Metabolomic Profiling Reveals Potential Markers and Mechanism for Bladder Cancer Progression

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List of Supplemental Materials

1) **Supplemental Methods**
2) **Supplemental Discussion**
3) **References**
4) **Supplementary Figures 1-6**
5) **Supplementary Tables S1-S11**

Supplemental Methods

Sample preparation for mass spectrometry-based examination of metabolome in tissues: Bladder tissues were stored at -140°C until analysis. For extraction of metabolome, 25 mg of tissue was homogenized in 1:4 ice cold water:methanol mixture containing equimolar mixture of 11 standard compounds [Epibrassinolide, [D3] Testosterone (mass difference from endogenous Testosterone = 3 Da), [15N] Anthranilic acid (mass difference from endogenous Anthranilic acid =1 Da), Zeatine, Jasmonic acid, Gibberelic acid, [D4] Estrone (mass difference from endogenous Estrone =4 Da), [15N]-Tryptophan (mass difference from endogenous Tryptophan =1 Da), [D4] Thymine (mass difference from endogenous Thymine =4 Da), [13C] Creatinine (mass difference from endogenous Creatinine =1 Da) and [15N] Arginine (mass difference from endogenous Arginine =1 Da)]. This was followed by sequential addition of ice cold chloroform and water in 3:1 ratio and separation of the organic (methanol and chloroform) and aqueous solvents (water:methanol:chloroform:water; ratio 1:4:3:1). The aqueous extract was de-proteinized using

a 3 KDa molecular filter (Amicon Ultracel -3K Membrane, Millipore Corporation, Billerica, MA) and the filtrate containing metabolites was dried under vacuum (Genevac EZ-2plus, Gardiner, NY). Prior to mass spectrometry, the dried extract was resuspended in identical volume of injection solvent composed of water:methanol (50:50) with 0.2% acetic acid and subjected to liquid chromatography (LC) mass spectrometry.

Liquid Chromatography/Mass Spectrometry (LC/MS): The chromatographic separation of metabolites was performed using either reverse phase (RP) separation or aqueous normal phase separation online with QTOF/QQQ mass spectrometers (both Agilent Technologies, Santa Clara, CA).

The RP separation associated with the unbiased profiling employed a gradient composed of water (solvent A) and methanol (MeOH, solvent B, with both solvents modified by the addition of 0.2% acetic acid). The binary pump flow rate was 0.6 ml/min with a gradient spanning 2% B to 98% B over a 24 minute period. A column system consisting of a guard column made of Zorbax SB-C8 (2.1X 30 mm, 3.5 um) attached to an analytical Zorbax SB-Aq (2.1x50 mm, 1.8 um, Agilent Technologies, Santa Clara, CA) was used for separating the metabolites.

For the targeted profiling (SRM), the RP chromatographic method employed a gradient containing water (solvent A) and acetonitrile (ACN, solvent B, with both solvents containing 0.2% Acetic acid and 0.1% formic acid). Separation of metabolites was performed on a Zorbax Eclipse XDB-C18 column (50 × 4.6 mm i.d.; 1.8 μm, Agilent Technologies, CA) maintained at 37°C. The binary pump flow rate was 0.2 ml/min with a gradient spanning 2% B to 95% B over a 25 minute time period.

In addition, an aqueous normal phase (ANP) chromatographic separation was also used for targeted identification of metabolites. This employed solvents containing acetonitrile (ACN, solvent A): water (solvent B), with both solvents modified by the addition of 0.2% Acetic acid and 0.1% formic acid. The binary pump flow rate was 0.4 ml/min with a gradient spanning 95 % B to 2 % B over a 20 minute period. Metabolites were separated on a Diamond Hydride column (4um, 100A 2.1x150mm, MicroSolv Technology, Eatontown, NJ), that was maintained in temperature controlled chamber (37^{o}C). All the columns used in this study were washed and reconditioned after every 50 injections.

As controls to monitor the profiling process, an equimolar mixture of 11 standard compounds (described under the section titled "Sample preparation for mass spectrometry-based examination of metabolome in tissues"), and a characterized pool of mouse liver tissue were extracted and analyzed in tandem with the clinical samples. These controls were incorporated multiple times into the randomization scheme such that sample preparation and analytical variability could be constantly monitored. Furthermore, two blank runs were performed following the analysis of each clinical sample to prevent any carryover of metabolites.

Metabolomic Mass Spectrometry The mass spectrometry portion of the unbiased profiling platform is based on a 1200 SL Rapid resolution LC and a 6520 Quadrapole Time Of Flight (Q-TOF) mass spectrometer (Agilent Technologies, Santa Clara, CA). The samples were independently examined in both positive and negative ionization modes using a dual Electrospray Ionization (ESI) source. Real time mass correction during mass spectrometry was achieved by infusion of a standard mixture of reference ions using an independent 1200 SL Rapid resolution LC isocratic pump equipped with 100:1 splitter to output a flow rate of 5 ml/min. This reference mixture supplied by the vendor contained ions with m/z 121.050873,

922.009798 and 119.03632, 966.000725 for mass correction in the positive (+) and negative (-) ionization modes respectively. A mass range between 50-1000 m/z was employed for the entire unbiased profiling process. The mass accuracy for the profiling study was below 10 ppm. The data acquisition during the analysis was controlled using the Mass Hunter workstation data acquisition software. Parameters used during the mass spectrometry analysis were 1) capillary voltage set at 4000 V (negative mode 3500 V); 2) source temperature set at 325 C; 3) drying gas used at 10 ml/min; 4) nebulizer pressure maintained at 45 psig (reference ion nebulizer 10 psig); 5) fragmentor voltage set at 140V and 6) skimmer voltage maintained at 65 V. Ultra high, pure nitrogen was used as the nebulizer and collision gas for the entire analysis. For collision induced dissociation (CID) experiments, the precursor ion was selected using the quadrupole analyzer set to high-resolution mode while the product ions were analyzed by the TOF analyzer. The collision energies in all the experiments were set between 10-40 eV unless otherwise specified. For the unbiased profiling experiments, mass spectral data was acquired in both centroid and profile modes.

Single Reaction Monitoring (SRM) experiments were performed using a Triple Quadrupole Mass Spectrometer (QQQ Agilent Technologies, Santa Clara CA, refer to **Supplementary Table S8** for SRM transitions). The operational parameters for this mass spectrometer included 1) source conditions capillary voltage of 3000 V and source temperature of 350^{o}C, 2) drying gas maintained at 10 ml/min, 3) nebulizer pressure set at 35 psig and 4) fragmentor voltage set at 70 V. The collision energies used for fragmentation was set at 10-40 eV unless otherwise stated.

Metabolomic Library, METLIN: This was used to search the mass spectral data. METLIN (Agilent Technologies, Santa Clara, CA), was created using approximately 1000

commercially available compounds whose retention time was defined using the RP and ANP chromatographic methods described above. Additionally, it also contained mass and fragment ion information for these compounds in both positive and negative ionization modes. Both mass and retention time information were employed to name the compounds detected in this study.

Metabolomic Data Analysis: Metabolites in the profiling data, with more than 75% missing values across samples were removed from the analysis. The above procedure resulted in 1509, 510 and 55 compounds in unbiased positive (+) and negative (-) ionization and Single Reaction Monitoring (SRM) data, respectively, resulting in 1905 unique compounds (listed in **Supplementary Table S9**) across platforms, from which 99 metabolites were named. For the remaining metabolites, the distribution of proportion of missing values in bladder cancer and benign samples were examined, and compounds with more than 90% missing values in each group, and less than 75% missing values overall, were considered to have biological missingness. Missing values for this group of metabolites were replaced (imputed) with the intensity value at the detection level (corresponding to a value of 2000). The missing measures in the remainder of metabolites were imputed using the nearest- neighbor algorithm with k=5, using the package "pamr" (1) in the R programming language (2). Imputed data from positive and negative ionization were log2 transformed and quantile normalized per sample using the R-package "limma" (3). To avoid bias due to a small number of compounds measured by targeted mass spectrometry, median centering was employed instead of quantile normalization for data pre-processing. Heat maps were drawn using R-packages "gplot" (4). Data obtained from different platforms were z-transformed and compared across samples. The samples from different platforms were then combined by averaging over duplicate samples for every given compound (eg. samples from positive and negative ionization and SRM). Hierarchical clustering

was performed using complete linkage with Pearson's correlation. A two-sided t-test was used to assess the association of each metabolite with the cancer status of the sample. Significance was determined using 10,000 sample permutations, and the resulting p-values were then adjusted for multiple testing using FDR with q*=0.2. Tests on all of the metabolites were adjusted by calculating the q-values for FDRs using the procedure implemented in the R-package fdrtool (5). FDR controlling procedure described in (6) was employed to correct the tests for named metabolites. The latter method was implemented to prevent the breakdown of the q-value based method in a small number of tests.

Data from urine samples were first normalized with respect to the osmolarity level of the sample, and then median centered and normalized using the inter-quartile range (IQR). Heat maps and hierarchical clustering were obtained as described above for tissue data. Partial Least Square Discriminant Analysis (PLS-DA) classification models in urine with two principal components (R-packages "pls" and "caret") (3, 7) were used to classify the benign and BCa samples in different datasets, as well as Muscle-Invasive and Non-Muscle-Invasive samples in the UM data set. Three-fold cross validation (CV) was used to assess the performance of the classification models in UM data. In order to obtain more reliable estimates, the process was repeated 1000 times, with random splitting of the data into three folds each time. In particular, we built a partial least squares discriminate analysis (PLS-DA)-based classifier with two principal components (PC1 and PC2) on a randomly selected set of two-thirds (n = 30, training set) of the urine specimens from the Group 2 (UM data) and assessed its performance on the remaining one-third (n = 14) of the samples in this group (test set). The process of training and testing was repeated 1,000 times to evaluate the performance of the PLS-DA classifier. ROC plots were drawn using the available functions in the R-package "caret" (7).

Integrative Molecular Concept Modeling of BCa Progression: We examined whether BCa-associated metabolites might be associated with altered biochemical processes fundamental to BCa development and progression using Oncomine Concept Maps (OCM), as described earlier (8). OCM compares the information within the BCa-associated metabolome with different biologic concepts represented by molecular signatures a.k.a. molecular concepts (i.e., lists of genes, proteins etc) (8). The latter is derived from cancer-related profiles including both gene and protein annotations from external databases, as well as computationally-derived regulatory networks. The regulatory networks were derived by scanning human promoters for known transcription factor motifs and by comparative genomics analyses, which identified the conserved promoter and 3'UTR elements. The compendia of molecular concepts for OCM analysis consisted of data from 13 databases and 335 high-throughput datasets (9).

For the OCM analysis, we used the premise that metabolites are end-products of gene/protein action and hence their levels will reflect the activity of the corresponding enzymes (both synthetic and breakdown). We derived a list of genes whose activity could potentially alter the levels of metabolites in the BCa-associated signature. These genes were used to carry out all-versus-all association analyses with the various cancer-related molecular signatures compiled from the external databases and computationally-derived regulatory networks. The genes associated with metabolic pathways in Homo sapiens and listed in KEGG (Kyoto Encyclopedia of Genes and Genomes) were used as the null set. To select concepts of potential interest, enrichment p-values derived using Fisher's exact test were adjusted for multiple comparisons and an FDR threshold of 10% was used. These "Molecular concepts" allowed us to link BCa-associated metabolomic signatures to biological processes, generating novel mechanistic insights

on BCa progression. A subset of molecular concepts is displayed in **Fig.4A**, and a list of all enriched concepts with their p-values is shown in **Supplementary Table S11**.

Immunoblot Analysis: Frozen bladder tissues (cancer and adjacent benign) tissue specimens were lysed in RIPA buffer (50 mM Tris-HCl, pH 7.4, 150 mM NaCl, 1 mM EDTA, 1% Triton X-100, 1% Sodium deoxycholate, 0.1% sodium dodecyl sulphate, protease and phosphatase inhibitors) and their protein concentration was determined by BCA protein assay kit as per manufacturer's instructions (Thermo Scientific, Rockford, IL). Equal amount of protein (30 µg) was separated by SDS-PAGE using pre-cast 4-20% mini-protean TGX gels (Bio-Rad laboratories, Hercules, CA) and transferred to Immobilon-PVDF (Polyvinylidene fluoride) membrane (Millipore Corp., Billerica, MA). The membranes were blocked in 3% non-fat dry milk (in TBST) for 1 h and incubated overnight with CYP1A1/CYP1B1 and/or GAPDH (loading control) primary antibodies (both from Santa Cruz Biotechnology Inc., Santa Cruz, CA). After washing the membranes with TBST, they were incubated with appropriate secondary antibodies (Cell Signaling, Danver, MA) for 1 h, washed, proteins detected by ECL chemiluminiscence detection kit (Thermo Scientific, Rockford, IL) and captured on autoradiography film (Denville Scientific Inc., Metuchen, NJ).

Supplemental Discussion:

Relevance of methylation-induced regulation of xenobiotic metabolizing enzymes: Using a data-driven approach, we confirmed a role for methylation as an additional contributing factor in regulating the expression of xenobiotic metabolizing enzymes. Importantly, this observation could be a consequence of elevated SAM levels within BCa tumors themselves. Interestingly, a

recent study demonstrated the existence of a novel epigenetic signature during BCa progression (10), supporting our metabolome-based findings. Furthermore, our findings provide additional rationale for the use of DNA hypomethylating agents like Zorbularin and Azacytidine in BCa, as shown by earlier studies using in vitro and in vivo models of the disease (11, 12).

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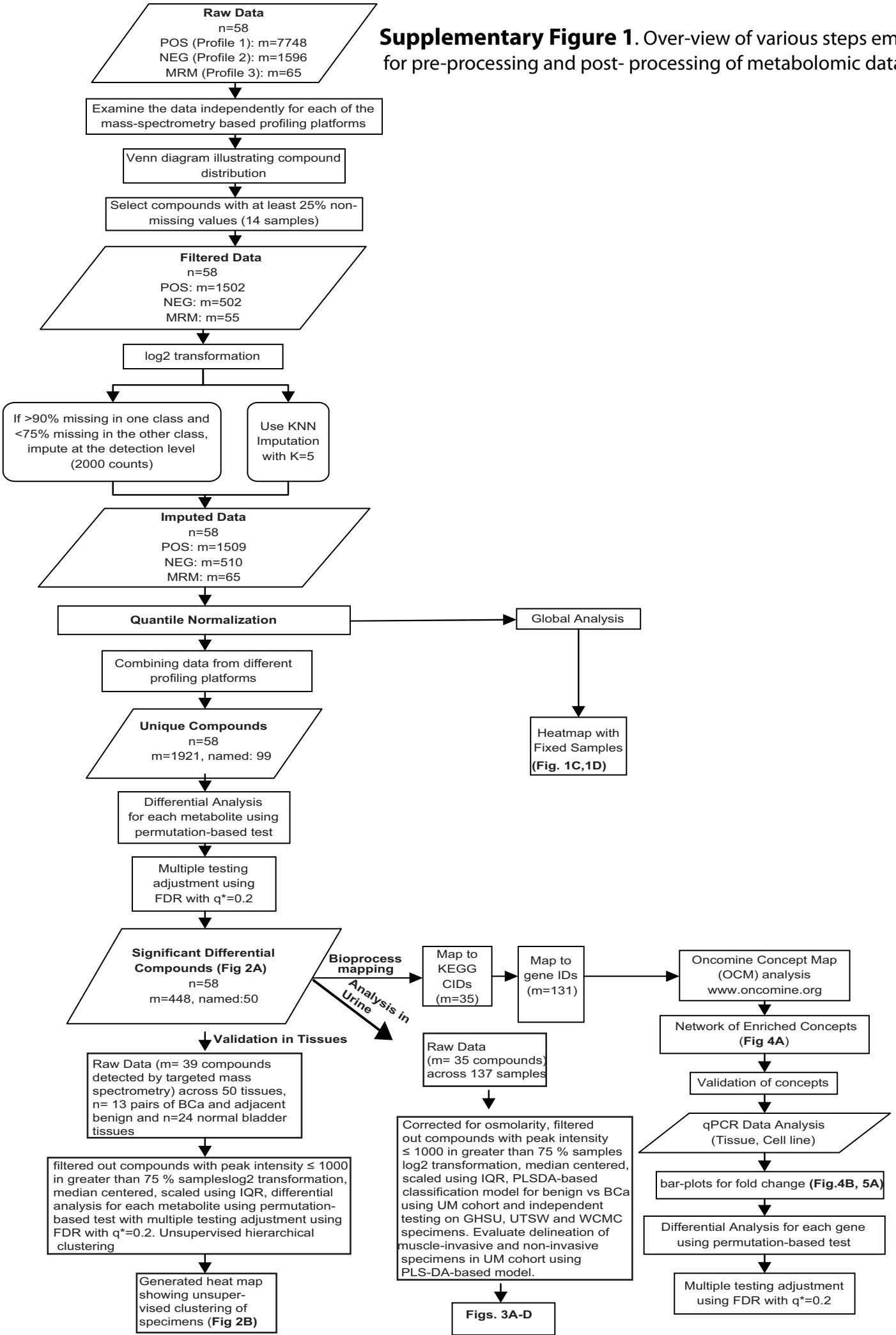
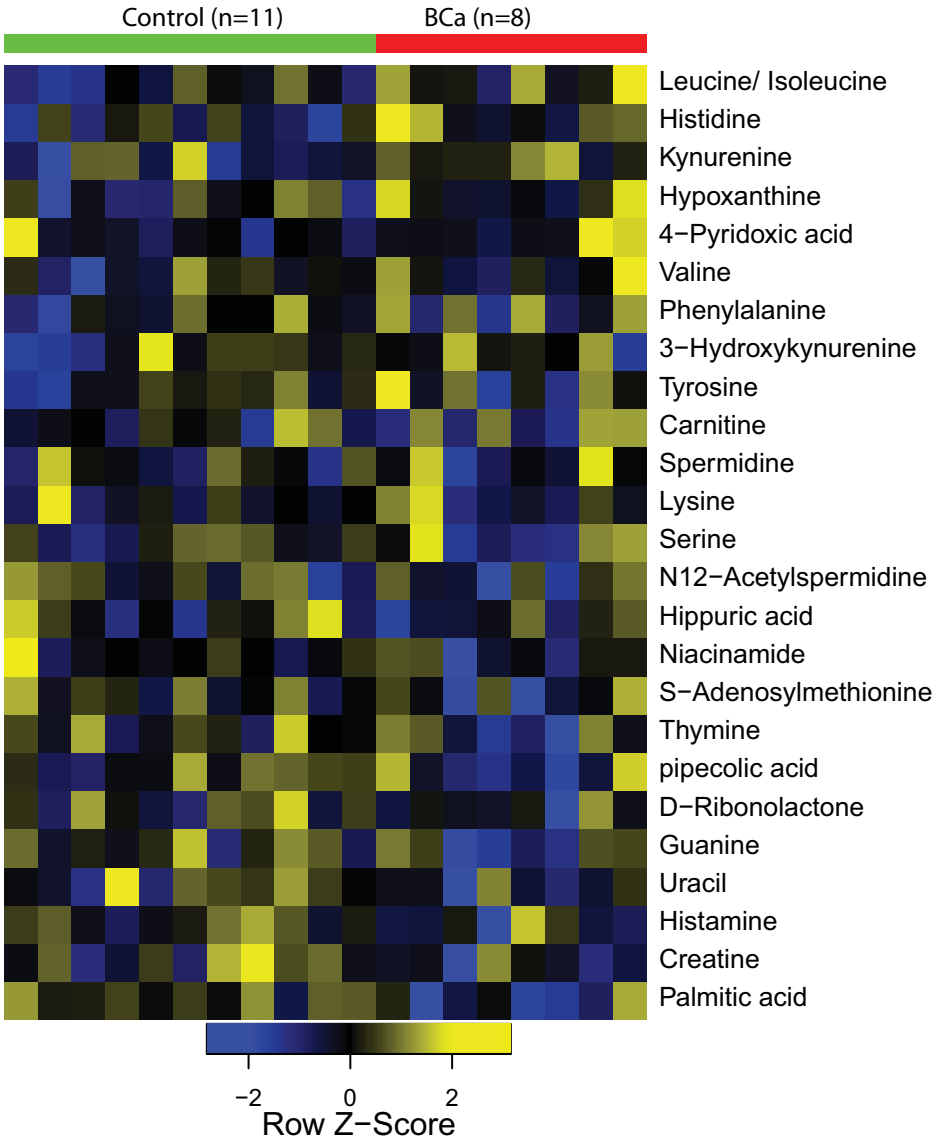
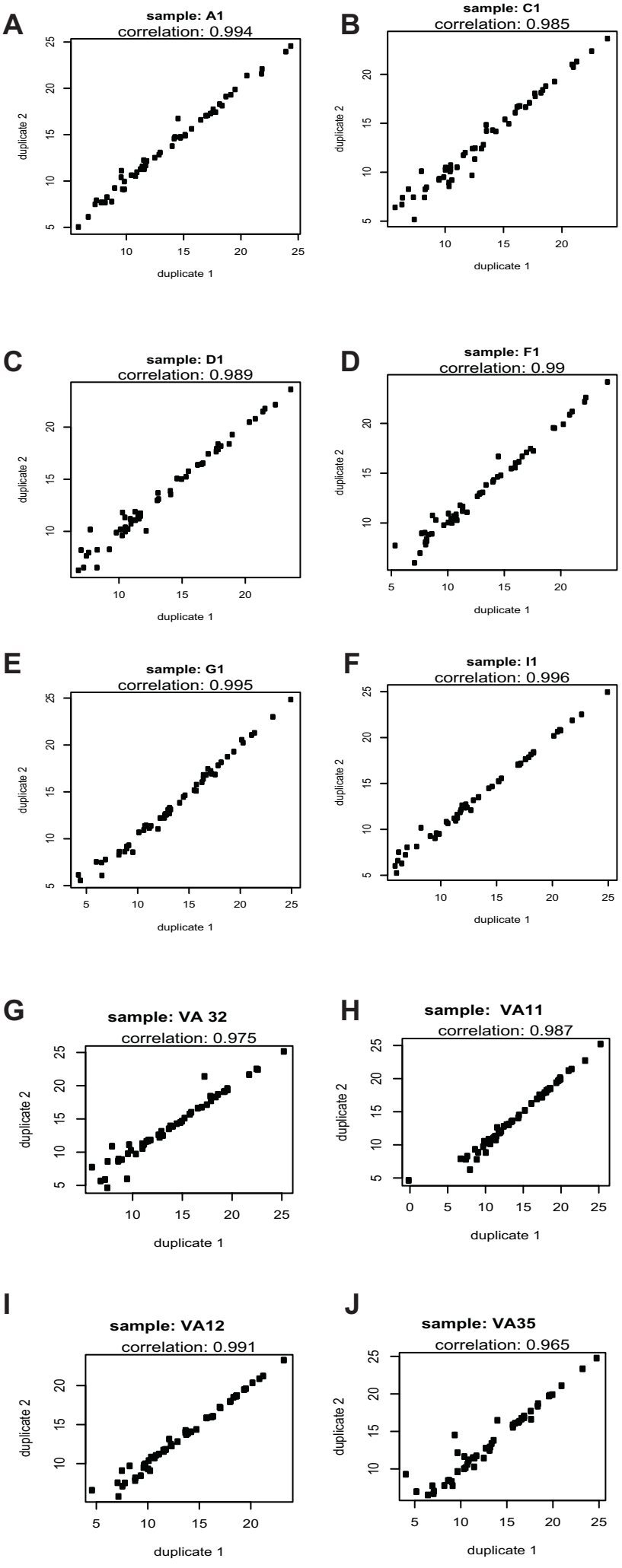
Supplementary Figure 1. Over-view of various steps employed for pre-processing and post- processing of metabolomic data.



Supplementary Figure 2 Heat map showing relative levels of 40 bladder-cancer associated metabolites in benign prostate (n=10) and prostate cancer (n=10). Only glyceraldehyde-3-phosphate levels (indicated by *) were significantly elevated in prostate cancer as was the case in bladder cancer.

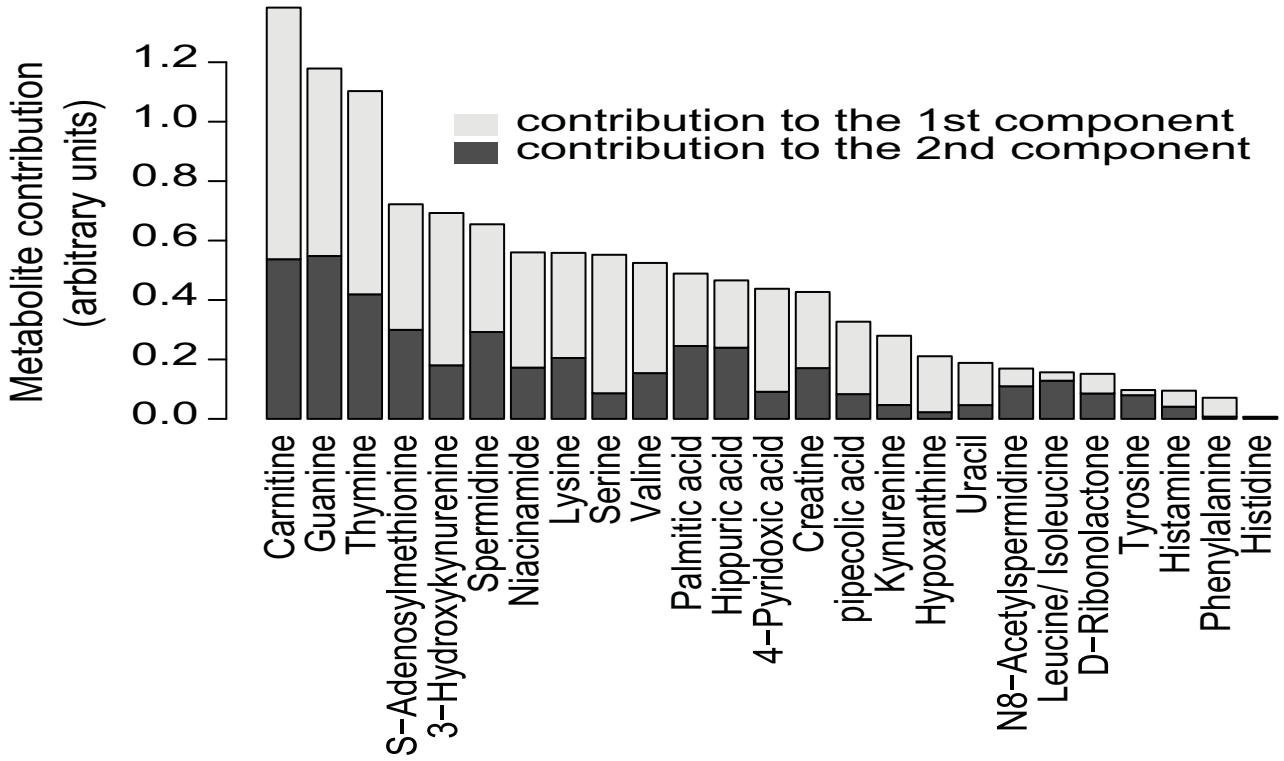


Supplementary Figure 3. Heat map showing relative levels of 25 bladder-cancer associated metabolites in urine from bladder cancer (n=8) and control (n=11) individuals. The control urine was collected from patients having no prior/current history of bladder cancer ad diagnosed with either prostate cancer or other non-cancer urological conditions like kidney stone, neurogenic bladder etc.



