

Supplementary Material

The carbamate esters as organocatalysts in asymmetric Michael addition reactions in aqueous media: when pyrrolidine backbone surpasses 1,2-diaminocyclohexane

Anirban Mondal and Kartick C. Bhowmick*

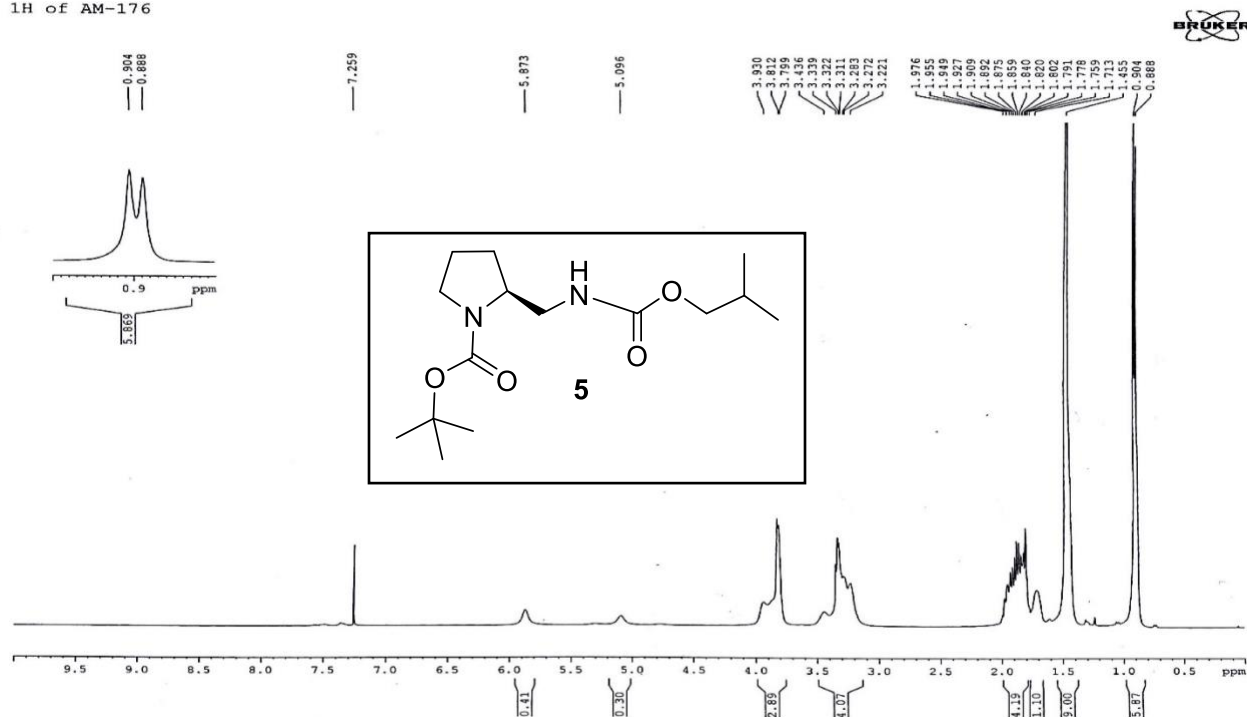
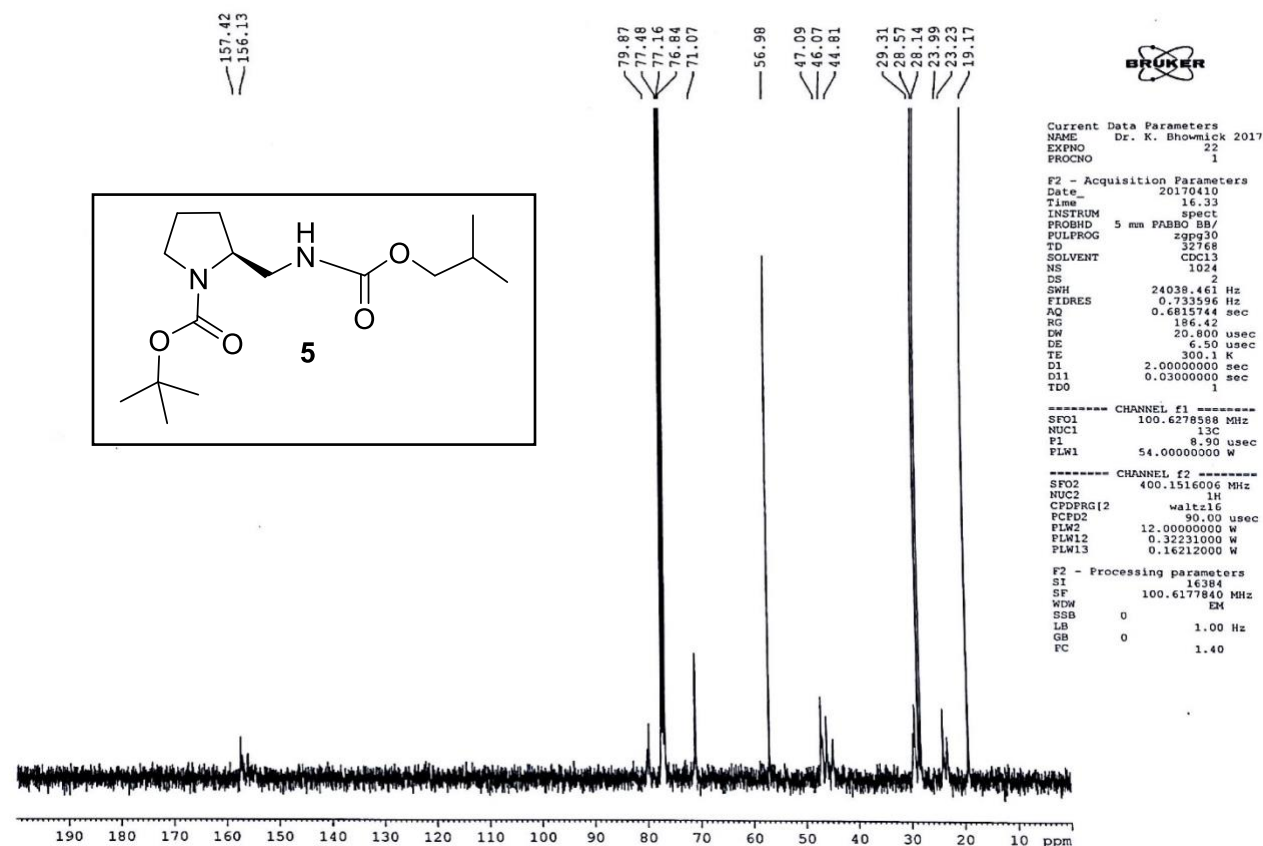
Division of Organic Synthesis, Department of Chemistry, Visva-Bharati (A Central University); Bolpur, West Bengal-731 235, India.

