

Supporting Materials

SM 1. Area percents (%) of *o*-nitrobenzoyl chloride and ethyl-*o*-nitrobenzoate (product) in 100% EtOH

Reat. time ^a (min.)	Area percent(%)	
	Ethyl- <i>o</i> -nitrobenzoate	<i>o</i> -Nitrobenzoyl chloride
	(5.3min) ^b	(6.0min) ^b
1	42.6	57.4
11	83.9	16.1
21	97.4	2.6
31	100.0	-
41	100.0	-
150	100.0	-

^aReaction time. ^bRetention time

SM 2. Area percents (%) of *o*-nitrobenzoyl chloride, *o*-nitrobenzoic acid (product), and trifluoroethyl *o*-nitrobenzoate (product) in 70% TFE

Reat. time ^a (min.)	Area percent(%)		
	<i>o</i> -Nitrobenzoic acid	<i>o</i> -Nitrobenzoyl chloride	Trifluoroethyl <i>o</i> -nitrobenzoate
	(2.4min)	(6.0min)	(7.0min)
1	44.2	29.5	26.3

11	45.3	0.1	54.6
21	45.3	-	54.7
31	45.3	-	54.7

^aReaction time. ^bRetention time

SM 3. Analyzing conditions of HPLC for products by solvolysis

Items	Analyzing conditions
System	Surveyor HPLC System (Thermo Finnigan Co. USA)
Detector	Surveyor PDA Detector
Pump	Finnigan Surveyor LC Pump
Column	150×4.6 mm 5μ Hypersill® GOLD C18
Wavelength	325 nm
Solvent	ACN 50% : H ₂ O 50% Isocratic
Flow Rate	1.0 mL/min
Injection Volume	2 μL

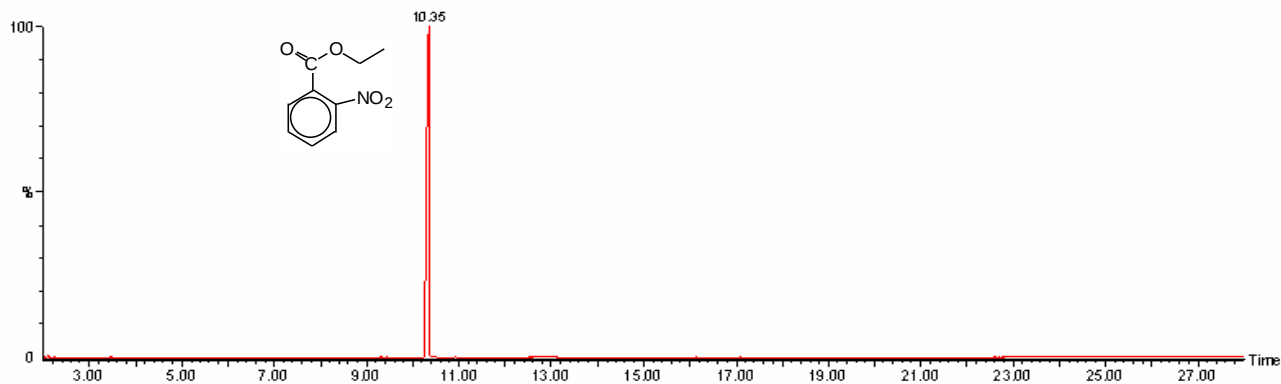
SM 3. Analyzing conditions of GC/mass for identification of products by solvolysis.

Items	Analyzing conditions
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GC	System	Clarus 500 GC-Mass System (Perkin-Elmer, USA)
	column	Elite-5MS, (30mx0.32 mm IDx 0.25 μ m DF)
	carrier gas	He
	flow rate	1 mL/min
	Oven Temp	initial : 70°C, 2min, ramp : 10°C min, 5min hold
	injection volume	1.0 μ l
	split ratio	50 : 1
	Ion mode	EI
Mass	mass range	30 amu ~ 500 amu
	solvent D. time	2 min

2. Nitrobenzoyl chloride in 100% EtOH

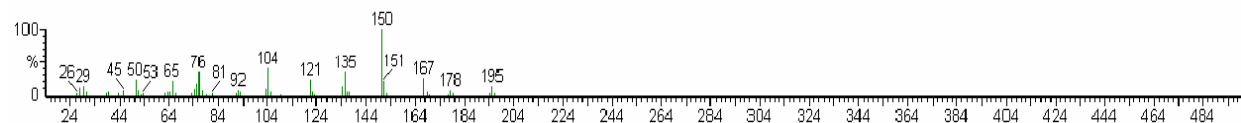
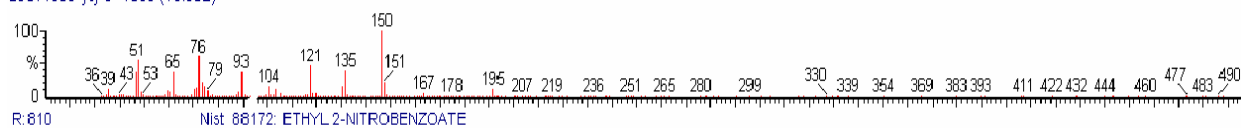
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2 EtOH

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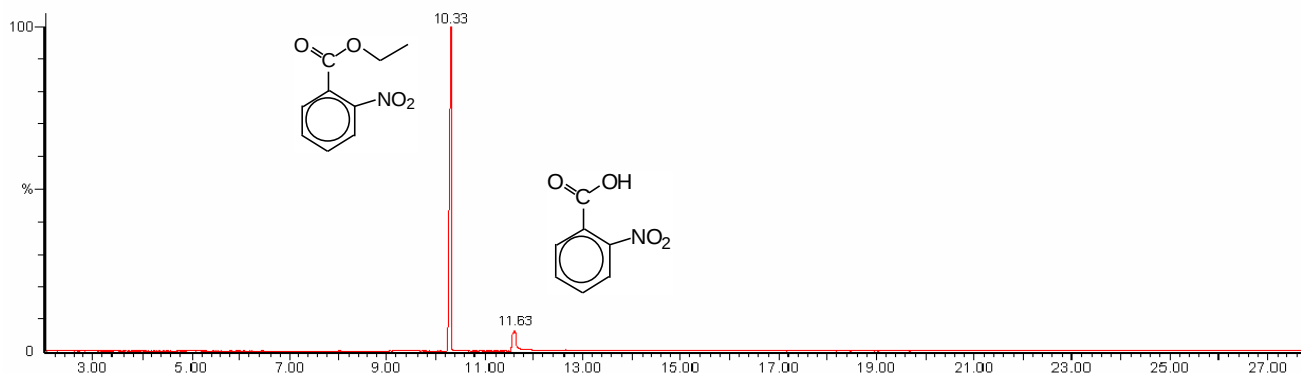
20071009-ycj-3- 1656 (10.352)



