#### Synthesis of Enantiomerically Pure 3-Substituted-Piperazine-2-Acetic Acid Esters as Intermediates for Library Production

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#### Supporting Information

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## Crystallographic data of 7d trans



Fig 1: ORTEP diagram for 7d trans (with ellipsoid contour 50%)

Empirical formula	C17 H25 N3 O6 S
Formula weight	399.46
Temperature	123(2) K
Wavelength, λ(Å)	1.54178 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 7.4329(2) A alpha = 90 deg.
	b = 14.0813(4) A beta = 90 deg.

	c = 18.3821(5) A gamma = 90 deg.
Volume	1923.96(9) A^3
Z, Calculated density	4, 1.379 Mg/m^3
Absorption coefficient	1.842 mm^-1
F(000)	848
Crystal color and shape	Colorless column
Crystal size	0.40 x 0.15 x 0.15 mm
Theta range for data collection	3.95 to 66.65 deg.
Limiting indices	-8<=h<=8, 0<=k<=16, 0<=l<=21
Reflections collected / unique	12918 / 3250 [R(int) = 0.0264]
Completeness to theta = 66.62	98.4 %
Absorption correction	Empirical
Max. and min. transmission	0.7528 and 0.5298
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3167 / 0 / 251
Goodness-of-fit on F^2	1.051
Final R indices [I>4sigma(I)]	R1 = 0.0207, wR2 = 0.0545
R indices (all data)	R1 = 0.0211, wR2 = 0.0552
Absolute structure parameter	0.053(11)
Extinction coefficient	0.0035(2)
Largest diff. peak and hole	0.194 and -0.202 e.A^-3

# Crystallographic data of 9g trans



Fig 2: ORTEP diagram for 9g trans (with ellipsoid contour 60%)

Empirical formula	C26 H33 N3 O8 S
Formula weight	547.61
Temperature	123(2) K
Wavelength, λ(Å)	1.54178 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.6172(2) A alpha = 90 deg.

	b = 11.8985(4) A beta = 90 deg.
	c = 27.2367(8) A gamma = 90 deg.
Volume	2792.63(14) A^3
Z, Calculated density	4, 1.302 Mg/m^3
Absorption coefficient	1.472 mm^-1
F(000)	1160
Crystal color and shape	Colorless thin plate
Crystal size	0.30 x 0.25 x 0.10 mm
Theta range for data collection	3.25 to 66.70 deg.
Limiting indices	-10<=h<=10, 0<=k<=13, 0<=l<=32
Reflections collected / unique	19320 / 4784 [R(int) = 0.0217]
Completeness to theta = 66.62	97%
Absorption correction	Empirical
Max. and min. transmission	0.7528 and 0.5816
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4729 / 0 / 348
Goodness-of-fit on F^2	1.055
Final R indices [I>4sigma(I)]	R1 = 0.0208, wR2 = 0.0561
R indices (all data)	R1 = 0.0210, wR2 = 0.0562
Absolute structure parameter	0.001(9)
Extinction coefficient	0.00128(9)
Largest diff. peak and hole	0.206 and -0.219 e.A^-3

## Crystallographic data of 10



Fig 3: ORTEP diagram for 10 (with ellipsoid contour 50%)

Empirical formula	C21 H26 N3 O6 S	+, Cl -		
Formula weight	483.96			
Temperature	123(2) K 1.54178 A			
Wavelength, λ(Å)				
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)			
Unit cell dimensions	a = 5.9955(1) A	alpha = 90 deg.		
	b = 13.9616(2) A	beta = 90 deg.		
	c = 27.0117(5) A	gamma = 90 deg.		

Volume	2261.06(6) A^3
Z, Calculated density	4, 1.422 Mg/m^3
Absorption coefficient	2.735 mm^-1
F(000)	1016
Crystal color and shape	Colorless flat column
Crystal size	0.35 x 0.10 x 0.06 mm
Theta range for data collection	3.27 to 66.62 deg.
Limiting indices	-6<=h<=6, 0<=k<=16, 0<=l<=32
Reflections collected / unique	15640 / 3832 [R(int) = 0.0223]
Completeness to theta = 66.62	96.7 %
Absorption correction	Empirical
Max. and min. transmission	0.7528 and 0.4961
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3786 / 1 / 297
Goodness-of-fit on F^2	1.054
Final R indices [I>4sigma(I)]	R1 = 0.0188, wR2 = 0.0509
R indices (all data)	R1 = 0.0189, wR2 = 0.0512
Absolute structure parameter	-0.003(8)
Extinction coefficient	0.00178(12)
Largest diff. peak and hole	0.199 and -0.182 e.A^-3

# <sup>13</sup>C chemical shifts identify the *cis* and *trans* diastereomers in each <u>set of products</u>

To determine which of the products corresponds to the *cis* or *trans* diastereomer, complete <sup>1</sup>H and <sup>13</sup>C chemical shift assignments were made using 1D <sup>1</sup>H, 1D <sup>13</sup>C spectra and 2D <sup>1</sup>H, <sup>13</sup>C HSQC and HMBC spectra. Chemical shifts were referenced to TMS, and select <sup>13</sup>C shifts are reported in **Table S1**; note that the shifts for the ethyl group carbons ( $E_1 = -OCH_2$ -,  $E_2 = -CH_3$ ) show little difference between diastereomers or across the family of compounds.

Summing the  $C_5$  and  $C_6$  shifts for the two Ser-derived mono-protected products reveals a ( $C_5$  +  $C_6$ ) chemical shift difference of about 7.35 ppm between the two diastereomers. Because this difference roughly matches the 6.3 ppm difference by which the *trans* compound shifts would be expected to be upfield of the *cis* compound shifts due to the gamma-gauche interaction, the species with the more upfield shift total is assigned as the *trans* diastereomer. A similar analysis is given for the Val-derived compound.

For each of the three sets of compounds analyzed as di-protected products, one diastereomer gives two sets of NMR resonances; chemical shift analysis and 2D NOESY data indicate that these correspond to rotamers of the Boc protecting group. Using the chemical shifts of the more populated rotamer, analysis as above in each case identifies the samples that show evidence of rotamers as the *trans* species (Table S1). The average  $(C_5 + C_6)$  chemical shift difference for these species, 9.36 ppm, is ~2 ppm greater than for the mono-substituted piperazines (average: 7.36). The direction of the difference leaves the analysis unaffected (note also that none of the minor rotamers show chemical shift differences with respect to the *cis* species of less than 7.37 ppm). This difference arises primarily from the *trans* states shifts: the  $(C_5 + C_6)$  totals for the *cis* species are all within 1.6 ppm of one another, whereas the  $(C_5 + C_6)$  totals for the di-protected *trans* species. We infer that the Boc protecting group rotamers can modestly perturb the piperazine ring shifts at  $C_5/C_6$  upfield for the cis species, but more significantly perturb them for the *trans* species. The additional upfield shifts reflect additional gauche interactions, suggesting that steric crowding of substituents is perturbing conformation and hence chemical shift.

