Supporting Information

Organic Base-Mediated Wittig Reaction of Perfluorohalogenated Benzaldehydes for Designing Halogen Bond-Driven Smart Polymer Materials: Toward Digitalization as Reliable Strategy in Organic Synthesis

momiyama@ims.ac.jp

Tatsuaki Hori,[1,2] Shuya Kakinuma,[1] Naoya Ohtsuka,[1,2] Takeshi Fujinami,[1] Toshiyasu, Suzuki,[1]

and Norie Momiyama[1,2]*

[1] Institute for Molecular Science, Okazaki, Aichi 444-8787, Japan

[2] SOKENDAI (The Graduate University for Advanced Studies), Okazaki, Aichi 444-8787, Japan

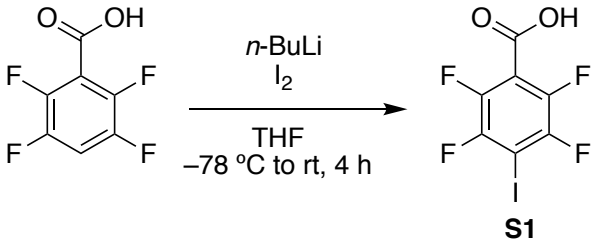
Table of Contents

1. General information

Unless otherwise noted, all reactions were carried out under an atmosphere of standard grade nitrogen gas (oxygen <10 ppm) in flame-dried glassware with magnetic stirring. Anhydrous THF, CH_2Cl_2, toluene and diethyl ether (Et_2O) were supplied from Kanto Chemical Co., Inc. as "Dehydrated solvent system". Other reagents were purchased from commercial suppliers and used without further purification. Purification of reaction products was carried out by column chromatography on silica gel 60 (spherical, neutral, 100-210 μm; KANTO and Merck). Analytical thin layer chromatography (TLC) was performed on E. Merck precoated (0.25 mm) silica gel 60-F254 plates. Visualization was accomplished with UV light and phosphomolybdic acid solution in ethanol by heating. ^{1}H NMR spectra were recorded on a JEOL ECA-400 (400 MHz) spectrometer at ambient temperature. NMR solvent was purchased from CIL ($CDCl_3$). Data are reported as follows: chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard ($CDCl_3$ 7.26 ppm), multiplicity (br = broad, s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, and m = multiplet), integration, coupling constant (Hz) and assignment. ^{13}C NMR spectra were recorded on a JEOL ECA-400 (100 MHz) spectrometer at ambient temperature. Chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard ($CDCl_3$ 77.0 ppm). ^{19}F NMR spectra were recorded on a JEOL ECS-400 (376 MHz) spectrometer. Chemical shifts are reported in ppm from the *α*,*α*,*α*-trifluorotoluene (–63.72 ppm) resonance as external standard. Infrared (IR) spectra were recorded on a Jasco FT/IR-460 plus using ATR. High-resolution mass spectra (HRMS) analysis was performed on a JEOL JMS-700 (double-focusing magnetic sector mass analyzer: EB) with the fast atom bombardment (FAB) using 3-nitrobenzyl alcohol as the matrix at the Instrument Center, Institute for Molecular Science.

2. Synthesis of 2,3,5,6-tetrafluoro-4-halobenzaldehydes

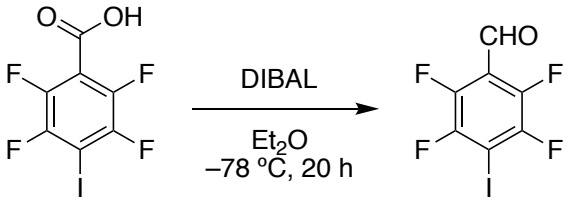
Synthesis of 2,3,5,6-tetrafluoro-4-iodobenzoic acid (S1)



S1

The **S1** was synthesized according to literature procedure.[1] To a solution of 2,3,5,6-tetrafluorobenzoic acid (2.91 g, 15.0 mmol, 1.0 equiv.) in THF (300 mL) was added *n*-BuLi (1.6 M in hexane, 18.3 mL, 29.3 mmol, 2.0 equiv.) dropwise over 15 min at –78 ºC under nitrogen atmosphere, then the mixture was stirred at –78 ºC for 1 h. A solution of iodine (3.70 g, 14.3 mmol, 0.95 equiv.) in THF (20 mL) was then slowly added to the reaction mixture. The mixture was allowed to slowly warm up to room temperature and stirred for 4 h. 2M HCl aq. (19 mL) was added to the mixture and the organic layer was separated. The aqueous layer was extracted with diethyl ether (3 x 50 mL). The combined organic layers were washed with sat. $Na_2S_2O_3$ aq. (50 mL) and brine (50 mL), dried over $MgSO_4$, and concentrated under reduced pressure after filtration to afford **S1** as white solid (4.56 g, 14.3 mmol, 95% yield). The **S1** was used in the next reaction without further purification.

Synthesis of 2,3,5,6-tetrafluoro-4-iodobenzaldehyde (1a)

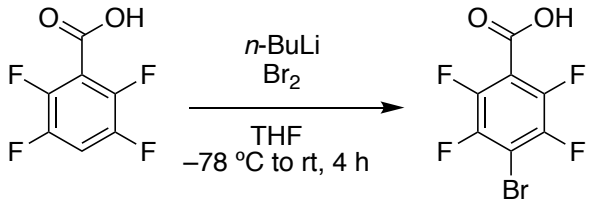


S1 **1a**

The **1a** was synthesized according to literature procedure.[2] To a solution of 2,3,5,6-tetrafluoro-4-iodobenzoic acid **S1** (4.64 g, 14.5 mmol, 1.0 equiv.) in diethyl ether (180 mL) was added DIBAL (1.0 M in *n*-hexane, 28.4 mL, 29.0 mmol, 2.0 equiv.) dropwise over 15 min at –78 °C under nitrogen atmosphere, then the mixture was stirred at –78 ºC for 14 h. Methanol (22.7 mL) was added to the mixture, and the mixture was allowed to warm to room temperature. Then 30% Rochelle's salt aq. (28.4 mL), celite (30 g), and sea sand (50 g) were added to the mixture, and the mixture was further stirred at room temperature for 1.5 h. The resulting suspension was filtered by celite and washed with

diethyl ether (50 mL). A filtrate was extracted with diethyl ether (3 x 50 mL). The combined organic layers were washed with sat. Rochelle's salt aq. (20 mL, 15 mL) and brine (30 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The obtained crude product was purified by silica gel chromatography (hexane/ethyl acetate = 30:1 to 8:1) to afford **1a** (1.36 g, 4.50 mmol, 31%) as white solid.
Rf = 0.42 (hexane/ethyl acetate = 8:1)
^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.32 (s, 1H). ^{19}F NMR ($CDCl_3$, 376 MHz) δ –118.18- –118.24 (m, 2F), –143.56- –143.65 (m, 2F). elemental analysis calcd (%) for C_7HF_4IO: C 27.66, H 0.33, F 25.00, I 41.75, found: C 27.67, H 0.56, F 24.77, I 41.70.

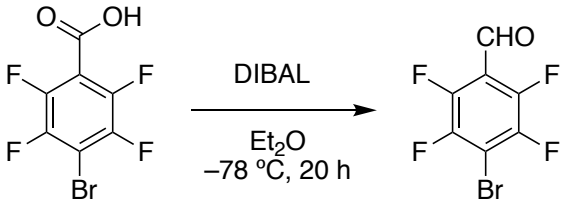
Synthesis of 4-bromo-2,3,5,6-tetrafluorobenzoic acid (S2)



S2

The **S2** was synthesized according to **Synthesis of 2,3,5,6-tetrafluoro-4-iodobenzoic acid (S1)**. To a solution of 2,3,5,6-tetrafluorobenzoic acid (584 mg, 3.01 mmol, 1.0 equiv) in THF (64 mL) was added *n*-BuLi (1.59 M in hexane, 3.80 mL, 6.04 mmol, 2.0 equiv) dropwise over 15 min at –78 ºC under nitrogen atmosphere, then the mixture was stirred at –78 ºC for 1 h. Bromine (310 μL, 6.10 mmol, 2.0 equiv.) was then added to the reaction mixture. The mixture was allowed to slowly warm up to room temperature and stirred for 4 h. 2 M HCl aq. (4.0 mL) was added to the mixture and the organic layer was separated. The aqueous layer was extracted with diethyl ether (3 x 30 mL). The combined organic layers were washed with sat. $Na_2S_2O_3$ aq. (50 mL) and brine (50 mL) and concentrated under reduced pressure after filtration. The residual product was dissolved in CH_2Cl_2 (40 mL) then the solution was back-extracted with 5% NaOH aq. (4 x 25 mL). The aqueous layer was acidified with 2 M HCl aq. (100 mL), then extracted with CH_2Cl_2 (4 x 25 mL). The combined organic layers were washed with H_2O (15 mL) and brine (20 mL), dried over $MgSO_4$, and concentrated under reduced pressure after filtration to afford **S2** as white solid (728 mg, 2.67 mmol, 89% yield). The **S2** was used in the next reaction without further purification.

Synthesis of 4-bromo-2,3,5,6-tetrafluorobenzaldehyde (1b)[3]



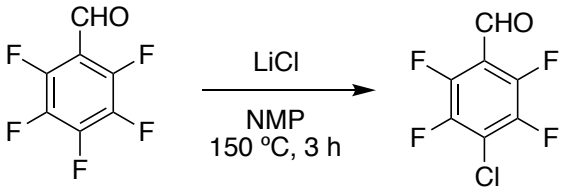
S2 **1b**

The **1b** was synthesized according to **Synthesis of 2,3,5,6-tetrafluoro-4-iodobenzaldehyde (1a)** using 4-bromo-2,3,5,6-tetrafluorobenzoic acid (**S2**) (728 mg, 2.67 mmol, 1.0 equiv.) to afford **1b** as white solid (286 mg, 1.11 mmol, 37%).

Rf = 0.42 (hexane/ethyl acetate = 8:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.30 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ –131.3- –131.4 (m, 2F), –141.0- –141.1 (m, 2F).

Synthesis of 4-chloro-2,3,5,6-tetrafluorobenzaldehyde (1c)



1c

The **1c** was synthesized according to literature procedure.[4]

A 100 mL three neck flask equipped with a magnetic stirring bar and a septum was charged with LiCl (466 mg, 11.0 mmol, 1.1 equiv.). The flask was flame-dried under vacuo then backfilled with nitrogen gas after cooling to room temperature. *N*-methylpyrrolidone (15 mL) and pentafluorobenzaldehyde (1.25 mL, 10.0 mmol, 1.0 equiv.) were added to the flask. The resulting suspension was warmed up to 150 ºC and stirred for 3 h. After cooling to room temperature, the mixture was poured into ice-water (50 mL) then extracted with CH_2Cl_2 (3 x 15 mL). The combined organic layers were washed with brine (15 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The residual crude product was purified by silica gel column chromatography (hexane/ethyl acetate = 10:1) to afford a **1c** as pale yellow solid (1.52 g, 7.10 mmol, 71% yield, 89% purity). The **1c** was further purified by washing with little amount of hexane to afford 99% purity of **1c** as white solid (891 mg, 4.20 mmol, 42% yield).

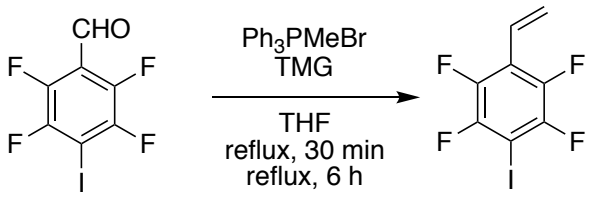
Rf = 0.20 (hexane/ethyl acetate = 10:1)

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.30 (s, 1H). ^{19}F NMR ($CDCl_3$, 376 MHz) δ –138.8- –138.9 (m, 2F), –144.1- –144.2 (m, 2F).

