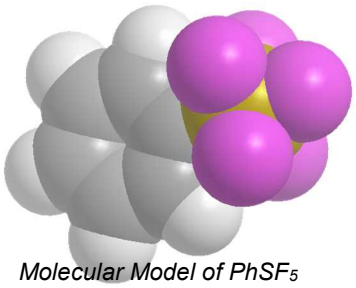
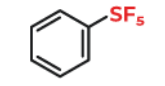


*Molecular Model of $PhSF_5$*

# *UBE Aromatic $SF_5$ Compounds*

*UBE Aromatic $SF_5$ compounds are applicable as Building blocks for pharmaceutical agents, pesticides, liquid crystals, conductive polymer, and higher performance organic materials.*



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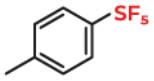

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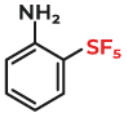

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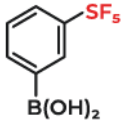

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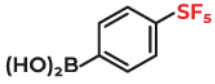

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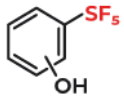

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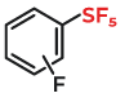

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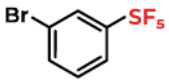

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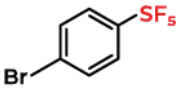

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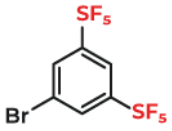
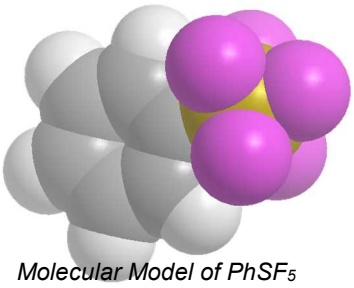


CAS# 432028-10-9

UBE / UBE INDUSTRIES,LTD.
**Pharmaceutical Division**
TEL: +81-3-5419-6178
FAX: +81-3-5419-6257
E-mail: fluorine@ube.com

# *UBE Aromatic $SF_5$ derivatives, prepared in high yield via highly versatile & cost competitive methods.*



*Molecular Model of $PhSF_5$*

***Introduction:*** *Concurrent with significant developments in the synthetic methodology for the preparation of $SF_5$ containing compounds, many potential applications, derived from the interesting and unique properties of the $SF_5$ function, have been proposed, particularly in certain advanced specialty chemical fields such as pharmaceuticals, agrochemicals and electronics.*

*The $SF_5$ function, one of the most electron-withdrawing groups known, imparts outstanding lipophilic properties to compounds which incorporate it, as well as added chemical and thermal stability. It is expected that the higher lipophilicity and other properties of $SF_5$ compounds will show interesting and unique influences on biological activities other than those observed with fluorine or trifluoromethyl-groups [1)].*

*Regarding electronics chemicals, it is reported that there has been a rapid increase in the number of patents which list the $SF_5$ group and other groups in liquid crystals due to the strong dipole moment which can be achieved by the $SF_5$ group [1), 2)].*

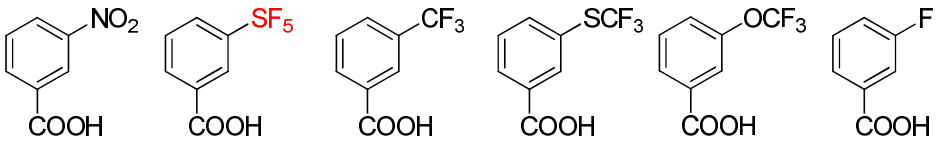
## *Properties of Aromatic $SF_5$ compounds:*

SF5 group is called **"Super-trifluoromethyl group"**[2)], and the expected properties of $SF_5$-containing compounds are similar to the ones which are seen in general fluorine compounds, although most of them are significantly enhanced by the increment of the number of fluorine atoms in $SF_5$ group.

### *A) Electron-withdrawing Effect[3)]*

$SF_5$ group is recognized as a strong electron-withdrawing group. Fig.1 below shows the comparative values of pKa in the substituted benzoic acid derivatives which have $SF_5$, $CF_3$, $SCF_3$, $OCF_3$ and F, respectively. In Fig.1, SF5 derivative is ranked as the second strongest group after the nitro-substituted one.

***Fig. 1***




| | | | | | | |
|---|---|---|---|---|---|---|
| pKa EtOH:$H_2O$ = 50:50 | 4.60 | 4.82 | 5.11 | 5.15 | 5.16 | 5.28 |
| $\sigma_m$ | 0.73 | 0.61 | 0.44 | 0.40 | 0.39 | 0.28 |

### *B) Lipophilicity [2)]*

It is well known that compounds which incorporate fluorine(s) show greater lipophilicity. Table 1 shows the comparative values of lipophilicity with varying substituents in the molecule. $SF_5$ substituted compounds are expected to show excellent lipophilicity compared with other fluorine-containing compounds.