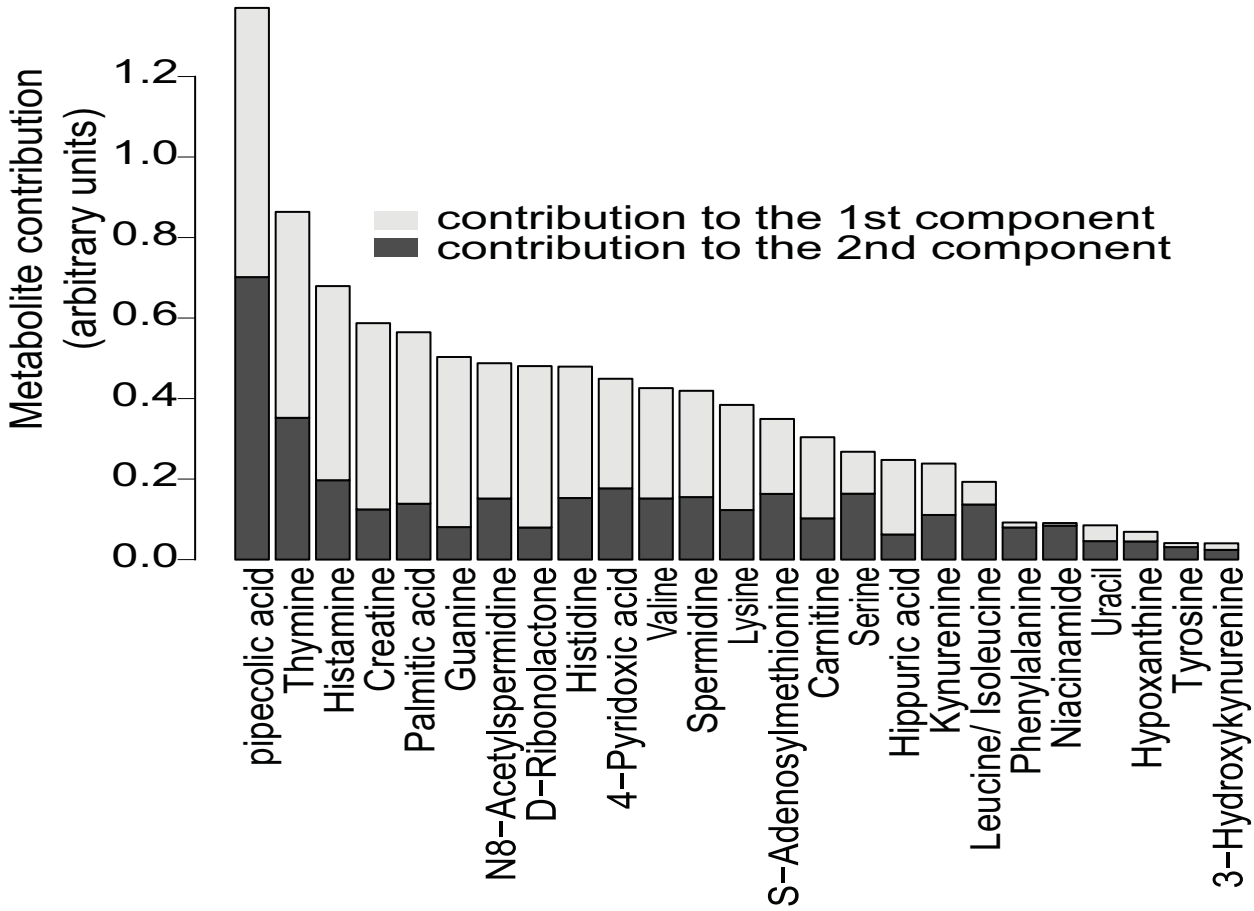
Supplementary Figure 4.

Correlation plots showing concordance in levels of BCa-specific metabolites (n=25 + 7 spiked standards) measured using targeted mass spectrometry across replicates of urine specimens from 10 patients



Supplementary Figure 5.

Plot showing the contribution of metabolites in a PLS-DA model used for classification of benign and BCa in urine in a model with two principal components (PCs). Contributions of each metabolite are calculated as the sum of the absolute value of the coefficient of each compound for the first (shown by black bars) and second (grey bars) PCs.



Supplementary Figure 6.

Plot showing the contribution of metabolites in a PLS-DA model used for classification of non-muscle-invasive and muscle-invasive BCa in urine in a model with two principal components (PCs). Contributions of each metabolite are calculated as the sum of the absolute value of the coefficient of each compound for the first (shown by black bars) and second (grey bars) PCs.

Supplementary Table S1. Detailed clinical information of bladder-derived tissues used for metabolomic profiling

Specimen ID	Age	Gender	Tissue	Specimen Type	Type of Carcinoma	Muscle Invasion Status (y/n)	Grade (high/low)	Grading	TNM staging
P1T-EU P1N-EU	71	M	Bladder	T N	Infiltrating,urothelial, TCC	y	high	G2	T3aN0Mx
P2T-EU P2N-EU	69	M	Bladder	T N	Urothelial,TCC	y	high	G2	T3bN2M1
P3T-EU P3N-EU	56	M	Bladder	T N	Urothelial, Invasive Papillary, TCC	y	high	G2	T2bN0Mx
P4T-EU P4N-EU	51	M	Bladder	T N	Urothelial,TCC	n			
P5T-EU P5N-EU	59	M	Bladder	T N	Urothelial,TCC	y	high	G2	T2bN2Mx
P6T-EU P6N-EU	57	M	Bladder	T N	Urothelial,TCC	y	high	G2	T2aN0Mx
P7T-EU P7N-EU	71	M	Bladder	T N	Urothelial,TCC	y	high	G2	T2aN0Mx
P8T-EU P8N-EU	80	M	Bladder	T N	Urothelial,TCC	y	high	G2	T3aN1Mx
P9T-EU P9N-EU	64	M	Bladder	T N	Urothelial,TCC	y	high	G2	T3aN Mx
P10T-EU P10N-EU	68	M	Bladder	T N	Urothelial,TCC	y	high	G2	T4aN0Mx
P11T-EU P11N-EU	67	M	Bladder	T 90% N	Urothelial,TCC	y	high	G2	T4aN2Mx
P12T-EU P12N-EU	62	M	Bladder	T N	Urothelial,TCC	n	high	G2	T3aN1Mx
P13T-EU P13N-EU	62	M	Bladder	T N	Urothelial,TCC	n	high	G1	TisN0Mx
P14T-EU P14N-EU	55	M	Bladder	T CIS	Urothelial,TCC, Invasive	y	high	G2	T3bN0Mx
P15T-EU P15N-EU	71	M	Bladder	T N	Urothelial,TCC	y	high	G2	T4aN2Mx
P16T-EU P16N-EU	56	M	Bladder w/ Prostate	T N	Urothelial,TCC	y	high	G2	T3aN2Mx
P7T-MCG P3N-MCG	83	F	Bladder	50% T N	Urothelial,TCC	n	high		T3aN1MX
P9T-MCG P4N-MCG	63	M	Bladder	55% T N	Urothelial,TCC	n			
P10T-MCG P5N-MCG	54	M	Bladder	40% T N	Urothelial,TCC	n			T2a
P11T-MCG P6N-MCG	78	M	Bladder	T N	Urothelial,TCC	n	high		n/a
P13T-MCG P8N-MCG	71	M	Bladder	40% T N	Urothelial,TCC	n			Unknown
P1T-MCG P1N-MCG	67	M	Bladder	T N	Urothelial,TCC, papillary	n	high		T2AN0MO
P2T-MCG P2N-MCG	74	M	Bladder	T N					T1N0
P8T-MCG P11N-MCG	68	F	Bladder	T N	Urothelial,TCC	n			
P12T-MCG P7N-MCG	71	M	Bladder	T N	Urothelial,TCC, papillary	n	high		T1
P15T-MCG P10N-MCG	50	M	Bladder	95% T N	Urothelial,TCC, papillary	n	high		T4N1
P16T-MCG	52	M	Bladder	T	Urothelial,TCC	n	low		T3NO
P9N-MCG	58	M	Bladder	N					
P3T-MCG	53	M	Bladder	T	Urothelial,TCC	n	low		T3N0M0
P5T-MCG	70	M	Bladder	T	Urothelial,TCC, papillary	n	high		
P4T-MCG	70	F	Bladder	60% T		n			
P6T-MCG	70	F	Bladder	T	Urothelial,TCC	n			

Supplemenary Table S2. Clinical characteristics of specimens used for validation of tissue-derived BCa signature

Speciman ID	Age	Gender	Tissue typ	Diagnosis	Path Review
EU-19N	70	M	Bladder	N	Benign adjacent
EU-19T			Bladder	T	Urothelial TCC
EU-20N	73	M	Bladder	N	Benign adjacent
EU-20T			Bladder	T	Urothelial TCC
EU-22N	83	M	Bladder	N	
EU-22T			Bladder	N	No malignancy
EU-23N	57	M	Bladder	N	ca in-situ
EU-23T			Bladder	T	Urothelial TCC
EU-24N	64	F	Bladder	N	
EU-24T			Bladder	N	No malignancy
EU-25N	75	M	Bladder	N	Benign adjacent
EU-25T			Bladder	T	Urothelial TCC
EU-26N	66	m	Bladder	N	Benign adjacent
EU-26T			Bladder	N	ca in-situ
EU-27N			Bladder	N	Benign adjacent
EU-27T			Bladder	T	Urothelial TCC
EU-28N			Bladder	N	Benign adjacent
EU-28T			Bladder	T	Urothelial TCC
EU-33N			Bladder	N	Benign adjacent
EU-33T			Bladder	T	Urothelial TCC
EU-34N			Bladder	N	Benign adjacent
EU-34T			Bladder	T	Urothelial TCC
EU-32N			Bladder	N	Benign adjacent
EU-17N	65	M	Bladder	N	Benign adjacent
EU-21T	63	M	Bladder	T	Urothelial TCC
EU-29N			Bladder	N	Benign adjacent
EU-30T			Bladder	T	Urothelial TCC
EU-32T			Bladder	T	Urothelial TCC
EU-35N			Bladder	N	Benign adjacent
0059678-07	80	F	Bladder	N	Normal Bladder
0060504-10*	76	F	Bladder	N	Normal Bladder
0060514-06	80	M	Bladder	N	Normal Bladder
0060530-03	61	M	Bladder	N	Normal Bladder
0060539-03	75	M	Bladder	N	Normal Bladder
0060684-07	63	F	Bladder	N	Normal Bladder
0060730-03*	78	M	Bladder	N	Normal Bladder
0060808-03*	85	F	Bladder	N	Normal Bladder
0060897-03	62	F	Bladder	N	Normal Bladder
0060910-02	69	M	Bladder	N	Normal Bladder
0060955-03*	76	M	Bladder	N	Normal Bladder
0060960-04	32	M	Bladder	N	Normal Bladder
0061011-03	65	M	Bladder	N	Normal Bladder
0061030-04	97	F	Bladder	N	Normal Bladder
0061060-03	49	F	Bladder	N	Normal Bladder
0061480-02	17	M	Bladder	N	Normal Bladder
0065242-05	20	F	Bladder	N	Normal Bladder
0065337-17	23	F	Bladder	N	Normal Bladder
0065349-03	15	F	Bladder	N	Normal Bladder
0065633-04	13	M	Bladder	N	Normal Bladder
0065936-10	44	F	Bladder	N	Normal Bladder
0065963-17	78	M	Bladder	N	Normal Bladder
0066130-16	48	F	Bladder	N	Normal Bladder
0066157-10	41	M	Bladder	N	Normal Bladder

* : predominently fibrous tissue, N: includes both benign adjacent and normal bladder tissue, T: BCa

Supplementary Table S3. Clinical information of the urine specimens from Georgia Health Science University used in the study.

Specimen ID	Gender	Age	Race	Urine Diagnosis	Histology	Init Clinical T-Stage	WHO Grade	Prior Therapy
VA32	M	60	Black	Bladder Cancer	Extravesical	T3aN0	High	Chemotherapy
VA33	M	53	White	Bladder Cancer	Muscle-Invasive	T4	High	None
VA34	M	87	White	Bladder Cancer	Non-Invasive	Ta	High	None
VA35	M	43	White	Bladder Cancer	Extravesical Extension	T4aN0	High	Chemotherapy
VA36	M	62	Black	Bladder Cancer	Lamina Propria Invasive	T1	High	Chemotherapy
VA37	M	45	White	Bladder Cancer	Extravesical Extension	T4aN0	High	Chemotherapy
VA38	M	58	White	Bladder Cancer	Non-Invasive	Ta	Low	None
VA41	F	59	White	Control				
VA42	M	66	White	Control				
VA43	F	40	Black	Control				
VA44	F	48	White	Control				
VA45	M	67	White	Control				
VA1	F	83	Black	Bladder Cancer	Lamina Propria invasive	T1	High	None
VA15	M	34	Black	Control				
VA2	M	56	White	Bladder Cancer	Lamina Propria invasive	T1	High	None
VA17	M	63	White	Control	Prostatitis,			None
VA3	F	45	White	Bladder Cancer	Muscle-Invasive		High	None
VA18	F	43	White	Control				
VA19	M	54	White	Control				
VA4	M	57	Black	Bladder Cancer		T3b	High	None
VA20	F	63	White	Control				None
VA5	M	62	White	Bladder Cancer			High	Chemotherapy
VA21	M	58	White	Control				
VA22	M	40	White	Control				
VA6	M	78	White	Bladder Cancer		T2		
VA23	M	48	Black	Control				

Abbreviations: cT: clinical staging pT: pathological staging Dx: diagnosis TURBT: Trans Urethral Resection of Bladder

Supplementary Table S4. Clinical information of urine specimens from University of Michigan used in this study

			Therapy administered		Post Chemotherapy and TuRBT			
ID	Sex	Age	Prior Chemotherapy	Prior Therapy	Urine_cT-stage	Urine_pT-Stage	Class Membership for the study	Urine_Cytology
A1	M	65	BCG	Intravesical	T0	T0	Down-staged Benign	Negative
A2	F	73	None	None	T0	T0	Down-staged Benign	Atypia or negative
A3	F	71	None	None	CIS	CIS	Non-muscle invasive	Positive
A4	F	40	None	None	T2	T1	Non-muscle invasive	Atypia or negative
C1	M	77	PCG + Herceptin	Systemic	T4	T1	Non-muscle invasive	Suspicious or negative
C2	M	88	None	None	T3b	T2	Muscle invasive	Suspicious or negative
C3	M	46	PCG	Systemic	T3	T1	Non-muscle invasive	Positive
C4	M	71	None	None	T2	T1 + CIS	Non-muscle invasive	Suspicious or negative
C5	M	52	BCG	Intravesical	CIS	T1 + CIS	Non-muscle invasive	Positive
C6	M	68	None	None	T1	CIS	Non-muscle invasive	Positive
C7	M	45	None	None	T3	T1	Non-muscle invasive	Atypia or negative
C8	M	67	BCG, MMC	Intravesical	Ta	T0	Down-staged Benign	Negative
D1	M	74	Gemcitabine	Systemic	T0	T0	Down-staged Benign	Negative
D2	F	92	BCG, MMC	Intravesical	Ta	T0	Down-staged Benign	Negative
D3	F	58	Carboplatin, Paclitaxel	Systemic	T0	T2	Muscle invasive	Suspicious or negative
D4	F	74	Methotrexate, Cytoxan, vincristine, 5-FU	Systemic	T2b	T2	Muscle invasive	Suspicious or negative
D5	F	77	None	None	T1 + CIS	T1 + CIS	Non-muscle invasive	Positive
D6	M	66	None	None	T1 + CIS	T1 + CIS	Non-muscle invasive	Atypia or negative
D7	M	74	MVAC	Systemic	T0	T0	Down-staged Benign	Atypia or negative
D8	M	71	Gemcitabine	Systemic	T0	T0	Down-staged Benign	Negative
F1	M	61	None	None	T3	Ta	Non-muscle invasive	Positive
F2	M	71	MMC	Intravesical	Ta	T0	Down-staged Benign	Negative
F3	M	57	PCG	Systemic	T3b	T1	Non-muscle invasive	Positive
F4	M	69	None	None	T2	T2	Muscle invasive	Positive
F5	M	81	None	None	T2	T2	Muscle invasive	Positive
F6	M	87	BCG, unknown systemic agent	Intravesical and Systemic	T2	T2	Muscle invasive	Suspicious or negative
F7	M	76	BCG	Intravesical	CIS	T0	Down-staged Benign	Negative
F8	M	51	None	None	T2/T3a	T2	Muscle invasive	Positive
G1	M	80	BCG	Intravesical	CIS	Ta + CIS	Non-muscle invasive	Atypia or negative
G2	M	74	5-FU, BCG, MMC	Intravesical and Systemic	Ta	T0	Down-staged Benign	Negative
G3	M	59	None	None	T2	T2	Muscle invasive	Positive
G4	M	55	None	None	T1/T2	T1 + CIS	Non-muscle invasive	Positive
G5	M	78	None	None	T1	Ta	Non-muscle invasive	Dysplasia or negative
G6	M	58	BCG, MMC	Intravesical	Ta	Ta	Non-muscle invasive	Atypia or negative
G7	M	82	BCG	Intravesical	CIS	T0	Down-staged Benign	Positive
G8	M	63	None	None	T2	T0	Down-staged Benign	Positive
I1	M	75	None	None	Tx	CIS	Non-muscle invasive	Positive
I2	F	41	BCG	Intravesical	CIS	T0	Down-staged Benign	Atypia or negative
I3	F	71	BCG, INF, MVAC	Intravesical and Systemic	T0	T0	Down-staged Benign	Atypia or negative
I4	M	51	BCG, PCG	Intravesical and Systemic	T0	T0	Down-staged Benign	Atypia or negative
I5	M	63	None	None	T0	Ta	Non-muscle invasive	Atypia or negative
I6	M	86	BCG	Intravesical	Ta	Ta	Non-muscle invasive	Positive
I7	M	61	MMC	Intravesical	Ta HG	Ta	Non-muscle invasive	Positive
I8	M	57	BCG	Intravesical	T1	T0	Down-staged Benign	Atypia or negative

Abbreviations: cT: clinical staging pT: pathological staging Dx: diagnosis TURBT: Trans Urethral Resection of Bladder

Table S5. Clinical information of the urine specimens used in the study from Weil Cornell Medical College

Sample ID	Age	Urine voided cytology	Clinical stage	Grade	p53 IHC	Ki67 IHC	Diagnosis used for the study
CU1	88	negative	0	0	neg	0	Benign
CU10	80	negative	0	0	neg	0	Benign
CU11	83	negative	0	0			Benign
CU2	49	negative	0	0	neg	0	Benign
CU25	62	Positive	Ta	G1	neg	0	BCa
CU26	64	negative	Ta	G1	neg	0	BCa
CU27	64	negative	Ta	G1	neg	<5%	BCa
CU28	77	Positive	Ta	G1	neg	5-10%	BCa
CU29	70	negative	Ta	G1	neg	0	BCa
CU3	74	negative	0	0	neg	20%	Benign
CU30	85	negative	Ta	G1	neg	3-5%	BCa
CU31	54	negative	Ta	G1	neg	3%	BCa
CU32	67	negative	Ta	G1			BCa
CU33	65	negative	Ta	G1			BCa
CU34	57	negative	Ta	G1	neg	5%	BCa
CU4	72	negative	0	0	neg	0	Benign
CU42	75	negative	Ta	G2	pos	30%	BCa
CU43	84	Positive	T1	G2	neg	10%	BCa
CU44	79	Positive	Ta	G2	neg	5-10%	BCa
CU45	82	negative	Ta	G2	neg	0	BCa
CU46	76	negative	Ta	G2	neg	0	BCa
CU47	64	negative	Ta	G2	neg	10%	BCa
CU48	68	negative	Ta	G2	neg	3-5%	BCa
CU49	73	negative	Ta	G2	neg	5%	BCa
CU5	54	negative	0	0	neg	0	Benign
CU50	50	negative	Ta	G2			BCa
CU6	63	negative	0	0			Benign
CU60	75	negative	T1	G3	pos	60%	BCa
CU61	87	negative	T1	G3	neg	0	BCa
CU62	82	Positive	T1	G3	neg	0	BCa
CU63	88	Positive	T1	G3	neg	30%	BCa
CU64	79	Positive	T1	G3	neg	60%	BCa
CU65	80	Positive	T1	G3	neg	0	BCa
CU66	73	negative	T1	G3	pos	60%	BCa
CU67	71	Positive	T1	G3	neg	0	BCa
CU68	79	negative	Tis	G3			BCa
CU7	64	negative	0	0			Benign
CU8	75	negative	0	0	neg	0	Benign
CU82	63	Positive	T4	G3	neg	0	BCa
CU83	54	Positive	T2	G3	pos	60%	BCa
CU84	72	Positive	T2	G3			BCa
CU85	65	Positive	T3	G3			BCa
CU86	70	Positive	T2	G3			BCa
CU87	58	negative	T2	G3			BCa
CU9	43	negative	0	0	neg	0	Benign

Supplementary Table S6. Clinical information of the urine specimens used in this study from University of Texas Southwestern Medical Center

Specimen ID	Race	Gender	Operative Procedure	Cancer Type	Path T	Path N	Path M	History	Diagnosis used in this study
2753	B	F	Cystectomy	TCC	T1	N0	M0	PRE-CYSTECTOMY	BCa
2658	C	M	Cystectomy	Adenocarcinoma	T2a/T3a	N0	Mx	PRE-CYSTECTOMY	BCa
2393	C	M	Cystoprostatectomy	TCC/TCIS	T1	N0	Mx	PRE-CYSTECTOMY	BCa
2332	C	M	TURBT	TCC	T1	NX	MX	PRE-CYSTECTOMY	BCa
2724	B	F	TURBT/Biopsy	TCC	Ta	NX	MX	PRE-TURBT	BCa
2136	C	F	TURBT	TCC	Ta	unk	unk	PRE-TURBT	BCa
2071	H	F	TURBT/Biopsy	TCC	T1c	NX	MX	PRE-TURBT	BCa
2032	C	M	TURBT	TCC	Ta	NX	MX	PRE-TURBT	BCa
2414	C	F						Normal	Benign
2406	C	F						Normal	Benign
2407	C	F						Normal	Benign
2410	B	F						Normal	Benign
2412	C	M						Normal	Benign
2420	C	M						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign
2401	C	F						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign
2402	Unk	M						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign
2404	Unk	M						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign
2409	C	M						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign
2417	C	F						Normal (SOME TYPE OF URO DIAGNOSIS)	Benign

Abbreviations: TURBT: Trans Urethral Resection of Bladder TCC: Transitional Cell Carcinoma B: Afro-American H: Hispanic C: Caucasian Unk : Unknown

Supplementary Table S7 : Summary of proportion of missingness and coefficient of variation (CV) in detection of spiked internal standards across the various profiling platforms.

Standard	Platform	missing %	CV
GIBBERELIC ACID	QTOF-neg	0.00%	0.01
GIBBERELIC ACID	QQQ-RP	0.00%	0.05
JASMONIC ACID	QQQ-RP	0.00%	0.10
L-(15N)2-TRYPTOPHAN	QQQ-RP	0.00%	0.02
L-(15N)2-TRYPTOPHAN	QTOF-neg	0.00%	0.02
L-(15N)2-TRYPTOPHAN	QTOF-pos	3.45%	0.02
L-(D4)THYMINE	QTOF-neg	0.00%	0.01
L-(D4)THYMINE	QQQ-RP	0.00%	0.07
L[13C]-CREATININE	QQQ-DH	0.00%	0.04
L-[15N] ANTHRANILIC ACID	QTOF-neg	0.00%	0.01
L-[15N] ANTHRANILIC ACID	QQQ-RP	0.00%	0.04
L-[15N] ANTHRANILIC ACID	QQQ-DH	0.00%	0.12
L-[15N]ARGININE	QQQ-RP	0.00%	0.02
L-[15N]ARGININE	QQQ-DH	0.00%	0.17
L-[D3]TESTOSTERONE	QQQ-RP	3.45%	0.06
L-[D4]-ESTRONE	QTOF-pos	3.57%	0.08
L-EPIBRASSINOLIDE	QTOF-pos	3.57%	0.15
ZEATINE	QTOF-neg	0.00%	0.01
ZEATINE	QQQ-DH	0.00%	0.05
ZEATINE	QTOF-pos	8.62%	0.02

Supplementary Table S8. List of SRM transitions used for targeted mass spectrometry-based examination of metabolites and isotopic standards in bladder-derived urine and tissue samples. Abbreviations: RP: reverse phase chromatography, ANP: Aqueous normal phase chromatography, +ve: positive ion mode, -ve: negative ion mode, m/z: mass : charge ratio.

Metabolite	Parent ion (m/z)	Product ion (m/z)	Retention time (min)	Chromatographic method and ion mode used for detection
Anilline	94.0651	77.051	4.56	RP +ve
Serine	106.0499	60.0451	2.7	RP +ve
Histamine	112.0869	95.0608	3.1	RP +ve
Uracil	113.0328	96.0082	3.1	RP +ve
Valine	118.0863	72.0819	2.8	RP +ve
Niacinamide	123.0553	80.04	3.3	RP +ve
Taurine	126.0219	85	2.02	RP +ve
Thymine	127.0502	110.024	3.7	RP +ve
2-Hydroxybutyric acid sodium salt	127.0366	98.9754	4.7	RP +ve
Pipecolic acid	130.0863	84.0818	3.39	RP +ve
Creatine	132.0768	90.01	2.4	RP +ve
Leucine / Isoleucine	132.1019	86.0969	4.7	RP +ve
Asparagine	133.0608	74.01	2.6	RP +ve
Homocysteine	136.0427	90	2.6	RP +ve
Hypoxanthine	137.0458	119.035	3.3	RP +ve
Spermidine	146.1652	72.0817	1.99	RP +ve
Lysine	147.1128	84.081	2.1	RP +ve
Guanine	152.0567	135.03	2.8	RP +ve
Histidine	156.07675	110.071	2.2	RP +ve
Carnitine	162.1125	103	2.4	RP +ve
Norepinephrine (noradrenaline)	170.0812	107	2.2	RP +ve
1,7-dimethylxanthine	181.072	124	11	RP +ve
Tyrosine	182.0812	91.0548	4.06	RP +ve
Lauric acid	201.1849	98.9758	16.4	RP +ve
Tryptophan	205.0972	118.065	11.1	RP +ve
Kynurenine	209.0921	191.9	7.8	RP +ve
3-Hydroxykynurenine	225.087	162.045	3.8	RP +ve
Palmitic acid	257.2475	98.9758	16.4	RP +ve
Oleic acid	283.2632	220.9	11	RP +ve
Phenylalanine	166.0863	120.081	8.55	RP +ve
Pantothenic acid	220.1179	184	2.95	RP +ve
Urocanic acid	137.0357	93.04	2.9	RP -ve
D-Ribonolactone	147.0299	129.02	2.56	RP -ve
Citramalic acid	147.0299	87.0101	3.9	RP -ve
DL-3-Phenyllactic acid	165.0557	147.045	11.01	RP -ve
4-Hydroxy Phenyllacticacid	181.0506	135	11.02	RP -ve
4-Pyridoxic acid	182.0459	138.05	5.5	RP -ve
5-Hydroxyindoleaceticacid	190.051	146.06	10.9	RP -ve
Phthalic acid Mono-2-ethylhexylEster	277.1455	134.038	13.3	RP -ve
Aminobutyric acid	104.0706	69.06	6.2	ANP +ve
Homoserine	120.0855	74.08	6.8	ANP +ve
Glyceraldehyde-3-phosphate	171.0053	112	8.6	ANP +ve
Cytidine monophosphate (CMP)	322.0446	96.02	7.2	ANP +ve
Hippuric acid	180.0655	105	0.6	ANP +ve
N-Acetylspermidine	188.1757	171.05	9.3	ANP +ve
N1-Acetylspermine	245.2336	171.002	9.9	ANP +ve
S-Adenosylmethionine	399.1445	136.021	9.4	ANP +ve
		Isotopic Standards		
(D4)Thymine	131.0753	113.9	3.7	RP +ve
L-(15N)2-Tryptophan	207.0912	147.057	11.1	RP +ve
[15N] Anthranilic acid	139.052	121.04	3.5	RP +ve
[15N]Arginine	177.113	116.07	2.2	RP +ve
Jasmonic acid	211.1329	118.946	10.949	RP +ve
L-[D3]Testosterone	292.235	197.079	12.2	RP +ve
L- Gibberelic acid	347.1489	180.087	10.8	RP +ve
L[13C]-Creatinine	115.0695	98.9762	2.013	RP +ve
L-[D4]-Estrone	275.1944	131.001	11.991	RP +ve
L-Zeatine	220.1193	136	2.115	RP +ve
L-(D3)-N-Acetyl Aspartic acid	177.0596	90.8	2.8	RP -ve
L-(D5)-Glutamic acid	151.0773	107.1	2.2	RP -ve
L-(15N)2-Tryptophan	205.0767	117	11	RP -ve
L- Gibberelic acid	345.1344	143	10.8	RP -ve
L-anthranilicacid	137.0374	93	3.5	RP -ve
L-(D4)Thymine	131.0753	113.9	7.3	ANP +ve
L-(15N)2-Tryptophan	207.0912	189	5.2	ANP +ve
L-[15N] Anthranilic acid	139.052	121	0.6	ANP +ve
L[15C]-Creatinine	115.0695	99	9.5	ANP +ve
L-[15N]Arginine	177.113	116	9.1	ANP +ve

