Crystallograhic Information for 1,1,1-Trifluoro-3-(octane-1-sulfonyl)-propan-2,2-diol (26)

Table 11. Crystal data and structure refinement for $OTFPdOHSO_2$.

Identification code	mn1104	
Empirical formula	C11 H21 F3 O4 S	
Formula weight	306.34	
Temperature	130(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 31.750(5) Å	α= 90°.
	b = 5.3684(8) Å	β= 106.583(14)°.
	c = 18.409(3) Å	γ = 90°.
Volume	3007.3(8) $Å^3$	
Z	8	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	2.310 mm^{-1}	
F(000)	1296	
Crystal size	0.80 x 0.16 x 0.02 mm^3	
Crystal color and habit	colorless plate	
Diffractometer	Siemens P4	
θ range for data collection	1.45 to 55.80°.	
Index ranges	-34≤h≤32, 0≤k≤5, 0≤l≤19	
Reflections collected	4528	
Independent reflections	3888 [R(int) = 0.0319]	
Observed reflections (I > 2σ(I))	2888	
Completeness to θ = 55.80°	100.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9553 and 0.2594	
Solution method	SHELXS-97 (Sheldrick, 1990)	
Refinement method	SHELXL-97 (Sheldrick, 1997) Full-matrix least-squares on F^2	
Data / restraints / parameters	3888 / 4 / 361	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2σ(I)]	R1 = 0.0453, wR2 = 0.1089	
R indices (all data)	R1 = 0.0667, wR2 = 0.1242	
Largest diff. peak and hole	0.498 and -0.310 $e.Å^{-3}$	

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $OTFPdOHSO_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4825(1)	8150(2)	3547(1)	23(1)
F(1)	6003(1)	3248(4)	3896(1)	47(1)
F(2)	6214(1)	3519(5)	5114(1)	49(1)
F(3)	6303(1)	6627(5)	4430(1)	48(1)
O(1)	5301(1)	3719(5)	4460(1)	31(1)
O(2)	5655(1)	7170(5)	5134(1)	32(1)
O(3)	4747(1)	8872(4)	4261(1)	28(1)
O(4)	4752(1)	10006(4)	2960(1)	29(1)
C(1)	6030(1)	4783(8)	4482(2)	35(1)
C(2)	5576(1)	5769(7)	4471(2)	26(1)
C(3)	5386(1)	7252(7)	3745(2)	26(1)
C(4)	4504(1)	5515(7)	3183(2)	28(1)
C(5)	4015(1)	6116(7)	2917(2)	32(1)
C(6)	3753(1)	3822(7)	2557(2)	35(1)
C(7)	3268(1)	4300(8)	2197(2)	41(1)
C(8)	3023(1)	1997(8)	1810(2)	42(1)
C(9)	2539(1)	2435(9)	1412(3)	54(1)
C(10)	2294(1)	117(9)	1028(3)	54(1)
C(11)	2437(2)	-776(11)	346(3)	85(2)
S(2)	130(1)	1993(2)	1439(1)	22(1)
F(4)	-1279(1)	6151(5)	-251(1)	51(1)
F(5)	-1119(1)	6489(5)	966(1)	49(1)
F(6)	-1352(1)	2998(5)	428(1)	54(1)
O(5)	-375(1)	6352(5)	499(1)	31(1)
O(6)	-656(1)	2765(5)	-171(1)	31(1)
O(7)	209(1)	228(4)	2051(1)	27(1)
O(8)	215(1)	1179(4)	742(1)	25(1)
C(12)	-1098(1)	4953(8)	403(2)	37(1)
C(13)	-626(1)	4201(6)	470(2)	25(1)
C(14)	-437(1)	2809(7)	1220(2)	26(1)
C(15)	436(1)	4715(6)	1767(2)	25(1)

C(16)	927(1)	4191(7)	2045(2)	31(1)
C(17)	1175(1)	6612(7)	2282(2)	31(1)
C(18)	1664(1)	6305(7)	2625(2)	35(1)
C(19)	1897(1)	8765(7)	2893(2)	36(1)
C(20)	2387(1)	8532(7)	3273(2)	38(1)
C(21)	2602(1)	11009(8)	3559(2)	46(1)
C(22)	3092(1)	10788(10)	3956(3)	65(1)

Table 13. Bond lengths [Å] and angles [°] for $OTFPdOHSO_2$.

S(1)-O(4)	1.439(2)	S(2)-O(7)	1.438(2)
S(1)-O(3)	1.456(2)	S(2)-O(8)	1.451(2)
S(1)-C(4)	1.761(3)	S(2)-C(15)	1.763(3)
S(1)-C(3)	1.779(3)	S(2)-C(14)	1.782(3)
F(1)-C(1)	1.341(4)	F(4)-C(12)	1.340(4)
F(2)-C(1)	1.331(4)	F(5)-C(12)	1.341(4)
F(3)-C(1)	1.338(4)	F(6)-C(12)	1.333(4)
O(1)-C(2)	1.400(4)	O(5)-C(13)	1.394(4)
O(2)-C(2)	1.394(4)	O(6)-C(13)	1.390(4)
C(1)-C(2)	1.530(5)	C(12)-C(13)	1.523(5)
C(2)-C(3)	1.526(5)	C(13)-C(14)	1.534(5)
C(4)-C(5)	1.521(5)	C(15)-C(16)	1.523(5)
C(5)-C(6)	1.528(5)	C(16)-C(17)	1.518(5)
C(6)-C(7)	1.515(5)	C(17)-C(18)	1.509(5)
C(7)-C(8)	1.526(5)	C(18)-C(19)	1.525(5)
C(8)-C(9)	1.521(5)	C(19)-C(20)	1.518(5)
C(9)-C(10)	1.529(6)	C(20)-C(21)	1.518(5)
C(10)-C(11)	1.529(6)	C(21)-C(22)	1.524(5)

O(4)-S(1)-O(3)	117.44(14)	O(1)-C(2)-C(3)	107.9(3)
O(4)-S(1)-C(4)	108.61(16)	O(2)-C(2)-C(1)	103.9(3)
O(3)-S(1)-C(4)	109.19(15)	O(1)-C(2)-C(1)	108.0(3)
O(4)-S(1)-C(3)	106.10(15)	C(3)-C(2)-C(1)	109.1(3)
O(3)-S(1)-C(3)	107.75(15)	C(2)-C(3)-S(1)	116.3(2)
C(4)-S(1)-C(3)	107.29(16)	C(5)-C(4)-S(1)	112.2(3)
F(2)-C(1)-F(3)	107.9(3)	C(4)-C(5)-C(6)	110.4(3)
F(2)-C(1)-F(1)	107.6(3)	C(7)-C(6)-C(5)	114.4(3)
F(3)-C(1)-F(1)	106.9(3)	C(6)-C(7)-C(8)	112.7(3)
F(2)-C(1)-C(2)	111.4(3)	C(9)-C(8)-C(7)	114.2(3)
F(3)-C(1)-C(2)	111.8(3)	C(8)-C(9)-C(10)	114.0(4)
F(1)-C(1)-C(2)	111.1(3)	C(9)-C(10)-C(11)	113.8(4)
O(2)-C(2)-O(1)	113.2(3)	O(7)-S(2)-O(8)	117.37(14)
O(2)-C(2)-C(3)	114.4(3)	O(7)-S(2)-C(15)	108.80(15)

O(8)-S(2)-C(15)	109.20(15)
O(7)-S(2)-C(14)	106.14(14)
O(8)-S(2)-C(14)	107.67(14)
C(15)-S(2)-C(14)	107.17(16)
F(6)-C(12)-F(4)	107.5(3)
F(6)-C(12)-F(5)	107.1(3)
F(4)-C(12)-F(5)	107.2(3)
F(6)-C(12)-C(13)	112.4(3)
F(4)-C(12)-C(13)	111.0(3)
F(5)-C(12)-C(13)	111.4(3)
O(6)-C(13)-O(5)	113.1(3)
O(6)-C(13)-C(12)	104.5(3)
O(5)-C(13)-C(12)	108.7(3)
O(6)-C(13)-C(14)	114.1(3)
O(5)-C(13)-C(14)	107.2(3)
C(12)-C(13)-C(14)	109.0(3)
C(13)-C(14)-S(2)	115.8(2)
C(16)-C(15)-S(2)	111.9(2)
C(17)-C(16)-C(15)	109.7(3)
C(18)-C(17)-C(16)	114.5(3)
C(17)-C(18)-C(19)	112.8(3)
C(20)-C(19)-C(18)	114.6(3)
C(21)-C(20)-C(19)	112.8(3)
C(20)-C(21)-C(22)	113.2(4)

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $OTFPdOHSO_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	28(1)	21(1)	22(1)	-1(1)	7(1)	-1(1)
F(1)	47(1)	54(2)	43(1)	-9(1)	18(1)	13(1)
F(2)	43(1)	60(2)	41(1)	11(1)	9(1)	22(1)
F(3)	28(1)	64(2)	52(1)	-1(1)	12(1)	-8(1)
O(1)	33(1)	29(1)	28(2)	2(1)	7(1)	-5(1)
O(2)	32(2)	35(2)	27(1)	-5(1)	7(1)	3(1)
O(3)	35(1)	23(1)	25(1)	-1(1)	9(1)	1(1)
O(4)	36(1)	26(1)	27(1)	5(1)	10(1)	3(1)
C(1)	32(2)	42(2)	30(2)	-4(2)	8(2)	3(2)
C(2)	29(2)	27(2)	22(2)	-4(2)	7(2)	-3(2)
C(3)	29(2)	26(2)	25(2)	-2(2)	10(2)	-7(2)
C(4)	31(2)	24(2)	31(2)	-7(2)	11(2)	-4(2)
C(5)	30(2)	31(2)	34(2)	-1(2)	8(2)	1(2)
C(6)	30(2)	33(2)	44(2)	-10(2)	13(2)	-2(2)
C(7)	27(2)	38(2)	55(3)	-7(2)	8(2)	-4(2)
C(8)	27(2)	45(3)	54(3)	-12(2)	13(2)	-4(2)
C(9)	31(2)	53(3)	68(3)	0(3)	0(2)	-3(2)
C(10)	30(2)	63(3)	63(3)	-1(3)	2(2)	-6(2)
C(11)	93(4)	101(5)	58(3)	-17(3)	18(3)	-52(4)
S(2)	23(1)	20(1)	24(1)	-1(1)	8(1)	-1(1)
F(4)	33(1)	70(2)	46(1)	13(1)	5(1)	21(1)
F(5)	45(1)	60(2)	47(1)	-5(1)	20(1)	19(1)
F(6)	26(1)	66(2)	70(2)	5(1)	13(1)	-9(1)
O(5)	35(1)	30(1)	25(1)	6(1)	5(1)	-6(1)
O(6)	29(2)	34(2)	29(1)	-4(1)	6(1)	2(1)
O(7)	33(1)	24(1)	24(1)	4(1)	9(1)	2(1)
O(8)	31(1)	22(1)	24(1)	-4(1)	11(1)	-2(1)
C(12)	31(2)	42(2)	36(2)	5(2)	8(2)	3(2)
C(13)	23(2)	25(2)	28(2)	-3(2)	8(2)	-5(2)
C(14)	29(2)	24(2)	26(2)	-2(2)	11(2)	-7(2)
C(15)	22(2)	22(2)	30(2)	-3(2)	6(2)	-1(2)
C(16)	29(2)	30(2)	32(2)	0(2)	7(2)	-1(2)

C(17)	25(2)	29(2)	40(2)	-4(2)	9(2)	-3(2)
C(18)	28(2)	33(2)	44(2)	-5(2)	10(2)	-3(2)
C(19)	25(2)	34(2)	48(2)	-5(2)	8(2)	-2(2)
C(20)	26(2)	37(2)	46(2)	-2(2)	5(2)	-4(2)
C(21)	31(2)	47(3)	52(3)	-7(2)	3(2)	-9(2)
C(22)	39(3)	67(3)	73(3)	2(3)	-12(2)	-15(2)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $OTFPdOHSO_2$.

	x	y	z	U(eq)
H(1)	5367(14)	3310(80)	4916(9)	59(15)
H(2)	5431(8)	8010(60)	5120(20)	43(13)
H(3A)	5418	6247	3313	31
H(3B)	5564	8778	3770	31
H(4A)	4596	4837	2752	34
H(4B)	4556	4216	3580	34
H(5A)	3963	7487	2542	38
H(5B)	3916	6676	3353	38
H(6A)	3881	3157	2165	43
H(6B)	3785	2524	2951	43
H(7A)	3234	5652	1819	49
H(7B)	3134	4872	2592	49
H(8A)	3167	1382	1434	50
H(8B)	3048	674	2195	50
H(9A)	2513	3751	1025	65
H(9B)	2394	3056	1787	65
H(10A)	1975	482	859	65
H(10B)	2342	-1247	1404	65
H(11A)	2381	537	-40	128
H(11B)	2271	-2273	132	128
H(11C)	2752	-1164	507	128
H(5)	-410(11)	6850(60)	55(9)	22(10)
H(6)	-419(9)	2050(80)	-150(30)	74(17)
H(14A)	-609	1265	1207	31
H(14B)	-479	3858	1636	31
H(15A)	378	5952	1351	29
H(15B)	338	5443	2186	29
H(16A)	989	3032	2481	37
H(16B)	1025	3396	1636	37
H(17A)	1124	7706	1832	37
H(17B)	1053	7462	2654	37

