

A Concise Synthesis towards Antimalarial Quinazolinedione TCMDC-125133 and Its Anti-Proliferative Activity against MCF-7

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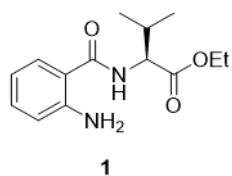
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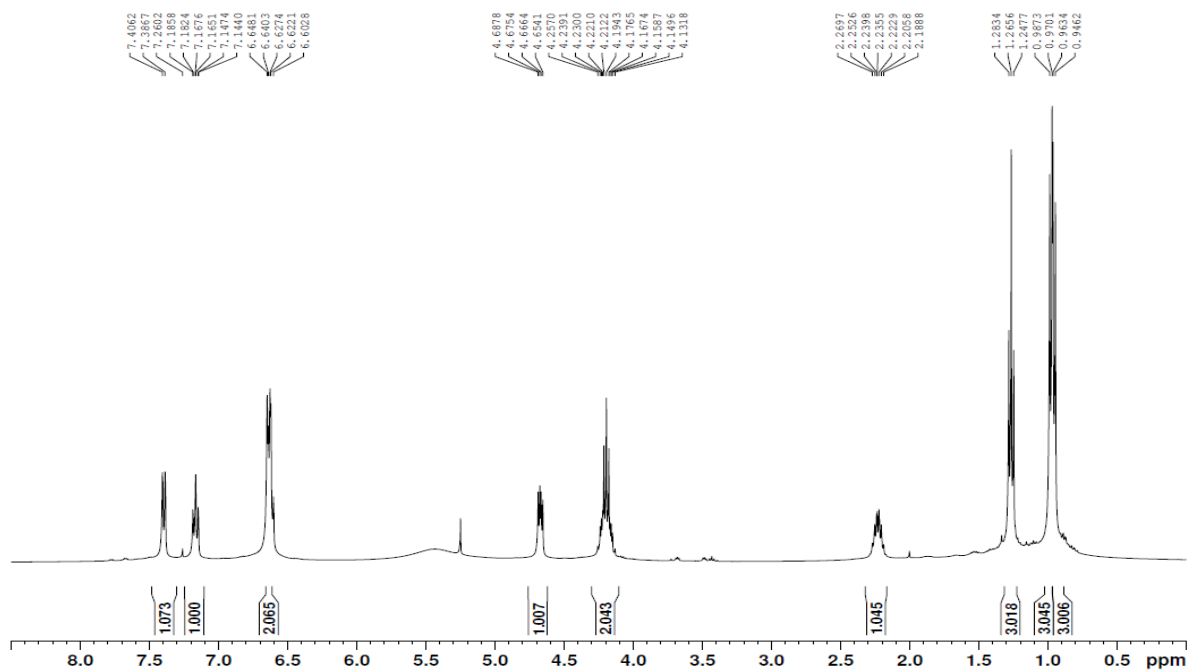
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Table of content

	page
¹ H NMR (400 MHz, CDCl ₃) and ¹³ C NMR (100 MHz, CDCl ₃) of compound 1	SI2
IR spectrum and mass spectrum of compound 1	SI3
¹ H NMR (400 MHz, MeOD-d ₄) and ¹³ C NMR (100 MHz, MeOD-d ₄) of compound 2	SI4
IR spectrum and mass spectrum of compound 2	SI5
¹ H NMR (400 MHz, DMSO-d ₆) and ¹³ C NMR (100 MHz, DMSO-d ₆) of compound 3	SI6
IR spectrum and mass spectrum of compound 3	SI7
¹ H NMR (500 MHz, CDCl ₃) and ¹³ C NMR (125 MHz, CDCl ₃) of compound 4	SI8
IR spectrum and mass spectrum of compound 4	SI9
Chiral HPLC traces of compound 1-4	SI10