3. Synthesis and Characterization of 2,3,5,6-tetrafluoro-4-halostyrenes

General procedure for Wittig reaction:

Synthesis of 2,3,5,6-tetrafluoro-4-iodostyrene (2a)



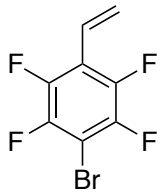
1a **2a**

To a solution of methyltriphenylphosphonium bromide (0.643 g, 1.80 mmol, 3.6 equiv.) in THF (5 mL) was added 1,1,3,3-tetramethylguanidine (282 µL, 2.25 mmol, 4.5 equiv.) and the reaction mixture was stirred at 80 ºC for 30 min. Then a solution of 2,3,5,6-tetrafluoro-4-iodobenzaldehyde **1a** (0.152 g, 0.50 mmol, 1.0 equiv.) in THF (1.5 mL) was added to the mixture. The mixture was stirred for 6 h. H_2O (10 mL) was added to the mixture and the organic layer was separated. The aqueous layer was extracted with dichloromethane (3 x 10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$. Small aliquots from the organic layers were analyzed by ^{19}F NMR using α,α,α-trifluorotoluene as standard (53% NMR yield). The organic layers were concentrated under reduced pressure to afford **2a** as colorless oil. *Due to stability of product, the **1c** was characterized as mixture and full date could not be collected.*

Rf = 0.53 (hexane)

^1H NMR ($CDCl_3$, 400 MHz) δ 6.69 (dd, *J* = 11.9, 6.2 Hz, 1H), 6.15 (d, *J* = 18.1 Hz, 1H), 5.76 (d, *J* = 11.9 Hz, 1H). ^{19}F NMR ($CDCl_3$, 376 MHz) δ –121.65—121.74 (m, 2F), –141.56—141.66 (m, 2F). ^{13}C NMR {^{19}F} ($CDCl_3$, 100 MHz) δ 147.24 (dd, *J* = 229, 15 Hz), 144.11 (dd, *J* = 239, 15 Hz), 124.40 (t, *J* = 160 Hz), 122.41 (d, *J* = 166 Hz), 117.51 (t, *J* = 13 Hz), 70.40. IR (ATR) 1471, 1416, 1259, 1101, 983, 953, 794.

4-bromo-2,3,5,6-tetrafluorostyrene (2b)



2b

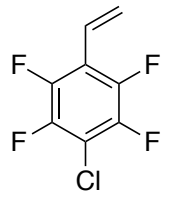
The **2b** was synthesized according to General Procedure using **1b** (128 mg, 0.500 mmol, 1.0 equiv.) to afford **2b** in 39% NMR yield. *Due to stability of product, the **2b** was*

characterized as mixture and full data could not be collected.

Rf = 0.58 (hexane)

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.67 (dd, *J* = 11.9, 18.1 Hz, 1H), 6.14 (d, *J* = 17.9 Hz, 1H), 5.76 (d, *J* = 11.9 Hz, 1H). ^{19}F NMR ($CDCl_3$, 376 MHz) δ –134.43- –134.50 (m, 2F), –142.10- –142.18 (m, 2F). ^{13}C NMR {^{19}F} ($CDCl_3$, 100 MHz) δ 145.02, 144.81, 124.42 (t, *J* = 161 Hz), 122.16 (d, *J* = 160 Hz), 116.36 (t, *J* = 13.4 Hz), 98.31. IR (ATR) 1481, 1457, 1421, 1398, 1267, 1122, 1072, 988, 957, 820, 741, 704.

4-chloro-2,3,5,6-tetrafluorostyrene (2c)



2c

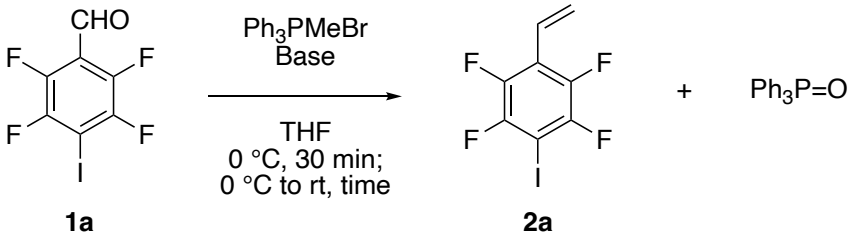
The **2c** was synthesized according to General Procedure using **1c** (106 mg, 0.500 mmol, 1.0 equiv.) to afford **2c** in 29% NMR yield. *Due to stability of product, the **2c** was characterized as mixture and full date could not be collected.*

Rf = 0.60 (hexane)

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.67 (dd, *J* = 11.5, 18.6 Hz, 1H), 6.12 (d, *J* = 18.6 Hz, 1H), 5.76 (d, *J* = 12.6 Hz, 1H). ^{19}F NMR ($CDCl_3$, 376 MHz) δ –142.11- –142.19 (m, 2F), –142.65- –142.71 (m, 2F). ^{13}C NMR {^{19}F} ($CDCl_3$, 100 MHz) δ 144.84, 144.18, 124.36 (t, *J* = 161 Hz), 121.94 (d, *J* = 162 Hz), 115.70 (t, *J* = 13.4 Hz), 110.74. IR (ATR) 1485, 1465, 1425, 1402, 1279, 1108, 1000, 989, 961, 939, 901, 859.

4. Initial study of Wittig reaction

Table S1. Wittig reaction of **1a** using conventional bases



1a **2a**

Entry	Ph_3PMeBr Equiv.	Base	Equiv.	time (h)	Yield (%)[b] **2a**	Yield (%)[b] $Ph_3P=O$
1	1.2	*n*-BuLi	1.2	2	31	64
2	1.2	*n*-BuLi	1.2	24	34	71
3	1.2	*t*-BuOK	1.2	2	2	28
4	1.2	*t*-BuOK	1.2	24	7	51
5	1.2	NaH	1.2	2	<1	2
6	1.2	NaH	1.2	24	2	4
7	1.2	K_2CO_3	1.2	2	<1	6
8	1.2	K_2CO_3	1.2	24	<1	10

a) The reaction was carried out using 0.50 mmol of **1a**, Ph_3PMeBr (1.2 equiv.) and indicated base in THF (6.5 mL) for indicated time. b) determined by ^{19}F and ^{31}P NMR using α,α,α-trifluorotoluene and triphenylphosphine as internal standards.

5. DFT Calculations

5-1. Computational analysis by DFT

All molecular geometries were optimized by the M06-2X functional with Grimme's D3 dispersion correction[5] using the 6-311+G(d,p) basis set. The SMD solvation model[6] was used with the solvents indicated. The stationary geometries were checked by the vibration analyses after the geometry optimization procedures. The stationary geometries and their energies were refined using Gaussian 16 software package.[7]

5-2. Computational details

The table shows total energy *E*, enthalpy *H*, and Gibbs free energy *G* (hartree) at the SMD/M06-2X-D3/6-311+G(d,p) level.

Table S2. Organic bases

compound	solvent	temp. (°C)	*E*	*H*	*G*
MTBD	THF	60	-478.0685409	-477.820122	-477.874209
DBN	THF	60	-383.4162621	-383.216875	-383.264765
DBU	THF	40	-462.0245018	-461.765565	-461.814401
DBU	THF	60	-462.0245018	-461.764137	-461.817565
DBU	THF	80	-462.0245018	-461.762611	-461.820816
DBU	CH_2Cl_2	55	-462.0271203	-461.767163	-461.819432
DBU	MeCN	95	-462.0265648	-461.763596	-461.825434
DBU	toluene	125	-462.0220921	-461.756142	-461.825920
DBU	Et_2O	45	-462.0242003	-461.764818	-461.814828
DBU	1,4-dioxane	115	-462.0179106	-461.752743	-461.819820
TMG	THF	60	-362.5440492	-362.341413	-362.394088
TMG	THF	80	-362.5440492	-362.340084	-362.397289
piperidine	THF	60	-251.8589684	-251.691224	-251.731886
quinuclidine	THF	60	-329.2536598	-329.048446	-329.092528
Et_3N	THF	60	-292.3478434	-292.128626	-292.180267

Table S3. (Organic base)·HBr salts

compound	solvent	temp. (°C)	*E*	*H*	*G*
MTBD·HBr	THF	60	-3052.9024750	-3052.635936	-3052.698567
DBN·HBr	THF	60	-2958.2499495	-2958.033479	-2958.091369
DBU·HBr	THF	40	-3036.8606171	-3036.584522	-3036.642610
DBU·HBr	THF	60	-3036.8606171	-3036.582886	-3036.646370
DBU·HBr	THF	80	-3036.8606171	-3036.581151	-3036.650232
DBU·HBr	CH_2Cl_2	55	-3036.8639084	-3036.586625	-3036.648763
DBU·HBr	MeCN	95	-3036.8654663	-3036.584698	-3036.658308
DBU·HBr	toluene	125	-3036.8508323	-3036.567264	-3036.650314
DBU·HBr	Et_2O	45	-3036.8576031	-3036.581161	-3036.640606
DBU·HBr	1,4-Dioxane	115	-3036.8452591	-3036.562597	-3036.641936
TMG·HBr	THF	60	-2937.3741575	-2937.154729	-2937.217686
TMG·HBr	THF	80	-2937.3741575	-2937.153162	-2937.221512
piperidine·HBr	THF	60	-2826.6854590	-2826.500219	-2826.550472
quinuclidine·HBr	THF	60	-2904.0849020	-2903.862007	-2903.915777
Et_3N·HBr	THF	60	-2867.1788689	-2866.941629	-2867.001054

Table S4. HBr

compound	solvent	temp. (°C)	*E*	*H*	*G*
HBr	THF	40	-2574.7712306	-2574.761714	-2574.785546
HBr	THF	60	-2574.7712306	-2574.761493	-2574.787075
HBr	THF	80	-2574.7712306	-2574.761271	-2574.788617
HBr	CH_2Cl_2	55	-2574.7716789	-2574.761997	-2574.787141
HBr	MeCN	95	-2574.7712393	-2574.761118	-2574.789796
HBr	toluene	125	-2574.7712645	-2574.760778	-2574.792136
HBr	Et_2O	45	-2574.7714449	-2574.761869	-2574.786137
HBr	1,4-Dioxane	115	-2574.7703863	-2574.760006	-2574.790467

6. Correlation analyses

6-1. Preparation of data sets

Data sets were prepared as csv. file using bellow descriptors.

Table S5. Descriptors for correlation analyses

Category	Descriptor	Physical meaning	Reference
Reaction	yield (%) of TFIS	Yield of 2,3,5,6-tetrafluoro-4-iodostyrene **2a**	
	yield (%) of $Ph_3P=O$	Yield of triphenylphosphine oxide	
	UDR-Pro	Undesired Reaction Product: 0: Not observed. -1:observed	
	temp. (deg C)	Reaction temperature	
	time (h)	Reaction time	
Basicity	pK_{BH}	Basicity of organic base.	Ref. 8
	Vs,min (kJ/mol)	Electrostatic potential energy for nitrogen atom center	
	NBO (a.u.)	NBO charge for nitrogen atom center	
	delta G (kcal/mol)	ΔG: Gibbs free energy for nitrogen atom center	
	HBD	Number of hydrogen-bonded donor centers connected to or conjugated with the basicity center	Ref. 8
Structure	NN	Number of Nitrogen atom in organic base	
	Cyclic/Acyclic	Type of structure for organic base (Equal to 1 if the structure is cyclic; equal to 0 if the structure is acyclic)	
	NRing	Number of ring in organic base	
	Ring Size of N	Size of the ring containing the basicity center (“0” if the center is not part of a ring)	
	Ring Size of S	Size of the ring that is out of the basicity center (“0” if the organic base is without ring structure or no	

		ring structure in the out of active center)	
Solvent	SVI-Et(30)	Solvent index: polarity index based on molar absorption energy (kcal/mol)	Ref. 9
	SVI-n	Solvent index: Reflective index	Ref. 10
	SVI-epsilon	Solvent index: dielectric constant	
	SVI-mu	Solvent index: dipole moment	
	SVI-pi*	Solvent index: polarity index based on solvatochromism	
	SVI-PC-1	Principal components which are reported in ACS solvent selection tool	Ref. 11
	SVI-PC-2		
	SVI-PC-3		
	SVI-PC-4		
	SVI-PC-5		
	SVI-DN	Solvent index: Number of Electron pair Donor	Ref. 12
	SVI-AN	Solvent index: Number of Electron pair Acceptor	
	SVI-dD	Solvent index: The energy from dispersion forces between molecules	Ref. 13
	SVI-dP	Solvent index: The energy from dipolar intermolecular forces between molecules	
	SVI-dH	The energy from hydrogen bonds between molecules	

6-2. Missing values

Some missing values such as $pK_{B\text{-}H}$ of DBU in CH_2Cl_2, toluene, diethyl ether, MTBE, glyme, and 1,4-dioxane, ΔG of DBU in MTBE and glyme, NBO of DBU in MTBE and glyme, Vs,min of DBU in MTBE and glyme, SVI-pi* of MTBE, SVI-DN of MTBE, and SVI-AN of MTBE, were complemented by Datachemical LAB[14] using VBGMR as prediction model.

