIC values defined as the concentrations to demonstrate measured absorbance to be equal or lower than that of the control.

9. Synthetic procedures

Synthesis of L-phenylalanine esters (1 – 8)

Product **1** was synthesized according to the procedure described in the previous papers [20, 21]. The following general technique was used for the synthesis of compounds (**1 – 8)**. To a stirred suspension of L-phenylalanine (10.00 g, 60.53 mmol) in toluene (100 ml) was added PTSA·H_2O (13.82 g, 72.64 mmol) and corresponding alcohol (72.64 mmol). The suspension was heated under reflux conditions for 12 hours using a Dean-Stark apparatus (after 1 hours, a homogenous solution was obtained). After 12 hours solution was allowed to cool to room temperature, which results in crystallization of the reaction mixture. Addition of diethyl ether (50 ml) can initiate precipitation of the product. The crude PTSA salt product was isolated by vacuum filtration, washed with petroleum ether (3 x 50 ml) and dried *in vacuo*. The PTSA salt of L-phenylalanine esters then was neutralised by stirring in mixture of an aqueous sodium carbonate solution (10.60 g [0.1 mol] Na_2CO_3 in 100 ml H_2O) with 100 ml dichloromethane and then transferred to a separating funnel. The organic layer was separated and washed with water (3 x 50 ml). The organic phase was dried over sodium sulphate, filtered and volatiles removed *in vacuo* to afford the title compound as a pale-yellow oil with 97 – 99 % yield. ^{1}H and ^{13}C NMR of L-phenylalanine esters is in agreement with the literature.[22]

Ethyl L-phenylalaninate (1). Yield 11.35 g (97 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 – 7.15 (m, 5H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.71 (dd, *J* = 7.9, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.4, 13.5, 6.6 Hz, 2H), 1.46 (s, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.16 (s), 137.43 (s), 129.41 (s), 128.63 (s), 126.89 (s), 61.02 (s), 55.99 (s), 41.29 (s), 14.29 (s).

Butyl L-phenylalaninate (2). Yield 13.00 g (97 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 – 7.16 (m, 5H), 4.10 (t, *J* = 6.7 Hz, 2H), 3.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.63 – 1.55 (m, 2H), 1.46 (s, 2H), 1.34 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.92 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.27 (s), 137.43 (s), 129.39 (s), 128.63 (s), 126.88 (s), 64.92 (s), 56.01 (s), 41.33 (s), 30.70 (s), 19.20 (s), 13.80 (s).

Hexyl L-phenylalaninate (3). Yield 14.80 g (98 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 – 7.16 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.64 – 1.55 (m, 2H), 1.46 (s, 2H), 1.36 – 1.24 (m, 6H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.26 (s), 137.42 (s), 129.39 (s), 128.62 (s), 126.88 (s), 65.22 (s), 56.00 (s), 41.32 (s), 31.50 (s), 28.61 (s), 25.64 (s), 22.61 (s), 14.10 (s).

Hexyl L-alaninate (3Ala). Following the procedure described above for L-phenylalanine derivatives procedure, product **3Ala** was synthesized using L-alanine (10.00 g, 0.112 mol) in toluene (100 ml), PTSA·H_2O (25.57 g, 0.134 mmol), and 1-hexanol (16.82 ml, 0.134 mmol). The title compound was obtained as colourless oil (yield 92 %) and consumed immediately for the next synthetic stage. ^{1}H NMR

(400 MHz, $CDCl_3$): δ 4.17 – 4.05 (m, 2H), 3.54 (q, *J* = 7.0 Hz, 1H), 1.68 – 1.60 (m, 2H), 1.54 (s, 2H), 1.39 – 1.26 (m, 9H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 176.75 (s), 65.06 (s), 50.12 (s), 31.40 (s), 28.58 (s), 25.54 (s), 22.52 (s), 20.76 (s), 13.99 (s).

Octyl L-phenylalaninate (4). Yield 16.45 g (98 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 – 7.14 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.65 – 1.55 (m, 2H), 1.46 (s, 2H), 1.35 – 1.22 (m, 10H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.26 (s), 137.43 (s), 129.39 (s), 128.62 (s), 126.88 (s), 77.48 (s), 77.16 (s), 76.84 (s), 65.23 (s), 56.01 (s), 41.32 (s), 31.88 (s), 29.29 (s), 29.25 (s), 28.65 (s), 25.98 (s), 22.74 (s), 14.19 (s).

Decyl L-phenylalaninate (5). Yield 18.30 g (99 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.16 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.59 (dd, *J* = 13.4, 6.7 Hz, 2H), 1.48 (s, 2H), 1.35 – 1.21 (m, 14H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.27 (s), 137.43 (s), 129.40 (s), 128.64 (s), 126.90 (s), 65.26 (s), 56.02 (s), 41.33 (s), 32.00 (s), 29.65 (s), 29.61 (s), 29.42 (s), 29.34 (s), 28.67 (s), 25.99 (s), 22.79 (s), 14.23 (s).

Dodecyl L-phenylalaninate (6). Yield 19.60 g (97 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 – 7.17 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.59 (dd, *J* = 13.4, 6.7 Hz, 2H), 1.47 (s, 2H), 1.36 – 1.19 (m, 18H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.28 (s), 137.44 (s), 129.41 (s), 128.64 (s), 126.90 (s), 65.26 (s), 56.02 (s), 41.34 (s), 32.03 (s), 29.77 (s), 29.75 (s), 29.69 (s), 29.62 (s), 29.47 (s), 29.35 (s), 28.67 (s), 26.00 (s), 22.81 (s), 14.24 (s).

Tetradecyl L-phenylalaninate (7). Yield 21.65 g (99 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 – 7.10 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.71 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.63 – 1.55 (m, 2H), 1.50 (s, 2H), 1.36 – 1.19 (m, 22H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 175.21 (s), 137.39 (s), 129.37 (s), 128.60 (s), 126.86 (s), 65.21 (s), 55.97 (s), 41.29 (s), 32.01 (s), 29.78 (s), 29.76 (s), 29.74 (s), 29.67 (s), 29.59 (s), 29.45 (s), 29.32 (s), 28.64 (s), 25.96 (s), 22.78 (s), 14.21 (s).

Hexadecyl L-phenylalaninate (8). Yield 23.10 g (98 %). ^{1}H NMR (400 MHz, $CDCl_3$): *δ*, ppm 7.33 – 7.16 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.71 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.97 (ddd, *J* = 21.3, 13.5, 6.6 Hz, 2H), 1.64 – 1.54 (m, 2H), 1.45 (s, 2H), 1.36 – 1.20 (m, 26H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): *δ*, ppm 175.23 (s), 137.41 (s), 129.37 (s), 128.60 (s), 126.86 (s), 65.20 (s), 55.99 (s), 41.31 (s), 32.02 (s), 29.79 (s), 29.77 (s), 29.75 (s), 29.68 (s), 29.59 (s), 29.46 (s), 29.33 (s), 28.65 (s), 25.97 (s), 22.79 (s), 14.21 (s).

Synthesis of alkyl (2-bromoacetyl)-L-phenylalaninates (9 - 16)

To a stirred solution of corresponding L-phenylalanine ester (**9 - 16**) (60.00 mmol) in dichloromethane (50 ml) was added solid Na_2CO_3 (9.54 g, 90 mmol). To this mixture, bromoacetyl bromide (6.8 ml, 78 mmol) was added dropwise and stirred for 12 hours. After 12 hours 50 ml of water was added carefully

and reaction mixture was transferred to a separating funnel. The organic layer was separated and washed with water (3 x 50 ml). The organic phase was dried over sodium sulphate, filtered and volatiles removed *in vacuo* to afford the title compound as a pale-yellow oil which was crystallized to a white solid product. The yields of the title compounds were 93–98 %.

Ethyl (2-bromoacetyl)-L-phenylalaninate (9). Yield 17.50 g (93 %); mp 74 – 75 ºC; $[\alpha]_D^{20}$: +41.14 º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3316.34; 3025.47; 2979.30; 1733.11; 1646.47; 1536.09; 1494.21; 1444.59; 1390.88; 1373.98; 1351.24; 1299.23; 1260.50; 1225.50; 1206.23; 1139.59; 1116.52; 1077.01; 1036.38; 1007.97; 963.09; 859.02; 741.34; 698.77; 646.32; 609.06; 556.17; 510.18. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.07 (m, 5H), 6.86 (d, *J* = 4.9 Hz, 1H), 4.88 – 4.77 (m, 1H), 4.19 (q, *J* = 7.0 Hz, 2H), 3.93 – 3.74 (m, 2H), 3.25 – 3.04 (m, 2H), 1.25 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.95 (s), 165.19 (s), 135.53 (s), 129.48 (s), 128.75 (s), 127.42 (s), 61.87 (s), 53.87 (s), 37.90 (s), 28.81 (s), 14.22 (s). ESI-MS (m/z): found $[M+H]^+$ 314.0395, $C_{13}H_{17}BrNO_3^+$ requires 314.0386.

Butyl (2-bromoacetyl)-L-phenylalaninate (10). Yield 19.50 g (95 %); mp 47 – 48 ºC; $[\alpha]_D^{20}$: +32.2º (1.0 c, $CHCl_3$). IR ($CHCl_3$, cm^{-1}): 3303.60; 3026.94; 2962.57; 1732.29; 1653.03; 1543.10; 1494.55; 1444.32; 1358.11; 1280.97; 1236.91; 1202.01; 1118.08; 1077.28; 1032.09; 974.04; 751.91; 696.57; 614.94; 574.71; 555.07. ^{1}H NMR (400 MHz, $CDCl_3$): *δ*, ppm 7.34 – 7.08 (m, 5H), 6.89 (d, *J* = 7.4 Hz, 1H), 4.84 (dt, *J* = 7.9, 5.9 Hz, 1H), 4.19 – 4.06 (m, 2H), 3.90 – 3.78 (m, 2H), 3.21 – 3.08 (m, 2H), 1.65 – 1.54 (m, 2H), 1.38 – 1.28 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): *δ*, ppm 171.02 (s), 165.22 (s), 135.52 (s), 129.44 (s), 128.75 (s), 127.40 (s), 65.71 (s), 53.89 (s), 37.93 (s), 30.55 (s), 28.80 (s), 19.15 (s), 13.76 (s). ESI-MS (m/z): found $[M+H]^+$ 342.0694, $C_{15}H_{21}BrNO_3^+$ requires 342.0699.;

Hexyl (2-bromoacetyl)-L-phenylalaninate (11). Yield 21.55 g (97 %); mp 50 – 51ºC; $[\alpha]_D^{20}$: +27.08º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3314.65; 2955.70; 2857.36; 1726.46; 1654.64; 1535.40; 1443.58; 1400.81; 1362.47; 1260.73; 1231.02; 1203.99; 1133.42; 1077.35; 974.90; 702.22; 616.29; 550.58. ^{1}H NMR (400 MHz, $CDCl_3$): *δ*, ppm 7.33 – 7.10 (m, 5H), 6.86 (d, *J* = 7.5 Hz, 1H), 4.84 (dt, *J* = 7.9, 5.8 Hz, 1H), 4.19 – 4.03 (m, 2H), 3.90 – 3.79 (m, 2H), 3.22 – 3.08 (m, 2H), 1.64 – 1.56 (m, 2H), 1.38 – 1.21 (m, 6H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): *δ*, ppm 171.01 (s), 165.16 (s), 135.53 (s), 129.46 (s), 128.77 (s), 127.43 (s), 66.04 (s), 53.91 (s), 37.97 (s), 31.47 (s), 28.83 (s), 28.52 (s), 25.61 (s), 22.63 (s), 14.13 (s). ESI-MS (m/z): found $[M+H]^+$ 370.1014, $C_{17}H_{25}BrNO_3^+$ requires 370.1012.

Hexyl (2-bromoacetyl)-L-alaninate (11Ala). To a stirred solution of hexyl L-alanine ester (17.3 g; 0.1 mol) in dichloromethane was added solid Na_2CO_3 (15.90 g, 0.15 mol). To this mixture was added dropwise bromoacetyl bromide (11.29 ml, 0.13 mol). After that it was stirred for 12 hours. Then 50 ml of water was added carefully to reaction mixture and then it was transferred to a separating funnel. The organic layer was separated and washed with water (3 x 50 ml). The organic phase was dried over sodium sulphate, filtered and volatiles removed *in vacuo* to afford the title compound as colorless oil which crystallized to a white solid product (mp 43-44 ºC) in 96 % yield. The titled compounds was crystallized

from petroleum ether. $[\alpha]_D^{20}$: +19º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3305.72; 2955.62; 2931.92; 2868.64; 1734.49; 1646.23; 1542.73; 1451.00; 1397.11; 1374.44; 1352.33; 1317.47; 1205.25; 1157.21; 1138.82; 1079.13; 1010.94; 971.68; 894.36; 726.89; 664.60; 562.60; 539.26; 447.30. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.05 (d, *J* = 4.9 Hz, 1H), 4.56 (p, *J* = 7.2 Hz, 1H), 4.23 – 4.10 (m, 2H), 3.89 (s, 2H), 1.70 – 1.61 (m, 2H), 1.45 (d, *J* = 7.1 Hz, 3H), 1.39 – 1.25 (m, 6H), 0.90 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 172.42 (s), 164.98 (s), 65.91 (s), 48.84 (s), 31.34 (s), 28.78 (s), 28.44 (s), 25.44 (s), 22.50 (s), 18.33 (s), 13.98 (s). ESI-MS (m/z): found $[M+H]^+$ 294.0696, $[C_{11}H_{20}BrNO_3+H]^+$ requires 294.0699.

Octyl (2-bromoacetyl)-L-phenylalaninate (12). Yield 22.70 g (95 %); mp 44 – 45 ºC; $[\alpha]_D^{20}$: +25.24º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3300.93; 3064.84; 2920.68; 2853.68; 1720.69; 1650.20; 1544.47; 1497.44; 1455.41; 1348.09; 1280.30; 1209.68; 1139.26; 1093.41; 944.95; 749.58; 700.48; 569.11; 546.56; 452.15. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.08 (m, 5H), 6.89 (d, *J* = 7.4 Hz, 1H), 4.84 (dt, *J* = 7.7, 5.9 Hz, 1H), 4.16 – 4.05 (m, 2H), 3.89 – 3.77 (m, 2H), 3.21 – 3.08 (m, 2H), 1.65 – 1.54 (m, 2H), 1.37–1.20 (m, 10H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 171.00 (s), 165.16 (s), 135.53 (s), 129.44 (s), 128.73 (s), 127.39 (s), 66.00 (s), 53.88 (s), 37.94 (s), 31.87 (s), 29.24 (s), 28.79 (s), 28.53 (s), 25.92 (s), 22.74 (s), 14.20 (s). ESI-MS (m/z): found $[M+H]^+$ 398.1327, $C_{19}H_{29}BrNO_3^+$ requires 398.1325.

Decyl (2-bromoacetyl)-L-phenylalaninate (13). Yield 25.10 g (98 %); mp 41 – 43 ºC; $[\alpha]_D^{20}$: +23.66º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3328.32; 3025.38; 2924.81; 2853.41; 1732.29; 1656.75; 1527.02; 1474.58; 1443.83; 1398.17; 1358.17; 1256.91; 1223.58; 1201.57; 1113.52; 1074.77; 971.13; 698.51; 604.78; 545.96; 474.57. ^{1}H NMR (400 MHz, $CDCl_3$): *δ*, ppm 7.34 – 7.08 (m, 5H), 6.87 (d, *J* = 7.6 Hz, 1H), 4.84 (dt, *J* = 7.8, 5.9 Hz, 1H), 4.17 – 4.04 (m, 2H), 3.91 – 3.78 (m, 2H), 3.23 – 3.06 (m, 2H), 1.64 – 1.56 (m, 2H), 1.36 – 1.20 (m, 14H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): *δ*, ppm 171.01 (s), 165.15 (s), 135.53 (s), 129.45 (s), 128.75 (s), 127.41 (s), 66.03 (s), 53.90 (s), 37.96 (s), 32.01 (s), 29.64 (s), 29.60 (s), 29.42 (s), 29.30 (s), 28.82 (s), 28.55 (s), 25.94 (s), 22.80 (s), 14.24 (s). ESI-MS (m/z): found $[M+H]^+$ 426.1650, $C_{21}H_{33}BrNO_3^+$ requires 426.1638.

Dodecyl (2-bromoacetyl)-L-phenylalaninate (14). Yield 26.45 g (97 %); mp 57 – 58 ºC; $[\alpha]_D^{20}$: +21.68º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3313.60; 3028.90; 2953.99; 2919.40; 2850.54; 1735.87; 1650.30; 1535.48; 1495.40; 1465.57; 1443.79; 1396.98; 1362.59; 1258.54; 1200.89; 1135.53; 1076.51; 1031.07; 986.11; 746.44; 699.58; 618.34; 551.90. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.08 (m, 5H), 6.86 (d, *J* = 7.2 Hz, 1H), 4.89 – 4.79 (m, 1H), 4.19 – 4.03 (m, 2H), 3.92 – 3.76 (m, 2H), 3.25 – 3.05 (m, 2H), 1.63 – 1.56 (m, 2H), 1.37 – 1.17 (m, 18H), 0.88 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 171.01 (s), 165.14 (s), 135.54 (s), 129.47 (s), 128.77 (s), 127.43 (s), 66.05 (s), 53.91 (s), 37.97 (s), 32.05 (s), 29.78 (s), 29.77 (s), 29.70 (s), 29.62 (s), 29.49 (s), 29.32 (s), 28.83 (s), 28.57 (s), 25.95 (s), 22.83 (s), 14.26 (s). ESI-MS (m/z): found $[M+H]^+$ 454.1952, $C_{23}H_{37}BrNO_3^+$ requires 454.1951.

Tetradecyl (2-bromoacetyl)-L-phenylalaninate (15) Yield 28.40 g (98 %); mp 66 – 67 ºC; $[\alpha]_D^{20}$: +20.10º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3314.57; 3029.02; 2954.00; 2919.25; 2850.40; 1735.95;

1650.14; 1536.25; 1495.54; 1465.27; 1443.92; 1396.99; 1362.00; 1258.65; 1201.51; 1135.75; 1076.91; 1034.98; 988.85; 975.84; 747.02; 699.67; 618.57; 552.24. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 – 7.09 (m, 5H), 6.87 (d, *J* = 7.7 Hz, 1H), 4.84 (dt, *J* = 7.8, 5.8 Hz, 1H), 4.16 – 4.05 (m, 2H), 3.89 – 3.80 (m, 2H), 3.20 – 3.09 (m, 2H), 1.63 – 1.55 (m, 2H), 1.34 – 1.19 (m, 22H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 171.01 (s), 165.15 (s), 135.54 (s), 129.45 (s), 128.75 (s), 127.41 (s), 66.03 (s), 53.90 (s), 37.96 (s), 32.05 (s), 29.82 (s), 29.80 (s), 29.78 (s), 29.70 (s), 29.61 (s), 29.49 (s), 29.31 (s), 28.82 (s), 28.56 (s), 25.94 (s), 22.82 (s), 14.25 (s). ESI-MS (m/z): found $[M+H]^+$ 482.2269, $C_{25}H_{41}BrNO_3^+$ requires 482.2264.

Hexadecyl (2-bromoacetyl)-L-phenylalaninate (16) Yield 29.40 g (96 %); mp 72 – 73 ºC; $[\alpha]_D^{20}$: +17.82º (1.0 c, $CHCl_3$). IR (KBr, cm^{-1}): 3315.01; 3029.11; 2919.01; 2850.11; 1736.10; 1650.28; 1536.26; 1495.55; 1465.00; 1443.74; 1396.81; 1361.33; 1258.99; 1201.60; 1135.57; 1077.83; 984.41; 746.73; 719.88; 699.56; 618.59; 552.00; 460.70. ^{1}H NMR (400 MHz, $CDCl_3$): *δ*, ppm 7.32 – 7.11 (m, 5H), 6.86 (d, *J* = 7.7 Hz, 1H), 4.84 (dt, *J* = 7.9, 5.8 Hz, 1H), 4.17 – 4.05 (m, 2H), 3.90 – 3.78 (m, 2H), 3.22 – 3.08 (m, 2H), 1.63 – 1.56 (m, 2H), 1.35 – 1.20 (m, 26H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): *δ*, ppm 171.01 (s), 165.14 (s), 135.54 (s), 129.47 (s), 128.77 (s), 127.43 (s), 66.05 (s), 53.91 (s), 37.98 (s), 32.07 (s), 29.84 (s), 29.82 (s), 29.80 (s), 29.71 (s), 29.63 (s), 29.50 (s), 29.33 (s), 28.83 (s), 28.57 (s), 25.96 (s), 22.83 (s), 14.27 (s). ESI-MS (m/z): found $[M+H]^+$ 510.2583, $C_{27}H_{45}BrNO_3^+$ requires 510.2577.

General method of synthesis of pyridinium salts (17 - 24)

Pyridine (4.04 ml, 50 mmol) was added to a stirred solution of corresponding alkyl (2-bromoacetyl)-L-phenylalaninate (50 mmol) in 100 mL of diethyl ether or in 1:1 dicloromethane/acetonitrile mixture (the latter was used in the cases of dodecyl, tetradecyl, and hexadecyl derivatives). The reaction mixture was stirred at room temperature for 48 hours. As a rule, a spontaneous crystallization was observed. If there were no crystals appeared, the reaction mixture was allowed to cool overnight in the fridge and then was crystallized. Solutions in mixture dicloromethane/acetonitrile were evaporated *in vacuo* to obtain viscous liquid residue which was crystallized under diethyl ether. The solid products were washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compounds as a white solids in 93 – 98 % yield.

(*S*)-1-(2-((1-(Ethyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (17). Yield 18.50 g (94 %); mp 104 – 105 ºC; $[\alpha]_D^{20}$: + 6.3º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3338.16; 3041.19; 2988.53; 2937.38; 2867.94; 2815.34; 1733.49; 1661.86; 1628.79; 1536.17; 1479.11; 1442.31; 1378.96; 1346.37; 1252.30; 1213.73; 1118.02; 1078.33; 1039.22; 964.92; 929.74; 847.12; 790.99; 755.10; 724.81; 702.20; 678.48; 598.52; 550.60; 495.73. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.25 (d, *J* = 7.5 Hz, 1H), 8.93 (d, *J* = 5.6 Hz, 2H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 7.5, 6.8 Hz, 2H), 7.38 – 7.19 (m, 5H), 5.61 – 5.39 (m, 2H), 4.53 (dd, *J* = 14.3, 7.6 Hz, 1H), 4.12 – 3.95 (m, 2H), 3.02 (qd, *J* = 13.7, 7.2 Hz, 2H), 1.09

(t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ, ppm 170.72 (s), 164.49 (s), 146.25 (s), 146.18 (s), 136.53 (s), 129.20 (s), 128.37 (s), 127.55 (s), 126.76 (s), 61.31 (s), 60.79 (s), 54.21 (s), 37.02 (s), 13.91 (s). ESI-MS (m/z): found $[M]^+$ 313.1549, $C_{18}H_{21}N_2O_3^+$ requires 313.1547.

(S)-1-(2-((1-(Butyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (18). Yield 19.60 g (93 %); mp 104 – 106 ºC; $[\alpha]_D^{20}$: + 1.7 º (1.0 c, MeOH).

IR (KBr, cm^{-1}): 3180.43; 3031.53; 2966.01; 1756.05; 1682.26; 1636.97; 1562.73; 1494.05; 1452.17; 1359.84; 1260.97; 1202.30; 1123.31; 1067.64; 1027.35; 972.52; 797.97; 724.04; 681.91; 575.83. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.24 (d, *J* = 7.5 Hz, 1H), 8.92 (d, *J* = 5.6 Hz, 2H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.24 – 8.13 (m, 2H), 7.34 – 7.20 (m, 5H), 5.61 – 5.40 (m, 2H), 4.54 (q, *J* = 7.4 Hz, 1H), 4.06 – 3.91 (m, 2H), 3.11 – 2.93 (m, 2H), 1.49 – 1.36 (m, 2H), 1.26 – 1.11 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.81 (s), 164.47 (s), 146.26 (s), 146.18 (s), 136.51 (s), 129.14 (s), 128.39 (s), 127.55 (s), 126.76 (s), 64.44 (s), 61.31 (s), 54.23 (s), 37.08 (s), 29.96 (s), 18.43 (s), 13.52 (s). ESI-MS (m/z): found $[M]^+$ 341.1864, $C_{20}H_{25}N_2O_3^+$ requires 341.1860.

(*S*)-1-(2-((1-(Hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (19). Yield 21.80 g (97 %); mp 85 – 86 ºC; $[\alpha]_D^{20}$: + 2.7 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3336.22; 3041.66; 2951.29; 2926.91; 2853.85; 2815.30; 1737.59; 1661.99; 1629.42; 1537.25; 1478.71; 1443.27; 1374.07; 1349.96; 1249.88; 1215.16; 1114.71; 1078.50; 974.69; 790.91; 755.99; 725.59; 702.37; 678.65; 596.50; 551.87. ^{1}H NMR (400 MHz, DMSO): δ 9.25 (d, *J* = 7.4 Hz, 1H), 8.93 (d, *J* = 5.9 Hz, 2H), 8.67 (t, *J* = 7.8 Hz, 1H), 8.24 – 8.10 (m, 2H), 7.36 – 7.17 (m, 5H), 5.62 – 5.40 (m, 2H), 4.53 (q, *J* = 7.4 Hz, 1H), 3.98 (td, *J* = 6.5, 2.1 Hz, 2H), 3.13 – 2.90 (m, 2H), 1.54 – 1.37 (m, 2H), 1.29 – 1.13 (m, 6H), 0.84 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO): δ 170.82 (s), 164.47 (s), 146.26 (s), 146.18 (s), 136.50 (s), 129.13 (s), 128.37 (s), 127.55 (s), 126.76 (s), 64.74 (s), 61.30 (s), 54.23 (s), 37.09 (s), 30.78 (s), 27.86 (s), 24.82 (s), 21.92 (s), 13.87 (s). ESI-MS (m/z): found $[M]^+$ 369.2178, $C_{22}H_{29}N_2O_3^+$ requires 369.2173.

(*S*)-1-(2-((1-(Hexyloxy)-1-oxopropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (19Ala) To a stirred solution of hexyl (2-bromoacetyl)-L-alaninate (8.00 g, 27.19 mmol) in diethyl ether (100 ml) was added pyridine (2.20 ml, 27.19 mmol). The reaction mixture was stirred at room temperature for 48 hours. To this time spontaneous layer formation was observed. The reaction mixture was left overnight in the fridge then solid amorphous product was triturated under diethyl ether. The product was washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compound as a colorless amorphous solid in 94 % yield. $[\alpha]_D^{20}$: – 48.9º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3420.02; 3052.54; 2932.25; 2859.55; 1739.68; 1688.07; 1635.87; 1551.62; 1489.39; 1456.38; 1204.16; 1160.24; 1055.79; 794.88; 676.61. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.19 (d, *J* = 6.8 Hz, 1H), 9.00 (d, *J* = 5.6 Hz, 2H), 8.68 (t, *J* = 7.8 Hz, 1H), 8.20 (dd, *J* = 7.6, 6.8 Hz, 2H), 5.56 (s, 2H), 4.31 (p, *J* = 7.2 Hz, 1H), 4.04 (qt, *J* = 10.8, 6.6 Hz, 2H), 1.59 – 1.49 (m, 2H), 1.34 (d, *J* = 7.3 Hz, 3H), 1.30 – 1.18 (m, 6H), 0.83 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.92 (s), 164.29 (s), 146.21 (s), 127.52 (s), 64.61 (s), 61.22 (s), 48.24 (s), 30.75 (s),

27.95 (s), 24.82 (s), 21.92 (s), 17.05 (s), 13.83 (s). ESI-MS (m/z): found $[M]^+$ 293.1854, $C_{16}H_{25}N_2O_3^+$ requires 293.1860.

(*S*)-1-(2-((1-(Octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (20). Yield 22.90 g (96 %); mp 98–99 ºC; $[\alpha]_D^{20}$: + 3.2 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3336.17; 3041.83; 2951.30; 2915.83; 2851.01; 1738.00; 1662.07; 1629.44; 1536.95; 1478.81; 1443.60; 1397.32; 1374.76; 1349.71; 1249.73; 1201.01; 1115.18; 1082.75; 1034.80; 975.48; 791.03; 756.39; 725.74; 702.63; 678.97; 596.58; 552.61. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.22 (d, *J* = 7.5 Hz, 1H), 8.91 (d, *J* = 5.6 Hz, 2H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 7.7, 6.8 Hz, 2H), 7.46 – 7.09 (m, 5H), 5.61 – 5.37 (m, 2H), 4.54 (q, *J* = 7.4 Hz, 1H), 4.12 – 3.85 (m, 2H), 3.13 – 2.88 (m, 2H), 1.52 – 1.37 (m, 2H), 1.34 – 1.09 (m, 10H), 0.85 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.83 (s), 164.47 (s), 146.26 (s), 146.19 (s), 136.49 (s), 129.13 (s), 128.37 (s), 127.55 (s), 126.77 (s), 64.75 (s), 61.31 (s), 54.20 (s), 37.12 (s), 31.18 (s), 28.54 (s), 28.51 (s), 27.90 (s), 25.17 (s), 22.06 (s), 13.96 (s).. ESI-MS (m/z): found $[M]^+$ 397.2495, $C_{24}H_{33}N_2O_3^+$ requires 397.2486.

(*S*)-1-(2-((1-(Decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (21). Yield 24.25 g (96 %); mp 105–107 ºC; $[\alpha]_D^{20}$: + 3.3 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3335.66; 3042.11 ; 2951.55; 2915.66; 2849.80; 1737.91; 1661.78; 1629.59; 1537.79; 1479.03; 1443.50; 1374.11; 1349.35; 1250.18; 1215.02; 1201.24; 1115.45; 972.36; 790.95; 756.57; 725.63; 702.78; 678.96; 596.88; 552.76. ^{1}H NMR (400 MHz, DMSO-d_6); δ 9.23 (d, *J* = 7.5 Hz, 1H), 8.91 (d, *J* = 5.5 Hz, 2H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 7.7, 6.8 Hz, 2H), 7.35 – 7.20 (m, 5H), 5.62 – 5.38 (m, 2H), 4.54 (q, *J* = 7.4 Hz, 1H), 4.08 – 3.88 (m, 2H), 3.11 – 2.89 (m, 2H), 1.54 – 1.36 (m, 2H), 1.29 – 1.10 (m, 14H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6); δ 170.83 (s), 164.47 (s), 146.25 (s), 146.19 (s), 136.49 (s), 129.13 (s), 128.37 (s), 127.55 (s), 126.77 (s), 64.76 (s), 61.31 (s), 54.20 (s), 37.12 (s), 31.28 (s), 28.91 (s), 28.86 (s), 28.68 (s), 28.57 (s), 27.90 (s), 25.16 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 425.2803, $C_{26}H_{37}N_2O_3^+$ requires 425.2799.

(*S*)-1-(2-((1-(Dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (22). Yield 26.15 g (98 %); mp 110–113 ºC; $[\alpha]_D^{20}$: +2.8º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3335.07; 3042.12; 2951.69; 2915.62; 2849.36; 1738.03; 1661.41; 1629.51; 1537.54; 1478.82; 1397.33; 1374.30; 1349.03; 1249.91; 1214.85; 1200.77; 1115.62; 1078.58; 1029.14; 971.50; 848.56; 790.90; 756.54; 725.75; 702.64; 678.89; 596.46; 553.03. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.22 (d, *J* = 7.5 Hz, 1H), 8.91 (d, *J* = 5.5 Hz, 2H), 8.66 (dd, *J* = 11.1, 4.5 Hz, 1H), 8.18 (dd, *J* = 7.7, 6.8 Hz, 2H), 7.37 – 7.18 (m, 5H), 5.61 – 5.37 (m, 2H), 4.54 (q, *J* = 7.5 Hz, 1H), 4.06 – 3.90 (m, 2H), 3.11 – 2.92 (m, 2H), 1.45 (dd, *J* = 13.7, 6.7 Hz, 2H), 1.23 (s, 18H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.83 (s), 164.46 (s), 146.25 (s), 146.20 (s), 136.48 (s), 129.13 (s), 128.37 (s), 127.55 (s), 126.76 (s), 64.76 (s), 61.32 (s), 54.19 (s), 37.13 (s), 31.29 (s), 29.02 (s), 29.01 (s), 28.95 (s), 28.85 (s), 28.70 (s), 28.57 (s), 27.90 (s), 25.16 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 453.3120, $C_{28}H_{41}N_2O_3^+$ requires 453.3112.

(*S*)-1-(2-((1-(Tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (23) Yield 26.95 g (96 %); mp 116–118 ºC; $[\alpha]_D^{20}$: +3.5 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3335.83; 3042.01; 2952.13; 2915.75; 2849.22; 1737.57; 1662.05; 1629.26; 1536.55; 1479.00; 1397.12; 1374.17; 1348.90; 1250.08; 1200.80; 1114.64; 1078.88; 1036.74; 971.25; 790.89; 756.85; 725.89; 702.95; 678.76; 597.15; 552.16 ^{1}H NMR (400 MHz, DMSO-d_6); δ 9.25 (d, *J* = 7.5 Hz, 1H), 8.93 (d, *J* = 5.6 Hz, 2H), 8.67 (t, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 7.6, 6.8 Hz, 2H), 7.38 – 7.17 (m, 5H), 5.62 – 5.41 (m, 2H), 4.53 (q, *J* = 7.4 Hz, 1H), 4.08 – 3.90 (m, 2H), 3.10 – 2.88 (m, 2H), 1.45 (dd, *J* = 13.5, 6.6 Hz, 2H), 1.23 (s, 22H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO); δ 170.80 (s), 164.46 (s), 146.24 (s), 146.18 (s), 136.50 (s), 129.13 (s), 128.35 (s), 127.54 (s), 126.73 (s), 64.74 (s), 61.30 (s), 54.21 (s), 37.10 (s), 31.29 (s), 29.04 (s), 29.01 (s), 28.95 (s), 28.86 (s), 28.70 (s), 28.58 (s), 27.90 (s), 25.17 (s), 22.09 (s), 13.94 (s). ESI-MS (m/z): found $[M]^+$ 481.3434, $C_{30}H_{45}N_2O_3^+$ requires 481.3425.

(*S*)-1-(2-((1-(Hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (24) Yield 28.60 g (97 %); mp 118–120 ºC; $[\alpha]_D^{20}$: + 3.0º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3335.87; 3042.03; 2916.46; 2849.46; 1737.55; 1661.63; 1629.46; 1536.78; 1478.98; 1443.47; 1396.83; 1373.99; 1348.82; 1250.37; 1200.68; 1116.35; 1079.45; 1047.13; 970.38; 848.53; 791.06; 756.81; 726.05; 702.96; 678.88; 597.23; 552.61. ^{1}H NMR (400 MHz, DMSO-d_6); δ 9.24 (d, *J* = 7.5 Hz, 1H), 8.92 (d, *J* = 5.5 Hz, 2H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.18 (dd, *J* = 7.7, 6.8 Hz, 2H), 7.34 – 7.18 (m, 5H), 5.61 – 5.40 (m, 2H), 4.54 (q, *J* = 7.4 Hz, 1H), 4.05 – 3.90 (m, 2H), 3.12 – 2.87 (m, 2H), 1.45 (dd, *J* = 13.6, 6.7 Hz, 2H), 1.23 (s, 26H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6); δ 170.81 (s), 164.46 (s), 146.24 (s), 146.18 (s), 136.49 (s), 129.12 (s), 128.35 (s), 127.54 (s), 126.74 (s), 64.74 (s), 61.31 (s), 54.20 (s), 37.12 (s), 31.28 (s), 29.03 (s), 29.01 (s), 29.00 (s), 28.95 (s), 28.86 (s), 28.70 (s), 28.58 (s), 27.90 (s), 25.17 (s), 22.09 (s), 13.94 (s). ESI-MS (m/z): found $[M]^+$ 509.3743, $C_{32}H_{49}N_2O_3^+$ requires 509.3738.

General method of synthesis of imidazolium salts (25-32)

1-Methylimidazole (3.98 ml, 50 mmol) was added to a stirred solution of corresponding alkyl (2-bromoacetyl)-L-phenylalaninate (50 mmol) in 100 mL of diethyl ether or 1:1 dicloromethane/acetonitrile mixture (the latter was used in the cases of dodecyl, tetradecyl and hexadecyl derivatives). The reaction mixture was stirred at room temperature for 48 hours. As a rule, spontaneous crystallization was observed. If crystallization did not occur, the reaction mixture was left overnight in the fridge and then was crystallized. Solutions in mixture dicloromethane/acetonitrile were evaporated *in vacuo* and then viscous liquid residue was crystallized under diethyl ether. In all cases except of butyl derivatives (a pale yellow viscous oil) was obtained white solid products. The crude product was washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compound of 91 – 97 % yield.

(*S*)-1-Methyl-3-(2-((1-(ethyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (25). Yield 18.00 g (91 %); mp 74–75 ºC; $[\alpha]_D^{20}$**:** + 7.7 º (1.0 c, MeOH). IR (KBr, cm^{-1}):

3397.97; 3228.89; 3029.51; 1736.48; 1680.32; 1530.22; 1454.32; 1374.76; 1346.52; 1264.43; 1219.80; 1181.60; 1109.54; 1030.15; 854.42; 750.56; 703.79; 618.77; 557.95; 466.46. ^{1}H NMR (400 MHz, DMSO-d_6); δ 9.09 (s, 1H), 9.04 (d, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 1.7 Hz, 1H), 7.62 (t, *J* = 1.7 Hz, 1H), 7.34 – 7.19 (m, 5H), 5.11 – 4.97 (m, 2H), 4.55 – 4.44 (m, 1H), 4.11 – 3.97 (m, 2H), 3.88 (s, 3H), 3.00 (qd, *J* = 13.8, 7.3 Hz, 2H), 1.09 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6); δ 170.92 (s), 165.08 (s), 137.72 (s), 136.65 (s), 129.15 (s), 128.35 (s), 126.73 (s), 123.66 (s), 123.01 (s), 60.75 (s), 54.08 (s), 50.29 (s), 36.89 (s), 35.82 (s), 13.93 (s). ESI-MS (m/z): found $[M]^+$ 316.1665, $C_{17}H_{22}N_3O_3^+$ requires 316.1656.

(*S*)-1-Methyl-3-(2-((1-(butyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (26). Yield 20.40 g (96 %); liquid at r.t.; $[\alpha]_D^{20}$: + 5.0º (1.0 c, MeOH).

IR (CH_3CN, cm^{-1}): 3034.13; 2959.57; 1737.39; 1687.61; 1559.38; 1455.40; 1177.74; 941.97; 747.20; 701.84; 622.20. ^{1}H NMR (400 MHz, DMSO-d_6); δ 9.09 (s, 1H), 9.05 (d, *J* = 7.4 Hz, 1H), 7.72–7.68 (m, 1H), 7.63 – 7.60 (m, 1H), 7.35 – 7.18 (m, 5H), 5.14 – 4.92 (m, 2H), 4.51 (dd, *J* = 14.4, 7.4 Hz, 1H), 3.99 (t, *J* = 5.9 Hz, 2H), 3.88 (s, 3H), 3.00 (qd, *J* = 13.7, 7.4 Hz, 2H), 1.44 (dd, *J* = 13.3, 6.9 Hz, 2H), 1.21 (dq, *J* = 14.7, 7.2 Hz, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.00 (s), 165.05 (s), 137.71 (s), 136.63 (s), 129.10 (s), 128.36 (s), 126.73 (s), 123.65 (s), 123.01 (s), 64.40 (s), 54.10 (s), 50.29 (s), 36.93 (s), 35.82 (s), 29.98 (s), 18.45 (s), 13.52 (s). ESI-MS (m/z): found $[M]^+$ 344.1979, $C_{19}H_{26}N_3O_3^+$ requires 344.1969.

(*S*)-1-Methyl-3-(2-((1-(hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (27). Yield 21.3 g (94 %); mp 62–65 ºC; $[\alpha]_D^{20}$: + 4.8 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3338.27; 3086.68; 2952.08; 2927.25; 2852.89; 1737.41; 1666.37; 1536.32; 1495.23; 1455.04; 1377.77; 1352.50; 1250.98; 1202.67; 1170.62; 1115.35; 1079.71; 1029.39; 973.70; 826.85; 752.13; 719.43; 702.23; 624.42; 598.45; 550.33. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.06 (s, 1H), 9.02 (d, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 1.6 Hz, 1H), 7.61 (t, *J* = 1.6 Hz, 1H), 7.34 – 7.19 (m, 5H), 5.11 – 4.94 (m, 2H), 4.51 (dd, *J* = 14.5, 7.6 Hz, 1H), 4.03 – 3.93 (m, 2H), 3.88 (s, 3H), 3.00 (qd, *J* = 13.7, 7.3 Hz, 2H), 1.44 (dd, *J* = 13.1, 6.6 Hz, 2H), 1.28 – 1.15 (m, 6H), 0.85 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.02 (s), 165.04 (s), 137.72 (s), 136.60 (s), 129.09 (s), 128.36 (s), 126.75 (s), 123.67 (s), 123.01 (s), 64.71 (s), 54.07 (s), 50.28 (s), 36.98 (s), 35.81 (s), 30.79 (s), 27.88 (s), 24.84 (s), 21.93 (s), 13.87 (s). ESI-MS (m/z): found $[M]^+$ 372.2279, $C_{21}H_{30}N_3O_3^+$ requires 372.2282.

(*S*)-3-(2-((1-(hexyloxy)-1-oxopropan-2-yl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium bromide (27Ala). To a stirred solution of hexyl (2-bromoacetyl)-L-alaninate (8.00 g, 27.19 mmol) in diethyl ether (100 ml) was added 1-methylimidazole (2.17 ml, 27.19 mmol). The reaction mixture was stirred at room temperature for 48 hours. To this time spontaneous crystallization was observed. The crude product was washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compound as a white solid product (mp 56 – 58 ºC) in 95 % yield. $[\alpha]_D^{20}$: – 44.9 º (1.0 c, MeOH). IR (KBr, cm–1): 3431.03; 3060.92; 2932.97; 2859.92; 1740.58; 1688.91; 1564.07; 1456.98; 1377.35; 1176.69; 1056.80;

756.07; 622.71. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.14 (s, 1H), 8.98 (d, J = 6.9 Hz, 1H), 7.82 – 7.60 (m, 2H), 5.07 (s, 2H), 4.29 (p, J = 7.2 Hz, 1H), 4.04 (qt, J = 10.8, 6.6 Hz, 2H), 3.90 (s, 3H), 1.61 – 1.49 (m, 2H), 1.32 (d, J = 7.3 Hz, 3H), 1.30 – 1.20 (m, 6H), 0.85 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 172.06 (s), 164.83 (s), 137.72 (s), 123.68 (s), 123.00 (s), 64.56 (s), 50.24 (s), 48.04 (s), 35.81 (s), 30.76 (s), 27.96 (s), 24.83 (s), 21.93 (s), 17.01 (s), 13.83 (s). ESI-MS (m/z): found $[M]^+$ 296.1970, $C_{15}H_{26}N_3O_3^+$ requires 296.1969.

(*S*)-1-Methyl-3-(2-((1-(octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (28). Yield 23.3 g (97 %); mp 83–84 ºC; $[\alpha]_D^{20}$: + 4.8 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3337.69; 3086.94; 2951.77; 2916.30; 2850.85; 1737.60; 1666.33; 1537.67; 1494.65; 1444.49; 1397.62; 1378.37; 1352.19; 1250.31; 1217.68; 1202.65; 1170.72; 1114.99; 1083.82; 1032.06; 975.11; 827.08; 752.39; 720.33; 702.46; 624.54; 599.30; 551.59. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.06 (s, 1H), 9.01 (d, J = 7.5 Hz, 1H), 7.69 (t, J = 1.6 Hz, 1H), 7.61 (t, J = 1.6 Hz, 1H), 7.33 – 7.20 (m, 5H), 5.12 – 4.90 (m, 2H), 4.51 (dd, J = 14.4, 7.7 Hz, 1H), 4.04 – 3.92 (m, 2H), 3.88 (s, 3H), 2.99 (qd, J = 13.7, 7.3 Hz, 2H), 1.52 – 1.38 (m, 2H), 1.33 – 1.12 (m, 10H), 0.86 (t, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.03 (s), 165.04 (s), 137.73 (s), 136.60 (s), 129.09 (s), 128.36 (s), 126.75 (s), 123.68 (s), 123.01 (s), 64.72 (s), 54.05 (s), 50.27 (s), 36.99 (s), 35.81 (s), 31.19 (s), 28.55 (s), 28.52 (s), 27.91 (s), 25.18 (s), 22.07 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 400.2591, $C_{23}H_{34}N_3O_3^+$ requires 400.2595.

(*S*)-1-Methyl-3-(2-((1-(decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (29). Yield 24.40 g (96 %); mp 90–91 ºC; $[\alpha]_D^{20}$: + 5.2 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3428.89; 3337.67; 3087.24; 2951.93; 2915.88; 2849.82; 1737.48; 1666.31; 1538.39; 1494.84; 1466.05; 1378.17; 1351.84; 1250.84; 1217.66; 1202.78; 1170.76; 1116.05; 1031.54; 970.91; 827.36; 752.52; 719.86; 702.63; 624.56; 599.13; 551.37. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.07 (s, 1H), 9.02 (d, J = 7.5 Hz, 1H), 7.69 (t, J = 1.7 Hz, 1H), 7.61 (t, J = 1.7 Hz, 1H), 7.33 – 7.20 (m, 5H), 5.08 – 4.97 (m, 2H), 4.51 (dd, J = 14.4, 7.7 Hz, 1H), 4.04 – 3.92 (m, 2H), 3.88 (s, 3H), 2.99 (qd, J = 13.7, 7.3 Hz, 2H), 1.51 – 1.39 (m, 2H), 1.30 – 1.15 (m, 14H), 0.85 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.02 (s), 165.04 (s), 137.72 (s), 136.60 (s), 129.09 (s), 128.35 (s), 126.73 (s), 123.67 (s), 123.00 (s), 64.72 (s), 54.05 (s), 50.28 (s), 36.99 (s), 35.81 (s), 31.29 (s), 28.92 (s), 28.87 (s), 28.68 (s), 28.58 (s), 27.91 (s), 25.18 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 428.2902, $C_{25}H_{38}N_3O_3^+$ requires 428.2908.

(*S*)-1-Methyl-3-(2-((1-(dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (30). Yield 25.50 g (95 %); mp 94–95 ºC; $[\alpha]_D^{20}$: + 4.7 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3335.57; 3086.54; 2951.97; 2915.80; 2849.45; 1738.00; 1665.55; 1537.65; 1494.72; 1465.61; 1397.79; 1378.31; 1351.19; 1250.55; 1218.06; 1202.03; 1170.88; 1116.86; 1030.01; 970.23; 827.13; 785.26; 752.01; 720.71; 702.32; 624.43; 600.14; 553.02. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.06 (s, 1H), 9.01 (d, J = 7.5 Hz, 1H), 7.69 (t, J = 1.7 Hz, 1H), 7.61 (t, J = 1.7 Hz, 1H), 7.33 – 7.20 (m, 5H), 5.07 – 4.96 (m,

2H), 4.52 (dd, J = 14.4, 7.7 Hz, 1H), 4.03 – 3.93 (m, 2H), 3.88 (s, 3H), 2.99 (qd, J = 13.8, 7.3 Hz, 2H), 1.51 – 1.39 (m, 2H), 1.31 – 1.12 (m, 18H), 0.85 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 171.02 (s), 165.04 (s), 137.73 (s), 136.60 (s), 129.09 (s), 128.35 (s), 126.73 (s), 123.68 (s), 123.00 (s), 64.73 (s), 54.04 (s), 50.27 (s), 37.00 (s), 35.81 (s), 31.29 (s), 29.03 (s), 29.01 (s), 28.96 (s), 28.86 (s), 28.71 (s), 28.58 (s), 27.91 (s), 25.18 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 456.3217, $C_{27}H_{42}N_3O_3^+$ requires 456.3221.

(*S*)-1-Methyl-3-(2-((1-(tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (31). Yield 27.40 g (97 %); mp 103–104 ºC; $[\alpha]_D^{20}$: + 4.6 º (1.0 c, MeOH);. IR (KBr, cm^{-1}): 3433.71; 3340.57; 3087.25; 2952.69; 2916.38; 2849.42; 1736.82; 1666.86; 1535.69; 1465.02; 1397.53; 1377.20; 1353.10; 1251.63; 1203.80; 1170.35; 1115.58; 1032.47; 970.33; 827.51; 753.33; 719.09; 703.11; 624.46; 598.38; 544.09. ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 9.08 (s, 1H), 9.03 (d, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 1.7 Hz, 1H), 7.61 (t, *J* = 1.7 Hz, 1H), 7.32 – 7.20 (m, 5H), 5.12 – 4.92 (m, 2H), 4.51 (dd, *J* = 14.4, 7.7 Hz, 1H), 4.03 – 3.92 (m, 2H), 3.88 (s, 3H), 3.00 (qd, *J* = 13.8, 7.3 Hz, 2H), 1.51 – 1.39 (m, 2H), 1.32 – 1.11 (m, 22H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 171.00 (s), 165.04 (s), 137.72 (s), 136.61 (s), 129.08 (s), 128.33 (s), 126.71 (s), 123.66 (s), 123.00 (s), 64.71 (s), 54.06 (s), 50.28 (s), 36.99 (s), 35.81 (s), 31.29 (s), 29.05 (s), 29.02 (s), 29.01 (s), 28.96 (s), 28.87 (s), 28.70 (s), 28.59 (s), 27.91 (s), 25.18 (s), 22.09 (s), 13.95 (s). ESI-MS (m/z): found $[M]^+$ 484.3528, $C_{29}H_{46}N_3O_3^+$ requires 484.3534.

(*S*)-1-Methyl-3-(2-((1-(hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (32). Yield 28.45 g (96 %); mp 105–107 ºC; $[\alpha]_D^{20}$: + 4.0 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3433.00; 3339.44; 3086.64; 2952.58; 2916.67; 2849.48; 1736.77; 1666.46; 1537.63; 1464.62; 1377.16; 1352.39; 1251.92; 1203.21; 1170.55; 1116.32; 969.24; 827.46; 753.22; 719.20; 703.01; 624.41; 598.94; 549.89. ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 9.07 (s, 1H), 9.03 (d, *J* = 7.5 Hz, 1H), 7.71–7.67 (m, 1H), 7.64 – 7.60 (m, 1H), 7.33 – 7.18 (m, 5H), 5.13 – 4.93 (m, 2H), 4.51 (dd, *J* = 14.5, 7.5 Hz, 1H), 4.03 – 3.92 (m, 2H), 3.88 (s, 3H), 2.99 (qd, *J* = 13.7, 7.3 Hz, 2H), 1.50 – 1.40 (m, 2H), 1.31 – 1.11(m, 26H), 0.85 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 171.00 (s), 165.04 (s), 137.72 (s), 136.60 (s), 129.08 (s), 128.33 (s), 126.71 (s), 123.66 (s), 123.00 (s), 64.71 (s), 54.05 (s), 50.28 (s), 36.99 (s), 35.81 (s), 31.29 (s), 29.04 (s), 29.00 (s), 28.96 (s), 28.87 (s), 28.70 (s), 28.59 (s), 27.92 (s), 25.18 (s), 22.09 (s), 13.95 (s). ESI-MS (m/z): found $[M]^+$ 512.3844, $C_{31}H_{50}N_3O_3^+$ requires 512.3847.

General method of synthesis of cholinium salts (33-40)

Dimethylethanolamine (5.03 ml, 50 mmol) was added to a stirred solution of corresponding alkyl (2-bromoacetyl)-L-phenylalaninate (50 mmol) in 100 mL of diethyl ether or 1:1 dicloromethane/acetonitrile mixture (the latter was used in the cases of dodecyl, tetradecyl and hexadecyl derivatives). Product was

observed precipitating as a white solid approximately after 30 min. The solution was stirred at room temperature for 48 hours. Solutions in mixture dicloromethane/acetonitrile were evaporated *in vacuo* and then viscous liquid residue was crystallized under diethyl ether. The solid product was washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compound as a white solid in 95 – 98 % yield.

(*S*)-2-((1-(Ethoxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (33). Yield 19.15 g (95 %); mp 104–105 ºC; $[\alpha]_D^{20}$: – 6.2 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3348.76; 3210.94; 3057.40; 2977.17; 2921.12; 1744.42; 1690.97; 1548.68; 1471.19; 1456.22; 1441.30; 1417.44; 1370.67; 1342.25; 1282.03; 1245.06; 1214.55; 1179.95; 1112.87; 1081.39; 1055.17; 1020.93; 979.99; 910.75; 858.57; 764.55; 740.87; 700.64; 588.78; 496.75. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.14 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.20 (m, 5H), 5.32 (t, *J* = 4.9 Hz, 1H), 4.56 (ddd, *J* = 9.1, 7.6, 5.7 Hz, 1H), 4.19 (dd, *J* = 31.5, 15.0 Hz, 2H), 4.12 – 4.04 (m, 2H), 3.79 (dd, *J* = 9.8, 4.8 Hz, 2H), 3.57 – 3.47 (m, 2H), 3.18 (s, 3H), 3.17 (s, 3H), 3.01 (ddd, *J* = 23.1, 13.9, 7.4 Hz, 2H), 1.13 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.65 (s), 163.41 (s), 136.67 (s), 129.14 (s), 128.33 (s), 126.71 (s), 66.02 (s), 62.46 (s), 60.91 (s), 54.94 (s), 53.64 (s), 52.04 (s), 52.00 (s), 36.47 (s), 13.94 (s). ESI-MS (m/z): found $[M]^+$ 323.1964, $C_{17}H_{27}N_2O_4^+$ requires 323.1965.

(*S*)-2-((1-(Butoxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (34). Yield 20.90 g (97 %); mp 91–93 ºC; $[\alpha]_D^{20}$: – 5.2 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3351.45; 3211.94; 3061.01; 2962.62; 1741.61; 1689.35; 1552.50; 1470.05; 1418.99; 1369.86; 1346.51; 1277.10; 1248.94; 1216.74; 1184.16; 1113.58; 1081.22; 1056.59; 1028.21; 982.15; 932.66; 911.78; 768.49; 704.24; 594.64; 496.90. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.11 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.20 (m, 5H), 5.32 (t, *J* = 4.9 Hz, 1H), 4.57 (ddd, *J* = 8.9, 7.7, 5.9 Hz, 1H), 4.16 (q, *J* = 15.0 Hz, 2H), 4.03 (t, *J* = 6.5 Hz, 2H), 3.79 (dd, *J* = 9.8, 4.8 Hz, 2H), 3.58 – 3.44 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.1, 13.9, 7.5 Hz, 2H), 1.54 – 1.43 (m, 2H), 1.31 – 1.19 (m, 2H), 0.85 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.76 (s), 163.39 (s), 136.63 (s), 129.10 (s), 128.35 (s), 126.72 (s), 66.02 (s), 64.55 (s), 62.46 (s), 54.97 (s), 53.62 (s), 52.03 (s), 51.99 (s), 36.53 (s), 30.01 (s), 18.46 (s), 13.53 (s). ESI-MS (m/z): found $[M]^+$ 351.2274, $C_{19}H_{31}N_2O_4^+$ requires 351.2278.

(*S*)-2-((1-(Hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (35). Yield 22.45 g (98 %); mp 57–59 ºC; $[\alpha]_D^{20}$: – 2.8 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3342.90; 3221.13; 3054.37; 2954.58; 1741.16; 1690.85; 1544.30; 1456.04; 1415.87; 1348.12; 1279.53; 1214.62; 1180.30; 1110.84; 1083.53; 979.14; 763.49; 702.11; 575.81; 496.10. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.14 (d, *J* = 7.5 Hz, 1H), 7.34 – 7.17 (m, 5H), 5.33 (t, *J* = 4.8 Hz, 1H), 4.57 (ddd, *J* = 8.8, 7.7, 6.0 Hz, 1H), 4.17 (q, *J* = 15.0 Hz, 2H), 4.02 (t, *J* = 6.6 Hz, 2H), 3.79 (dd, *J* = 9.3, 4.5 Hz, 2H), 3.57 – 3.47 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.0, 13.9, 7.5 Hz, 2H), 1.53 – 1.43 (m, 2H), 1.32 – 1.14 (m, 6H), 0.86 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6: δ 170.77 (s), 163.39 (s), 136.63 (s), 129.09 (s), 128.34 (s), 126.73 (s), 66.04 (s), 64.85 (s), 62.48 (s), 54.96 (s), 53.65

(s), 52.02 (s), 51.98 (s), 36.54 (s), 30.81 (s), 27.92 (s), 24.86 (s), 21.95 (s), 13.88 (s). ESI-MS **(**m/z): found $[M]^+$ 379.2592, $C_{21}H_{35}N_2O_4^+$ requires 379.2591.

(*S*)-2-((1-(Hexyloxy)-1-oxopropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (35Ala). To a stirred solution of hexyl (2-bromoacetyl)-L-alaninate (8.00 g, 27.19 mmol) in diethyl ether (100 ml) was added dimethylethanolamine (2.74 ml, 27.19 mmol). Product was observed precipitating as a white solid approximately after 30 min. The solution was stirred at room temperature for 48 hours. The solid product was washed with diethyl ether (3 x 50 ml) and dried *in vacuo* to afford the title compound as a white solid (mp 62 – 65 ºC) in 97 % yield. $[\alpha]_D^{20}$: – 21.6 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3367.44; 3052.54; 2932.97; 1741.62; 1685.11; 1549.74; 1458.17; 1210.90; 1165.65; 1057.24; 924.46; 544.58. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.13 (d, *J* = 6.6 Hz, 3H), 5.34 (t, *J* = 4.9 Hz, 3H), 4.34 – 4.19 (m, 9H), 4.05 (qt, *J* = 10.8, 6.6 Hz, 6H), 3.85 (dd, *J* = 9.6, 4.7 Hz, 6H), 3.61 (t, *J* = 4.5 Hz, 6H), 3.27 (s, 18H), 1.54 (dd, *J* = 14.0, 6.8 Hz, 6H), 1.31 (d, *J* = 7.3 Hz, 9H), 1.27 (d, *J* = 14.1 Hz, 17H), 0.85 (t, *J* = 6.8 Hz, 9H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.82 (s), 163.27 (s), 66.06 (s), 64.65 (s), 62.50 (s), 54.93 (s), 52.08 (s), 51.94 (s), 47.97 (s), 30.76 (s), 27.98 (s), 24.83 (s), 21.94 (s), 16.53 (s), 13.83 (s). ESI-MS (m/z): found $[M]^+$ 303.2280, $C_{15}H_{31}N_2O_4^+$ requires 303.2278

(*S*)-2-((1-(Octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (36). Yield 23.40 g (96 %); mp 81–83 ºC; $[\alpha]_D^{20}$: – 2.6 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3330.93; 3223.91; 3062.77; 2922.29; 2854.88; 1741.60; 1691.09; 1547.54; 1476.77; 1416.43; 1348.04; 1279.98; 1244.92; 1215.74; 1181.27; 1112.33; 1084.05; 1030.24; 980.31; 956.06; 908.33; 763.62; 703.34; 575.83; 495.93.^{1}H NMR (400 MHz, DMSO-d_6): δ 9.08 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.20 (m, 5H), 5.32 (t, *J* = 4.9 Hz, 1H), 4.61 – 4.53 (m, 1H), 4.14 (q, *J* = 15.1 Hz, 2H), 4.02 (t, *J* = 6.3 Hz, 2H), 3.79 (dd, *J* = 9.8, 4.8 Hz, 2H), 3.57 – 3.45 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.0, 13.9, 7.5 Hz, 2H), 1.57 – 1.41 (m, 2H), 1.31 – 1.18 (m, 10H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.76 (s), 163.37 (s), 136.58 (s), 129.06 (s), 128.32 (s), 126.71 (s), 66.02 (s), 64.85 (s), 62.44 (s), 54.97 (s), 53.57 (s), 52.03 (s), 51.98 (s), 36.55 (s), 31.18 (s), 28.54 (s), 28.52 (s), 27.93 (s), 25.18 (s), 22.05 (s), 13.94 (s). ESI-MS (m/z): found $[M]^+$ 407.2904, $C_{23}H_{39}N_2O_4^+$ requires 407.2904.

(*S*)-2-((1-(Decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (37). Yield 25.00 g (97 %); mp 64–65 ºC; $[\alpha]_D^{20}$: – 1.8 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3324.41; 3234.57; 3060.35; 2954.14; 2921.15; 2853.08; 1736.83; 1673.31; 1548.75; 1469.35; 1369.62; 1201.15; 1123.54; 1087.74; 996.57; 920.31; 887.16; 738.39; 698.25; 534.16.^{1}H NMR (400 MHz, DMSO-d_6): δ 9.10 (d, *J* = 7.6 Hz, 1H), 7.33 – 7.20 (m, 5H), 5.32 (t, *J* = 4.9 Hz, 1H), 4.57 (ddd, *J* = 8.9, 7.7, 5.9 Hz, 1H), 4.16 (q, *J* = 15.0 Hz, 2H), 4.08 – 3.96 (m, 2H), 3.79 (dd, *J* = 9.8, 4.8 Hz, 2H), 3.60 – 3.44 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.0, 13.9, 7.4 Hz, 2H), 1.55 – 1.42 (m,

2H), 1.29 – 1.18 (m, 14H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.77 (s), 163.39 (s), 136.61 (s), 129.08 (s), 128.33 (s), 126.72 (s), 66.04 (s), 64.86 (s), 62.46 (s), 54.97 (s), 53.61 (s), 52.03 (s), 51.99 (s), 36.56 (s), 31.29 (s), 28.92 (s), 28.89 (s), 28.69 (s), 28.59 (s), 27.95 (s), 25.19 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 435.3219, $C_{25}H_{43}N_2O_4^+$ requires 435.3217.

