Supporting Information

Are the Sublimation Thermodynamics of Organic Molecules Predictable?

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Table S1, The sublimation 48 molecule dataset used in this work with reference to the experimental sublimation data next to the refcodes.

Molecule Name	CSD refcode	ΔH sub exp (kJ mol^{-1})	ΔS sub exp (J K^{-1} mol^{-1})	ΔG sub exp (kJ mol^{-1})
acetanilide	ACANIL01[1]	99.80	197.00	40.50
aspirin (acetylsalicylic acid)	ACSALA15[2]	109.70	222.00	43.60
benzoic acid	BENZAC01[3 4]	89.2 ± 0.8	185.5 ± 2.7	33.9 ± 1.1
isophthalic acid	BENZDC01[5]	143.4 ± 1.7	234.3 ± 4.5	73.5 ± 2.2
2,4-dinitrobenzoic acid	BIPJUF[6]	134 ± 3	244 ± 8	61.00
benzophenone	BPHENO03[7 8]	89.1 ± 0.3	182.89	34.60
atenolol	CEZVIN[9]	140.0 ± 3.7	215 ± 9	71.10
2-chlorobenzoic acid	CLBZAC01[3]	106.3 ± 0.5	217.3 ± 1.6	41.5 ± 0.7
4-chlorobenzoic acid	CLBZAP03[3]	105.2 ± 0.7	199.4 ± 2.1	45.8 ± 1.0
2,6-dichloro-4-nitroaniline	CLNOAN[10]	109.2 ± 0.9	203.0 ± 2.6	48.7 ± 1.2
3-fluorobenzoic acid	COVJIG[3 11]	93.6 ± 0.6	199 ± 2	34.4 ± 0.9
naproxen	COYRUD11[12]	128.30	234.23	58.50
2,4-dichlorophenoxy acetic acid	CPXACA[13]	122 ± 5	239 ± 4	51.78
1,8-diphenylnaphthalene	DPNAPH01[14]	126.4± 0.5	230.9 ± 1.4	57.56
2-fluorobenzoic acid	FBENZA02[3 11]	94.7 ± 0.5	198.6 ± 1.6	35.5 ± 0.7
flurbiprofen	FLUBIP[15]	110.20 ± 0.5	191.00 ± 2	53.30
flufenamic acid	FPAMCA17[16]	121.20 ± 0.7	224.00 ± 2	54.30
2,4,6-trinitromesitylene (tnm)	HEXTIN01[17]	103.6 ± 1.2	117.3 ± 1.6	68.6 ± 2.8
4-amino-n-(4-ethylphenyl)benzenesulfonamide	HUNXIY[18]	143.6 ± 0.9	233 ± 2	74.20
4-amino-n-(4-methoxyphenyl)benzenesulfonamide	HUNXOE[18]	124 ± 1	173 ± 2	72.40
4-amino-n-(5-chloro-2-methylphenyl)benzenesulfonamide	HUNXUK[18]	130 ± 1	206 ± 3	68.50
paracetamol	HXACAN27[19]	117.9 ± 0.7	190 ± 2	60.00
ibuprofen	IBPRAC01[20]	115.80	240.00	44.20
4-hydroxybenzoic acid	JOZZIH[21]	121.1 ± 0.4	218.0 ± 1.4	56.1 ± 0.1
tolfenamic acid	KAXXAI01[22]	128.4 ± 0.8	216 ± 4	53.9 ± 0.4
ketoprofen	KEMRUP[8]	110.1 ± 0.5	178 ± 1	57.00
9-methylanthracene	MANTHR01[23]	101.8 ± 1.0	199.7 ± 3.0	42.2 ± 1.3
2,4,6-n-tetranitro-n-methylaniline (tetryl)	MTNANL[17]	133.8 ± 1.6	155.8 ± 2.0	87.3 ± 3.2
1-naphthol	NAPHOL01[12]	91.20	187.50	35.30
4-nitrobenzoic acid	NBZOAC01[21 24]	116.6 ± 0.6	210.0 ± 2.0	54.0 ± 0.1
niflumic acid	NIFLUM10[16]	130.2 ± 0.8	231 ± 2	61.30
nitroguanidine	NTRGUA01[17]	142.7 ± 2.0	116.8 ± 3.4	107.9 ± 4.6
2,2-dimethylsuccinic acid	OLENIC[25]	122.7 ± 2.7	241 ± 8	50.8 ± 3.6
4-methylbenzoic acid	PTOLIC01[26]	98.6 ± 0.6	196.1 ± 1.8	40.1 ± 0.8
phenacetin	PYRAZB21[1]	121.8 ± 0.7	226 ± 2	52.30
5-chloro-2-nitroaniline	RAPKUP[27]	100.8 ± 0.3	200.0 ± 0.9	41.2 ± 0.4
salicylic acid(2 hydroxybenzoic	SALIAC15[28]	96.60 ± 0.8	191.00 ± 3	38.50

acid)				
diclofenac	SIKLIH01[29]	115.60 ± 1.3	222.00 ± 4	49.30
4-cyanobenzoic acid	TAGNAR[21]	111.2 ± 0.4	202.9 ± 1.4	50.7 ± 0.1
o-terphenyl	TERPHO02[30]	103.0 ± 0.4	210.6 ± 1.3	40.2 ± 0.6
2,4,6-trinitroaniline (tna)	TNIOAN[17]	125.3 ± 0.8	140.7 ± 0.3	83.3 ± 1.2
1,3,5-triphenylbenzene	TPHBEN01[31]	147.8 ± 0.7	254 ± 2	72.1 ± 0.9
n-(4-nitrophenyl)-benzene-sulfonamide	UVEMOY[32]	132.5 ± 1.6	217 ± 7	67.70
4-amino-n-(4-nitrophenyl)benzenesulfonamide	UVEMUE[32]	131.4 ± 2.6	179 ± 7	78.00
4-hydroxybenzamide	VIDMAX[33]	117.8 ± 0.6	198 ± 2	58.90
2-methylglutaric acid	XIBVIO[25]	126.5 ± 2.1	259 ± 8	49.2 ± 3.2
mefenamic acid	XYANAC[22]	136.2 ± 0.8	213 ± 3	59.2 ± 0.1
4-heptylbenzoic acid (cr, ii)	ZIKWOF[26]	130.0 ± 0.9	255.3 ± 2.6	53.9 ± 1.2

Table S2. SUB-158 dataset with original references and SMILES structural representations.

Molecule	Enthalpy of sublimation (kJ/mol)	Entropy of sublimation (J/K.mol)	Temperature (K)	G sub (kJ/mol)	CSD reference code	*Reference*	Smiles (in red are duplicates)
(±)-Ibuprofen	115.8 ± 0.6	240 ± 2	298	44.2	IBPRAC01	[20]	CC(C)Cc1ccc(cc1)C(C)C(=O)O
1-([1,1-biphenyl]-4-yl)-naphthalene	138.9 ± 0.8	245.0 ± 2.1	298.15	65.85		[14]	C12=CC=CC(C3=CC=C(C4=CC=CC=C4)C=C3)=C1C=CC=C2
1,2,3,4-tetraphenylnaphthalene	154.2 ± 0.8	246.9 ± 2.1	298.15	80.59		[14]	c15ccccc1c(c2ccccc2)c(c3ccccc3)c(c4ccccc4)c5c6ccccc6
1,2,3-Triphenylbenzene	134.1 ± 0.7	245 ± 3.2	298.15	61 ± 1.5		[34]	c1cc(ccc1)c3c(cccc3c2ccccc2)c4ccccc4
1,2-Diphenylethane	93.2 ± 0.9	211 ± 3	298.15	30.2 ± 1.3	DIBENZ* (polymorphs)	[35]	c1ccc(cc1)CCc2ccccc2
1,3,5-trinitrobenzene (TNB)	107.3±0.6	116.6±0.5	298.15	72.5 ± 1.2	TNBENZ*	[17]	c1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
1,3,5-Triphenylbenzene	147.8 ± 0.7	254 ± 2	298.15	72.1 ± 0.9	TPHBEN*	[31]	c1cc(ccc1)c2cc(cc(c2)c3ccccc3)c4ccccc4
1,4-diphenylnaphthalene	132.5 ± 0.6	237.4 ± 1.6	298.15	70.78		[14]	c2cc(c1ccccc1c2c3ccccc3)c4ccccc4
1,8-di([1,1-biphenyl]-4-yl)naphthalene	178.5 ± 1.1	280.2 ± 2.7	298.15	94.96		[14]	C1(C2=CC=C(C3=CC=CC=C3)C=C2)=C4C(C5=CC=C(C6=CC=CC=C6)C=C5)=CC=CC4=CC=C1
1,8-diphenylnaphthalene	126.4 ± 0.5	230.9 ± 1.4	298.15	57.56	DPNAPH01	[14]	c3cc(c2c(c1ccccc1)ccc2c3)c4ccccc4
1-[(5-Phenylamino)-1,2,4-Thiadiazol-3-yl]-Propan-2-ol	123.8 ± 1.1	220 ± 6	298	58.3		[36]	CC(O)CC1=NSC(NC2=CC=CC=C2)=N1

1-[(5-p-Tolylamino)-1,2,4-thiadiazol-3-yl]-propan-2-ol	142.0 ± 1.6	267 ± 8	298	62.5		[36]	CC(O)CC1=NSC(NC2=CC=C(C)C=C2)=N1
1-[5-(4-Ethoxy-phenylamino)-1,2,4-thiadiazol-3-yl]-propan-2-ol	152.8 ± 2.2	311 ± 7	298	60.2		[36]	CC(O)CC1=NSC(NC2=CC=C(OCC)C=C2)=N1
1-naphthol	91.2	187.5	298.15	35.3	NAPHOL01	[12]	Oc2cccc1ccccc12
1-Nitronaphthalene	95.1 ± 0.4	196.7 ± 1.3	298.15	36.4 ± 1.4		[37]	[O-][N+](=O)c2cccc1ccccc12
2-([1,1-biphenyl]-4-yl)naphthalene	140.2 ± 1.3	228.0 ± 3.6	298.15	72.22		[38]	C1(C2=CC=C(C3=CC=CC=C3)C=C2)=CC=C4C=CC=CC4=C1
2,2-Dimethylglutaric acid	126.8 ± 2.1	257 ± 9	298.15	50.2 ± 3.4		[25]	O=C(O)CCC(C(=O)O)(C)C
2,2-Dimethylsuccinic acid	122.7 ± 2.7	241 ± 8	298.15	50.8 ± 3.6	OLENIC	[25]	O=C(O)CC(C(=O)O)(C)C
2,4,6-N-tetranitro-N-methylaniline (Tetryl)	133.8±1.6	155.8±2.0	298.15	87.3±3.2	MTNANL	[17]	CN(c1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
2,4,6-trinitroaniline (TNA)	125.3 ± 0.8	140.7±0.3	298.15	83.3±1.2	TNIOAN	[17]	c1c(cc(c(c1[N+](=O)[O-])N)[N+](=O)[O-])[N+](=O)[O-]
2,4,6-trinitro-m-cresol (TNC)	111.2± 2.1	126.0± 5.0	298.15	73.6±6.7		[17]	O=[N+]([O-])c1cc(c(c([N+]([O-])=O)c1O)C)[N+]([O-])=O
2,4,6-trinitromesitylene (TNM)	103.6±1.2	117.3± 1.6	298.15	68.6±2.8	HEXTIN01	[17]	Cc1c(c(c(c(c1[N+](=O)[O-])C)[N+](=O)[O-])C)[N+](=O)[O-]
2,4,6-trinitro-m-phenylene diamine (DATB)	143.5±2.3	148.5 ± 4.5	298.15	99.2±5.8	DATNBZ	[17]	c1c(c(c(c(c1[N+](=O)[O-])N)[N+](=O)[O-])N)[N+](=O)[O-]

2,4,6-trinitro-m-xylene (TNX)	129.8±1.1	167.0±1.8	298.15	80.0±2 .7	TNOXYL*	[17] Cc1c(cc(c(c1[N+](=O)[O-])C)[N+](=O)[O-])[N+](=O)[O-]
2,4,6-trinitrophenol (picric acid)	105.1±1.6	99.1±1.8	298.15	75.6±3.8	PICRAC*	[17] O=[N+]([O-])c1cc(cc([N+]([O-])=O)c1O)[N+]([O-])=O
2,4,6-trinitroresorcinol (styphnic acid, TNR)	120.8±1.1	135.0± 1.8	298.15	80.6±2.5		[17] c1c(c(c(c(c1[N+](=O)[O-])O)[N+](=O)[O-])O)[N+](=O)[O-]
2,4,6-trinitrotoluene (TNT)	113.2±1.5	146.2±1.3	298.15	69.6±3.0	ZZZMUC*	[17] Cc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
2,4-dichlorophenoxy acetic acid	122 ± 5	239± 4	298	51.78	CPXACA	[13] Clc1cc(Cl)ccc1OCC(=O)O
2,4-dichlorophenoxy butyric acid	137 ± 10	294± 4	298	50.39		[13] Clc1cc(Cl)ccc1OC(C(=O)O)CC
2,4-dichlorophenoxy propionic acid	127 ± 8	263± 4	298	49.63		[13] Clc1cc(Cl)ccc1OC(C(=O)O)C
2,4-Dinitrobenzoic acid	134 ± 3	244 ± 8	298.15	61.00	BIPJUF	[6] O=[N+]([O-])c1cc(ccc1C(=O)O)[N+]([O-])=O
2,5-Dichloro-4-nitroaniline	114.3 ± 0.9	209.9 ± 2.6	298.15	51.7 ± 1.2		[10] Clc1c(cc(Cl)c(N)c1)[N+]([O-])=O
2,6-Dichloro-4-nitroaniline	109.2 ± 0.9	203.0 ± 2.6	298.15	48.7 ± 1.2	CLNOAN	[10] Clc1cc(cc(Cl)c1N)[N+]([O-])=O
2-acetaminophen	121.8±0.9	227±3	298	52.8		[19] O=C(Nc1ccccc1O)C
2-Bromobenzoic acid	108.5 ± 0.6	215.8 ± 1.9	298.15	44.1 ± 0.8	BRBZAC	[3] O=C(O)c1ccccc1Br
2-Chlorobenzoic acid	106.3 ± 0.5	217.3 ± 1.6	298.15	41.5 ± 0.7	CLBZAC01	[3] O=C(O)c1ccccc1Cl
2-Ethylanthracene	107.6 ± 0.6	203.0 ± 1.7	298.15	47.1 ± 0.8		[23] c3ccc2cc1ccc(cc1cc2c3)CC
2-Fluorobenzoic acid	94.7 ± 0.5	198.6 ± 1.6	298.15	35.5 ± 0.7	FBENZA02	[3 11] O=C(O)c1ccccc1F

2-Iodobenzoic acid	113.8 ± 1.0	221.3 ± 3.0	298.15	47.8 ± 1.4	OIBZAC01	[3 11]	O=C(O)c1ccccc1I
2-methoxybenzoic acid	110.7 ± 0.8	225 ± 2	298	43.7		[39]	O=C(O)c1ccccc1OC
2-methyl-3-nitrobenzoic acid	119.5 ± 2.3	227 ± 9	298.15	51.8 ± 3.5		[40]	O=[N+]([O-])c1cccc(C(=O)O)c1C
2-methyl-6-nitrobenzoic acid	120.0 ± 2.2	228 ± 9	298.15	52.0 ± 3.5		[40]	O=C(O)c1c(cccc1C)[N+]([O-])=O
2-Methylglutaric acid	126.5 ± 2.1	259 ± 8	298.15	49.2 ± 3.2	XIBVIO	[25]	O=C(O)CCC(C(=O)O)C
2-phenylnaphthalene	107.8 ± 0.6	211.5	298.15	44.74		[38]	c1cc(cc2ccccc12)c3ccccc3
2-Thiopheneacetamide	109.2 ± 0.5	211.6 ± 1.4	298.15	46.1 ± 0.6		[41]	O=C(N)Cc1sccc1
2-Thiophenecarboxamide	107.1 ± 0.4	204.6 ± 1.3	298.15	46.1 ± 0.6	TUKPOF	[41]	O=C(N)c1sccc1
3-(2-methoxyphenyl) propionic acid	117.8 ± 1.4	245 ± 6	298.15	44.8 ± 2.3		[42]	O=C(O)CCc1ccccc1OC
3-(3,4-dimethoxyphenyl) propionic acid	143.6 ± 2.2	290 ± 9	298.15	57.0 ± 3.4		[42]	O=C(O)CCc1cc(OC)c(OC)cc1
3-(4-methoxyphenyl) propionic acid	124.5 ± 1.7	255 ± 7	298.15	48.6 ± 2.7		[42]	COc1ccc(cc1)CCC(=O)O
3,4-Dinitrobenzoic acid	129 ± 3	234 ± 8	298.15	59.00	YADKOF	[6]	O=[N+]([O-])c1cc(ccc1[N+]([O-])=O)C(=O)O
3-acetaminophen	111±1	179±3	298	56.4		[19]	CC(=O)Nc1cccc(c1)O
3-Bromobenzoic acid	105.9 ± 0.7	209.3 ± 2.1	298.15	43.5 ± 0.9	MBBNZA	[3]	O=C(O)c1cc(Br)ccc1
3-Chlorobenzoic acid	102.5 ± 0.5	205.8 ± 1.6	298.15	41.1 ± 0.7	MCBZAC01	[3]	O=C(O)c1cc(Cl)ccc1
3-Fluorobenzoic acid	93.8 ± 0.5	199.4 ± 1.6	298.15	34.4 ± 0.7	COVJIG01	[3 11]	O=C(O)c1cc(F)ccc1
3-hydroxybenzoic acid	105.2 ± 0.8	180 ± 2	298	50.6	BIDLOP*	[28]	O=C(O)c1cc(O)ccc1
3-Iodobenzoic acid	112.2 ± 0.8	213.6 ± 2.4	298.15	48.5 ± 1.1	ZZZOAE	[3 11]	O=C(O)c1cc(I)ccc1
3-methoxybenzoic acid	114.7 ± 0.8	245 ± 3	298	41.8		[39]	O=C(O)c1cc(OC)ccc1
3-methyl-2-nitrobenzoic acid	124.4 ± 2.7	228 ± 11	298.15	56.4 ± 4.2		[40]	Cc1cccc(c1[N+](=O)[O-])C(=O)O
3-methyl-4-nitrobenzoic acid	119.3 ± 2.5	218 ± 10	298.15	54.3 ± 3.9		[40]	O=C(O)C1=CC=C([N+]([O-])=O)C(C)=C1