Table S1. <sup>13</sup> C chemical shifts for diastereomer products											
	Ser		Val		Ala		Leu		Pł	Phe	
	cis	trans	cis	trans	cis	trans <sup>1</sup>	cis	trans <sup>1</sup>	cis	trans <sup>1</sup>	
E1	60.71	60.74	60.95	60.75	61.03	60.92	61.08	60.84	61.12	60.88	
E <sub>2</sub>	14.16	14.31	14.03	14.21	14.24	14.18	14.26	14.16	14.09	14.12	
C <sub>5</sub>	46.03	39.02	46.99	39.33	41.75	36.85	42.51	40.92	41.56	37.11	
C <sub>6</sub>	42.21	41.87	41.56	41.84	45.21	40.90	44.96	37.10	45.80	40.84	
C <sub>5</sub> + C <sub>6</sub>	88.24	80.91	88.55	81.17	86.96	77.75	87.47	78.02	87.36	77.95	
	$\Delta = 7.35$ $\Delta = 7.38$		Δ =	Δ = 9.21		<b>∆</b> = 9.45		Δ = 9.41			

<sup>1</sup>these compounds exhibit two conformers in slow exchange due to slow rotation about the Boc-*N*<sub>4</sub> bond; the <sup>13</sup>C shifts for the more populated rotamer are reported here.

All species identified as trans show canonical NOE peaks and  ${}^{3}J_{HH}$  and  ${}^{3}J_{HC}$  couplings consistent with diaxial substituents at positions 2 and 3.







S12











S17










































































S54







S57






















































































S97


























S110





























S124







































S143








S147

Data File C:\Chem32\...\_AlaWittig\_050616\chiral\_test\_011116 2016-05-06 09-00-09\061-0201.D Sample Name: BCM-GSK-140Rac



CHIRAL 5/6/2016 11:20:23 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...\_AlaWittig\_050616\chiral\_test\_011116 2016-05-06 09-00-09\064-0301.D Sample Name: BCM-GSK-124-Wittig-L

Acq. Operator : SYSTEM	Seq. Line : 3
Acq. Instrument : CHIRAL	Location : 64
Injection Date : 5/6/2016 9:34:30 AM	Inj: 1
	Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry! Actual	Inj Volume : 10.000 μl
Method : C:\Chem32\1\Data\GSK_AlaWitti	g_050616\chiral_test_011116 2016-05-06 09-00-
09\FAST_Chiral_Scout_ID_nHep_	Ethanol.M (Sequence Method)
Last changed : 5/6/2016 9:00:09 AM by SYSTEM	1
Method Info : Scouting method for normal ph Heptane and Ethanol	ase chiral separations ChiralPak ID with n-

Sample Info : BCM-GSK-124-Wittig-L





Area Percent Report


Sorted By	:	Sig	nal		
Multiplier	:	1.0	996		
Dilution		1.0	990		
Do not use M	Multiplier &	Dilution	Factor	with	ISTDs



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.799	MM	0.1639	29.20967	2.97001	1.0849
2	5.230	MM	0.2941	2663.06348	150.89680	98.9151

Data File C:\Chem32\...\_AlaWittig\_050616\chiral\_test\_011116 2016-05-06 10-57-48\066-0201.D Sample Name: BCM-GSK-153C-Wittig-D



S150

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\074-0601.D Sample Name: Rac-Val-Bottom



CHIRAL 6/30/2017 3:03:21 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\074-0601.D Sample Name: Rac-Val-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.659	MM	0.3788	3.79414e4	1669.32178	46.1820
2	12.713	MM	0.4486	4.42149e4	1642.87720	53.8180

8.21563e4 3312.19897 Totals :

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.658	MM	0.3780	2.87438e4	1267.26550	47.5243
2	12.712	MM	0.4315	3.17385e4	1225.80908	52.4757

6.04823e4 2493.07458





Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.659	MM	0.3709	9549.31934	429.07864	47.2600
2	12.714	MM	0.4264	1.06566e4	416.54224	52.7400

Totals : 2.02059e4 845.62088

..... \*\*\* End of Report \*\*\*

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\075-0701.D Sample Name: L-Val-Bottom



Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\075-0701.D Sample Name: L-Val-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12,632	MM	0,4929	8.57091e4	2898,06006	100.0000

Totals : 8.57091e4 2898.06006

Signal 2: DAD1 B, Sig=220,4 Ref=off

 Peak RetTime Type Width
 Area
 Height
 Area

 # [min]
 [min]
 [mAU\*s]
 [mAU]
 %

 ----|-----|-----|------|
 -----|------|------|
 -----|-----|
 1

 1
 12.632
 MM
 0.4475
 7.00560e4
 2609.25854
 100.0000

Totals : 7.00560e4 2609.25854



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.634	MM	0.4292	2.35800e4	915.64758	100.0000

Totals : 2.35800e4 915.64758

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\076-0801.D Sample Name: D-Val-Bottom



Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\076-0801.D Sample Name: D-Val-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.591	MM	0,4121	7,03671e4	2845,76709	100.0000

Totals : 7.03671e4 2845.76709

Signal 2: DAD1 B, Sig=220,4 Ref=off

![](_page_155_Figure_6.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.590	MM	0.3745	1.99844e4	889.32953	100.0000

Totals : 1.99844e4 889.32953

\*\*\* End of Report \*\*\*

![](_page_156_Figure_0.jpeg)

![](_page_156_Figure_1.jpeg)

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CHIRAL 6/30/2017 3:01:50 PM SYSTEM
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Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\071-0201.D Sample Name: Rac-Val-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.360	MM	0.1760	3.46235e4	3278.70728	48.1611
2	9.477	MM	0.2426	3.72676e4	2560.61548	51.8389

Totals : 7.18911e4 5839.32275

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
	[		[	[	[]	
1	7.359	MM	0.1544	3.11400e4	3362.17480	50.6660
2	9.476	MM	0.2375	3.03213e4	2128.10376	49.3340

6.14612e4 5490.27856

![](_page_157_Figure_6.jpeg)

![](_page_157_Figure_7.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak	RetTime	Туре	Width	Area	Height	Area
**	furul		furul	[mwo.z]	[ mayo ]	/0
1	7.359	MM	0.1456	1.09450e4	1252.71252	51.7262
2	9.477	MM	0.2421	1.02144e4	703.09052	48.2738

Totals : 2.11594e4 1955.80304

\*\*\* End of Report \*\*\*

CHIRAL 6/30/2017 3:01:50 PM SYSTEM

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\072-0301.D Sample Name: L-Val-Top

![](_page_158_Figure_1.jpeg)

CHIRAL 6/30/2017 3:02:35 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\072-0301.D Sample Name: L-Val-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.461	MM	0.4078	7.97546e4	3259.58008	100.0000

Totals : 7.97546e4 3259.58008

Signal 2: DAD1 B, Sig=220,4 Ref=off

Totals : 7.18107e4 3254.91162

![](_page_159_Figure_7.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals : 2.44784e4 1156.94116

\*\*\* End of Report \*\*\*

![](_page_160_Figure_0.jpeg)

CHIRAL 6/30/2017 3:02:58 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Val 2017-06-30 12-34-20\073-0401.D Sample Name: D-Val-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.330	MM	0.2235	4.65298e4	3470.05884	100.0000

Totals : 4.65298e4 3470.05884

Signal 2: DAD1 B, Sig=220,4 Ref=off

 Peak RetTime Type Width
 Area
 Height
 Area

 # [min]
 [min]
 [mAU\*s]
 [mAU]
 %

----	-----
 -----|
 -----|
 1

 1
 7.331
 MM
 0.1994
 4.62491e4
 3866.16284
 100.0000

Totals : 4.62491e4 3866.16284

![](_page_161_Figure_7.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals : 2.22667e4 2396.88232

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...\Demo\Kevin\_Isopropanol\_Prime 2017-05-18 10-48-08\IA-Ethanol--002.D Sample Name: Racemic Serine

