

# **Enantiomeric scaffolding of $\alpha$ -tetralone and related scaffolds by EKR (Enzymatic Kinetic Resolution) and stereoselective ketoreduction with ketoreductases**

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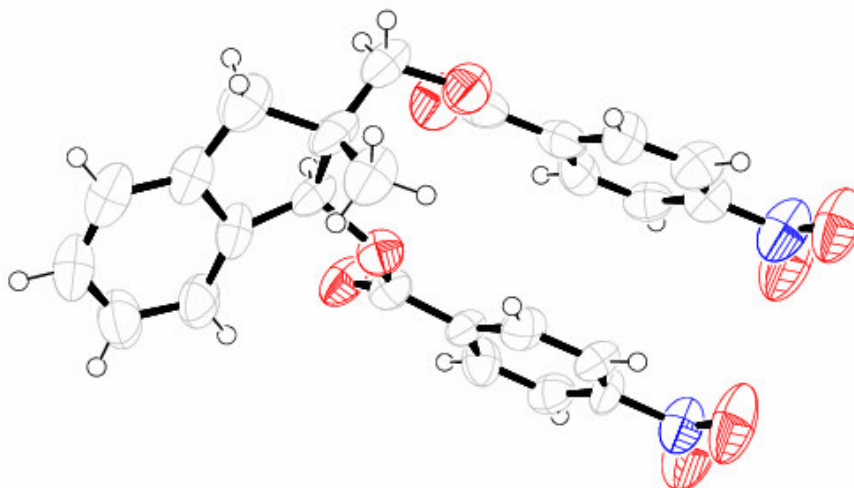
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## **Supporting Information Part II**

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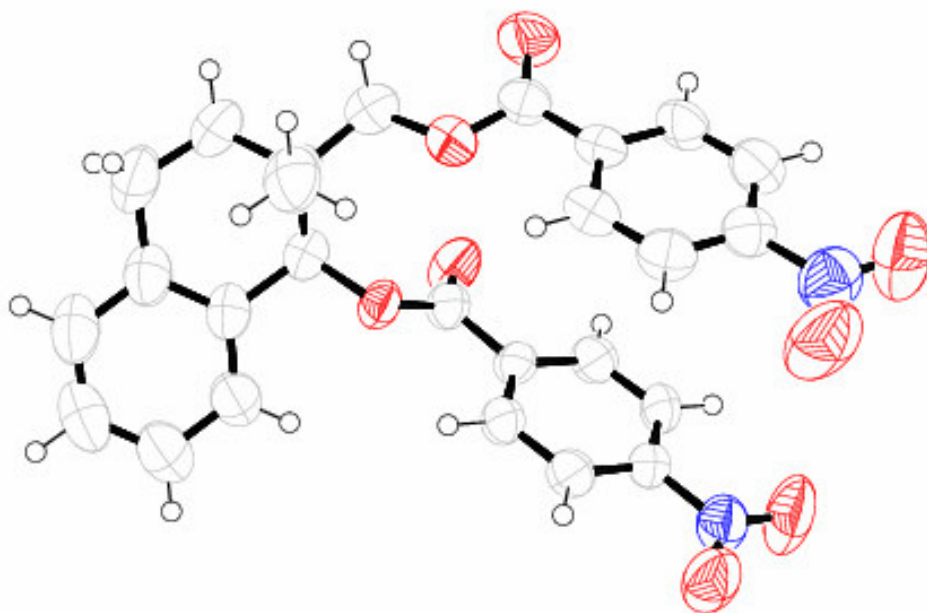
X-ray crystal data of bis-paranitrobenzoate derivative of compound **27** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 830578).



Empirical formula	C <sub>25</sub> H <sub>20</sub> N <sub>2</sub> O <sub>8</sub>
Formula weight	476.43
Temperature	293 K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P 1
Unit cell dimensions	a = 6.717(3) Å b = 7.176(3) Å c = 12.147(4) Å α = 99.024(11)° β = 99.364(12)° γ = 91.872(11)°
Volume, Z	569.5(4) Å <sup>3</sup> , 1
Density	1.389 Mg/m <sup>3</sup>
Crystal description	Prism
Crystal color	Colorless
Absorption coefficient	0.105 mm <sup>-1</sup>
F (000)	248

Crystal size	0.2 x 0.2 x 0.1 mm <sup>3</sup>
Reflections collected	5184
$\theta$ range for data collection	1.72 to 22.39°
Independent reflections	2942 [R (int) = 0.0654]
Goodness -of-fit on F <sup>2</sup>	0.997
Limiting indices	-6<= <i>h</i> <=7, -7<= <i>k</i> <=7, -12<= <i>l</i> <=13
Data/ restraints/parameters	2942/3/317
Final R indices [1>2 $\sigma$ (I)]	R1 = 0.0769, wR2 = 0.1893
R indices (all data)	R1 = 0.1285, wR2 = 0.2251
Absolute structure parameter	-1(4)

X-ray crystal data of bis-paranitrobenzoate derivative of compound **18** (the following crystal has been deposited at the Cambridge Crystallographic Data Centre and has the deposition number CCDC 830577).

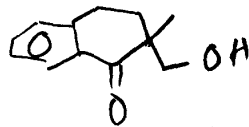


Empirical formula	C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub>
Formula weight	490.46
Temperature	293 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P 21
Unit cell dimensions	a = 6.805(5) Å b = 13.163(5) Å c = 13.478(5) Å $\alpha$ = 90.000(5)° $\beta$ = 99.373(5)° $\gamma$ = 90.000(5)°
Volume, Z	1191.2 (11) Å <sup>3</sup> , 2
Density	1.367 Mg/m <sup>3</sup>
Crystal description	Prism
Crystal color	Colorless
Absorption coefficient	0.103 mm <sup>-1</sup>
F (000)	512
Crystal size	0.2 x 0.2 x 0.1 mm <sup>3</sup>
Reflections collected	12580
$\theta$ range for data collection	1.53 to 23.75°
Independent reflections	3609 [R (int) = 0.0524]
Goodness -of-fit on F <sup>2</sup>	0.985
Limiting indices	-7<= $h$ <=7, -14<= $k$ <=14, -15<= $l$ <=15
Data/ restraints/parameters	3609/1/329
Final R indices [I>2 $\sigma$ (I)]	R1 = 0.0459, wR2 = 0.0823
R indices (all data)	R1 = 0.0973, wR2 = 0.1016
Absolute structure parameter	-0.5(15)

# HPLC chromatogram of racemic 1

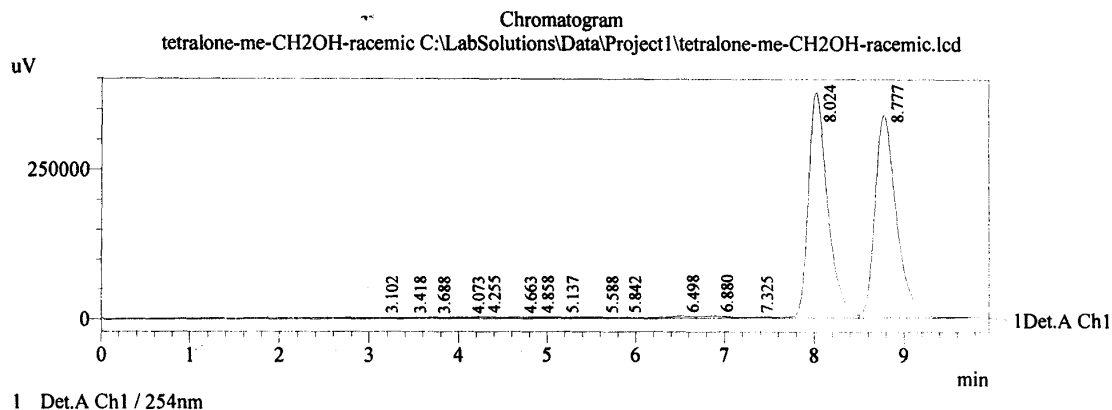
Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : tetralone-me-CH2OH-racemic  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : tetralone-me-CH2OH-racemic.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/29/2008 2:29:46 PM  
Data Processed : 10/29/2008 2:39:51 PM



(I)

hex: iPr n: 9:1  
1ml/min



PeakTable

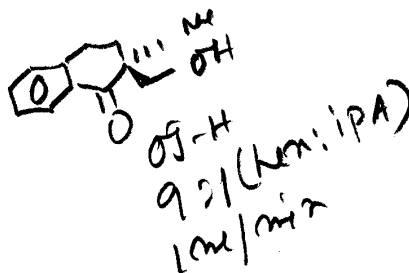
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.102	184600	1421	1.561	0.193
2	3.418	17959	1278	0.152	0.173
3	3.688	17005	1316	0.144	0.179
4	4.073	30087	1470	0.254	0.199
5	4.255	35428	2398	0.300	0.325
6	4.663	21817	1519	0.185	0.206
7	4.858	19749	1466	0.167	0.199
8	5.137	27106	1511	0.229	0.205
9	5.588	37566	1453	0.318	0.197
10	5.842	19553	1411	0.165	0.192
11	6.498	71566	3533	0.605	0.480
12	6.880	71525	3092	0.605	0.420
13	7.325	11699	1050	0.099	0.143
14	8.024	5623002	376092	47.562	51.052
15	8.777	5633781	337681	47.653	45.838
Total		11822441	736691	100.000	100.000

## HPLC chromatogram of (S)- 1

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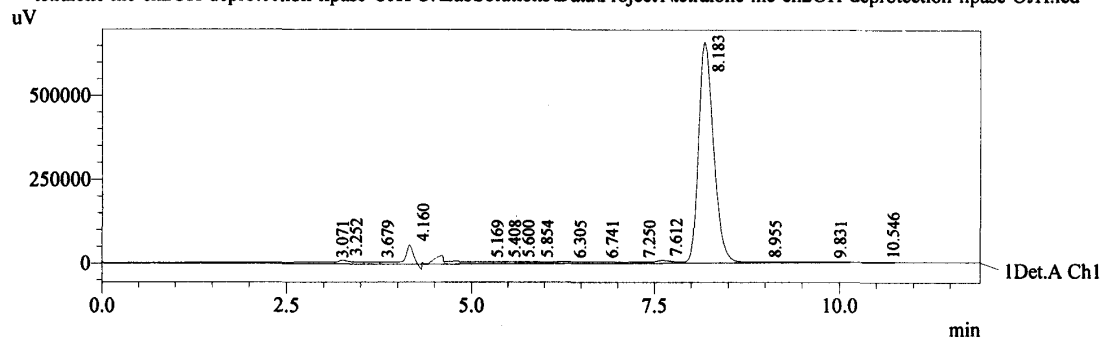
#### Sample Information

Acquired by : Admin  
Sample Name : tetralone-me-ch2OH-deprotection-lipase-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : tetralone-me-ch2OH-deprotection-lipase-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/4/2009 4:27:33 PM  
Data Processed : 5/4/2009 4:39:28 PM



#### Chromatogram

tetralone-me-ch2OH-deprotection-lipase-OJH C:\LabSolutions\Data\Project1\tetralone-me-ch2OH-deprotection-lipase-OJH.lcd



1 Det.A Ch1 / 254nm

#### PeakTable

Detector A Ch1 254nm

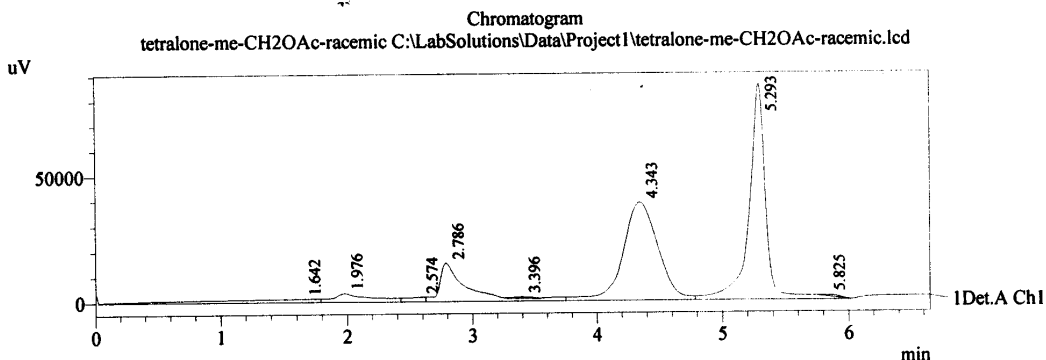
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.071	453356	4451	3.899	0.573
2	3.252	156010	10793	1.342	1.390
3	3.679	62813	4944	0.540	0.637
4	4.160	418146	55507	3.596	7.151
5	5.169	445196	5558	3.829	0.716
6	5.408	49058	5145	0.422	0.663
7	5.600	74754	4986	0.643	0.642
8	5.854	81433	4753	0.700	0.612
9	6.305	137945	4775	1.186	0.615
10	6.741	114132	4402	0.982	0.567
11	7.250	66711	3239	0.574	0.417
12	7.612	154494	8209	1.329	1.058
13	8.183	9407646	659167	80.915	84.921
14	8.955	1403	45	0.012	0.006
15	9.831	1938	114	0.017	0.015
16	10.546	1561	122	0.013	0.016
Total		11626597	776210	100.000	100.000