SM 4. GC/mass total ion chromatogram and mass spectrum of product of *o*-nitrobenzoyl chloride in 100% ethanol.

3. *o*-Nitrobenzoyl chloride in 80% EtOH

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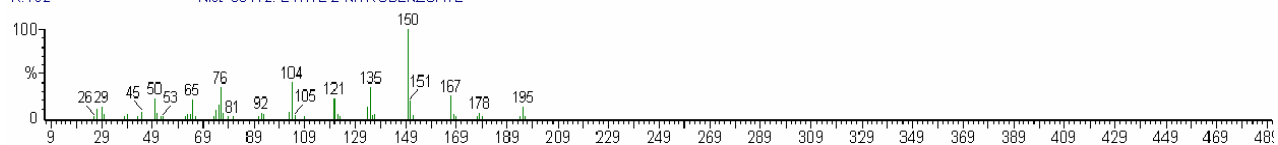
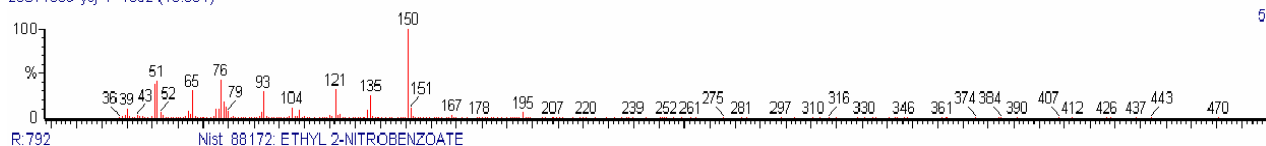


3 EtOH 80%

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20071009-ycj-4- 1652 (10.331)

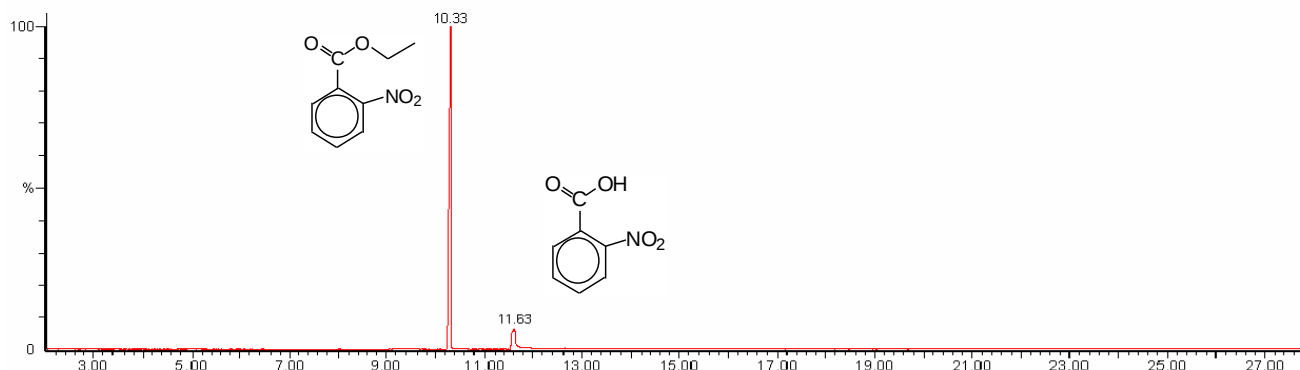
5.8



SM 5. GC/mass total ion chromatogram and mass spectrum of product of *o*-nitrobenzoyl chloride in 80% aqueous ethanol at 10.33 min.

3. *o*-Nitrobenzoyl chloride in 80% EtOH

10-OCT-200723

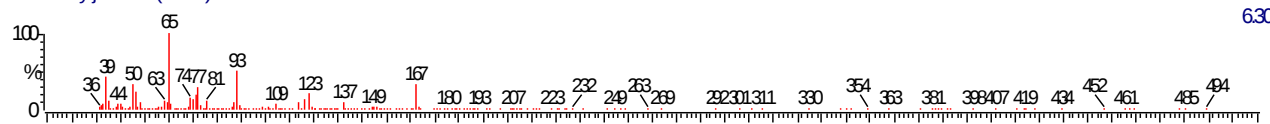


3 EtOH80%

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20071009-yg-4 1910 (11.632)