Acq. Operator	:	SYSTEM	Seq.	Line	:	2		
Acq. Instrument	:	CHIRAL	Loca	tion	:	91		
Injection Date	:	5/18/2017 11:10:38 AM		Inj	:	1		
			Inj Vo	lume	:	10.000 µl		
Method	:	C:\Chem32\1\Data\Demo\Kevin_	Isopropa	nol_	Pri	ime 2017-05-18	10-48-08\FAS	ST_
		Chiral_Scout_IC_nHep_2Propan	ol.M (Se	quen	ce	Method)		
Last changed	:	5/18/2017 10:48:08 AM by SYS	TEM					
Method Info	:	Scouting method for normal p	hase chi	ral :	sep	oarations Chira	alPak IC with	h n-
		Heptane and Isopropanol						

![](_page_162_Figure_2.jpeg)

![](_page_162_Figure_3.jpeg)

CHIRAL 5/19/2017 2:49:50 PM SYSTEM

Data File C:\Chem32\...\Demo\Kevin\_Isopropanol\_Prime 2017-05-18 10-48-08\IA-Ethanol--002.D Sample Name: Racemic Serine

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.007	MM	0.2564	2.74118e4	1781.83386	51.2233
2	6.469	MM	0.2412	2.61025e4	1803.95007	48.7767

Totals : 5.35142e4 3585.78394

Racemic SER-*O*-Bn ether

![](_page_163_Figure_6.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak   #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.007	MM	0.1768	949.08167	89.46393	53.8695
2	6.467	MM	0.1777	812.73590	76.21669	46.1305
Total	s :			1761.81757	165.68062	

\*\*\* End of Report \*\*\*

1.61258e4 1427.33051

CHIRAL 5/19/2017 2:49:50 PM SYSTEM

Data File C:\Chem32\1\Data\Srinivas\ELS\_chiral\_scout 2017-05-04 15-44-23\091-0201.D Sample Name: L-Serine

Acq. Operator	:	SYSTEM	Seq. Line	:	2		
Acq. Instrument	:	CHIRAL	Location	:	91		
Injection Date	:	5/4/2017 4:06:53 PM	Inj	:	1		
			Inj Volume	:	10.000 µl		
Method	:	C:\Chem32\1\Data\Srinivas\ELS	S_chiral_scou	it :	2017-05-04 15-44-23\FAST_Chiral_		
<pre>Scout_IC_nHep_2Propanol.M (Sequence Method)</pre>							
Last changed	:	5/4/2017 3:44:23 PM by SYSTEM	4				
Method Info	:	Scouting method for normal ph	hase chiral s	ep	arations ChiralPak IC with n-		
		Heptane and Isopropanol					

![](_page_164_Figure_2.jpeg)

![](_page_164_Figure_3.jpeg)

CHIRAL 5/19/2017 2:48:15 PM SYSTEM

Data File C:\Chem32\1\Data\Srinivas\ELS\_chiral\_scout 2017-05-04 15-44-23\091-0201.D Sample Name: L-Serine

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.105	MM	0.2936	3.37022e4	1912.97864	100.0000

Totals : 3.37022	2e4 1912.97864
------------------	----------------

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.104	MM	0.2026	1.43042e4	1176.63611	98.3166
2	6.517	MM	0.2130	244.91501	19.16068	1.6834

1.45491e4 1195.79679

![](_page_165_Figure_6.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.104	MM	0.1692	1811.26855	178.39732	96.4560
2	6.523	MM	0.2418	66.54992	4.58628	3.5440

Totals : 1877.81847 182.98360

\*\*\* End of Report \*\*\*

Data File C:\Chem32\1\Data\Srinivas\ELS\_chiral\_scout 2017-05-04 09-58-50\051-0701.D Sample Name: D-Serine

![](_page_166_Figure_1.jpeg)

Data File C:\Chem32\1\Data\Srinivas\ELS\_chiral\_scout 2017-05-04 09-58-50\051-0701.D Sample Name: D-Serine

Signal 1: DAD1 A, Sig=210,4 Ref=off

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak Ret	Time Type	Width	Area	Height	Area
# [m	in]	[min]	[mAU*s]	[mAU]	%
1 6	.191 MM	0.2832	2219.65576	130.64211	6.3629
2 6	.632 MM	0.2861	3.26646e4	1902.94104	93.6371

Totals : 3.48843e4 2033.58315

(S)-SER-O-Bn ether

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.208	MM	0.2157	566.64063	43.77433	4.4311
2	6.633	MM	0.2106	1.22210e4	967.06311	95.5689

![](_page_167_Figure_6.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.214	MM	0.2274	125.75787	9.21786	8.4842
2	6.634	MM	0.1832	1356.49536	123.41334	91.5158
Total	s :			1482.25323	132.63120	

\*\*\* End of Report \*\*\*

1.27877e4 1010.83744

CHIRAL 5/19/2017 2:48:49 PM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\054-0201.D Sample Name: 23-Ser-Cis-Rac

Acq. Operator	:	SYSTEM	Seq. Lir	ne	:	2
Acq. Instrument	:	CHIRAL	Locatio	on	:	54
Injection Date	:	8/22/2017 6:13:12 PM	Ir	nj	:	1
			Inj Volum	ne	:	10.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krish	nna_Reddy_Gu	udu	Iri	J\GSK-23-Ser 2017-08-22 17-50-42
		\FAST_Chiral_Scout_IC_nHep_2	Propanol.M	(9	Sec	quence Method)
Last changed	:	8/22/2017 5:50:42 PM by SYST	(EM			
Method Info	:	Scouting method for normal p	hase chiral	1 9	sep	parations ChiralPak IC with n-
		Heptane and Isopropanol				

## Additional Info : Peak(s) manually integrated

![](_page_168_Figure_3.jpeg)

racemic

CHIRAL 8/23/2017 9:56:29 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\054-0201.D Sample Name: 23-Ser-Cis-Rac

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.075	MM	0.4082	6.06526e4	2476.30469	54.0836
2	14.414	MM	0.4482	5.14933e4	1914.85754	45.9164

Totals : 1.12146e5 4391.16223

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %	
1	13.075	MM	0.3677	3.56526e4	1615.93127	55.4656	
2	14.414	MM	0.4278	2.86261e4	1115.31750	44.5344	
Total	ls :			6.42787e4	2731.24878		

![](_page_169_Figure_6.jpeg)

Cis racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.076	MM	0.3654	1.13579e4	518.00879	55.7752
2	14.414	MM	0.4249	9005.81836	353.27780	44.2248

Totals : 2.03637e4 871.28659

\*\*\* End of Report \*\*\*

CHIRAL 8/23/2017 9:56:29 AM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\055-0301.D Sample Name: 23-L-Ser-Cis

Acq. Operator	:	SYSTEM	Seq. Line : 3	
Acq. Instrument	:	CHIRAL	Location : 55	
Injection Date	:	8/22/2017 6:34:25 PM	Inj : 1	
			Inj Volume : 10.000 µl	
Method	:	C:\Chem32\1\Data\Shiva_Kri	shna_Reddy_Guduru\GSK-23-Ser 2017-08-22 17-	-50-42
		\FAST_Chiral_Scout_IC_nHep	_2Propanol.M (Sequence Method)	
Last changed	:	8/22/2017 5:50:42 PM by SY	STEM	
Method Info	:	Scouting method for normal	phase chiral separations ChiralPak IC with	hn-
		Heptane and Isopropanol		
Additional Info	:	Peak(s) manually integrate	d	
DAD1 A, Si	g=:	210,4 Ref=off (Shiva_Krishna_Reddy_Guo	uru\GSK-23-Ser 2017-08-22 17-50-42\055-0301.D)	
mAU -			8 x2	
0000			A 400	