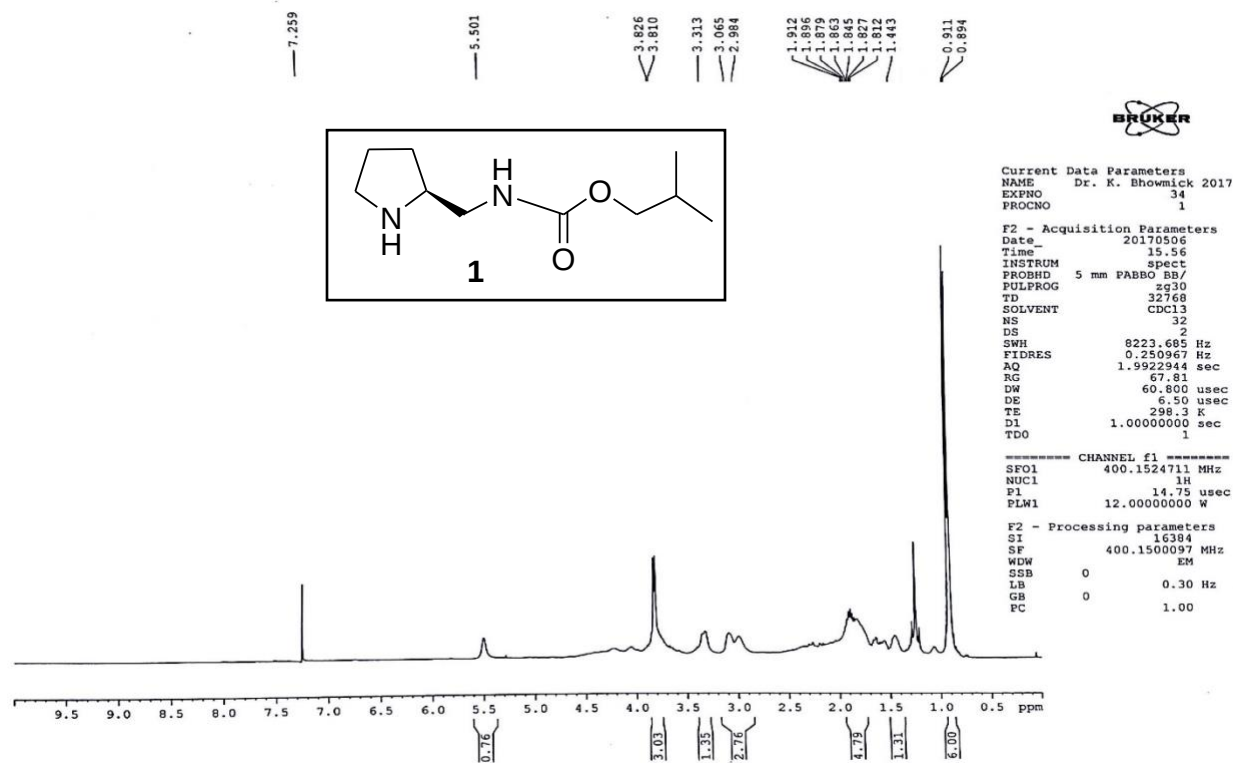
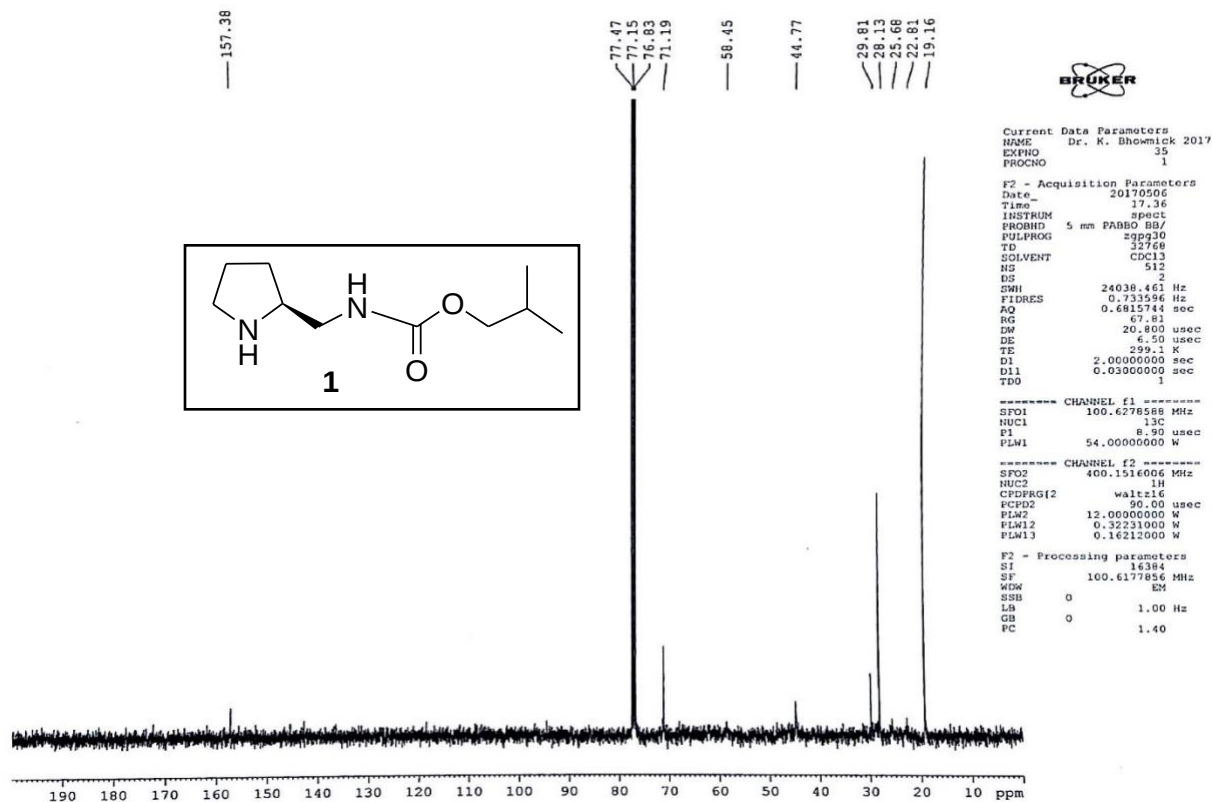
E-mail: kartickc.bhowmick@visva-bharati.ac.in

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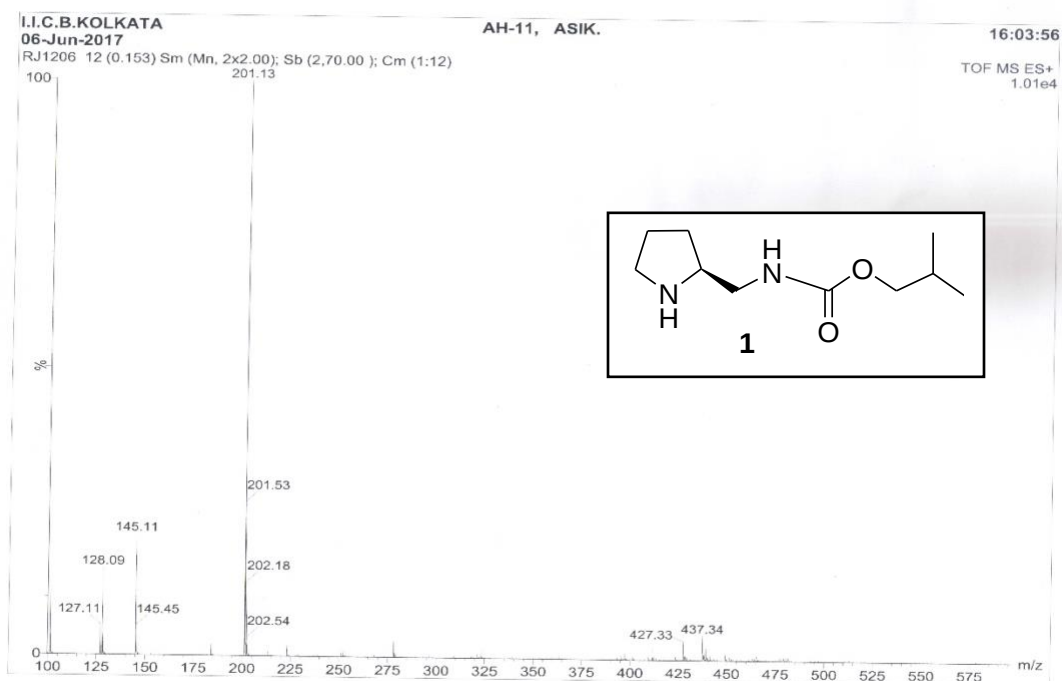
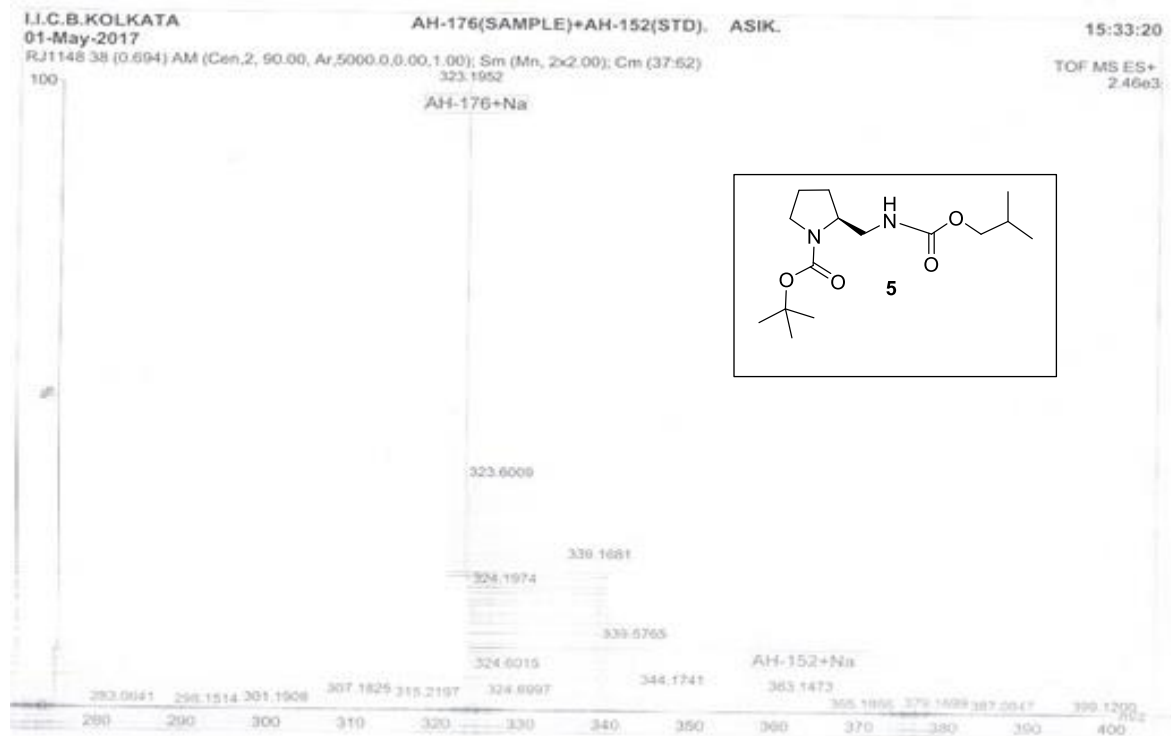
1. NMR spectra of compounds 1 & 5	S2
2. Mass spectra of compounds 1 & 5	S4
3. HPLC chromatogram of Michael Addition Products	S5