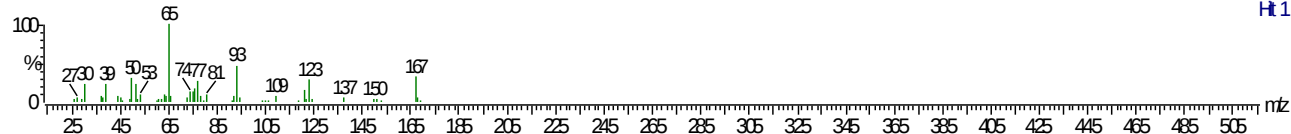
6.30e7



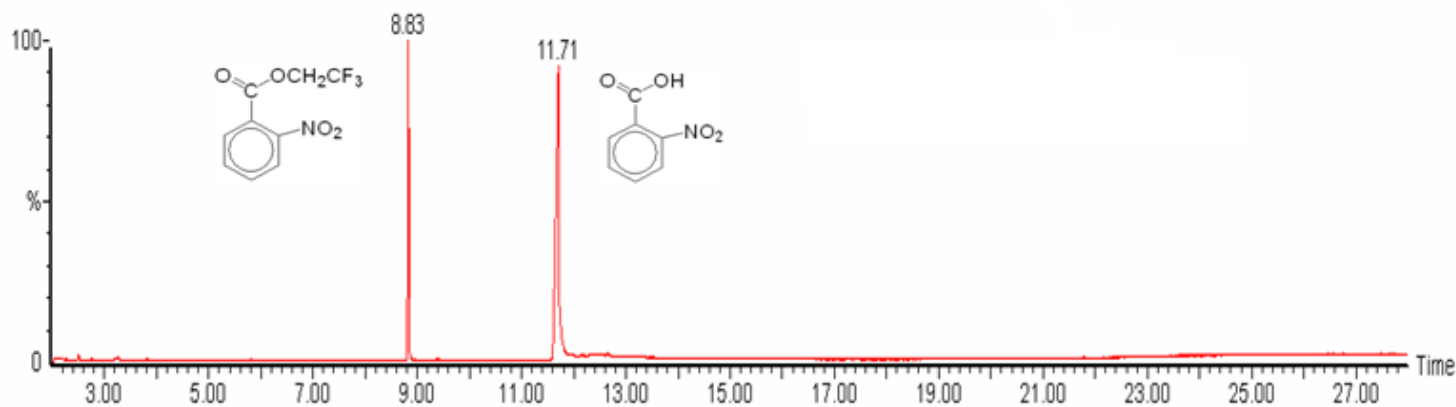
R967

VILEY 54167: BENZOIC ACID, 2-NITRO- (CAS) \$O\$NITROBENZOIC ACID\$2-NITROBENZOIC ACID

H1



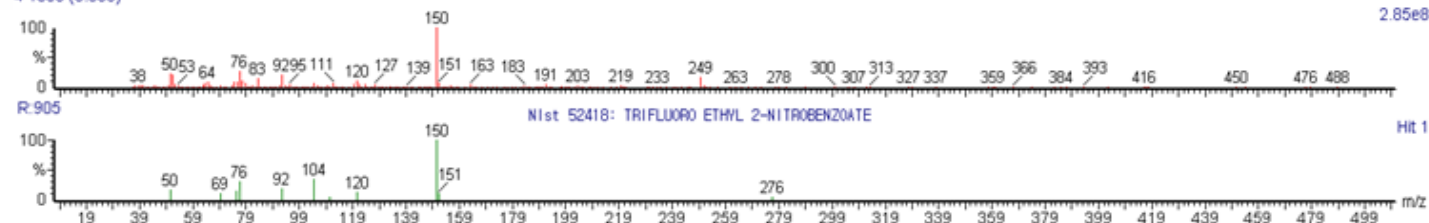
SM 6. GC/mass total ion chromatogram and mass spectrum of product of *o*-nitrobenzoyl chloride in 80% aqueous EtOH at 11.63 min.

4. *o*-Nitrobenzoyl chloride in 70% TFE

4 TFE 70

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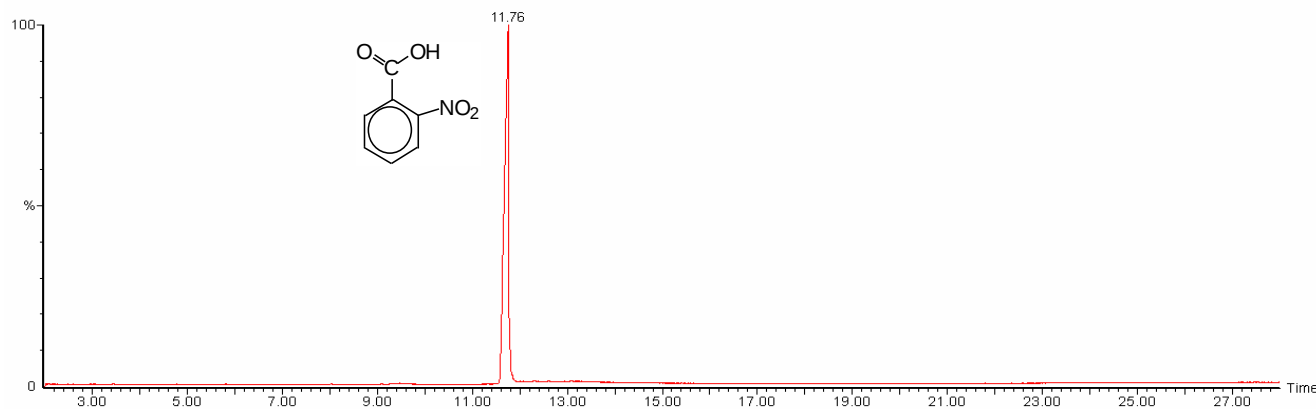
4 1356 (8.838)

SM 7. GC/mass total ion chromatogram and mass spectrum of product of *o*-nitrobenzoyl chloride

in 60% aqueous TFE.

