

Supporting Information

Synthesis, Structure-Activity Relationship, and Mechanistic Investigation of Lithocholic Acid Amphiphiles for Colon Cancer Therapy

Manish Singh,^{a,†} Sandhya Bansal,^{a,†} Somanath Kundu,^{a,c,†} Priyanshu Bhargava,^a Ashima Singh,^a Rajender K. Motiani,^{a,§} Radhey Shyam,^b Vedagopuram Sreekanth,^{a,c} Sagar Sengupta,^b and Avinash Bajaj^{a,*}

^a*The Laboratory of Nanotechnology and Chemical Biology, Regional Centre for Biotechnology, 180 Udyog Vihar, Phase 1, Gurgaon-122016, Haryana, India.* ^b*National Institute of Immunology, Aruna Asif Ali Marg, New Delhi 110067, India.* ^c*Manipal University, Manipal, Karnataka, India.*

[§] *Current address: Institute of Genomics and Integrative Biology, New Delhi-110025.*

[†]*These Authors contributed equally.*

**Corresponding Author:*

Avinash Bajaj, Email: bajaj@rcb.res.in, Ph: +91-124-2848831, Fax: +91-124-4038117.

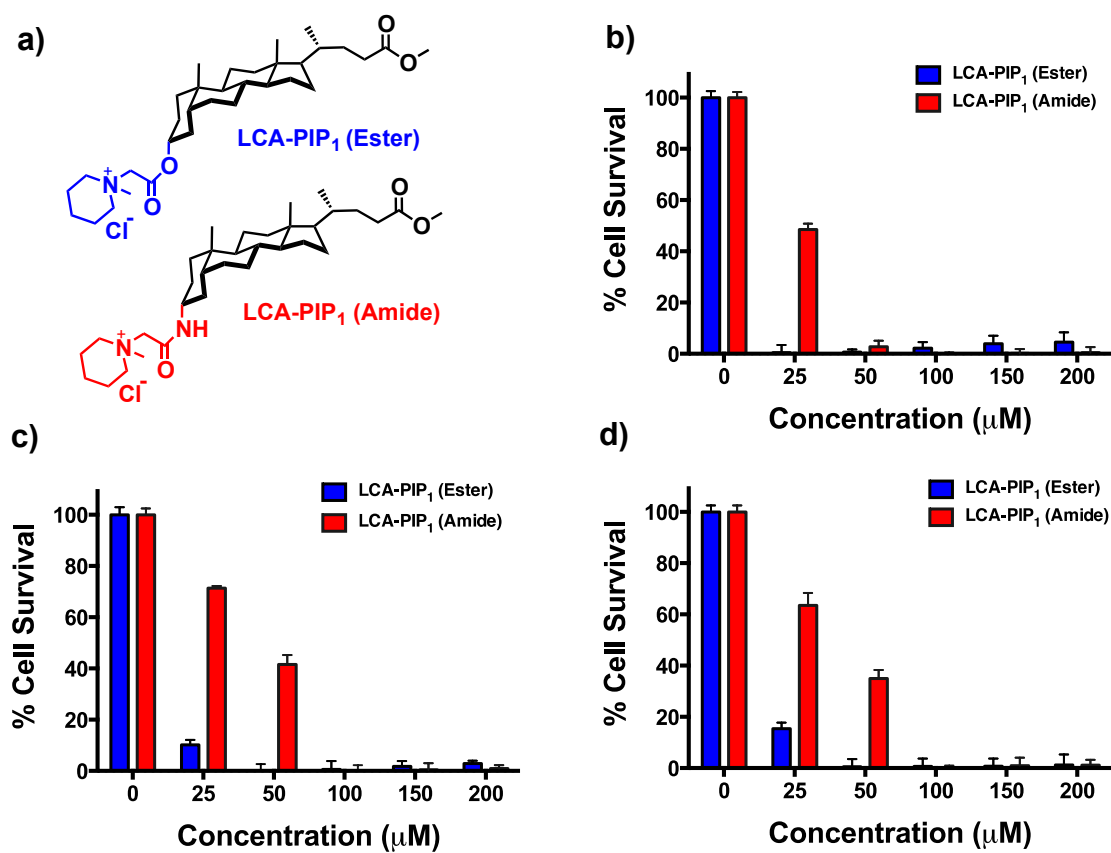
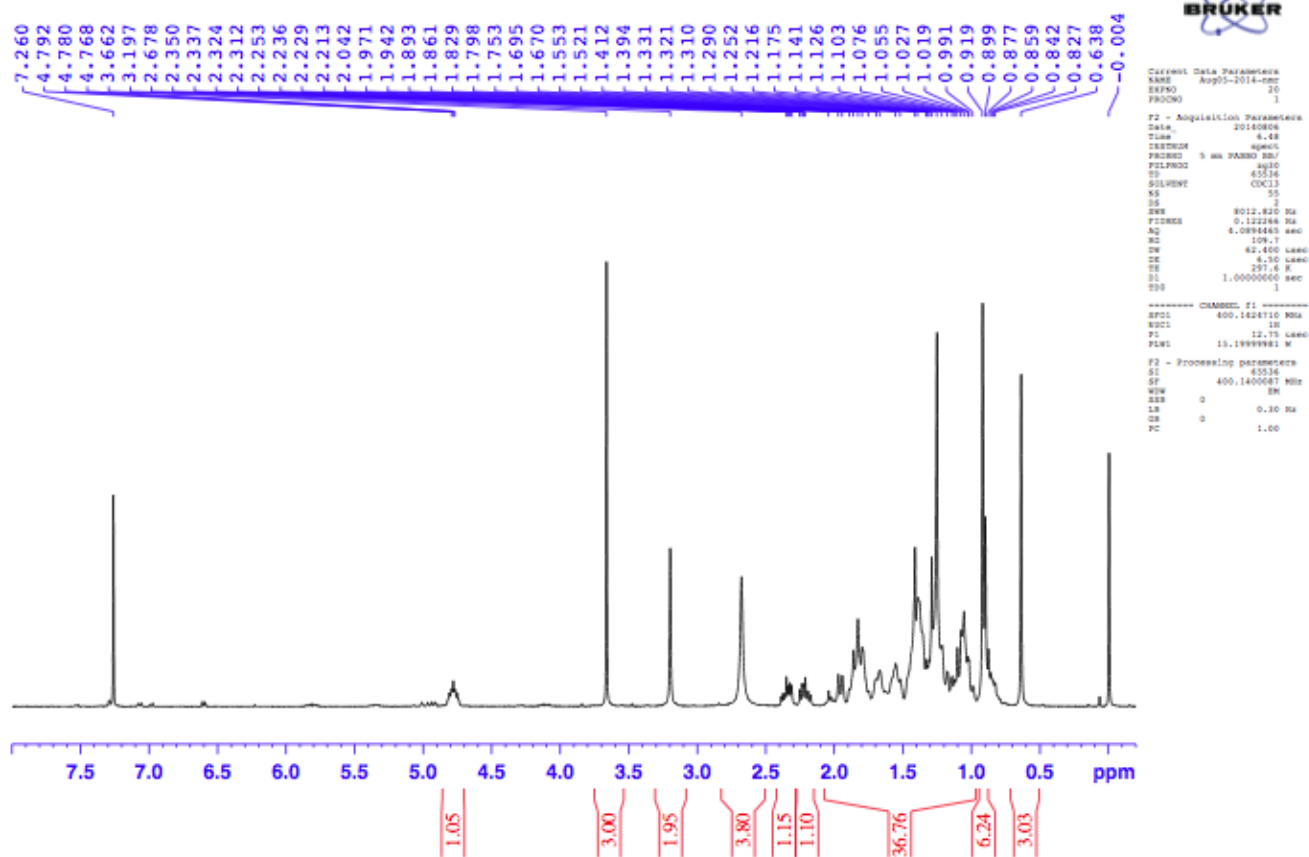