H(18A)	1791	5550	2244	42
H(18B)	1718	5147	3060	42
H(19A)	1851	9891	2452	43
H(19B)	1759	9550	3254	43
H(20A)	2436	7363	3705	45
H(20B)	2530	7820	2907	45
H(21A)	2454	11738	3915	55
H(21B)	2559	12165	3124	55
H(22A)	3137	9730	4406	98
H(22B)	3214	12447	4110	98
H(22C)	3241	10045	3609	98

Table 16. Hydrogen bonds for OTFPdOHSO$_2$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(3)#1	0.835(10)	2.03(2)	2.778(3)	149(4)
O(1)-H(1)...S(1)#1	0.835(10)	3.16(2)	3.933(3)	155(4)
O(2)-H(2)...O(3)#2	0.837(10)	2.19(3)	2.864(3)	138(4)
O(2)-H(2)...O(3)	0.837(10)	2.34(3)	3.015(3)	138(3)
O(2)-H(2)...O(1)#1	0.837(10)	2.81(3)	3.363(3)	125(3)
O(2)-H(2)...S(1)	0.837(10)	2.99(4)	3.372(3)	111(3)
O(5)-H(5)...O(8)#3	0.837(10)	2.044(18)	2.812(3)	152(3)
O(5)-H(5)...S(2)#3	0.837(10)	3.184(16)	3.965(2)	156(3)
O(6)-H(6)...O(8)#4	0.836(10)	2.24(3)	2.898(3)	136(4)
O(6)-H(6)...O(8)	0.836(10)	2.25(3)	2.923(3)	137(4)
O(6)-H(6)...O(5)#3	0.836(10)	2.91(4)	3.528(3)	133(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y+2,-z+1 #3 -x,-y+1,-z

#4 -x,-y,-z

Table 17A. Purity Assessment

Compound No.	GC/EI-MS[a]	HPLC[b] C-18	HPLC[c] cyanopropyl	^{1}H NMR	Melting Point (°C)
6	>99	>98	>98	>97	N.A.[d]
7	>99	>98	>98	>97	85-87
8	>99	>98	>98	>97	N.A.
9	>99	>98	>98	>97	N.A.
10	>99	>98	>98	>97	N.A.
11	>99	>98	>98	>97	N.A.

[a]Data are shown as percent of the GC/MS total ion chromatogram (TIC). See the Experimental Section for a complete description of the GC/EI-MS methods.
[b]Percent purity is shown as determined by UV detection at 205 nm using a C-18 column as described in the Experimental section.
[c]Percent purity is shown as determined by UV detection at 205 nm using a cyanopropyl column as described in the Experimental section.
[d]N.A. indicates not applicable as the compound was an oil.

These data are for the six compounds that were used for correlation analysis. The GC/MS total ion chromatograms (TIC) and electron impact (EI) mass spectra are displayed in the following pages to support this information. The starting materials for the synthesis of all compounds listed are analyzable by GC/MS (volatile and thermally stabile). The TIC therefore shows no detectable presence of any starting materials. All NMR data (^{1}H NMR, ^{13}C NMR, and ^{19}F NMR) contained no detectable impurities and all data supported the assigned structures. As discussed in the next, it was not possible to obtain accurate elemental analyses for these compounds due to their hygroscopic nature. The ketones are highly hydrated, thus providing a large source of error in the mass percentage determinations. These results have been reported by other authors for compounds of similar structure.[1,2]

Table 17B. High Resolution Mass Spectrometry Results (negative mode)

Compound No	Elementary Composition	Theoretical Mass $(M-H)^+$ (Th)	Measured Mass $(M-H)^+$ (Th)	Error (mDa)	Error (ppm)
6	$C_9H_{15}F_3OS$	227.0718	227.0708	1.0	4.4
7	$C_9H_{15}F_3O_3S$	259.0616	259.0597	1.9	7.3
9	$C_9H_{18}O_3S$	205.0899	205.0913	1.4	6.8
10	$C_9H_{15}F_3O_2$	211.0946	211.0945	0.1	0.5

Table 17C. High Resolution Mass Spectrometry Results (positive mode)

Compound No	Elementary Composition	Theoretical Mass $(M-H)^+$ (Th)	Measured Mass $(M-H)^+$ (Th)	Error (mDa)	Error (ppm)
8	$C_9H_{18}OS$	175.1156	175.1113	4.3	25
11	$C_9H_{18}O_2$	159.1385	159.1407	2.2	14

High resolution mass spectrometry was performed on orthogonal time of flight mass spectrometer (LCT, Micromass UK Limited, Manchester, UK) equipped with a Z-flow electrospray ionization source using MassLynx 3.5 software. Sodium trifluoroacetate (Sigma, T0757) was used for external multipoint calibration. Mass accuracy was typically better than 10 ppm and resolution was typically better than 4500 FWHM. The flow rate applied was 25 μL/min. The experiment was performed either negative mode (Table 17B) or positive mode (Table 17C), with the following parameters: capillary 2880 V; sample cone 30 V, RF lens 250 V, extraction cone 10 V, acceleration 180 V, pusher cycle time 50/s, ion energy 30 V, reflectron 1794 V. Analog-digital converter was operated at 3.6 GHz frequency.

The resulting spectra are the averages of 20-40 consecutive spectra. MassLynx software was used for data processing and accurate mass measurement.

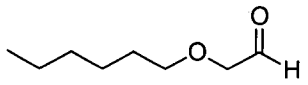
GC/EI-MS Spectral Data

The following pages provide the GC/EI-MS data for the compounds whose synthesis is described in the text. There are no data for compounds 1,1,1-trifluoro-3-(hexane-1-sulfonyl)-propan-2,2-diol (**7**) and 1,1,1-trifluoro-3-(octane-1-sulfonyl)-propan-2,2-diol (**26**) because the EI MS spectra of these two compounds have been previously reported by Wheelock et al.

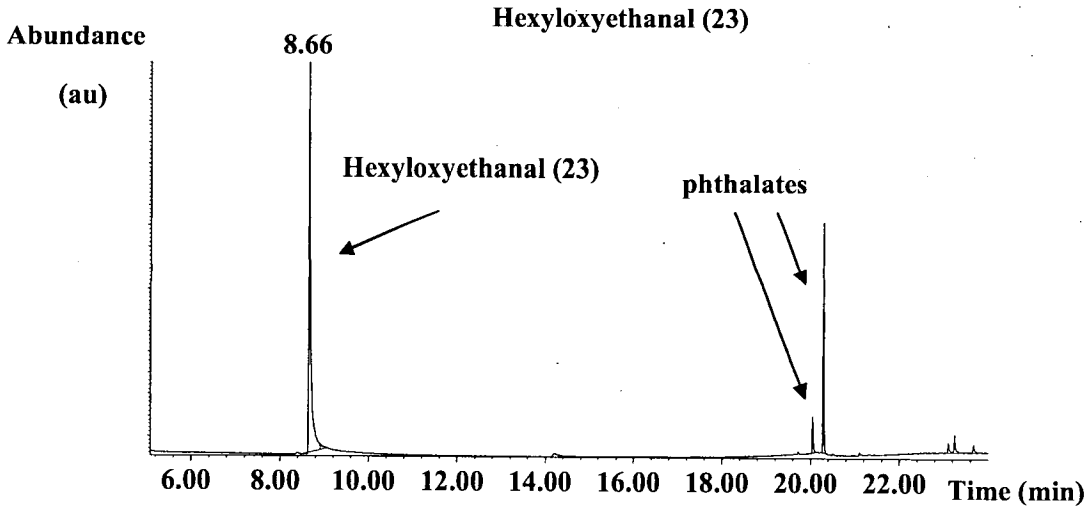
Structural characterization and purity was provided by GC/MS (Agilent Technologies; Engelwood, CO). For GC analysis, samples were analyzed on a HP 6890 GC equipped with a 30 m DB-17MS column (J&W Scientific; Folsom, CA) with a 0.25 mm internal diameter and a 0.25 μm film thickness with a He carrier gas at a flow rate of 0.8 mL/min. The injector temperature was 250°C and the initial column temperature was 50°C and was held for 5.00 min and then ramped at 15°C/min to 320°C and held for 2.00 min. The GC was interfaced with a HP 5973 MS that was run in full scan mode from 50-550 *m/z* with a quadrapole temperature of 186°C and a source temperature of 240°C.

All spectral data supported the reported structures.

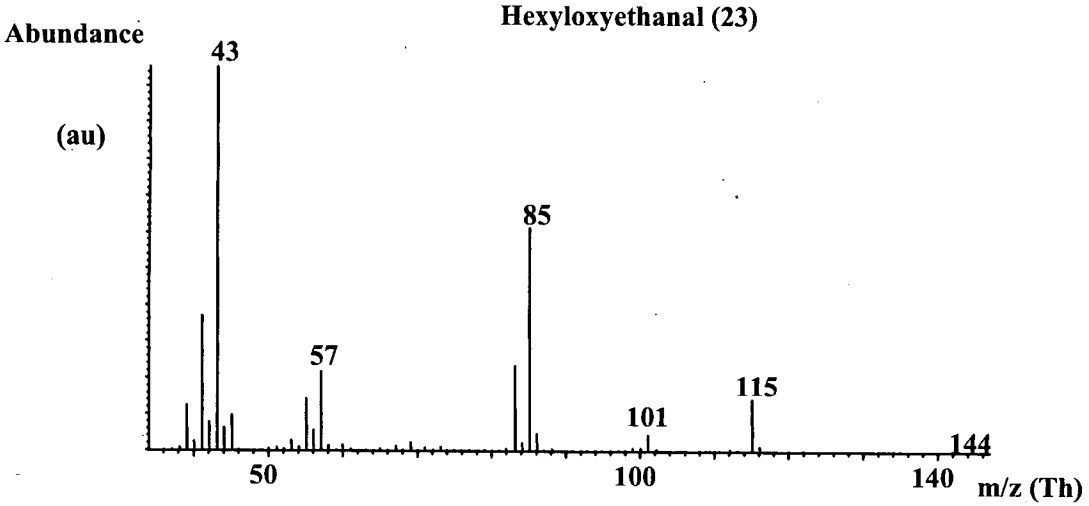
Hexyloxyethanal (23)



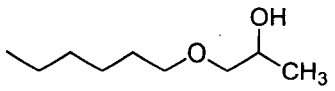
TIC



EI MS



1-Hexyloxy-propan-2-ol (24)



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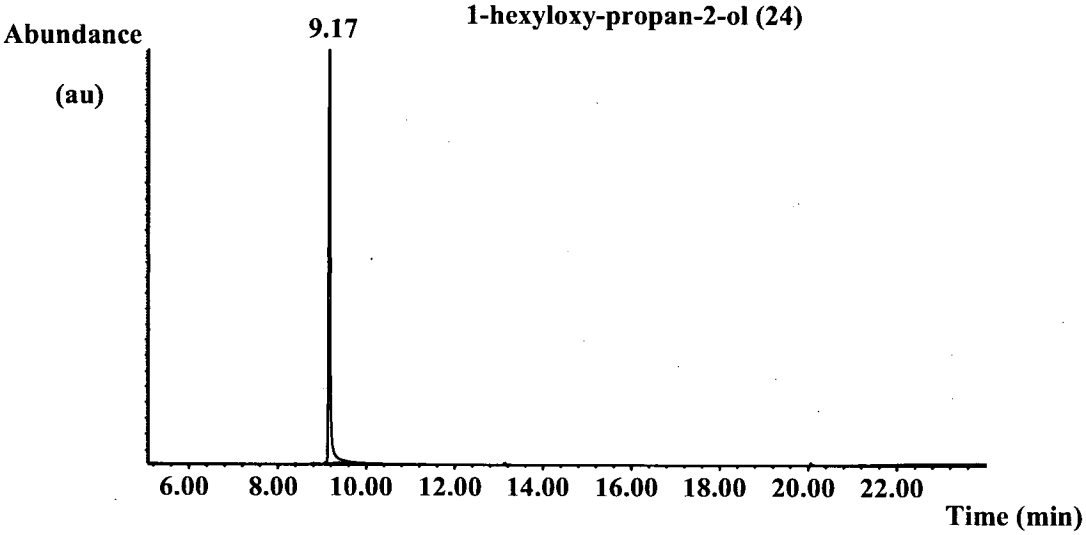