6-3. Heatmaps

Correlation analyses were performed by Datachemical LAB[14] using the prepared data sets.

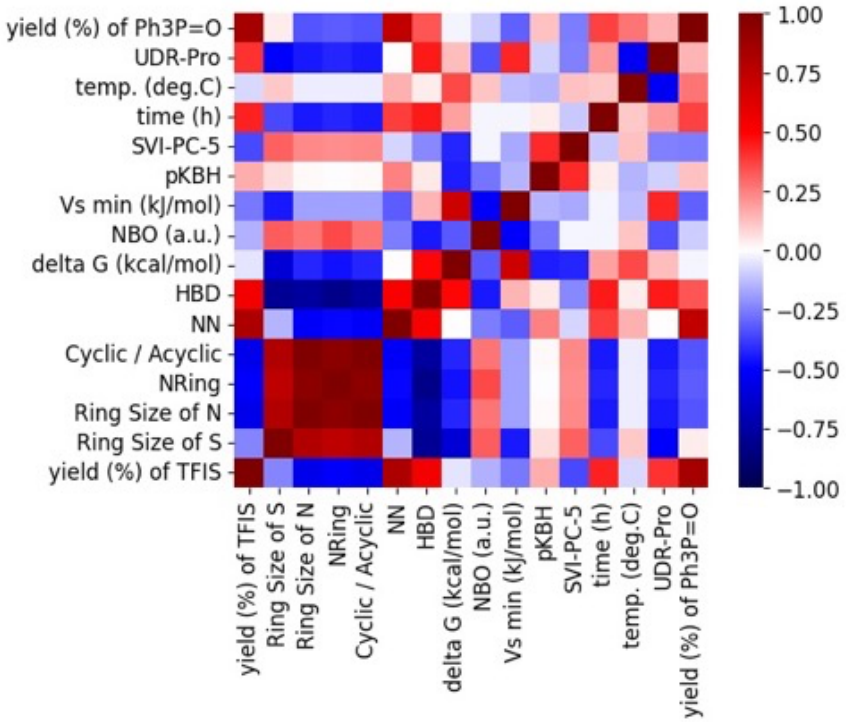


Figure S1. Heatmap for reaction, basicity, and structure.

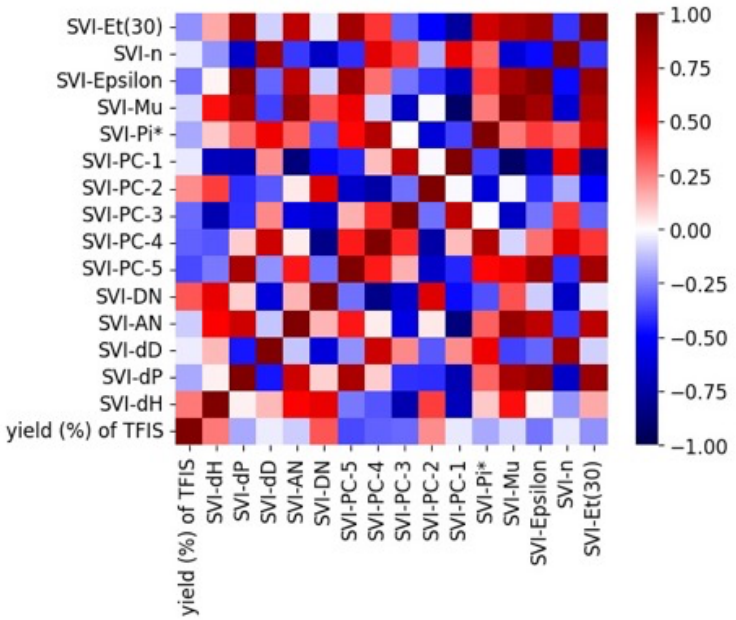


Figure S2. Heatmap for solvent index.

Table S6. Absolute value of coefficients |*r*| between yield of TFIS and other descriptors

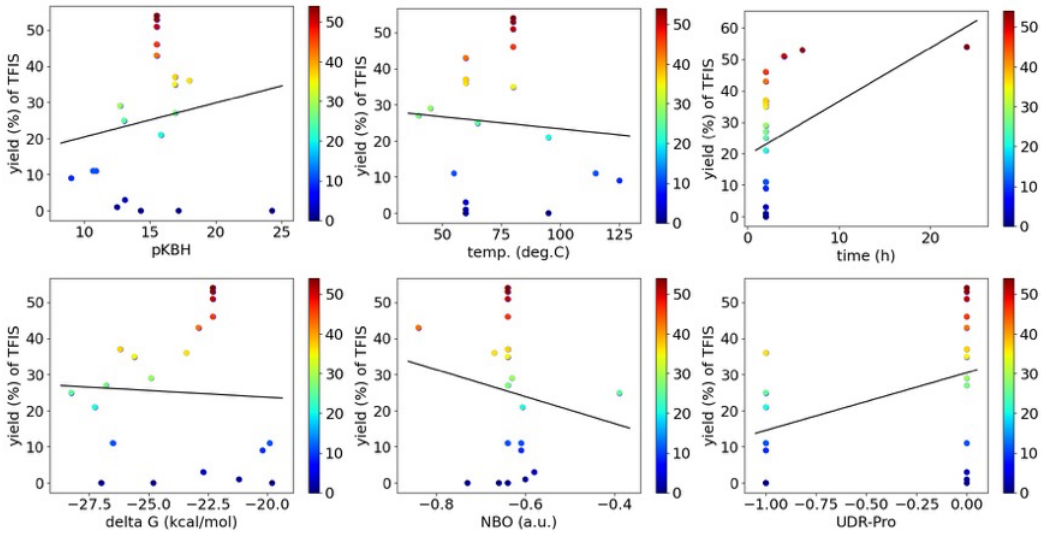
a) |*r*| with reaction, basicity, and structure

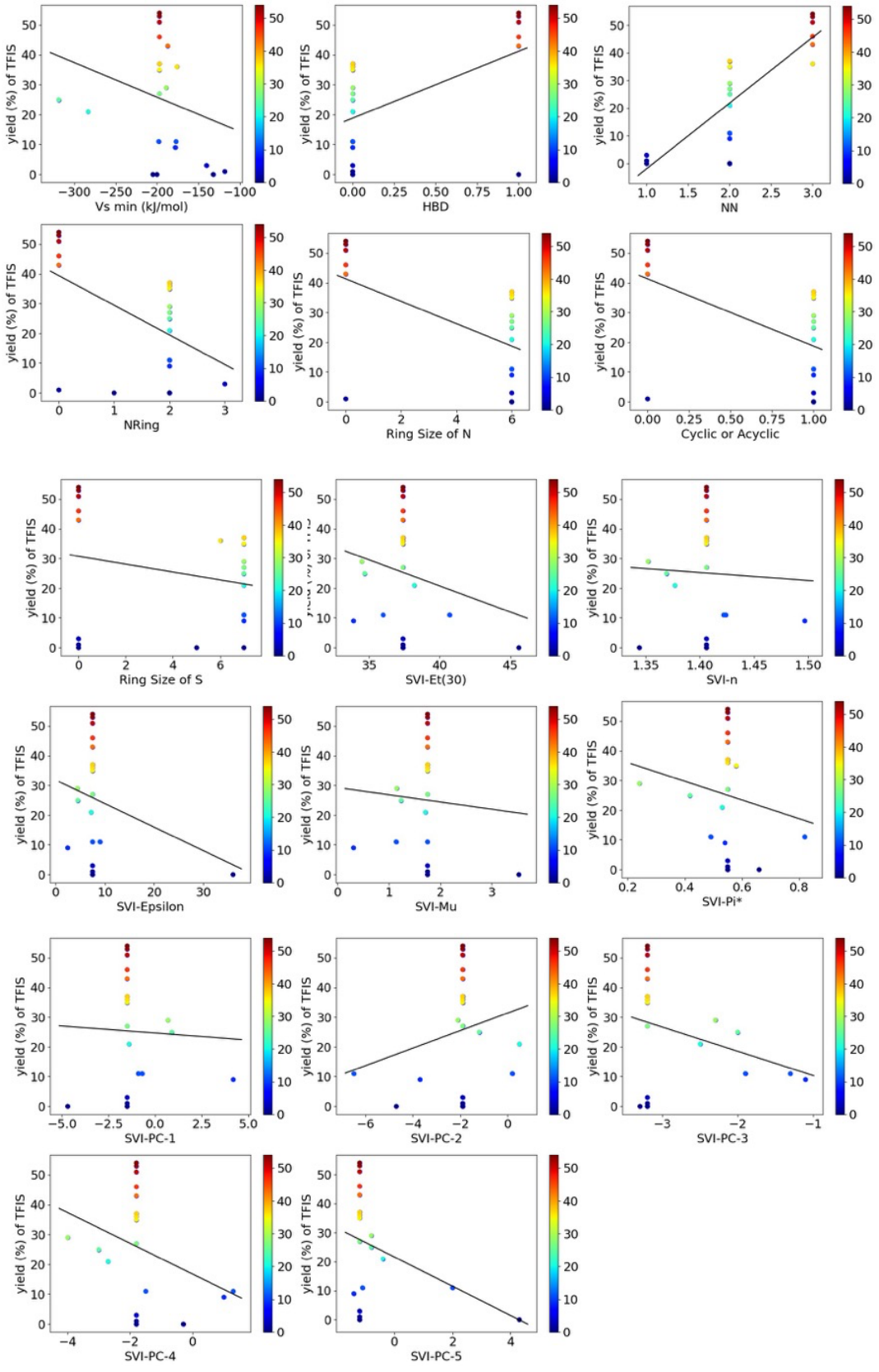
yield (%) of Ph3P=O	0.84831668
NN	0.81926259
Ring Size of N	0.55164264
Cyclic / Acyclic	0.55164264
HBD	0.54594722
NRing	0.51394616
time (h)	0.43482153
UDR-Pro	0.40571214
SVI-PC-5	0.35895377
Vs min (kJ/mol)	0.26216825
Ring Size of S	0.23785348
pKBH	0.16004195
NBO (a.u.)	0.15235514
temp. (deg.C)	0.07632792
delta G (kcal/mol)	0.05130469

b) |*r*| with solvent index

SVI-PC-5	0.35895377
SVI-DN	0.33311941
SVI-PC-4	0.31192379
SVI-PC-3	0.29447727
SVI-epsilon	0.27164037
SVI-dH	0.26296359
SVI-PC-2	0.22569313
SVI-Et(30)	0.21588364
SVI-dP	0.16739549
SVI-pi*	0.16669091
SVI-AN	0.09911477
SVI-mu	0.07085037
SVI-n	0.04178254
SVI-PC-1	0.03975838
SVI-dD	0.03536133

6-4. Scatter plots between yield of TFIS and other descriptors




yield (%) of TFIS
Vs min (kJ/mol)
HBD
NN
NRing
Ring Size of N
Cyclic or Acyclic
Ring Size of S
SVI-Et(30)
SVI-n
SVI-Epsilon
SVI-Mu
SVI-Pi*
SVI-PC-1
SVI-PC-2
SVI-PC-3
SVI-PC-4
SVI-PC-5

7. References

[1] Biot, N.; Bonifazi, D. *Chem. Eur. J.* **2020**, *26*, 2904.

[2] Dumele, O.; Trapp, N.; Diederich, F. *Angew. Chem. Int. Ed.* **2015**, *54*, 12339.

[3] Koehne, I.; Lik, A.; Gerstel, M.; Bruhn, C.; Reithmaier, J. P.; Benyoucef, M.; Pietschnig, R. *Dalton Trans.* **2020**, *49*, 16683.

[4] a) Mariaca, P.; Labat, G.; Behrnd, N.-R.; Bonin, M.; Helbling, F.; Eggli, P.; Couderc, G.; Neels, A.; Stoeckli-Evans, H.; Hulliger, J. *J. Fluorine Chem.* **2009**, *130*, 175. b) Senaweera, S.; Weaver, J. D. *Chem. Commun.* **2017**, *53*, 7545.