5. *o*-Nitrobenzoyl chloride in 60% Acetone

11-OCT-200700:30:08

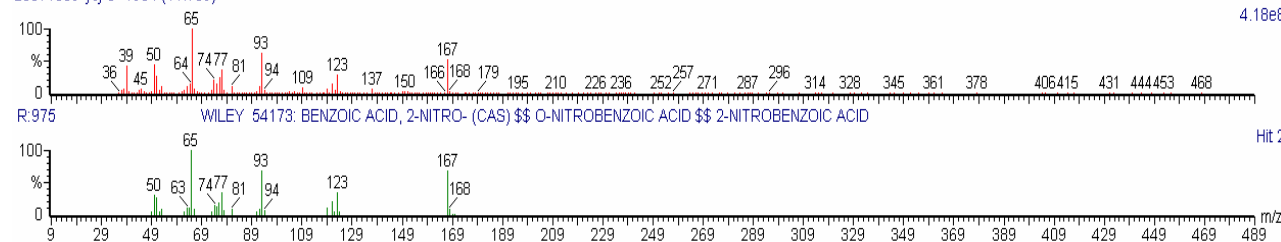


5 ACETONE 60

11-OCT-2007 + 00:30:08

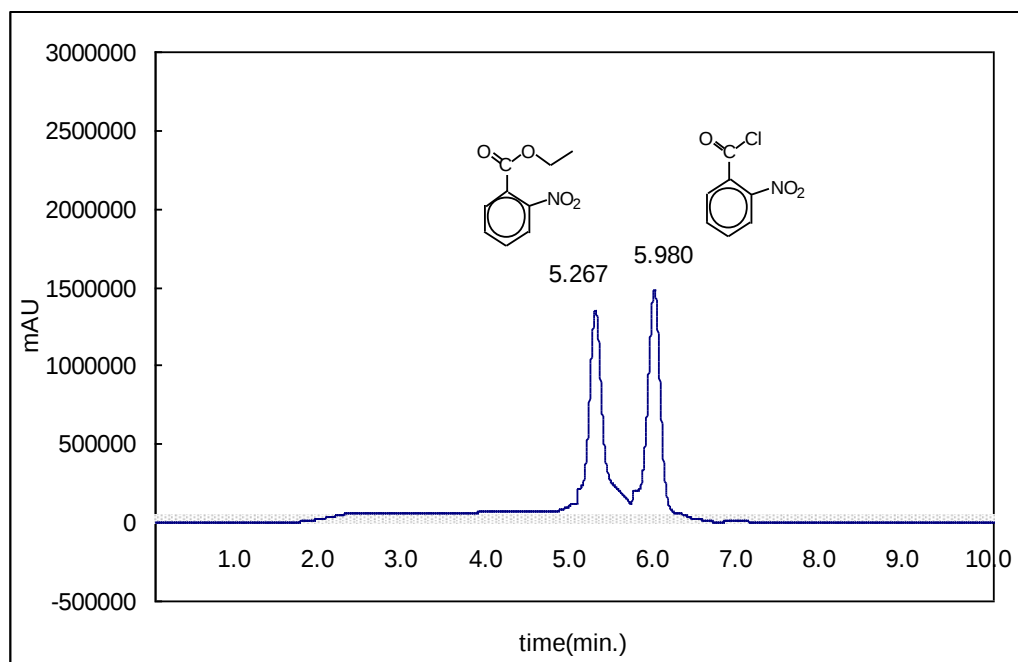
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4.18e8