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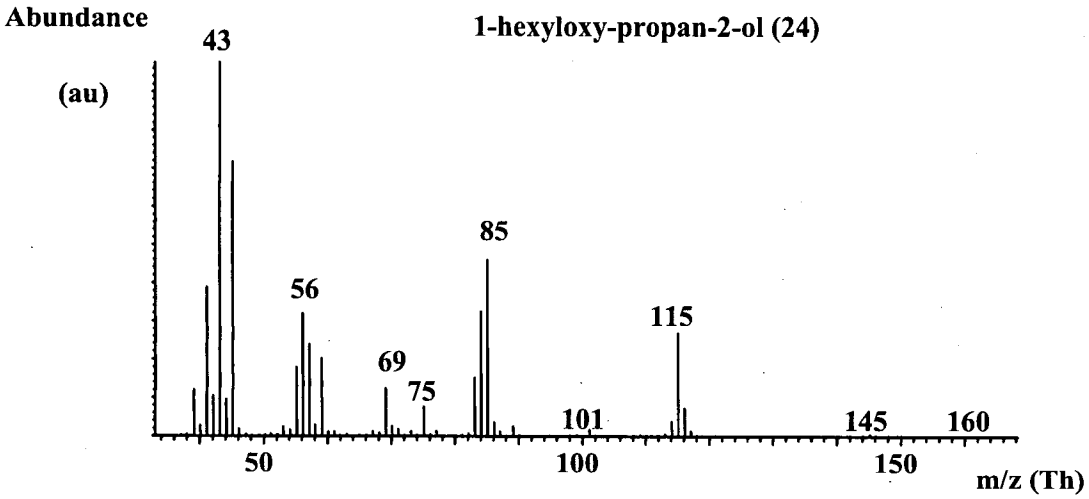
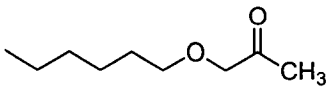


1-Hexyloxy-propan-2-one (11)



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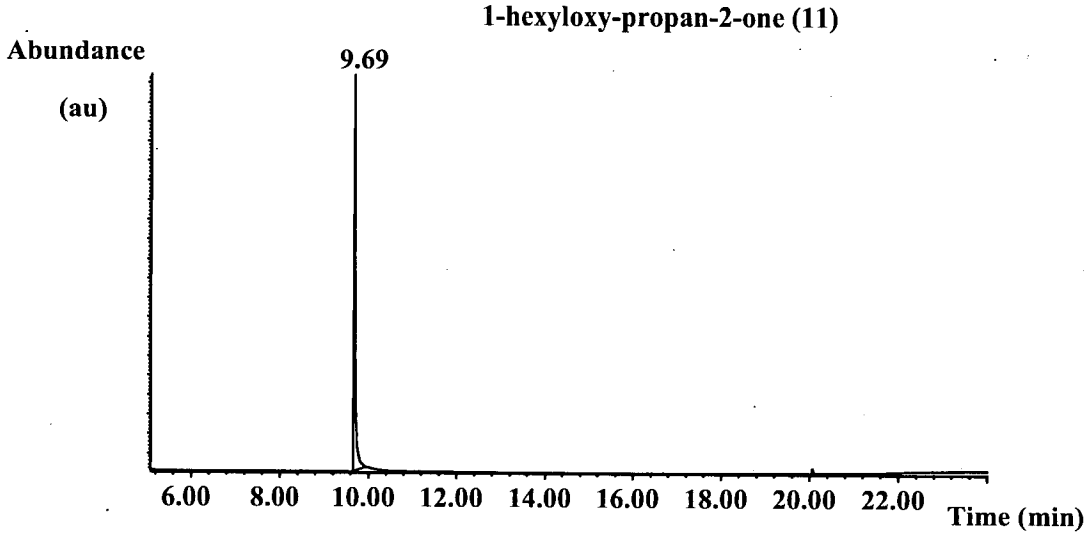

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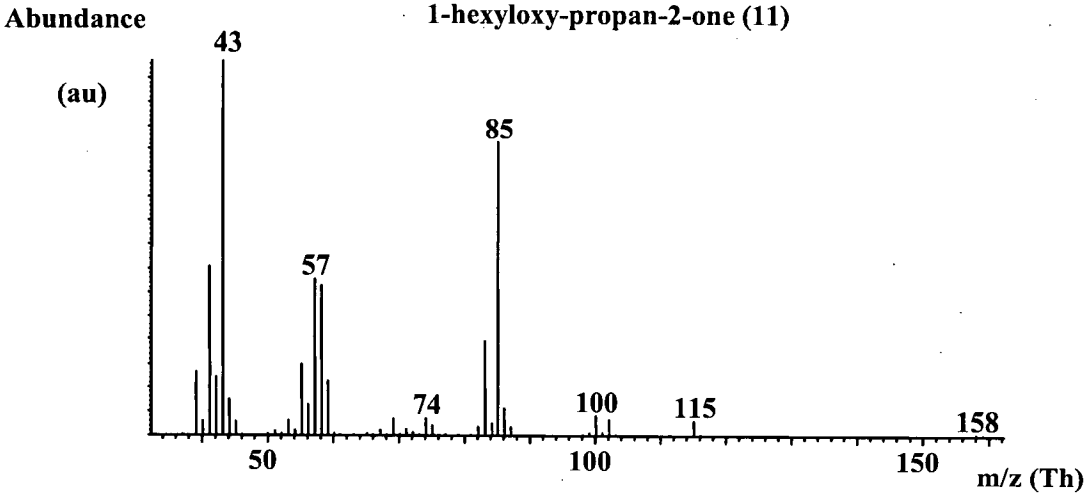
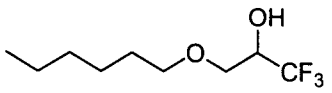


1,1,1-Trifluoro-3-hexyloxy-propan-2-ol (25)



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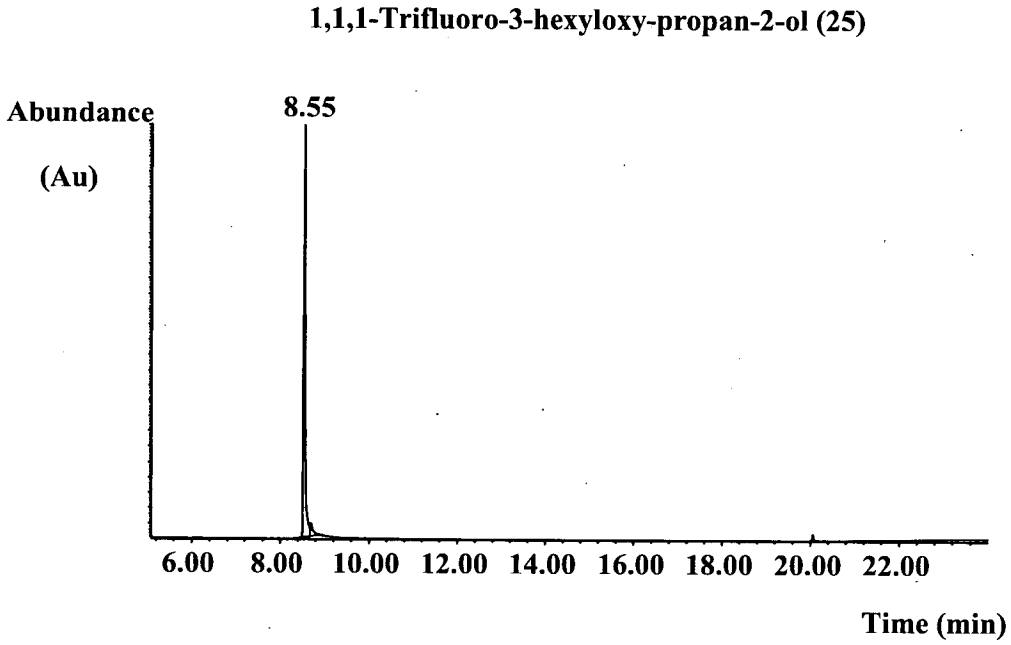

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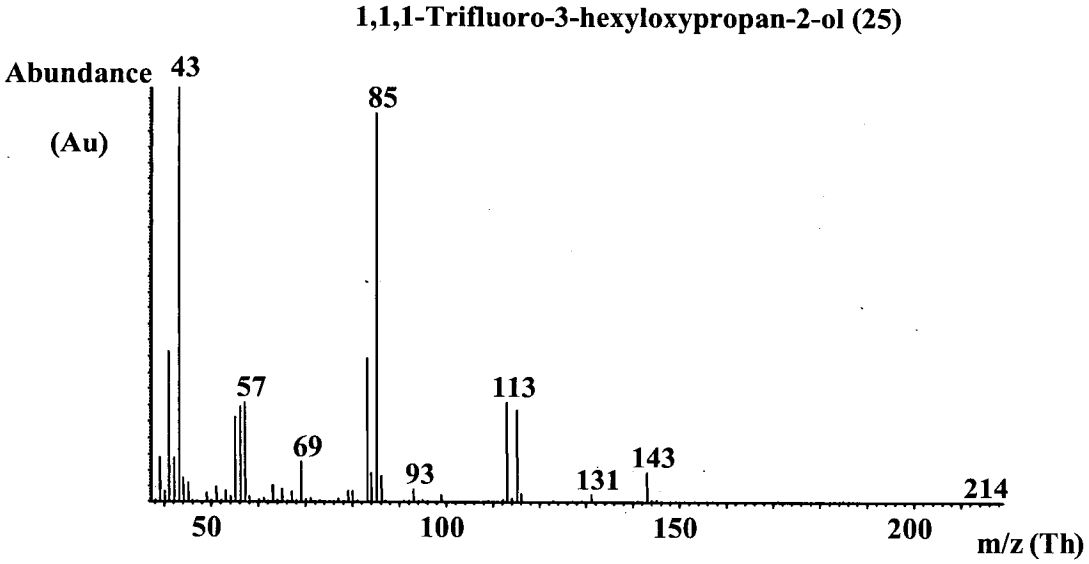

1,1,1-Trifluoro-3-hexyloxy-propan-2,2-diol

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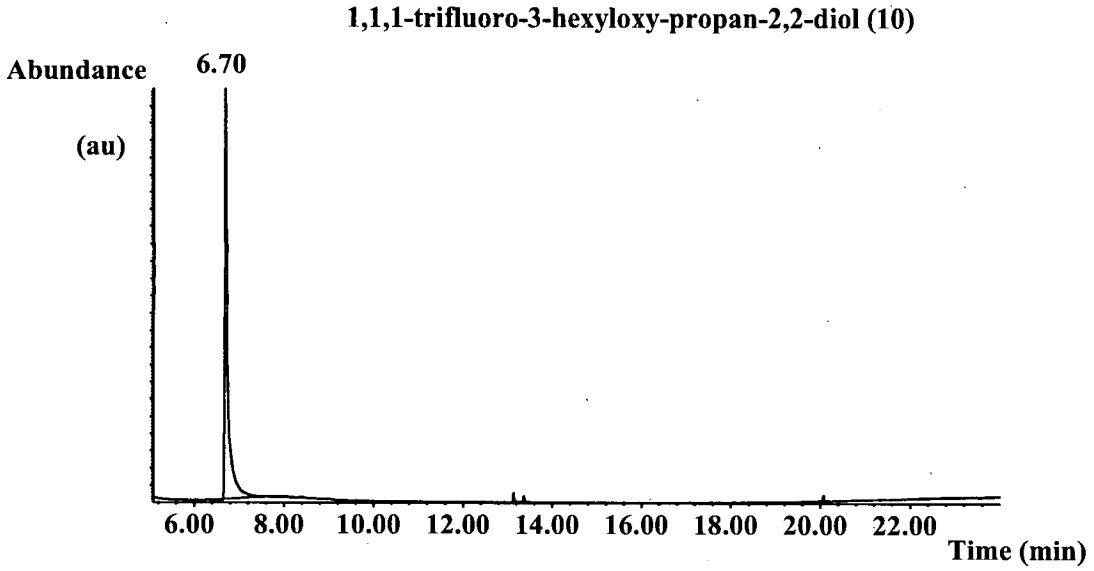

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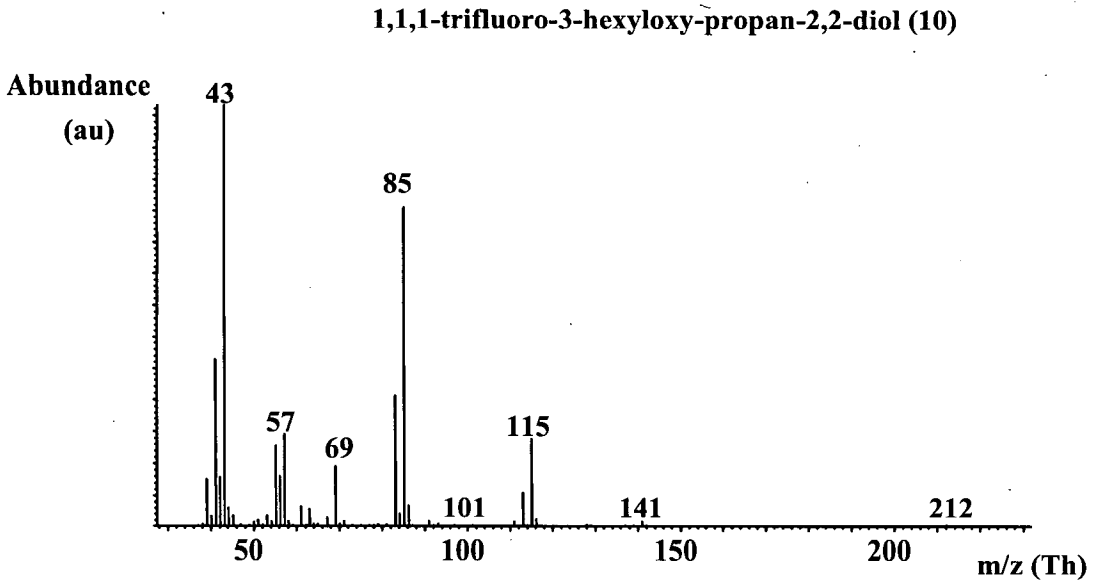
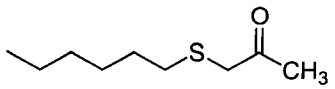


