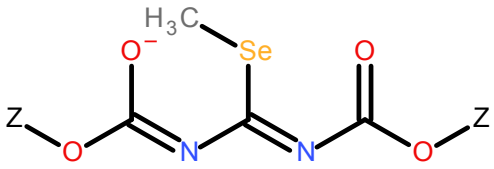
Electronic Supplementary Material (ESI) for Metallomics.

Table 1: 2D dreiding descriptors for aliphatic derivatives[a]



Ref	Z	JX	JY	Wiener	Zagreb	CHI_1	CHI_2	CHI_{V1}	CHI_{V2}	CHI_{V3P}	BIC	E.ADJ.equ	E.ADJ.mag	E.DIST.equ
1	CH_3CH_2	4.1135	4.4836	428	60	7.1338	5.5334	6.8845	3.7308	2.2412	0.7804	125.845	160.000	594.342
2	$CH_3(CH_2)_2$	4.0644	4.3999	630	68	8.1337	6.2405	7.8845	4.5617	2.5649	0.7856	149.984	186.117	837.994
3	$CH_3(CH_2)_3$	4.0016	4.3054	892	76	9.1337	6.9476	8.9373	5.3713	3.2666	0.7424	174.706	212.877	1129.760
4	$CH_3(CH_2)_5$	3.7278	3.9681	1628	92	11.1337	8.3618	10.8845	6.6830	4.1525	0.6487	225.723	268.078	1861.630
5	$(CH_3)_2CHCH_2$	4.1575	4.4707	860	80	8.8454	7.8984	8.6489	6.3770	2.9001	0.7754	185.697	240.215	1097.400
6	CH_2=CH-CH_2	4.1531	4.4951	630	68	8.1337	6.2405	7.1560	4.1667	2.4691	0.7967	149.984	186.117	837.994
7	$C_6H_5CH_2$	1.7842	1.8822	1874	116	12.1690	10.1188	10.0515	6.5159	4.2301	0.6284	305.473	384.000	2587.450
8	NO_2-C_6H_4-CH_2	1.7932	1.9252	3536	148	14.7781	13.1604	11.0504	7.3918	4.8387	0.6202	419.119	536.955	4205.460
9	fmoc[b]	1.084	1.120	5786	212	19.135	16.887	15.303	11.043	8.491	0.584	664.657	862.320	7872.150

	4	2			4	1	6	5	9	6			
R(HT29)[c]	0.825	0.827	-0.644	-0.709	-0.686	-0.685	-0.643	-0.655	-0.694	0.672	-0.706	-0.706	-0.686
R^2(HT29)[c]	0.681	0.684	0.415	0.503	0.471	0.469	0.413	0.429	0.482	0.452	0.498	0.498	0.471

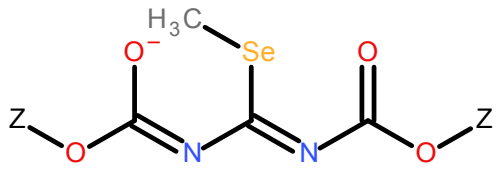
Table 1: Cont.

Ref	Z	E.DIST.mag	V.ADJ.equ	V.ADJ.mag	V.DIST.equ	V.DIST.mag	SC_0	SC_1	SC_2	SC_{3P}	Mol.SASA	Mol.SAVol	logS
1	CH_3CH_2	1427.410	121.951	134.606	720.053	1687.040	15	14	16	16	423.836	371.352	-1.286
2	$CH_3(CH_2)_2$	1961.230	145.108	160.000	987.060	2269.350	17	16	18	18	473.396	412.375	-1.816
3	$CH_3(CH_2)_3$	2590.090	168.990	186.117	1302.880	2947.980	19	18	20	20	525.362	455.386	-1.999
4	$CH_3(CH_2)_5$	4144.310	218.621	240.215	2084.680	4604.960	23	22	24	24	609.008	526.744	-4.583
5	$(CH_3)_2CHCH_2$	2592.080	168.990	186.117	1270.520	2951.250	19	18	22	20	505.977	438.461	-1.781
6	CH_2=CH-CH_2	1961.230	145.108	160.000	987.060	2269.350	17	16	18	18	460.945	407.775	-1.338
7	$C_6H_5CH_2$	6124.480	258.347	296.423	2413.220	5599.060	25	26	32	36	584.488	517.848	-3.720
8	NO_2-C_6H_4-CH_2	9878.370	339.324	384.000	4007.580	9193.700	31	32	42	48	638.246	572.641	-4.785

9	fmoc[b]	20505.100	485.012	568.430	6255.730	15598.400	39	44	62	88	773.117	687.571	-8.332
	R(HT29)[c]	-0.691	-0.693	-0.706	-0.656	-0.668	-0.673	-0.707	-0.710	-0.718	-0.637	-0.651	0.647
	R^2(HT29)[c]	0.477	0.480	0.498	0.430	0.446	0.453	0.500	0.504	0.516	0.406	0.424	0.419

[a] See text for details. [b] 9-fluorenylmethyl. [c]R, R^2= Regression coefficients (cell line).