## HPLC chromatogram of acetate derivative of racemic 1

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### Sample Information

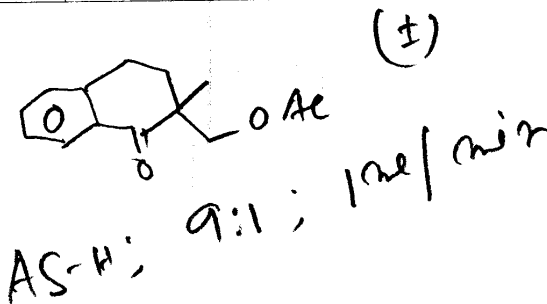
Acquired by : Admin  
Sample Name : tetralone-me-CH2OAc-racemic  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : tetralone-me-CH2OAc-racemic.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/29/2008 4:04:59 PM  
Data Processed : 10/29/2008 4:11:42 PM



### PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	1.642	80789	1172	4.127	0.799
2	1.976	70669	3357	3.610	2.289
3	2.574	18210	1637	0.930	1.116
4	2.786	239421	15161	12.232	10.337
5	3.396	4177	457	0.213	0.312
6	4.343	751793	38695	38.409	26.383
7	5.293	787501	85820	40.233	58.513
8	5.825	4794	368	0.245	0.251
Total		1957353	146668	100.000	100.000

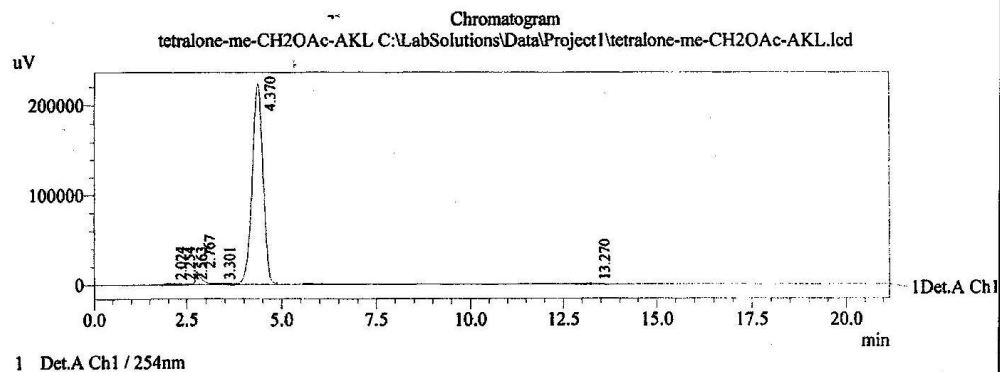
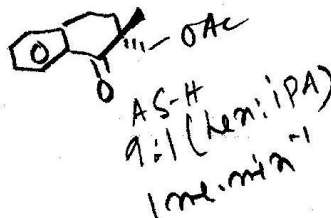


## HPLC chromatogram of (*R*)-acetate derivative of 1

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Sample Information

Acquired by : Admin  
Sample Name : tetralone-me-CH<sub>2</sub>OAc-AKL  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5  $\mu$ L  
Data Filename : tetralone-me-CH<sub>2</sub>OAc-AKL.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/29/2008 4:31:24 PM  
Data Processed : 10/29/2008 4:54:25 PM

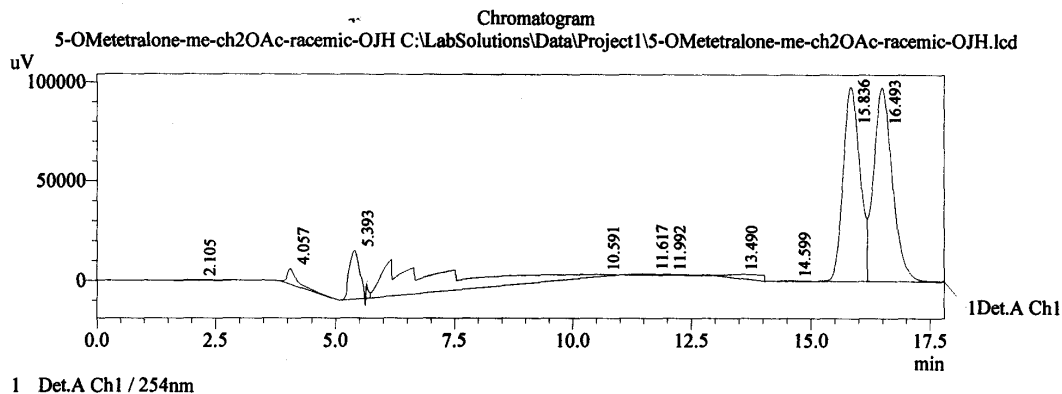




# HPLC chromatogram of acetate derivative of racemic 2

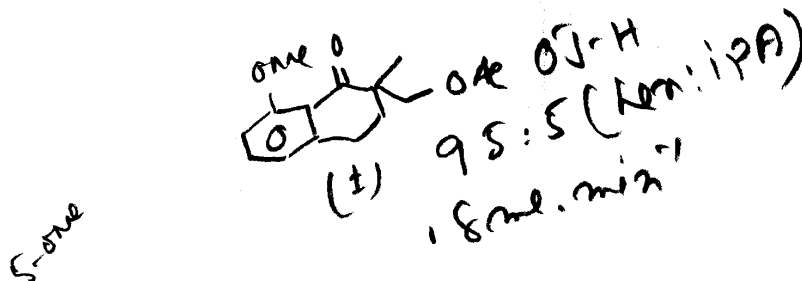
Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 5-OMetetalone-me-ch2OAc-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 5-OMetetalone-me-ch2OAc-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/11/2009 3:18:45 PM  
Data Processed : 5/11/2009 3:37:21 PM



PeakTable

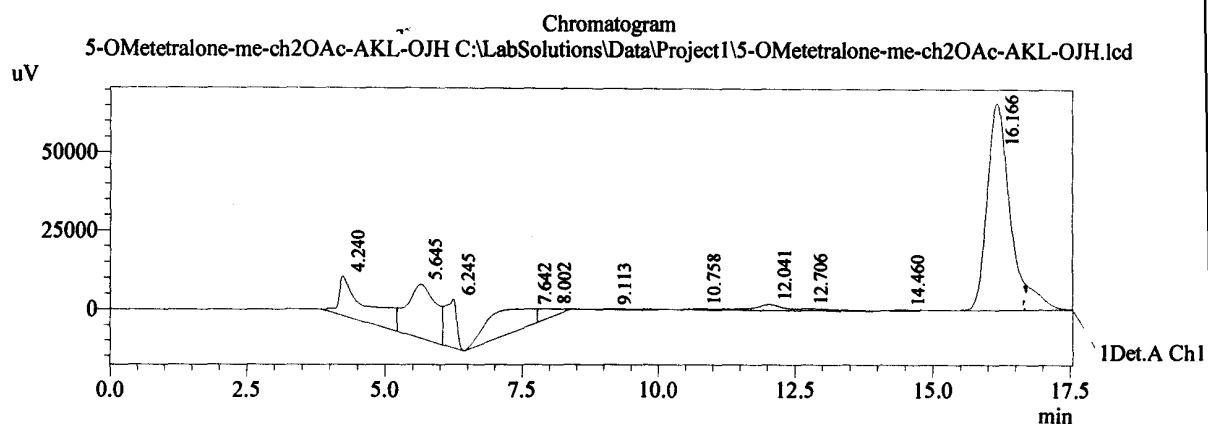
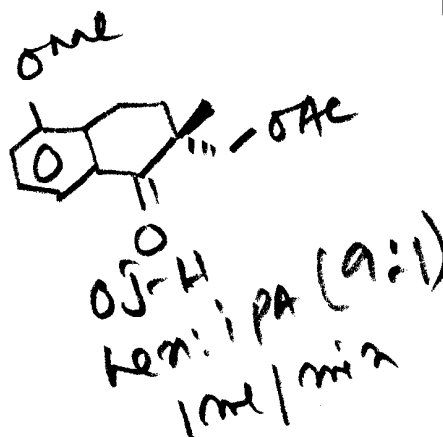
Peak#	Ret. Time	Area	Height	Area %	Height %
1	2.105	8711	266	0.118	0.115
2	4.057	105547	7782	1.426	3.363
3	5.393	384721	24258	5.199	10.483
4	10.591	1694525	816	22.901	0.352
5	11.617	13998	460	0.189	0.199
6	11.992	8095	280	0.109	0.121
7	13.490	107142	1851	1.448	0.800
8	14.599	1806	83	0.024	0.036
9	15.836	2392447	97998	32.333	42.350
10	16.493	2682330	97609	36.251	42.182
Total		7399322	231402	100.000	100.000



# HPLC chromatogram of (R)-acetate derivative of 2

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Sample Information  
Acquired by : Admin  
Sample Name : 5-OMetetalone-me-ch2OAc-AKL-OJH  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : 5-OMetetalone-me-ch2OAc-AKL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/11/2009 3:39:38 PM  
Data Processed : 5/11/2009 3:58:23 PM



Detector A Ch1 254nm

PeakTable

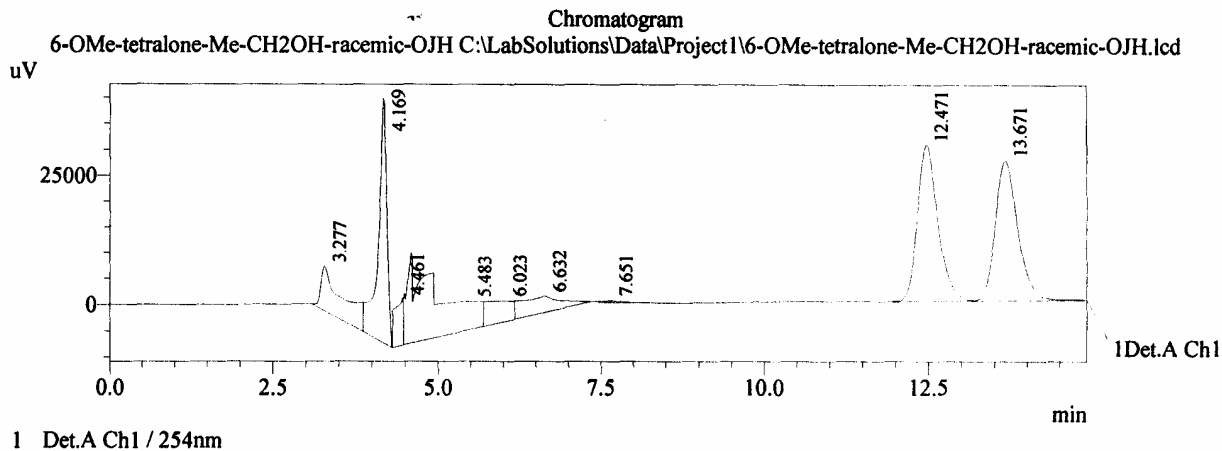
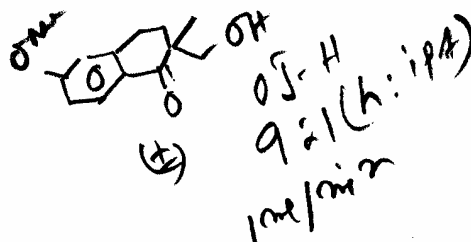
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.240	453496	12399	11.631	10.179
2	5.645	633500	17077	16.248	14.019
3	6.245	224736	15555	5.764	12.769
4	7.642	446486	5130	11.452	4.211
5	8.002	74632	2668	1.914	2.191
6	9.113	4007	138	0.103	0.113
7	10.758	7499	228	0.192	0.187
8	12.041	58059	1699	1.489	1.395
9	12.706	21604	524	0.554	0.430
10	14.460	4443	231	0.114	0.190
11	16.166	1970427	66165	50.538	54.317
Total		3898890	121814	100.000	100.000

## HPLC chromatogram of racemic 3

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Sample Information

Acquired by : Admin  
Sample Name : 6-OMe-tetralone-Me-CH<sub>2</sub>OH-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 µL  
Data Filename : 6-OMe-tetralone-Me-CH<sub>2</sub>OH-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 7/8/2009 8:46:24 AM  
Data Processed : 7/8/2009 9:02:35 AM