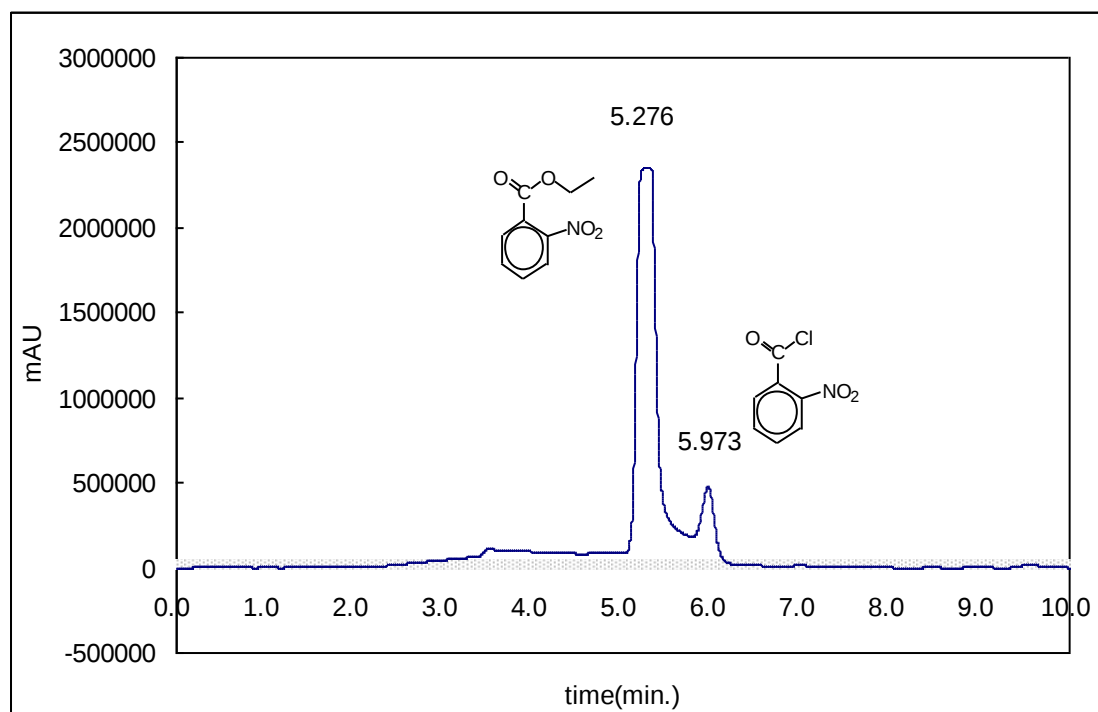


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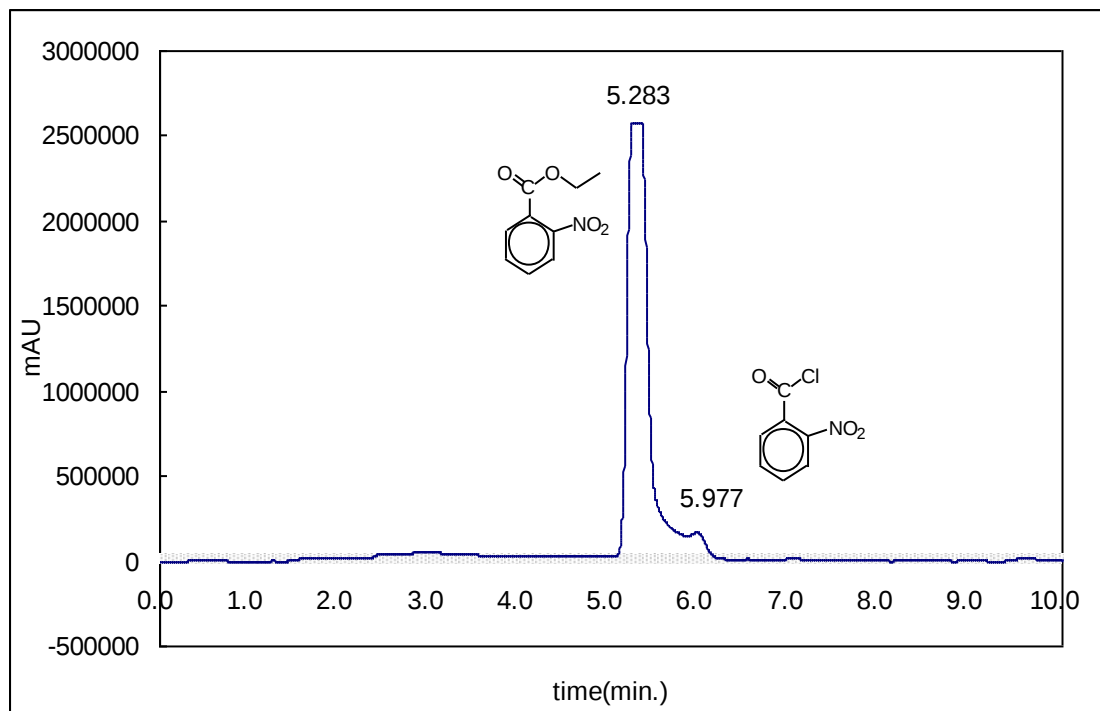
SM 8. GC/mass total ion chromatogram and mass spectrum of product of *o*-nitrobenzoyl chloride in 60% aqueous acetone.



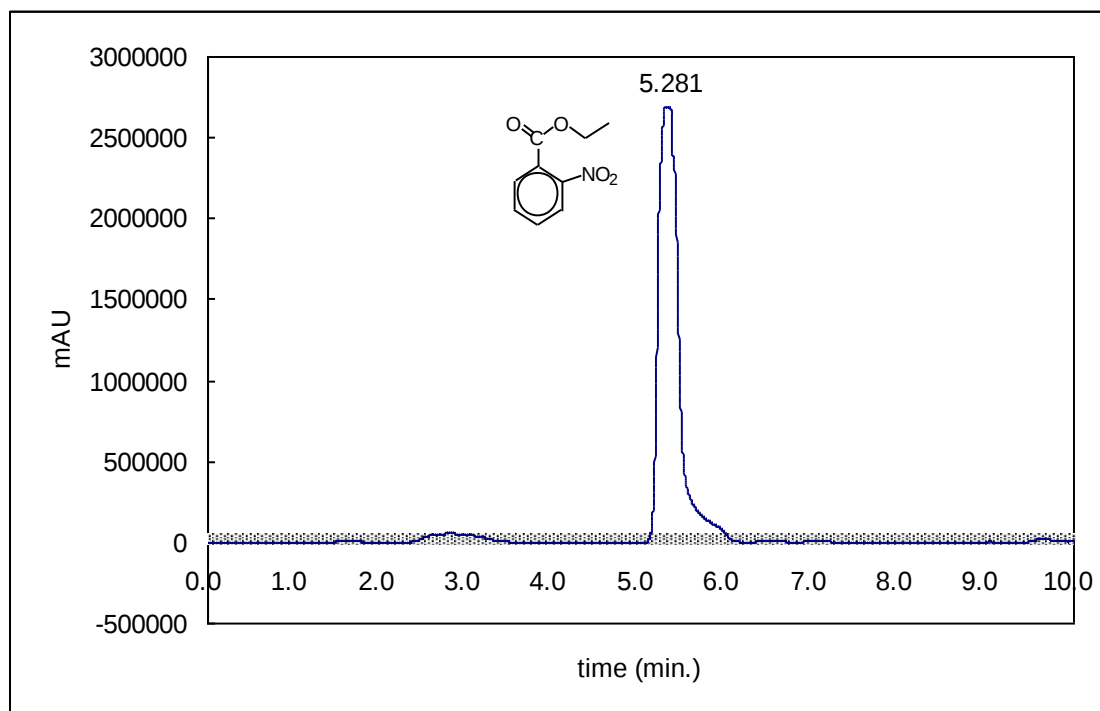
SM 9. HPLC chromatogram of *o*-nitrobenzoyl chloride in 100%EtOH at 1 minute.



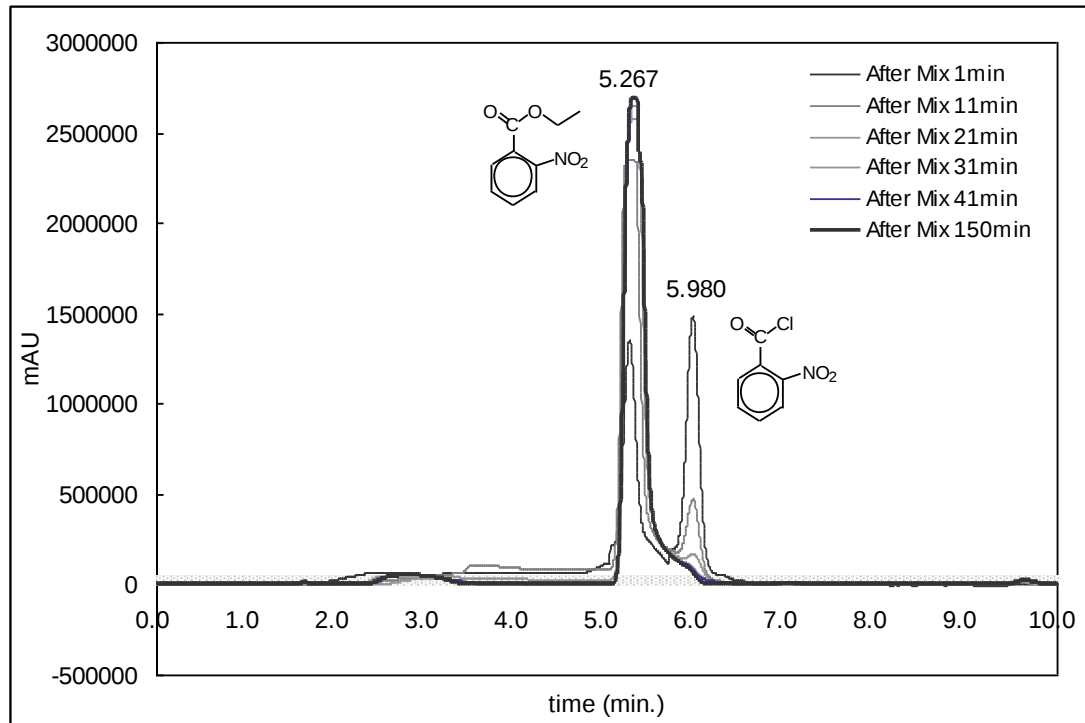
SM 10. HPLC chromatogram of *o*-nitrobenzoyl chloride in 100%EtOH at 11 minute.