Fig. S1 a) Molecular structures of LCA-PIP₁ amphiphile having ester or amide linkage; **b-d)** Cytotoxicity of ester and amide derivatives of LCA-PIP₁ against three colon cancer cell lines **b)** HCT-116, **c)** DLD-1, and **d)** HCT-8.

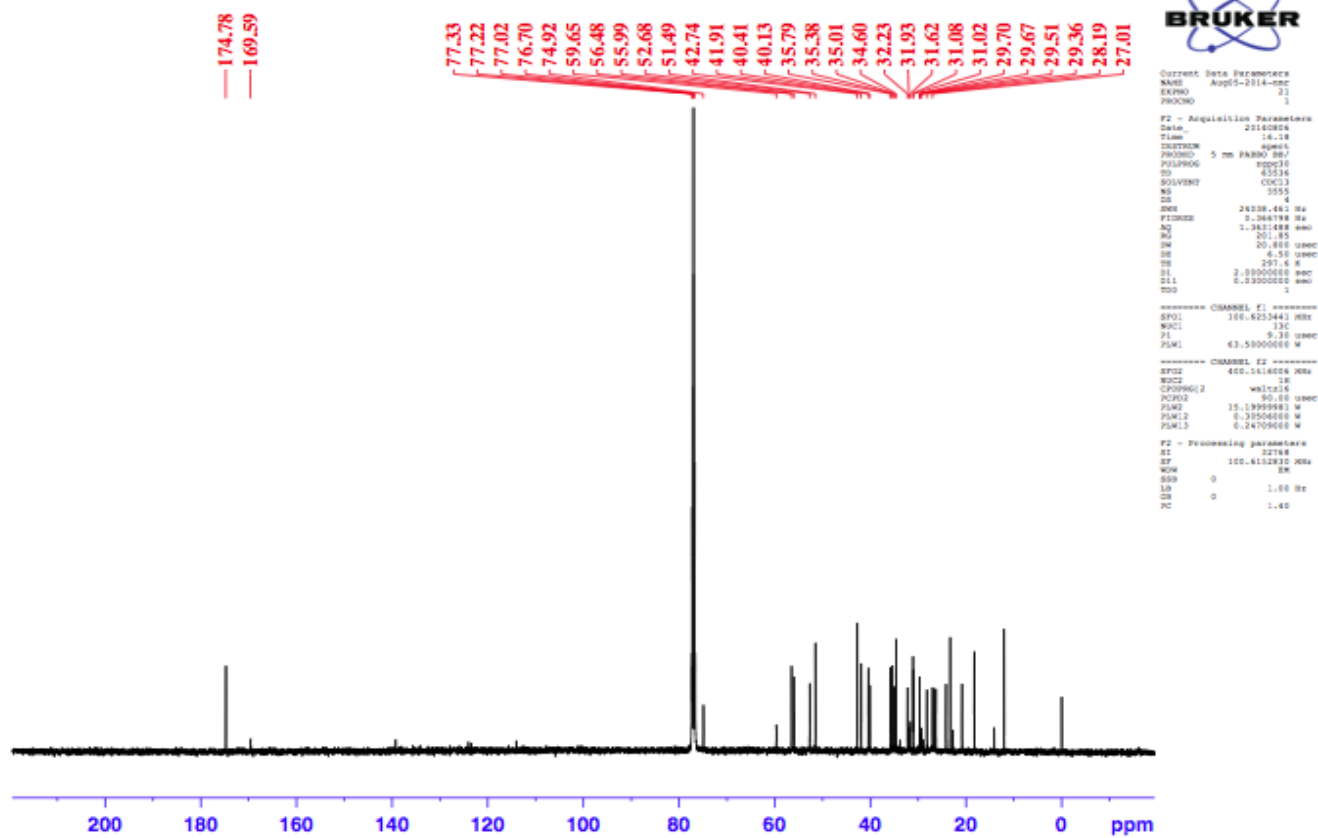
¹H-NMR Spectra, LCA-PPZ₁

Exp-221, LCA-Piperazine



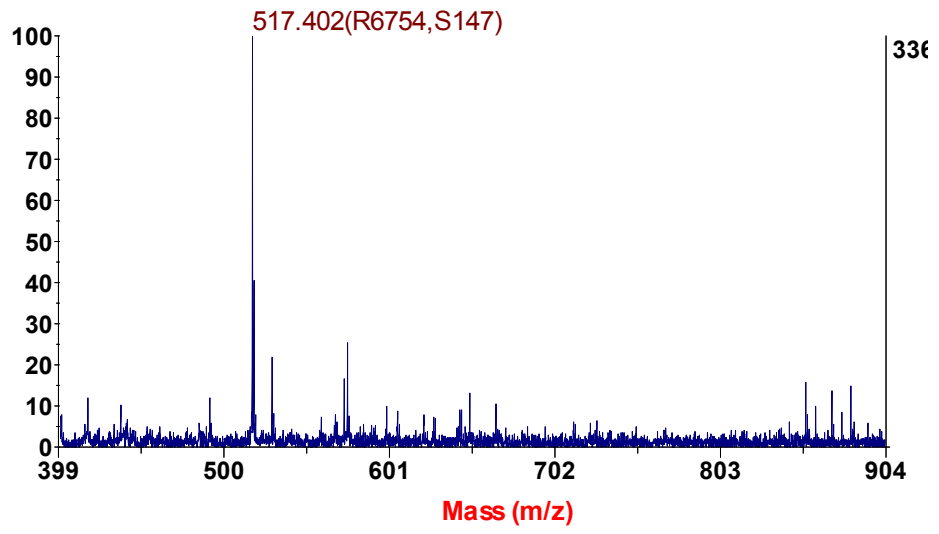
¹³C-NMR Spectra, LCA-PPZ₁

Exp-221, LCA-Piperazine



