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Supporting Information

The Affinity of Some Lewis Bases for Hexafluoroisopropanol as a Reference Lewis Acid: An ITC/DFT Study**

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S.1. ITC data.

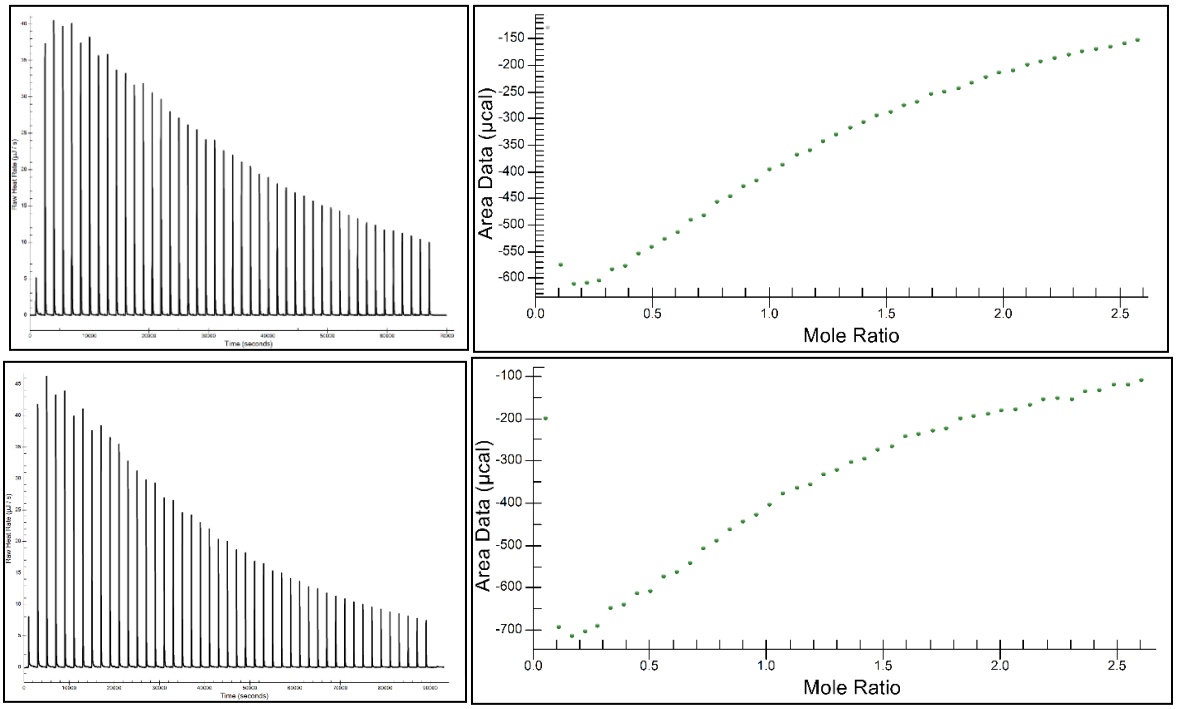


Figure SI 1. *up-left* – ITC thermogram of the reaction between **2a** (sample call, c=4.09 mM) and **1** (syringe, c=108.43 mM) in chlorobenzene. The titration was performed at 25°C through 45 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s. *up-right* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections. *down-left* – ITC thermogram of the reaction between **1** (sample call, c=4.09 mM) and **2a** (syringe, c=106.85 mM) in chlorobenzene. The titration was performed at 25°C through 45 sequential additions (of 2.06 µL each). Time between two consecutive injections was 2000 s. Heat released is expressed in µJ/s versus time in s. *down-right* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections.

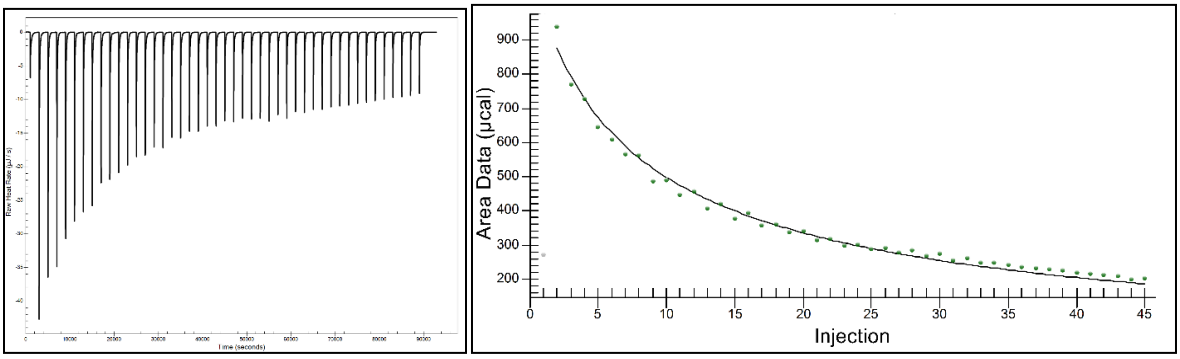


Figure SI 2. *left side* – ITC thermogram of the dissociation of the complex **1/2b** (syringe, c=129.99 mM) in chlorobenzene. The titration was performed at 25°C through 45 sequential

additions (of 2.06 µL each). Time between two consecutive injections was 2000 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by dimer dissociation model implemented in NanoAnalyze software.

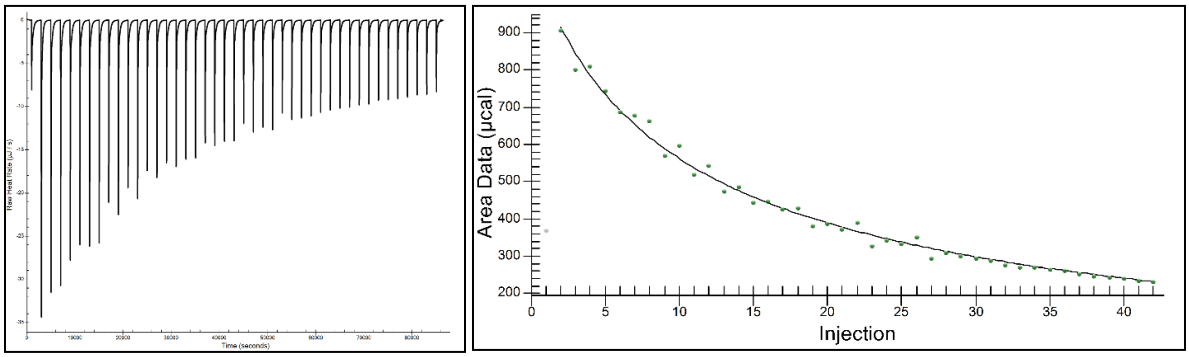


Figure SI 3. *left side* – ITC thermogram of the dissociation of the complex **1/2c** (syringe, c=131.36 mM) in chlorobenzene. The titration was performed at 25°C through 43 sequential additions (of 2.06 µL each). Time between two consecutive injections was 2000 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by the dimer dissociation model implemented in NanoAnalyze software.

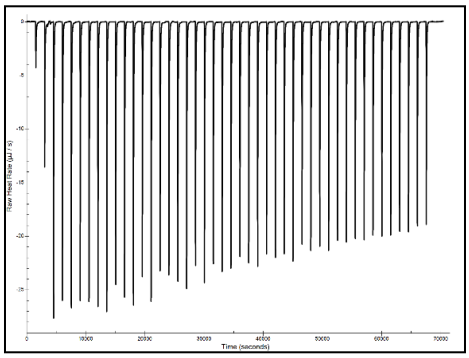


Figure SI 4. *left side* – ITC thermogram of the dissociation of the complex **1/2d** (syringe, c=132.07 mM) in chlorobenzene. The titration was performed at 25°C through 45 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s.

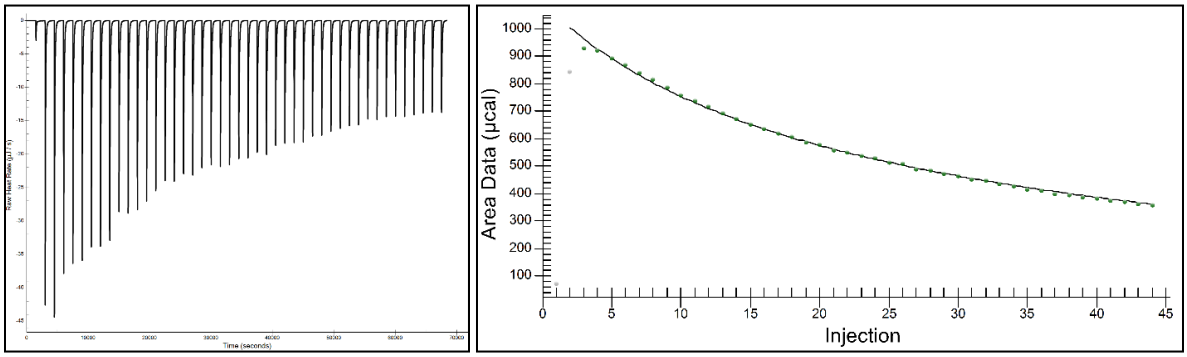


Figure SI 5. *left side* – ITC thermogram of the dissociation of the complex **1/2e** (syringe, c=132.11 mM) in chlorobenzene. The titration was performed at 25°C through 44 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by dimer dissociation model implemented in NanoAnalyze software.

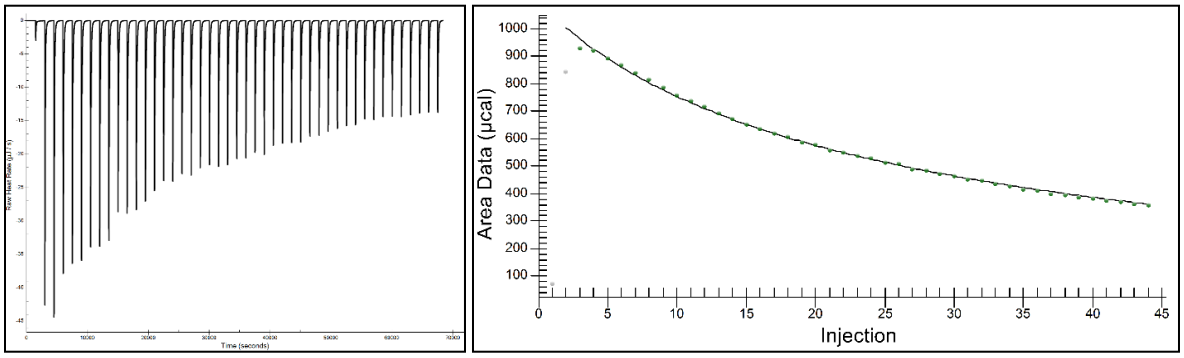


Figure SI 6. *left side* – ITC thermogram of the dissociation of the complex **1/2f** (syringe, c=129.14 mM) in chlorobenzene. The titration was performed at 25°C through 44 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by dimer dissociation model implemented in NanoAnalyze software.

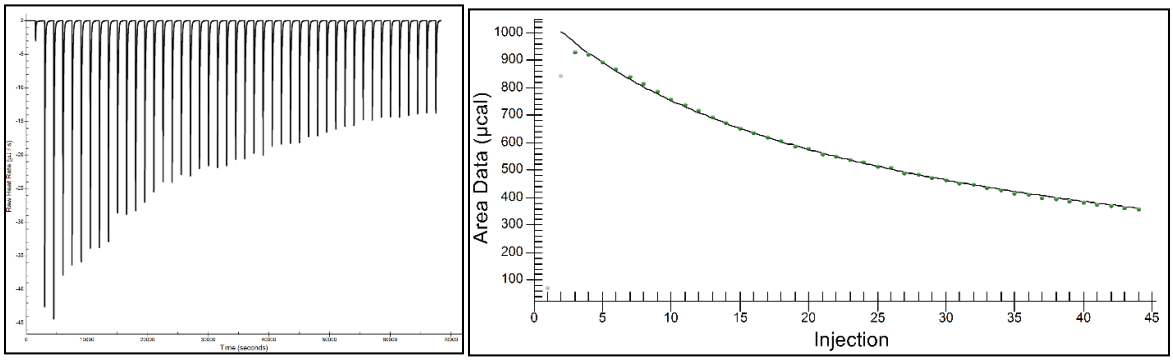


Figure SI 7. *left side* – ITC thermogram of the dissociation of the complex **1/2g** (syringe, c=129.14 mM) in chlorobenzene. The titration was performed at 25°C through 44 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by dimer dissociation model implemented in NanoAnalyze software.