1-Hexylsulfanyl-propan-2-one (8)



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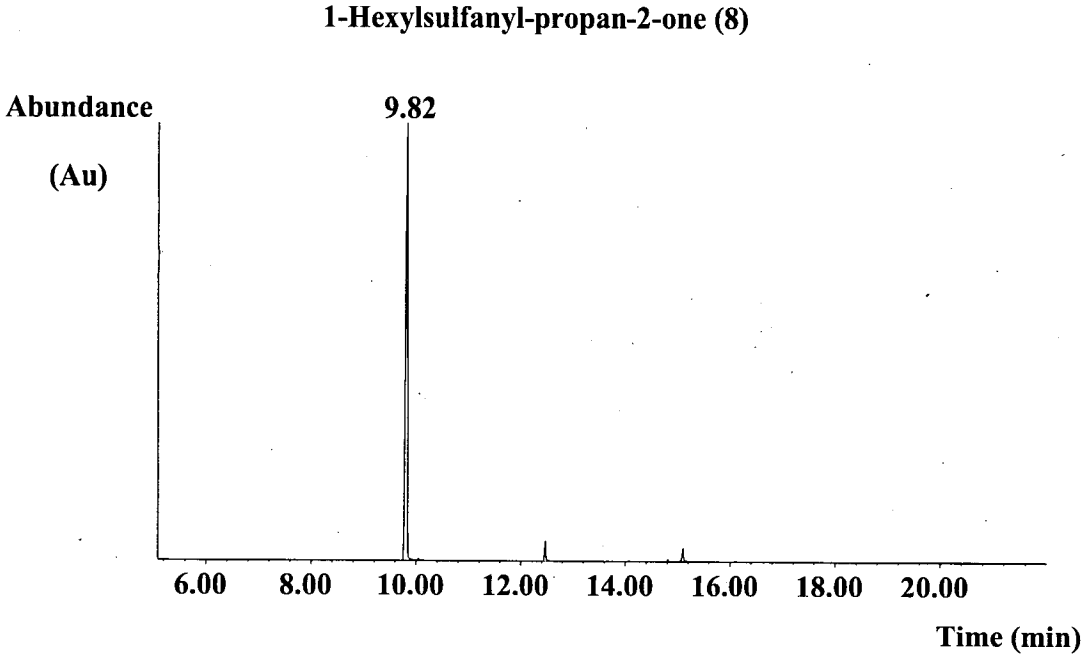

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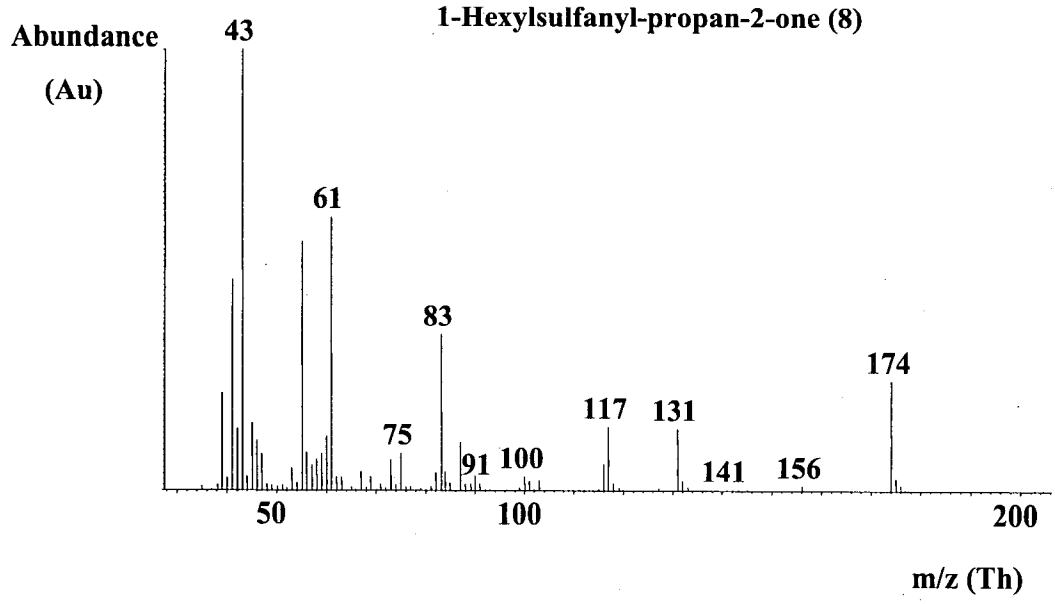
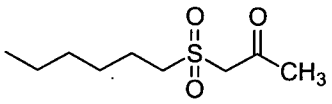


1-(Hexane-1-sulfonyl)-propan-2-one (9)



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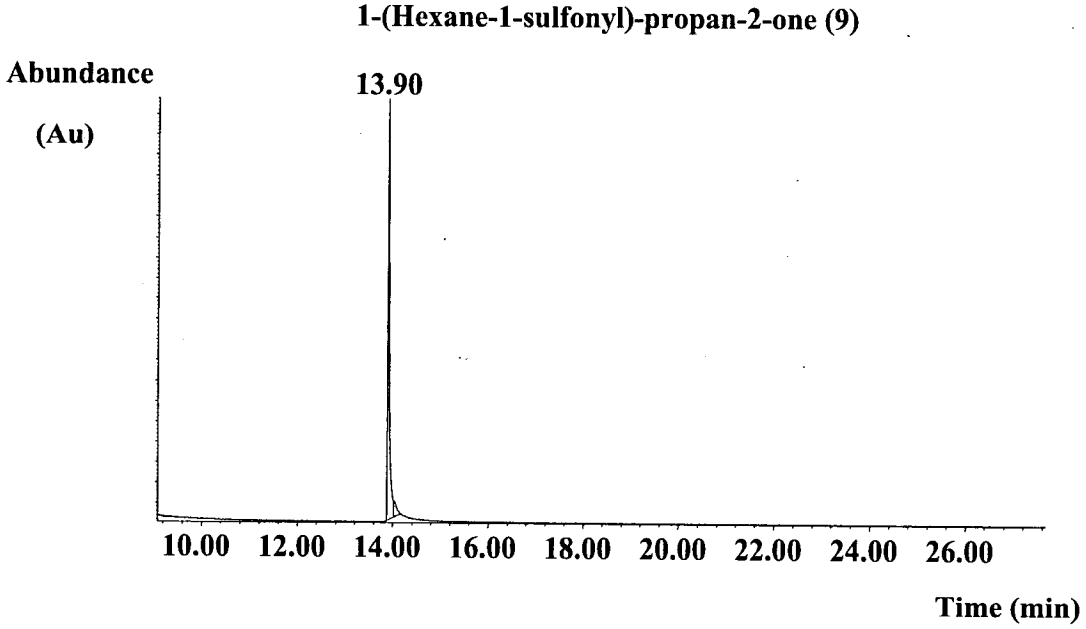

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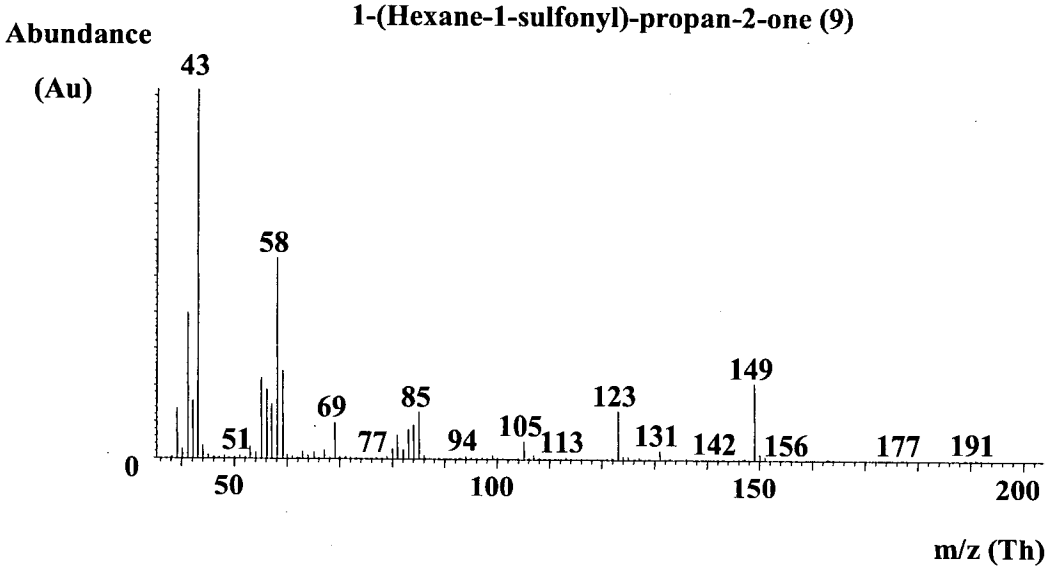
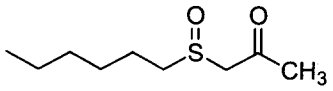


1-(Hexane-1-sulfinyl)-propan-2-one (13)



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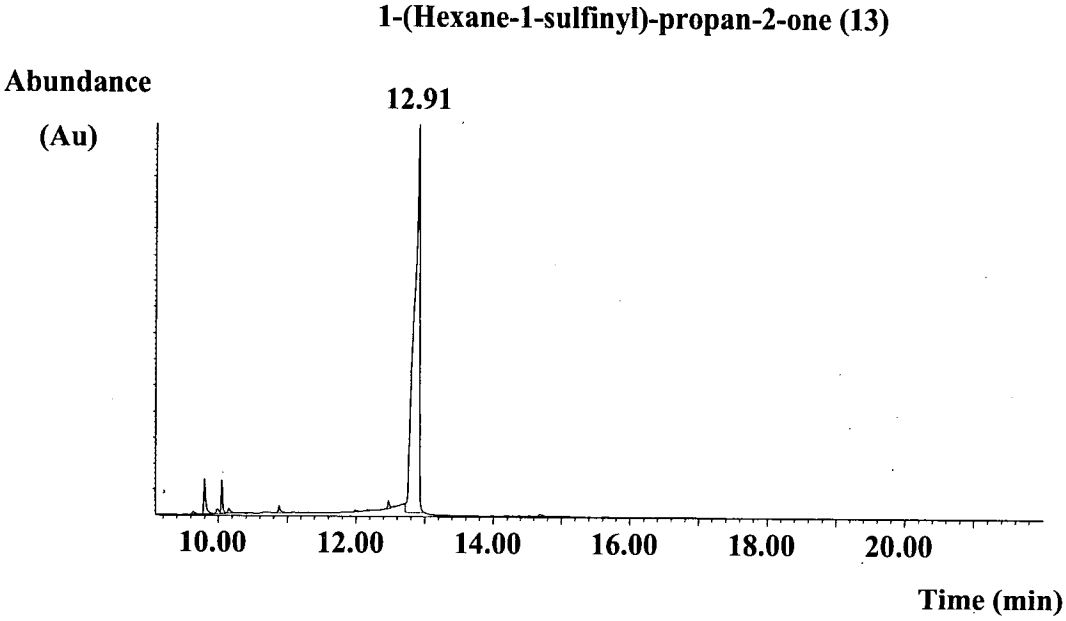

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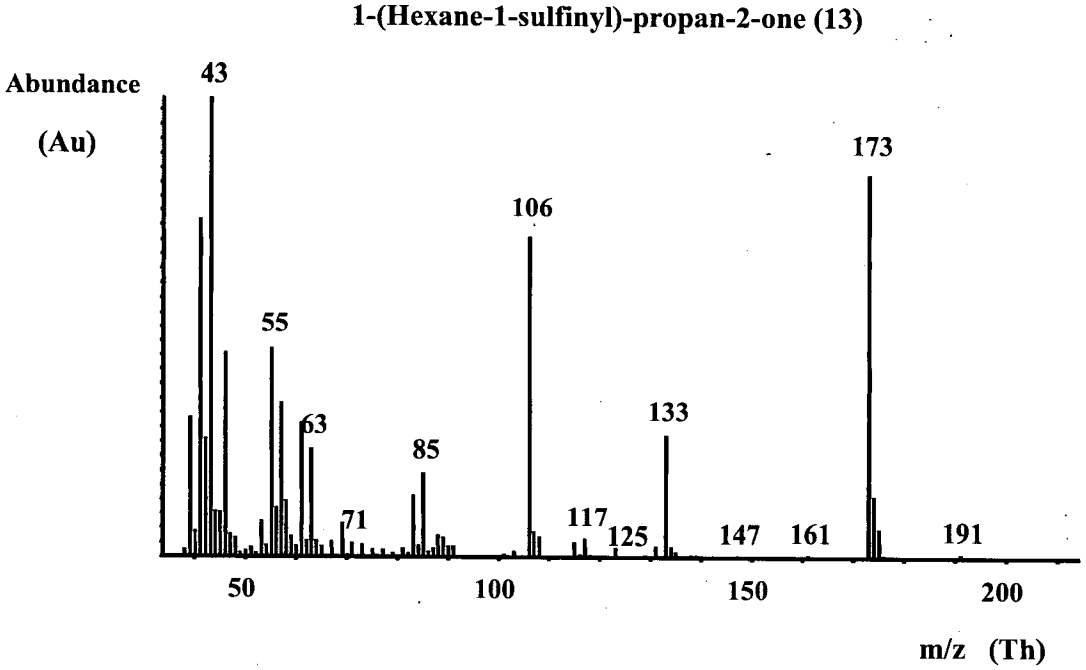
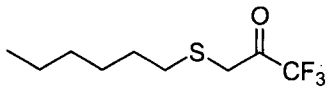