3-Phenylpropiolic acid	105.0 ± 1.4	211 ± 6	298.15	42.1 ± 2.3	PHPLAC*	[35]	O=C(C#Cc1ccccc1)O
3-phenylpropionic acid	102.4 ± 0.8	223 ± 3	298.15	35.9 ± 1.2		[42]	OC(=O)CCc1ccccc1
4-(acetylamino)benzoic acid	148.9 ± 1.1	243.2 ± 3.8	298.15	76.4 ± 0.3	DIXFAR02	[21]	CC(=O)Nc1ccc(cc1)C(=O)O
4-(dimethylamino)benzoic acid	120.3 ± 0.5	213.0 ± 1.7	298.15	56.8 ± 0.1		[21]	O=C(O)c1ccc(N(C)C)cc1
4-(methylamino)benzoic acid (cr I)	123.9 ± 0.4	230.1 ± 1.4	298.15	55.3 ± 0.1	BUFDOW	[21]	O=C(O)c1ccc(NC)cc1
4-acetoxybenzoic acid (cr II)	116.1 ± 0.3	216.7 ± 1.1	298.15	51.5 ± 0.1		[21]	O=C(Oc1ccc(cc1)C(=O)O)C
4-aminobenzoic acid	115.1 ± 1	205.9	298.15	53.7	AMBNAC*	[21 43]	O=C(O)c1ccc(N)cc1
4-amino-N-(2,3-dichlorophenyl)-benzene-sulfonamide	141.1 ± 0.7	266 ± 2	298	61.7		[44]	c1cc(c(c(c1)Cl)Cl)NS(=O)(=O)c2ccc(cc2)N
4-amino-N-(2,5-dichlorophenyl)-benzene-sulfonamide	155.4 ± 1.6	268 ± 4	298	75.7		[44]	Clc2ccc(Cl)cc2NS(=O)(=O)c1ccc(N)cc1
4-amino-N-(3,4-dichlorophenyl)-benzene-sulfonamide	167.5 ± 3.6	274 ± 8	298	85.8		[44]	Clc2ccc(NS(=O)(=O)c1ccc(N)cc1)cc2Cl
4-amino-N-(4-chlorophenyl)-benzene-sulfonamide	134.1 ± 1.2	202 ± 3	298	74.0		[44]	Clc2ccc(NS(=O)(=O)c1ccc(N)cc1)cc2
4-amino-N-(4-cyanophenyl)benzenesulfonamide	168.3 ± 2.3	269 ± 9	298	88.0	UVENAL	[32]	O=S(=O)(Nc1ccc(cc1)C#N)c2ccc(N)cc2
4-amino-N-(4-ethylphenyl)benzenesulfonamide	143.6 ± 0.9	233 ± 2	298	74.2	HUNXIY	[18]	O=S(=O)(Nc1ccc(cc1)CC)c2ccc(N)cc2
4-Amino-N-(4-methoxyphenyl)benzenesulfonamide	124 ± 1	173 ± 2	298	72.4	HUNXOE	[18]	O=S(=O)(Nc1ccc(OC)cc1)c2ccc(N)cc2
4-Amino-N-(4-nitrophenyl)benzenesulfonami	131.4 ± 2.6	179 ± 7	298	78.0	UVEMUE	[32]	O=S(=O)(Nc1ccc(cc1)[N+]([O-

de							])=O)c2ccc(N)cc3
4-Amino-N-(5-chloro-2-methylphenyl)benzenesulfonamide	130 ± 1	206 ± 3	298	68.5	HUNXUK	[18]	Cc1ccc(cc1NS(=O)(=O)c2ccc(cc2)N)Cl
4-Bromoacetanilide	110 ± 4	204 ± 10	298.15	49 ± 6		[45]	Brc1ccc(NC(=O)C)cc1
4-Bromobenzoic acid	110.1 ± 0.8	204.4 ± 2.5	298.15	49.0 ± 1.1	BRBZAP*	[3]	O=C(O)c1ccc(Br)cc1
4-Butylbenzoic acid (cr, II)	110.5±0.7	221.4±2.1	298.15	44.5±0.9		[26]	O=C(O)c1ccc(cc1)CCCC
4-chloro-3-nitroaniline	105.4 ± 0.4	205.9 ± 1.2	298.15	44.0 ± 0.5		[27]	O=[N+]([O-])c1cc(ccc1Cl)N
4-Chlorobenzoic acid	105.2 ± 0.7	199.4 ± 2.1	298.15	45.8 ± 1.0	CLBZAP03	[3]	O=C(O)c1ccc(Cl)cc1
4-cyanobenzoic acid	111.2 ± 0.4	202.9 ± 1.4	298.15	50.7 ± 0.1	TAGNAR	[21]	N#Cc1ccc(C(=O)O)cc1
4-Ethylbenzoic acid	101.2±0.8	206.6±2.4	298.15	39.6±1.1		[26]	O=C(O)c1ccc(cc1)CC
4-Fluorobenzoic acid	94.1 ± 1.1	191.6 ± 3.1	298.15	37.0 ± 1.4	PFBZAD*	[3 46]	O=C(O)c1ccc(F)cc1
4-Heptylbenzoic acid (cr, II)	130.0±0.9	255.3±2.6	298.15	53.9±1.2	ZIKWOF	[26]	O=C(O)c1ccc(cc1)CCCCCCC
4-Hexylbenzoic acid	123.6±1.0	245.1±2.8	298.15	50.5±1.3	APOCOY	[26]	O=C(O)c1ccc(cc1)CCCCCC
4-Hydroxybenzamide	117.8 ± 0.6	198 ± 2	298	58.9	VIDMAX	[33]	O=C(c1ccc(O)cc1)N
4-hydroxybenzoic acid	121.1 ± 0.4	218.0 ± 1.4	298.15	56.1 ± 0.1	JOZZIH	[21]	c1cc(ccc1C(=O)O)O
4-Iodobenzoic acid	114.2 ± 0.9	206.1 ± 2.8	298.15	52.8 ± 1.2	BENMOW	[3 11]	O=C(O)c1ccc(I)cc1
4-methoxybenzoic acid	111.2 ± 0.6	212.0 ± 2.0	298.15	48.0 ± 0.1	ANISIC*	[21 47]	COc1ccc(cc1)C(O)=O
4-methoxycarbonylbenzoic acid	123.5 ± 0.5	228.4 ± 1.7	298.15	55.4 ± 0.1		[21 5]	O=C(OC)c1ccc(C(=O)O)cc1
4-methyl-3-nitrobenzoic acid	118.6 ± 2.5	219 ± 10	298.15	53.3 ± 3.9		[40]	O=[N+]([O-])c1cc(ccc1C)C(=O)O
4-Methylbenzoic acid	98.6 ± 0.7	196.1±1.8	298.15	40.1±0.8	PTOLIC01	[26]	Cc1ccc(cc1)C(=O)O
4-nitrobenzoic acid	116.6 ± 0.6	210.0 ± 2.0	298.15	54.0 ± 0.1	NBZOAC02	[21 24]	O=[N+]([O-])c1ccc(C(=O)O)cc1
4-Octylbenzoic acid (cr, II)	134.7±1.5	262.5±4.2	298.15	56.4±1.9		[26]	O=C(O)c1ccc(cc1)CCCCCCCC (cr2)

4-Octylbenzoic acid (cr, III)	135.4±1.3	264.1±3.6	298.15	56.6±1.7		[26]	O=C(O)c1ccc(cc1)CCCCCCCC (cr3)
4-Pentylbenzoic acid	118.2±1.0	236.8±2.9	298.15	47.6±1.3		[26]	O=C(O)c1ccc(cc1)CCCCC
4-Propylbenzoic acid (cr, II)	109.1±0.8	219.0±2.6	298.15	43.8±1.1		[26]	O=C(O)c1ccc(cc1)CCC
5-chloro-2-nitroaniline	100.8 ± 0.3	200.0 ± 0.9	298.15	41.2 ± 0.4	RAPKUP	[27]	O=[N+]([O-])c1c(cc(Cl)cc1)N
5-methyl-2-nitrobenzoic acid	118.7 ± 2.2	225 ± 9	298.15	51.6 ± 3.5		[40]	O=[N+]([O-])c1c(cc(cc1)C)C(=O)O
9,10-Dimethylanthracene	113.0 ± 1.7	204.3 ± 4.6	298.15	52.1 ± 2.2	DMANTR	[23]	c23c(c1ccccc1c(c2cccc3)C)C
9-Methylanthracene	101.8 ± 1.0	199.7 ± 3.0	298.15	42.2 ± 1.3	MANTHR01	[23]	Cc1c2ccccc2cc3c1cccc3
9-Nitroanthracene	115.4 ± 0.6	211.1 ± 1.6	298.15	52.5 ± 0.8	NTRANT	[37]	[O-][N+](=O)c2c3c(cc1c2cccc1)cccc3
Acetanilide	99.8 ± 0.8	197 ± 2	298	40.5	ACANIL01	[1]	O=C(Nc1ccccc1)C
ametryn (N-ethyl-N¢-(1-methylethyl)-6-(methylthio)-2,4-diamine-1,3,5-triazine)	121 ± 5	244 ± 10	298	48.29		[48]	S(c1nc(nc(n1)NC(C)C)NCC)C
Anthracene	100.2 ± 0.4	183 ± 1	298.15	45.6 ± 0.3	ANTCEN*	[31]	c1ccc2cc3ccccc3cc2c1
aspirin (acetylsalicylic acid)	109.7 ± 0.5	222 ± 2	298	43.6	ACSALA09	[2]	CC(=O)Oc1ccccc1C(=O)O
atenolol (2-{4-[2-Hydroxy-3-(isopropylamino)propoxy]phenyl}acetamide)	140.0 ± 3.7	215 ± 9	298	71.1	CEZVIN	[9]	CC(C)NCC(COc1ccc(cc1)CC(=O)N)O
Benzanthrone	125.6 ± 0.6	211 ± 2	298.15	62.7 ± 0.8	BATCAA*	[31]	O=C3c4c(c2cccc1cccc3c12)cccc4
Benzil (Benzyl) (TdS was given in this reference)	98.4 ± 1.1	188.2550336	298	42.3	BENZIL*	[49] [8]	c1ccc(cc1)C(=O)C(=O)c2ccccc2
Benzoic acid	89.2 ± 0.8	185.5 ± 2.7	298.15	33.9 ± 1.1	BENZAC*	[3] [4]	c1ccc(cc1)C(=O)O

Benzophenone (TdS was given in this reference)	89.1 ± 0.3	182.885906	298	34.6	BPHENO01	[7 8]	O=C(c1ccccc1)c2ccccc2
cyclotrimethylenetrinitramine (RDX)	134.3±0.7	153.6±0.4	298.15	88.5±1.2		[17]	C1N(CN(CN1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
Diclofenac Form 2	115.6 ± 1.3	222 ± 4	298	49.3	SIKLIH01	[29]	c1ccc(c(c1)CC(=O)O)Nc2c(cccc2Cl)Cl
Diflunisal	120.1 ± 0.6	210 ± 2	298	57.6	FAFWIS*	[15]	O=C(O)c1cc(ccc1O)c2ccc(F)cc2F
dimethyl isophthalate	100.9 ± 0.2	224.6 ±0.7	298.15	33.9		[5 50]	O=C(OC)c1cccc(C(=O)OC)c1
dimethyl terephthalate	104.6 ±0.3	217.00	298.15	39.9	DMTPAL	[5]	O=C(OC)c1ccc(cc1)C(=O)OC
Diphenylamine	110.0 ± 1.0	211 ± 4	298	35.9 ± 0.1	QQQBVP*	[22]	c1ccc(cc1)Nc2ccccc2
Diphenylmethane (TdS was given in this reference)	82.5 ± 0.6	186.2416107	298	27	ZZZMKS*	[49 8]	c1c(cccc1)Cc2ccccc2
Fenbufen	155.0 ± 0.8	272 ± 3	298	74.0	SAFNIW	[15]	O=C(O)CCC(=O)c2ccc(c1ccccc1)cc2
Flufenamic acid	121.2 ± 0.7	224 ± 2	298	54.3	FPAMCA	[16]	FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)O
flurbiprofen	110.2 ± 0.5	191.0 ± 2	298	53.3	FLUBIP	[15]	Fc2cc(ccc2c1ccccc1)C(C(=O)O)C
Hexachlorobenzene	81 ± 6	114 ± 6	298.15	47 ± 6	HCLBNZ*	[51]	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl
Imidazolidin-2-one	96.6 ± 0.8	181.2 ± 3.3	298.15	42.6 ± 1.2		[52]	C1CNC(=O)N1
isophthalic acid	143.4 ±1.7	234.3 ±4.5	298.15	73.5 ± 2.2	BENZDC*	[5]	O=C(O)c1cccc(C(=O)O)c1
Ketoprofen	110.1 ± 0.5	178 ± 1	298	57	KEMRUP	[8]	CC(c1cccc(c1)C(=O)c2ccccc2)C(=O)O
Lindane	96 ± 9	156 ± 9	298.15	50 ± 6		[51]	Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H]1Cl
Mefenamic acid (form 1)	136.2 ± 0.8	213 ± 3	298	59.2 ± 0.1	XYANAC	[22]	O=C(O)c2c(Nc1cccc(c

							1C)C)cccc2
Methylsuccinic acid	121.7 ± 2.3	245 ± 6	298.15	48.6 ± 2.9	DLMSUC*	[25]	O=C(O)CC(C(=O)O)C
monomethyl isophthalate	125.6 ± 1.0	238.0 ± 3	298.15	54.6 ± 1.3		[5]	O=C(OC)c1cccc(C(=O)O)c1
monomethyl phthalate	117.9 ± 0.8	238.2 ±1.7	298.15	46.9 ± 1.0		[5]	O=C(OC)c1ccccc1C(=O)O
m-Terphenyl	118.6 ± 0.7	233.1 ± 2.2	298.15	49.1 ± 1.0	ZZZMTW	[30]	c1cc(ccc1)c2cccc(c2)c3ccccc3
N - phenyl - anthranilic acid *(N-Phenyl 2-Aminobenzoic Acid)*	126.0 ± 1.3	193 ± 6	298	58.9 ± 0.5	QQQBTY*	[22]	O=C(O)c2ccccc2Nc1ccccc1
N-(2,3-dichlorophenyl)-benzene-sulfonamide	124.9 ± 1.6	237 ± 5	298	54.1		[53]	Clc2c(NS(=O)(=O)c1ccccc1)cccc2Cl
N-(2-chlorophenyl)-benzene-sulfonamide	114 ±1	213 ± 3	298	50.4		[53]	Clc2ccccc2NS(=O)(=O)c1ccccc1
N-(4-chlorophenyl)-benzene-sulfonamide	98.6 ± 1.9	163 ± 5	298	49.9		[53]	Clc2ccc(NS(=O)(=O)c1ccccc1)cc2
N-(4-nitrophenyl)-benzene-sulfonamide	132.5 ± 1.6	217 ± 7	298	67.7	UVEMOY	[32]	O=S(=O)(Nc1ccc(cc1)[N+]([O-])=O)c2ccccc2
N,N-Trimethyleneurea	113.4 ± 0.7	200.2 ± 4.9	298.15	53.7 ± 1.6		[52]	O=C1NCCCN1
Naphthalene	72.70 ± 0.04	168.1 ± 0.1	298.15	22.58	NAPHTA*	[54]	c1ccc2ccccc2c1
naproxen	128.3	234.23	298.15	58.5	COYRUD11	[12]	C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O
Niflumic acid	130.2 ± 0.8	231 ± 2	298	61.3	NIFLUM10	[16]	FC(F)(F)c1cc(ccc1)Nc2ncccc2C(=O)O
Nitroguanidine (2-Nitroguanidine)	142.7±2.0	116.8± 3.4	298.15	107.9±4.6	NTRGUA	[17]	C(=N)(N)N[N+](=O)[O-]
N-phenylbenzenesulfonamide	111.5 ± 1.1	195 ± 6	298	53.4	TEQYUK*	[32]	O=S(=O)(Nc1ccccc1)c2ccccc2
o-Terphenyl	103.0 ± 0.4	210.6 ± 1.3	298.15	40.2 ± 0.6	TERPHO*	[30]	c1cc(ccc1)c3ccccc3c2ccccc2

Paracetamol	117.9±0.7	190±2	298	60.00	HXACAN04	[19]	CC(=O)Nc1ccc(cc1)O
pentaerythritoltetranitrate (PETN)	150.4±1.3	215.4±2.6	298.15	86.2±2.9		[17]	C(C(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-])O[N+](=O)[O-]
Phenacetin	121.8 ± 0.7	226 ± 2	298	52.3	PYRAZB21	[1]	O=C(Nc1ccc(OCC)cc1)C
Phenanthrene	92.5 ± 0.4	182 ± 1	298.15	38.2 ± 0.3	PHENAN*	[31]	c1ccc2c(c1)ccc3c2cccc3
phthalic acid	143.3 ± 1.5	248.4 ±4.1	298.15	69.2 ±1.9	PHTHAC*	[5]	c1ccc(c(c1)C(=O)O)C(=O)O
Pindolol	146 ± 1.2	251 ± 3	298	68.00	PINDOL	[9]	OC(CNC(C)C)COc1cccc2c1ccn2
p-Terphenyl	125.6 ± 0.8	224.3 ± 2.2	298.15	58.7 ± 1.0	TERPHE*	[30]	c1cc(ccc1)c2ccc(cc2)c3ccccc3
salicylic acid (2-hydroxybenzoic acid)	96.6 ± 0.8	191 ± 3	298	38.5	SALIAC03	[28]	c1ccc(c(c1)C(=O)O)O
simetryn (N,N¢-diethyl-6-(methylthio)-2,4-diamine-1,3,5-triazine)	117 ± 5	243 ± 10	298	44.59		[48]	S(c1nc(nc(n1)NCC)NCC)C
Succinic acid	123.2 ± 2.6	232 ± 8	298.15	54.0 ± 3.5	SUCACB*	[25]	C(CC(=O)O)C(=O)O
sym-cyclotetramethylene-tetramitramine (HMX)	161.0±0.3	152.7± 4.0	298.15	115.5±1.9		[17]	C1N(CN(CN(CN1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
terbutryn (N-(1,1-dimethylethyl)-N¢-ethyl-6-(methylthio)-2,4-diamine-1,3,5-triazine)	112 ± 5	214 ± 10	298	48.23		[48]	S(c1nc(nc(n1)NC(C)(C)C)NCC)C
terephthalic acid	152.2 ± 1.7	237.2 ±4.8	298.15	81.5 ± 2.2	TEPHTH*	[5]	c1cc(ccc1C(=O)O)C(=O)O
Tolfenamic acid (form 1)	128.4 ± 0.8	216 ± 4	298	53.9 ± 0.4	KAXXAI*	[22]	Clc2cccc(Nc1ccccc1C(

							=O)O)c2C
Triphenyl methane (TdS was given in this reference)	100.1 ± 0.6	187.2483221	298	44.3	TPHMET*	[49] [8]	c1c(cccc1)C(c2ccccc2)c3ccccc3

Table S3. The names number and description of all descriptors used.[55–59]

Category	Number of descriptors in the category	Name	Description
Enthalpy of sublimation	1	ΔH sub kJ/mol	The enthalpy of sublimation Ulatt - 2RT
Entropy of the crystal	1	scrys (J K-1 mol-1)	The entropy of the crystal calculated by DMACRYS
Entropy of gas phase rotation	1	srot (J mol-1 K-1)	The rotational entropy of a single molecule in the gas phase, as calculated by Gaussian 09
Entropy of translation	1	strans (J mol-1 K-1)	The translation entropy of a single molecule in the gas phase, as calculated by Gaussian 09
Entropy of sublimation	1	ΔS sub J mol-1 K-1	The entropy of sublimation ΔS sub = Scrys - (Srot + Strans)
Free energy of sublimation	1	ΔG sub	The free energy of sublimation ΔG sub = ΔH sub - TΔS sub
XlogP	1	XLogP:XLogP	Atom type calculation estimating Log P
Number of rotatable bonds	1	RotatableBondsCount:nRotB	Count the number of rotatable bonds
Molecular weight	1	MolWt:MWt	Calculation of molecular weight
Longest aliphatic chain	1	LongestAliphaticChain:nAtomLAC	The number of atoms in the longest aliphatic group
Largest Pi system	1	LargestPiSystem:nAtomP	The number of atoms in the largest pi system
Largest chain	1	LargestChain:nAtomLC	The number of atoms in the longest chain of atoms

Hydrogen bond donor count	1	HBondDonorCount:nHBDon	A count of the number H bond donors
Hydrogen bond acceptor count	1	HBondAcceptorCount:nHBAcc	A count of the number H bond acceptors
Number of Carbon atoms	1	No. of C	Count of the number of Carbon atoms
Number of Hydrogen atoms	1	No. of H	Count of the number of Hydrogen atoms
Number of Fluorine atoms	1	No. of F	Count of the number of Fluorine atoms
Number of Chlorine atoms	1	No. of Cl	Count of the number of Chlorine atoms
Number of Nitrogen atoms	1	No. of N	Count of the number of Nitrogen atoms
Number of Oxygen atoms	1	No. of O	Count of the number of Oxygen atoms
Number of Sulphur atoms	1	No. of S	Count of the number of Sulphur atoms
Carbon types	7	CarbonTypes:C1SP1	Topologically describes the connectivity between Carbon atoms
		CarbonTypes:C1SP2	
		CarbonTypes:C2SP2	
		CarbonTypes:C1SP3	
		CarbonTypes:C2SP3	
		CarbonTypes:C3SP3	
		CarbonTypes:C4SP3	
Number of bonds	1	BondCount:nB	Counts the number of bonds
Number of basic groups	1	BasicGroupCount:nBase	Counts the number of basic groups
Number of atoms	1	AtomCount:nAtom	Counts the number of atoms
Number of aromatic bonds	1	AromaticBondsCount:nAromBond	Counts the number of aromatic bonds

Number of aromatic atoms	1	AromaticAtomsCount:naAromAtom	Counts the number of aromatic atoms
Number of acid groups	1	AcidicGroupCount:nAcid	Counts the number of acid groups
Fraction of Carbon atom hybrids	1	HybridizationRatio:HybRatio	Calculates the fraction of Carbon atoms sp3 to sp2 hybidised
Topological descriptor	1	EccentricConnectivityIndex:ECCEN	Topological descriptor for atom distances and adjacency
Atomic polarizability differences	1	BPol:bpol	The sum of squared difference between atomic polarizabilities
Intermolecular interaction	6	BCUT:BCUTw-1l	Used for defining chemical diversity by encoding intermolecular interactions
		BCUT:BCUTw-1h	
		BCUT:BCUTc-1l	
		BCUT:BCUTc-1h	
		BCUT:BCUTp-1l	
		BCUT:BCUTp-1h	
Atomic polarizability	1	APol:apol	Sum of the atomic polarizabilities
Complexity descriptor	1	ZagrebIndex:Zagreb	Sum of the squares of an atom's degree (number of heavy atoms bonded) over all heavy atoms, complexity descriptor
Branching Descriptor	5	WeightedPath:WTPT-1	Calculated the path lengths between different atoms, branching descriptor
		WeightedPath:WTPT-2	
		WeightedPath:WTPT-3	
		WeightedPath:WTPT-4	
		WeightedPath:WTPT-5	
Topological graph	1	PetitjeanShapeIndex:topoShape	Calculates a values based on radii and diameters within a molecule to give information on the topology of a molecule

Elements spread	17	MDE:MDEC-11	Calculate the molecular distance edge between the same elements in a molecule
		MDE:MDEC-12	
		MDE:MDEC-13	
		MDE:MDEC-14	
		MDE:MDEC-22	
		MDE:MDEC-23	
		MDE:MDEC-24	
		MDE:MDEC-33	
		MDE:MDEC-34	
		MDE:MDEO-11	
		MDE:MDEO-12	
		MDE:MDEN-11	
		MDE:MDEN-12	
		MDE:MDEN-13	
		MDE:MDEN-22	
		MDE:MDEN-23	
		MDE:MDEN-33	
Molecular shape	3	KappaShapeIndices:Kier1	Compares a molecules graph with a minimal and maximal graph
		KappaShapeIndices:Kier2	
		KappaShapeIndices:Kier3	
Fragments of a molecule	8	ChiCluster:SC-3	Isomorphism code is used to identify molecular subgraphs of clusters from the main molecular graph
		ChiCluster:SC-4	
		ChiCluster:SC-5	
		ChiCluster:SC-6	
		ChiCluster:VC-3	
		ChiCluster:VC-4	
		ChiCluster:VC-5	