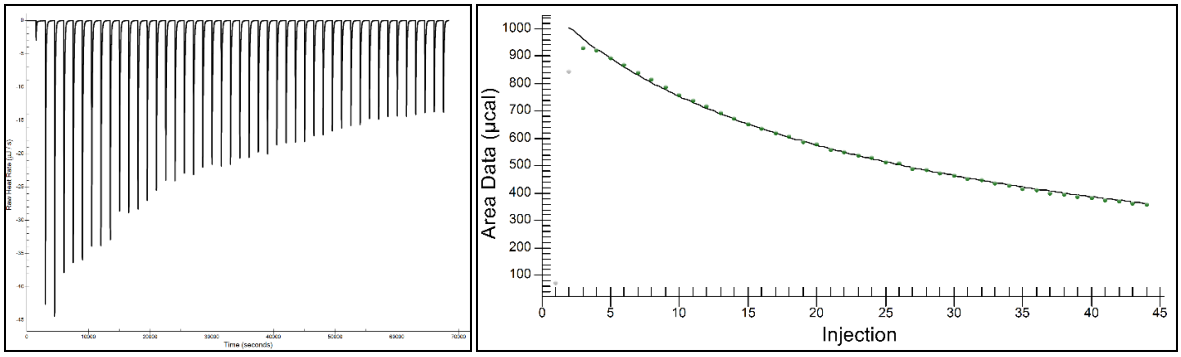
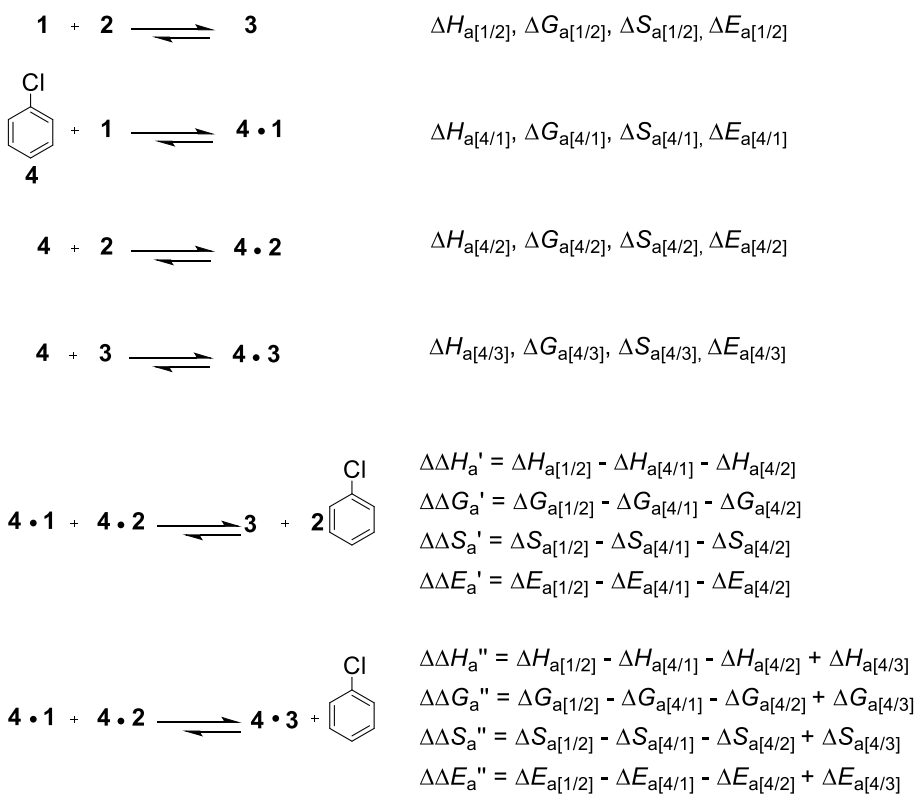


Figure SI 8. *left side* – ITC thermogram of the dissociation of the complex **1/2h** (syringe, c=124.84 mM) in chlorobenzene. The titration was performed at 25°C through 44 sequential additions (of 2.06 µL each). Time between two consecutive injections was 1500 s. Heat released is expressed in µJ/s versus time in s. *right side* – ITC integrated heat peaks of the thermogram shown on the left side. Integrated heats are expressed in µcal versus number of injections and fitted by dimer dissociation model implemented in NanoAnalyze software.

S.2. DFT-D calculation data.



Scheme SI 1. Static DFT calculations preformed at PBE-D3(BJ)/def2-TZVP level of theory with implicit solvation (PCM) provided the corrective enthalpy terms for the explicit solvation of both the reactants **1** and **2a-h** and corresponding reaction products (**3a-h**) by PhCl (**4**) (Scheme 1, Table 1-2, Table SI 1, Figure 1, Figure SI 9-10) and the equations used to correct calculated association values.

Table SI 1. Supplementary to thermodynamic data obtained by ITC experiments and DFT (PBE-D3-BJ/def2-TZVP) calculations of the affinity of the Lewis donors (**2a-h**) to HFIP (**1**) (Scheme 1) including explicit solvation interactions of **1**, **2a-h** and **3a-h** with the solvent (chlorobenzene, **4**) (Scheme 1, Scheme SI 1). All the values are in kcal mol^{-1} except ΔS_a values (in cal/mol K) and were acquired and computed at T= 298.15 K.

	Thermodynamic data from model fitting[a]		**DFT with implicit solvation[b]**		**DFT with implicit and explicit solvation**															
					PhCl with Lewis donors[c]				**PhCl with the pairs[e]**				**corrected values[f]**							
Donor	$K_{a[1/2]}$ **(fit)**	$\Delta S_{a[1/2]}$ **(fit)**	$\Delta S_{a[1/2]}$	$\Delta E_{a[1/2]}$	$\Delta H_{a[4/2]}$	$\Delta G_{a[4/2]}$	$\Delta S_{a[4/2]}$	$\Delta E_{a[4/2]}$	$\Delta H_{a[4/3]}$	$\Delta G_{a[4/3]}$	$\Delta S_{a[4/3]}$	$\Delta E_{a[4/3]}$	$\Delta\Delta H_{a[1/2]}'$	$\Delta\Delta G_{a[1/2]}'$	$\Delta\Delta S_{a[1/2]}'$	$\Delta\Delta E_{a[1/2]}'$	$\Delta\Delta H_{a[1/2]}''$	$\Delta\Delta G_{a[1/2]}''$	$\Delta\Delta S_{a[1/2]}''$	$\Delta\Delta E_{a[1/2]}''$
2a	230 ± 40	-32 ± 6	-34.2	-11.3	-4.5	4.5	-30.1	-5.6	-5.9	3.8	-32.6	-7.1	-2.0	-8.1	20.5	-0.7	-7.9	-4.3	-12.1	-7.8
2b	130 ± 20	-24 ± 4	-34.2	-11.1	-4.9	3.4	-27.8	-5.8	-6.8	3.7	-35.0	-8.0	-1.6	-7.7	20.3	-0.3	-8.4	-4.0	-14.7	-8.3
2c	89 ± 10	-25 ± 4	-35.4	-11.9	-4.6	4.3	-30.0	-6.0	-6.6	2.4	-30.2	-7.7	-2.3	-7.4	17.0	-1.0	-8.8	-4.9	-13.2	-8.7
2d	n.a.	n.a.	-33.4	-10.7	-2.8	5.0	-26.0	-3.9	-4.6	4.4	-30.1	-5.8	-2.9	-8.0	17.3	-1.8	-7.4	-3.6	-12.8	-7.7
2e	220 ± 50	-37 ± 9	-29.1	-12.8	-2.9	3.7	-22.1	-4.0	-5.0	5.1	-33.8	-6.2	-5.3	-10.6	17.6	-3.9	-10.3	-5.4	-16.2	-10.0
2f	27 ± 5	-33 ± 6	-34.4	-13.6	-4.2	3.3	-25.3	-5.4	-5.5	3.7	-30.9	-6.7	-4.7	-9.4	15.6	-3.3	-10.2	-5.7	-15.3	-10.0
2g	11 ± 2	-36 ± 8	-37.5	-12.5	-5.5	3.0	-28.7	-6.7	-6.2	2.6	-29.4	-7.4	-2.1	-6.8	15.8	-0.8	-8.3	-4.3	-13.5	-8.3
2h	10 ± 1	-27 ± 3	-31.2	-9.9	-3.0	4.6	-25.5	-4.3	-3.4	4.9	-27.9	-4.7	-1.8	-7.4	18.9	-0.7	-5.2	-2.5	-9.1	-5.4
					PhCl with HFIP[d]															
					$\Delta H_{a[4/1]}$	$\Delta G_{a[4/1]}$	$\Delta S_{a[4/1]}$	$\Delta E_{a[4/1]}$												
1					-3.7	3.6	-24.6	-4.9												

[a] values were obtained by the whole thermogram (ITC trace) with Cooper's model for dimer dissociation.[15] [b] $\Delta S_{a[1/2]}$ and $\Delta E_{a[1/2]}$ are data on the association of HFIP (**1**) and Lewis donors (**2a-h**), forming adducts **3a-h** (by OH···O bonding at the sulfoxide) (Scheme 1, Figure 2). [c] $\Delta H_{a[4/2]}$, $\Delta G_{a[4/2]}$, $\Delta S_{a[4/2]}$ and $\Delta E_{a[4/2]}$ are data obtained from the *optimized* geometries of [**4**/**2a-h**] (Figure SI 9). [d] $\Delta H_{a[4/1]}$, $\Delta G_{a[4/1]}$, $\Delta S_{a[4/1]}$ and $\Delta E_{a[4/1]}$ are data obtained from the *optimized* geometry of [**4**/**1**] (Figure SI 9). [e] $\Delta H_{a[4/3]}$, $\Delta G_{a[4/3]}$, $\Delta S_{a[4/3]}$ and $\Delta E_{a[4/3]}$ are data obtained from the *optimized* geometry of [**4**/**3**] (Figure SI 10). [f] $\Delta\Delta H_{a[1/2]}'$, $\Delta\Delta G_{a[1/2]}'$, $\Delta\Delta S_{a[1/2]}'$ and $\Delta\Delta E_{a[1/2]}'$ are corrected data for the association of **1** and **2a-h** including explicit solvation, i.e. [**4**/**1**] and [**4**/**2a-h**] (see Scheme SI 1), considering the *optimized* geometries of [**4**/**1**], [**4**/**2a-h**] (Figure SI 9, Scheme SI 1), while $\Delta\Delta H_{a[1/2]}''$, $\Delta\Delta G_{a[1/2]}''$, $\Delta\Delta S_{a[1/2]}''$ and $\Delta\Delta E_{a[1/2]}''$ are corrected data for the association of **1** and **2a-h** including explicit solvation, i.e. [**4**/**1**], [**4**/**2a-h**] and [**4**/**3a-h**] (see Scheme SI 1), considering the *optimized* geometries of [**4**/**1**], [**4**/**2a-h**] and [**4**/**3a-h**] (Figure SI 9-10, Scheme SI 1).

Table SI 2. Supplementary to thermodynamic data obtained by DFT (ZORA-GGAPBE-D3-BJ/TZP) calculations of affinity of the sulfoxide' centers (oxygen and sulphur) of the Lewis donors (**2a-c**) to HFIP (**1**) (Scheme 1) All the values are in kcal mol^{-1} except ΔS_a values (in cal/mol K) and were acquired were computed at T= 298.15 K in gas phase.

Donor	Type of main interaction	$\Delta H_{a[1/2]}$	$\Delta G_{a[1/2]}$	$\Delta S_{a[1/2]}$
2a	OH-S	-6.0	5.5	-38.8
	OH-O	-11.5	0.7	-41.0
2b	OH-S	-6.8	6.0	-42.9
	OH-O	-12.4	2.5	-50.3
2c	OH-S	-5.9	6.5	-41.6
	OH-O	-13.0	0.1	-44.0

The computations were performed using Amsterdam Density Functional package (ADF2013 version)[1]

[1] a) G. te Velde, F.M. Bickelhaupt, S. J. A. van Gisbergen, C. Fonseca Guerra, E. J. Baerends, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* **2001**, *22*, 931; b) C. Fonseca Guerra, J. G. Snijders, G. te Velde, E. J. Baerends, *Theor. Chem. Acc.* **1998**, *99*, 391; c) ADF2013, SCM, Theorical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
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E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J.A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, M. Pavanello, P. H. T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev.

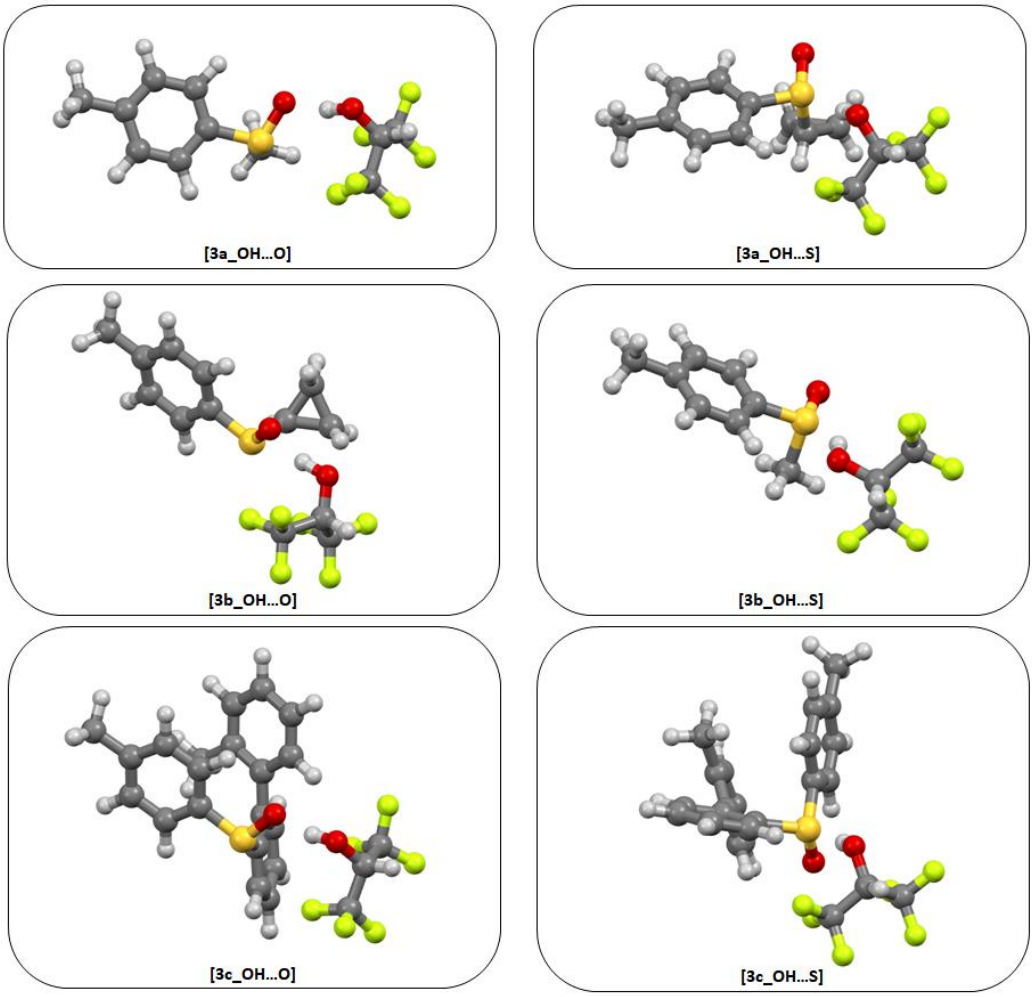

Figure SI 9. Graphic representations **1/2a-c** adducts show the difference in thermochemical parameters (Table SI 2) of the two approaches of HFIP: to oxygen atom (OH…O) and to sulfur atom (OH…S). The calculations were performed at ZORA-GGAPBE-D3-BJ/TZP level of theory in gas phase. S: orange; O: red; F: yellowish; C: grey; H: white. The computations were performed using Amsterdam Density Functional package (ADF2013 version)[2]