1. NMR spectra of the compound 5

 ^1H NMR ^1H of AM-176 ^{13}C NMR ^{13}C of AM-176

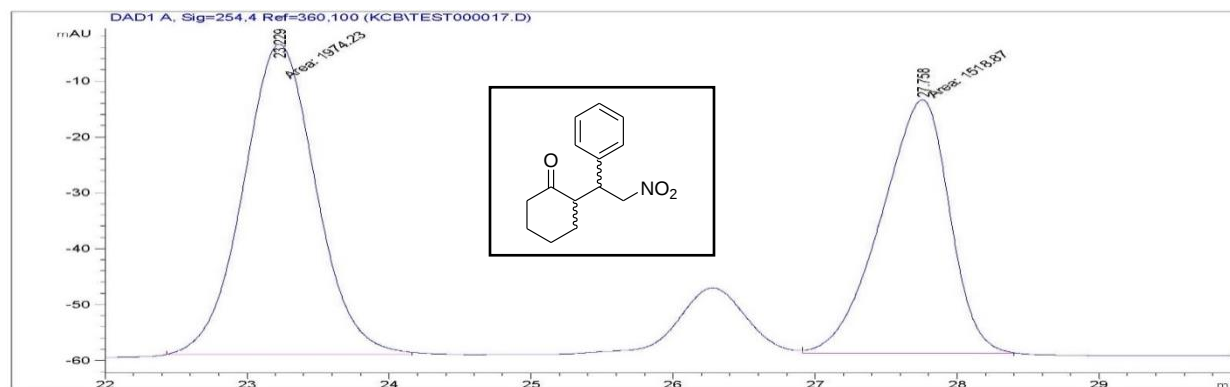
¹H NMR of organocatalyst 1¹H of AM-181¹³C NMR of organocatalyst 1¹³C of AM-181

2. Mass spectra of the compound 1 and 5



3. HPLC Data of Michael addition Products

Racemic



Area Percent Report

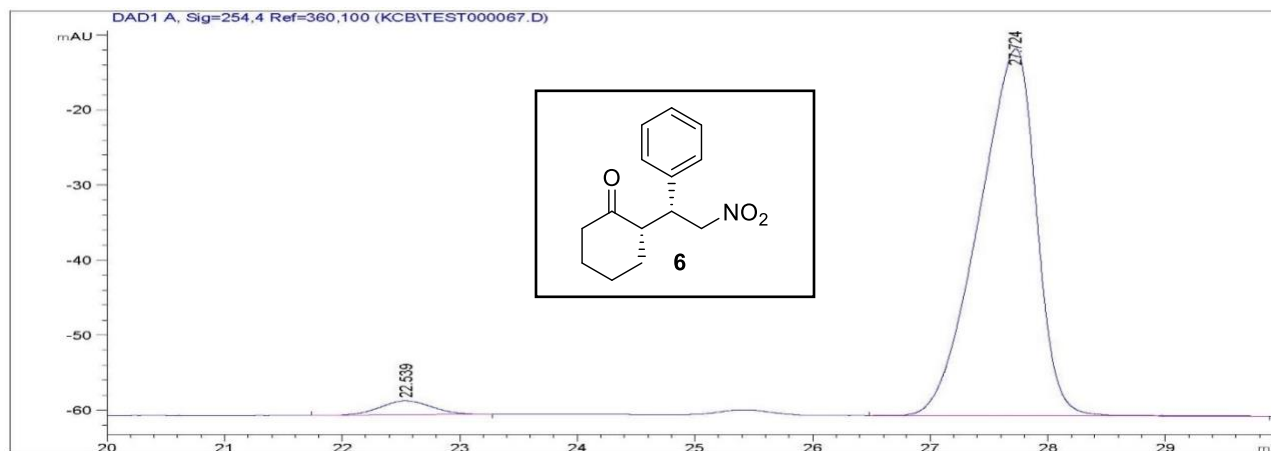
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 Use Multiplier & Dilution Factor with ISTDs

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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.229	MM	0.5926	1974.23474	55.52208	56.5180
2	27.758	MM	0.5581	1518.87329	45.36180	43.4820

Totals : 3493.10803 100.00388

Chiral



Area Percent Report

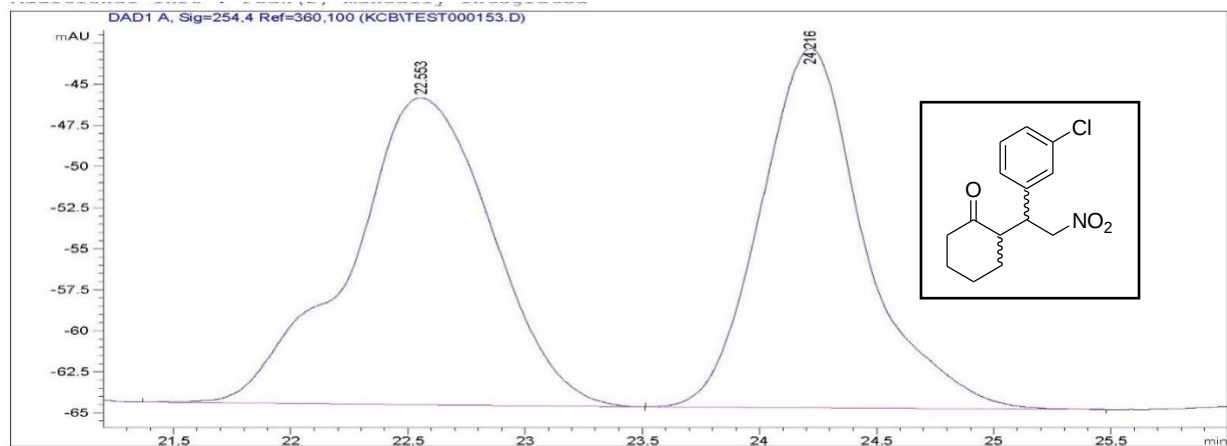
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.539	BB	0.4762	56.43361	1.84831	3.2943
2	27.724	BBA	0.5197	1656.62549	48.83812	96.7057