		ChiCluster:VC-6	
Fragments of a molecule	1	ChiChain:VCH-7	Isomorphism code is used to identify molecular subgraphs of chain from the main molecular graph
Fragments of a molecule	16	ChiPath:SP-0	Isomorphism code is used to identify molecular subgraphs of paths from the main molecular graph
		ChiPath:SP-1	
		ChiPath:SP-2	
		ChiPath:SP-3	
		ChiPath:SP-4	
		ChiPath:SP-5	
		ChiPath:SP-6	
		ChiPath:SP-7	
		ChiPath:VP-0	
		ChiPath:VP-1	
		ChiPath:VP-2	
		ChiPath:VP-3	
		ChiPath:VP-4	
		ChiPath:VP-5	
		ChiPath:VP-6	
		ChiPath:VP-7	
Molecular complexity descriptor	1	FMF:FMF	Ratio of the number of heavy atoms in a Murcko framework (ring system defined as rings sharing an edge, a framework is defined as a union of rings with linker atoms) and all heavy atoms
Fragment complexity	1	FragmentComplexity:fragC	Represents the complexity of a fragment in terms of bond number number of hydrogen atoms and hetroatoms
Fragments descriptor	22	KierHallSmarts:khs.sCH3	A fragment count descriptor based on fragmentation via E-states
		KierHallSmarts:khs.ssCH2	
		KierHallSmarts:khs.aaCH	
		KierHallSmarts:khs.sssCH	

		KierHallSmarts:khs.tsC	
		KierHallSmarts:khs.dssC	
		KierHallSmarts:khs.aasC	
		KierHallSmarts:khs.aaaC	
		KierHallSmarts:khs.ssssC	
		KierHallSmarts:khs.sNH2	
		KierHallSmarts:khs.dNH	
		KierHallSmarts:khs.ssNH	
		KierHallSmarts:khs.tN	
		KierHallSmarts:khs.aaN	
		KierHallSmarts:khs.sssN	
		KierHallSmarts:khs.ddsN	
		KierHallSmarts:khs.sOH	
		KierHallSmarts:khs.dO	
		KierHallSmarts:khs.ssO	
		KierHallSmarts:khs.sF	
		KierHallSmarts:khs.ddssS	
		KierHallSmarts:khs.sCl	
LogP calculated	1	MannholdLogP:MLogP	Calculates logP using an atomic contribution based method
Toplogicial descriptor	1	PetitjeanNumber:PetitjeanNumber	A measure of the maximum separating distance between the two most distant vertices
Failures of the rule of 5	1	RuleOfFive:LipinskiFailures	Counts the number of Lipinski's rules a molecule does not meet.
Toplogicial descriptor	1	TPSA:TopoPSA	Estimate of the topological polar surface area
Topological descriptor	1	VAdjMa:VAdjMat	1 + log2 x here x is the number of heavy atom bonds to heavy atoms
Topological descriptor	2	WienerNumbers:WPATH	Information is encoded on the size of paths and polarity
		WienerNumbers:WPOL	

Toplogicial and branching descriptor	6	ChiPathCluster:SPC-4	Descriptors providing information on molecular branching and size
		ChiPathCluster:SPC-5	
		ChiPathCluster:SPC-6	
		ChiPathCluster:VPC-4	
		ChiPathCluster:VPC-5	
		ChiPathCluster:VPC-6	
Fragments of a molecule	4	ChiChain:SCH-6	Isomorphism code is used to identify molecular subgraphs of chain from the main molecular graph

Table S4. Predicted values by DMACRYS-G09

Molecule chemical name	Refcode	ΔH sub (kJ/mol)	ΔS sub (J/mol. K)	T (k)	TΔS (kJ/mol)	ΔG sub (kJ/mol)
Acetanilide	ACANIL01	88.57	191.00	298	56.92	31.65
aspirin (acetylsalicylic acid)	ACSALA15	112.76	202.68	298	60.40	52.36
Benzoic acid	BENZAC01	90.85	189.64	298.15	56.54	34.31
isophthalic acid	BENZDC01	131.03	197.14	298.15	58.78	72.25
2,4-Dinitrobenzoic acid	BIPJUF	119.89	201.20	298.15	59.99	59.90
Benzophenone	BPHENO03	91.65	195.88	298	58.37	33.28
atenolol (2-{4-[2-Hydroxy-3-(isopropylamino)propoxy]phenyl}acetamide)	CEZVIN	162.28	211.09	298	62.90	99.38
2-Chlorobenzoic acid	CLBZAC01	98.67	185.35	298.15	55.26	43.41
4-Chlorobenzoic acid	CLBZAP03	98.52	191.15	298.15	56.99	41.53
2,6-Dichloro-4-nitroaniline	CLNOAN	101.14	186.65	298.15	55.65	45.49
3-Fluorobenzoic acid	COVJIG	94.65	188.16	298.15	56.10	38.55
naproxen	COYRUD11	126.79	208.00	298.15	62.02	64.77
2,4-dichlorophenoxy acetic acid	CPXACA	125.00	209.75	298	62.51	62.50
1,8-diphenylnaphthalene	DPNAPH01	125.37	203.64	298.15	60.72	64.65
2-Fluorobenzoic acid	FBENZA02	92.80	182.23	298.15	54.33	38.46
flurbiprofen	FLUBIP	149.21	214.48	298	63.91	85.29
Flufenamic acid	FPAMCA17	137.98	215.24	298	64.14	73.83
2,4,6-trinitromesitylene (TNM)	HEXTIN01	111.52	206.66	298.15	61.62	49.90
4-amino-N-(4-ethylphenyl)benzenesulfonamide	HUNXIY	162.32	213.84	298	63.73	98.59
4-Amino-N-(4-methoxyphenyl)benzenesulfonamide	HUNXOE	164.16	213.33	298	63.57	100.59
4-Amino-N-(5-chloro-2-methylphenyl)benzenesulfonamide	HUNXUK	152.77	214.21	298	63.84	88.93

Paracetamol	HXACAN27	114.05	200.85	298	59.85	54.20
Ibuprofen	IBPRAC01	116.14	206.76	298	61.62	54.52
4-hydroxybenzoic acid	JOZZIH	116.34	201.41	298.15	60.05	56.29
Tolfenamic acid	KAXXAI01	131.35	205.23	298	61.16	70.19
Ketoprofen	KEMRUP	142.44	213.68	298	63.68	78.76
9-Methylanthracene	MANTHR01	97.71	193.71	298.15	57.75	39.96
2,4,6-N-tetranitro-N-methylaniline (Tetryl)	MTNANL	126.38	205.34	298.15	61.22	65.16
1-naphthol	NAPHOL01	90.47	192.19	298.15	57.30	33.17
4-nitrobenzoic acid	NBZOAC01	107.42	199.05	298.15	59.35	48.07
Niflumic acid	NIFLUM10	157.87	209.03	298	62.29	95.58
nitroguanidine	NTRGUA01	116.43	190.71	298.15	56.86	59.57
2,2-Dimethylsuccinic acid	OLENIC	113.90	197.84	298.15	58.99	54.91
4-Methylbenzoic acid	PTOLIC01	92.76	195.27	298.15	58.22	34.54
Phenacetin	PYRAZB21	107.89	201.44	298	60.03	47.86
5-chloro-2-nitroaniline	RAPKUP	94.80	192.40	298.15	57.36	37.44
salicylic acid	SALIAC15	91.28	194.22	298	57.88	33.40
Diclofenac	SIKLIH01	132.19	209.96	298	62.57	69.62
4-cyanobenzoic acid	TAGNAR	79.06	183.25	298.15	54.64	24.42
o-Terphenyl	TERPHO02	107.36	198.34	298.15	59.14	48.22
2,4,6-trinitroaniline (TNA)	TNIOAN	109.74	200.65	298.15	59.82	49.91
1,3,5-Triphenylbenzene	TPHBEN01	147.68	214.98	298.15	64.10	83.58
N-(4-nitrophenyl)-benzene-sulfonamide	UVEMOY	138.63	210.03	298	62.59	76.05
4-Amino-N-(4-nitrophenyl)benzenesulfonamide	UVEMUE	161.00	211.08	298	62.90	98.10
4-Hydroxybenzamide	VIDMAX	117.10	199.67	298	59.50	57.60

2-Methylglutaric acid	XIBVIO	121.16	204.44	298.15	60.95	60.21
Mefenamic acid	XYANAC	132.07	212.60	298	63.36	68.71
4-Heptylbenzoic acid (cr, II)	ZIKWOF	136.82	210.77	298.15	62.84	73.98

The next set of figure present the same machine learning and regression method predicting the sublimation thermodynamics of the SUB-158 dataset with CDK descriptors only.