Table 2: 3D dreiding descriptors for aliphatic derivatives[a]

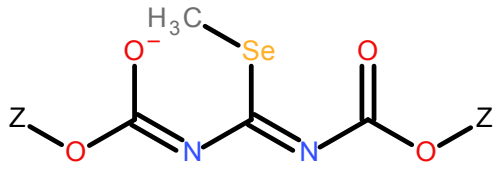


Ref	Z	JursPPSA3	JursWPSA3	ShadYZ
1	CH_3CH_2	18.1395	8.8539	38.2684
2	$CH_3(CH_2)_2$	18.4464	10.0685	42.6970
3	$CH_3(CH_2)_3$	24.8708	15.1755	46.8645
4	$CH_3(CH_2)_5$	20.8778	15.5347	46.3870
5	$(CH_3)_2CHCH_2$	23.3740	13.9356	46.2255
6	CH_2=CH-CH_2	25.6778	13.3979	40.6497
7	$C_6H_5CH_2$	30.8694	20.2047	51.9143
8	NO_2-C_6H_4-CH_2	32.1951	23.4517	58.8028

9	fmoc[b]	35.2453	29.5656	73.7709
	R(HT29)[c]	-0.712	-0.704	-0.696
	R^2(HT29)[c]	0.507	0.496	0.484

[a] See text for details. [b] 9-fluorenylmethyl. [c]R, R^2= Regression coefficient (cell line).

Table 3: 2D dreiding descriptors for aromatic derivatives[a]



Ref.	Z	JY	Wiener	Zagreb	CHI_0	CHI_1	CHI_{3P}	CHI_{V0}	CHI_{V1}	CHI_{V2}	CHI_{V3P}	BIC	CIC	IAC_Total	IC	SIC	E.ADJ.equ
10	C_6H_5	2.0313	1408	108	16.4933	11.1690	6.9696	13.9750	9.1753	5.7975	3.7143	0.6424	1.2830	65.4468 0	3.24052	0.71636	277.670
11	CH_3O-C_6H_4	2.0254	2280	128	19.6481	13.0327	8.6075	16.6368	10.2214	6.5225	4.3467	0.5892	1.6855	79.5063 0	3.06934	0.64551	346.976
12	CH_3-C_6H_4	2.0355	1802	120	18.2338	11.9567	7.7910	15.8203	9.9967	6.7975	4.2698	0.6187	1.4702	73.2121 0	3.17366	0.68341	318.307
13	Cl-C_6H_4	2.0347	1802	120	18.2338	11.9567	7.7910	16.0881	10.1306	6.9521	4.3591	0.6187	1.4702	73.7302 0	3.17366	0.68341	318.307
14	F-C_6H_4	2.0424	1802	120	18.2338	11.9567	7.7910	14.5763	9.3746	6.0793	3.8551	0.6187	1.4702	73.7302 0	3.17366	0.68341	318.307
	R(HT29)[b]	-0.635	0.749	0.709	0.726	0.753	0.740	0.889	0.874	0.676	0.845	-0.750	0.747	0.694	-0.755	-0.747	0.715
	R^2(HT29)[b]	0.403	0.561	0.503	0.527	0.567	0.548	0.790	0.764	0.457	0.714	0.563	0.558	0.482	0.570	0.558	0.511

Table 3: Cont.