Totals : 1713.05910 50.68643

Racemic



Area Percent Report

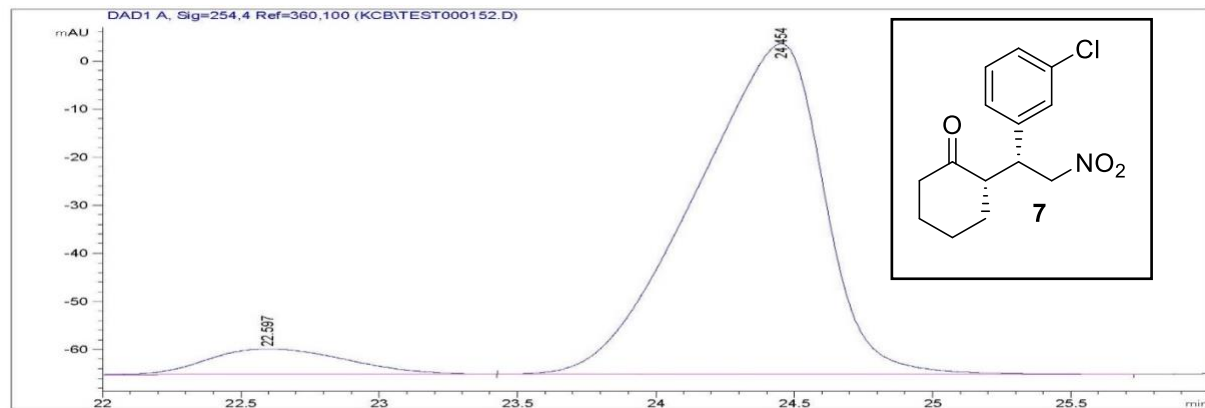
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.553	BB	0.6466	786.47101	18.70302	53.8725
2	24.216	BB	0.4668	673.40454	21.89748	46.1275

Totals : 1459.87555 40.60051

Chiral



Area Percent Report

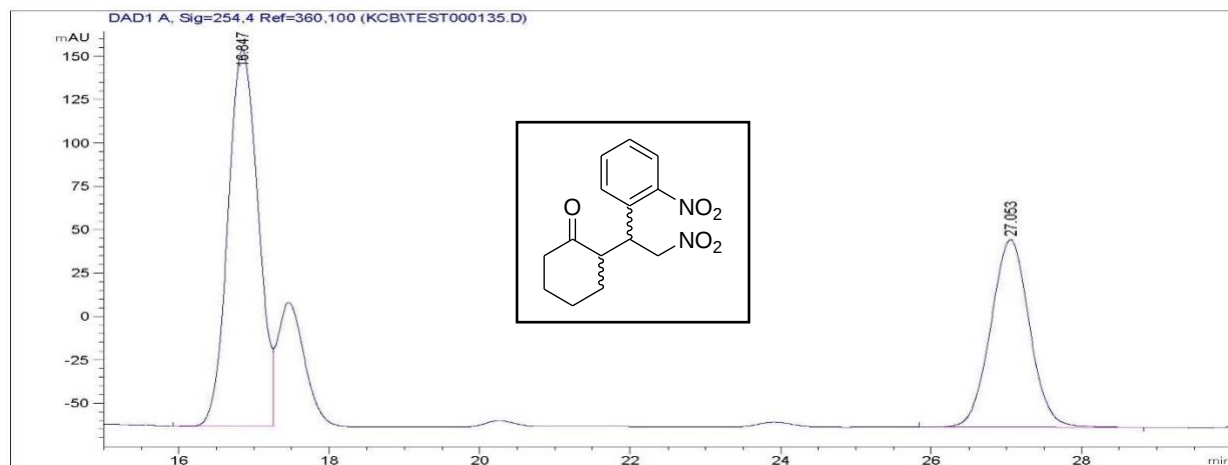
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.597	BB	0.5517	187.23883	5.33140	7.7684
2	24.454	BB	0.4796	2223.01758	68.69134	92.2316

Totals : 2410.25641 74.02274

Racemic



Area Percent Report

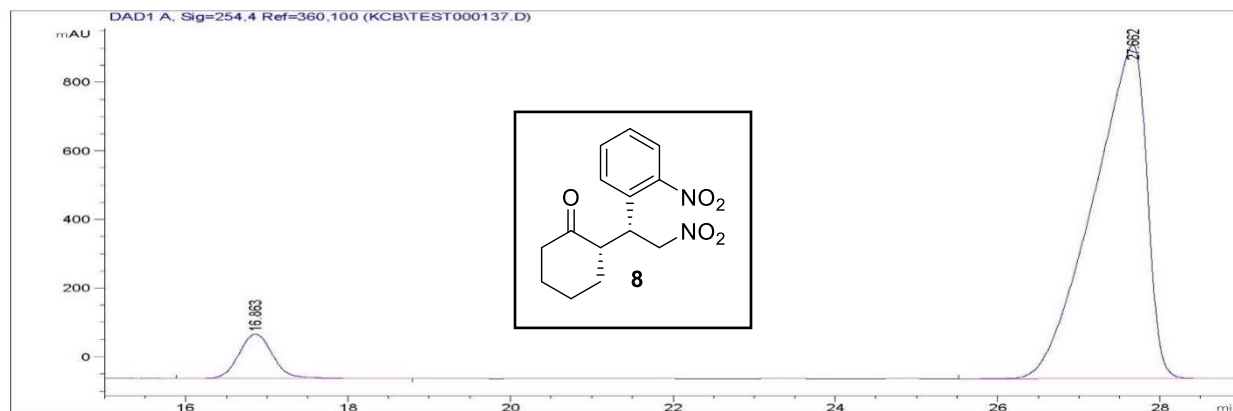
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.847	BV	0.4415	6046.09961	216.71820	61.0787
2	27.053	BB	0.5522	3852.76709	107.99067	38.9213

Totals : 9898.86670 324.70887

Chiral



Area Percent Report

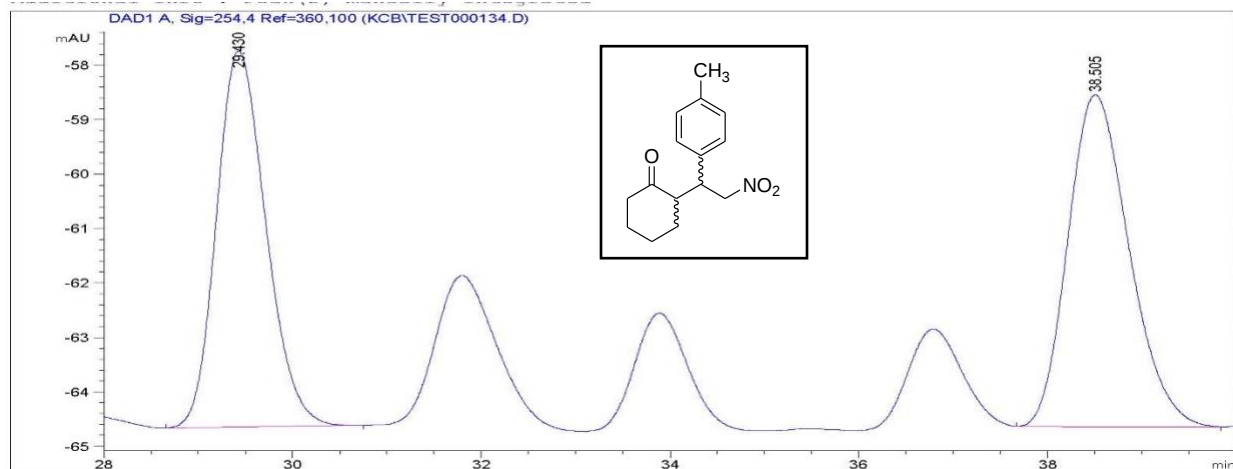
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.863	BB	0.4538	3748.36035	129.44632	7.7380
2	27.662	BBA	0.6809	4.46925e4	971.21509	92.2620