(a) ^1H -NMR



(b) ^{13}C -NMR

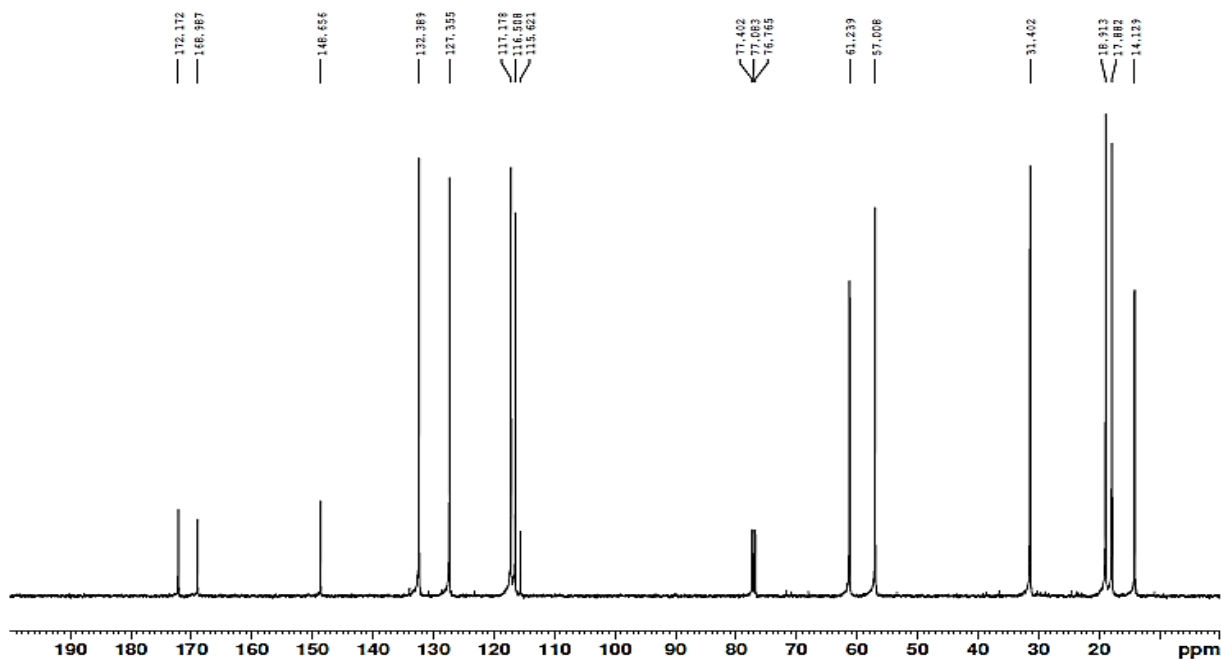


Figure S1 (1): Representative (a) ^1H -NMR (b) ^{13}C -NMR of *(-)-(Ethyl (2-aminobenzoyl)-L-valinate 1*

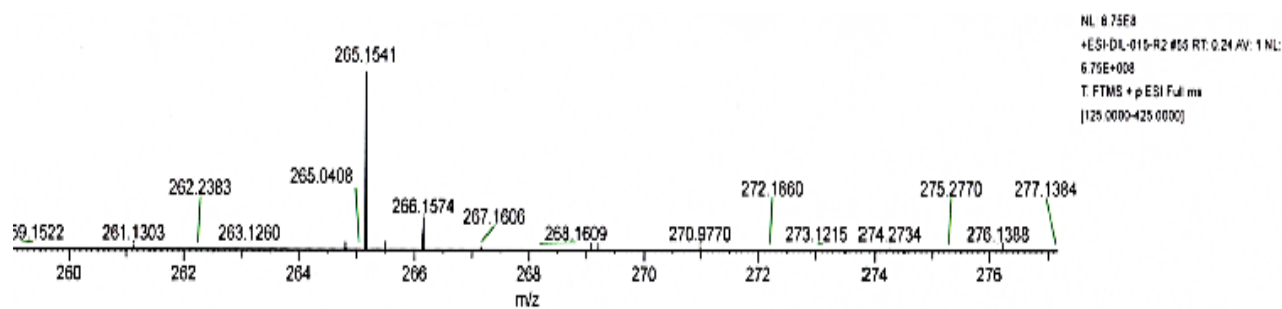
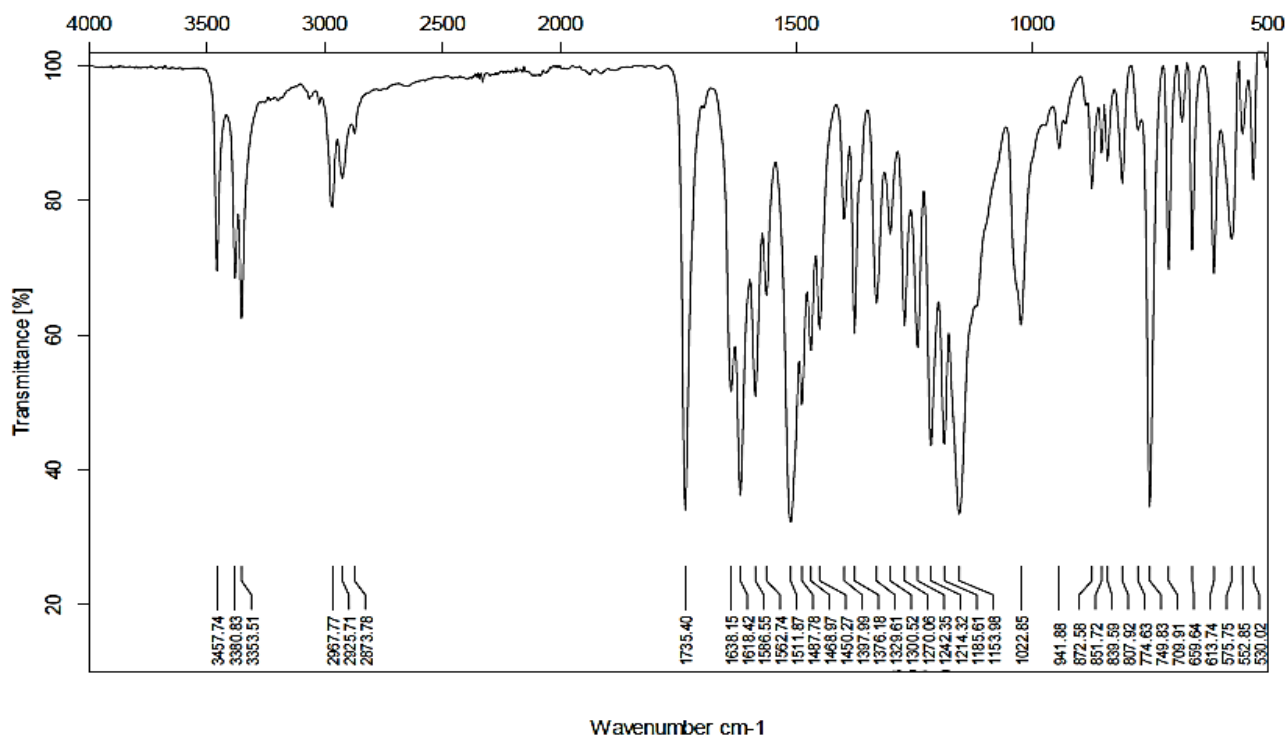
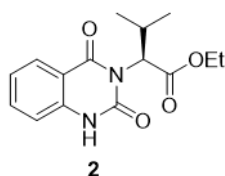
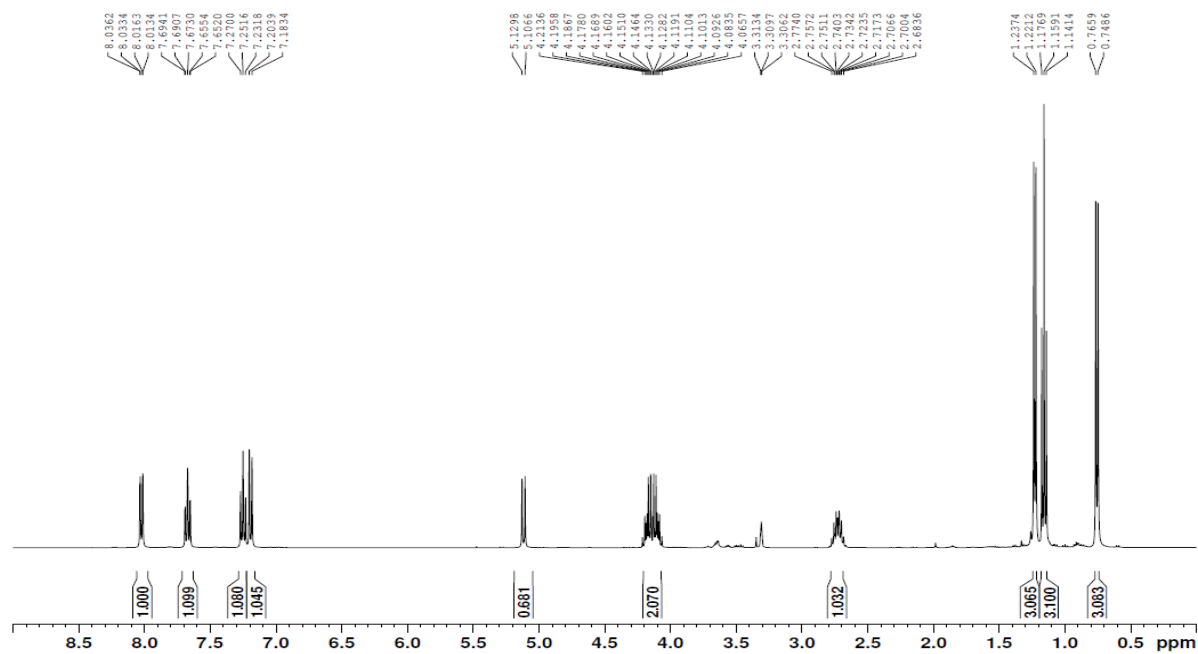