[5] Grimme, S.; Antony, J.; Ehrlich S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

[6] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378−6396.

[7] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J.V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[8] Tshepelevitsh, S.; Kütt, A.; Lõkov, M.; Kaljirand, I.; Saame, J.; Heering, A.; Plieger, P. G.; Vianello, R.; Leito, I. *Eut. J. Org. Chem.* **2019**, *2019*, 6735.

[9] Reichardt, C. *Chem. Rev.* **1994**, *94*, 2319.

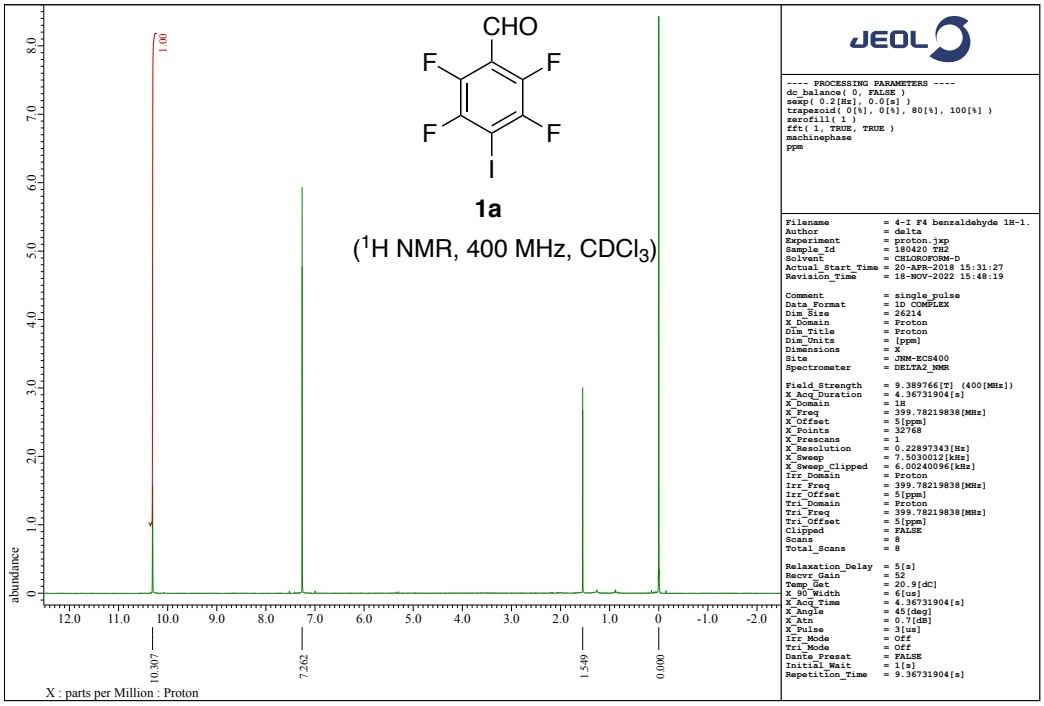
[10] a) Laurence, C.; Nicolet, P.; Dalati, T. *J. Phys. Chem.* **1994**, *98*, 5807. b) Spingler, B.; Schnidrig, S.; Todorova, T.; Wild, F. *CrystEngComm* **2012**, *14*, 751.

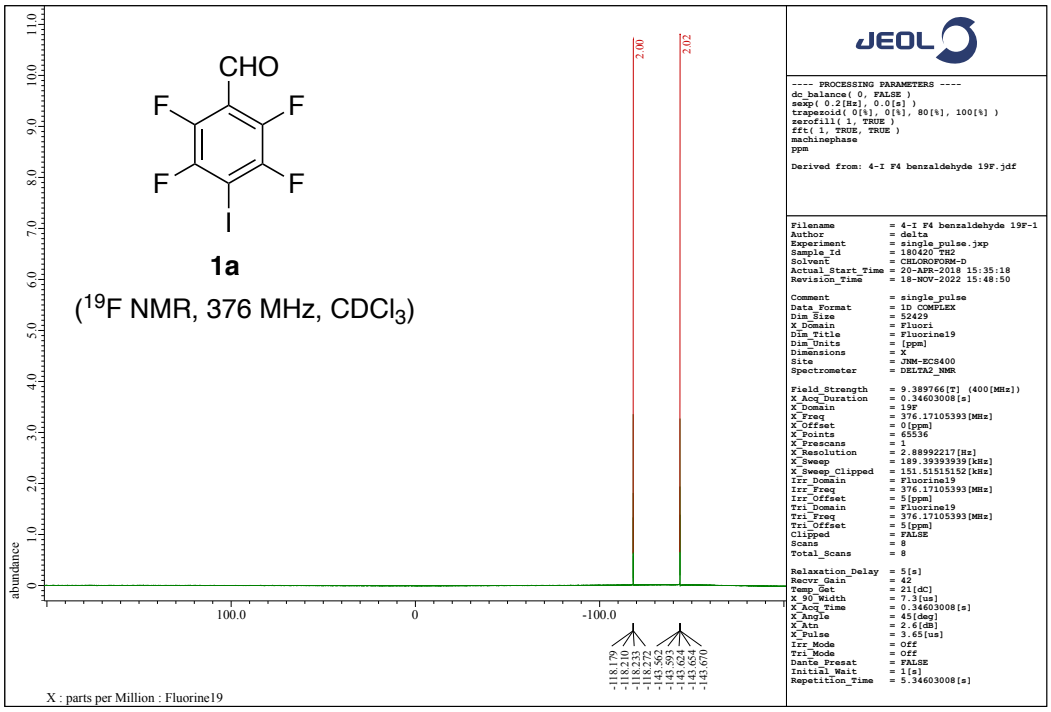
[11] a) Diorazio, L. J.; Hose, D. R. J.; Adlington, N. K. *Org. Process Res. Des.* **2016**, *20*, 760. b) ACS solvent selection tool: https://www.acs.org/greenchemistry/research-innovation/tools-for-green-chemistry/solvent-selection-tool.html

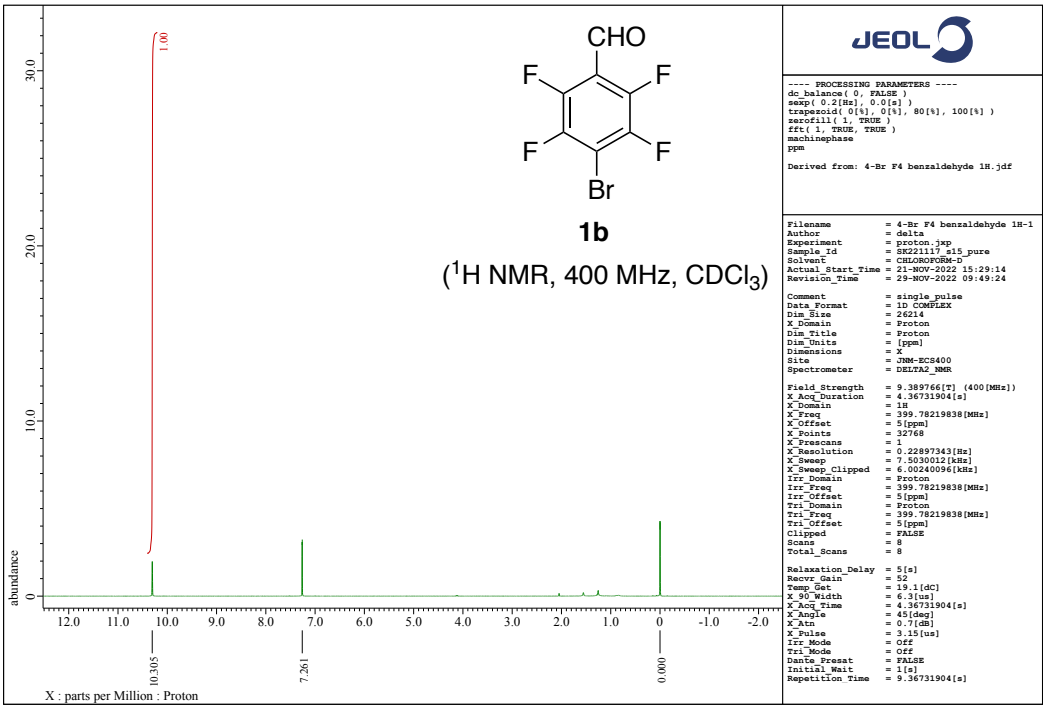
[12] a) Mayer, U.; Gutmann, V.; Gerger, W. *Monatsh. Chem.* **1975**, *106*, 1235. b) Gutmann, V. *Coord. Chem. Rev.* **1976**, *18*, 225. c) Marcus, Y. *J. Solution Chem.* **1984**, *13*, 599.

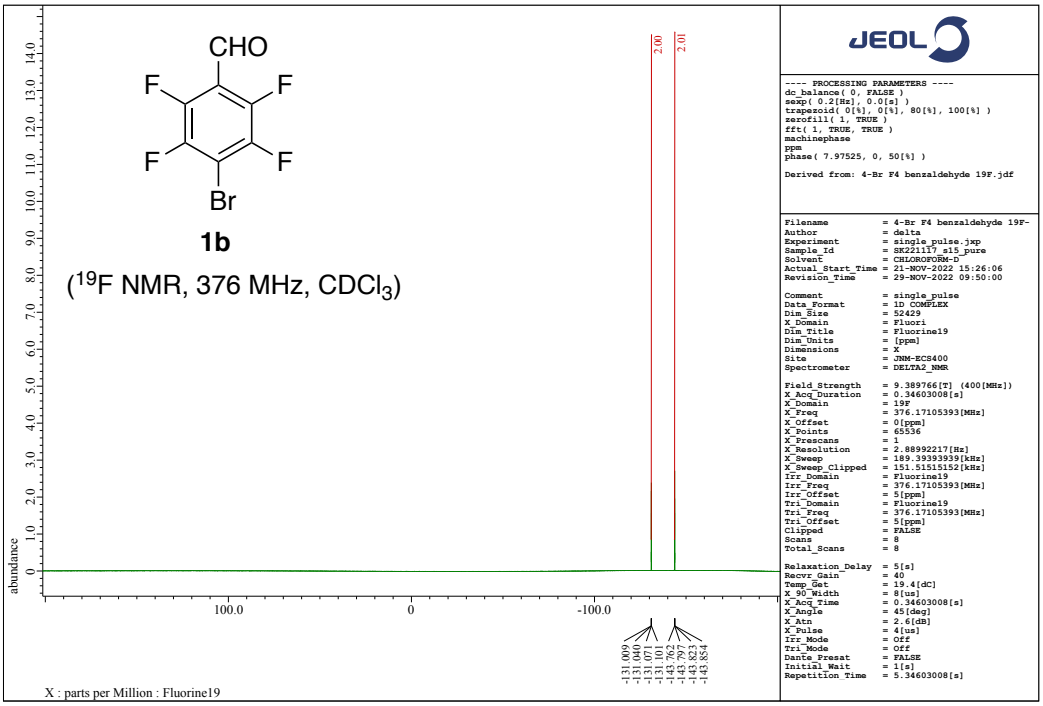
[13] Takebayashi, Y.; Morii, N.; Sue, K.; Furuya, T.; Yoda, S.; Ikemizu, D.; Taka, H. *Ind. Eng. Chem. Res.* **2015**, *54*, 8801. b) Ruwoldt, J.; Tanase-Opedal, M.; Syverud, K. *ACS Omega* **2022**, *7*, 46371.
[14] Datachemical LAB: https://www.datachemicallab.com/