(*S*)-2-((1-(Dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (38). Yield 26.10 g (96 %); mp 67–68 ºC; $[\alpha]_D^{20}$: –1.3º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3324.06; 3234.67; 3060.67; 2954.59; 2921.19; 2852.41; 1737.02; 1673.42; 1549.48; 1469.60; 1370.43; 1199.33; 1123.66; 1087.79; 996.33; 920.48; 887.22; 738.12; 698.27; 534.50; 501.73. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.10 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.16 (m, 5H), 5.32 (t, *J* = 4.9 Hz, 1H), 4.57 (ddd, *J* = 8.9, 7.7, 6.0 Hz, 1H), 4.16 (q, *J* = 15.0 Hz, 2H), 4.08 – 3.96 (m, 2H), 3.79 (dd, *J* = 9.8, 4.8 Hz, 2H), 3.57 – 3.46 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.0, 13.9, 7.5 Hz, 2H), 1.57 – 1.41 (m, 2H), 1.30 – 1.16 (m, 18H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ170.77 (s), 163.39 (s), 136.61 (s), 129.08 (s), 128.33 (s), 126.72 (s), 66.04 (s), 64.86 (s), 62.46 (s), 54.98 (s), 53.60 (s), 52.03 (s), 51.99 (s), 36.57 (s), 31.29 (s), 29.03 (s), 29.02 (s), 28.96 (s), 28.88 (s), 28.71 (s), 28.59 (s), 27.95 (s), 25.19 (s), 22.09 (s), 13.96 (s). ESI-MS (m/z): found $[M]^+$ 463.3529, $C_{27}H_{47}N_2O_4^+$ requires 463.3530.

(*S*)-2-((1-(Tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (39). Yield 28.00 g (98 %); mp 74–75 ºC; $[\alpha]_D^{20}$: – 2.0º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3323.56; 3234.74; 3061.60; 2954.98; 2921.15; 2851.89; 1737.18; 1673.33; 1549.79; 1469.88; 1370.36; 1209.89; 1123.98; 1088.04; 996.45; 920.43; 886.98; 738.09; 698.30; 534.73. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.12 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.19 (m, 5H), 5.33 (t, *J* = 4.9 Hz, 1H), 4.57 (ddd, *J* = 8.9, 7.6, 5.9 Hz, 1H), 4.17 (q, *J* = 15.0 Hz, 2H), 4.07 – 3.96 (m, 2H), 3.79 (dd, *J* = 9.8, 4.9 Hz, 2H), 3.58 – 3.46 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 22.9, 13.9, 7.4 Hz, 2H), 1.57 – 1.41 (m, 2H), 1.32 – 1.15 (m, 22H), 0.85 (t, *J* = 6.8 Hz, 3H).
^{13}C NMR (101 MHz, DMSO-d_6): δ 170.76 (s), 163.39 (s), 136.61 (s), 129.08 (s), 128.32 (s), 126.71 (s), 66.04 (s), 64.85 (s), 62.46 (s), 54.97 (s), 53.62 (s), 52.02 (s), 51.98 (s), 36.56 (s), 31.29 (s), 29.05 (s), 29.02 (s), 29.01 (s), 28.96 (s), 28.88 (s), 28.70 (s), 28.59 (s), 27.95 (s), 25.19 (s), 22.09 (s), 13.95 (s). ESI-MS (m/z): found $[M]^+$ 491.3843, $C_{27}H_{47}N_2O_4^+$ requires 491.3843.

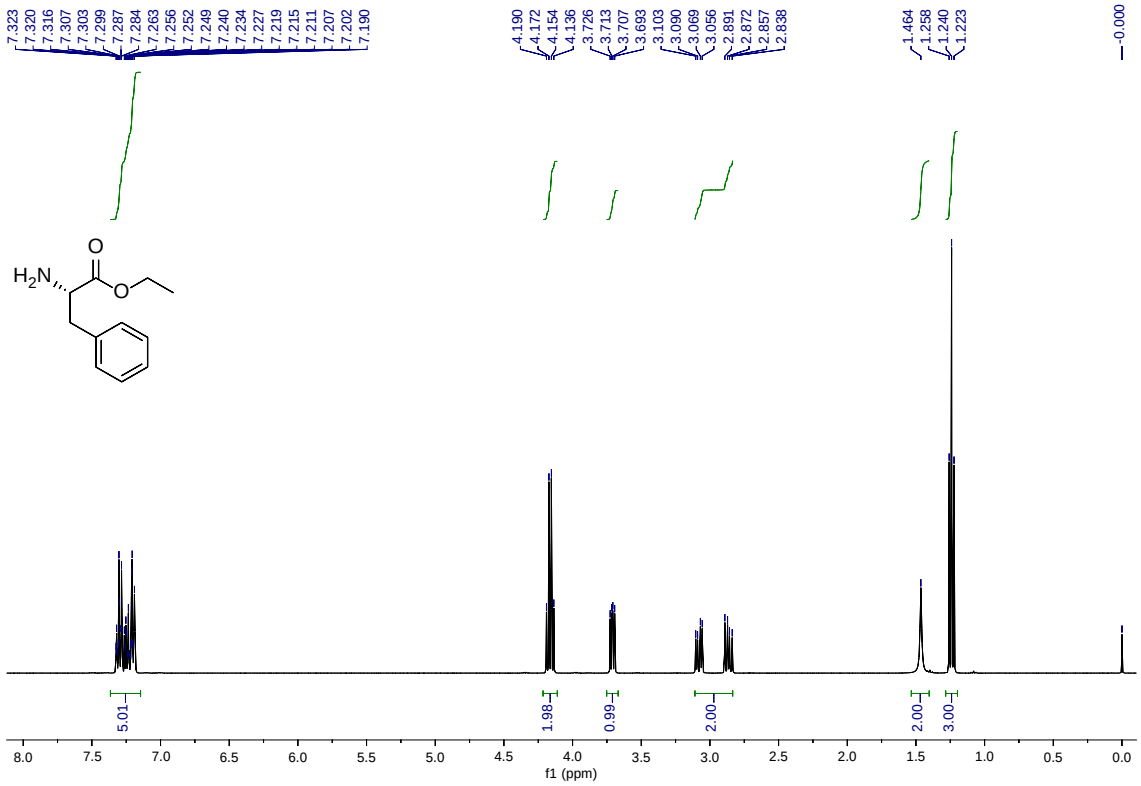
(*S*)-2-((1-(Hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (40). Yield 29.10 g (97 %); mp 80–81 ºC ; $[\alpha]_D^{20}$: – 2.2 º (1.0 c, MeOH). IR (KBr, cm^{-1}): 3322.92; 3234.32; 3061.49; 2955.13; 2920.77; 2851.42; 1737.24; 1673.16; 1549.81; 1470.18; 1369.69; 1204.38; 1123.54; 1088.06; 996.78; 955.64; 920.18; 887.01; 738.05; 719.28; 698.24; 534.52. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.12 (d, *J* = 7.5 Hz, 1H), 7.32 – 7.20 (m, 5H), 5.33 (t, *J* = 4.8 Hz, 1H), 4.57 (ddd, *J* = 8.8, 7.7, 6.0 Hz, 1H), 4.16 (q, *J* = 15.0 Hz, 2H), 4.07 – 3.96 (m, 2H), 3.79 (dd, *J*

= 9.5, 4.7 Hz, 2H), 3.57 – 3.46 (m, 2H), 3.17 (s, 3H), 3.16 (s, 3H), 3.01 (ddd, *J* = 23.0, 13.9, 7.5 Hz, 2H), 1.56 – 1.41 (m, 2H), 1.32 – 1.15 (m, 26H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 170.76 (s), 163.39 (s), 136.61 (s), 129.08 (s), 128.32 (s), 126.71 (s), 66.05 (s), 64.86 (s), 62.46 (s), 54.97 (s), 53.61 (s), 52.03 (s), 51.98 (s), 36.57 (s), 31.29 (s), 29.06–29.02 (m), 29.00 (s), 28.96 (s), 28.88 (s), 28.70 (s), 28.60 (s), 27.95 (s), 25.19 (s), 22.09 (s), 13.95 (s). ESI-MS (m/z): found $[M]^+$ 519.4155, $C_{29}H_{51}N_2O_4^+$ requires 519.4156.

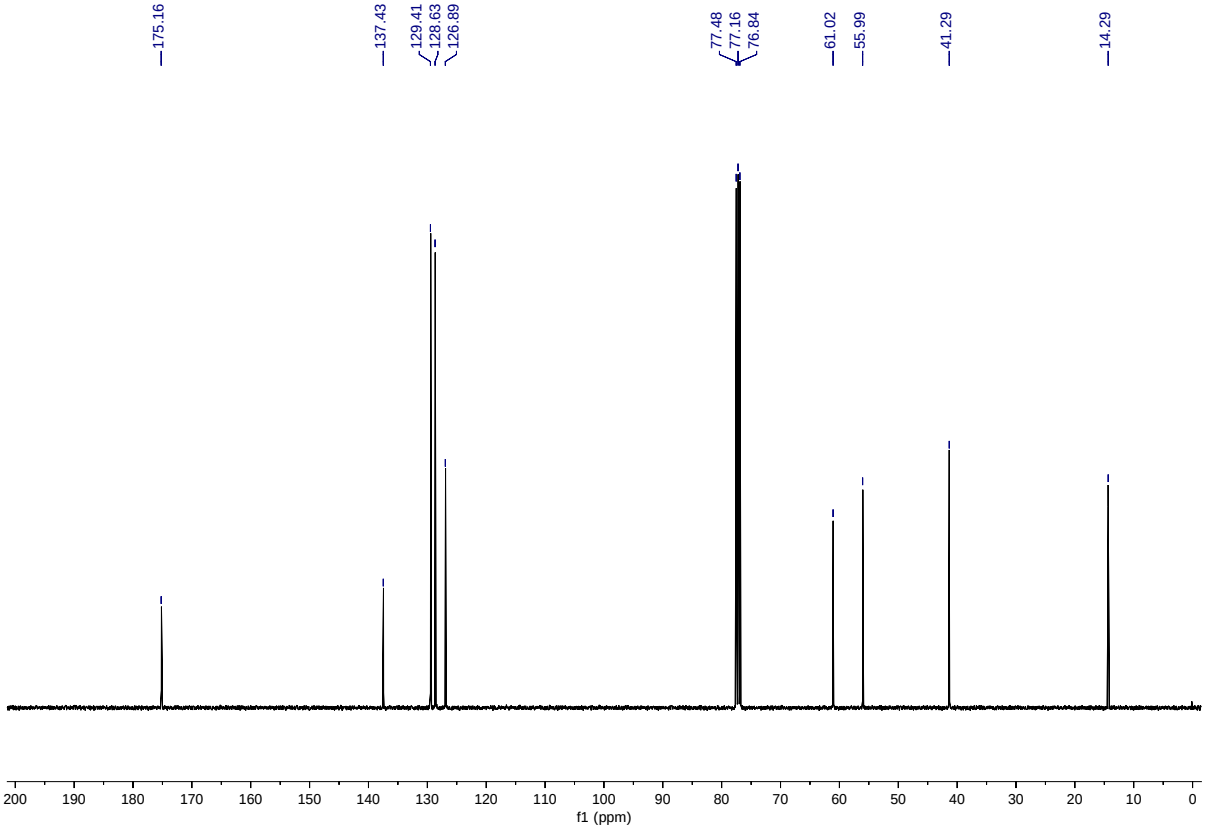
9. NMR spectra of *n*-alkyl L-phenylalaninate

Ethyl L-phenylalaninate (1)

^{1}H NMR

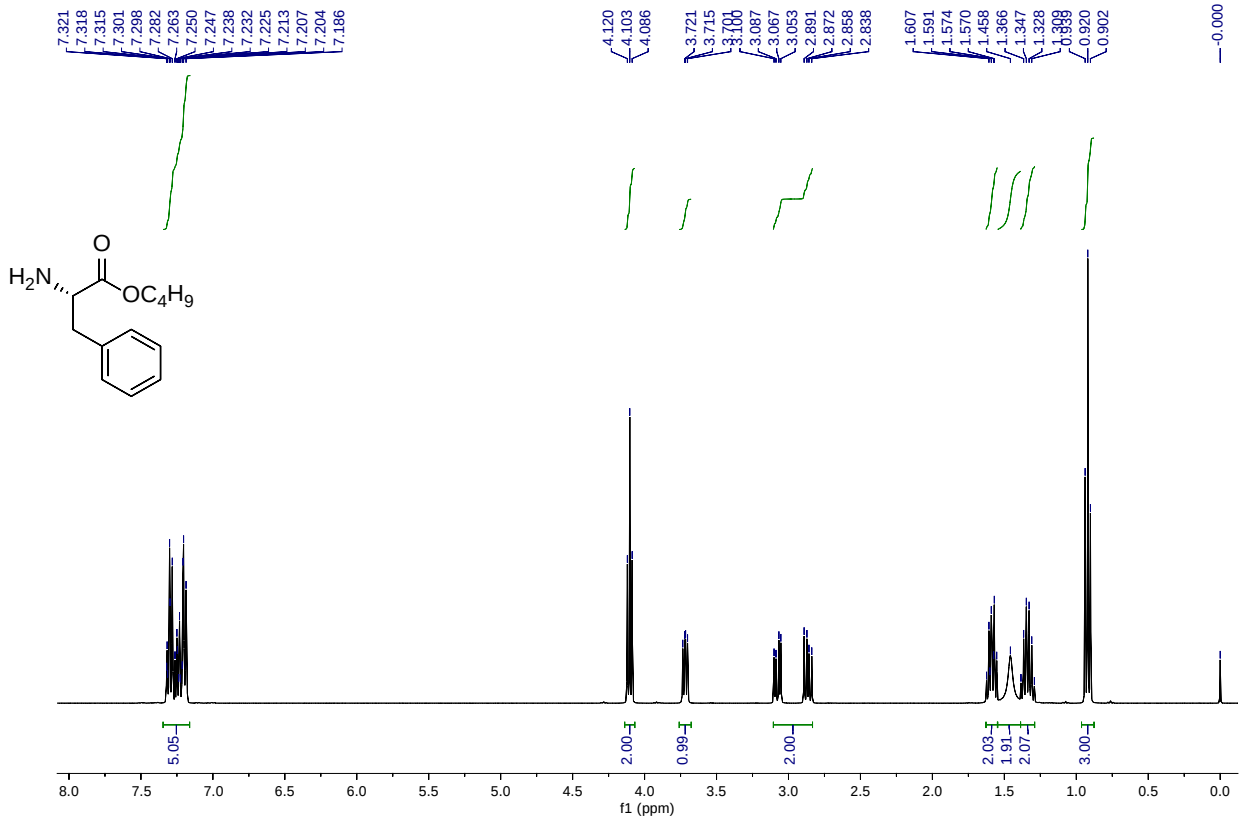


^{13}C NMR

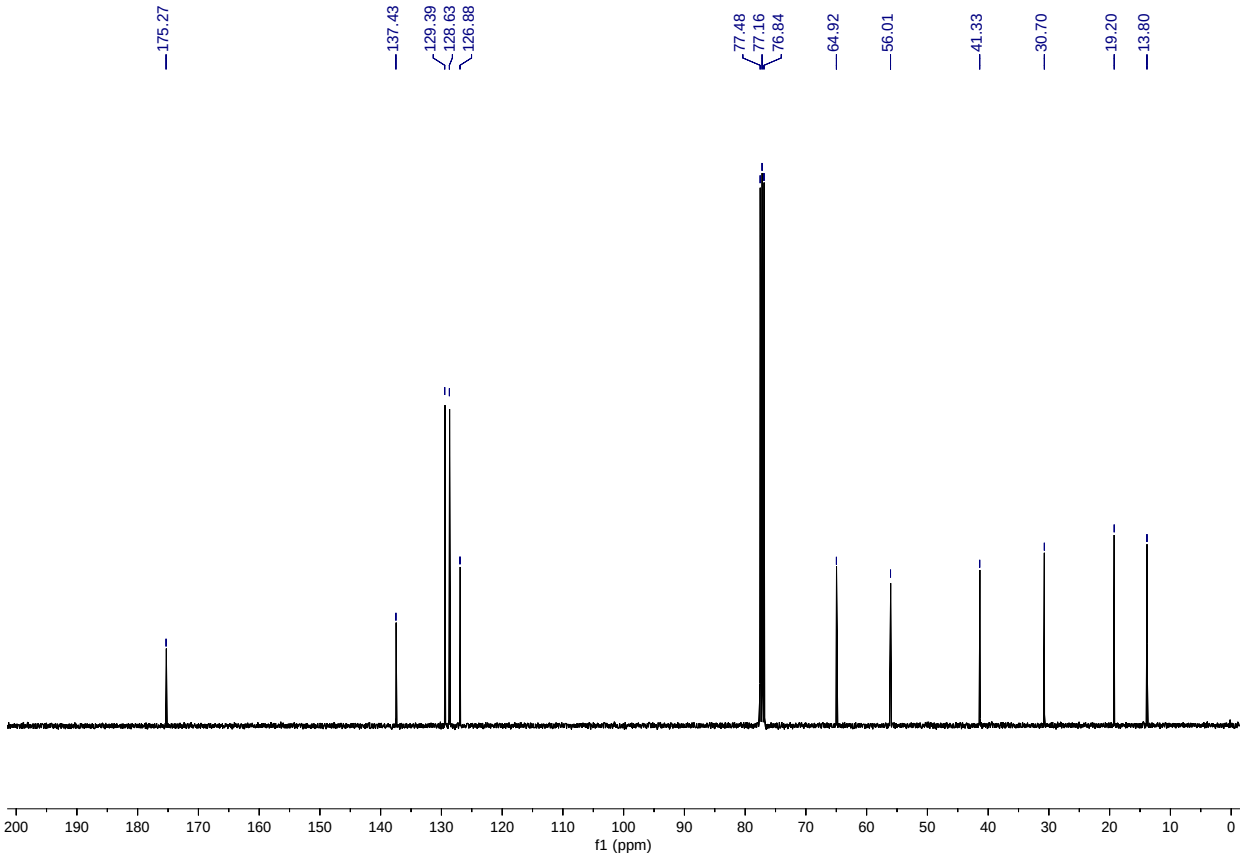


Butyl L-phenylalaninate (2)

^{1}H NMR

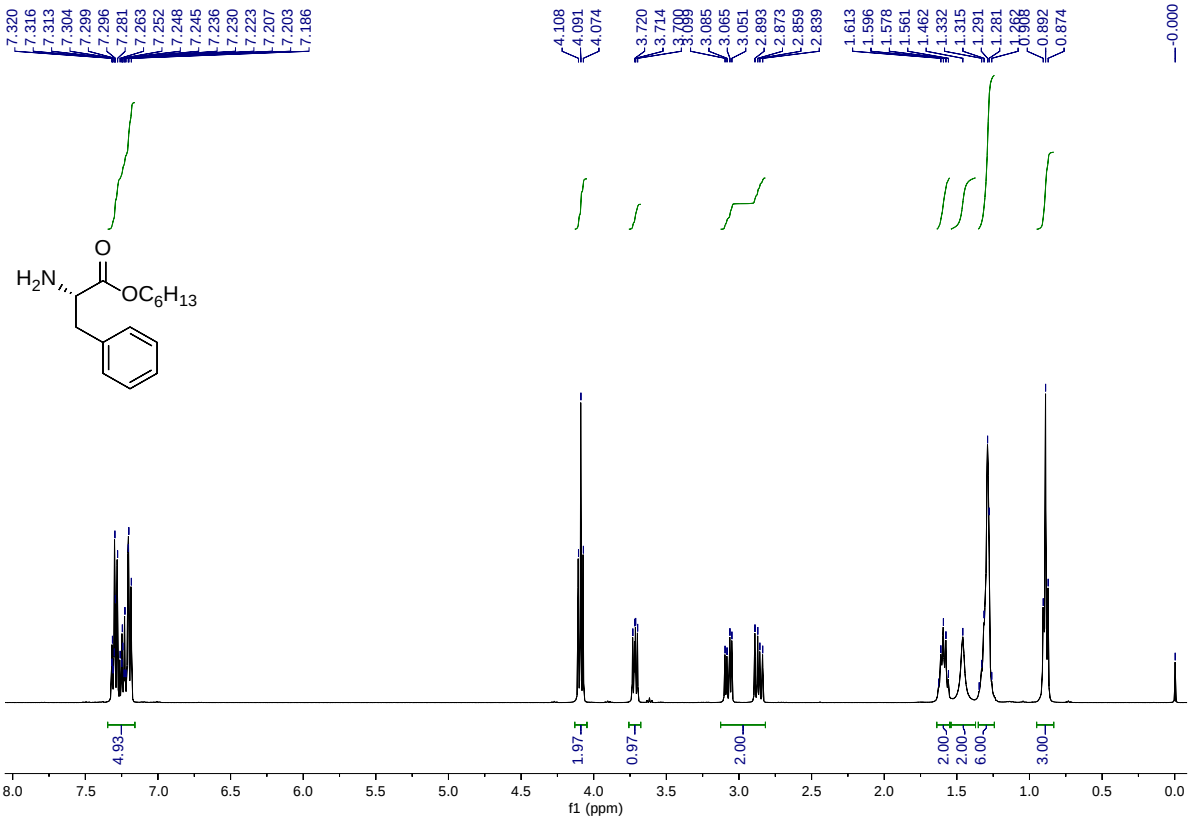


^{13}C NMR

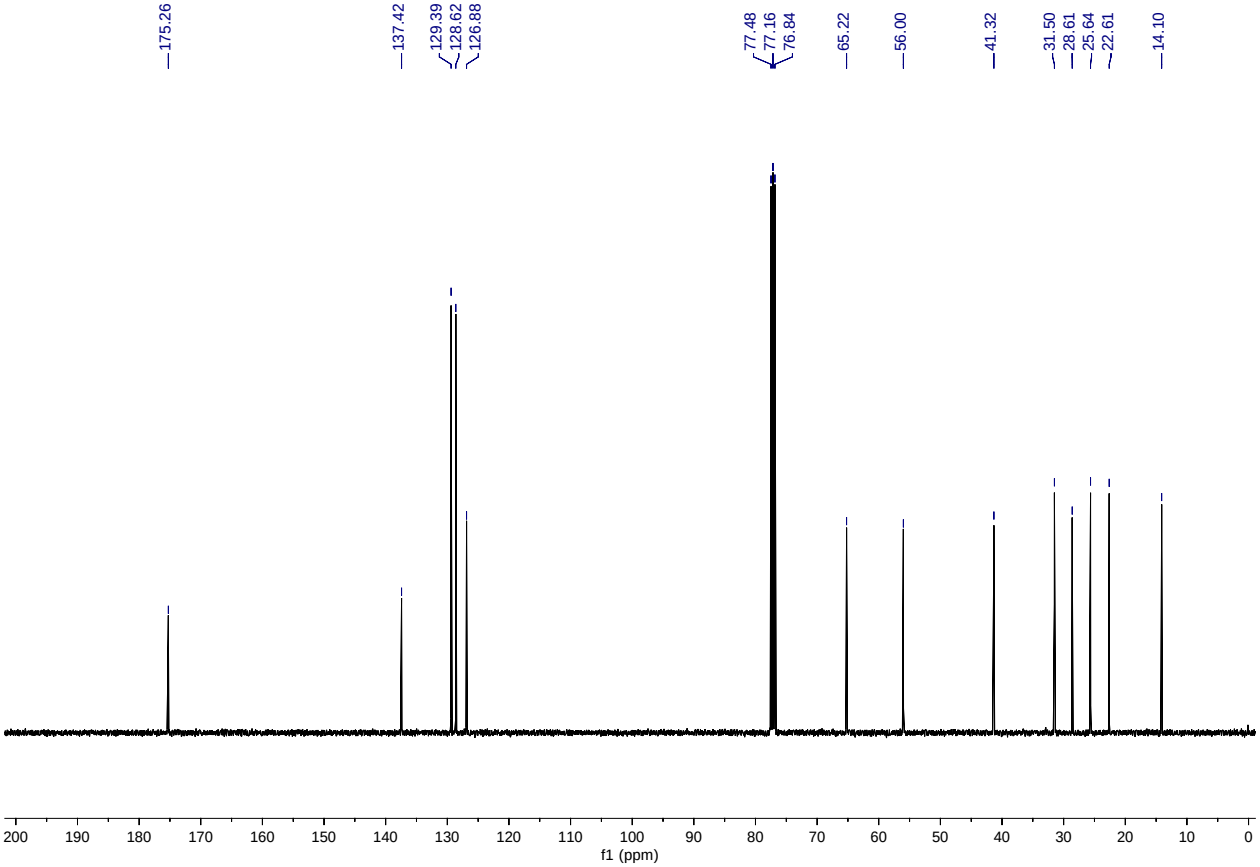


Hexyl L-phenylalaninate (3)

^{1}H NMR

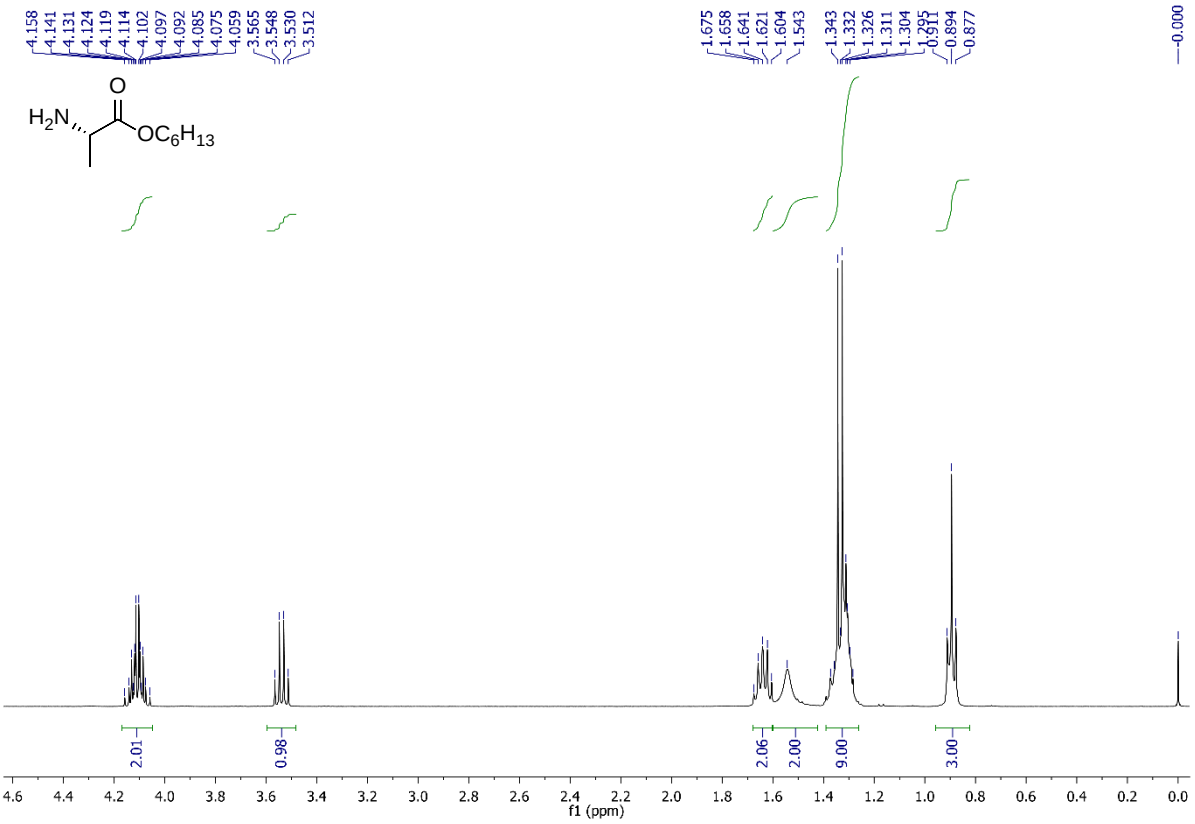


^{13}C NMR

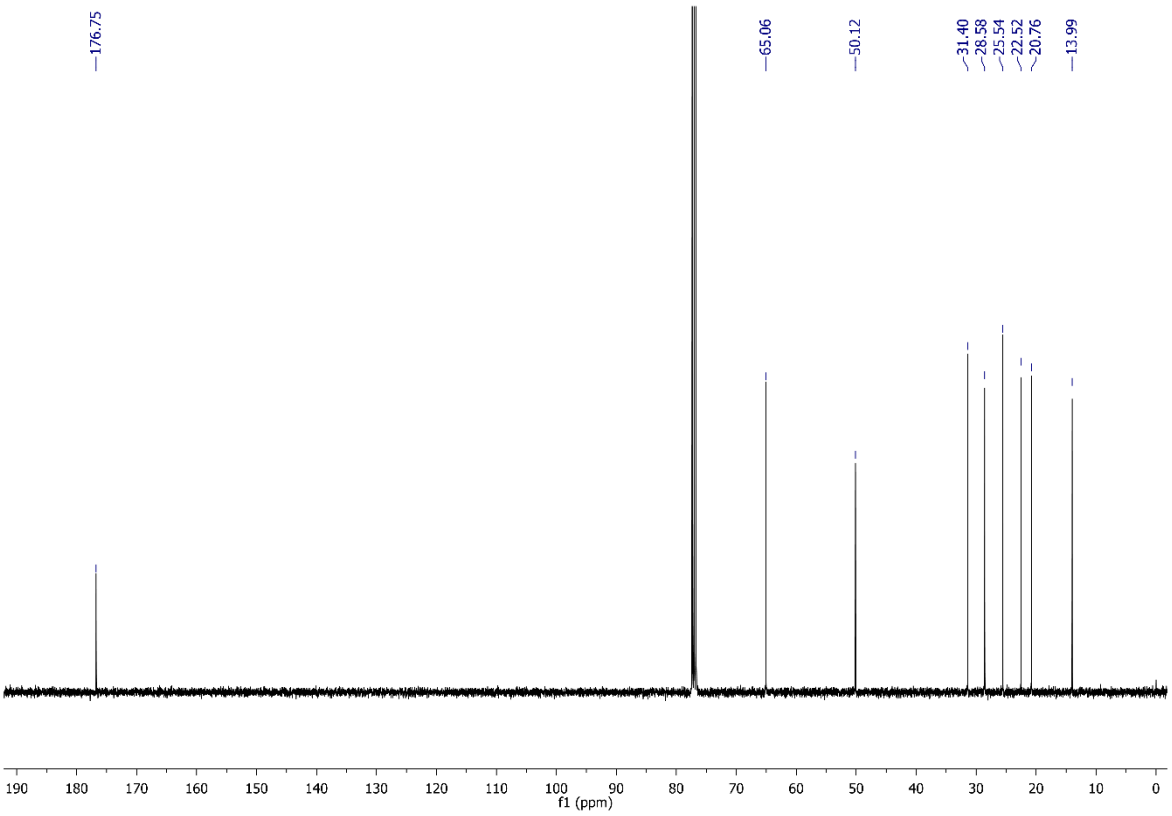


Hexyl L-alaninate (3Ala)

^{1}H NMR

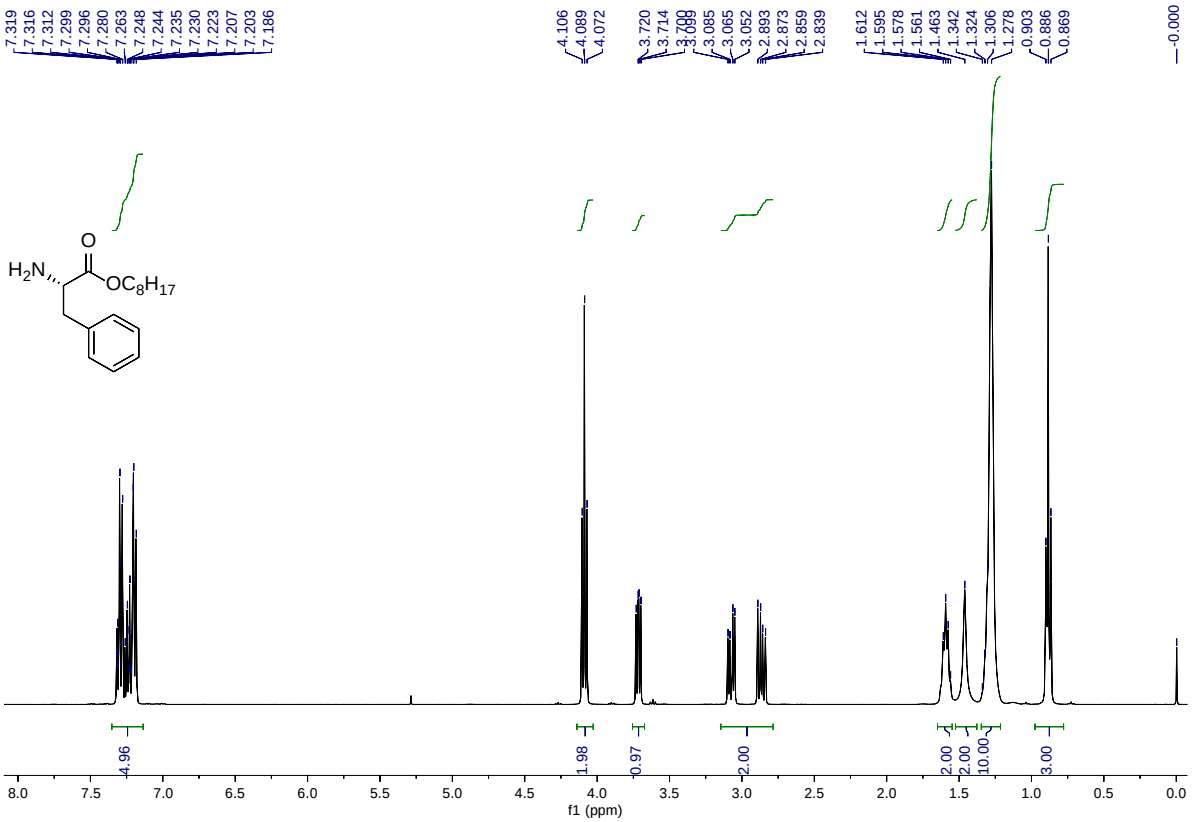


^{13}C NMR

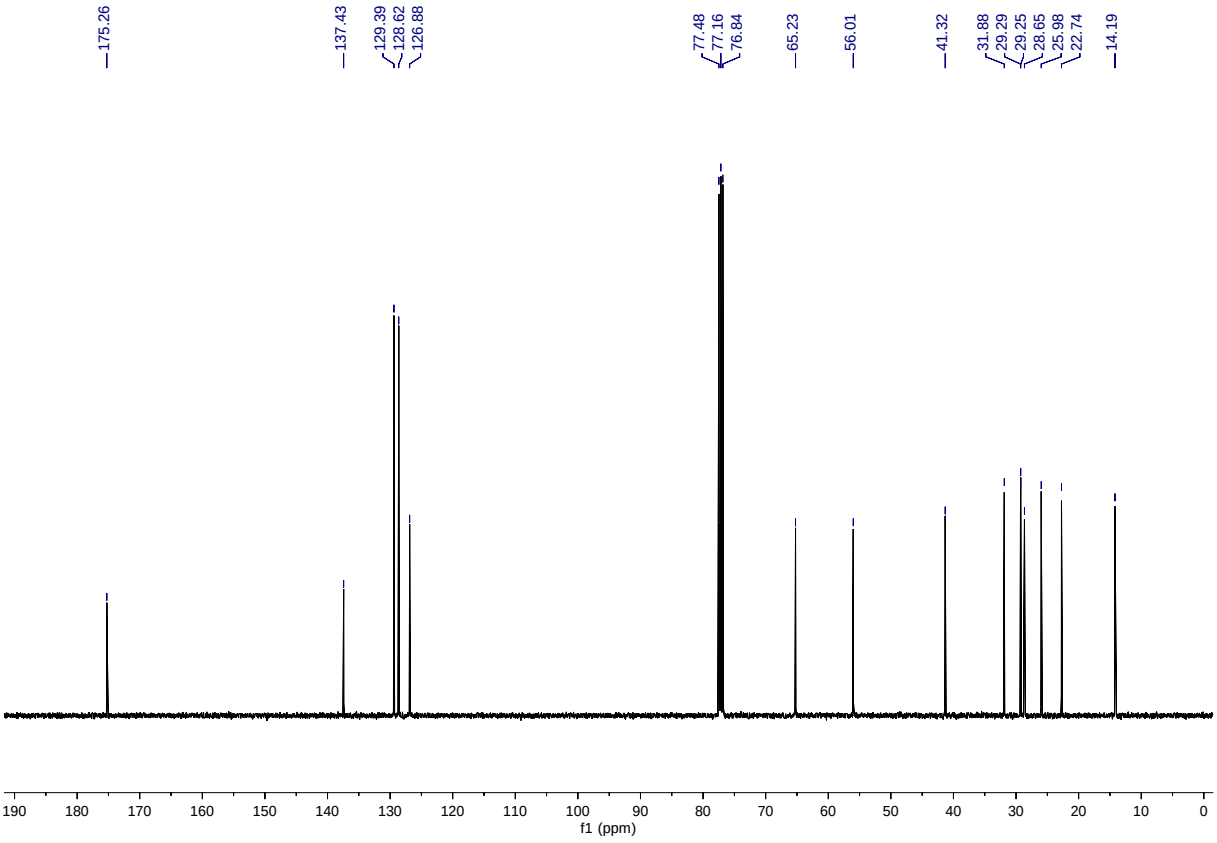


Octyl L-phenylalaninate (4)

^{1}H NMR

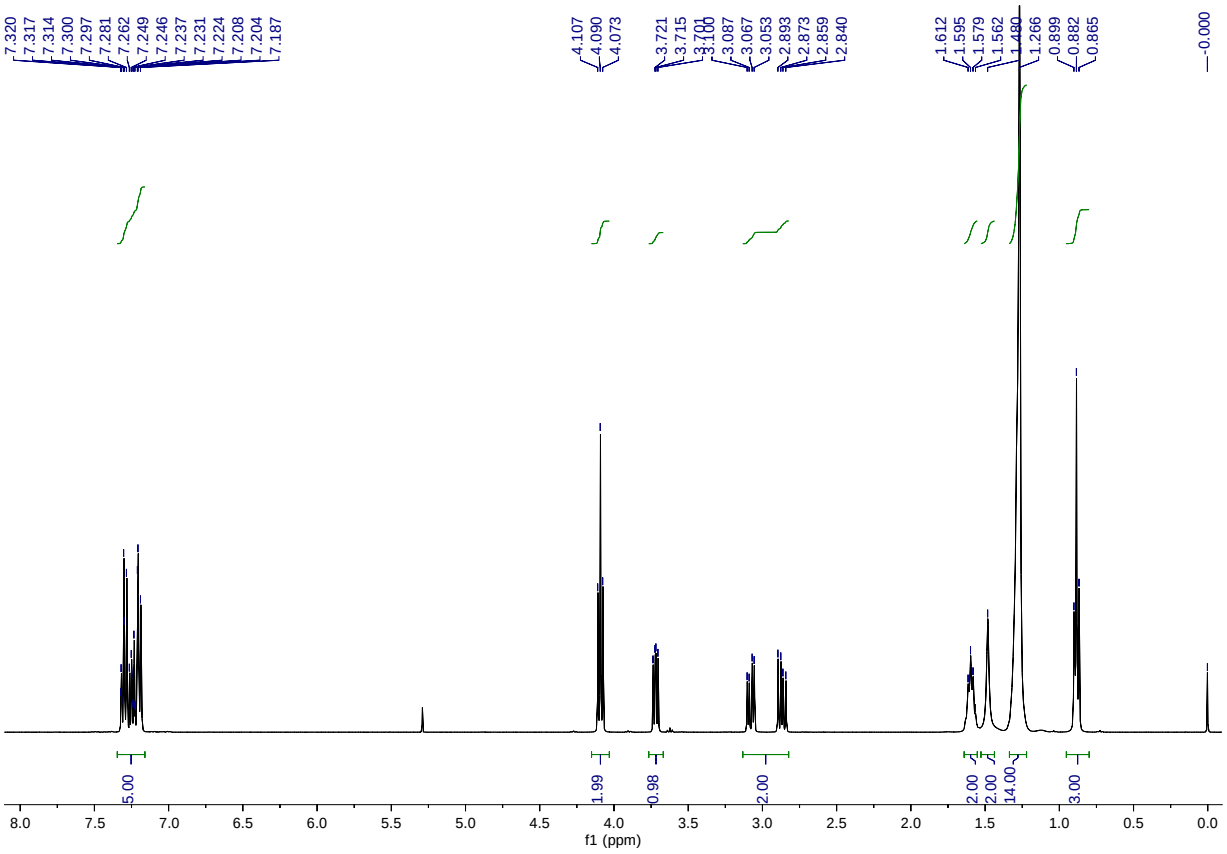


^{13}C NMR

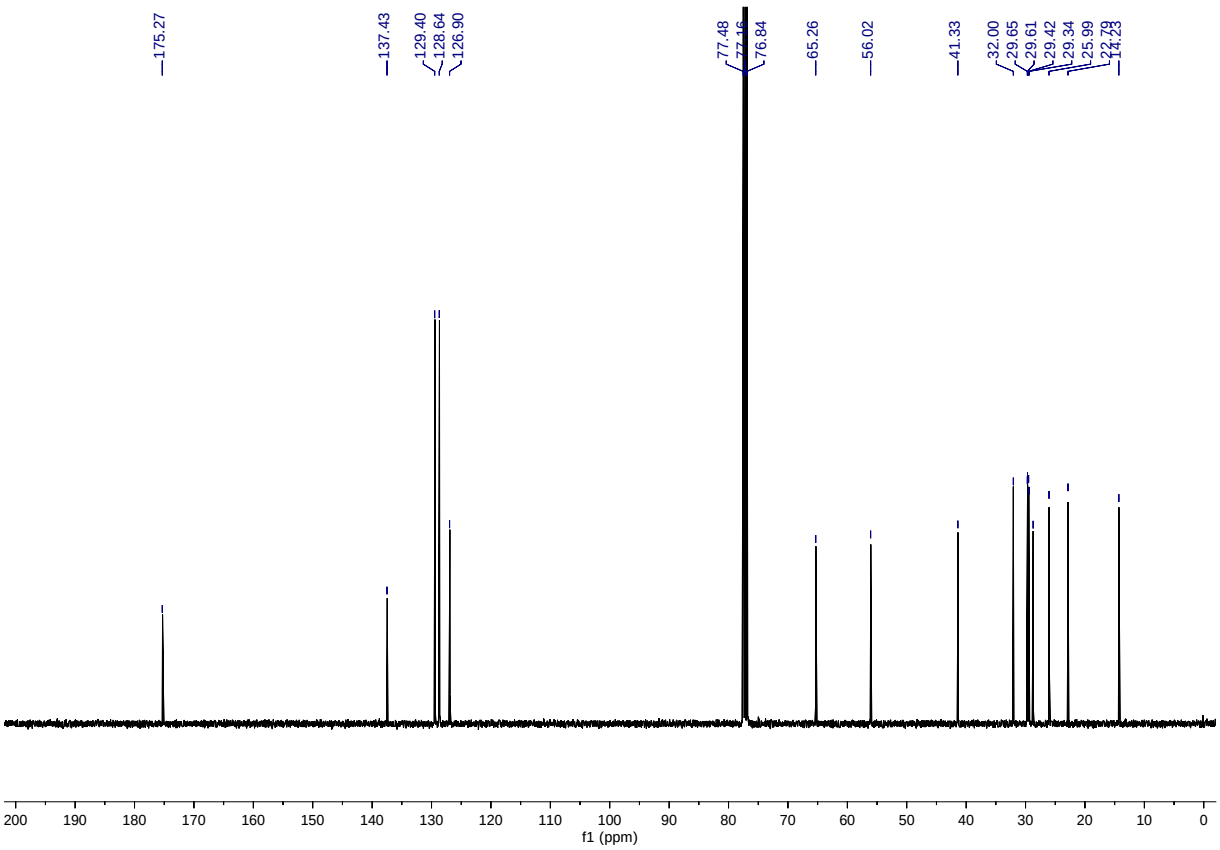


Decyl L-phenylalaninate (5)

^{1}H NMR

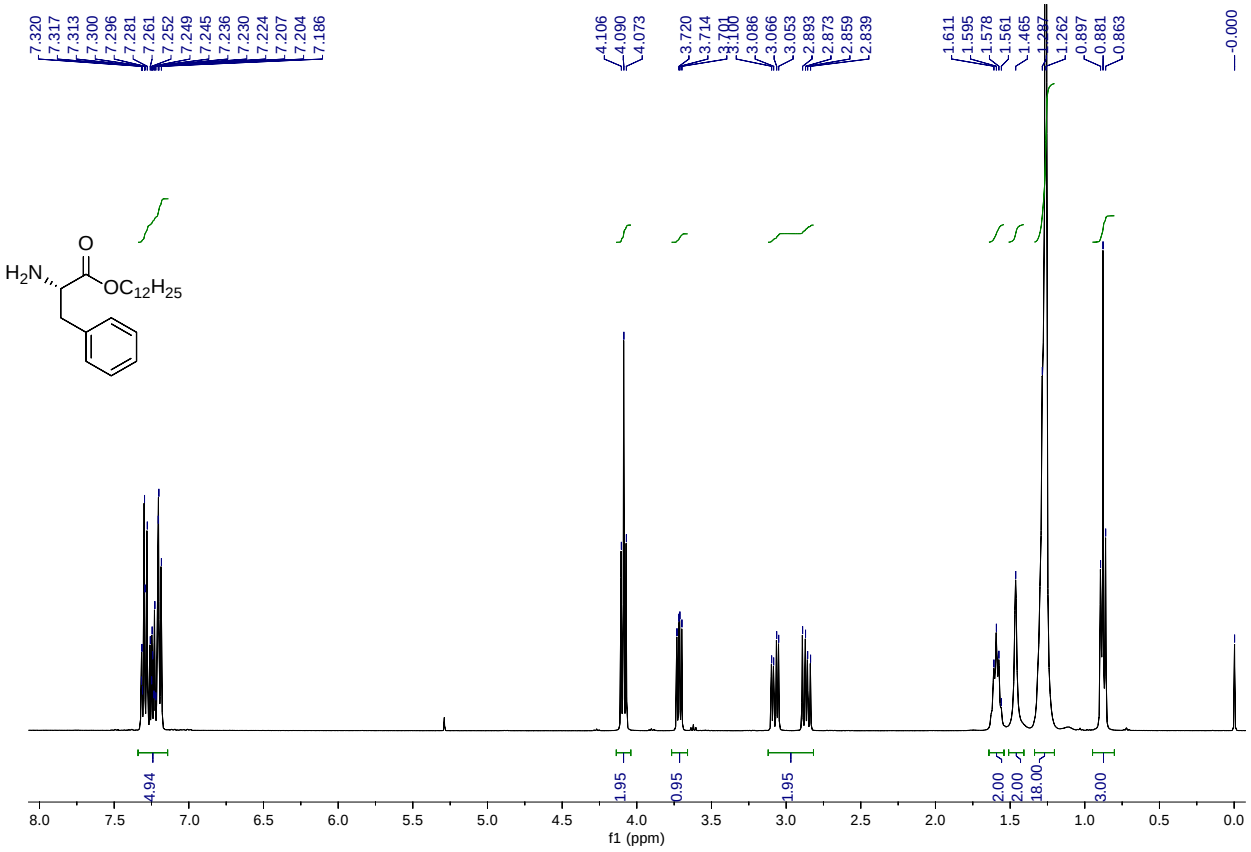


^{13}C NMR

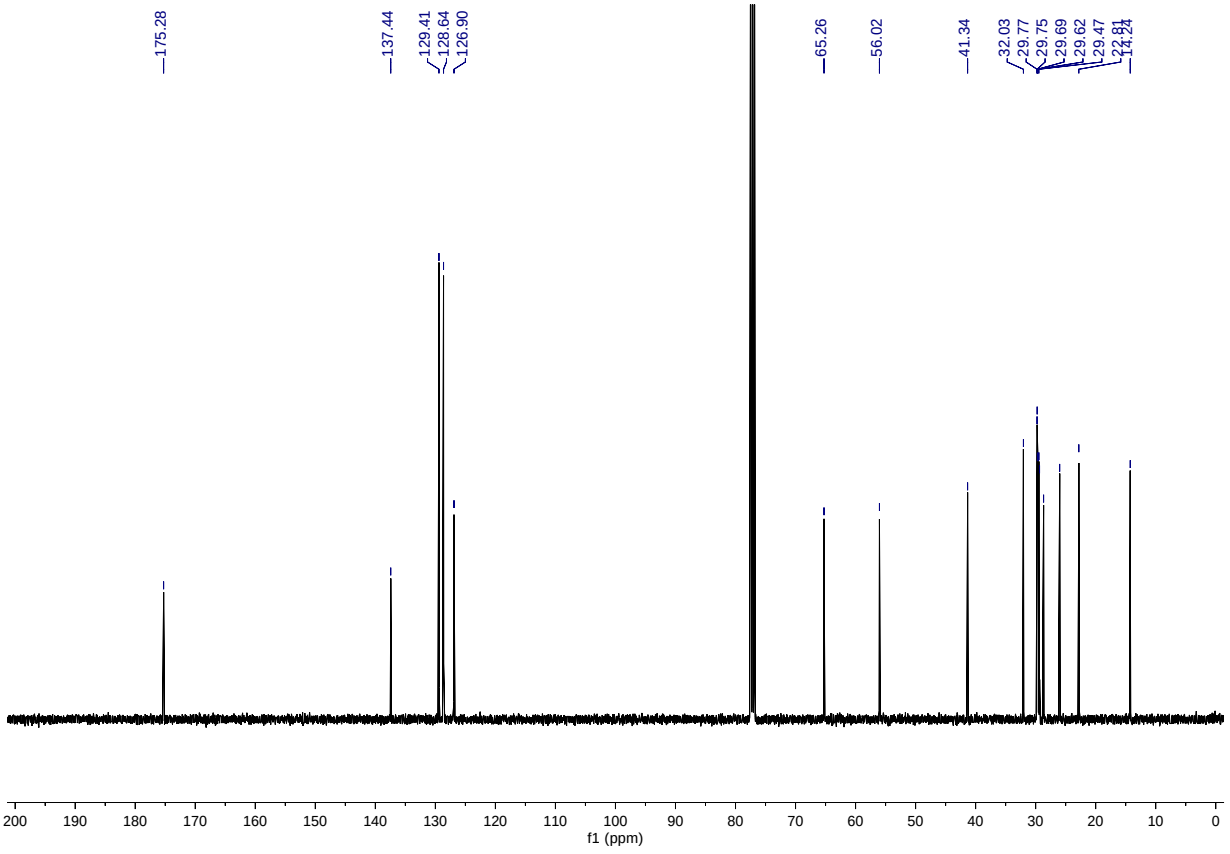


Dodecyl L-phenylalaninate (6)

^{1}H NMR

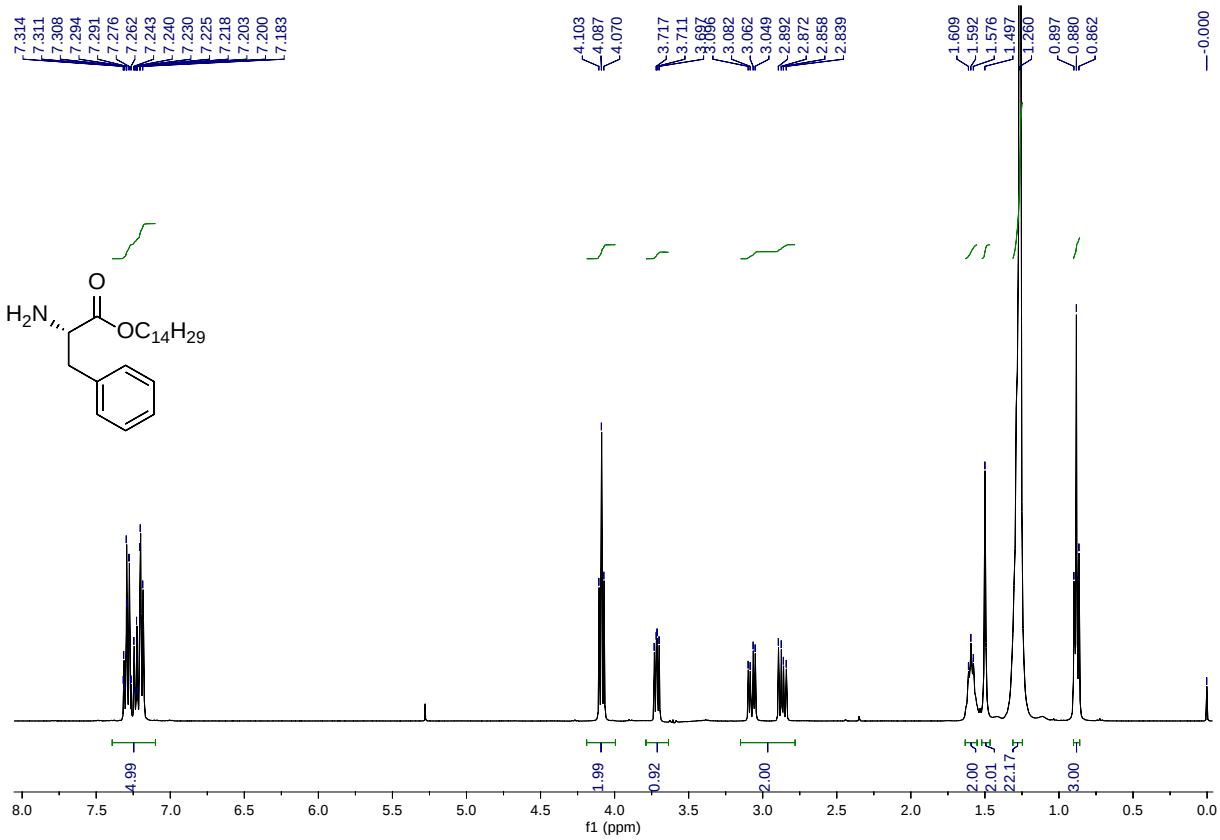


^{13}C NMR

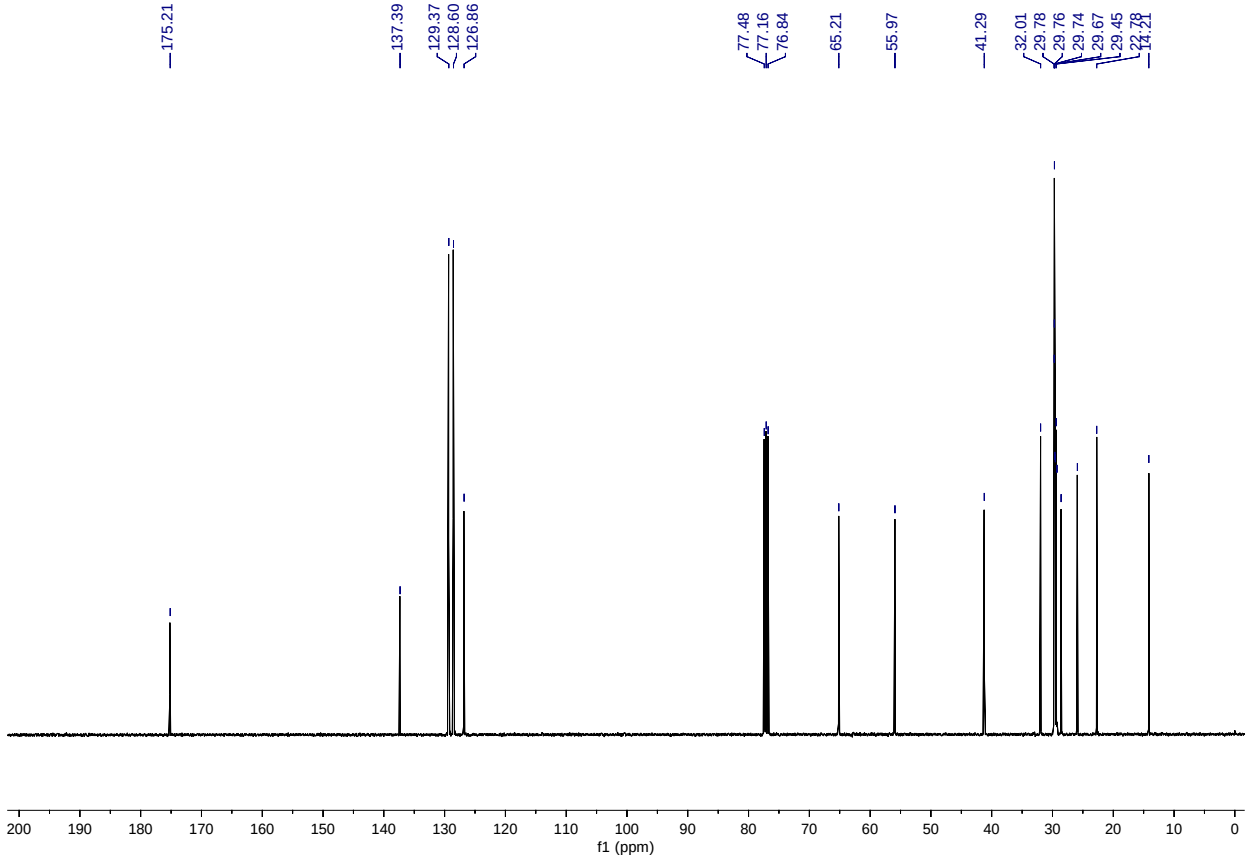


Tetradecyl L-phenylalaninate (7)

^{1}H NMR

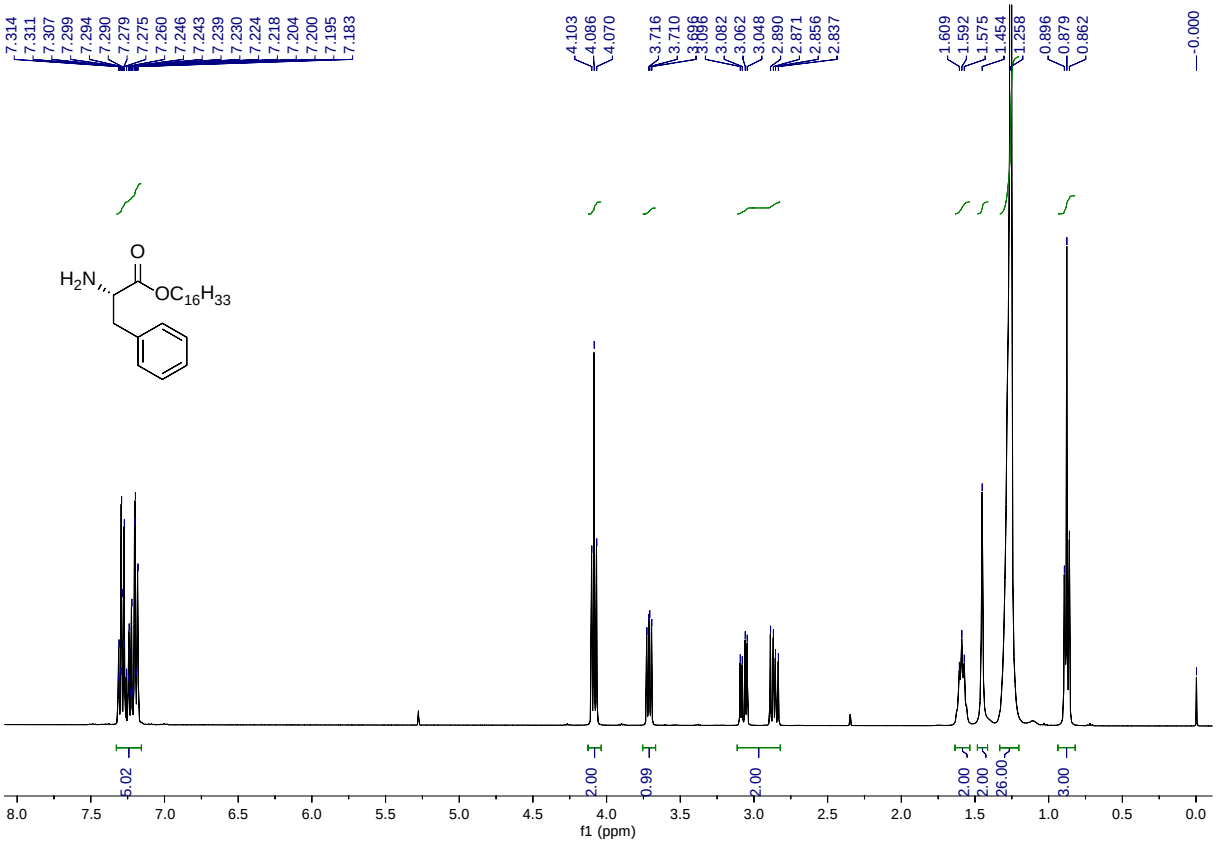


^{13}C NMR

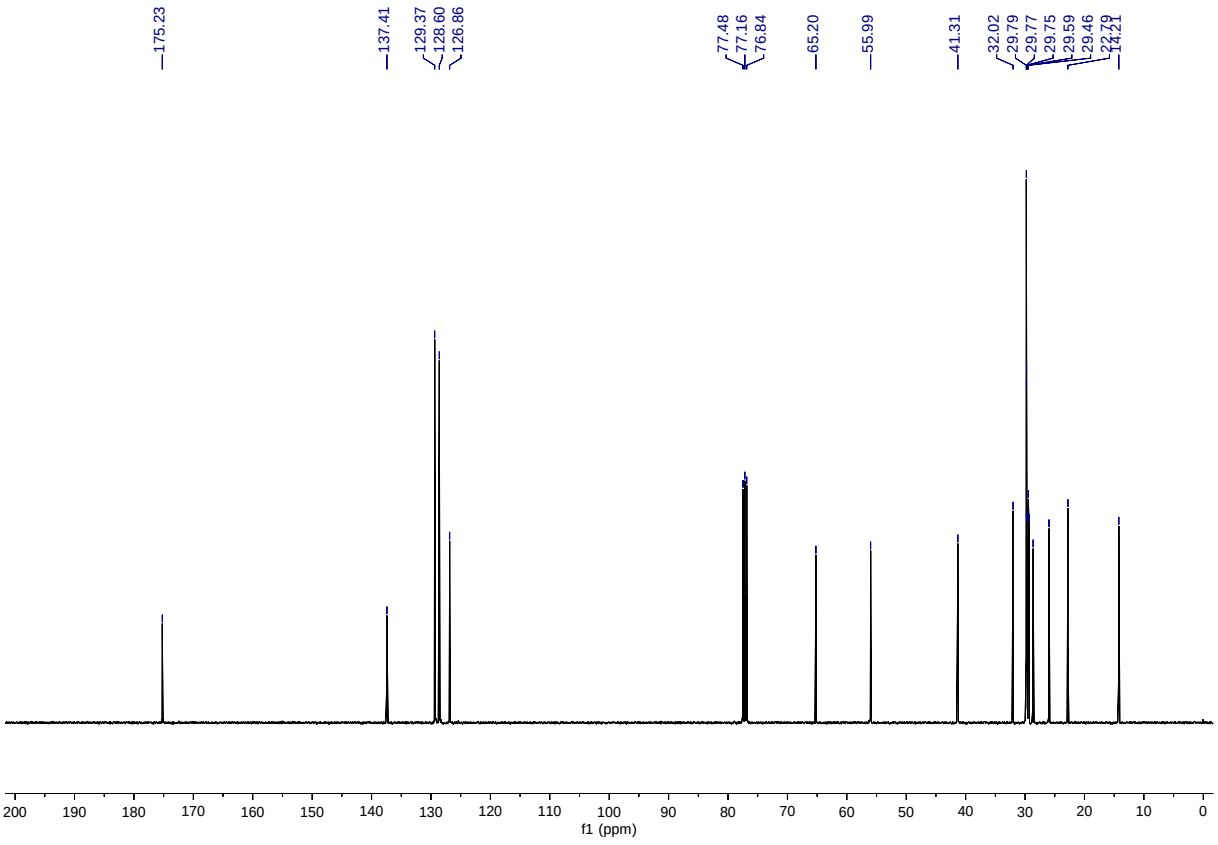


Hexadecyl L-phenylalaninate (8)