Figure S1 (2): Representative (c) IR spectrum (d) Mass spectrum of (–)-(Ethyl (2-aminobenzoyl)-L-valinate **1**



(a) ^1H -NMR



(b) ^{13}C -NMR

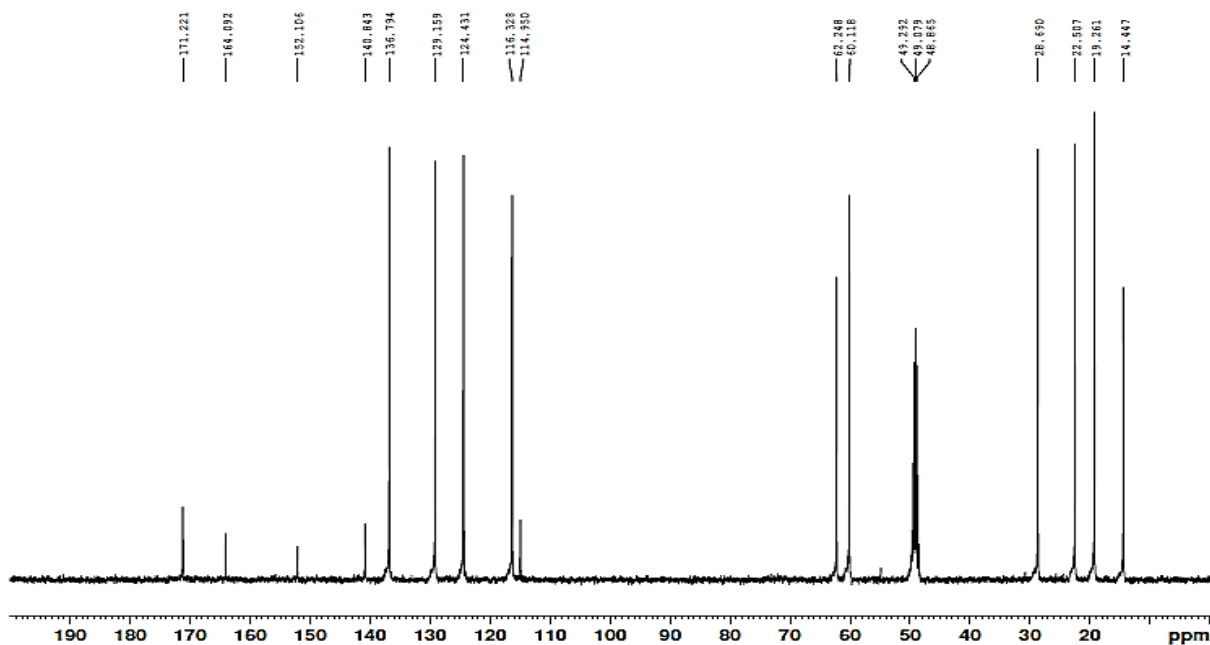
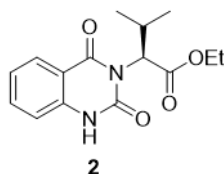
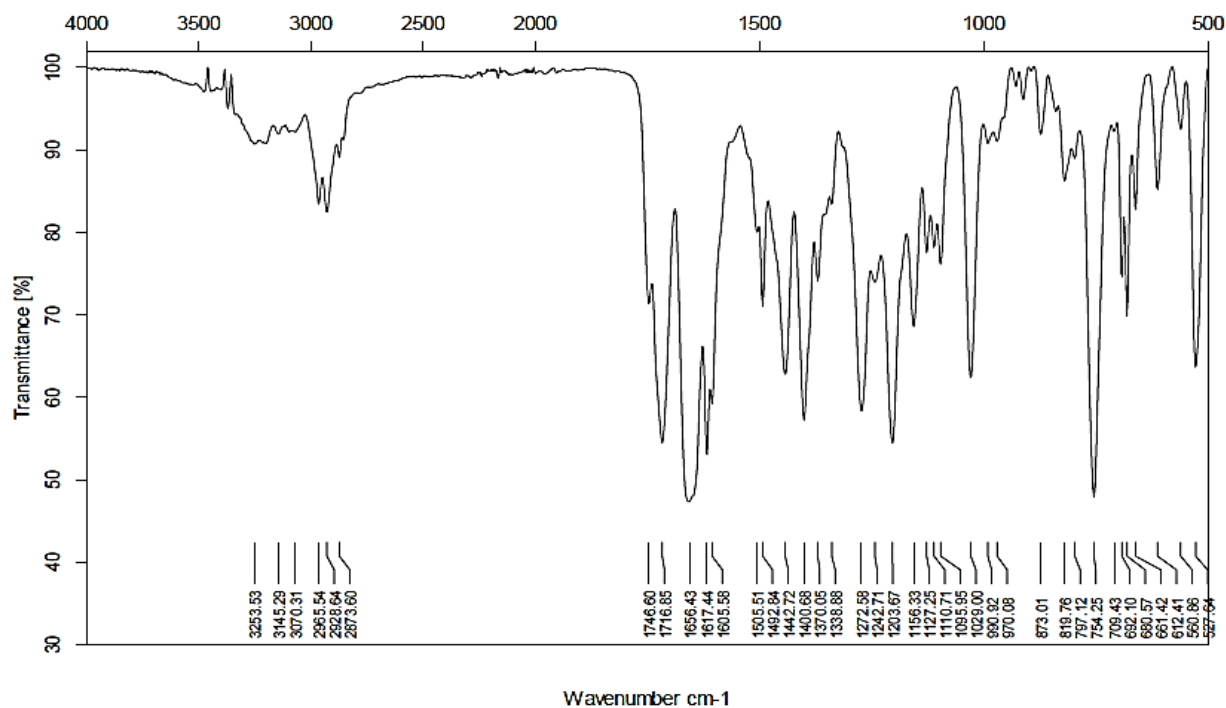