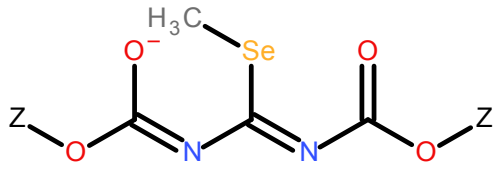
Ref.	Z	E.ADJ.mag	E.DIST.equ	E.DIST.mag	V.ADJ.equ	V.ADJ.mag	V.DIST.equ	V.DIST.mag	$Kappa_1$	Kappa1AM	Kappa2	Kappa2AM	Kappa3
10	C_6H_5	354.413	2092.780	5091.700	232.192	268.078	1945.750	4617.410	19.3264	16.6963	10.7800	8.6952	7.6125
11	CH_3O-C_6H_4	444.235	3032.600	7270.180	284.941	325.212	2872.190	6691.230	23.2806	20.5606	12.5386	10.4112	8.4898
12	CH_3-C_6H_4	413.947	2533.330	6127.270	258.347	296.423	2381.310	5601.520	21.3018	18.6656	10.9827	8.9814	8.0443
13	Cl-C_6H_4	413.947	2533.330	6127.270	258.347	296.423	2381.310	5601.520	21.3018	19.2376	10.9827	9.4080	8.0443
14	F-C_6H_4	413.947	2533.330	6127.270	258.347	296.423	2381.310	5601.520	21.3018	18.5275	10.9827	8.8792	8.0443
	R(HT29)	0.682	0.747	0.746	0.742	0.741	0.747	0.746	0.741	0.744	0.711	0.753	0.742
	R^2(HT29) [b]	0.465	0.558	0.557	0.551	0.549	0.558	0.557	0.549	0.554	0.506	0.567	0.551

Table 3: Cont.

Ref.	Z	Kappa3 AM	PHI	SC0	SC1	SC2	SC3P	Mol.Surf.Area	Mol.PolarSurf.Area	Mol.SASA	Mol.PolarSASA	Mol.Fract.PolarSASA	Mol.SAVol
10	C_6H_5	5.9144	6.31202	23	24	30	34	314.390	86.540	534.928	149.145	0.278	476.825
11	CH_3O-C_6H_4	6.8149	7.92813	27	28	36	42	379.480	105.010	607.300	161.206	0.265	538.461
12	CH_3-C_6H_4	6.3851	6.70572	25	26	34	38	353.220	86.540	573.919	149.145	0.259	508.650
13	Cl-C_6H_4	6.7353	7.23948	25	26	34	38	360.530	86.540	577.738	149.145	0.258	534.514
14	F-C_6H_4	6.3015	6.58037	25	26	34	38	331.280	86.540	553.127	149.145	0.269	495.259
	R(HT29)[b]	0.695	0.754	0.741	0.741	0.680	0.741	0.876	0.675	0.887	0.675	-0.617	0.739
	R^2(HT29)[b]	0.483	0.569	0.549	0.549	0.462	0.549	0.767	0.456	0.787	0.456	0.381	0.546

[a] See text for details. [b] R, R^2= Regression coefficient (cell line).

Table 4: 3D dreiding descriptors, aromatic derivatives[a]



Ref.	Z	Mol.Vol.	Dipole_mag	JursDPSA1	JursDPSA2	JursFNSA3	JursFPSA2	JursPPSA1	JursPPSA2	JursSASA	JursTASA	JursWPSA1
10	C_6H_5	196.470	9.74788	154.25867	1458.98148	-0.08305	1.48873	372.66926	880.05930	591.07959	492.24452	220.33285
11	CH_3O-C_6H_4	237.342	9.45944	269.51023	2004.10128	-0.07959	1.94709	481.22218	1349.28205	692.93413	565.70182	333.50444
12	CH_3-C_6H_4	223.096	9.67384	234.19052	1629.38852	-0.07381	1.63485	443.15819	1066.21037	652.12611	552.83470	289.04881
13	Cl-C_6H_4	228.724	10.18916	-4.47812	1578.47296	-0.09019	1.15426	317.18981	737.53144	638.85756	539.94885	202.70159
14	F-C_6H_4	206.061	10.43779	50.96737	1601.57815	-0.10517	1.35221	330.14244	824.04000	609.31741	419.11841	201.21967
	R(HT29)[b]	0.876	-0.725	0.684	0.772	0.732	0.694	0.823	0.802	0.947	0.885	0.897
	R^2(HT29)[b]	0.767	0.526	0.468	0.596	0.536	0.482	0.677	0.643	0.897	0.783	0.805

Table 4: Cont.

Ref.	Z	JursWPSA2	JursWPSA3	Shad.nu	Shad.Xleng.	Shad.XY	Shad.XYfrac	Shad.XZ	Shad.XZfrac
10	C_6H_5	520.31641	17.18127	3.21016	17.65453	103.59011	0.53580	59.04959	0.60766
11	CH_3O-C_6H_4	935.10167	23.95072	3.82840	21.42878	121.54672	0.49384	73.55308	0.61370
12	CH_3-C_6H_4	695.43278	18.62704	3.53599	19.48750	113.89056	0.52180	68.17310	0.63396
13	Cl-C_6H_4	471.32304	16.27966	3.55633	19.56504	113.01252	0.51473	66.42369	0.61650
14	F-C_6H_4	502.24711	16.87461	3.36092	18.48275	107.33585	0.52434	61.71918	0.60663
	R(HT29)[b]	0.851	0.776	0.891	0.889	0.925	-0.781	0.950	0.652
	R^2(HT29)[b]	0.724	0.602	0.794	0.790	0.856	0.610	0.903	0.425

Table 4: Cont.