^{1}H NMR



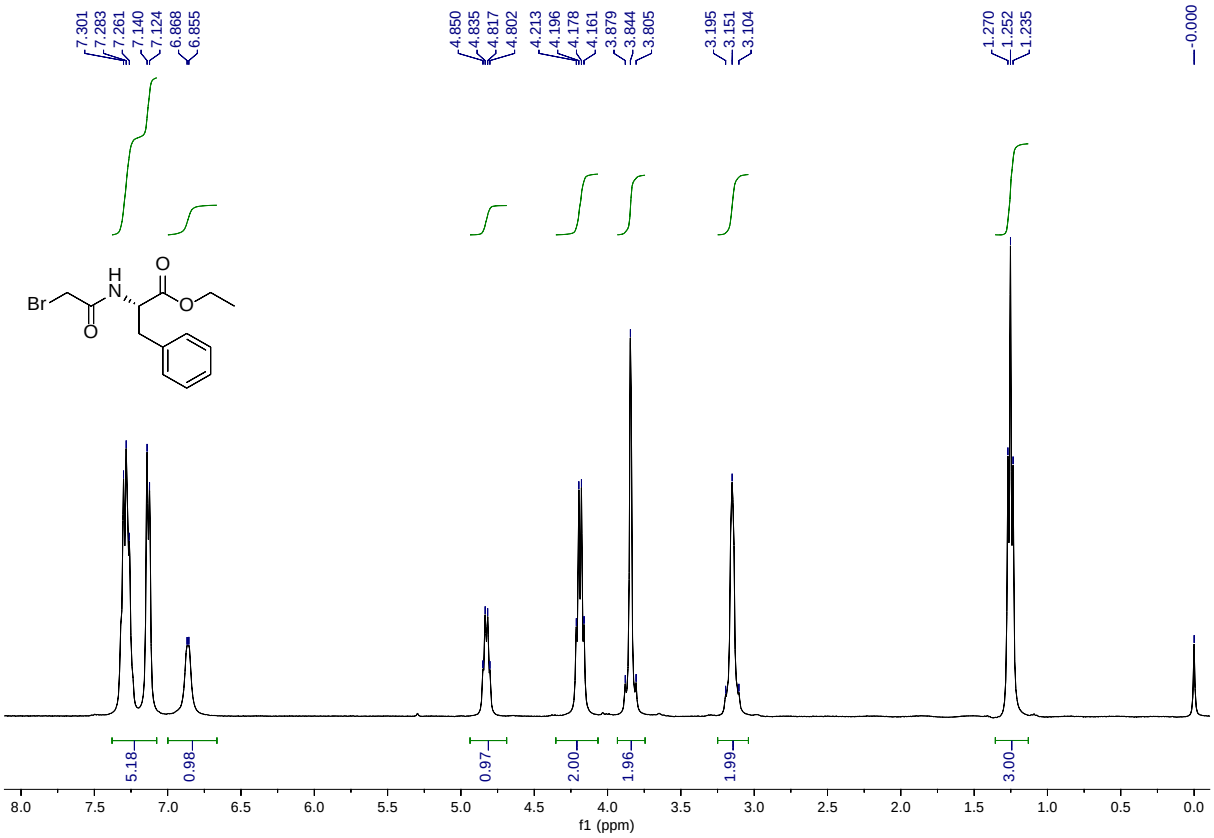
^{13}C NMR



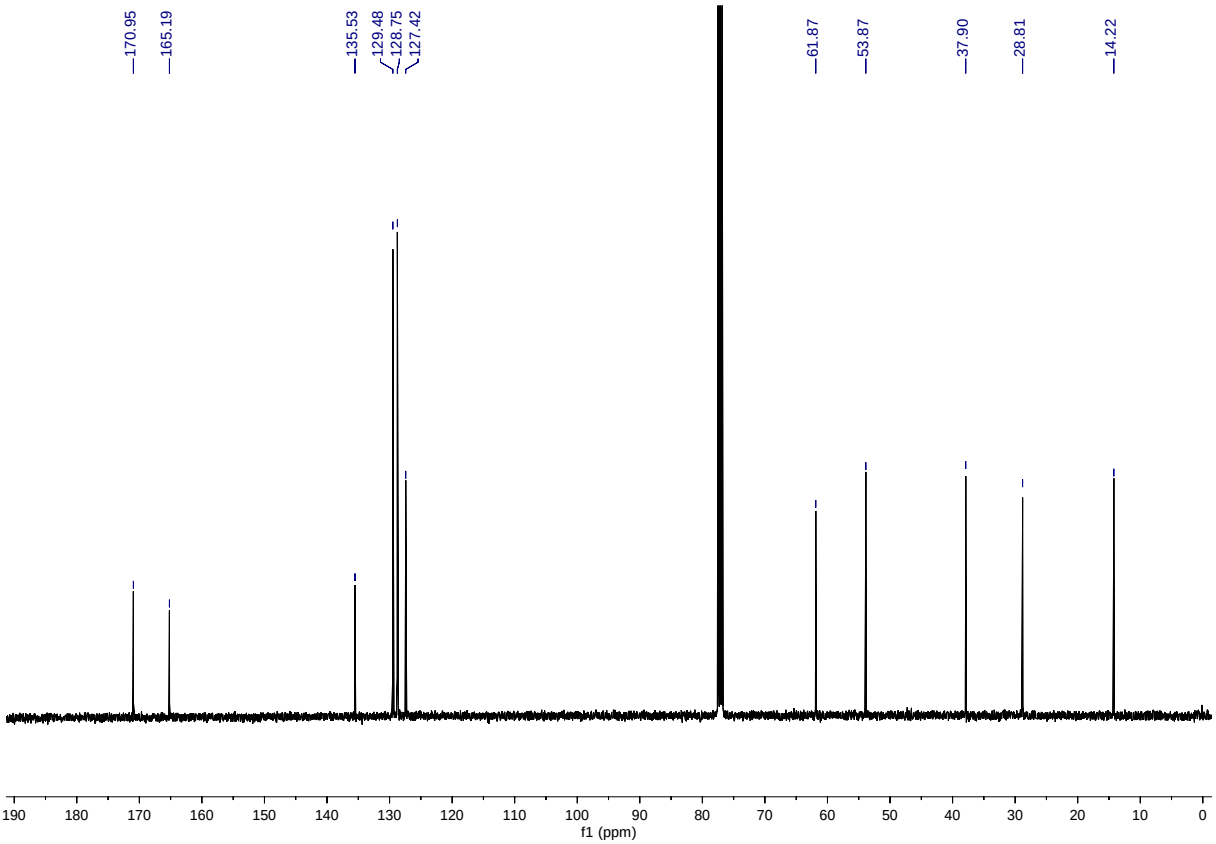
10. NMR and IR spectra of 2-bromoacetyl-L-phenylalaninates

Ethyl (2-bromoacetyl)-L-phenylalaninate (9)

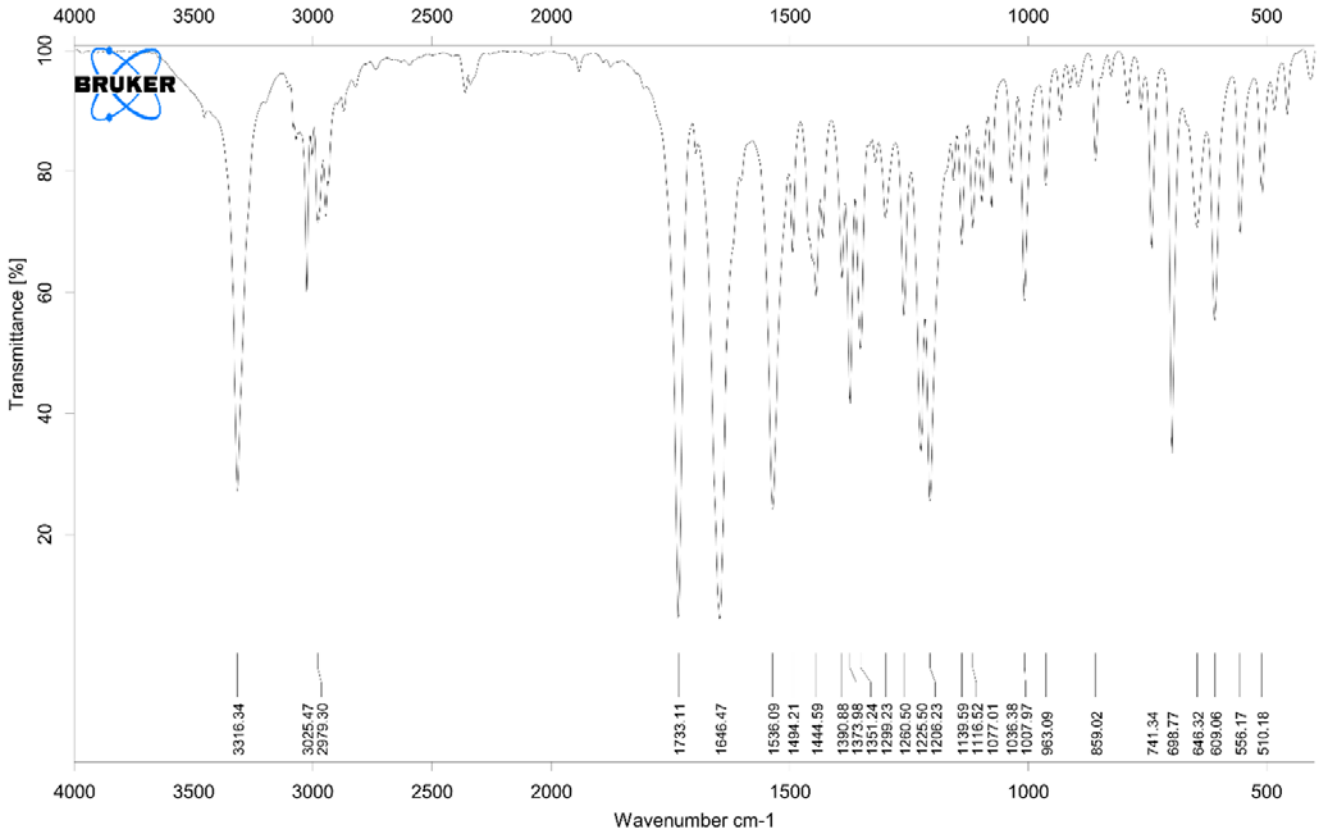
^{1}H NMR



^{13}C NMR

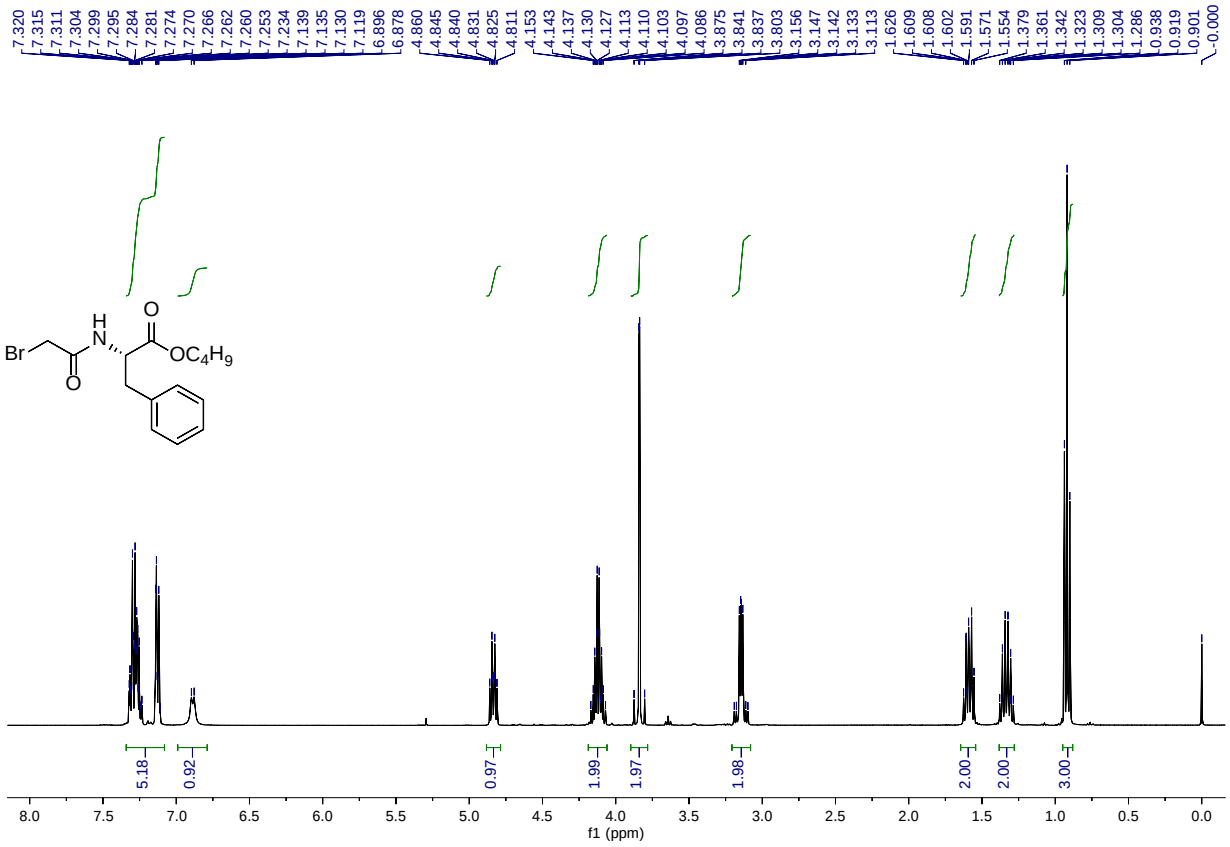


IR (KBr, cm^{-1})

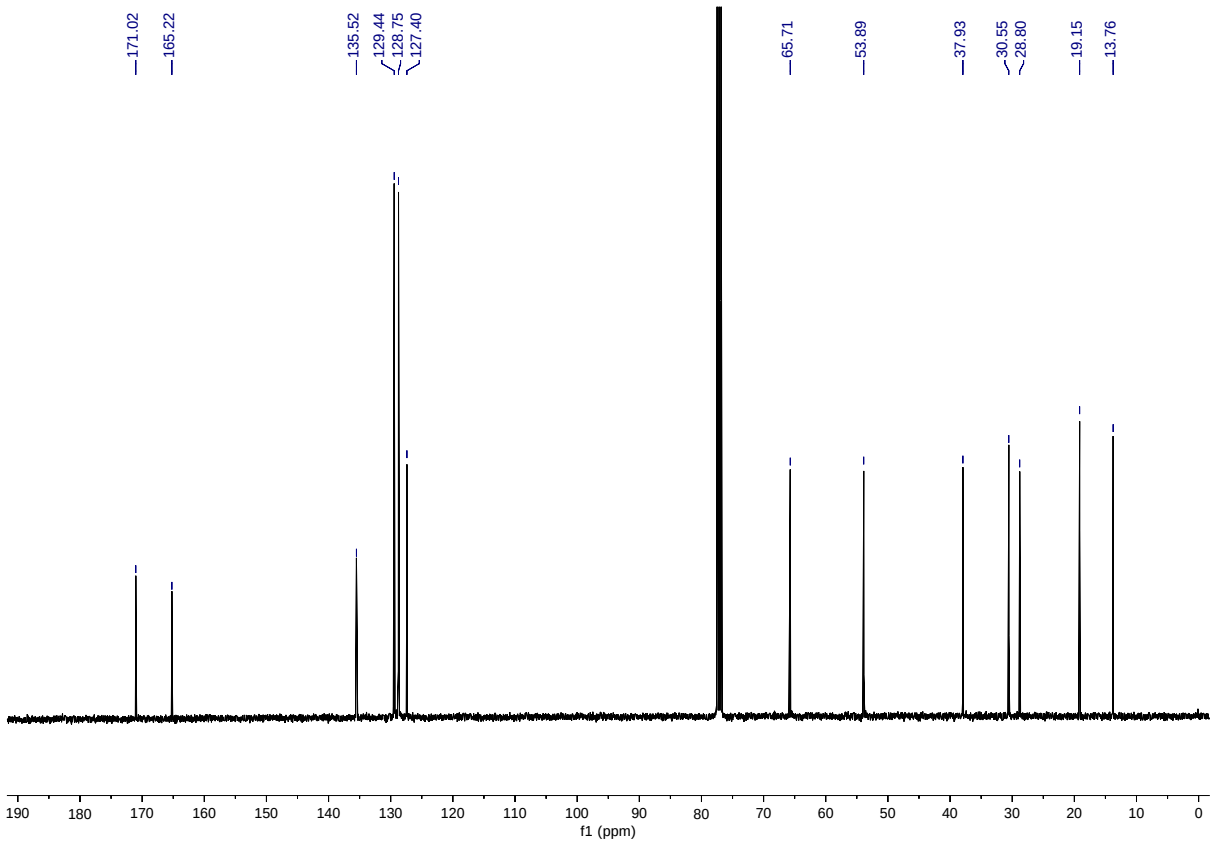

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3316.34
3025.47
2979.30
1733.11
1646.47
1536.09
1494.21
1444.59
1390.88
1373.98
1351.24
1299.23
1260.50
1225.50
1206.23
1139.59
1116.52
1077.01
1036.38
1007.97
983.09
859.02
741.34
698.77
646.32
609.06
556.17
510.18
Wavenumber cm-1

Butyl (2-bromoacetyl)-L-phenylalaninate (10)

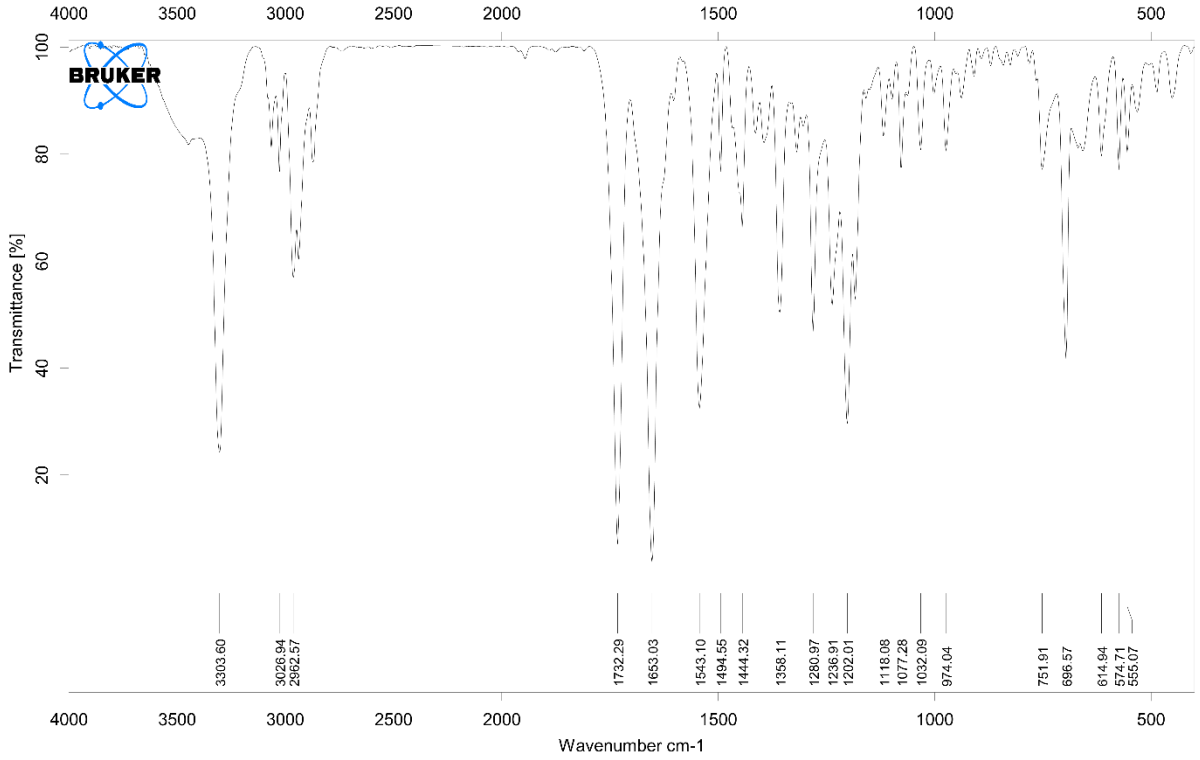
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
3500
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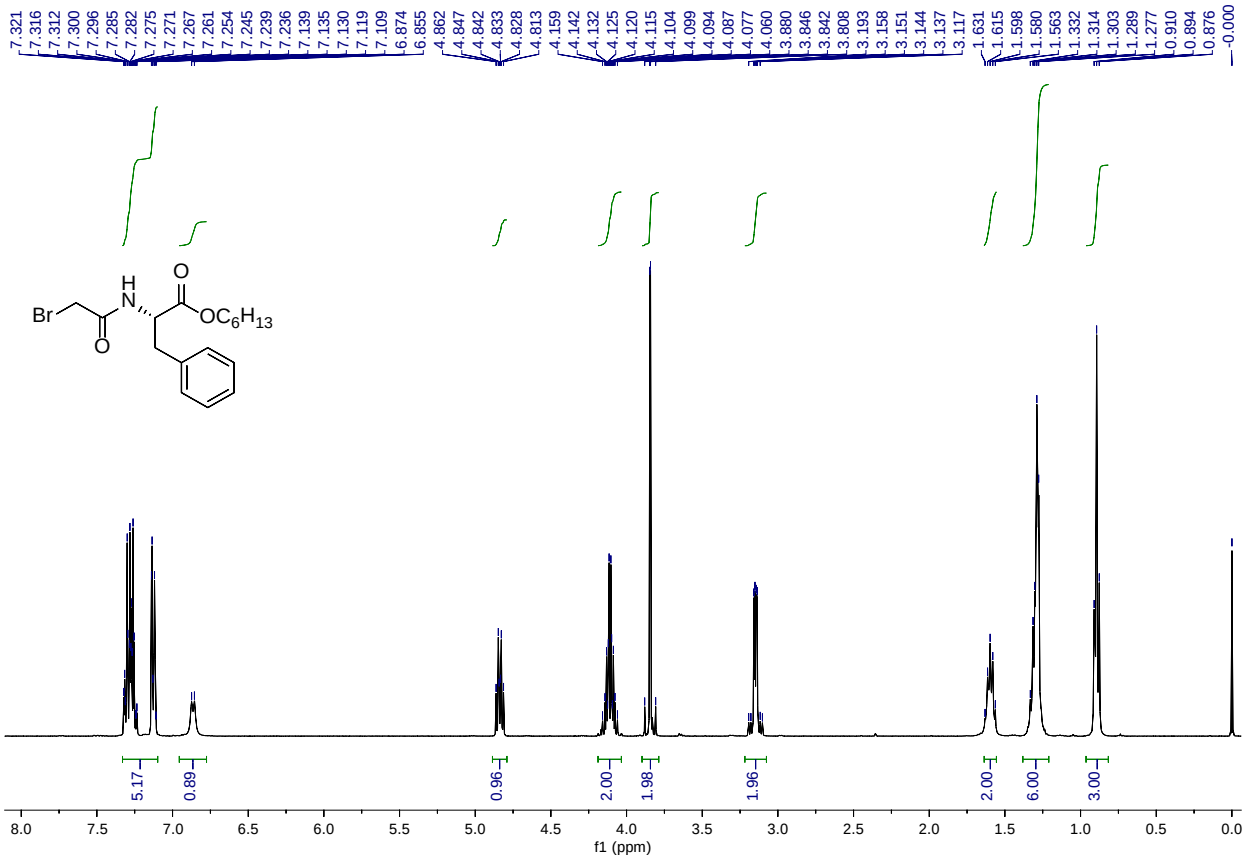
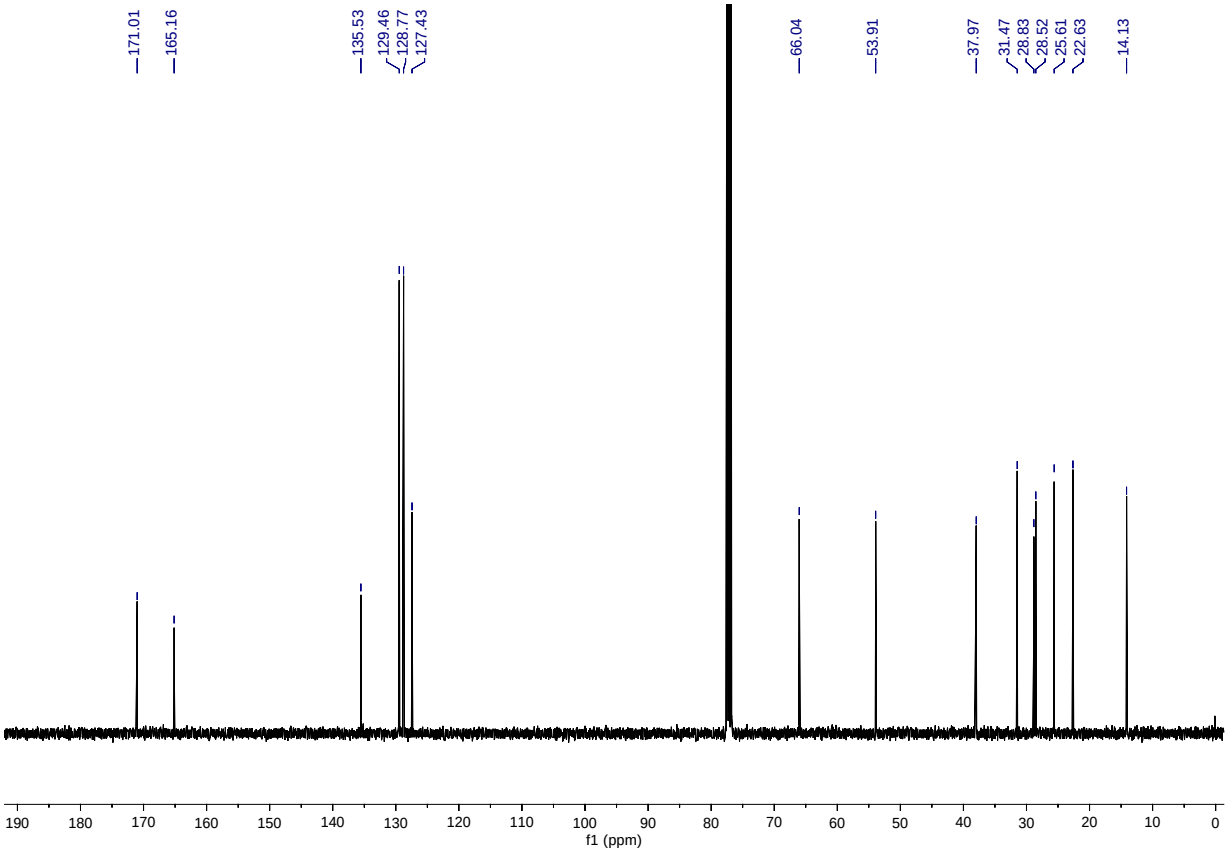
80
60
40
20
Transmittance [%]
BRUKER
3303.60
3026.94
2962.57
1732.29
1653.03
1543.10
1494.55
1444.32
1358.11
1280.97
1236.91
1202.01
1118.08
1077.28
1032.09
974.04
751.91
696.57
614.94
574.71
555.07
Wavenumber cm-1

Hexyl (2-bromoacetyl)-L-phenylalaninate (11)

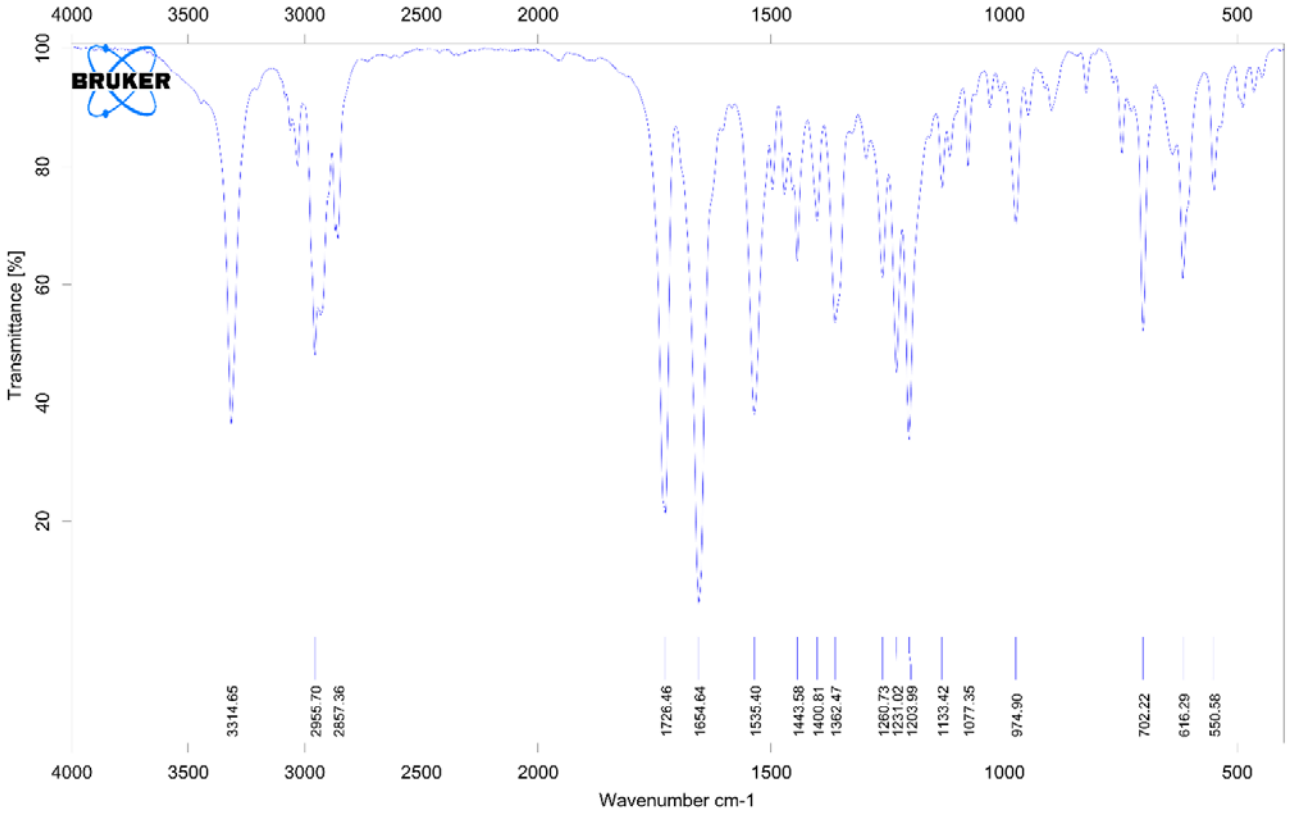
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
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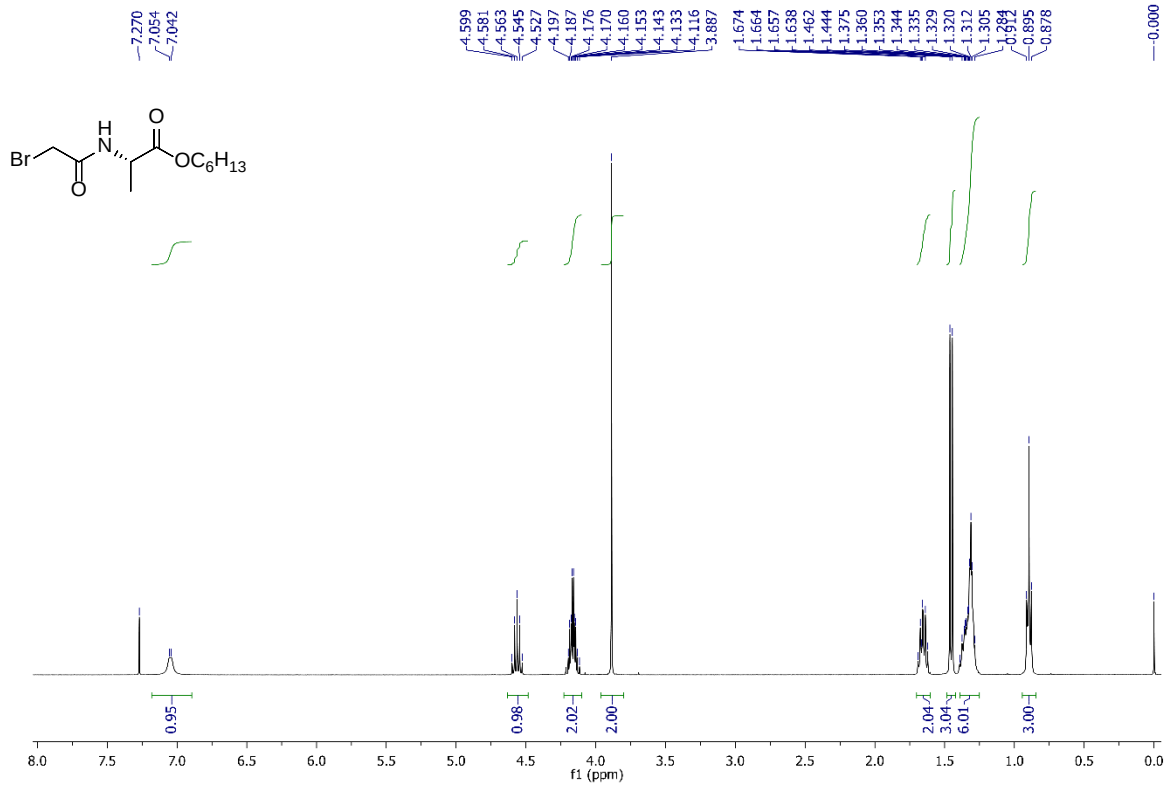
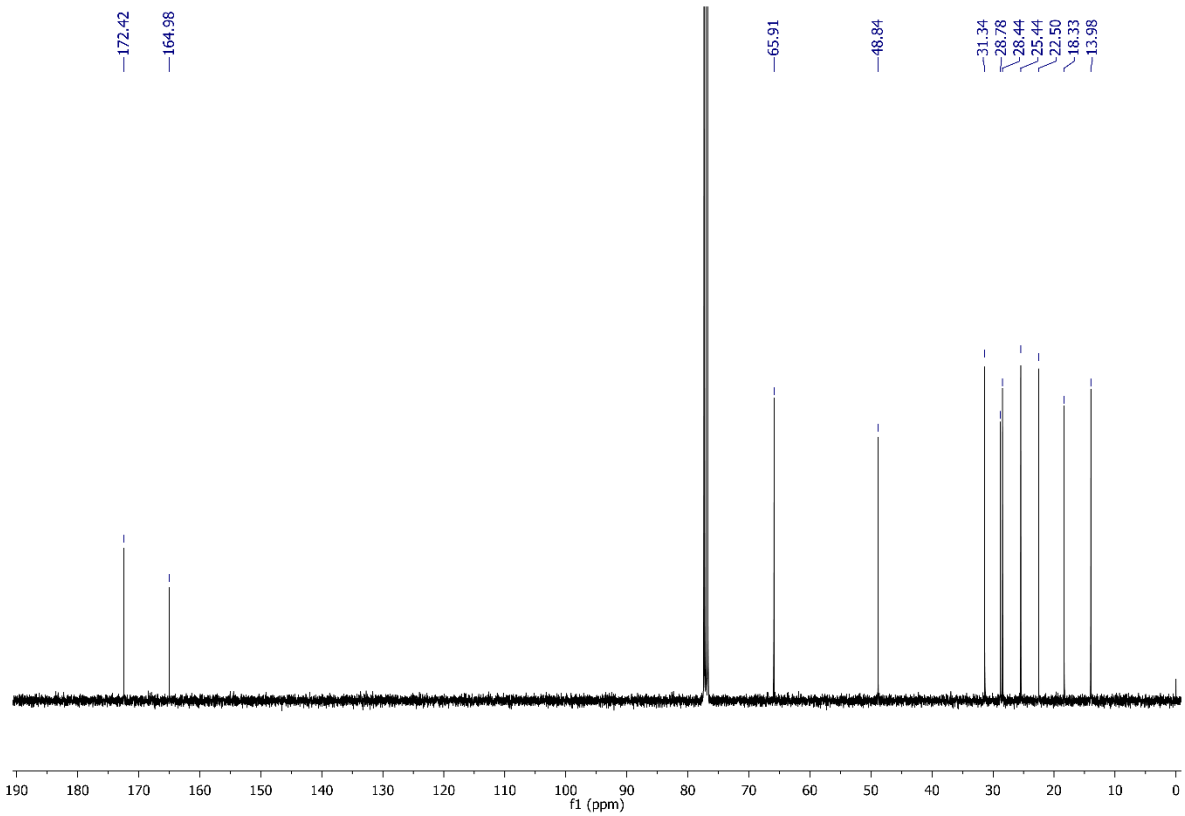
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3314.65
2955.70
2857.36
1726.46
1654.64
1535.40
1443.58
1400.81
1362.47
1260.73
1231.02
1203.99
1133.42
1077.35
974.90
702.22
616.29
550.58
Wavenumber cm-1

Hexyl (2-bromoacetyl)-L-alaninate (11Ala)

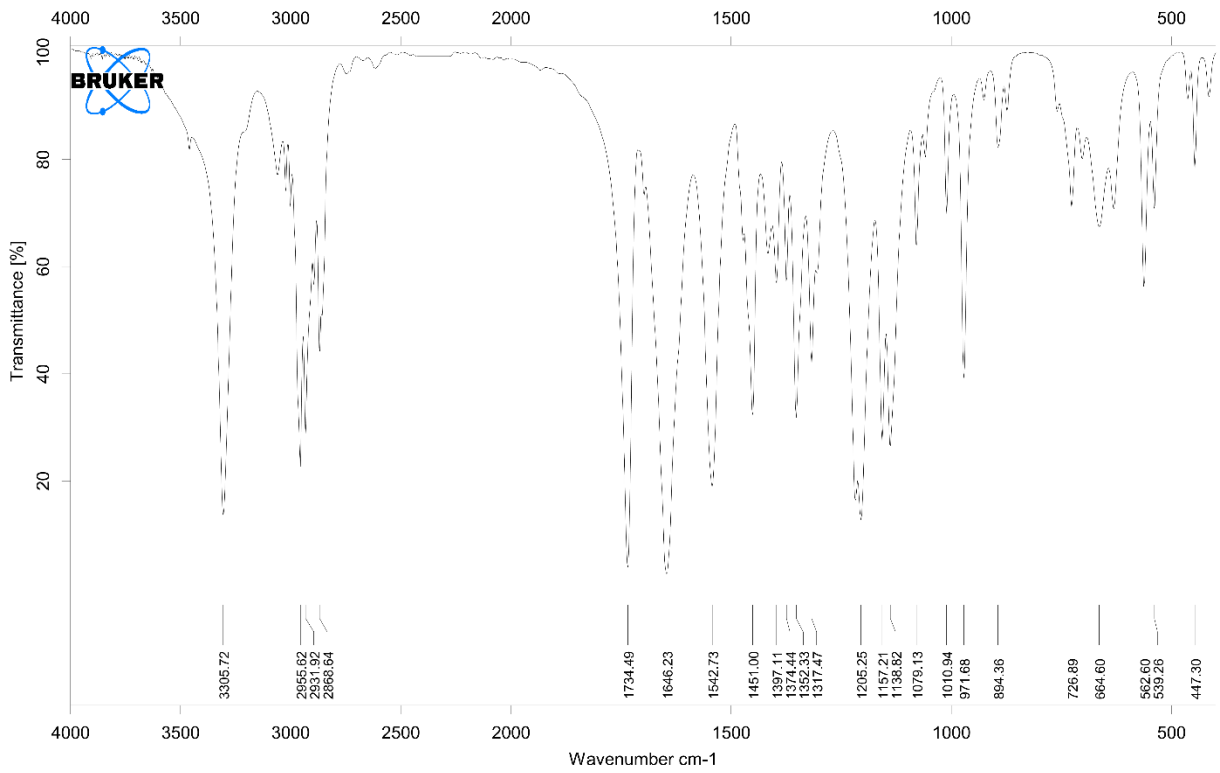
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
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1500
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100
80
60
40
20
Transmittance [%]
BRUKER
3305.72
2955.62
2931.92
2868.64
1734.49
1646.23
1542.73
1451.00
1397.11
1374.44
1352.33
1317.47
1205.25
1157.21
1138.82
1079.13
1010.94
971.68
894.36
726.89
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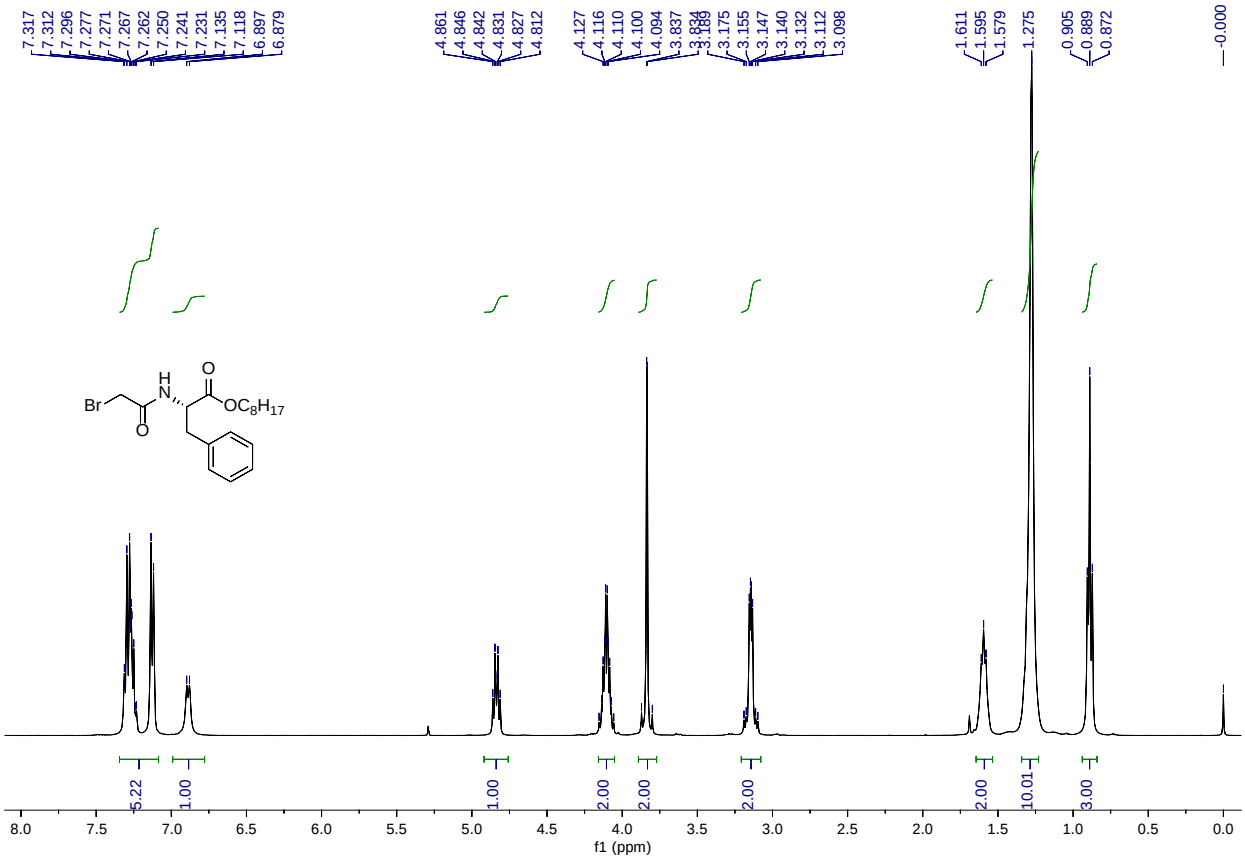
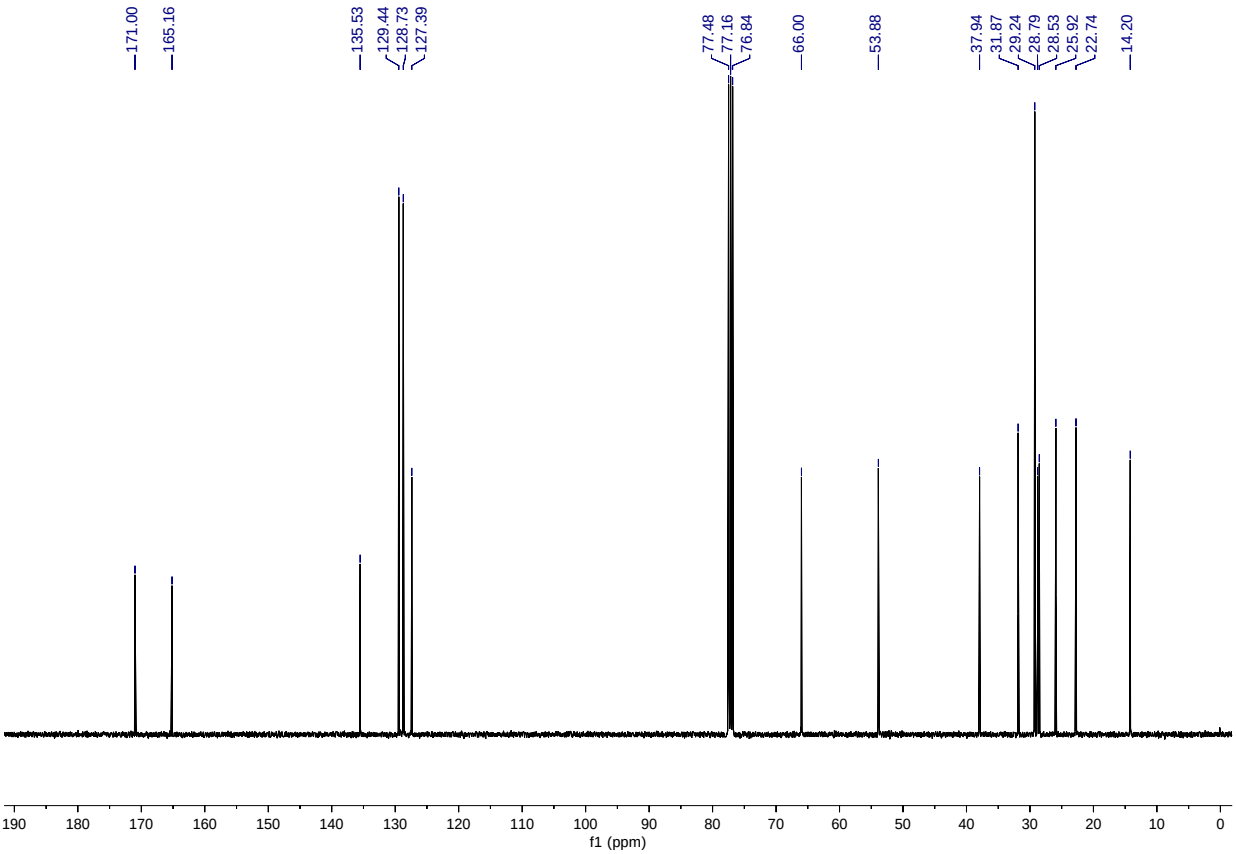
562.60
539.26
447.30
Wavenumber cm-1

Octyl (2-bromoacetyl)-L-phenylalaninate (12)

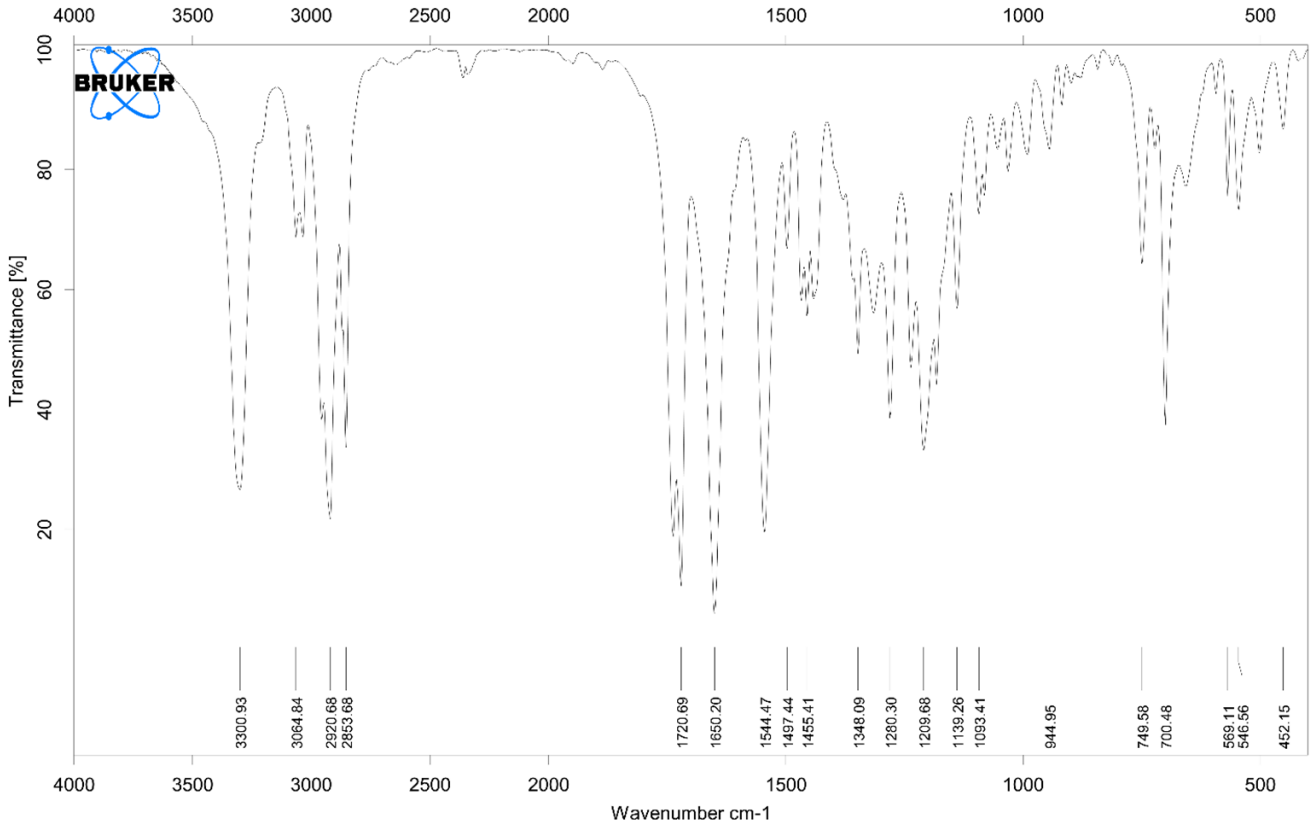
^{1}H NMR



^{13}C NMR

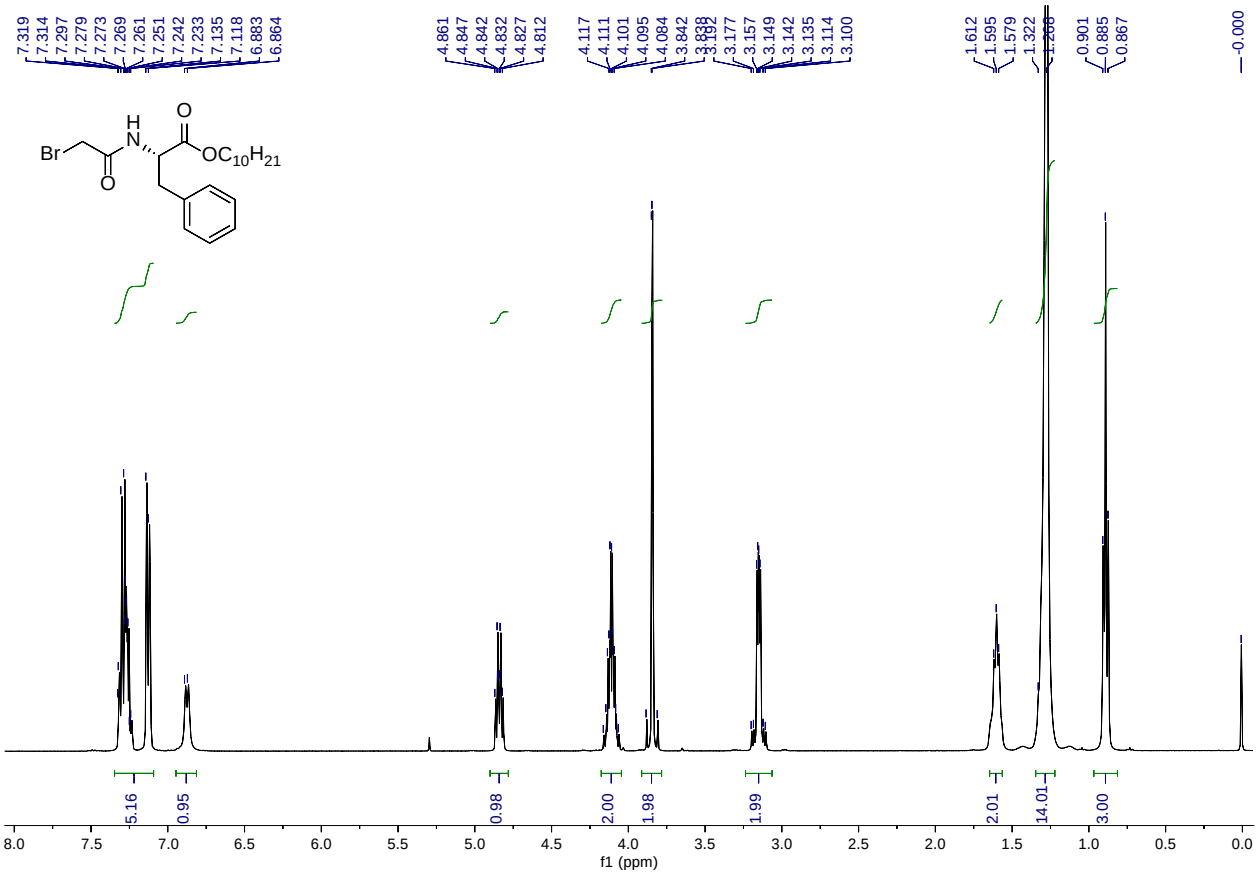


IR (KBr, cm^{-1})

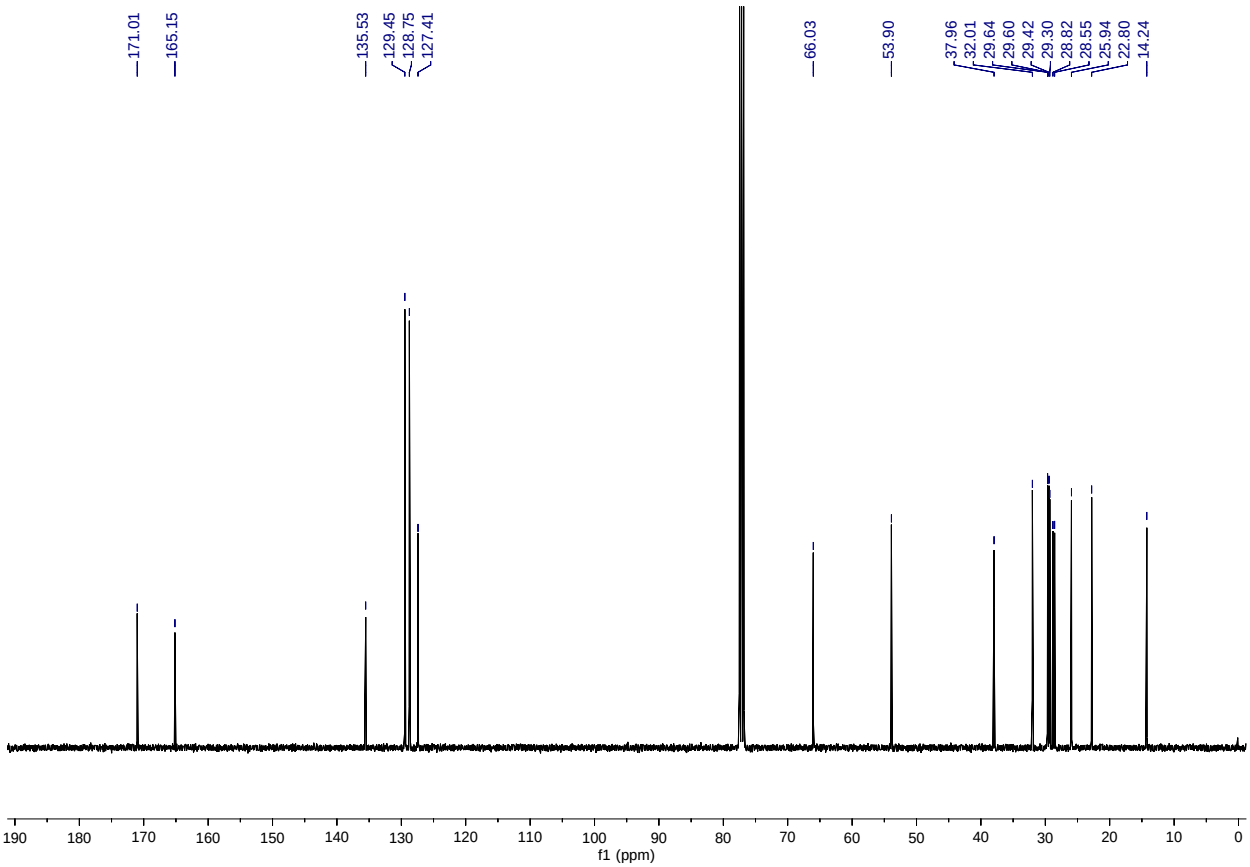

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3300.93
3064.84
2920.68
2853.68
1720.69
1650.20
1544.47
1497.44
1455.41
1348.09
1280.30
1209.68
1139.26
1093.41
944.95
749.58
700.48
569.11
546.56
452.15
Wavenumber cm-1

Decyl (2-bromoacetyl)-L-phenylalaninate (13)

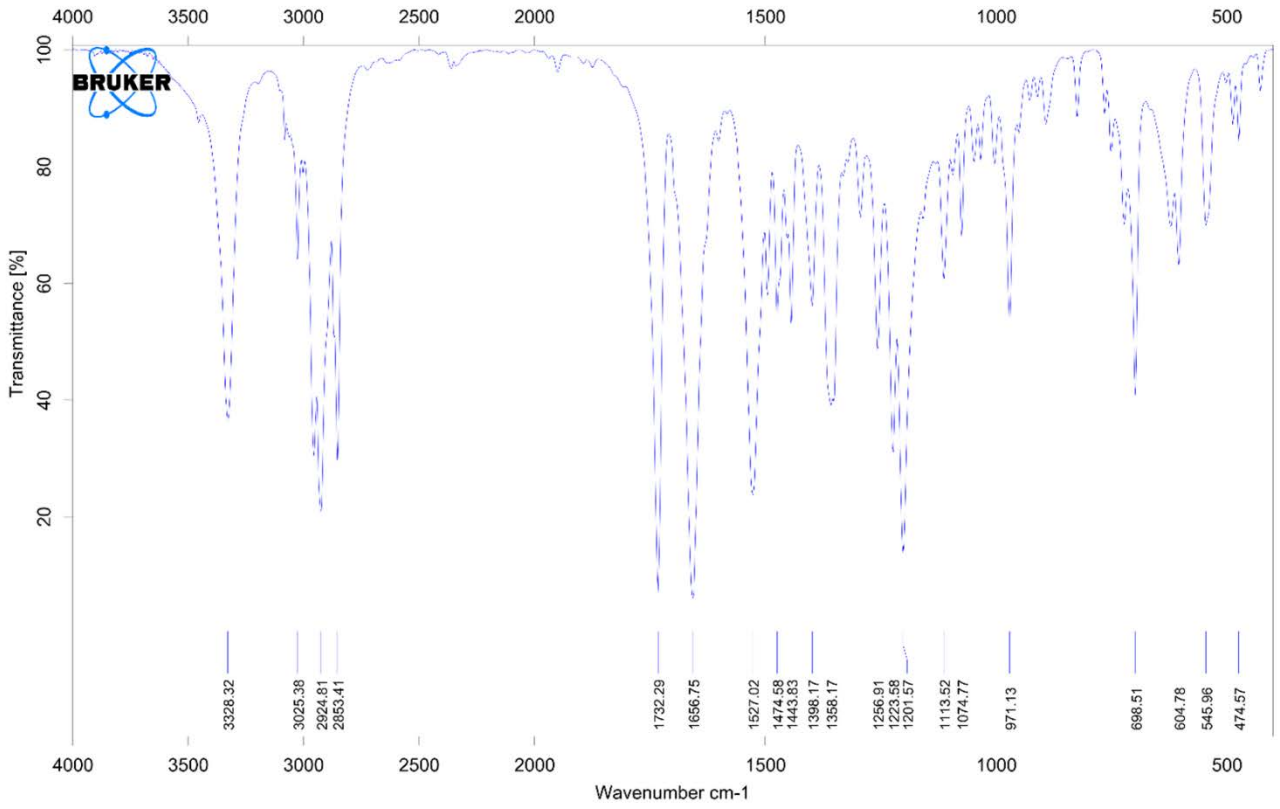
^{1}H NMR



^{13}C NMR

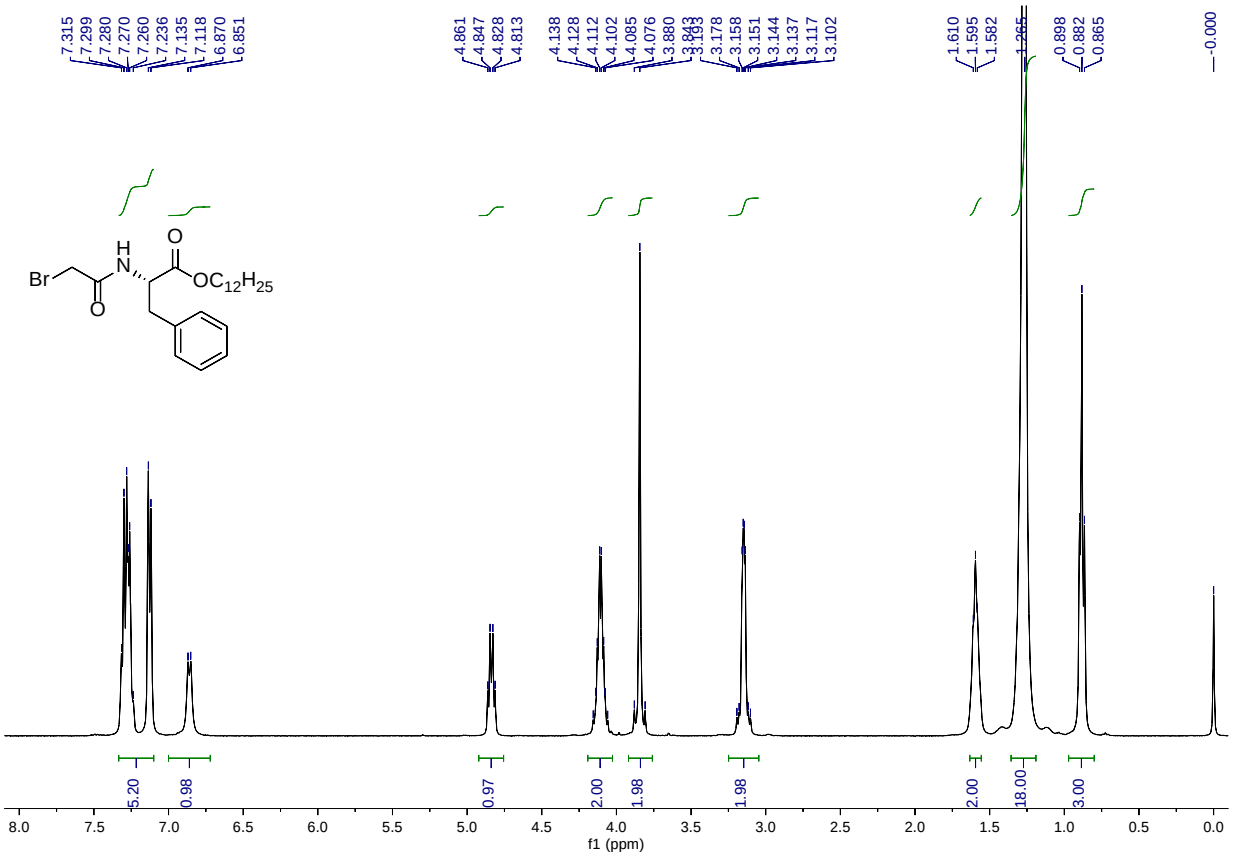


IR (KBr, cm^{-1})