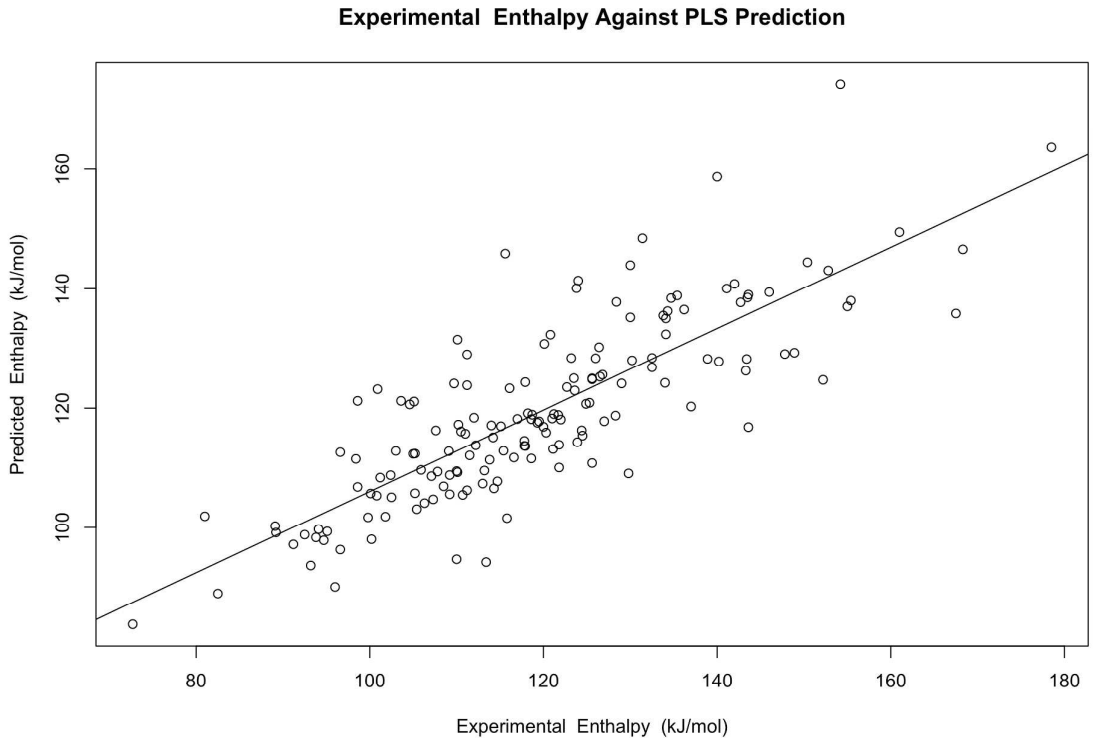

Figure S1. SUB-158 PLS prediction of the enthalpy of sublimation

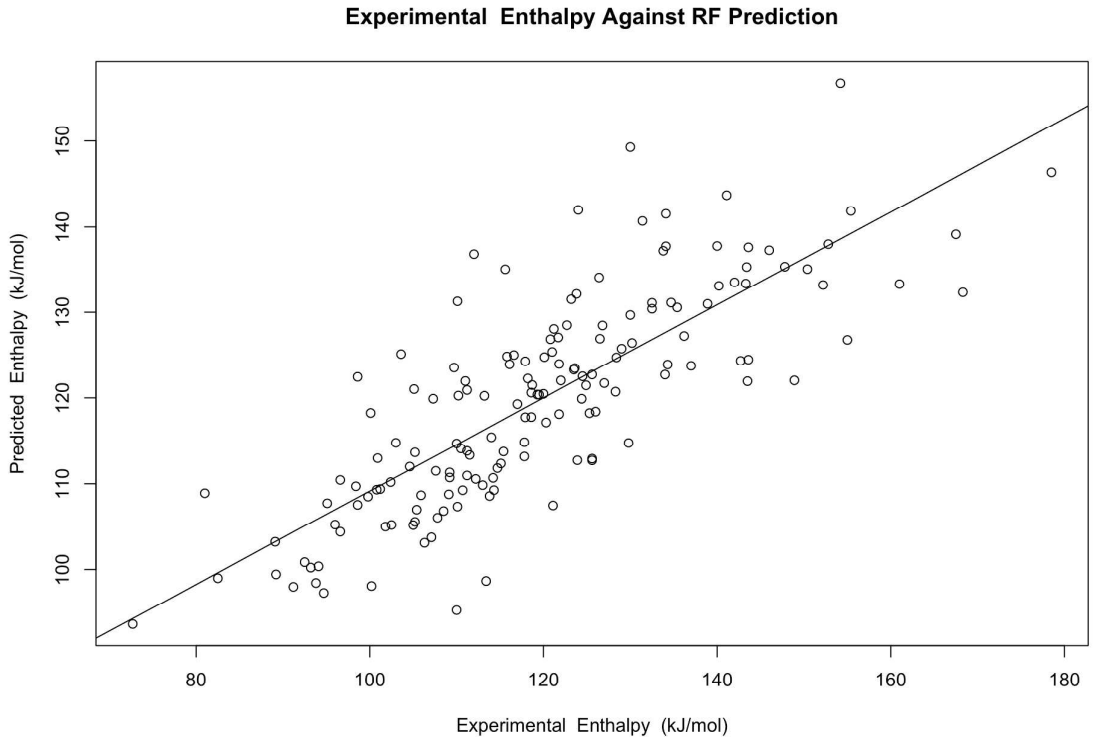

Figure S2. SUB-158 RF prediction the enthalpy of sublimation

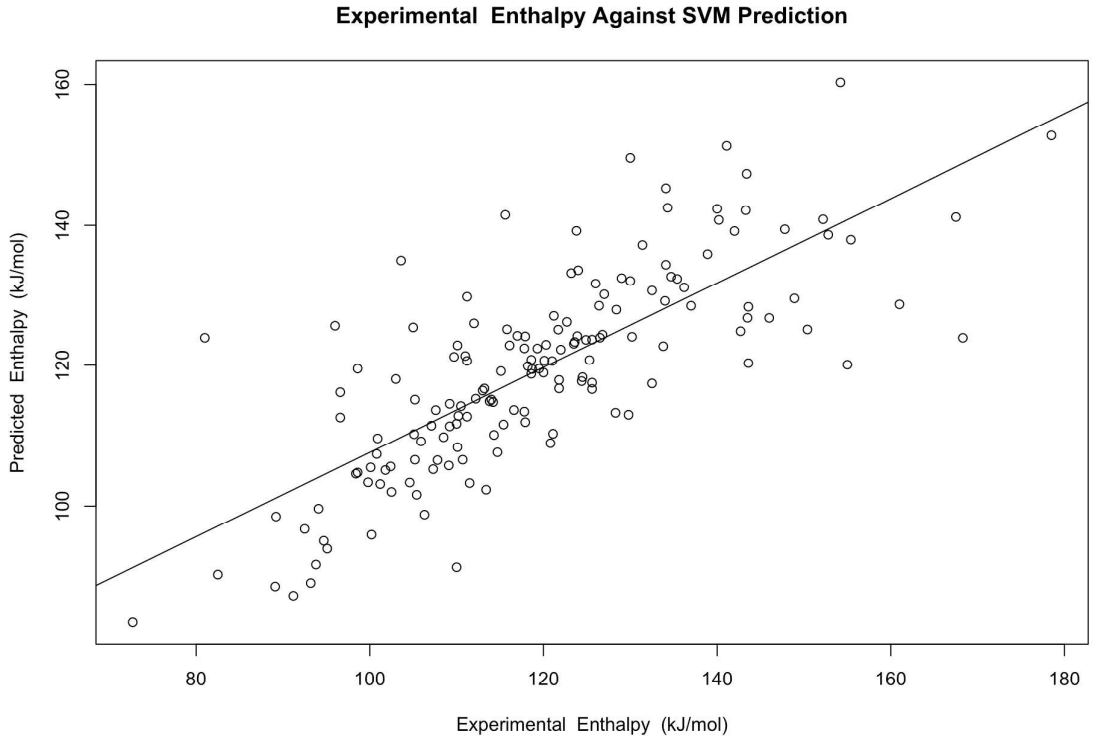

Figure S3. SUB-158 SVM prediction the enthalpy of sublimation

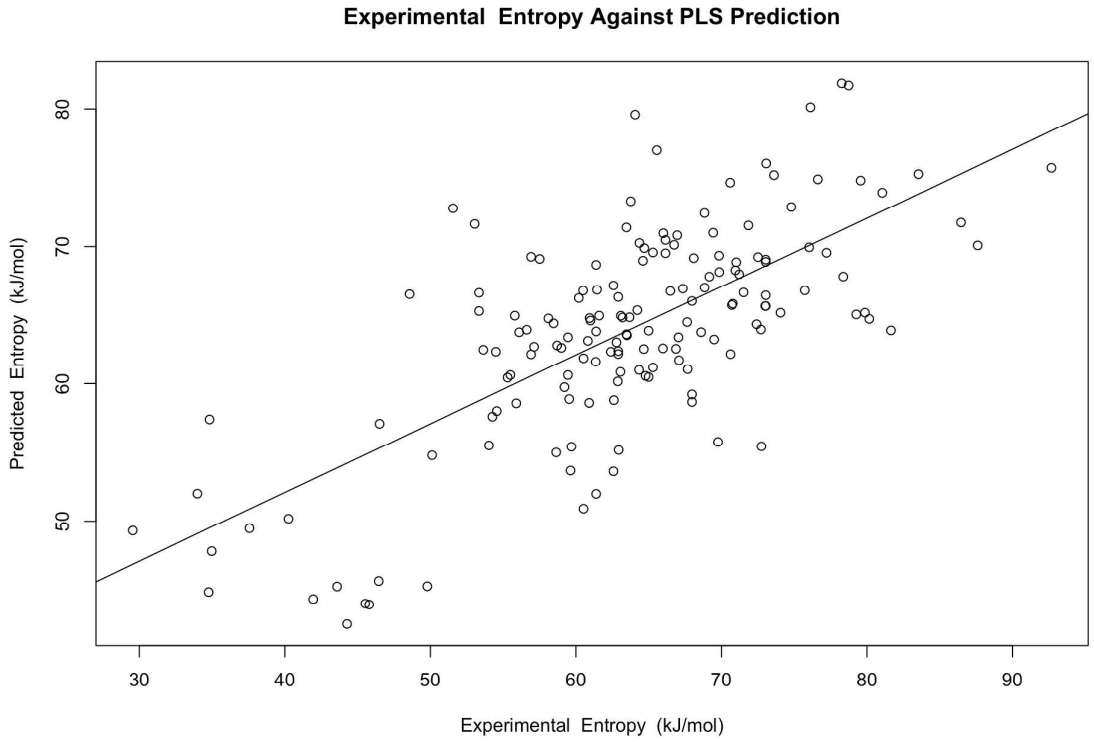

Figure S4. SUB-158 PLS prediction the entropy of sublimation

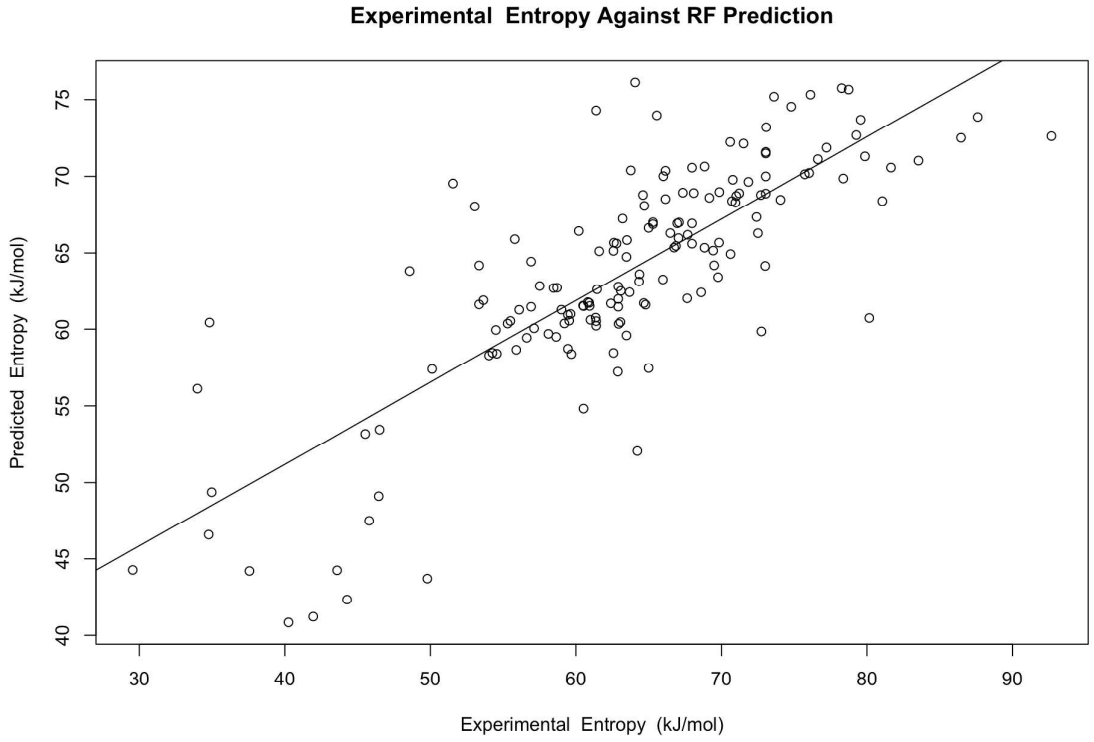

Figure S5. SUB-158 RF prediction the entropy of sublimation

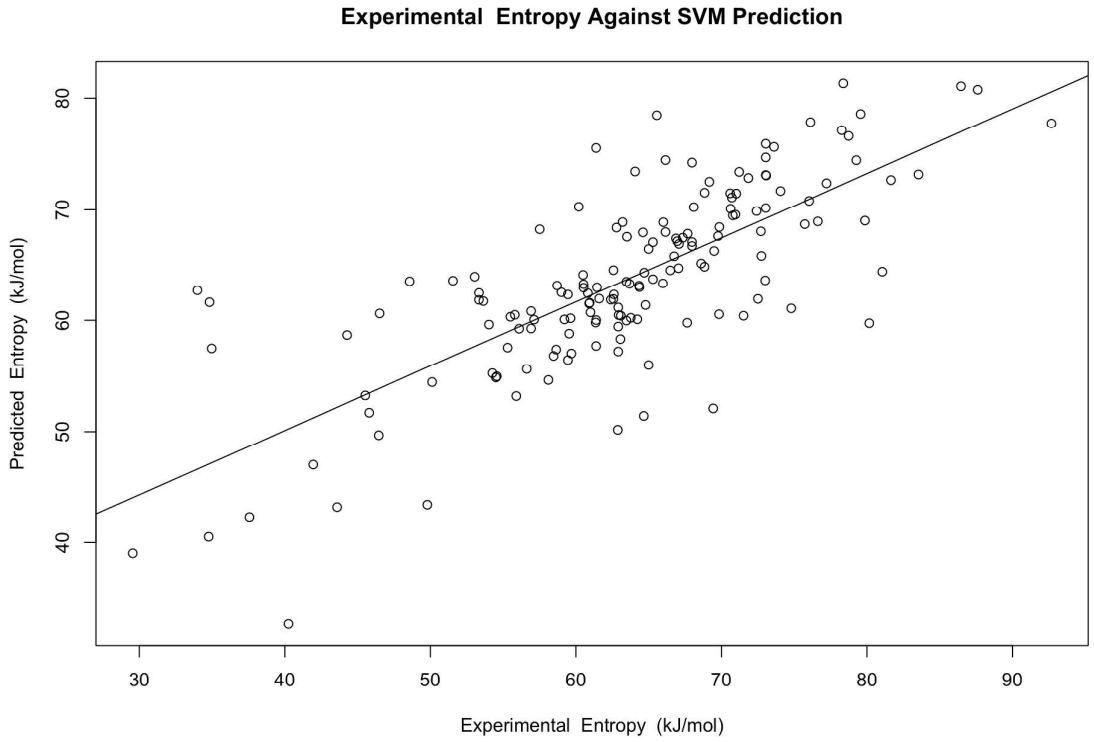

Figure S6. SUB-158 SVM prediction the entropy of sublimation

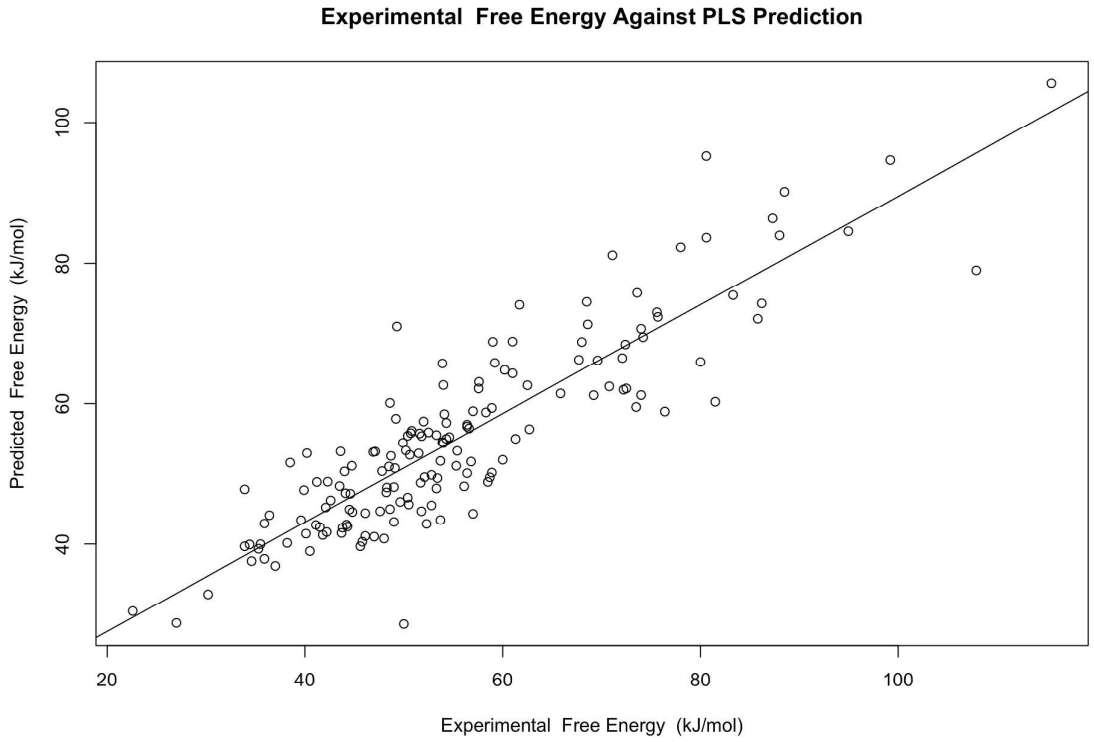

Figure S7. SUB-158 PLS prediction the free energy of sublimation

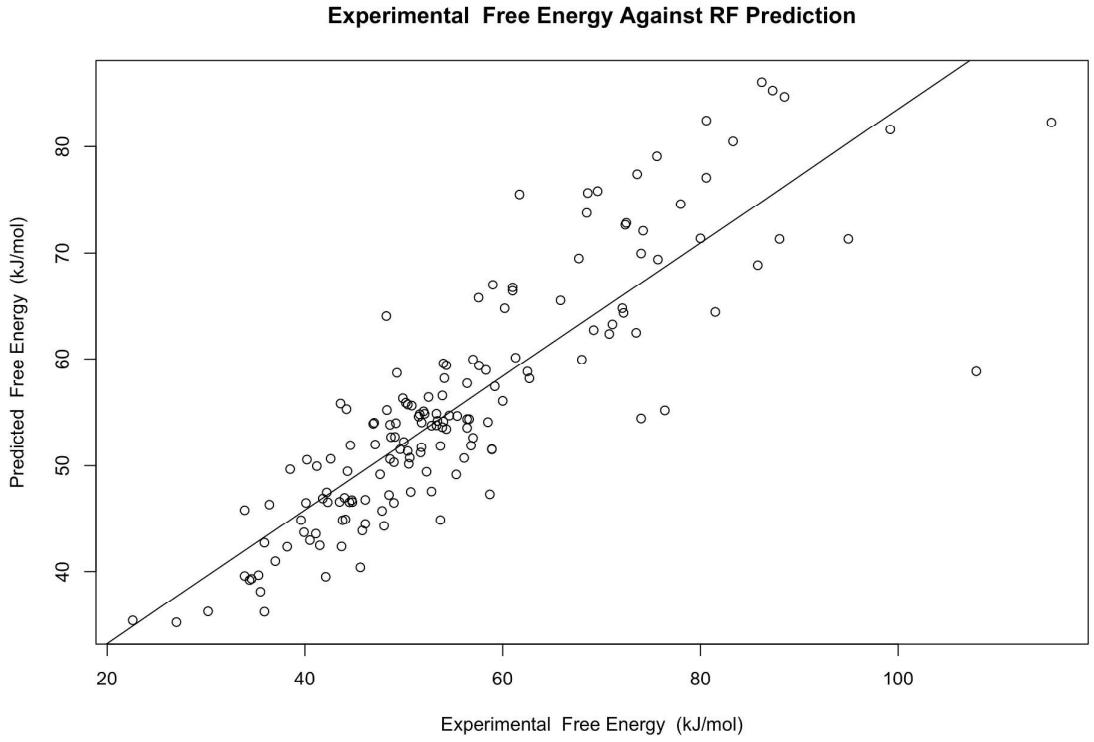

Figure S8. SUB-158 RF prediction the free energy of sublimation

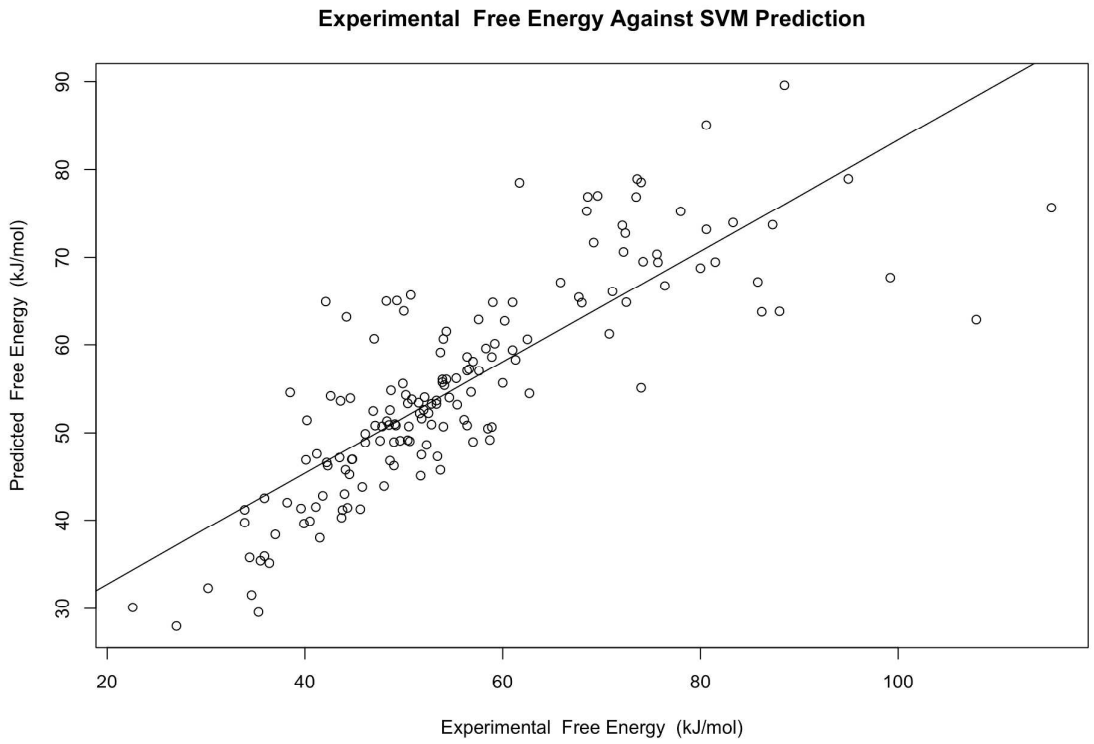

Figure S9. SUB-158 SVM prediction the free energy of sublimation

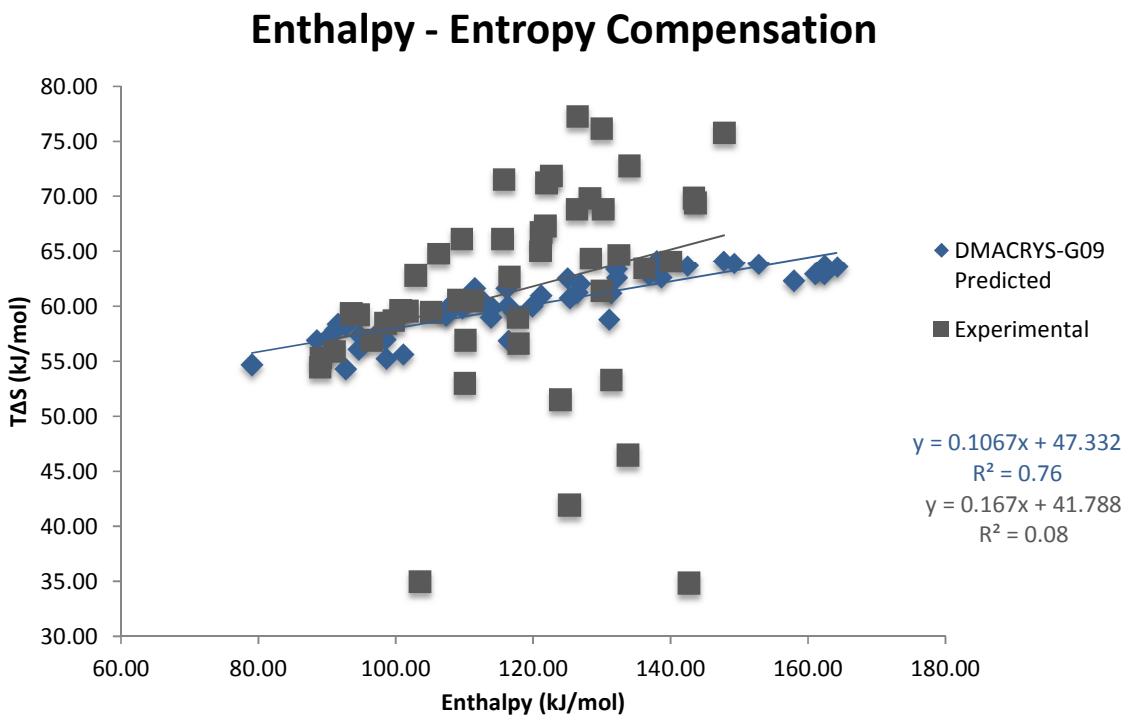

Figure S10. DMACRYS-G09 enthalpy Entropy compensation

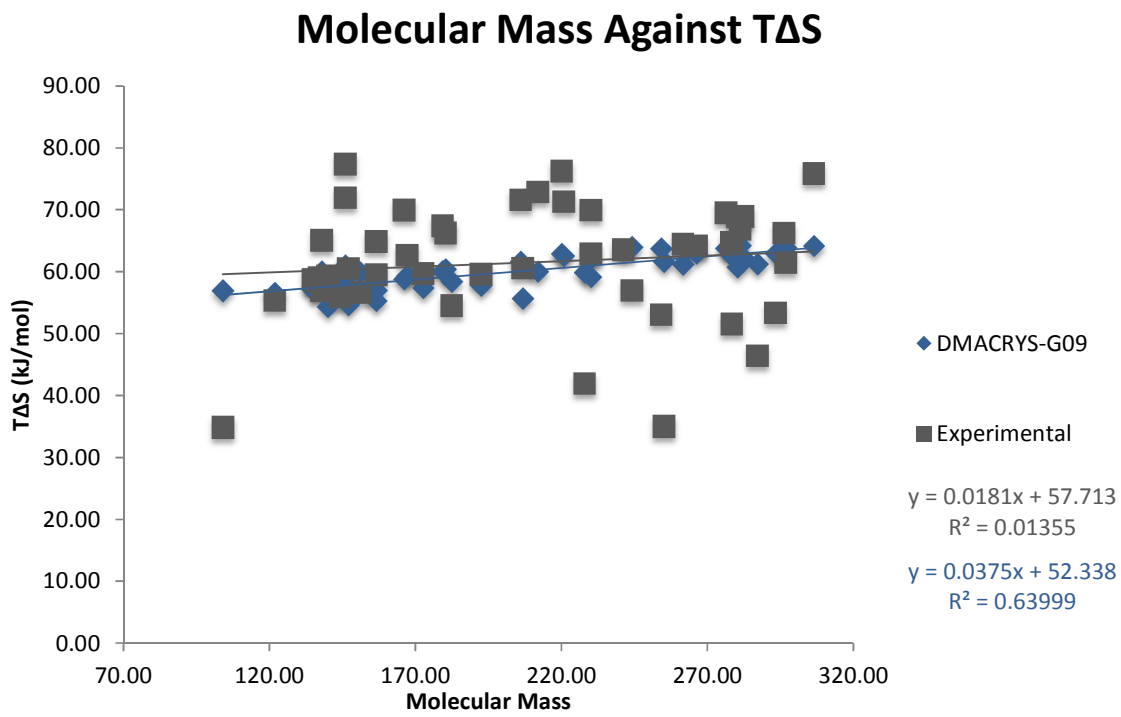

Figure S11. DMACRYS-G09 molecular weight against entropy.

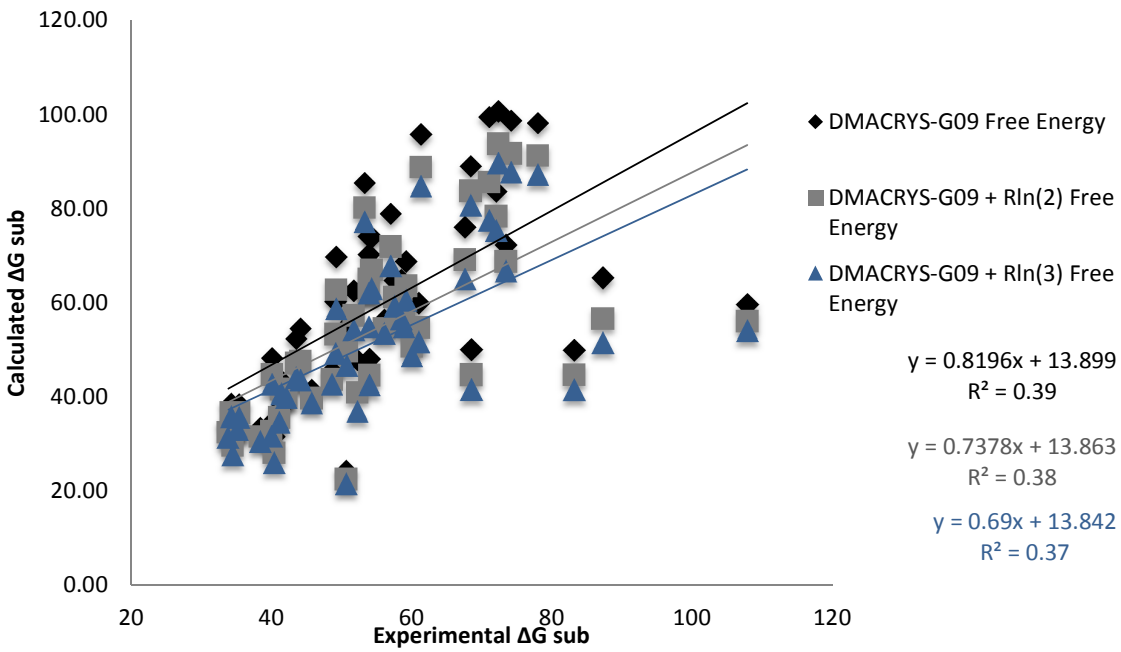

Figure S12. DMACRYS-G09 including a correction for rotational bonds in the predictions of ΔG of sublimation.

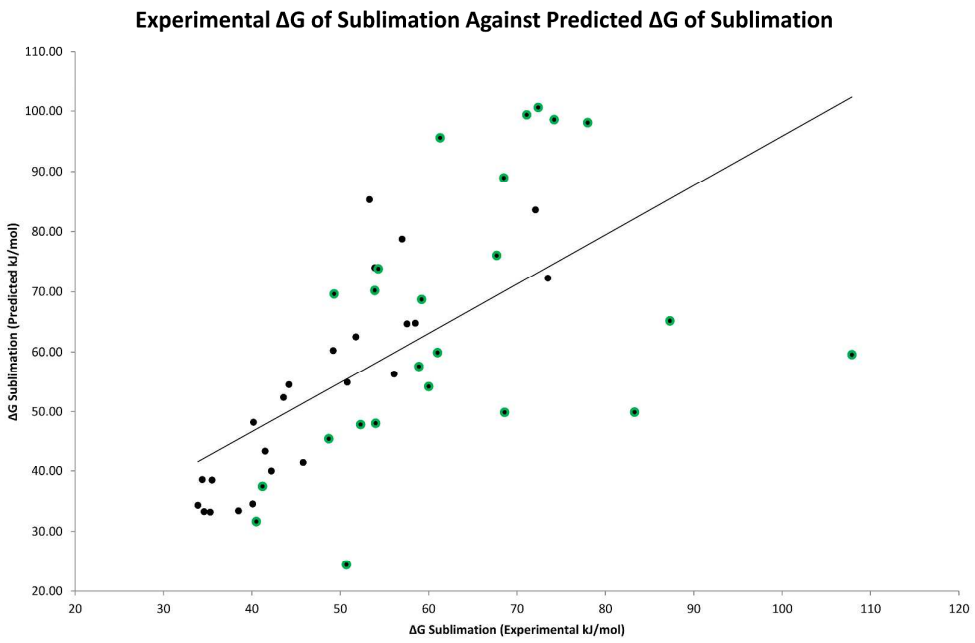

Figure S13. The free energy of sublimation experimental data plotted against the DMACRYS-G09 predictions. The molecules containing nitrogen are shown with the green lines.

The following plots present the QSPR predictions of the SUB-48 sublimation thermodynamics against the experiment. Predicted thermodynamic (PT), Chemistry Development Kit (CDK) and a combination of the two (All) are used as descriptors for the QSPR models. Random Forest (RF), Partial Least Squares (PLS) and Support Vector Machines (SVM) are.