Ref.	Z	Shad.Yleng.	Shad.YZ	Shad.YZfrac	Shad.Zleng.
10	C_6H_5	11.05162	37.61844	0.61666	5.52002
11	CH_3O-C_6H_4	11.67455	42.27212	0.64673	5.60130
12	CH_3-C_6H_4	11.34460	40.75131	0.64858	5.53139
13	Cl-C_6H_4	11.37357	39.10453	0.62159	5.52440
14	F-C_6H_4	11.19467	38.13779	0.61687	5.52100
	R(HT29)[b]	0.877	0.972	0.944	0.762
	R^2(HT29)[b]	0.769	0.945	0.891	0.581

[a] See text for details. [b] R, R^2= Regression coefficient (cell line).

QuaSAR_Contingency Analysis

Database : contingencia_alifaticos
Date : Thu May 04 09:30:15 2017
Activity Field : HT29
Sample Size : 9

C : Contingency Coefficient (above 0.6 is useful)
V : Cramer's V (above 0.2 is useful)
U : Entropic Uncertainty (above 0.2 is useful)
R : Linear Correlation R**2 (above 0.2 is useful)

Database fields

#	C	V	U	R	Field
1	0.82717	0.42492	0.65122	0.32896	ALogP
2	0.78551	0.36641	0.55726	0.45990	Molecular_Solubility
3	0.82717	0.42492	0.68353	0.38123	Molecular_Volume
4	0.84908	0.46398	0.74577	0.32160	Molecular_SurfaceArea
5	0.44721	0.14434	0.15912	0.00985	Molecular_PolarSurfaceArea
6	0.79057	0.37268	0.58428	0.26570	Molecular_FractionalPolarSurfaceArea
7	0.82717	0.42492	0.65122	0.38197	Molecular_SASA
8	0.44721	0.14434	0.15912	0.00712	Molecular_PolarSASA
9	0.81264	0.40254	0.65840	0.14085	Molecular_FractionalPolarSASA
10	0.82717	0.42492	0.65122	0.40699	Molecular_SAVol
11	0.84908	0.46398	0.71210	0.45161	BIC
12	0.82717	0.42492	0.65122	0.38650	CIC
13	0.77021	0.34861	0.53848	0.49780	E_ADJ_equ
14	0.77021	0.34861	0.53848	0.49810	E_ADJ_mag
15	0.78446	0.36515	0.58597	0.47092	E_DIST_equ
16	0.78446	0.36515	0.58597	0.47707	E_DIST_mag
17	0.82199	0.41667	0.68353	0.14434	IAC_Mean
18	0.84908	0.46398	0.74577	0.25831	IAC_Total
19	0.84242	0.45134	0.72298	0.01946	IC
20	0.82199	0.41667	0.65122	0.32530	SIC
21	0.81837	0.41107	0.65840	0.47996	V_ADJ_equ
22	0.81837	0.41107	0.65840	0.49817	V_ADJ_mag
23	0.82717	0.42492	0.71922	0.43061	V_DIST_equ
24	0.72375	0.30277	0.49947	0.44576	V_DIST_mag
25	0.84242	0.45134	0.72298	0.39591	CHI_0
26	0.81837	0.41107	0.65840	0.47109	CHI_1
27	0.81837	0.41107	0.65840	0.46866	CHI_2
28	0.77799	0.35746	0.58597	0.22564	CHI_3_C
29	0.00000	0.00000	0.00000	0.00000	CHI_3_CH
30	0.78446	0.36515	0.58597	0.51615	CHI_3_P
31	0.84908	0.46398	0.74577	0.40048	CHI_V_0
32	0.82717	0.42492	0.68353	0.41015	CHI_V_1
33	0.82717	0.42492	0.68353	0.42416	CHI_V_2
34	0.77799	0.35746	0.58597	0.22195	CHI_V_3_C
35	0.00000	0.00000	0.00000	0.00000	CHI_V_3_CH
36	0.79057	0.37268	0.64866	0.47312	CHI_V_3_P