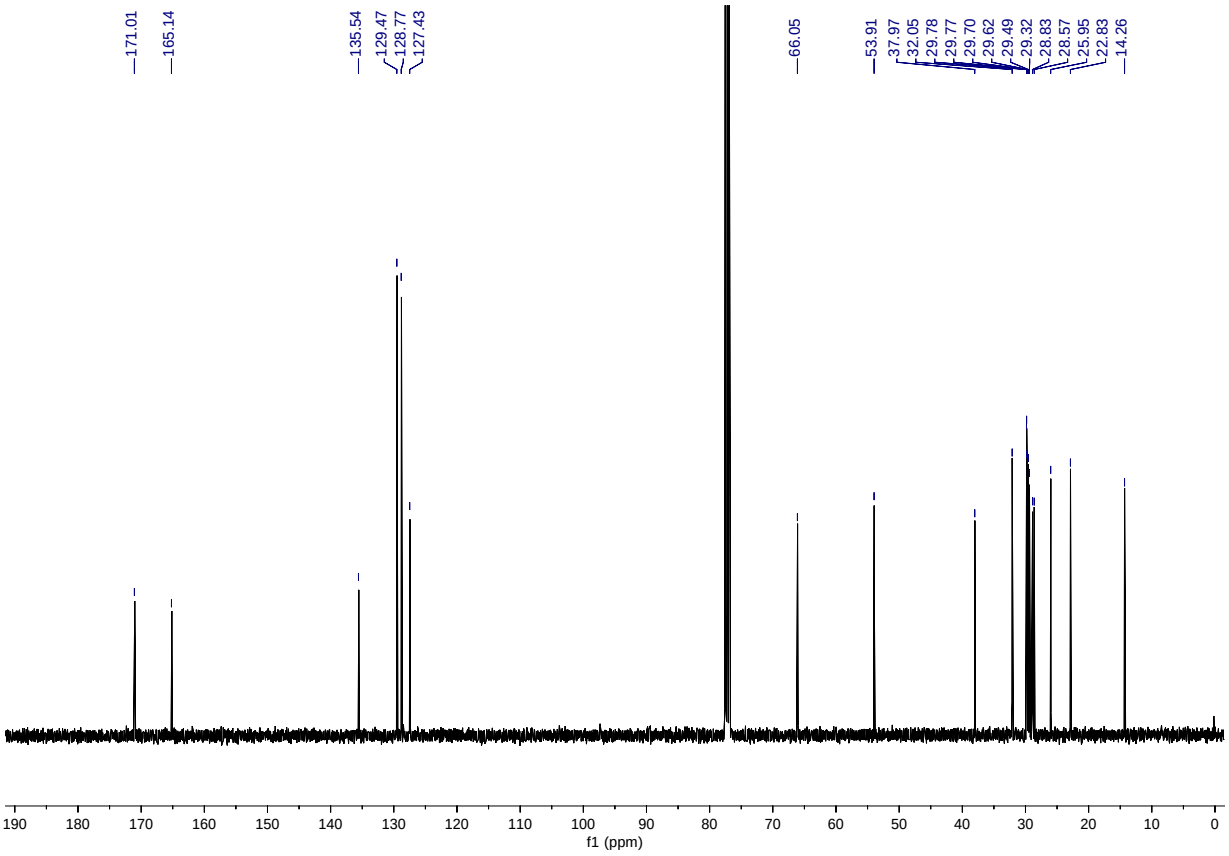

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3328.32
3025.38
2924.81
2853.41
1732.29
1656.75
1527.02
1474.58
1443.83
1398.17
1358.17
1256.91
1223.58
1201.57
1113.52
1074.77
971.13
698.51
604.78
545.96
474.57
Wavenumber cm-1

Dodecyl (2-bromoacetyl)-L-phenylalaninate (14)

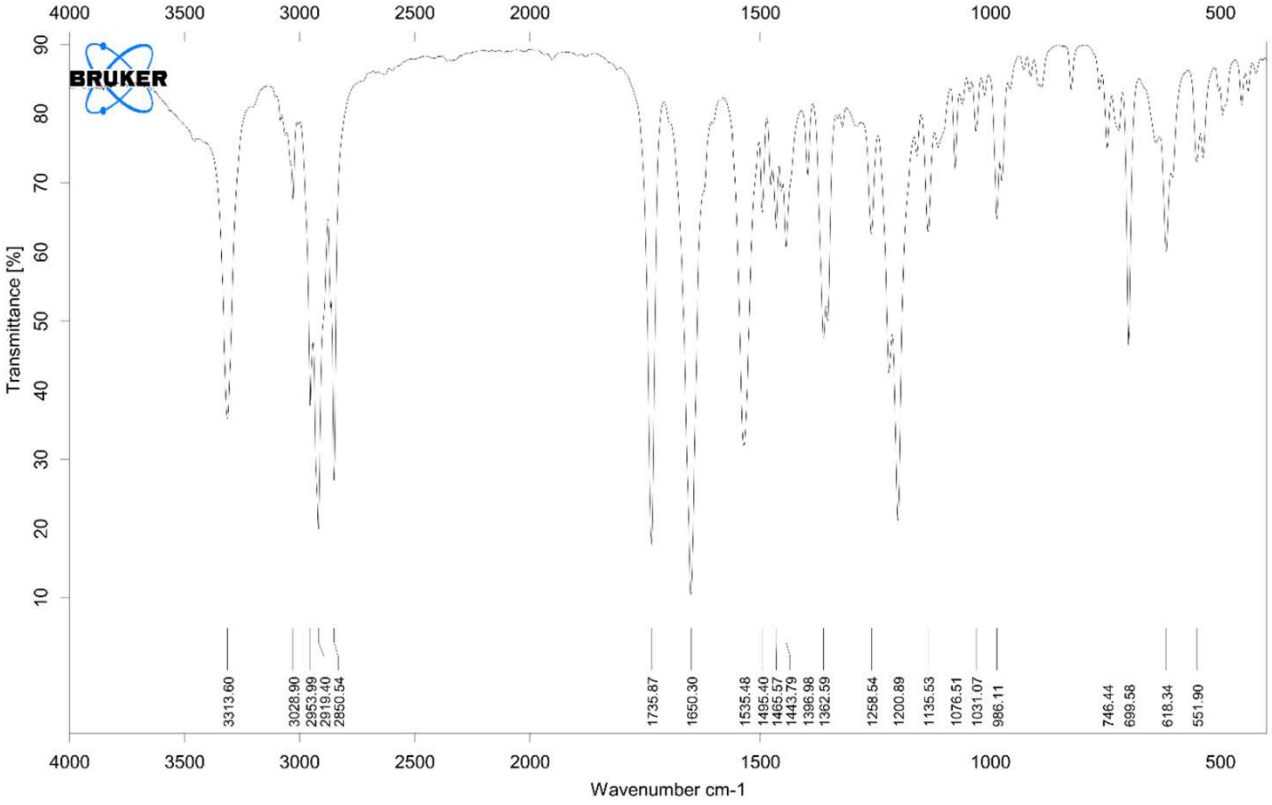
^{1}H NMR



^{13}C NMR (BA-PheC12)

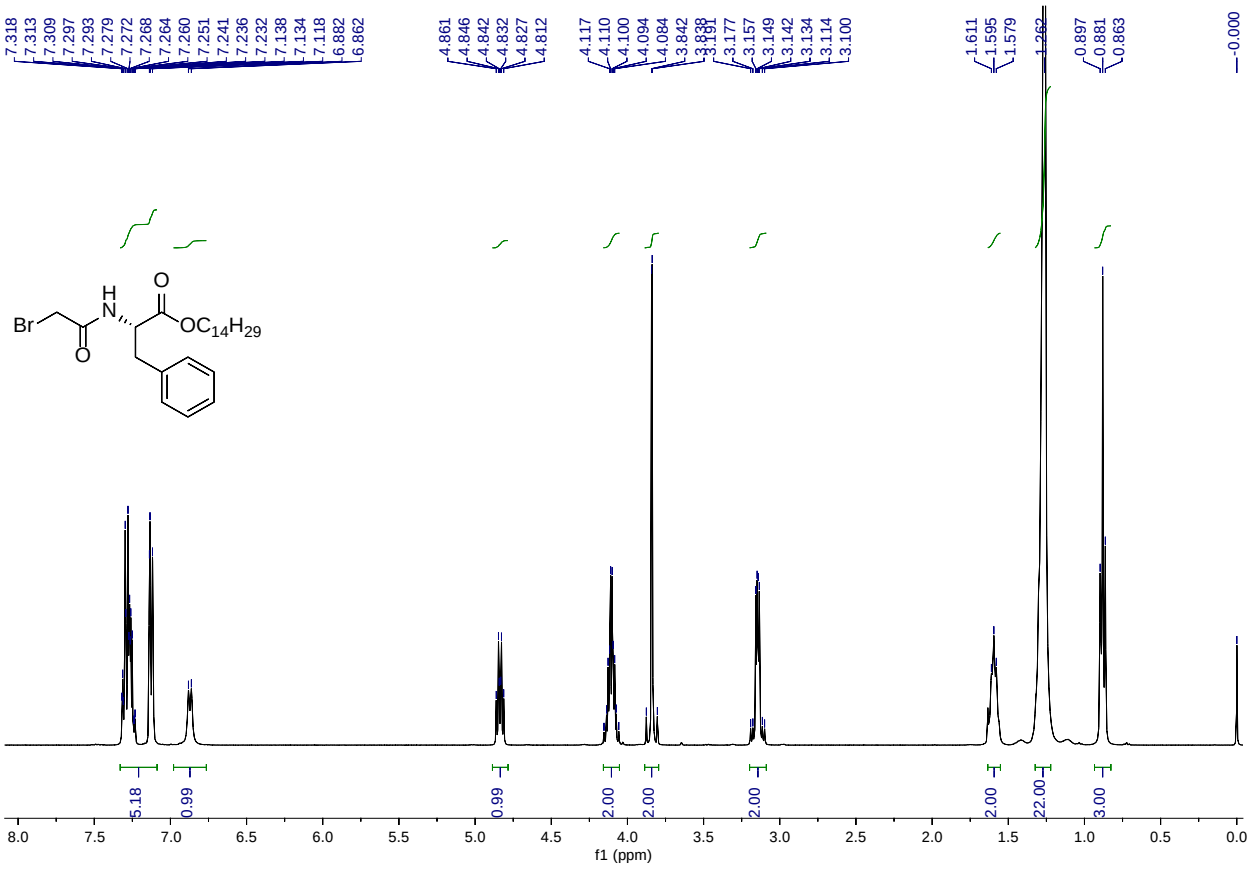


IR (KBr, cm^{-1})

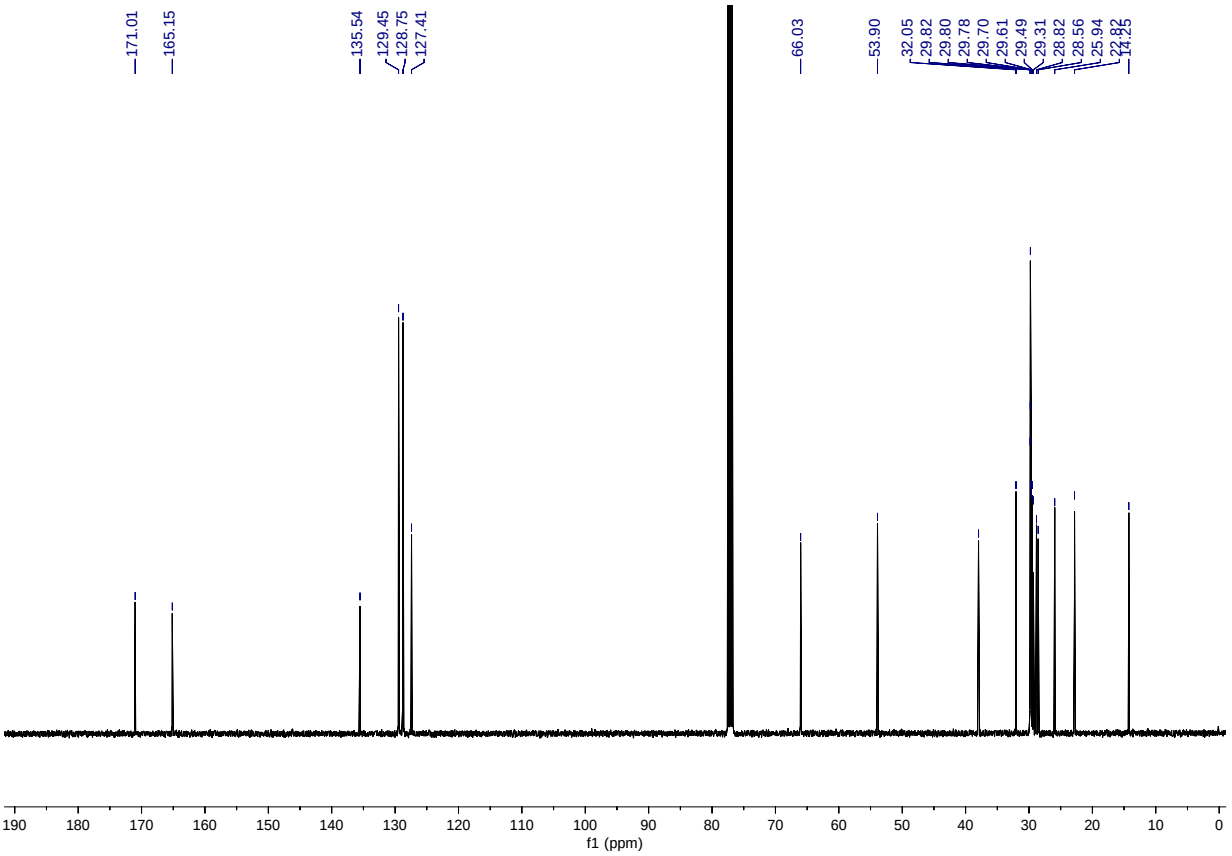

BRUKER
Transmittance [%]
Wavenumber cm-1
3313.60
3028.90
2953.99
2919.40
2850.54
1735.87
1650.30
1535.48
1495.40
1465.57
1443.79
1396.98
1362.59
1258.54
1200.89
1135.53
1076.51
1031.07
986.11
746.44
699.58
618.34
551.90

Tetradecyl (2-bromoacetyl)-L-phenylalaninate (15)

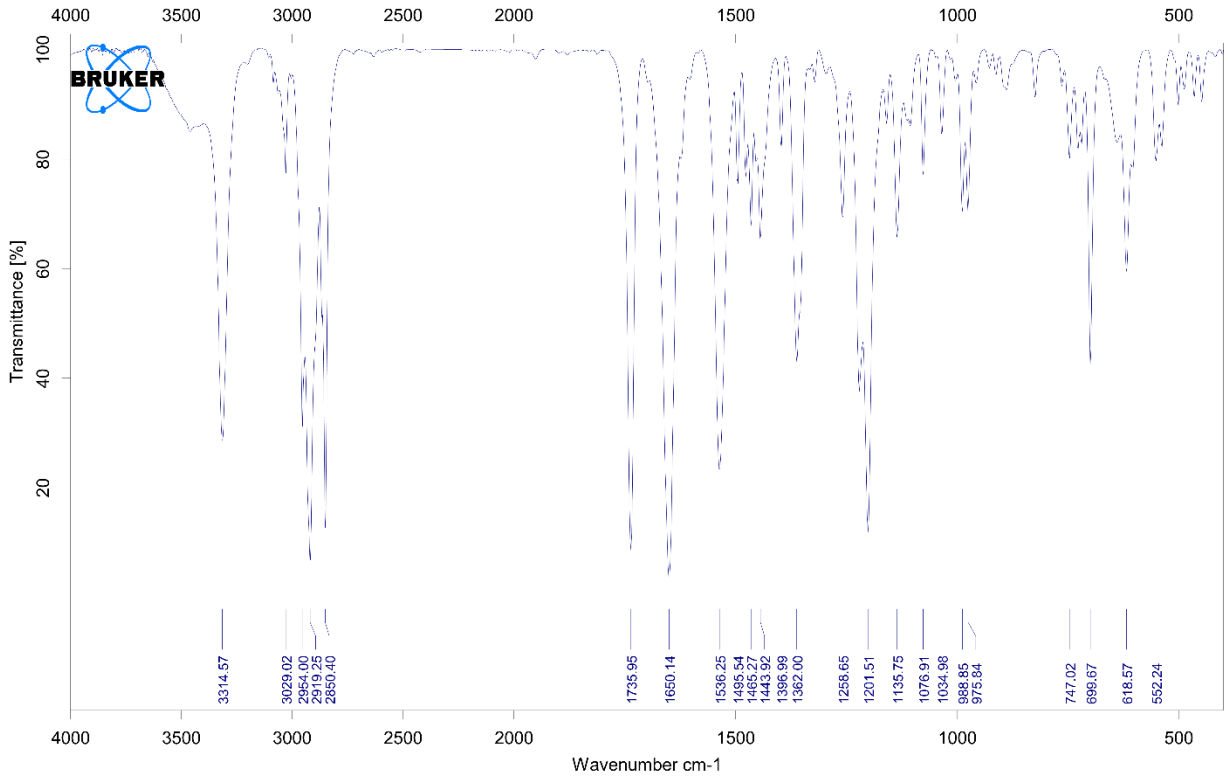
^{1}H NMR



^{13}C NMR

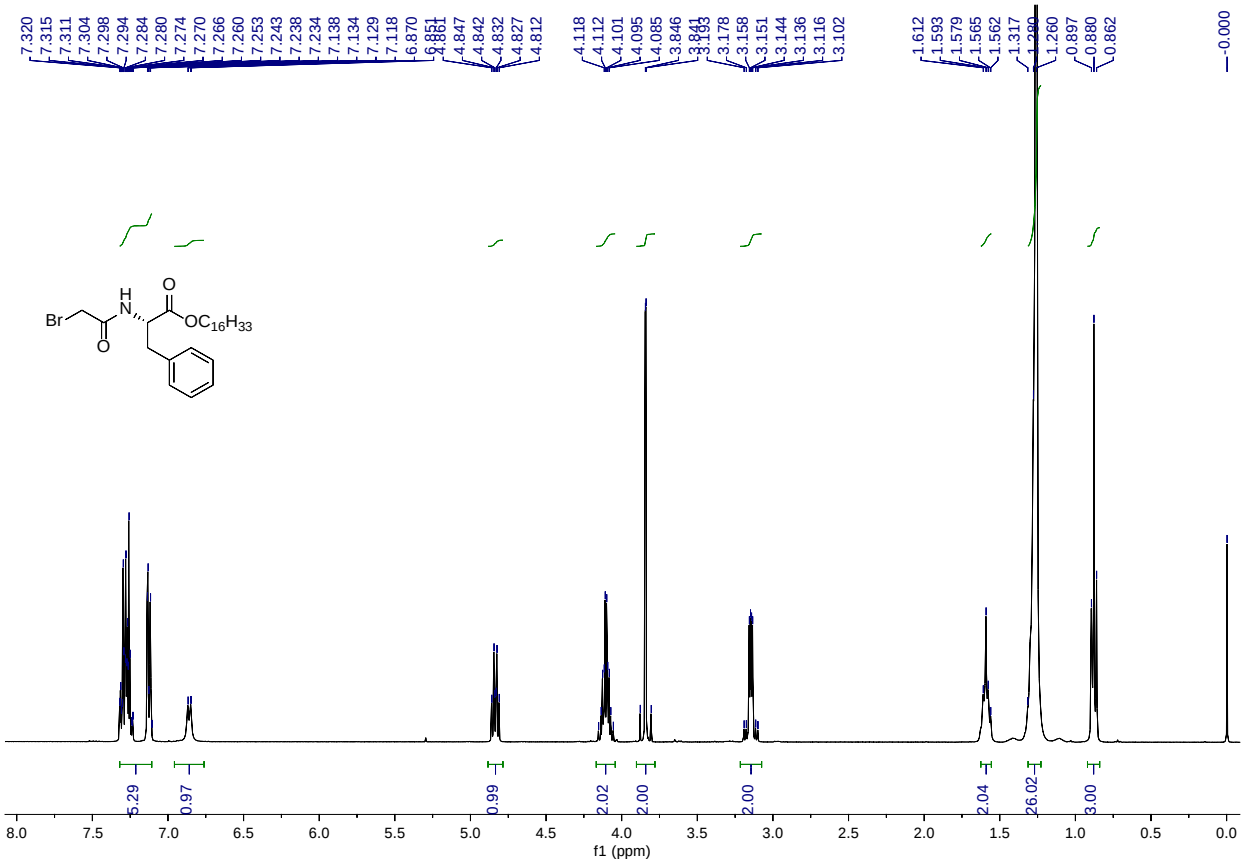


IR (KBr, cm^{-1})

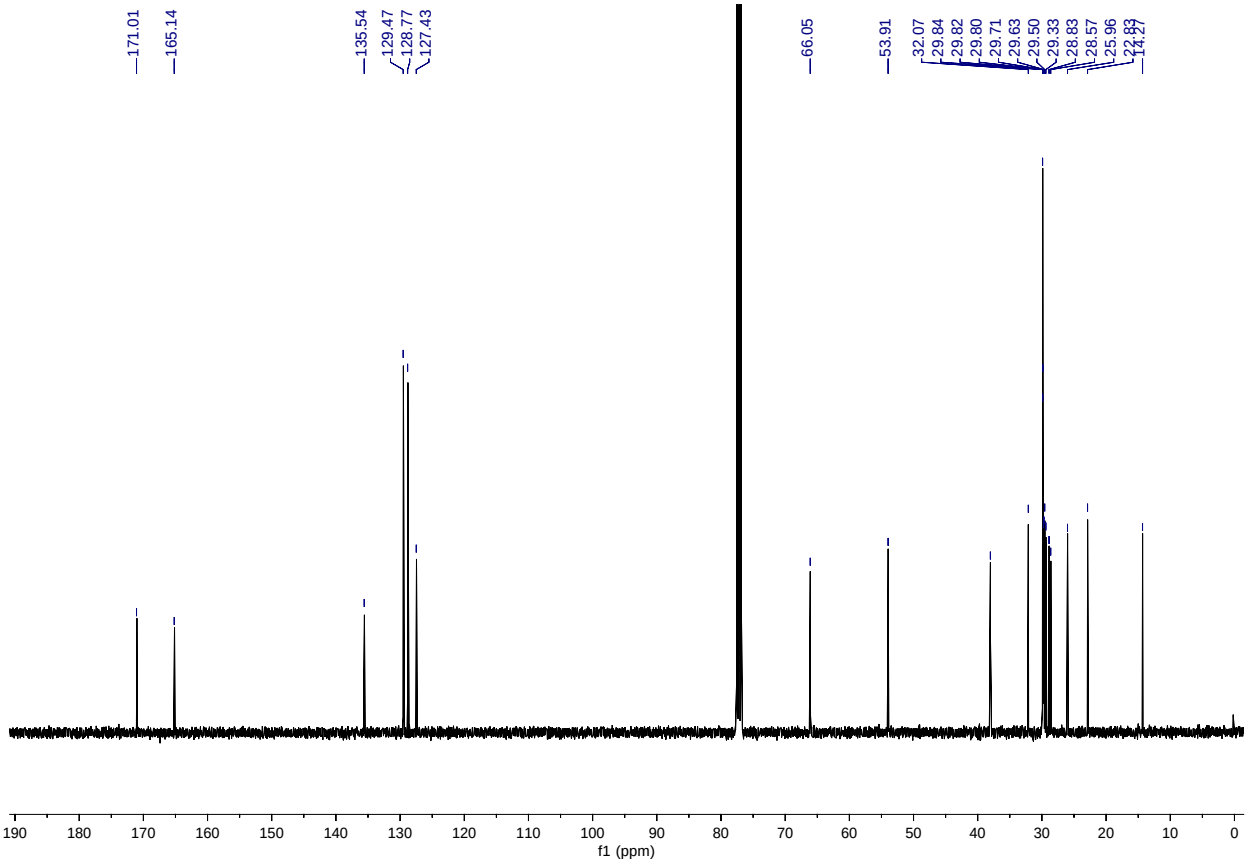

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3314.57
3029.02
2954.00
2919.25
2850.40
1735.95
1650.14
1536.25
1495.54
1465.27
1443.92
1396.99
1362.00
1258.65
1201.51
1135.75
1076.91
1034.98
988.85
975.84
747.02
699.67
618.57
552.24
Wavenumber cm-1

Hexadecyl (2-bromoacetyl)-L-phenylalaninate (16)

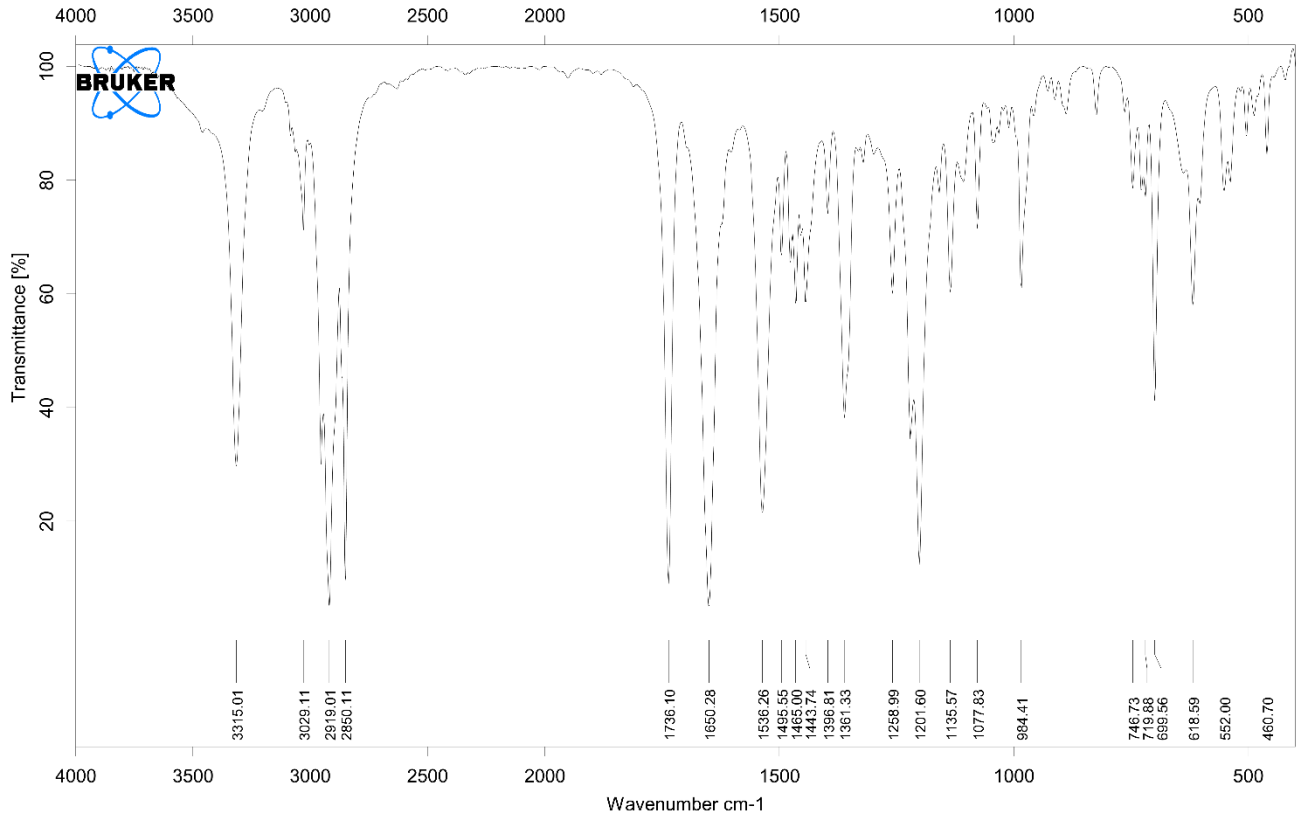
^{1}H NMR



^{13}C NMR



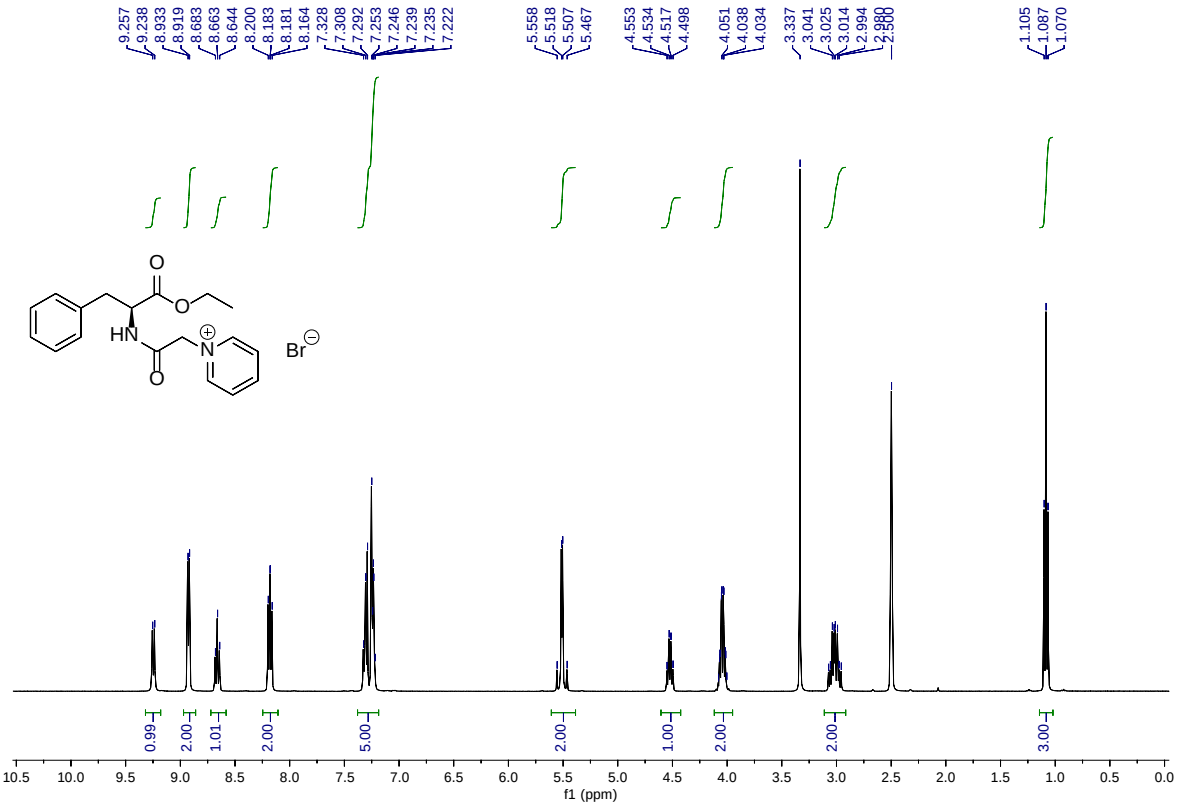
IR (KBr, cm^{-1})


BRUKER
Transmittance [%]
Wavenumber cm-1
3315.01
3029.11
2919.01
2850.11
1736.10
1650.28
1536.26
1495.55
1465.00
1443.74
1396.81
1361.33
1258.99
1201.60
1135.57
1077.83
984.41
746.73
719.88
699.56
618.59
552.00
460.70

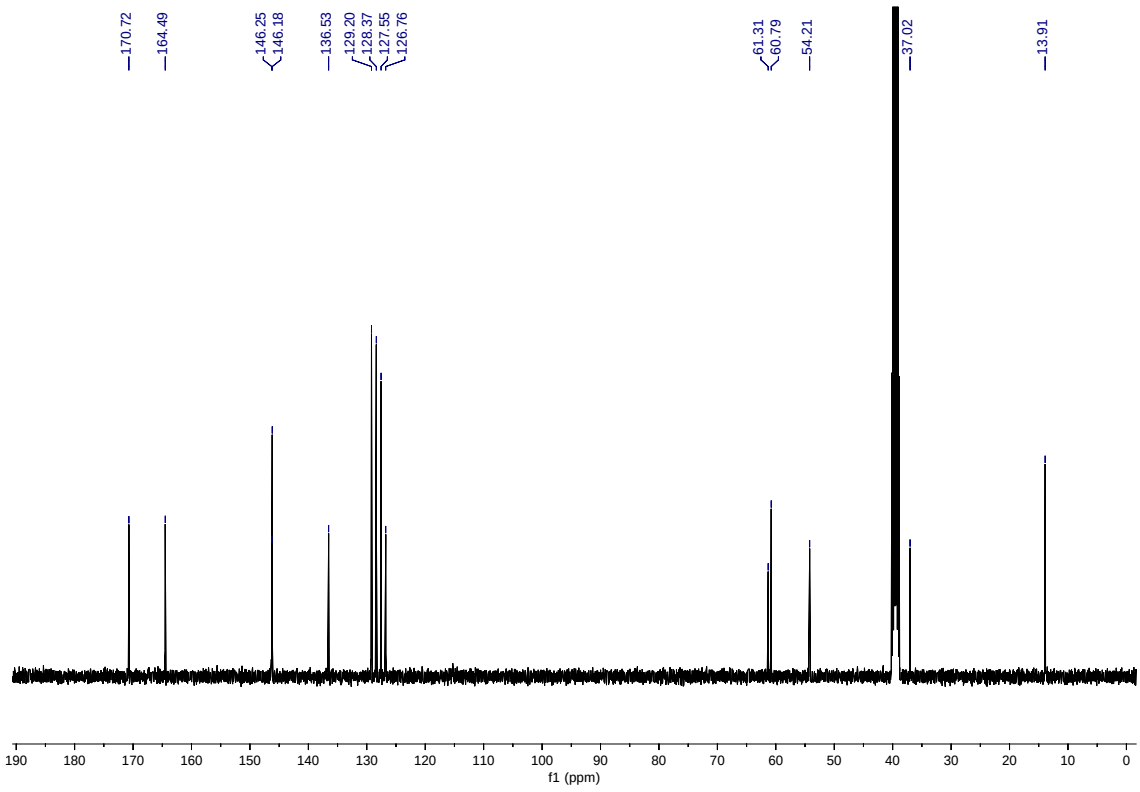
11. NMR and IR spectra of pyridinium ILs (17 - 24)

(*S*)-1-(2-((1-(Ethyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (17)

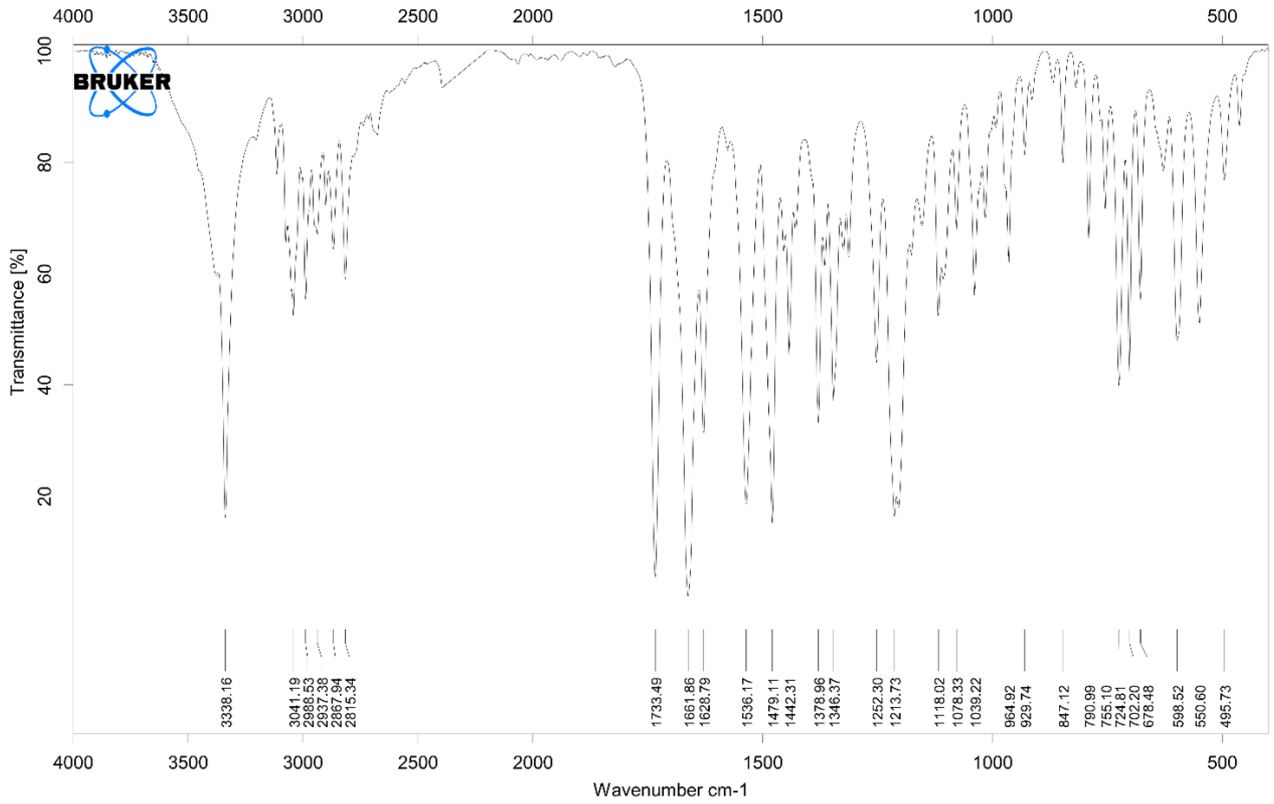
^{1}H NMR **(17)**



^{13}C NMR **(17)**

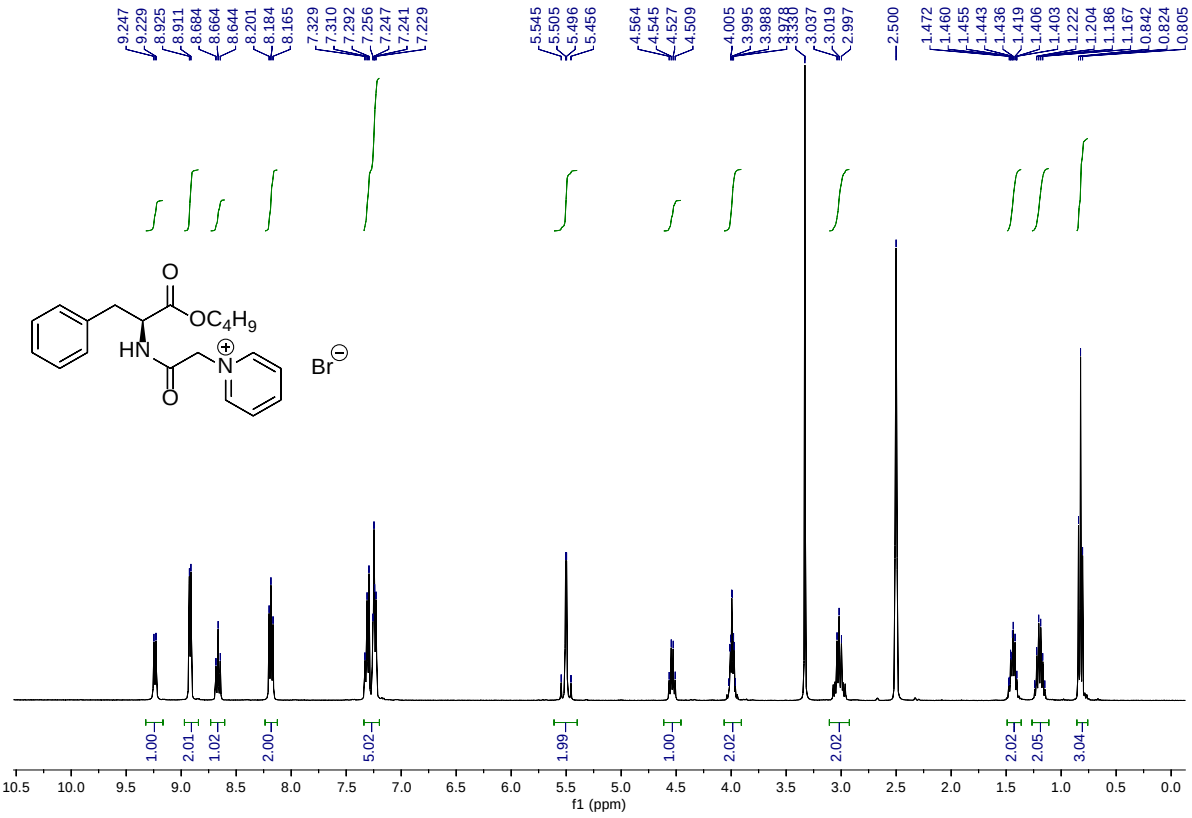


IR (KBr, cm^{-1})

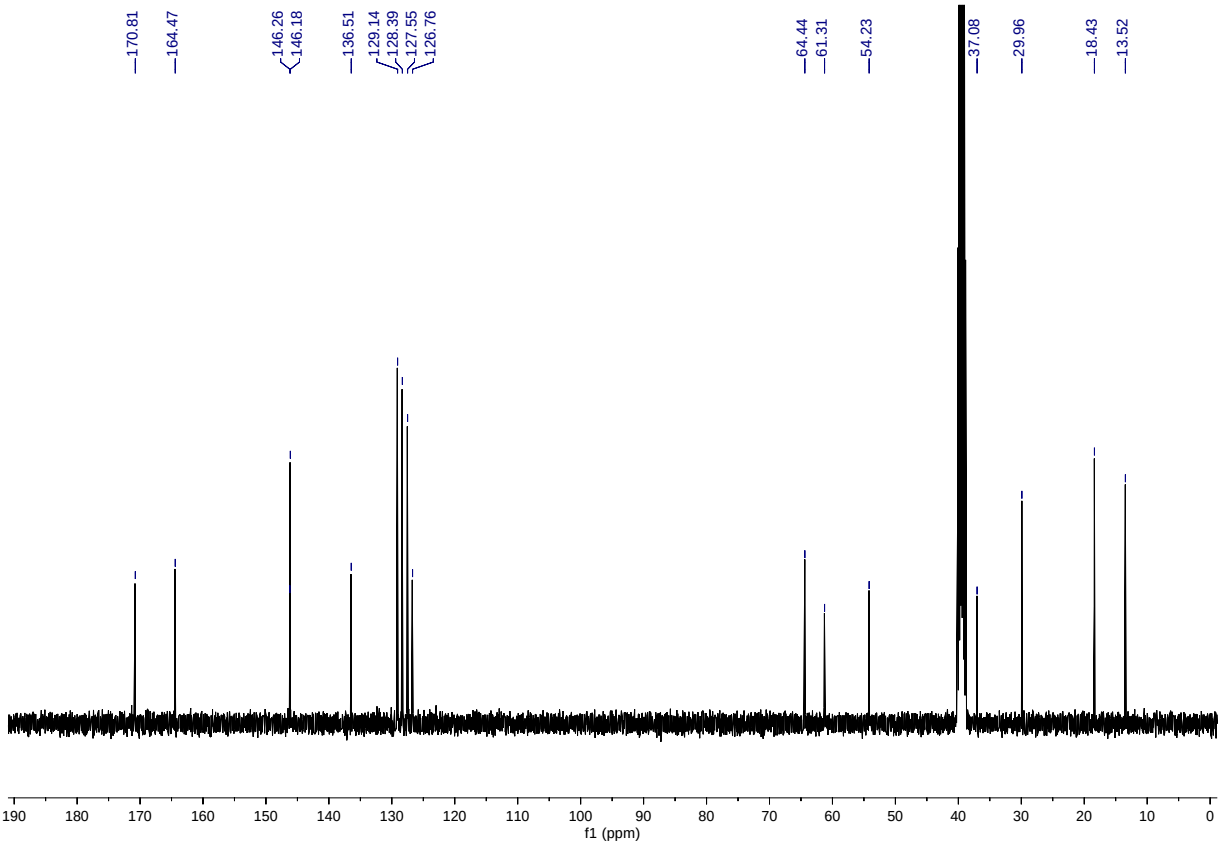

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3338.16
3041.19
2988.53
2937.38
2867.94
2815.34
1733.49
1661.86
1628.79
1536.17
1479.11
1442.31
1378.96
1346.37
1252.30
1213.73
1118.02
1078.33
1039.22
964.92
929.74
847.12
790.99
755.10
724.81
702.20
678.48
598.52
550.60
495.73
Wavenumber cm-1

(*S*)-1-(2-((1-(Butyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (18)

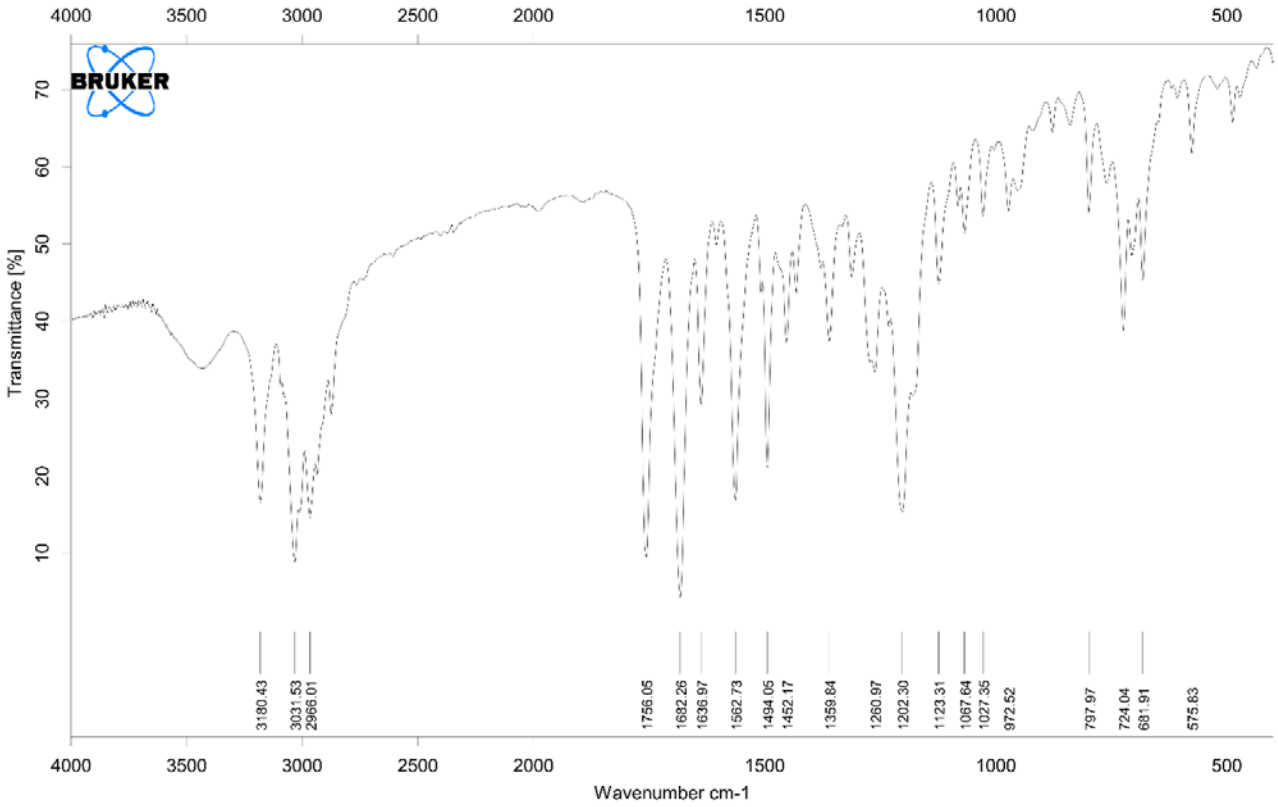
^{1}H NMR



^{13}C NMR

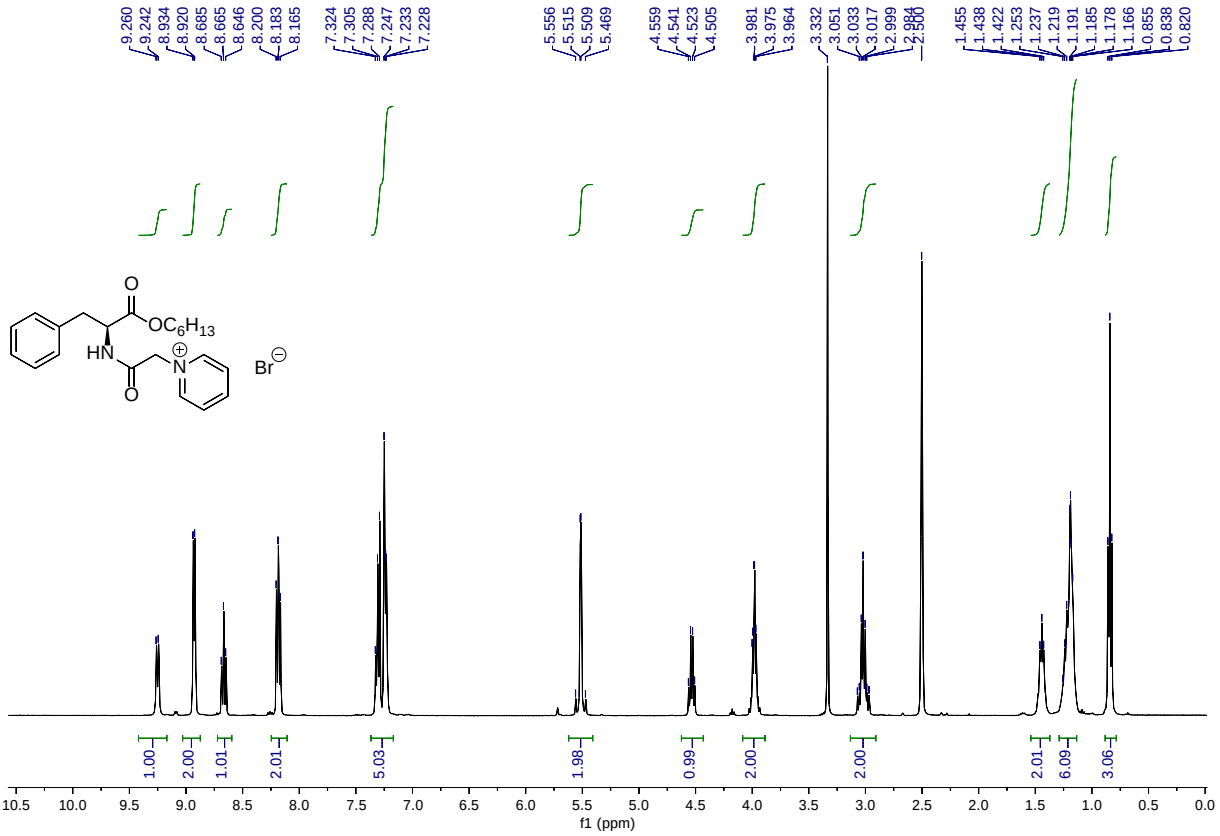


IR (KBr, cm^{-1})

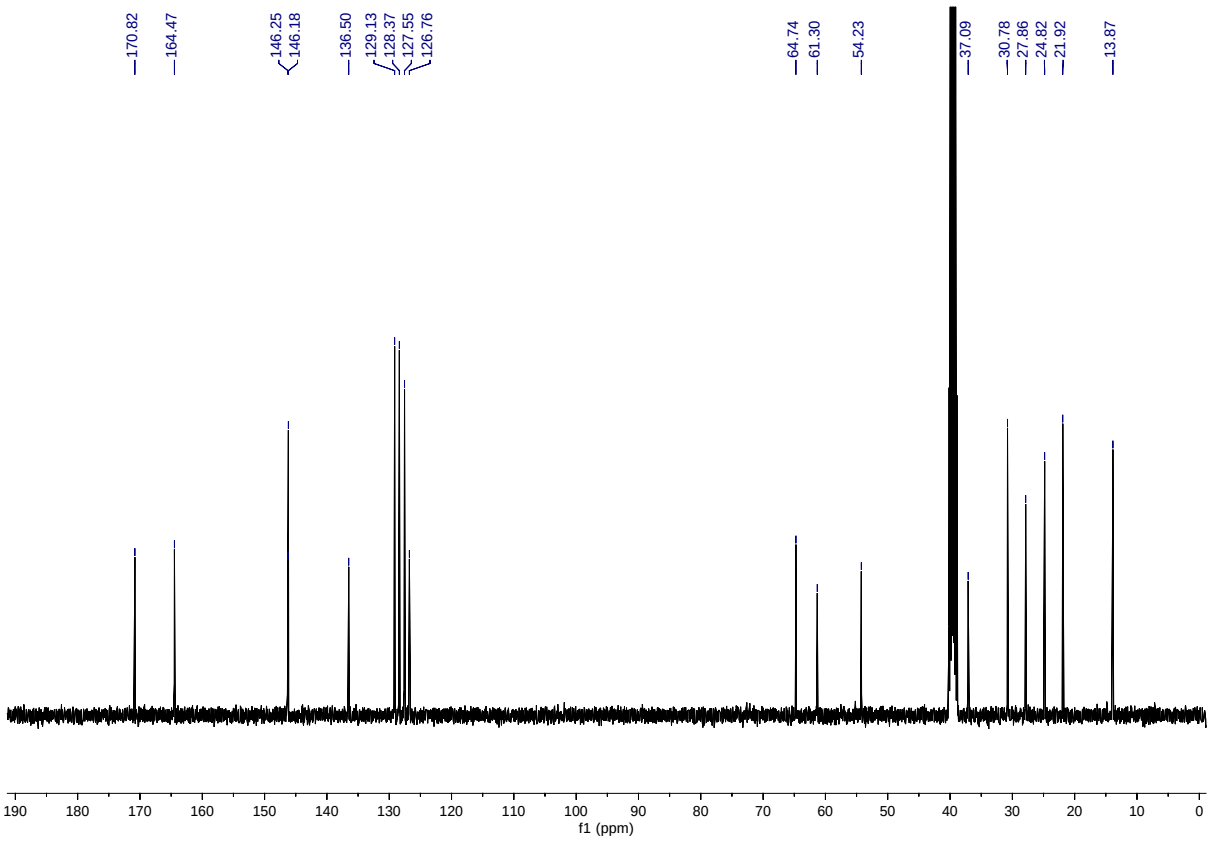

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
10
20
30
40
50
60
70
3180.43
3031.53
2966.01
1756.05
1682.26
1636.97
1562.73
1494.05
1452.17
1359.84
1260.97
1202.30
1123.31
1067.64
1027.35
972.52
797.97
724.04
681.91
575.63
Wavenumber cm-1

(*S*)-1-(2-((1-(Hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (19)

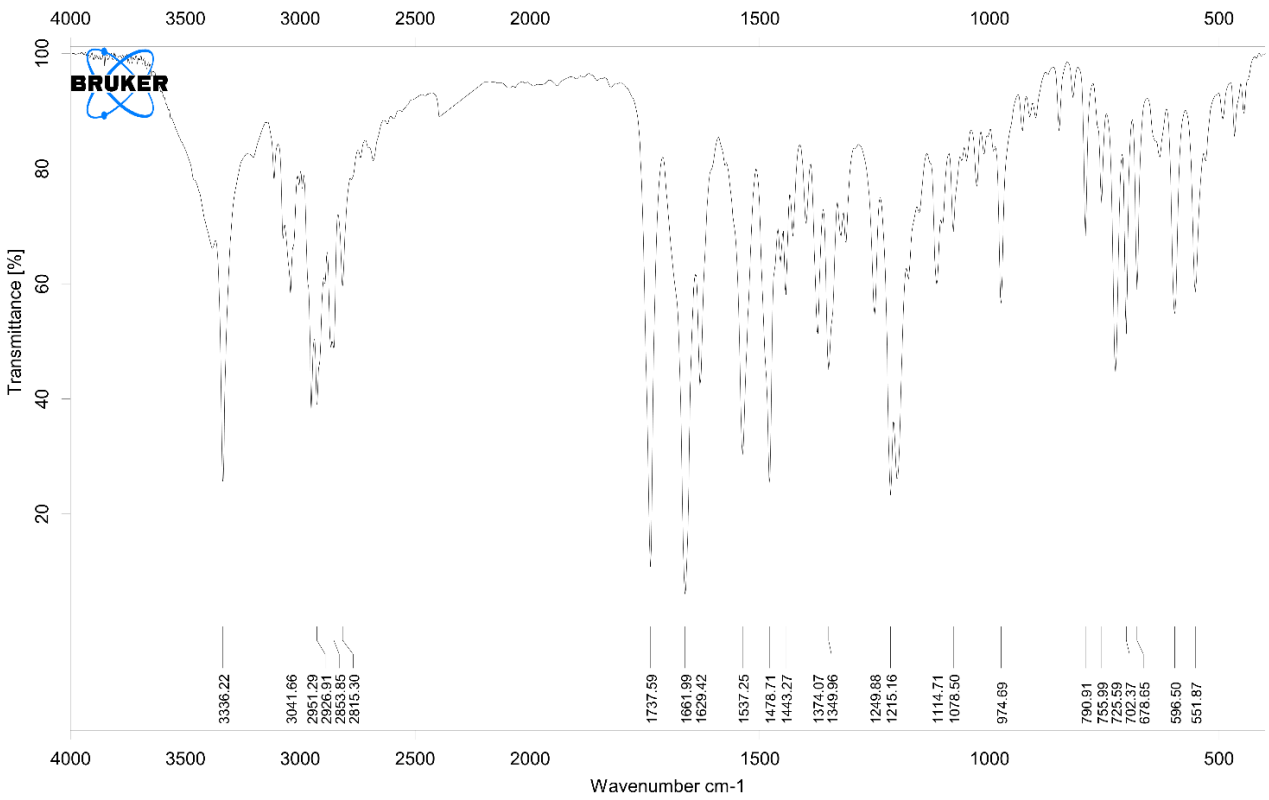
^{1}H NMR



^{13}C NMR

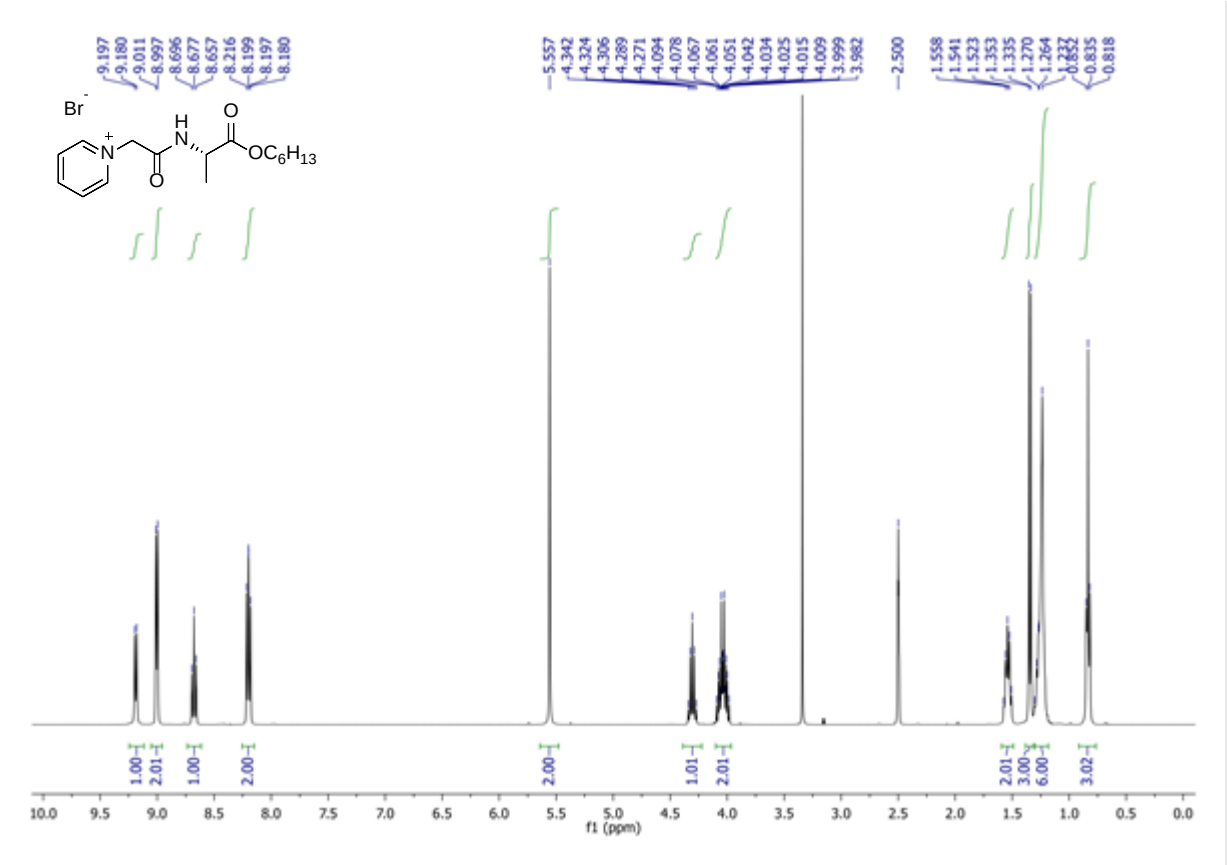


IR (KBr, cm^{-1})