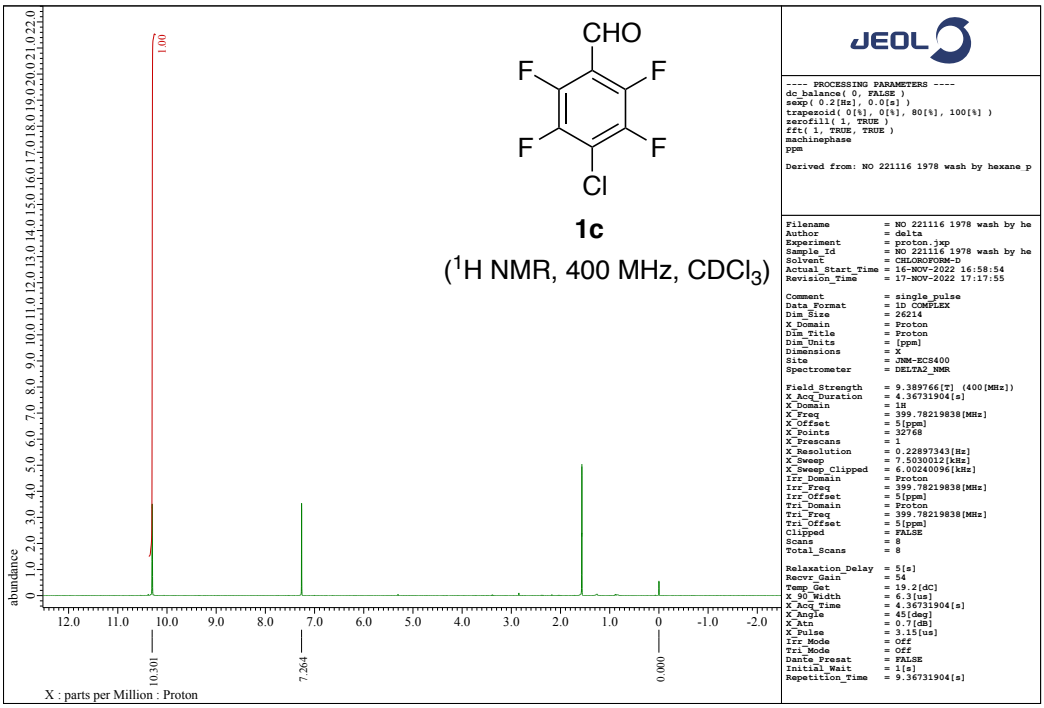
8. NMR spectra

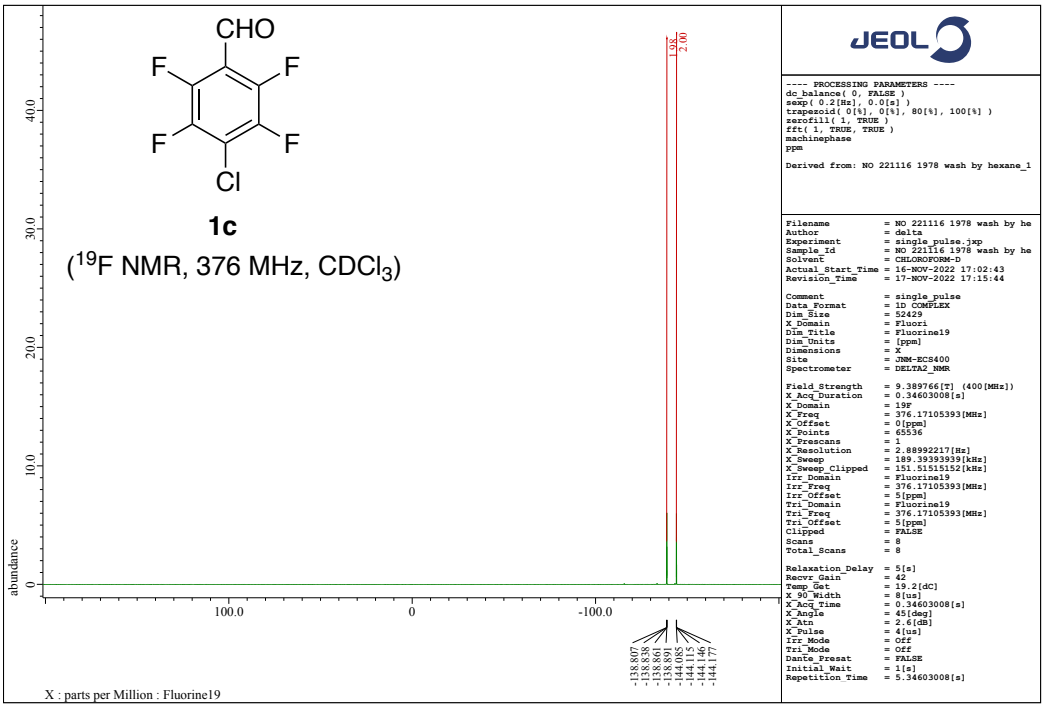


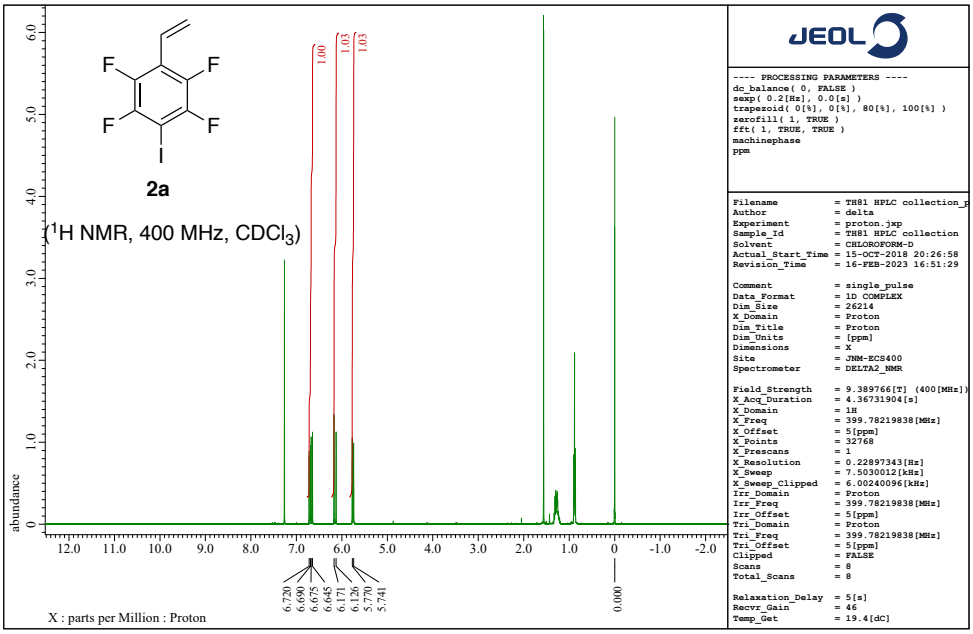


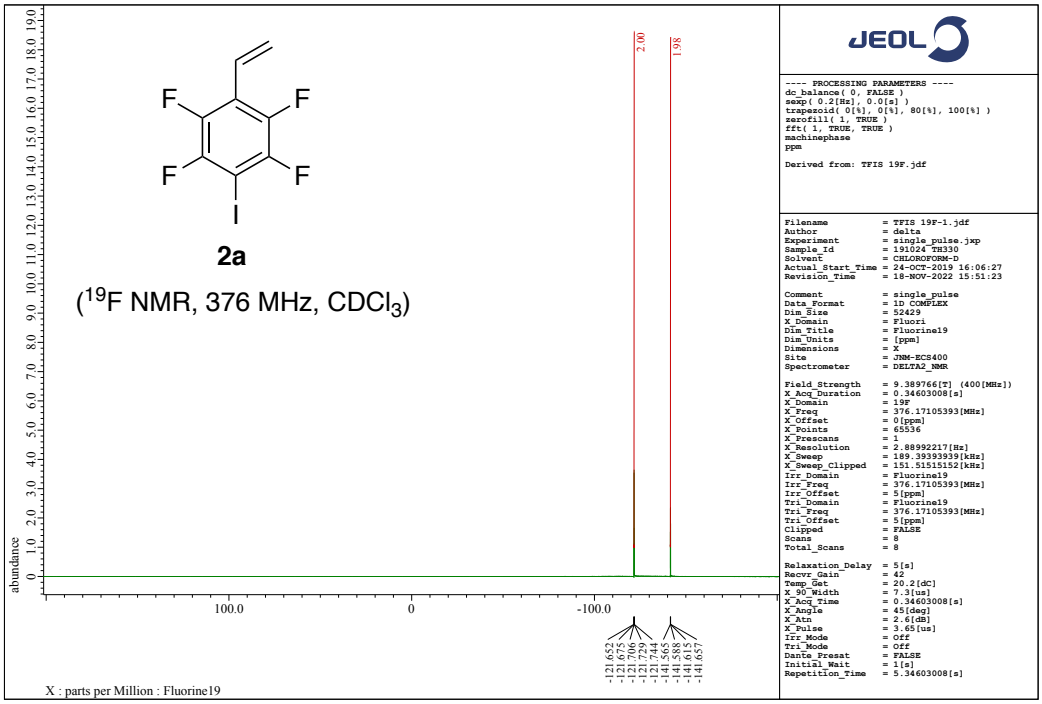

CHO
F
F
F
F
Br
1b
(1H NMR, 400 MHz, CDCl3)
abundance
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 4-Br F4 benzaldehyde 1H.jdf
Filename = 4-Br F4 benzaldehyde 1H-1
Author = delta
Experiment = proton.jxp
Sample_Id = SK221117_s15_pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2022 15:29:14
Revision_Time = 29-NOV-2022 09:49:24
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 52
Temp_Get = 19.1[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

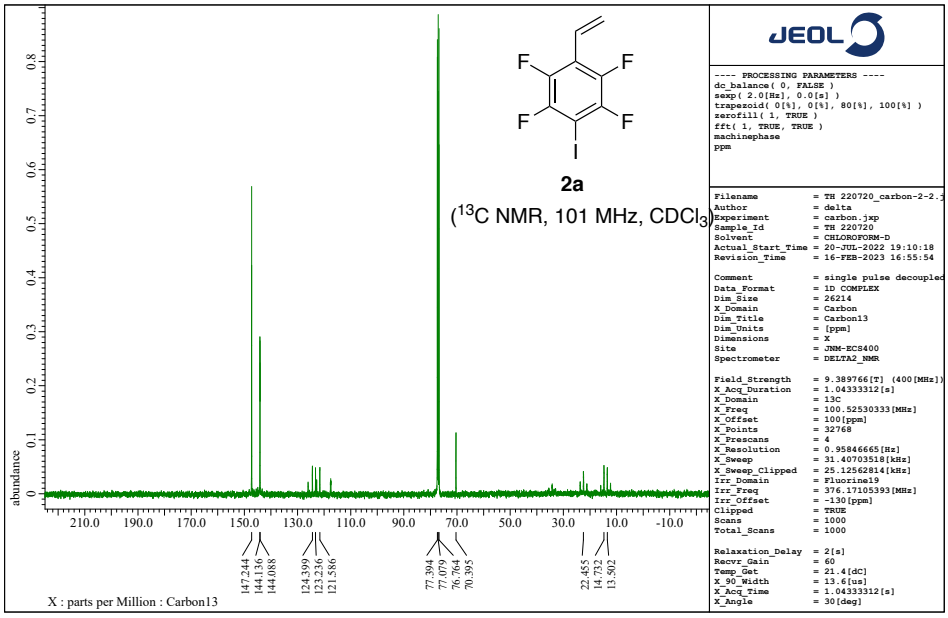

CHO
F
F
F
F
Br
1b
(19F NMR, 376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(7.97525, 0, 50[%])
Derived from: 4-Br F4 benzaldehyde 19F.jdf
Filename = 4-Br F4 benzaldehyde 19F-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SK221117_s15_pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2022 15:26:06
Revision_Time = 29-NOV-2022 09:50:00
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[Hz]
X_Sweep = 189.39393939[kHz]
X_Sweep_Clipped = 151.51515152[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 19.4[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