Supplementary Table S9: List of all compounds detected in bladder-derived tissues in the profiling study. For each compound the method of detection (Source) is indicated. POS and NEG represent positive and negative ionization modes on the Q-TOF while QQQ RP and QQQ DH signify compounds detected using reverse phase and normal phase separation coupled to a triple quadrupole mass spectrometer. Also for each compound the Z-normalized value, regulation, p-value and the q-value are described

CPDname	Source	Z-score	Regulation	pvalue	FDR-qvalue
1,7-dimethylxanthine	POS	-2.47763	DOWN	0.011905	0.068814
100.0168@0.57277274	NEG	-1.41516	DOWN	0.158845	0.312488
103.0336@0.28384486	POS	-3.51581	DOWN	0.00023	0
113.0927@2.5536594	POS	1.566165	UP	0.11817	0.276383
117.0803@3.9238045	POS	-1.4463	DOWN	0.14971	0.305346
129.045@0.59635705	POS	1.572584	UP	0.116636	0.264513
132.0269@0.2923104	POS	-1.47839	DOWN	0.140713	0.291296
134.1@2.4993749	POS	-0.0872	DOWN	0.931431	0.684015
158.0581@3.3400626	POS	-0.46548	DOWN	0.645687	0.579202
187.0651@2.281147	POS	-0.08284	DOWN	0.93485	0.683806
1-Methyl-L-tryptophan	QQQ-RP	0.75365	UP	0.45594	0.524434
216.0889@1.8678421	NEG	-3.85558	DOWN	4.21E-05	0
235.1432@0.7777501	POS	1.077889	UP	0.285015	0.424139
256.1404@5.1234703	POS	-0.12051	DOWN	0.905336	0.663611
262.1364@2.3729749	POS	-1.78033	DOWN	0.074748	0.210335
276.1718@9.966183	NEG	0.691061	UP	0.49438	0.532073
2-Hydroxy caprylic acid	NEG	0.662016	UP	0.512775	0.53486
2-Hydroxybutyric acid sodium salt	QQQ-RP	-2.84501	DOWN	0.003549	0.027763
2-Methylglutaric acid	NEG	-0.6462	DOWN	0.522936	0.552695
2-Phenylacetamide	NEG	1.57586	UP	0.115859	0.273169
366.1443@1.6363891	POS	-1.20688	DOWN	0.230666	0.384441
3-Deoxyguanosie	NEG	-0.35303	DOWN	0.727424	0.627761
3-Hydroxy-2-methylvalerate	NEG	0.248875	UP	0.805953	0.650979
3-hydroxy-3-methyl-Glutaric acid	NEG	-0.10997	DOWN	0.91358	0.679567
3-Hydroxykynurenine	QQQ-RP	3.213507	UP	0.000865	0.005943
410.1731@1.3699316	NEG	2.457164	UP	0.012669	0.068225
438.1979@5.5332	POS	0.32673	UP	0.747029	0.637757
4-Hydroxy Phenyllacticacid	NEG	3.258845	UP	0.000717	0.007706
4-Isopropylbenzyl alcohol	POS	0.175039	UP	0.86285	0.667356
4-Pyridoxic acid	NEG	-1.74836	DOWN	0.080273	0.216259
530.2662@9.085779	POS	1.865957	UP	0.061427	0.197597
5-Hydroxyindoleaceticacid	POS	2.497757	UP	0.011194	0.060604

60.0228@0.30110717	POS	-2.88958	DOWN	0.003025	0.021365
60.0235@0.16182351	POS	-1.21325	DOWN	0.228182	0.371607
60.0236@0.079937495	POS	-1.27071	DOWN	0.206613	0.357578
64.0398@2.5860255	POS	-1.34465	DOWN	0.18103	0.333824
64.9988@0.27988	POS	3.438897	UP	0.000327	0.005021
6-hydroxy caproic acid	POS	1.090851	UP	0.279202	0.41427
70.0287@4.2837	NEG	-1.25428	DOWN	0.212627	0.365566
72.015@0.28444737	POS	2.059957	UP	0.038246	0.13427
750.3672@4.1218805	POS	2.418129	UP	0.014242	0.072497
753.4114@12.266687	POS	0.727025	UP	0.472089	0.523534
754.3449@11.782734	POS	0.545916	UP	0.589609	0.584244
754.3457@11.340474	POS	1.105374	UP	0.272782	0.417586
754.4003@3.386621	POS	-0.27518	DOWN	0.785908	0.647894
755.3575@5.2760997	POS	2.731389	UP	0.005263	0.029321
756.3404@6.889419	NEG	-1.74815	DOWN	0.080312	0.220893
756.3645@11.795263	NEG	-0.19673	DOWN	0.846052	0.662529
757.3563@3.2076316	POS	0.606486	UP	0.548883	0.559788
758.36@12.2238	POS	0.266415	UP	0.792571	0.647606
759.4142@11.160056	POS	-0.45501	DOWN	0.653139	0.603074
760.3736@4.7362	NEG	1.49648	UP	0.135822	0.294671
760.3773@4.720982	POS	-2.75502	DOWN	0.004856	0.032264
764.3584@3.9436092	NEG	2.264285	UP	0.02218	0.096279
764.3633@3.9458647	POS	-0.35054	DOWN	0.729278	0.629364
764.4118@11.392766	POS	-0.7231	DOWN	0.474494	0.529111
766.3585@2.5847504	POS	0.494106	UP	0.625482	0.590962
767.4206@11.839601	POS	0.966743	UP	0.338109	0.465834
768.3646@2.8198273	POS	2.424536	UP	0.013973	0.06486
770.4133@4.5698066	POS	2.628312	UP	0.007409	0.05261
771.3677@4.721745	POS	-2.75062	DOWN	0.00493	0.034108
771.3892@5.867258	POS	2.418864	UP	0.014211	0.07167
771.4048@4.3835006	POS	0.176568	UP	0.861663	0.666918
772.3724@2.5775266	POS	2.85242	UP	0.003457	0.028289
775.4246@12.276001	POS	-0.12361	DOWN	0.902915	0.677357
776.4163@9.0227995	POS	0.807471	UP	0.42424	0.507476
777.3656@2.9937139	POS	1.525663	UP	0.128203	0.28553
779.3512@4.735277	POS	1.366862	UP	0.173813	0.324522
780.4218@12.024667	POS	-0.28874	DOWN	0.775624	0.646099
781.4279@11.185354	POS	-2.1957	DOWN	0.026775	0.116483
782.3542@5.7417016	POS	0.333781	UP	0.741757	0.632623
782.3774@11.816346	POS	0.575707	UP	0.569408	0.573235
783.3722@4.8025913	POS	0.77216	UP	0.444894	0.510571
784.4052@7.1533523	POS	0.163371	UP	0.871913	0.669958
786.3864@3.2027922	POS	0.594914	UP	0.556558	0.563184

787.4301@8.905766	POS	-0.24187	DOWN	0.811315	0.650355
788.4072@7.10579	POS	1.801314	UP	0.071288	0.198796
792.4273@10.432442	POS	0.020128	UP	0.984153	0.6954
794.4366@9.206	POS	-0.78253	DOWN	0.438774	0.514477
796.419@8.471875	POS	3.185356	UP	0.000971	0.01186
799.4053@6.667	POS	4.043444	UP	1.48E-05	0
807.3766@3.445722	POS	2.985551	UP	0.002124	0.017926
808.437@11.431645	POS	-0.50193	DOWN	0.620008	0.588813
809.4439@8.9874	POS	-0.21109	DOWN	0.834964	0.654897
810.3831@1.6731874	NEG	-0.14152	DOWN	0.888929	0.675899
810.3948@6.664263	POS	3.313632	UP	0.000568	0.009476
814.4125@4.7368827	POS	-0.59063	DOWN	0.559411	0.565522
817.3772@4.0255003	NEG	2.888038	UP	0.003042	0.022902
817.4288@6.576334	POS	1.847713	UP	0.064091	0.181386
82.0739@0.30744445	POS	1.916807	UP	0.054468	0.174604
820.3976@4.80545	POS	0.896604	UP	0.374597	0.473371
820.444@9.145	POS	1.065526	UP	0.290633	0.429559
824.4478@12.023251	POS	0.019307	UP	0.9848	0.696217
828.4201@6.5789104	POS	0.689348	UP	0.495456	0.533614
828.4321@7.3547106	POS	0.420987	UP	0.677598	0.611214
831.3913@4.8034396	POS	-1.55578	DOWN	0.120683	0.262079
833.4346@4.7315555	POS	2.009576	UP	0.043426	0.149409
834.3874@2.8491783	POS	2.376785	UP	0.016089	0.084366
836.3847@9.701072	POS	-0.94625	DOWN	0.348531	0.461799
836.4537@10.526853	POS	-0.77046	DOWN	0.445903	0.514295
847.3903@5.328473	NEG	-0.78371	DOWN	0.438076	0.50514
847.3956@5.295215	POS	0.164204	UP	0.871265	0.668687
850.4431@10.510401	NEG	-0.16828	DOWN	0.868098	0.669476
852.4589@12.496999	POS	-0.55027	DOWN	0.586635	0.580597
852.4636@11.468491	POS	-0.66678	DOWN	0.509735	0.541356
854.4027@5.578471	POS	1.674535	UP	0.094268	0.229076
858.4429@3.6281762	POS	0.166322	UP	0.869619	0.663374
859.4417@5.863267	POS	2.357944	UP	0.016996	0.067927
864.4693@9.250286	POS	2.398025	UP	0.015116	0.072497
868.4733@12.065002	POS	0.272461	UP	0.787972	0.650412
872.4588@7.5399413	POS	-1.1331	DOWN	0.260803	0.404126
880.4797@10.596551	POS	-0.93553	DOWN	0.354061	0.467673
900.4261@6.876948	NEG	0.35709	UP	0.724414	0.62731
900.4367@3.8994994	POS	1.899909	UP	0.056706	0.177209
903.4604@2.8666189	POS	1.005911	UP	0.318734	0.442637
916.475@9.699421	POS	-0.6699	DOWN	0.507746	0.542348
920.4598@10.184614	POS	0.043944	UP	0.965412	0.691535
922.4924@9.710158	POS	-2.62888	DOWN	0.007395	0.046308

924.4625@4.148	POS	-2.1768	DOWN	0.028174	0.104895
94.0787@9.358134	POS	0.927352	UP	0.358319	0.470427
992.4871@3.8786316	POS	1.367303	UP	0.173671	0.331032
Adenine	QQQ-RP	-1.2716	DOWN	0.206289	0.352375
Adenosine	QQQ-RP	-0.59654	DOWN	0.555477	0.563627
Alanine	QQQ-DH	-2.7058	DOWN	0.005737	0.03794
Allose	NEG	-0.20189	DOWN	0.84206	0.661813
alpha-hydroxyisobutyric acid	NEG	1.322293	UP	0.188511	0.344273
Aminobutyric acid	QQQ-DH	1.657539	UP	0.097744	0.242361
Aniline	POS	3.202885	UP	0.000904	0.009476
Arginine	POS	1.553339	UP	0.12128	0.276029
Arginine	QQQ-RP	0.695409	UP	0.491657	0.537678
Asparagine	QQQ-RP	2.767327	UP	0.004656	0.013969
Aspartic Acid	QQQ-RP	-0.55613	DOWN	0.58265	0.580556
Atenolol	POS	-0.80824	DOWN	0.423794	0.504996
Avobenzene	NEG	-0.5282	DOWN	0.601775	0.583278
Benzoic acid	NEG	-0.9842	DOWN	0.329384	0.451682
Benzyl alcohol	NEG	-0.75164	DOWN	0.457148	0.520628
Betaine	QQQ-DH	0.616296	UP	0.542416	0.555238
b-Hydroxyisovaleric acid	NEG	0.479821	UP	0.635532	0.60245
C10 H10 O2	POS	1.09915	UP	0.275521	0.410729
C10 H11 N5	POS	-0.44506	DOWN	0.660258	0.608455
C10 H13 N	POS	0.571383	UP	0.572321	0.572004
C10 H13 N O3	POS	-1.86955	DOWN	0.060913	0.181564
C10 H13 N5 O	POS	-0.59065	DOWN	0.559396	0.56631
C10 H13 N5 O	NEG	0.424664	UP	0.674938	0.610299
C10 H13 N7	POS	-0.03482	DOWN	0.972591	0.693556
C10 H14 Cl N5 O	NEG	-1.55239	DOWN	0.121512	0.274128
C10 H14 N2	POS	-1.01118	DOWN	0.316181	0.445102
C10 H14 N2 O	POS	1.450961	UP	0.148378	0.302822
C10 H14 N2 O2 S	POS	0.039451	UP	0.968947	0.690492
C10 H14 N8 O3	NEG	4.469099	UP	9.88E-07	0
C10 H14 O4	NEG	1.102585	UP	0.274007	0.413221
C10 H15 N O	POS	0.730115	UP	0.4702	0.5266
C10 H15 N3	POS	-1.8051	DOWN	0.070677	0.206158
C10 H15 N9	POS	-0.63898	DOWN	0.527607	0.548281

C10 H16 N8	NEG	-0.76788	DOWN	0.447434	0.519443
C10 H16 N8 O5	POS	2.917362	UP	0.002735	0.02339
C10 H18 N2 O S	POS	-0.03333	DOWN	0.97376	0.693512
C10 H18 N2 O4 S	POS	0.210442	UP	0.835464	0.657643
C10 H18 N4 O2	POS	-0.33653	DOWN	0.739701	0.630953
C10 H18 N6 O2	POS	0.611674	UP	0.545458	0.551857
C10 H18 O5	NEG	0.089412	UP	0.929692	0.682546
C10 H19 N O S2	POS	0.324157	UP	0.748955	0.634837
C10 H19 N O3	POS	0.564657	UP	0.576864	0.572429
C10 H19 N3 O S - 4.273033	NEG	-1.63109	DOWN	0.10335	0.258425
C10 H19 N5 O5	POS	-1.84225	DOWN	0.064908	0.182809
C10 H19 N7 O	POS	-0.41152	DOWN	0.684465	0.614971
C10 H20 N2 O3 S	POS	1.099395	UP	0.275413	0.417062
C10 H20 N2 O4 - 0.9845834	NEG	-2.54357	DOWN	0.009709	0.054898
C10 H20 N2 O4 + 1.0626875	POS	1.161963	UP	0.248712	0.396901
C10 H20 N2 O4 S	POS	-1.19328	DOWN	0.236031	0.384124
C10 H20 N2 O6	POS	0.488277	UP	0.629575	0.595575
C10 H20 N4 O S	NEG	1.606274	UP	0.108836	0.256567
C10 H20 N4 S + 1.3510385	POS	-2.71586	DOWN	0.005547	0.035514
C10 H21 N3 O9	POS	3.407869	UP	0.000376	0.003989
C10 H22 O4 S	NEG	2.412587	UP	0.014479	0.066108
C10 H23 Cl N14 O	POS	0.353022	UP	0.727432	0.628404
C10 H23 Cl N4 O S	POS	-2.03678	DOWN	0.040562	0.140855
C10 H23 N O3 S	POS	-0.75721	DOWN	0.453802	0.521501
C10 H23 N9 O S	POS	-1.74207	DOWN	0.081399	0.217917
C10 H24 N2 O5 S	NEG	-0.98887	DOWN	0.327074	0.444638
C10 H24 N4 O S2	POS	0.50355	UP	0.618875	0.590417
C10 H24 N4 O6 S	NEG	5.366719	UP	4.06E-10	0
C10 H24 N6 O S	POS	-1.7962	DOWN	0.072119	0.201162
C10 H25 Cl N8 O2	NEG	-0.31492	DOWN	0.755887	0.635887
C10 H25 N9 O5 + 10.031215	POS	-0.30578	DOWN	0.762761	0.637818
C10 H26 N10 O S	POS	0.990049	UP	0.326493	0.456931
C10 H26 N10 O2 S	POS	-2.48261	DOWN	0.011726	0.061948
C10 H30 N10 O2 S2	POS	-0.08813	DOWN	0.930697	0.683991
C10 H6 N6	NEG	-0.11686	DOWN	0.90819	0.677695
C10 H9 N5	POS	-1.2729	DOWN	0.205818	0.358272
C10 H9 N5	NEG	-0.6063	DOWN	0.549004	0.558251
C11 H12	NEG	-2.70757	DOWN	0.005703	0.031308
C11 H12 N10	POS	1.475775	UP	0.141431	0.28806
C11 H12 N2 O2	NEG	-0.54535	DOWN	0.589993	0.578543
C11 H12 N2 O2 + 4.1904817	POS	-0.26939	DOWN	0.790305	0.648153
C11 H12 O S	POS	3.425231	UP	0.000348	0
C11 H12 O2	POS	-0.1908	DOWN	0.850639	0.664372

C11 H14 N6 O2	POS	0.260296	UP	0.797233	0.649186
C11 H14 O3	NEG	-1.44462	DOWN	0.150192	0.286636
C11 H15 Cl N2 O2	POS	-2.26861	DOWN	0.021914	0.082743
C11 H15 N O5	POS	-1.78971	DOWN	0.073185	0.180128
C11 H15 N13 O2	POS	0.253599	UP	0.802343	0.652444
C11 H15 N3 O3	NEG	-0.71366	DOWN	0.480312	0.52936
C11 H15 N3 O4	POS	0.414584	UP	0.682239	0.613554
C11 H15 N5	POS	-0.29051	DOWN	0.774282	0.643164
C11 H15 N9	POS	0.094294	UP	0.925863	0.68362
C11 H16 N4	POS	-2.44878	DOWN	0.012994	0.06852
C11 H16 N8 O4	NEG	0.516807	UP	0.609651	0.584685
C11 H16 O	NEG	1.813747	UP	0.069299	0.206334
C11 H17 N3 O4	POS	0.033324	UP	0.973767	0.693534
C11 H17 N5 O4	POS	-0.48099	DOWN	0.634707	0.596788
C11 H18 Cl N3	POS	-2.57617	DOWN	0.00876	0.049918
C11 H18 N10 O	NEG	1.052692	UP	0.296541	0.427261
C11 H18 N2 O2 S	NEG	-0.58239	DOWN	0.564922	0.574879
C11 H18 N2 O4	NEG	1.797974	UP	0.07183	0.202064
C11 H18 N8 O2	NEG	-2.21331	DOWN	0.025525	0.090024
C11 H18 O3 S	POS	-1.26543	DOWN	0.208531	0.362719
C11 H19 N3 O6	POS	-0.53281	DOWN	0.598596	0.582266
C11 H19 N9 O S	POS	-1.64139	DOWN	0.10114	0.242941
C11 H20 N2 O3	POS	2.695089	UP	0.005947	0.033655
C11 H20 N2 O4	POS	-0.57458	DOWN	0.570168	0.566921
C11 H20 N2 O5 - 0.72262496	NEG	3.990474	UP	2.00E-05	0
C11 H20 N6 O2	POS	-2.712	DOWN	0.005619	0.032734
C11 H20 N6 O2 S	POS	0.695148	UP	0.49182	0.530558
C11 H21 Cl N8	NEG	1.650681	UP	0.099175	0.244383
C11 H21 Cl O3	POS	-2.53019	DOWN	0.010124	0.060263
C11 H21 N O5	POS	3.987875	UP	2.03E-05	0
C11 H21 N5 O3	POS	-3.61534	DOWN	0.000143	0.00158
C11 H21 N7 S2	POS	2.048264	UP	0.0394	0.135429
C11 H22 N2 O2 S	POS	2.268661	UP	0.021911	0.093047
C11 H22 N2 O3 S	POS	-1.64623	DOWN	0.100111	0.248076
C11 H22 N2 O4 S	NEG	-3.0938	DOWN	0.001401	0.013293
C11 H22 N2 O6 S	NEG	0.088799	UP	0.930173	0.683852
C11 H22 N2 O9	POS	-0.7378	DOWN	0.465517	0.521501
C11 H22 O S	POS	3.364495	UP	0.000456	0.005021
C11 H22 S2 + 5.079705	POS	0.450821	UP	0.656135	0.604932
C11 H23 N5 O6	NEG	0.769235	UP	0.44663	0.516687
C11 H24 Cl N9 O2	NEG	0.894527	UP	0.375713	0.480781
C11 H24 N10 O S	NEG	0.347897	UP	0.731238	0.631207
C11 H24 N2 O3 S2	POS	-0.01251	DOWN	0.990149	0.696987

C11 H24 N8 O S	NEG	1.865506	UP	0.061492	0.184393
C11 H25 Cl N4 O S	NEG	0.201214	UP	0.842585	0.660961
C11 H26 N2 O4 S	POS	0.377451	UP	0.709378	0.626566
C11 H27 N13 S2	POS	0.584013	UP	0.563835	0.564951
C11 H27 N3 O7	POS	0.572749	UP	0.5714	0.568614
C11 H27 N3 S2	POS	-1.64639	DOWN	0.100079	0.260393
C11 H27 N5 O2 S2	POS	1.862258	UP	0.06196	0.18986
C11 H27 N9 O2 S	POS	1.232669	UP	0.220724	0.383966
C11 H28 Cl N5 O5	POS	-0.0962	DOWN	0.92437	0.680874
C11 H28 Cl N9 O3	POS	-1.61074	DOWN	0.107832	0.258821
C11 H28 Cl2 N6 O2	POS	0.985311	UP	0.328834	0.449944
C11 H28 N10 O2 S	POS	-2.63766	DOWN	0.007187	0.039348
C11 H29 N13 O S2	NEG	-1.50277	DOWN	0.134153	0.287295
C11 H29 N9 O2 S2	POS	1.427564	UP	0.155159	0.309209
C11 H32 N10 O4 S2	POS	-0.12165	DOWN	0.904448	0.67873
C11 H6	NEG	-0.81722	DOWN	0.418635	0.508231
C11 H9 N O2	POS	-1.38224	DOWN	0.168939	0.329239
C12 H10	POS	-0.65621	DOWN	0.516494	0.547854
C12 H10 N4	POS	-0.54363	DOWN	0.591171	0.577799
C12 H12 N2 O	POS	-0.41141	DOWN	0.684544	0.614661
C12 H12 O3	POS	-1.77582	DOWN	0.075509	0.212898
C12 H12 O3	NEG	-0.48079	DOWN	0.634848	0.594928
C12 H12 O4	POS	0.785168	UP	0.437221	0.513109
C12 H13 N O2	POS	-0.71618	DOWN	0.478753	0.526558
C12 H14 N4	POS	-0.6474	DOWN	0.522163	0.551296
C12 H14 N6 + 3.0640671	POS	-0.72895	DOWN	0.470914	0.527902
C12 H15 N O2	POS	-2.20563	DOWN	0.026065	0.098002
C12 H15 N5 S	POS	-1.01776	DOWN	0.313015	0.435751
C12 H16 N2	NEG	-0.64901	DOWN	0.521125	0.54866
C12 H16 N2 O3	POS	0.593213	UP	0.557691	0.564113
C12 H16 N2 O4	POS	1.047745	UP	0.298839	0.43436
C12 H16 O2 S	POS	-0.07632	DOWN	0.93997	0.687094
C12 H16 O3	POS	-1.21603	DOWN	0.227105	0.370723
C12 H16 O3	NEG	-1.76261	DOWN	0.077773	0.21709
C12 H16 O4	POS	-2.0308	DOWN	0.041177	0.144347
C12 H16 O4 - 4.2537827	NEG	-0.30118	DOWN	0.766229	0.638882
C12 H16 O5	NEG	-2.04757	DOWN	0.039469	0.144347
C12 H17 Cl N2	POS	0.284983	UP	0.778469	0.642066
C12 H17 Cl O2	POS	-1.20739	DOWN	0.230468	0.38452
C12 H17 N O4	POS	0.803672	UP	0.426435	0.504515
C12 H17 N5	POS	4.145168	UP	8.09E-06	0
C12 H17 N7	POS	-2.02625	DOWN	0.041651	0.145845
C12 H18 N10	POS	-0.90785	DOWN	0.368593	0.476269

C12 H18 N2 O	POS	1.350634	UP	0.179065	0.330844
C12 H18 N8 O5	POS	0.463963	UP	0.646765	0.596561
C12 H18 O2 S	POS	0.474059	UP	0.639604	0.60234
C12 H18 O3	POS	-0.19545	DOWN	0.847037	0.665234
C12 H19 Cl O3	NEG	0.420607	UP	0.677873	0.609202
C12 H19 N O3	POS	-0.69558	DOWN	0.49155	0.540073
C12 H19 N11 O	POS	0.232994	UP	0.818117	0.655174
C12 H20 N16 O	POS	-1.56251	DOWN	0.11905	0.276619
C12 H20 N16 S	NEG	1.276812	UP	0.204409	0.352196
C12 H20 N2 O S2 + 9.56347	POS	-1.96201	DOWN	0.048832	0.138847
C12 H20 N2 O3	POS	-0.23027	DOWN	0.820207	0.65534
C12 H20 N2 O4	NEG	0.673329	UP	0.505569	0.540882
C12 H20 N2 O6	POS	-0.84303	DOWN	0.404004	0.497638
C12 H20 O3	POS	-0.01143	DOWN	0.990999	0.696923
C12 H20 O5 - 6.208647	NEG	-1.24817	DOWN	0.214896	0.360766
C12 H21 N O3	POS	-0.41188	DOWN	0.684204	0.616344
C12 H21 N7 O2	POS	-0.56103	DOWN	0.579319	0.575466
C12 H22 N14 O	NEG	-0.75981	DOWN	0.452248	0.515789
C12 H22 N2 O3 S	POS	1.600486	UP	0.110147	0.260132
C12 H22 N2 O4	NEG	-0.13693	DOWN	0.892506	0.674551
C12 H23 N O2 S	NEG	-1.82023	DOWN	0.06828	0.197253
C12 H23 N O6	POS	-0.61927	DOWN	0.540464	0.555468
C12 H23 N O8	NEG	1.129541	UP	0.26232	0.404963
C12 H24 Cl N5	POS	-0.66424	DOWN	0.511353	0.542537
C12 H24 N14 O2	POS	0.202897	UP	0.841285	0.662026
C12 H24 N2 O S2	POS	1.786271	UP	0.073755	0.215425
C12 H24 N2 O5	POS	2.423548	UP	0.014014	0.071111
C12 H24 N2 O8	POS	-0.43811	DOWN	0.665246	0.607168
C12 H24 N6 O4 S	NEG	0.368178	UP	0.716212	0.623264
C12 H25 N11 O S	POS	-0.01115	DOWN	0.991221	0.697349
C12 H25 N11 O3	POS	-2.64746	DOWN	0.00696	0.045485
C12 H25 N13 O4 S	NEG	-1.20866	DOWN	0.229972	0.384362
C12 H25 N15 O3	POS	-1.24896	DOWN	0.214601	0.359996
C12 H25 N3 O9	POS	-0.40759	DOWN	0.687319	0.615796
C12 H25 N5 S2	POS	-1.68202	DOWN	0.092768	0.228762
C12 H26 N2 O2 S2	NEG	1.475348	UP	0.141548	0.292888
C12 H26 N2 S3	POS	-2.78162	DOWN	0.004432	0.031789
C12 H26 N6 O2 S	POS	-1.80425	DOWN	0.070815	0.198796
C12 H26 O3 S	NEG	-0.91354	DOWN	0.365578	0.475535
C12 H26 O4 S - 10.587432	NEG	-1.11497	DOWN	0.268595	0.409619
C12 H27 N5 S2	POS	-0.25079	DOWN	0.804489	0.653061
C12 H31 N15 O S2	NEG	-1.75273	DOWN	0.0795	0.213068
C12 H32 Cl N9 O3	POS	-0.623	DOWN	0.538021	0.546273