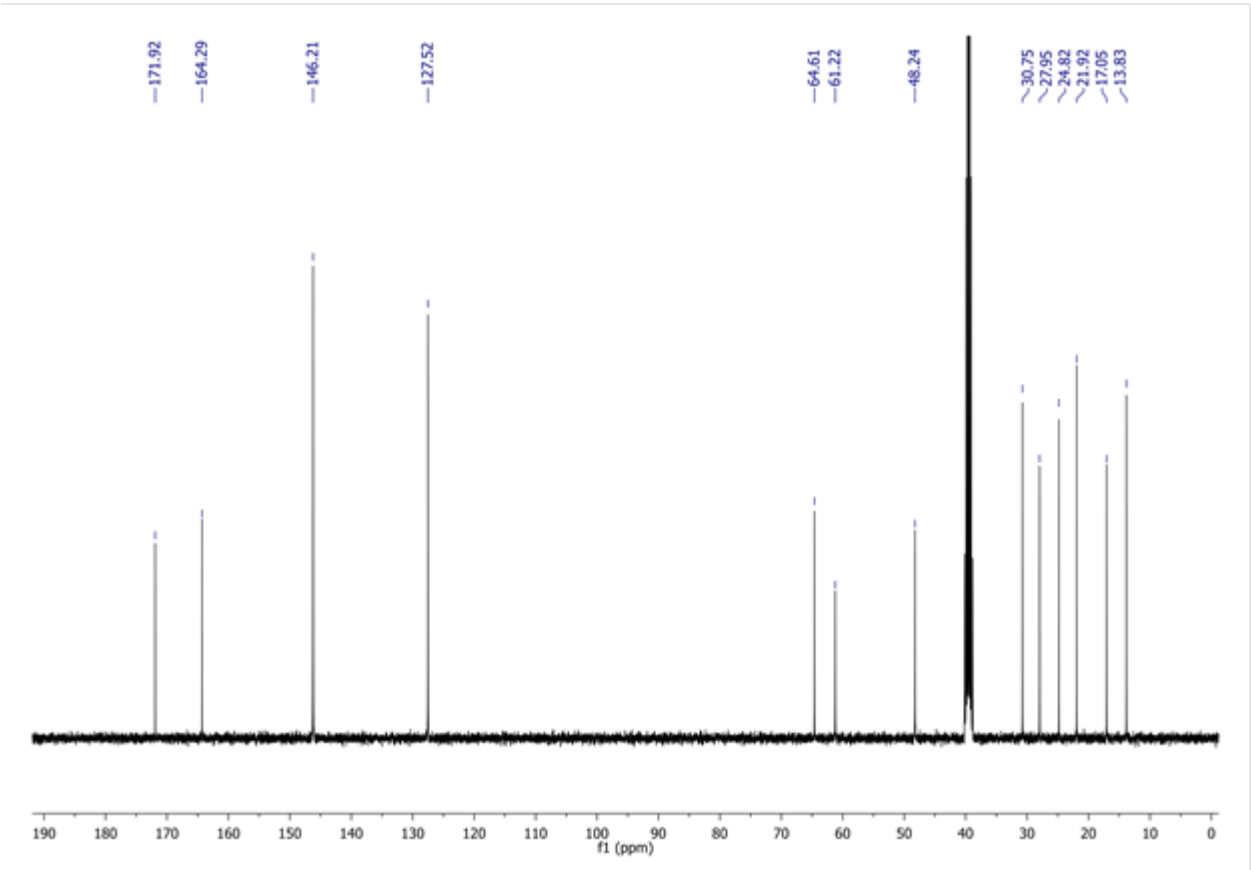

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3336.22
3041.66
2951.29
2926.91
2853.85
2815.30
1737.59
1661.99
1629.42
1537.25
1478.71
1443.27
1374.07
1349.96
1249.88
1215.16
1114.71
1078.50
974.69
790.91
755.99
725.59
702.37
678.65
596.50
551.87
Wavenumber cm-1

(*S*)-1-(2-((1-(hexyloxy)-1-oxopropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (19Ala)

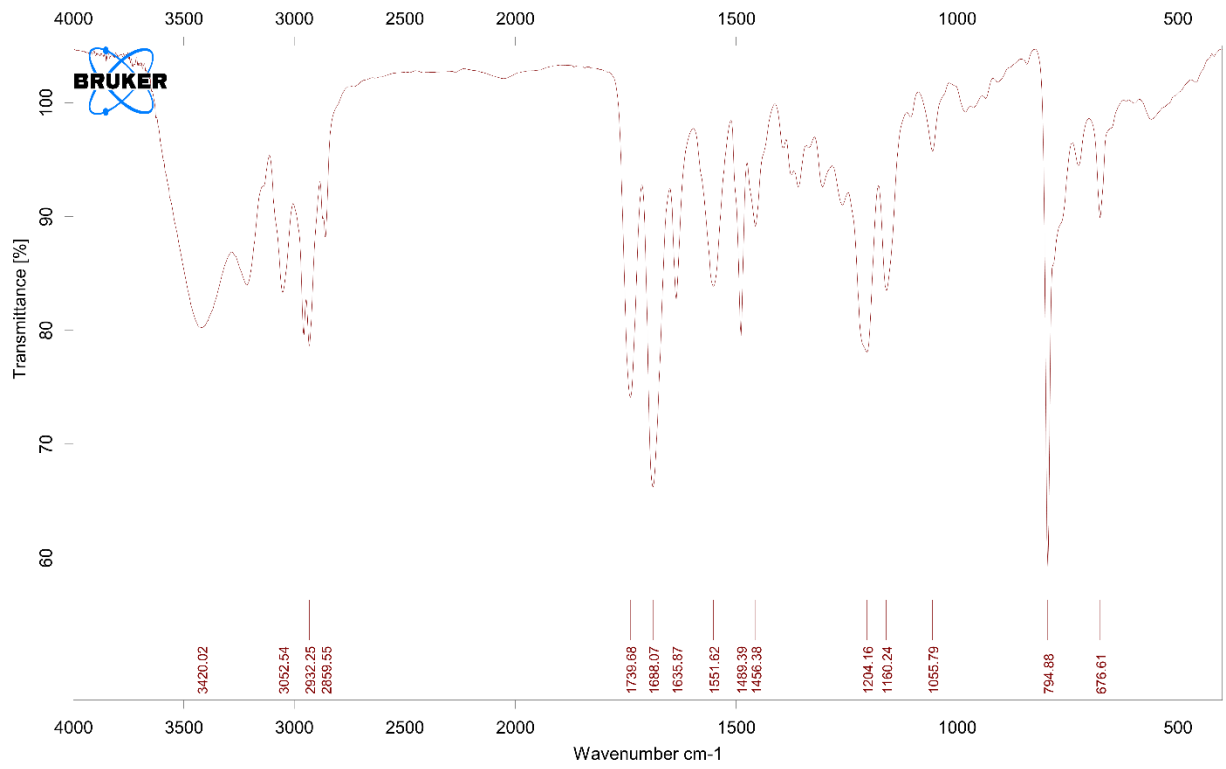
^{1}H NMR



^{13}C NMR

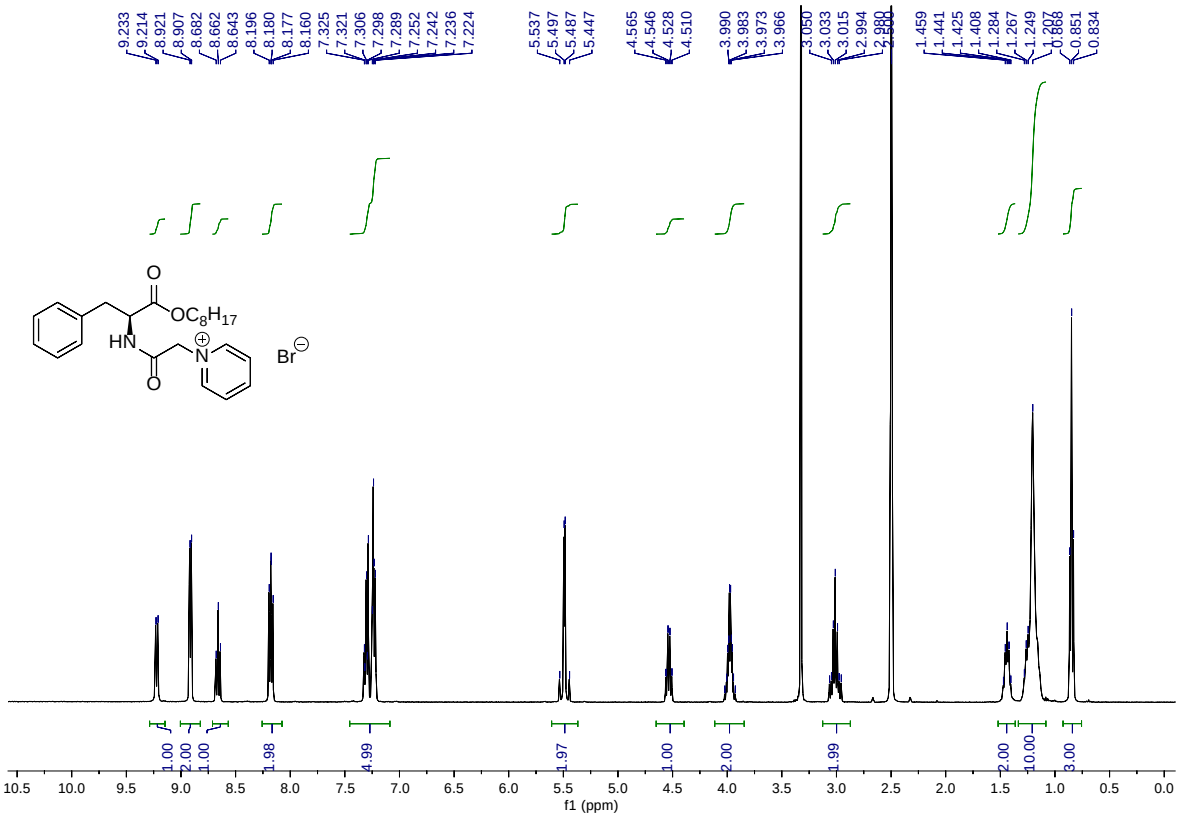


IR (KBr, cm^{-1}):

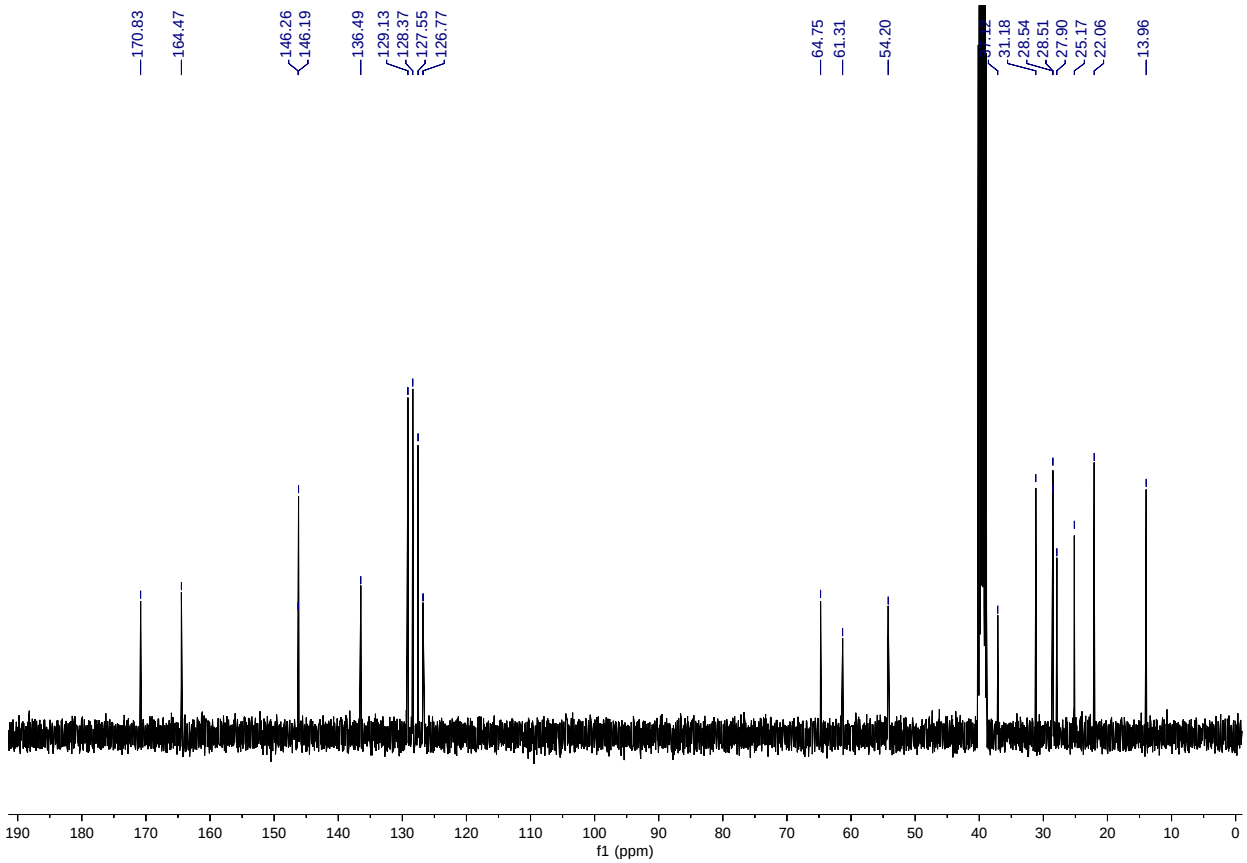

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
100
90
80
70
60
3420.02
3052.54
2932.25
2859.55
1739.68
1688.07
1635.87
1551.62
1489.39
1456.38
1204.16
1160.24
1055.79
794.88
676.61
Wavenumber cm-1

(*S*)-1-(2-((1-(Octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (20)

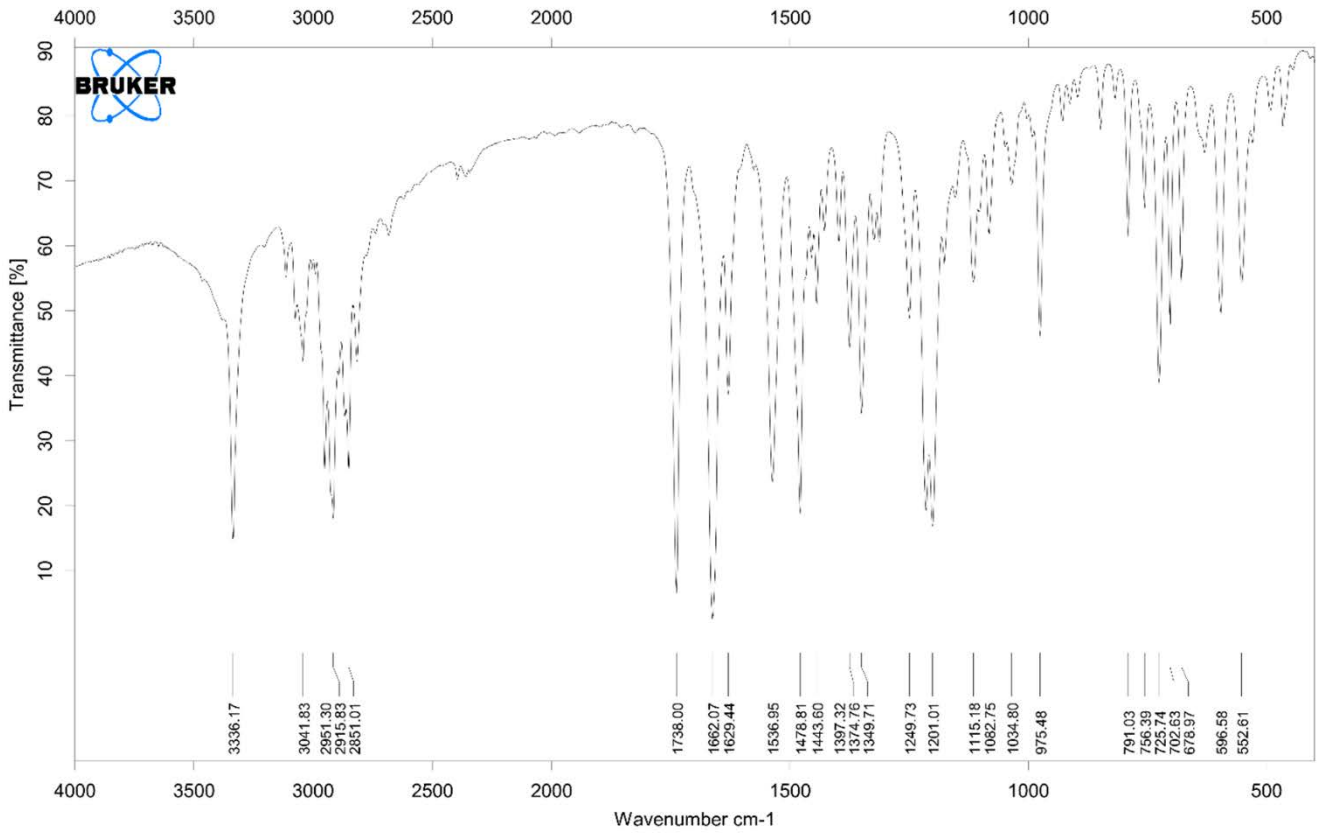
^{1}H NMR



^{13}C NMR **(20)**

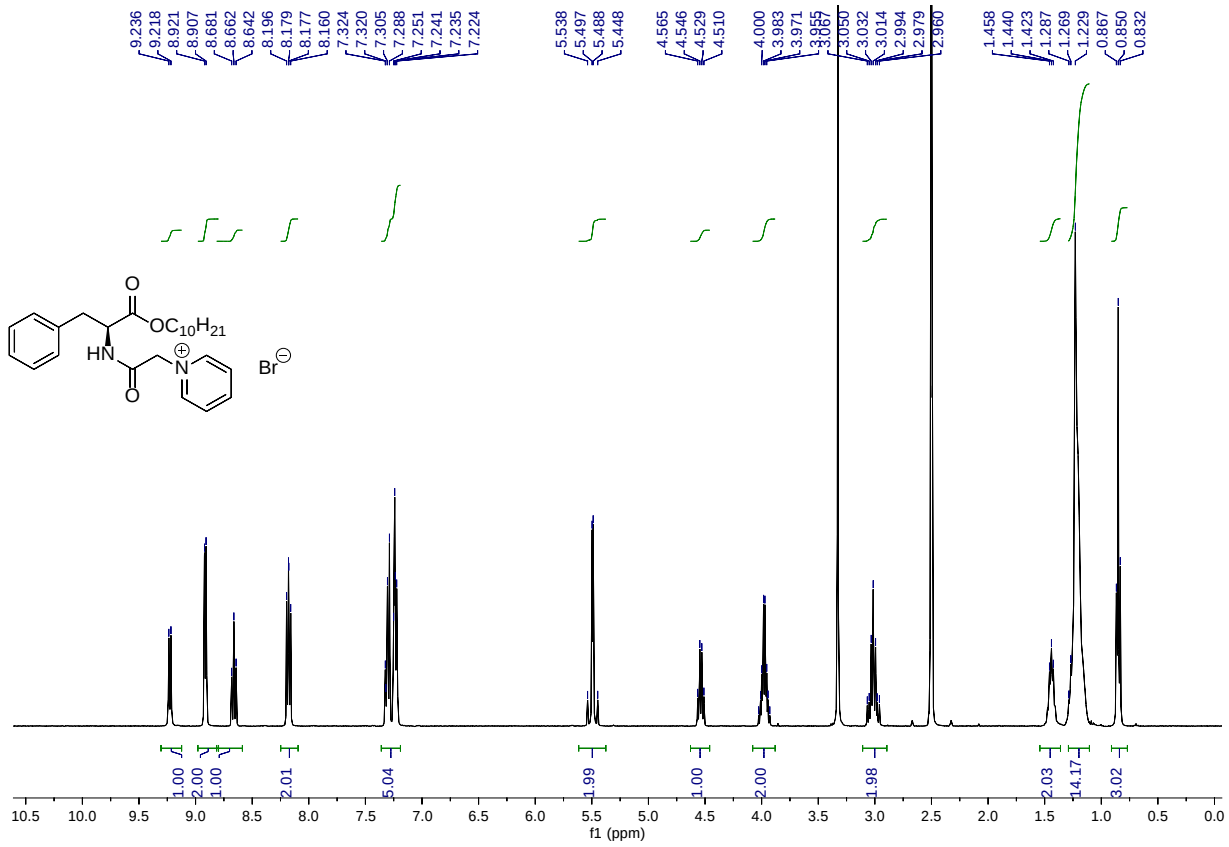


IR (KBr, cm^{-1})

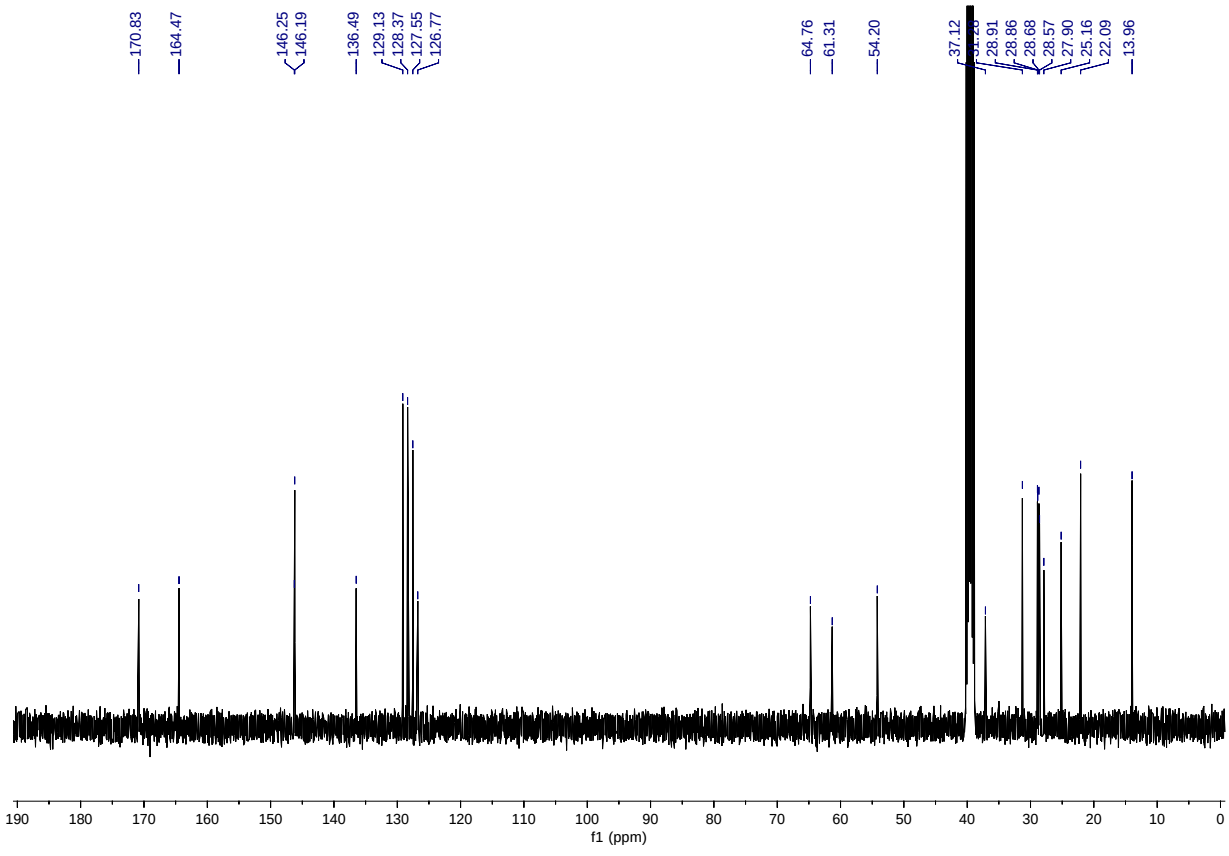

BRUKER
Transmittance [%]
Wavenumber cm-1
3336.17
3041.83
2951.30
2915.83
2851.01
1738.00
1662.07
1629.44
1536.95
1478.81
1443.60
1397.32
1374.76
1349.71
1249.73
1201.01
1115.18
1082.75
1034.80
975.48
791.03
756.39
725.74
702.63
678.97
596.58
552.61

(*S*)-1-(2-((1-(Decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (21)

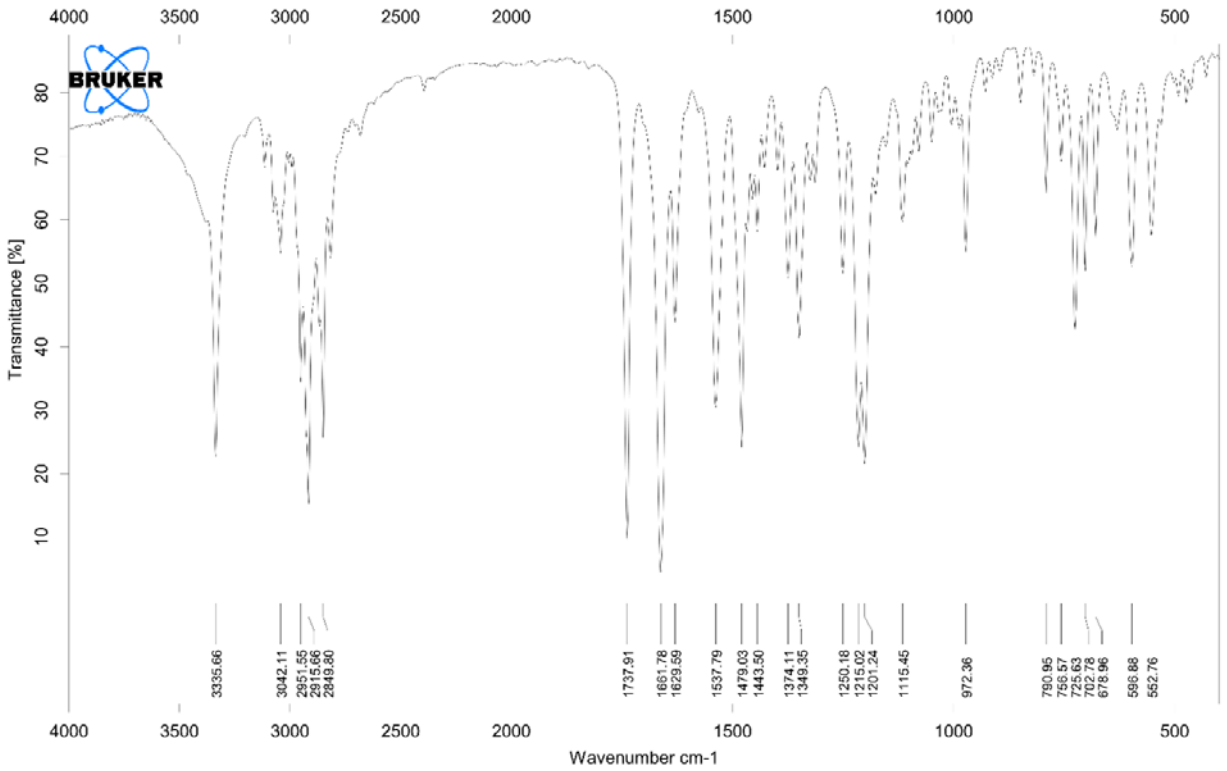
^{1}H NMR



^{13}C NMR

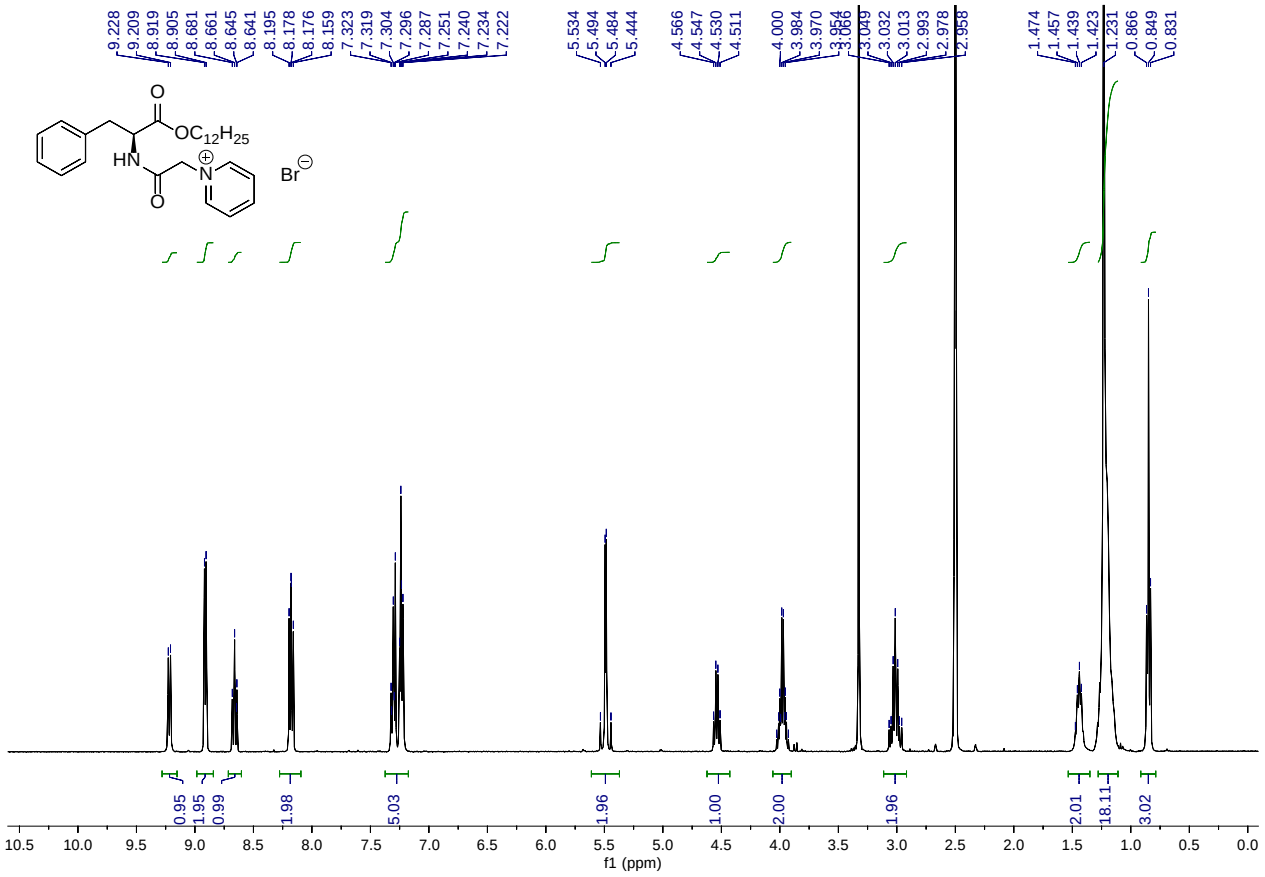


IR (KBr, cm^{-1})

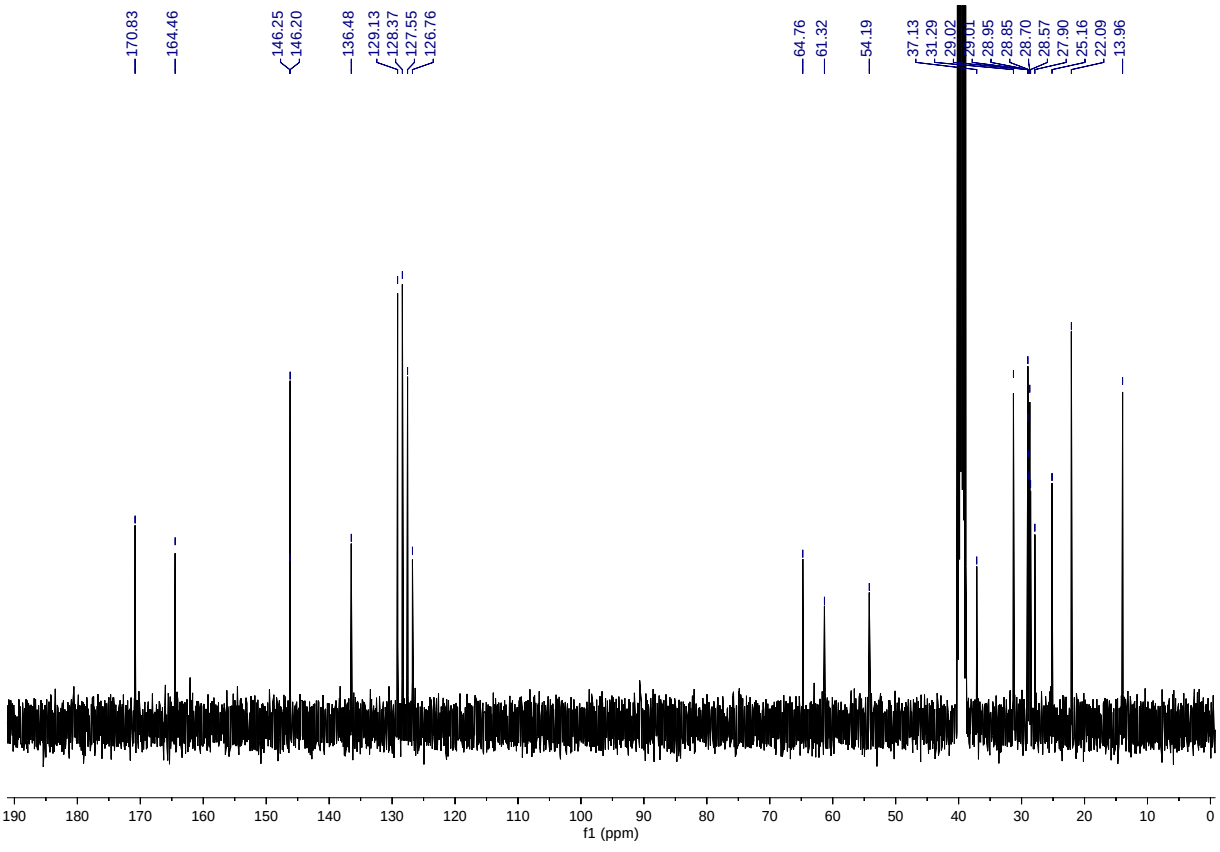

BRUKER
Transmittance [%]
Wavenumber cm-1
3335.66
3042.11
2951.55
2915.66
2849.80
1737.91
1661.78
1629.59
1537.79
1479.03
1443.50
1374.11
1349.35
1250.18
1215.02
1201.24
1115.45
972.36
790.95
756.57
725.63
702.78
678.96
596.88
552.76

(*S*)-1-(2-((1-(Dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (22)

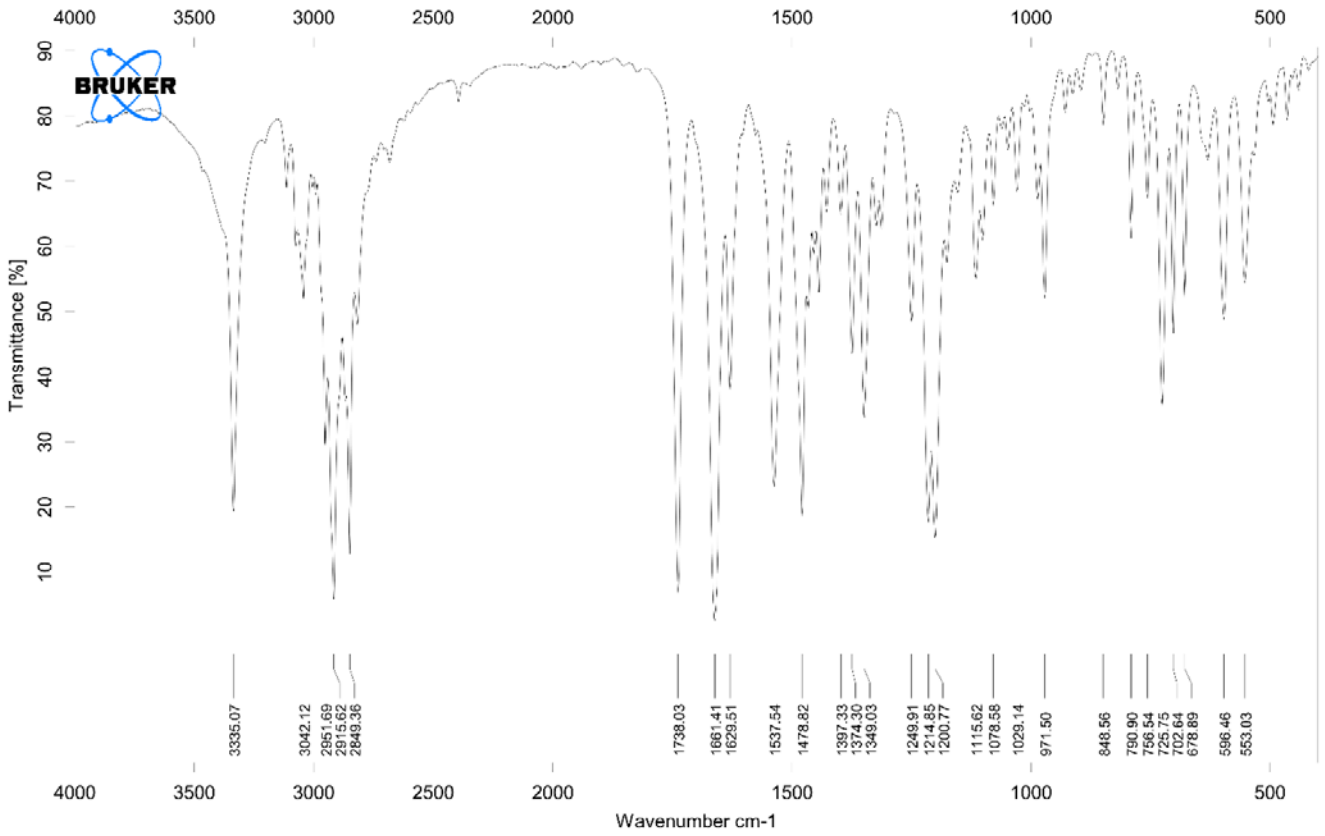
^{1}H NMR



^{13}C NMR

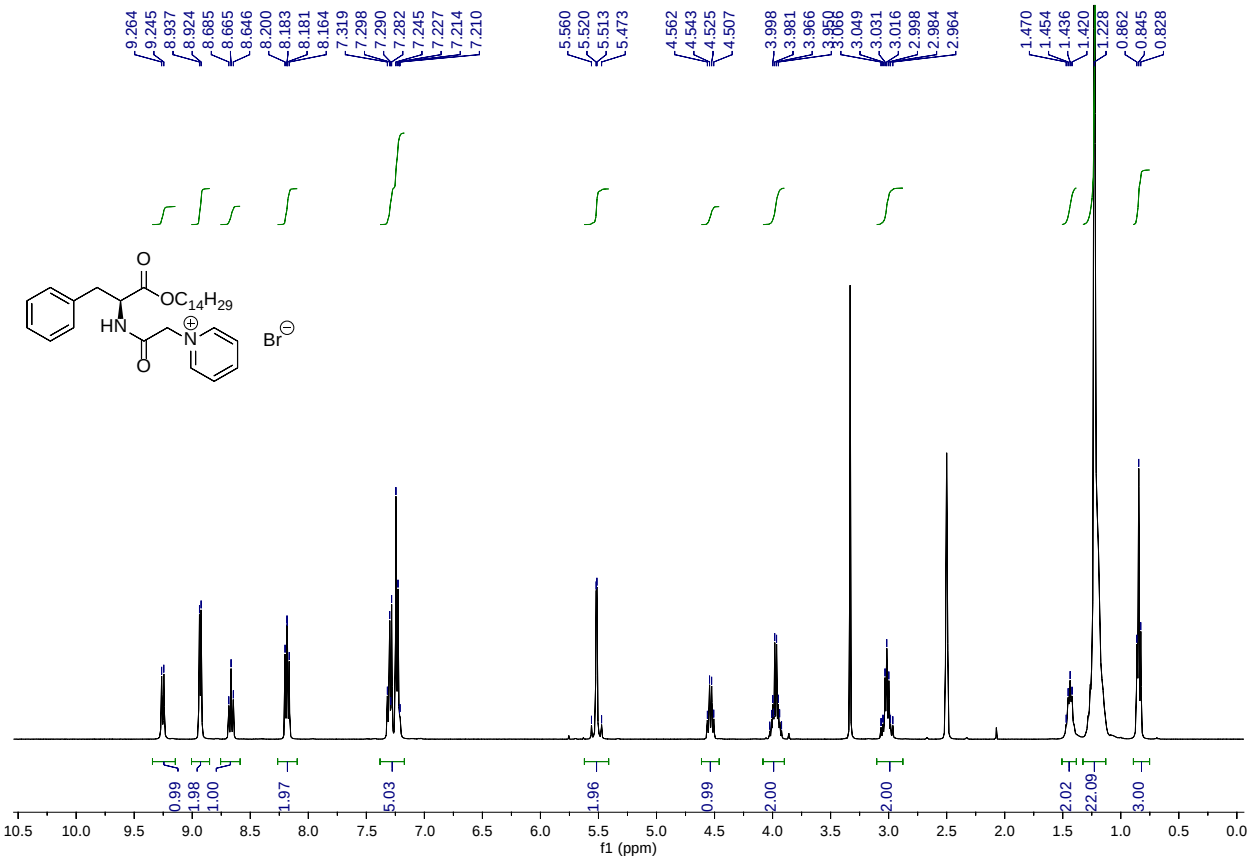


IR (KBr, cm^{-1})

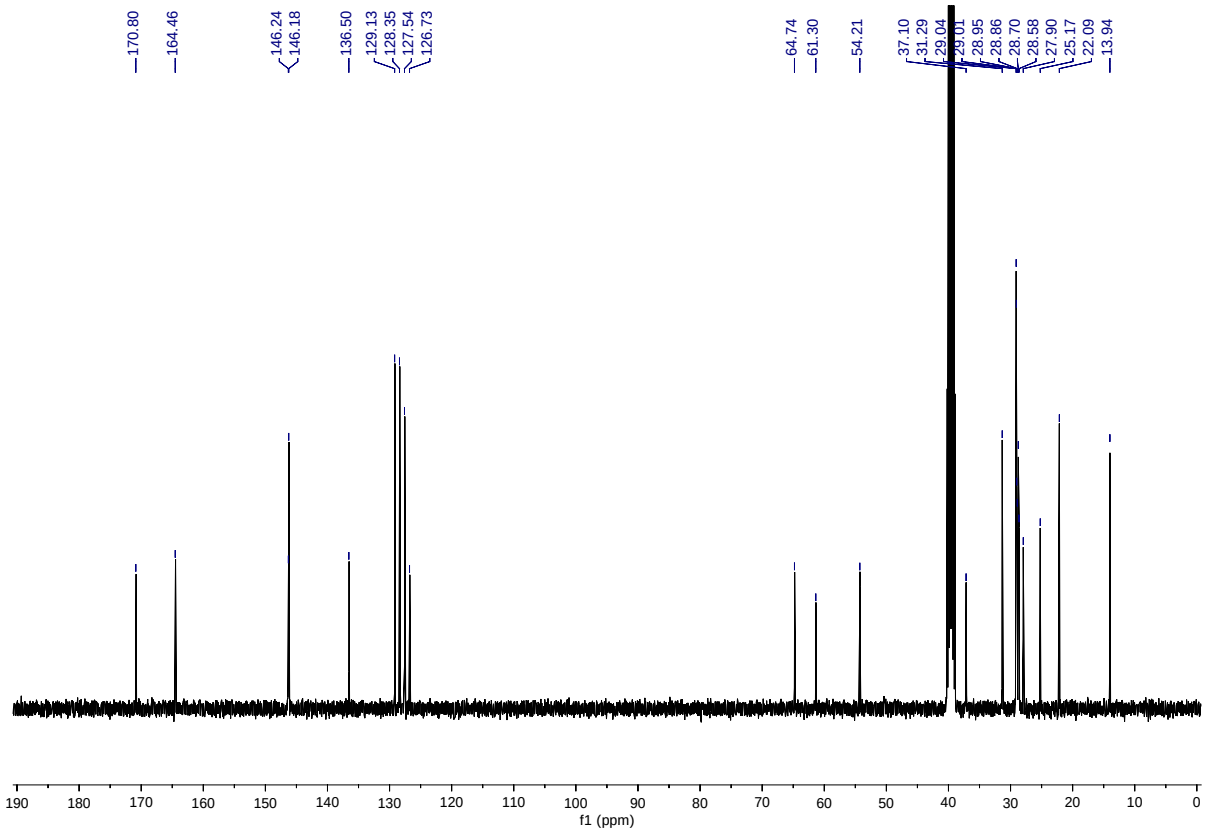

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
90
80
70
60
50
40
30
20
10
3335.07
3042.12
2951.69
2915.62
2849.36
1738.03
1681.41
1629.51
1537.54
1478.82
1397.33
1374.30
1349.03
1249.91
1214.85
1200.77
1115.62
1078.58
1029.14
971.50
848.56
790.90
756.54
725.75
702.64
678.89
596.46
553.03
Wavenumber cm-1

(*S*)-1-(2-((1-(Tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (23)

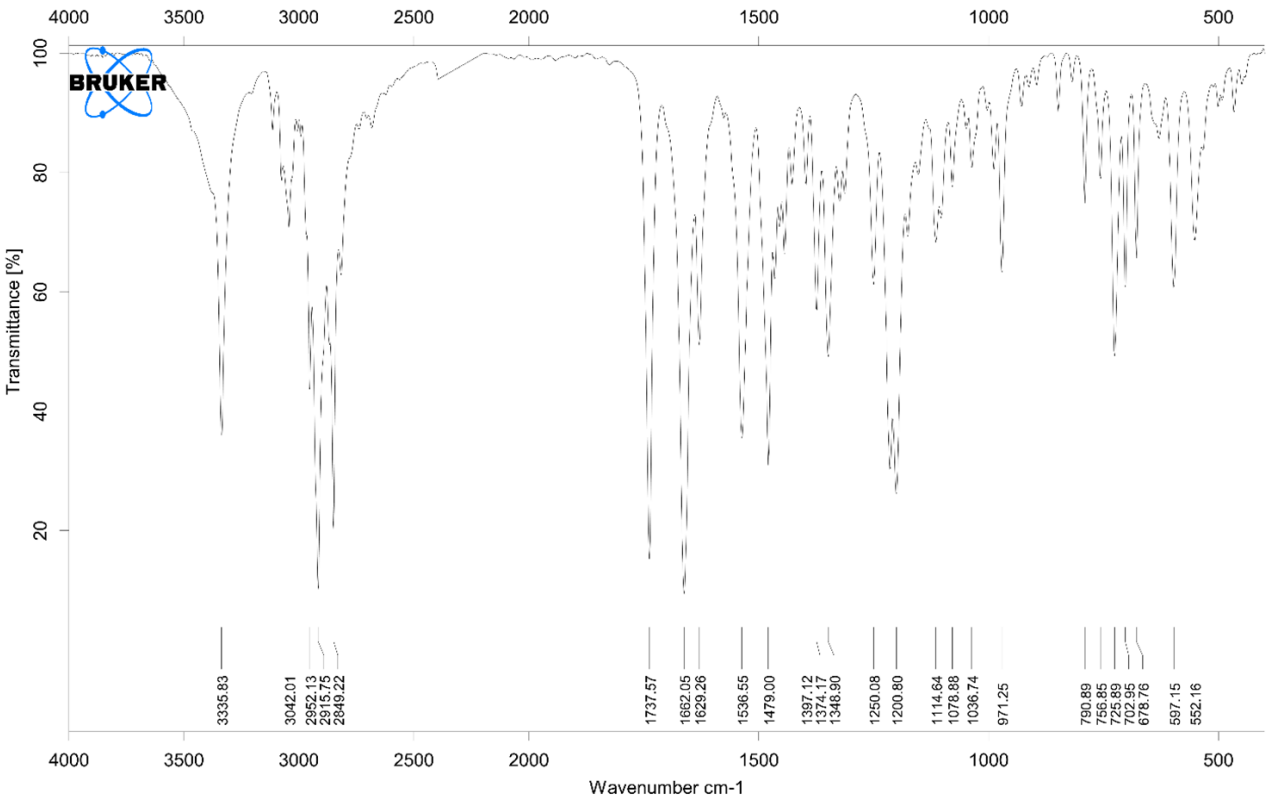
^{1}H NMR



^{13}C NMR

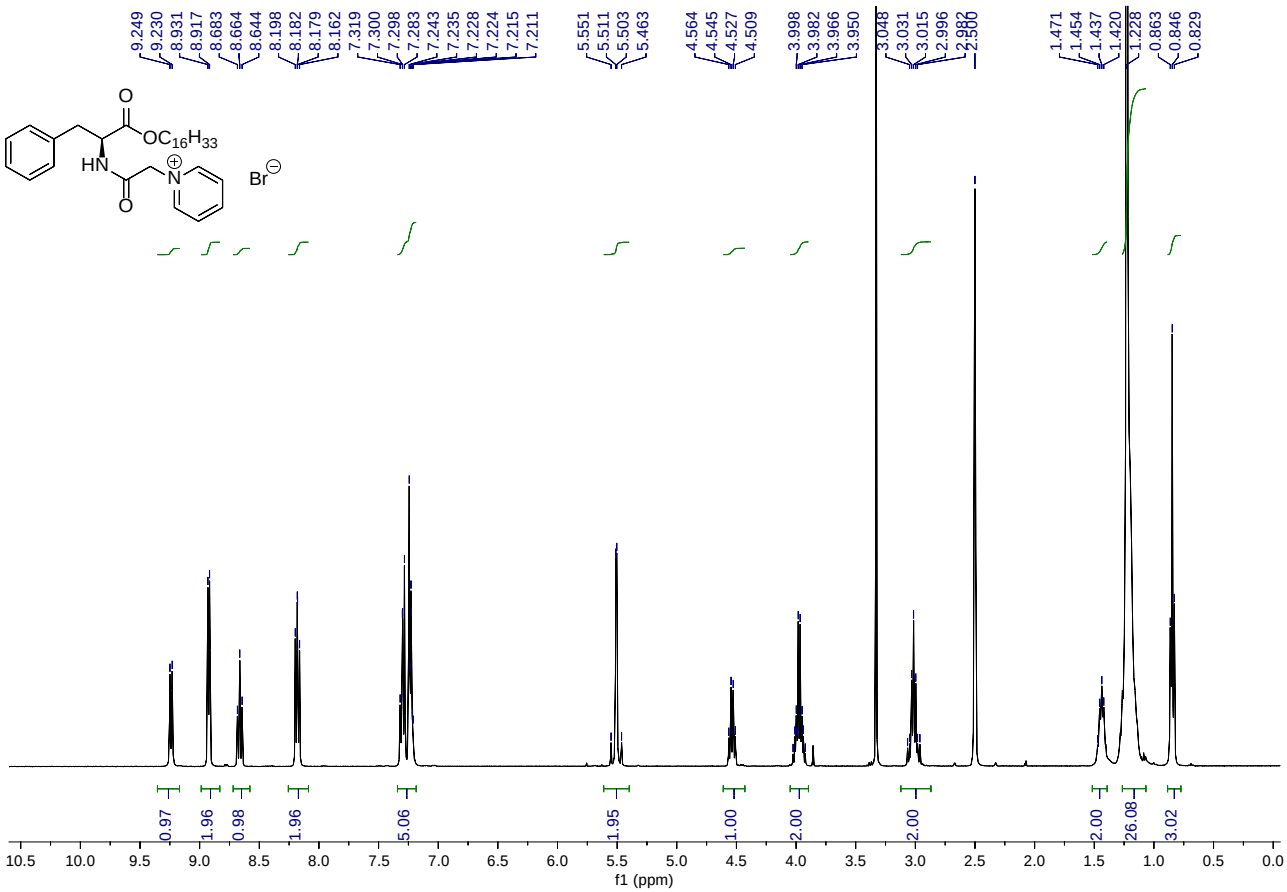


IR (KBr, cm^{-1})

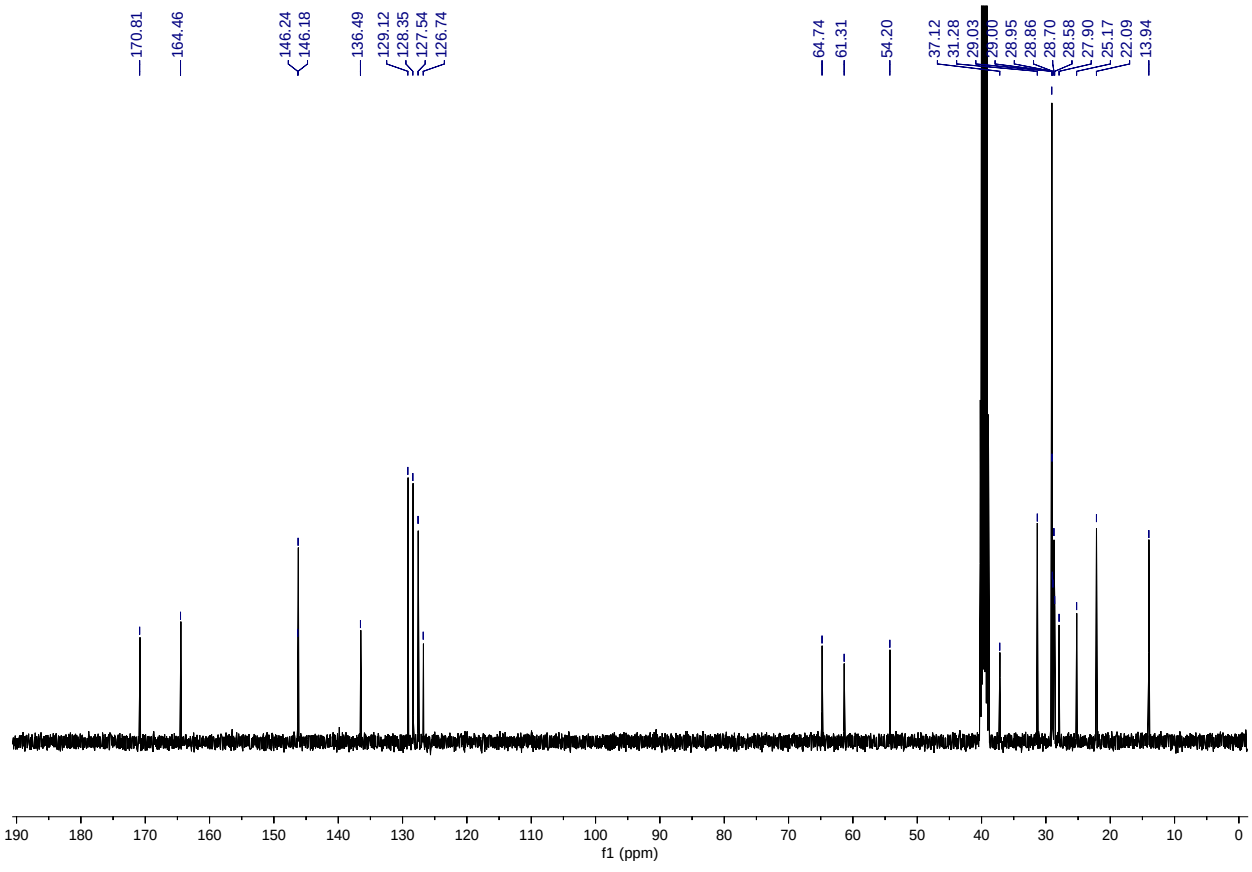

BRUKER
Transmittance [%]
Wavenumber cm-1
3335.83
3042.01
2952.13
2915.75
2849.22
1737.57
1662.05
1629.26
1536.55
1479.00
1397.12
1374.17
1348.90
1250.08
1200.80
1114.64
1078.88
1036.74
971.25
790.89
756.85
725.89
702.95
678.76
597.15
552.16

(*S*)-1-(2-((1-(Hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)pyridin-1-ium bromide (24)

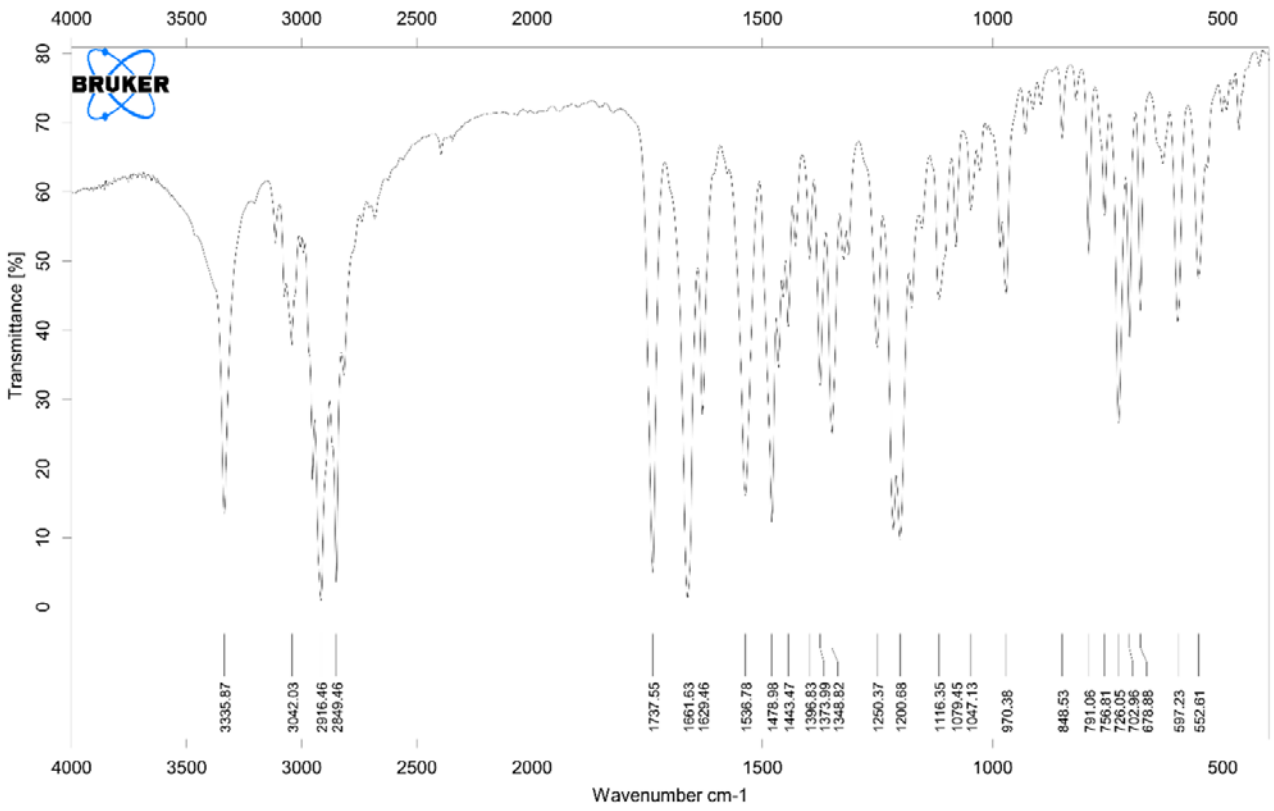
^{1}H NMR



^{13}C NMR



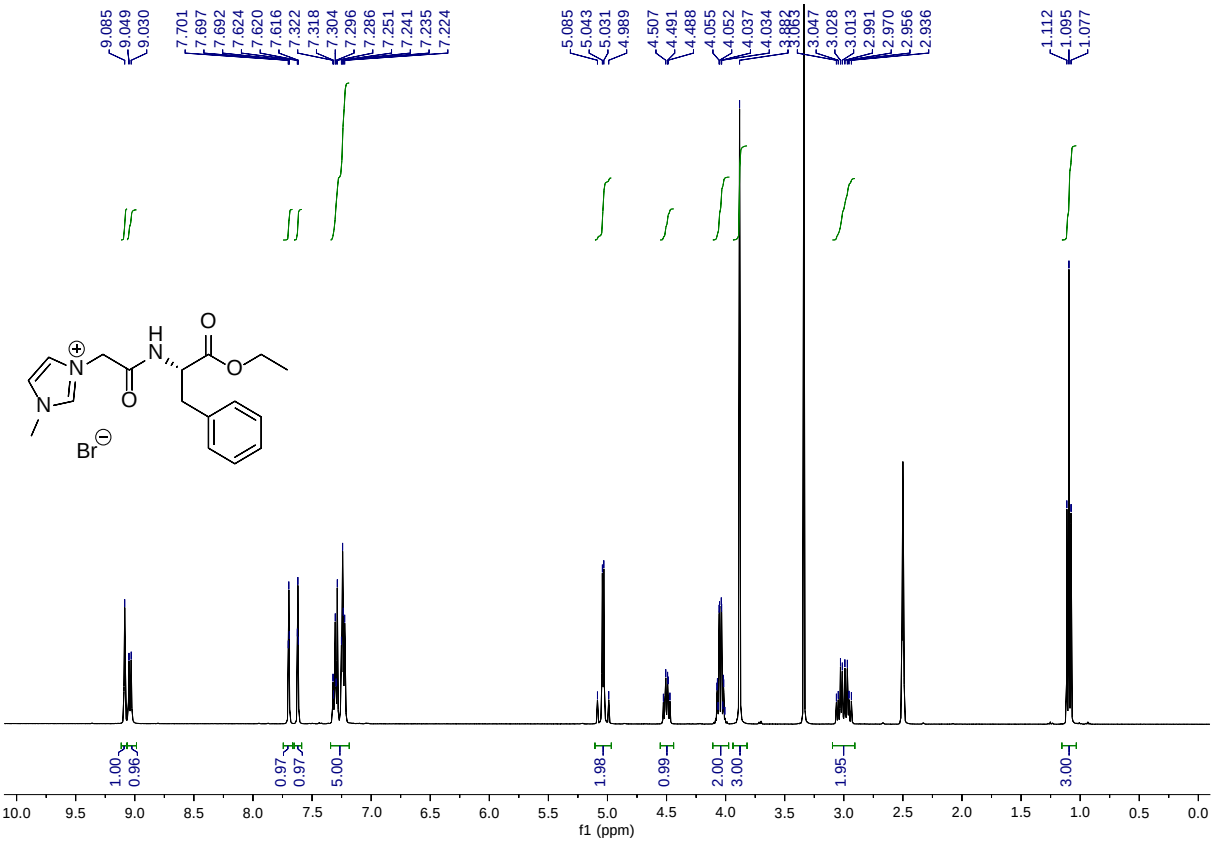
IR (KBr, cm^{-1})