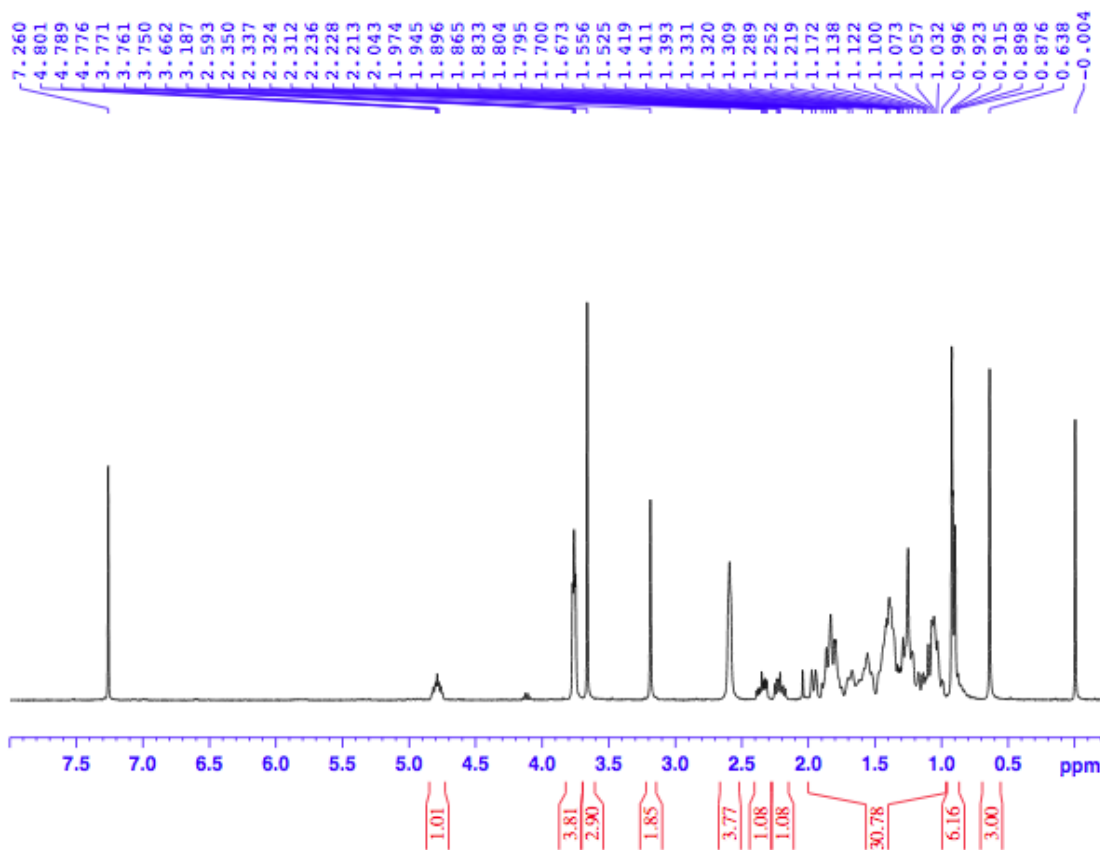
MALDI Mass Spectra, LCA-PPZ₁

Final - Shots 400 - 19082014; Label J2



¹H-NMR Spectra, LCA-MOR₁

Exp-218, LCA-OMe- Morpholine



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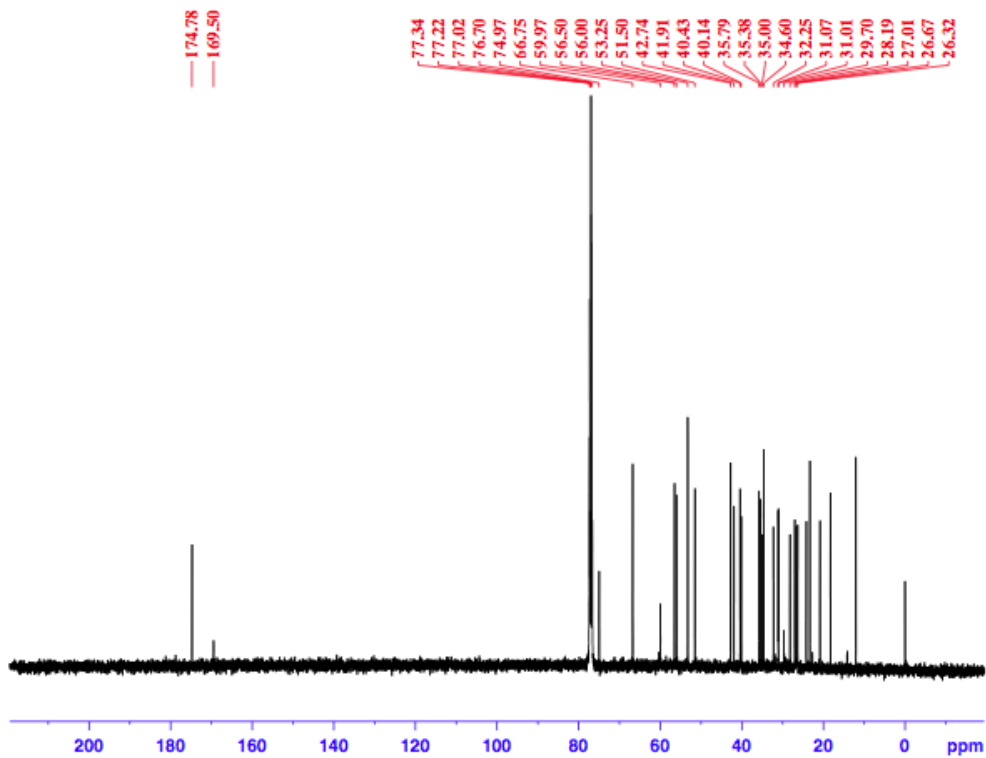
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 F2DRMS 0.122266 Hz
 AQ 4.028460 sec
 RG 124.78
 DW 62.400 usec
 DE 4.50 usec
 TE 299.7 K
 D1 1.0000000 sec
 TDO 1