C12 H32 N16 S2	POS	-1.59347	DOWN	0.111753	0.26464
C12 H32 N6 O2 S2	POS	-0.39407	DOWN	0.697183	0.613935
C12 H34 N8 O8 S	POS	-4.31424	DOWN	2.80E-06	0
C12 H35 N9 O9	POS	-0.21014	DOWN	0.835701	0.6608
C12 H36 N10 S4	POS	-1.2598	DOWN	0.210591	0.36959
C12 H8 N2	POS	0.469507	UP	0.642829	0.598256
C13 H10 O + 5.9442377	POS	-2.16484	DOWN	0.02909	0.107529
C13 H14 N2 O3	POS	-0.10186	DOWN	0.919934	0.681418
C13 H14 N2 O3	NEG	-0.92434	DOWN	0.359895	0.470194
C13 H14 N2 O4	NEG	-0.99854	DOWN	0.322327	0.447014
C13 H14 N4	POS	-0.01508	DOWN	0.988129	0.696901
C13 H15 Cl N4	POS	0.567125	UP	0.575195	0.574374
C13 H16 Cl N O	POS	-0.87667	DOWN	0.385385	0.493378
C13 H16 N2 O4	NEG	-0.60151	DOWN	0.552175	0.568051
C13 H16 N2 O5	POS	1.968425	UP	0.048072	0.160189
C13 H16 N6	POS	-0.20783	DOWN	0.837475	0.659242
C13 H17 N3 O4	POS	1.205964	UP	0.231025	0.380525
C13 H17 N3 O4	NEG	3.251776	UP	0.000738	0.006772
C13 H18 N10	POS	3.835986	UP	4.67E-05	0
C13 H18 N2 O	POS	0.190844	UP	0.850603	0.664738
C13 H18 N2 O4	NEG	-2.93492	DOWN	0.002564	0.022402
C13 H18 N6 O4	NEG	0.894566	UP	0.375692	0.477897
C13 H20 N2 O4	POS	-1.21514	DOWN	0.22745	0.370561
C13 H20 O S2	NEG	1.494814	UP	0.136267	0.292677
C13 H21 N7 O5	POS	0.118266	UP	0.907091	0.67885
C13 H22 N2 O3	POS	-1.06957	DOWN	0.288785	0.419744
C13 H22 N2 O4	POS	-0.41488	DOWN	0.682027	0.609344
C13 H22 N2 O4	NEG	-0.73405	DOWN	0.467799	0.525542
C13 H22 O2 S2	POS	-1.30973	DOWN	0.192811	0.342971
C13 H22 O6	POS	1.385959	UP	0.167777	0.303879
C13 H23 Cl N6 O	NEG	0.610156	UP	0.546459	0.556887
C13 H23 Cl S	POS	-0.13105	DOWN	0.897102	0.67663
C13 H23 N O5	POS	0.2761	UP	0.785207	0.647317
C13 H23 N11 O3 S	NEG	0.077606	UP	0.938956	0.686043
C13 H23 N19	POS	1.119801	UP	0.266504	0.413585
C13 H24 Cl N3 O2	POS	-2.03777	DOWN	0.04046	0.133334
C13 H24 N2 O3 S	POS	1.656419	UP	0.097977	0.24467
C13 H24 N4 O5 S	NEG	1.89517	UP	0.057346	0.174979
C13 H24 S2	NEG	0.916883	UP	0.363812	0.474911
C13 H25 Cl N14	POS	-2.2133	DOWN	0.025526	0.102738
C13 H25 N O5	POS	-1.17765	DOWN	0.242305	0.390391
C13 H25 N7 O5	POS	-0.55049	DOWN	0.586486	0.579079
C13 H26 Cl2 N2 O	POS	-2.64891	DOWN	0.006928	0.040721

C13 H26 N10 S	NEG	-0.32735	DOWN	0.746566	0.634247
C13 H27 N O4 S2	POS	-1.19517	DOWN	0.23528	0.380848
C13 H28 N2 O3 S2	POS	-1.34324	DOWN	0.181496	0.332248
C13 H28 N4 O3 S2	NEG	-0.56927	DOWN	0.573748	0.571322
C13 H28 O11	POS	0.500151	UP	0.62125	0.59255
C13 H28 O3 S2	POS	1.866229	UP	0.061388	0.183515
C13 H29 N O7	POS	-0.07505	DOWN	0.940964	0.686387
C13 H29 N7 O9	POS	0.960212	UP	0.34141	0.457118
C13 H30 N8 O4 S	POS	2.403762	UP	0.014862	0.073916
C13 H31 N13 S2	POS	1.732455	UP	0.083141	0.228919
C13 H31 N15 O2 S	POS	-2.31875	DOWN	0.019023	0.082743
C13 H31 N5 O9 S	POS	-2.96455	DOWN	0.002297	0.0173
C13 H31 N7 O9	POS	-0.25787	DOWN	0.799084	0.650752
C13 H31 N9 O2 S2	POS	0.778162	UP	0.441345	0.511683
C13 H32 N14 O5	POS	0.995936	UP	0.3236	0.444372
C13 H33 N11 O8	POS	1.659829	UP	0.09727	0.239577
C13 H35 N7 O11	POS	1.285346	UP	0.201356	0.361532
C13 H36 N16 S3	POS	0.395055	UP	0.696464	0.620339
C13 H37 N13 O5 S	POS	-0.32471	DOWN	0.748539	0.634589
C13 H39 N11 S4	POS	2.158548	UP	0.029582	0.116245
C14 H10 N2	NEG	-4.21834	DOWN	5.16E-06	0
C14 H12 N6	POS	-2.52254	DOWN	0.010368	0.05069
C14 H12 N6 O	POS	-0.98363	DOWN	0.329665	0.446225
C14 H14 N4	POS	0.696707	UP	0.490845	0.534017
C14 H15 N5 S	POS	-0.07386	DOWN	0.941894	0.670363
C14 H16	POS	-0.46004	DOWN	0.64956	0.600976
C14 H16 N2 O4	POS	-0.35451	DOWN	0.726331	0.628885
C14 H16 N6 O2	NEG	-1.29757	DOWN	0.197038	0.337744
C14 H16 O4	POS	-2.38174	DOWN	0.015857	0.077732
C14 H17 N5	POS	0.977034	UP	0.332949	0.463012
C14 H18 O4	POS	-1.01659	DOWN	0.313575	0.445763
C14 H20 Cl N3 O3	POS	-0.76416	DOWN	0.449653	0.517045
C14 H20 N10 S	NEG	-0.66451	DOWN	0.511184	0.539548
C14 H20 N2 O2	POS	-2.4546	DOWN	0.012767	0.069398
C14 H20 N2 O3 + 2.4299998	POS	2.050839	UP	0.039143	0.135198
C14 H20 N2 O3 S	NEG	-4.02227	DOWN	1.67E-05	0
C14 H20 N2 O4	POS	1.094073	UP	0.277769	0.415708
C14 H20 N6 O	POS	0.370493	UP	0.714504	0.625102
C14 H20 N6 O4	NEG	-0.98969	DOWN	0.326673	0.449556
C14 H21 N O3 + 7.6616955	POS	-2.17079	DOWN	0.028632	0.114804
C14 H21 N3 O2	POS	2.127732	UP	0.032093	0.116006
C14 H22 N2 O3	NEG	-0.06443	DOWN	0.949306	0.688588
C14 H22 N2 O7	POS	-1.25952	DOWN	0.210694	0.367055

C14 H22 N8 O	POS	-0.20984	DOWN	0.835927	0.663163
C14 H22 N8 O5	NEG	-0.21562	DOWN	0.831471	0.657942
C14 H22 O3 S	POS	0.525558	UP	0.603594	0.584605
C14 H23 N3 O4	POS	-0.44122	DOWN	0.663016	0.607096
C14 H24 N2 S2	NEG	1.101303	UP	0.274572	0.410359
C14 H24 N4 O7	POS	-0.44369	DOWN	0.661238	0.607527
C14 H24 N4 S	NEG	-0.60857	DOWN	0.547505	0.558976
C14 H24 O7	POS	0.037542	UP	0.970449	0.692965
C14 H25 N3 O5	POS	0.999548	UP	0.321833	0.444837
C14 H25 N5 O3	POS	0.510215	UP	0.61423	0.586481
C14 H25 N5 O5	POS	0.587021	UP	0.561822	0.565741
C14 H25 N7 O3	POS	-1.3952	DOWN	0.164912	0.318965
C14 H25 N9 S + 10.1726675	POS	-2.03364	DOWN	0.040884	0.109589
C14 H26 N2 O7 S	NEG	-0.41742	DOWN	0.680181	0.610193
C14 H27 N17 O3	POS	-0.00533	DOWN	0.995801	0.698431
C14 H28 N6 O4 S	NEG	1.098021	UP	0.27602	0.414877
C14 H28 N8 S2	POS	1.942844	UP	0.051161	0.162045
C14 H28 O3 S	NEG	1.882702	UP	0.05906	0.176284
C14 H28 O9	POS	-0.77262	DOWN	0.44462	0.515969
C14 H29 Cl O3	NEG	-0.26127	DOWN	0.796493	0.650184
C14 H29 Cl O4	POS	0.130914	UP	0.897205	0.675972
C14 H29 N O5 S	POS	0.22778	UP	0.82212	0.655533
C14 H29 N15 O2 S	POS	5.018394	UP	1.27E-08	0
C14 H29 N7 O S2	POS	-1.3551	DOWN	0.177609	0.332991
C14 H29 N7 S2	POS	-2.11633	DOWN	0.033066	0.116006
C14 H30 Cl N S2	POS	-0.25781	DOWN	0.799125	0.649329
C14 H30 O4 S	NEG	1.811883	UP	0.069595	0.197081
C14 H31 N11 O5	POS	0.176072	UP	0.862048	0.66666
C14 H31 N7 O S2	POS	-0.12958	DOWN	0.898246	0.675361
C14 H31 N9 O S2	POS	-0.20352	DOWN	0.840807	0.659969
C14 H31 N9 O9	POS	-4.49137	DOWN	8.45E-07	0
C14 H32 Cl2 N4 O5	POS	-1.83543	DOWN	0.065937	0.186131
C14 H32 N12 O3 S2	NEG	0.073852	UP	0.941904	0.685768
C14 H32 N6 O8 S	POS	-2.07126	DOWN	0.037156	0.132156
C14 H32 N8 O12	NEG	1.260978	UP	0.21016	0.361362
C14 H32 N8 O6	POS	-0.7166	DOWN	0.478497	0.52936
C14 H33 Cl N4 O5	POS	0.903997	UP	0.370643	0.479511
C14 H33 N11 O4 S	POS	0.280052	UP	0.782208	0.645253
C14 H34 N10 O7 S	POS	1.702004	UP	0.088854	0.230482
C14 H34 N4 O3 S3	POS	0.27374	UP	0.787	0.646564
C14 H34 N6 O11	POS	0.554094	UP	0.584032	0.574079
C14 H35 N13 O3 S2	POS	2.221185	UP	0.024982	0.094234
C14 H35 N5 O8 S	POS	4.120405	UP	9.39E-06	0

C14 H35 N7 O7 S	POS	-4.66589	DOWN	2.36E-07	0
C14 H37 N11 O2 S3	POS	-0.82443	DOWN	0.414516	0.494605
C14 H37 N11 O5 S	POS	0.971677	UP	0.335629	0.456993
C14 H37 N11 O6 S2	POS	0.046086	UP	0.963727	0.691092
C14 H37 N13 O5 S	POS	-4.53838	DOWN	6.05E-07	0
C14 H38 N8 O2 S3	POS	0.389246	UP	0.700716	0.619735
C14 H39 N9 O8 S	POS	-0.44983	DOWN	0.656843	0.606378
C14 H40 N14 O2 S3	POS	0.435493	UP	0.667129	0.609273
C14 H41 N11 O7 S	POS	-0.49049	DOWN	0.628018	0.594585
C15 H10 N2	POS	-2.90765	DOWN	0.002833	0.02339
C15 H11 N	POS	-2.60353	DOWN	0.008026	0.045485
C15 H13 N7	POS	-2.24116	DOWN	0.023649	0.097717
C15 H14 N2 O3	POS	2.372412	UP	0.016295	0.079427
C15 H16 O4	POS	-2.55051	DOWN	0.0095	0.050305
C15 H17 N7 O	POS	2.229667	UP	0.024408	0.09857
C15 H18 N10 O2	NEG	0.332114	UP	0.743002	0.633218
C15 H18 N2	POS	-0.33311	DOWN	0.742257	0.633843
C15 H18 N4 O2	POS	0.088112	UP	0.930711	0.687684
C15 H18 N8 S	POS	0.074053	UP	0.941746	0.685355
C15 H19 N9 S	NEG	0.430569	UP	0.670676	0.607741
C15 H20 N2 O6	POS	1.727722	UP	0.084009	0.221876
C15 H20 N8 O	NEG	-2.05667	DOWN	0.038567	0.129525
C15 H20 O2 + 1.6722274	POS	-2.4377	DOWN	0.013433	0.062608
C15 H21 Cl N6 O	NEG	0.512066	UP	0.612943	0.585645
C15 H21 N O3	POS	1.289693	UP	0.199813	0.356182
C15 H23 Cl N4 O4	NEG	-0.47315	DOWN	0.640249	0.599192
C15 H23 N O4	NEG	-0.313	DOWN	0.757324	0.639759
C15 H23 N5 O S	NEG	-1.69184	DOWN	0.090828	0.230948
C15 H23 N7 O6	POS	1.394126	UP	0.165242	0.322064
C15 H24 N2 S	POS	1.303988	UP	0.1948	0.348032
C15 H24 N6 O4 + 1.474389	POS	3.31069	UP	0.000575	0.006772
C15 H24 O3 S	NEG	0.211071	UP	0.834979	0.659135
C15 H24 O7	POS	0.534765	UP	0.597252	0.579614
C15 H26 N10 O4 S	NEG	0.018266	UP	0.985619	0.696174
C15 H26 N2 O3 S2	POS	-0.53292	DOWN	0.59852	0.576885
C15 H26 N6 O2 S2	NEG	0.5926	UP	0.558099	0.561805
C15 H26 O S2	POS	-1.24692	DOWN	0.215361	0.360851
C15 H26 O8	POS	-0.90252	DOWN	0.37143	0.477001
C15 H27 N O6	POS	-0.48805	DOWN	0.629737	0.595233
C15 H27 N3 O S2	POS	-1.58999	DOWN	0.112555	0.256567
C15 H28 N16 O3 + 4.0208	POS	1.488648	UP	0.137923	0.295399
C15 H28 N2 O3 S	POS	0.253859	UP	0.802144	0.652276
C15 H28 N2 O3 S2	NEG	-1.24492	DOWN	0.216107	0.368123

C15 H28 N4 O5	POS	-0.24693	DOWN	0.807444	0.654065
C15 H29 Cl N2 O S2	NEG	0.645954	UP	0.523094	0.546874
C15 H29 N S3	POS	-2.19815	DOWN	0.026598	0.10622
C15 H30 N6 O S2	POS	1.492137	UP	0.136984	0.293205
C15 H31 N3 O5 S2	POS	-1.6162	DOWN	0.106617	0.252376
C15 H32 N2 O12	POS	-0.7752	DOWN	0.443095	0.512006
C15 H32 N2 O3 S3	NEG	-2.60774	DOWN	0.007919	0.044227
C15 H32 N8 O4 S	POS	0.92356	UP	0.360303	0.470892
C15 H32 O4 S2	POS	0.235092	UP	0.816507	0.654315
C15 H33 N17 O4	NEG	-0.27419	DOWN	0.786657	0.646273
C15 H33 N9 O5 S	POS	0.812237	UP	0.421494	0.503888
C15 H35 N17 O2 S2	NEG	-1.39504	DOWN	0.164959	0.316628
C15 H35 N7 O10	POS	0.346925	UP	0.731961	0.632529
C15 H37 Cl N12 S2	POS	1.881905	UP	0.059171	0.174604
C15 H37 N11 O9	POS	-2.26093	DOWN	0.022388	0.086916
C15 H37 N9 O11	POS	1.358268	UP	0.17658	0.336024
C15 H37 N9 O7 S	POS	0.851067	UP	0.399507	0.496885
C15 H39 N7 O12	POS	-1.47105	DOWN	0.142733	0.307522
C15 H40 N8 O5 S2	POS	-0.7702	DOWN	0.446057	0.515021
C16 H14 N4 O2	POS	-0.79448	DOWN	0.431772	0.507191
C16 H14 N6 O	NEG	2.144278	UP	0.030724	0.1186
C16 H15 N5 O2	POS	-0.26993	DOWN	0.789893	0.647837
C16 H16 N10 O	NEG	-2.76921	DOWN	0.004626	0.02339
C16 H16 N12 O	POS	0.024679	UP	0.980571	0.693599
C16 H16 N2 O	POS	0.223266	UP	0.82559	0.657888
C16 H16 N2 O3	NEG	0.155253	UP	0.878228	0.671043
C16 H16 N4 O	POS	-0.12701	DOWN	0.900258	0.67492
C16 H18 N2 O2	POS	-1.33141	DOWN	0.185433	0.343754
C16 H18 N4	POS	-1.27595	DOWN	0.204717	0.355128
C16 H19 N5 + 3.5305	POS	1.170922	UP	0.245038	0.405494
C16 H20 N6 O5	POS	-0.48561	DOWN	0.631453	0.595271
C16 H20 O6	POS	-2.11946	DOWN	0.032797	0.119064
C16 H21 N O3 S	NEG	2.031287	UP	0.041127	0.149202
C16 H21 N13 O2	POS	0.425909	UP	0.674038	0.610475
C16 H22 Cl N5	POS	0.628165	UP	0.534642	0.55611
C16 H22 N6 O2	POS	-0.13241	DOWN	0.896035	0.681865
C16 H22 N6 O3	NEG	-0.07064	DOWN	0.944431	0.686889
C16 H22 N8 O2 S	NEG	0.891104	UP	0.377555	0.47672
C16 H22 O S	POS	-1.86667	DOWN	0.061325	0.186476
C16 H23 N S	POS	1.757265	UP	0.078703	0.210335
C16 H23 N5 O3	POS	0.45337	UP	0.654313	0.607204
C16 H24 Cl N3 S	POS	-0.56485	DOWN	0.576734	0.571535
C16 H24 N12 O S	NEG	-0.25806	DOWN	0.79894	0.650724

C16 H24 N2 O S2	POS	-2.03251	DOWN	0.041001	0.137491
C16 H24 N2 O5 S	POS	-1.42141	DOWN	0.156979	0.311858
C16 H24 N6 O3 S	NEG	-0.73549	DOWN	0.466921	0.523749
C16 H24 N6 S2	NEG	-1.35899	DOWN	0.176348	0.332434
C16 H24 O3 S	NEG	0.959356	UP	0.341844	0.460456
C16 H24 O7	POS	-0.12355	DOWN	0.902958	0.677768
C16 H24 O8	POS	1.427751	UP	0.155103	0.313532
C16 H25 N3 O8	NEG	3.631764	UP	0.000132	0
C16 H25 N5 O6	POS	-1.39361	DOWN	0.165403	0.314259
C16 H26 N10 O2	POS	-2.1153	DOWN	0.033156	0.116957
C16 H26 N4 O S2	POS	1.013183	UP	0.315217	0.441359
C16 H26 O3 S	POS	-0.00317	DOWN	0.997502	0.698705
C16 H26 O3 S	NEG	-1.22459	DOWN	0.223804	0.371848
C16 H26 O4 S	POS	-0.26098	DOWN	0.796711	0.648383
C16 H27 N7 O S	POS	-0.86869	DOWN	0.389753	0.488117
C16 H28 N14 S	POS	-0.73227	DOWN	0.468886	0.526558
C16 H29 Cl N4 O2	NEG	-2.60264	DOWN	0.008049	0.051451
C16 H29 N5 O S2	POS	0.203685	UP	0.840677	0.661999
C16 H29 N5 O2 S	POS	0.86162	UP	0.39365	0.491209
C16 H29 N9 O S2	POS	0.270682	UP	0.789324	0.64697
C16 H30 N12 O2 S2	NEG	0.207308	UP	0.837881	0.661308
C16 H30 N2 O8 S	NEG	0.945242	UP	0.349051	0.463254
C16 H31 Cl N12 O	POS	1.352179	UP	0.17856	0.331219
C16 H31 Cl N4 O4	POS	0.642855	UP	0.525096	0.548944
C16 H31 N O S2	POS	1.544024	UP	0.123577	0.270988
C16 H31 N5 O S2	POS	2.726115	UP	0.005358	0.024455
C16 H31 N5 S2	POS	2.964095	UP	0.002301	0.020276
C16 H34 N12 O6 S	POS	-0.05582	DOWN	0.956072	0.689823
C16 H35 N11 O S2	NEG	-0.69927	DOWN	0.489245	0.531747
C16 H35 N11 S2	POS	0.140249	UP	0.88992	0.673167
C16 H35 N3 S4	POS	-0.2083	DOWN	0.837119	0.662159
C16 H36 N10 O3 S2	POS	-0.46118	DOWN	0.648745	0.606125
C16 H36 N2 O3 S2	NEG	-1.66699	DOWN	0.095799	0.240314
C16 H36 N6 O8	POS	-0.18653	DOWN	0.85394	0.664503
C16 H37 N5 O8 S	POS	0.330693	UP	0.744064	0.635733
C16 H38 N2 O6 S2	POS	1.900026	UP	0.05669	0.177209
C16 H39 N15 O3 S2	POS	-0.59217	DOWN	0.558388	0.56451
C16 H39 N9 O13	POS	-1.76407	DOWN	0.077519	0.207387
C16 H39 N9 O9	POS	-1.1753	DOWN	0.243256	0.398005
C16 H40 Cl N15 O S	POS	0.9508	UP	0.346201	0.460884
C16 H41 N11 O6 S	POS	1.575822	UP	0.115868	0.275082
C16 H42 N14 O7 S	POS	1.809551	UP	0.069966	0.187163
C16 H43 N9 O11	POS	1.387352	UP	0.167342	0.327905

C16 H43 N9 O9 S	POS	0.390264	UP	0.69997	0.617878
C16 H45 N11 O10 S	POS	-0.60798	DOWN	0.547892	0.560417
C17 H11 N O	POS	-0.85464	DOWN	0.397516	0.486471
C17 H16 N10	NEG	0.367531	UP	0.71669	0.62184
C17 H18	NEG	0.430814	UP	0.670499	0.608882
C17 H18 N10	NEG	0.093714	UP	0.926318	0.688971
C17 H18 N4 - 9.8863735	NEG	-0.02778	DOWN	0.978134	0.694686
C17 H18 N4 + 10.218596	POS	0.267387	UP	0.791831	0.647837
C17 H18 O	POS	-0.00098	DOWN	0.999227	0.699106
C17 H18 O2	NEG	0.191436	UP	0.850144	0.663032
C17 H18 O5 + 8.7336	POS	1.348574	UP	0.17974	0.341219
C17 H20 N10 - 6.0427375	NEG	-0.53993	DOWN	0.593707	0.578337
C17 H20 N10 - 6.4647493	NEG	-1.39604	DOWN	0.164653	0.325496
C17 H21 N O3	POS	0.338515	UP	0.738224	0.631364
C17 H21 N5 O	POS	-0.11675	DOWN	0.908274	0.678226
C17 H22 N2 O3	NEG	0.969026	UP	0.33696	0.461312
C17 H22 N2 O7	POS	3.276214	UP	0.000666	0.002828
C17 H22 N4 O2	POS	-1.69997	DOWN	0.089247	0.242796
C17 H22 O6	POS	0.880462	UP	0.383319	0.491209
C17 H22 S2	POS	0.311453	UP	0.758489	0.637024
C17 H24 N12 O S	NEG	0.662504	UP	0.512463	0.547058
C17 H24 N14 S	POS	-0.13565	DOWN	0.893511	0.675141
C17 H24 N6 O2	POS	-1.1085	DOWN	0.271412	0.4061
C17 H24 N6 O3	NEG	-0.38111	DOWN	0.706684	0.621274
C17 H24 O3	POS	0.230609	UP	0.819948	0.657125
C17 H25 N7 O3	POS	2.735005	UP	0.005199	0.034555
C17 H26 N10 O3 S	NEG	-1.84948	DOWN	0.063829	0.185265
C17 H26 N2 O5 S	POS	0.469579	UP	0.642778	0.603914
C17 H26 N6 O3 S	NEG	-0.78657	DOWN	0.436399	0.507995
C17 H26 O S2	POS	1.207087	UP	0.230585	0.371367
C17 H26 O3 S - 10.53332	NEG	0.235058	UP	0.816534	0.656413
C17 H26 O5	NEG	-1.15165	DOWN	0.252988	0.396505
C17 H27 Cl O4	NEG	1.699614	UP	0.089315	0.229233
C17 H27 N7 O2 S - 4.379	NEG	-0.49287	DOWN	0.626352	0.5917
C17 H28 N6 O8	POS	1.019188	UP	0.312331	0.449621
C17 H28 O3 S	POS	-1.19755	DOWN	0.234337	0.38333
C17 H28 O3 S - 11.375057	NEG	0.852577	UP	0.398666	0.491313
C17 H29 N O8 + 5.1114116	POS	-0.19658	DOWN	0.846164	0.663005
C17 H29 N15 O	NEG	-3.90515	DOWN	3.22E-05	0.00158
C17 H29 N15 S	POS	-1.45454	DOWN	0.147362	0.306386
C17 H29 N5 O5	POS	0.24741	UP	0.807073	0.653033
C17 H30 N10 O S	NEG	-0.89324	DOWN	0.376405	0.481879
C17 H30 N2 O7	POS	-2.16336	DOWN	0.029205	0.111608

C17 H30 N2 O8	NEG	1.466231	UP	0.144073	0.294149
C17 H31 N13 O2 S	POS	-2.25425	DOWN	0.022807	0.096279
C17 H31 N5 O3 S	POS	0.867008	UP	0.390679	0.490271
C17 H32 N14 O2 S2	POS	-0.54629	DOWN	0.589351	0.578254
C17 H32 N2 O8 S	NEG	0.430055	UP	0.671046	0.610299
C17 H32 N2 S3	POS	1.994263	UP	0.04511	0.150232
C17 H33 N7 O11	POS	1.576494	UP	0.11571	0.265273
C17 H33 N9 O4 S	POS	0.411515	UP	0.684467	0.614108
C17 H34 N4 O S2	POS	0.37136	UP	0.713865	0.622404
C17 H34 O5 S	NEG	-0.19339	DOWN	0.848631	0.663058
C17 H34 O5 S2	POS	-0.8236	DOWN	0.414987	0.49547
C17 H35 Cl N6 O4 S	POS	-0.83557	DOWN	0.408198	0.494452
C17 H35 N3 O11	POS	2.30718	UP	0.01966	0.08372
C17 H35 N7 O9	POS	1.283401	UP	0.202049	0.35948
C17 H36 N2 O5 S2	POS	-1.06942	DOWN	0.288857	0.422976
C17 H37 Cl N8 O7	POS	0.015414	UP	0.987865	0.696452
C17 H37 N9 O6 S	POS	0.021308	UP	0.983225	0.695938
C17 H38 N8 O13	POS	2.210201	UP	0.025742	0.105427
C17 H39 N7 O11	POS	0.106039	UP	0.91666	0.680732
C17 H40 N8 O8 S	POS	2.277494	UP	0.021376	0.093938
C17 H41 N11 O10	POS	1.860056	UP	0.062279	0.192357
C17 H41 N17 O S2	POS	-1.01803	DOWN	0.312886	0.438643
C17 H41 N21 S2	POS	1.593231	UP	0.111807	0.266909
C17 H42 N6 O S3	NEG	-0.49367	DOWN	0.625786	0.592743
C17 H42 N6 O5 S2	NEG	-2.54765	DOWN	0.009586	0.055271
C17 H43 N7 O13	POS	-0.34289	DOWN	0.734966	0.632655
C17 H45 N11 O8 S2	POS	2.851398	UP	0.003469	0.02339
C17 H45 N17 O3 S2	POS	0.980371	UP	0.331286	0.448647
C17 H46 N10 S4	POS	-1.03085	DOWN	0.306775	0.437064
C17 H48 N12 O7 S2	POS	-0.30454	DOWN	0.763691	0.637818
C18 H10	POS	-1.99405	DOWN	0.045133	0.145205
C18 H14 O + 3.5519335	POS	2.95451	UP	0.002385	0.019131
C18 H14 O2	POS	0.401555	UP	0.691717	0.615831
C18 H16 N2 O	POS	-2.34748	DOWN	0.017518	0.082743
C18 H16 S	POS	-4.01959	DOWN	1.69E-05	0
C18 H18 N6 O3 + 6.8881874	POS	-0.83098	DOWN	0.410799	0.516149
C18 H18 O2	POS	-1.18409	DOWN	0.239706	0.384678
C18 H20 N2 O3	POS	0.602029	UP	0.551833	0.564246
C18 H20 O4	POS	-0.69846	DOWN	0.489752	0.533937
C18 H20 S	NEG	-3.31415	DOWN	0.000567	0.005943
C18 H21 N3 O3	POS	0.439624	UP	0.664158	0.610299
C18 H22 N14 O	NEG	-4.64306	DOWN	2.80E-07	0
C18 H22 N4	NEG	-0.76175	DOWN	0.45109	0.519927