37 0.72633 0.30505 0.49947 0.69116 JX
38 0.73620 0.31402 0.49947 0.69521 JY
39 0.72375 0.30277 0.49947 0.41495 Wiener
40 0.81837 0.41107 0.65840 0.50321 Zagreb
41 0.82717 0.42492 0.65122 0.27665 Kappa_1
42 0.82717 0.42492 0.65122 0.20109 Kappa_1_AM
43 0.82199 0.41667 0.65122 0.00975 Kappa_2
44 0.81837 0.41107 0.65840 0.01404 Kappa_2_AM
45 0.82717 0.42492 0.65122 0.31446 Kappa_3
46 0.79057 0.37268 0.58428 0.35411 Kappa_3_AM
47 0.81064 0.39965 0.69347 0.26174 PHI
48 0.82717 0.28868 0.65122 0.45328 SC_0
49 0.82717 0.26021 0.65122 0.50021 SC_1
50 0.84908 0.23199 0.71210 0.50348 SC_2
51 0.72633 0.30505 0.49947 0.39142 SC_3_C
52 0.00000 0.00000 0.00000 0.00000 SC_3_CH
53 0.82717 0.17111 0.65122 0.51533 SC_3_P
54 0.75593 0.33333 0.47067 0.06108 Dipole_mag
55 0.71660 0.29659 0.40688 0.01803 Dipole_X
56 0.76089 0.33850 0.53848 0.00574 Dipole_Y
57 0.79301 0.37577 0.55726 0.45953 Dipole_Z
58 0.81064 0.39965 0.65840 0.07256 Jurs_DPSA_1
59 0.79301 0.37577 0.55726 0.18399 Jurs_DPSA_2
60 0.72375 0.30277 0.49947 0.02015 Jurs_DPSA_3
61 0.84242 0.45134 0.72298 0.20209 Jurs_FNSA_1
62 0.79301 0.37577 0.55726 0.10106 Jurs_FNSA_2
63 0.77021 0.34861 0.53848 0.01706 Jurs_FNSA_3
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65 0.82199 0.41667 0.68353 0.04098 Jurs_FPSA_2
66 0.84908 0.46398 0.71210 0.19344 Jurs_FPSA_3
67 0.78446 0.36515 0.58597 0.30621 Jurs_PNSA_1
68 0.82717 0.42492 0.71922 0.14862 Jurs_PNSA_2
69 0.70211 0.28464 0.40688 0.00015 Jurs_PNSA_3
70 0.84242 0.45134 0.72298 0.02880 Jurs_PPSA_1
71 0.79057 0.37268 0.58428 0.16094 Jurs_PPSA_2
72 0.82199 0.41667 0.65122 0.46211 Jurs_PPSA_3
73 0.77021 0.34861 0.53848 0.11353 Jurs_RASA
74 0.82199 0.41667 0.65122 0.22245 Jurs_RNCG
75 0.77460 0.35355 0.58694 0.07523 Jurs_RNCS
76 0.79301 0.37577 0.55726 0.21011 Jurs_RPCG
77 0.78551 0.36641 0.55726 0.10065 Jurs_RPCS
78 0.77021 0.34861 0.53848 0.11353 Jurs_RPSA
79 0.84908 0.46398 0.74577 0.30392 Jurs_SASA
80 0.82717 0.42492 0.65122 0.39306 Jurs_TASA
81 0.63246 0.23570 0.30939 0.02682 Jurs_TPSA
82 0.76564 0.34359 0.53848 0.34637 Jurs_WNSA_1
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84 0.78446 0.36515 0.58597 0.00541 Jurs_WNSA_3
85 0.84242 0.45134 0.75954 0.15508 Jurs_WPSA_1
86 0.81837 0.41107 0.65840 0.21910 Jurs_WPSA_2
87 0.79057 0.37268 0.58428 0.43413 Jurs_WPSA_3
88 0.81837 0.41107 0.65840 0.23711 PMI_mag

89 0.84242 0.45134 0.75954 0.33521 PMI_X
90 0.81837 0.41107 0.65840 0.24028 PMI_Y
91 0.84242 0.45134 0.72298 0.22916 PMI_Z
92 0.73620 0.31402 0.49947 0.13168 Shadow_nu
93 0.70413 0.28626 0.37712 0.04322 Shadow_Xlength
94 0.84908 0.46398 0.74577 0.28747 Shadow_XY
95 0.78551 0.36641 0.58694 0.17722 Shadow_XYfrac
96 0.82717 0.42492 0.65122 0.36213 Shadow_XZ
97 0.79057 0.37268 0.58428 0.28057 Shadow_XZfrac
98 0.86603 0.50000 0.80239 0.23686 Shadow_Ylength
99 0.82717 0.42492 0.68353 0.50423 Shadow_YZ
100 0.82375 0.41944 0.62671 0.15175 Shadow_YZfrac
101 0.79057 0.37268 0.58428 0.52557 Shadow_Zlength