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 VPC1 28
 P1 12.75 usec
 FWH1 15.1595981 Hz

F2 - Processing parameters
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 GB 0
 PC 1.00

¹³C-NMR Spectra, LCA-MOR₁

Exp-218, LCA-OMe- Morpholine



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EXPNO 151
PROCNO 1

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DS 4
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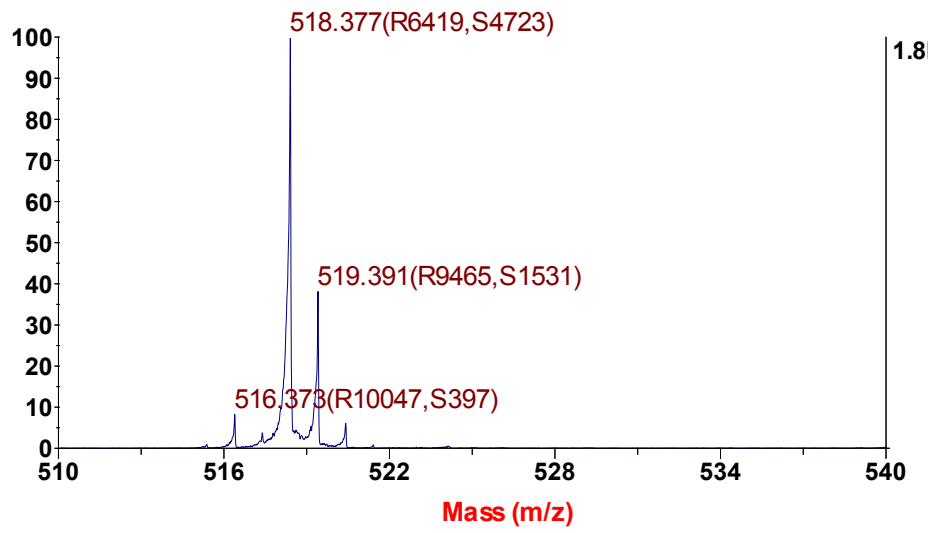
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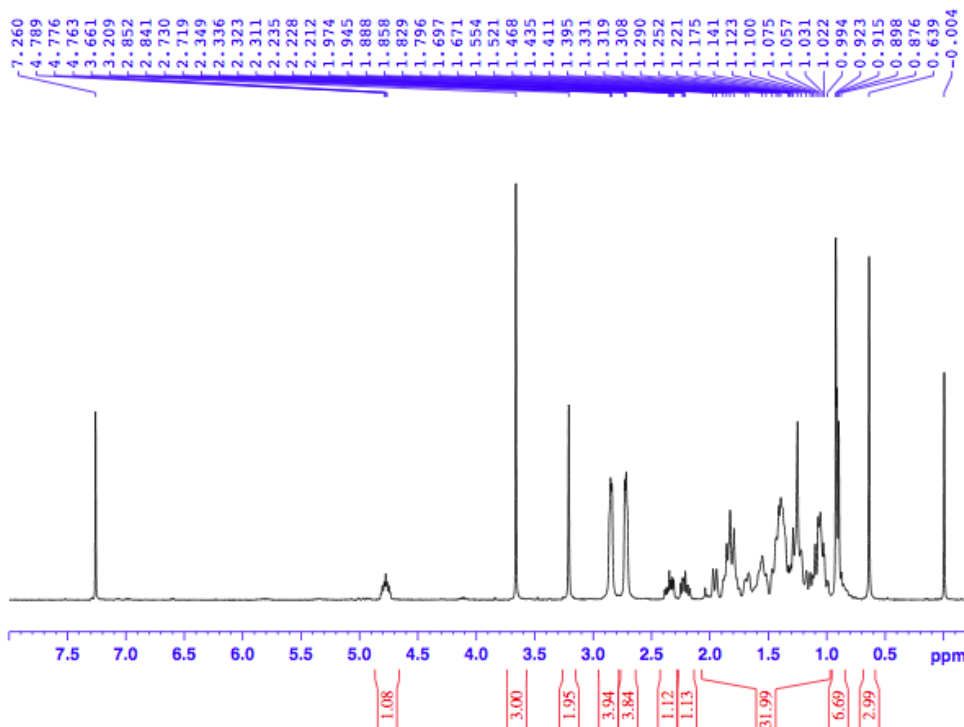
MALDI Mass Spectra, LCA-MOR₁