C18 H22 N4 O	NEG	0.174546	UP	0.863233	0.666763
C18 H22 O3	POS	1.291758	UP	0.199083	0.349125
C18 H23 N15 O3	NEG	-0.86922	DOWN	0.389461	0.483404
C18 H23 N3 O S	POS	0.740607	UP	0.463813	0.52319
C18 H23 N5	POS	1.431074	UP	0.154127	0.309848
C18 H23 N9 O	POS	-1.04084	DOWN	0.302067	0.428053
C18 H24 Cl N	POS	0.675252	UP	0.504349	0.539262
C18 H24 N12 O S	NEG	-1.48042	DOWN	0.140157	0.292994
C18 H24 O4 S	POS	1.188807	UP	0.237815	0.387264
C18 H24 O6	POS	0.339773	UP	0.737286	0.634434
C18 H25 Cl O3	POS	-2.46631	DOWN	0.012323	0.057102
C18 H25 N O3	POS	1.748639	UP	0.080224	0.211877
C18 H25 N5 O S	POS	0.06806	UP	0.946453	0.688114
C18 H26 N12 + 12.657447	POS	-1.23822	DOWN	0.218626	0.367384
C18 H26 N6 O5	POS	3.029396	UP	0.001798	0.008611
C18 H26 O7	NEG	-1.67345	DOWN	0.094486	0.246098
C18 H26 O8 - 4.7898607	NEG	-0.9984	DOWN	0.322395	0.44975
C18 H26 O8 - 6.1956897	NEG	0.805396	UP	0.425438	0.506002
C18 H27 Cl N4 O	POS	-0.41783	DOWN	0.679883	0.611986
C18 H28 N12 O3 S	NEG	2.123853	UP	0.032422	0.117193
C18 H28 N12 O6	POS	2.90885	UP	0.002821	0.019131
C18 H28 N2 O5 S	POS	-0.09866	DOWN	0.922439	0.680495
C18 H28 N6 O3 S	NEG	-0.98349	DOWN	0.329737	0.450976
C18 H28 N6 O8	POS	-0.86712	DOWN	0.390616	0.486631
C18 H30 N12 O S2	NEG	0.781091	UP	0.439618	0.512052
C18 H30 N2 O6 S	POS	-1.61061	DOWN	0.107861	0.258161
C18 H30 O3 S	POS	0.317396	UP	0.754025	0.638336
C18 H30 O3 S	NEG	0.639928	UP	0.526991	0.549935
C18 H30 O9	POS	0.312437	UP	0.75775	0.636993
C18 H31 N15 O2	POS	2.574152	UP	0.008816	0.051828
C18 H31 N3 O8	POS	0.076161	UP	0.940091	0.685906
C18 H32 N10 S2	POS	0.089631	UP	0.92952	0.683782
C18 H33 N5 O2 S2	POS	0.302422	UP	0.76529	0.639759
C18 H34 N2 O2 S2	POS	1.160767	UP	0.249205	0.390554
C18 H34 N2 O3 S2	POS	-0.58386	DOWN	0.563937	0.566877
C18 H34 N2 O4 S2	POS	1.333579	UP	0.184708	0.339624
C18 H34 N2 O7 S	NEG	-0.34129	DOWN	0.736156	0.630827
C18 H34 N2 O8 S	NEG	0.302231	UP	0.765433	0.639638
C18 H35 Cl N16 O4	POS	3.119105	UP	0.001268	0.014618
C18 H35 N3 O3 S2	POS	-2.03752	DOWN	0.040486	0.145632
C18 H35 N5 O S2	POS	0.096508	UP	0.924128	0.68163
C18 H36 N2 O3 S2	POS	1.043313	UP	0.300908	0.431973
C18 H36 N4 O13	POS	-1.80344	DOWN	0.070946	0.197253

C18 H37 N O S3	POS	-1.7585	DOWN	0.078487	0.214755
C18 H37 N3 O2 S2	POS	-0.24179	DOWN	0.811374	0.650922
C18 H38 N4 O5 S2	POS	0.373186	UP	0.712518	0.625036
C18 H39 N O3 S3	POS	1.638768	UP	0.101699	0.251277
C18 H39 N S4	POS	-1.33646	DOWN	0.183747	0.34236
C18 H39 N11 O S2	POS	0.327189	UP	0.746685	0.634496
C18 H40 N14 O7 S	POS	-1.03351	DOWN	0.305514	0.438643
C18 H40 N2 O2 S4	POS	0.021031	UP	0.983443	0.69583
C18 H41 N11 O7 S	POS	0.255956	UP	0.800544	0.651233
C18 H43 N11 O12	POS	1.641082	UP	0.101205	0.24709
C18 H44 N6 O13	POS	0.345493	UP	0.733027	0.631238
C18 H44 N8 O4 S3	POS	0.93064	UP	0.356604	0.471182
C18 H47 N9 O10 S	POS	1.337121	UP	0.183525	0.33575
C18 H48 N10 O6 S3	POS	0.939572	UP	0.351972	0.462103
C19 H16 O2	POS	-3.07934	DOWN	0.001483	0.013293
C19 H17 N5 O	POS	1.57968	UP	0.114959	0.266909
C19 H18 N4	POS	0.534999	UP	0.597091	0.578626
C19 H18 O	POS	-0.9394	DOWN	0.352062	0.467614
C19 H22 N14	POS	1.901449	UP	0.056499	0.174604
C19 H22 N8 O	POS	-1.17045	DOWN	0.24523	0.400352
C19 H22 O3	POS	0.761721	UP	0.451106	0.515608
C19 H23 N3 O S	POS	-1.09822	DOWN	0.27593	0.415935
C19 H24 S2	POS	1.754866	UP	0.079124	0.213913
C19 H25 N O S	POS	-0.4317	DOWN	0.669862	0.609698
C19 H25 N O3	POS	0.445147	UP	0.660196	0.595727
C19 H25 N17 O	NEG	-0.64132	DOWN	0.526087	0.550499
C19 H26 N10 O5	POS	-1.13666	DOWN	0.259291	0.404659
C19 H26 N4 O6	POS	-0.93244	DOWN	0.355668	0.470136
C19 H26 N6 O	POS	-1.32997	DOWN	0.185918	0.339713
C19 H26 O S	POS	-0.00747	DOWN	0.994123	0.697604
C19 H26 S2	POS	2.182162	UP	0.027771	0.111608
C19 H27 N7 O4 + 5.2991037	POS	-1.00437	DOWN	0.319484	0.425375
C19 H28 Cl N7	POS	0.146201	UP	0.885279	0.673489
C19 H28 N14 O2 S	NEG	-0.70883	DOWN	0.483299	0.530681
C19 H28 N4 O5 S	POS	-2.12181	DOWN	0.032596	0.119295
C19 H28 O2 S2	POS	0.254197	UP	0.801886	0.651148
C19 H28 O5 S	NEG	-1.37323	DOWN	0.171783	0.331874
C19 H29 Cl N10	NEG	2.602418	UP	0.008055	0.046715
C19 H29 N21 O3	POS	3.02868	UP	0.001803	0.019711
C19 H29 N7 S2	POS	-0.79756	DOWN	0.429981	0.504226
C19 H30 N10 O3	POS	1.03588	UP	0.304398	0.434709
C19 H30 N24	POS	-3.95561	DOWN	2.43E-05	0
C19 H30 N6 O9	POS	0.180918	UP	0.858291	0.664921

C19 H30 N8 O3 S	POS	-1.48246	DOWN	0.139602	0.292783
C19 H30 O3 S	NEG	-1.39316	DOWN	0.16554	0.329807
C19 H30 O5 S	NEG	0.742766	UP	0.462505	0.520278
C19 H31 Cl N22 O	POS	-2.48983	DOWN	0.011469	0.069975
C19 H31 N11 O6	POS	1.590269	UP	0.11249	0.270009
C19 H32 O3 S	POS	1.435992	UP	0.15269	0.308995
C19 H32 O3 S	NEG	-1.03543	DOWN	0.304609	0.432889
C19 H33 Cl N14 O3	NEG	-1.97827	DOWN	0.046925	0.16569
C19 H33 Cl N2 S	NEG	-0.52112	DOWN	0.606665	0.581982
C19 H33 N3 O9	POS	1.015321	UP	0.314188	0.449556
C19 H34 Cl2 O5	POS	-0.82878	DOWN	0.412045	0.498388
C19 H34 N2 O5 S2	POS	0.920118	UP	0.36211	0.474456
C19 H34 N6 O4 S2	POS	-1.64896	DOWN	0.099536	0.246523
C19 H35 N O3 S2	POS	0.630472	UP	0.533137	0.553484
C19 H36 N10 O S3	NEG	-0.79052	DOWN	0.434086	0.507854
C19 H36 N10 O8 S	NEG	-2.43789	DOWN	0.013426	0.071391
C19 H36 N2 O8 S	NEG	-1.67219	DOWN	0.094741	0.245671
C19 H36 N4 O13	POS	0.215357	UP	0.831676	0.660318
C19 H36 N6 O S2	NEG	-0.09643	DOWN	0.924192	0.681724
C19 H36 O10 S	POS	-1.78435	DOWN	0.074076	0.192357
C19 H37 Cl N8 O5	POS	-0.72546	DOWN	0.47305	0.524221
C19 H37 N O4 S2	POS	-0.49156	DOWN	0.627267	0.592627
C19 H37 N7 O S3	POS	-0.87313	DOWN	0.38732	0.485186
C19 H37 N9 O5 S	POS	1.187267	UP	0.238431	0.389573
C19 H38 Cl N9 O7	POS	3.258774	UP	0.000717	0.006772
C19 H38 N12 S3	POS	-0.57922	DOWN	0.567046	0.570423
C19 H38 N16 S2	NEG	-0.70013	DOWN	0.488707	0.531583
C19 H38 N2 O S4	NEG	0.910862	UP	0.366995	0.472279
C19 H38 N2 O6 S2	POS	-0.92308	DOWN	0.360552	0.475195
C19 H38 N2 O8 S2	POS	-1.4048	DOWN	0.161972	0.319971
C19 H38 N4 O4 S2	POS	-0.93168	DOWN	0.356064	0.465357
C19 H39 N O13	POS	-0.99813	DOWN	0.322524	0.450138
C19 H39 N15 O5 S	POS	-1.51038	DOWN	0.132152	0.288496
C19 H39 N7 O10	POS	0.061089	UP	0.951931	0.688768
C19 H40 N12 S3	POS	1.355685	UP	0.177418	0.333639
C19 H40 N4 O3 S2	POS	1.478412	UP	0.140707	0.297326
C19 H43 N7 O12	POS	0.939789	UP	0.35186	0.462407
C19 H44 N10 O15	POS	-1.24283	DOWN	0.216891	0.369102
C19 H44 N10 O15	NEG	-0.20629	DOWN	0.838668	0.662026
C19 H44 N16 O9	POS	-0.82607	DOWN	0.413585	0.499135
C19 H46 N8 O13	POS	-2.59499	DOWN	0.008249	0.049527
C19 H47 N13 O4 S2	POS	-2.61218	DOWN	0.007806	0.041619
C19 H48 N8 S4	POS	-0.93211	DOWN	0.35584	0.467673

C20 H14 N2 O	POS	1.051292	UP	0.29719	0.430556
C20 H16 N4	POS	1.486149	UP	0.138599	0.303034
C20 H16 N4 O	POS	-1.81073	DOWN	0.069778	0.190756
C20 H18 N4 O	POS	1.060639	UP	0.292873	0.407455
C20 H20 N4 O	NEG	-1.5293	DOWN	0.127277	0.274606
C20 H21 Cl N2	POS	-1.41028	DOWN	0.160312	0.321766
C20 H23 N O2	POS	-1.86525	DOWN	0.061528	0.185785
C20 H23 N15	POS	1.27049	UP	0.206692	0.361277
C20 H23 N3 O	POS	1.619015	UP	0.105993	0.247936
C20 H24 O7	POS	-0.5445	DOWN	0.590579	0.580801
C20 H26 N10 O	NEG	-0.40232	DOWN	0.691159	0.618081
C20 H27 N S2	POS	0.008602	UP	0.993228	0.697626
C20 H29 Cl O3 S	NEG	0.39694	UP	0.695087	0.617878
C20 H29 N3 O6	POS	-0.15281	DOWN	0.880126	0.673489
C20 H30 N8 O4	POS	-0.80721	DOWN	0.424388	0.511452
C20 H30 O7 + 10.545896	POS	-0.22691	DOWN	0.822786	0.658404
C20 H31 N O S2	POS	1.378783	UP	0.170027	0.331594
C20 H31 N9 O3 S	NEG	-0.33321	DOWN	0.742181	0.633967
C20 H31 N9 S	POS	1.516946	UP	0.130444	0.285197
C20 H32 N10 S2	POS	-0.94169	DOWN	0.350877	0.461799
C20 H32 N14 O S	POS	-3.56921	DOWN	0.000179	0.002828
C20 H32 N2 O7 S	NEG	-0.44292	DOWN	0.661789	0.604678
C20 H32 O10	POS	0.84761	UP	0.401437	0.495013
C20 H33 N3 O9	POS	-1.44892	DOWN	0.148961	0.306074
C20 H34 N2 O8 S	POS	1.377521	UP	0.170424	0.335568
C20 H34 N6 O4 S2	POS	-1.06137	DOWN	0.292538	0.424573
C20 H34 S3	NEG	0.758213	UP	0.453204	0.519443
C20 H35 N19 O4	POS	1.140652	UP	0.257601	0.408801
C20 H35 N3 O3 S2	POS	-1.43452	DOWN	0.15312	0.300689
C20 H35 N9 S2	POS	2.17461	UP	0.02834	0.106484
C20 H36 Cl N23	POS	1.580104	UP	0.114859	0.266408
C20 H36 N10 O6 S	NEG	-1.48786	DOWN	0.138136	0.288496
C20 H36 N12 O7 S	NEG	-1.05589	DOWN	0.29506	0.424284
C20 H36 N2 O3 S3	POS	0.77744	UP	0.441771	0.515202
C20 H36 N4 O4 S	POS	-0.24309	DOWN	0.810381	0.652781
C20 H36 N6 S2	POS	2.429772	UP	0.013756	0.063261
C20 H37 N O9	POS	-0.75325	DOWN	0.456183	0.519971
C20 H37 N S3	POS	0.867272	UP	0.390534	0.490114
C20 H38 N2 O5 S2	POS	1.710828	UP	0.087168	0.229858
C20 H39 N3 O S3	POS	0.829473	UP	0.41165	0.499184
C20 H39 N5 O5 S2	POS	0.401064	UP	0.692076	0.617979
C20 H40 N4 O8 S	POS	0.690105	UP	0.49498	0.535061
C20 H40 N6 O14	POS	0.466163	UP	0.645202	0.600976

C20 H40 N6 S3	POS	-0.59718	DOWN	0.555052	0.563937
C20 H41 N3 O S3	POS	2.99269	UP	0.002067	0.018537
C20 H42 Cl N O S3	POS	0.235548	UP	0.816158	0.652865
C20 H42 N2 O S4	POS	-1.75765	DOWN	0.078636	0.220893
C20 H42 N6 S4	POS	1.755432	UP	0.079024	0.211365
C20 H43 N O8 S2	POS	-0.25404	DOWN	0.80201	0.648928
C20 H43 N11 O10	POS	-0.25947	DOWN	0.797865	0.649729
C20 H44 N12 O11 S	POS	-1.03869	DOWN	0.303077	0.437477
C20 H44 N8 O12	POS	-0.71709	DOWN	0.478192	0.526895
C20 H44 N8 O8 S	POS	0.716538	UP	0.478533	0.529484
C20 H45 N11 O7 S2	POS	-0.49765	DOWN	0.623	0.592897
C20 H45 N9 O12 S	POS	-4.30742	DOWN	2.93E-06	0
C20 H46 N8 O6 S3	POS	2.7781	UP	0.004486	0.028289
C20 H48 N14 O12	POS	-0.01337	DOWN	0.989473	0.696901
C20 H50 Cl N17 O S2	POS	0.886223	UP	0.380192	0.484324
C20 H50 N6 O2 S4	POS	1.159308	UP	0.249808	0.392099
C20 H51 N9 O11 S	POS	3.0725	UP	0.001523	0.0173
C21 H18 N4 O	POS	0.962723	UP	0.340138	0.456368
C21 H20 O S	POS	0.126603	UP	0.900573	0.677091
C21 H21 N O2	POS	0.168884	UP	0.867629	0.667561
C21 H21 N5 O2	POS	1.467515	UP	0.143716	0.298528
C21 H22 N4 S	POS	-0.74	DOWN	0.464181	0.521414
C21 H25 Cl N2	POS	1.972014	UP	0.047652	0.151672
C21 H26 N10	POS	1.784119	UP	0.074113	0.209127
C21 H30 N2 O4 S	POS	1.178607	UP	0.241916	0.384678
C21 H30 N2 O4 S	NEG	0.515931	UP	0.610259	0.585126
C21 H30 O2 S2	NEG	0.653064	UP	0.518513	0.55064
C21 H31 N13 O2	POS	-0.66092	DOWN	0.513472	0.546689
C21 H31 N27	POS	1.593958	UP	0.111639	0.260393
C21 H31 N5 O6 S	POS	0.880599	UP	0.383244	0.481988
C21 H32 N2 O2 S2	POS	-0.76803	DOWN	0.447348	0.513657
C21 H32 N2 O7 S	NEG	3.095928	UP	0.001389	0.011099
C21 H32 O6 S	NEG	-1.26905	DOWN	0.207216	0.365067
C21 H34 N6 S2	POS	0.380971	UP	0.706789	0.620439
C21 H35 N17 O5	POS	2.562186	UP	0.009157	0.058528
C21 H35 N5 O S2	NEG	3.55823	UP	0.000188	0.003989
C21 H35 N9 O2 S	POS	2.04787	UP	0.039439	0.138622
C21 H36 Cl2 N4 O2	POS	-0.28859	DOWN	0.77574	0.643401
C21 H36 N20 O S	POS	-3.51592	DOWN	0.00023	0.00158
C21 H36 N6 O S2	NEG	0.437248	UP	0.665866	0.608277
C21 H36 N8 O7	POS	0.795736	UP	0.431042	0.516687
C21 H36 O2 S2	NEG	0.782059	UP	0.439048	0.512558
C21 H38 O6 S2	POS	0.297665	UP	0.768878	0.642274

C21 H39 N21 O4	POS	2.836875	UP	0.003653	0.017926
C21 H39 N7 O9	POS	0.643252	UP	0.524839	0.55316
C21 H40 N4 O10	POS	1.857839	UP	0.062601	0.183867
C21 H40 N6 O14	POS	-0.60042	DOWN	0.552898	0.563406
C21 H41 N9 O6 S	POS	0.038629	UP	0.969594	0.692571
C21 H42 N6 O6 S	POS	0.333823	UP	0.741725	0.645224
C21 H42 O12 S	POS	-3.98409	DOWN	2.07E-05	0
C21 H43 N15 O2 S2	POS	3.060179	UP	0.001597	0.01186
C21 H43 N7 O11	POS	-0.14002	DOWN	0.890102	0.674107
C21 H44 N12 S3	POS	0.324417	UP	0.74876	0.63378
C21 H44 N8 O3 S2	POS	0.181445	UP	0.857882	0.666841
C21 H45 N21 O3 S2	POS	3.812952	UP	5.28E-05	0
C21 H46 N4 O17	POS	-1.29185	DOWN	0.199052	0.350305
C21 H46 N6 O10 S	POS	1.549541	UP	0.122213	0.277791
C21 H48 N16 O10	POS	-1.79259	DOWN	0.072711	0.202244
C21 H48 N18 O8 S	POS	-1.02483	DOWN	0.309637	0.440819
C21 H49 Cl N6 O15	POS	-1.1006	DOWN	0.274881	0.413512
C21 H49 N13 O14	POS	-0.89319	DOWN	0.376432	0.479788
C21 H49 N5 O18	POS	1.91555	UP	0.054632	0.167281
C21 H49 N7 O15	POS	0.829815	UP	0.411456	0.502334
C21 H51 N15 O10 S2	POS	2.111826	UP	0.033458	0.125104
C21 H52 N12 O11 S2	POS	2.40577	UP	0.014774	0.071111
C22 H19 N3	POS	0.255016	UP	0.801261	0.649386
C22 H21 N5 O2	POS	1.182164	UP	0.24048	0.386267
C22 H22 O	POS	-0.06676	DOWN	0.947473	0.687116
C22 H23 N5	POS	-2.3361	DOWN	0.018102	0.078073
C22 H23 N5 O	POS	0.756937	UP	0.453968	0.519707
C22 H24 N16 O + 3.8080628	POS	-0.35904	DOWN	0.722968	0.632874
C22 H24 N8 O	POS	3.303308	UP	0.000594	0.005943
C22 H26 N2 O	NEG	-0.35147	DOWN	0.728582	0.623462
C22 H26 O3 S	NEG	0.516461	UP	0.609891	0.589558
C22 H28 O4 + 10.355622	POS	-2.45535	DOWN	0.012738	0.06852
C22 H29 N O6	POS	1.187412	UP	0.238373	0.383807
C22 H30 N4 S	NEG	0.699252	UP	0.489256	0.5345
C22 H30 O S	POS	0.164031	UP	0.8714	0.671746
C22 H30 O9	POS	0.214238	UP	0.832538	0.6608
C22 H32 N10 O3	POS	-0.05809	DOWN	0.954285	0.689554
C22 H33 Cl N14 S	POS	-2.12348	DOWN	0.032454	0.116245
C22 H33 Cl N6 O	POS	-1.00794	DOWN	0.317752	0.441359
C22 H33 N13 O5	POS	2.803406	UP	0.004109	0.02723
C22 H33 N15 O	POS	1.498847	UP	0.135192	0.29236
C22 H34 N16 O2	POS	-2.2897	DOWN	0.020656	0.092449
C22 H34 N6 O S	POS	-2.26862	DOWN	0.021914	0.091848

C22 H34 O9	POS	-1.66417	DOWN	0.096376	0.240608
C22 H36 N2 O3 S2	POS	1.478474	UP	0.14069	0.299071
C22 H36 N2 O9 S	POS	-0.75225	DOWN	0.45678	0.522845
C22 H36 S3	NEG	-0.38362	DOWN	0.70484	0.621174
C22 H37 N3 O7	POS	0.610023	UP	0.546547	0.558569
C22 H38 N6 O S2	NEG	0.658251	UP	0.515184	0.542442
C22 H38 O2 S2	NEG	-1.31143	DOWN	0.192227	0.347185
C22 H39 N O3 S2	NEG	-2.25129	DOWN	0.022996	0.094822
C22 H39 N11 O S3	NEG	2.267767	UP	0.021966	0.086916
C22 H39 N21 S	POS	-3.14939	DOWN	0.001123	0.011099
C22 H40 N16 O5 S	POS	0.834405	UP	0.408858	0.494758
C22 H40 N2 O6 S2	POS	1.393757	UP	0.165356	0.320071
C22 H41 N5 O4 S2	POS	-0.42531	DOWN	0.674475	0.609627
C22 H41 N7 O5 S	NEG	0.069224	UP	0.945539	0.686911
C22 H42 N4 O S3	POS	-0.86052	DOWN	0.394259	0.488855
C22 H43 N5 S4	POS	-1.19057	DOWN	0.237111	0.382693
C22 H44 N18 O7 S	POS	-4.25739	DOWN	4.04E-06	0
C22 H44 N6 O11	POS	-2.42466	DOWN	0.013968	0.064226
C22 H44 N6 S4	POS	-0.46258	DOWN	0.64775	0.600865
C22 H45 N5 O9 S	POS	0.75084	UP	0.45763	0.521675
C22 H46 N6 O12	POS	-4.0952	DOWN	1.09E-05	0
C22 H48 N16 O3 S3	POS	1.522336	UP	0.129055	0.287623
C22 H52 N14 O13	POS	0.267799	UP	0.791518	0.648125
C23 H20 N10	POS	-0.05009	DOWN	0.960581	0.691866
C23 H20 O2	POS	0.410235	UP	0.685398	0.614039
C23 H20 O3 + 1.7308096	POS	-0.86916	DOWN	0.389496	0.485883
C23 H22 N4 O	NEG	-2.14056	DOWN	0.031028	0.118832
C23 H22 N4 O2	POS	0.388503	UP	0.701261	0.618081
C23 H22 O S	NEG	-0.43543	DOWN	0.667173	0.605295
C23 H24 O5 - 10.727	NEG	-1.54222	DOWN	0.124026	0.277674
C23 H25 Cl	POS	1.235008	UP	0.219838	0.374285
C23 H26 N10 O2	NEG	1.206098	UP	0.230972	0.380202
C23 H26 N4 O5	POS	0.273896	UP	0.786881	0.647894
C23 H26 N8 O	POS	0.875031	UP	0.38628	0.485883
C23 H28 N4 O5	POS	-1.75031	DOWN	0.079928	0.211194
C23 H29 N3 O3 S	POS	0.746112	UP	0.460482	0.517135
C23 H30 O S2	NEG	3.259275	UP	0.000715	0.005943
C23 H32 N14 O6	POS	0.303549	UP	0.764439	0.639033
C23 H32 N6 O5 S	NEG	1.57138	UP	0.116923	0.274128
C23 H33 N S2	POS	-0.04938	DOWN	0.961136	0.689957
C23 H34 N12 O4	POS	3.159318	UP	0.001079	0.006772
C23 H34 N2 O5	POS	-0.27391	DOWN	0.786867	0.647865
C23 H36 Cl N11	POS	-0.79896	DOWN	0.429167	0.501061

C23 H36 Cl2	NEG	-0.41806	DOWN	0.679721	0.61244
C23 H36 S2	POS	-0.10282	DOWN	0.919181	0.680258
C23 H37 N11 O8	POS	0.587366	UP	0.561592	0.568095
C23 H37 N3 S3	POS	-1.37032	DOWN	0.172709	0.329144
C23 H38 N10 O2 S	NEG	-0.88475	DOWN	0.380992	0.486417
C23 H38 N6 O9	NEG	-1.46271	DOWN	0.145059	0.300259
C23 H38 N8 O3 S	POS	-1.45043	DOWN	0.148528	0.312697
C23 H40 O8 S	POS	0.776068	UP	0.442581	0.51265
C23 H41 N5 O8	POS	-1.28563	DOWN	0.201253	0.350305
C23 H42 N8 S4	POS	0.654773	UP	0.517415	0.544319
C23 H43 Cl N2 O6	POS	0.450551	UP	0.656328	0.600568
C23 H43 N21 O5	POS	1.926175	UP	0.053259	0.166487
C23 H43 N7 O10	POS	1.551113	UP	0.121826	0.279878
C23 H44 N12 O3 S2	POS	-1.01457	DOWN	0.314548	0.442637
C23 H44 N16 O3 S2	POS	-0.60429	DOWN	0.550336	0.564995
C23 H44 N24 S2	POS	2.868468	UP	0.003264	0.021889
C23 H44 N6 O13	POS	-0.98283	DOWN	0.330064	0.449621
C23 H44 O15	POS	0.655562	UP	0.516909	0.543007
C23 H46 N20 O3 S2	POS	3.107595	UP	0.001327	0.012591
C23 H46 N8 O12	POS	3.617852	UP	0.000141	0
C23 H47 N3 O9 S2	POS	-1.05714	DOWN	0.294484	0.428915
C23 H47 N7 O12	POS	0.152495	UP	0.880376	0.671946
C23 H48 N6 O2 S4	POS	-1.16931	DOWN	0.245698	0.387678
C23 H50 Cl N17 O S2	POS	0.038096	UP	0.970012	0.692768
C23 H52 N18 O7 S	POS	0.054788	UP	0.956884	0.690692
C23 H53 N7 O16 S	POS	-0.39741	DOWN	0.694745	0.621607
C24 H23 N5	POS	2.967918	UP	0.002269	0.015317
C24 H24 N2 O2	POS	2.203051	UP	0.026248	0.107269
C24 H25 N5 O2	POS	1.842952	UP	0.064802	0.187505
C24 H25 N5 O3	POS	0.210134	UP	0.835701	0.661813
C24 H26 Cl N	NEG	-1.4757	DOWN	0.141451	0.291935
C24 H26 N2 O5	POS	1.978395	UP	0.046911	0.150846
C24 H27 Cl O3	NEG	-1.2989	DOWN	0.196572	0.346931
C24 H27 N3 O S	POS	0.316115	UP	0.754986	0.635208
C24 H28 O5	POS	0.520797	UP	0.606887	0.584926
C24 H28 S	NEG	-0.30036	DOWN	0.766846	0.638457
C24 H30 N2 S2	POS	3.843878	UP	4.48E-05	0.005943
C24 H30 O8	NEG	1.535803	UP	0.125632	0.282051
C24 H31 Cl N2	NEG	-1.13454	DOWN	0.260191	0.403744
C24 H31 Cl N4 O	POS	-1.06895	DOWN	0.289071	0.424718
C24 H32 N6 O5	POS	0.936801	UP	0.353405	0.474627
C24 H32 N6 S2	POS	-0.21536	DOWN	0.83167	0.658051
C24 H32 O5	POS	0.070949	UP	0.944184	0.686432