QuaSAR_Contingency Analysis

Database : contingencia_aromaticos
Date : Thu May 04 09:48:40 2017
Activity Field : HT29
Sample Size : 5

C : Contingency Coefficient (above 0.6 is useful)
V : Cramer's V (above 0.2 is useful)
U : Entropic Uncertainty (above 0.2 is useful)
R : Linear Correlation R**2 (above 0.2 is useful)

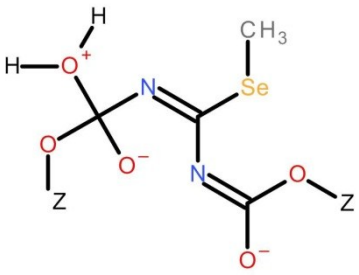
Database fields

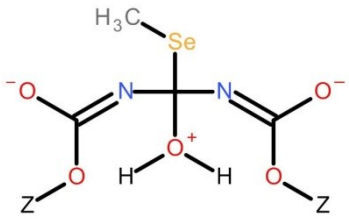
#	C	V	U	R	Field
1	0.83205	0.43301	0.79188	0.00900	ALogP
2	0.86603	0.50000	0.90575	0.01557	Molecular_Solubility
3	0.86603	0.50000	0.90575	0.78323	Molecular_Volume
4	0.86603	0.50000	0.90575	0.76806	Molecular_SurfaceArea
5	0.70711	0.28868	0.54612	0.45614	Molecular_PolarSurfaceArea
6	0.86603	0.50000	0.90575	0.00007	Molecular_FractionalPolarSurfaceArea
7	0.81650	0.40825	0.79188	0.78622	Molecular_SASA
8	0.70711	0.28868	0.54612	0.45614	Molecular_PolarSASA
9	0.86603	0.50000	0.90575	0.11375	Molecular_FractionalPolarSASA
10	0.86603	0.50000	0.90575	0.54612	Molecular_SAVol
11	0.70711	0.28868	0.54612	0.45614	BIC
12	0.75593	0.33333	0.58973	0.52930	CIC
13	0.75593	0.33333	0.58973	0.51062	E_ADJ_equ
14	0.75593	0.33333	0.58973	0.46538	E_ADJ_mag
15	0.75593	0.33333	0.58973	0.55772	E_DIST_equ
16	0.75593	0.33333	0.58973	0.55598	E_DIST_mag
17	0.77460	0.35355	0.65155	0.30370	IAC_Mean
18	0.75593	0.33333	0.58973	0.48191	IAC_Total
19	0.75593	0.33333	0.58973	0.32068	IC
20	0.75593	0.33333	0.58973	0.49890	SIC
21	0.75593	0.33333	0.58973	0.54984	V_ADJ_equ
22	0.75593	0.33333	0.58973	0.54975	V_ADJ_mag
23	0.75593	0.33333	0.58973	0.55737	V_DIST_equ
24	0.75593	0.33333	0.58973	0.55620	V_DIST_mag
25	0.75593	0.33333	0.58973	0.52779	CHI_0
26	0.75593	0.33333	0.58973	0.56668	CHI_1
27	0.75593	0.33333	0.58973	0.38131	CHI_2
28	0.75593	0.33333	0.58973	0.09440	CHI_3_C
29	0.00000	0.00000	0.00000	0.00000	CHI_3_CH
30	0.75593	0.33333	0.58973	0.54795	CHI_3_P
31	0.86603	0.50000	0.90575	0.79047	CHI_V_0
32	0.86603	0.50000	0.90575	0.76446	CHI_V_1
33	0.86603	0.50000	0.90575	0.45661	CHI_V_2
34	0.83205	0.43301	0.79188	0.19162	CHI_V_3_C
35	0.00000	0.00000	0.00000	0.00000	CHI_V_3_CH
36	0.86603	0.50000	0.90575	0.71452	CHI_V_3_P