PeakTable

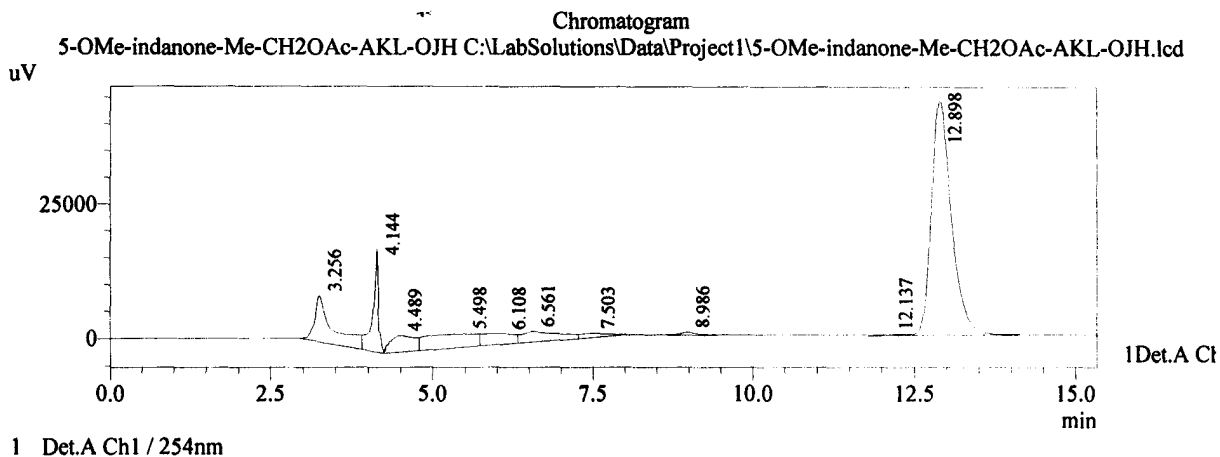
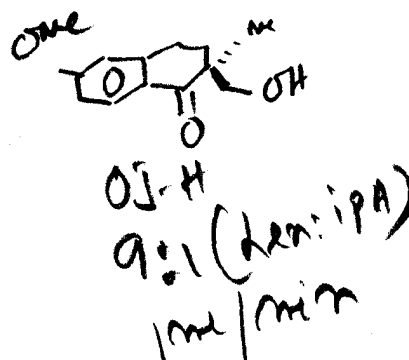
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.277	203172	8464	7.134	6.289
2	4.169	426918	47140	14.990	35.026
3	4.461	77876	9001	2.734	6.688
4	5.483	581109	5301	20.404	3.939
5	6.023	118640	3887	4.166	2.888
6	6.632	136762	3117	4.802	2.316
7	7.651	3114	249	0.109	0.185
8	12.471	652369	30337	22.906	22.540
9	13.671	648045	27092	22.754	20.130
Total		2848005	134588	100.000	100.000

# HPLC chromatogram of (S)-3

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Sample Information  
Acquired by : Admin  
Sample Name : 5-OMe-indanone-Me-CH2OAc-AKL-OJH  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : 5-OMe-indanone-Me-CH2OAc-AKL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 8/7/2009 3:27:37 PM  
Data Processed : 8/7/2009 3:44:06 PM



PeakTable

Detector A Ch1 254nm

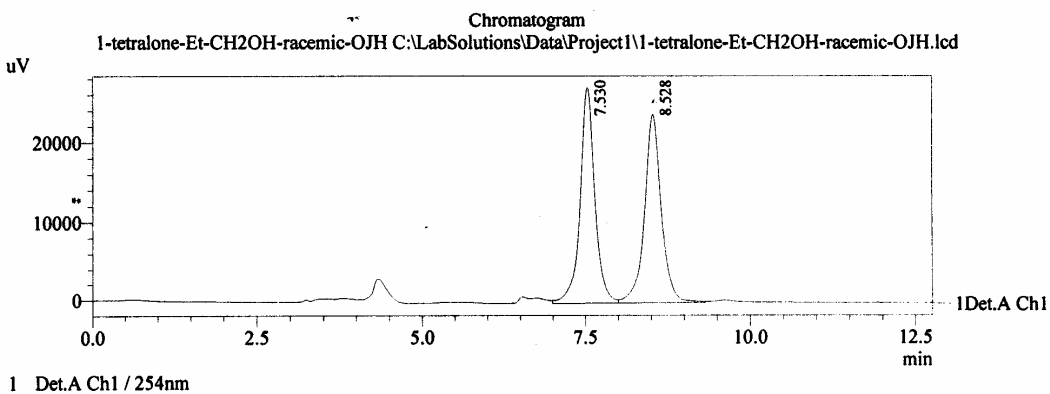
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.256	162498	8447	10.172	10.338
2	4.144	109528	19096	6.856	23.371
3	4.489	77146	2947	4.829	3.607
4	5.498	136804	2363	8.564	2.893
5	6.108	66803	1858	4.182	2.274
6	6.561	75401	1909	4.720	2.337
7	7.503	19715	719	1.234	0.881
8	8.986	7851	450	0.491	0.551
9	12.137	3239	163	0.203	0.200
10	12.898	938480	43752	58.748	53.549
Total		1597464	81705	100.000	100.000

## HPLC chromatogram of racemic 4

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### Sample Information

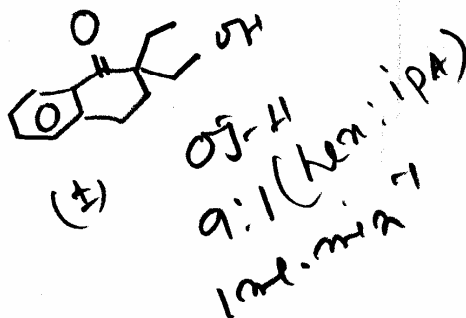
Acquired by : Admin  
Sample Name : 1-tetralone-Et-CH<sub>2</sub>OH-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-tetralone-Et-CH<sub>2</sub>OH-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/1/2010 2:27:08 PM  
Data Processed : 1/1/2010 2:41:17 PM



### PeakTable

Detector A Ch1 254nm

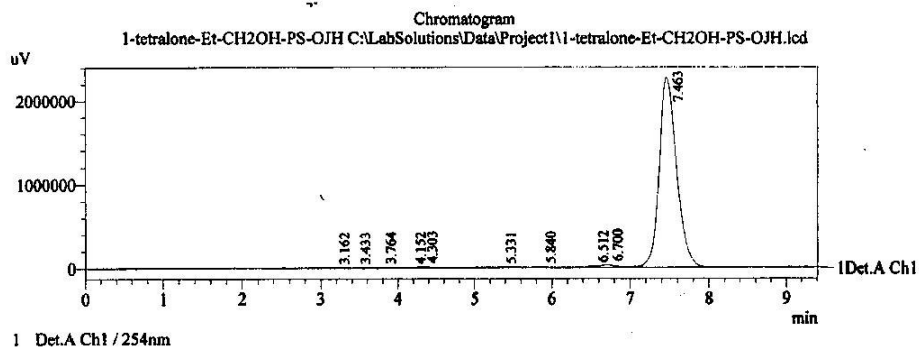
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.530	429843	27266	50.076	53.325
2	8.528	428539	23866	49.924	46.675
Total		858382	51132	100.000	100.000



## HPLC chromatogram of (S)-4

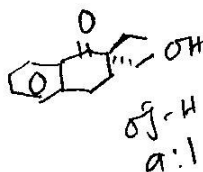
### Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 1-tetralone-Et-CH<sub>2</sub>OH-PS-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 µL  
Data Filename : 1-tetralone-Et-CH<sub>2</sub>OH-PS-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/1/2010 2:45:22 PM  
Data Processed : 1/1/2010 2:54:53 PM



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.162	56461	479	0.130	0.017
2	3.433	16735	1531	0.039	0.054
3	3.764	66896	4522	0.154	0.160
4	4.152	55366	6137	0.128	0.218
5	4.303	188948	17798	0.436	0.631
6	5.331	158619	4021	0.366	0.143
7	5.840	143157	5389	0.330	0.191
8	6.512	187974	16850	0.434	0.597
9	6.700	427359	32258	0.986	1.143
10	7.463	34611897	2272201	79.892	80.541
11	8.446	7409752	460000	17.103	16.305
Total		43323163	2821187	100.000	100.000

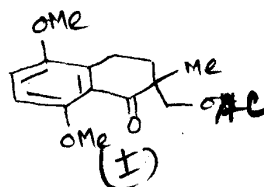


# HPLC chromatogram of acetate derivative of racemic 5

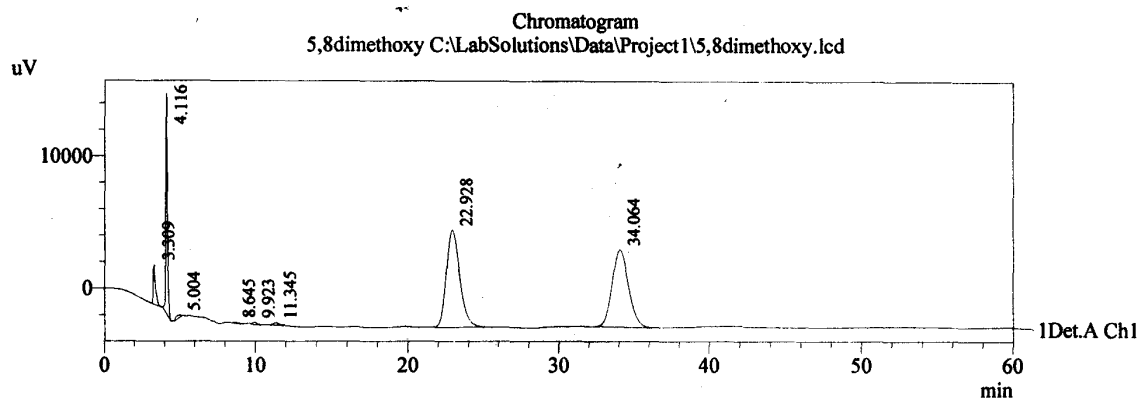
Department of Chemistry, IIT-Kharagpur

Acquired by : Admin  
Sample Name : 5,8dimethoxy  
Sample ID : monohydroxylation  
Vial# :  
Injection Volume : 10 uL  
Data Filename : 5,8dimethoxy.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 12/27/2007 10:07:22 AM  
Data Processed : 12/27/2007 11:07:25 AM

## Sample Information



Flow rate = 1 ml/min  
0.5-H  
9:1 (Hex: IPA)



1 Det.A Ch1 / 254nm

## PeakTable

Detector A Ch1 254nm

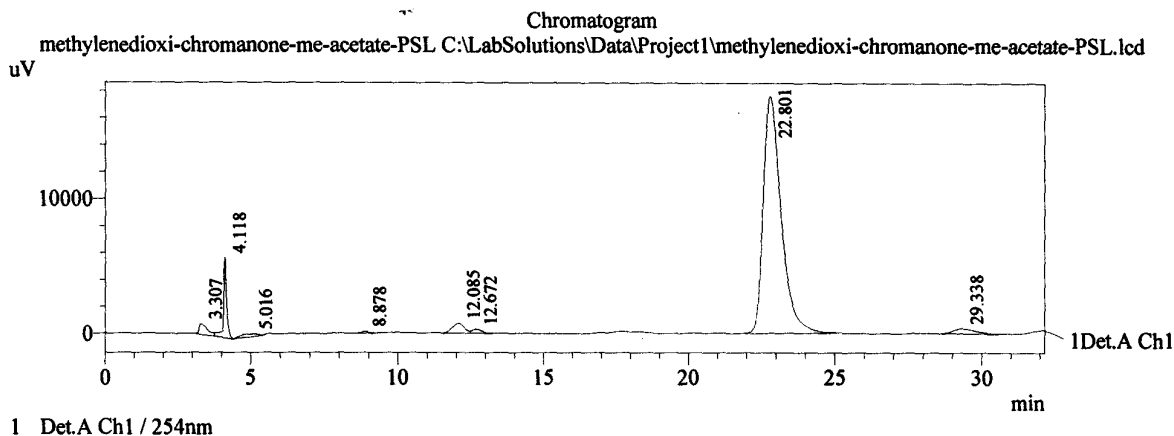
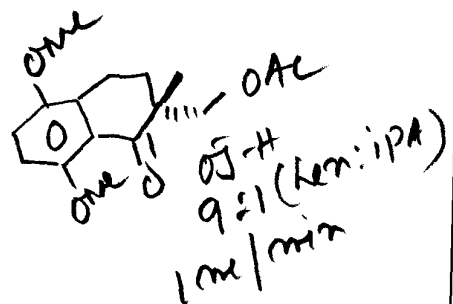
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.309	30978	2988	2.929	8.977
2	4.116	125674	16631	11.882	49.959
3	5.004	4372	145	0.413	0.437
4	8.645	1040	69	0.098	0.208
5	9.923	2502	146	0.237	0.437
6	11.345	3637	165	0.344	0.496
7	22.928	453015	7332	42.832	22.027
8	34.064	436429	5812	41.264	17.459
Total		1057647	33289	100.000	100.000

# HPLC chromatogram of (R)-acetate derivative of 5

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Sample Information

Acquired by : Admin  
Sample Name : methylenedioxi-chromanone-me-acetate-PSL  
Sample ID : transesterification  
Vail# :  
Injection Volume : 10 uL  
Data Filename : methylenedioxi-chromanone-me-acetate-PSL.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/29/2008 4:01:59 PM  
Data Processed : 1/29/2008 4:34:10 PM