Final - Shots 400 - 19082014; Run #4; Label H1



¹H-NMR Spectra, LCA-TMOR₁

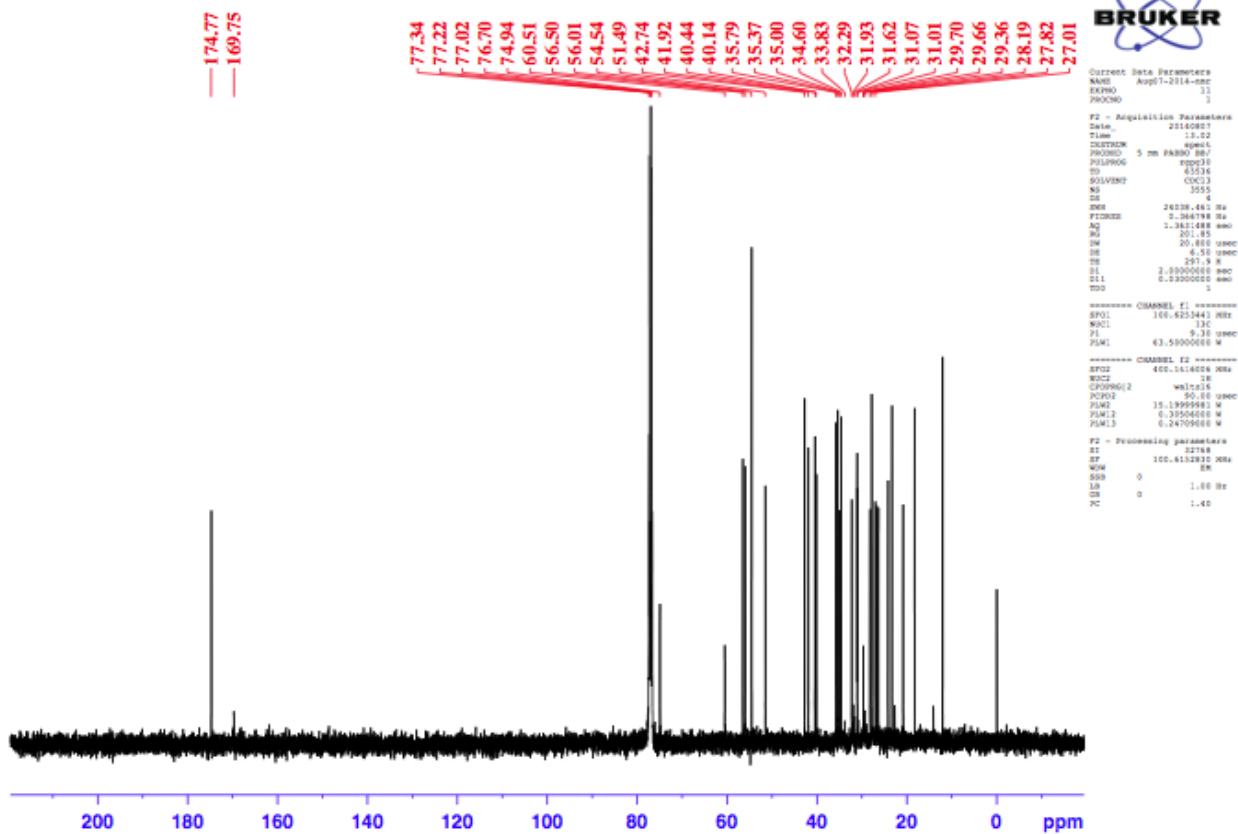
Exp-222, LCA-OMe-Thiomorpholine



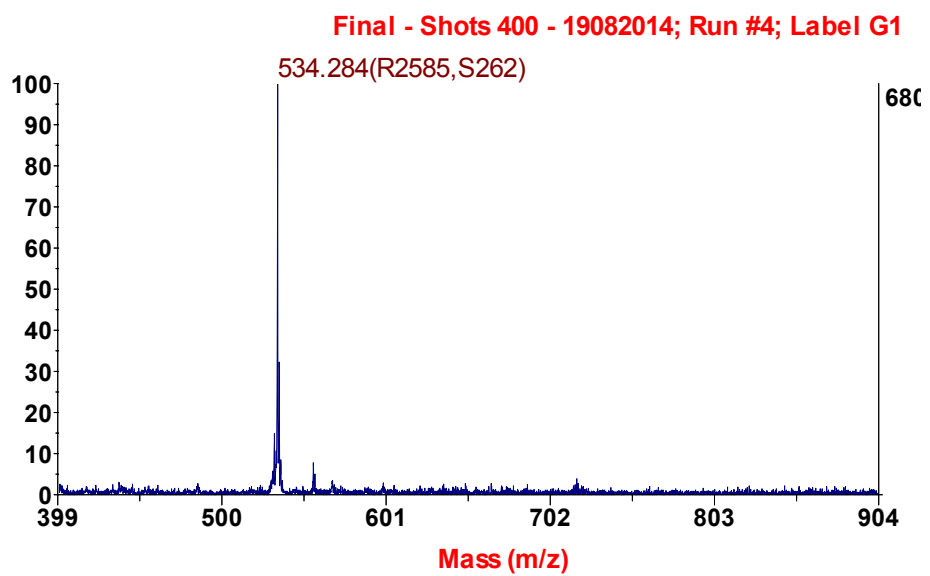
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 DE 4.50 umsec
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 D2 1
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¹³C-NMR Spectra, LCA-TMOR₁