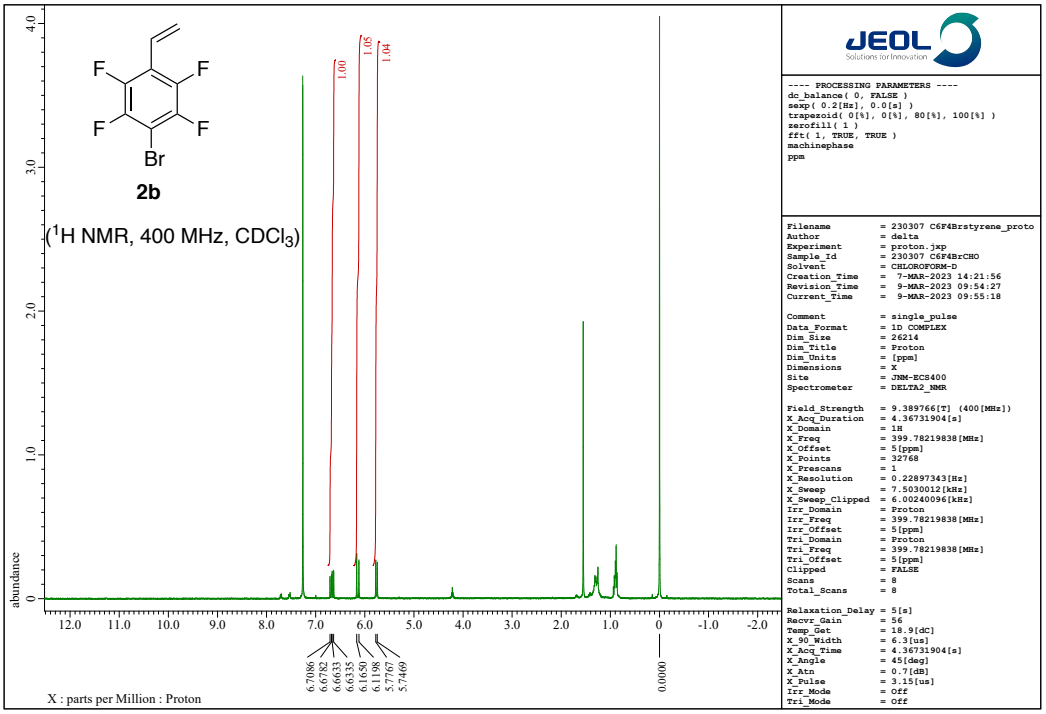

CHO
F
F
F
F
Cl
1c
(1H NMR, 400 MHz, CDCl3)
abundance
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 221116 1978 wash by hexane_p
Filename = NO 221116 1978 wash by he
Author = delta
Experiment = proton.jxp
Sample_Id = NO 221116 1978 wash by he
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-NOV-2022 16:58:54
Revision_Time = 17-NOV-2022 17:17:55
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 54
Temp_Get = 19.2[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

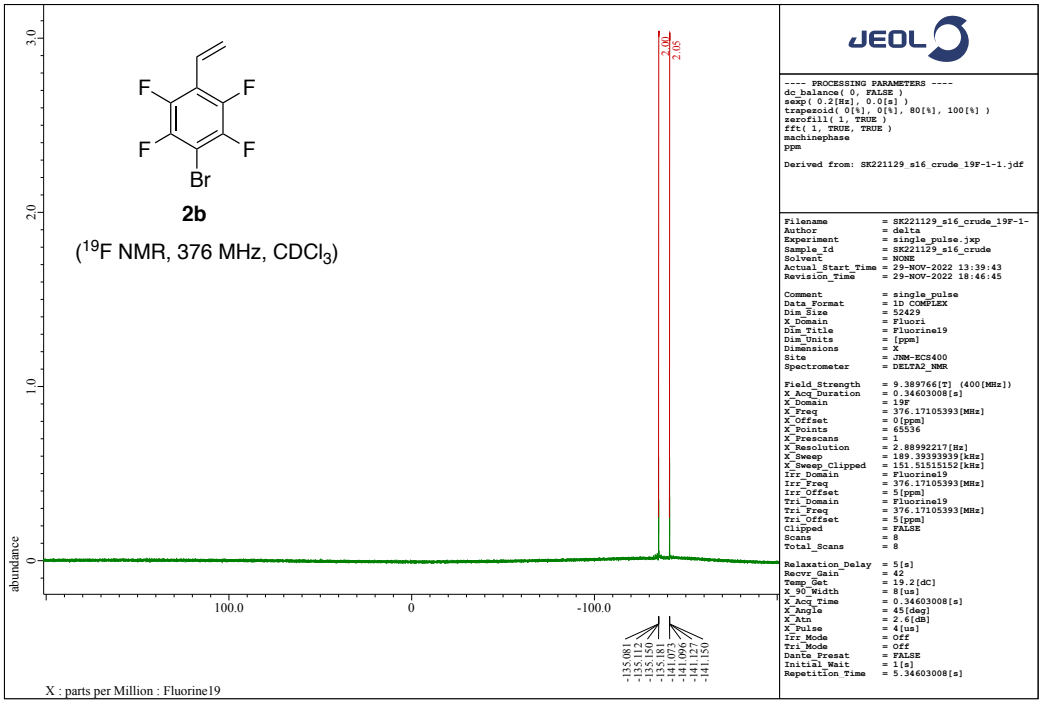

CHO
F
F
F
F
Cl
1c
(19F NMR, 376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 221116 1978 wash by hexane_1
Filename = NO 221116 1978 wash by he
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 221116 1978 wash by he
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-NOV-2022 17:02:43
Revision_Time = 17-NOV-2022 17:15:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[Hz]
X_Sweep = 189.39393939[kHz]
X_Sweep_Clipped = 151.51515152[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 19.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

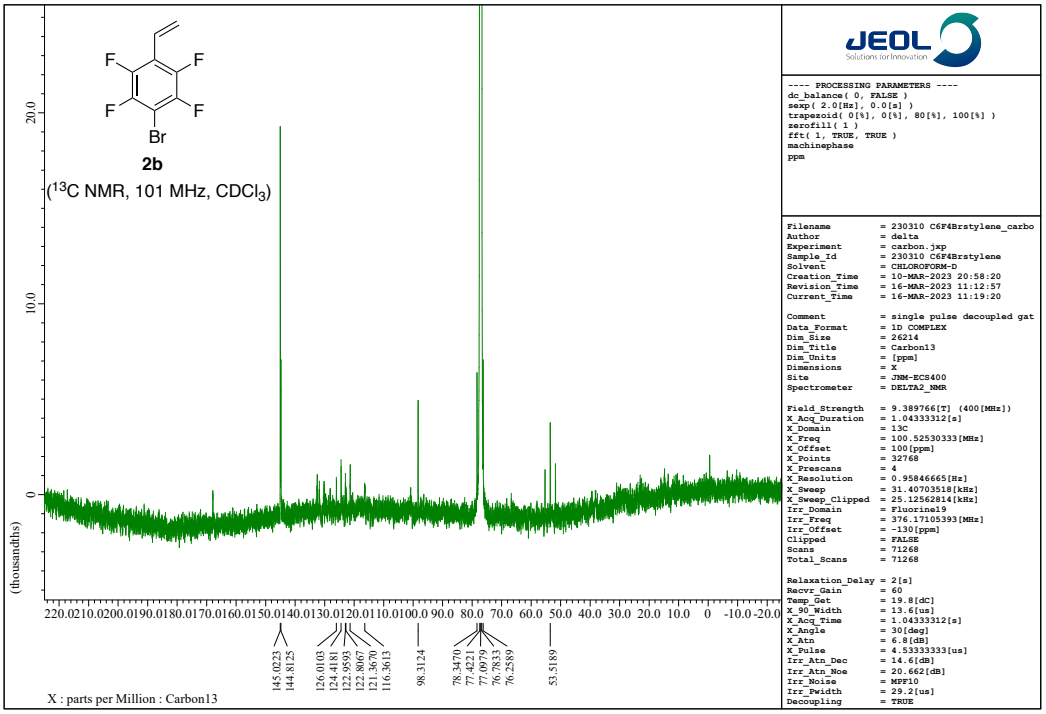

F
F
F
F
I
2a
(^{1}H NMR, 400 MHz, $CDCl_3$)
1.00
1.03
1.03
abundance
X : parts per Million : Proton
6.720
6.690
6.675
6.645
6.171
6.126
5.770
5.741
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = TH81 HPLC collection_p
Author = delta
Experiment = proton.jxp
Sample_Id = TH81 HPLC collection
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-OCT-2018 20:26:58
Revision_Time = 16-FEB-2023 16:51:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 19.4[dC]

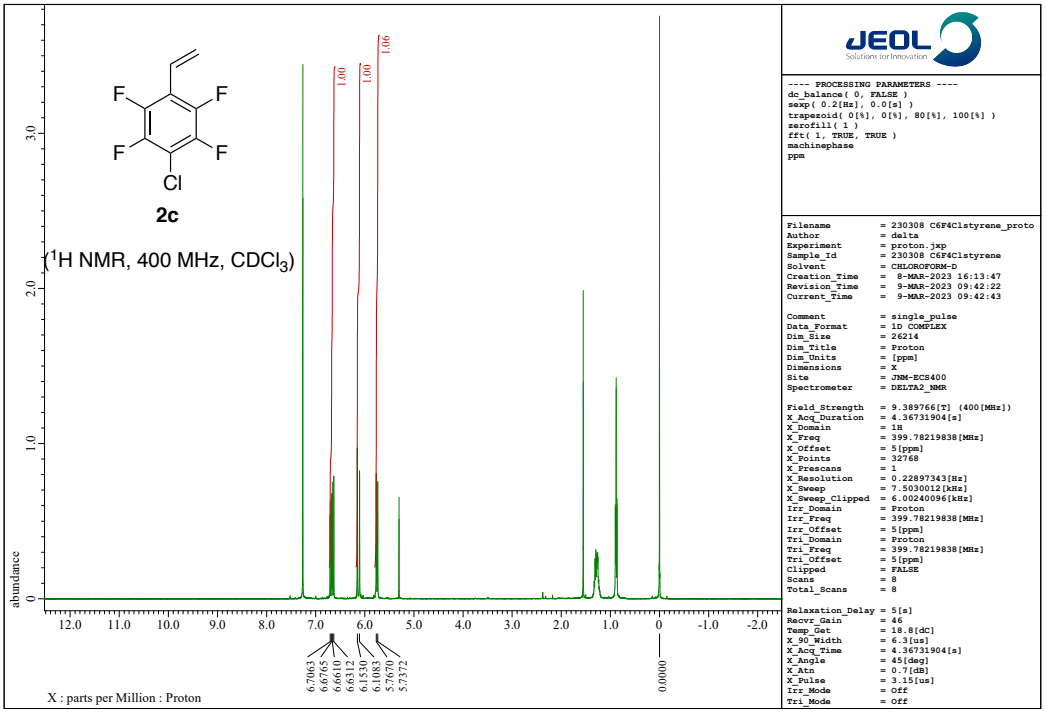

F
F
F
F
I
2a
(^{19}F NMR, 376 MHz, $CDCl_3$)
2.00
1.98
abundance
X : parts per Million : Fluorine19
-121.652
-121.675
-121.706
-121.729
-121.744
-141.565
-141.588
-141.615
-141.657
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TFIS 19F.jdf
Filename = TFIS 19F-1.jdf
Author = delta
Experiment = single_pulse.jxp
Sample_Id = 191024 TH330
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-OCT-2019 16:06:27
Revision_Time = 18-NOV-2022 15:51:23
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[Hz]
X_Sweep = 189.39393939[kHz]
X_Sweep_Clipped = 151.51515152[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 20.2[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

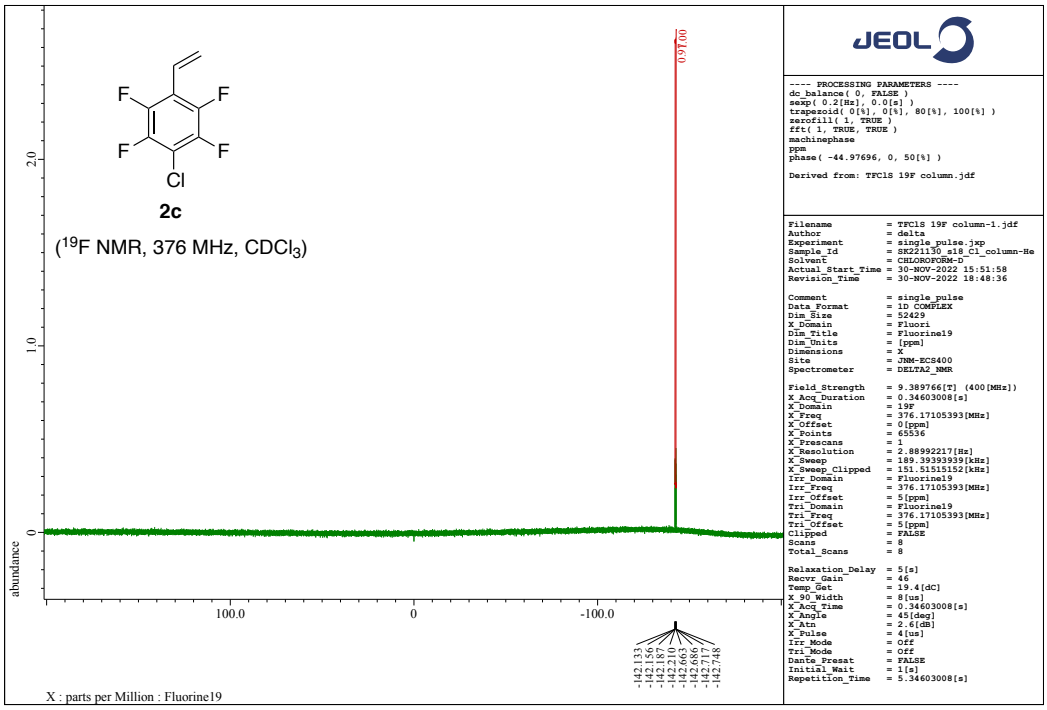

F
F
F
F
I
2a
(13C NMR, 101 MHz, CDCl3)
abundance
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
-10.0
147.244
144.136
144.088
124.399
123.236
121.586
77.394
77.079
76.764
70.395
22.455
14.732
13.502
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
traperoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = TH 220720_carbon-2-2.
Author = delta
Experiment = carbon.jxp
Sample_Id = TH 220720
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-JUL-2022 19:10:18
Revision_Time = 16-FEB-2023 16:55:54
Comment = single pulse decoupled
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = TRUE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]