C24 H33 N O S2	POS	0.283729	UP	0.77942	0.645428
C24 H33 N17 O	POS	-0.69825	DOWN	0.489884	0.536809
C24 H34 N4 O2 S	NEG	0.088421	UP	0.930469	0.68355
C24 H35 N O7	POS	2.236153	UP	0.023977	0.112354
C24 H35 N25	POS	-3.56635	DOWN	0.000181	0.002828
C24 H36 N6 O2 S2	POS	-0.56067	DOWN	0.579564	0.574164
C24 H38 N10 S2	POS	1.373715	UP	0.171629	0.334285
C24 H39 Cl N6 O2 S	NEG	1.540849	UP	0.124368	0.273649
C24 H40 N10 O2 S2	POS	-0.69266	DOWN	0.493379	0.534259
C24 H40 N10 O7 S	NEG	-0.37963	DOWN	0.707775	0.62997
C24 H40 N2 O6 S2	POS	-1.17913	DOWN	0.241704	0.383807
C24 H40 N6 O4 S2	NEG	0.887944	UP	0.379261	0.482534
C24 H41 N3 O10	POS	1.570914	UP	0.117034	0.2654
C24 H41 N5 O7 S	POS	-0.12509	DOWN	0.901757	0.677551
C24 H42 N4 O7 S2	POS	0.471536	UP	0.641391	0.599825
C24 H43 N O14	POS	-1.12738	DOWN	0.263244	0.402594
C24 H43 N17 O5 S	POS	0.982041	UP	0.330456	0.45149
C24 H44 N14 O11	NEG	-5.80468	DOWN	1.82E-12	0
C24 H46 N6 O12	POS	0.049343	UP	0.961165	0.690781
C24 H47 N5 O8 S	POS	-0.83618	DOWN	0.407858	0.493018
C24 H50 N2 O3 S4	NEG	1.753221	UP	0.079413	0.217586
C24 H50 N2 O9 S2	POS	0.954415	UP	0.344356	0.465058
C24 H52 N12 O8 S2	POS	-0.4833	DOWN	0.633082	0.596448
C24 H53 N3 O3 S4	POS	1.319659	UP	0.189407	0.346335
C24 H57 N7 O17 S	POS	-4.65121	DOWN	2.64E-07	0
C25 H18	POS	-1.06687	DOWN	0.290017	0.424066
C25 H22 N4 O2	POS	3.525011	UP	0.00022	0.002828
C25 H25 N S	POS	-0.42186	DOWN	0.676967	0.610122
C25 H27 N3 S	POS	-0.33285	DOWN	0.742449	0.631017
C25 H27 N9 O2	POS	-0.46729	DOWN	0.644405	0.596977
C25 H28 N2 O3	POS	-0.85814	DOWN	0.395575	0.486257
C25 H29 N15 O3	NEG	-0.11905	DOWN	0.906477	0.672096
C25 H29 N5 O4	POS	2.050401	UP	0.039187	0.132156
C25 H29 N9 O + 5.2830625	POS	-2.0794	DOWN	0.036389	0.131681
C25 H30 N2 O5	POS	-3.32623	DOWN	0.000538	0.002828
C25 H33 N3 O5 S	POS	-0.64742	DOWN	0.522146	0.558478
C25 H34 S2	NEG	-2.8593	DOWN	0.003373	0.029321
C25 H38 N2 O8	POS	-0.2532	DOWN	0.802646	0.650837
C25 H38 N24 S	POS	2.538957	UP	0.009851	0.060604
C25 H38 N8 O3 S	NEG	-0.94181	DOWN	0.350818	0.464398
C25 H38 N8 S3	POS	0.363143	UP	0.719933	0.624415
C25 H38 S3	POS	0.650094	UP	0.520424	0.547427
C25 H39 N21 O2	POS	2.221138	UP	0.024986	0.102192

C25 H40 N8 O3 S2	POS	2.61305	UP	0.007784	0.046715
C25 H41 N13 O6	POS	-1.44682	DOWN	0.149562	0.313636
C25 H41 N3 O3 S2	POS	0.849534	UP	0.400363	0.493326
C25 H42 N10 O5 S	NEG	1.997545	UP	0.044744	0.150642
C25 H43 N9 O5 S2	POS	-4.11774	DOWN	9.54E-06	0
C25 H44 N2 O2 S3	POS	-0.24669	DOWN	0.807624	0.653229
C25 H44 N6 O4 S2	POS	0.911042	UP	0.366899	0.473199
C25 H46 N6 O3 S2	POS	2.393639	UP	0.015313	0.07083
C25 H46 N8 O10	POS	-1.40177	DOWN	0.162897	0.320071
C25 H47 N21 O6	POS	0.457941	UP	0.651052	0.605331
C25 H47 N3 O7 S2	POS	-0.09624	DOWN	0.924337	0.68299
C25 H47 N7 O11	POS	1.981645	UP	0.046537	0.149409
C25 H48 N6 O2 S3	NEG	-1.52961	DOWN	0.127197	0.276029
C25 H48 N6 O3 S3	POS	0.391151	UP	0.699321	0.621508
C25 H51 N7 O13	POS	0.370519	UP	0.714485	0.625949
C25 H52 N2 O8 S3	POS	-1.98143	DOWN	0.046562	0.153609
C25 H52 N4 O12 S	POS	0.937083	UP	0.353259	0.464218
C25 H57 N11 O14	POS	0.372766	UP	0.712828	0.622967
C26 H20 N2 O	POS	-1.1268	DOWN	0.263495	0.398005
C26 H25 N5 O	NEG	-0.03494	DOWN	0.972498	0.689263
C26 H26 N2 S	POS	-0.7116	DOWN	0.481586	0.530063
C26 H26 O5	POS	0.599391	UP	0.553582	0.560328
C26 H28 N2 O3	POS	2.431183	UP	0.013698	0.070546
C26 H29 N9 S	POS	0.671645	UP	0.506639	0.546365
C26 H30 O S	POS	0.735331	UP	0.467019	0.52362
C26 H30 O S2	POS	-0.96722	DOWN	0.33787	0.460333
C26 H31 N3 O4 S	POS	-2.72529	DOWN	0.005373	0.032264
C26 H32 N6 O2	POS	-0.70012	DOWN	0.488713	0.539596
C26 H34 N6 O2 S	POS	0.708359	UP	0.483591	0.53321
C26 H34 N8 O5	POS	2.181218	UP	0.027842	0.105957
C26 H35 N9 O4 S	POS	-0.36964	DOWN	0.715133	0.624938
C26 H36 N4 O S	POS	-0.42667	DOWN	0.673492	0.613032
C26 H37 Cl N2 O2 S	POS	-1.12948	DOWN	0.262345	0.400196
C26 H37 N9 O5 S	POS	0.655259	UP	0.517103	0.543945
C26 H38 N14 S	POS	-0.37193	DOWN	0.713444	0.623363
C26 H40 N10 O5	POS	-0.23887	DOWN	0.813613	0.653508
C26 H40 N2 O3 S2	NEG	-0.65146	DOWN	0.519547	0.545902
C26 H40 N2 O8	NEG	-3.46846	DOWN	0.000286	0.005021
C26 H40 N6 O10	POS	1.707633	UP	0.087775	0.231722
C26 H41 N3 O9	POS	-0.21913	DOWN	0.828768	0.659053
C26 H42 O12	POS	-0.44093	DOWN	0.663218	0.609733
C26 H43 N O11	POS	-1.59913	DOWN	0.110454	0.259871
C26 H44 N12 O S3	NEG	1.627203	UP	0.104196	0.247231

C26 H44 N18 S2	POS	2.161787	UP	0.029328	0.110351
C26 H44 N2 O8 S	POS	0.837345	UP	0.407199	0.499184
C26 H45 N13 O2 S2	NEG	2.464511	UP	0.01239	0.06486
C26 H45 N17 S2	POS	2.687271	UP	0.006104	0.038882
C26 H46 N14 O5 S	POS	-4.72356	DOWN	1.51E-07	0
C26 H47 N3 O12 S	POS	0.574344	UP	0.570326	0.565039
C26 H47 N5 O11	POS	0.287366	UP	0.776665	0.643902
C26 H48 N10 S4	POS	-3.71392	DOWN	8.79E-05	0
C26 H50 N4 O3 S3	POS	-2.28485	DOWN	0.02094	0.08307
C26 H50 N6 O13	POS	0.305978	UP	0.76261	0.639245
C26 H55 N3 O3 S4	POS	-3.03403	DOWN	0.001767	0.016657
C26 H57 N11 O S5	POS	1.956424	UP	0.049502	0.16589
C27 H22 N4 O	POS	1.886538	UP	0.058529	0.153392
C27 H25 N7	POS	-0.29104	DOWN	0.773884	0.642304
C27 H27 N5 O	POS	2.702153	UP	0.005808	0.023877
C27 H28 N2 O	POS	0.081014	UP	0.936281	0.685171
C27 H30 O5	POS	1.457417	UP	0.146547	0.296124
C27 H31 N O S	POS	-1.08058	DOWN	0.283803	0.422684
C27 H31 N O5	POS	-0.85178	DOWN	0.399107	0.491935
C27 H31 N5 O S	POS	1.30471	UP	0.194549	0.345907
C27 H33 N5 O3	POS	0.549214	UP	0.587357	0.582023
C27 H34 N10 O5	POS	0.359309	UP	0.722771	0.633062
C27 H34 N6 O S2	NEG	-1.06754	DOWN	0.289711	0.423122
C27 H36 Cl N3 O S	POS	-0.66246	DOWN	0.512488	0.554501
C27 H36 N2 O6 S	POS	-1.90996	DOWN	0.055365	0.169634
C27 H38 N4 O7 S	POS	-0.76567	DOWN	0.448752	0.516283
C27 H39 N19 O6	POS	0.045127	UP	0.964482	0.691291
C27 H39 N23 S	POS	2.948028	UP	0.002443	0.021889
C27 H40 N4 O5 S2	NEG	0.009486	UP	0.992532	0.697859
C27 H40 N6 O S2	POS	1.327934	UP	0.186603	0.347185
C27 H41 N O S2	POS	-0.80334	DOWN	0.426625	0.505571
C27 H42 N2 O6 S2	POS	1.578126	UP	0.115324	0.267285
C27 H43 N21 O3	POS	1.826534	UP	0.0673	0.192887
C27 H44 Cl2 O6	POS	-2.6915	DOWN	0.006018	0.030821
C27 H44 N16 O4 S	POS	-0.53117	DOWN	0.599728	0.580964
C27 H45 N19 O3 S2	POS	-2.06539	DOWN	0.037719	0.130727
C27 H48 N2 O S3	POS	-0.72381	DOWN	0.474057	0.527567
C27 H48 N2 O15	POS	-4.17061	DOWN	6.93E-06	0
C27 H48 N2 O7 S2	POS	2.527716	UP	0.010202	0.064226
C27 H48 N4 O4 S3	POS	-4.67577	DOWN	2.19E-07	0
C27 H49 N O2 S3	POS	-1.346	DOWN	0.180585	0.331781
C27 H50 N6 O3 S3	POS	-1.01006	DOWN	0.316722	0.446817
C27 H50 N8 O11	POS	-1.67319	DOWN	0.094539	0.240461

C27 H51 Cl N10 O7 S	POS	1.209829	UP	0.229514	0.382133
C27 H51 N O3 S3	POS	-0.1095	DOWN	0.913951	0.680756
C27 H54 N10 O8 S2	POS	-0.35187	DOWN	0.728289	0.62834
C27 H54 N4 O2 S4	POS	1.316056	UP	0.190637	0.341307
C27 H55 N7 O14	POS	0.699352	UP	0.489193	0.530434
C27 H58 N2 O3 S5	POS	-0.05052	DOWN	0.960237	0.69107
C28 H24 O	POS	-2.84471	DOWN	0.003553	0.02669
C28 H30 N4 O2 S	POS	-0.73404	DOWN	0.467808	0.526769
C28 H31 N5 O S	POS	-0.36344	DOWN	0.719714	0.619028
C28 H32 N22 O	POS	0.85179	UP	0.399104	0.48427
C28 H33 N11	POS	-0.2927	DOWN	0.772633	0.642155
C28 H36 O6 S	POS	-1.49968	DOWN	0.13497	0.284417
C28 H37 N3 O6	POS	0.274262	UP	0.786603	0.648699
C28 H40 N2 O S3	POS	0.555559	UP	0.583035	0.575382
C28 H40 O7 S	POS	-2.18157	DOWN	0.027816	0.113095
C28 H41 Cl N12	POS	0.812708	UP	0.421223	0.500323
C28 H43 N3 O7 S	NEG	1.903536	UP	0.056219	0.167281
C28 H44 N8 O4 S2	NEG	0.752527	UP	0.456615	0.517135
C28 H44 O11 S	POS	-0.30179	DOWN	0.765766	0.638639
C28 H45 N3 O10	POS	-0.14509	DOWN	0.886141	0.674379
C28 H45 N3 O11	POS	0.201295	UP	0.842522	0.662238
C28 H46 N4 S3	POS	-1.19196	DOWN	0.236558	0.380525
C28 H51 N13 O9	POS	1.214368	UP	0.227748	0.379472
C28 H52 N16 O4 S2	POS	-0.51938	DOWN	0.607867	0.587156
C28 H54 N6 O14	POS	0.536486	UP	0.596069	0.579901
C28 H56 N6 O10 S2	POS	-0.75324	DOWN	0.456185	0.517045
C28 H60 N2 O8 S4	POS	1.354767	UP	0.177716	0.329712
C29 H36 N4 O3 S	POS	-0.38308	DOWN	0.70524	0.621973
C29 H37 N7 O S	NEG	-0.55707	DOWN	0.582009	0.577093
C29 H37 N9 O3	POS	0.341484	UP	0.736011	0.628243
C29 H38 O3 S	NEG	0.007727	UP	0.993917	0.697732
C29 H38 O4 S	NEG	2.612937	UP	0.007787	0.045899
C29 H40 N4 O7 S	POS	-3.51381	DOWN	0.000232	0.002828
C29 H42 N2 S2	POS	-0.52104	DOWN	0.60672	0.582469
C29 H43 N7 O3 S	POS	-0.11416	DOWN	0.910303	0.679066
C29 H45 N15 O7 S	NEG	-2.4382	DOWN	0.013413	0.067327
C29 H46 N4 O6 S	POS	0.803452	UP	0.426562	0.50466
C29 H46 O3 S3	POS	0.90666	UP	0.369226	0.471182
C29 H48 N2 O10	POS	-2.14085	DOWN	0.031003	0.123092
C29 H48 N6 O11 S	POS	1.093067	UP	0.278216	0.409247
C29 H50 N18 O2 S2	POS	1.148676	UP	0.254229	0.396029
C29 H50 N2 O8 S2	NEG	-0.47526	DOWN	0.638758	0.598556
C29 H55 N3 O14	POS	2.537613	UP	0.009892	0.054144

C29 H56 N2 O15 S	POS	3.541189	UP	0.000204	0.002828
C3 H10 N2 O3 S	POS	0.140273	UP	0.889901	0.673464
C3 H10 N2 O3 S	NEG	1.179942	UP	0.241376	0.391531
C3 H10 N2 O5	POS	-1.02795	DOWN	0.308152	0.440616
C3 H10 N2 O6	POS	-0.20515	DOWN	0.839546	0.660184
C3 H10 N6 S	POS	1.202477	UP	0.232394	0.376937
C3 H10 N8	POS	-2.95886	DOWN	0.002347	0.013969
C3 H12 N4 O4	POS	-0.91666	DOWN	0.36393	0.472452
C3 H12 N6 O S + 7.8712277	POS	1.827224	UP	0.067194	0.184917
C3 H13 N7 S	POS	1.298673	UP	0.196653	0.345651
C3 H6 O	POS	-0.73892	DOWN	0.464836	0.522066
C3 H6 O2	NEG	-2.66075	DOWN	0.006663	0.046715
C3 H6 O2 + 0.20226668	POS	-0.14783	DOWN	0.88401	0.672769
C3 H6 O3 - 1.1123182	NEG	-0.48869	DOWN	0.629286	0.596372
C3 H6 O3 - 6.876823	NEG	-0.06234	DOWN	0.950946	0.688159
C3 H7 N O	POS	0.091805	UP	0.927815	0.682944
C3 H7 N O2	POS	-0.32718	DOWN	0.746691	0.635456
C3 H8 N2 O4	POS	-3.34663	DOWN	0.000492	0.005021
C3 H8 O3	POS	0.09314	UP	0.926768	0.683759
C3 H9 Cl N4 O	NEG	-1.20426	DOWN	0.231694	0.378903
C3 H9 N O	POS	2.096479	UP	0.034819	0.128798
C3 H9 N7 S	POS	-3.39923	DOWN	0.000391	0.003989
C30 H26 N2 O	POS	-4.16987	DOWN	6.96E-06	0.00158
C30 H28 N4 O3	NEG	-2.48254	DOWN	0.011728	0.061615
C30 H28 O S	POS	1.310739	UP	0.192463	0.343667
C30 H32 N12 + 10.165411	POS	2.294628	UP	0.020371	0.081097
C30 H36 O2 S	POS	3.418987	UP	0.000358	0.003989
C30 H36 O5 S	NEG	-0.78975	DOWN	0.434536	0.509499
C30 H38 N2 O6 S	NEG	0.139742	UP	0.890315	0.671921
C30 H40 N4 O7 S	POS	-1.15466	DOWN	0.251734	0.39331
C30 H42 N2 O2 S3	POS	-0.04641	DOWN	0.963473	0.691513
C30 H44 N18 O S2	POS	-1.44253	DOWN	0.150795	0.301225
C30 H44 N18 O3	POS	-4.2544	DOWN	4.11E-06	0
C30 H45 N3 O9	POS	-0.31535	DOWN	0.755562	0.637452
C30 H45 N9 O7 S	NEG	4.058679	UP	1.35E-05	0
C30 H46 N6 O3 S3	POS	0.694382	UP	0.4923	0.533897
C30 H46 O9	POS	0.391726	UP	0.6989	0.626371
C30 H49 N3 O11	POS	0.217791	UP	0.829802	0.657834
C30 H52 N2 O2 S3	POS	0.209386	UP	0.836278	0.659053
C30 H52 N2 O8 S2	NEG	0.792113	UP	0.433155	0.512925
C30 H55 N11 O11	POS	2.172121	UP	0.02853	0.108821
C30 H55 N3 O5 S4	POS	1.120333	UP	0.266274	0.404583
C30 H58 N6 O15	POS	-1.26014	DOWN	0.210467	0.363224

C30 H61 N5 O S5	POS	2.931669	UP	0.002595	0.023877
C31 H28 N4 O3	POS	-2.37789	DOWN	0.016037	0.070546
C31 H33 N S	POS	1.062846	UP	0.29186	0.420778
C31 H34 Cl N9 O	POS	-0.05965	DOWN	0.95306	0.688836
C31 H34 N12 O4	POS	-1.10889	DOWN	0.271242	0.413367
C31 H34 N22 + 12.284333	POS	0.097947	UP	0.923	0.680922
C31 H36 N14 O4	POS	0.01526	UP	0.987986	0.696859
C31 H36 N4 O S	POS	-0.41836	DOWN	0.6795	0.6139
C31 H40 N10 O4	POS	-0.52918	DOWN	0.601097	0.584685
C31 H40 N4 O2 S2	POS	0.640026	UP	0.526928	0.553577
C31 H42 O5 S	NEG	1.614859	UP	0.106914	0.254417
C31 H42 O6 S	NEG	-1.14067	DOWN	0.257592	0.403897
C31 H43 N11 O S2	POS	0.057905	UP	0.954434	0.68843
C31 H43 N3 O3 S2	POS	2.826628	UP	0.003787	0.021889
C31 H44 N2 O11	NEG	-0.11228	DOWN	0.911771	0.679305
C31 H44 N2 O8 S	POS	2.616086	UP	0.007708	0.044227
C31 H44 O4 S2	POS	-2.97369	DOWN	0.00222	0.021365
C31 H46 N18 S	NEG	1.63903	UP	0.101643	0.248357
C31 H46 N4 O S2	POS	0.937951	UP	0.35281	0.467141
C31 H50 N2 O10	POS	-0.44018	DOWN	0.663757	0.608597
C31 H51 N5 O2 S3	POS	3.328089	UP	0.000534	0.008611
C31 H52 N2 O13	POS	1.581545	UP	0.114521	0.288169
C31 H54 N2 O8 S2	NEG	-0.46457	DOWN	0.646336	0.598593
C31 H56 N8 O10 S	POS	-0.86764	DOWN	0.390334	0.486417
C31 H61 Cl3 N6 O S2	POS	-0.49157	DOWN	0.627258	0.591118
C32 H28 N6 O2 + 3.4709504	POS	-0.48068	DOWN	0.634929	0.592936
C32 H31 N O3	POS	0.855029	UP	0.397302	0.489118
C32 H36 N2 O S2	POS	-0.68413	DOWN	0.498737	0.538255
C32 H36 N20 O	POS	-4.42746	DOWN	1.32E-06	0
C32 H36 N8 S	POS	-0.96697	DOWN	0.337996	0.449297
C32 H40 N6 O5	POS	0.644214	UP	0.524218	0.553993
C32 H41 N O4 S	POS	-3.8997	DOWN	3.31E-05	0
C32 H43 N3 O6	POS	0.179909	UP	0.859073	0.665416
C32 H44 N10 O6 S	NEG	1.151323	UP	0.253123	0.394434
C32 H44 N4 O7 S	POS	0.437641	UP	0.665584	0.60792
C32 H45 N3 O8	POS	1.989832	UP	0.045607	0.152082
C32 H46 N8 O4 S	POS	-2.54745	DOWN	0.009592	0.056376
C32 H48 N6 O4 S	POS	-0.31582	DOWN	0.755206	0.635764
C32 H48 N6 O9	POS	-0.20926	DOWN	0.836373	0.661228
C32 H48 O4 S2	NEG	0.47407	UP	0.639596	0.596031
C32 H49 Cl3 N4 O	POS	1.140961	UP	0.25747	0.39595
C32 H49 N3 O10 + 11.723135	POS	1.222248	UP	0.224705	0.374285
C32 H50 O8 S	POS	-0.09183	DOWN	0.927792	0.68299

C32 H52 N12 O5 S	POS	-1.4346	DOWN	0.153097	0.306489
C32 H52 N12 O6 S	POS	-2.5198	DOWN	0.010457	0.057462
C32 H52 N6 O4 S3	POS	1.284439	UP	0.201679	0.35662
C32 H53 N3 O12	POS	0.836704	UP	0.40756	0.499184
C33 H27 N O2	POS	-3.27874	DOWN	0.000659	0.00158
C33 H42 N12 O7	POS	-0.11404	DOWN	0.910396	0.681016
C33 H45 N O11	POS	0.745545	UP	0.460824	0.524006
C33 H45 N7 O4 S	POS	0.272937	UP	0.78761	0.647433
C33 H48 N2 O10	POS	-0.0409	DOWN	0.967806	0.692461
C33 H48 N2 O6 S	POS	-0.37066	DOWN	0.714383	0.624906
C33 H51 N O8 S2	POS	0.828546	UP	0.412177	0.497838
C33 H52 N2 O8 S2	POS	-0.07631	DOWN	0.939971	0.685539
C33 H54 N10 O8 S	NEG	-2.19258	DOWN	0.027003	0.111608
C33 H54 N14 S3	POS	1.21133	UP	0.228929	0.380283
C33 H54 O5 S3	POS	0.787842	UP	0.435653	0.512098
C33 H57 N5 O11 S	POS	-0.75607	DOWN	0.454488	0.515608
C33 H58 N2 O8 S2	NEG	1.071947	UP	0.287706	0.424573
C33 H60 N6 O8 S2	POS	1.108287	UP	0.271507	0.416537
C34 H26 O	POS	0.515831	UP	0.610328	0.61869
C34 H28 N2 O	POS	-2.6224	DOWN	0.007552	0.045485
C34 H33 N3 O3	POS	-0.9893	DOWN	0.326865	0.449037
C34 H36 N4 O2 S	POS	2.627971	UP	0.007417	0.046308
C34 H39 N S2	POS	-1.4309	DOWN	0.154177	0.319368
C34 H42 N6 O4	NEG	0.872281	UP	0.387784	0.485025
C34 H43 N O2 S2	POS	-0.11658	DOWN	0.908412	0.678514
C34 H43 N9 O5	POS	0.280877	UP	0.781582	0.645603
C34 H44 N6 O6	POS	1.468334	UP	0.143488	0.304928
C34 H44 N8 O9	POS	-0.03713	DOWN	0.970774	0.693184
C34 H48 O7 S	POS	2.776784	UP	0.004506	0.034108
C34 H49 N3 O9	POS	2.476455	UP	0.011948	0.060263
C34 H49 N3 O9 S	POS	3.685256	UP	0.000102	0
C34 H53 N3 O11	POS	1.560108	UP	0.119631	0.272928
C34 H57 N3 O13	POS	1.027334	UP	0.308443	0.438027
C35 H28 N4	POS	-0.0148	DOWN	0.988348	0.696581
C35 H46 N14 O3 S	NEG	-1.25055	DOWN	0.21401	0.360167
C35 H49 N13 O5	POS	0.65029	UP	0.520298	0.54715
C35 H49 N9 O6 S	POS	3.069186	UP	0.001543	0.01186
C35 H52 N6 O5 S2	POS	-2.26869	DOWN	0.021909	0.093047
C35 H52 N8 O3 S3	NEG	-0.43088	DOWN	0.670453	0.608526
C35 H52 O6 S2	POS	2.978341	UP	0.002182	0.019711
C36 H26 N2	POS	-1.18258	DOWN	0.240312	0.383807
C36 H37 Cl	POS	3.006892	UP	0.001959	0.021889
C36 H38 N12	POS	-0.05639	DOWN	0.955623	0.689016