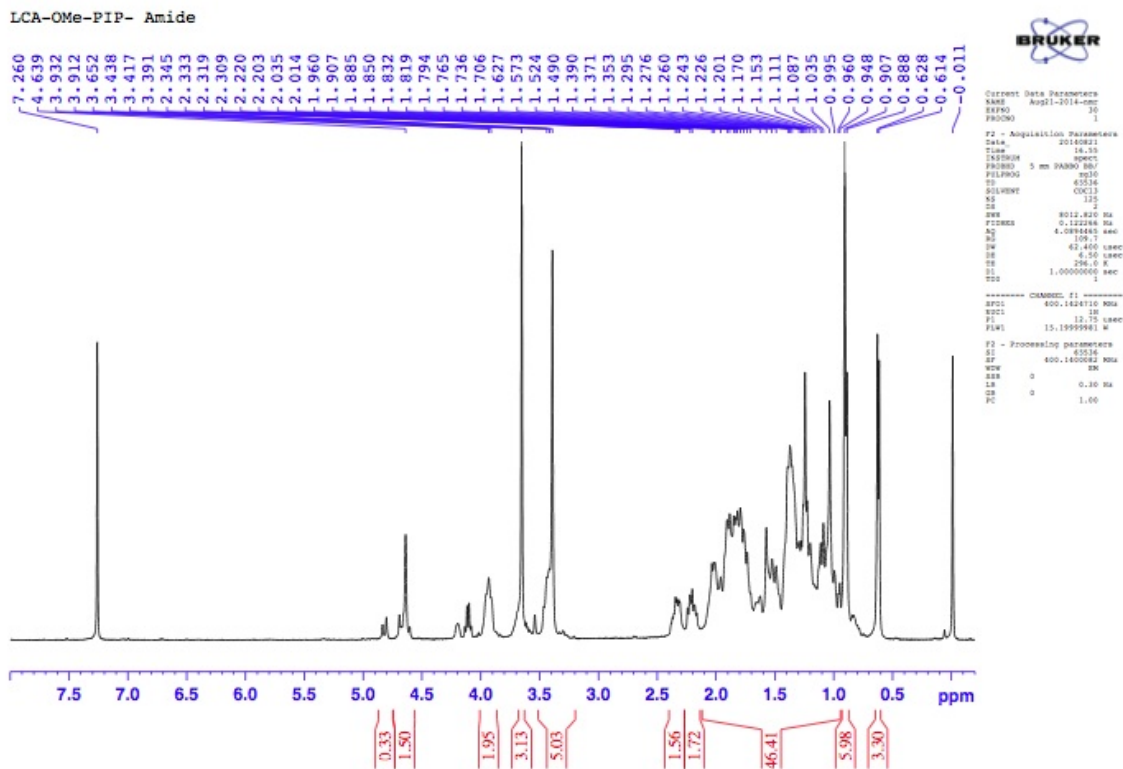
Exp-222, LCA-OMe-Thiomorpholine



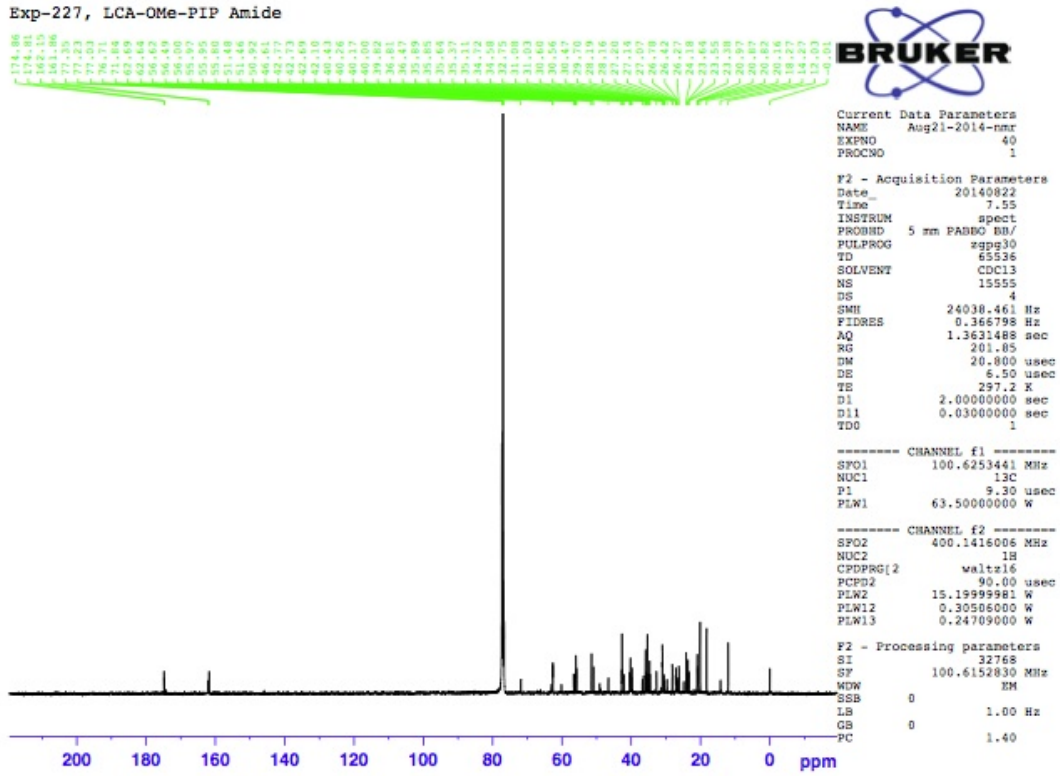
MALDI Mass Spectra, LCA-TMOR₁



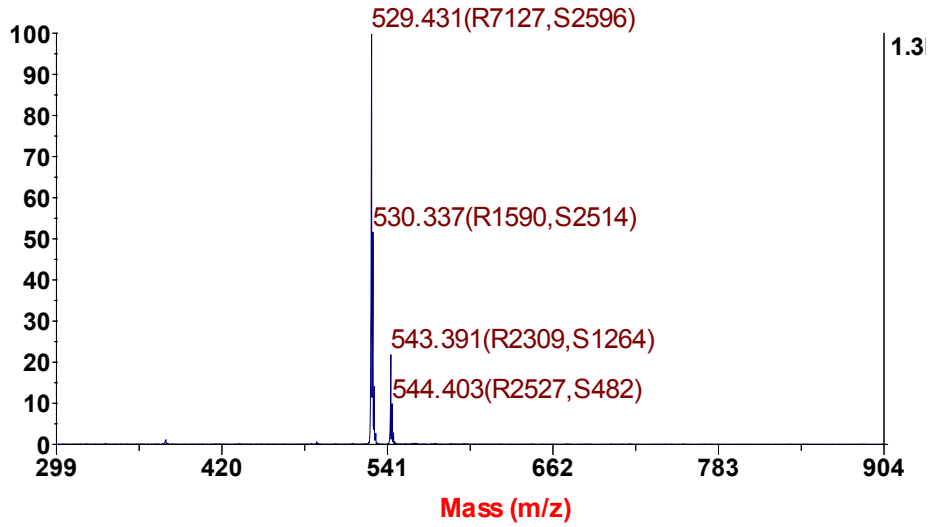
¹H-NMR Spectra, LCA-PIP₁ (Amide)



¹³C-NMR Spectra, LCA-PIP₁ (Amide)



Final - Shots 400 - 21082014; Run #1; Label L1

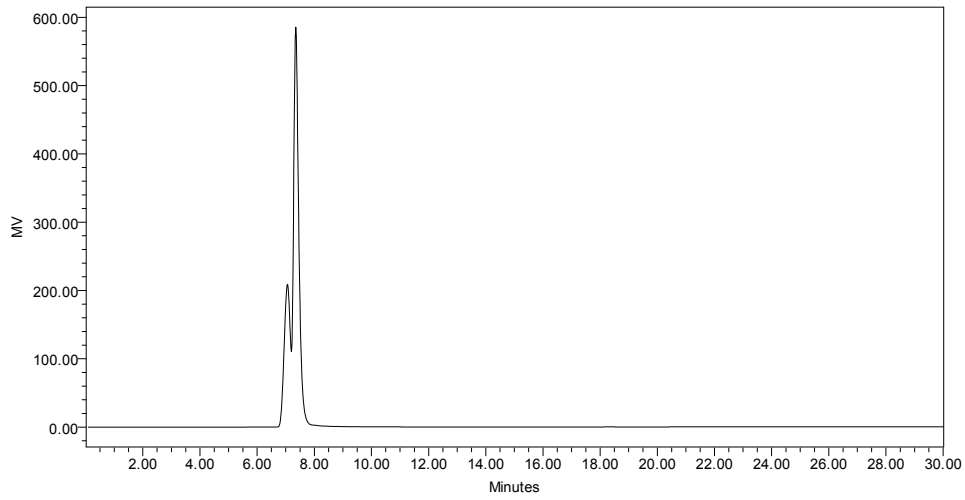


HPLC Profile, Mobile Phase



Default Individual Report

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Injection#:	1	Processing Method:	****
Injection Volume:	5.00µl	Channel Name:	****
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	****
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Date Processed:	****		