[2] a) G. te Velde, F.M. Bickelhaupt, S. J. A. van Gisbergen, C. Fonseca Guerra, E. J. Baerends, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* **2001**, *22*, 931; b) C. Fonseca Guerra, J. G. Snijders, G. te Velde, E. J. Baerends, *Theor. Chem. Acc.* **1998**, *99*, 391; c) ADF2013, SCM, Theorical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
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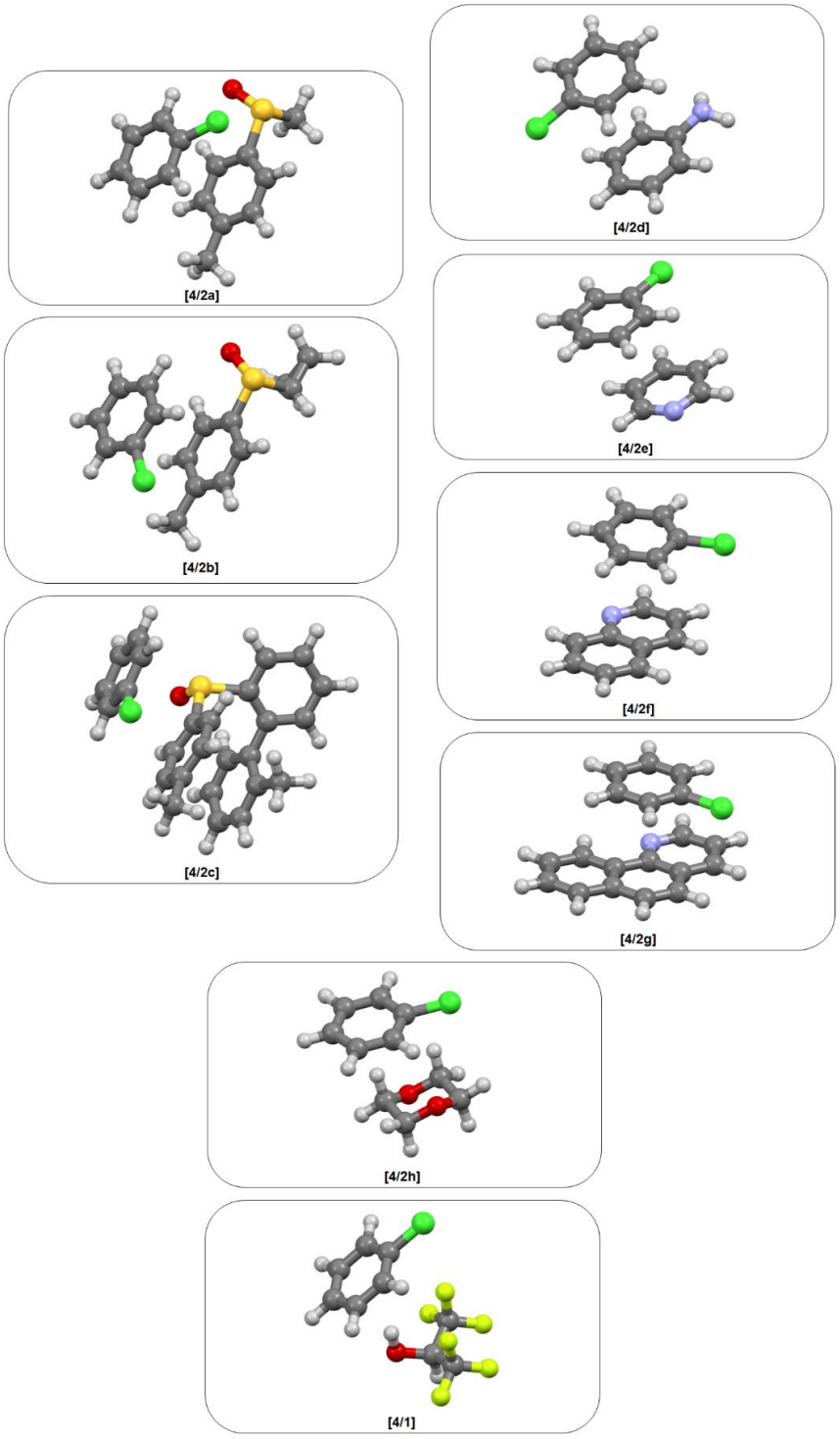


Figure SI 10. Graphic representations of optimized geometries of the systems **4/1** and **4/2a-h** at PBE-D3(BJ)/def2-TZVP level of theory in chlorobenzene solution (PCM) phase. S: orange; O: red; N: violet; F: yellowish; Br: brown; C: grey; H: white. Corresponding thermodynamic parameters ($\Delta H_{a[4/1]}$, $\Delta G_{a[4/1]}$, $\Delta S_{a[4/1]}$,$\Delta E_{a[4/1]}$, $\Delta H_{a[4/2]}$, $\Delta G_{a[4/2]}$, $\Delta S_{a[4/2]}$ and $\Delta E_{a[4/2]}$) are shown in Table SI 1.

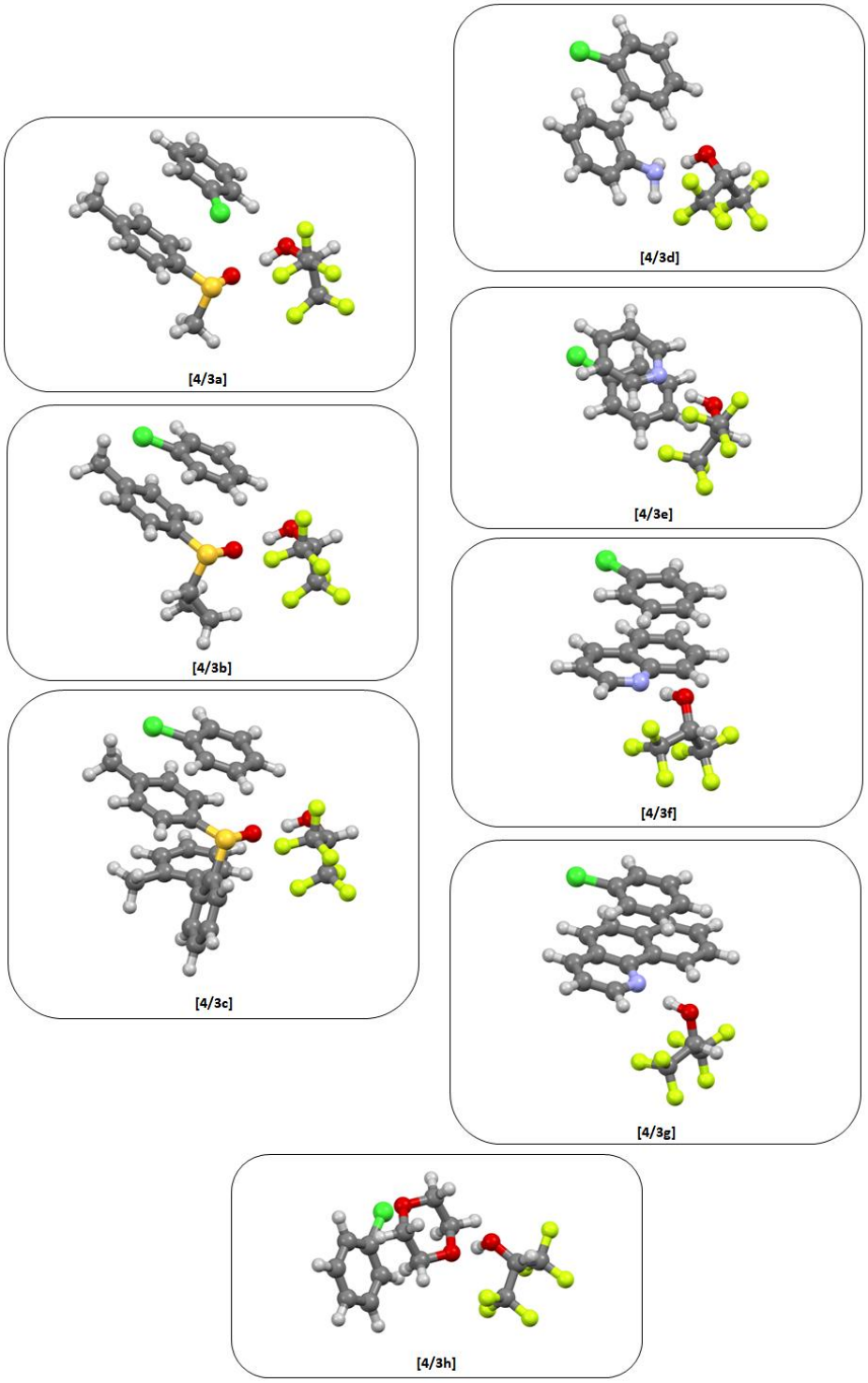


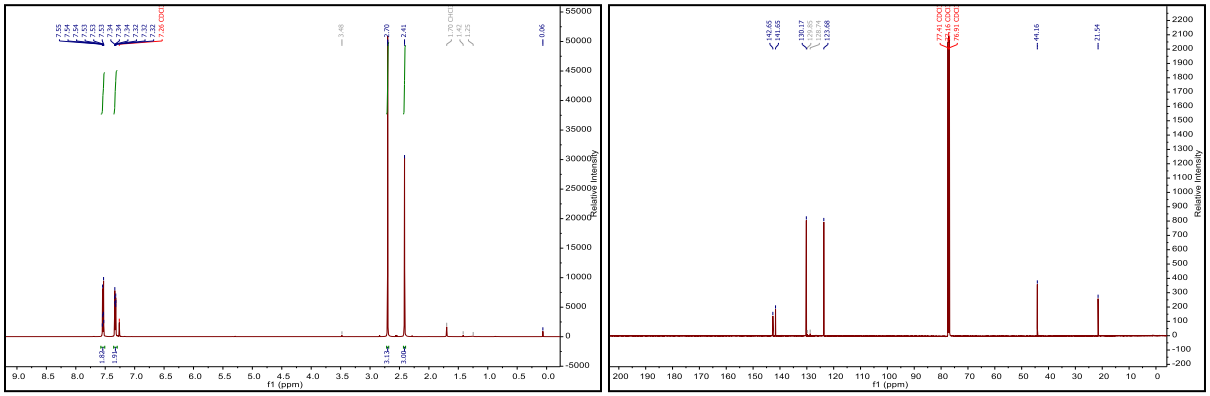
Figure SI 11. Graphic representations of optimized geometries of the systems **4/3** at PBE-D3(BJ)/def2-TZVP level of theory in chlorobenzene solution (PCM) phase. S: orange; O: red; N: violet; F: yellowish; Br: brown; C: grey; H: white. Corresponding thermodynamic parameters ($\Delta H_{a[\mathbf{4/3}]}$, $\Delta G_{a[\mathbf{4/3}]}$, $\Delta S_{a[\mathbf{4/3}]}$ and $\Delta E_{a[\mathbf{4/3}]}$) are shown in Table SI 1.

S.3. Analytical data for substrates 2a-c.

2a

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 7.57 – 7.51 (m, 2H), 7.33 (dt, *J* = 8, 1 Hz, 2H), 2.70 (s, 3H), 2.41 (s, 3H).

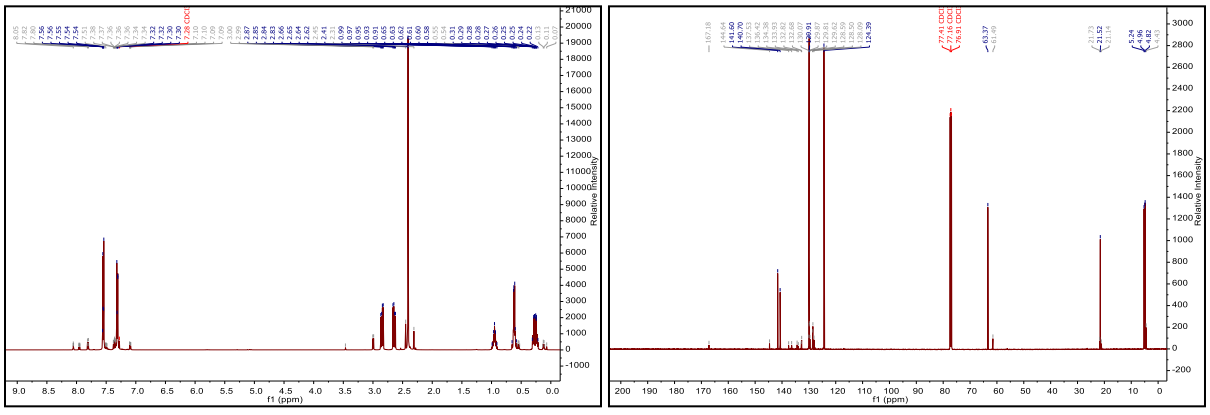
^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 142.65, 141.65, 130.17, 123.68, 44.16, 21.54.



2b

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 7.58 – 7.52 (m, 2H), 7.34 – 7.29 (m, 2H), 2.85 (dd, *J* = 13, 7 Hz, 1H), 2.64 (dd, *J* = 13, 7 Hz, 1H), 2.41 (s, 3H), 1.03 – 0.89 (m, 1H), 0.67 – 0.56 (m, 2H), 0.34 – 0.18 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 141.60, 140.70, 129.91, 124.39, 63.37, 21.52, 5.24, 4.96, 4.82.