PeakTable

Detector A Ch1 254nm

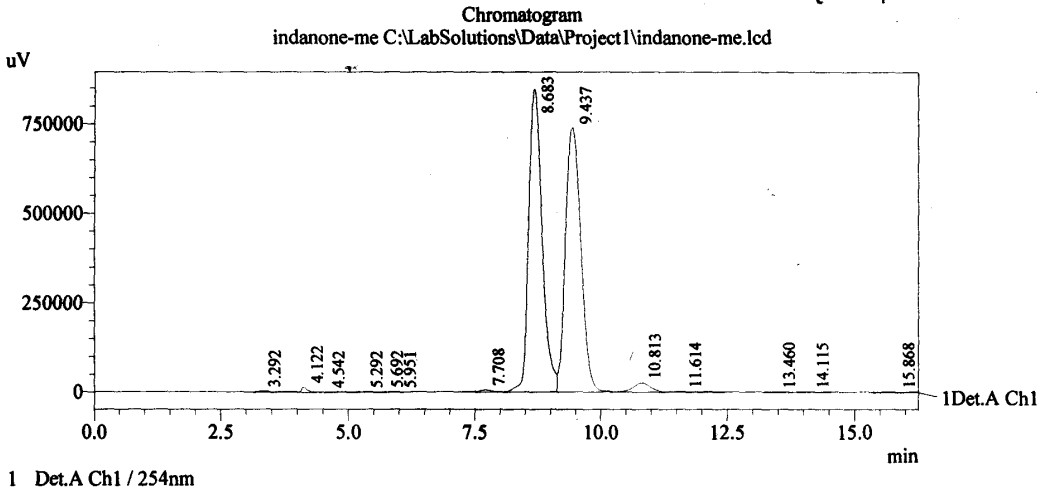
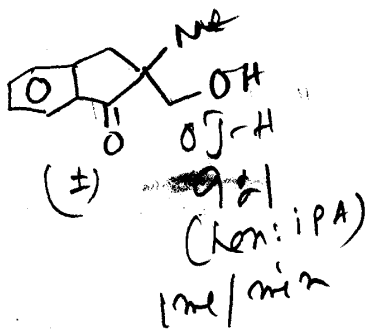
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.307	15194	793	1.762	3.048
2	4.118	44067	5991	5.111	23.041
3	5.016	7960	196	0.923	0.755
4	8.878	1591	113	0.185	0.434
5	12.085	19251	686	2.233	2.640
6	12.672	6270	277	0.727	1.064
7	22.801	749790	17577	86.956	67.599
8	29.338	18139	369	2.104	1.418
Total		862263	26002	100.000	100.000



HPLC chromatogram of racemic 6

IIT

Sample Information  
Acquired by : Admin  
Sample Name : indanone-me  
Sample ID : monohydroxylation  
Vial# :  
Injection Volume : 10 uL  
Data Filename : indanone-me.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 12/27/2007 11:20:49 AM  
Data Processed : 12/27/2007 11:37:12 AM



PeakTable

Detector A Ch1 254nm

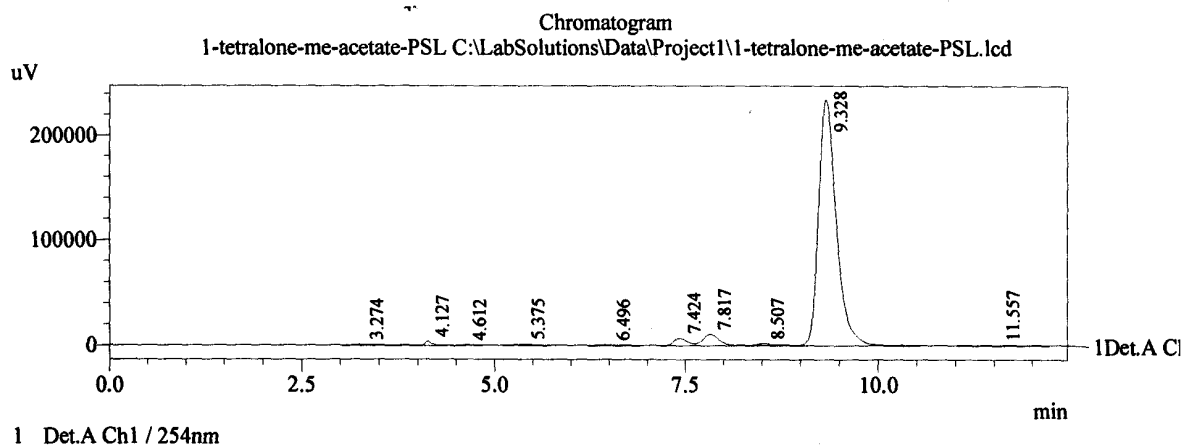
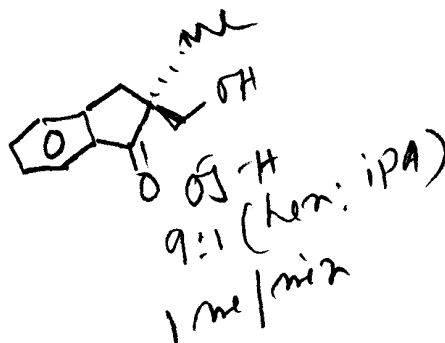
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.292	31560	1972	0.097	0.121
2	4.122	105063	13987	0.323	0.855
3	4.542	1018	127	0.003	0.008
4	5.292	17390	321	0.053	0.020
5	5.692	3399	172	0.010	0.011
6	5.951	1396	98	0.004	0.006
7	7.708	89095	5790	0.274	0.354
8	8.683	15800321	846864	48.564	51.775
9	9.437	15833492	739433	48.666	45.207
10	10.813	606331	25340	1.864	1.549
11	11.614	38819	1256	0.119	0.077
12	13.460	1452	87	0.004	0.005
13	14.115	1303	68	0.004	0.004
14	15.868	4201	155	0.013	0.009
Total		32534839	1635668	100.000	100.000

# HPLC chromatogram of (S)-6

Department of Chemistry, IIT-Kharagpur

Sample Information

Acquired by : Admin  
Sample Name : 1-tetralone-me-acetate-PSL  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-tetralone-me-acetate-PSL.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/29/2008 10:14:06 AM  
Data Processed : 1/29/2008 10:26:36 AM



PeakTable

Detector A Ch1 254nm

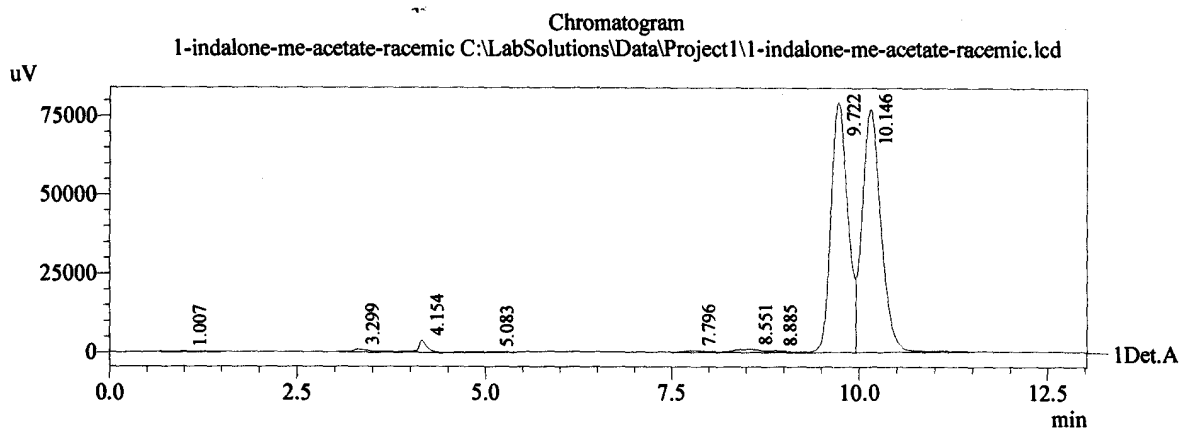
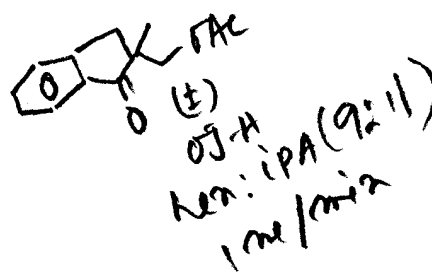
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.274	14889	789	0.368	0.304
2	4.127	27090	3781	0.670	1.456
3	4.612	4005	366	0.099	0.141
4	5.375	13165	1051	0.325	0.405
5	6.496	4154	324	0.103	0.125
6	7.424	80334	6799	1.986	2.618
7	7.817	151210	10516	3.739	4.049
8	8.507	27110	1411	0.670	0.543
9	9.328	3714698	234465	91.846	90.278
10	11.557	7823	213	0.193	0.082
Total		4044477	259714	100.000	100.000

# HPLC chromatogram of acetate derivative of racemic 6

Department of Chemistry, IIT-Kharagpur

Sample Information

Acquired by : Admin  
Sample Name : 1-indalone-me-acetate-racemic  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : 1-indalone-me-acetate-racemic.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/29/2008 9:36:37 AM  
Data Processed : 1/29/2008 9:49:43 AM



1 Det.A Ch1 / 254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	1.007	1243	49	0.047	0.030
2	3.299	13950	821	0.525	0.503
3	4.154	29043	3802	1.094	2.330
4	5.083	4486	121	0.169	0.074
5	7.796	8572	464	0.323	0.284
6	8.551	21440	873	0.808	0.535
7	8.885	6999	443	0.264	0.271
8	9.722	1245254	79448	46.906	48.688
9	10.146	1323796	77155	49.865	47.283
Total		2654782	163176	100.000	100.000

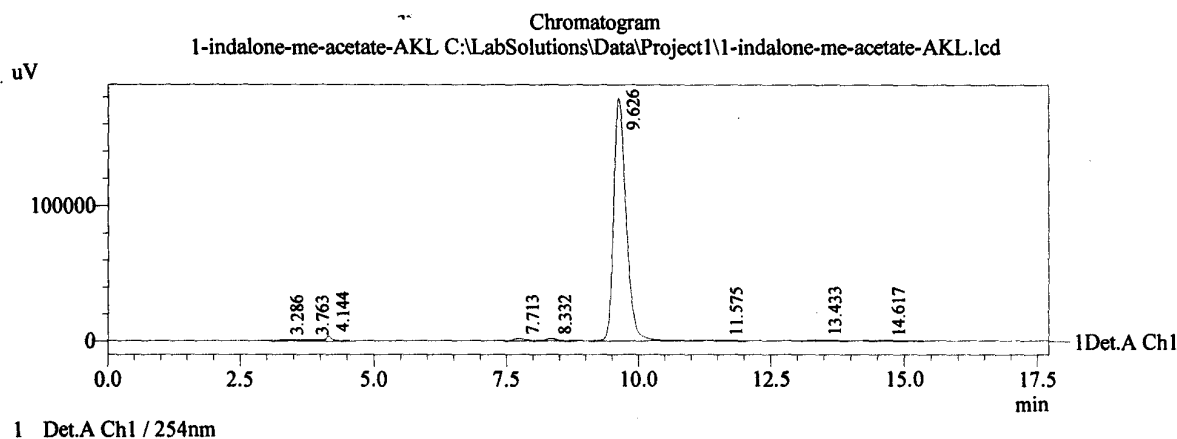
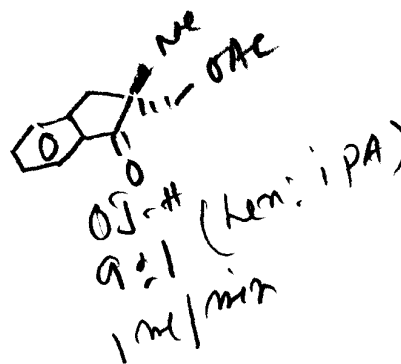
11

# HPLC chromatogram of (R)-acetate derivative of 6

Department of Chemistry, IIT-Kharagpur

Sample Information

Acquired by : Admin  
Sample Name : 1-indalone-me-acetate-AKL  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : 1-indalone-me-acetate-AKL.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/29/2008 9:52:50 AM  
Data Processed : 1/29/2008 10:10:42 AM



PeakTable

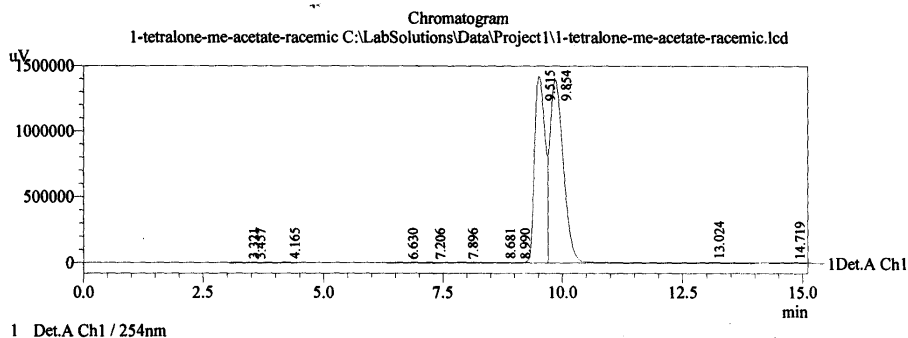
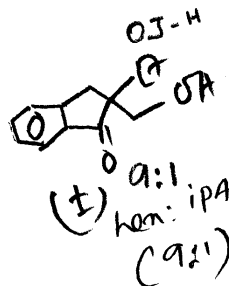
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.286	9421	686	0.308	0.364
2	3.763	26338	851	0.861	0.452
3	4.144	24782	3600	0.810	1.910
4	7.713	27594	1671	0.902	0.887
5	8.332	22101	1473	0.723	0.782
6	9.626	2926642	179156	95.693	95.069
7	11.575	2003	96	0.065	0.051
8	13.433	12160	615	0.398	0.326
9	14.617	7338	300	0.240	0.159
Total		3058378	188448	100.000	100.000