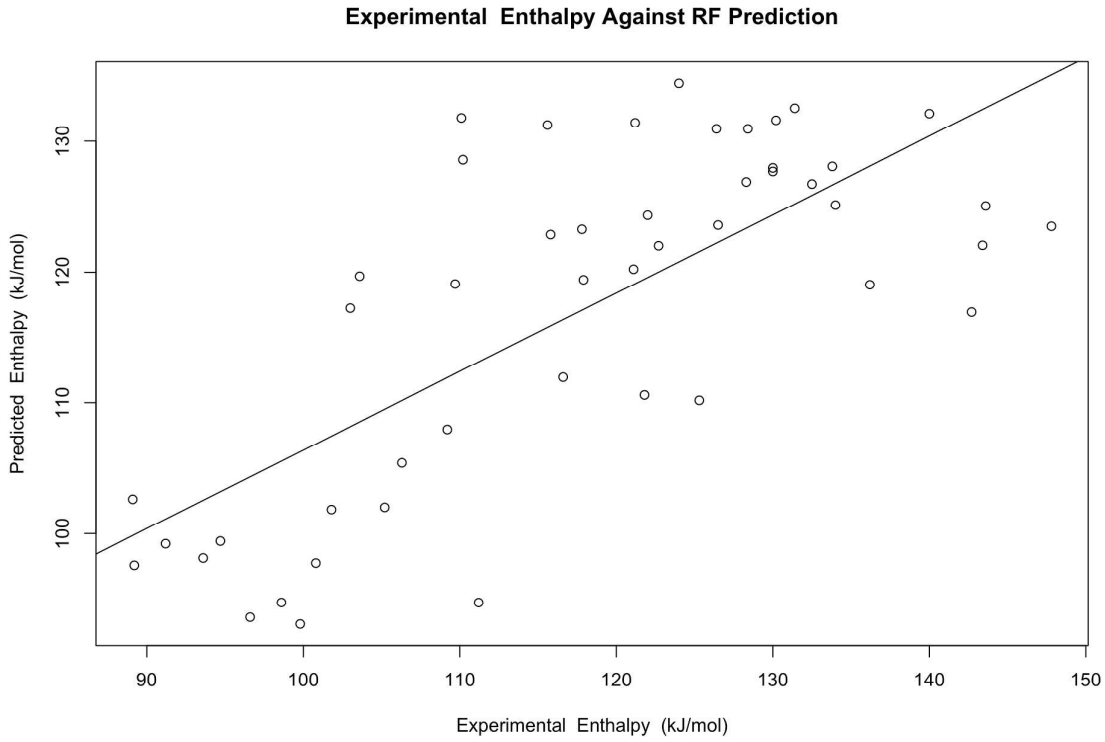

Figure S 14. RF prediction of enthalpy of sublimation using PT descriptors against the experiment.

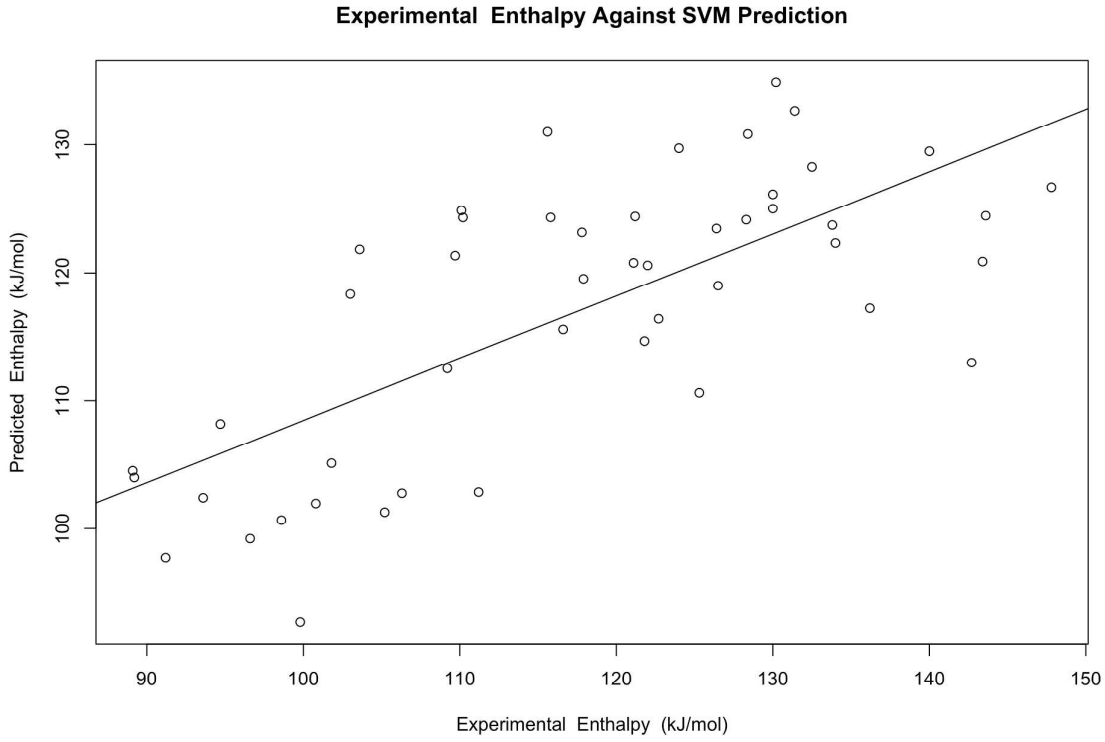

Figure S 15. SVM prediction of enthalpy of sublimation using PT descriptors against the experiment.

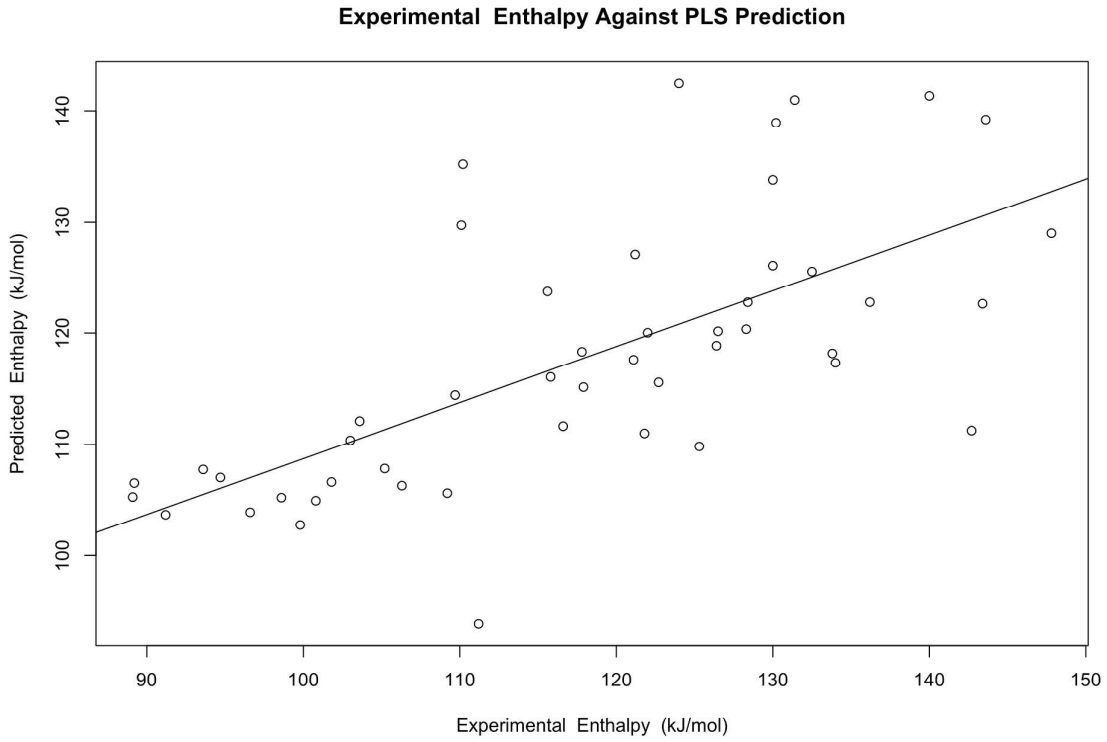

Figure S 16. PLS prediction of enthalpy of sublimation using PT descriptors against the experiment.

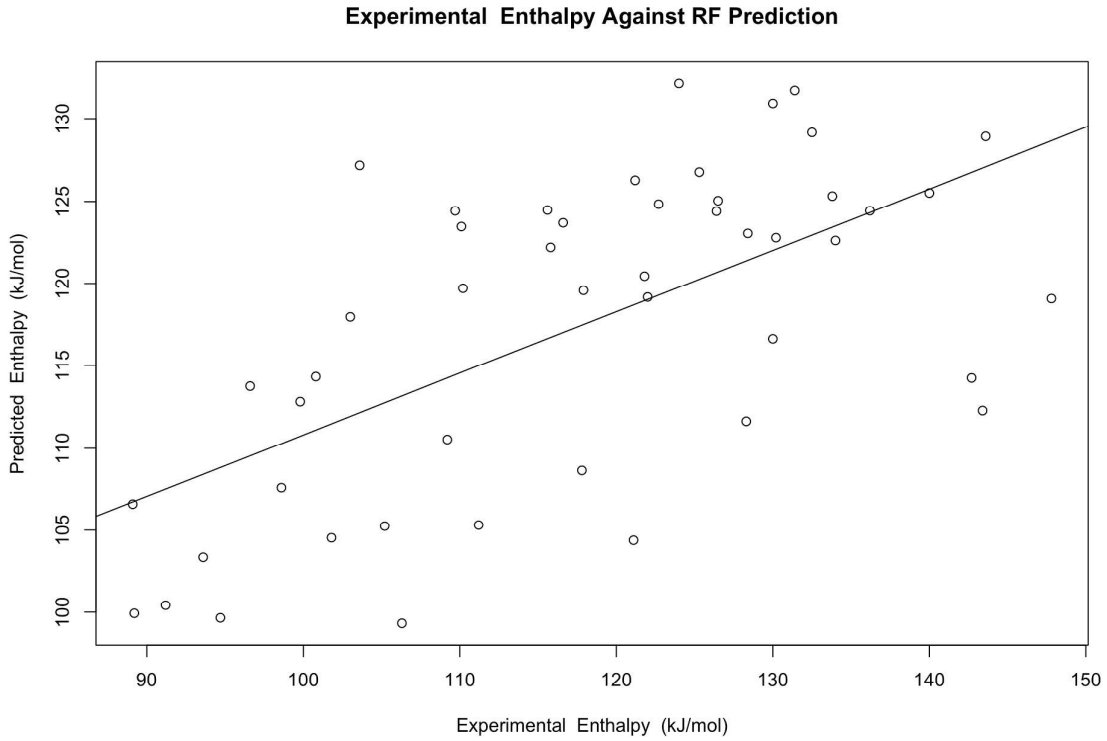

Figure S 17. RF prediction of enthalpy of sublimation using CDK descriptors against the experiment.

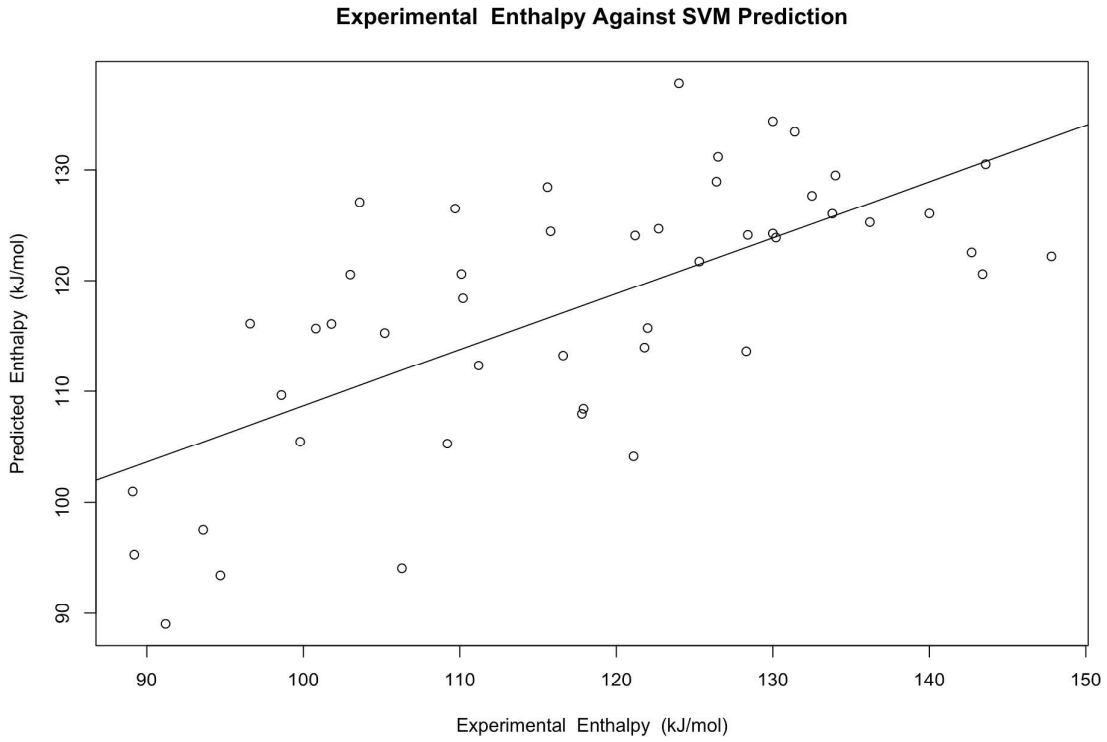

Figure S 18. SVM prediction of enthalpy of sublimation using CDK descriptors against the experiment

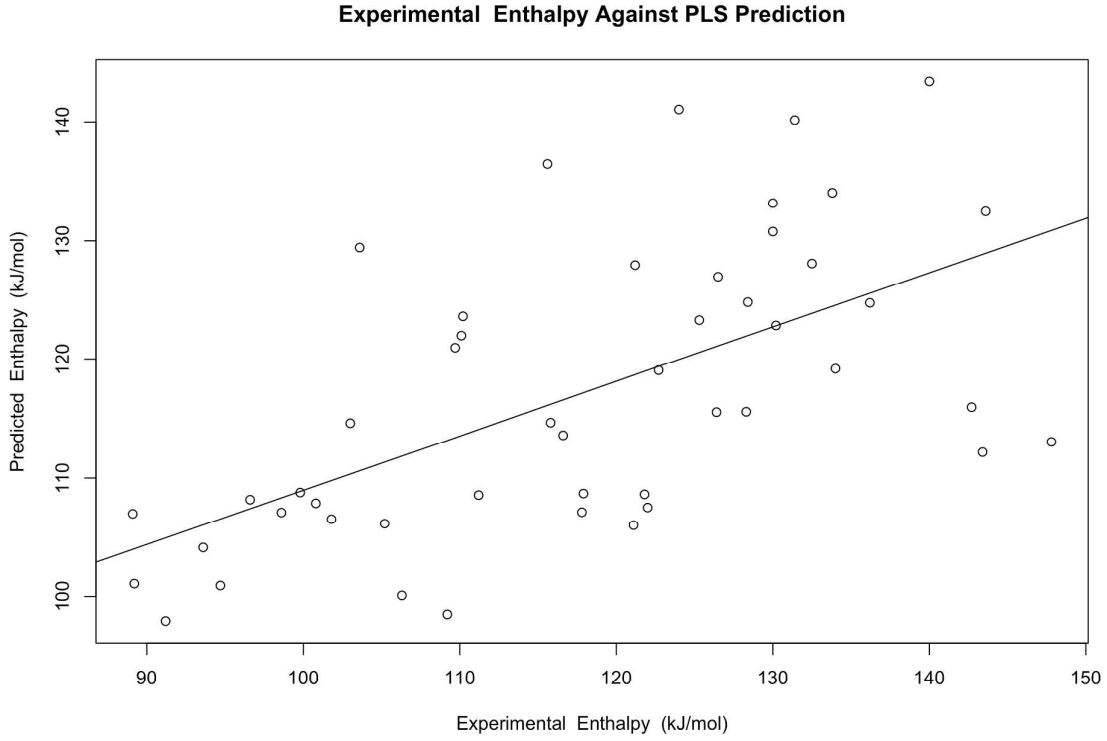

Figure S 19. PLS prediction of enthalpy of sublimation using CDK descriptors against the experiment.

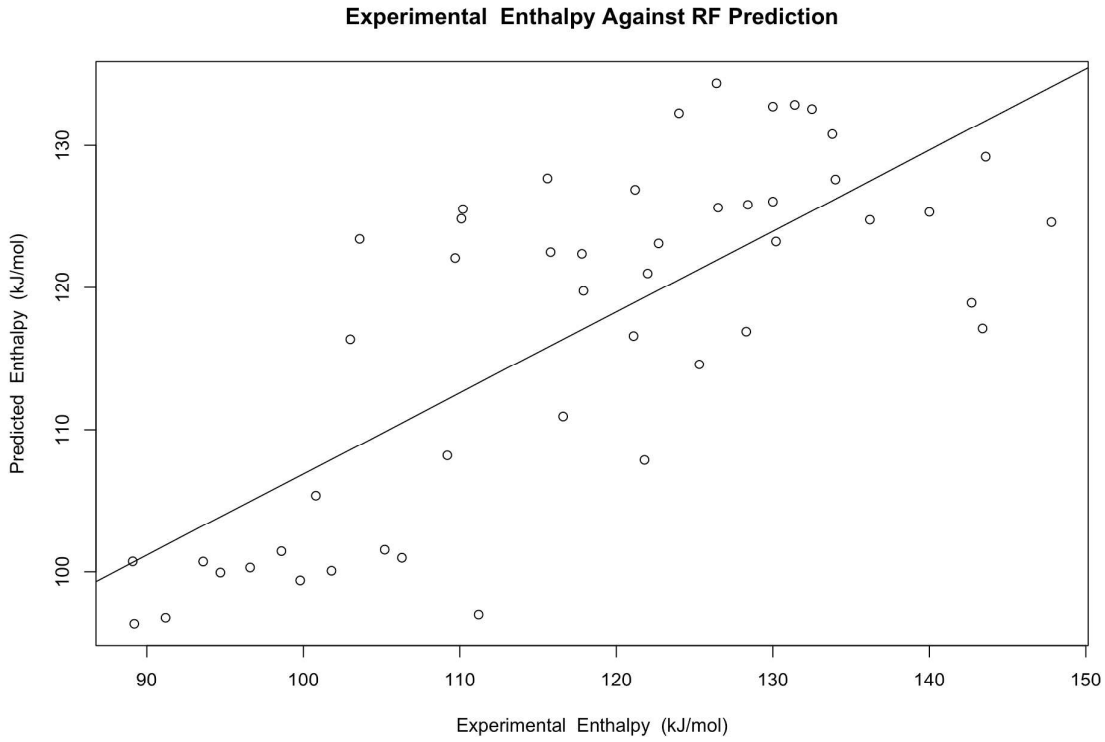

Figure S 20. RF prediction of enthalpy of sublimation using All descriptors against the experiment.

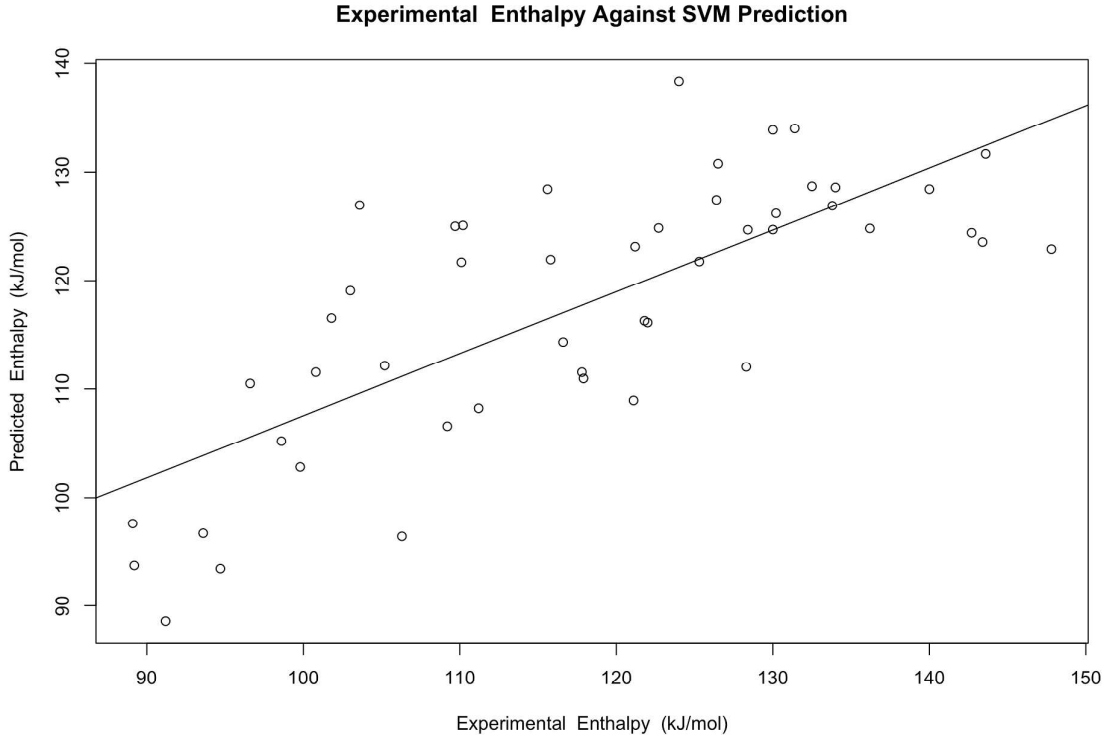

Figure S 21. SVM prediction of enthalpy of sublimation using All descriptors against the experiment.