1,1,1-Trifluoro-3-hexylsulfanyl-propan-2-one (6)



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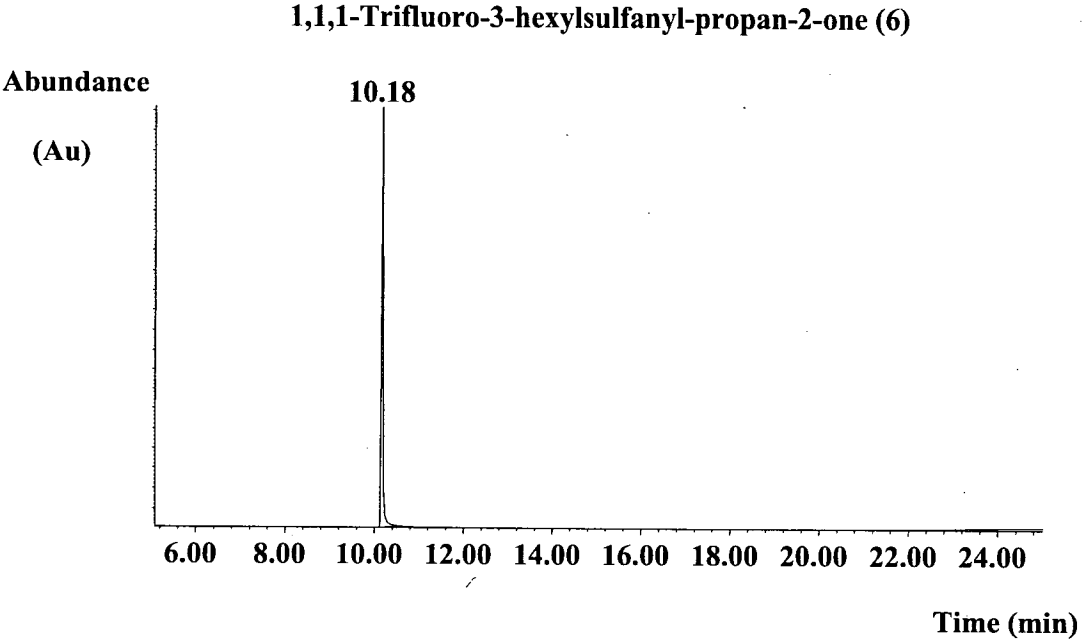

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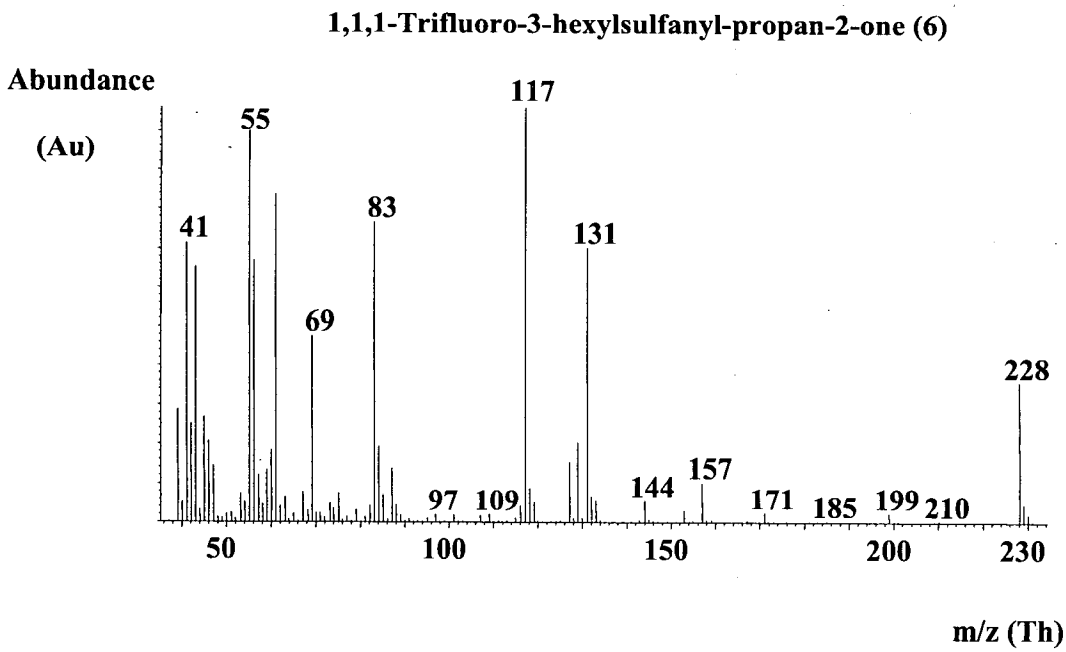
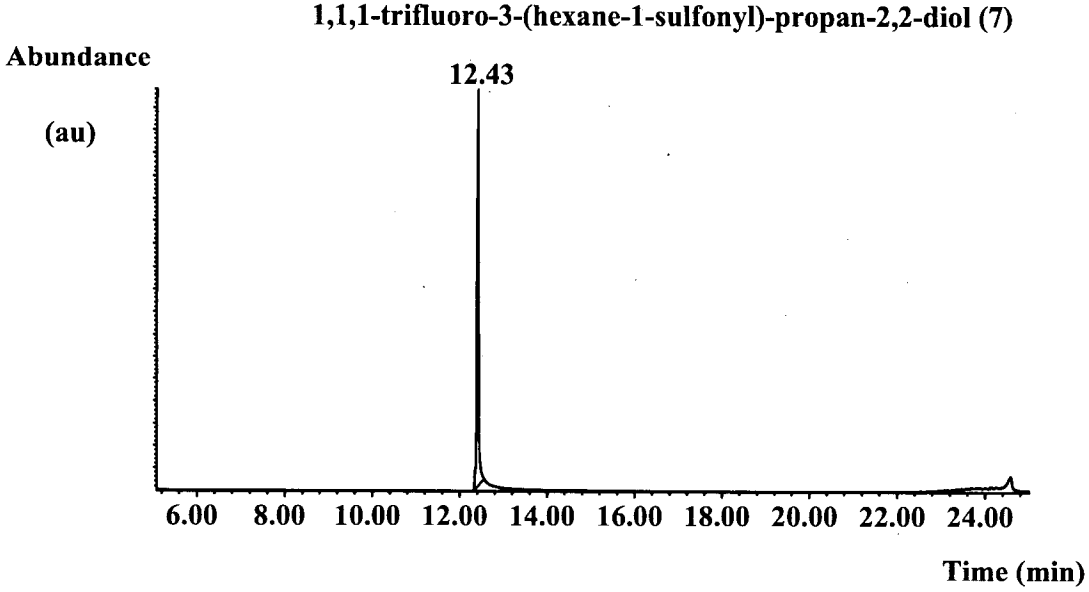


1,1,1-Trifluoro-3-(hexane-1-sulfonyl)-propan-2,2-diol (7)

TIC



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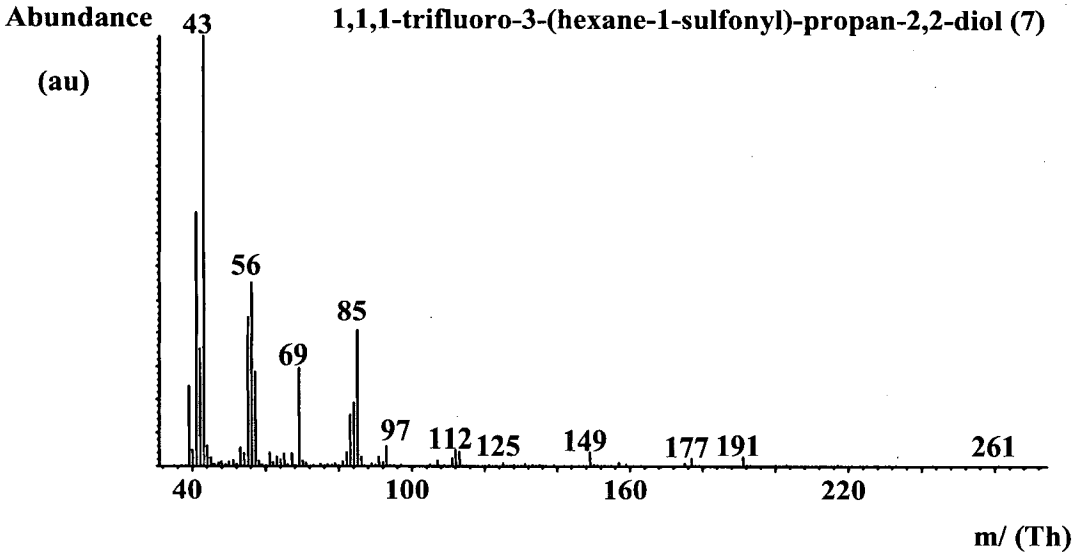
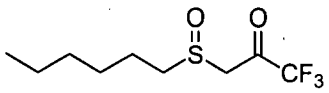


1,1,1-Trifluoro-3-(hexane-1-sulfinyl)-propan-2-one (12)



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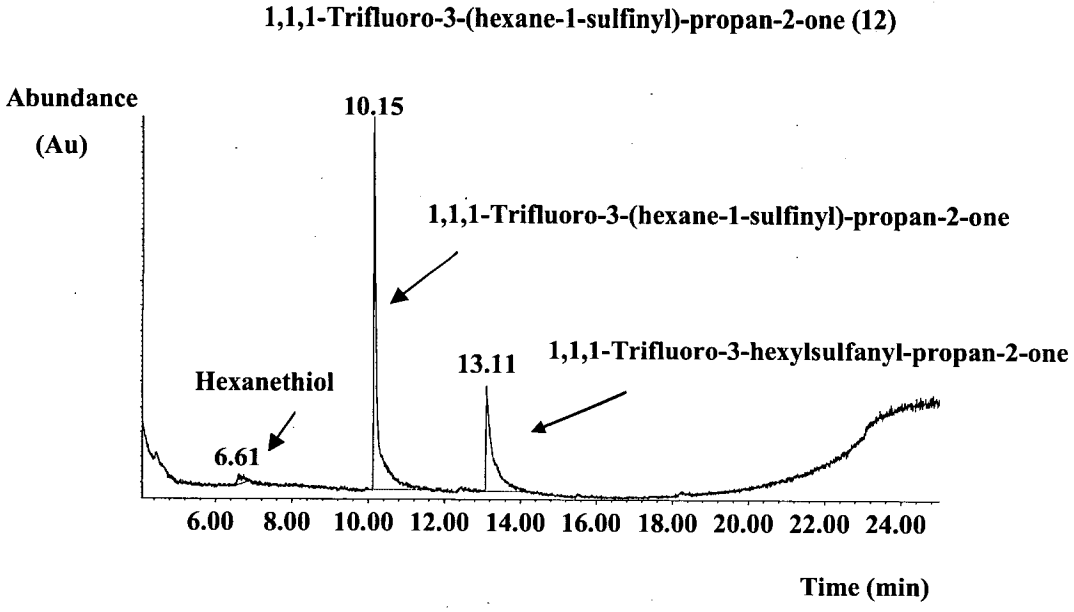