![](_page_170_Figure_2.jpeg)

7e cis

### CHIRAL 8/23/2017 9:58:44 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\055-0301.D Sample Name: 23-L-Ser-Cis

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.232	MM	0.2956	4329.78613	244.12048	4.6540
2	14.359	MM	0.5195	8.87035e4	2845.98071	95.3460

Totals :	0 2022204	2000 10120
lotals :	9.3033304	3090.10120

![](_page_171_Figure_4.jpeg)

6.13669e4 2378.52106

H N CO<sub>2</sub>Et Ns 7e cis

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.237	MM	0.3026	745.33337	41.04734	3.7502
2	14.357	MM	0.4360	1.91292e4	731.18427	96.2498
Total	ls :			1.98746e4	772.23160	

\*\*\* End of Report \*\*\*

CHIRAL 8/23/2017 9:58:44 AM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\056-0401.D Sample Name: 23-D-Ser-Cis

Acq. Operator	:	SYSTEM Seq. Line : 4
Acq. Instrument	:	CHIRAL Location : 56
Injection Date	:	8/22/2017 6:55:37 PM Inj: 1
		Inj Volume : 10.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krishna_Reddy_Guduru\GSK-23-Ser 2017-08-22 17-50-42
		<pre>\FAST_Chiral_Scout_IC_nHep_2Propanol.M (Sequence Method)</pre>
Last changed	:	8/22/2017 5:50:42 PM by SYSTEM
Method Info	:	Scouting method for normal phase chiral separations ChiralPak IC with n-
		Heptane and Isopropanol

# Additional Info : Peak(s) manually integrated

![](_page_172_Figure_3.jpeg)

7k cis

#### CHIRAL 8/23/2017 9:57:59 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\056-0401.D Sample Name: 23-D-Ser-Cis

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.041	MM	0.4738	8.88093e4	3123.79102	97.8860
2	14.653	MM	0.3583	1917.96570	89.21995	2.1140

Totals : 9.07273e4 3213.01096

![](_page_173_Figure_4.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.039	MM	0.3677	2.16248e4	980.06012	97.4960
2	14.653	MM	0.3546	555.38751	26.10575	2.5040

Totals : 2.21802e4 1006.16587

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\051-1001.D Sample Name: 23-Ser-Trans-Rac

			-
Acq. Operator	: SYSTEM	Seq. Line : 10	
Acq. Instrument	: CHIRAL	Location : 51	
Injection Date	: 8/22/2017 8:58:38 PM	Inj : 1	
		Inj Volume : 10.000	μl
Method	: C:\Chem32\1\Data\Shiva_Kr	ishna Reddy Guduru\GSK-23	-Ser 2017-08-22 17-50-42
	\FAST Chiral Scout IF nHe	p 2Propanol.M (Sequence M	lethod)
Last changed	: 8/22/2017 5:50:42 PM by S	YSTEM	
Method Info	: Scouting method for normal	l phase chiral separation	s ChiralPak IF with n-
	Heptane and Isopropanol		
Additional Info	: Peak(s) manually integrate	ed	
DAD1 A, Sig	=210,4 Ref=off (Shiva_Krishna_Reddy_Gu	duru\GSK-23-Ser 2017-08-22 17-50-42	051-1001.D)
mAU =			8 .2
2500			2 15h 2 30 <sup>54</sup>
2000			est Cast
			Ma Ve
1500			
1000			
500			
0			
	2 4	6 8	10 12 14 "
DAD1 B, Sig	=220,4 Ref=off (Shiva_Krishna_Reddy_Gu	duru\GSK-23-Ser 2017-08-22 17-50-42	051-1001.D)
mAU			1 A A
1/50			P . 43' 8 . 30''
1500			xea
1200 -			
750			
500			
260			
200			
°=		· · · · · · · ·	
DAD1 C. Sin	2 4 =254.4 Ref=off (Shiva Krishna Reddy Gu	6 8 dum//GSK-23-Ser 2017-08-22 17-50-42	10 12 14 n (051-1001 D)
mAll 7	-204,4 rel-on (onna_relaina_reduy_ou		3
			a white the
500 -			Treat 8 NOT
400 -			Theo.
300			
200			
100			
0			
	2 4	6 8	10 12 14 "
	Anna Dansant Dansar		-
	Area Percent Report	t	, OBn
Control Di			
Sorted By	: Signal		
Multiplier	: 1.0000		
Dilution	: 1.0000		i.
Do not use Multip	niier & Dilution Factor wit	n ISTDC	Nc
	piler a bildelon raccor with	15103	113

Trans racemic

CHIRAL 8/23/2017 9:46:30 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\051-1001.D Sample Name: 23-Ser-Trans-Rac

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.695	MM	0.4357	7.15413e4	2736.92065	54.7900
2	13.730	MM	0.5146	5.90324e4	1912.07947	45.2100

Totals :	1.30574e5	4649,00012
IVLais .	1.303/463	4049.00012

![](_page_175_Figure_4.jpeg)

![](_page_175_Figure_5.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.694	MM	0.3883	1.44200e4	618.89899	57.3895
2	13.730	MM	0.4969	1.07065e4	359.08862	42.6105
Total	s :			2.51266e4	977.98761	

\*\*\* End of Report \*\*\*

CHIRAL 8/23/2017 9:46:30 AM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\052-1101.D Sample Name: 23-L-Ser-Trans

Acq. Operator	:	SYSTEM Seq. Line : 11
Acq. Instrument	:	CHIRAL Location : 52
Injection Date	:	8/22/2017 9:14:50 PM Inj: 1
		Inj Volume : 10.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krishna_Reddy_Guduru\GSK-23-Ser 2017-08-22 17-50-42
		\FAST_Chiral_Scout_IF_nHep_2Propanol.M (Sequence Method)
Last changed	:	8/22/2017 5:50:42 PM by SYSTEM
Method Info	:	Scouting method for normal phase chiral separations ChiralPak IF with n-
		Heptane and Isopropanol

### Additional Info : Peak(s) manually integrated

![](_page_176_Figure_3.jpeg)

CHIRAL 8/23/2017 9:54:45 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\052-1101.D Sample Name: 23-L-Ser-Trans

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.750	MM	0.2306	1956.07568	141.36531	1.8757
2	13.632	MM	0.5933	1.02328e5	2874.72485	98.1243

Totals : 1.04285e5 3016.09016

![](_page_177_Figure_4.jpeg)

H N N Ns 7e trans

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.750	MM	0.2311	421.59326	30.41113	1.9262
2	13.634	MM	0.5079	2.14655e4	704.39465	98.0738
Tota]	ls :			2.18871e4	734.80578	

\*\*\* End of Report \*\*\*

7.10660e4 2329.70559

CHIRAL 8/23/2017 9:54:45 AM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\053-1201.D Sample Name: 23-D-Ser-Trans

Acq. Operator	:	SYSTEM	Seq. L	ine	:	12			
Acq. Instrument	:	CHIRAL	Locat	ion	:	53			
Injection Date	:	8/22/2017 9:31:01 PM	1	Inj	:	1			
			Inj Vol	ume	:	10.000 µl			
Method	:	C:\Chem32\1\Data\Shiva_Krishna	_Reddy_(	Gudu	ıru	\GSK-23-Ser 2017-08-22 17-50-42			
		\FAST_Chiral_Scout_IF_nHep_2Pr	opanol.	M (S	ieq	uence Method)			
Last changed	:	8/22/2017 5:50:42 PM by SYSTEM	1						
Method Info	:	Scouting method for normal pha	ise chira	al s	sep	arations ChiralPak IF with n-			
		Heptane and Isopropanol							