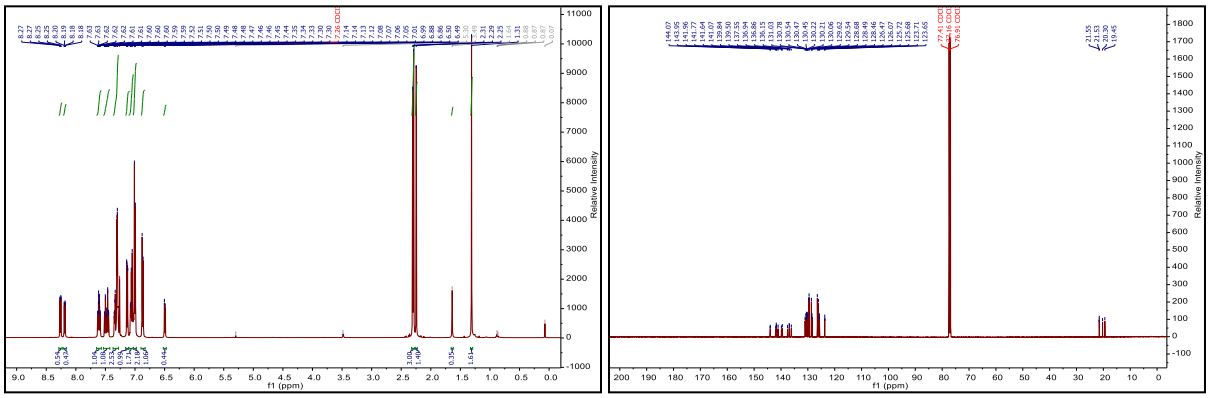


2c

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 8.22 (ddd, *J* = 36, 8, 1 Hz, 1H), 7.61 (tdd, *J* = 8, 5, 1 Hz, 1H), 7.48 (dtd, *J* = 19, 8, 1 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.13 (dd, *J* = 8, 1 Hz, 1H), 7.09 – 7.02 (m, 2H), 7.00 (d, *J* = 8 Hz, 2H), 6.87 (d, *J* = 8 Hz, 1H), 6.50 (d, *J* = 7 Hz, 1H), 2.30 (d, *J* = 9 Hz, 3H), 1.78 (d, *J* = 467 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 143.95, 141.96, 141.77, 141.64, 141.07, 139.50, 137.55, 136.94, 136.86, 136.15, 131.03, 130.78, 130.54, 130.47, 130.45, 130.22, 130.21, 130.06, 129.62, 129.54, 128.68, 128.49, 128.46, 126.47, 126.07, 125.72, 125.68, 123.71, 123.65, 21.55, 21.53, 20.30, 19.45.

^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 144.01 (d, *J* = 15 Hz), 141.96, 141.70 (d, *J* = 16 Hz), 141.07, 139.84, 139.50, 137.55, 136.90 (d, *J* = 10 Hz), 136.15, 131.03, 130.78, 130.54, 130.46 (d, *J* = 3 Hz), 130.21 (d, *J* = 1 Hz), 130.06, 129.58 (d, *J* = 10 Hz), 128.68, 128.48 (d, *J* = 3 Hz), 126.47, 126.07, 125.70 (d, *J* = 4 Hz), 123.68 (d, *J* = 8 Hz), 21.54 (d, *J* = 3 Hz), 19.87 (d, *J* = 107 Hz).



S.4. Purity verifications by NMR spectroscopy

2d, Aniline

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 7.26 – 7.18 (m, 2H), 6.82 (tt, *J* = 7, 1 Hz, 1H), 6.73 – 6.67 (m, 2H), 3.64 (s, 2H).
^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 146.45, 129.26, 118.42, 115.06, 77.41, 77.16, 76.90.

2e, Pyridine

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 8.61 (dt, *J* = 4, 2 Hz, 2H), 7.66 (tt, *J* = 8, 2 Hz, 1H), 7.27 (ddd, *J* = 8, 4, 2 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 149.94, 135.99, 123.78.

2f, 2-Phenylpyridine

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 8.70 (dt, *J* = 5, 1 Hz, 1H), 8.03 – 7.97 (m, 2H), 7.78 – 7.69 (m, 2H), 7.52 – 7.46 (m, 2H), 7.46 – 7.38 (m, 1H), 7.22 (ddd, *J* = 6, 5, 3 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 157.55, 149.77, 139.50, 136.83, 129.04, 128.84, 127.00, 122.19, 120.65.

2g, Benzo[*h*]quinoline

^{1}H NMR (500 MHz, $CDCl_3$, δ ppm) 9.33 – 9.27 (m, 1H), 9.01 (dd, *J* = 4, 2 Hz, 1H), 8.18 (dd, *J* = 8, 2 Hz, 1H), 7.95 – 7.89 (m, 1H), 7.82 (d, *J* = 9 Hz, 1H), 7.76 (dd, *J* = 7, 1 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.53 (dd, *J* = 8, 4 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$, δ ppm) 148.98, 146.73, 135.98, 133.75, 131.65, 128.35, 127.97, 127.92, 127.23, 126.56, 125.50, 124.49, 121.95.

2h, Dioxane

^{1}H NMR (300 MHz, $CDCl_3$, δ ppm) 3.71 – 3.64 (m, 8H).

S.5. Cartesian's coordinates of the optimized geometries of the investigated systems within the study of the affinity of Lewis donors to HFIP

[**1**] - HFIP - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

9	-1.198077	-1.883437	5.112496
9	-2.099961	-0.772511	3.460311
8	0.066811	-2.420963	2.670030
1	-1.031007	-3.900721	3.518560
9	-3.148921	-2.486478	4.336707
6	-1.193536	-2.946533	2.996106
1	-0.058809	-1.567026	2.212695
6	-2.001185	-3.269214	1.717466
9	-1.302166	-4.138930	0.952672
9	-2.217040	-2.153952	0.971812
9	-3.200462	-3.829656	1.987787
6	-1.933051	-2.015209	3.984277

[**2a**] - 1-methyl-4-(methylsulfinyl)benzene - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-2.874274	0.203968	-1.020917
8	-0.212078	-0.069562	0.216092
16	-1.212709	1.028948	0.476457
1	-2.008805	3.801958	0.994065
1	-2.929217	2.001626	-0.918701
6	-2.275524	1.123485	-1.003173
1	-1.633129	1.193107	-1.890446
6	-0.367901	2.612351	0.220820
6	0.933439	2.611920	-0.274270
6	1.601539	3.828471	-0.437901
6	0.988827	5.045307	-0.107474
6	-0.320661	5.013526	0.404506
6	-0.998105	3.808430	0.578566
1	1.410140	1.661224	-0.521445
1	2.622090	3.831079	-0.828161
1	2.725579	6.207141	-0.668908
1	-0.812951	5.949680	0.679055
6	1.708405	6.355876	-0.283680
1	1.170285	7.010773	-0.986150
1	1.780662	6.900312	0.670152

[**2b**] - 1-(cyclopropylsulfinyl)-4-methylbenzene - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-3.910928	0.154077	-2.188224
8	-0.491199	0.036637	0.153114
16	-1.424442	1.194550	0.414408
1	-2.014346	3.977096	1.074864
1	-2.567441	-0.803311	-1.363019
1	-0.819128	0.611250	-2.401539
1	-2.087314	1.625725	-3.279157
6	-0.464677	2.719681	0.227955
6	0.825538	2.657173	-0.295563
6	1.566584	3.833298	-0.423260

6	1.039322	5.072732	-0.028934
6	-0.260003	5.103645	0.504285
6	-1.010588	3.936360	0.644618
1	1.235850	1.689741	-0.591425
1	2.576668	3.788357	-0.837874
1	2.604427	6.257037	-0.940050
1	-0.687360	6.057825	0.821698
6	1.856929	6.332017	-0.138555
1	1.222366	7.207435	-0.334453
1	2.400754	6.527199	0.799896
6	-2.425023	1.399268	-1.093806
6	-2.901054	0.149062	-1.778291
6	-1.834887	1.010082	-2.416200
1	-3.089617	2.262293	-1.020097

[**2c**] - 2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	3.205213	4.184769	-2.730207
8	0.214398	-0.477994	1.083104
16	-0.331602	0.927944	1.052321
1	-0.511949	3.685963	0.085672
1	2.801746	4.135714	-3.754978
1	3.244336	5.246045	-2.447536
1	-2.289143	2.236884	-3.997186
6	0.678363	1.883885	-0.107896
6	1.821655	1.298606	-0.646611
6	2.642680	2.054217	-1.484530
6	2.344546	3.391588	-1.783722
6	1.203457	3.965446	-1.197994
6	0.373612	3.225050	-0.358193
1	2.040385	0.253222	-0.425184
1	3.529296	1.590706	-1.923734
1	4.231732	3.795290	-2.763703
1	0.959481	5.009774	-1.407253
6	-1.926440	0.972621	0.171101
6	-2.986032	1.372119	0.995652
6	-4.284231	1.456707	0.491712
6	-4.517207	1.135263	-0.846040
6	-3.459478	0.736255	-1.665433
6	-2.143578	0.641802	-1.184860
1	-2.781705	1.622715	2.039060
1	-5.104134	1.768347	1.140304
1	-5.526924	1.190204	-1.256544
1	-3.650949	0.478559	-2.709029
6	-1.067495	0.194960	-2.113669
6	-0.449472	-1.047281	-1.904087
6	0.536259	-1.513978	-2.773276
6	0.919593	-0.731510	-3.863751
6	0.309223	0.505378	-4.075971
6	-0.692430	0.988303	-3.222708
1	-0.737039	-1.638897	-1.035418
1	1.007691	-2.481394	-2.591872
1	1.697662	-1.079253	-4.546115
1	0.622006	1.124013	-4.920893
6	-1.316112	2.334093	-3.490251

1	-1.491103	2.891363	-2.560103
1	-0.665322	2.939317	-4.135551

[**2d**] - aniline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.215816	-2.114551	1.187796
6	-0.013193	-0.000490	0.001054
6	0.149902	-0.721840	1.200846
6	0.121677	-2.826053	-0.012996
1	0.172611	-3.915565	-0.018333
1	0.225969	-0.178834	2.146329
7	-0.015117	1.391900	0.001716
6	-0.108904	-0.722134	-1.205799
6	-0.041660	-2.114894	-1.206532
1	0.340041	-2.649991	2.131559
1	-0.235546	-0.179713	-2.146201
1	-0.120581	-2.650593	-2.155012
1	-0.284153	1.829277	0.878816
1	-0.464060	1.830581	-0.797644

[**2e**] - pyridine - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	0.000000	-0.123340	-2.069650
1	0.000000	-3.910502	0.000000
1	0.000000	-2.617594	-2.162789
6	0.000000	-2.819062	0.000000
6	0.000000	-2.105614	-1.199426
6	0.000000	-0.709544	-1.145458
7	0.000000	-0.007252	0.000000
6	0.000000	-0.709544	1.145458
6	0.000000	-2.105614	1.199426
1	0.000000	-0.123340	2.069650
1	0.000000	-2.617594	2.162789

[**2f**] - quinoline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.000000	-2.046690	3.660911
6	0.000000	0.030640	2.400719
6	0.000000	-0.630781	3.612036
6	0.000000	-2.783687	2.494516
6	0.000000	-2.121293	-1.178971
6	0.000000	-0.705484	-1.120214
7	0.000000	-0.004598	0.002422
6	0.000000	-0.697853	1.182580
6	0.000000	-2.133478	1.232824
6	0.000000	-2.833297	0.000032
1	0.000000	-3.925981	0.002281
1	0.000000	-2.623557	-2.147130
1	0.000000	-0.128931	-2.051474
1	0.000000	-2.552752	4.627775
1	0.000000	-3.875925	2.524915
1	0.000000	-0.061491	4.543301
1	0.000000	1.120657	2.344976

[**2g**] - benzo[h]quinoline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.000000	-2.074723	3.658181
6	0.000000	0.066902	2.417796
6	0.000000	-0.640711	3.658173
6	0.000000	-2.783697	2.491199
6	0.000000	-2.107443	-1.188674
6	0.000000	-0.699655	-1.129874
7	0.000000	-0.003943	0.002287
6	0.000000	-0.685792	1.176235
6	0.000000	-2.113265	1.225453
6	0.000000	-2.813838	-0.000862
6	0.000000	0.094056	4.868294
1	0.000000	-2.615429	-2.153727
1	0.000000	-0.115942	-2.056225
1	0.000000	2.031998	5.798525
6	0.000000	1.479193	2.433382
1	0.000000	-3.906440	0.006037
6	0.000000	2.173912	3.631787
6	0.000000	1.478099	4.858043
1	0.000000	-3.876160	2.502475
1	0.000000	-0.451951	5.814521
1	0.000000	-2.593160	4.619766
1	0.000000	3.265428	3.627794
1	0.000000	2.005959	1.479013

[**2h**] - dioxane - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

8	-0.005657	-2.860244	0.000000
6	-0.341769	-0.755652	-1.173092
6	0.341769	-2.114191	-1.173092
6	0.341769	-2.114191	1.173092
6	-0.341769	-0.755652	1.173092
8	0.005657	-0.009599	0.000000
1	-1.440800	-0.890860	1.220065
1	-1.440800	-0.890860	-1.220065
1	-0.019598	-0.156805	-2.037324
1	1.440800	-1.978983	-1.220065
1	0.019598	-2.713038	-2.037324
1	1.440800	-1.978983	1.220065
1	0.019598	-2.713038	2.037324
1	-0.019598	-0.156805	2.037324