37 0.83205 0.43301 0.79188 0.00213 JX
38 0.81650 0.40825 0.79188 0.03494 JY
39 0.75593 0.33333 0.58973 0.56167 Wiener
40 0.75593 0.24618 0.58973 0.50321 Zagreb
41 0.75593 0.33333 0.58973 0.54860 Kappa_1
42 0.86603 0.50000 0.90575 0.55382 Kappa_1_AM
43 0.75593 0.33333 0.58973 0.50597 Kappa_2
44 0.83205 0.43301 0.79188 0.56772 Kappa_2_AM
45 0.75593 0.33333 0.58973 0.55101 Kappa_3
46 0.86603 0.50000 0.90575 0.48478 Kappa_3_AM
47 0.86603 0.50000 0.90575 0.56915 PHI
48 0.75593 0.33333 0.58973 0.54846 SC_0
49 0.75593 0.33333 0.58973 0.54846 SC_1
50 0.75593 0.33333 0.58973 0.46289 SC_2
51 0.52223 0.17678 0.24353 0.24560 SC_3_C
52 0.00000 0.00000 0.00000 0.00000 SC_3_CH
53 0.75593 0.33333 0.58973 0.54846 SC_3_P
54 0.83205 0.43301 0.79188 0.00365 Dipole_mag
55 0.86603 0.50000 0.90575 0.58699 Dipole_X
56 0.86603 0.50000 0.90575 0.58251 Dipole_Y
57 0.86603 0.50000 0.90575 0.66395 Dipole_Z
58 0.86603 0.50000 0.90575 0.46543 Jurs_DPSA_1
59 0.83205 0.43301 0.79188 0.58574 Jurs_DPSA_2
60 0.86603 0.50000 0.90575 0.00373 Jurs_DPSA_3
61 0.81650 0.40825 0.79188 0.38330 Jurs_FNSA_1
62 0.77460 0.35355 0.65155 0.26875 Jurs_FNSA_2
63 0.86603 0.50000 0.90575 0.32175 Jurs_FNSA_3
64 0.86603 0.50000 0.90575 0.38330 Jurs_FPSA_1
65 0.86603 0.50000 0.90575 0.47944 Jurs_FPSA_2
66 0.86603 0.50000 0.90575 0.00526 Jurs_FPSA_3
67 0.75593 0.33333 0.58973 0.17263 Jurs_PNSA_1
68 0.86603 0.50000 0.90575 0.05428 Jurs_PNSA_2
69 0.86603 0.50000 0.90575 0.12166 Jurs_PNSA_3
70 0.83205 0.43301 0.79188 0.68231 Jurs_PPSA_1
71 0.86603 0.50000 0.90575 0.63597 Jurs_PPSA_2
72 0.86603 0.50000 0.90575 0.33287 Jurs_PPSA_3
73 0.83205 0.43301 0.79188 0.26185 Jurs_RASA
74 0.86603 0.50000 0.90575 0.48129 Jurs_RNCG
75 0.70711 0.28868 0.54612 0.47813 Jurs_RNCS
76 0.86603 0.50000 0.90575 0.28431 Jurs_RPCG
77 0.83205 0.43301 0.79188 0.24377 Jurs_RPCS
78 0.75593 0.33333 0.58973 0.26185 Jurs_RPSA
79 0.86603 0.50000 0.90575 0.89808 Jurs_SASA
80 0.86603 0.50000 0.90575 0.77598 Jurs_TASA
81 0.75593 0.33333 0.58973 0.14787 Jurs_TPSA
82 0.83205 0.43301 0.79188 0.02662 Jurs_WNSA_1
83 0.86603 0.50000 0.90575 0.00547 Jurs_WNSA_2
84 0.86603 0.50000 0.90575 0.00783 Jurs_WNSA_3
85 0.83205 0.43301 0.79188 0.81517 Jurs_WPSA_1
86 0.81650 0.40825 0.83268 0.71672 Jurs_WPSA_2
87 0.83205 0.43301 0.79188 0.59550 Jurs_WPSA_3
88 0.83205 0.43301 0.79188 0.27167 PMI_mag

 89 0.86603 0.50000 0.90575 0.40758 PMI_X
 90 0.86603 0.50000 0.90575 0.25982 PMI_Y
 91 0.83205 0.43301 0.79188 0.27641 PMI_Z
 92 0.86603 0.50000 0.90575 0.83464 Shadow_nu
 93 0.86603 0.50000 0.90575 0.83781 Shadow_Xlength
 94 0.81650 0.40825 0.79188 0.85166 Shadow_XY
 95 0.81650 0.40825 0.79188 0.69125 Shadow_XYfrac
 96 0.86603 0.50000 0.90575 0.90875 Shadow_XZ
 97 0.81650 0.40825 0.88385 0.65466 Shadow_XZfrac
 98 0.70711 0.28868 0.54612 0.46638 Shadow_Ylength
 99 0.81650 0.40825 0.83268 0.80256 Shadow_YZ
100 0.81650 0.40825 0.83268 0.88420 Shadow_YZfrac
101 0.83205 0.43301 0.79188 0.01636 Shadow_Zlength

Table 5: Energy (Kcal/mol) data of the theoretical chemical species formed after the proposed nucleophilic attack[a]





ref	Z	C_2	C_4
1	CH_3CH_2	-3159.1482	-3159.1290
10	C_6H_5	-3458.3197	-3458.3468

[a]. Equilibrium geometry, STO-3G, water solvent continuum model.