Totals : 4.84408e4 1100.66141

Racemic



Area Percent Report

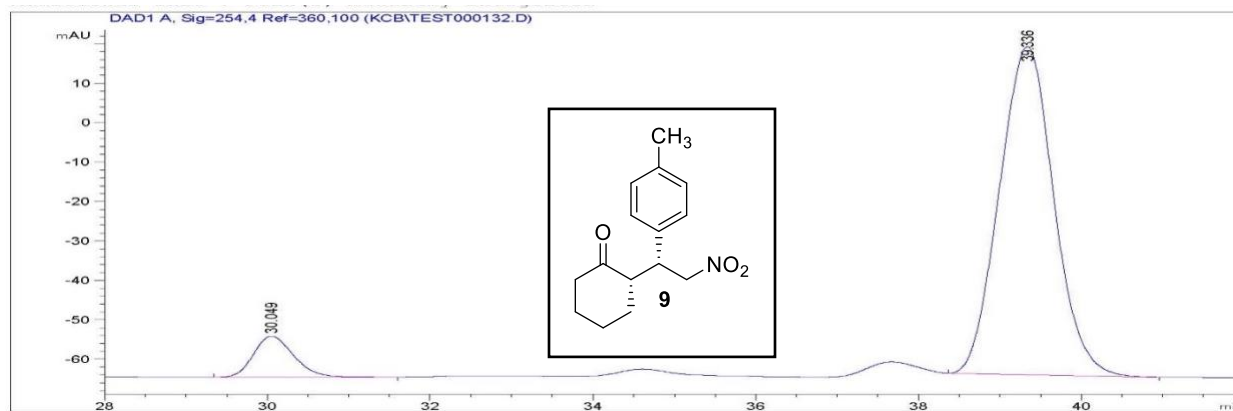
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.430	BB	0.5432	250.64798	6.90930	47.7257
2	38.505	BB	0.6693	274.53613	6.09692	52.2743

Totals : 525.18411 13.00622

Chiral



Area Percent Report

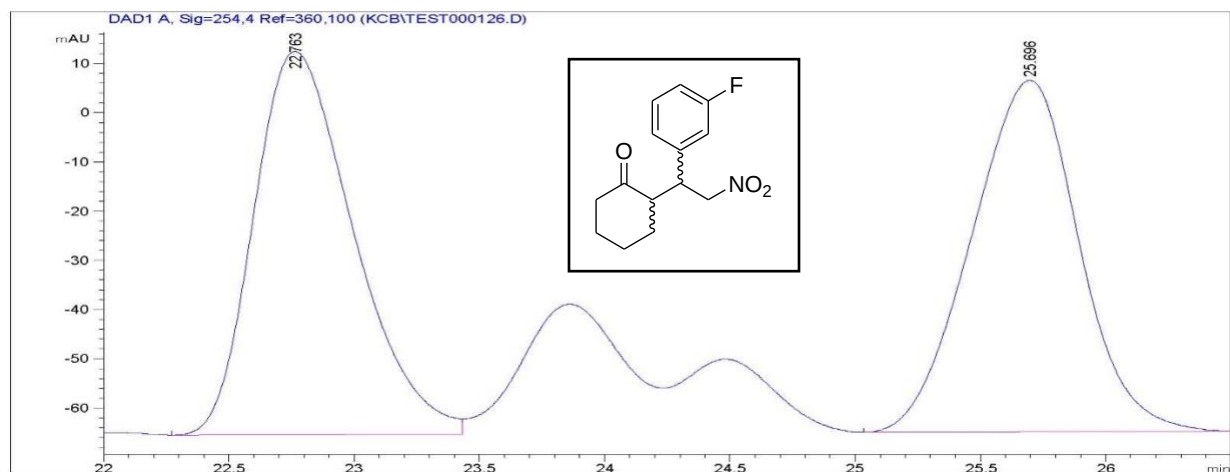
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.049	BB	0.5246	358.16095	10.43052	8.4898
2	39.336	BB	0.7250	3860.58301	83.25861	91.5102

Totals : 4218.74396 93.68913

Racemic



Area Percent Report

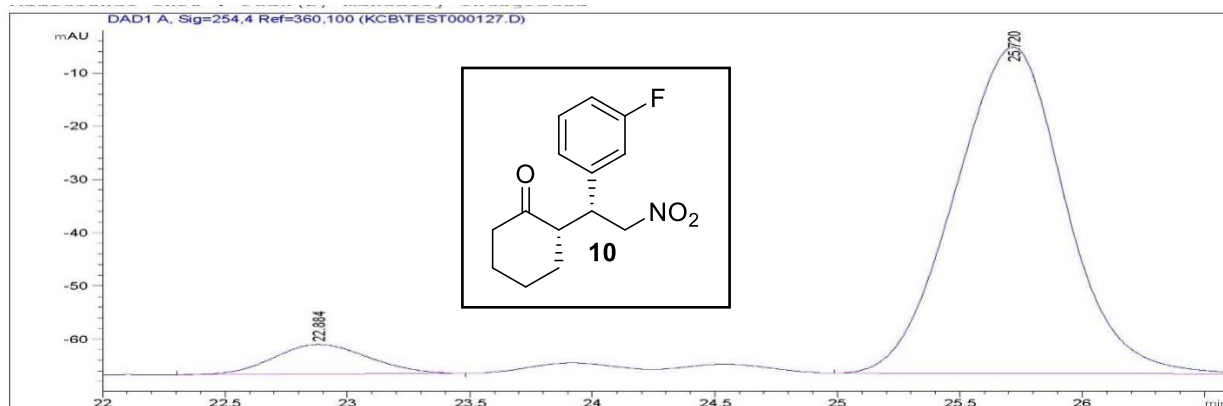
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.763	BV	0.4239	2147.28906	77.82543	50.3129
2	25.696	BB	0.4624	2120.58228	71.43094	49.6871

Totals : 4267.87134 149.25637

Chiral



Area Percent Report

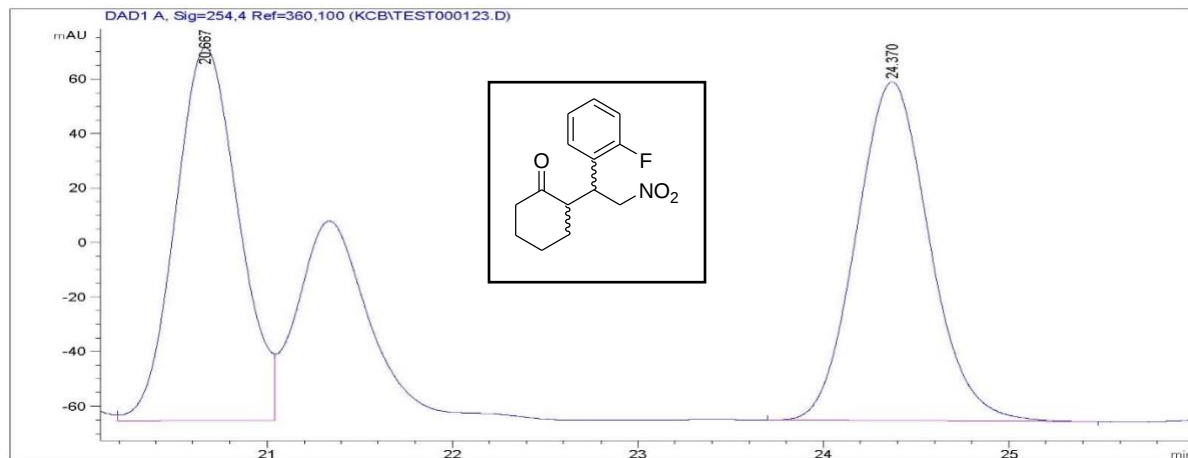
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 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.884	BB	0.4135	149.17635	5.55099	7.1885
2	25.720	BBA	0.4863	1926.02612	61.34002	92.8115