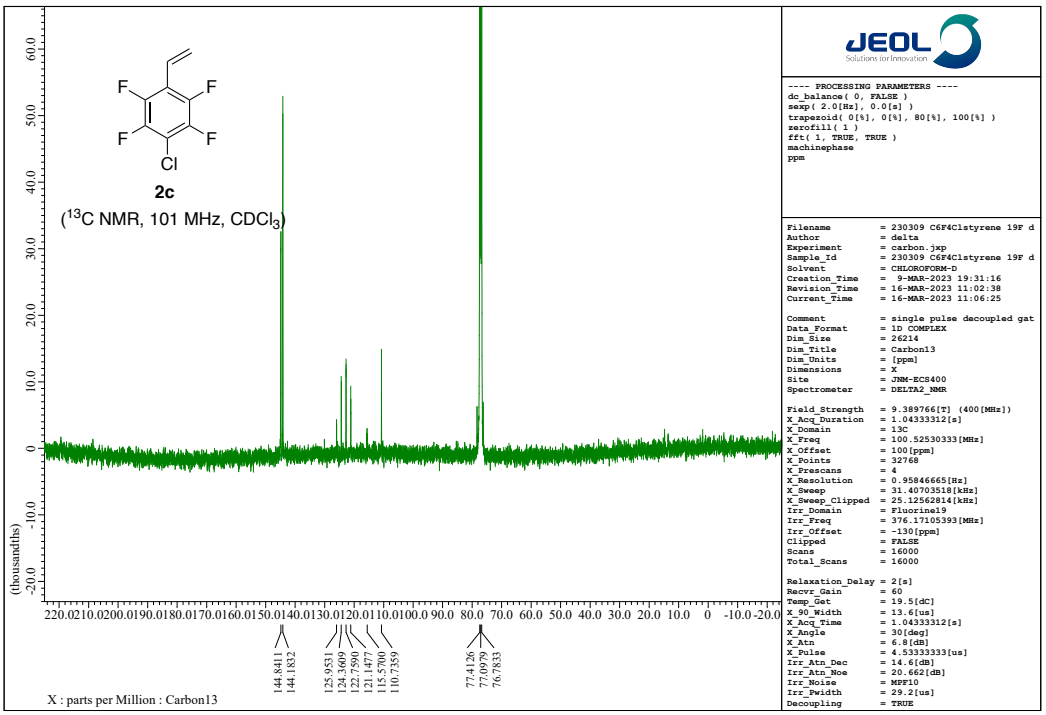

F
F
F
F
Br
2b
(1H NMR, 400 MHz, CDCl3)
1.00
1.05
1.04
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
6.7086
6.6782
6.6633
6.6335
6.1650
6.1198
5.7767
5.7469
0.0000
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
traperoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 230307 C6F4Brstyrene_proto
Author = delta
Experiment = proton.jxp
Sample_Id = 230307 C6F4BrCHO
Solvent = CHLOROFORM-D
Creation_Time = 7-MAR-2023 14:21:56
Revision_Time = 9-MAR-2023 09:54:27
Current_Time = 9-MAR-2023 09:55:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 18.9[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off


F
F
F
F
Br
2b
(19F NMR, 376 MHz, CDCl3)
abundance
3.0
2.0
1.0
0
100.0
0
-100.0
-135.081
-135.112
-135.150
-135.181
-141.073
-141.096
-141.127
-141.150
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: SK221129_s16_crude_19F-1-1.jdf
Filename = SK221129_s16_crude_19F-1-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SK221129_s16_crude
Solvent = NONE
Actual_Start_Time = 29-NOV-2022 13:39:43
Revision_Time = 29-NOV-2022 18:46:45
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[Hz]
X_Sweep = 189.39393939[kHz]
X_Sweep_Clipped = 151.51515152[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 19.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]


F
F
F
F
Br
2b
(13C NMR, 101 MHz, CDCl3)
(thousandths)
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
145.0223
144.8125
126.0103
124.4181
124.1698
122.8067
121.3670
116.3613
98.3124
78.3470
77.4221
77.0979
76.7833
76.2589
53.5189
X : parts per Million : Carbon13
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 230310 C6F4Brstylene_carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = 230310 C6F4Brstylene
Solvent = CHLOROFORM-D
Creation_Time = 10-MAR-2023 20:58:20
Revision_Time = 16-MAR-2023 11:12:57
Current_Time = 16-MAR-2023 11:19:20
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 71268
Total_Scans = 71268
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.8[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE


F
F
F
F
Cl
2c
(1H NMR, 400 MHz, CDCl3)
1.00
1.00
1.06
abundance
3.0
2.0
1.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
6.7063
6.6765
6.6610
6.6312
6.1530
6.1083
5.7670
5.7372
0.0000
X : parts per Million : Proton
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 230308 C6F4Clstyrene_proto
Author = delta
Experiment = proton.jxp
Sample_Id = 230308 C6F4Clstyrene
Solvent = CHLOROFORM-D
Creation_Time = 8-MAR-2023 16:13:47
Revision_Time = 9-MAR-2023 09:42:22
Current_Time = 9-MAR-2023 09:42:43
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 18.8[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off


F
F
F
F
Cl
2c
(19F NMR, 376 MHz, CDCl3)
0.97
0.00
abundance
2.0
1.0
0
100.0
0
-100.0
-142.133
-142.155
-142.187
-142.210
-142.663
-142.686
-142.717
-142.748
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-44.97696, 0, 50[%])
Derived from: TFClS 19F column.jdf
Filename = TFClS 19F column-1.jdf
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SK221130_s18_Cl_column-He
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-NOV-2022 15:51:58
Revision_Time = 30-NOV-2022 18:48:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[Hz]
X_Sweep = 189.39393939[kHz]
X_Sweep_Clipped = 151.51515152[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 19.4[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
RepetitIon_Time = 5.34603008[s]


F
F
F
F
Cl
2c
(13C NMR, 101 MHz, CDCl3)
(thousandths)
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
144.8411
144.1832
125.9531
124.3609
122.7590
121.1477
115.5700
110.7359
77.4126
77.0979
76.7833
X : parts per Million : Carbon13
JEOL
Solutions for Innovation
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 230309 C6F4Clstyrene 19F d
Author = delta
Experiment = carbon.jxp
Sample_Id = 230309 C6F4Clstyrene 19F d
Solvent = CHLOROFORM-D
Creation_Time = 9-MAR-2023 19:31:16
Revision_Time = 16-MAR-2023 11:02:38
Current_Time = 16-MAR-2023 11:06:25
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 16000
Total_Scans = 16000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.5[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE

9. Cartesian coordinates

SMD(THF)/M06-2X-D3/6-311+G(d,p)

MTBD	C	2.0070400	-1.506412	-0.292040
	C	2.3327910	-0.110016	0.196553
	N	1.2851200	0.822431	-0.210660
	C	-0.0534970	0.477837	-0.036416
	N	-0.3519410	-0.879547	-0.113837
	C	0.6397190	-1.893801	0.230145
	N	-0.9170250	1.424617	0.097599
	C	-2.3355060	1.103661	0.187886
	C	-2.6897980	-0.261040	-0.385280
	C	-1.7225590	-1.277964	0.188443
	C	1.6276240	2.222664	-0.026893
	H	2.7566380	-2.215676	0.063929
	H	2.0062600	-1.521448	-1.385327
	H	2.4536920	-0.109576	1.291172
	H	3.2708990	0.240120	-0.237344
	H	0.6792050	-2.032792	1.321426
	H	0.3078270	-2.837747	-0.208641
	H	-2.8950890	1.889157	-0.327814
	H	-2.6443580	1.146868	1.240368
	H	-3.7180920	-0.532701	-0.136861
	H	-2.5948190	-0.248695	-1.475216
	H	-1.8666380	-1.368331	1.275794
	H	-1.8796330	-2.266852	-0.249039
	H	1.5227180	2.543531	1.017916
	H	2.6649390	2.359023	-0.335443
	H	0.9884910	2.853038	-0.641027
DBN	C	-0.1995640	-0.735012	0.027013
	N	-0.2272640	0.632734	0.009436
	N	0.8327260	-1.493327	0.058036
	C	2.1315060	-0.816749	0.146787
	C	2.1347940	0.605709	-0.413682
	C	0.9841570	1.405757	0.188915
	C	-1.5637440	1.174287	0.199331
	C	-2.4532640	0.026377	-0.294031
	C	-1.6320900	-1.225593	0.043109
	H	2.8692320	-1.424816	-0.382199
	H	2.4429380	-0.795921	1.198750
	H	3.0866550	1.095798	-0.199784
	H	2.0100420	0.571406	-1.500124
	H	0.8646940	2.368862	-0.314084
	H	1.1639630	1.601758	1.254669
	H	-1.6888910	2.093391	-0.377284
	H	-1.7471400	1.402050	1.258290
	H	-3.4370930	0.032675	0.173385

	H	-2.5817590	0.109030	-1.375259
	H	-1.7780240	-2.055963	-0.646741
	H	-1.8536190	-1.582778	1.053423
DBU	C	-0.3996040	0.779957	-0.362430
	N	-0.3237180	-0.584729	-0.445636
	N	-1.4775850	1.451142	-0.134876
	C	-2.7021520	0.673102	0.010899
	C	-2.4503380	-0.619957	0.778252
	C	-1.4234370	-1.437073	0.015015
	C	0.9033620	-1.287631	-0.811225
	C	1.9608660	-1.310327	0.294824
	C	2.7555870	-0.008392	0.385790
	C	1.9099220	1.245609	0.613626
	C	0.8950360	1.548091	-0.502897
	H	-3.4465720	1.289885	0.518301
	H	-3.1075880	0.430495	-0.981621
	H	-3.3670780	-1.199732	0.901906
	H	-2.0677010	-0.373145	1.773368
	H	-1.8876840	-1.928247	-0.848267
	H	-1.0022550	-2.220133	0.653789
	H	0.6057720	-2.307472	-1.063400
	H	1.3236230	-0.852905	-1.722962
	H	1.4650750	-1.524798	1.248846
	H	2.6526250	-2.135613	0.099504
	H	3.4929540	-0.091525	1.189852
	H	3.3210160	0.118704	-0.545832
	H	2.5840830	2.102315	0.697998
	H	1.3787460	1.172049	1.569665
	H	1.3509470	1.353609	-1.479851
	H	0.6177120	2.601354	-0.478841
TMG	C	-2.3980710	0.548984	-0.372276
	N	-1.1717170	-0.189521	-0.124589
	C	-0.0069810	0.554755	-0.007916
	N	1.1543680	-0.202238	0.114045
	C	2.3885290	0.502159	0.409433
	C	-1.3778950	-1.352177	0.734058
	N	-0.0646900	1.842669	-0.007767
	C	1.3575560	-1.363736	-0.748421
	H	-2.7347870	1.097671	0.516623
	H	-2.2529620	1.261711	-1.181852
	H	-3.1730510	-0.164657	-0.658555
	H	2.2455850	1.192539	1.241622
	H	3.1414560	-0.231858	0.700618
	H	2.7712870	1.060134	-0.457015
	H	-1.9299490	-1.066957	1.639136
	H	-1.9592120	-2.107104	0.198967
	H	-0.4297760	-1.788903	1.037322