## HPLC chromatogram of racemic 7

Department of Chemistry, IIT-Kharagpur

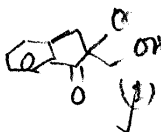
Sample Information  
Acquired by : Admin  
Sample Name : 1-tetralone-me-acetate-racemic  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-tetralone-me-acetate-racemic.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/29/2008 9:17:40 AM  
Data Processed : 1/29/2008 9:32:52 AM



PeakTable  
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.321	8722	795	0.018	0.028
2	3.457	8963	702	0.018	0.025
3	4.165	38407	4501	0.078	0.159
4	6.630	1753	150	0.004	0.005
5	7.206	6052	400	0.012	0.014
6	7.896	37576	1655	0.077	0.059
7	8.681	22488	1189	0.046	0.042
8	8.990	12338	891	0.025	0.032
9	9.515	21728734	1419635	44.270	50.256
10	9.854	27159401	1392355	55.334	49.290
11	13.024	36772	1518	0.075	0.054
12	14.719	21201	1042	0.043	0.037
Total		49082406	2824834	100.000	100.000

tr = 9.5 (ma)  
tr = 9.85 (mi)

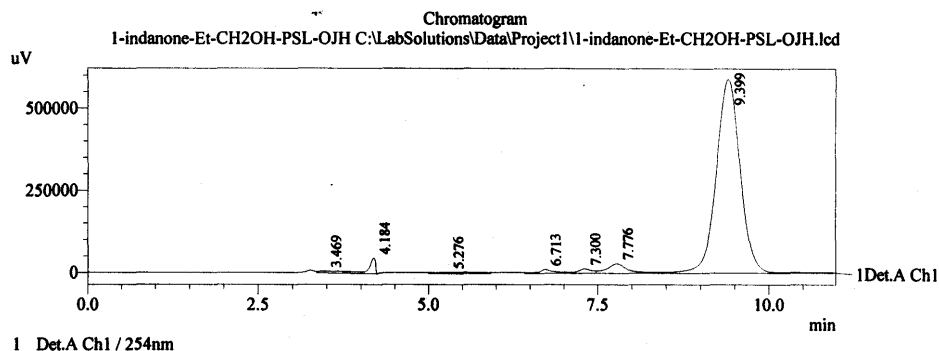


## HPLC chromatogram of (S)-7

Department of Chemistry, IIT-Kharagpur

Sample Information

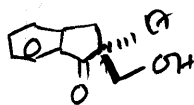
Acquired by : Admin  
Sample Name : 1-indanone-Et-CH2OH-PSL-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-indanone-Et-CH2OH-PSL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 9/9/2009 9:56:27 AM  
Data Processed : 9/9/2009 10:08:43 AM



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.469	185329	5126	1.171	0.736
2	4.184	269826	46713	1.705	6.709
3	5.276	134963	2756	0.853	0.396
4	6.713	179870	11224	1.137	1.612
5	7.300	184051	12914	1.163	1.855
6	7.776	577626	28621	3.651	4.110
7	9.399	14289994	588962	90.319	84.583
Total		15821661	696315	100.000	100.000



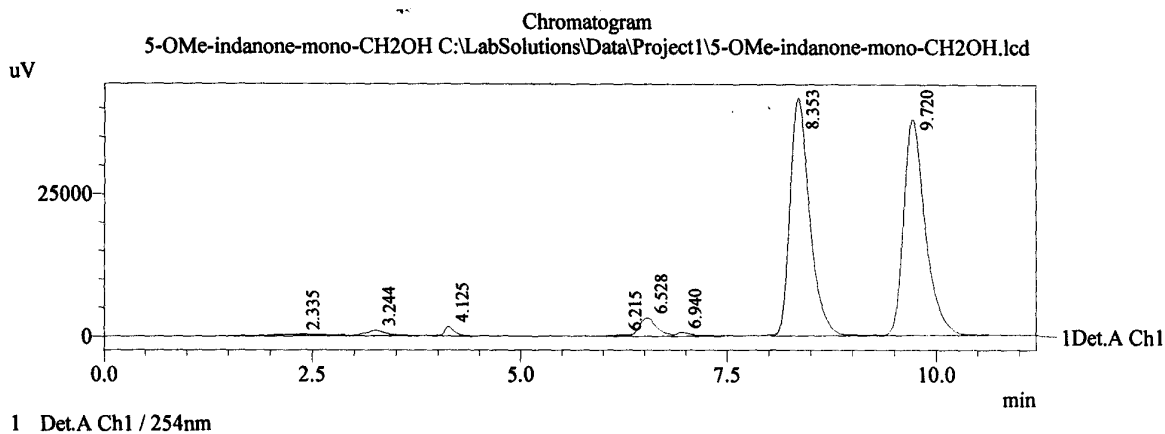
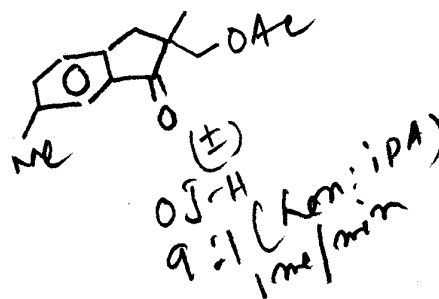
OS-4  
9.1  
1ml/min

# HPLC chromatogram of acetate derivative of racemic 8

## Department of Chemistry, IIT-Kharagpur

Sample Information

Acquired by : Admin  
Sample Name : 5-OMe-indanone-mono-CH2OH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 10 uL  
Data Filename : 5-OMe-indanone-mono-CH2OH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 4/14/2008 3:31:48 PM  
Data Processed : 4/14/2008 3:43:05 PM



PeakTable

Detector A Ch1 254nm

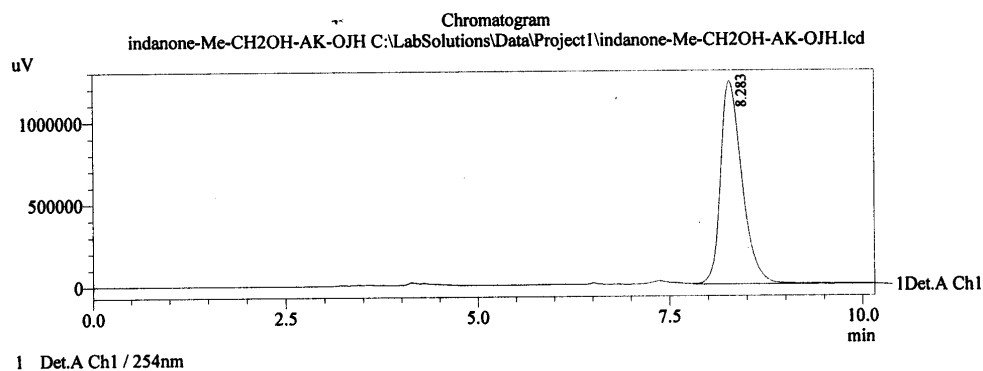
Peak#	Ret. Time	Area	Height	Area %	Height %
1	2.335	12773	262	0.876	0.304
2	3.244	14671	901	1.006	1.043
3	4.125	12409	1530	0.851	1.771
4	6.215	1935	201	0.133	0.232
5	6.528	45297	3125	3.106	3.618
6	6.940	7386	603	0.506	0.698
7	8.353	681134	41763	46.709	48.347
8	9.720	682651	37997	46.813	43.987
Total		1458258	86383	100.000	100.000

# HPLC chromatogram of (R)-acetate derivative of 8

Department of Chemistry, IIT-Kharagpur

## Sample Information

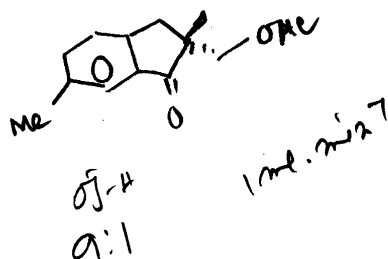
Acquired by : Admin  
Sample Name : indanone-Me-CH2OH-AK-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : indanone-Me-CH2OH-AK-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/1/2010 3:52:06 PM  
Data Processed : 1/1/2010 4:03:44 PM



## PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.283	23712343	1231381	100.000	100.000
Total		23712343	1231381	100.000	100.000

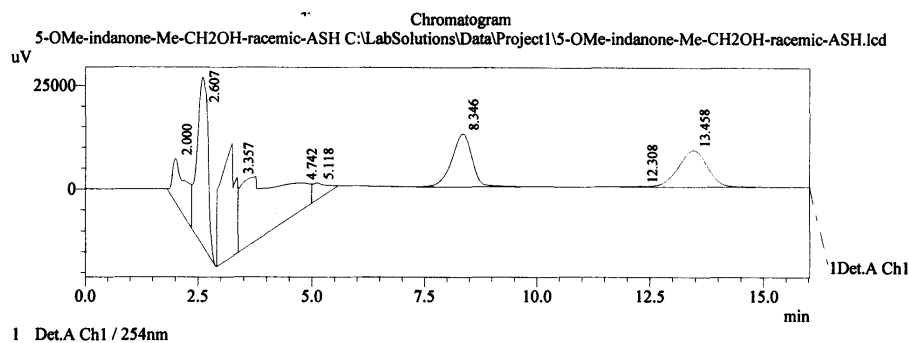




## HPLC chromatogram of racemic 9

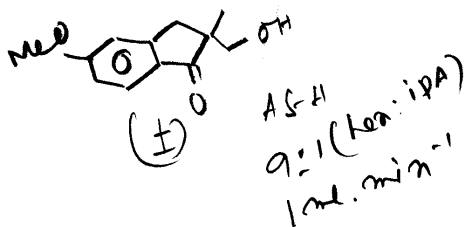
Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 5-OMe-indanone-Me-CH2OH-racemic-ASH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 5-OMe-indanone-Me-CH2OH-racemic-ASH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/29/2009 5:31:16 PM  
Data Processed : 5/29/2009 5:48:17 PM



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	2.000	240218	10422	7.122	10.305
2	2.607	672364	40561	19.935	40.105
3	3.357	583983	17981	17.314	17.778
4	4.742	1006837	6654	29.851	6.579
5	5.118	81842	3953	2.426	3.909
6	8.346	395977	12696	11.740	12.553
7	12.308	1745	83	0.052	0.082
8	13.458	389879	8788	11.559	8.689
Total		3372843	101138	100.000	100.000



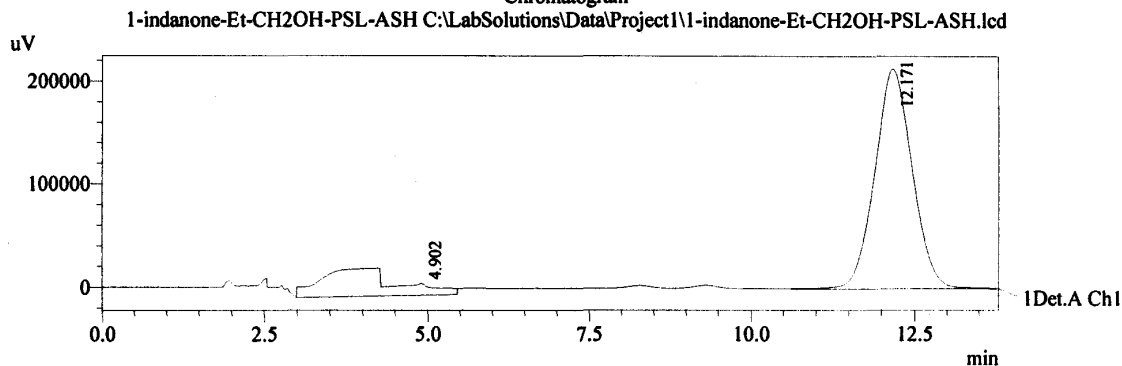
# HPLC chromatogram of (S)- 9

Department of Chemistry, IIT-Kharagpur

## Sample Information

Acquired by : Admin  
Sample Name : 1-indanone-Et-CH2OH-PSL-ASH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-indanone-Et-CH2OH-PSL-ASH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 9/9/2009 10:29:06 AM  
Data Processed : 9/9/2009 10:43:45 AM

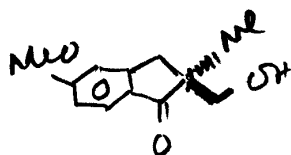
## Chromatogram



## PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.902	2170868	10993	20.355	4.890
2	12.171	8494242	213820	79.645	95.110
Total		10665111	224813	100.000	100.000