Figure S2 (1): Representative (a) ^1H -NMR (b) ^{13}C -NMR of (–)-Ethyl (S)-2-(2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-3-methylbutanoate **2**



(c) IR Spectrum



(d) Mass spectrum

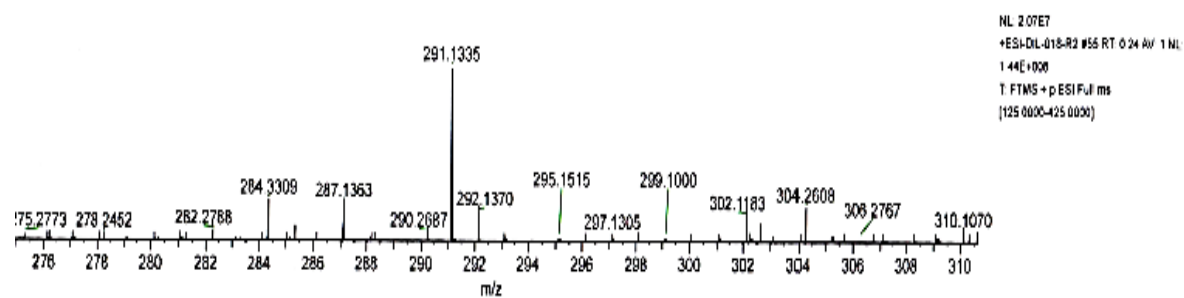
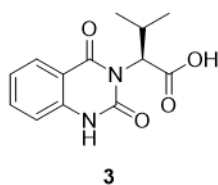
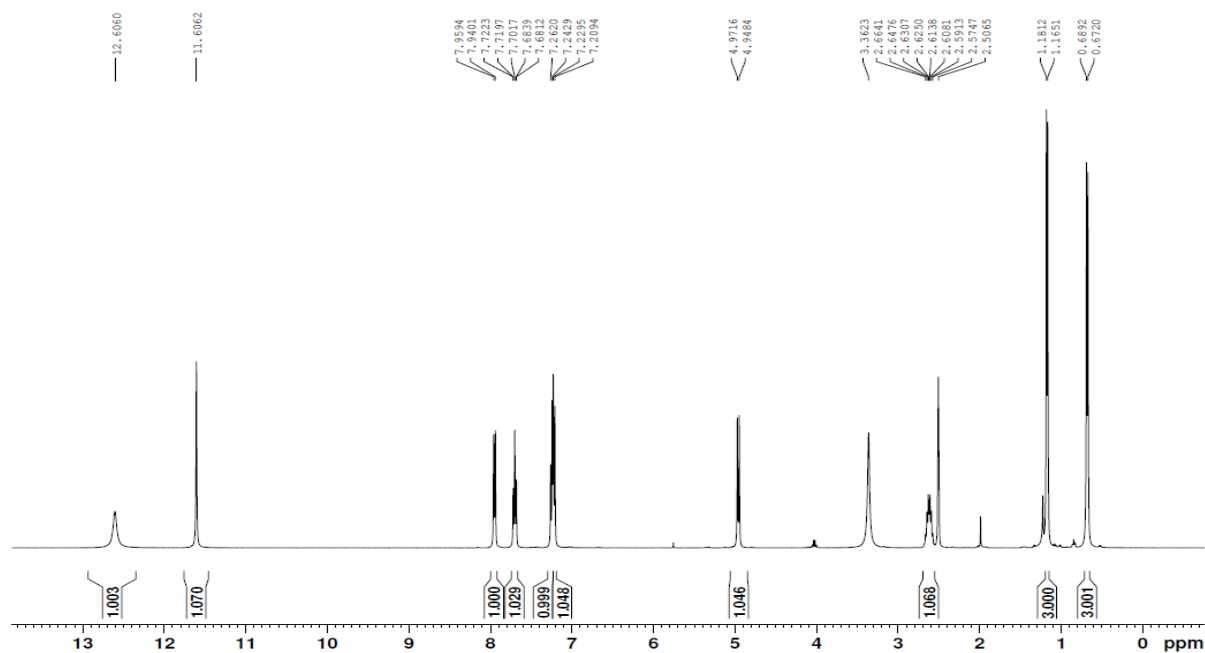