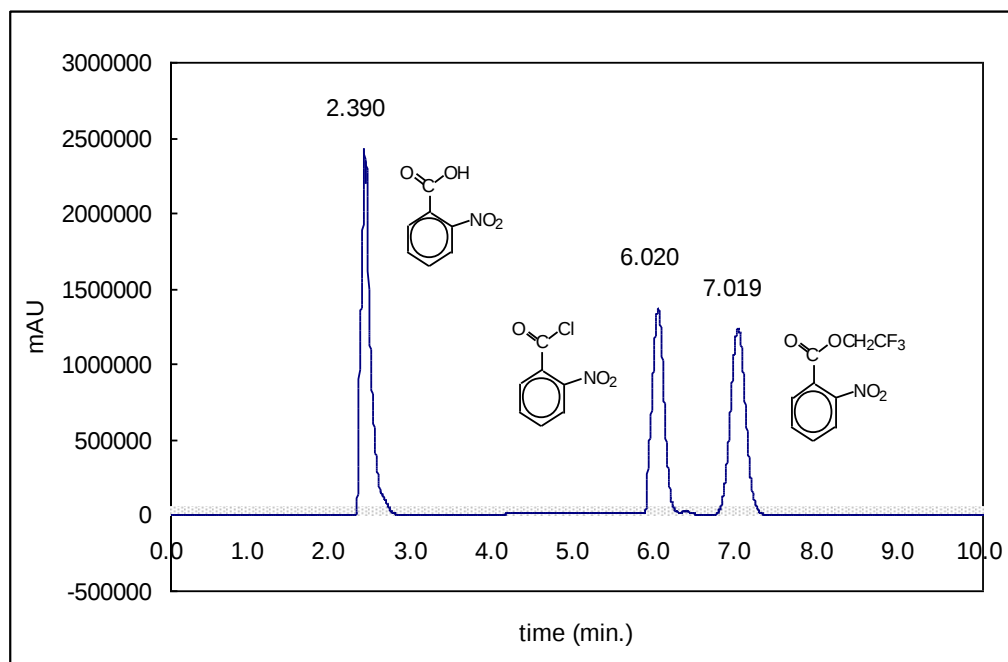
SM 11. HPLC chromatogram of *o*-nitrobenzyl chloride in 100%EtOH at 21 minute.



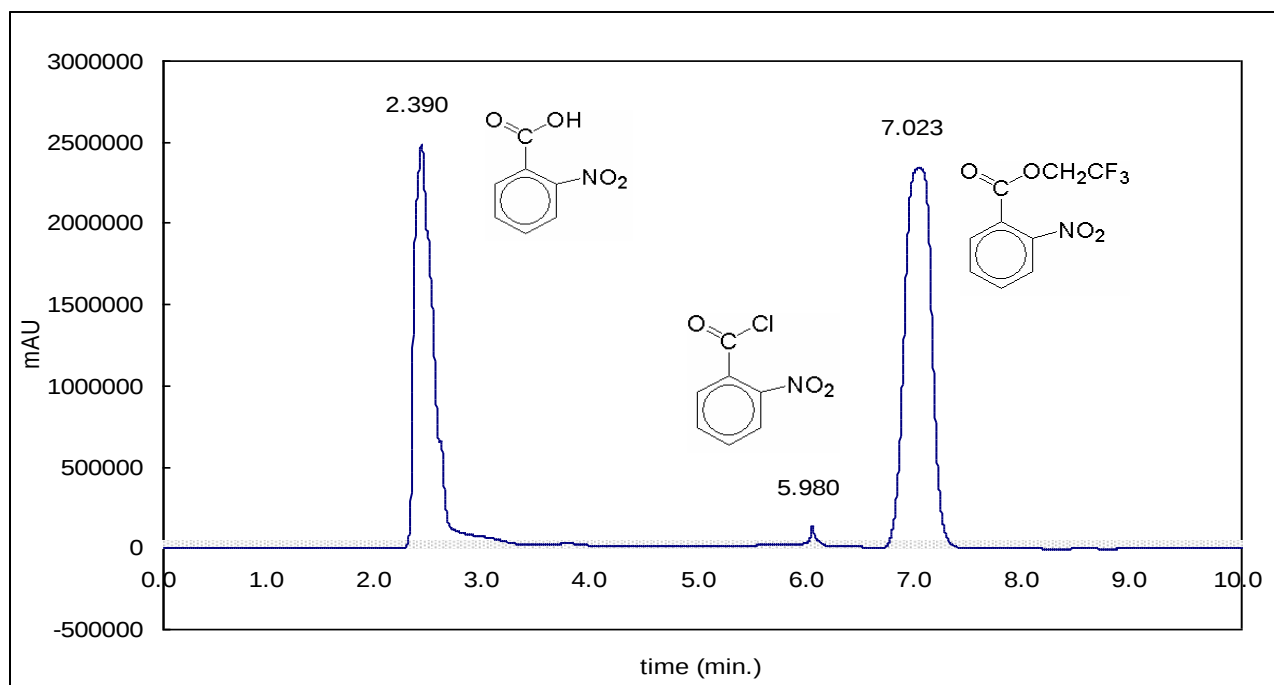
SM 12. HPLC chromatogram of *o*-nitrobenzyl chloride in 100%EtOH at 150 minute.