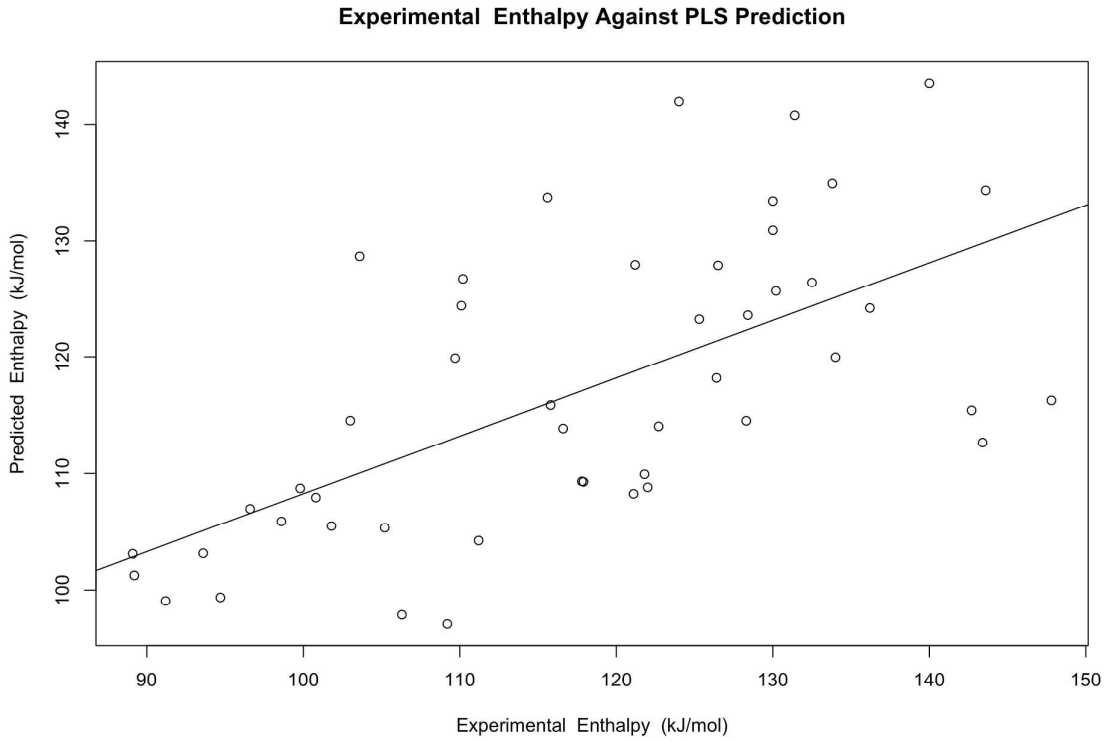

Figure S 22. PLS prediction of enthalpy of sublimation using All descriptors against the experiment.

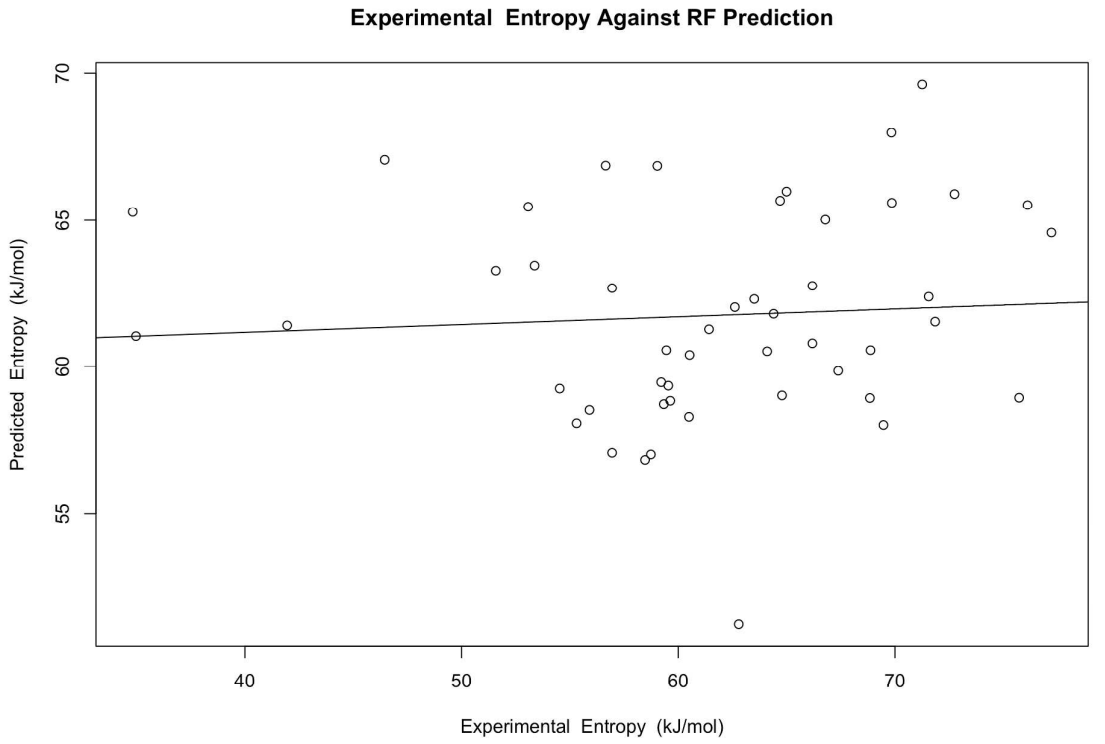

Figure S 23. RF prediction of TΔS of sublimation using PT descriptors against the experiment.

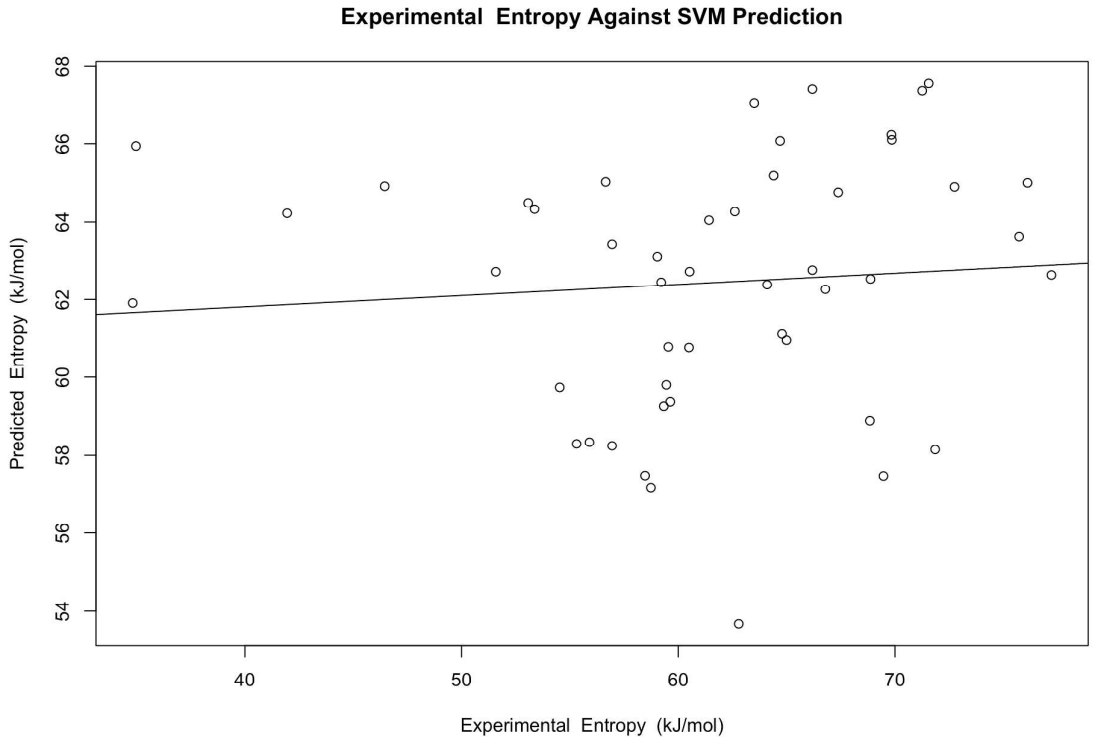

Figure S 24. SVM prediction of TΔS of sublimation using PT descriptors against the experiment.

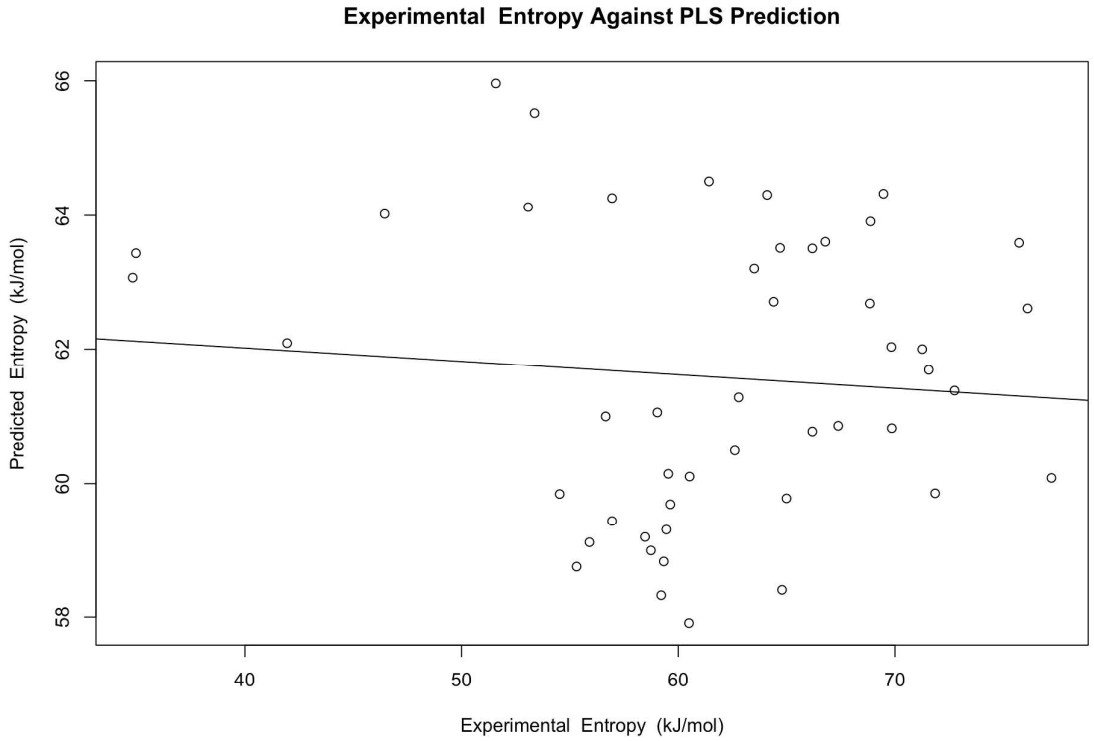

Figure S 25. PLS prediction of TΔS of sublimation using PT descriptors against the experiment.

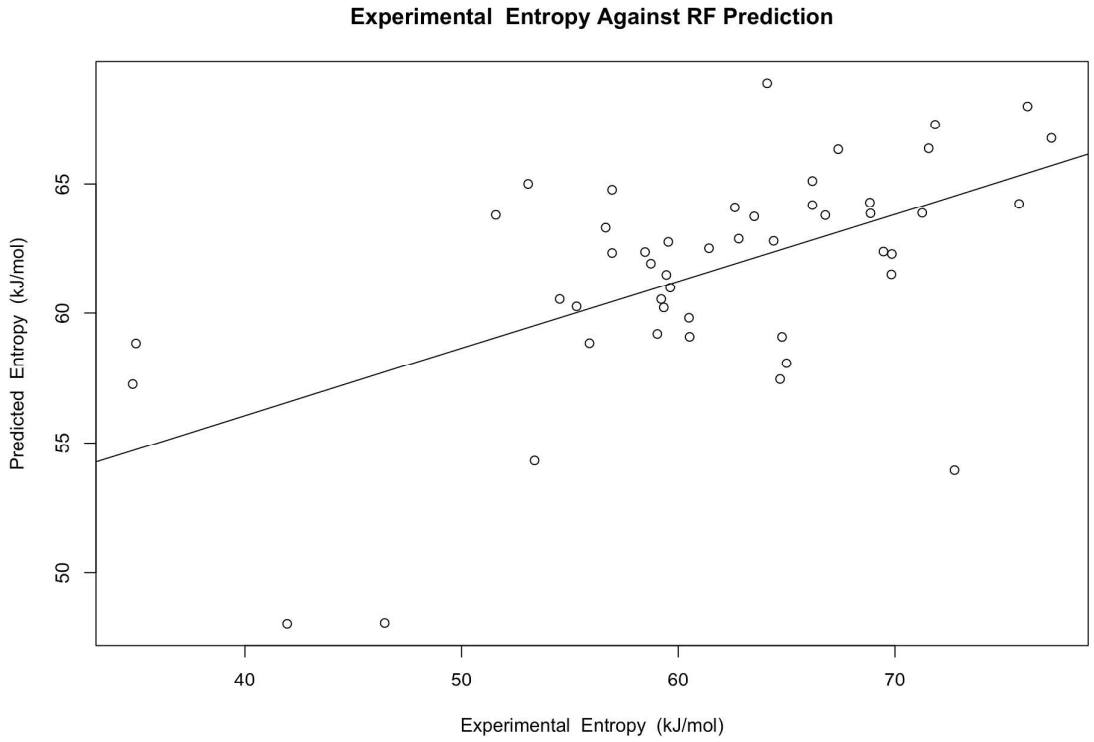

Figure S 26. RF prediction of TΔS of sublimation using CDK descriptors against the experiment.

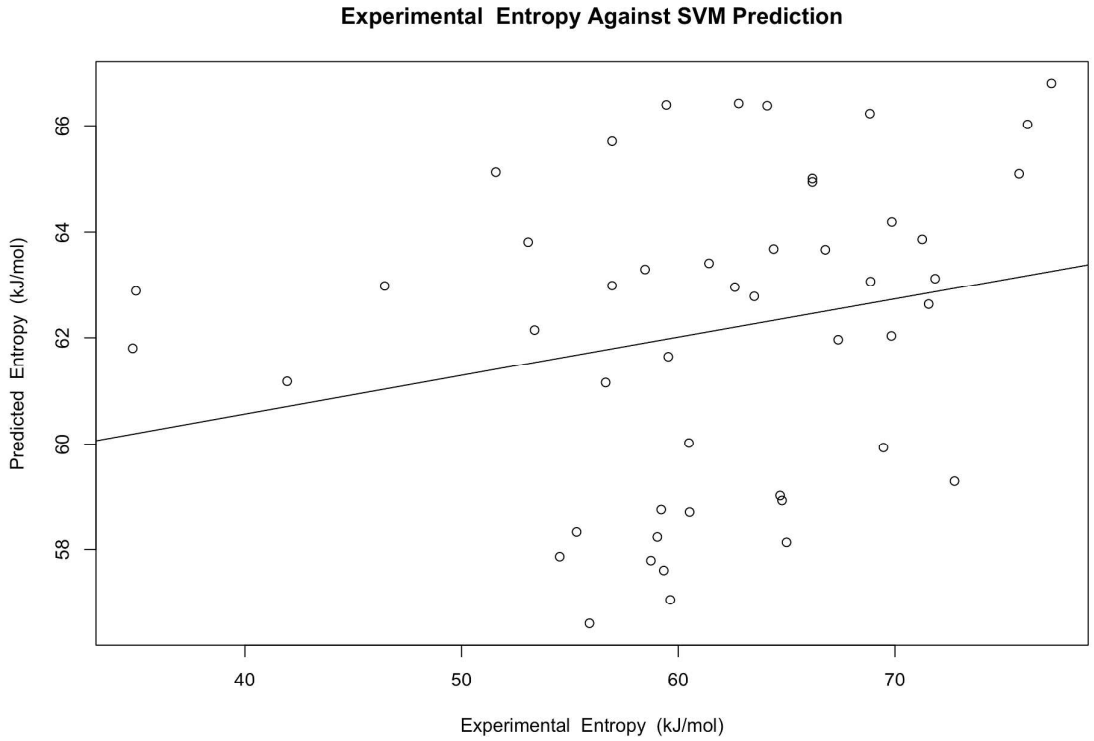

Figure S 27. SVM prediction of TΔS of sublimation using CDK descriptors against the experiment.

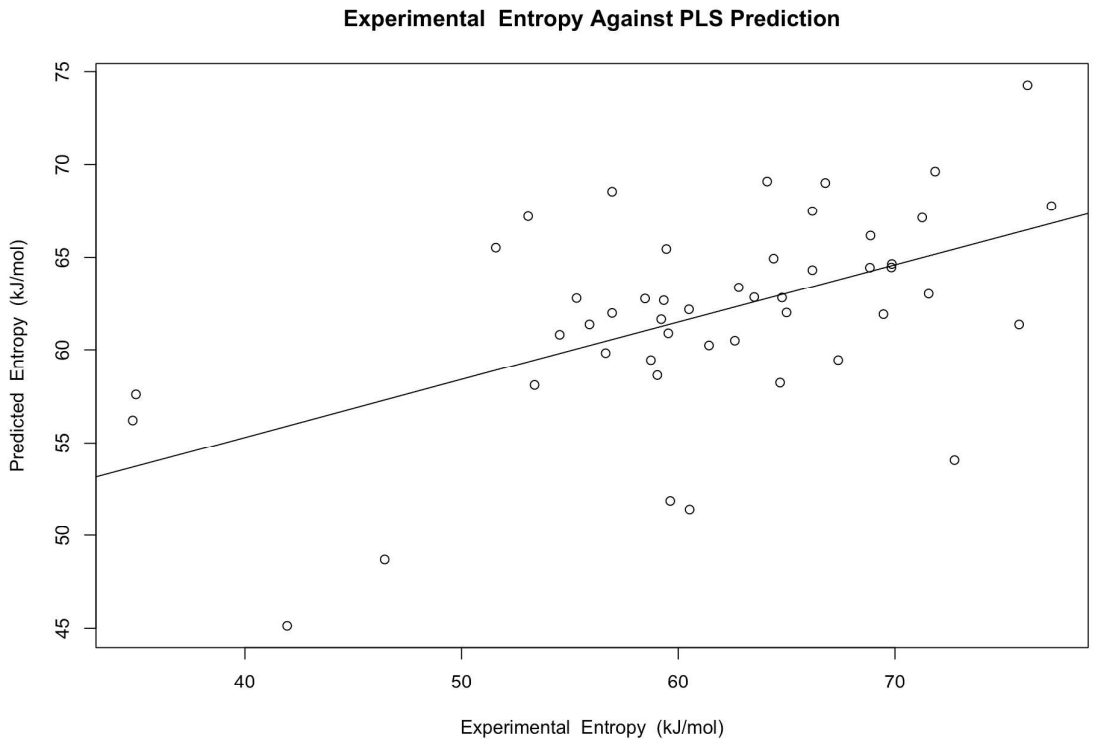

Figure S 28. PLS prediction of TΔS of sublimation using CDK descriptors against the experiment.

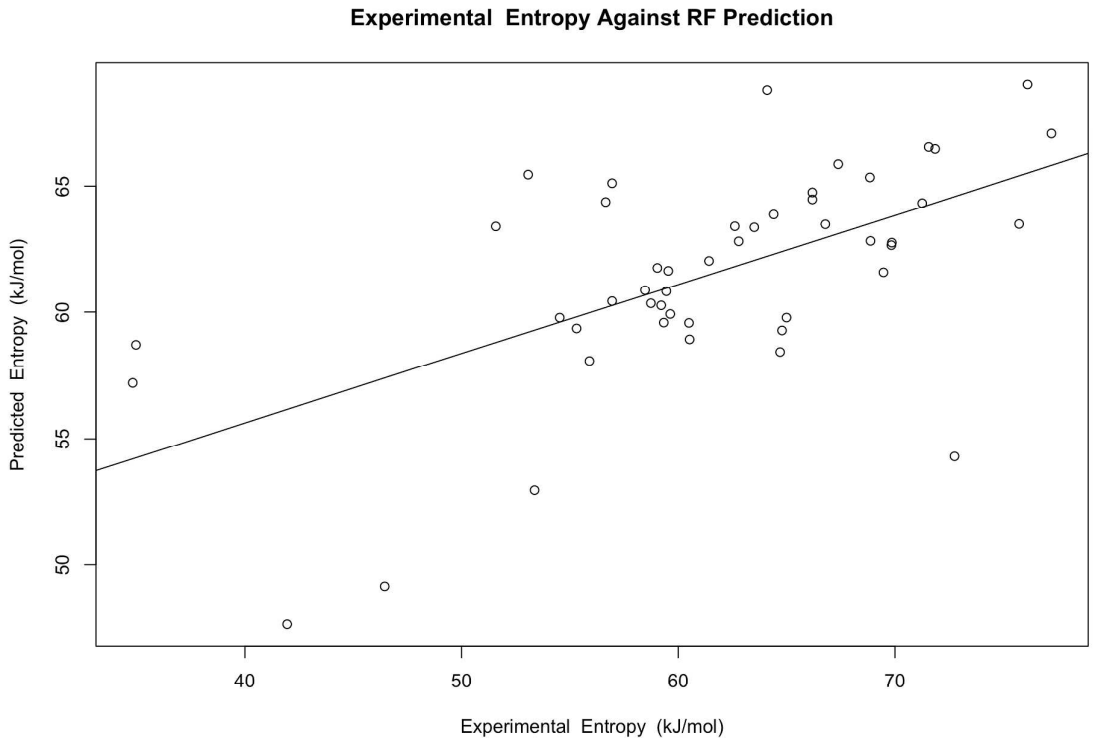

Figure S 29. RF prediction of TΔS of sublimation using All descriptors against the experiment.