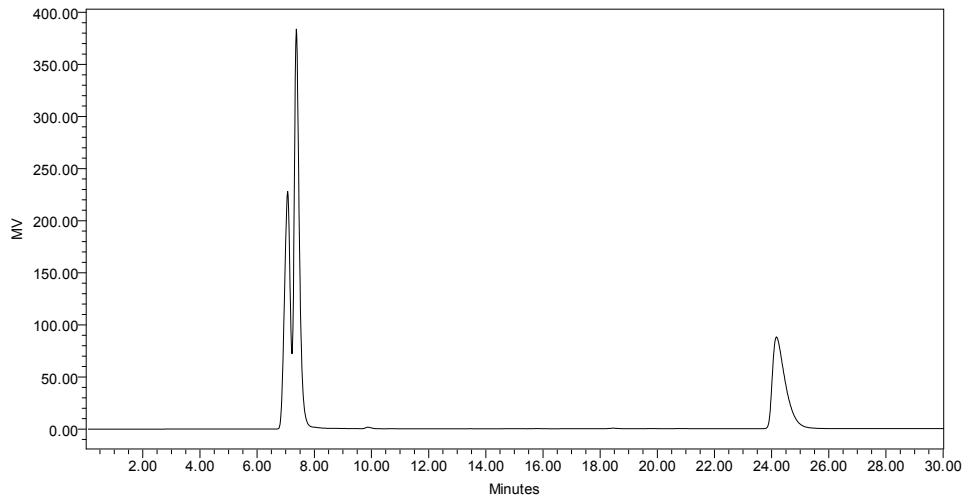


HPLC Profile, LCA-MOR₁



Default Individual Report

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Sample Type:	Unknown	Sample Set Name:	LCA-MOR
Vial:	1:B,3	Acq. Method Set:	5jsep2014
Injection#:	1	Processing Method:	****
Injection Volume:	5.00 µl	Channel Name:	****
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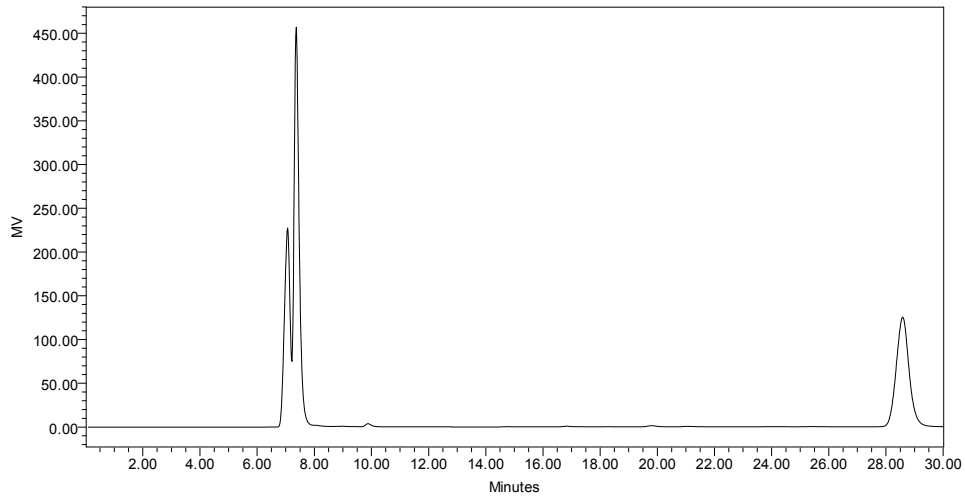


HPLC Profile, LCA-TMOR₁



Default Individual Report

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Sample Type:	Unknown	Sample Set Name:	LCA-TMOR
Vial:	1:B,4	Acq. Method Set:	5/sep/2014
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Injection Volume:	5.00 µl	Channel Name:	****
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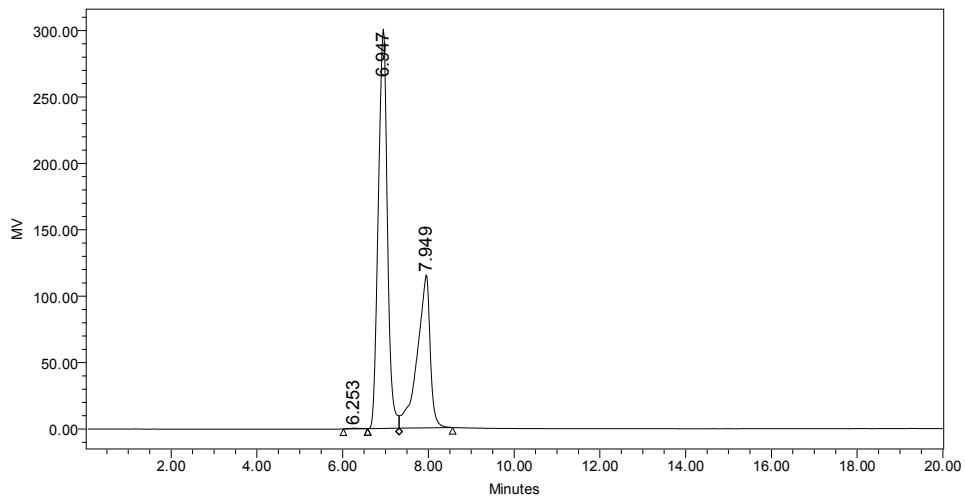


HPLC Profile, LCA-TMA₁



Default Individual Report

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Injection#:	1	Processing Method:	LyTMA
Injection Volume:	10.00 µl	Channel Name:	410j
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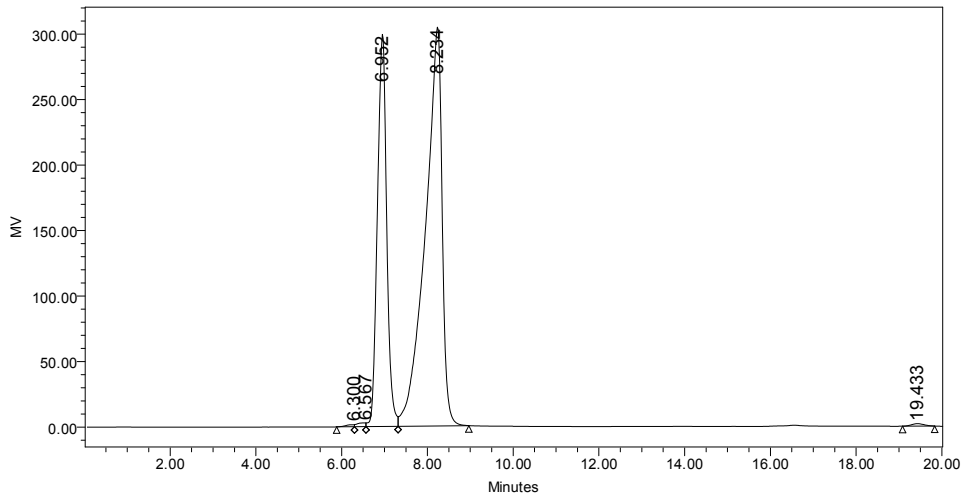