[**4**] - PhCl - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.000000	-2.887334	0.098000
6	0.000000	-2.204334	1.315735
6	0.000000	-0.807211	1.306800
6	0.000000	-0.105982	0.098000
6	0.000000	-0.807211	-1.110800
6	0.000000	-2.204334	-1.119735
1	0.000000	-2.759377	2.253873

1	0.000000	-0.267688	2.255400
1	0.000000	0.984886	0.098000
1	0.000000	-0.267688	-2.059400
1	0.000000	-2.759377	-2.057873
17	0.000000	-4.636749	0.098000

[**3a**] - HFIP/1-methyl-4-(methylsulfinyl)benzene_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

9	0.589357	1.584320	2.801446
6	1.922891	2.462199	0.991759
1	1.345903	3.601162	-0.541326
6	2.049577	1.129978	0.213530
9	3.254957	1.084133	-0.403912
9	1.099322	0.999463	-0.744241
9	1.967705	0.045628	1.025192
6	0.631276	2.542964	1.843190
9	0.572923	3.742845	2.466953
9	-0.496080	2.420930	1.093937
8	2.071866	3.562107	0.154836
1	2.753390	2.465249	1.716717
1	-1.511281	4.394843	-4.015296
8	0.331291	3.970676	-1.809373
16	-1.189742	3.963862	-1.699931
1	-3.578468	4.204113	-0.081722
1	-2.833653	5.108397	-3.020275
6	-1.749012	4.962852	-3.107107
1	-1.217799	5.922882	-3.089223
6	-1.636273	5.114075	-0.384552
6	-0.720155	6.077539	0.037134
6	-1.066795	6.927804	1.086276
6	-2.314318	6.828202	1.723431
6	-3.213321	5.845367	1.279352
6	-2.878701	4.979599	0.238099
1	0.257735	6.143824	-0.443056
1	-0.352182	7.683147	1.421320
1	-2.163324	8.700439	2.796421
1	-4.186339	5.747659	1.766077
6	-2.662407	7.725393	2.880181
1	-3.746080	7.891330	2.948895
1	-2.338993	7.273381	3.831749

[**3b**] - HFIP/1-(cyclopropylsulfinyl)-4-methylbenzene_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

9	2.392319	0.428907	2.425550
6	2.529607	1.522515	0.276585
1	1.689899	3.272328	-0.192828
6	1.527587	0.562029	-0.410471
9	1.801756	0.499648	-1.736370
9	0.239716	0.978085	-0.286939
9	1.599320	-0.699236	0.079022
6	2.313830	1.632686	1.805282
9	3.272514	2.427213	2.338263
9	1.113209	2.179962	2.120222

8	2.552055	2.769982	-0.336349
1	3.520077	1.055669	0.148363
6	-4.062902	9.020317	1.505025
8	0.452744	4.366077	-0.172868
16	-1.017709	3.970662	-0.082135
1	-3.706008	4.382236	0.906894
1	-4.744494	8.834625	2.346828
1	-0.161724	5.396146	-2.521264
1	-3.385344	9.839854	1.779124
6	-1.903971	5.467876	0.382135
6	-1.264095	6.705054	0.322188
6	-1.968206	7.850084	0.697287
6	-3.301597	7.777742	1.129376
6	-3.913658	6.514831	1.193287
6	-3.222587	5.359017	0.831868
1	-0.222604	6.758664	0.001603
1	-1.469444	8.821282	0.658211
1	-4.678316	9.368792	0.659905
1	-4.944264	6.434116	1.546374
6	-1.595503	3.865572	-1.798076
6	-0.669714	3.254630	-2.812871
6	-0.967224	4.735588	-2.845721
1	-2.662926	3.639703	-1.837392
1	-1.115058	2.598871	-3.560600
1	0.328286	2.968479	-2.478341
1	-1.622093	5.136322	-3.618816

[**3c**] - HFIP/2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	3.239308	4.235630	-2.695465
8	0.281317	-0.494403	0.988348
16	-0.280715	0.920589	1.032925
1	-0.409132	3.701861	0.201505
1	4.247565	3.811146	-2.792212
1	2.794397	4.261029	-3.703665
1	-2.243397	2.273311	-3.892579
6	0.734632	1.883999	-0.102939
6	1.845961	1.293094	-0.699149
6	2.659424	2.066155	-1.528152
6	2.385233	3.421560	-1.761480
6	1.274943	3.996196	-1.119822
6	0.451653	3.240584	-0.287839
1	2.047568	0.235150	-0.530093
1	3.521477	1.601282	-2.011965
1	3.329971	5.276566	-2.355019
1	1.050585	5.053767	-1.276742
6	-1.879872	0.974103	0.181530
6	-2.921684	1.394187	1.018271
6	-4.225687	1.479646	0.531467
6	-4.480335	1.137160	-0.796949
6	-3.438101	0.718733	-1.626713
6	-2.115946	0.624301	-1.165861
1	-2.702016	1.650445	2.056477
1	-5.033976	1.804628	1.187709
1	-5.496168	1.189755	-1.192186

1	-3.646782	0.445327	-2.662918
6	-1.056025	0.159293	-2.105063
6	-0.481232	-1.107917	-1.925650
6	0.488734	-1.585151	-2.806956
6	0.896696	-0.789710	-3.879079
6	0.324593	0.469802	-4.063851
6	-0.659114	0.964874	-3.197051
1	-0.794658	-1.715173	-1.077316
1	0.927193	-2.572033	-2.649650
1	1.662368	-1.146742	-4.570565
1	0.654107	1.096120	-4.896569
6	-1.245608	2.333325	-3.430177
1	-1.359882	2.889381	-2.489568
1	-0.603185	2.920749	-4.099653
9	-3.262857	-2.340397	4.195504
6	-1.258322	-2.934835	2.973635
1	0.017077	-1.673393	2.106167
6	-2.084925	-3.251701	1.701061
9	-1.337800	-3.984347	0.841948
9	-2.487035	-2.137292	1.038680
9	-3.195297	-3.975224	1.993635
6	-1.987745	-1.961327	3.931420
9	-1.325125	-1.910117	5.112221
9	-2.029630	-0.695922	3.440370
8	0.028302	-2.493325	2.691934
1	-1.184572	-3.890145	3.518907

[**3d**] - HFIP/aniline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-0.814463	4.268215	-2.423783
6	-0.575980	6.659886	-2.743345
6	-1.305551	5.563929	-2.259838
6	0.406845	4.046838	-3.066832
1	0.787819	3.032626	-3.193417
1	-2.258674	5.730470	-1.752234
7	-1.034920	7.982339	-2.511925
6	0.650633	6.439606	-3.387409
6	1.133826	5.140362	-3.546290
1	-1.394844	3.424853	-2.045008
1	1.227457	7.289911	-3.757871
1	2.089096	4.983966	-4.050839
1	-2.050560	8.044141	-2.431503
1	-0.712772	8.645749	-3.217342
9	2.876604	10.773199	-0.899386
6	0.775856	9.891682	-0.104156
1	-0.377874	8.535230	-1.004119
6	-0.073291	11.146442	-0.422884
9	-1.034958	11.289747	0.520060
9	-0.701855	11.047209	-1.624760
9	0.658174	12.286604	-0.436637
6	2.006495	9.743454	-1.032972
9	2.670117	8.605320	-0.729569
9	1.660696	9.670029	-2.348726
8	-0.007499	8.743589	-0.080657
1	1.186909	10.056016	0.905655

[**3e**] - HFIP/pyridine_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

9	2.199960	-0.693696	1.643598
6	2.087095	1.454078	0.527369
1	0.587106	2.798739	0.631174
6	1.649954	0.823119	-0.817617
9	1.967992	1.659827	-1.834052
9	0.310428	0.602023	-0.882104
9	2.269998	-0.359357	-1.057117
6	1.729817	0.573913	1.750577
9	2.274167	1.115096	2.867115
9	0.388411	0.496504	1.956303
8	1.615702	2.748715	0.681627
1	3.189850	1.476911	0.493803
1	-1.795904	1.335409	0.893364
1	-4.656600	4.480696	0.135083
1	-4.180208	2.068703	0.677192
6	-3.630712	4.123847	0.238434
6	-3.370893	2.785994	0.539310
6	-2.045011	2.372840	0.662114
7	-1.006093	3.209768	0.503745
6	-1.261388	4.496575	0.212299
6	-2.554870	4.997008	0.071119
1	-0.389584	5.143768	0.088812
1	-2.710169	6.049719	-0.165787

[**3f**] - HFIP/quinoline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-1.177740	5.678727	-1.780451
6	0.546456	7.033391	-2.830759
6	-0.647672	6.940468	-2.145447
6	-0.506033	4.519411	-2.107894
6	2.648695	3.566007	-3.866803
6	3.101461	4.866340	-4.181764
7	2.443663	5.968673	-3.854998
6	1.258798	5.857750	-3.177704
6	0.724288	4.577601	-2.812842
6	1.461557	3.425000	-3.181231
1	1.078109	2.437003	-2.916407
1	3.240520	2.701175	-4.166257
1	4.042884	5.007317	-4.719021
1	-2.123138	5.628346	-1.238140
1	-0.909363	3.542777	-1.831473
1	-1.191802	7.848443	-1.880366
1	0.961246	8.000478	-3.118198
9	4.946256	9.802556	-1.661635
6	4.361407	8.941711	-3.843564
1	3.053756	7.448376	-4.239442
6	5.683666	8.159278	-4.038190
9	5.978335	8.096084	-5.359697
9	5.603657	6.881398	-3.583801
9	6.735047	8.748497	-3.416495
6	3.989703	9.133736	-2.352209

9	2.846776	9.860467	-2.264503
9	3.767346	7.958148	-1.712418
8	3.321717	8.387248	-4.575526
1	4.563213	9.956765	-4.226599

[**3g**] - HFIP/benzo[h]quinoline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-1.865989	4.964628	-2.942025
6	-0.147268	6.551078	-2.118752
6	-1.461345	5.993730	-2.030507
6	-1.012380	4.485099	-3.891785
6	2.475163	5.089457	-5.093507
6	2.803584	6.148419	-4.233004
7	1.974007	6.632958	-3.310202
6	0.740623	6.075495	-3.163143
6	0.308574	5.020580	-4.024329
6	1.212649	4.536983	-4.994501
6	-2.343669	6.458867	-1.026644
1	3.200338	4.735418	-5.825863
1	3.779695	6.635926	-4.303030
1	-2.636238	7.780358	0.643697
6	0.239062	7.527535	-1.173268
1	0.899676	3.726944	-5.657078
6	-0.643140	7.961219	-0.197816
6	-1.945986	7.430733	-0.125898
1	-1.320865	3.688048	-4.571546
1	-3.347018	6.030720	-0.972315
1	-2.875928	4.559024	-2.850071
1	-0.323694	8.719164	0.519327
1	1.244648	7.942557	-1.206245
9	3.677794	11.122128	-5.157276
6	3.037659	10.030332	-3.103969
1	2.617009	8.074276	-2.763124
6	1.589226	10.574839	-3.049483
9	1.237386	10.787330	-1.757090
9	0.690804	9.706912	-3.575966
9	1.454488	11.754731	-3.705109
6	3.574648	9.913099	-4.552994
9	4.813583	9.362708	-4.533210
9	2.798307	9.125732	-5.341378
8	3.176686	8.849169	-2.386894
1	3.662175	10.803165	-2.625089

[**3h**] - HFIP/dioxane_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

8	1.741205	6.577561	-0.252419
6	2.671218	8.280472	1.219894
6	1.518558	7.887622	0.311389
6	3.003779	6.531934	-0.950490
6	4.139383	6.941070	-0.027739
8	3.914238	8.249102	0.509675
1	4.237533	6.206173	0.795632
1	2.715034	7.594139	2.088624
1	2.538321	9.308079	1.586776

1	1.412012	8.614752	-0.513275
1	0.572520	7.829548	0.867192
1	2.951499	7.209150	-1.821536
1	3.126487	5.498314	-1.302341
1	5.088246	6.981624	-0.581159
9	-1.966202	3.571961	1.293954
6	0.443707	3.730619	1.350338
1	1.522802	5.321464	0.850773
6	0.663870	2.921380	0.049694
9	1.852829	2.274128	0.121878
9	0.704542	3.716396	-1.049223
9	-0.296418	1.987444	-0.150632
6	-0.931494	4.438066	1.410400
9	-1.058809	5.066707	2.604693
9	-1.068852	5.380019	0.443184
8	1.488098	4.625740	1.574383
1	0.438095	2.991878	2.167999

[**4**/**1**] - PhCl/HFIP_in ring_pH - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	1.436603	0.190770	-0.683450
6	0.282140	-0.463590	-0.249440
6	0.306634	-1.854642	-0.101915
6	1.472869	-2.576740	-0.380356
6	2.619737	-1.902134	-0.809407
6	2.608572	-0.514472	-0.965770
1	-0.619411	0.106591	-0.026935
1	-0.593979	-2.372001	0.233227
1	1.487355	-3.660258	-0.257350
1	3.534456	-2.456702	-1.023737
1	3.499864	0.018934	-1.295863
17	1.417672	1.926826	-0.863428
9	2.972214	0.947338	4.465706
6	1.726255	-1.019522	3.847250
1	1.357880	-1.673723	2.028562
6	0.325816	-0.419221	4.111772
9	-0.505254	-1.395334	4.547347
9	-0.218558	0.101089	2.981521
9	0.345904	0.553552	5.050167
6	2.796488	0.035944	3.481324
9	3.983416	-0.581112	3.275876
9	2.482930	0.704108	2.343415
8	1.662528	-2.038047	2.887482
1	2.053462	-1.476087	4.793468

[**4**/**2a**] - PhCl/1-methyl-4-(methylsulfinyl)benzene - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-1.352816	3.859700	-3.433537
8	-0.093831	3.700459	-0.777648
16	-1.569728	3.855037	-1.057527
1	-4.246646	4.736130	-0.310010
1	-2.749411	4.868225	-2.904661
6	-1.699348	4.611121	-2.712567
1	-1.063513	5.505547	-2.740007