4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
0
10
20
30
40
50
60
70
80
3335.87
3042.03
2916.46
2849.46
1737.55
1661.63
1629.46
1536.78
1478.98
1443.47
1396.83
1373.99
1348.82
1250.37
1200.68
1116.35
1079.45
1047.13
970.38
848.53
791.06
756.81
726.05
702.96
678.88
597.23
552.61
Wavenumber cm-1

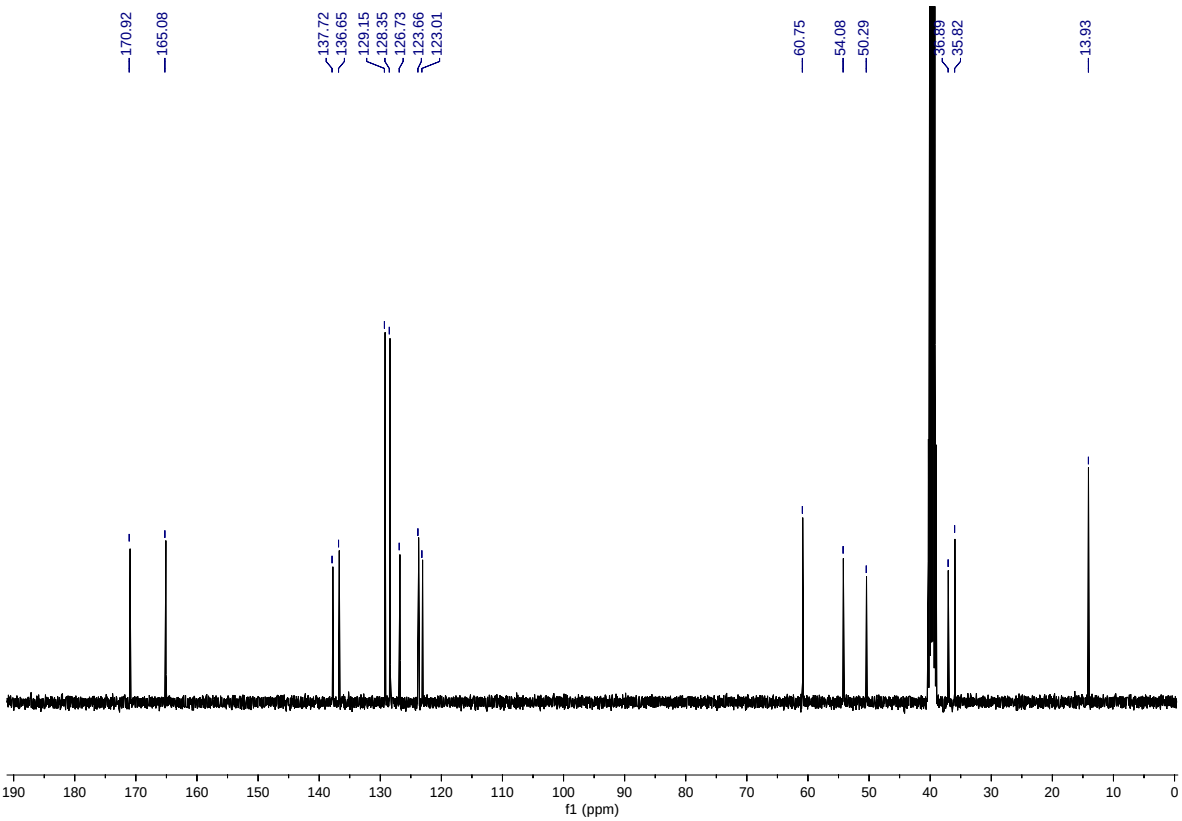
12. NMR and IR spectra of imidazolium ILs (25 - 32)

(*S*)-1-Methyl-3-(2-((1-(ethyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2- oxoethyl)-1H- imidazol-3- ium bromide (25)

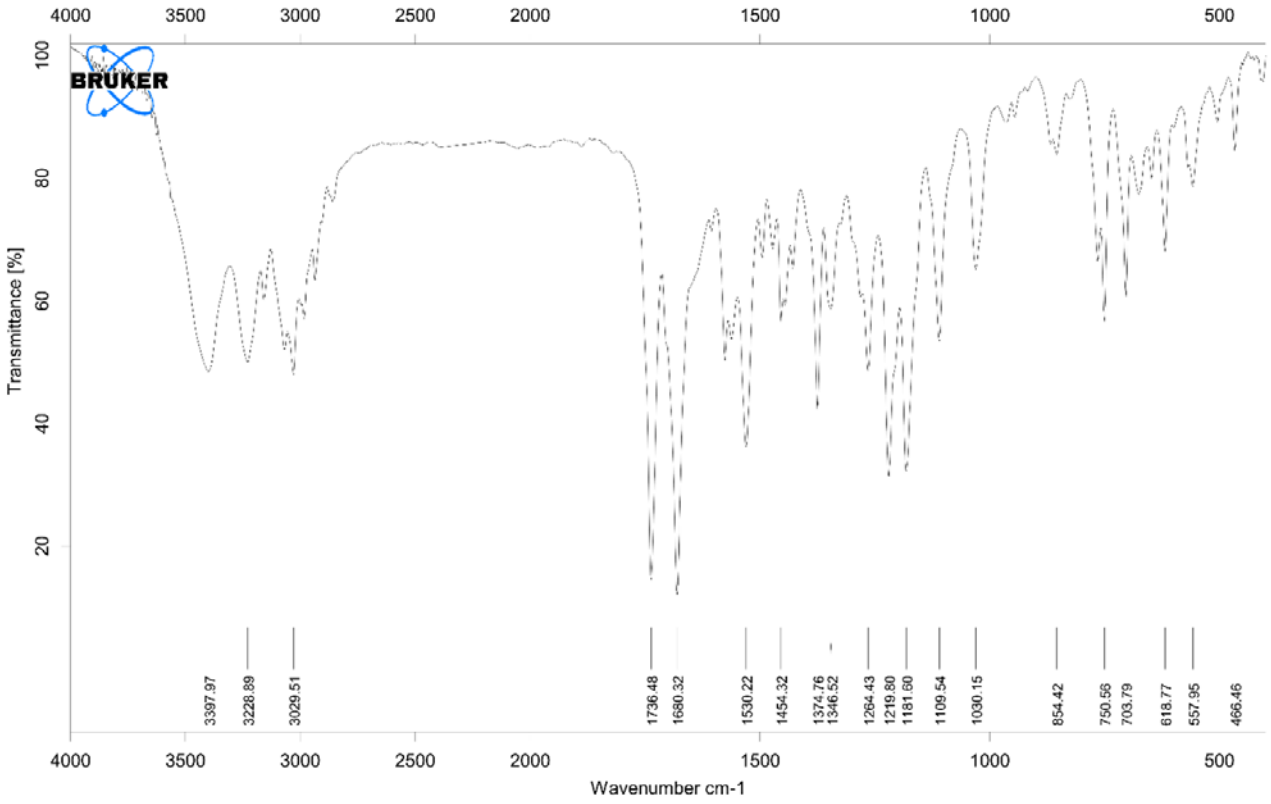
^{1}H NMR



^{13}C NMR

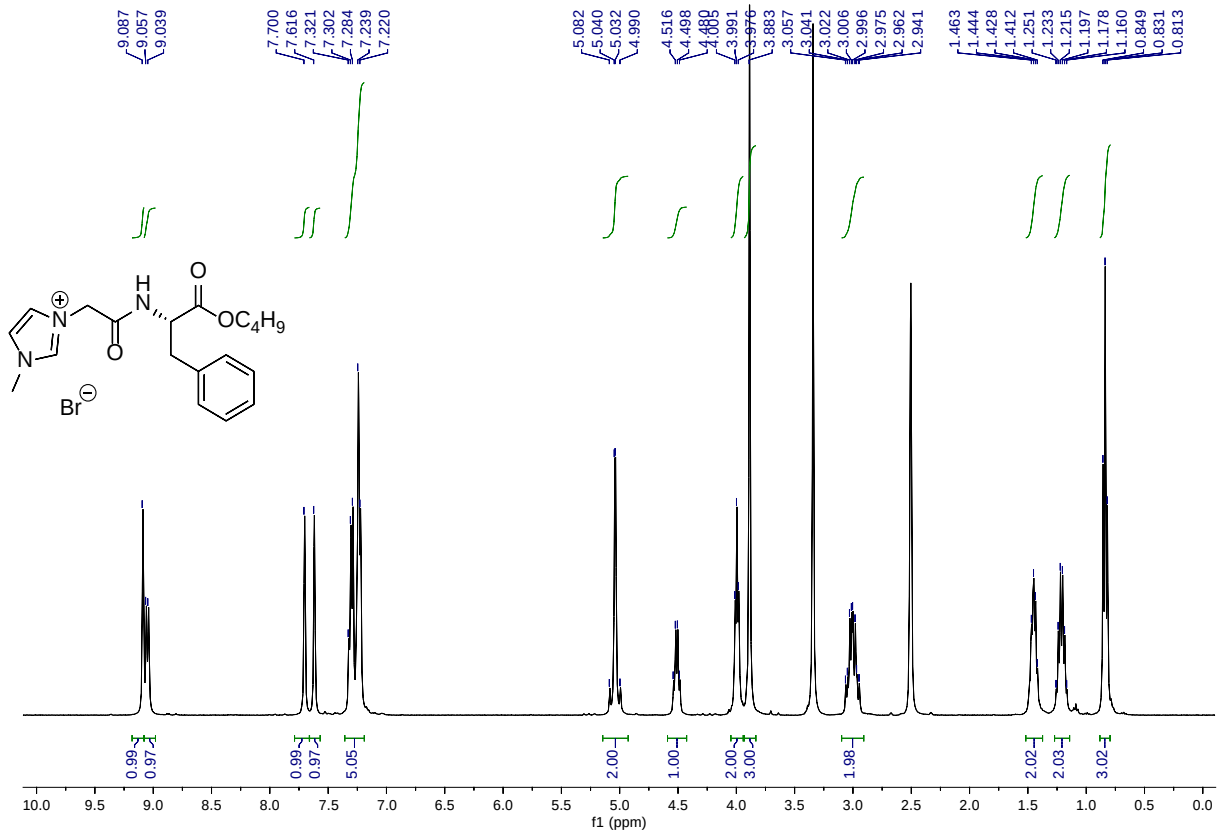


IR (KBr, cm^{-1})

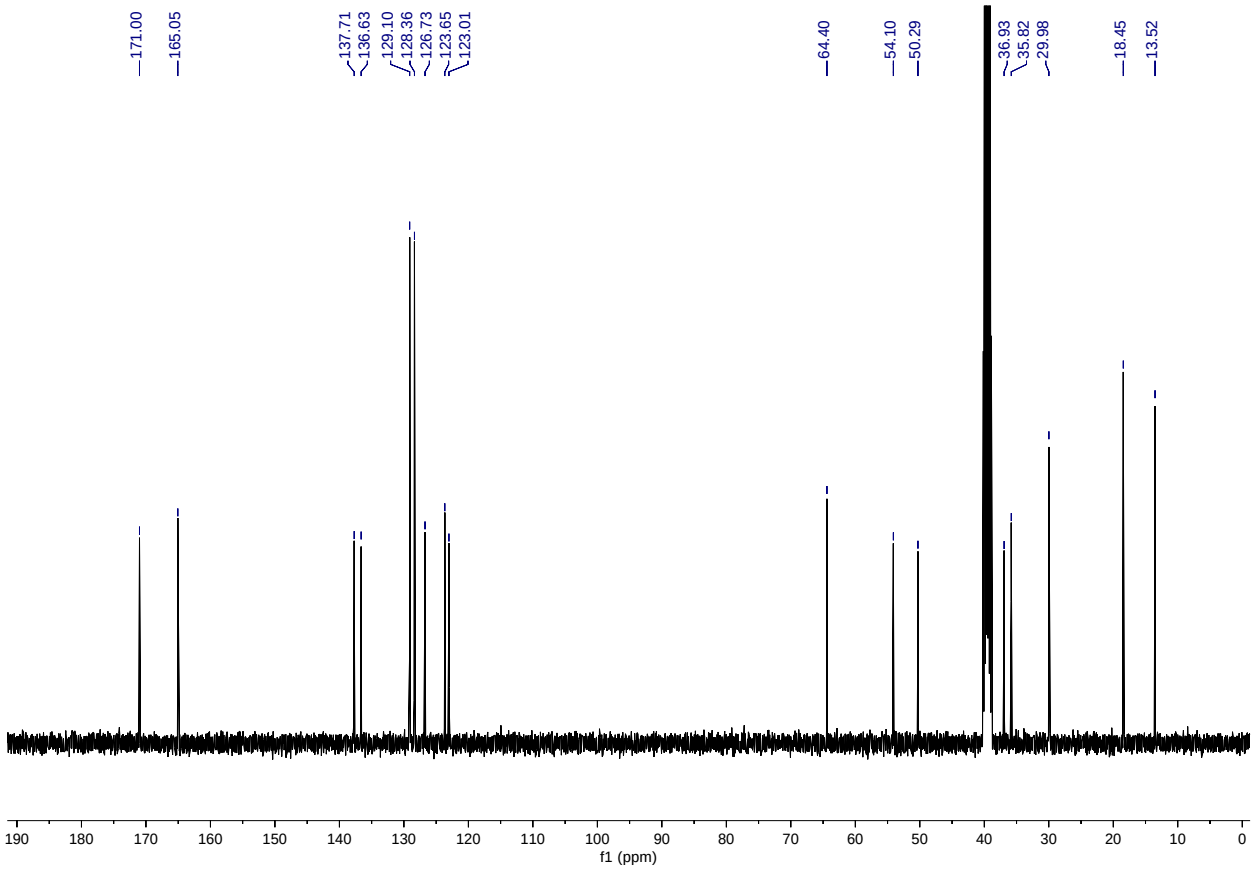

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3397.97
3228.89
3029.51
1736.48
1680.32
1530.22
1454.32
1374.76
1346.52
1264.43
1219.80
1181.60
1109.54
1030.15
854.42
750.56
703.79
618.77
557.95
466.46
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(butyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (26)

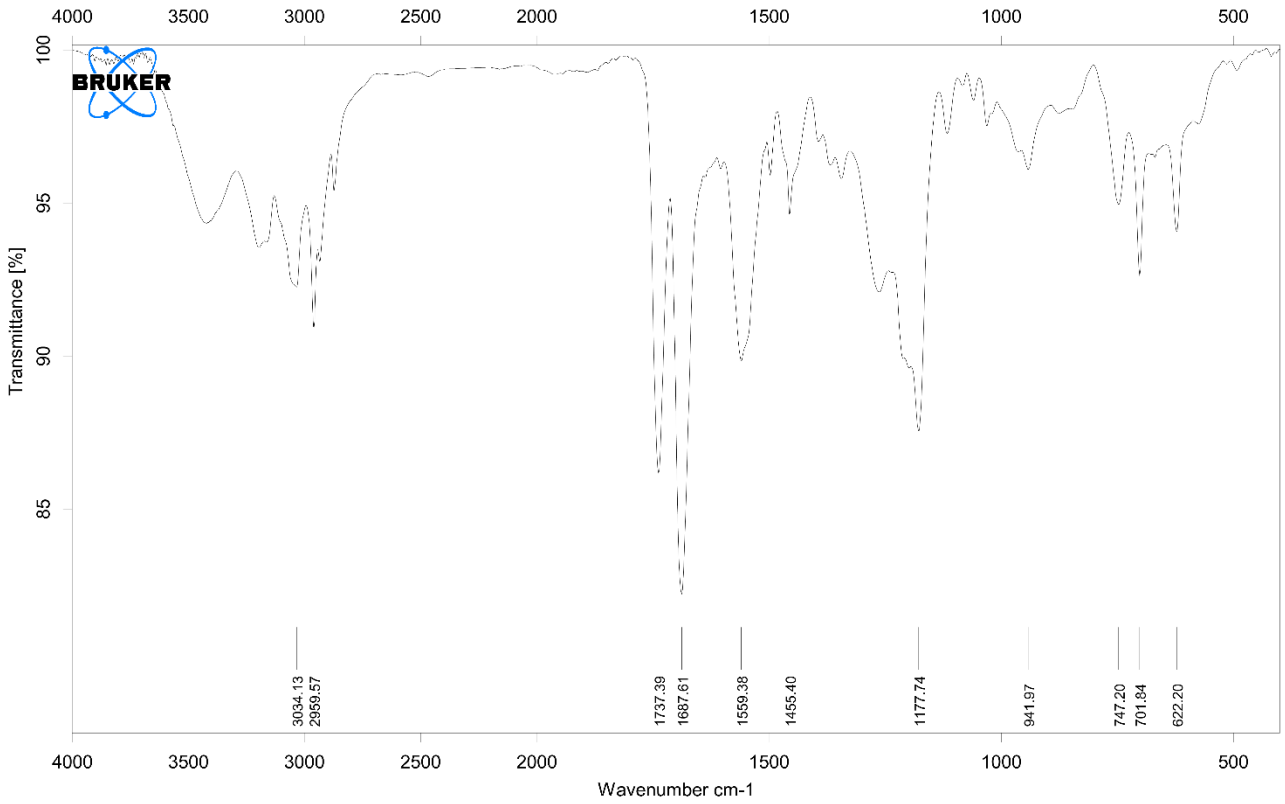
^{1}H NMR



^{13}C NMR

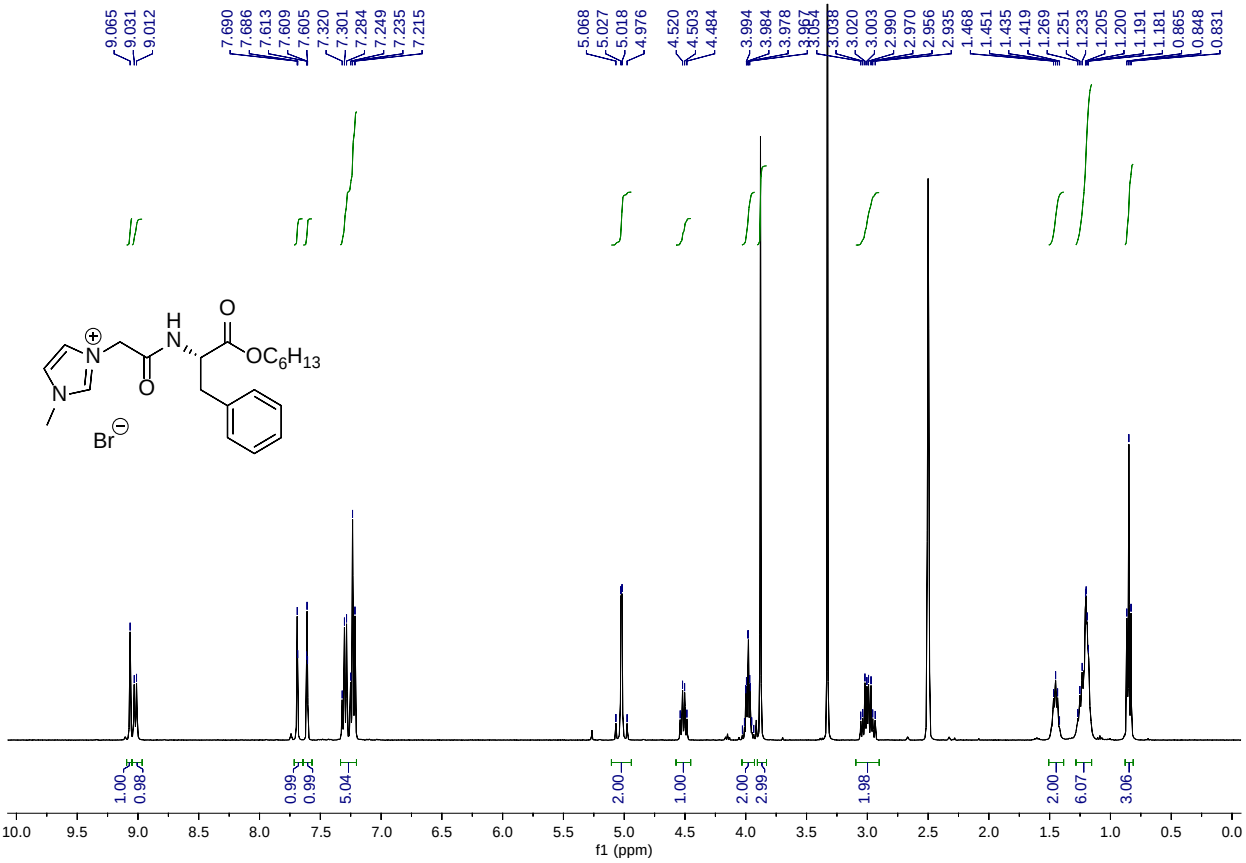


IR (KBr, cm^{-1})

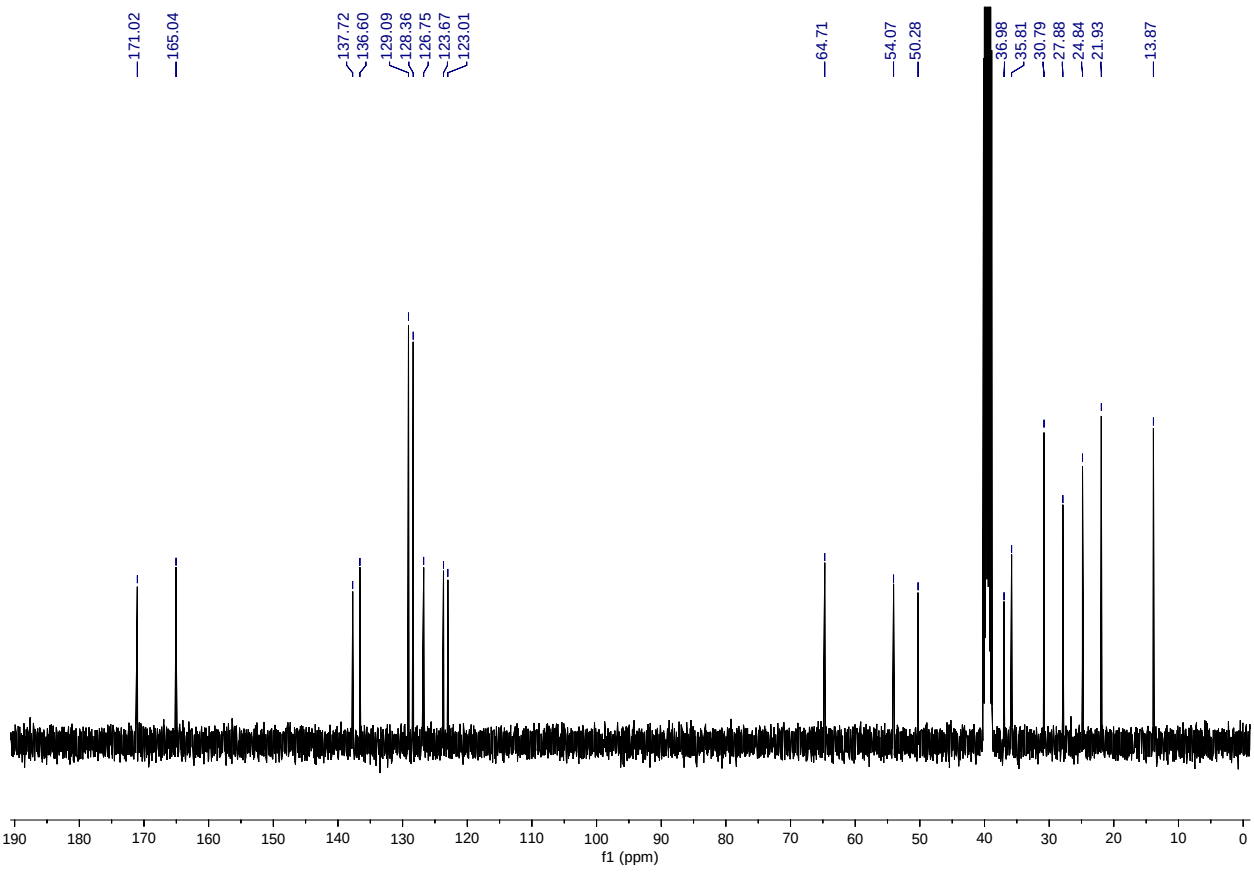

4000
3500
3000
2500
2000
1500
1000
500
100
95
90
85
Transmittance [%]
BRUKER
3034.13
2959.57
1737.39
1687.61
1559.38
1455.40
1177.74
941.97
747.20
701.84
622.20
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium bromide (27)

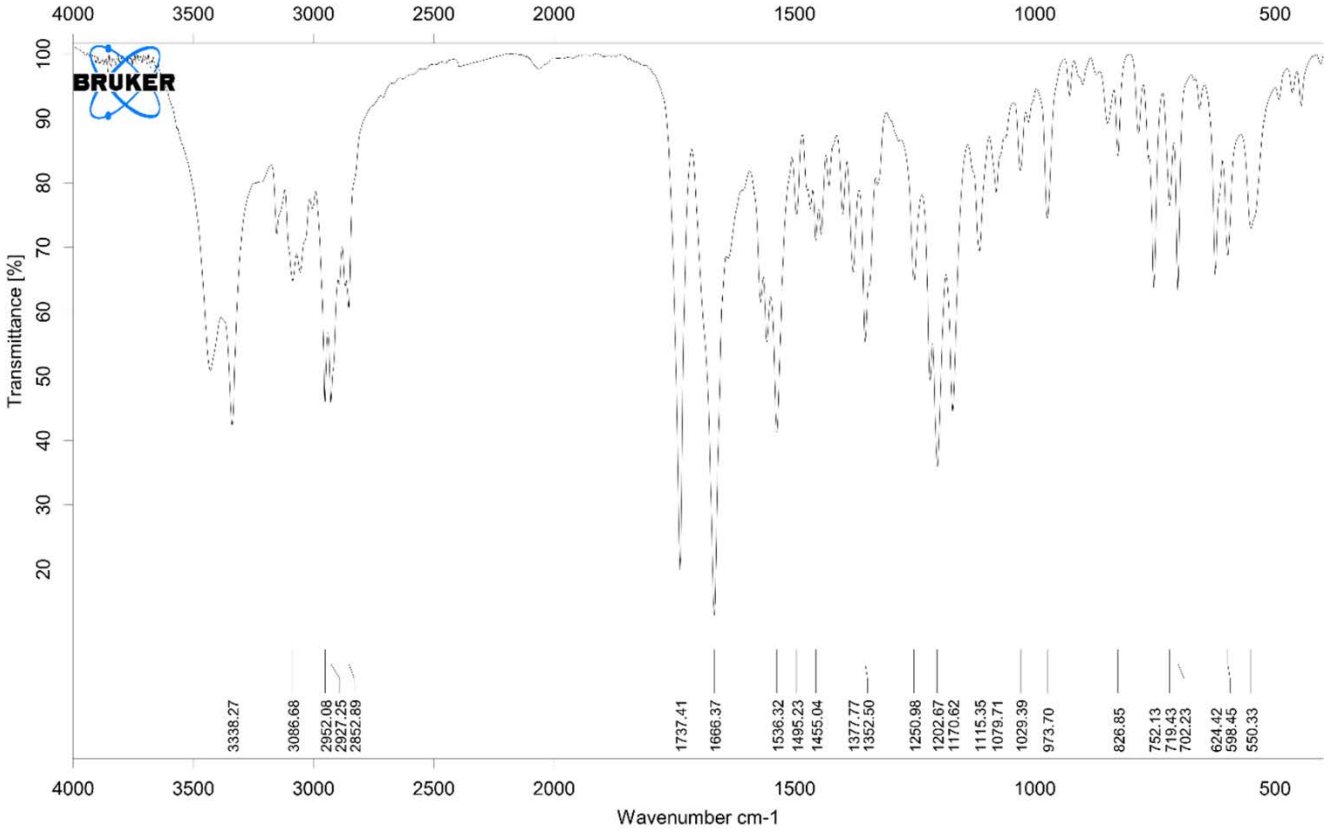
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
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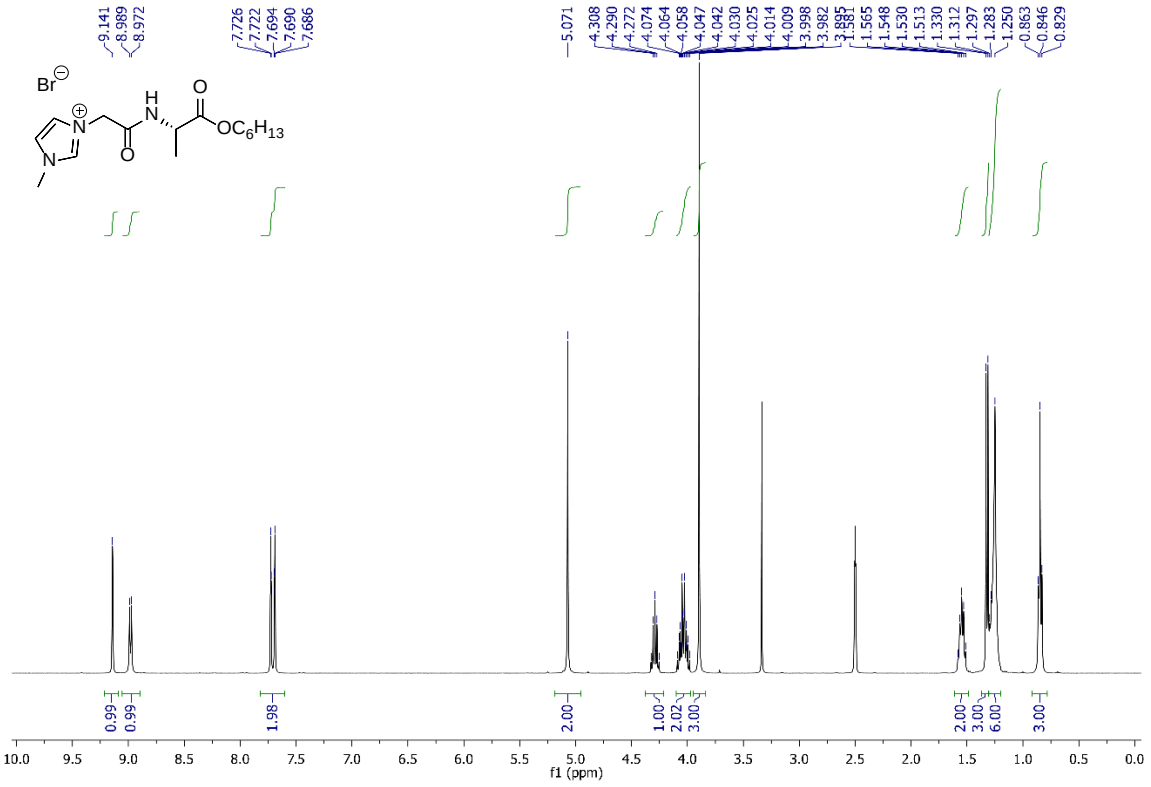
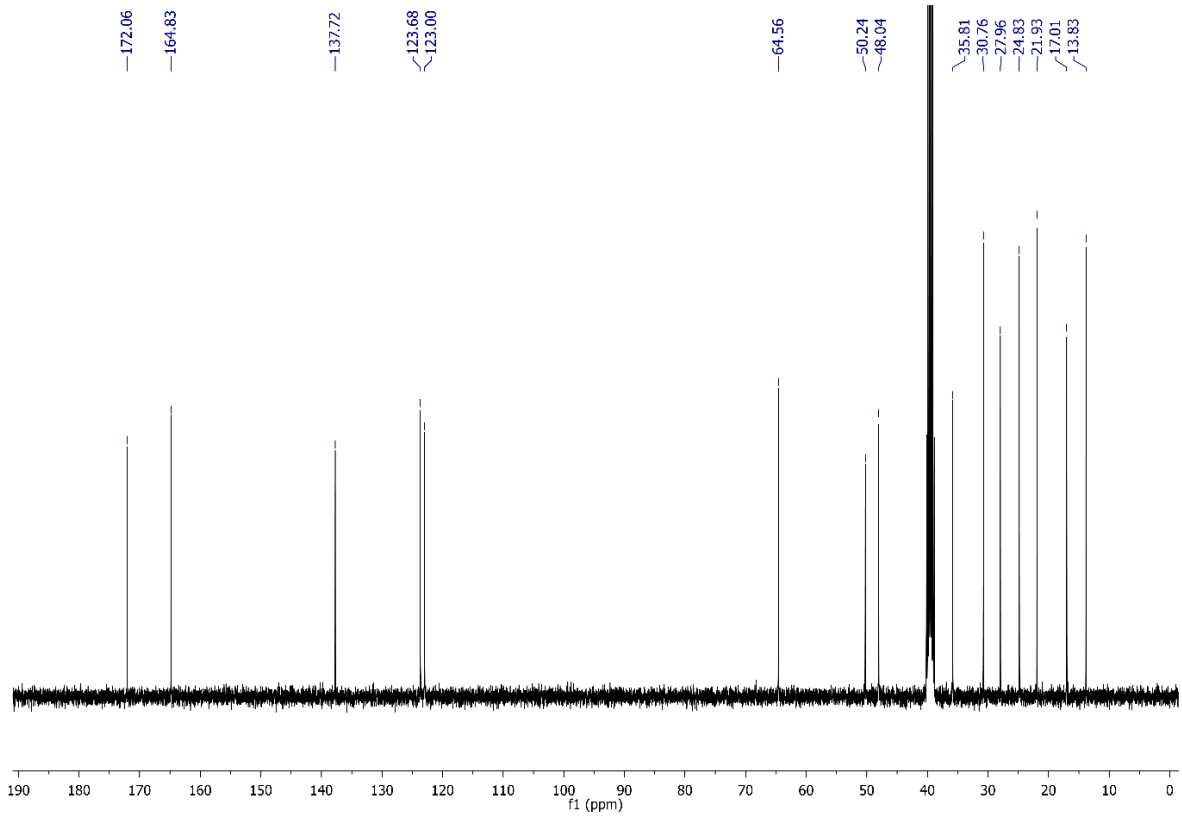
90
80
70
60
50
40
30
20
3338.27
3086.68
2952.08
2927.25
2852.89
1737.41
1666.37
1536.32
1495.23
1455.04
1377.77
1352.50
1250.98
1202.67
1170.62
1115.35
1079.71
1029.39
973.70
826.85
752.13
719.43
702.23
624.42
598.45
550.33
Wavenumber cm-1

(*S*)-3-(2-((1-(hexyloxy)-1-oxopropan-2-yl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium bromide (27Ala)

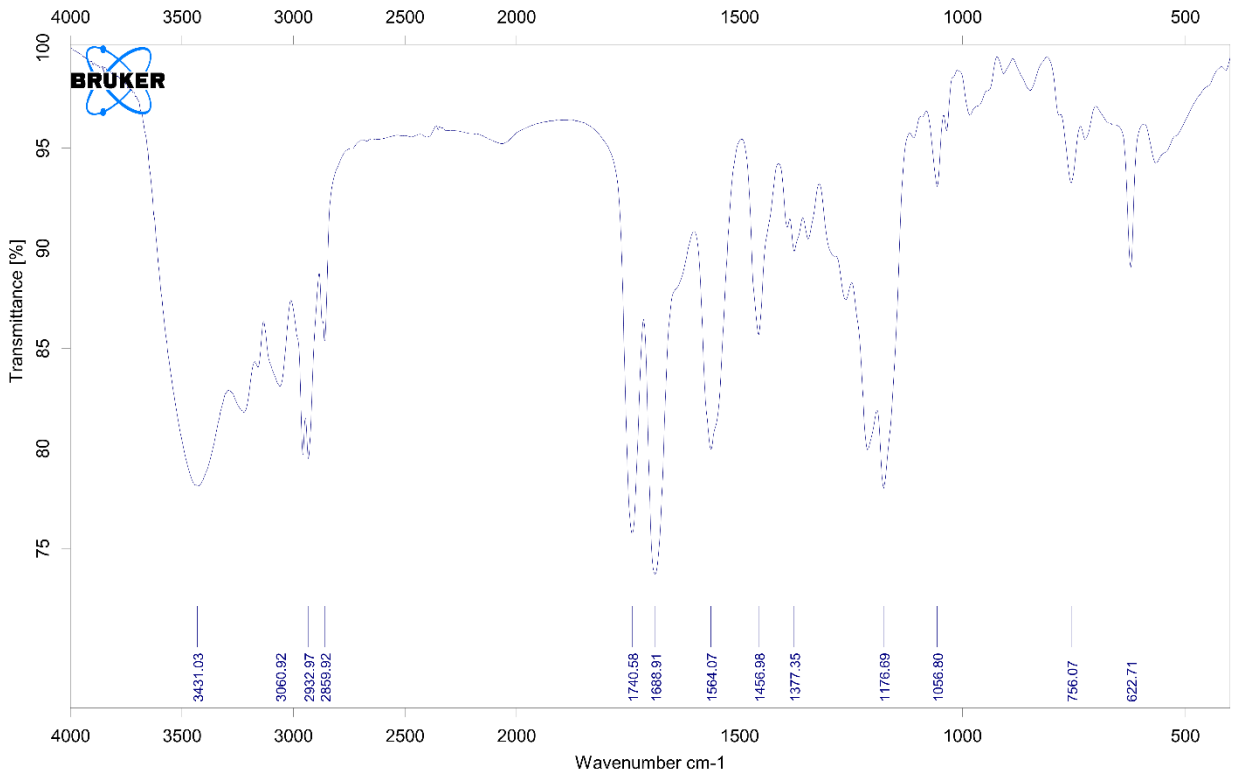
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1}):


4000
3500
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2000
1500
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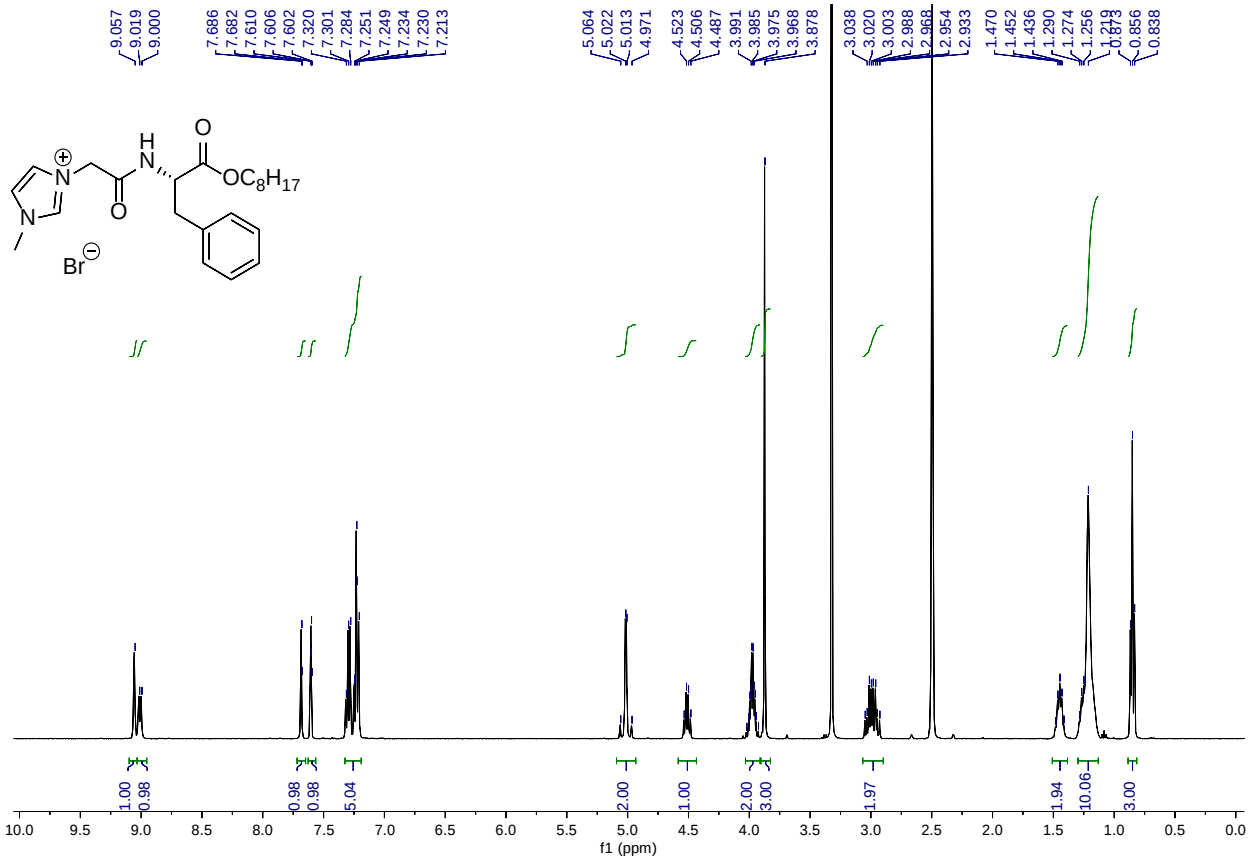
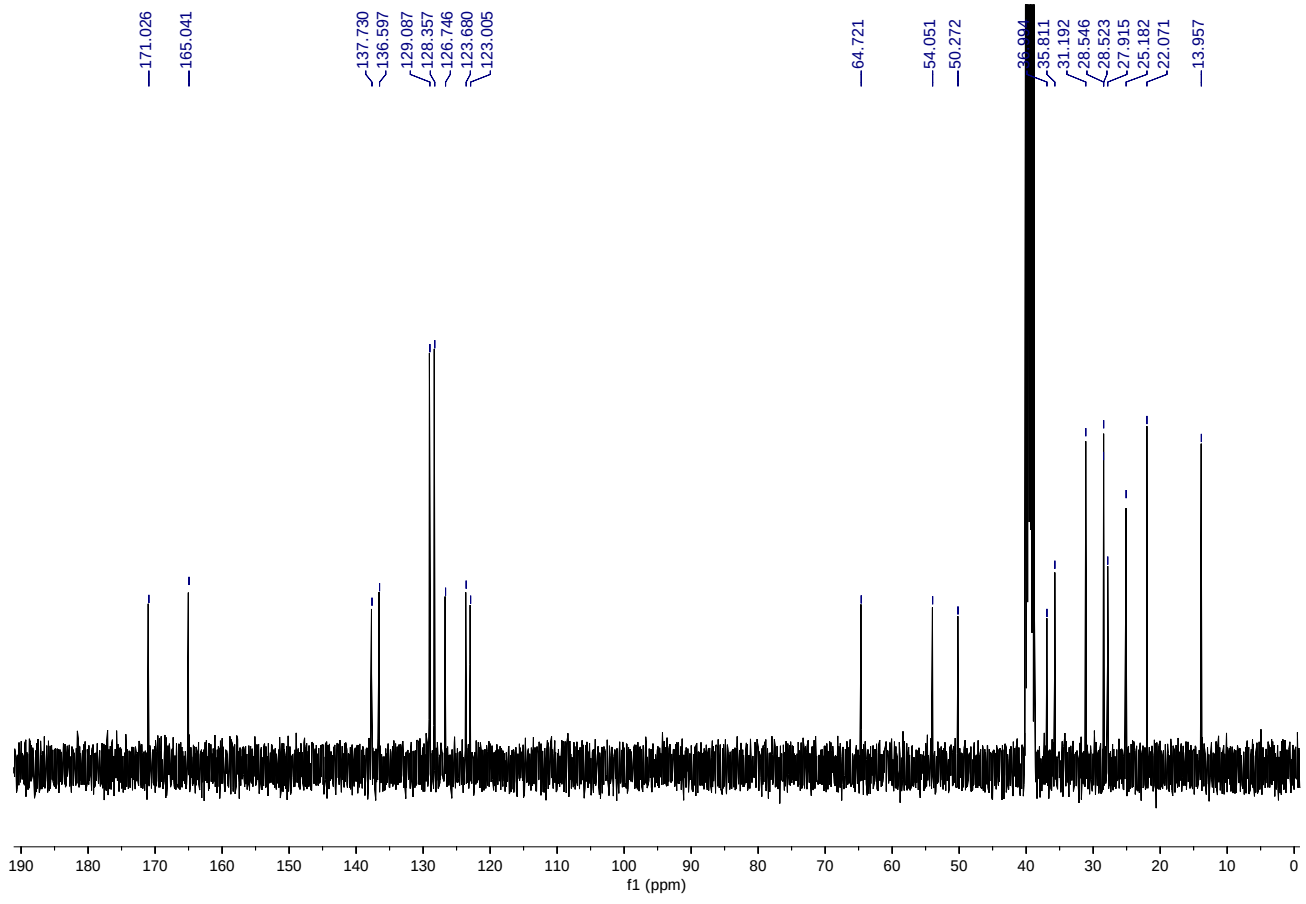
500
100
95
90
85
80
75
Transmittance [%]
BRUKER
3431.03
3060.92
2932.97
2859.92
1740.58
1688.91
1564.07
1456.98
1377.35
1176.69
1056.80
756.07
622.71
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium (28)

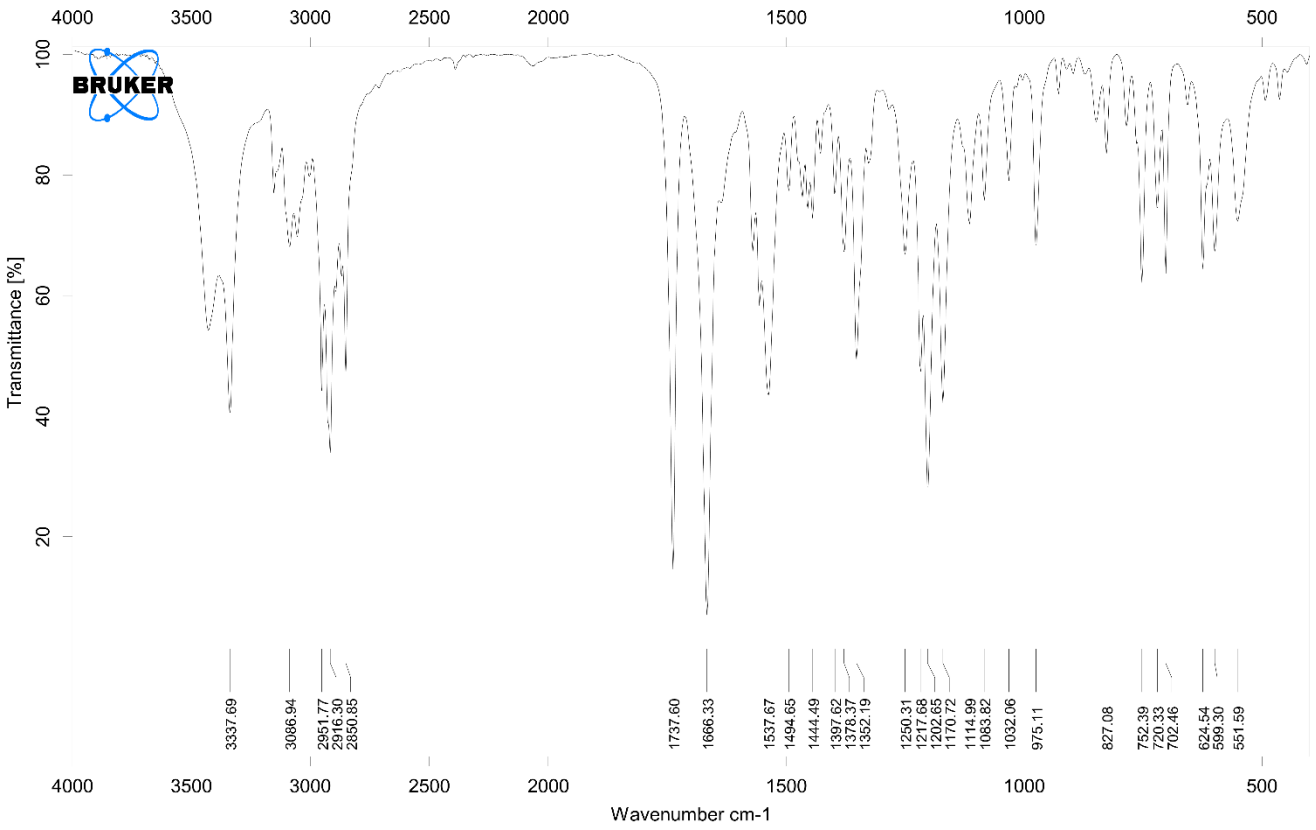
^{1}H NMR



^{13}C NMR

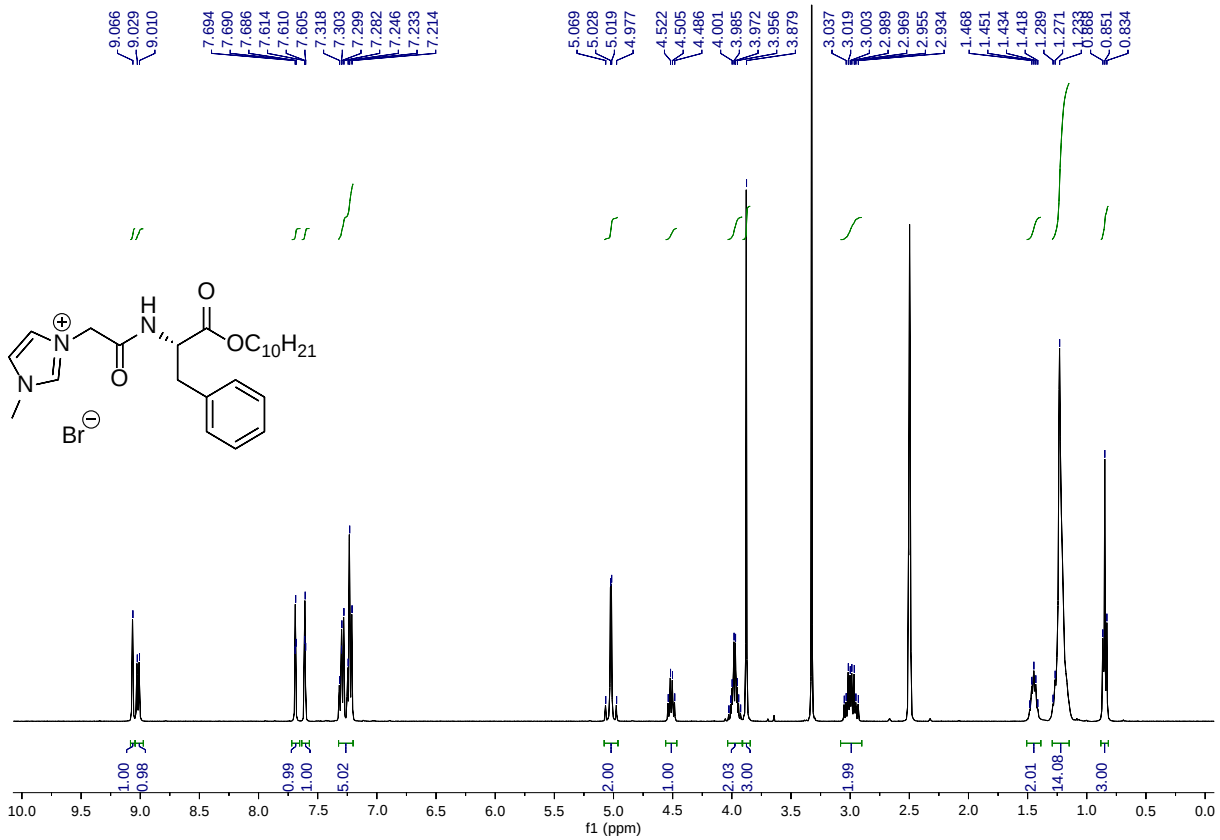


IR (KBr, cm^{-1})

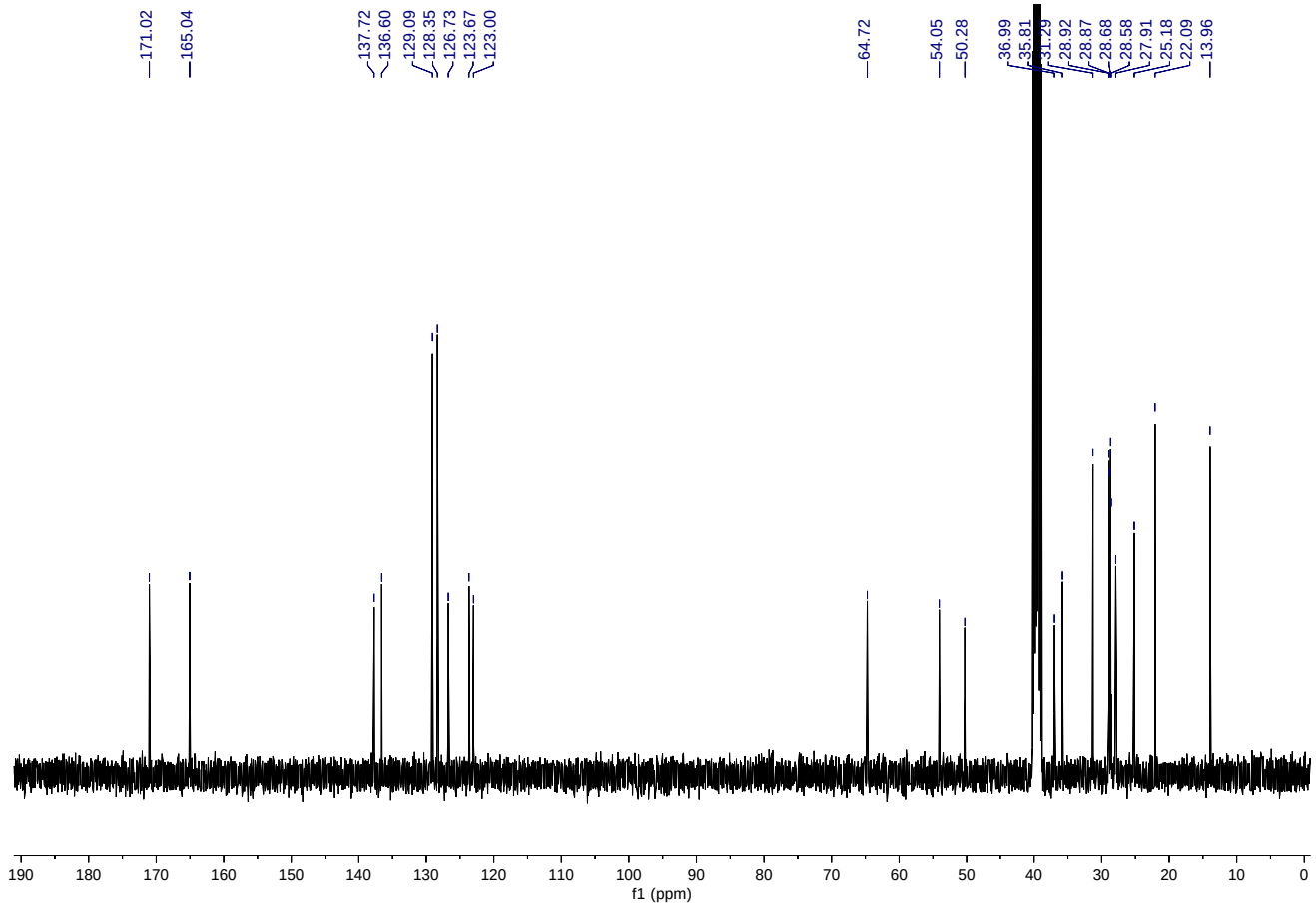

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3337.69
3086.94
2951.77
2916.30
2850.85
1737.60
1666.33
1537.67
1494.65
1444.49
1397.62
1378.37
1352.19
1250.31
1217.68
1202.65
1170.72
1114.99
1083.82
1032.06
975.11
827.08
752.39
720.33
702.46
624.54
599.30
551.59
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium (29)