Figure S2 (2): Representative (c) IR spectrum (d) Mass spectrum of *(-)-Ethyl (S)-2-(2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-3-methylbutanoate 2*



(a) ^1H -NMR



(b) ^{13}C -NMR

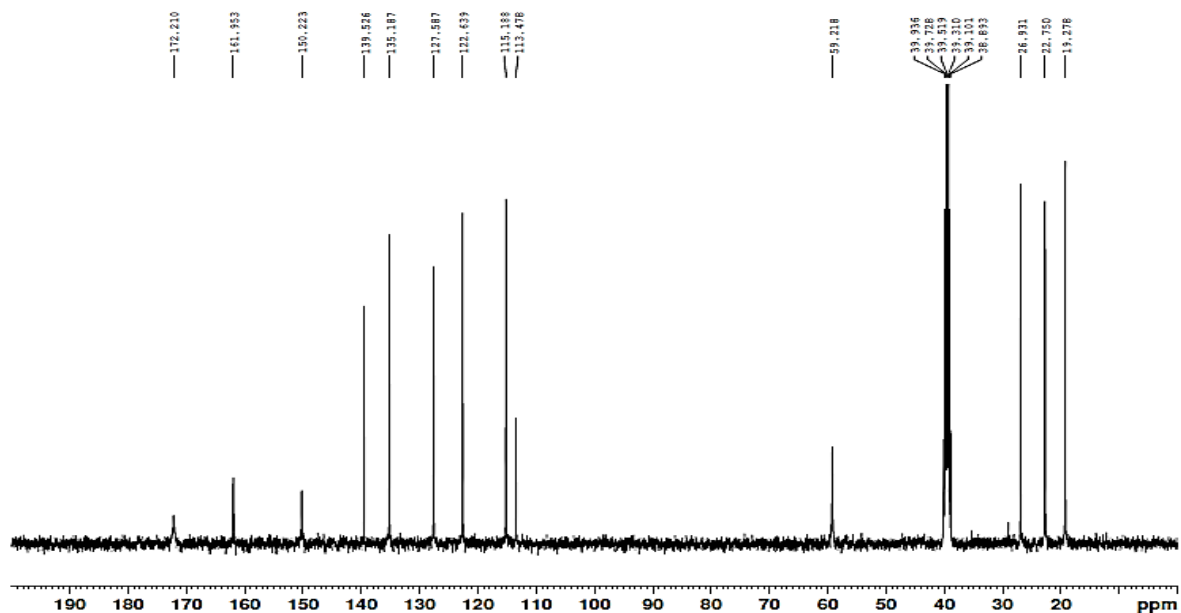
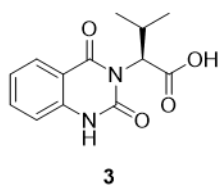
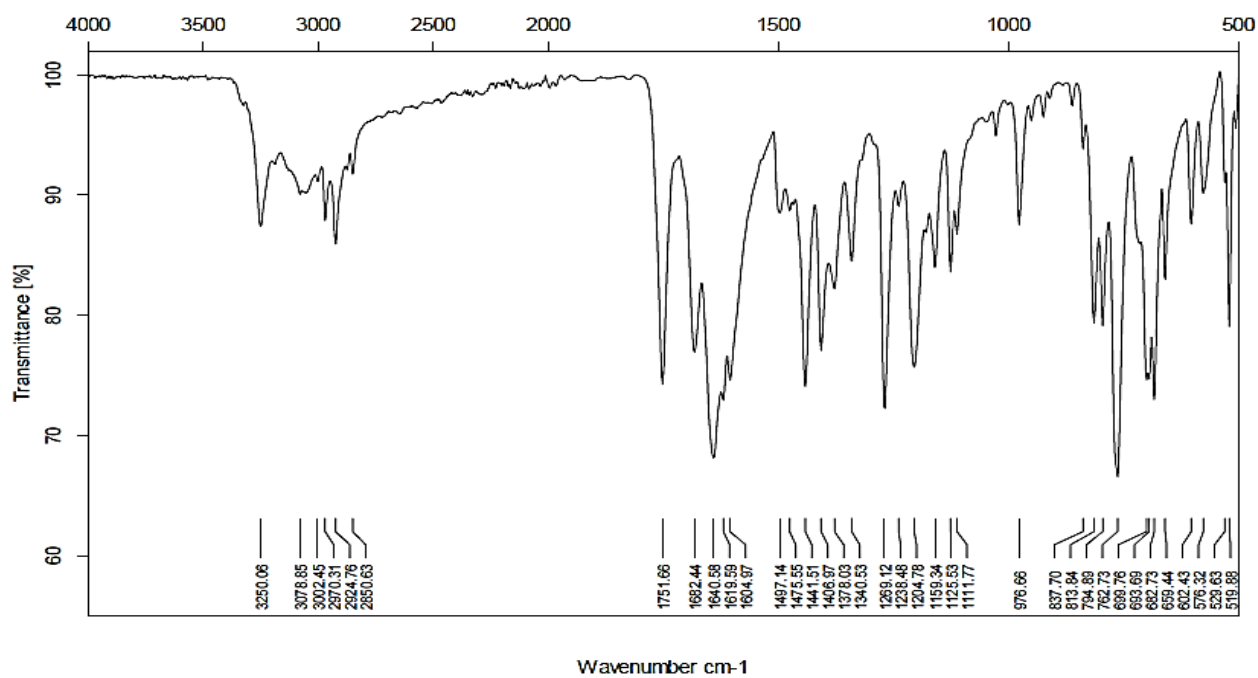