6	-2.161339	5.290233	-0.126025
6	-1.236216	6.175145	0.425589
6	-1.691101	7.239903	1.201809
6	-3.060297	7.427823	1.446656
6	-3.969690	6.522753	0.877458
6	-3.529099	5.450161	0.101062
1	-0.170495	6.005694	0.261369
1	-0.967638	7.928227	1.644903
1	-2.922712	9.443734	2.221646
1	-5.039309	6.648924	1.061102
6	-3.532183	8.537644	2.346199
1	-4.583042	8.794651	2.156585
1	-3.450222	8.234996	3.403299
6	-1.806405	3.882301	3.218440
6	-2.386504	4.828094	4.065004
6	-1.573319	5.806305	4.641804
6	-0.202175	5.835605	4.373958
6	0.358816	4.881566	3.521058
6	-0.439956	3.897198	2.935005
1	-3.458193	4.801295	4.261834
1	-2.020645	6.550717	5.302952
1	0.427293	6.603590	4.825945
1	1.426966	4.902430	3.298521
1	-0.016406	3.166109	2.246806
17	-2.815836	2.654084	2.489475

[**4**/**2b**] - PhCl/1-(cyclopropylsulfinyl)-4-methylbenzene - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-4.259973	8.173256	1.881177
8	0.306318	3.853787	-0.478875
16	-1.153738	3.651753	-0.811776
1	-3.990115	4.028329	-0.294996
1	-4.360671	7.917299	2.948897
1	0.319436	5.599064	-2.447318
1	-3.741335	9.139654	1.820293
6	-2.078362	5.025660	-0.085206
6	-1.393754	6.142560	0.390053
6	-2.111065	7.169093	1.003500
6	-3.503869	7.093605	1.156480
6	-4.167590	5.956991	0.667230
6	-3.463482	4.918793	0.057431
1	-0.306908	6.182796	0.301142
1	-1.576583	8.040400	1.389227
1	-5.275606	8.294619	1.479650
1	-5.250366	5.874950	0.786397
6	-1.357417	4.153994	-2.549844
6	-0.282094	3.747751	-3.517618
6	-0.441728	5.196924	-3.118006
1	-2.404706	4.116209	-2.856039
1	-0.594678	3.427764	-4.511512
1	0.585568	3.227698	-3.108253
1	-0.867453	5.905865	-3.827633
6	-2.641632	5.241739	4.168813
6	-1.915075	6.324353	4.667433
6	-0.537100	6.372655	4.442248

6	0.099795	5.354718	3.727926
6	-0.645085	4.279772	3.236820
6	-2.022775	4.214854	3.455352
1	-2.422105	7.115931	5.219383
1	0.037088	7.217411	4.826783
1	1.174454	5.401899	3.546769
1	-0.157556	3.493464	2.658509
1	-2.614066	3.387419	3.063861
17	-4.369563	5.175974	4.438671

[**4/2c**] - PhCl/2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	3.096893	4.486243	-3.168546
8	0.628998	-0.405021	0.729206
16	0.017390	0.973626	0.767883
1	-0.270563	3.771011	0.009886
1	3.694927	3.896729	-3.876299
1	2.445969	5.161992	-3.742115
1	-2.470994	2.170753	-3.930121
6	0.850417	1.981591	-0.481371
6	1.890059	1.428639	-1.223118
6	2.600313	2.240151	-2.108578
6	2.298277	3.601780	-2.249839
6	1.250438	4.134882	-1.480054
6	0.532057	3.338440	-0.592042
1	2.121148	0.368731	-1.109655
1	3.407367	1.804923	-2.702922
1	3.788774	5.119578	-2.589760
1	1.004449	5.195475	-1.569061
6	-1.664284	0.944767	0.063264
6	-2.640676	1.342268	0.985729
6	-3.986776	1.383736	0.621085
6	-4.352374	1.018940	-0.675236
6	-3.377523	0.619511	-1.591611
6	-2.016217	0.569960	-1.251618
1	-2.333029	1.625875	1.994865
1	-4.741039	1.694830	1.345272
1	-5.400988	1.039403	-0.976997
1	-3.671163	0.326772	-2.601779
6	-1.035233	0.120265	-2.279621
6	-0.395034	-1.118389	-2.126801
6	0.497206	-1.588369	-3.090678
6	0.761076	-0.812836	-4.220918
6	0.128532	0.421641	-4.376215
6	-0.777306	0.908786	-3.424451
1	-0.591190	-1.705794	-1.230109
1	0.988231	-2.553284	-2.953163
1	1.463253	-1.164354	-4.979443
1	0.350094	1.035629	-5.252664
6	-1.418343	2.258671	-3.619106
1	-1.405062	2.845106	-2.689602
1	-0.888356	2.830371	-4.392438
6	3.328405	4.482647	1.512536
6	3.970994	3.299380	1.149966
6	3.642113	2.119693	1.821836

6	2.689010	2.126837	2.842728
6	2.057607	3.323251	3.193474
6	2.372227	4.511208	2.529678
1	4.701807	3.298997	0.341768
1	4.126330	1.186451	1.530414
1	2.428859	1.198825	3.353305
1	1.306656	3.336465	3.985219
1	1.879924	5.447991	2.791104
17	3.718848	5.963029	0.664511

[**4/2d**] - PhCl/aniline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-0.238294	-2.192741	0.915589
6	-0.276429	-0.047694	-0.232581
6	-0.095367	-0.807013	0.939780
6	-0.569761	-2.859153	-0.268596
1	-0.671226	-3.944936	-0.283577
1	0.177527	-0.300888	1.869118
7	-0.059006	1.328759	-0.231509
6	-0.612217	-0.722496	-1.422441
6	-0.756209	-2.109674	-1.434242
1	-0.077607	-2.760979	1.834131
1	-0.754134	-0.149163	-2.342187
1	-1.015655	-2.610018	-2.369840
1	-0.151432	1.783466	0.672787
1	-0.532359	1.846235	-0.967317
6	3.286550	-2.828762	0.435822
6	3.814053	-2.160675	1.541712
6	4.004974	-0.778230	1.466852
6	3.671990	-0.079642	0.303642
6	3.145533	-0.767931	-0.792267
6	2.950633	-2.148832	-0.735076
1	4.065727	-2.714025	2.446581
1	4.414699	-0.248676	2.328817
1	3.812660	1.000992	0.253789
1	2.865260	-0.227353	-1.697420
1	2.519532	-2.689216	-1.576959
17	3.023356	-4.556655	0.526992

[**4/2e**] - PhCl/pyridine - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-0.050228	0.500005	-0.915533
1	-0.455039	-3.790092	-0.709321
1	0.025440	-1.716257	-2.056880
6	-0.491006	-2.801472	-0.248744
6	-0.224153	-1.655274	-0.996868
6	-0.264567	-0.415267	-0.355290
7	-0.552024	-0.257871	0.947324
6	-0.805898	-1.372599	1.653421
6	-0.787642	-2.657852	1.107144
1	-1.034753	-1.229018	2.714097
1	-0.994138	-3.525145	1.735752
6	3.019817	-3.053699	0.211111
6	2.895436	-1.943151	1.046615

6	3.164520	-0.675053	0.527627
6	3.556085	-0.522674	-0.805019
6	3.677937	-1.647046	-1.625419
6	3.409004	-2.922713	-1.122863
1	2.578018	-2.069512	2.081345
1	3.054508	0.198445	1.172033
1	3.761677	0.471462	-1.204389
1	3.981909	-1.537245	-2.667828
1	3.496470	-3.805513	-1.756315
17	2.665028	-4.645062	0.845600

[**4/2f**] - PhCl/quinoline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-0.171283	-1.701866	3.833964
6	-0.153738	0.148297	2.258362
6	-0.109561	-0.313137	3.559242
6	-0.278753	-2.611886	2.801056
6	-0.419320	-2.544766	-0.936111
6	-0.351210	-1.138324	-1.107757
7	-0.276439	-0.263381	-0.104708
6	-0.257151	-0.761581	1.173504
6	-0.323241	-2.169388	1.452592
6	-0.408177	-3.057931	0.345814
1	-0.448543	-4.135369	0.523648
1	-0.466972	-3.196319	-1.809519
1	-0.354844	-0.719330	-2.120685
1	-0.133717	-2.049277	4.867896
1	-0.325043	-3.684404	3.005461
1	-0.025839	0.394658	4.386062
1	-0.103442	1.213884	2.028078
6	3.283643	-2.770740	-0.892578
6	3.196308	-2.488774	0.471297
6	3.338642	-1.166215	0.897914
6	3.573104	-0.144855	-0.026062
6	3.667203	-0.448365	-1.386753
6	3.520925	-1.765247	-1.831149
1	3.003991	-3.290628	1.184030
1	3.247796	-0.936494	1.960972
1	3.672492	0.887079	0.312968
1	3.847659	0.343725	-2.115388
1	3.582594	-2.010006	-2.891577
17	3.068917	-4.419460	-1.438677

[**4/2g**] - PhCl/benzo[h]quinoline - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.196473	-2.195917	3.325539
6	0.038058	-0.079362	2.054082
6	0.252091	-0.763884	3.288039
6	-0.042874	-2.925259	2.196570
6	-0.653206	-2.318284	-1.442313
6	-0.622070	-0.910113	-1.414955
7	-0.416002	-0.193163	-0.315630
6	-0.220469	-0.853160	0.854072
6	-0.249734	-2.278280	0.936338

6	-0.470887	-3.002003	-0.255240
6	0.533711	-0.009064	4.452064
1	-0.821362	-2.844439	-2.382764
1	-0.772441	-0.344273	-2.340349
1	0.824706	1.941866	5.307243
6	0.109191	1.330443	2.029593
1	-0.485646	-4.093794	-0.223850
6	0.387935	2.045662	3.182460
6	0.603585	1.372516	4.402571
1	-0.068194	-4.016644	2.231884
1	0.699569	-0.537744	5.393676
1	0.362226	-2.696490	4.282378
1	0.444081	3.135240	3.147108
1	-0.049691	1.837777	1.077986
6	3.247141	-2.364298	0.465063
6	3.467587	-1.724764	1.685756
6	3.551744	-0.331093	1.711285
6	3.418361	0.408117	0.533595
6	3.198577	-0.250266	-0.678469
6	3.110991	-1.643663	-0.722023
1	3.554737	-2.309130	2.601340
1	3.703207	0.177115	2.665015
1	3.469858	1.497197	0.563662
1	3.080032	0.320693	-1.600685
1	2.925557	-2.165616	-1.660565
17	3.122760	-4.109322	0.424726

[**4/2h**] - PhCl/dioxane - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

8	-0.303175	-2.815559	-0.090119
6	0.016797	-0.515599	-0.817034
6	0.414269	-1.971854	-1.001561
6	-0.056740	-2.390261	1.256348
6	-0.455367	-0.934784	1.445739
8	0.245993	-0.085782	0.529782
1	-1.548513	-0.825215	1.297187
1	-1.053302	-0.383942	-1.075213
1	0.622810	0.135635	-1.463700
1	1.503408	-2.085768	-0.841263
1	0.164938	-2.316499	-2.015850
1	1.015707	-2.518105	1.500663
1	-0.652218	-3.043860	1.910406
1	-0.195548	-0.589860	2.457035
6	3.781809	-1.228645	1.086464
6	3.681223	-0.134218	0.226399
6	3.964074	-0.313483	-1.129451
6	4.338652	-1.569098	-1.616392
6	4.431500	-2.653602	-0.740089
6	4.153581	-2.490726	0.619757
1	3.371295	0.836331	0.611887
1	3.884033	0.537594	-1.807864
1	4.554631	-1.702860	-2.677253
1	4.718911	-3.638398	-1.111954
1	4.219482	-3.331621	1.310172
17	3.418150	-1.018323	2.783904

[**4/3a**] - PhCl/HFIP/1-methyl-4-(methylsulfinyl)benzene_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-0.946344	4.658774	-3.730627
8	0.412673	4.597980	-1.149380
16	-1.082538	4.391782	-1.373991
1	-3.845210	4.538446	-0.507241
1	-2.518021	5.264254	-3.089096
6	-1.430979	5.242289	-2.937779
1	-1.018448	6.257672	-2.882930
6	-1.933813	5.532314	-0.269892
6	-1.213172	6.536901	0.374443
6	-1.875696	7.378101	1.266774
6	-3.245384	7.224658	1.531772
6	-3.943538	6.203685	0.868186
6	-3.295606	5.348497	-0.022855
1	-0.142415	6.635695	0.189668
1	-1.313412	8.159435	1.782922
1	-3.501053	9.104759	2.571797
1	-5.008316	6.062832	1.067191
6	-3.932125	8.094419	2.548707
1	-5.009224	8.177340	2.350309
1	-3.814838	7.667513	3.558555
6	-1.339209	3.729318	2.874717
6	-1.971179	4.596424	3.767419
6	-1.219778	5.605343	4.374209
6	0.140909	5.744666	4.088238
6	0.754133	4.866691	3.190716
6	0.018904	3.849852	2.577020
1	-3.035403	4.486556	3.975691
1	-1.708175	6.289121	5.070925
1	0.721229	6.537559	4.562514
1	1.814731	4.969534	2.954872
1	0.495789	3.170390	1.870791
17	-2.273935	2.466250	2.104608
9	0.865162	0.579524	0.956339
9	-0.136699	1.240387	-0.868512
8	2.081877	2.883335	-0.069776
1	3.098882	1.132467	-0.193557
9	1.165722	-0.519600	-0.908944
6	2.237282	1.635688	-0.662888
1	1.375787	3.438557	-0.536619
6	2.585254	1.734541	-2.168350
9	3.631282	2.577503	-2.336651
9	1.557028	2.210542	-2.915256
9	2.944631	0.532862	-2.685946
6	1.018736	0.721843	-0.383494