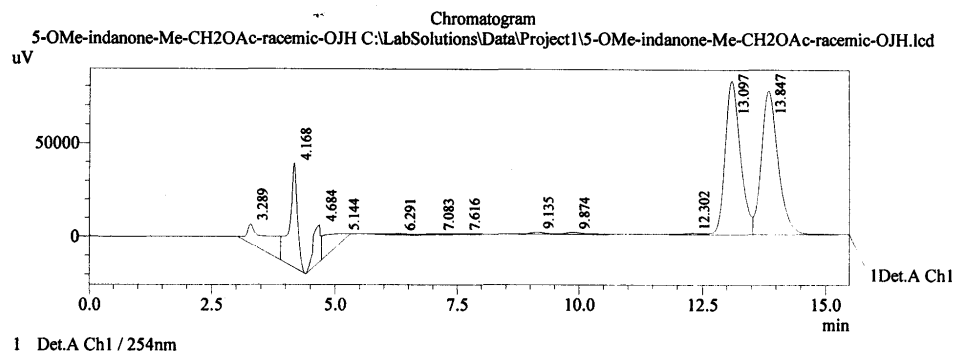


AS-H  
9:1  
1ml. mix<sup>-1</sup>

# HPLC chromatogram of acetate derivative of racemic 9

Department of Chemistry, IIT-Kharagpur

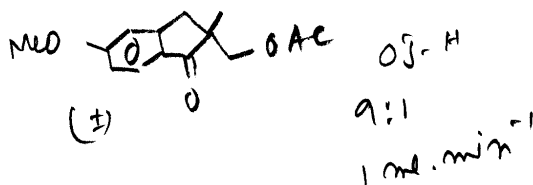
Sample Information  
Acquired by : Admin  
Sample Name : 5-OMe-indanone-Me-CH2OAc-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 5-OMe-indanone-Me-CH2OAc-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/29/2009 5:03:55 PM  
Data Processed : 5/29/2009 5:20:16 PM



PeakTable

Detector A Ch1 254nm

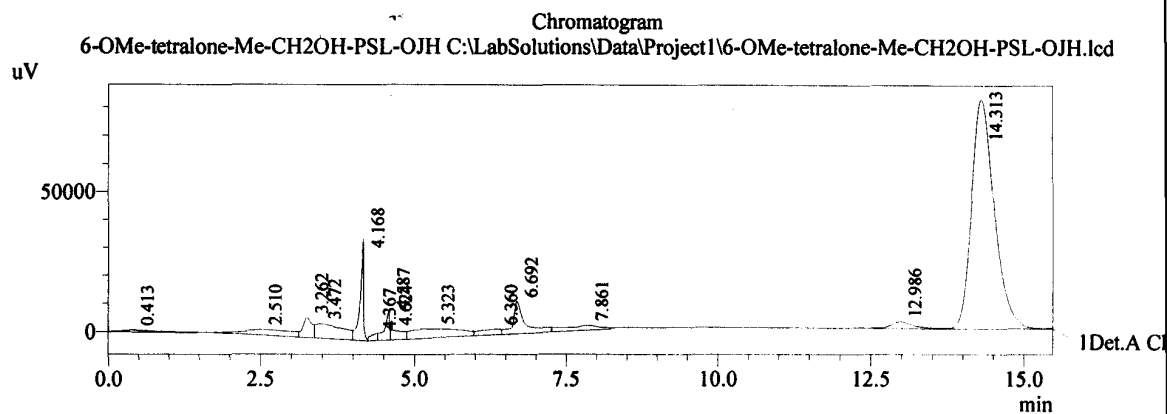
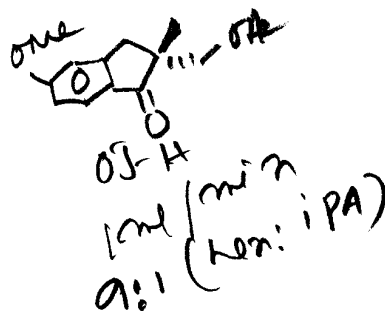
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.289	381973	10353	7.488	4.114
2	4.168	617046	55837	12.096	22.188
3	4.684	212638	19643	4.168	7.805
4	5.144	233761	3926	4.582	1.560
5	6.291	12871	444	0.252	0.176
6	7.083	8849	322	0.173	0.128
7	7.616	9327	282	0.183	0.112
8	9.135	18328	997	0.359	0.396
9	9.874	20065	955	0.393	0.379
10	12.302	14490	614	0.284	0.244
11	13.097	1762253	81761	34.544	32.489
12	13.847	1809822	76522	35.477	30.407
Total		5101423	251657	100.000	100.000



# HPLC chromatogram of (R)-acetate of 9

Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 6-OMe-tetralone-Me-CH2OH-PSL-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 6-OMe-tetralone-Me-CH2OH-PSL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 9/9/2009 9:37:15 AM  
Data Processed : 9/9/2009 9:54:04 AM



PeakTable

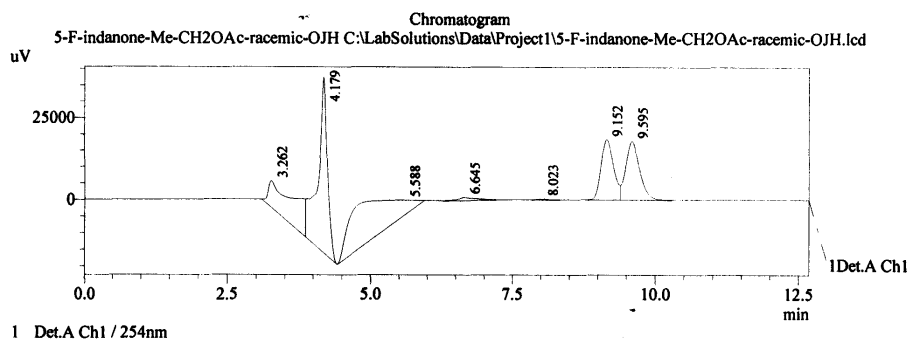
Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	0.413	17807	533	0.555	0.317
2	2.510	100337	1776	3.130	1.057
3	3.262	71020	6863	2.215	4.086
4	3.472	155561	4954	4.852	2.950
5	4.168	134851	36178	4.206	21.543
6	4.367	17365	2271	0.542	1.353
7	4.587	54794	10312	1.709	6.140
8	4.624	46335	3271	1.445	1.948
9	5.323	166796	2873	5.202	1.711
10	6.360	44971	1746	1.403	1.040
11	6.692	155931	11343	4.864	6.754
12	7.861	66638	1646	2.078	0.980
13	12.986	53964	2299	1.683	1.369
14	14.313	2119729	81870	66.116	48.751
Total		3206100	167933	100.000	100.000

# HPLC chromatogram of acetate derivative of racemic 10

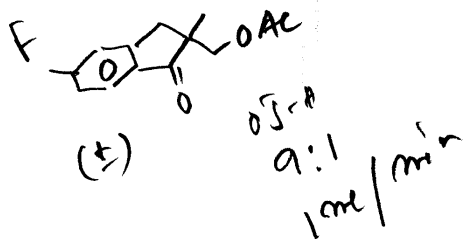
Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 5-F-indanone-Me-CH2OAc-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 5-F-indanone-Me-CH2OAc-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 7/13/2009 9:42:10 AM  
Data Processed : 7/13/2009 9:55:58 AM



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.262	317882	7990	14.298	7.738
2	4.179	625790	53368	28.147	51.686
3	5.588	682211	4592	30.685	4.447
4	6.645	18676	907	0.840	0.879
5	8.023	3032	214	0.136	0.208
6	9.152	276901	18372	12.455	17.793
7	9.595	298777	17811	13.439	17.250
Total		2223270	103255	100.000	100.000



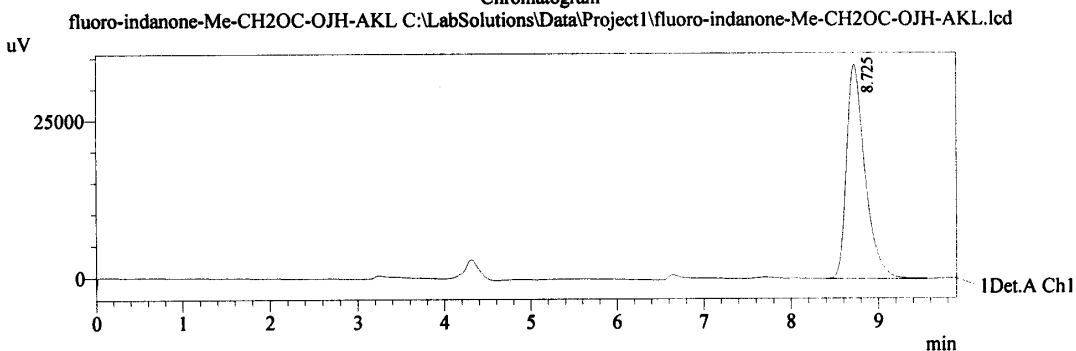
## HPLC chromatogram of (*R*)-acetate derivative of 10

### Department of Chemistry, IIT-Kharagpur

#### Sample Information

Acquired by : Admin  
Sample Name : fluoro-indanone-Me-CH2OC-OJH-AKL  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : fluoro-indanone-Me-CH2OC-OJH-AKL.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/15/2009 4:06:20 PM  
Data Processed : 10/15/2009 4:18:17 PM

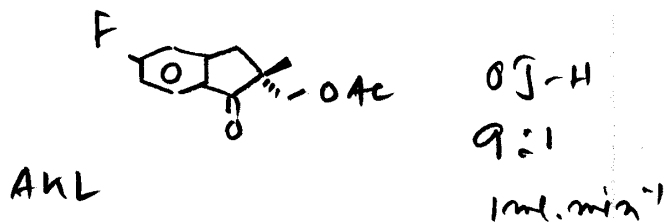
#### Chromatogram



#### PeakTable

Detector A Ch1 254nm

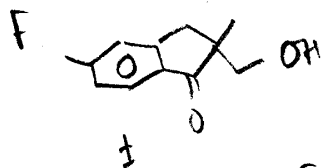
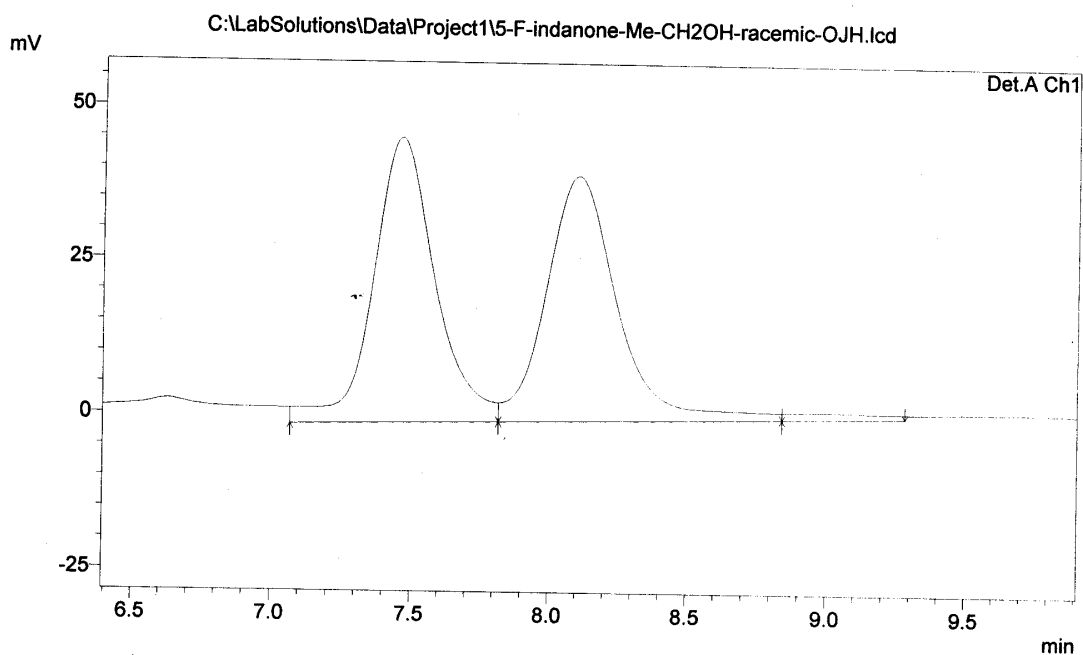
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.725	496932	34048	100.000	100.000
Total		496932	34048	100.000	100.000