Totals : 2075.20247 66.89101

Racemic



Area Percent Report

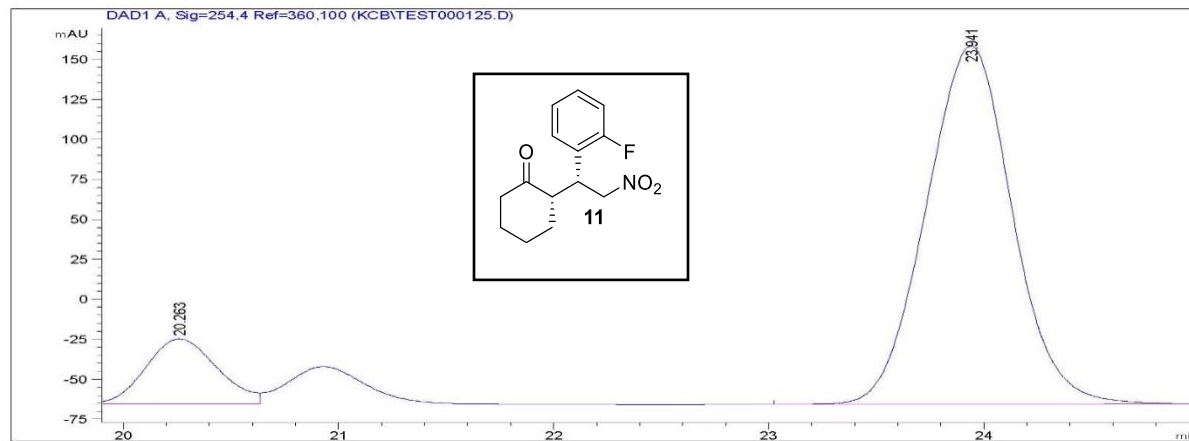
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.667	VV	0.3660	3233.63184	136.69766	48.7702
2	24.370	BB	0.4232	3396.71021	124.16700	51.2298

Totals : 6630.34204 260.86466

Chiral



Area Percent Report

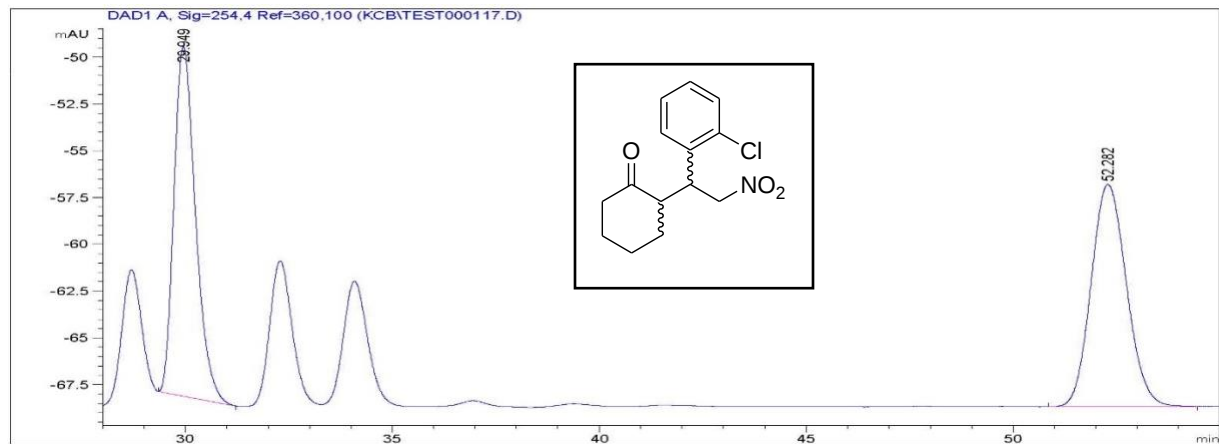
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.263	VV	0.3574	928.23480	40.50366	12.9971
2	23.941	BB	0.4318	6213.62061	223.85617	87.0029

Totals : 7141.85541 264.35983

Racemic



Area Percent Report

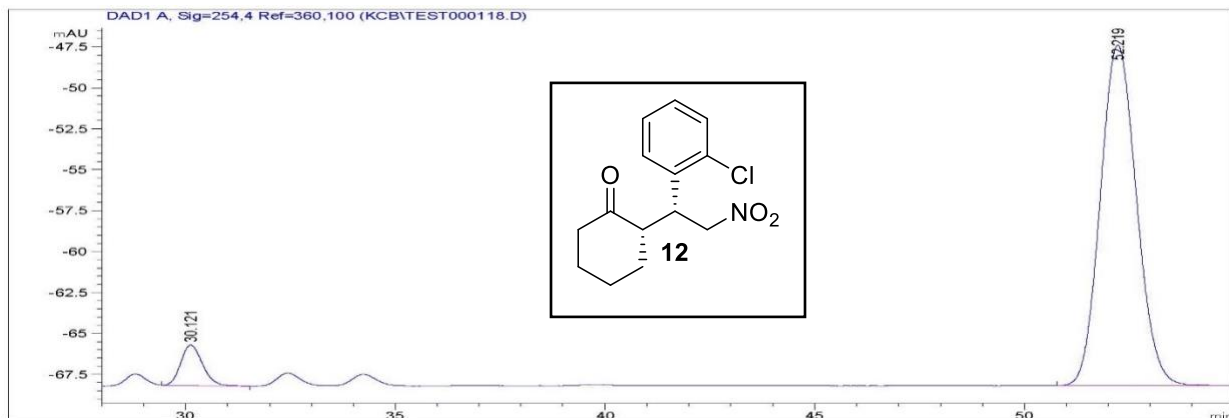
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.949	BB	0.5528	673.95917	18.68406	48.8994
2	52.282	BB	0.8822	704.29700	11.86974	51.1006

Totals : 1378.25616 30.55381

Chiral



Area Percent Report

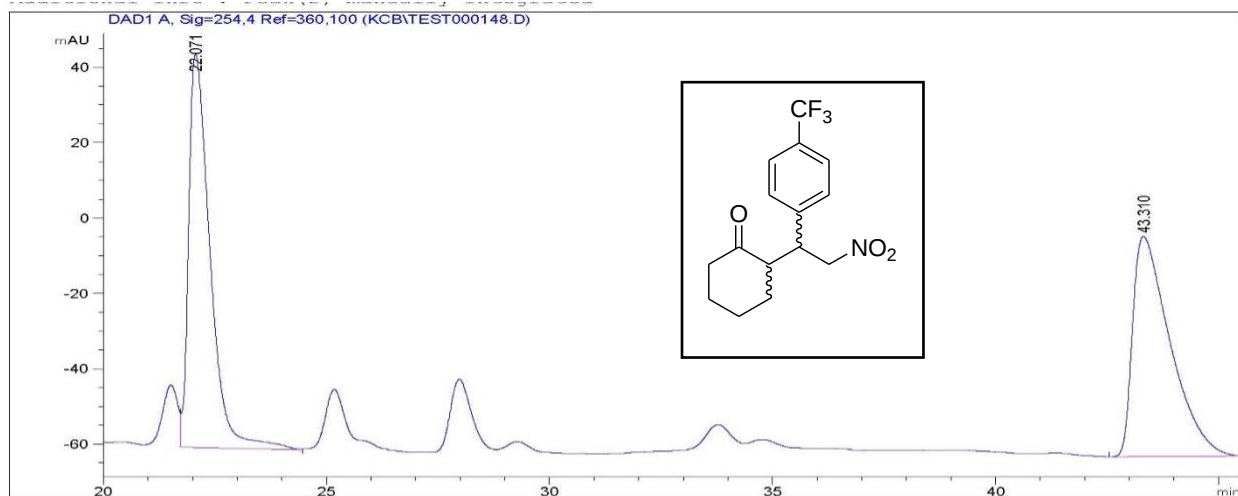
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.121	BB	0.5222	88.57727	2.47092	6.6317
2	52.219	BBA	0.9076	1247.08484	20.79625	93.3683

Totals : 1335.66211 23.26717

Racemic



Area Percent Report

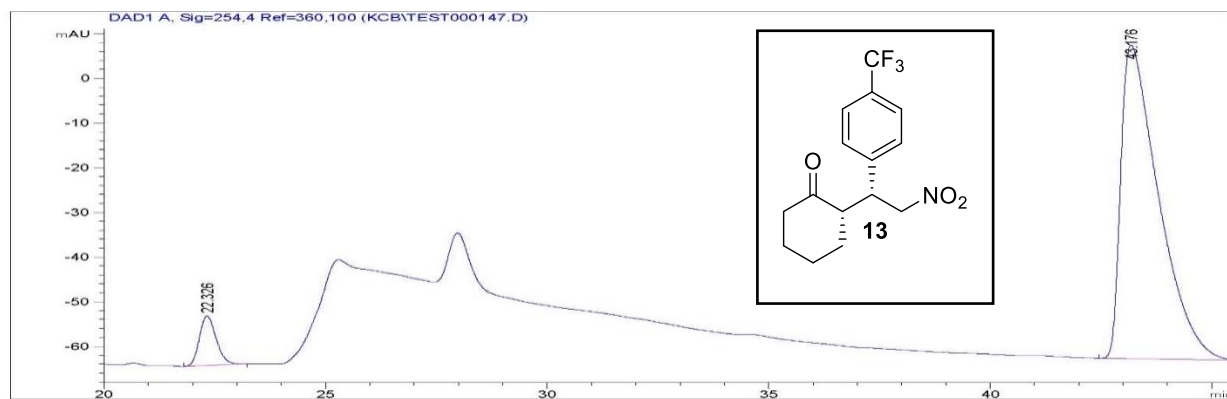
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.071	VV	0.5066	3459.63647	104.41255	50.3926
2	43.310	BB	0.8721	3405.72583	58.42039	49.6074