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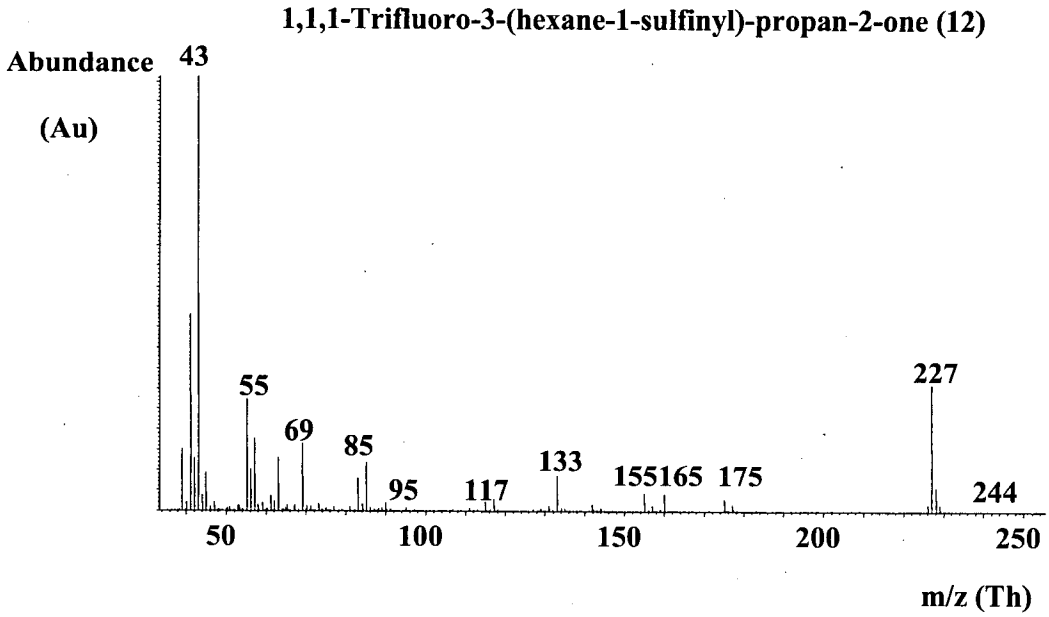
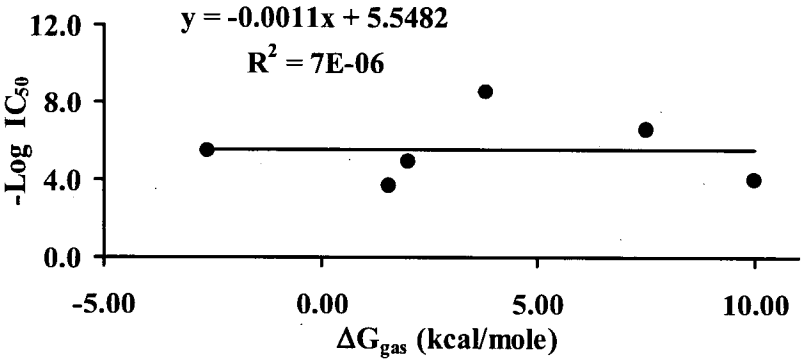


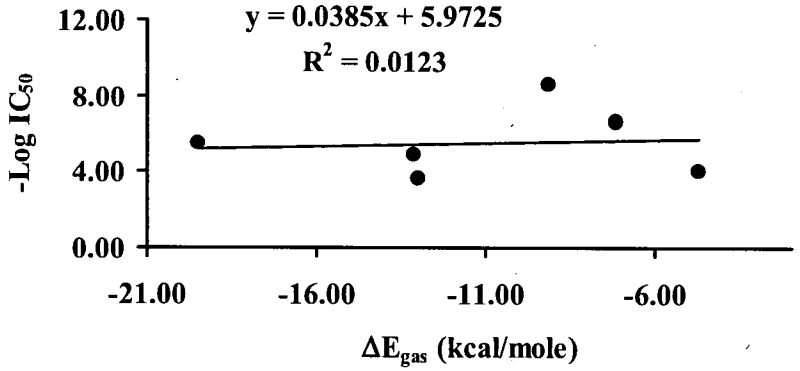
Table 18. Summary of regression and correlation analysis.

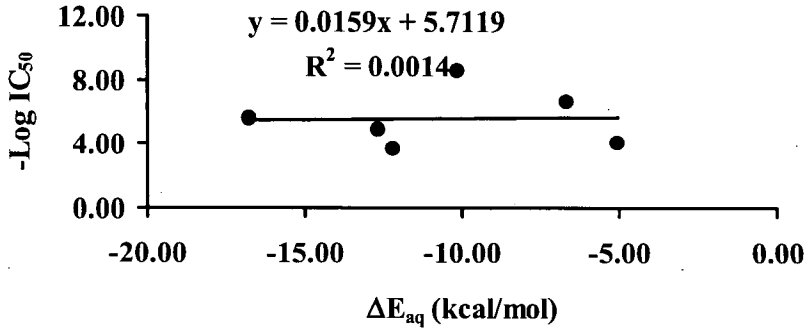
	Equation	R^2	r_s[a]	P(F)[b]	*p*-value
Human Carboxylesterase[c]					
ΔE_{gas}[d]	y=-0.39x+0.23	0.94	0.98	0.47	<0.01
ΔG_{gas}[e]	y=-0.40x+6.27	0.92	0.96	0.47	<0.01
ΔE_{aq}[f]	y=-0.36x+1.48	0.92	0.99	0.46	<0.01
ΔG_{aq}(COSMO)[g]	y=-0.38x+7.21	0.89	0.94	0.45	<0.01
ΔG_{aq}(ChemSol)[h]	y=-0.33x+8.27	0.85	0.92	0.45	<0.01
Murine Carboxylesterase[c]					
ΔE_{gas}[d]	y=-0.43x-1.28	0.90	0.98	0.45	<0.01
ΔG_{gas}[e]	y=-0.45x+5.53	0.88	0.94	0.45	<0.01
ΔE_{aq}[f]	y=-0.41x+0.14	0.87	0.99	0.44	<0.01
ΔG_{aq}(COSMO)[g]	y=-0.42x+6.59	0.85	0.92	0.43	<0.01
ΔG_{aq}(ChemSol)[h]	y=-0.37x+7.83	0.85	0.92	0.43	<0.01
Porcine Carboxylesterase[c]					
ΔE_{gas}[d]	y=-0.42x-0.78	0.84	0.98	0.42	<0.01
ΔG_{gas}[e]	y=-0.42x+5.74	0.84	0.91	0.42	<0.05
ΔE_{aq}[f]	y=-0.39x+0.57	0.81	0.99	0.41	<0.01
ΔG_{aq}(COSMO)[g]	y=-0.41x+6.75	0.81	0.90	0.41	<0.05
ΔG_{aq}(ChemSol)[h]	y=-0.37x+7.99	0.82	0.91	0.42	<0.05
Juvenile Hormone Esterase[i]					
ΔE_{gas}[d]	y=-0.34x+0.43	0.82	0.90	0.38	<0.01
ΔG_{gas}[e]	y=-0.37x+5.71	0.85	0.92	0.41	<0.01
ΔE_{aq}[f]	y=-0.39x+0.48	0.87	0.93	0.42	<0.01
ΔG_{aq}(COSMO)[g]	y=-0.42x+6.52	0.87	0.94	0.42	<0.01
ΔG_{aq}(ChemSol)[h]	y=-0.34x+7.71	0.85	0.92	0.41	<0.01

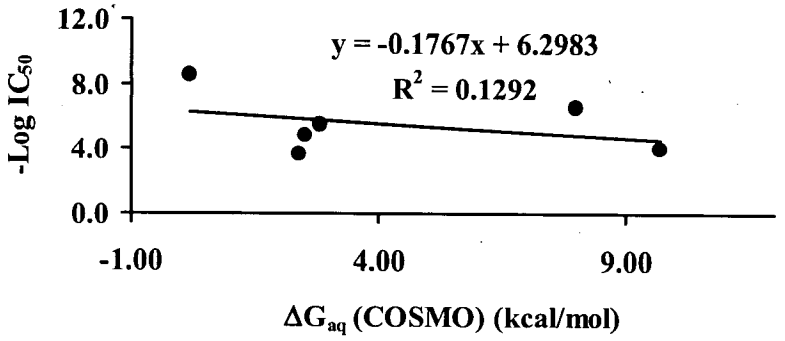
[a]The Spearman Rank correlation coefficient. [b]F test probability value. [c]n=6 (compounds **6-11**). [d]Energy of hydration in the gas phase (kcal/mole). [e]Free energy of hydration in the gas phase (kcal/mole). [f]Energy of hydration in the aqueous phase using the COSMO solvation model (kcal/mole).[3] [g]Free energy of hydration in the aqueous phase using COSMO solvation model[3] [h]Free Energy of hydration in the aqueous phase using the Langevin dipole (ChemSol) solvation model[4] [i]n=10 (compounds **1-11**, excluding compound **5**).

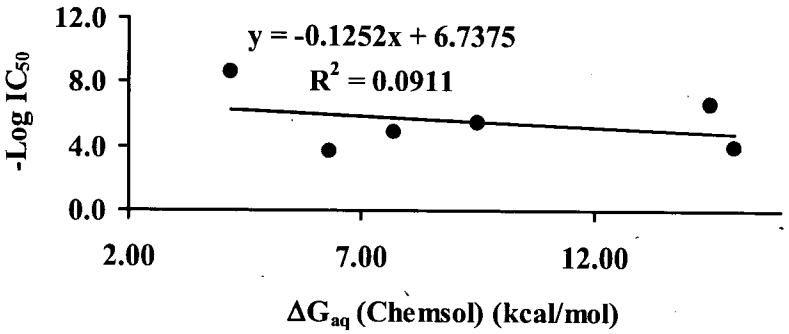
The following graphs show the correlations between inhibition of electric eel acetylcholinesterase activity and the various calculated energy values. There is no correlation between any of the values. The IC_{50} values were taken from Székács et al. (1992).



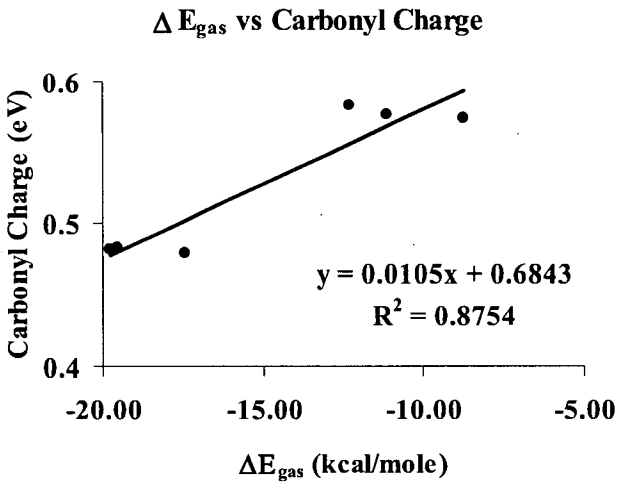


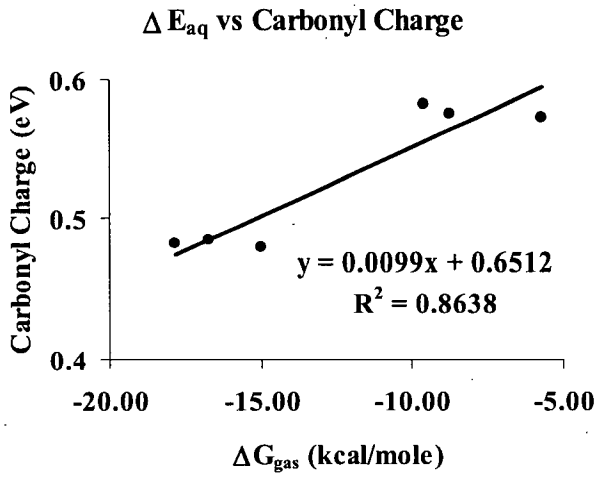


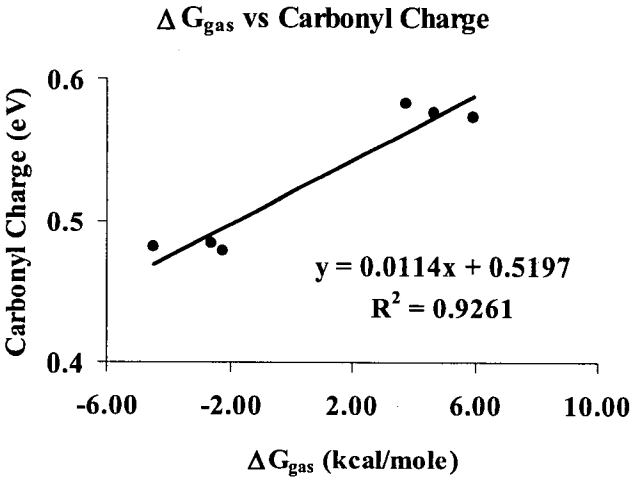


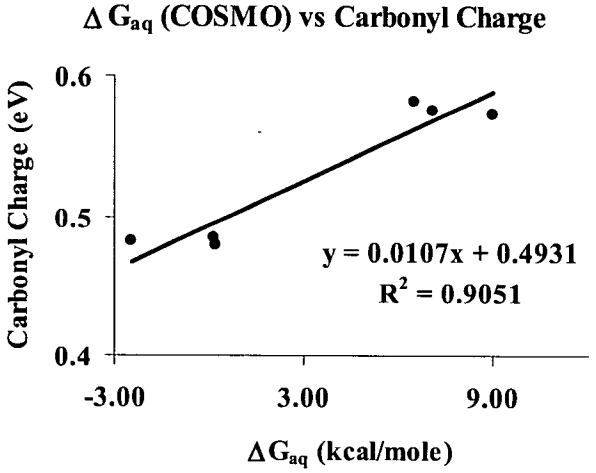


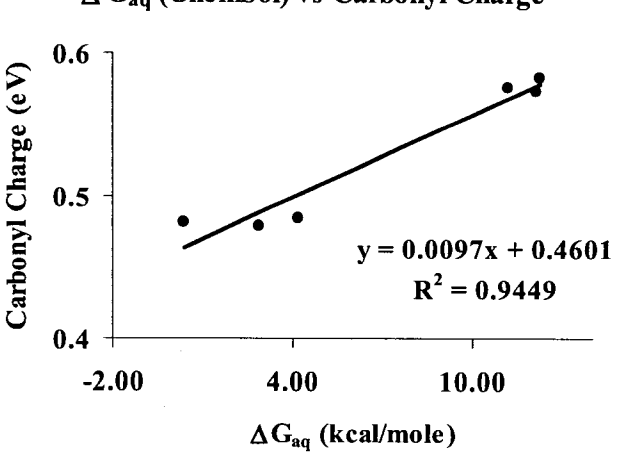
The following graphs provide the correlations between calculated carbonyl charge and the different calculated quantum chemical energies for compounds **6-11**.