## HPLC chromatogram of racemic 10

==== Shimadzu LCsolution LC Data Image ====

<Chromatogram>



OJ-H

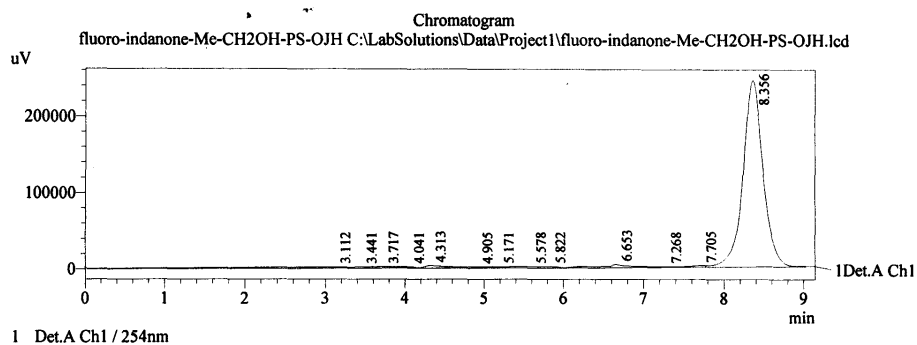
921

1 ml/min

## HPLC chromatogram of (S)- 10

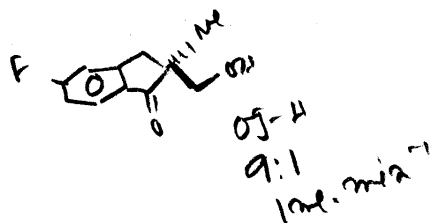
### Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : fluoro-indanone-Me-CH<sub>2</sub>OH-PS-OJH  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : fluoro-indanone-Me-CH<sub>2</sub>OH-PS-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/23/2009 9:47:26 AM  
Data Processed : 10/23/2009 9:56:44 AM



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.112	175177	1410	3.617	0.530
2	3.441	22896	1525	0.473	0.573
3	3.717	30836	1653	0.637	0.621
4	4.041	22591	1477	0.466	0.555
5	4.313	59430	3174	1.227	1.193
6	4.905	21566	1358	0.445	0.510
7	5.171	22968	1448	0.474	0.544
8	5.578	40666	1548	0.840	0.582
9	5.822	20819	1504	0.430	0.565
10	6.653	98398	4079	2.032	1.533
11	7.268	18798	852	0.388	0.320
12	7.705	29203	1942	0.603	0.730
13	8.356	4279727	244172	88.368	91.745
Total		4843075	266143	100.000	100.000

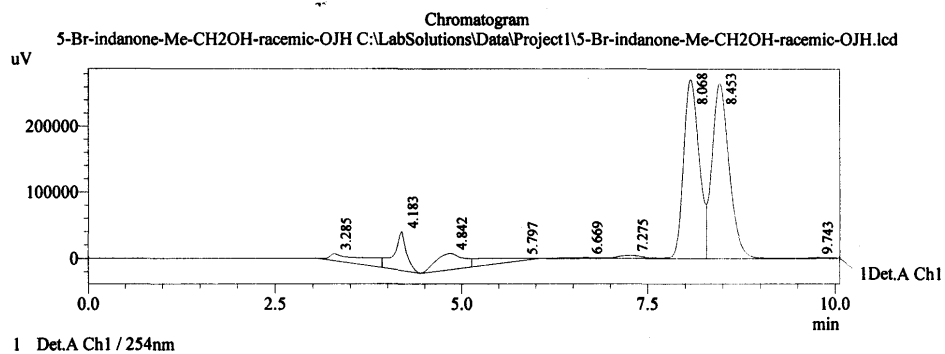




## HPLC chromatogram of racemic 11

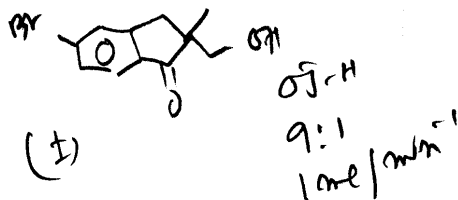
### Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : 5-Br-indanone-Me-CH<sub>2</sub>OH-racemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 5-Br-indanone-Me-CH<sub>2</sub>OH-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 7/8/2009 9:40:55 AM  
Data Processed : 7/8/2009 9:51:48 AM



PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.285	428020	10048	4.183	1.574
2	4.183	656208	57531	6.413	9.011
3	4.842	621074	23930	6.070	3.748
4	5.797	332699	3375	3.252	0.529
5	6.669	17744	1069	0.173	0.167
6	7.275	89094	4190	0.871	0.656
7	8.068	3876692	271567	37.888	42.535
8	8.453	4196583	265809	41.014	41.633
9	9.743	13909	940	0.136	0.147
Total		10232023	638458	100.000	100.000



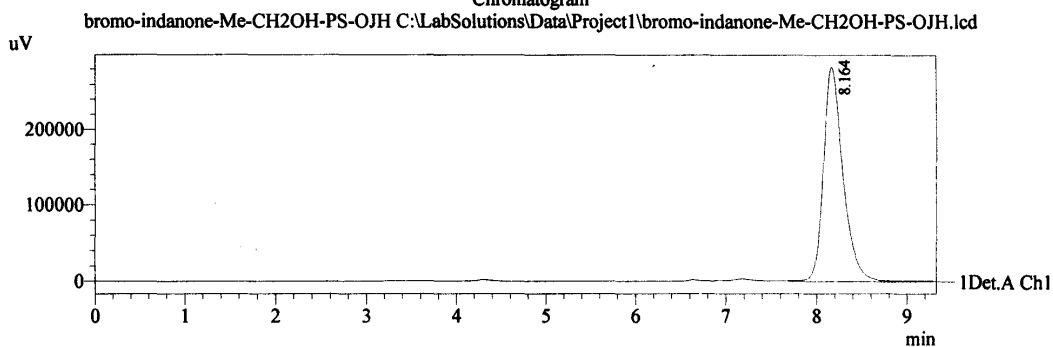
## HPLC chromatogram of (S)-11

### Department of Chemistry, IIT-Kharagpur

#### Sample Information

Acquired by : Admin  
Sample Name : bromo-indanone-Me-CH2OH-PS-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : bromo-indanone-Me-CH2OH-PS-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/23/2009 9:34:46 AM  
Data Processed : 10/23/2009 9:45:22 AM

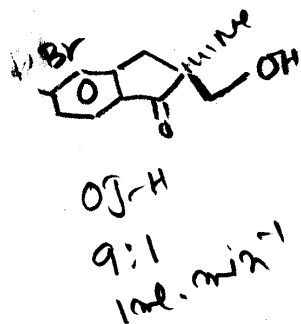
#### Chromatogram



#### PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.164	4226319	283269	100.000	100.000
Total		4226319	283269	100.000	100.000



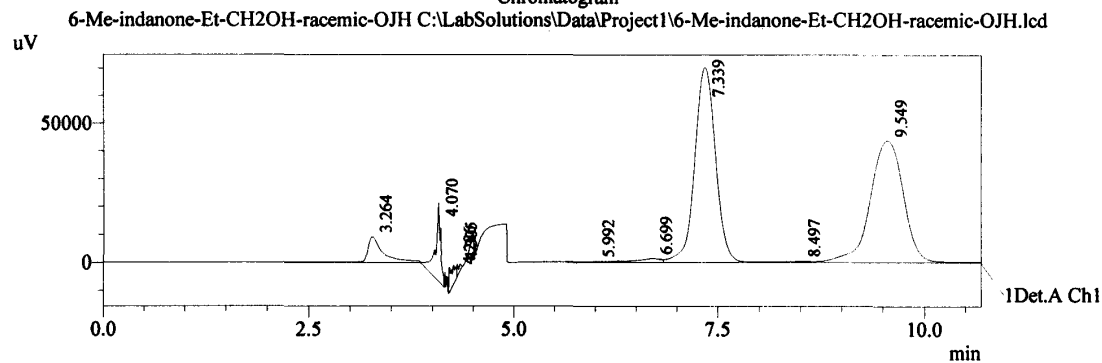
## HPLC chromatogram of racemic 12

### Department of Chemistry, IIT-Kharagpur

#### Sample Information

Acquired by : Admin  
Sample Name : 6-Me-indanone-Et-CH2OH-racemic-OJH  
Sample ID : transesterification  
Vail# :  
Injection Volume : 5 uL  
Data Filename : 6-Me-indanone-Et-CH2OH-racemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 6/5/2009 9:50:41 AM  
Data Processed : 6/5/2009 10:02:57 AM

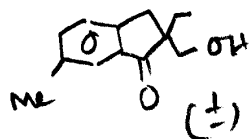
#### Chromatogram



#### PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.264	119113	9108	4.323	5.667
2	4.070	120064	27681	4.358	17.223
3	4.286	34580	4520	1.255	2.813
4	4.305	7756	4279	0.281	2.663
5	5.992	2497	155	0.091	0.096
6	6.699	28741	1337	1.043	0.832
7	7.339	1229128	69994	44.609	43.550
8	8.497	1423	107	0.052	0.067
9	9.549	1212015	43538	43.988	27.090
Total		2755317	160719	100.000	100.000



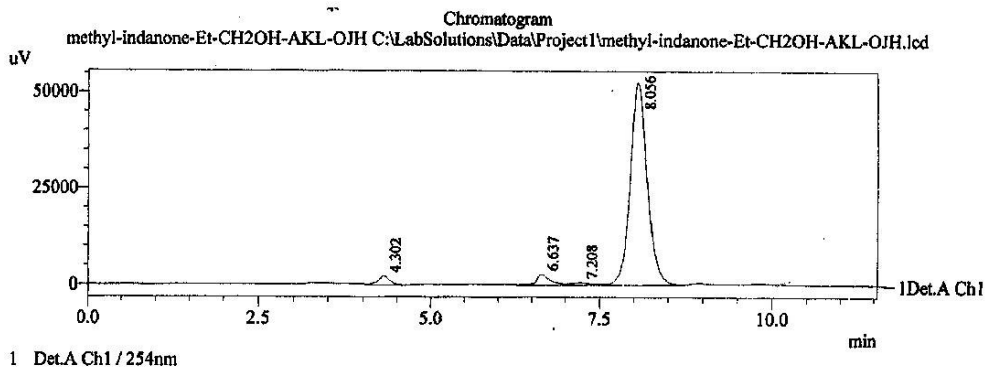
OJ-H  
9:1  
1ml.min<sup>-1</sup>

## HPLC chromatogram of (S)-12

### Department of Chemistry, IIT-Kharagpur

Sample Information

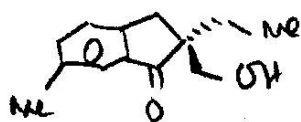
Acquired by : Admin  
Sample Name : methyl-indanone-Et-CH2OH-AKL-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : methyl-indanone-Et-CH2OH-AKL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/15/2009 4:53:21 PM  
Data Processed : 10/15/2009 4:55:57 PM



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.302	26839	2279	2.517	3.661
2	6.637	37816	2753	3.547	4.422
3	7.208	10063	544	0.944	0.874
4	8.056	897068	52504	84.143	84.345
5	10.604	94331	4170	8.848	6.698
Total		1066118	62249	100.000	100.000



OJ-H  
9:1  
1ml/min

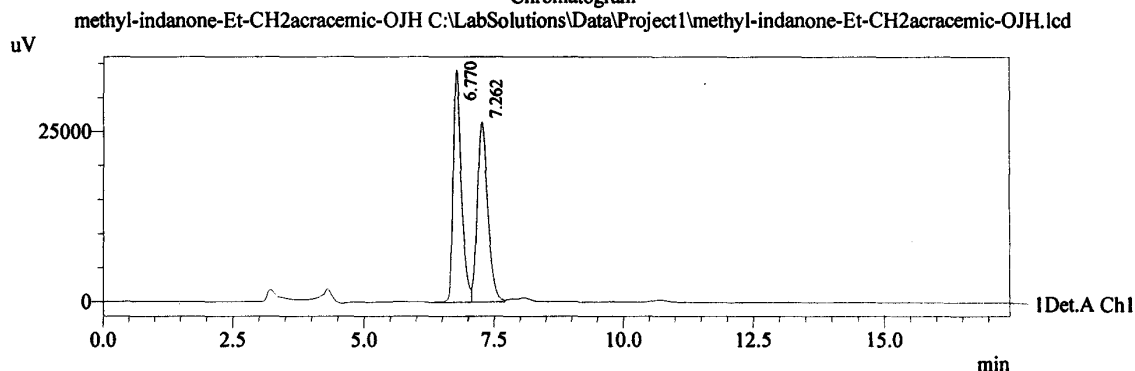
# HPLC chromatogram acetate derivative of racemic 12

Department of Chemistry, IIT-Kharagpur

## Sample Information

Acquired by : Admin  
Sample Name : methyl-indanone-Et-CH2acracemic-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : methyl-indanone-Et-CH2acracemic-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/15/2009 4:59:07 PM  
Data Processed : 10/15/2009 5:17:42 PM

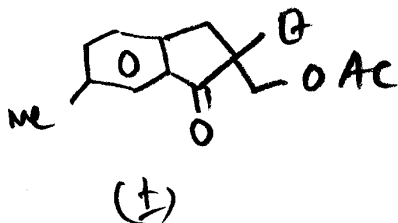
## Chromatogram



## PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.770	372530	34155	49.939	56.333
2	7.262	373435	26475	50.061	43.667
Total		745965	60630	100.000	100.000