# Additional Info : Peak(s) manually integrated

![](_page_178_Figure_3.jpeg)

7k trans

#### CHIRAL 8/23/2017 9:48:18 AM SYSTEM

Data File C:\Chem32\...hiva\_Krishna\_Reddy\_Guduru\GSK-23-Ser 2017-08-22 17-50-42\053-1201.D Sample Name: 23-D-Ser-Trans

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.589	MM	0.5150	9.87932e4	3197.27783	98.1562
2	13.910	MM	0.3068	1855.78186	100.82298	1.8438

Totals : 1.00649e5 3298.10081

![](_page_179_Figure_4.jpeg)

![](_page_179_Figure_5.jpeg)

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.583	MM	0.3754	2.62209e4	1164.08154	97.7245
2	13.912	MM	0.3664	610.55963	27.77085	2.2755

Totals : 2.68315e4 1191.85239

\*\*\* End of Report \*\*\*
Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\071-0201.D Sample Name: Rac-Ala-Major

Acq. Operator : SYS	STEM	Seq. Line	:	2
Acq. Instrument : CHI	IRAL	Location	:	71
Injection Date : 6/2	29/2017 9:21:15 AM	Inj	:	1
		Inj Volume	:	5.000 µl
Different Inj Volume	from Sample Entry! Actual	Inj Volume	:	10.000 µl
Method : C:\	\Chem32\1\Data\Shiva_Krishna	_Reddy_Gudu	uru	1\23-Ala 2017-06-29 08-58-47\FAST
_Ch	hiral_Scout_IF_nHep_Ethanol.	M (Sequence	e M	lethod)
Last changed : 6/2	29/2017 8:58:47 AM by SYSTEM			
Method Info : Sco	outing method for normal pha	se chiral s	sep	arations ChiralPak IF with n-
Hep	ptane and Ethanol			

#### Additional Info : Peak(s) manually integrated



racemic

CHIRAL 6/29/2017 1:44:29 PM SYSTEM

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\071-0201.D Sample Name: Rac-Ala-Major

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.164	MM	0.3461	4.23157e4	2037.70325	50.3374
2	12.486	MM	0.3975	4.17484e4	1750.56311	49.6626

Totals :	8.40640e4	3788.26636

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Boc CH <sub>3</sub>
 1 2	11.163 12.486	 ММ ММ	0.3400 0.3948	3.03751e4 2.98793e4	1488.82935 1261.34692	50.4115 49.5885	CO₂Et Ns
Total	ls :			6.02544e4	2750.17627		Cis racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.164	MM	0.3397	9783.59082	480.05774	49.7764
2	12.486	MM	0.4023	9871.48535	408.99603	50.2236

Totals : 1.96551e4 889.05377

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\072-0301.D Sample Name: L-Ala-Major



Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\072-0301.D Sample Name: L-Ala-Major

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.406	MM	0.4733	8.35906e4	2943.65479	100.0000

Totals : 8.35906e4 2943.65479

Signal 2: DAD1 B, Sig=220,4 Ref=off



Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.405	MM	0.4286	2.07786e4	807.99927	100.0000

Totals : 2.07786e4 807.99927

\*\*\* End of Report \*\*\*

6.45318e4 2462.64453

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\073-0401.D Sample Name: D-Ala-Major



Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\073-0401.D Sample Name: D-Ala-Major

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.083	MM	0.4055	7.76617e4	3192.32715	100.0000

Totals : 7.76617e4 3192.32715

Signal 2: DAD1 B, Sig=220,4 Ref=off

Boc Peak RetTime Type Width Height Area Area CH3 Ń. # [min] [min] [mAU\*s] [mAU] % CO<sub>2</sub>Et 1 11.082 MM 0.3632 5.84432e4 2682.02783 100.0000 N Ńs Totals : 5.84432e4 2682.02783 8f cis

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.082	MM	0.3645	1.96961e4	900.70404	100.0000

Totals : 1.96961e4 900.70404

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\074-0601.D Sample Name: Rac-Ala-Minor



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CHIRAL 6/29/2017 1:47:12 PM SYSTEM
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Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\074-0601.D Sample Name: Rac-Ala-Minor

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.789	MM	0.3994	4.70097e4	1961.77551	50.2524
2	13.334	MM	0.6535	4.65375e4	1186.87866	49.7476

Totals :	9.35472e4	3148.65417

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Boc N_CH <sub>3</sub>
1 2	11.789 13.334	мм мм	0.3953 0.6621	3.47105e4 3.45233e4	1463.60791 869.02081	50.1352 49.8648	CO <sub>2</sub> Et
Tota	ls :			6.92338e4	2332.62872		Trans racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.789	MM	0.3967	1.19117e4	500.46402	50.8285
2	13.334	MM	0.6478	1.15233e4	296.45627	49.1715
Total	s :			2.34350e4	796.92029	

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\075-0701.D Sample Name: L-Ala-Minor



Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\075-0701.D Sample Name: L-Ala-Minor

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.185	MM	0.7123	9.47576e4	2217.15601	100.0000

Totals : 9.47576e4 2217.15601

Signal 2: DAD1 B, Sig=220,4 Ref=off



Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.185	MM	0.7035	2.41510e4	572.13873	100.0000

Totals : 2.41510e4 572.13873

\*\*\* End of Report \*\*\*

6.99576e4 1663.90283

Page 2 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\076-0801.D Sample Name: D-Ala-Minor



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CHIRAL 6/29/2017 1:49:12 PM SYSTEM
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Page 1 of 2

Data File C:\Chem32\...ta\Shiva\_Krishna\_Reddy\_Guduru\23-Ala 2017-06-29 08-58-47\076-0801.D Sample Name: D-Ala-Minor

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.699	MM	0.4762	8.64976e4	3027.30200	100.0000

Totals : 8.64976e4 3027.30200

Signal 2: DAD1 B, Sig=220,4 Ref=off



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.700	MM	0.4302	2.30411e4	892.68848	100.0000

Totals : 2.30411e4 892.68848

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...dris\_Raji\_PhD\ELS\_chiral\_scout 2017-03-03 15-51-08\ID-Isopropanol.D Sample Name: EXP-17-PHE\_2,3\_Lower\_spot\_Racemic



CHIRAL 6/23/2017 5:02:42 PM SYSTEM

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Data File C:\Chem32\...dris\_Raji\_PhD\ELS\_chiral\_scout 2017-03-03 15-51-08\ID-Isopropanol.D Sample Name: EXP-17-PHE\_2,3\_Lower\_spot\_Racemic

Area

%

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Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.220	MM	0.4707	5.88010e4	2082.09180	46.9310
2	14.783	MM	0.6832	6.64915e4	1622.15784	53.0690

Totals :	1.25292e5	3704,24963
IVLais .	1.2323203	3704.24903

1	12.220	MM	0.4360	3.76335e4	1438.63794	47.2523
2	14.783	MM	0.6767	4.20102e4	1034.65637	52.7477
Total	s :			7.96438e4	2473.29431	



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.220	MM	0.4300	9957.72461	385.99615	47.4028
2	14.783	MM	0.6670	1.10489e4	276.07495	52.5972
Total	ls :			2.10066e4	662.07111	

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:02:42 PM SYSTEM

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-02-13 09-57-47\021-0302.D Sample Name: L-Pheala-Major-Bottom