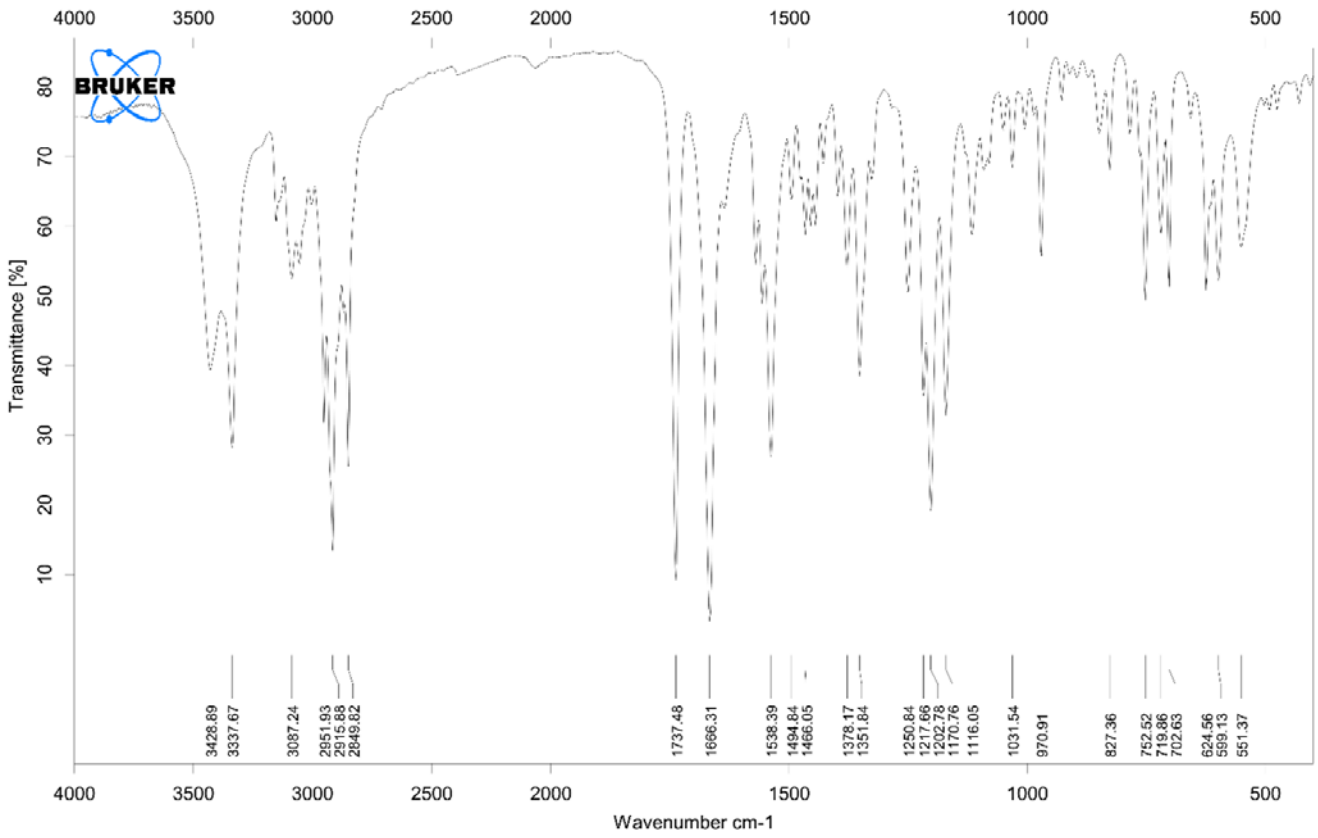
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
3500
3000
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1500
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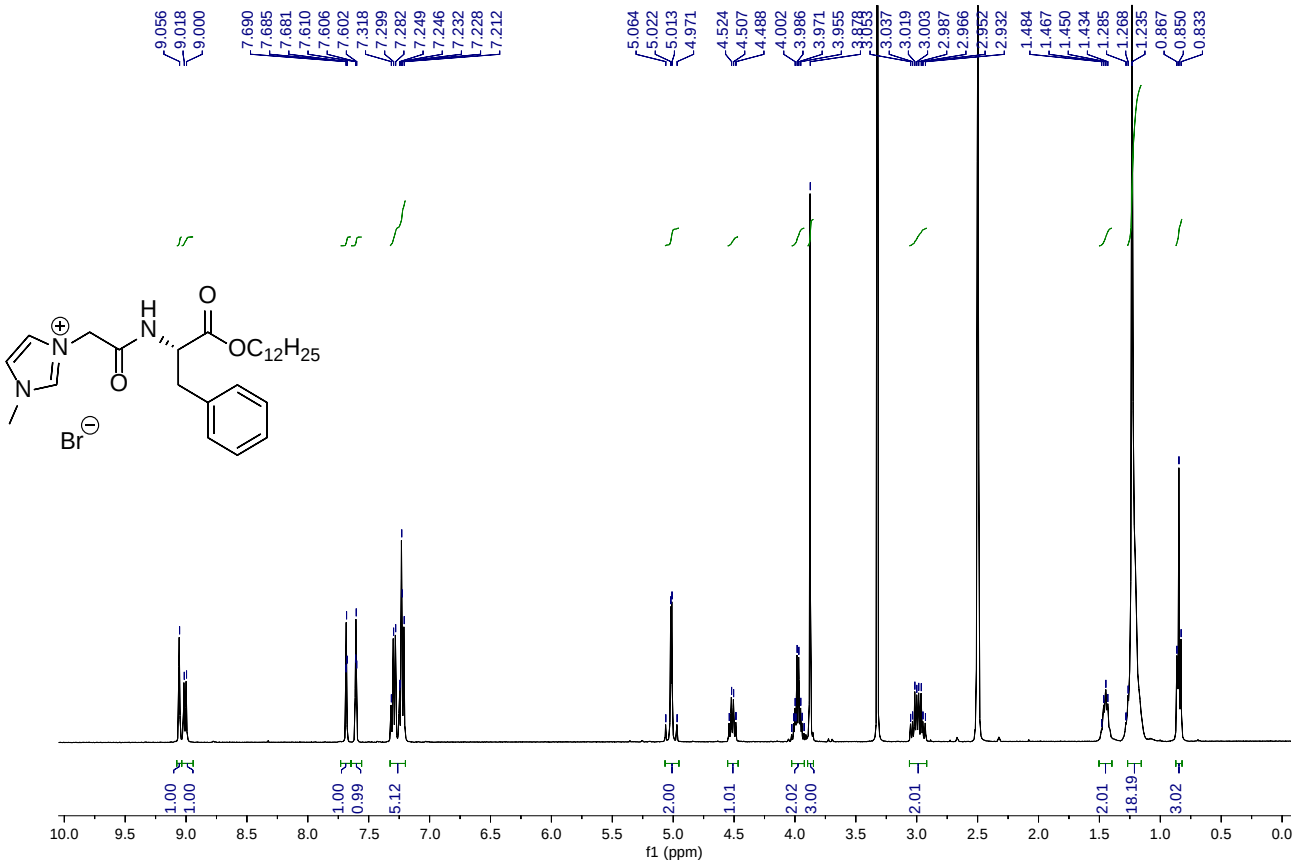
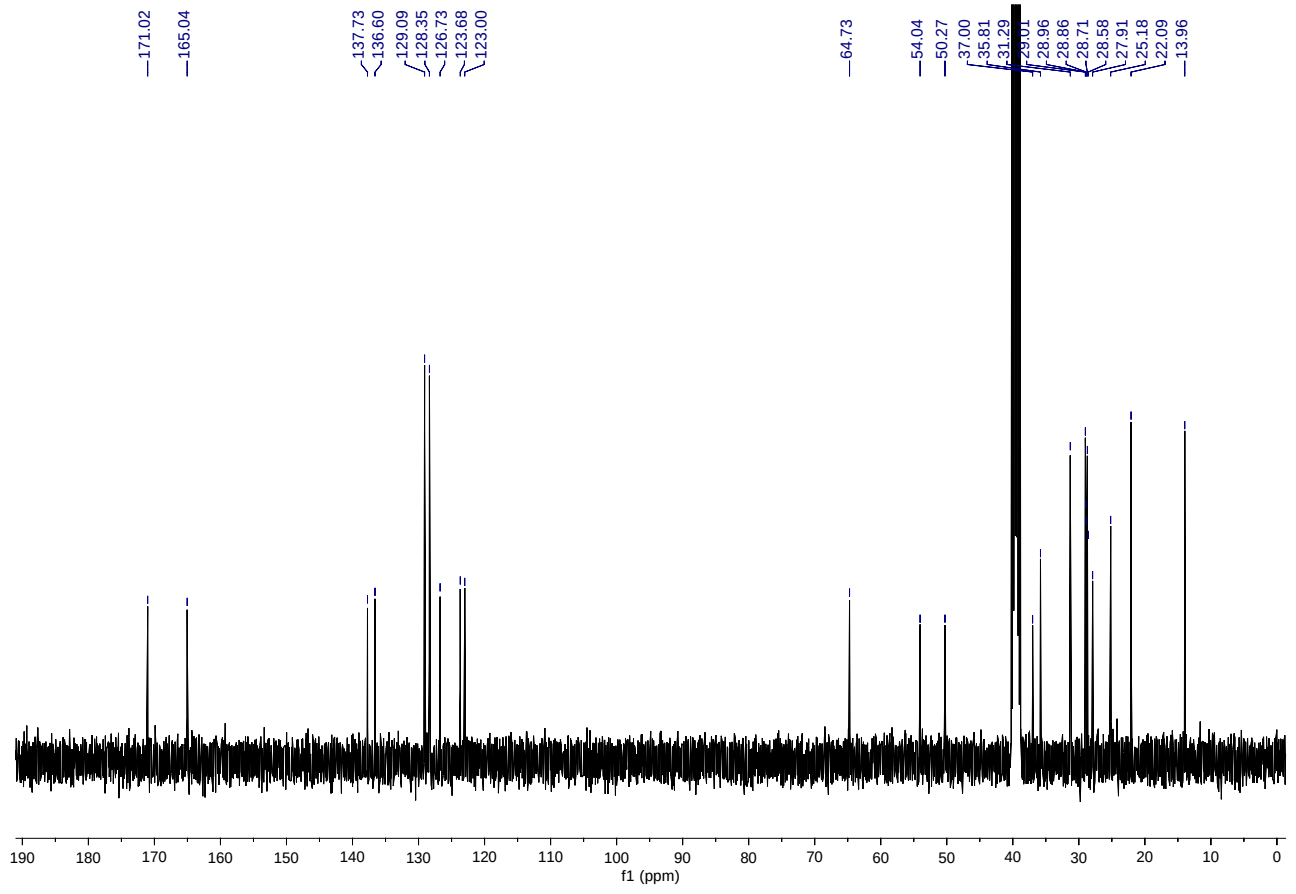
500
BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
3428.89
3337.67
3087.24
2951.93
2915.88
2849.82
1737.48
1686.31
1538.39
1494.84
1466.05
1378.17
1351.84
1250.84
1217.66
1202.78
1170.76
1116.05
1031.54
970.91
827.36
752.52
719.86
702.63
624.56
599.13
551.37
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium (30)

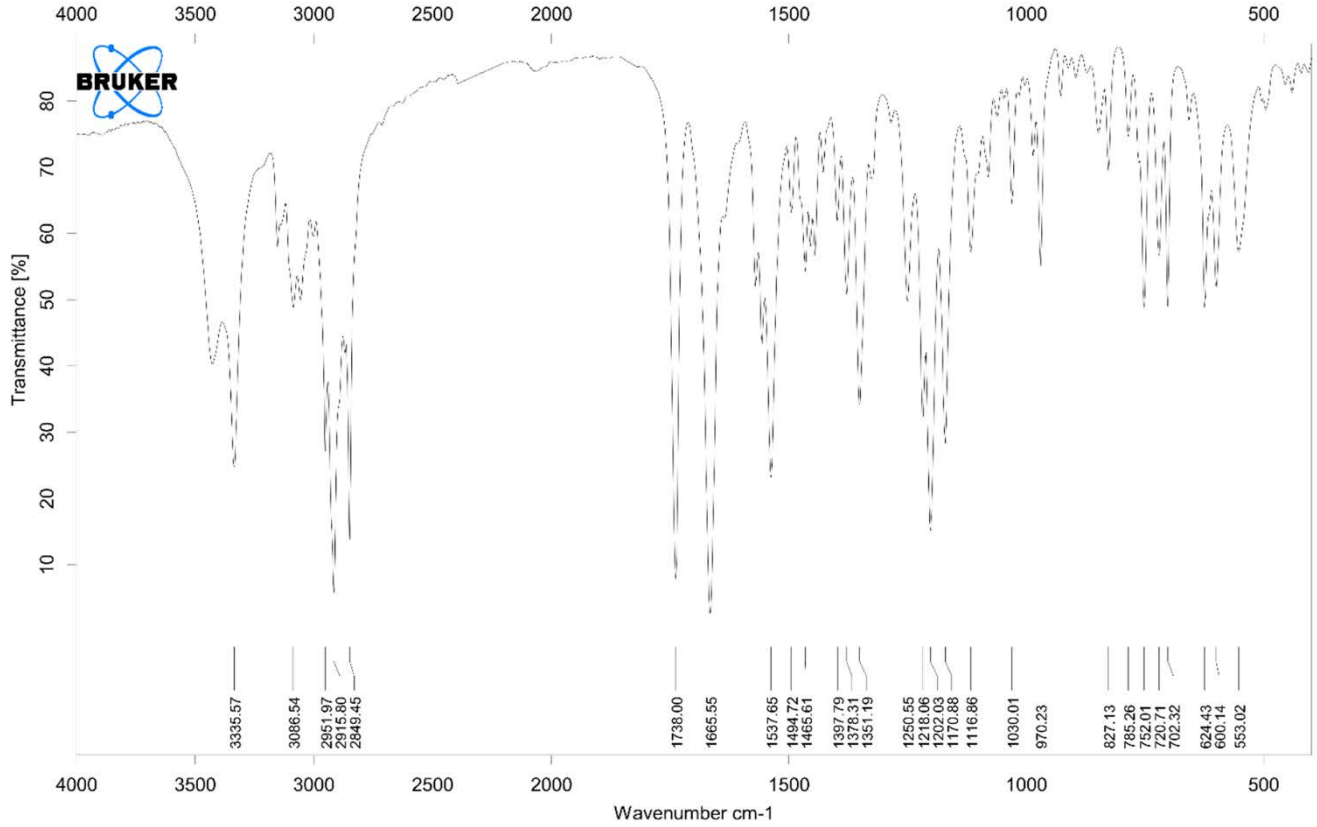
^{1}H NMR



^{13}C NMR

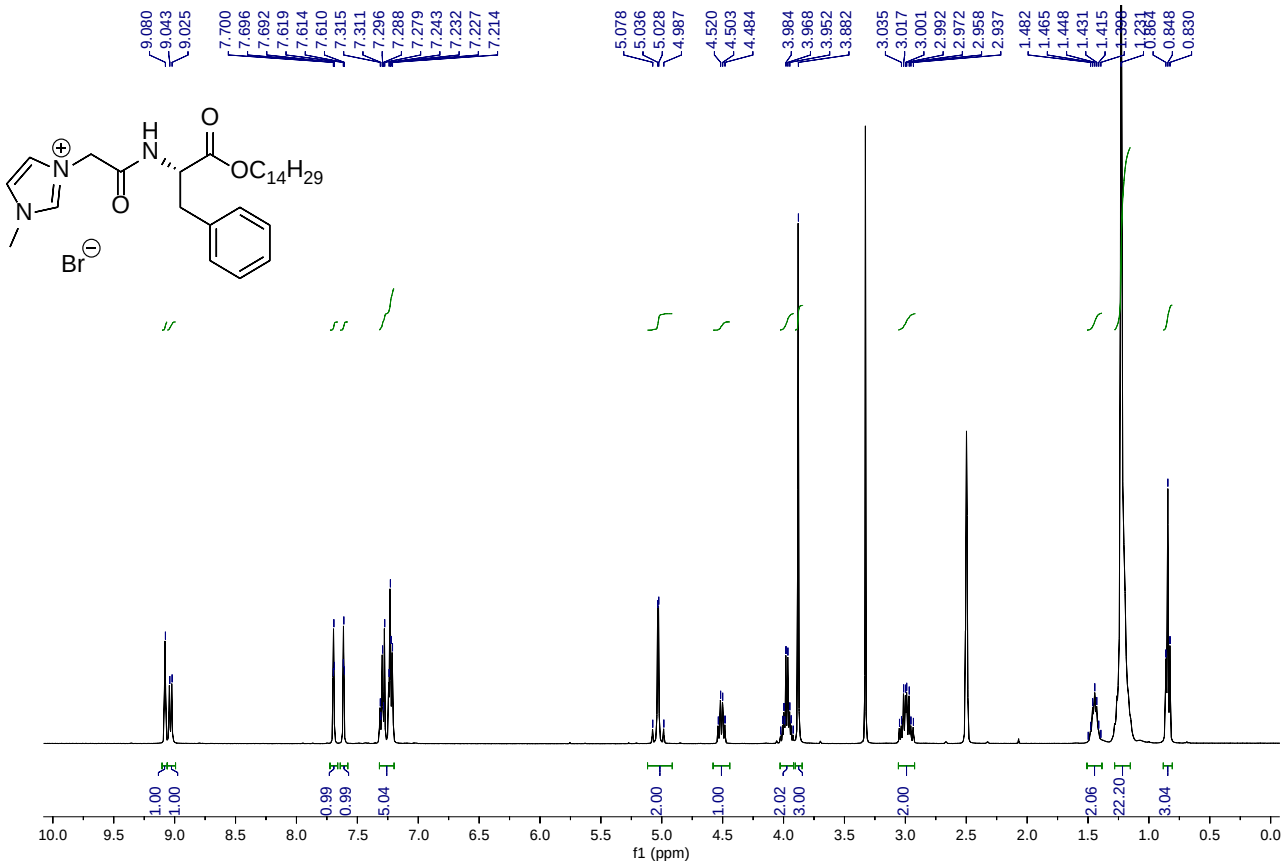


IR (KBr, cm^{-1})

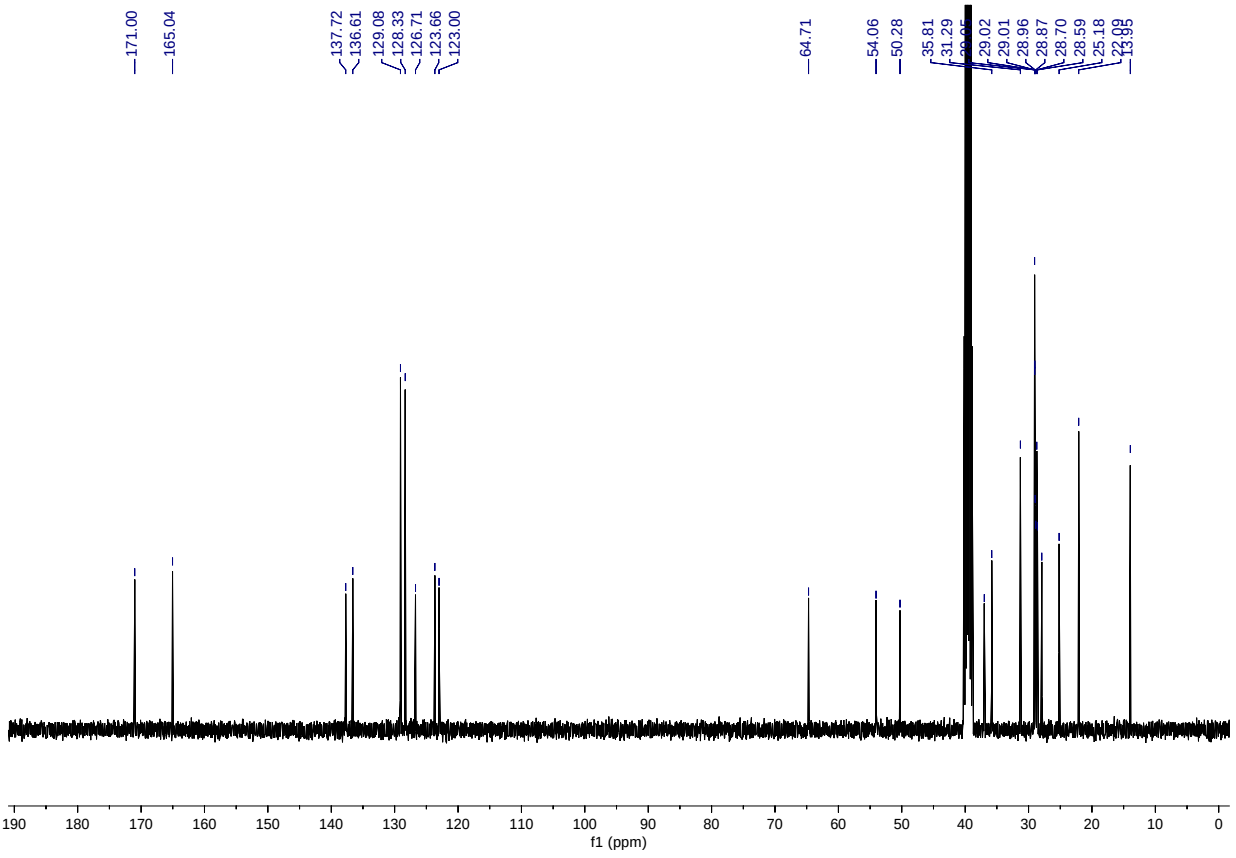

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
3335.57
3086.54
2951.97
2915.80
2849.45
1738.00
1665.55
1537.65
1494.72
1465.61
1397.79
1378.31
1351.19
1250.55
1218.06
1202.03
1170.88
1116.86
1030.01
970.23
827.13
785.26
752.01
720.71
702.32
624.43
600.14
553.02
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium (31)

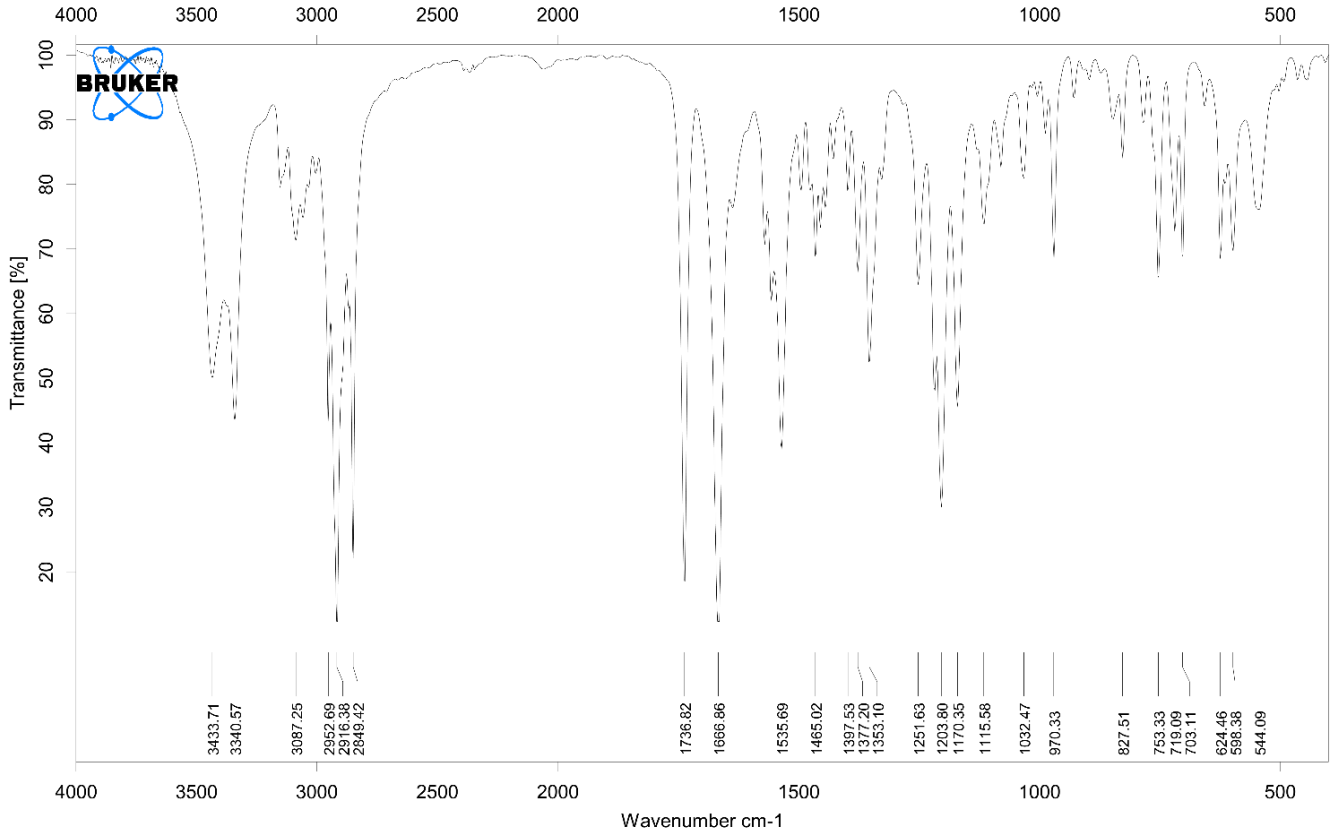
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
3500
3000
2500
2000
1500
1000
500
Transmittance [%]
100
90
80
70
60
50
40
30
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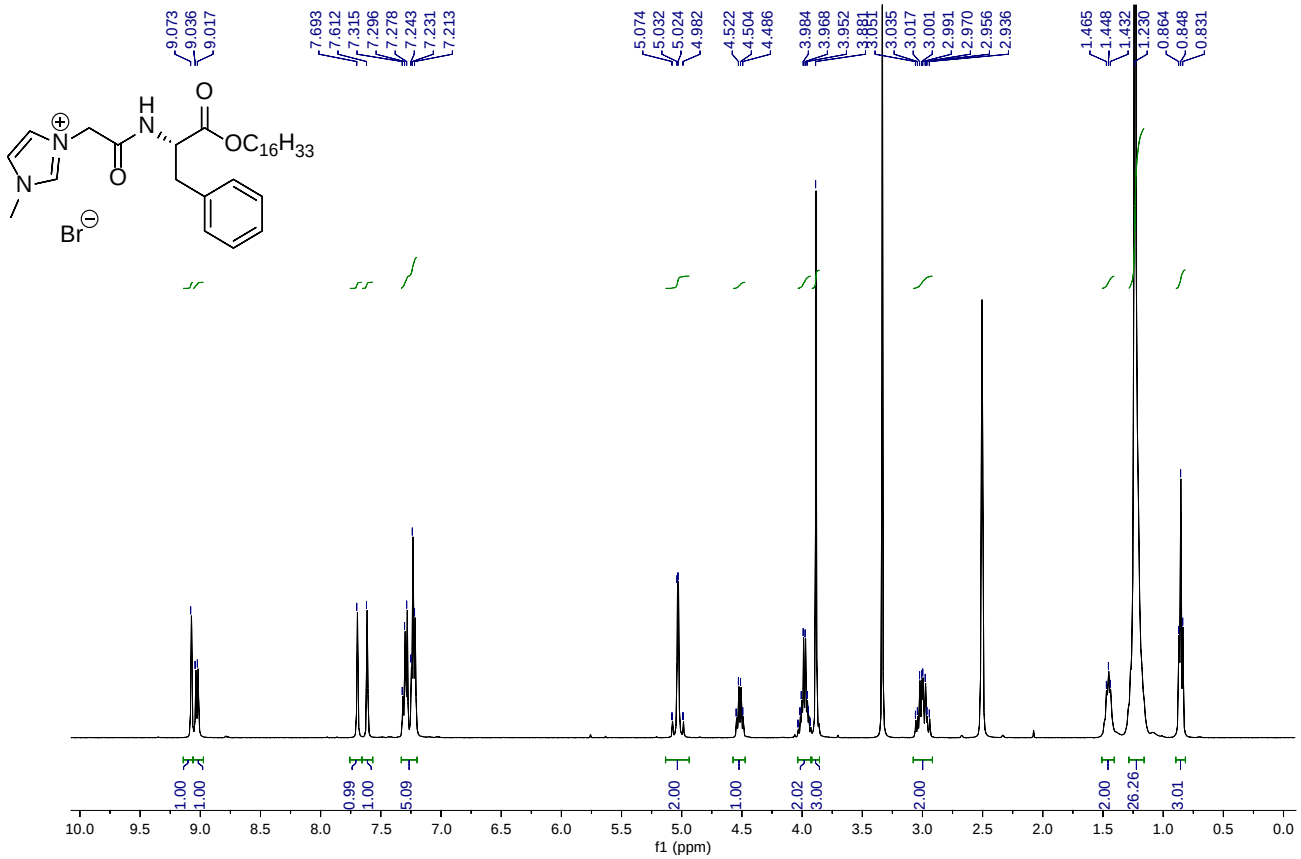
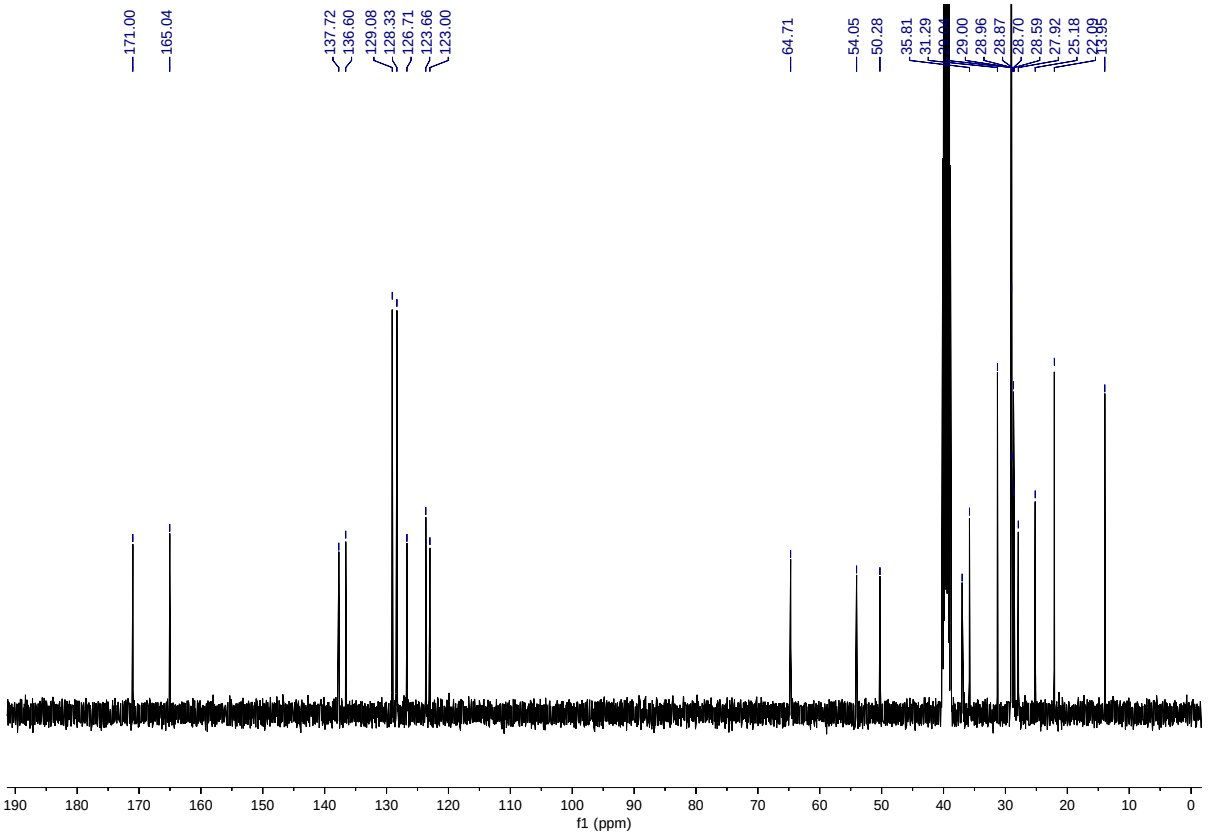
3433.71
3340.57
3087.25
2952.69
2916.38
2849.42
1736.82
1666.86
1535.69
1465.02
1397.53
1377.20
1353.10
1251.63
1203.80
1170.35
1115.58
1032.47
970.33
827.51
753.33
719.09
703.11
624.46
598.38
544.09
Wavenumber cm-1

(*S*)-1-Methyl-3-(2-((1-(hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-2-oxoethyl)-1H-imidazol-3-ium (32)

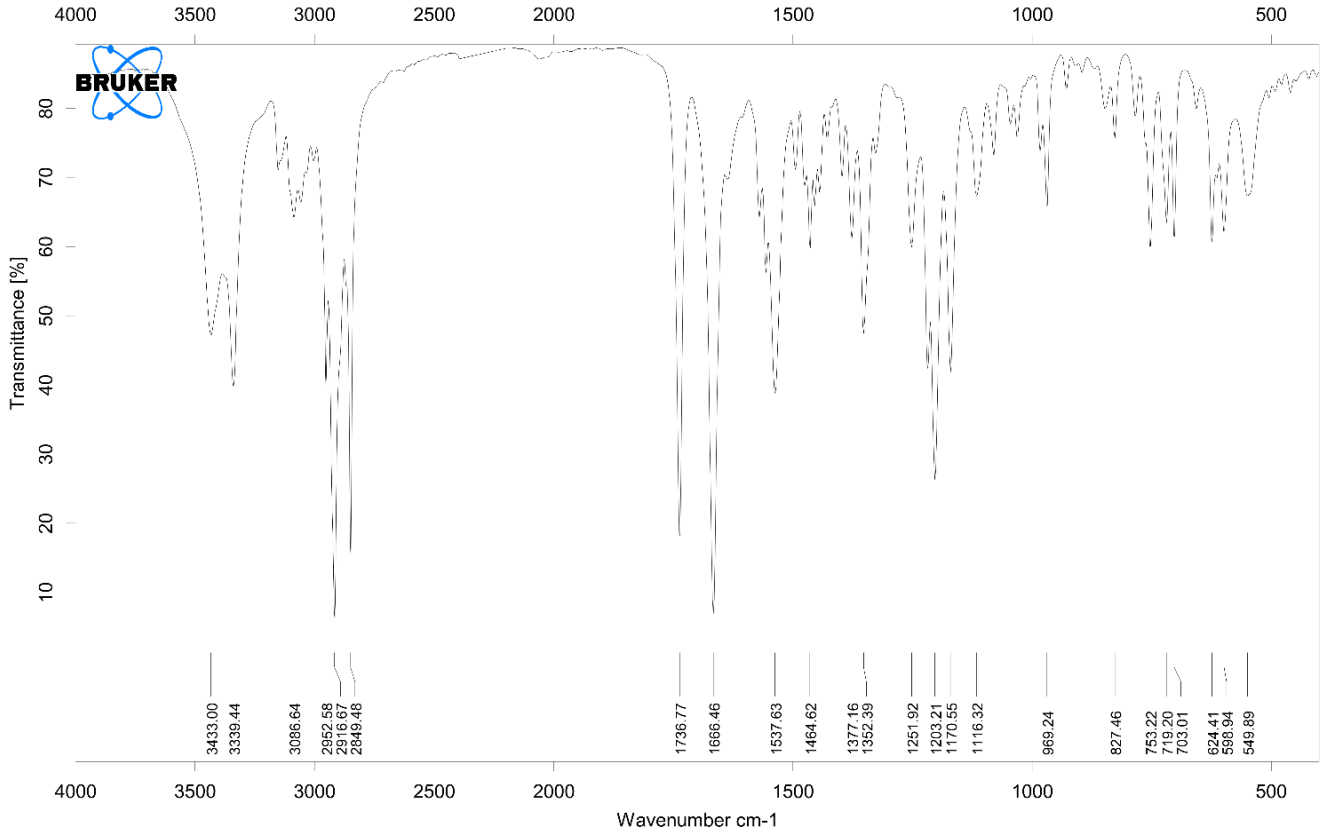
^{1}H NMR



^{13}C NMR



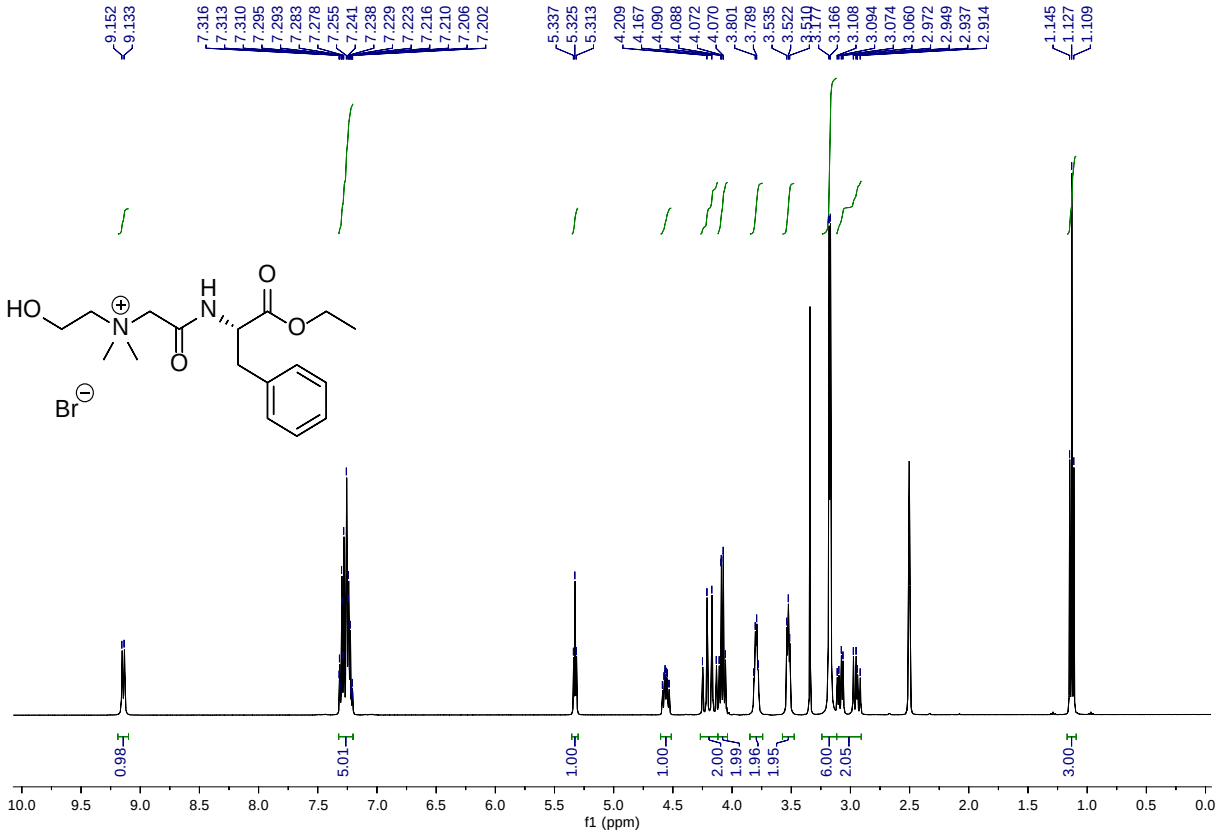
IR (KBr, cm^{-1})


4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
3433.00
3339.44
3086.64
2952.58
2916.67
2849.48
1736.77
1666.46
1537.63
1464.62
1377.16
1352.39
1251.92
1203.21
1170.55
1116.32
969.24
827.46
753.22
719.20
703.01
624.41
598.94
549.89
Wavenumber cm-1

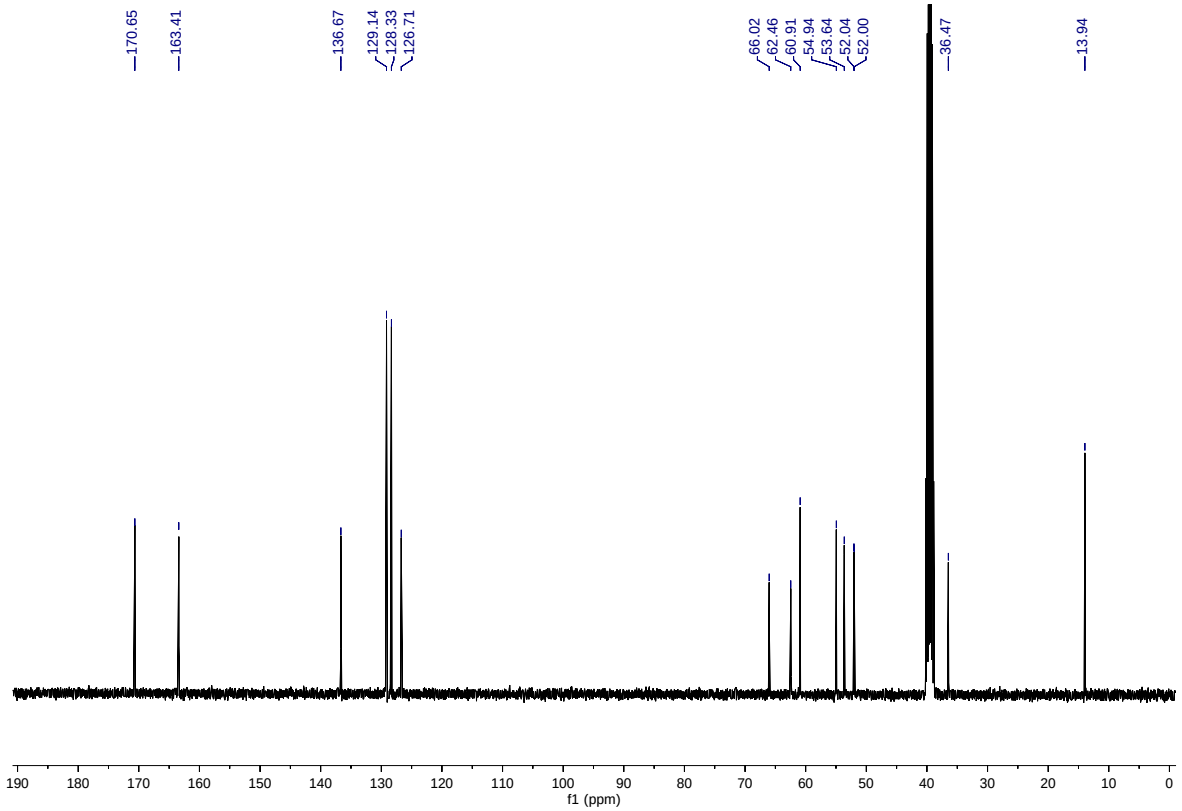
13. NMR and IR Spectra of cholinium ILs (33 - 40)

(*S*)-2-((1-(ethoxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (33)

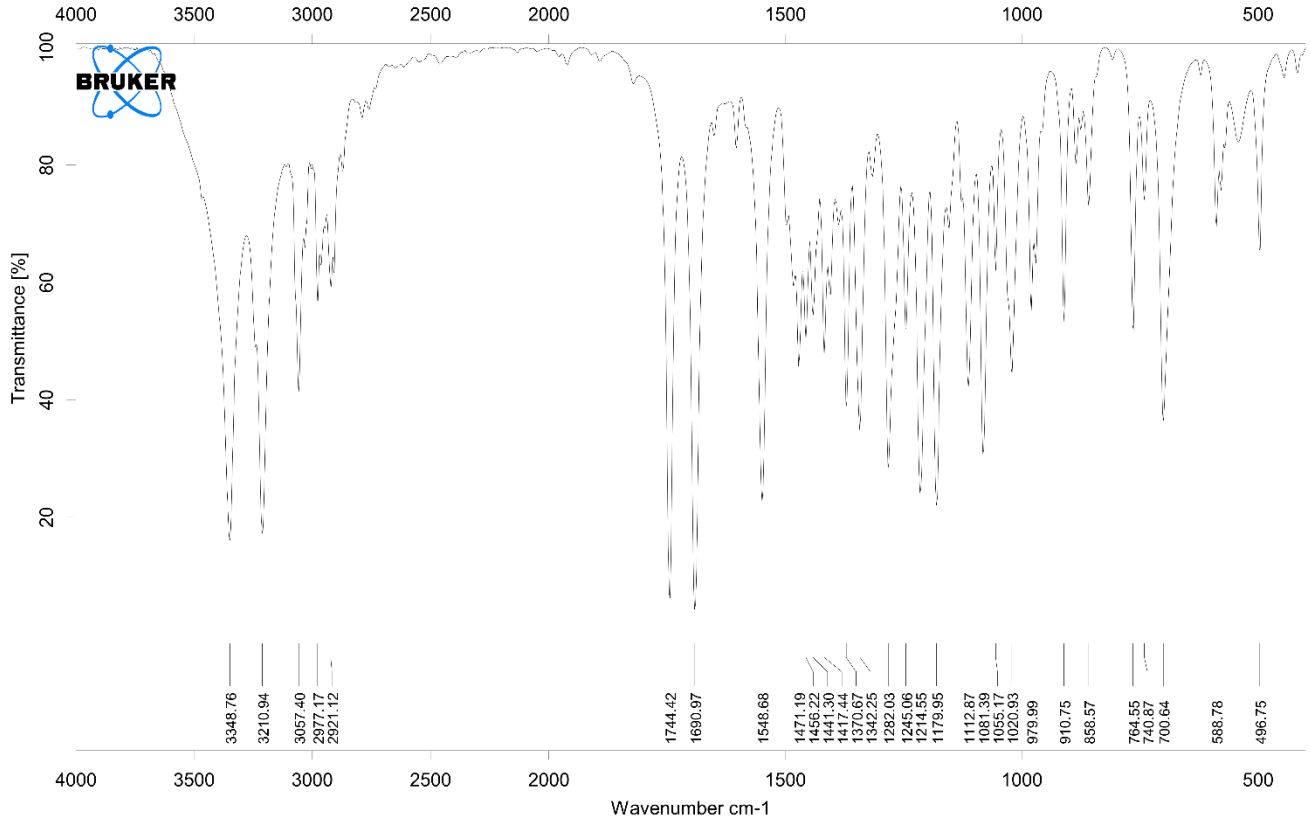
^{1}H NMR



^{13}C NMR

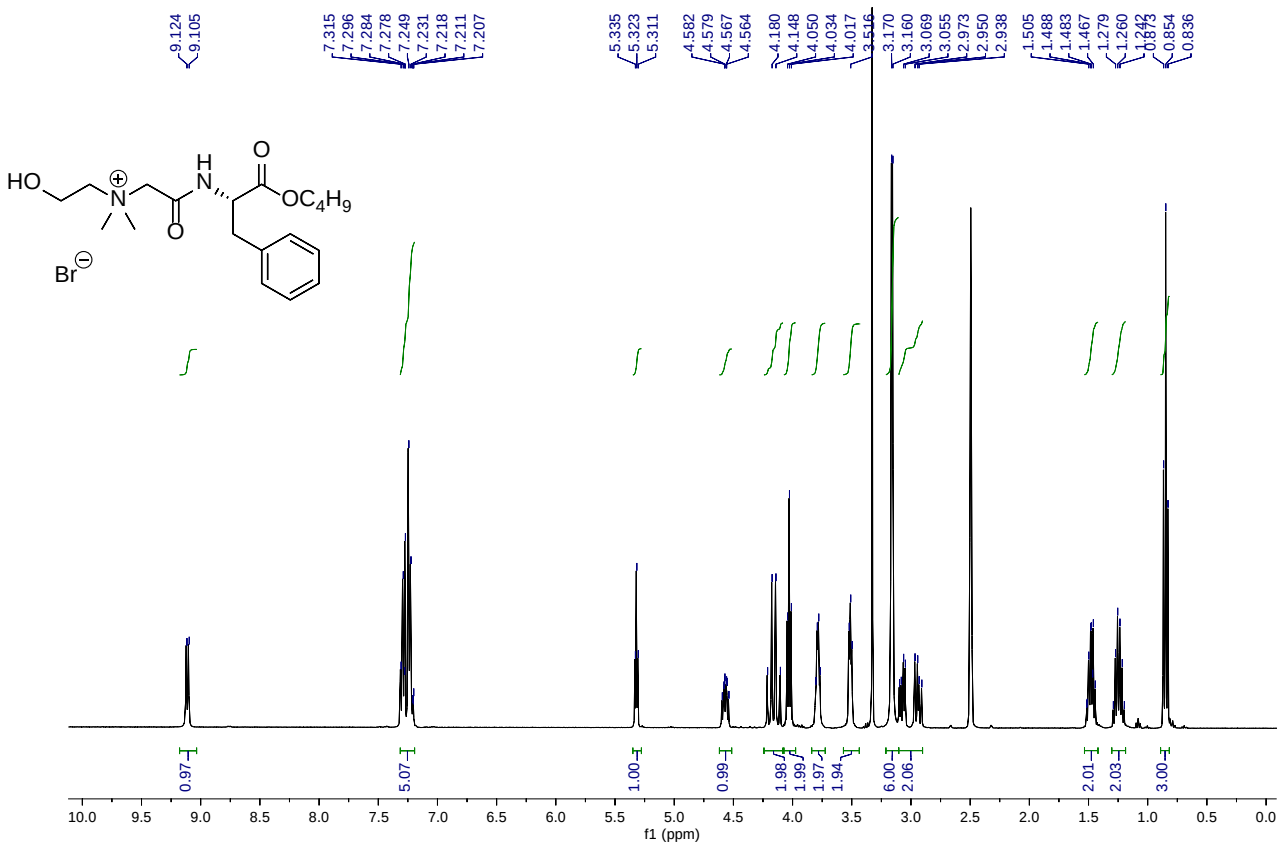


IR (KBr, cm^{-1})

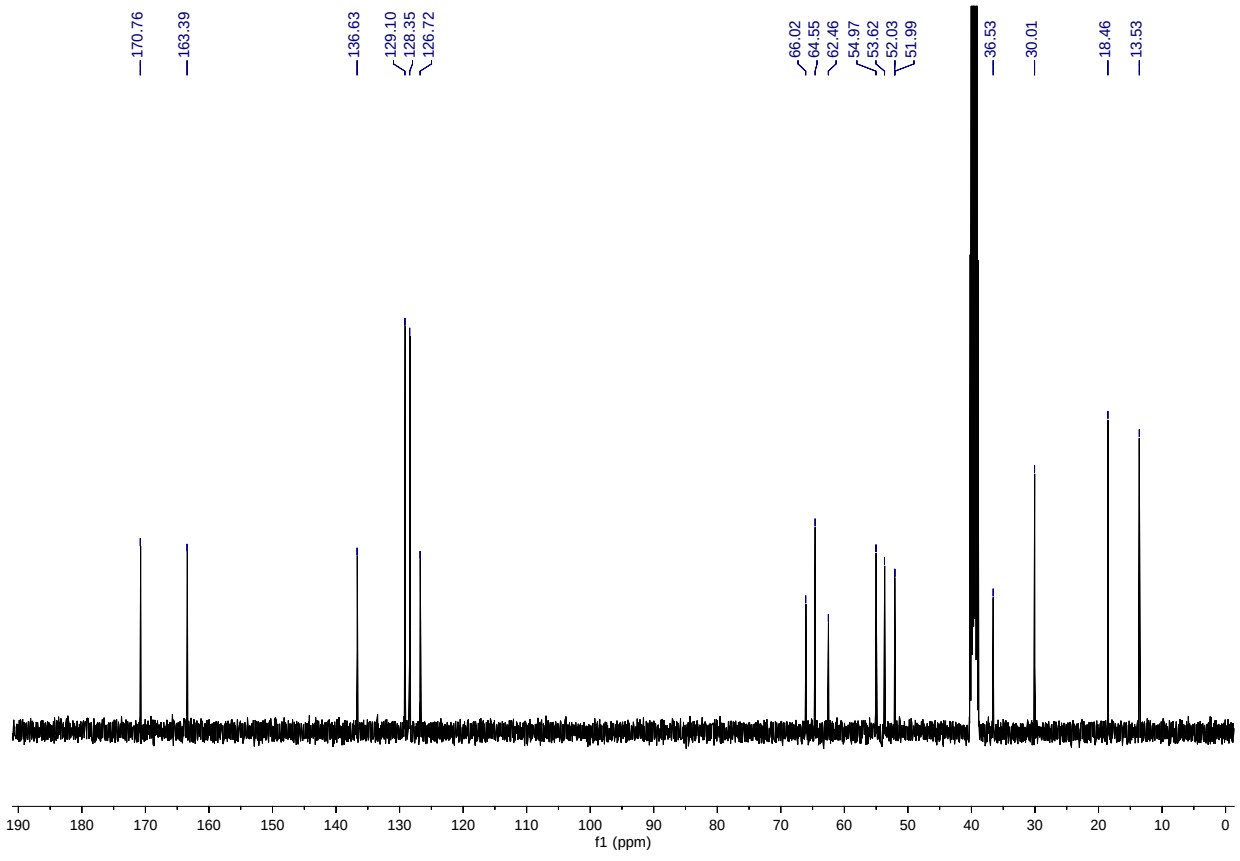

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3348.76
3210.94
3057.40
2977.17
2921.12
1744.42
1690.97
1548.68
1471.19
1456.22
1441.30
1417.44
1370.67
1342.25
1282.03
1245.06
1214.55
1179.95
1112.87
1081.39
1055.17
1020.93
979.99
910.75
858.57
764.55
740.87
700.64
588.78
496.75
Wavenumber cm-1

(*S*)-2-((1-(butoxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (34)

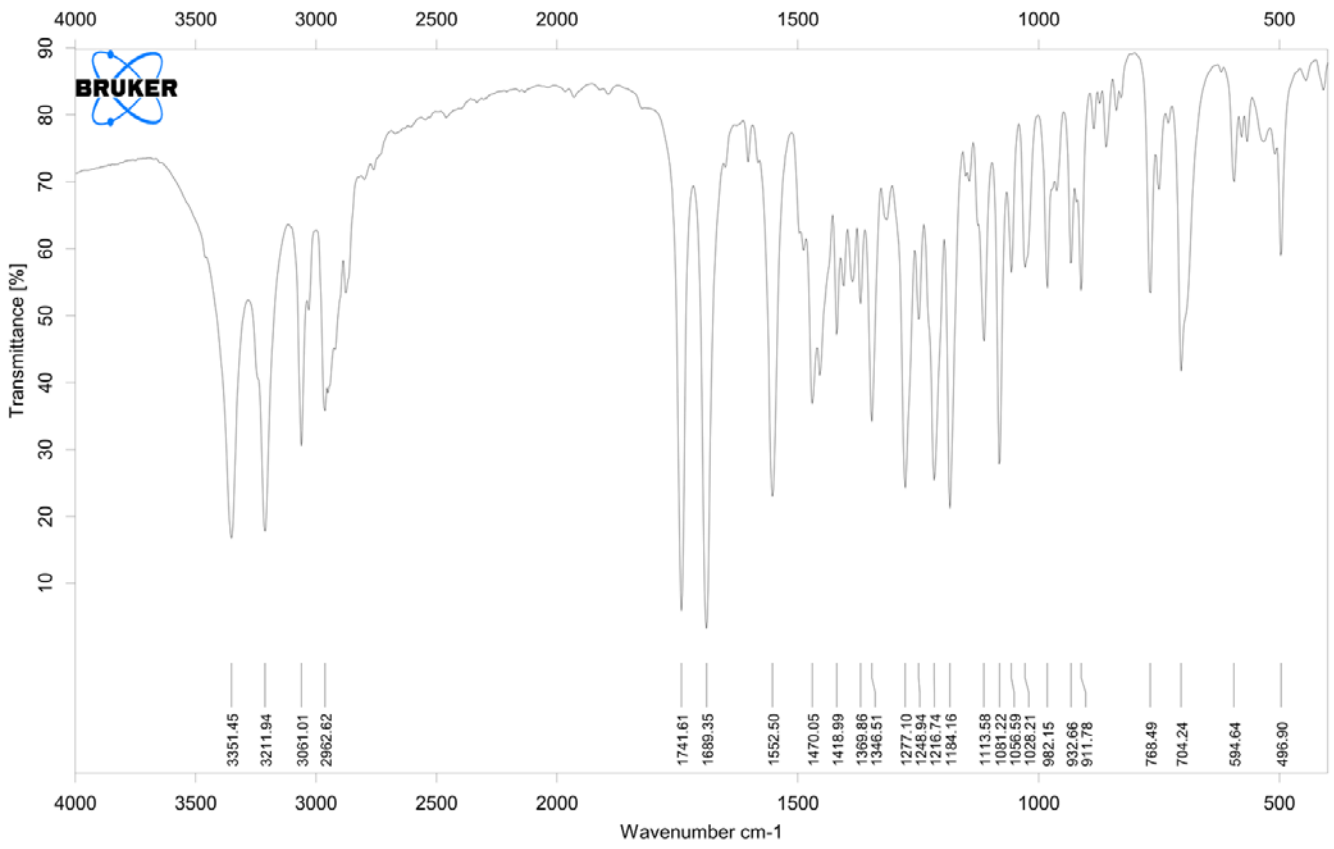
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


BRUKER
Transmittance [%]
Wavenumber cm-1
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3211.94
3061.01
2962.62
1741.61
1689.35
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1277.10
1248.94
1216.74
1184.16
1113.58
1081.22
1056.59
1028.21
982.15
932.66
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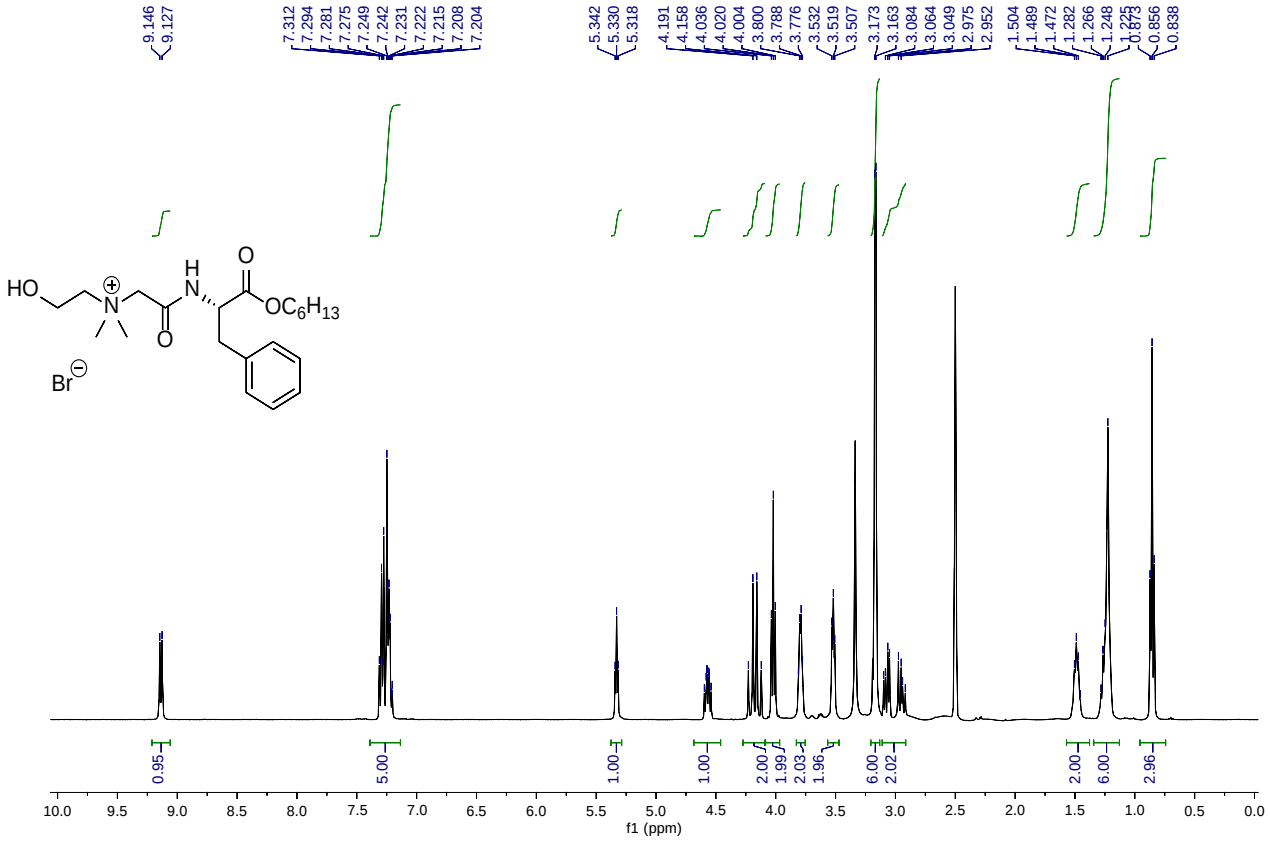
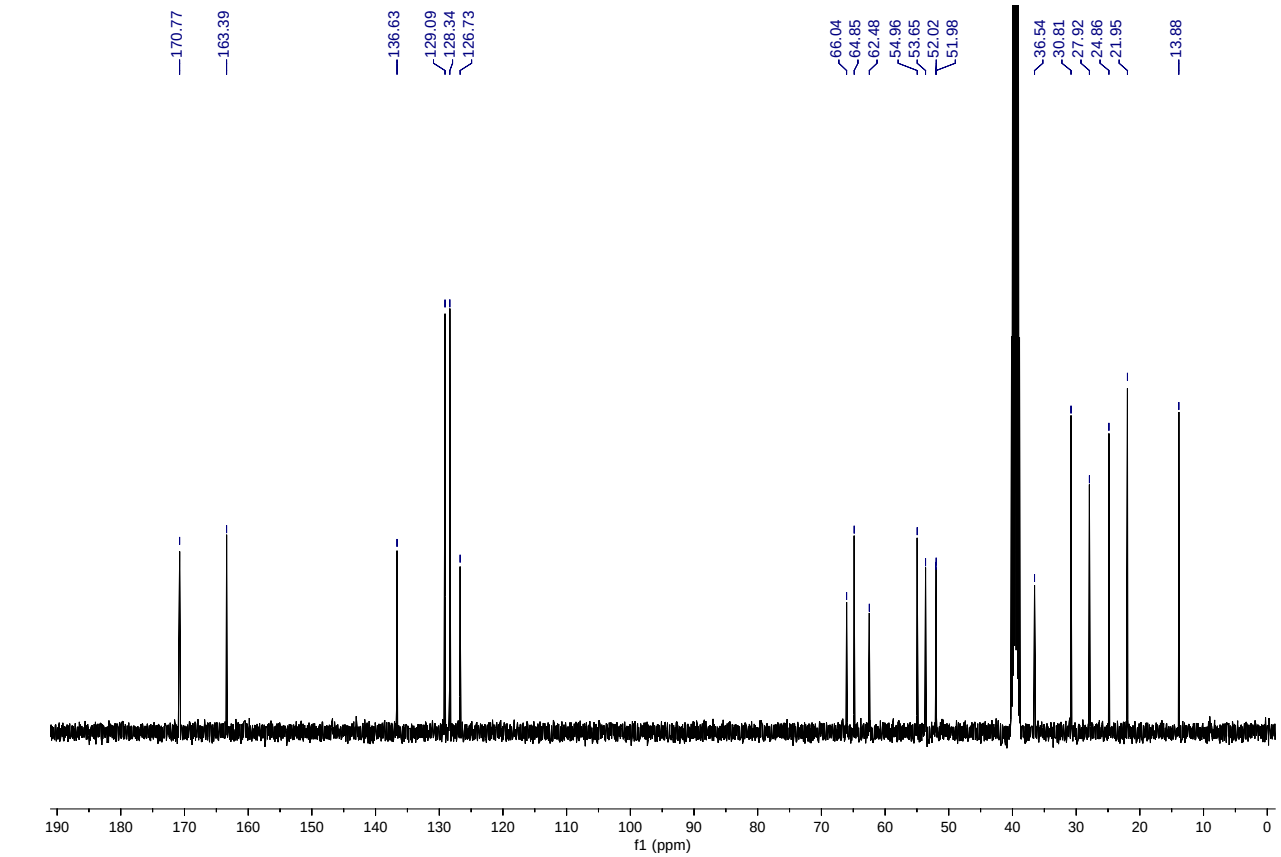
768.49
704.24
594.64
496.90

(*S*)-2-((1-(hexyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (35)

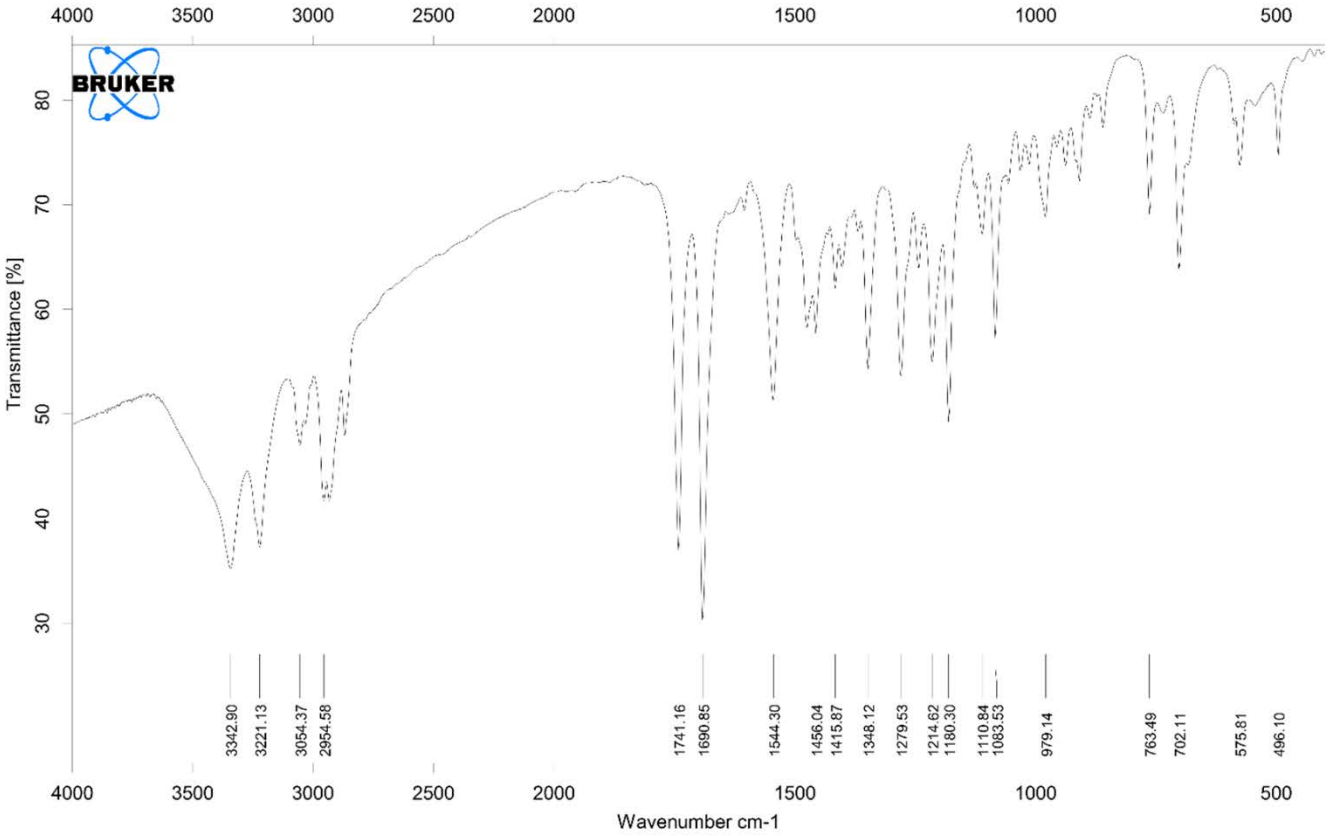
^{1}H NMR



^{13}C NMR

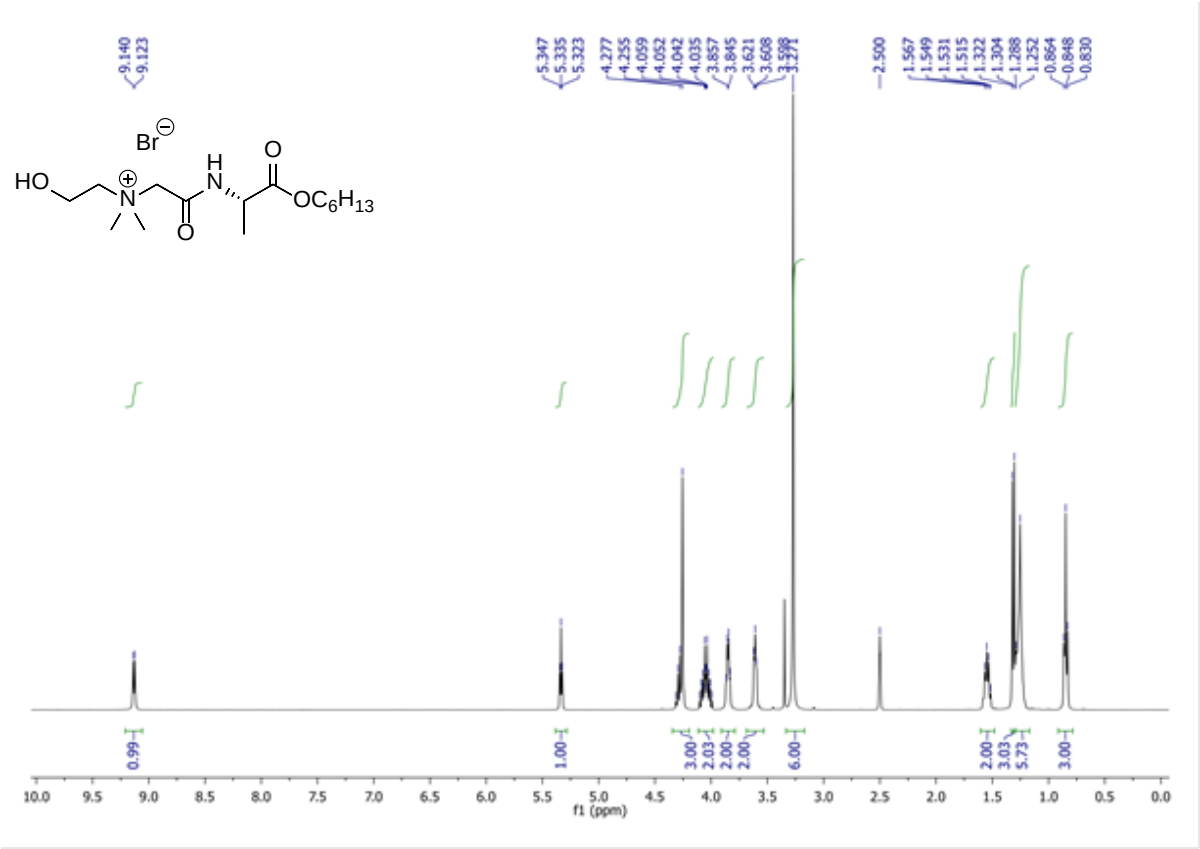


IR (KBr, cm^{-1})