C36 H41 N O2 S2	POS	1.077754	UP	0.285075	0.422757
C36 H43 N5 O3 S	POS	-4.81743	DOWN	7.13E-08	0
C36 H48 N6 O7	POS	-0.11772	DOWN	0.907521	0.677671
C36 H50 N2 O7 S	POS	1.002676	UP	0.320308	0.445367
C36 H52 O8 S	POS	1.850885	UP	0.063622	0.186992
C36 H53 N3 O10	POS	2.463353	UP	0.012434	0.060604
C36 H56 N6 O11	POS	0.023071	UP	0.981837	0.694903
C36 H57 N3 O12	POS	1.265351	UP	0.20856	0.360936
C37 H32 N6 O	POS	0.09041	UP	0.928909	0.683968
C37 H39 N13	POS	-1.70007	DOWN	0.089227	0.241048
C37 H42 O4	POS	-0.87874	DOWN	0.384255	0.488486
C37 H43 N9 O7	NEG	-0.49014	DOWN	0.628268	0.59309
C37 H45 N O S2	POS	2.998639	UP	0.002022	0.021365
C37 H48 N8 O6 S	POS	-1.22614	DOWN	0.223214	0.363897
C37 H49 Cl N2 O3 S	NEG	-0.81575	DOWN	0.419475	0.503161
C37 H50 N2 O7 S	POS	-0.07566	DOWN	0.940483	0.683177
C37 H50 N8 O S2	POS	0.441811	UP	0.662589	0.608847
C37 H53 N7 O4 S2	POS	1.725145	UP	0.084485	0.220236
C37 H55 Cl N2 O8	POS	0.38508	UP	0.703771	0.622039
C37 H56 Cl N O2 S2	POS	1.608857	UP	0.108255	0.253468
C38 H30 N4 O	POS	0.213756	UP	0.83291	0.658485
C38 H33 N O	POS	-0.9416	DOWN	0.350925	0.467318
C38 H42 Cl N O	POS	-1.65748	DOWN	0.097757	0.242361
C38 H42 O9	POS	0.60998	UP	0.546576	0.555192
C38 H47 N9 O5	POS	-0.15997	DOWN	0.87456	0.670059
C38 H48 N2 O S2	NEG	0.941579	UP	0.350936	0.460762
C38 H48 O12	POS	0.824907	UP	0.414245	0.501699
C38 H48 O3 S	POS	1.355543	UP	0.177464	0.333362
C38 H50 O S3	POS	-3.85698	DOWN	4.18E-05	0.00158
C38 H52 N6 O8	POS	0.551677	UP	0.585678	0.579161
C38 H52 O6 S2	NEG	-0.05495	DOWN	0.95676	0.689509
C38 H54 O5 S2	POS	0.057173	UP	0.955009	0.691358
C38 H56 O9 S	POS	1.325593	UP	0.187393	0.351388
C38 H57 Cl N2 O S3	POS	0.41801	UP	0.679754	0.61044
C39 H45 N11 O2 S	POS	3.391673	UP	0.000404	0.006772
C39 H46 O4 S2	POS	1.690837	UP	0.091025	0.232647
C39 H47 N O2 S2	POS	-1.45904	DOWN	0.146089	0.307522
C39 H48 O3 S2	NEG	0.447737	UP	0.658341	0.602487
C39 H49 N O2 S2	POS	-0.99424	DOWN	0.324431	0.449297
C39 H50 O13	POS	1.421184	UP	0.157047	0.307419
C4 H10 N2 S	POS	-1.52355	DOWN	0.128742	0.28352
C4 H10 O3 + 5.2717648	POS	-0.82141	DOWN	0.416239	0.503016
C4 H11 N O2	POS	0.571279	UP	0.57239	0.571961

C4 H12 N2 O2 S	POS	-2.02479	DOWN	0.041804	0.144347
C4 H12 N2 O3 S	POS	0.741283	UP	0.463404	0.525372
C4 H12 N2 O3 S	NEG	1.351818	UP	0.178678	0.329712
C4 H13 N3 O4 S	POS	0.140637	UP	0.889617	0.674231
C4 H14 N4 O4 S	POS	-1.79037	DOWN	0.073077	0.190577
C4 H3 N3 O	POS	1.211188	UP	0.228984	0.392261
C4 H4 O2	POS	-0.28664	DOWN	0.777218	0.642215
C4 H4 O3 - 0.469625	NEG	-1.03701	DOWN	0.303864	0.439257
C4 H5 N3 O2	NEG	0.226501	UP	0.823103	0.658756
C4 H6 N6 + 0.6443889	POS	-0.77545	DOWN	0.442945	0.521022
C4 H6 O4	NEG	-0.08593	DOWN	0.932421	0.684293
C4 H7 N3 O	POS	0.49524	UP	0.624687	0.593704
C4 H8 + 9.6981945	POS	-1.48183	DOWN	0.139772	0.299504
C4 H8 N4 O2	POS	1.270993	UP	0.206509	0.35948
C4 H8 N4 O2	NEG	-1.22472	DOWN	0.223755	0.36845
C4 H8 N6 O	POS	0.429744	UP	0.67127	0.611003
C4 H8 O	POS	0.063102	UP	0.950349	0.687661
C4 H8 O S	POS	0.719371	UP	0.476788	0.535548
C4 H8 O2	POS	0.415197	UP	0.681794	0.614454
C4 H9 N	POS	0.485649	UP	0.631424	0.595993
C4 H9 N + 0.7567741	POS	0.45482	UP	0.653278	0.601899
C4 H9 N3 O2	POS	-0.67047	DOWN	0.507384	0.541451
C40 H42 N10 O S	POS	-1.11439	DOWN	0.268848	0.403667
C40 H56 N6 O3 S2	POS	0.655412	UP	0.517005	0.542819
C40 H56 N6 O4 S2	POS	-0.25281	DOWN	0.802947	0.656879
C41 H46 N6 S	POS	-0.1884	DOWN	0.852491	0.6639
C42 H39 N9 O	POS	-1.53614	DOWN	0.125546	0.281368
C42 H45 N O5	POS	-1.13983	DOWN	0.257949	0.406024
C43 H39 N3 S	POS	-0.80109	DOWN	0.427932	0.506097
C44 H49 Cl N2 O4	POS	-0.47215	DOWN	0.640959	0.596788
C44 H49 N O6	POS	-1.35541	DOWN	0.177507	0.341042
C5 H10 O S	NEG	-0.71607	DOWN	0.478821	0.530146
C5 H10 O3 - 1.3391999	NEG	0.868675	UP	0.389763	0.490062
C5 H12 N2 S	POS	-2.23143	DOWN	0.024291	0.091546
C5 H12 N4 S	POS	-3.87184	DOWN	3.85E-05	0
C5 H12 N6	POS	-0.65503	DOWN	0.517248	0.544039
C5 H12 N6 O S	NEG	1.621906	UP	0.105356	0.255764
C5 H12 O3 S - 3.6071332	NEG	-0.60026	DOWN	0.553005	0.564907
C5 H16 N6 O S	POS	-1.81098	DOWN	0.069739	0.198112
C5 H16 N6 O2	POS	-1.83901	DOWN	0.065395	0.19377
C5 H4 N4 O	POS	-1.35064	DOWN	0.179062	0.340954
C5 H5 N5	POS	0.118846	UP	0.906637	0.678754
C5 H6 N2	POS	-0.67654	DOWN	0.503534	0.543758

C5 H6 N2	NEG	-0.13027	DOWN	0.897712	0.675801
C5 H6 O3	POS	-4.06627	DOWN	1.29E-05	0
C5 H7 N S	NEG	-2.65833	DOWN	0.006717	0.045485
C5 H7 N5 O2	POS	0.895324	UP	0.375285	0.48679
C5 H8 N6	POS	-0.87473	DOWN	0.386447	0.48427
C5 H9 N O	POS	-1.40667	DOWN	0.161403	0.322558
C5 H9 N3	POS	1.775671	UP	0.075534	0.202603
C5 H9 N5 O3	NEG	-0.04532	DOWN	0.964332	0.691424
C6 H10 N6	POS	-0.99957	DOWN	0.32182	0.449362
C6 H10 O3	NEG	-2.06951	DOWN	0.037324	0.130727
C6 H11 N O2 + 3.938733	POS	-1.36418	DOWN	0.174674	0.33575
C6 H12 N2 O3	POS	-0.38952	DOWN	0.700516	0.621774
C6 H12 O3	POS	0.968771	UP	0.337088	0.45867
C6 H13 N O2 S	POS	3.056624	UP	0.00162	0.01186
C6 H13 N O3 S	POS	1.22051	UP	0.225374	0.373699
C6 H14 N2 O2	POS	-0.63019	DOWN	0.533321	0.553484
C6 H14 N2 O4	POS	0.962808	UP	0.340095	0.459473
C6 H14 N4 S	NEG	1.49957	UP	0.134999	0.287185
C6 H14 N8 O	POS	-0.1531	DOWN	0.879902	0.673092
C6 H14 O3	POS	-1.91036	DOWN	0.055312	0.169049
C6 H14 O4	POS	0.003044	UP	0.997604	0.698811
C6 H15 N O4	POS	2.122295	UP	0.032554	0.111608
C6 H15 N O5 S	POS	-1.17299	DOWN	0.244197	0.395791
C6 H15 N5 S	POS	6.280545	UP	6.04E-16	0
C6 H16 Cl N5 O2	POS	-2.38501	DOWN	0.015706	0.068225
C6 H16 N2 O S2 + 4.5088425	POS	1.309915	UP	0.192747	0.340423
C6 H16 N2 O8	POS	0.838633	UP	0.406473	0.496885
C6 H16 N8 O2 + 0.9335556	POS	1.480006	UP	0.140271	0.296227
C6 H16 O2 S2	POS	-0.24005	DOWN	0.812704	0.652893
C6 H19 N5 O S2	POS	-0.56888	DOWN	0.574008	0.572938
C6 H4	POS	-2.09878	DOWN	0.034612	0.128555
C6 H6	POS	-1.29838	DOWN	0.196757	0.350667
C6 H6 N2 O3	NEG	-0.97406	DOWN	0.334435	0.454798
C6 H6 N4 O2	NEG	2.063627	UP	0.037889	0.13589
C6 H6 O	NEG	1.034881	UP	0.304869	0.433591
C6 H6 O3	POS	0.828141	UP	0.412407	0.499135
C6 H7 N3 O2	POS	-2.68138	DOWN	0.006224	0.042502
C6 H7 N3 O3	NEG	-0.35529	DOWN	0.725751	0.626209
C6 H8 O2	POS	-1.53321	DOWN	0.126286	0.279301
C6 H9 N O4	POS	-0.72836	DOWN	0.471273	0.524092
C6 H9 N3 O4	NEG	-1.52885	DOWN	0.12739	0.282278
C7 H10 N2 O S	POS	-2.1609	DOWN	0.029398	0.119295
C7 H10 N2 O4	POS	0.054924	UP	0.956777	0.691092

C7 H10 O2 S	NEG	2.964942	UP	0.002294	0.016657
C7 H11 N O2	POS	0.867586	UP	0.390361	0.487322
C7 H12 O4 - 3.0801935	NEG	-0.14064	DOWN	0.889618	0.673018
C7 H13 N O2	POS	-1.29804	DOWN	0.196875	0.348116
C7 H13 N11 O2	POS	-1.39176	DOWN	0.165974	0.331407
C7 H13 N5	POS	0.228042	UP	0.821919	0.657234
C7 H14 N2 S + 4.1905837	POS	0.401859	UP	0.691496	0.618013
C7 H14 N4 O2 S	NEG	-3.16418	DOWN	0.001058	0.006772
C7 H14 N4 O3	POS	0.018303	UP	0.98559	0.695981
C7 H14 N6	POS	1.2738	UP	0.205494	0.356357
C7 H15 N O2	POS	4.113665	UP	9.78E-06	0
C7 H15 N3 O3	POS	-1.33931	DOWN	0.182799	0.34332
C7 H16 N2 O S	POS	-0.53059	DOWN	0.600127	0.584163
C7 H16 N4 O3	POS	-0.65167	DOWN	0.519412	0.550358
C7 H16 N8 O2	NEG	0.70396	UP	0.486323	0.533291
C7 H16 O6	POS	1.62509	UP	0.104657	0.247936
C7 H18 N2 O3 S	POS	0.826476	UP	0.413352	0.496582
C7 H18 N2 O3 S	NEG	1.648338	UP	0.099667	0.236447
C7 H18 N6 O6	POS	-1.74396	DOWN	0.081059	0.218081
C7 H19 Cl N4 O2	POS	-1.15352	DOWN	0.252208	0.389982
C7 H21 Cl N6 O	POS	0.991639	UP	0.325711	0.450203
C7 H4 N4	POS	-0.71309	DOWN	0.480659	0.531174
C7 H4 O	POS	-1.13533	DOWN	0.259853	0.404202
C7 H6 N2 O	NEG	-0.8307	DOWN	0.410955	0.499085
C7 H6 O	POS	-1.3849	DOWN	0.168108	0.322064
C7 H6 O2	NEG	1.019854	UP	0.312012	0.438164
C7 H7 N3	POS	3.319948	UP	0.000553	0.007706
C7 H7 N5 O2	POS	-0.18617	DOWN	0.854221	0.664529
C7 H8 N2 O2	POS	0.932195	UP	0.355795	0.468027
C7 H8 N4 O3 - 2.622133	NEG	-1.51728	DOWN	0.130356	0.294149
C7 H9 N O2	POS	-0.72748	DOWN	0.471812	0.529733
C7 H9 N O2	NEG	0.354922	UP	0.726022	0.626436
C8 H10	POS	0.05781	UP	0.954508	0.689106
C8 H10 N2 O3	POS	1.628876	UP	0.103832	0.243952
C8 H10 N2 O3 - 3.5058272	NEG	-1.88693	DOWN	0.058474	0.177761
C8 H10 N8 O2	NEG	-1.00137	DOWN	0.320945	0.450912
C8 H12 N2 O4	POS	1.694949	UP	0.090221	0.225911
C8 H12 N8 O	NEG	-2.67715	DOWN	0.006312	0.035514
C8 H12 N8 O2	NEG	-1.98769	DOWN	0.045849	0.15469
C8 H13 Cl	NEG	-1.80754	DOWN	0.070287	0.197425
C8 H13 N3 O5	NEG	0.741487	UP	0.46328	0.51909
C8 H14 N8 O2	POS	0.467518	UP	0.64424	0.595765
C8 H14 O3 - 6.071393	NEG	-2.17143	DOWN	0.028582	0.114561

C8 H14 O4	POS	-0.98471	DOWN	0.329132	0.451874
C8 H15 N3 O3 + 3.8022223	POS	-1.08501	DOWN	0.281811	0.421366
C8 H15 N3 O3 + 4.178133	POS	0.785668	UP	0.436928	0.509499
C8 H16 N2 O3	POS	3.78898	UP	5.98E-05	0
C8 H16 N6 O	POS	0.498918	UP	0.622112	0.590884
C8 H16 O3 - 5.7483726	NEG	2.804055	UP	0.004099	0.034555
C8 H16 O3 S	NEG	-1.23284	DOWN	0.220658	0.370481
C8 H16 O8	NEG	-0.58812	DOWN	0.561085	0.565828
C8 H17 Cl N2	POS	-1.21627	DOWN	0.227011	0.377841
C8 H17 N O2 S	POS	0.333032	UP	0.742316	0.634713
C8 H17 N7 O2 S	NEG	-0.52708	DOWN	0.602547	0.58259
C8 H17 N7 S	POS	-1.07112	DOWN	0.28808	0.420188
C8 H20 Cl2 N2 O2	POS	0.257808	UP	0.79913	0.649415
C8 H20 N2 O3 S	POS	-0.0802	DOWN	0.936924	0.685263
C8 H20 N2 O4 - 3.5148826	NEG	1.464623	UP	0.144522	0.30545
C8 H21 N5 O5	POS	-0.05117	DOWN	0.959729	0.691092
C8 H22 N8 O S	POS	3.398957	UP	0.000391	0.003989
C8 H22 N8 O2 S	POS	0.361302	UP	0.721295	0.629492
C8 H25 N7 O5 S	POS	1.512739	UP	0.131536	0.292041
C8 H8 N2 O3	NEG	-1.88692	DOWN	0.058475	0.174792
C8 H8 O2	NEG	-0.42478	DOWN	0.674853	0.60817
C8 H9 N O2	POS	0.422975	UP	0.67616	0.61345
C9 H10 N4	POS	-1.62675	DOWN	0.104294	0.252376
C9 H10 O3	POS	-1.87247	DOWN	0.060498	0.182277
C9 H12 N10 O	NEG	0.867952	UP	0.39016	0.491157
C9 H12 N4 + 5.0588694	POS	0.387299	UP	0.702143	0.618115
C9 H12 N8	POS	-1.69305	DOWN	0.090592	0.24002
C9 H12 O	POS	0.238415	UP	0.81396	0.653842
C9 H12 O3	POS	-2.29339	DOWN	0.020442	0.092149
C9 H13 Cl N2	POS	0.720328	UP	0.476199	0.525287
C9 H13 N9 O	POS	0.439782	UP	0.664045	0.604569
C9 H14 O2	POS	1.135266	UP	0.259881	0.40105
C9 H15 Cl N4 O2 + 3.7597144	POS	0.090283	UP	0.929009	0.68334
C9 H15 N O5	POS	0.193362	UP	0.848654	0.664293
C9 H15 N11	POS	0.110563	UP	0.913118	0.680139
C9 H15 N7 O4	NEG	4.995015	UP	1.57E-08	0
C9 H15 N7 O5	NEG	0.513594	UP	0.611881	0.584926
C9 H16 N10	POS	-0.17383	DOWN	0.86379	0.6681
C9 H16 N6 O2	POS	0.280292	UP	0.782025	0.646535
C9 H17 Cl N4 O2	POS	0.381286	UP	0.706557	0.583076
C9 H17 N O4	POS	-0.84292	DOWN	0.404061	0.494605
C9 H17 N7 O	POS	1.07014	UP	0.288527	0.422319
C9 H18 N2 O3	POS	2.057618	UP	0.038474	0.13589

C9 H18 N2 O6	POS	0.244855	UP	0.809028	0.655063
C9 H18 N4 O3	POS	0.310246	UP	0.759397	0.638852
C9 H18 N4 S + 0.62561905	POS	-2.61961	DOWN	0.007621	0.051828
C9 H19 Cl2 N3	POS	-0.7083	DOWN	0.483629	0.52965
C9 H19 N O4	POS	-1.22237	DOWN	0.22466	0.374201
C9 H19 N O4 S	NEG	1.545759	UP	0.123147	0.281824
C9 H19 N3 O5	NEG	1.087023	UP	0.28091	0.419003
C9 H20 N2 O2 S	POS	-3.65125	DOWN	0.00012	0
C9 H20 N4 O4	POS	3.402232	UP	0.000386	0.002828
C9 H20 O3 S	POS	1.421324	UP	0.157005	0.308138
C9 H22 N2 O4 S	POS	0.466547	UP	0.644929	0.595841
C9 H23 N11 S2	POS	2.913406	UP	0.002774	0.019131
C9 H23 N3 O2 S2	NEG	-2.62397	DOWN	0.007514	0.044227
C9 H23 N3 O5 S	POS	-0.72407	DOWN	0.473899	0.529443
C9 H25 N11 S2	NEG	1.048732	UP	0.29838	0.429058
C9 H26 Cl2 N8 O	NEG	-0.08702	DOWN	0.931567	0.686112
C9 H6 N6	NEG	0.107225	UP	0.915731	0.6804
C9 H8 O2	POS	-0.05934	DOWN	0.953305	0.689487
C9 H8 O3	POS	0.636088	UP	0.529483	0.54655
Caffeine	QQQ-DH	0.419057	UP	0.678996	0.61244
Carnitine	POS	2.117473	UP	0.032968	0.119756
Carvone	POS	-0.9199	DOWN	0.362222	0.473771
Cinnamic acid	POS	0.19266	UP	0.849197	0.664372
Cinnamic acid	QQQ-DH	-2.48686	DOWN	0.011574	0.066108
Citramalic acid	NEG	1.864675	UP	0.061611	0.184218
Citrulline	QQQ-RP	-1.47053	DOWN	0.142879	0.296124
Cortisol	POS	-1.20928	DOWN	0.229728	0.373783
Coumarin	QQQ-RP	-5.14027	DOWN	4.09E-09	0
Creatine	NEG	3.761566	UP	6.89E-05	0
Cytidine monophosphate (CMP)	QQQ-DH	1.846725	UP	0.064238	0.184042
Dimethylglycine	QQQ-RP	-1.48544	DOWN	0.13879	0.29352
DL-3-Phenyllactic acid - 3.2354286	NEG	4.893727	UP	3.78E-08	0
DL-Indole-3-lactic acid (3-Indolelactic acid)	POS	-1.12468	DOWN	0.264403	0.406477
D-Ribonolactone	NEG	3.03561	UP	0.001756	0.013293
Epinephrine (adrenaline)	POS	-0.35046	DOWN	0.729335	0.6307
Glutamic Acid	POS	0.874452	UP	0.386597	0.488803
Glutamine or lysine or glutamic acid	QQQ-	-1.11145	DOWN	0.270124	0.410876

glyceraldehyde-3-phosphate	RP QQQ-DH	-3.69238	DOWN	9.80E-05	0.00158
Glycerophosphocholine	POS	1.379105	UP	0.169925	0.322657
Guanine	POS	3.420655	UP	0.000355	0.006772
Guanine	QQQ-RP	5.028301	UP	1.16E-08	0
Hippuric acid	NEG	1.878469	UP	0.059651	0.177209
Histamine	QQQ-RP	-3.65966	DOWN	0.000115	0.00158
Histidine	NEG	2.989602	UP	0.002092	0.018537
Histidine	QQQ-RP	2.957812	UP	0.002356	0.014618
Homocysteine	QQQ-RP	-2.72936	DOWN	0.0053	0.031308
Homoserine	QQQ-DH	1.973149	UP	0.047519	0.160603
Hypoxanthine	POS	0.713697	UP	0.480287	0.538303
Hypoxanthine	NEG	3.547924	UP	0.000198	0
Hypoxanthine	QQQ-RP	2.513751	UP	0.010655	0.046715
Isobutyryl carnitine	POS	2.740017	UP	0.005111	0.028289
Kynurenic acid	QQQ-RP	0.78979	UP	0.434513	0.508702
Kynurenine	POS	5.870501	UP	7.03E-13	0
Kynurenine	NEG	4.887923	UP	3.97E-08	0
Kynurenine	QQQ-RP	5.813717	UP	1.60E-12	0
Lauric acid	QQQ-RP	-3.3951	DOWN	0.000398	0.00158
Leucine	QQQ-RP	1.932761	UP	0.052421	0.150437
Liver Unknown 100	POS	-0.08378	DOWN	0.934109	0.685171
Liver Unknown 100	NEG	1.244123	UP	0.216406	0.371367
Liver Unknown 1005	POS	1.178661	UP	0.241894	0.39088
Liver Unknown 1034	POS	-0.39487	DOWN	0.696602	0.622669
Liver Unknown 1093	POS	-0.33332	DOWN	0.742104	0.633062
Liver Unknown 1128	POS	-0.57431	DOWN	0.57035	0.565126
Liver Unknown 1130	POS	-1.52437	DOWN	0.128534	0.284305
Liver Unknown 1141	POS	-0.53954	DOWN	0.593975	0.580556
Liver Unknown 1143	POS	-0.83091	DOWN	0.410833	0.495875
Liver Unknown 1155	POS	1.542422	UP	0.123976	0.280109
Liver Unknown 1192	POS	-2.17063	DOWN	0.028644	0.110855
Liver Unknown 121	NEG	0.68577	UP	0.497705	0.531828
Liver Unknown 122	POS	0.295309	UP	0.770658	0.64144

Liver Unknown 122	NEG	6.146594	UP	7.79E-15	0
Liver Unknown 1237	POS	-0.50877	DOWN	0.615233	0.590923
Liver Unknown 1239	POS	1.860885	UP	0.062158	0.189139
Liver Unknown 126	POS	-0.50932	DOWN	0.614853	0.587946
Liver Unknown 1260	POS	-0.97299	DOWN	0.334971	0.459411
Liver Unknown 131 + 5.727112	POS	0.320823	UP	0.751454	0.635394
Liver Unknown 133	POS	0.604941	UP	0.549905	0.559157
Liver Unknown 136	POS	-2.15477	DOWN	0.029881	0.106746
Liver Unknown 137	POS	1.940604	UP	0.051439	0.16225
Liver Unknown 138	NEG	0.627942	UP	0.534788	0.558976
Liver Unknown 1416	POS	-0.10916	DOWN	0.914217	0.680756
Liver Unknown 143	POS	-2.70475	DOWN	0.005757	0.038413
Liver Unknown 143	NEG	-0.57008	DOWN	0.573197	0.575173
Liver Unknown 149	POS	-0.23875	DOWN	0.813704	0.654037
Liver Unknown 15	POS	0.346985	UP	0.731917	0.627697
Liver Unknown 1504	POS	-3.1782	DOWN	0.001	0.007706
Liver Unknown 1537	POS	0.283115	UP	0.779885	0.644931
Liver Unknown 1655	POS	-0.92379	DOWN	0.360183	0.470659
Liver Unknown 1658	POS	1.97923	UP	0.046815	0.148163
Liver Unknown 1674	NEG	-3.94682	DOWN	2.56E-05	0.00158
Liver Unknown 1676	POS	-0.80951	DOWN	0.423064	0.500372
Liver Unknown 1696	POS	1.379599	UP	0.169769	0.324718
Liver Unknown 176	POS	0.028718	UP	0.977392	0.694621
Liver Unknown 1762	POS	-2.85315	DOWN	0.003448	0.02669
Liver Unknown 1769	POS	1.679526	UP	0.093266	0.23326
Liver Unknown 1771	POS	-1.44152	DOWN	0.151086	0.314881
Liver Unknown 1788	POS	-0.7056	DOWN	0.485304	0.531706
Liver Unknown 1796 + 3.5135784	POS	-0.54873	DOWN	0.587687	0.576594
Liver Unknown 1803	POS	2.156824	UP	0.029718	0.113095
Liver Unknown 1812	POS	-1.21635	DOWN	0.22698	0.371286
Liver Unknown 1815	POS	0.891143	UP	0.377535	0.477113
Liver Unknown 1829	POS	3.340119	UP	0.000507	0.00158
Liver Unknown 1832	POS	2.755829	UP	0.004843	0.033197
Liver Unknown 1835	POS	-0.70699	DOWN	0.484441	0.534981
Liver Unknown 1838	POS	1.595477	UP	0.111291	0.263108
Liver Unknown 184	POS	0.656992	UP	0.515992	0.547997
Liver Unknown 1840	POS	-0.08211	DOWN	0.935424	0.684038
Liver Unknown 1841	POS	0.833573	UP	0.409329	0.49435
Liver Unknown 1844	POS	-0.72718	DOWN	0.471994	0.522543
Liver Unknown 1845	POS	-0.99789	DOWN	0.322642	0.443573
Liver Unknown 1852	POS	-1.16934	DOWN	0.245682	0.388091
Liver Unknown 1853	POS	1.347341	UP	0.180144	0.3341
Liver Unknown 1857	POS	-0.99368	DOWN	0.324708	0.452705

Liver Unknown 1866	POS	-0.20396	DOWN	0.840464	0.66245
Liver Unknown 1868	POS	1.419241	UP	0.157625	0.314156
Liver Unknown 1869	POS	1.03217	UP	0.30615	0.441089
Liver Unknown 187	POS	-0.61772	DOWN	0.541483	0.555238
Liver Unknown 1880	NEG	-0.39612	DOWN	0.695689	0.620238
Liver Unknown 1881	NEG	-0.42557	DOWN	0.674282	0.60991
Liver Unknown 1884	POS	-1.48915	DOWN	0.137789	0.295917
Liver Unknown 190	POS	-1.52334	DOWN	0.128796	0.285641
Liver Unknown 1907 - 2.3064	NEG	3.799703	UP	5.65E-05	0.00158
Liver Unknown 1926	NEG	0.633372	UP	0.531249	0.550076
Liver Unknown 1930	NEG	0.521888	UP	0.606132	0.581779
Liver Unknown 1931	NEG	2.325809	UP	0.018644	0.081758
Liver Unknown 1937	NEG	-0.48597	DOWN	0.631198	0.596031
Liver Unknown 195	POS	0.283626	UP	0.779497	0.645982
Liver Unknown 195	NEG	-0.92831	DOWN	0.357818	0.467732
Liver Unknown 1959	NEG	3.793098	UP	5.85E-05	0.00158
Liver Unknown 1996	NEG	-1.33728	DOWN	0.183473	0.338194
Liver Unknown 2007	NEG	1.193381	UP	0.235991	0.377513
Liver Unknown 2020	POS	-1.53543	DOWN	0.125726	0.282957
Liver Unknown 2027	NEG	-1.11414	DOWN	0.268957	0.409989
Liver Unknown 2027 + 0.9195554	POS	0.141839	UP	0.88868	0.673934
Liver Unknown 2097	POS	-0.65462	DOWN	0.517511	0.54655
Liver Unknown 2125	NEG	1.021399	UP	0.311273	0.433731
Liver Unknown 2134	NEG	-2.00369	DOWN	0.044067	0.140411
Liver Unknown 2167	NEG	-1.76368	DOWN	0.077587	0.204745
Liver Unknown 2168	NEG	3.871734	UP	3.86E-05	0
Liver Unknown 2178	NEG	-1.70617	DOWN	0.088054	0.225432
Liver Unknown 2234	NEG	1.135484	UP	0.259788	0.403131
Liver Unknown 2260	NEG	-1.12506	DOWN	0.26424	0.405039
Liver Unknown 2263	NEG	-0.43615	DOWN	0.666659	0.605403
Liver Unknown 2300	NEG	0.64832	UP	0.521568	0.546458
Liver Unknown 2335	NEG	1.348747	UP	0.179683	0.328573
Liver Unknown 2367	NEG	0.024602	UP	0.980632	0.695227
Liver Unknown 2368	NEG	0.044974	UP	0.964602	0.69138
Liver Unknown 2369	NEG	-2.4006	DOWN	0.015002	0.059229
Liver Unknown 2372	NEG	-1.53582	DOWN	0.125627	0.277323
Liver Unknown 238	POS	-2.32158	DOWN	0.01887	0.084044
Liver Unknown 2386	NEG	-0.00853	DOWN	0.993284	0.697541
Liver Unknown 2398	NEG	-1.35582	DOWN	0.177374	0.326174
Liver Unknown 2403	NEG	-0.10922	DOWN	0.914171	0.679615
Liver Unknown 2414	NEG	-0.38737	DOWN	0.702088	0.620473
Liver Unknown 2426	NEG	-0.93338	DOWN	0.355179	0.470834
Liver Unknown 2429	NEG	1.086675	UP	0.281066	0.412345