Acq. Operator	:	SYSTEM	Seq.	Line	:	3
Acq. Instrument	:	CHIRAL	Loca	ation	:	21
Injection Date	:	2/13/2018 10:40:19 AM		Inj	:	2
			Inj Vo	olume	:	5.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krish	na_Reddy	_Gud	uri	u\Shiva 2018-02-13 09-57-47\FAST_
		Chiral_Scout_ID_nHep_2Propan	ol.M (Se	equen	ce	Method)
Last changed	:	2/13/2018 9:57:48 AM by SYST	EM			
Method Info	:	Scouting method for normal pl	hase chi	iral	sep	parations ChiralPak ID with n-
		Heptane and Isopropanol				

Sample Info : L-Pheala-Major-Bottom

Additional Info : Peak(s) manually integrated



### CHIRAL 2/13/2018 11:02:15 AM SYSTEM

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-02-13 09-57-47\021-0302.D Sample Name: L-Pheala-Major-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.880	MM	0.4159	566.52661	22.70391	1.2680
2	14.896	MM	0.6467	4.41121e4	1136.79004	98.7320

Totals :	4.46786e4	1159.49395

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.890	MM	0.3968	350.64880	14.72691	1.2562
2	14.896	MM	0.6572	2.75635e4	699.00690	98.7438
Total	ls :			2.79142e4	713.73380	



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.915	MM	0.4000	60.42810	2.51806	0.8360
2	14.896	MM	0.6442	7167.91943	185.44417	99.1640
Total	ls :			7228.34753	187.96223	

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\078-0301.D Sample Name: D-Pheala-Major-Bottom



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CHIRAL 6/24/2017 1:02:19 PM SYSTEM
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Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\078-0301.D Sample Name: D-Pheala-Major-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.006	MM	0.5638	8.12404e4	2401.37231	100.0000

Totals : 8.12404e4 2401.37231



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.004	MM	0.5069	1.45057e4	476.93921	100.0000

Totals : 1.45057e4 476.93921

\*\*\* End of Report \*\*\*

Data File C:\Chem32\...ir\_Idris\_Raji\_PhD\ELS\_chiral\_scout 2017-03-03 17-01-36\ID-Ethanol.D Sample Name: EXP-17-PHE\_2,3\_Upper\_spot\_Racemic



CHIRAL 6/23/2017 5:06:28 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...ir\_Idris\_Raji\_PhD\ELS\_chiral\_scout 2017-03-03 17-01-36\ID-Ethanol.D Sample Name: EXP-17-PHE\_2,3\_Upper\_spot\_Racemic

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.359	MM	0.2643	4.15149e4	2617.46729	52.0952
2	10.352	MM	0.3252	3.81755e4	1956.52515	47.9048

Totals :	7,96903e4	4573,99243
IVLais .	7.3030364	4373.33243





Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.360	MM	0.2127	9600.75781	752.13861	57.1689
2	10.352	MM	0.3256	7192.91797	368.15021	42.8311

Totals : 1.67937e4 1120.28882

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:06:28 PM SYSTEM

Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\079-0501.D Sample Name: L-Pheala-Minor-Top



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CHIRAL 6/24/2017 12:13:42 PM SYSTEM
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Page 1 of 2

Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\079-0501.D Sample Name: L-Pheala-Minor-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.515	MM	0.3941	8.19827e4	3467.22705	96.3295
2	10.768	MM	0.3112	3123.86279	167.29315	3.6705

Totals : 8.51066e4 3634.52020



Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.499	MM	0.2450	3.38780e4	2304.94043	96.9902
2	10.969	MM	0.3047	1051.28992	57.51159	3.0098

Totals : 3.49293e4 2362.45202

\*\*\* End of Report \*\*\*

8.34559e4 4034.79152

CHIRAL 6/24/2017 12:13:42 PM SYSTEM

Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\080-0601.D Sample Name: D-Pheala-Minor-Top



9g trans

CHIRAL 6/24/2017 12:12:05 PM SYSTEM

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Data File C:\Chem32\...Shiva\_Krishna\_Reddy\_Guduru\23-Pheala 2017-06-23 17-44-56\080-0601.D Sample Name: D-Pheala-Minor-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.575	MM	0.2261	1991.00879	146.75478	1.7800
2	10.429	MM	0.5588	1.09863e5	3276.56323	98.2200

Totals : 1.11854e5 3423.31801





Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.565	MM	0.2393	307.92880	21.44879	1.0331
2	10.419	MM	0.3997	2.94977e4	1229.89990	98.9669

Totals : 2.98056e4 1251.34869

\*\*\* End of Report \*\*\*

CHIRAL 6/24/2017 12:12:05 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\074-0601.D Sample Name: 23-Leu-Rac-Major-Bottom



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CHIRAL 6/23/2017 5:48:02 PM SYSTEM
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Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\074-0601.D Sample Name: 23-Leu-Rac-Major-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.532	MM	0.2630	4.23951e4	2686.44409	49.4902
2	13.736	MM	0.3318	4.32685e4	2173.30469	50.5098

Totals :	8,56635e4	4859,74878
ICCOLD .	0.0000000	

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.532	MM	0.2501	3.02077e4	2013.37488	49.5913
2	13.736	MM	0.3302	3.07056e4	1549.74744	50.4087

6.09133e4 3563.12231



Cis racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.532	MM	0.2513	1.02583e4	680.44391	49.5724
2	13.736	MM	0.3312	1.04352e4	525.12274	50.4276

Totals : 2.06935e4 1205.56665

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:48:02 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\075-0701.D Sample Name: 23-Leu-L-Major-Bottom

	-						
Acq. Operator	:	SYSTEM		Seq	. Line	:	7
Acq. Instrument	:	CHIRAL		Lo	cation	:	75
Injection Date	:	6/23/2017 12:13:16 PM			Inj	:	1
				Inj	Volume	:	5.000 µl
Different Inj V	010	ume from Sample Entry!	Actual	Inj	Volume	:	10.000 µl
Method	:	C:\Chem32\1\Data\Shiva	_Krishna	_Red	dy_Gud	uri	u\Default_chiral_scout 2017-06-23
		10-05-25\FAST_Chiral_S	cout_IE_	nHep	Ethan	01	.M (Sequence Method)
Last changed	:	6/23/2017 10:05:25 AM	by SYSTE	M			
Method Info	:	Scouting method for nor	rmal pha	se cl	hiral	sep	parations ChiralPak IE with n-
		Heptane and Ethanol					





Do not use Multiplier & Dilution Factor with ISTDs



CHIRAL 6/23/2017 5:53:00 PM SYSTEM

1 of 2 Page

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\075-0701.D Sample Name: 23-Leu-L-Major-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.102	MM	0.2397	1675.78064	116.51774	1.5936
2	13.538	MM	0.5088	1.03484e5	3390.05029	98.4064

Totals : 1.05160e5 3506.56803

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.116	MM	0.2441	1295.50171	88.45919	1.4165
2	13.537	MM	0.4247	9.01607e4	3538.09033	98.5835
Tota]	s :			9.14562e4	3626.54952	



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.109	MM	0.2454	508.90936	34.57028	1.4976
2	13.537	MM	0.3943	3.34731e4	1415.00806	98.5024

Totals : 3.39820e4 1449.57833

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:53:00 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\076-0801.D Sample Name: 23-Leu-D-Major-Bottom

Acq. Operator	:	SYSTEM	Seq. Line	:	8
Acq. Instrument	:	CHIRAL	Location	:	76
Injection Date	:	6/23/2017 12:34:28 PM	Inj	:	1
		I	nj Volume	:	5.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krishna_	Reddy_Gud	ur	u\Default_chiral_scout 2017-06-23
		10-05-25\FAST_Chiral_Scout_IE_n	Hep_Ethan	01	.M (Sequence Method)
Last changed	:	6/23/2017 10:05:25 AM by SYSTEM			
Method Info	:	Scouting method for normal phas	e chiral	se	parations ChiralPak IE with n-
		Heptane and Ethanol			