Figure S3 (1): Representative (a) ^1H -NMR (b) ^{13}C -NMR of *(-)-(S)*-2-(2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-3-methylbutanoic acid **3**



(c) IR Spectrum



(d) Mass spectrum

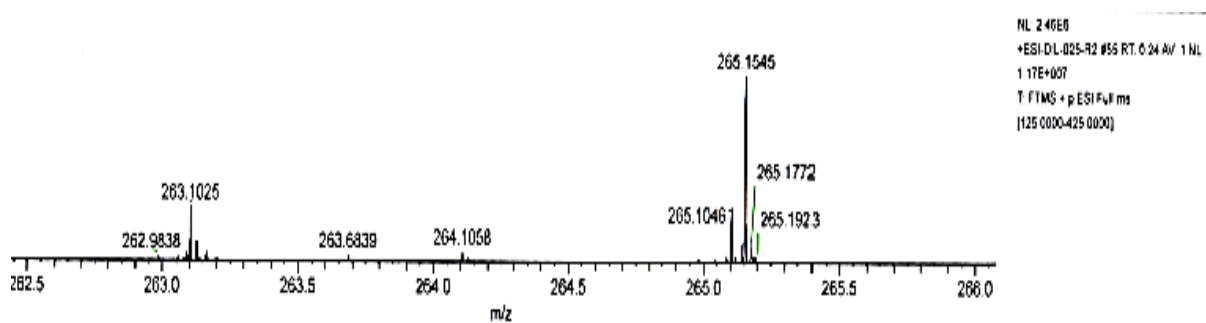
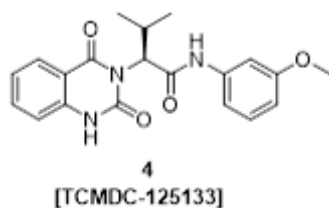
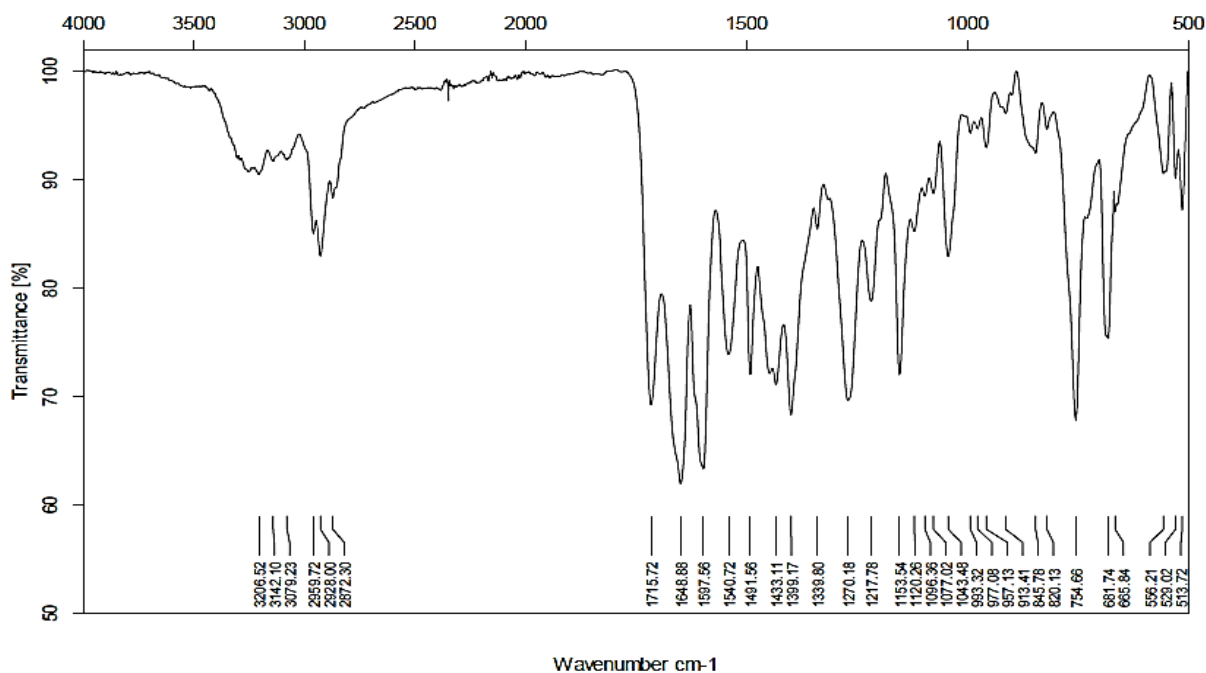