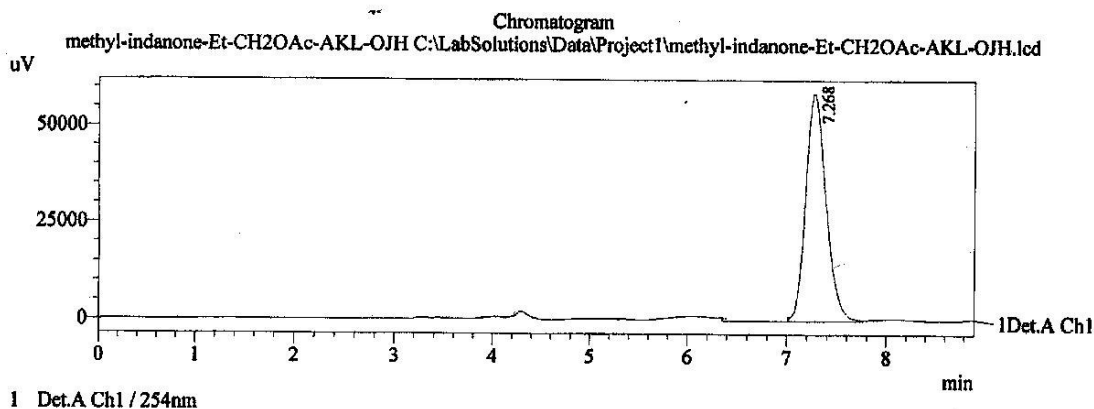


OJ-H  
9:1  
1 ml. min<sup>-1</sup>

# HPLC chromatogram (*R*)-acetate derivative of 12

## Department of Chemistry, IIT-Kharagpur

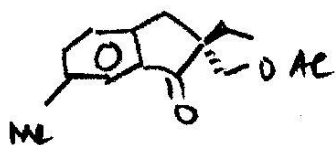
Sample Information  
Acquired by : Admin  
Sample Name : methyl-indanone-Et-CH<sub>2</sub>OAc-AKL-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : methyl-indanone-Et-CH<sub>2</sub>OAc-AKL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 10/15/2009 5:20:18 PM  
Data Processed : 10/15/2009 5:30:18 PM



Detector A Ch1 254nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.622	209951	13284	20.195	18.418
2	7.268	829659	58842	79.805	81.582
Total		1039611	72127	100.000	100.000

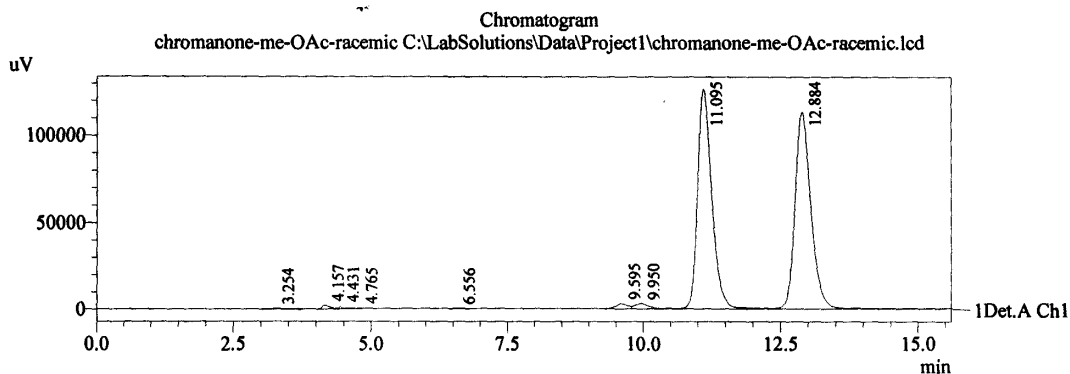
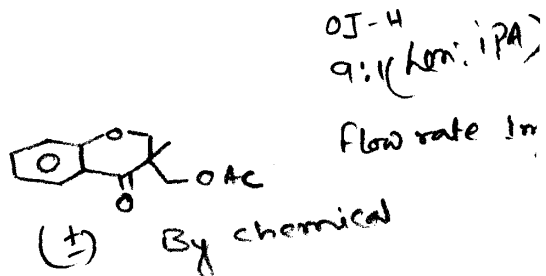


05-H  
9:1 (Hex:IPA)  
1 ml/min

## HPLC chromatogram of acetate derivative of racemic 13

Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : chromanone-me-OAc-racemic  
Sample ID : monohydroxylation  
Vial# :  
Injection Volume : 5 uL  
Data Filename : chromanone-me-OAc-racemic.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/15/2008 4:20:02 PM  
Data Processed : 1/15/2008 4:35:38 PM



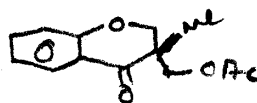
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.254	5981	389	0.129	0.156
2	4.157	19370	2077	0.417	0.834
3	4.431	3110	1289	0.067	0.518
4	4.765	1180	88	0.025	0.035
5	6.556	1198	125	0.026	0.050
6	9.595	41627	2800	0.895	1.124
7	9.950	49158	2898	1.057	1.163
8	11.095	2264668	126357	48.704	50.736
9	12.884	2263540	113024	48.680	45.383
Total		4649833	249047	100.000	100.000

# HPLC chromatogram of (R)-acetate derivative of 13

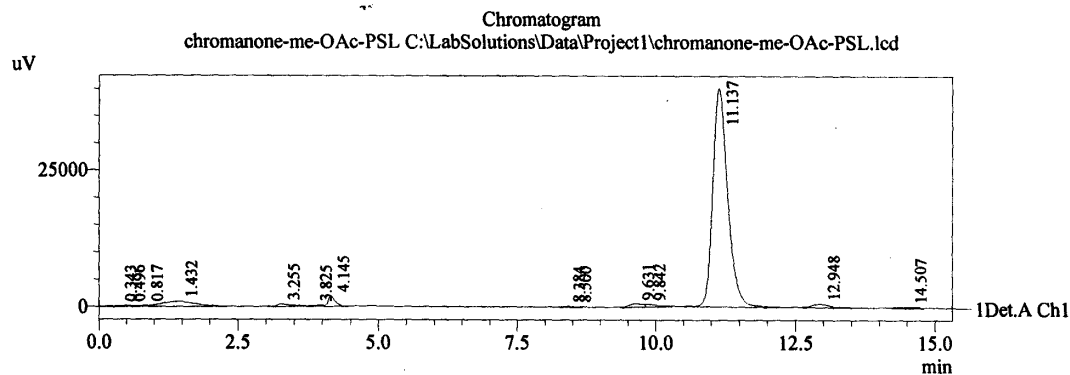
Department of Chemistry, IIT-Kharagpur

Sample Information  
Acquired by : Admin  
Sample Name : chromanone-me-OAc-PSL  
Sample ID : monohydroxylation  
Vial# :  
Injection Volume : 5 uL  
Data Filename : chromanone-me-OAc-PSL.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 1/15/2008 4:40:16 PM  
Data Processed : 1/15/2008 4:55:44 PM



OJ-4  
9:1 (hex:IPA)  
1ml/min

From PS-Lipase  
trans esterification



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	0.343	1772	134	0.210	0.292
2	0.496	1577	146	0.187	0.319
3	0.817	2153	157	0.255	0.342
4	1.432	37102	889	4.399	1.937
5	3.255	7963	420	0.944	0.915
6	3.825	1619	120	0.192	0.262
7	4.145	16308	1927	1.934	4.197
8	8.384	1144	116	0.136	0.253
9	8.500	1069	107	0.127	0.233
10	9.631	9858	539	1.169	1.174
11	9.842	5960	449	0.707	0.978
12	11.137	738318	40021	87.543	87.175
13	12.948	13299	646	1.577	1.408
14	14.507	5239	237	0.621	0.517
Total		843381	45909	100.000	100.000



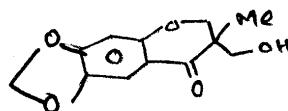
# HPLC chromatogram of racemic 14

## Department of Chemistry, IIT-Kharagpur

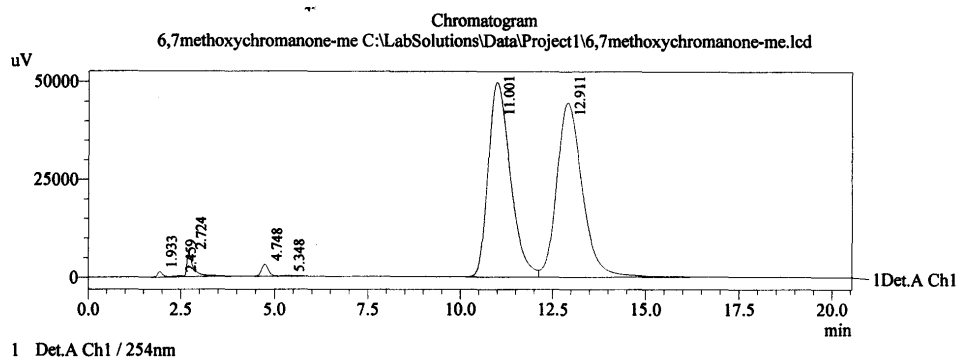
Acquired by : Admin  
Sample Name : 6,7methoxychromanone-me  
Sample ID : monohydroxylation  
Vail# :  
Injection Volume : 10 uL  
Data Filename : 6,7methoxychromanone-me.lcd  
Method Filename : tetralone 6 methoxy.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 12/28/2007 12:10:03 PM  
Data Processed : 12/28/2007 12:30:38 PM

### Sample Information

ODH



(D) 1ml/min



### PeakTable

Detector A Ch1 254nm

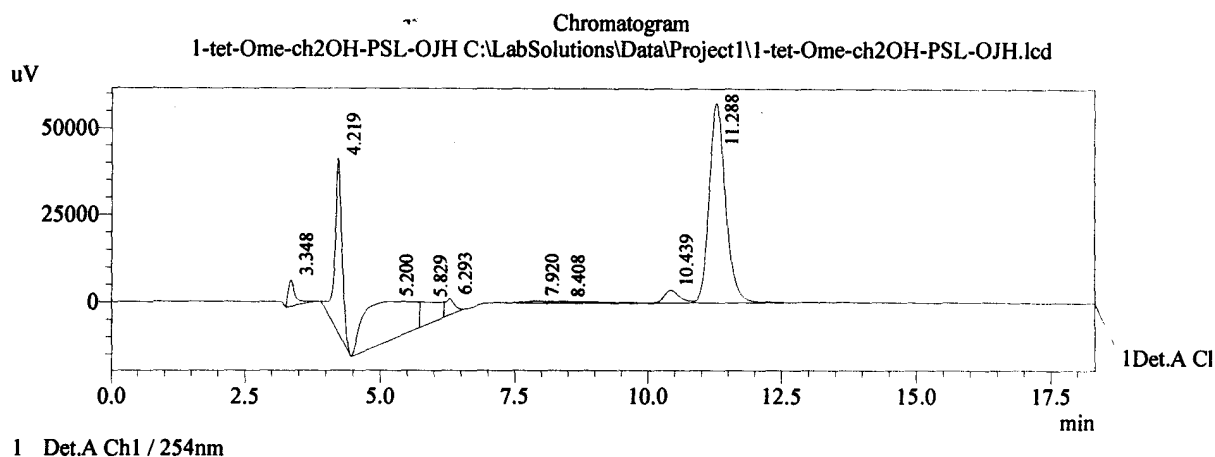
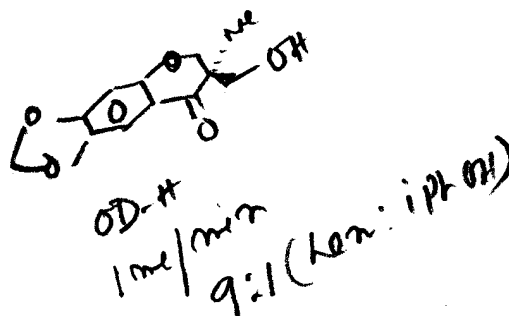
Peak#	Ret. Time	Area	Height	Area %	Height %
1	1.933	12162	1311	0.281	1.250
2	2.459	2567	224	0.059	0.214
3	2.724	71762	5955	1.658	5.678
4	4.748	37139	2955	0.858	2.818
5	5.348	1894	119	0.044	0.113
6	11.001	2074847	49775	47.928	47.465
7	12.911	2128714	44527	49.172	42.461
Total		4329084	104865	100.000	100.000

# HPLC chromatogram of (S)- 14

Department of Chemistry, IIT-Kharagpur

Acquired by : Admin  
Sample Name : 1-tet-Ome-ch2OH-PSL-OJH  
Sample ID : transesterification  
Vial# :  
Injection Volume : 5 uL  
Data Filename : 1-tet-Ome-ch2OH-PSL-OJH.lcd  
Method Filename : adduct1.lcm  
Batch Filename :  
Report Filename : Default.lcr  
Date Acquired : 5/18/2009 5:18:59 PM  
Data Processed : 5/18/2009 5:38:00 PM

## Sample Information



## PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.348	65351	7461	2.357	5.266
2	4.219	456621	50127	16.466	35.375
3	5.200	715631	10955	25.806	7.731
4	5.829	156147	6634	5.631	4.681
5	6.293	53973	4521	1.946	3.190
6	7.920	12325	531	0.444	0.374
7	8.408	17466	351	0.630	0.248
8	10.439	72548	3641	2.616	2.570
9	11.288	1223004	57480	44.103	40.564
Total		2773066	141702	100.000	100.000