# Additional Info : Peak(s) manually integrated



8h cis

### CHIRAL 6/23/2017 5:53:58 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\076-0801.D Sample Name: 23-Leu-D-Major-Bottom

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.442	MM	0.3444	7.01070e4	3392.46631	99.0193
2	13.347	MM	0.1828	694.33185	63.31287	0.9807

Totals :	7,08013e4	3455,77918
IULdis .	7.0001304	2422111210

Signal 2: DAD1 B, Sig=220,4 Ref=off

Boc Peak RetTime Type Width Area Height Area # [min] [min] [mAU\*s] [mAU] % 1 11.444 MM 0.2833 6.02815e4 3546.79297 100.0000 Ńs Totals : 6.02815e4 3546.79297 8h cis Signal 3: DAD1 C, Sig=254,4 Ref=off Peak RetTime Type Width Area Height Area # [min] [min] [mAU\*s] [mAU] % 1 11.443 MM 0.2691 2.32255e4 1438.21118 100.0000 Totals : 2.32255e4 1438.21118

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:53:58 PM SYSTEM

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CO<sub>2</sub>Et

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\071-0201.D
Sample Name: 23-Leu-Rac-Minor-Top



racemic

CHIRAL 6/23/2017 5:46:56 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\071-0201.D Sample Name: 23-Leu-Rac-Minor-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak RetTim	е Туре	Width	Area	Height	Area
# [min]		[min]	[mAU*s]	[mAU]	%
	-				
1 11.24	6 MM	0.3565	4.24095e4	1982.46899	49.5871
2 14.01	9 MM	0.4335	4.31158e4	1657.66113	50.4129

Totals : 8.55253e4 3640.13013

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.246	MM	0.3573	3.12359e4	1456.96436	50.5855
2	14.019	MM	0.4272	3.05129e4	1190.37231	49.4145

6.17488e4 2647.33667



Trans racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Totals :

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.246	MM	0.3571	1.09842e4	512.69775	50.1303
2	14.019	MM	0.4324	1.09271e4	421.14539	49.8697
Total	s :			2.19113e4	933.84314	

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:46:56 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\072-0301.D Sample Name: 23-Leu-L-Minor-Top

Acq. Operator	:	SYSTEM	Seq. Line	:	3
Acq. Instrument	:	CHIRAL	Location	:	72
Injection Date	:	6/23/2017 10:49:05 AM	Inj	:	1
			Inj Volume	: 5	.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krishn	a_Reddy_Gud	uru\	Default_chiral_scout 2017-06-23
		10-05-25\FAST_Chiral_Scout_IE	_nHep_Ethan	ol.M	(Sequence Method)
Last changed	:	6/23/2017 10:05:25 AM by SYST	EM		
Method Info	:	Scouting method for normal ph	ase chiral	sepa	rations ChiralPak IE with n-
		Heptane and Ethanol			

## Additional Info : Peak(s) manually integrated



9c trans

## CHIRAL 6/23/2017 5:52:22 PM SYSTEM

Page 1 of 2

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\072-0301.D Sample Name: 23-Leu-L-Minor-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.216	MM	0.4480	9.01583e4	3353.95239	97.5981
2	14.042	MM	0.3126	2218.83350	118.28944	2.4019

Totals : 9.23771e4 3472.24184

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.203	MM	0.3785	7.91387e4	3484.97729	97.2817
2	14.017	MM	0.3074	2211.31494	119.90569	2.7183
Total	ls :			8.13500e4	3604.88299	



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.203	MM	0.3479	2.87882e4	1379.16504	98.7094
2	14.042	MM	0.2849	376.39276	22.02021	1.2906

Totals : 2.91646e4 1401.18525

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:52:22 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\073-0401.D Sample Name: 23-Leu-D-Minor-Top

Aca Operator · SYSTEM	Sea line : 4	
Acq. Instrument : CHIRAL	location : 73	
Injection Date : 6/23/2017 11:10:	15 AM Ini: 1	
Injection bace : 0, 10, 101, 1110.	Ini Volume : 5.000 ul	
Different Inj Volume from Sample B	ntry! Actual Inj Volume : 10.000 ul	
Method : C:\Chem32\1\Data	A\Shiva Krishna Reddy Guduru\Default chiral scou	ut 2017-06-23
10-05-25\FAST C	niral Scout IE nHep Ethanol.M (Sequence Method)	
Last changed : 6/23/2017 10:05:	25 AM by SYSTEM	
Method Info : Scouting method	for normal phase chiral separations ChiralPak 1	IE with n-
Heptane and Etha	anol	
Additional Info : Peak(s) manually	/ integrated	
DAD1 A, Sig=210,4 Ref=off (Shiva_Kris.	Reddy_Guduru\Default_chiral_scout 2017-08-23 10-05-25\073-0401.D)	
mAU	ă "v	
3000 -	E 201	
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1500	22	
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500-	Tpsee.	
0		
2 4	6 8 10 12 14	16 18 min
DAD1 B, Sig=220,4 Ref=off (Shiva_Kris.	Reddy_Guduru\Default_chiral_scout 2017-06-23 10-05-25\073-0401.D)	
mAU =	^ى. 🕺	
3000 -	2 . 10 <sup>n</sup>	
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2000		
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1000-	S ST	
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0		
2 4	6 8 10 12 14	16 18 min
DAD1 C, Sig=254,4 Ref=off (Shiva_Kris.	Reddy_Guduru\Default_chiral_scout 2017-06-23 10-05-25/073-0401.D)	
mAU	<u>الم الم الم الم الم الم الم الم الم الم </u>	
1200-	P	
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200	in see	
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2 4	6 8 10 12 14	16 18 min
Area Pero	ent Report	
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		N
Sorted By : Signa	1	
Multiplier : 1.000	90	COLET
Dilution : 1.000	90	

Do not use Multiplier & Dilution Factor with ISTDs



CHIRAL 6/23/2017 5:53:25 PM SYSTEM

Data File C:\Chem32\...na\_Reddy\_Guduru\Default\_chiral\_scout 2017-06-23 10-05-25\073-0401.D Sample Name: 23-Leu-D-Minor-Top

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area	
#	[min]		[min]	[mAU*s]	[mAU]	%	
1	11.629	MM	0.2529	3975.23706	261.93579	3.1753	
2	13.782	MM	0.5926	1.21219e5	3409.51587	96.8247	

Totals : 1.25194e5 3671.45166

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.635	MM	0.2570	2672.71851	173.35158	2.5039
2	13.766	MM	0.4895	1.04071e5	3543.80933	97.4961
Total	s :			1.06744e5	3717.16090	



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.629	MM	0.2366	878.48553	61.89431	2.1839
2	13.766	MM	0.4492	3.93471e4	1459.81360	97.8161

Totals : 4.02256e4 1521.70791

\*\*\* End of Report \*\*\*

CHIRAL 6/23/2017 5:53:25 PM SYSTEM
Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-29 15-47-02\021-0201.D Sample Name: BCM-GSK-470