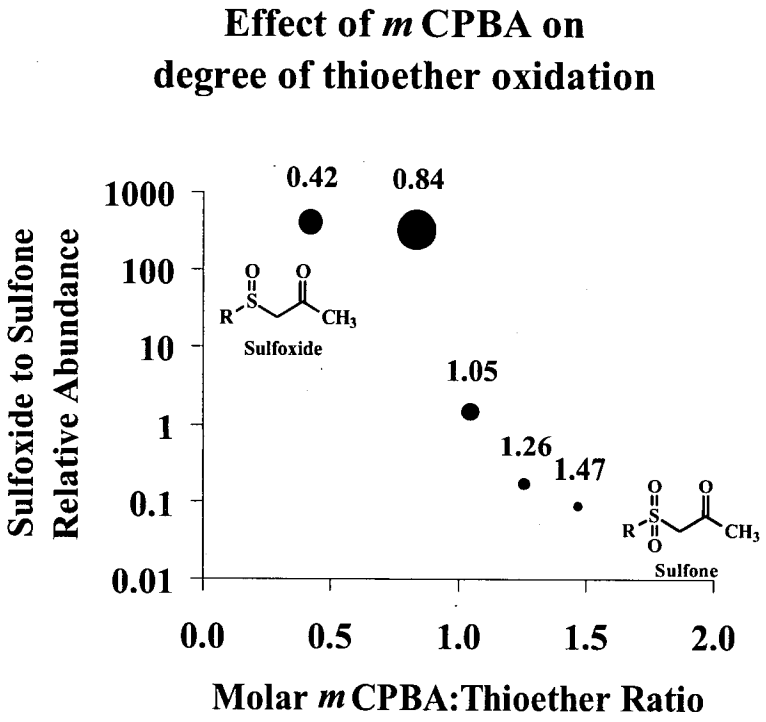












This figure shows the dependence of sulfur oxidation upon the quantity of *m*-CPBA added to the reaction. The relative size of the spots indicates the ratio of *m*-CPBA used. The figure therefore shows that a ratio of 0.84 moles of *m*-CPBA to 1 mole of thioether was the optimal ratio for selective sulfoxide production.

Definition of Energy Terms Used in Regressions.

The ΔE_{gas} for the hydration reactions derived from the total electronic energies of the reactants and products as calculated from the Molecular Schrödinger equation within the Density Functional Theory formalism.[5] This electronic energy includes the kinetic energy of the electrons, the electron-nuclear electrostatic attraction and the nuclear-nuclear and electron-electron electrostatic repulsions. Conceptually, this is the total energy of an isolated molecule in a vacuum at 0K and excluding quantum mechanical zero-point vibrational motion.

The ΔG_{gas} for the hydration reactions is derived from the predicted molecular Gibb's Free Energies (G_{gas}). This is calculated from the predicted enthalpies H_{gas}, and entropies S_{gas}. The enthalpy is calculated by including the quantum mechanical zero-point energy (ZPE) calculated from the predicted harmonic vibrational frequencies and other temperature-dependent corrections (calculated here at 298K) using standard equations from statistical mechanics.[6]

$$H_{gas} = E_{gas} + ZPE + H_{trans}(T) + H_{rot}(T) + H_{vib}(T)$$

The molecular entropy S_{gas} is also calculated from standard statistical mechanics equations using the predicted harmonic vibrational frequencies and the molecular structure.[7]

The aqueous-phase electronic and free energies, E_{aq} and G_{aq}, are calculated from the gas-phase energies described above and the predicted solvation free energy:

$$E_{aq} = E_{gas} + \Delta G_{solv}$$
$$G_{aq} = G_{gas} + \Delta G_{solv}$$

The solvation free energy, ΔG_{solv} is calculated using either the conductor-like screening solvation model(COSMO)[3] or the Langevin Dipole method(LD). [4] The electrostatic

portion of the solvation energy is calculated from the interaction of the solute charges with either the solvent modeled as polarization charges distributed on the solvent exposed surface of the molecule (COSMO), or as a large set of polarizable dipoles on a fixed three-dimensional grid (LD). The non-electrostatic terms, including the cavitation energy, the solute-solvent dispersive interaction, and the solvent reorganization free energy, are included using empirical approximations.[8]

The following pages give the predicted IC_{50} values for all inhibitors using the regressions given in Table 7 of the text.

ND indicates value not determined as ChemSol lacks parameters for the selenium atom.

Human CaE		Energies		ΔGaq	ΔGaq		IC_{50} (M)			ΔGaq	ΔGaq
Compound #	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol
1	-4.72	10.01	-5.05	9.69	15	8.5E-03	5.4E-03	5.0E-04	3.0E-04	4.8E-04
2	-12.99	1.58	-12.17	2.4	6.3	5.1E-06	2.3E-06	1.4E-06	5.0E-07	6.4E-07
3	-13.15	2	-12.65	2.51	7.7	4.4E-06	3.4E-06	9.2E-07	5.5E-07	1.9E-06
4	-7.17	7.5	-6.67	8.01	14.5	9.4E-04	5.4E-04	1.3E-04	6.8E-05	3.3E-04
5	-9.16	3.81	-10.14	2.82	9.5	1.6E-04	1.8E-05	7.4E-06	7.3E-07	7.3E-06
6	-19.51	-2.6	-16.74	0.17	4.2	1.4E-08	4.9E-08	3.1E-08	7.2E-08	1.3E-07
7	-17.42	-2.23	-14.98	0.21	2.9	9.5E-08	6.9E-08	1.3E-07	7.4E-08	4.9E-08
8	-12.3	3.78	-9.58	6.5	12.28	9.4E-06	1.7E-05	1.2E-05	1.8E-05	6.1E-05
9	-8.73	5.95	-5.69	8.99	12.15	2.3E-04	1.3E-04	3.0E-04	1.6E-04	5.5E-05
10	-19.77	-4.46	-17.8	-2.49	0.4	1.1E-08	8.8E-09	1.3E-08	7.0E-09	7.3E-09
11	-11.11	4.69	-8.75	7.05	11.19	2.7E-05	4.0E-05	2.3E-05	2.9E-05	2.6E-05
12	-25.06	-10.25	-21.69	-6.88	-0.35	9.9E-11	4.3E-11	5.1E-10	1.5E-10	4.1E-09
13	-15.05	1.38	-11.06	5.37	10.88	8.0E-07	1.9E-06	3.5E-06	6.8E-06	2.1E-05
14	-17.35	-2.16	-15.05	0.14	ND	1.0E-07	7.3E-08	1.3E-07	7.0E-08	ND
15	-24.4	-9.47	-21.55	-6.61	ND	1.8E-10	8.7E-11	5.8E-10	1.9E-10	ND
16	-21.12	-5.71	-17.61	-2.2	ND	3.4E-09	2.8E-09	1.5E-08	9.0E-09	ND
17	-11.06	4.04	-8.88	6.22	ND	2.9E-05	2.2E-05	2.1E-05	1.4E-05	ND
18	-14.01	1.27	-10.31	4.97	ND	2.0E-06	1.7E-06	6.4E-06	4.8E-06	ND
19	-12.05	3.10	-9.48	5.67	ND	1.2E-05	9.3E-06	1.3E-05	8.8E-06	ND
20	-20.6	-5.42	-16.62	-1.45	-1.0	5.4E-09	3.6E-09	3.4E-08	1.7E-08	2.5E-09
21	-18.61	-3.53	-19.29	-4.21	0.4	3.3E-08	2.1E-08	3.8E-09	1.5E-09	7.3E-09
22	-9.29	5.47	-6.94	7.82	12.6	1.4E-04	8.3E-05	1.1E-04	5.8E-05	7.7E-05

Murine CaE	Energies			ΔGaq	ΔGaq	IC_{50} (M)			ΔGaq	ΔGaq
Compound #	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol
1	-4.72	10.01	-5.05	9.69	15	1.7E-01	1.1E-01	6.3E-03	3.4E-03	6.1E-03
2	-12.99	1.58	-12.17	2.4	6.3	4.4E-05	1.5E-05	7.8E-06	2.7E-06	3.4E-06
3	-13.15	2	-12.65	2.51	7.7	3.8E-05	2.4E-05	5.0E-06	3.0E-06	1.1E-05
4	-7.17	7.5	-6.67	8.01	14.5	1.5E-02	7.6E-03	1.4E-03	6.5E-04	4.0E-03
5	-9.16	3.81	-10.14	2.82	9.5	2.0E-03	1.6E-04	5.3E-05	4.1E-06	5.3E-05
6	-19.51	-2.6	-16.74	0.17	4.2	6.6E-08	1.9E-07	1.1E-07	3.1E-07	5.5E-07
7	-17.42	-2.23	-14.98	0.21	2.9	5.3E-07	2.9E-07	5.6E-07	3.2E-07	1.8E-07
8	-12.3	3.78	-9.58	6.5	12.28	8.8E-05	1.5E-04	8.9E-05	1.5E-04	5.9E-04
9	-8.73	5.95	-5.69	8.99	12.15	3.1E-03	1.5E-03	3.5E-03	1.7E-03	5.2E-04
10	-19.77	-4.46	-17.8	-2.49	0.4	5.1E-08	2.8E-08	3.9E-08	2.3E-08	2.1E-08
11	-11.11	4.69	-8.75	7.05	11.19	2.9E-04	4.0E-04	2.0E-04	2.5E-04	2.3E-04
12	-25.06	-10.25	-21.69	-6.88	-0.35	2.6E-10	6.4E-11	1.0E-09	3.1E-10	1.1E-08
13	-15.05	1.38	-11.06	5.37	10.88	5.7E-06	1.3E-05	2.2E-05	4.9E-05	1.7E-04
14	-17.35	-2.16	-15.05	0.14	ND	5.7E-07	3.1E-07	5.2E-07	3.0E-07	ND
15	-24.4	-9.47	-21.55	-6.61	ND	5.0E-10	1.5E-10	1.2E-09	4.1E-10	ND
16	-21.12	-5.71	-17.61	-2.2	ND	1.3E-08	7.5E-09	4.7E-08	3.0E-08	ND
17	-11.06	4.04	-8.88	6.22	ND	3.0E-04	2.0E-04	1.7E-04	1.1E-04	ND
18	-14.01	1.27	-10.31	4.97	ND	1.6E-05	1.1E-05	4.5E-05	3.3E-05	ND
19	-12.05	3.10	-9.48	5.67	ND	1.1E-04	7.6E-05	9.8E-05	6.6E-05	ND
20	-20.6	-5.42	-16.62	-1.45	-1.0	2.2E-08	1.0E-08	1.2E-07	6.3E-08	6.2E-09
21	-18.61	-3.53	-19.29	-4.21	0.4	1.6E-07	7.3E-08	9.7E-09	4.2E-09	2.1E-08
22	-9.29	5.47	-6.94	7.82	12.6	1.8E-03	9.1E-04	1.1E-03	5.4E-04	7.7E-04