[**4/3b**] - PhCl/HFIP/1-(cyclopropylsulfinyl)-4-methylbenzene_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-3.978516	9.029997	1.815408
8	0.189812	4.386338	-0.641009
16	-1.312928	4.117176	-0.631606

1	-4.001435	4.594299	0.312080
1	-4.071582	8.866816	2.901479
1	-0.237031	5.805162	-2.802588
1	-3.393623	9.946883	1.664174
6	-2.095571	5.591138	0.042954
6	-1.355991	6.759025	0.216147
6	-1.978675	7.877103	0.772790
6	-3.326733	7.842849	1.159982
6	-4.047001	6.652926	0.965887
6	-3.437912	5.523304	0.423609
1	-0.301570	6.775889	-0.063765
1	-1.401923	8.793275	0.919952
1	-4.993832	9.195968	1.427814
1	-5.093539	6.601381	1.273329
6	-1.835664	4.333812	-2.353098
6	-0.941899	3.795367	-3.434441
6	-1.091453	5.286899	-3.240120
1	-2.918690	4.230261	-2.444634
1	-1.423979	3.313670	-4.284834
1	0.009740	3.361561	-3.126200
1	-1.679215	5.865465	-3.952155
6	-2.957661	4.841564	3.888094
6	-1.858749	5.700304	3.852572
6	-0.632049	5.206202	3.404189
6	-0.506162	3.874513	3.000667
6	-1.619529	3.030945	3.042709
6	-2.855167	3.508436	3.487424
1	-1.967803	6.741054	4.157039
1	0.228628	5.875538	3.359461
1	0.451888	3.499538	2.638690
1	-1.530398	1.992127	2.721055
1	-3.730263	2.859142	3.518822
17	-4.503828	5.456243	4.432133
9	0.978665	0.789592	2.082219
9	-0.065836	1.150734	0.199347
8	2.006392	3.034815	0.700954
1	3.158365	1.378255	0.893214
9	1.348683	-0.512479	0.365458
6	2.276304	1.723542	0.329046
1	1.254226	3.436737	0.157244
6	2.665723	1.590948	-1.164528
9	3.594792	2.522387	-1.478094
9	1.610574	1.771729	-2.001094
9	3.199238	0.374284	-1.439052
6	1.122878	0.772285	0.732775

[**4/3c**] - PhCl/HFIP/2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	2.887900	4.704550	-2.965113
8	0.758420	-0.732174	0.319044
16	0.042789	0.599625	0.526807
1	-0.481497	3.398653	0.017675
1	3.506974	4.240518	-3.744550
1	2.196001	5.411938	-3.444087

1	-2.611508	2.149778	-3.982104
6	0.816288	1.772318	-0.594712
6	1.921804	1.384325	-1.345568
6	2.574556	2.336431	-2.128752
6	2.149362	3.671625	-2.158692
6	1.037159	4.034773	-1.380427
6	0.374362	3.099008	-0.591329
1	2.250758	0.345582	-1.319923
1	3.434833	2.033054	-2.729867
1	3.555317	5.293653	-2.315093
1	0.693073	5.071389	-1.384745
6	-1.628376	0.487502	-0.159523
6	-2.619527	0.643527	0.818815
6	-3.968560	0.584569	0.470775
6	-4.319186	0.367715	-0.862521
6	-3.327838	0.209844	-1.833040
6	-1.962376	0.260701	-1.512255
1	-2.322775	0.811736	1.856086
1	-4.736456	0.704256	1.236058
1	-5.370093	0.314394	-1.151768
1	-3.610405	0.028676	-2.871930
6	-0.957461	0.058001	-2.593280
6	-0.196870	-1.120699	-2.612341
6	0.725538	-1.361106	-3.630690
6	0.897917	-0.413702	-4.641178
6	0.143556	0.760510	-4.625876
6	-0.795615	1.018197	-3.618221
1	-0.325506	-1.845036	-1.808183
1	1.310859	-2.282150	-3.627974
1	1.622794	-0.584743	-5.439400
1	0.291665	1.507932	-5.409193
6	-1.578958	2.305460	-3.632185
1	-1.642693	2.748731	-2.628703
1	-1.107394	3.037866	-4.300680
6	3.383635	3.557525	1.671985
6	4.240930	2.571223	1.183225
6	4.073693	1.255025	1.619719
6	3.067181	0.931300	2.532970
6	2.220298	1.934222	3.012804
6	2.371437	3.255573	2.584656
1	5.016448	2.829683	0.462401
1	4.732392	0.476252	1.231706
1	2.929679	-0.101347	2.855860
1	1.427227	1.687445	3.720371
1	1.710505	4.042688	2.947763
17	3.578680	5.208390	1.124287
9	1.193298	-1.156516	4.839658
9	-0.450051	-0.569730	3.528124
8	1.535707	-2.271556	2.298976
1	1.025699	-3.518077	3.814456
9	-0.774322	-2.077186	5.082793
6	0.570603	-2.736799	3.183061
1	1.145702	-1.642758	1.607001
6	-0.615908	-3.427365	2.465267
9	-0.142387	-4.345360	1.590244
9	-1.387077	-2.558648	1.764472

9	-1.424712	-4.078270	3.339718
6	0.115814	-1.628140	4.164528

[**4/3d**] - PhCl/HFIP/aniline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	-0.050504	-2.183471	1.018474
6	-0.213474	-0.084095	-0.181378
6	0.047489	-0.792534	0.999887
6	-0.407938	-2.886210	-0.135237
1	0.339869	-0.250567	1.902298
7	-0.053109	1.327449	-0.223098
6	-0.567046	-0.787437	-1.341831
6	-0.663577	-2.179508	-1.313333
1	-0.759766	-0.241257	-2.267844
1	-0.939558	-2.714520	-2.224002
1	-0.176837	1.763258	0.691912
1	-0.685968	1.774128	-0.888283
1	0.166712	-2.722690	1.942088
1	-0.472262	-3.974883	-0.118649
9	2.436656	0.890202	-3.535906
9	0.546694	1.956910	-3.279920
9	2.120860	2.800480	-4.546692
6	2.514563	2.829025	-2.167101
6	1.907740	4.228867	-1.902838
9	2.603361	4.839476	-0.914315
9	0.611858	4.157388	-1.496025
9	1.951006	5.033840	-2.991112
6	1.893113	2.122687	-3.397348
8	2.474127	2.035719	-1.026535
1	3.569996	3.005796	-2.432317
1	1.516127	1.803955	-0.767037
6	3.306416	-3.320496	0.542049
6	3.742013	-2.751385	1.739357
6	3.975860	-1.373921	1.785178
6	3.772761	-0.583545	0.651362
6	3.340309	-1.174111	-0.538927
6	3.106700	-2.548655	-0.603065
1	3.889301	-3.376097	2.620528
1	4.313646	-0.921307	2.719291
1	3.934235	0.494404	0.688365
1	3.162522	-0.553092	-1.417316
1	2.751446	-3.014827	-1.521671
17	2.978762	-5.039577	0.481289

[**4/3e**] - PhCl/HFIP/pyridine_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

1	-0.196734	-0.621954	-1.444441
1	-0.704304	-4.616193	0.111521
1	-0.219309	-3.094386	-1.832836
6	-0.697677	-3.532811	0.239260
6	-0.430126	-2.692675	-0.841744
6	-0.417893	-1.315424	-0.629933
7	-0.655944	-0.761160	0.570239
6	-0.915943	-1.573577	1.607844

6	-0.946008	-2.962087	1.488421
1	-1.100554	-1.085331	2.566668
1	-1.157541	-3.579725	2.361572
6	3.037481	-2.618652	-0.308419
6	2.832572	-2.067720	0.957401
6	2.789148	-0.678211	1.089357
6	2.950315	0.145945	-0.026968
6	3.161779	-0.424228	-1.284785
6	3.207190	-1.812791	-1.435315
1	2.694905	-2.718066	1.821098
1	2.612132	-0.239482	2.072092
1	2.893312	1.229075	0.083529
1	3.286416	0.211919	-2.162750
1	3.364176	-2.266862	-2.413802
17	3.063578	-4.359049	-0.489194
9	-2.837009	2.870490	1.049004
9	-2.360162	1.288865	2.478198
8	-0.305722	1.875780	0.484862
1	-0.385587	3.703054	1.370740
9	-2.301171	3.386997	3.102739
6	-0.545709	2.638862	1.615853
1	-0.477680	0.868521	0.643211
6	0.463913	2.323355	2.747392
9	1.726556	2.522665	2.293120
9	0.389261	1.031606	3.164936
9	0.297818	3.113924	3.835736
6	-2.020578	2.542924	2.078795

[**4/3f**] - PhCl/HFIP/quinoline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.136843	-1.864338	3.389713
6	-0.119450	0.003466	1.855792
6	0.120109	-0.472705	3.128122
6	-0.094594	-2.767538	2.373302
6	-0.824124	-2.666897	-1.287011
6	-0.804636	-1.265138	-1.455059
7	-0.582440	-0.413251	-0.465845
6	-0.358020	-0.902571	0.792329
6	-0.351453	-2.312203	1.054514
6	-0.593948	-3.187650	-0.031970
1	-0.587770	-4.266236	0.138643
1	-1.012183	-3.311048	-2.145889
1	-0.972236	-0.825349	-2.441667
1	0.335224	-2.219800	4.402078
1	-0.079564	-3.842447	2.565418
1	0.306264	0.229124	3.942793
1	-0.117581	1.072672	1.641217
6	3.068801	-2.342010	0.130911
6	3.337524	-1.539551	1.240451
6	3.326458	-0.151370	1.086266
6	3.049742	0.422185	-0.157127
6	2.788160	-0.398556	-1.256596
6	2.797943	-1.788720	-1.121478
1	3.535598	-1.995493	2.210198
1	3.521443	0.482521	1.952727

1	3.017264	1.506540	-0.266990
1	2.557099	0.043263	-2.227135
1	2.583351	-2.437217	-1.970672
17	3.054086	-4.082075	0.317659
9	-0.862949	2.639917	-3.571738
9	-2.366390	1.427232	-2.552365
8	-0.030296	2.141673	-0.966483
1	-0.683013	4.022316	-1.375354
9	-2.736144	3.554466	-2.915907
6	-1.082757	3.002828	-1.237907
1	-0.346606	1.172270	-0.786456
6	-2.071191	3.107516	-0.050264
9	-1.389855	3.462520	1.069383
9	-2.695645	1.933511	0.216550
9	-3.029082	4.045928	-0.253167
6	-1.781884	2.653411	-2.574787

[**4/3g**] - PhCl/HFIP/benzo[h]quinoline_OH-N - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

6	0.045395	-2.096876	3.321580
6	0.088725	-0.039847	1.938269
6	0.180596	-0.674621	3.215781
6	-0.150394	-2.871997	2.216797
6	-0.501118	-2.456594	-1.477853
6	-0.432946	-1.056314	-1.530903
7	-0.277238	-0.283783	-0.457311
6	-0.155344	-0.862608	0.768853
6	-0.248778	-2.280286	0.917822
6	-0.423279	-3.066136	-0.240650
6	0.433265	0.113664	4.363663
1	-0.623962	-3.032823	-2.394634
1	-0.512918	-0.535301	-2.488553
1	0.798199	2.078990	5.155797
6	0.280058	1.357542	1.862953
1	-0.483568	-4.152019	-0.142913
6	0.528544	2.105566	3.001294
6	0.602197	1.483101	4.262710
1	-0.228673	-3.957842	2.299763
1	0.499222	-0.382268	5.334676
1	0.121014	-2.552480	4.311383
1	0.672837	3.184005	2.916713
1	0.251638	1.854297	0.895804
6	3.245421	-2.376871	0.455960
6	3.447526	-1.699564	1.659757
6	3.548697	-0.307064	1.640832
6	3.447126	0.394540	0.436990
6	3.245266	-0.300901	-0.757225
6	3.144519	-1.694360	-0.757039
1	3.508223	-2.254133	2.595875
1	3.686741	0.230837	2.580200
1	3.508956	1.483427	0.432173
1	3.150455	0.241321	-1.699359
1	2.975324	-2.245134	-1.682088
17	3.098834	-4.120393	0.470767
9	-1.690781	1.734706	-3.747105

9	-2.905225	0.866166	-2.152851
8	-0.339925	2.213005	-1.403734
1	-1.383739	3.802247	-2.108897
9	-3.501029	2.759124	-3.077241
6	-1.565641	2.821126	-1.638271
1	-0.416093	1.286748	-0.956740
6	-2.323353	3.126367	-0.322657
9	-1.562917	3.936555	0.456025
9	-2.585756	2.006696	0.394642
9	-3.501720	3.762618	-0.538517
6	-2.434679	2.037069	-2.654139

[**4/3h**] - PhCl/HFIP/dioxane_OH-O - PBE-D3(BJ)/def2-TZVP_PhCl solution phase

8	-0.129664	-2.826882	-0.112649
6	0.117618	-0.518146	-0.849882
6	0.577909	-1.955497	-1.022726
6	0.044517	-2.380469	1.249687
6	-0.409064	-0.938293	1.401384
8	0.297121	-0.079092	0.500426
1	-1.499434	-0.866065	1.216542
1	-0.948615	-0.426768	-1.138093
1	0.715551	0.151681	-1.484063
1	1.660305	-2.041779	-0.827366
1	0.361782	-2.323998	-2.035127
1	1.109336	-2.480254	1.522186
1	-0.555530	-3.054764	1.876309
1	-0.195968	-0.576374	2.417123
6	3.810366	-1.123552	1.126990
6	3.705754	-0.027246	0.269586
6	4.030860	-0.192023	-1.078695
6	4.450549	-1.435292	-1.560916
6	4.546979	-2.521832	-0.687423
6	4.227654	-2.373277	0.665101
1	3.360076	0.932824	0.650894
1	3.948469	0.660414	-1.755086
1	4.699202	-1.557825	-2.615917
1	4.869790	-3.496917	-1.055668
1	4.296779	-3.215773	1.353260
17	3.392644	-0.932253	2.814100
9	-2.586645	-3.914458	-3.427059
9	-1.058401	-4.934818	-2.246541
8	-2.711696	-3.051367	-0.786909
1	-4.195879	-4.284650	-1.420128
9	-2.861996	-6.009834	-2.871065
6	-3.126766	-4.328882	-1.156695
1	-1.736099	-3.048770	-0.541866
6	-3.023517	-5.320055	0.027291
9	-3.759499	-4.853589	1.065867
9	-1.748534	-5.461893	0.469071
9	-3.493245	-6.552156	-0.283233
6	-2.397408	-4.815575	-2.432011