HPLC Profile, LCA-PYROL₁



Default Individual Report

Sample: LCA-PYROL ₁			
Sample Name:	L-Pyrolidine	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	L-Pyrolidine
Vial:	1:B,8	Acq. Method Set:	195% ACN/5 %Methanol 150420
Injection#:	1	Processing Method:	L-pyrolidine
Injection Volume:	10.00 µl	Channel Name:	410
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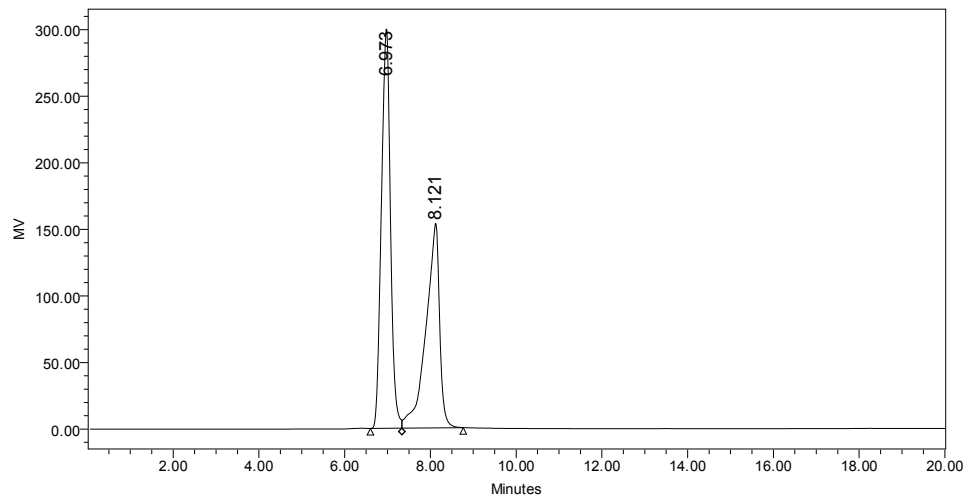


HPLC Profile, LCA-PIP₁



Default Individual Report

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Injection#:	1	Processing Method:	LyPiperidine
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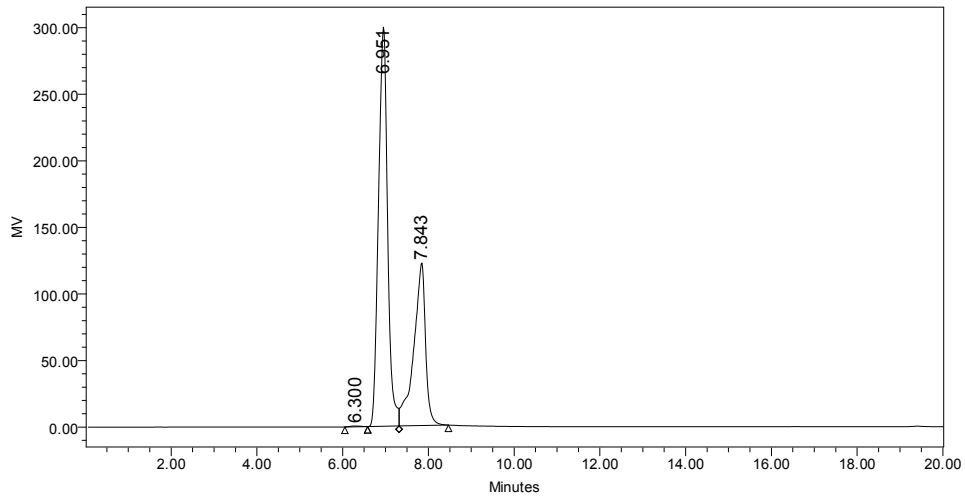


HPLC Profile, LCA-PYR₁



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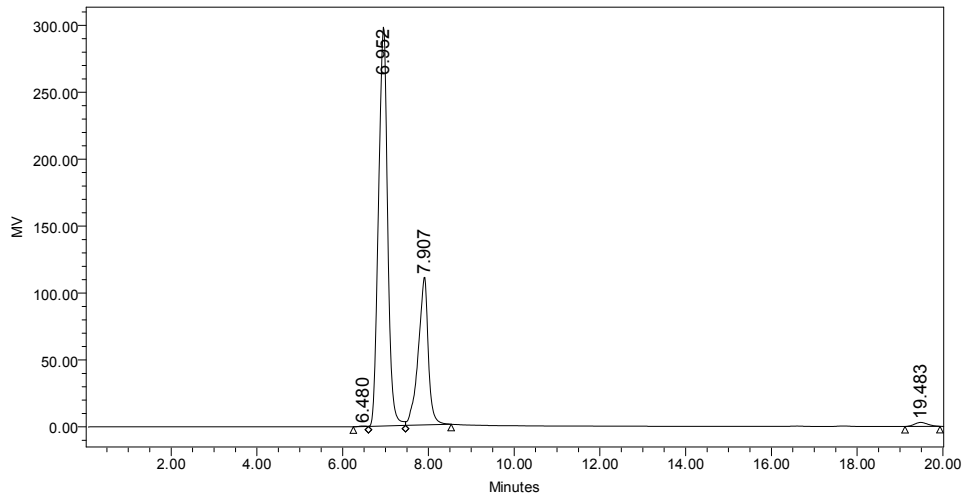


HPLC Profile, LCA-DMAP₁



Default Individual Report

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Injection#:	1	Processing Method:	L-DMAP
Injection Volume:	10.00 µl	Channel Name:	410j
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HPLC Profile, LCA-DABCO₁



Default Individual Report

Sample Entry			
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Sample Type:	Unknown	Sample Set Name:	L-DABCO
Vial:	1:B,4	Acq. Method Set:	195% ACN 5 % Methanol 150420
Injection#:	1	Processing Method:	L-DABCO
Injection Volume:	10.00 µl	Channel Name:	410j
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	
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