Totals : 6865.36230 162.83294

Chiral



Area Percent Report

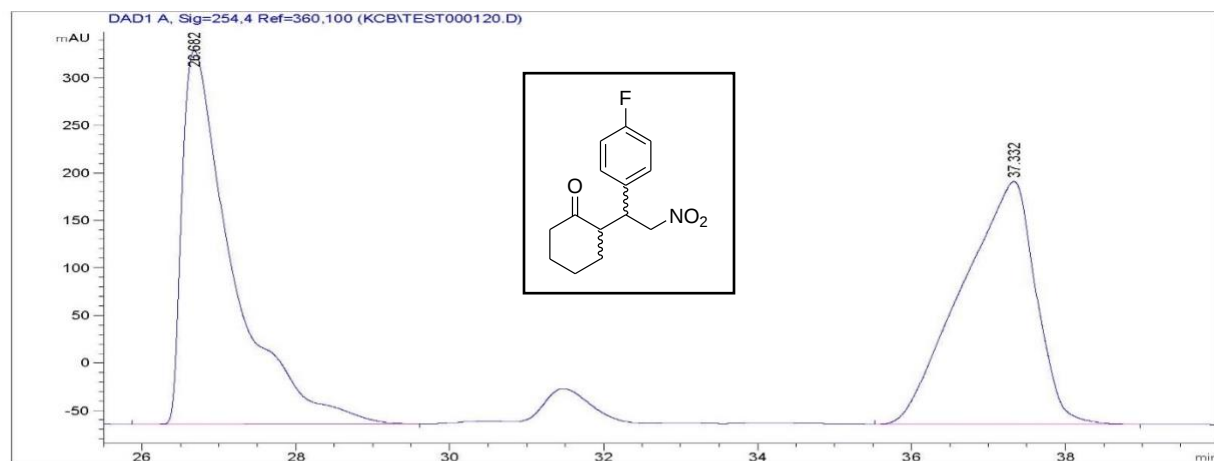
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Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.326	BB	0.4036	291.16653	11.11613	6.5592
2	43.176	BBA	0.8534	4147.91113	70.19157	93.4408

Totals : 4439.07767 81.30771

Racemic



Area Percent Report

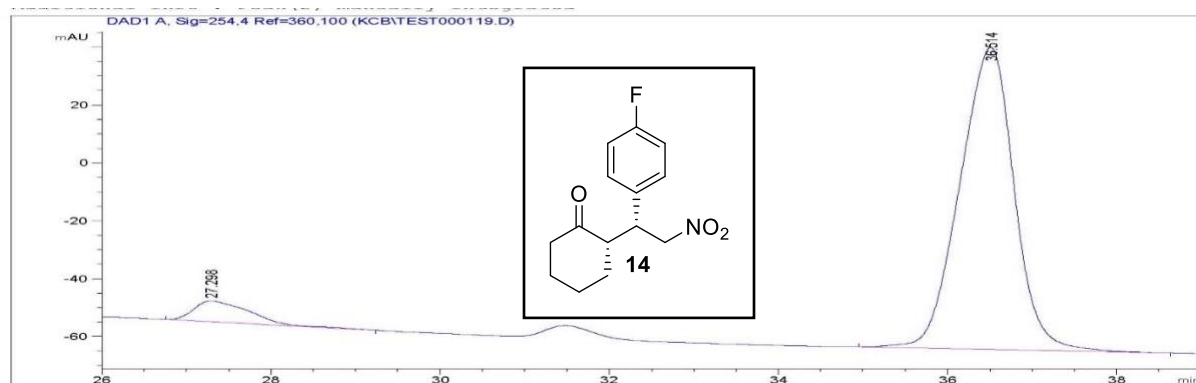
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.682	BB	0.6540	1.79314e4	393.20734	51.2681
2	37.332	BB	0.8994	1.70444e4	255.79810	48.7319

Totals : 3.49758e4 649.00543

Chiral



Area Percent Report

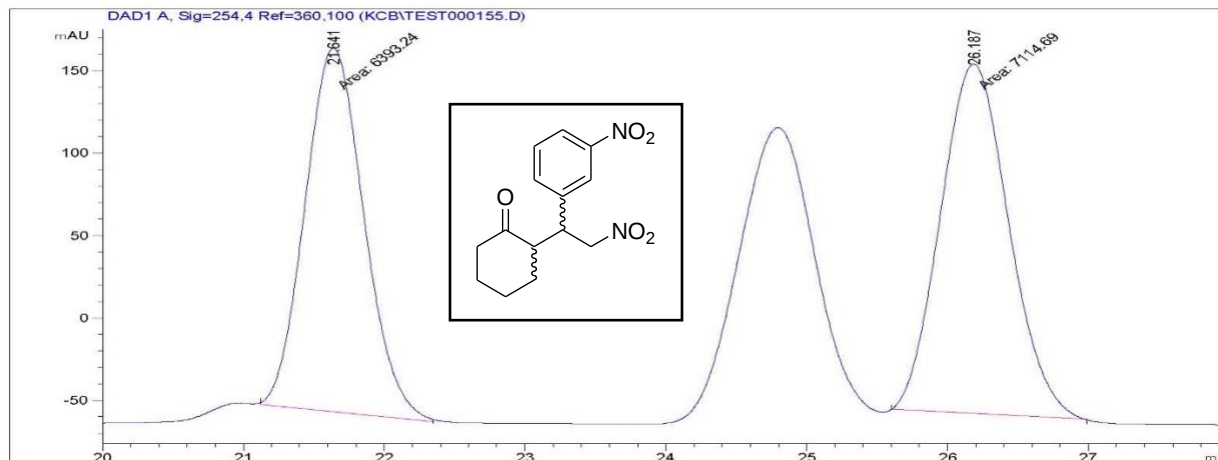
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.298	BB	0.6345	329.17538	7.15839	6.5901
2	36.514	BB	0.6934	4665.82764	104.39725	93.4099

Totals : 4995.00302 111.55564

Racemic



Area Percent Report

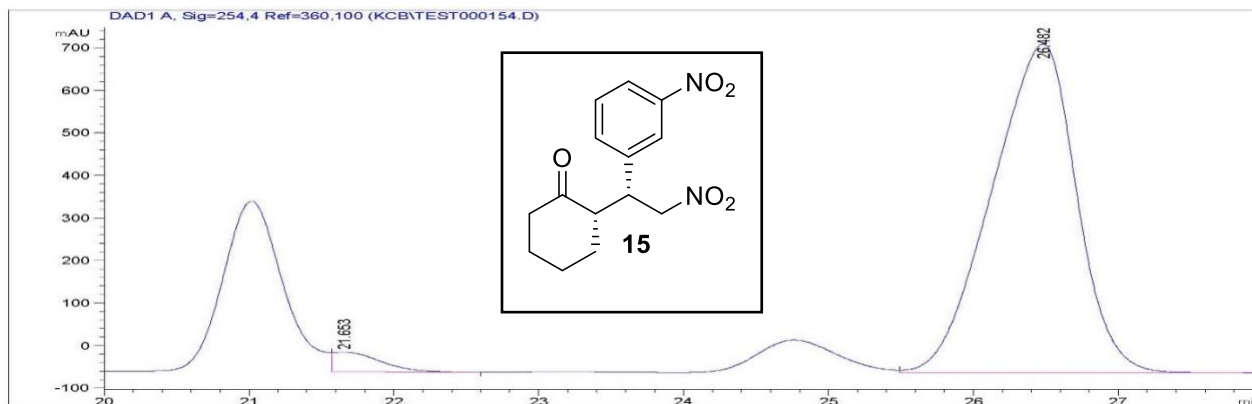
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.641	MM	0.4833	6393.24023	220.47656	47.3295
2	26.187	MM	0.5595	7114.69189	211.95001	52.6705