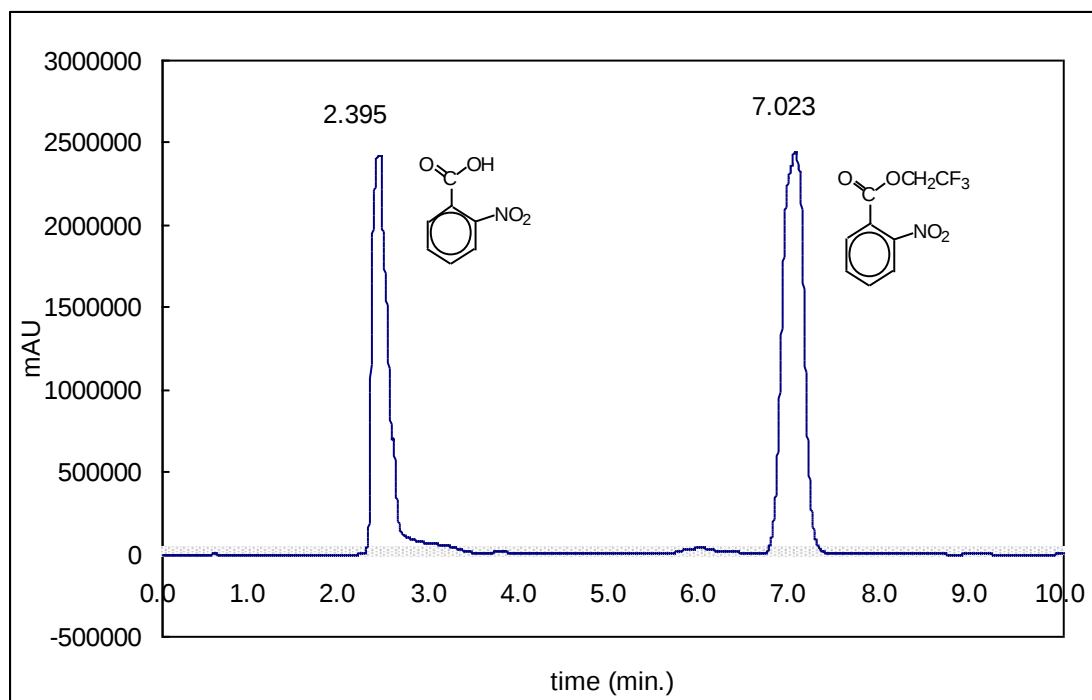
SM 13. HPLC chromatogram of *o*-nitrobenzoyl chloride in 100%EtOH at various times.



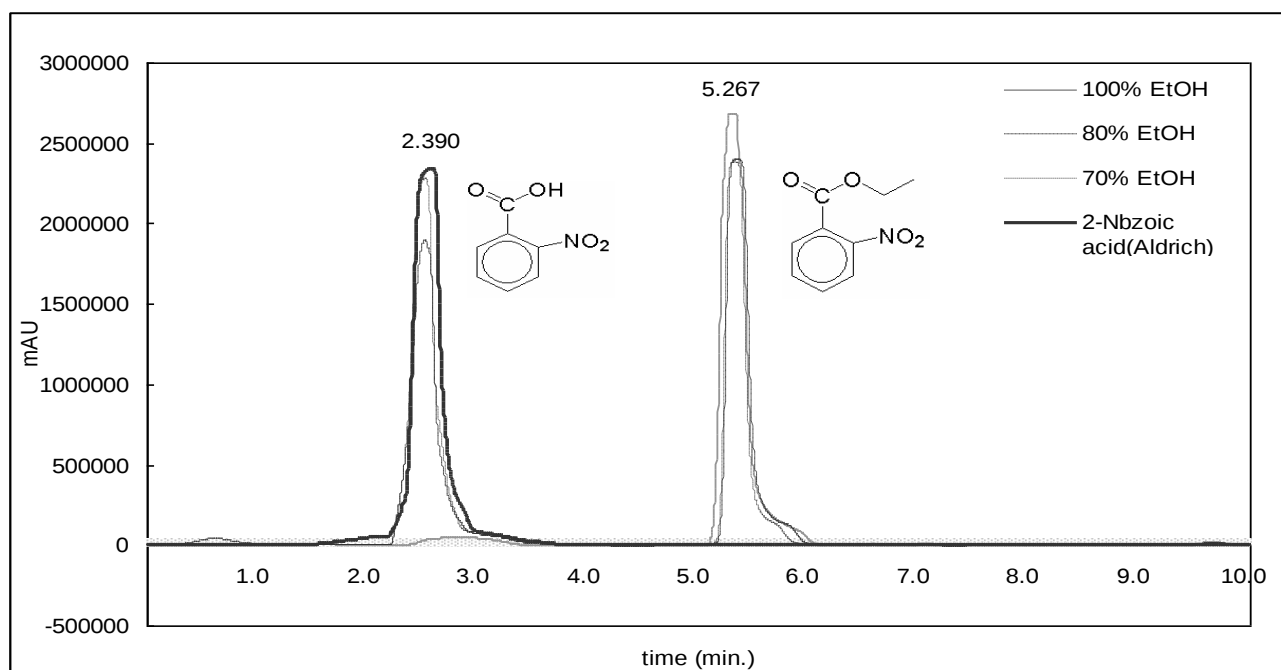
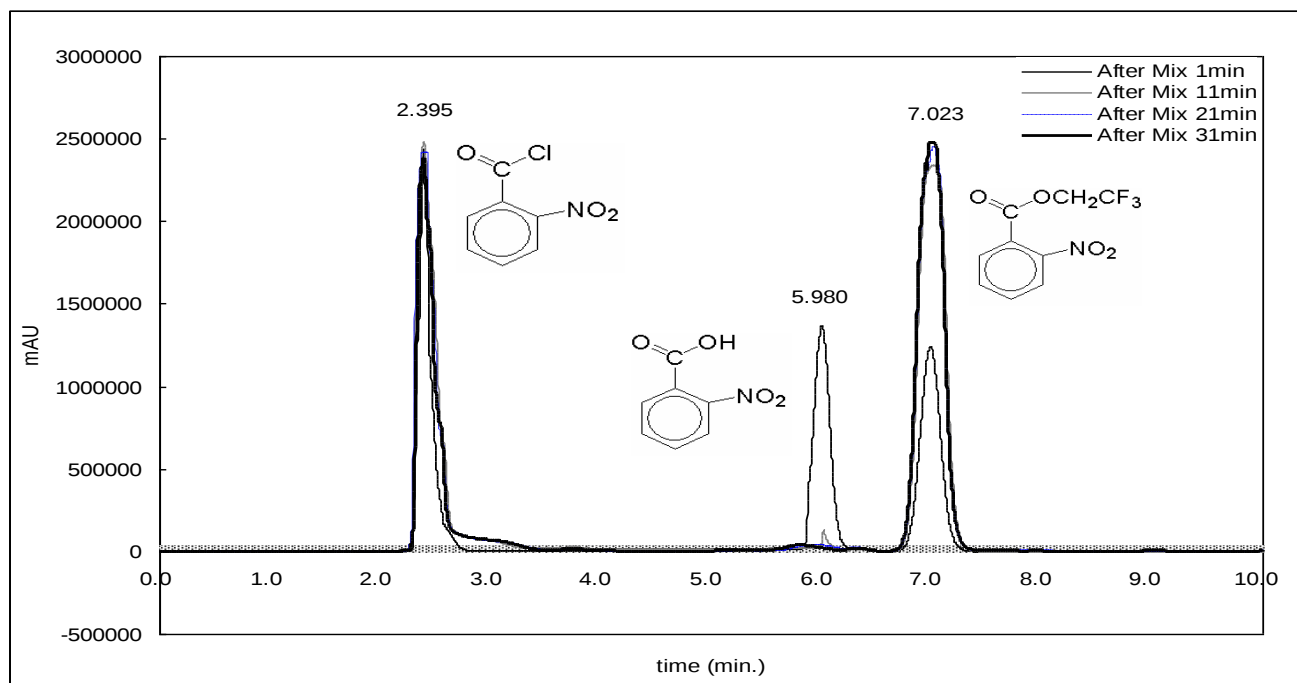
SM 14. HPLC chromatogram of *o*-nitrobenzoyl chloride in 70%TFE at 1 minute.