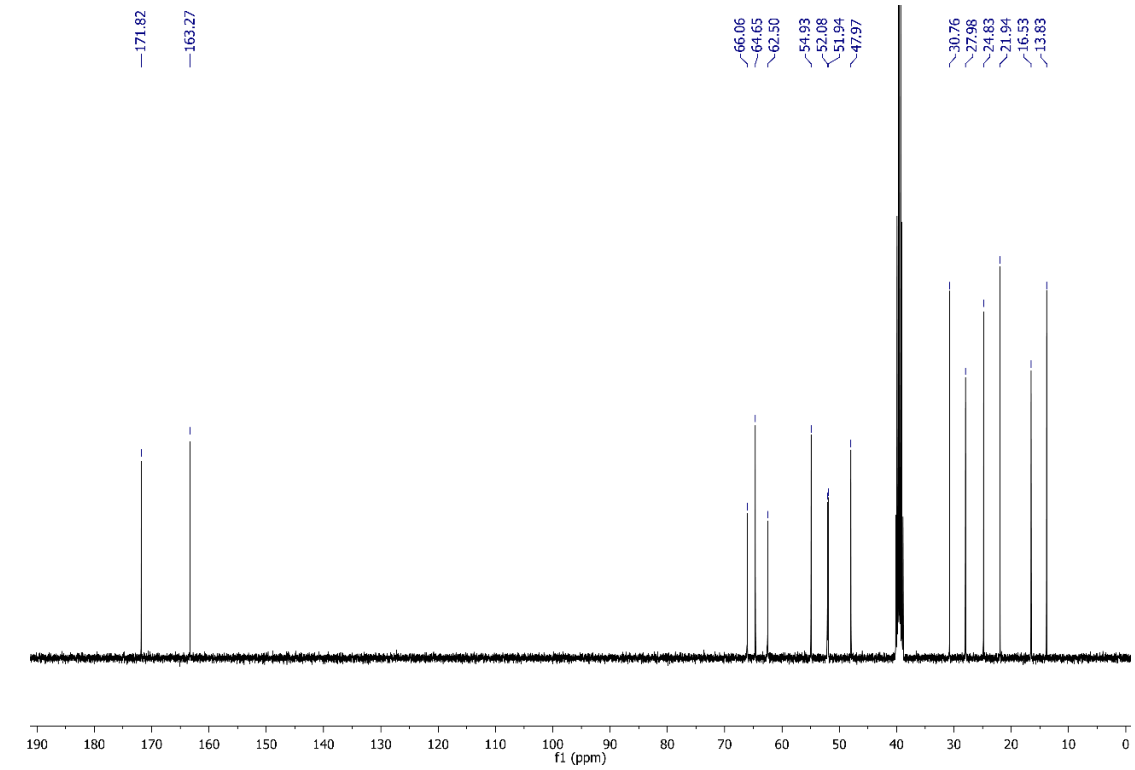

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
80
70
60
50
40
30
3342.90
3221.13
3054.37
2954.58
1741.16
1690.85
1544.30
1456.04
1415.87
1348.12
1279.53
1214.62
1180.30
1110.84
1083.53
979.14
763.49
702.11
575.81
496.10
Wavenumber cm-1

(*S*)-2-((1-(hexyloxy)-1-oxopropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (35Ala)

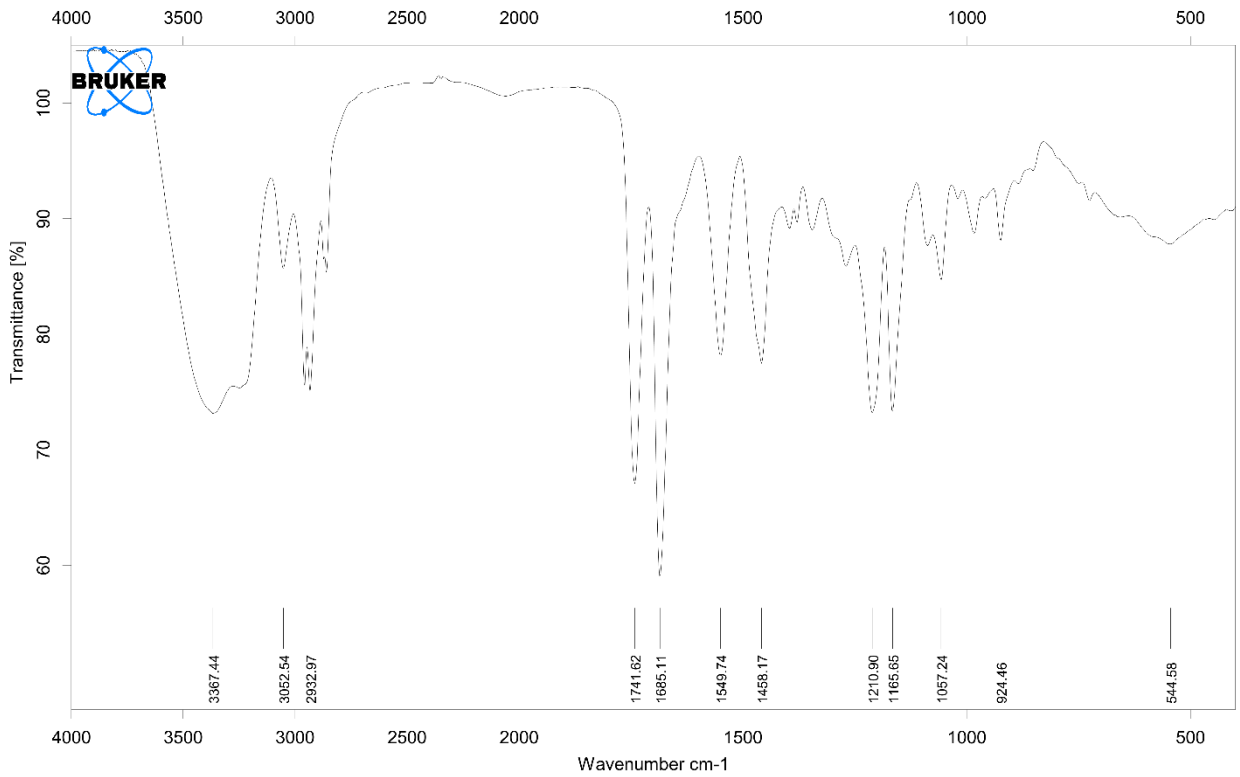
^{1}H NMR



^{13}C NMR

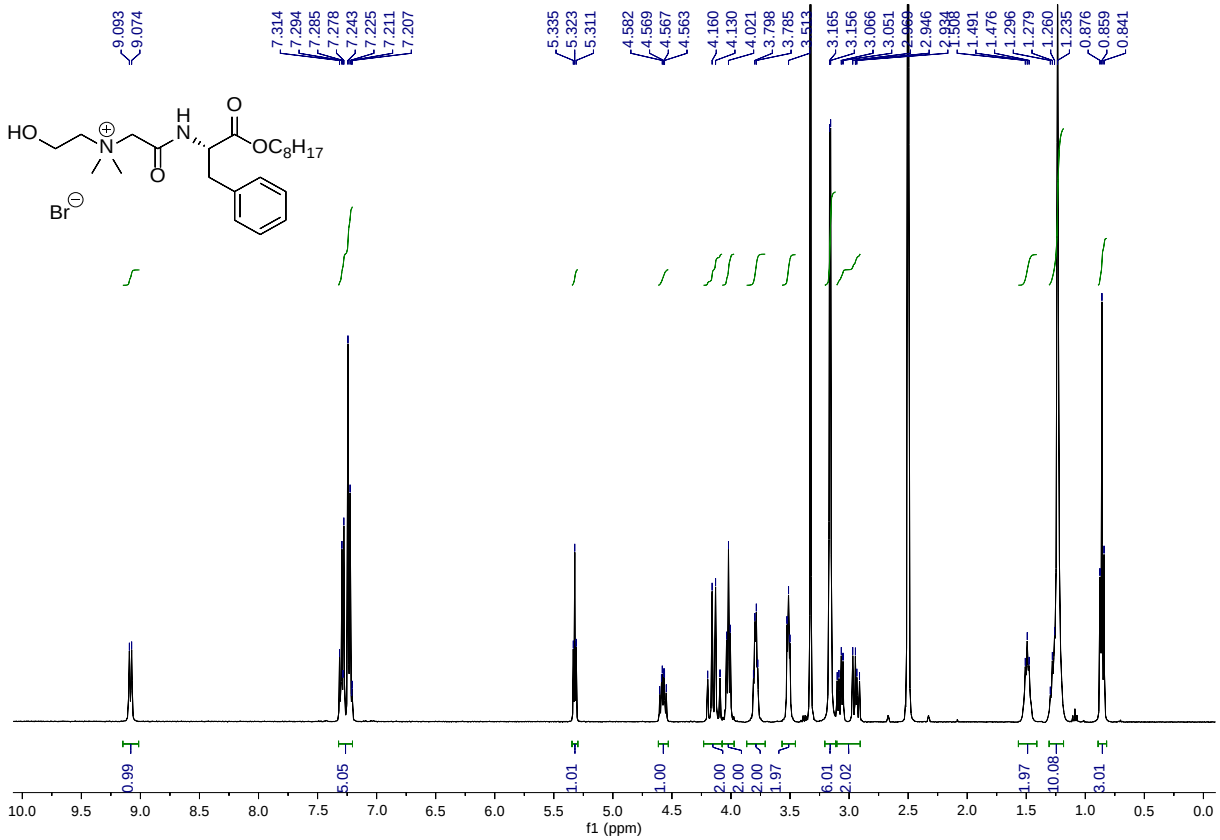


IR (KBr, cm^{-1})

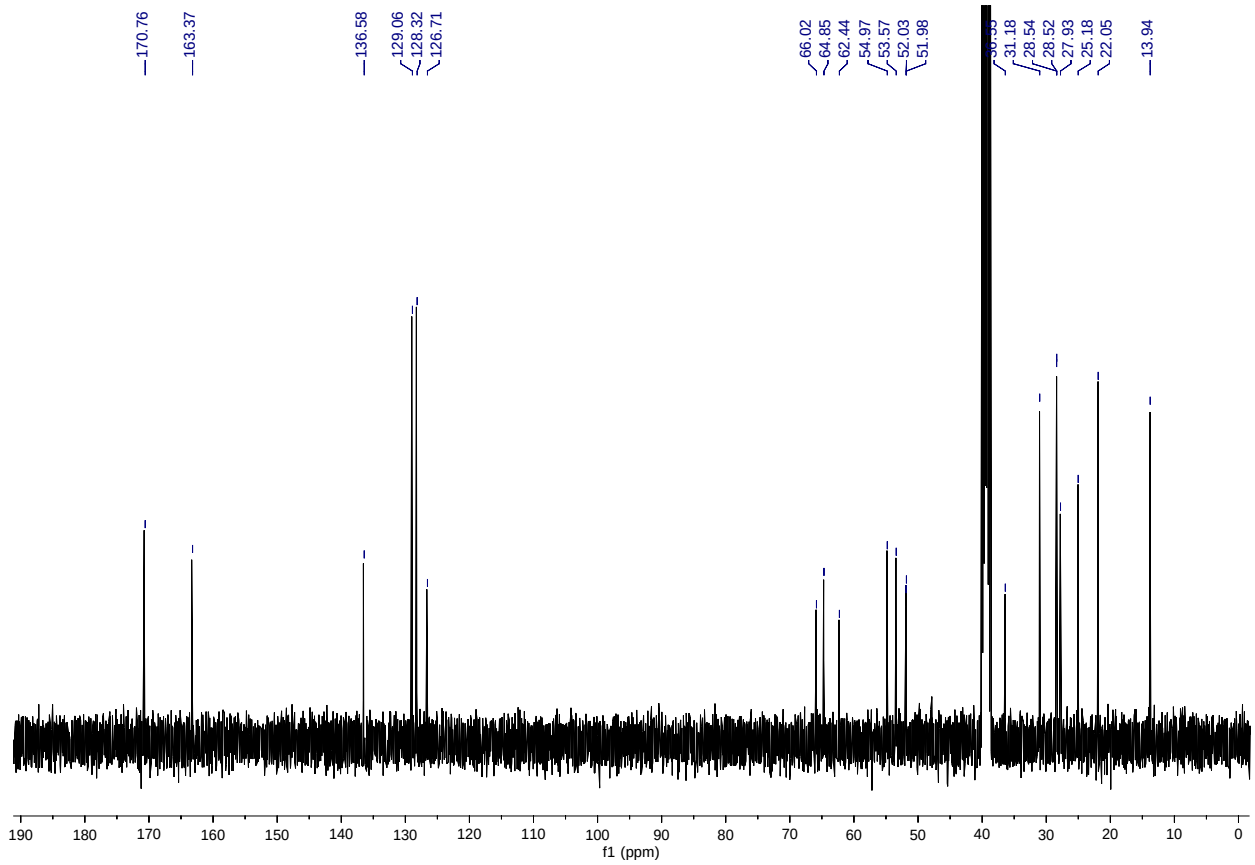

BRUKER
Transmittance [%]
Wavenumber cm-1
3367.44
3052.54
2932.97
1741.62
1685.11
1549.74
1458.17
1210.90
1165.65
1057.24
924.46
544.58

(*S*)-2-((1-(octyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (36)

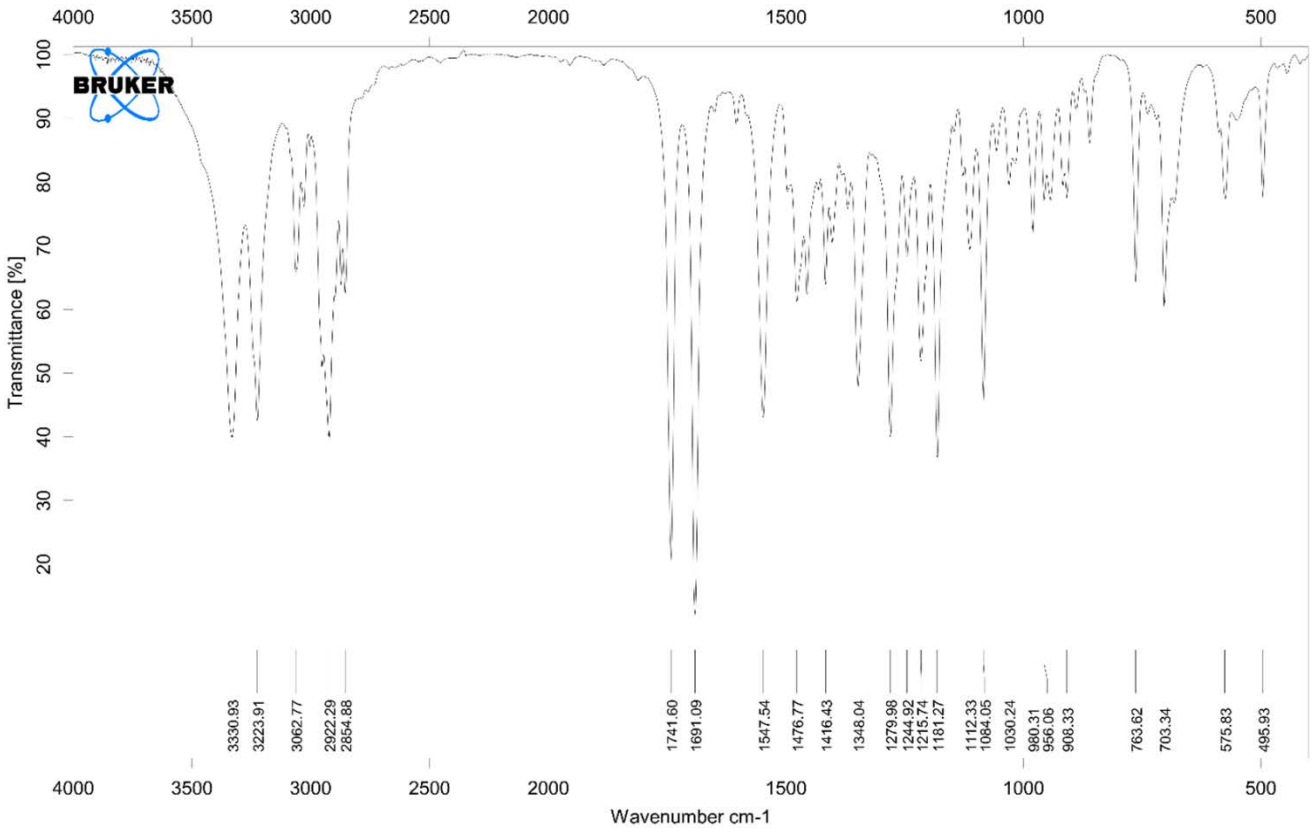
^{1}H NMR



^{13}C NMR

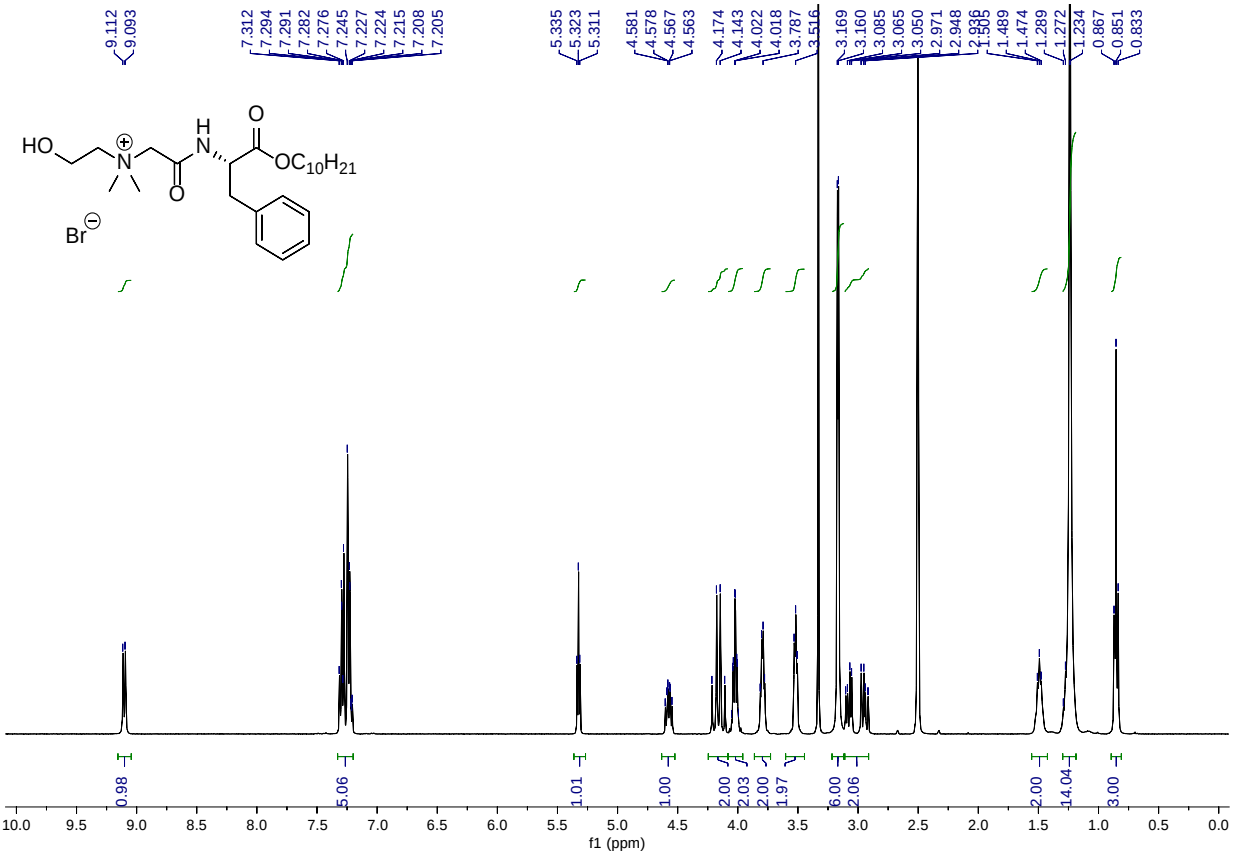


IR (KBr, cm^{-1})

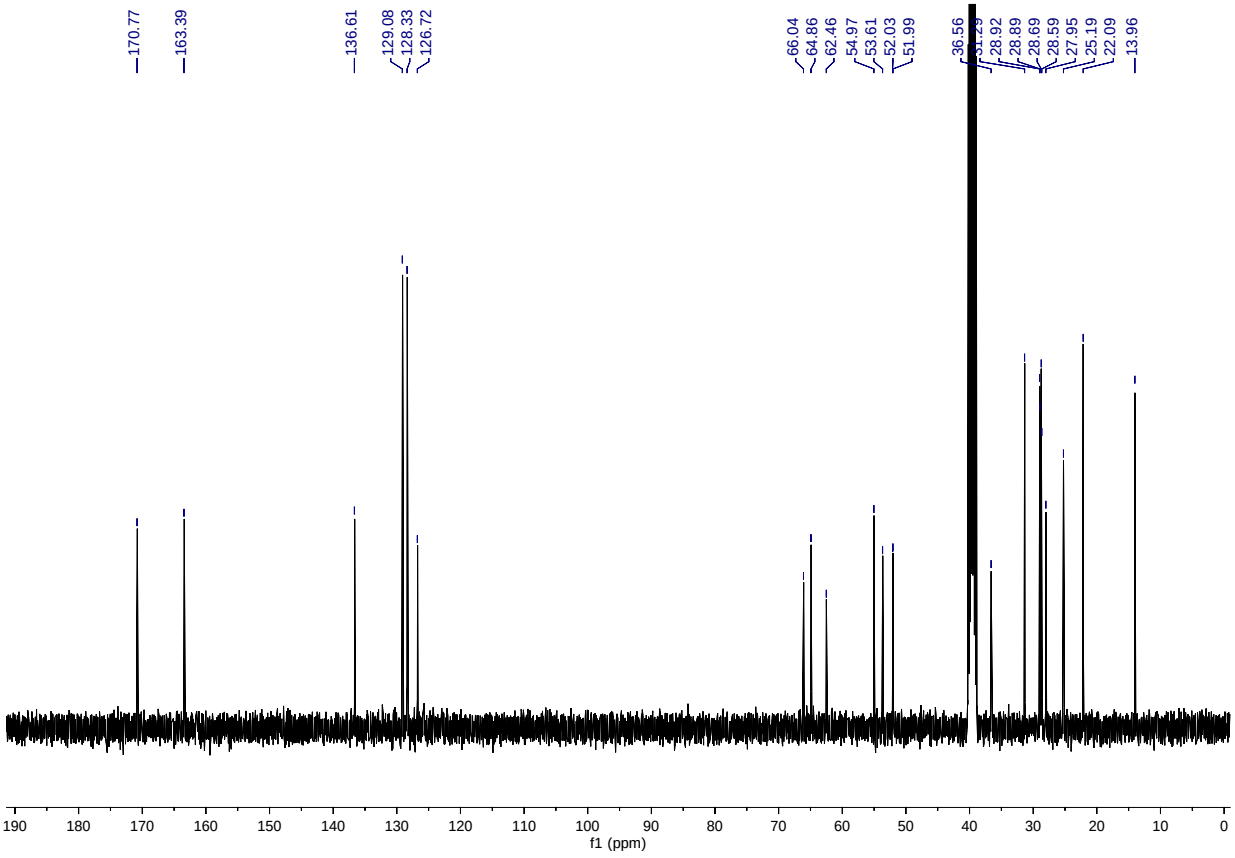

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
20
3330.93
3223.91
3062.77
2922.29
2854.88
1741.60
1691.09
1547.54
1476.77
1416.43
1348.04
1279.98
1244.92
1215.74
1181.27
1112.33
1084.05
1030.24
980.31
956.06
908.33
763.62
703.34
575.83
495.93
Wavenumber cm-1

(*S*)-2-((1-(decyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (37)

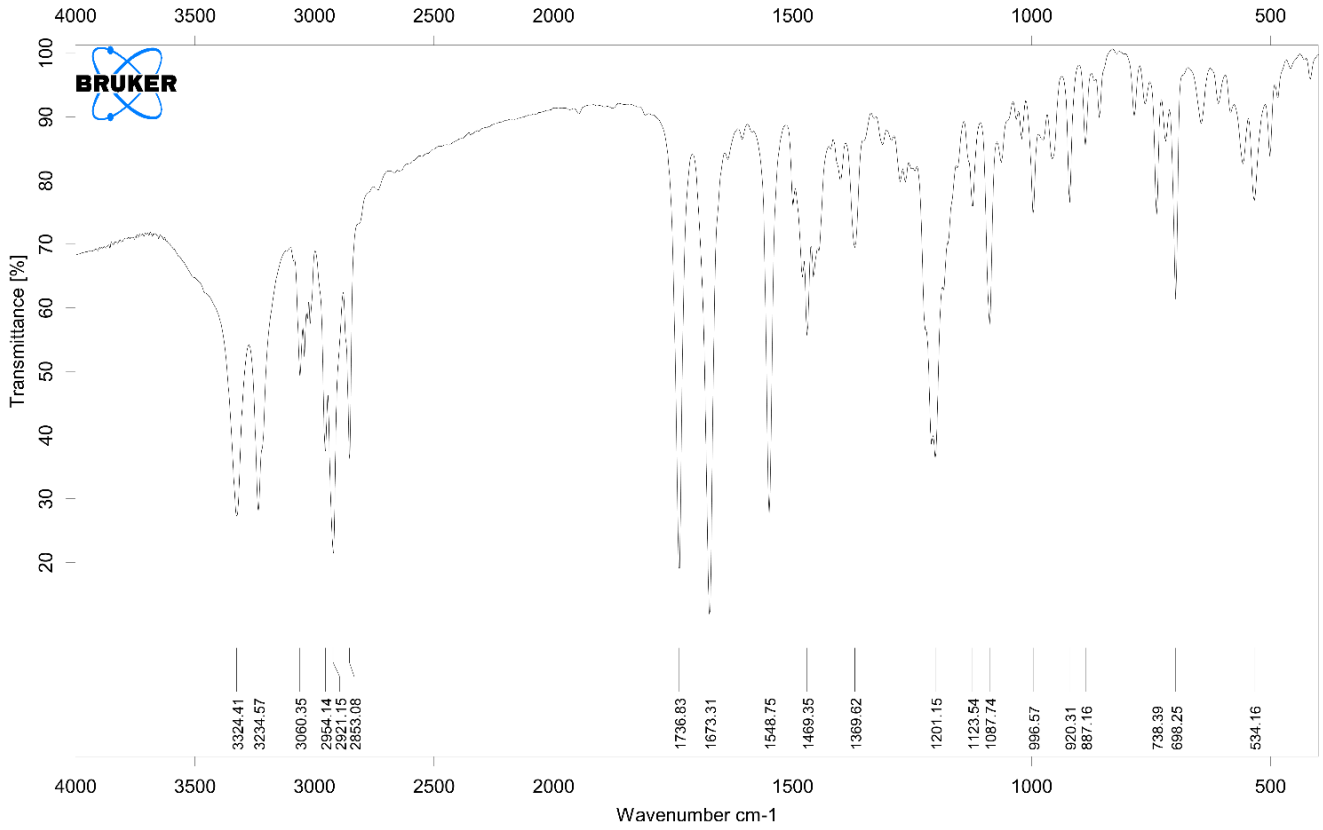
^{1}H NMR



^{13}C NMR

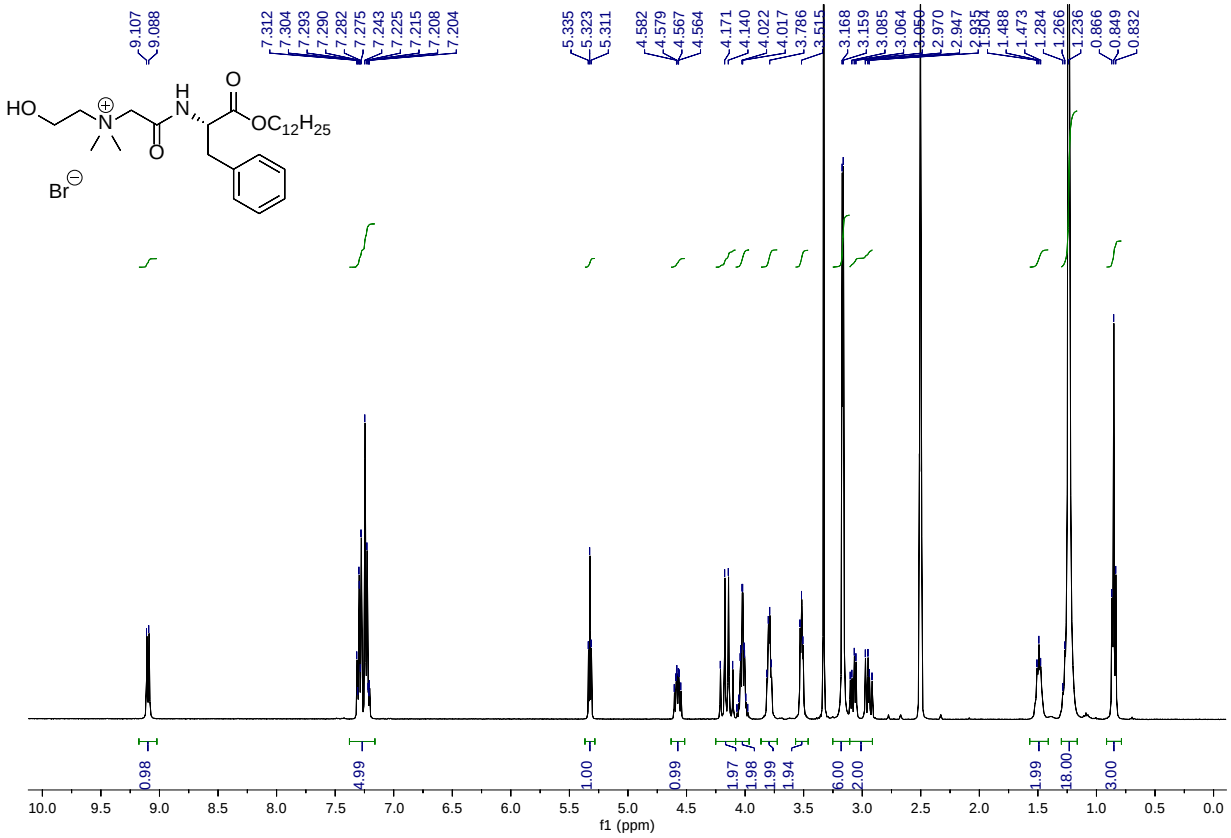


IR (KBr, cm^{-1})

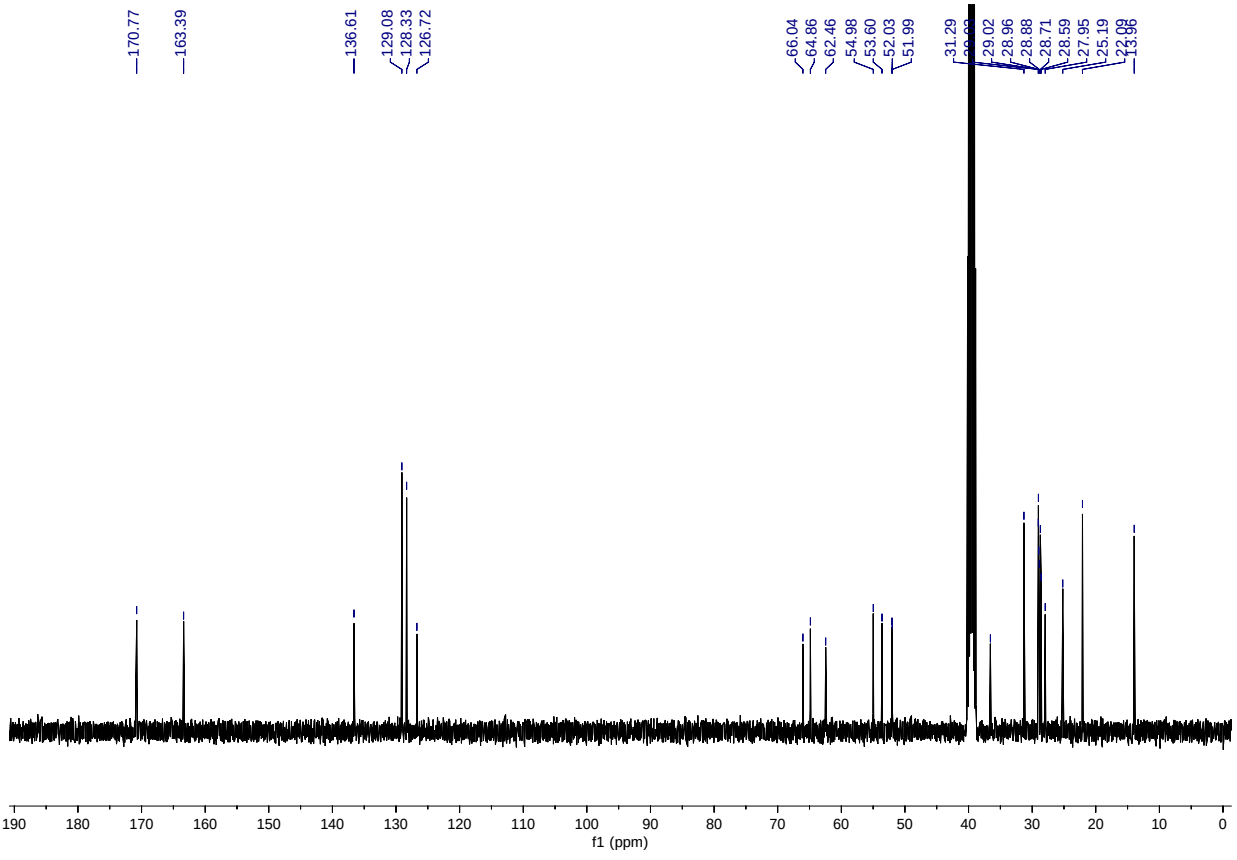

4000
3500
3000
2500
2000
1500
1000
500
BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
20
3324.41
3234.57
3060.35
2954.14
2921.15
2853.08
1736.83
1673.31
1548.75
1469.35
1369.62
1201.15
1123.54
1087.74
996.57
920.31
887.16
738.39
698.25
534.16
Wavenumber cm-1

(*S*)-2-((1-(dodecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (38)

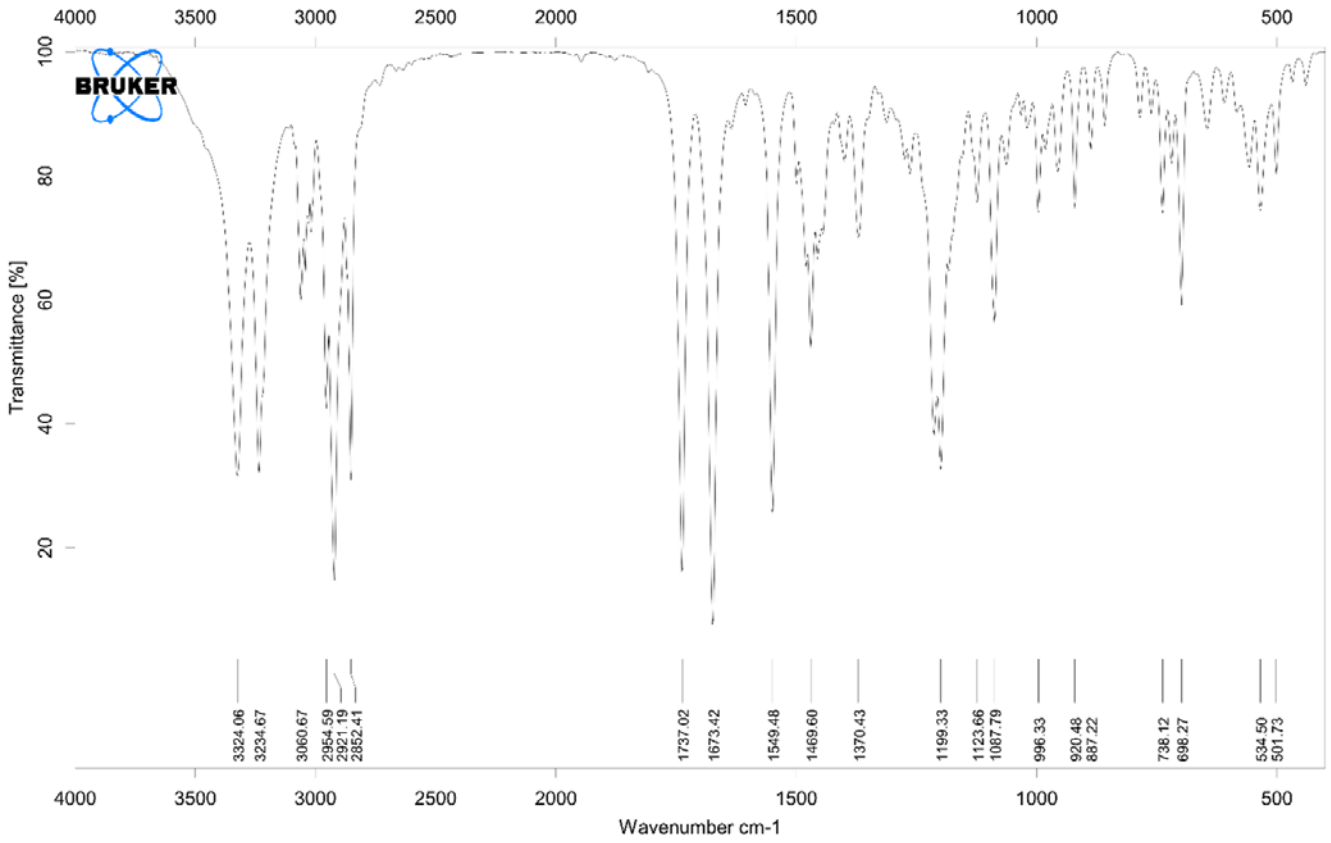
^{1}H NMR



^{13}C NMR

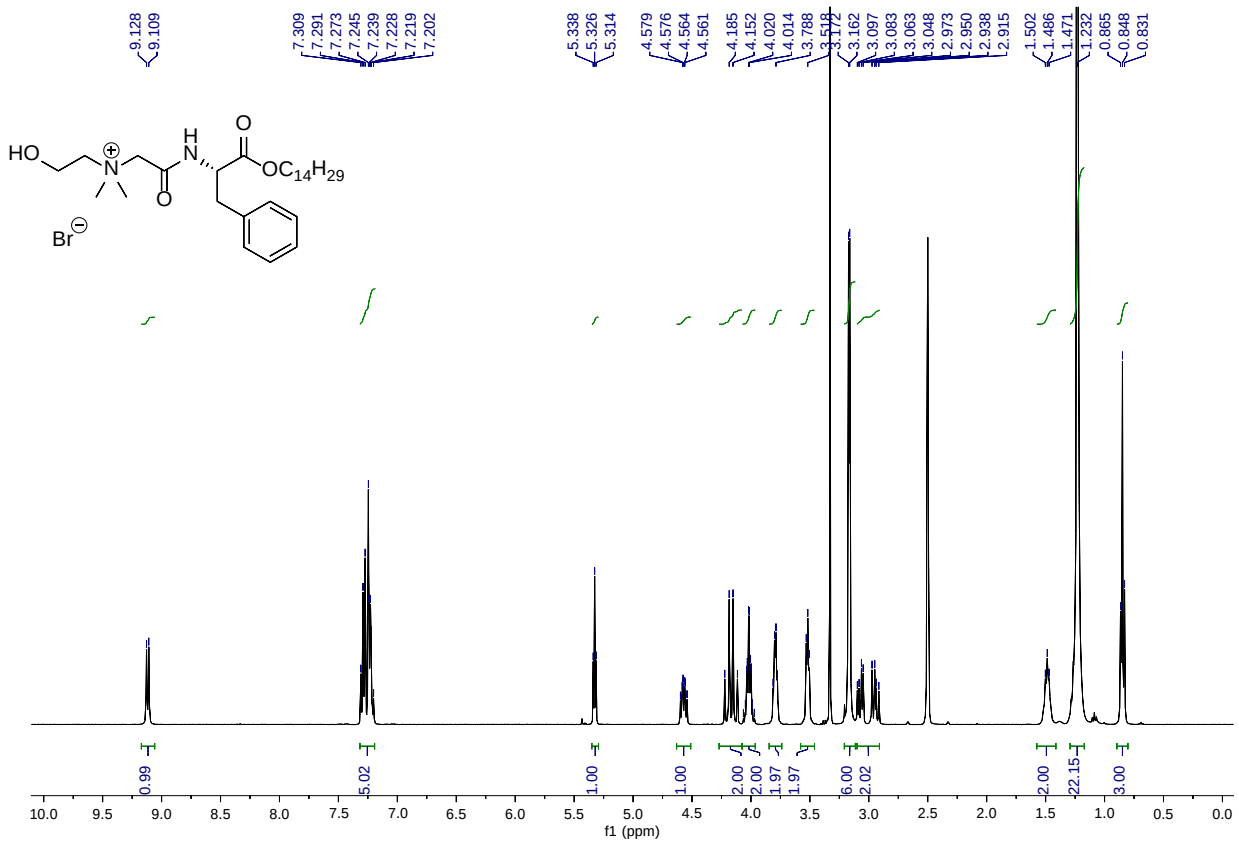


IR (KBr, cm^{-1})

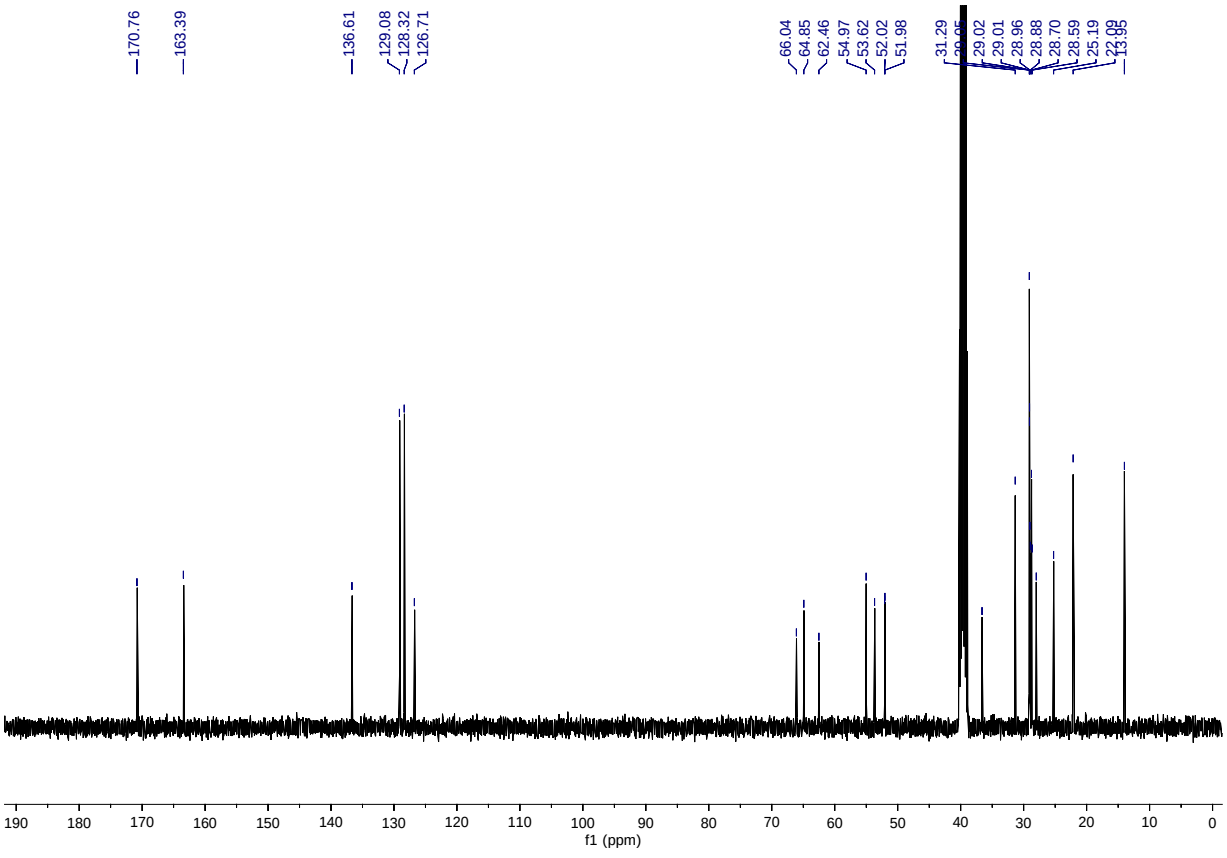

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3324.06
3234.67
3060.67
2954.59
2921.19
2852.41
1737.02
1673.42
1549.48
1469.60
1370.43
1199.33
1123.66
1087.79
996.33
920.48
887.22
738.12
698.27
534.50
501.73
Wavenumber cm-1

(*S*)-2-((1-(tetradecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (39)

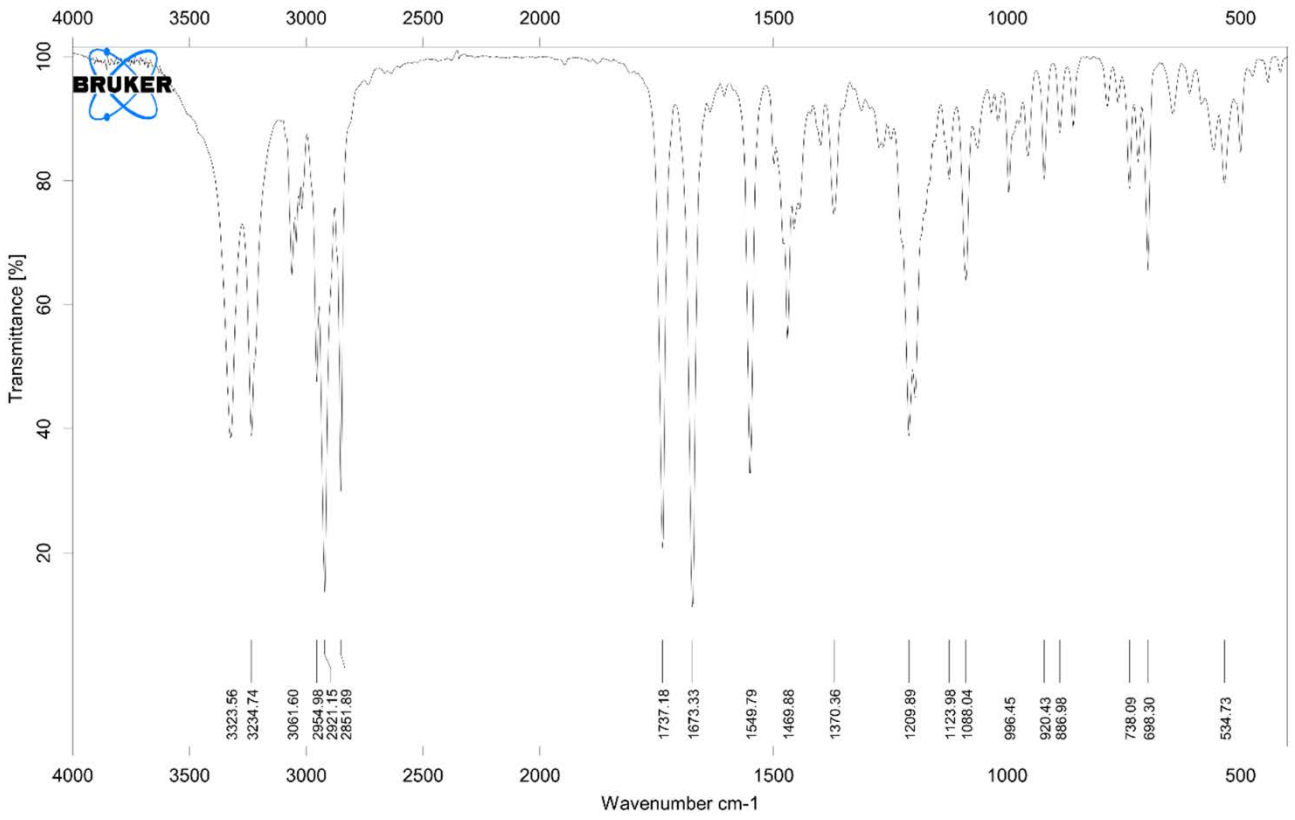
^{1}H NMR



^{13}C NMR

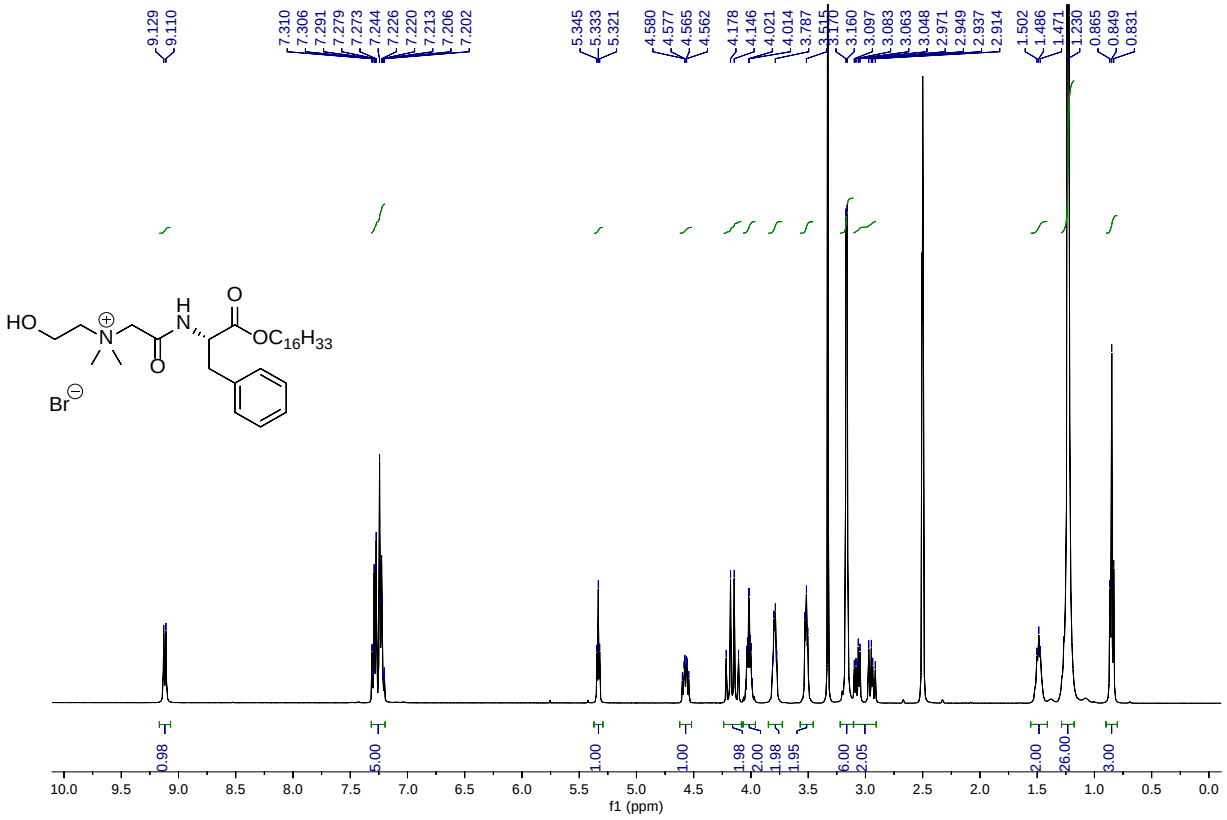


IR (KBr, cm^{-1})

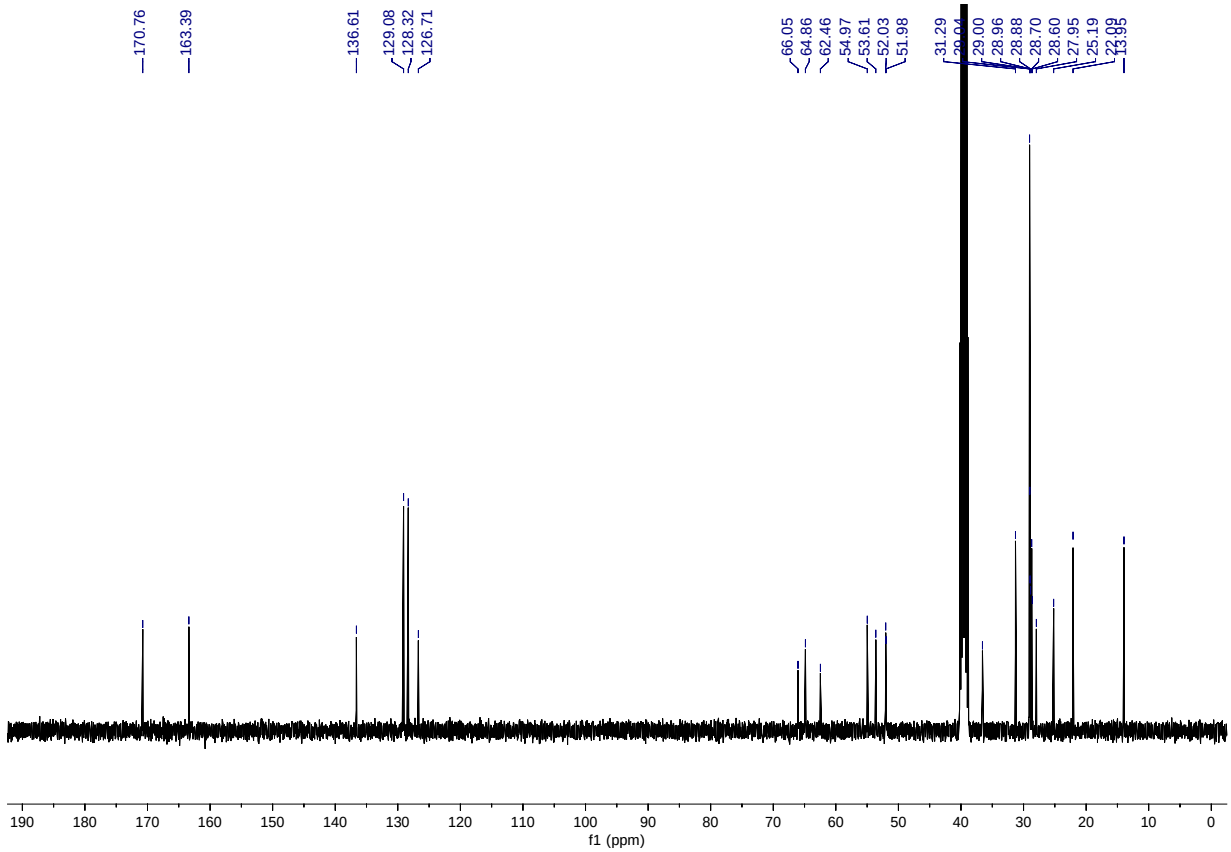

4000
3500
3000
2500
2000
1500
1000
500
100
80
60
40
20
Transmittance [%]
BRUKER
3323.56
3234.74
3061.60
2954.98
2921.15
2851.89
1737.18
1673.33
1549.79
1469.88
1370.36
1209.89
1123.98
1088.04
996.45
920.43
886.98
738.09
698.30
534.73
Wavenumber cm-1

(*S*)-2-((1-(hexadecyloxy)-1-oxo-3-phenylpropan-2-yl)amino)-*N*-(2-hydroxyethyl)-*N*,*N*-dimethyl-2-oxoethan-1-aminium bromide (40)

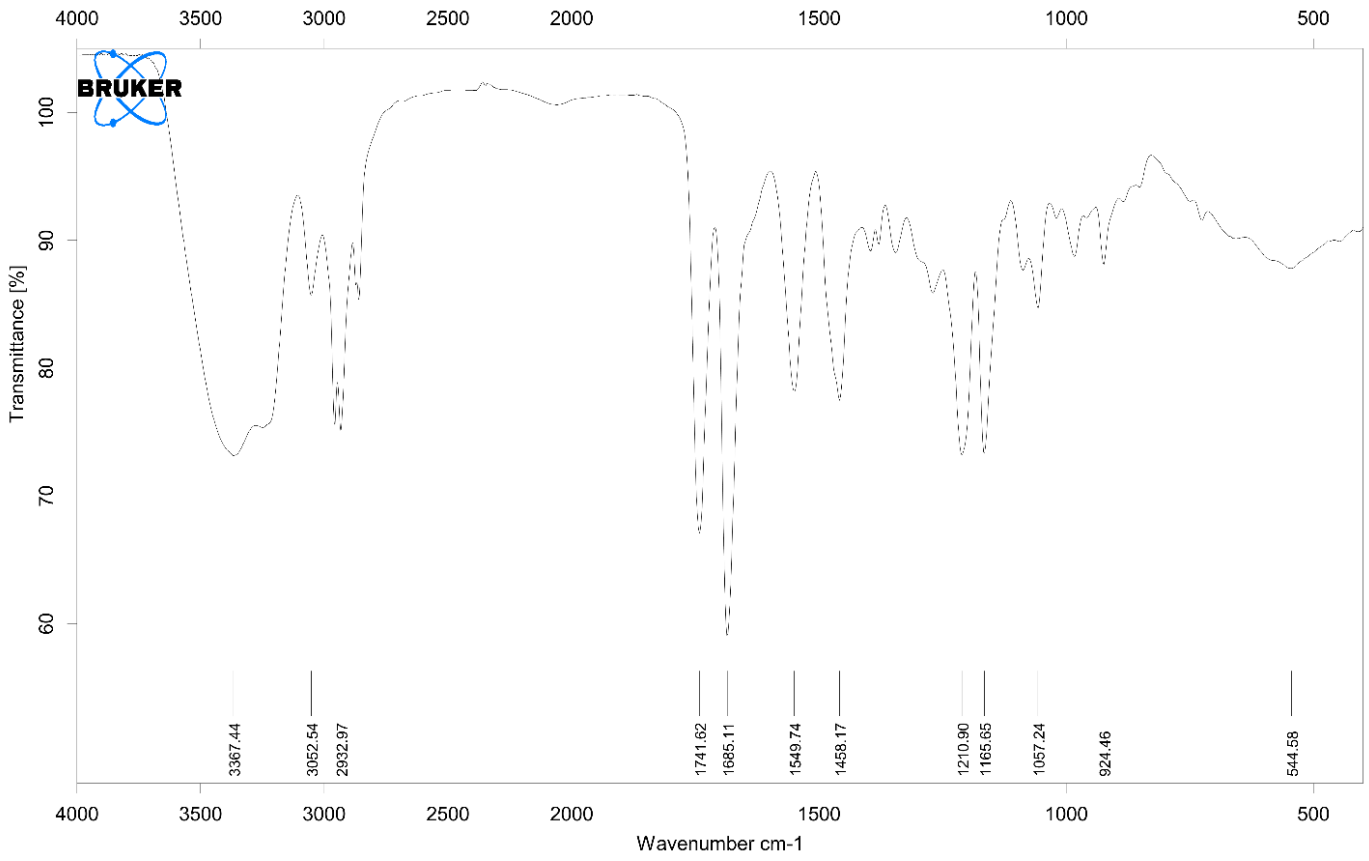
^{1}H NMR



^{13}C NMR



IR (KBr, cm^{-1})


4000
3500
3000
2500
2000
1500
1000
500
BRUKER
100
90
80
70
60
Transmittance [%]
3367.44
3052.54
2932.97
1741.62
1685.11
1549.74
1458.17
1210.90
1165.65
1057.24
924.46
544.58
Wavenumber cm-1

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