Totals : 1.35079e4 432.42657

Chiral



Area Percent Report

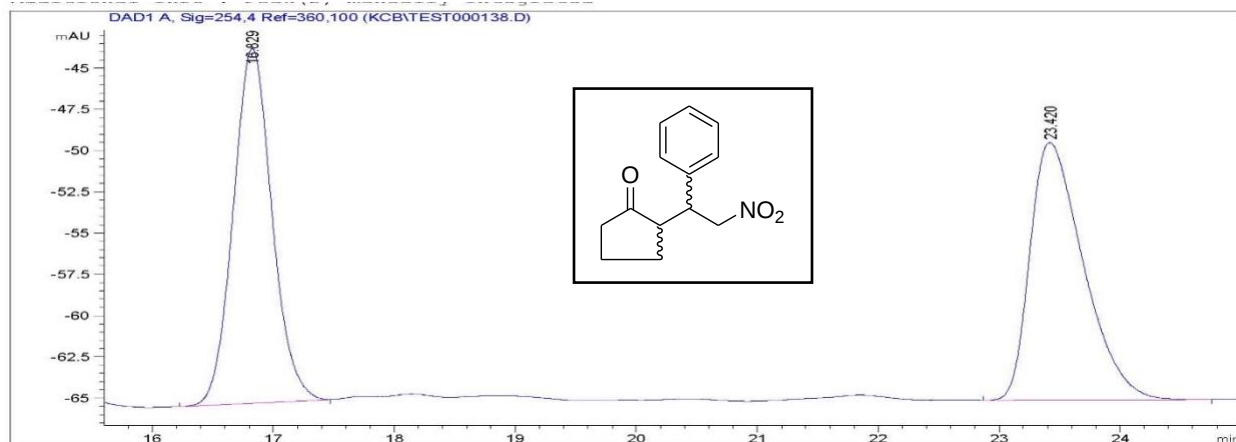
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.653	VB	0.3428	1050.89331	46.30445	3.2475
2	26.482	VB	0.6386	31309.1e4	772.96631	96.7525

Totals : 3.23600e4 819.27076

Racemic



Area Percent Report

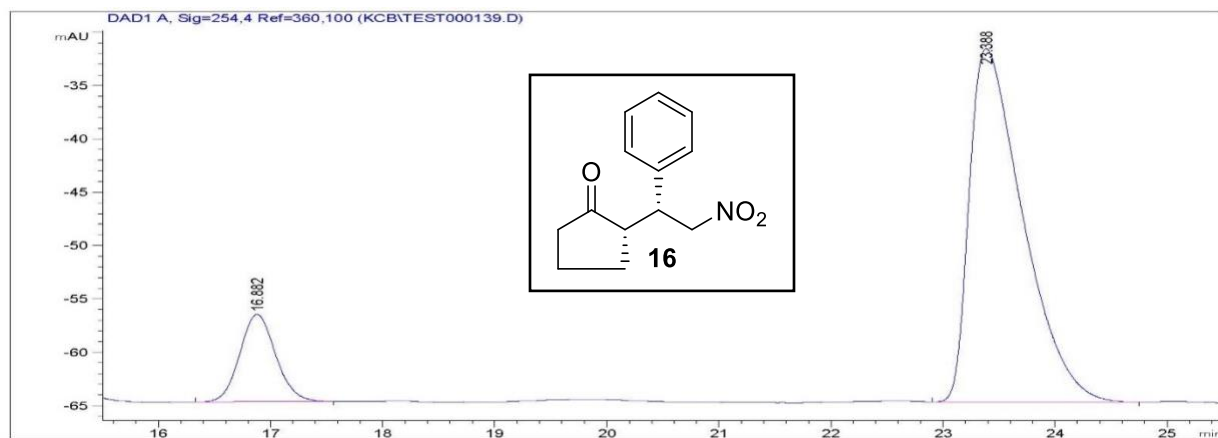
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.829	BB	0.3414	478.75424	21.52957	50.0531
2	23.420	BB	0.4690	477.73895	15.61443	49.9469

Totals : 956.49319 37.14400

Chiral



Area Percent Report

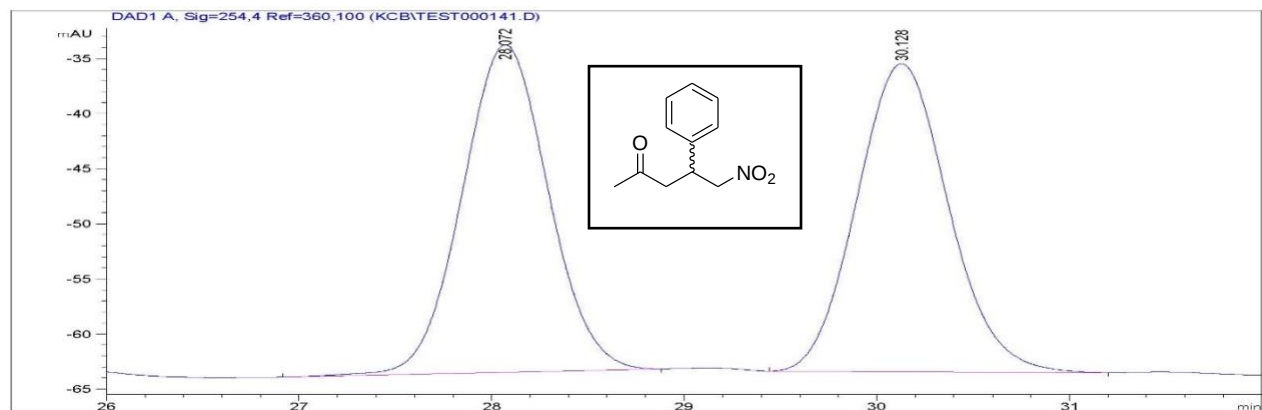
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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.882	BB	0.3426	181.25787	8.17723	14.1850
2	23.388	BB	0.4965	1096.55823	33.09870	85.8150

Totals : 1277.81610 41.27593

Racemic



Area Percent Report

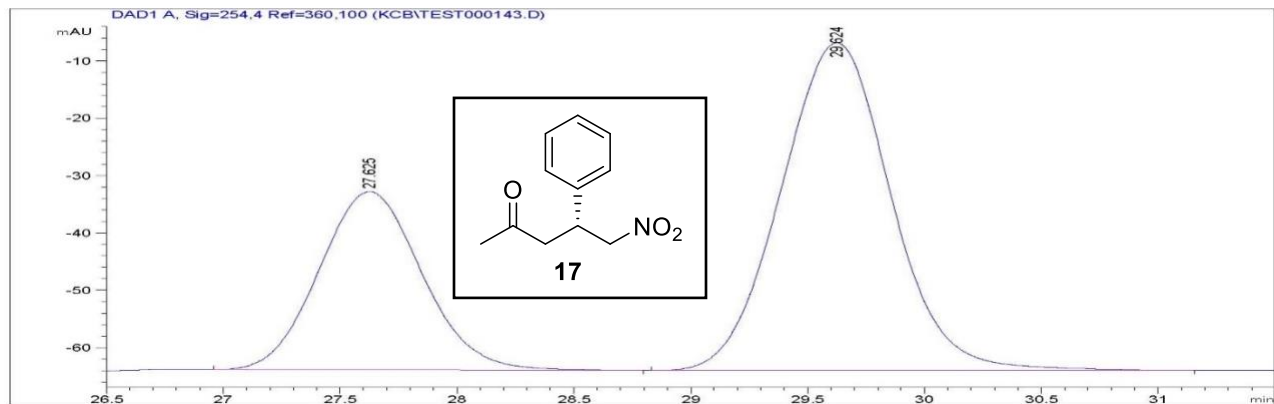
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Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.072	BB	0.4845	922.46887	29.68477	50.0144
2	30.128	BB	0.5131	921.93939	27.92962	49.9856

Totals : 1944.40826 57.61439

Chiral



Area Percent Report

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.625	BB	0.4751	950.46588	31.05261	33.7824
2	29.624	BB	0.5024	1863.02625	57.14528	66.2176

Totals : 2813.49213 88.19789