[**3a**] - HFIP/1-methyl-4-(methylsulfinyl)benzene_OH-S - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

F	-2.50760123	0.02552363	3.58573274
C	-2.14720777	2.38448406	3.95844489
H	-1.69066537	3.74335809	2.61208676
C	-0.72775357	2.25994768	4.56196358
F	-0.57340510	3.19763818	5.53350652
F	0.23354792	2.47493771	3.62515384
F	-0.50622149	1.04349723	5.12430235
C	-2.51433427	1.24068361	2.98345528
F	-3.76952957	1.45107027	2.49922636
F	-1.67086475	1.18581554	1.91428136
O	-2.32917488	3.64165373	3.36567855
H	-2.85102228	2.30431576	4.79992589
H	-2.06410728	2.50322427	-0.61651923
O	0.15004524	4.43318707	-0.33722285
S	-1.13868672	4.42651318	0.44133682
H	-3.41504248	5.68910405	1.82355837
H	-3.35994841	3.63462674	-0.07355568
C	-2.38344658	3.55151333	-0.56868910
H	-2.39815927	4.01146293	-1.56426215
C	-1.87773765	6.07938844	0.33880099
C	-1.27868372	7.01259025	-0.50121193
C	-1.81121468	8.30295304	-0.56719826
C	-2.92491029	8.66882740	0.20213935
C	-3.49555034	7.70672276	1.05529461
C	-2.97537268	6.41691751	1.13777026
H	-0.40241153	6.71764854	-1.07995492
H	-1.34847298	9.04122471	-1.22616195
H	-3.01329669	10.65432313	-0.65235484
H	-4.35533859	7.97724770	1.67269434
C	-3.48787063	10.06607969	0.14259194
H	-4.57129057	10.05022708	-0.04227158
H	-3.32807151	10.59436718	1.09446988

[**3a**] - HFIP/1-methyl-4-(methylsulfinyl)benzene_OH-O - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

F	1.73342064	-0.13877913	2.02611217
C	2.53346354	1.67731784	0.63982344
H	1.75347928	3.47224335	0.22439150
C	2.18101915	1.02514950	-0.71938865
F	3.10752806	1.38105735	-1.64548017
F	0.96334794	1.42466822	-1.19069387
F	2.16650660	-0.33519165	-0.65661375
C	1.61820417	1.19910759	1.79753375
F	1.96822805	1.83743827	2.94270391
F	0.29783218	1.46301199	1.57151126
O	2.61070519	3.06163610	0.55832165
H	3.53527515	1.29409461	0.89391262
H	-1.51173188	2.48821013	-1.27787824
O	0.49910128	4.42713255	-0.36212159
S	-0.85881288	4.15989016	0.28571512
H	-3.10790864	4.99126022	1.90202700
H	-2.93829648	3.42851798	-0.68797150
C	-1.90329317	3.48714745	-1.04991647
H	-1.82250592	4.15448974	-1.91668812

C	-1.69176360	5.75436628	0.44953667
C	-1.22184037	6.85984507	-0.25392369
C	-1.87339036	8.08508480	-0.09644939
C	-2.97790694	8.21807094	0.75889816
C	-3.41556473	7.08684967	1.46921220
C	-2.77387578	5.85831633	1.32826927
H	-0.34881360	6.75154836	-0.89853226
H	-1.51394959	8.95757653	-0.64655851
H	-3.34020921	10.27352343	0.18863153
H	-4.26351206	7.17399767	2.15237496
C	-3.66506657	9.54673079	0.94324661
H	-4.75672812	9.44259062	0.87463912
H	-3.43976825	9.96822907	1.93459100

[**3b**] - HFIP/1-(cyclopropylsulfinyl)-4-methylbenzene_OH-S - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

F	-3.68856436	1.22032569	3.89788043
C	-1.67435824	2.53326775	4.16320269
H	-0.99814173	3.97943877	3.00496783
C	-0.69075134	1.44681112	3.66564514
F	0.47164599	1.54478250	4.35933943
F	-0.39553402	1.59926876	2.34468605
F	-1.17326053	0.18839622	3.84301572
C	-3.10076362	2.39893734	3.57765901
F	-3.88396129	3.39663698	4.06875366
F	-3.11274209	2.51605469	2.21484574
O	-1.15858071	3.81857000	3.97160053
H	-1.78111552	2.37408437	5.24699934
C	-5.06004483	8.89416029	-0.47939141
O	0.62745031	5.37292842	0.35544284
S	-0.69294406	4.82482534	0.83714967
H	-3.41631156	5.16316496	1.84228153
H	-6.06168322	8.44597155	-0.43996984
H	0.02499204	4.46965871	-1.95021905
H	-5.03975366	9.71707489	0.25184353
C	-1.99157755	6.02355658	0.45107733
C	-1.72602059	7.02797833	-0.47691729
C	-2.73071866	7.94684344	-0.78318057
C	-3.99070209	7.87829965	-0.16696386
C	-4.22106729	6.86273270	0.77642250
C	-3.22720381	5.93833800	1.09719106
H	-0.73725712	7.08198793	-0.93368175
H	-2.53394801	8.73418655	-1.51476650
H	-4.91588711	9.33342021	-1.47475380
H	-5.19160118	6.79964280	1.27385049
C	-1.19779462	3.54819427	-0.35695632
C	-0.13419770	2.58301159	-0.79875322
C	-0.65328946	3.63878477	-1.75118924
H	-2.21587365	3.19916050	-0.17883719
H	-0.42983639	1.54268075	-0.93146685
H	0.87233959	2.74492555	-0.41047407
H	-1.31647202	3.35148426	-2.56639223

[**3b**] - HFIP/1-(cyclopropylsulfinyl)-4-methylbenzene_OH-O - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

F	2.42539316	0.53933829	2.44196163
C	2.40637403	1.46188864	0.20847293
H	1.69979844	3.27376992	-0.26511728
C	1.29486961	0.51431797	-0.31090784
F	1.47041084	0.31260527	-1.64678923
F	0.04413807	1.02751815	-0.14225716
F	1.32445376	-0.70592824	0.28890796
C	2.34284127	1.70151742	1.73575583
F	3.39079925	2.48051010	2.11155590
F	1.20215384	2.33660486	2.11651814
O	2.45163936	2.65007284	-0.51467621
H	3.34943493	0.91866905	0.03544496
C	-4.24244254	8.88703112	1.54646966
O	0.59012019	4.52697246	-0.16042745
S	-0.86929081	4.06777226	-0.09279939
H	-3.57128500	4.29540396	0.86894667
H	-5.27819380	8.79019501	1.19399715
H	0.11135845	5.40273830	-2.50283460
H	-4.27652707	8.96217033	2.64426939
C	-1.84627433	5.50978645	0.37476034
C	-1.28994342	6.78508835	0.32799260
C	-2.07744199	7.87660722	0.69973686
C	-3.40630122	7.70784506	1.11912690
C	-3.93373617	6.40625381	1.16690342
C	-3.15906920	5.30490962	0.80786750
H	-0.25176726	6.90379380	0.01705456
H	-1.65091524	8.88170879	0.66475047
H	-3.83272998	9.82916204	1.16157255
H	-4.96250573	6.25325165	1.50090505
C	-1.42150924	3.96277953	-1.82401121
C	-0.49709637	3.29345976	-2.80353942
C	-0.71794929	4.78985342	-2.85857872
H	-2.49872327	3.79541067	-1.88743714
H	-0.95486382	2.65390794	-3.55777585
H	0.47523884	2.96160812	-2.43717254
H	-1.32557530	5.21864146	-3.65481636

[**3c**] - HFIP/2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl_OH-S - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

C	3.27137763	4.47606054	-2.72835609
O	-0.56664646	0.95793128	1.52289532
S	-1.08783867	2.23736658	0.92637284
H	-1.04368516	4.54943917	-0.89417923
H	2.89492664	4.68353323	-3.74021051
H	3.65491031	5.42511323	-2.32399991
H	-1.65086106	1.49724407	-4.62166391
C	0.16661391	2.88284051	-0.21074146
C	1.39866554	2.24028788	-0.25577418
C	2.39934449	2.75806413	-1.08218616
C	2.18580185	3.91334568	-1.84617430
C	0.93489931	4.55153444	-1.76126485
C	-0.07492316	4.04884496	-0.94517481
H	1.54745859	1.33711599	0.33595747
H	3.36365180	2.24797577	-1.13767723

H	4.11662205	3.78181158	-2.81267775
H	0.74950885	5.45473681	-2.34756210
C	-2.43533322	1.97479646	-0.27590611
C	-3.61018504	2.66245289	0.05336231
C	-4.71430671	2.61372219	-0.79767361
C	-4.63587355	1.86653910	-1.97371014
C	-3.46483790	1.17491703	-2.29051845
C	-2.33638969	1.20585047	-1.45585042
H	-3.65695948	3.24537356	0.97436212
H	-5.62703996	3.15031112	-0.53722878
H	-5.49379770	1.81146305	-2.64573966
H	-3.41753951	0.57603474	-3.20105245
C	-1.12416962	0.42426026	-1.82752405
C	-0.70113117	-0.61526549	-0.98471378
C	0.41157069	-1.39119301	-1.30510605
C	1.11935843	-1.12903925	-2.47872757
C	0.70168360	-0.09895041	-3.32270076
C	-0.41994686	0.68768095	-3.02589854
H	-1.24708045	-0.80184346	-0.06212098
H	0.72430491	-2.19169937	-0.63389572
H	1.99635820	-1.72431418	-2.73869722
H	1.26300054	0.11309871	-4.23572387
C	-0.81769228	1.79763458	-3.96790767
H	-1.13920236	2.69381049	-3.42045718
H	0.02665374	2.07099671	-4.61370913
F	-4.16706123	2.00146906	5.37628139
C	-2.76200107	3.68053926	4.35216877
H	-1.94016993	3.64280494	2.56263449
C	-1.46761978	3.30784005	5.11278140
F	-0.75193830	4.44021456	5.35208737
F	-0.68399480	2.46959645	4.38854253
F	-1.72094823	2.72190726	6.31276894
C	-3.75176286	2.50229710	4.18454450
F	-4.85974100	2.94900158	3.52386376
F	-3.22378124	1.48682261	3.45591232
O	-2.46720742	4.27715813	3.11712166
H	-3.28162000	4.42711242	4.97053566

[**3c**] - HFIP/2-methyl-2'-(p-tolylsulfinyl)-1,1'-biphenyl_OH-O - ZORA-GGAPBE-D3(BJ)/TZP_gas phase

C	3.23383459	4.35798062	-2.54551103
O	0.30179651	-0.55054529	0.92518649
S	-0.29495961	0.85445547	0.99816730
H	-0.53573247	3.63249250	0.15178897
H	2.66958573	5.16749296	-3.02707925
H	4.01136755	4.82549419	-1.92137768
H	-2.29003782	2.17113110	-4.02964575
C	0.69286823	1.86679544	-0.12626743
C	1.83779136	1.31844508	-0.69717940
C	2.64688825	2.13059452	-1.49376460
C	2.33506499	3.48111484	-1.71113222
C	1.18052787	4.00699114	-1.10703313
C	0.35985449	3.21211579	-0.30973102
H	2.06620403	0.26659777	-0.52744935
H	3.53636697	1.70176003	-1.96106904

H	3.74420718	3.77882920	-3.32604638
H	0.91970072	5.05598775	-1.26480209
C	-1.90274629	0.94237208	0.15310108
C	-2.92659266	1.38056989	1.00255347
C	-4.22120879	1.54748545	0.51386744
C	-4.48209488	1.26718966	-0.82840342
C	-3.45783365	0.82436955	-1.66775956
C	-2.14484732	0.64614056	-1.20469605
H	-2.69845215	1.58693590	2.04946951
H	-5.01759660	1.88296981	1.17861171
H	-5.49196870	1.38276671	-1.22478252
H	-3.67378956	0.58906103	-2.71095690
C	-1.09655225	0.14246124	-2.13503645
C	-0.51835037	-1.11368288	-1.89750745
C	0.45082463	-1.62915640	-2.75700817
C	0.85379421	-0.88525203	-3.86699610
C	0.27656001	0.36205139	-4.11177774
C	-0.70666385	0.89556693	-3.26721173
H	-0.83119425	-1.68372774	-1.02529081
H	0.88904721	-2.60672472	-2.55320654
H	1.61643201	-1.27418233	-4.54386411
H	0.59907351	0.94759481	-4.97602983
C	-1.29373033	2.25257576	-3.56866513
H	-1.40634334	2.85267906	-2.65542635
H	-0.64917369	2.80260248	-4.26610321
F	-3.20585550	-2.33578046	4.19252249
C	-1.17988202	-2.94630692	2.99776472
H	0.08362493	-1.70127017	2.09953905
C	-2.01167406	-3.28434745	1.73244073
F	-1.24915522	-3.99737713	0.86101437
F	-2.45689213	-2.17954108	1.07459690
F	-3.09840621	-4.04755947	2.03871771
C	-1.91500318	-1.97403024	3.95422738
F	-1.27082882	-1.94991610	5.15190499
F	-1.92741157	-0.69516971	3.47928355
O	0.10461669	-2.49769636	2.71602194
H	-1.09944082	-3.89604565	3.55072458