Acq. Operator	:	SYSTEM	Seq	. Lir	ne	:	: 2
Acq. Instrument	:	CHIRAL	Lo	catio	on	:	: 21
Injection Date	:	1/29/2018 4:08:30 PM		Ir	nj	:	: 1
			Inj	Volur	ne	:	: 10.000 µl
Method	:	C:\Chem32\1\Data\Shiva_Krishna	_Red	dy_Gu	udu	uru	ru\Shiva 2018-01-29 15-47-02\FAST_
		Chiral_Scout_IC_nHep_2Propanol	.M (	Seque	end	ce	e Method)
Last changed	:	1/29/2018 3:47:02 PM by SYSTEM	1				
Method Info	:	Scouting method for normal pha	se c	hiral	1 :	sep	eparations ChiralPak IC with n-
		Heptane and Isopropanol					

Sample Info : BCM-GSK-470 Rac-Trans

Additional Info : Peak(s) manually integrated



CHIRAL 1/30/2018 9:23:46 AM SYSTEM

Page 1 of 2

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-29 15-47-02\021-0201.D Sample Name: BCM-GSK-470

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.129	MF	0.5085	5.65670e4	1854.17371	51.2945
2	11.812	FM	0.4340	5.37119e4	2062.45703	48.7055

Totals :	1.10279e5	3916,63074
		22201020/ ···

Signal 2: DAD1 B, Sig=220,4 Ref=off

							Me
Peak	RetTime	Туре	Width	Area	Height	Area	
#	[min]		[min]	[mAU*s]	[mAU]	%	
1	11.130	MF	0.4724	3.42104e4	1207.09009	50.0127	
2	11.812	FM	0.3693	3.41930e4	1543.31262	49.9873	Ï
							o 13
Tota	ls :			6.84034e4	2750.40271		racemic

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.136	MF	0.4623	1135.58533	40.93751	50.5640
2	11.813	FM	0.3396	1110.25159	54.48027	49.4360
Tota]	s:			2245.83691	95.41778	

\*\*\* End of Report \*\*\*

CHIRAL 1/30/2018 9:23:46 AM SYSTEM

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-29 15-47-02\022-0301.D Sample Name: BCM-GSK-445D

							-
Acq. Operator	:	SYSTEM	Seq.	Line	:	3	
Acq. Instrument	:	CHIRAL	Loca	tion	:	22	
Injection Date	:	1/29/2018 4:29:39 PM		Inj	:	1	
			Inj Vo	lume	:	10.000	μl
Method	:	C:\Chem32\1\Data\Shiva_Kris	shna_Reddy	_Gudu	uru	u\Shiva	2018-01-29 15-47-02\FAST_
		Chiral_Scout_IC_nHep_2Propa	anol.M (Se	quen	ce	Method)	)
Last changed	:	1/29/2018 3:47:02 PM by SYS	STEM				
Method Info	:	Scouting method for normal	phase chi	ral :	sep	paration	ns ChiralPak IC with n-
		Heptane and Isopropanol					

Sample Info : BCM-GSK-445D D-Trans

## Additional Info : Peak(s) manually integrated



CHIRAL 1/30/2018 9:27:57 AM SYSTEM

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Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-29 15-47-02\022-0301.D Sample Name: BCM-GSK-445D

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.349	MM	0.5338	4.07467e4	1272.24268	100.0000

Totals :	4.07467e4	1272.24268

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak RetTime Type	Width Area	Height Area	Me
# [min]	[min] [mAU*s]	[mAU] %	N Bn
1 11.348 MM	0.5076 2.27162e4	745.91541 100.0000	CO <sub>2</sub> Et
Totals :	2.27162e4	745.91541	o 13

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak #	RetTime [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %	
1	11.361	 MM	0.5017	779.88776	25.90947	100.0000	
Total	ls :			779.88776	25,90947		

\*\*\* End of Report \*\*\*

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-30 09-53-07\021-0201.D Sample Name: BCM-GSK-463C

							-
Acq. Operator	:	SYSTEM	Seq. L	ine	:	2	
Acq. Instrument	:	CHIRAL	Locat	tion	:	21	
Injection Date	:	1/30/2018 10:14:35 AM		Inj	:	1	
			Inj Vol	lume	: 1	10.000	μl
Method	:	C:\Chem32\1\Data\Shiva_Krishr	a_Reddy_	Gudu	Iru\	\Shiva	2018-01-30 09-53-07\FAST_
		Chiral_Scout_IC_nHep_2Propand	l.M (Seq	quenc	e M	Method)	)
Last changed	:	1/30/2018 9:53:07 AM by SYSTE	M				
Method Info	:	Scouting method for normal ph	hase chir	al s	sepa	aration	ns ChiralPak IC with n-
		Heptane and Isopropanol					

Sample Info : BCM-GSK-463C Rac-Trans



Do not use Multiplier & Dilution Factor with ISTDs



CHIRAL 1/30/2018 11:18:16 AM SYSTEM

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Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-30 09-53-07\021-0201.D Sample Name: BCM-GSK-463C

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.693	MM	0.5912	7.67771e4	2164.37671	52.9255
2	13.167	MM	0.5024	6.82893e4	2265.48022	47.0745

Totals :	1.45066e5	4429.85693
TOTALS :	1.45000005	4429.80093

Signal 2: DAD1 B, Sig=220,4 Ref=off

0							<b></b> 0
Peak	RetTime	Туре	Width	Area	Height	Area	Ť
#	[min]		[min]	[mAU*s]	[mAU]	%	_NBn
1	11.693	MM	0.5323	4.81435e4	1507.34009	52.5801	N CO2
2	13.167	MM	0.4312	4.34187e4	1678.05872	47.4199	Me
Total	ls :			9.15623e4	3185.39880		16
				212302304	5205155000		racer

Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.694	MM	0.5215	1066.89661	34.09945	51.6941
2	13.167	MM	0.4184	996.96692	39.71299	48.3059
Total	s :			2063.86353	73.81244	

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\*\*\* End of Report \*\*\*

Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-30 09-53-07\022-0301.D Sample Name: BCM-GSK-447D

Acq. Operator	:	SYSTEM	Seq.	Line	:	3		
Acq. Instrument	:	CHIRAL	Loca	ation	:	22		
Injection Date	:	1/30/2018 10:35:44 AM		Inj	:	1		
			Inj Vo	olume	:	10.000	μl	
Method	:	C:\Chem32\1\Data\Shiva_Krishr	a_Reddy	_Gud	uri	u\Shiva	2018-01-30 09-53-07\FAST_	
Chiral_Scout_IC_nHep_2Propanol.M (Sequence Method)								
Last changed	:	1/30/2018 9:53:07 AM by SYSTE	M					
Method Info	Info : Scouting method for normal phase chiral separations ChiralPak IC with n- Heptane and Isopropanol							

Sample Info : BCM-GSK-447D Rac-Trans

Additional Info : Peak(s) manually integrated



CHIRAL 1/30/2018 11:19:36 AM SYSTEM

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Data File C:\Chem32\1\Data\Shiva\_Krishna\_Reddy\_Guduru\Shiva 2018-01-30 09-53-07\022-0301.D Sample Name: BCM-GSK-447D

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.075	MM	0.5460	7.75903e4	2368.44629	100.0000

Totals :	7.75903e4	2368.44629

Signal 2: DAD1 B, Sig=220,4 Ref=off

Peak RetTime # [min]	Туре	Width [min]	Area [mAU*s]	Height [mAU]	Area %	
1 13.072	 MM	0.4537	5.46944e4	2009.13867	100.0000	[
Totals :			5.46944e4	2009.13867		



Signal 3: DAD1 C, Sig=254,4 Ref=off

Peak	RetTime	Туре	Width	Area	Height	Area	
#	[min]		[min]	[mAU*s]	[mAU]	%	
1	13.072	MM	0.4200	1298.06445	51.51447	100.0000	

Totals : 1298.06445 51.51447

\*\*\* End of Report \*\*\*