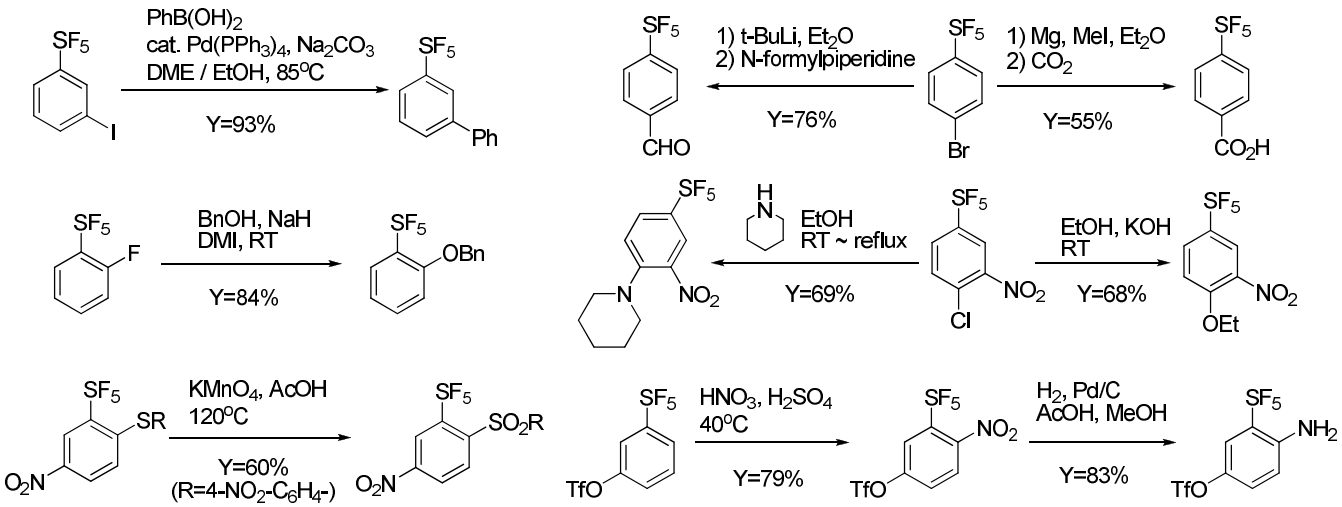
**Table 1** Lipophilicity(π) of substituent X

| Substituent X | $SCF_3$ | **$SF_5$** | $OCF_3$ | $CF_3$ | F | H | $NO_2$ |
|---|---|---|---|---|---|---|---|
| $\pi_p$ | 1.44 | **1.23** | 1.04 | 0.88 | 0.14 | 0 | -0.28 |

## C) Thermal and Chemical Stability

Aromatic $SF_5$ compounds provide excellent thermal and chemical stability.

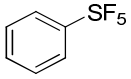
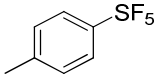
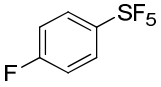
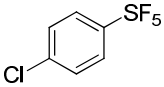
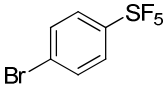
For example, it was demonstrated that the thermal decomposition rate of $PhSF_5$ (PSF) was less than 20% when heated in a sealed tube at 400°C for 7 hours [3a]. It was also demonstrated that aromatic $SF_5$ compound shows the better tolerance in either strong acid or base conditions than the corresponding $CF_3$ one [3a, 4a], thus it is widely applicable for common synthetic transformations that mostly proceed in high yield. Examples of reactions for Aromatic $SF_5$ compounds are shown below [4].




## D) Toxicity

We evaluated the health hazards of the aromatic $SF_5$ compounds by conducting mutagenicity test (Ames test) and acute oral toxicity test (rat). Table 2 below shows both results including the empirical data obtained from the acute oral toxicity tests.

**Table 2 Safety testing of Aromatic $SF_5$ compounds**

| NAME | PSF | 4MPSF | 4FPSF | 4CPSF | 4BPSF |
|---|---|---|---|---|---|
| Structure |  |  |  |  |  |
| Ames Test | Negative | Negative | Negative | Negative | Negative |
| ACUTE ORAL TOXICITY (Rat): $LD_{50}$ | >2000mg/Kg | 50-300mg/Kg | >2000mg/Kg | 300-2000mg/Kg | 300-2000mg/Kg |

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2) P. Kirsch, *Modern Fluoroorganic Chemistry; WILEY-VCH,* Weinheim, p.146, 2004
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5) *R.D. Bowden et al., WO 97/05106, 1997*
6) *T. Umemoto et al., US 7592491, 2009*