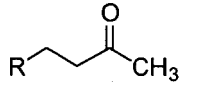
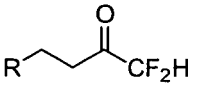
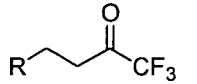
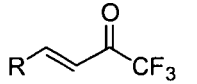
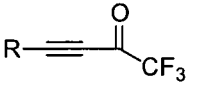
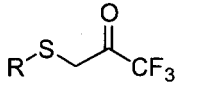
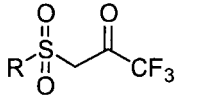
Porcine CaE	Energies			ΔGaq	ΔGaq	IC_{50} (M)			ΔGaq	ΔGaq
Compound #	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol
1	-4.72	10.01	-5.05	9.69	15	6.7E-02	4.5E-02	2.9E-03	1.6E-03	3.2E-03
2	-12.99	1.58	-12.17	2.4	6.3	2.5E-05	9.1E-06	4.7E-06	1.7E-06	2.1E-06
3	-13.15	2	-12.65	2.51	7.7	2.1E-05	1.4E-05	3.1E-06	1.9E-06	6.7E-06
4	-7.17	7.5	-6.67	8.01	14.5	6.4E-03	3.6E-03	6.7E-04	3.3E-04	2.1E-03
5	-9.16	3.81	-10.14	2.82	9.5	9.6E-04	8.6E-05	2.9E-05	2.5E-06	3.1E-05
6	-19.51	-2.6	-16.74	0.17	4.2	4.9E-08	1.3E-07	7.7E-08	2.1E-07	3.5E-07
7	-17.42	-2.23	-14.98	0.21	2.9	3.6E-07	1.9E-07	3.7E-07	2.2E-07	1.2E-07
8	-12.3	3.78	-9.58	6.5	12.28	4.8E-05	8.4E-05	4.8E-05	8.0E-05	3.2E-04
9	-8.73	5.95	-5.69	8.99	12.15	1.4E-03	7.5E-04	1.6E-03	8.4E-04	2.9E-04
10	-19.77	-4.46	-17.8	-2.49	0.4	3.8E-08	2.0E-08	3.0E-08	1.7E-08	1.4E-08
11	-11.11	4.69	-8.75	7.05	11.19	1.5E-04	2.1E-04	1.0E-04	1.3E-04	1.3E-04
12	-25.06	-10.25	-21.69	-6.88	-0.35	2.4E-10	5.9E-11	8.9E-10	2.7E-10	7.6E-09
13	-15.05	1.38	-11.06	5.37	10.88	3.5E-06	7.4E-06	1.3E-05	2.8E-05	9.8E-05
14	-17.35	-2.16	-15.05	0.14	ND	3.8E-07	2.1E-07	3.5E-07	2.0E-07	ND
15	-24.4	-9.47	-21.55	-6.61	ND	4.5E-10	1.3E-10	1.0E-09	3.5E-10	ND
16	-21.12	-5.71	-17.61	-2.2	ND	1.0E-08	5.8E-09	3.5E-08	2.2E-08	ND
17	-11.06	4.04	-8.88	6.22	ND	1.6E-04	1.1E-04	9.1E-05	6.2E-05	ND
18	-14.01	1.27	-10.31	4.97	ND	9.3E-06	6.6E-06	2.5E-05	1.9E-05	ND
19	-12.05	3.10	-9.48	5.67	ND	6.1E-05	4.2E-05	5.3E-05	3.7E-05	ND
20	-20.6	-5.42	-16.62	-1.45	-1.0	1.7E-08	7.7E-09	8.6E-08	4.5E-08	4.4E-09
21	-18.61	-3.53	-19.29	-4.21	0.4	1.2E-07	5.2E-08	7.7E-09	3.3E-09	1.4E-08
22	-9.29	5.47	-6.94	7.82	12.6	8.5E-04	4.6E-04	5.2E-04	2.8E-04	4.2E-04

JHE Regressions Without Alkyne (5)	Energies			ΔGaq	ΔGaq	IC_{50} (M)			ΔGaq	ΔGaq
Compound #	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol
1	-4.72	10.01	-5.05	9.69	15	9.3E-03	1.1E-02	3.7E-03	3.3E-03	2.8E-03
2	-12.99	1.58	-12.17	2.4	6.3	1.5E-05	7.6E-06	6.6E-06	3.0E-06	2.9E-06
3	-13.15	2	-12.65	2.51	7.7	1.3E-05	1.1E-05	4.3E-06	3.3E-06	8.7E-06
4	-7.17	7.5	-6.67	8.01	14.5	1.4E-03	1.2E-03	8.9E-04	6.5E-04	1.9E-03
5	-9.16	3.81	-10.14	2.82	9.5	2.9E-04	5.2E-05	4.0E-05	4.5E-06	3.6E-05
6	-19.51	-2.6	-16.74	0.17	4.2	9.1E-08	2.1E-07	1.1E-07	3.5E-07	5.5E-07
7	-17.42	-2.23	-14.98	0.21	2.9	4.7E-07	2.9E-07	5.5E-07	3.7E-07	2.0E-07
8	-12.3	3.78	-9.58	6.5	12.28	2.5E-05	5.1E-05	6.7E-05	1.5E-04	3.3E-04
9	-8.73	5.95	-5.69	8.99	12.15	4.1E-04	3.3E-04	2.1E-03	1.7E-03	2.9E-04
10	-19.77	-4.46	-17.8	-2.49	0.4	7.5E-08	4.2E-08	4.4E-08	2.8E-08	2.7E-08
11	-11.11	4.69	-8.75	7.05	11.19	6.4E-05	1.1E-04	1.4E-04	2.6E-04	1.4E-04
12	-25.06	-10.25	-21.69	-6.88	-0.35	1.2E-09	2.9E-10	1.4E-09	4.1E-10	1.5E-08
13	-15.05	1.38	-11.06	5.37	10.88	3.0E-06	6.4E-06	1.8E-05	5.2E-05	1.1E-04
14	-17.35	-2.16	-15.05	0.14	ND	4.9E-07	3.0E-07	5.1E-07	3.4E-07	ND
15	-24.4	-9.47	-21.55	-6.61	ND	2.0E-09	5.6E-10	1.6E-09	5.3E-10	ND
16	-21.12	-5.71	-17.61	-2.2	ND	2.6E-08	1.4E-08	5.3E-08	3.6E-08	ND
17	-11.06	4.04	-8.88	6.22	ND	6.6E-05	6.3E-05	1.2E-04	1.2E-04	ND
18	-14.01	1.27	-10.31	4.97	ND	6.7E-06	5.8E-06	3.5E-05	3.5E-05	ND
19	-12.05	3.10	-9.48	5.67	ND	3.1E-05	2.8E-05	7.3E-05	6.9E-05	ND
20	-20.6	-5.42	-16.62	-1.45	-1.0	3.9E-08	1.8E-08	1.3E-07	7.5E-08	8.9E-09
21	-18.61	-3.53	-19.29	-4.21	0.4	1.8E-07	9.4E-08	1.2E-08	5.3E-09	2.7E-08
22	-9.29	5.47	-6.94	7.82	12.6	2.6E-04	2.2E-04	7.0E-04	5.4E-04	4.2E-04

JHE Regressions With Alkyne (5)	Energies			ΔGaq	ΔGaq	IC_{50} (M)			ΔGaq	ΔGaq
Compound #	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol	ΔEgas	ΔGgas	ΔEaq	COSMO	ChemSol
1	-4.72	10.01	-5.05	9.69	15	2.6E-03	5.7E-03	2.2E-03	2.9E-03	1.7E-03
2	-12.99	1.58	-12.17	2.4	6.3	8.5E-06	5.0E-06	4.5E-06	2.3E-06	2.0E-06
3	-13.15	2	-12.65	2.51	7.7	7.7E-06	7.2E-06	2.9E-06	2.6E-06	5.9E-06
4	-7.17	7.5	-6.67	8.01	14.5	4.8E-04	7.0E-04	5.4E-04	5.7E-04	1.2E-03
5	-9.16	3.81	-10.14	2.82	9.5	1.2E-04	3.2E-05	2.6E-05	3.5E-06	2.4E-05
6	-19.51	-2.6	-16.74	0.17	4.2	9.3E-08	1.5E-07	8.4E-08	2.6E-07	3.9E-07
7	-17.42	-2.23	-14.98	0.21	2.9	4.0E-07	2.1E-07	3.9E-07	2.7E-07	1.4E-07
8	-12.3	3.78	-9.58	6.5	12.28	1.4E-05	3.2E-05	4.3E-05	1.3E-04	2.1E-04
9	-8.73	5.95	-5.69	8.99	12.15	1.6E-04	1.9E-04	1.3E-03	1.5E-03	1.9E-04
10	-19.77	-4.46	-17.8	-2.49	0.4	7.8E-08	3.3E-08	3.3E-08	1.9E-08	2.0E-08
11	-11.11	4.69	-8.75	7.05	11.19	3.1E-05	6.8E-05	8.8E-05	2.2E-04	8.8E-05
12	-25.06	-10.25	-21.69	-6.88	-0.35	2.0E-09	2.6E-10	1.1E-09	2.6E-10	1.1E-08
13	-15.05	1.38	-11.06	5.37	10.88	2.1E-06	4.3E-06	1.2E-05	4.3E-05	6.9E-05
14	-17.35	-2.16	-15.05	0.14	ND	4.2E-07	2.2E-07	3.6E-07	2.5E-07	ND
15	-24.4	-9.47	-21.55	-6.61	ND	3.2E-09	5.0E-10	1.3E-09	3.4E-10	ND
16	-21.12	-5.71	-17.61	-2.2	ND	3.1E-08	1.1E-08	3.9E-08	2.6E-08	ND
17	-11.06	4.04	-8.88	6.22	ND	3.3E-05	3.9E-05	7.8E-05	9.8E-05	ND
18	-14.01	1.27	-10.31	4.97	ND	4.2E-06	3.9E-06	2.3E-05	2.9E-05	ND
19	-12.05	3.10	-9.48	5.67	ND	1.6E-05	1.8E-05	4.6E-05	5.7E-05	ND
20	-20.6	-5.42	-16.62	-1.45	-1.0	4.4E-08	1.5E-08	9.3E-08	5.4E-08	6.8E-09
21	-18.61	-3.53	-19.29	-4.21	0.4	1.7E-07	7.1E-08	9.1E-09	3.6E-09	2.0E-08
22	-9.29	5.47	-6.94	7.82	12.6	1.1E-04	1.3E-04	4.2E-04	4.7E-04	2.6E-04

The following tables provide all of the quantum chemical data from the energy of hydration calculations.

Table 19. Quantum chemical data for synthesized compounds.

n°	Compound[a]	E_{gas} (Hartrees)	E_{aq} (COSMO) (Hartrees)	Free E corrections (Hartrees)	ΔG_{solv} (ChemSol) (kcal/mol)
1		-468.35283	-468.35407	0.24103	-4.3
		-544.76931	-544.78043	0.26802	-8.0
2		-666.81347	-666.81307	0.22422	-0.9
		-743.24312	-743.25077	0.25095	-4.9
3		-766.06155	-766.05920	0.21481	-1.2
		-842.49146	-842.49766	0.24246	-4.2
4		-764.83539	-764.83430	0.19126	-3.4
		-841.25578	-841.26323	0.21815	-5.1
5		-763.57757	-763.57511	0.16985	-3.8
		-840.00111	-840.00958	0.19401	-6.8
6		-1124.92437	-1124.92562	0.18352	-3.9
		-1201.36440	-1201.37060	0.21397	-5.8
7		-1275.31296	-1275.31899	0.19357	-8.6
		-1351.74967	-1351.76116	0.22127	-12.2

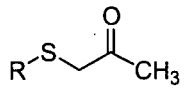
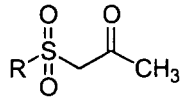
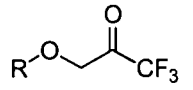
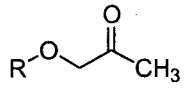
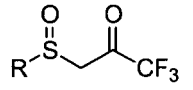
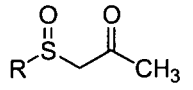
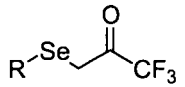
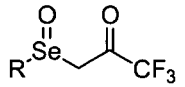
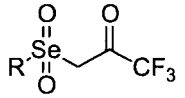
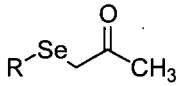
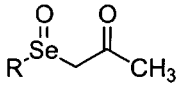
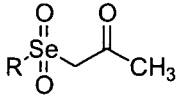
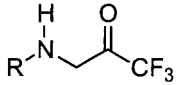
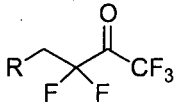
8		-827.21895	-827.22307	0.21157	-5.7
		-903.64751	-903.65664	0.24070	-5.9
9		-977.61114	-977.61987	0.22092	-9.9
		-1054.03400	-1054.04724	0.24782	-12.4
10		-801.94378	-801.94545	0.19063	-2.9
		-878.38423	-878.39212	0.21853	-6.7
11		-504.24052	-504.24456	0.21694	-4.4
		-580.66718	-580.67681	0.24563	-6.6
12		-1200.09780	-1200.09773	0.19093	-11.8
		-1276.54668	-1276.55060	0.21804	-10.6
13		-902.39675	-902.39938	0.21547	-11.7
		-978.82968	-978.83531	0.24516	-10.9

Table 20. Quantum chemical data for theoretical compounds.

n°	Compound[a]	E_{gas} (Hartrees)	E_{aq} (COSMO) (Hartrees)	Free E corrections (Hartrees)	ΔG_{solv} (ChemSol) (kcal/mol)
14		-3126.12583	-3126.12034	0.18419	NA
		-3202.56242	-3202.56262	0.21190	NA
15		-3201.29185	-3201.29073	0.18724	NA
		-3277.73970	-3277.74337	0.21455	NA
16		-3276.46260	-3276.46559	0.18869	NA
		-3352.90521	-3352.91196	0.21675	NA
17		-2828.41869	-2828.41544	0.21060	NA
		-2904.84527	-2904.84789	0.23817	NA
18		-2903.59089	-2903.59310	0.21303	NA
		-2980.02216	-2980.02783	0.24089	NA
19		-2978.76126	-2978.76648	0.21508	NA
		-3055.18942	-3055.19989	0.24273	NA
20		-782.08320	-782.08969	0.20413	-1.9
		-858.52498	-858.53448	0.23182	-6.2
21		-964.52585	-964.52070	0.19676	0.7
		-1040.96445	-1040.96975	0.22429	-4.1