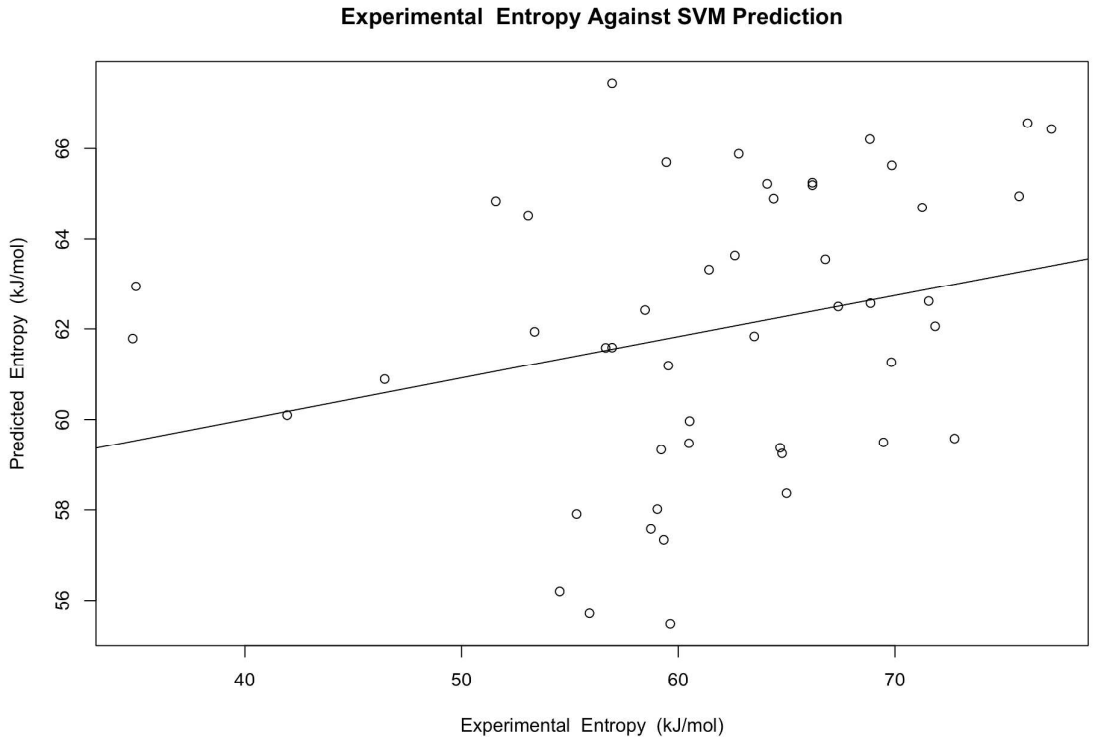

Figure S 30. SVM prediction of TΔS of sublimation using All descriptors against the experiment.

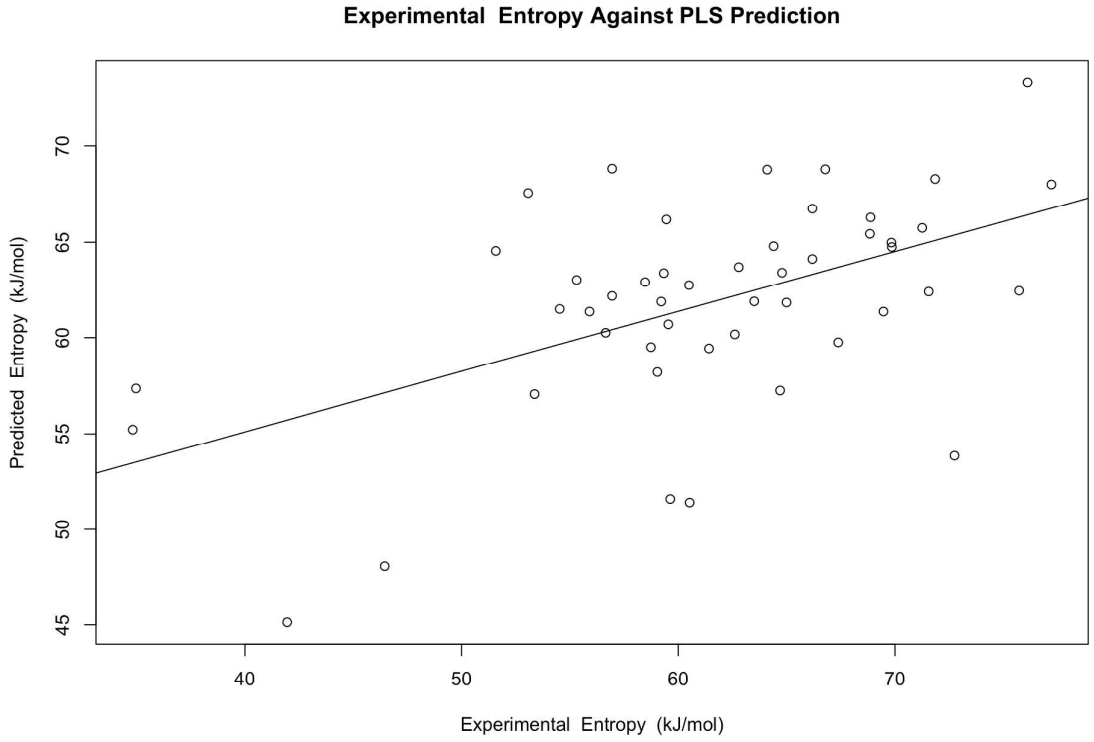

Figure S 31. PLS prediction of TΔS of sublimation using All descriptors against the experiment.

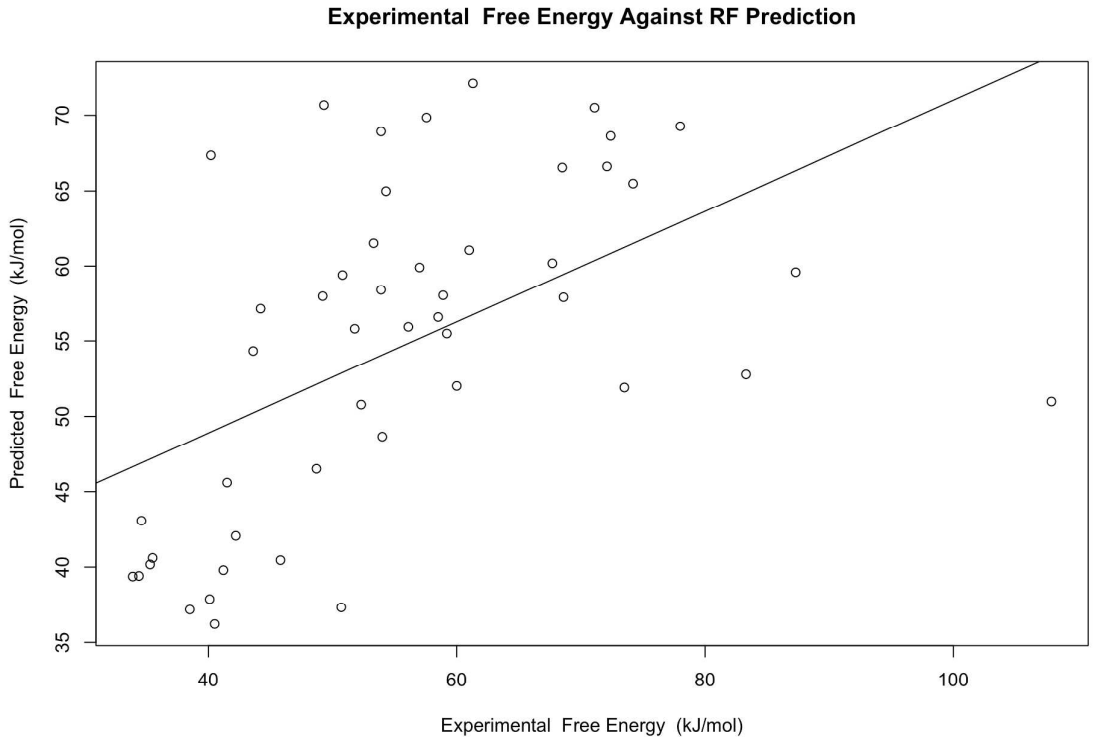

Figure S 32. RF prediction of free energy of sublimation using PT descriptors against the experiment.

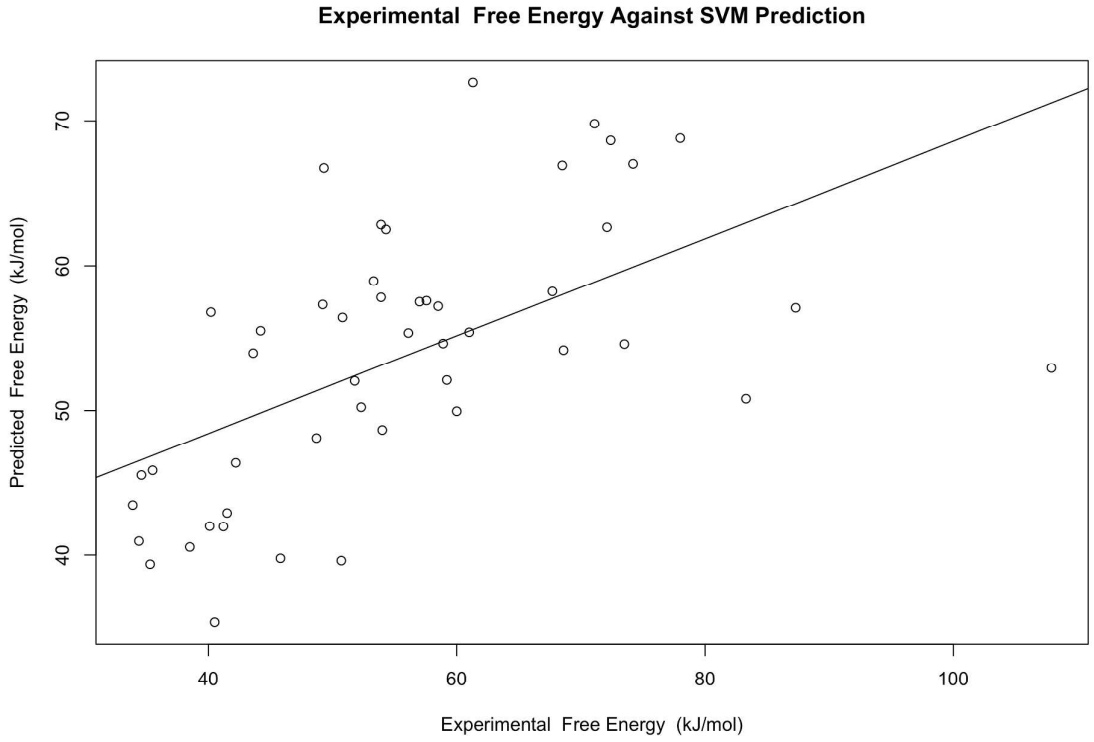

Figure S 33. SVM prediction of free energy of sublimation using PT descriptors against the experiment

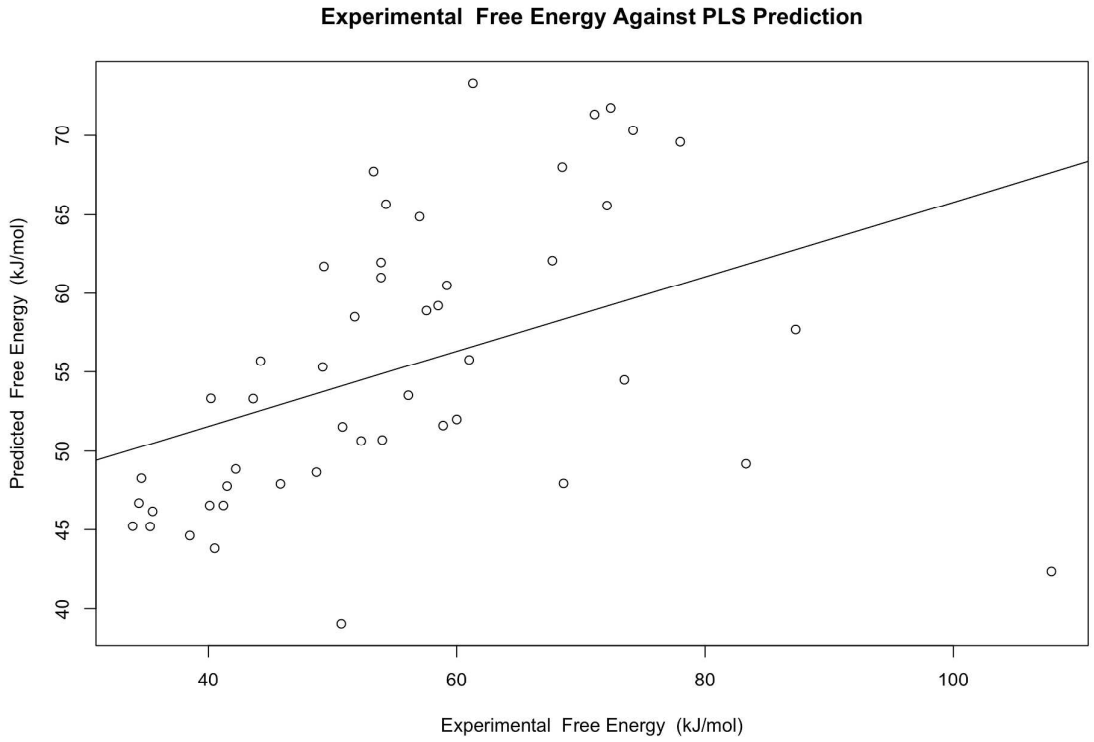

Figure S 34. PLS prediction of free energy of sublimation using PT descriptors against the experiment.

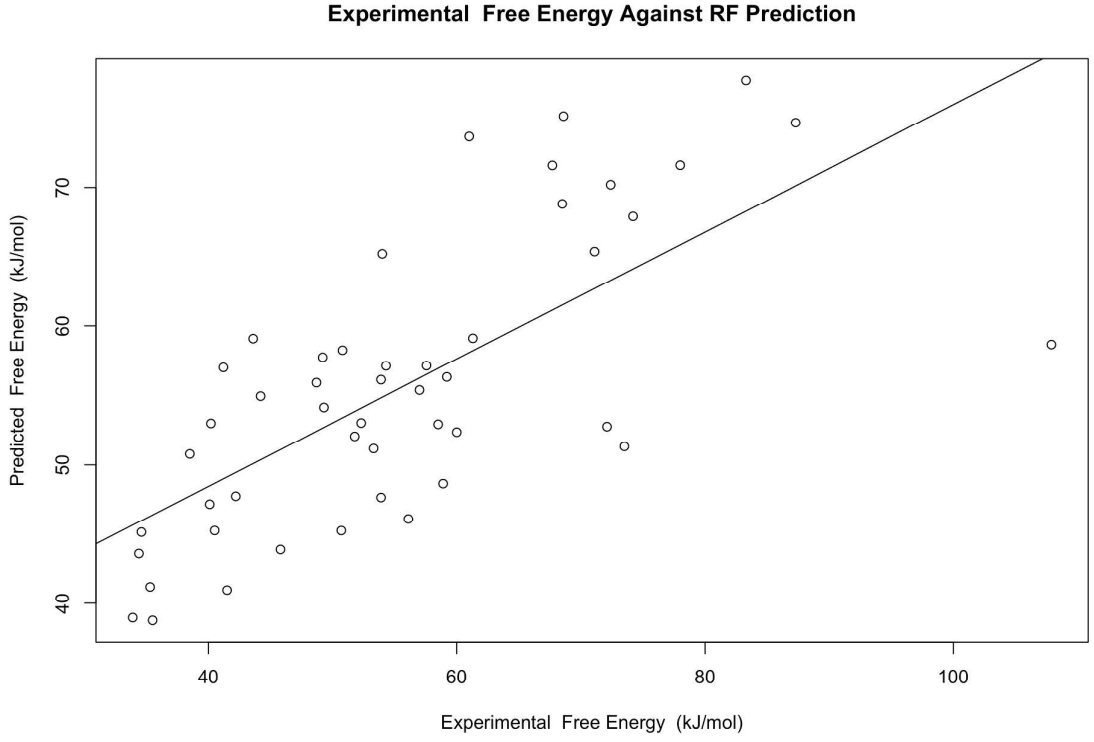

Figure S 35. RF prediction of free energy of sublimation using CDK descriptors against experiment.

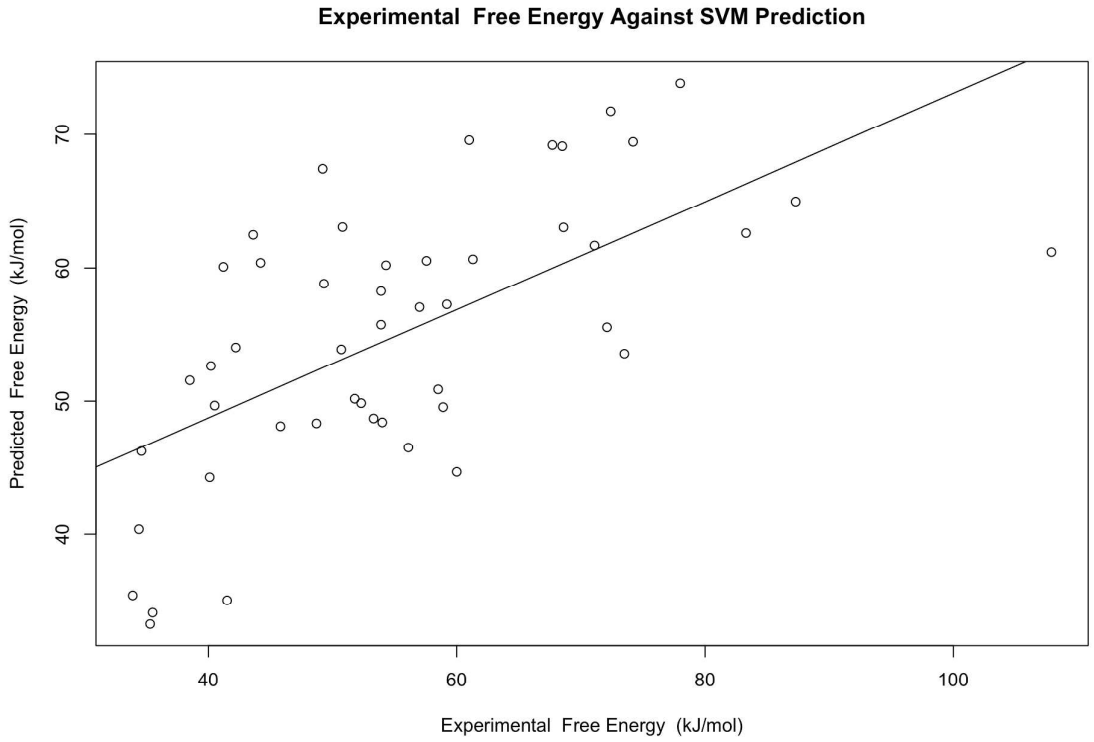

Figure S 36. SVM prediction of free energy of sublimation using CDK descriptors against experiment.

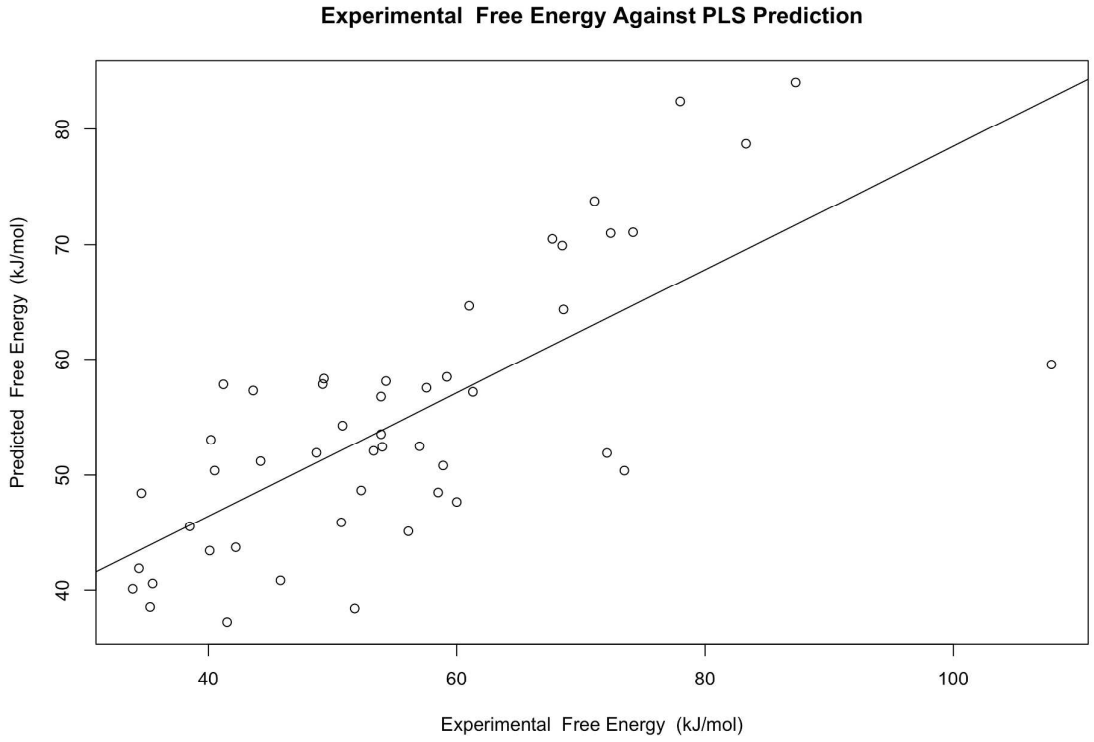

Figure S 37. PLS prediction of free energy of sublimation using CDK descriptors against experiment.