Figure S3 (2): Representative (c) IR spectrum (b) Mass spectrum of *(-)-(S)-2-(2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-3-methylbutanoic acid 3*



(c) IR Spectrum



(d) Mass spectrum

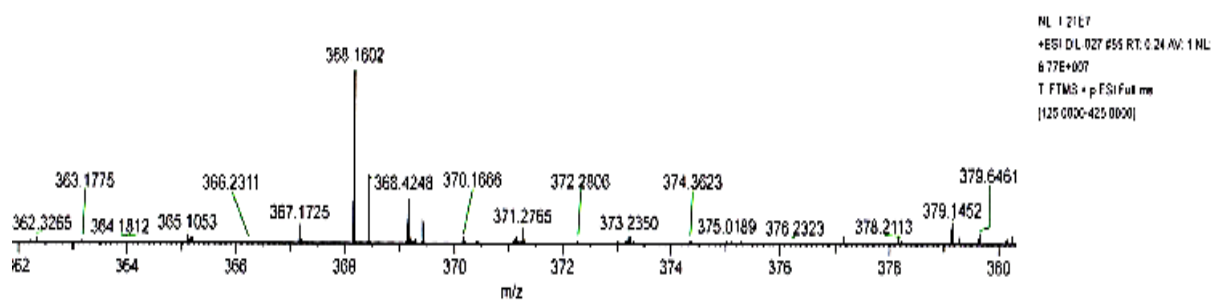


Figure S4 (2): Representative (c) IR spectrum (b) Mass spectrum of *(-)-(S)-2-(2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-N-(3-methoxyphenyl)-3-methylbutanamide 4* [TCMDC-125133]

Chiral HPLC analysis

Instrument: Waters Alliance e2695 HPLC system with Waters 2489 UV/Vis Detector

Column: CHIRALPAK® AD-H COLUMNS (Dimensions(Ø) 4.6 mm × 250 mm)

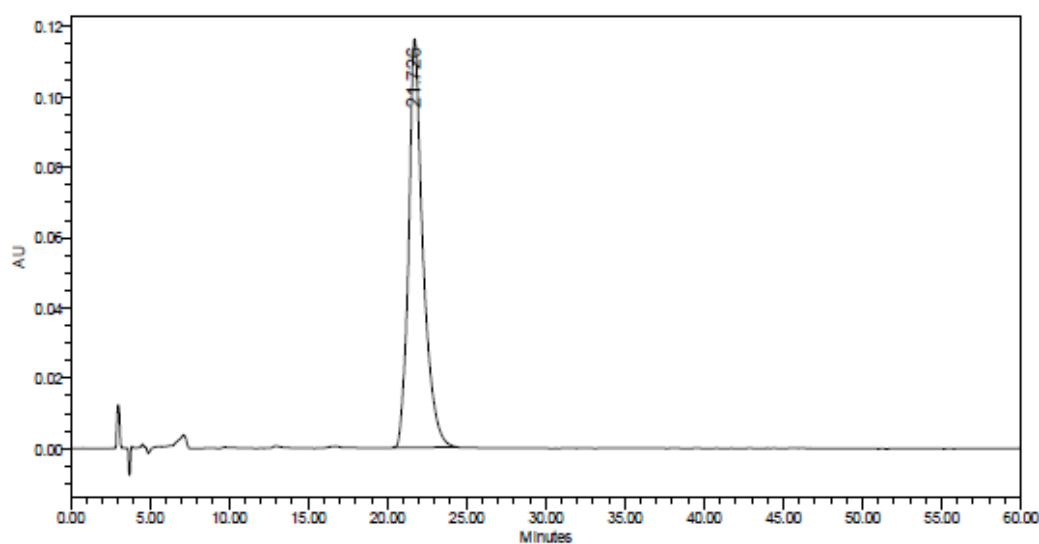
Compound 1



Default Individual Report

SAMPLE INFORMATION

Sample Name:	015-500ppm	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	
Vial:	4	Acq. Method Set:	Valine product
Injection #:	1	Processing Method	4
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired:	3/23/2022 11:57:01 AM ICT		
Date Processed:	3/23/2022 4:03:14 PM ICT		



	RT	Area	% Area	Height
1	21.726	7314232	100.00	116247

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Report Method IC1097
Page: 1 of 1

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Date Printed: 3/23/2022
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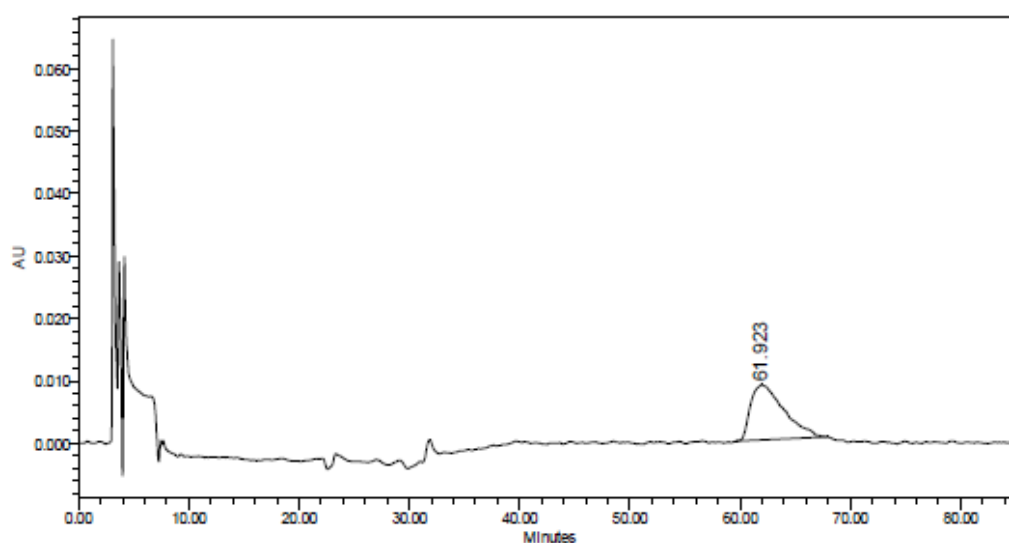
Compound 2