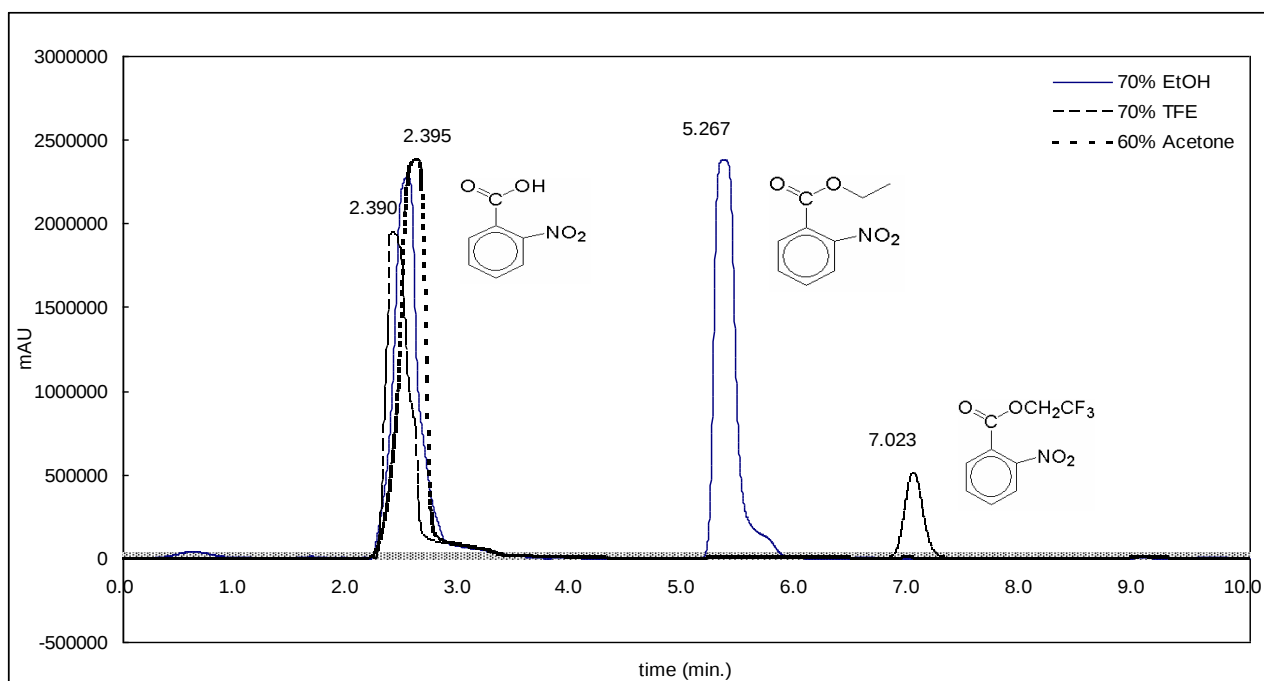
SM 15. HPLC chromatogram of *o*-nitrobenzoyl chloride in 70%TFE at 11 mnute.



SM 16. HPLC chromatogram of *o*-nitrobenzoyl chloride in 70%TFE at 31 minute.



SM 17. HPLC chromatogram of *o*-nitrobenzoyl chloride in various concentrations of pure and aqueous ethanol



SM 18. HPLC chromatogram of *o*-nitrobenzoyl chloride in various aqueous solvents.