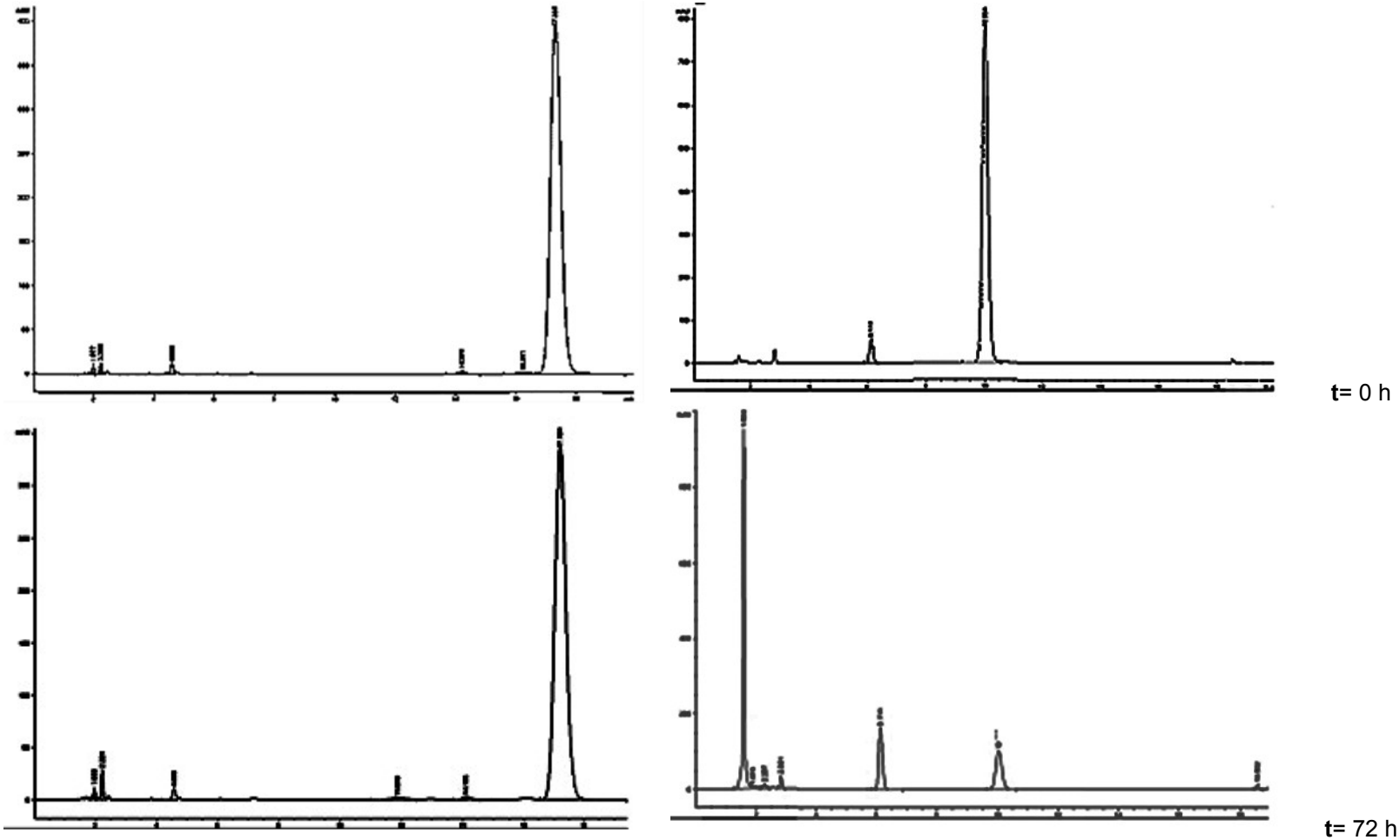


Figure 1: Chromatographic analysis of compounds (a) **4** and (b) **14** taken as representatives of aliphatic and aromatic derivatives respectively.