Default Individual Report

SAMPLE INFORMATION

Sample Name:	018-1000ppm-5_2%(flow1)-27m	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	
Vial:	11	Acq. Method Set:	Valine product_5_2%IPA_27m
Injection #:	1	Processing Method	21
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	120.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired:	4/8/2022 12:25:25 PM ICT		
Date Processed:	4/8/2022 3:37:24 PM ICT		



	RT	Area	% Area	Height
1	61.923	1848199	100.00	8855

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4/8/2022
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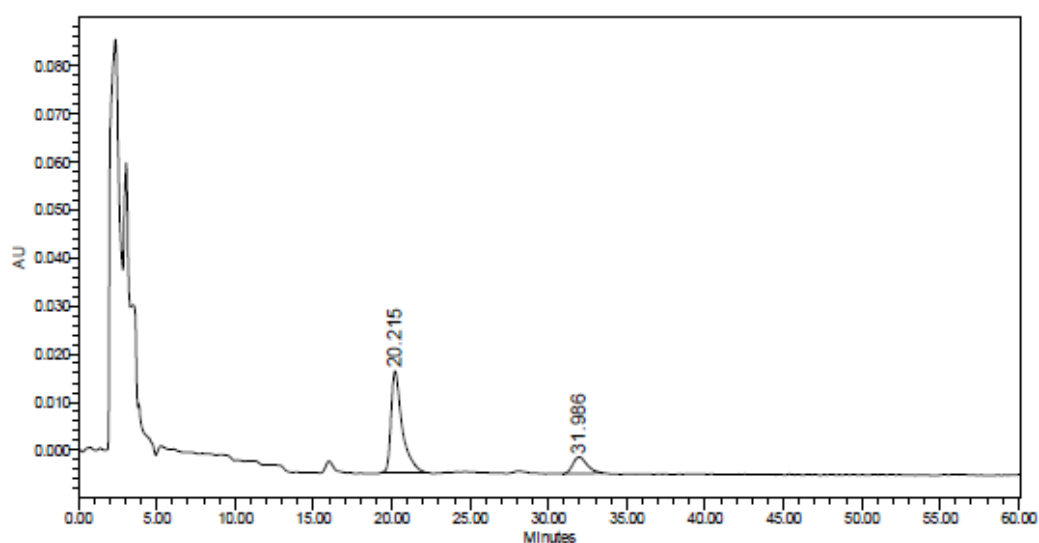
Compound 3

Empower³
SOFTWARE

Default Individual Report

SAMPLE INFORMATION

Sample Name:	025-60c-3h-500ppm	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	
Vial:	12	Acq. Method Set:	Valine product
Injection #:	1	Processing Method	22
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	120.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
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Date Processed:	4/8/2022 4:38:15 PM ICT		



	RT	Area	% Area	Height
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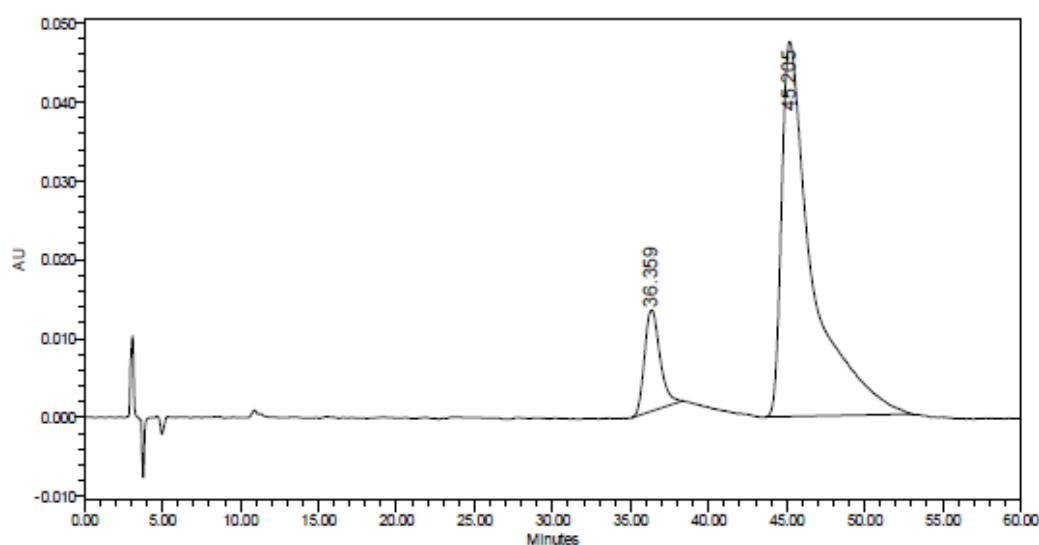
Compound 4



Default Individual Report

SAMPLE INFORMATION

Sample Name:	027-R1-SPE-500ppm	Acquired By:	System
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Vial:	7	Acq. Method Set:	Valine product
Injection #:	1	Processing Method	19
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
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Date Processed:	4/8/2022 12:43:36 PM ICT		



	RT	Area	% Area	Height
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Page: 1 of 1

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