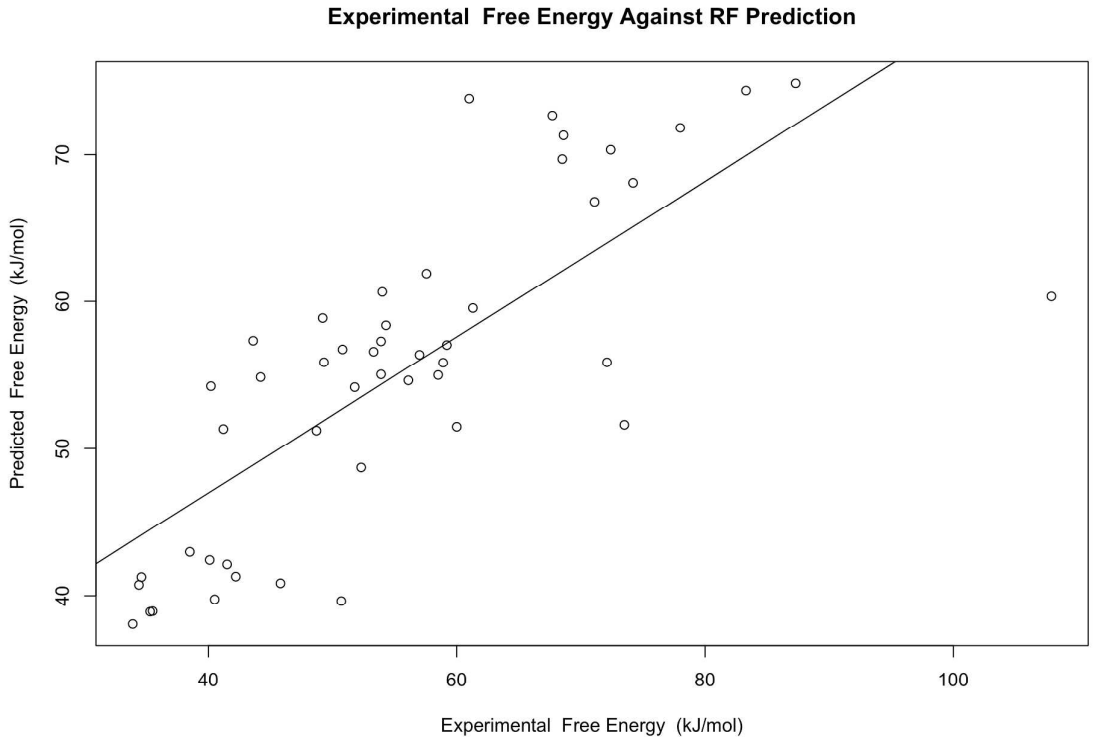

Figure S 38. RF prediction of free energy of sublimation using All descriptors against experiment.

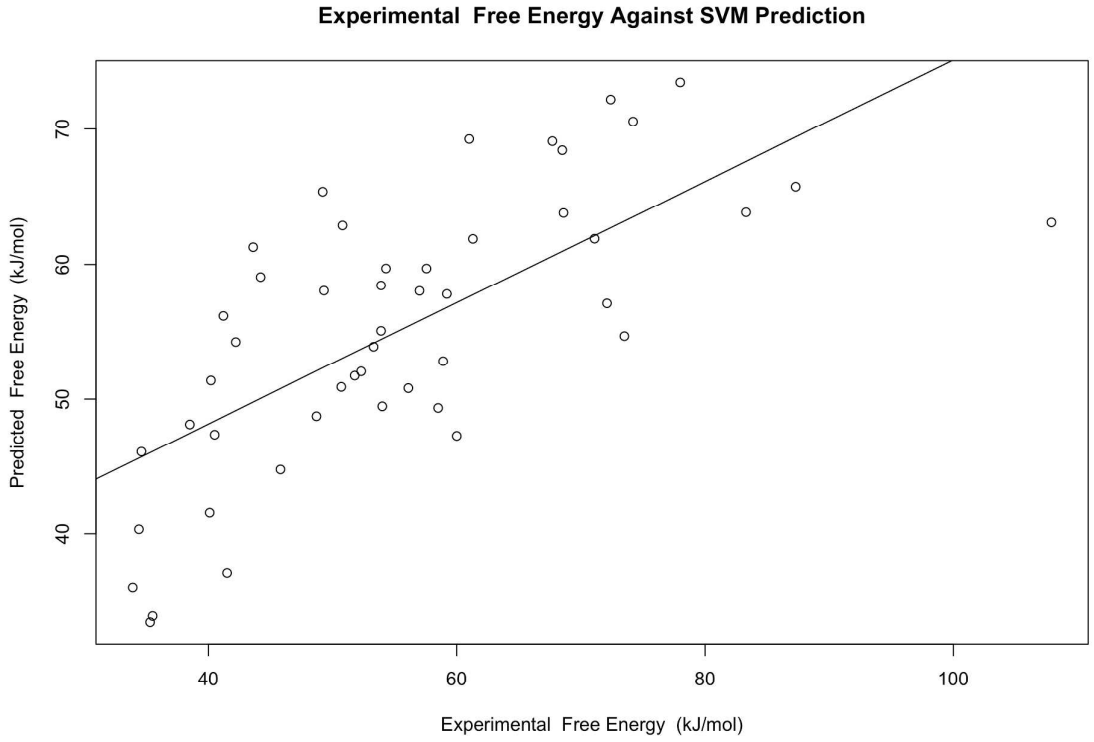

Figure S 39. SVM prediction of free energy of sublimation using All descriptors against experiment.

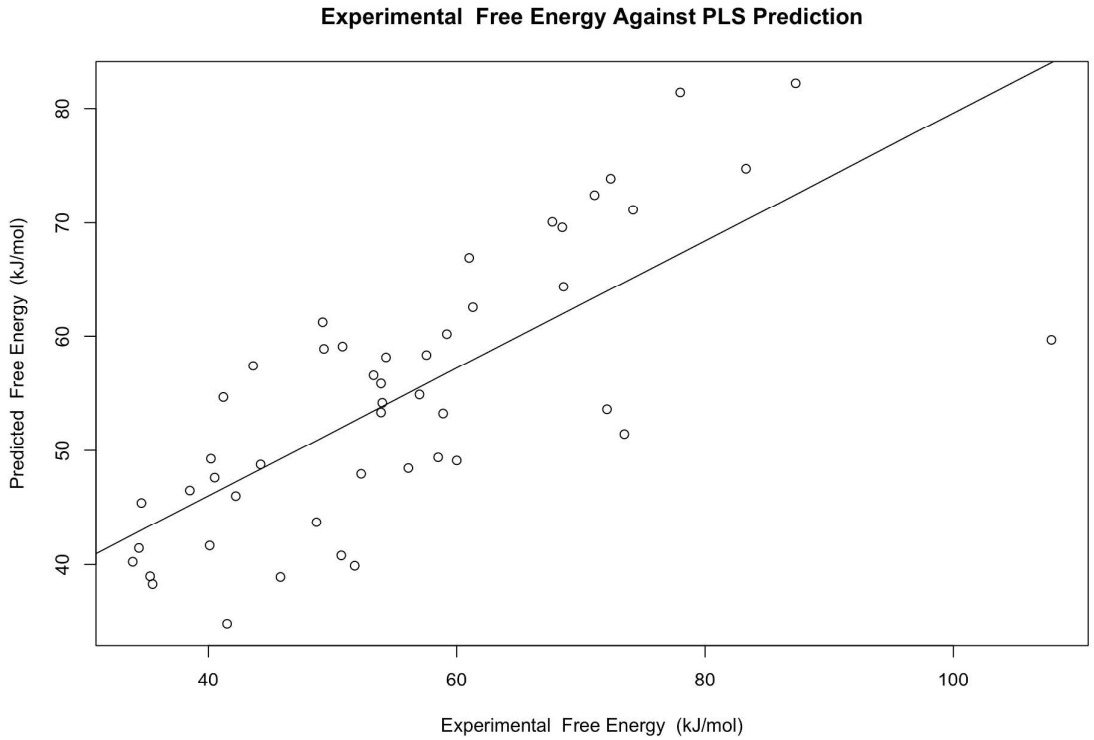

Figure S 40. PLS prediction of free energy of sublimation using all descriptors against experiment.

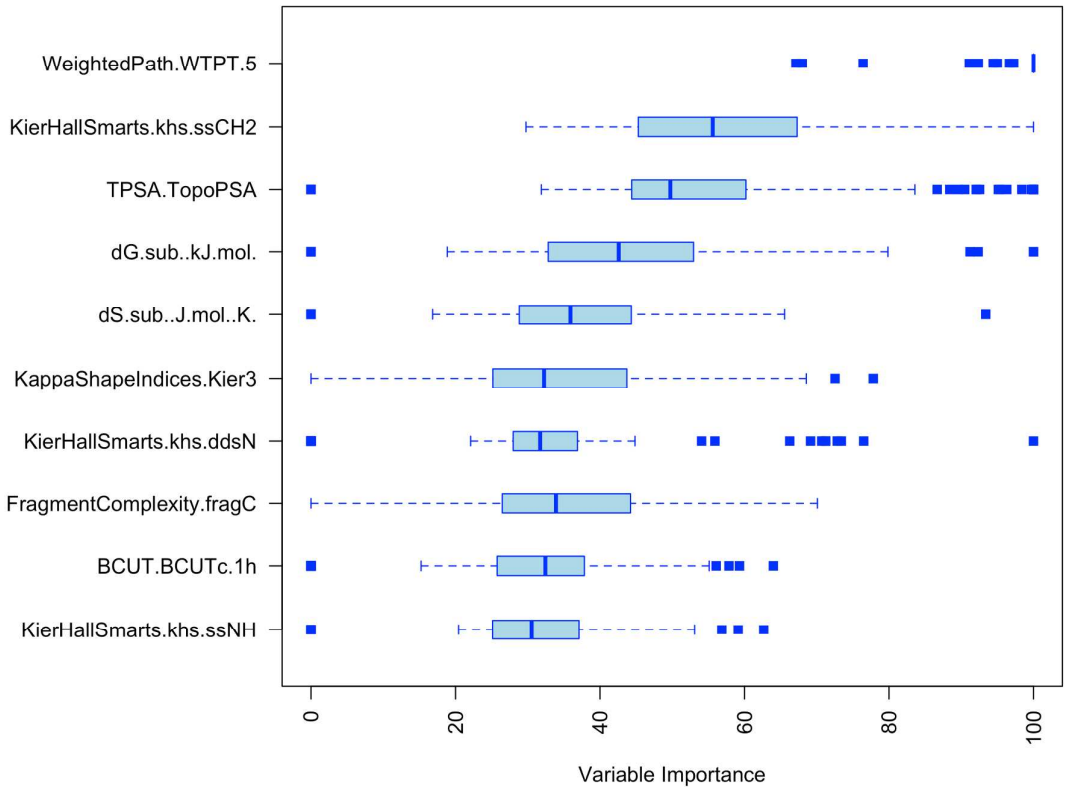

Figure S 41. Entropy all descriptors variable importance from RF.

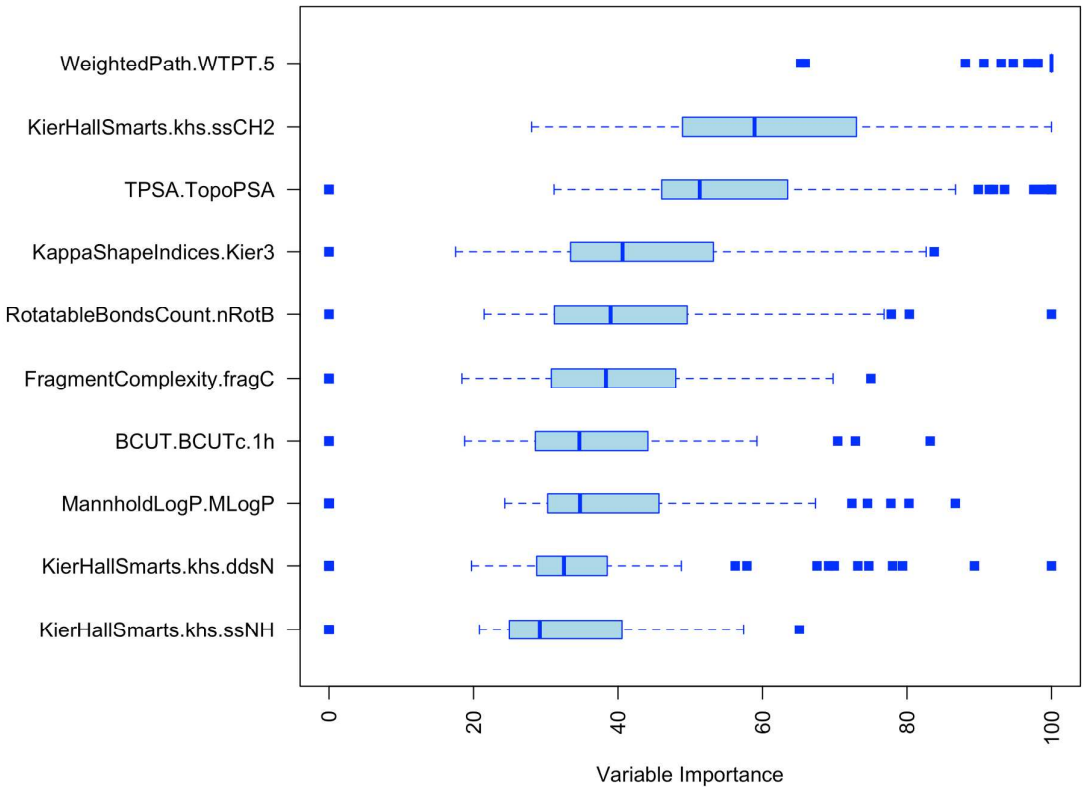

Figure S 42. Entropy CDK descriptors variable importance from RF.

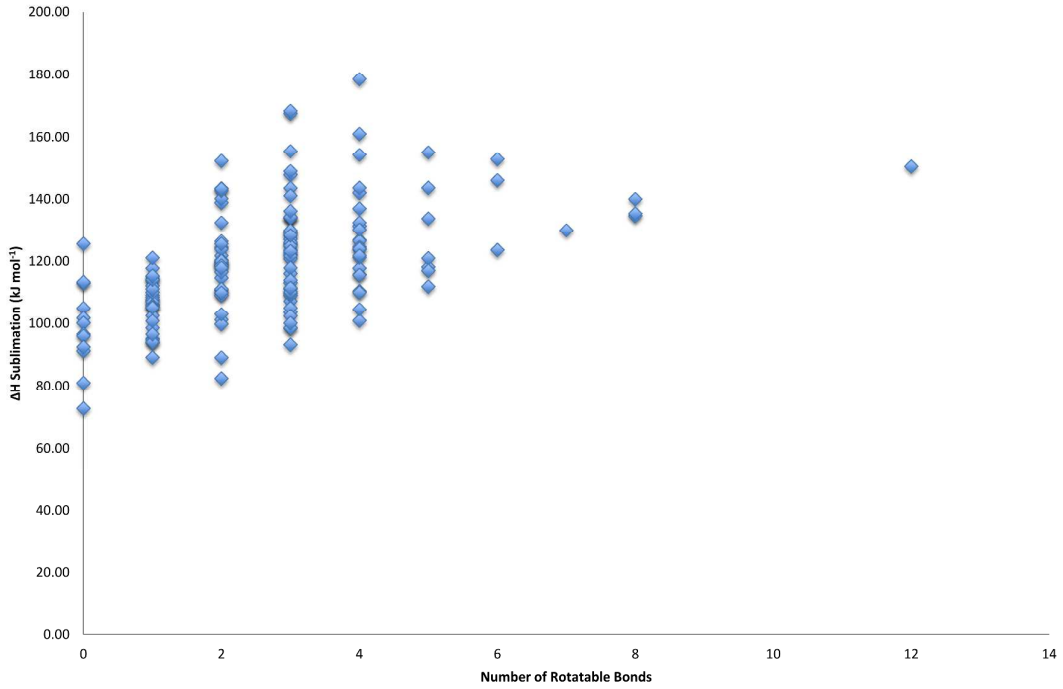

Figure S 43. Number of rotatable bonds against the experimental enthalpy of sublimation.

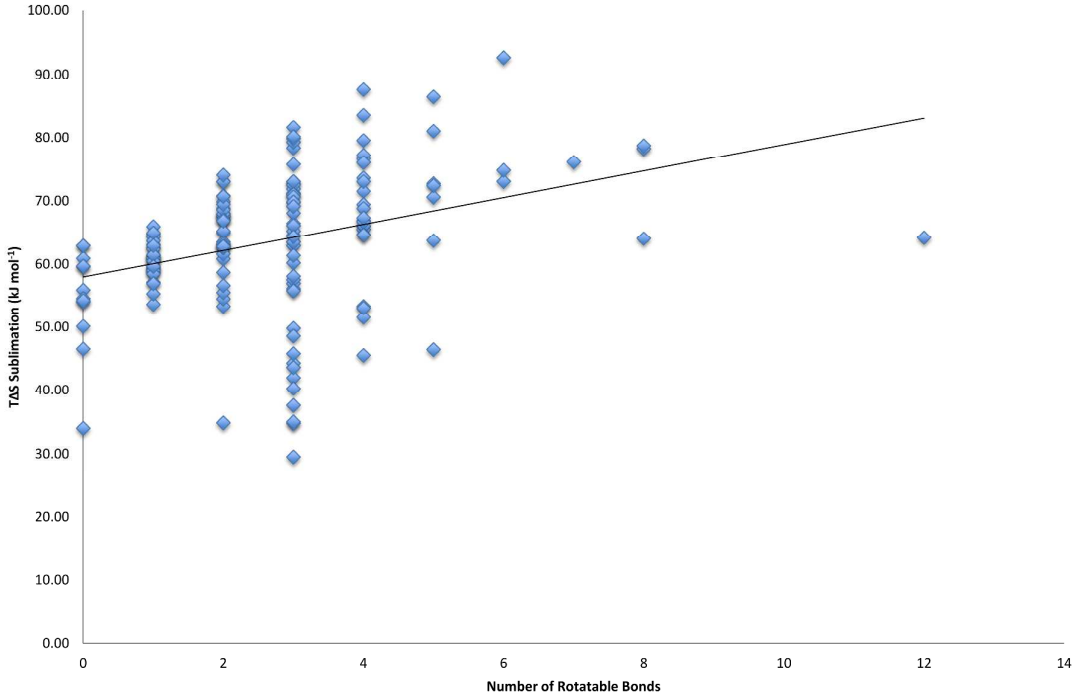

Figure S 44. Number of rotatable bonds against the experimental TΔS.

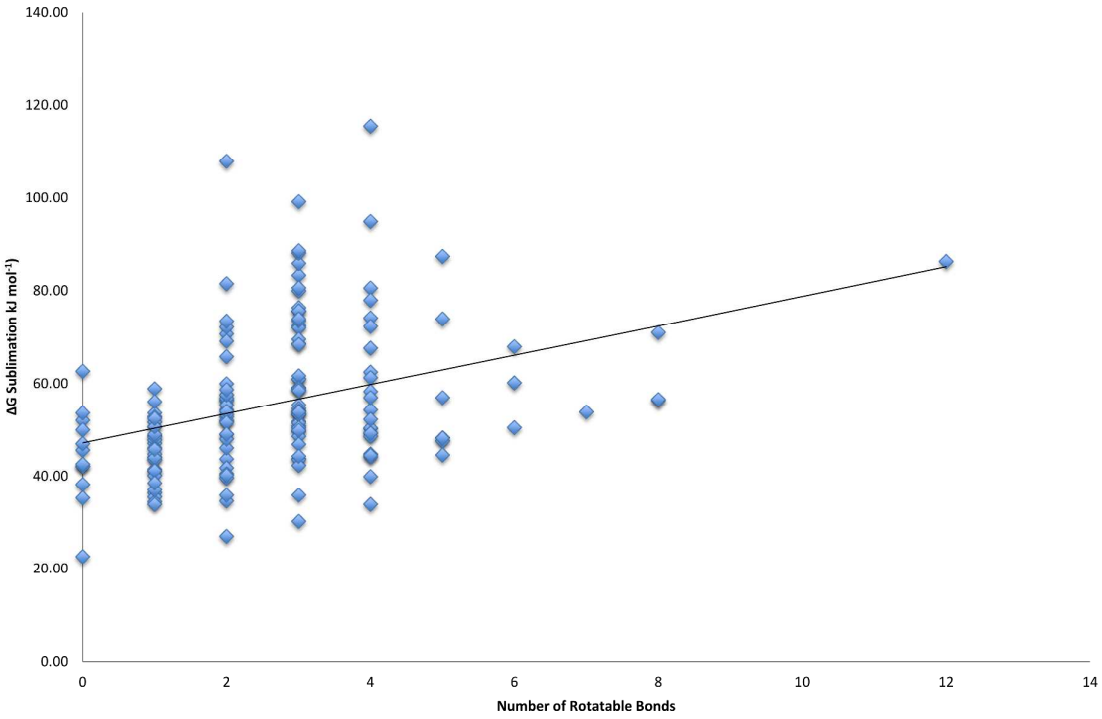

Figure S 45. Number of rotatable bonds against the experimental free energy of sublimation.

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