	H	0.8655960	2.244795	-0.076923
	H	0.4066680	-1.760604	-1.094876
	H	1.9554060	-1.087828	-1.626526
	H	1.8891780	-2.145219	-0.199631
piperidine	C	0.7473950	-1.210570	0.206149
	C	-0.7145130	-1.258097	-0.229077
	N	1.3803360	-0.000001	-0.321053
	C	0.7473960	1.210569	0.206149
	C	-0.7145120	1.258097	-0.229077
	C	-1.4515220	0.000001	0.236373
	H	1.2892020	-2.080501	-0.171684
	H	0.7911170	-1.240158	1.308618
	H	-0.7547310	-1.324686	-1.321773
	H	-1.1907660	-2.155378	0.175484
	H	2.3654050	-0.000001	-0.077509
	H	1.2892040	2.080501	-0.171684
	H	0.7911180	1.240157	1.308618
	H	-1.1907640	2.155379	0.175483
	H	-0.7547300	1.324687	-1.321773
	H	-2.4809560	0.000001	-0.131719
	H	-1.5019230	0.000001	1.332208
quinuclidine	H	1.0147230	-2.086630	0.509705
	H	-1.2959800	-1.902641	0.861284
	H	1.2028050	-1.035674	1.913119
	H	-1.0881450	-0.562444	1.987590
	H	1.0134820	1.482512	1.555453
	H	-1.2958830	1.700368	1.212826
	H	1.2083860	2.171486	-0.056033
	H	-1.0816300	2.005164	-0.510328
	H	1.0216360	0.603706	-2.057890
	H	-1.2882040	0.202703	-2.083600
	H	1.2121210	-1.136864	-1.848821
	H	-1.0795520	-1.442127	-1.484432
	H	2.3827590	-0.000645	0.005820
	C	1.2910160	-0.000337	0.003118
	C	0.7505480	-1.107306	0.920362
	C	-0.7915000	-0.944349	1.007013
	C	0.7523040	1.348875	0.501228
	C	-0.7891830	1.346303	0.311720
	C	0.7565800	-0.242131	-1.416200
	C	-0.7855340	-0.401336	-1.324321
	N	-1.2902720	0.000395	-0.003173
Et_3N	C	-0.4749240	-1.308636	0.284321
	N	-0.0001130	0.000282	-0.172069
	C	-0.8964540	1.065502	0.284894

	C	0.3407890	-2.482232	-0.246538
	C	-2.3202550	0.946142	-0.246833
	C	1.3704630	0.243746	0.285500
	C	1.9803460	1.535420	-0.247163
	H	-1.5016630	-1.428805	-0.062703
	H	-0.5020430	-1.342421	1.389589
	H	-0.9128670	1.104662	1.390189
	H	-0.4866610	2.015039	-0.060729
	H	-0.2003310	-3.413166	-0.062373
	H	1.3167000	-2.572148	0.232666
	H	0.4915930	-2.383693	-1.325019
	H	-2.8558630	1.880296	-0.062843
	H	-2.3098700	0.766353	-1.325315
	H	-2.8863380	0.146008	0.232161
	H	1.9876370	-0.586292	-0.059396
	H	1.4122490	0.239185	1.390789
	H	3.0568750	1.531742	-0.061521
	H	1.5704740	2.426804	0.229883
	H	1.8211190	1.614812	-1.325986
MTBT·HBr	C	-1.0068240	-2.460757	-1.097889
	C	-1.7306070	-1.774405	0.040751
	N	-0.7650340	-1.247760	1.011102
	C	0.4062580	-0.733036	0.596751
	N	0.8827370	-0.975494	-0.635382
	C	0.0047440	-1.499346	-1.683288
	N	1.1548020	-0.050298	1.484781
	C	2.2823050	0.787246	1.076883
	C	3.0212060	0.096342	-0.050052
	C	2.0282060	-0.217373	-1.151314
	C	-1.3291950	-0.802749	2.280801
	H	-1.7234350	-2.754074	-1.866009
	H	-0.5040110	-3.360684	-0.734225
	H	-2.3400500	-0.941727	-0.327903
	H	-2.3714760	-2.477618	0.572930
	H	-0.4953780	-0.650972	-2.165040
	H	0.6414920	-1.997481	-2.415959
	H	2.9198870	0.927184	1.949511
	H	1.9020660	1.758666	0.745763
	H	3.8037040	0.748410	-0.439786
	H	3.4868190	-0.823960	0.312189
	H	1.6474950	0.705071	-1.605293
	H	2.4879840	-0.829153	-1.928659
	H	-1.5421420	0.271577	2.251504
	H	-2.2609460	-1.341169	2.439704
	H	-0.6633080	-1.039318	3.112933
	H	0.6627570	0.276674	2.302520
	Br	-1.0461590	1.916226	-0.437244

DBN·HBr	C	-0.9097890	0.272460	-0.081282
	N	-2.2246700	0.140883	-0.073546
	N	-0.0841440	-0.740733	-0.113131
	C	-0.5681330	-2.120670	-0.184151
	C	-1.9524030	-2.212454	0.447291
	C	-2.8838530	-1.158613	-0.144643
	C	-2.9216430	1.430084	-0.137570
	C	-1.8314530	2.419138	0.295597
	C	-0.5173050	1.719672	-0.088989
	H	0.1471960	-2.750996	0.343277
	H	-0.5965900	-2.435135	-1.230932
	H	-2.3689470	-3.205234	0.277423
	H	-1.8708940	-2.056074	1.525751
	H	-3.8145700	-1.094772	0.420623
	H	-3.1271160	-1.383621	-1.187694
	H	-3.7834030	1.414837	0.530031
	H	-3.2666190	1.607135	-1.160773
	H	-1.9435430	3.389539	-0.183452
	H	-1.8723610	2.556276	1.376976
	H	0.3198740	1.912672	0.580446
	H	-0.1980360	1.971357	-1.104782
	H	0.9333280	-0.540060	-0.087416
	Br	3.0603100	0.077581	0.016278
DBU·HBr	C	-0.6348050	0.189540	-0.408120
	N	-1.8630840	0.688273	-0.394588
	N	0.4212110	0.948594	-0.207686
	C	0.3428440	2.382042	0.047829
	C	-0.9667000	2.675250	0.759743
	C	-2.1178770	2.095981	-0.044250
	C	-3.0406850	-0.137676	-0.705519
	C	-3.3900680	-1.130789	0.401117
	C	-2.5182030	-2.385837	0.385278
	C	-1.0180000	-2.129207	0.526923
	C	-0.4095390	-1.282232	-0.605115
	H	1.2061600	2.655177	0.654081
	H	0.4010720	2.924717	-0.900005
	H	-1.1080200	3.750249	0.871782
	H	-0.9477680	2.224983	1.755531
	H	-2.2804190	2.661666	-0.966575
	H	-3.0403950	2.118701	0.537863
	H	-3.8603880	0.562945	-0.862056
	H	-2.8762890	-0.656171	-1.653730
	H	-3.3166710	-0.620125	1.367716
	H	-4.4354640	-1.423767	0.271050
	H	-2.8393870	-3.053804	1.189000
	H	-2.6927270	-2.919322	-0.556638
	H	-0.4970600	-3.089197	0.528909
	H	-0.8005660	-1.654143	1.489533

	H	-0.8292450	-1.582091	-1.570372
	H	0.6691100	-1.439259	-0.650844
	H	1.3503470	0.494077	-0.168580
	Br	3.3859720	-0.402147	0.020913
TMG·HBr	C	-0.0308540	1.878926	0.683299
	N	1.1146830	1.187171	0.096466
	C	1.2237470	-0.147932	0.168299
	N	2.4058470	-0.745910	-0.068828
	C	2.4744480	-2.182813	-0.310901
	C	1.9137430	1.988357	-0.827798
	N	0.1594150	-0.878504	0.489604
	C	3.6779280	-0.115829	0.281171
	H	-0.8643890	1.940968	-0.020782
	H	-0.3673710	1.358011	1.578361
	H	0.2931740	2.883468	0.958103
	H	1.6259080	-2.510131	-0.910627
	H	3.3881460	-2.386969	-0.868950
	H	2.5041790	-2.746840	0.627605
	H	1.2313510	2.572056	-1.449708
	H	2.5708370	2.672271	-0.285650
	H	2.5081050	1.348800	-1.476260
	H	0.2766370	-1.852629	0.726987
	H	3.5083290	0.825936	0.797703
	H	4.2198720	-0.785548	0.953177
	H	4.2854190	0.060005	-0.609220
	H	-0.8078390	-0.554217	0.327230
	Br	-3.0196010	-0.236821	-0.112374
piperidine·HBr	C	1.0839030	-1.243801	0.001518
	C	2.6014360	-1.256828	0.096221
	N	0.5376680	-0.000087	0.619343
	C	1.0837410	1.243719	0.001552
	C	2.6012710	1.256919	0.096267
	C	3.2005970	0.000096	-0.536810
	H	0.6246090	-2.088369	0.514213
	H	0.7467770	-1.238533	-1.037402
	H	2.8951160	-1.319902	1.150198
	H	2.9700390	-2.158029	-0.397594
	H	-0.5159650	-0.000166	0.498557
	H	0.6243350	2.088207	0.514275
	H	0.7466190	1.238427	-1.037369
	H	2.9697690	2.158185	-0.397509
	H	2.8949360	1.319988	1.150248
	H	4.2858610	0.000166	-0.417879
	H	2.9900470	0.000105	-1.612014
	H	0.7373240	-0.000082	1.623695
	Br	-2.5473950	-0.000001	-0.081123

quinuclidine·HBr	H	2.5624050	1.814239	1.141931
	H	0.2662270	1.997477	0.623412
	H	2.8233060	2.096060	-0.580093
	H	0.5599450	1.756376	-1.107163
	H	2.5645630	0.080587	-2.140642
	H	0.2678200	-0.456959	-2.043065
	H	2.8226690	-1.552228	-1.523950
	H	0.5578690	-1.835326	-0.968315
	H	2.5608470	-1.895764	1.002097
	H	0.2635210	-1.539021	1.414804
	H	2.8190800	-0.545364	2.107801
	H	0.5550010	0.080293	2.072008
	H	3.9693150	-0.001146	0.002536
	C	2.8793960	-0.000636	0.001424
	C	2.3446700	1.432654	0.141685
	C	0.8244390	1.412121	-0.106784
	C	2.3451190	-0.594855	-1.310498
	C	0.8244220	-0.797402	-1.170316
	C	2.3424270	-0.838840	1.171375
	C	0.8219440	-0.613839	1.274532
	N	0.3455560	0.000576	-0.001348
	H	-0.7119100	0.001003	-0.002042
	Br	-2.8169730	0.000015	0.000046
Et_3N·HBr	C	1.4908260	-0.412473	1.378027
	N	1.0665400	-0.000564	0.001847
	C	1.5049420	1.392893	-0.327458
	C	1.0954160	-1.836691	1.727304
	C	1.1101770	2.411698	0.727306
	C	1.4975630	-0.987785	-1.038692
	C	1.1174480	-0.578221	-2.450945
	H	1.0045890	0.277667	2.065319
	H	2.5717730	-0.261131	1.436286
	H	2.5868600	1.358899	-0.478673
	H	1.0277790	1.645956	-1.272608
	H	1.2573760	-1.981673	2.796768
	H	1.6890220	-2.579859	1.194989
	H	0.0357380	-2.005732	1.520258
	H	1.2817010	3.408242	0.316825
	H	0.0484920	2.324168	0.970857
	H	1.6975240	2.320972	1.640955
	H	1.0063220	-1.926379	-0.787544
	H	2.5770290	-1.117082	-0.926888
	H	1.2805590	-1.434214	-3.107940
	H	1.7196560	0.249609	-2.824740
	H	0.0599260	-0.307750	-2.503904
	H	0.0072220	0.003600	-0.003010
	Br	-2.1204450	0.002632	-0.004090

HBr	Br	0.0000000	0.000000	0.039511
	H	0.0000000	0.000000	-1.382876