Liver Unknown 2432 - 3.3879032	NEG	-0.65051	DOWN	0.520155	0.545019
Liver Unknown 2435	NEG	0.338129	UP	0.738512	0.632937
Liver Unknown 2456	NEG	-0.10406	DOWN	0.918213	0.679639
Liver Unknown 247	POS	-0.22194	DOWN	0.826606	0.658891
Liver Unknown 2481	NEG	0.498823	UP	0.622179	0.591157
Liver Unknown 2499 - 6.208662	NEG	-0.08853	DOWN	0.930385	0.684154
Liver Unknown 25	NEG	-1.02246	DOWN	0.310767	0.441427
Liver Unknown 2500	POS	-1.69932	DOWN	0.089373	0.228762
Liver Unknown 2500	NEG	-0.11869	DOWN	0.906757	0.677526
Liver Unknown 2503	NEG	-2.03578	DOWN	0.040664	0.143266
Liver Unknown 2504	NEG	0.110305	UP	0.91332	0.6794
Liver Unknown 2541	POS	0.41315	UP	0.68328	0.615934
Liver Unknown 2542	NEG	-0.09181	DOWN	0.927812	0.680874
Liver Unknown 2550	NEG	-0.63562	DOWN	0.529785	0.549605
Liver Unknown 2551	NEG	1.226822	UP	0.222952	0.370803
Liver Unknown 2552	NEG	-0.60269	DOWN	0.551392	0.561582
Liver Unknown 2563	POS	-0.76597	DOWN	0.448572	0.52362
Liver Unknown 2567	NEG	1.638119	UP	0.101838	0.248217
Liver Unknown 2568	NEG	-3.25073	DOWN	0.000741	0.009476
Liver Unknown 2569	NEG	-1.69448	DOWN	0.090311	0.231103
Liver Unknown 2573	NEG	-1.9608	DOWN	0.048976	0.161635
Liver Unknown 2578	POS	2.050134	UP	0.039213	0.145205
Liver Unknown 2578	NEG	-2.08171	DOWN	0.036173	0.131681
Liver Unknown 2579	NEG	-0.0034	DOWN	0.997326	0.698663
Liver Unknown 2583	NEG	-1.30402	DOWN	0.194787	0.346846
Liver Unknown 2599	NEG	-0.9775	DOWN	0.332715	0.454924
Liver Unknown 2601	POS	0.32134	UP	0.751066	0.637574
Liver Unknown 2607	NEG	1.045563	UP	0.299856	0.434709
Liver Unknown 2611	NEG	-0.12452	DOWN	0.902198	0.676192
Liver Unknown 2616	NEG	-2.05616	DOWN	0.038618	0.071391
Liver Unknown 2630	NEG	-1.85392	DOWN	0.063174	0.176099
Liver Unknown 2637	NEG	0.941336	UP	0.351061	0.461495
Liver Unknown 2649	NEG	0.995113	UP	0.324004	0.447669
Liver Unknown 2652	NEG	-0.59502	DOWN	0.556491	0.562117
Liver Unknown 2653	NEG	-1.39566	DOWN	0.164769	0.323052
Liver Unknown 2680	NEG	-1.55672	DOWN	0.120453	0.276148
Liver Unknown 2688	POS	3.787082	UP	6.04E-05	0
Liver Unknown 2688	NEG	4.994918	UP	1.57E-08	0
Liver Unknown 2693	NEG	-1.02179	DOWN	0.311084	0.436028
Liver Unknown 2699	NEG	-0.27341	DOWN	0.787254	0.646883
Liver Unknown 2706	POS	-0.10466	DOWN	0.917739	0.680377
Liver Unknown 2707	POS	-1.36699	DOWN	0.173772	0.328573
Liver Unknown 2707	NEG	-2.3479	DOWN	0.017497	0.084366

Liver Unknown 2708	NEG	1.509206	UP	0.132458	0.291829
Liver Unknown 2711	NEG	0.109398	UP	0.91403	0.681087
Liver Unknown 2713	POS	0.456924	UP	0.651777	0.599378
Liver Unknown 2714	NEG	3.249421	UP	0.000746	0.010305
Liver Unknown 2724	NEG	-0.67578	DOWN	0.504014	0.537388
Liver Unknown 2735	NEG	2.035287	UP	0.040714	0.132156
Liver Unknown 2739	NEG	-0.17726	DOWN	0.861127	0.666169
Liver Unknown 2750	NEG	-1.25032	DOWN	0.214094	0.365234
Liver Unknown 2751	NEG	1.756905	UP	0.078766	0.216758
Liver Unknown 2754	NEG	0.413936	UP	0.682709	0.613519
Liver Unknown 2755	NEG	2.766807	UP	0.004664	0.034108
Liver Unknown 2771	NEG	0.527213	UP	0.602452	0.581576
Liver Unknown 2779	POS	0.704798	UP	0.485802	0.531379
Liver Unknown 2779	NEG	-3.67525	DOWN	0.000107	0.002828
Liver Unknown 2794	NEG	-2.91421	DOWN	0.002766	0.022402
Liver Unknown 2806	NEG	-3.12495	DOWN	0.001239	0.013969
Liver Unknown 2807	NEG	1.429826	UP	0.154493	0.308138
Liver Unknown 29	POS	0.83426	UP	0.408941	0.502724
Liver Unknown 290	POS	1.0351	UP	0.304766	0.438301
Liver Unknown 290	NEG	1.171321	UP	0.244875	0.389982
Liver Unknown 294	POS	0.081859	UP	0.935618	0.684154
Liver Unknown 3	POS	0.494107	UP	0.625481	0.593128
Liver Unknown 304	POS	1.484877	UP	0.138944	0.299179
Liver Unknown 311	POS	-0.68881	DOWN	0.495796	0.537002
Liver Unknown 34	POS	-0.17186	DOWN	0.865314	0.66907
Liver Unknown 348	POS	1.579104	UP	0.115094	0.263748
Liver Unknown 349	POS	-1.11631	DOWN	0.268012	0.408652
Liver Unknown 367	POS	-0.49223	DOWN	0.626798	0.592203
Liver Unknown 399	POS	-1.56042	DOWN	0.119556	0.270621
Liver Unknown 40	POS	-0.85193	DOWN	0.399026	0.489171
Liver Unknown 400	POS	1.318802	UP	0.189699	0.348621
Liver Unknown 401	POS	-1.23714	DOWN	0.219031	0.368041
Liver Unknown 416	POS	-0.29563	DOWN	0.770416	0.642036
Liver Unknown 420	POS	0.51724	UP	0.609351	0.586839
Liver Unknown 420	NEG	-3.5575	DOWN	0.000189	0
Liver Unknown 421	POS	0.49734	UP	0.623217	0.59282
Liver Unknown 44	POS	0.87303	UP	0.387374	0.483078
Liver Unknown 46	POS	1.595546	UP	0.111275	0.258161
Liver Unknown 48	POS	1.544372	UP	0.123491	0.276266
Liver Unknown 485	POS	-2.48827	DOWN	0.011524	0.060263
Liver Unknown 486	POS	-2.14172	DOWN	0.030933	0.115527
Liver Unknown 487	POS	-1.95785	DOWN	0.04933	0.168462
Liver Unknown 49	POS	-0.48143	DOWN	0.634398	0.594202

Liver Unknown 493	POS	-0.60483	DOWN	0.549978	0.559382
Liver Unknown 494	POS	-1.90377	DOWN	0.056188	0.16549
Liver Unknown 5	POS	2.246877	UP	0.023278	0.102192
Liver Unknown 5	NEG	-0.62353	DOWN	0.537674	0.55464
Liver Unknown 520	POS	0.488569	UP	0.62937	0.592704
Liver Unknown 531	POS	-0.52007	DOWN	0.607392	0.586004
Liver Unknown 55	POS	0.863385	UP	0.392675	0.492709
Liver Unknown 559	POS	-1.25273	DOWN	0.213201	0.367467
Liver Unknown 560	POS	-0.90169	DOWN	0.371875	0.474968
Liver Unknown 564	POS	-1.85945	DOWN	0.062367	0.184568
Liver Unknown 566	POS	-2.87658	DOWN	0.00317	0.022402
Liver Unknown 572	POS	0.089635	UP	0.929517	0.684131
Liver Unknown 573	POS	-0.68699	DOWN	0.496939	0.5347
Liver Unknown 574	POS	-1.93052	DOWN	0.052704	0.16225
Liver Unknown 576	POS	-0.24662	DOWN	0.807674	0.651685
Liver Unknown 6	POS	1.646833	UP	0.099985	0.253195
Liver Unknown 607	POS	-1.25194	DOWN	0.213495	0.36255
Liver Unknown 63	POS	-0.58635	DOWN	0.562271	0.568787
Liver Unknown 643	POS	-1.92751	DOWN	0.053088	0.168069
Liver Unknown 651	POS	1.592153	UP	0.112055	0.261044
Liver Unknown 657	POS	1.193129	UP	0.236091	0.387098
Liver Unknown 686	POS	-0.91394	DOWN	0.365365	0.480506
Liver Unknown 690	POS	-0.33752	DOWN	0.738967	0.63278
Liver Unknown 691	POS	0.549683	UP	0.587037	0.580352
Liver Unknown 697	POS	1.105388	UP	0.272776	0.411612
Liver Unknown 7	POS	0.291551	UP	0.773498	0.64346
Liver Unknown 718	POS	0.887238	UP	0.379643	0.481001
Liver Unknown 734	POS	-0.95064	DOWN	0.346284	0.459842
Liver Unknown 735	POS	-0.14201	DOWN	0.888543	0.673042
Liver Unknown 740	POS	2.733087	UP	0.005233	0.033197
Liver Unknown 77	POS	1.305841	UP	0.194156	0.347609
Liver Unknown 795	POS	-0.95536	DOWN	0.343876	0.457927
Liver Unknown 80	POS	-2.19176	DOWN	0.027062	0.109078
Liver Unknown 837	POS	-1.30357	DOWN	0.194946	0.34659
Liver Unknown 839	POS	2.433729	UP	0.013594	0.067927
Liver Unknown 846	POS	-0.82458	DOWN	0.414429	0.495419
Liver Unknown 862	POS	1.36155	UP	0.175519	0.324522
Liver Unknown 877	NEG	2.005369	UP	0.043883	0.150232
Liver Unknown 883	POS	0.272676	UP	0.787808	0.646622
Liver Unknown 904	POS	0.859336	UP	0.394913	0.48615
Liver Unknown 910	POS	0.142093	UP	0.888481	0.675239
Liver Unknown 910	NEG	-1.73547	DOWN	0.082591	0.227184
Liver Unknown 911	POS	-2.53773	DOWN	0.009888	0.049918

Liver Unknown 912	POS	0.738977	UP	0.464802	0.523061
Liver Unknown 913	POS	0.470868	UP	0.641864	0.59893
Liver Unknown 914	POS	-0.83917	DOWN	0.406169	0.49486
Liver Unknown 916	POS	-2.01562	DOWN	0.042776	0.147535
Liver Unknown 919	POS	-1.55307	DOWN	0.121344	0.270009
Liver Unknown 97	POS	-0.72514	DOWN	0.473245	0.527063
Liver Unknown 97	NEG	1.309046	UP	0.193047	0.352911
Liver Unknown 975	POS	-1.29816	DOWN	0.196833	0.348957
Liver Unknown 990	POS	-0.82044	DOWN	0.416792	0.498786
Liver-10-hydroxy-2E-decenoic acid	POS	-0.42075	DOWN	0.677771	0.61153
Liver-11-Dehydrodexamethasone	POS	-1.08247	DOWN	0.282949	0.42004
Liver-2,4,6,8,10-dodecapentaenal	POS	3.058764	UP	0.001606	0.013969
Liver-2,6-Diisopropylhydroquinone	POS	-1.26353	DOWN	0.209225	0.358186
Liver-2E,4E,8Z,10E-dodecatetraenoic acid	POS	-0.65911	DOWN	0.514633	0.547712
Liver-2-hydroxy pelargonic acid	NEG	-0.42176	DOWN	0.677042	0.612719
Liver-2-Hydroxyfelbamate	POS	-0.72416	DOWN	0.473845	0.531092
Liver-2-Propylglutaric acid	NEG	0.397952	UP	0.694348	0.616686
Liver-3Capryloylglycine	NEG	-0.83965	DOWN	0.405899	0.498836
Liver-3Capryloylglycine + 5.732313	POS	-1.52323	DOWN	0.128826	0.281368
Liver-3-hydroxy-phenylglycol	POS	-0.29336	DOWN	0.772128	0.64266
Liver-6-Ketoestriol	NEG	-3.09695	DOWN	0.001384	0.010305
Liver-8-Amino-7-oxononanoate	POS	1.147828	UP	0.254584	0.39587
Liver-8-Amino-7-oxononanoate	NEG	0.890886	UP	0.377673	0.47773
Liver-Albuterol	POS	0.650879	UP	0.519919	0.545531
Liver-alpha-Phenylcyclohexylglycolic acid	POS	0.960951	UP	0.341035	0.457492
Liver-Artemether	POS	-0.83898	DOWN	0.406279	0.491572
Liver-Canrenoate	POS	-1.32613	DOWN	0.187211	0.337564
Liver-cyclandelate	POS	0.383229	UP	0.70513	0.624938
Liver-Cys Pro Ile	POS	-1.0937	DOWN	0.277935	0.412711
Liver-Cys Pro Ile	NEG	-1.454	DOWN	0.147513	0.300797
Liver-Descarboethoxyloratadine	POS	-2.52111	DOWN	0.010414	0.051072
Liver-Didesmethylloperamide	POS	-0.87499	DOWN	0.386301	0.490636
Liver-Didrovaltratum	POS	-1.15508	DOWN	0.251561	0.39218
Liver-Dienestrol	POS	-0.82769	DOWN	0.412665	0.500175
Liver-Gibberellin A3	POS	-0.75433	DOWN	0.455532	0.52124
Liver-Gibberellin A3	NEG	-0.45704	DOWN	0.651695	0.604932
Liver-Glu Ile	NEG	-1.99529	DOWN	0.044995	0.157887
Liver-Isoleucine	POS	2.147425	UP	0.030469	0.113831
Liver-Isoleucine	NEG	3.685254	UP	0.000102	0
Liver-Isopentenyladenine	POS	2.565278	UP	0.009068	0.049527
Liver-Isopentenyladenine - 4.017848	NEG	3.970051	UP	2.25E-05	0

Liver-Leu Trp Arg	POS	-2.71697	DOWN	0.005526	0.037463
Liver-Lys Lys Met	POS	-1.45755	DOWN	0.14651	0.301439
Liver-m-Coumaric acid	POS	0.83079	UP	0.410904	0.502188
Liver-N2,N2-Dimethylguanosine	POS	0.916445	UP	0.364043	0.473428
Liver-Oleandolide	POS	-0.51066	DOWN	0.613917	0.588459
Liver-Pantothenic Acid	NEG	1.826601	UP	0.06729	0.192534
Liver-Pentamidine	POS	2.057432	UP	0.038493	0.13589
Liver-Phe Ile	POS	3.746323	UP	7.45E-05	0
Liver-Phe Ile	NEG	0.78633	UP	0.43654	0.513292
Liver-Pro Gln Leu	POS	-1.27575	DOWN	0.204792	0.35905
Liver-Probenecid	POS	-3.0603	DOWN	0.001597	0.014618
Liver-Purine	POS	-3.4815	DOWN	0.000269	0.006772
Liver-Ramiprilat	NEG	0.987808	UP	0.327599	0.442972
Liver-Ser Trp Pro	POS	-2.00517	DOWN	0.043905	0.149409
Liver-sodium chlorovulone II	POS	-1.36571	DOWN	0.174182	0.325204
Liver-sodium chlorovulone II	NEG	-0.32559	DOWN	0.74788	0.634309
Liver-Sodium tetradecyl sulfate	POS	-1.3135	DOWN	0.191513	0.3482
Liver-thymol	POS	-2.06695	DOWN	0.037569	0.130966
Liver-Trp Lys Pro	POS	-0.2202	DOWN	0.827949	0.65767
Liver-Trp Trp Gln	POS	0.92475	UP	0.35968	0.466548
Lysine	POS	1.956209	UP	0.049528	0.15512
Methionine	QQQ-RP	1.542736	UP	0.123898	0.260263
Methyl alanine	QQQ-RP	0.084029	UP	0.933915	0.685562
N12-Acetylthermospermidine	QQQ-DH	4.032929	UP	1.57E-05	0.00158
N1-Acetylspermine	QQQ-DH	3.311078	UP	0.000574	0.003989
N-Acetyl Valine	QQQ-RP	0.224373	UP	0.824738	0.65962
Niacinamide	POS	1.875027	UP	0.060136	0.182809
Nonanedioic acid	NEG	-0.34596	DOWN	0.732681	0.63051
Norepinephrine (noradrenaline)	QQQ-RP	-1.92273	DOWN	0.0537	0.162659
Oleic acid	QQQ-DH	-1.86171	DOWN	0.062039	0.184742
Palmitic acid	QQQ-RP	-4.52478	DOWN	6.67E-07	0
Pantothenic acid	POS	2.396565	UP	0.015181	0.072497
Phenylalanine	POS	3.797334	UP	5.73E-05	0.00158
Phenylalanine	NEG	5.297555	UP	8.47E-10	0
Phenylalanine	QQQ-RP	3.091633	UP	0.001413	0.015996
Phthalic acid Mono-2-ethylhexyl Ester	POS	-2.63852	DOWN	0.007167	0.049918

pipecolic acid	QQQ-RP	-1.73555	DOWN	0.082576	0.217421
Proline	QQQ-RP	0.185253	UP	0.854931	0.680851
Pyroglutamic acid	NEG	0.736763	UP	0.466148	0.527902
S-Adenosylmethionine	QQQ-DH	4.018038	UP	1.71E-05	0
Sarcosine	QQQ-DH	0.788127	UP	0.435486	0.512466
Serine	QQQ-RP	1.943221	UP	0.051114	0.150232
Spermidine	QQQ-RP	3.160728	UP	0.001073	0.012591
Spermine	QQQ-RP	-0.62076	DOWN	0.539487	0.555284
Suberic acid	QQQ-RP	-1.44099	DOWN	0.151239	0.313219
Succinic acid	NEG	-0.19622	DOWN	0.846445	0.663243
Succinicanhydride	NEG	-1.62642	DOWN	0.104367	0.256567
Taurine	QQQ-RP	-3.68964	DOWN	9.93E-05	0
Theophylline	NEG	-0.7101	DOWN	0.482509	0.528278
Threonine	QQQ-RP	1.603086	UP	0.109556	0.259871
Thymine	QQQ-RP	2.115848	UP	0.033108	0.129041
Trans-4 Hydroxytamoxifen	POS	-0.34735	DOWN	0.731643	0.63089
Trans-4 Hydroxytamoxifen	NEG	-1.14667	DOWN	0.25507	0.397217
Tryptophan	POS	2.438634	UP	0.013396	0.064226
Tryptophan	NEG	4.047586	UP	1.44E-05	0
Tryptophan	QQQ-RP	1.179704	UP	0.241473	0.407155
Tyrosine	POS	2.797767	UP	0.00419	0.032734
Tyrosine	NEG	2.559282	UP	0.009241	0.056741
Tyrosine	QQQ-RP	-1.17228	DOWN	0.244484	0.405646
Uracil	QQQ-RP	4.834633	UP	6.19E-08	0
Urocanic acid	QQQ-DH	-3.57535	DOWN	0.000174	0.002828
Valine	POS	3.260993	UP	0.00071	0.006772
Valine	QQQ-RP	0.599006	UP	0.553838	0.563228
Vidarabine	POS	0.139244	UP	0.890703	0.676557
Xanthine	QQQ-RP	-1.31289	DOWN	0.191723	0.354244

Supplementary Table S10. Gene-specific primers used for qRT-PCR

	Primer sequence (5'-3')	
Gene	Sense	Anti-sense
GAPDH	GAGTCAACGGATTTGGTCGT	TTGATTTTGGAGGGATCTCG
CYP2E1	GACAGAGACCACCAGCACAA	GGTGATGAACCGCTGAATCT
AHR	CTTCCAAGCGGCATAGAGAC	AGTTATCCTGGCCTCCGTTT
COMT	TCCTGGAATACAGGGAGGTG	CGAGGTGTGCTTTGCATTTA
CYP1A1	GACAGATCCCATCTGCCCTA	GGTTGATCTGCCACTGGTTT
EPHX1	CTGTACCCCGTCAAGGAGAA	CCAGGGAGAACTTCCTTTCC
ABCB1	GCTCCTGACTATGCCAAAGC	TCTTCACCTCCAGGCTCAGT
PTGS2	TGAGCATCTACGGTTTGCTG	TGCTTGTCTGGAACAACTGC
CYP1B1	GACCCCCAGTCTCAATCTCA	CTCCCACTCGAGTCTCTTGG
GSTK1	CCAGAGATGCTGGAGAAAGC	GCCTCAGTGGTCTCCTTGAG
CYP2D6	AGATCGACGACCGTGATAGG	CAGGTTGGTGATGAGTGTCG
NAT1	ATTCAAGCCAGGAAGAAGCA	CCCCACAATGGATGTTAAGG
NAT2	GGGATCATGGACATTGAAGC	CACCCCGGTTTCTTCTTACA
GSTT1	GGCCTTCCTTACTGGTCCTC	TTGGCCTTCAGAATGACCTC

Supplementary Table S11. List of all molecular concepts enriched by BCa-specific metabolome

Database	Molecular Concept	P-Value	Q-Value
InterPro	Nuclear protein SET	4.10E-19	1.9155E-15
KEGG Pathway	Tryptophan metabolism	7.10E-19	1.20355E-16
GO Molecular Function	methyltransferase activity	3.00E-18	6.25802E-15
GO Molecular Function	unspecific monooxygenase activity	1.20E-16	1.29887E-13
InterPro	E-class P450, group I	4.00E-14	9.43082E-11
InterPro	Cytochrome P450	3.20E-13	4.98E-10
InterPro	SET-related region	1.20E-12	1.39964E-09
GO Molecular Function	oxygen binding	3.40E-12	2.36E-09
KEGG Pathway	gamma-Hexachlorocyclohexane degradation	4.30E-12	3.63165E-10
KEGG Pathway	Fatty acid metabolism	7.20E-11	4.05E-09
GO Biological Process	chromatin modification	1.20E-10	2.24195E-07
KEGG Pathway	Methionine metabolism	5.60E-10	2.36884E-08
GO Molecular Function	histone-lysine N-methyltransferase activity	1.40E-09	7.3094E-07
InterPro	Glycosyl transferase, family 29	1.70E-09	1.65379E-06
GO Molecular Function	monooxygenase activity	7.70E-09	3.22692E-06
GO Cellular Component	microsome	8.70E-09	3.82139E-06
Literature-defined Concepts	Up-regulated genes in normal liver compared to other normal tissues	8.00E-08	5.28402E-05
Literature-defined Concepts	Experimental Drug Targets	2.00E-07	6.54136E-05
InterPro	Pre-SET	2.10E-07	1.66E-04
Oncomine Clusters	Co-expressed across 62 Normal samples (Hsiao_Normal)	7.00E-07	0.007992168
InterPro	Nuclear protein Zn2+-binding	2.20E-06	1.52E-03
Literature-defined Concepts	Up-regulated genes in liver compared to brain, kidney, lung, muscle, prostate, and vulva	2.50E-06	5.59E-04
HPRD Interaction Sets	DNMT3A	3.00E-06	0.01644257
Oncomine Gene Expression Signatures	Normal Type - Top 5% over-expressed in Liver (Hsiao)	8.30E-06	0.046484876
HPRD Interaction Sets	HDAC1	1.00E-05	0.027718545

Biocarta Pathway	SARS Coronavirus Protease	1.30E-05	0.003464399
Oncomine Gene Expression Signatures	Normal Type - Top 10% over-expressed in Liver (Hsiao)	1.40E-05	0.039665105
KEGG Pathway	Aminoacyl-tRNA biosynthesis	1.50E-05	0.000516995
InterPro	SAM (and some other nucleotide) binding motif	1.60E-05	0.009160212
GO Molecular Function	L-lactate dehydrogenase activity	2.10E-05	7.18E-03
GO Biological Process	DNA methylation	2.10E-05	0.019036188
GO Molecular Function	5-nucleotidase activity	2.10E-05	7.18E-03
GO Biological Process	tricarboxylic acid cycle intermediate metabolism	2.10E-05	0.019036188
InterPro	PWWP	2.30E-05	1.22E-02
InterPro	Pyridoxal-dependent decarboxylase	2.30E-05	1.22E-02
InterPro	AWS	2.30E-05	1.22E-02
InterPro	L-lactate/malate dehydrogenase	2.30E-05	1.22E-02
KEGG Pathway	Alkaloid biosynthesis I	2.90E-05	8.28E-04
Oncomine Gene Expression Signatures	Normal Type - Top 10% under-expressed in Vulvar (Hsiao)	3.60E-05	0.067553012
Oncomine Clusters	Co-expressed across 36 Multi-cancer samples (Ge_Multi-cancer)	3.70E-05	0.139717635
HPRD Interaction Sets	DNMT1	4.70E-05	0.085493793
HPRD Interaction Sets	DNMT3B	4.70E-05	0.085493793
HPRD Interaction Sets	CBX1	4.70E-05	0.085493793
KEGG Pathway	Tyrosine metabolism	5.60E-05	1.36E-03
GO Biological Process	electron transport	6.50E-05	0.030099927
GO Molecular Function	long-chain-fatty-acid-CoA ligase activity	6.70E-05	0.01757878
Oncomine Clusters	Co-expressed across 101 Normal samples (Su_Normal)	6.80E-05	0.156390159
InterPro	Lactate/malate dehydrogenase	7.60E-05	0.027623397
Literature-defined Concepts	Trimethylated H3K27 occupancy in embryonic fibroblasts	8.50E-05	0.014027468
Oncomine Gene Expression Signatures	Normal Type - Top 10% under-expressed in Prostate (Hsiao)	9.60E-05	0.135052655
Oncomine Gene Expression Signatures	Cancer Type - Top 5% under-expressed in Prostate Adenocarcinoma (Su)	1.20E-04	0.134268958
GO Cellular Component	endoplasmic reticulum	1.20E-04	0.026741963
KEGG Pathway	Phenylalanine, tyrosine and tryptophan biosynthesis	1.40E-04	0.003036203

GO Molecular Function	S-adenosylmethionine-dependent methyltransferase activity	1.70E-04	3.89E-02
GO Biological Process	protein biosynthesis	1.80E-04	0.066755622
Oncomine Clusters	Co-expressed across 54 Sarcoma samples (Detwiller_Sarcoma)	2.10E-04	0.238874229
GO Molecular Function	DNA (cytosine-5-)-methyltransferase activity	2.10E-04	0.044390242
GO Molecular Function	creatine kinase activity	2.10E-04	0.044390242
GO Molecular Function	hydrolase activity, acting on ester bonds	2.10E-04	0.044390242
GO Biological Process	nucleotide catabolism	2.10E-04	6.54E-02
GO Molecular Function	oxidoreductase activity, acting on paired donors, with incorporation or reduction of molecular oxygen,	2.10E-04	0.044390242
GO Molecular Function	palmitoyl-CoA hydrolase activity	2.10E-04	0.044390242
GO Biological Process	catecholamine biosynthesis	2.10E-04	6.54E-02
Oncomine Clusters	Co-expressed across 30 Prostate samples (Luo_Prostate_2)	2.30E-04	0.219913392
Oncomine Clusters	Co-expressed across 25 Pancreas samples (Grutzmann_Pancreas)	2.30E-04	0.203341554
Oncomine Clusters	Co-expressed across 107 Seminoma samples (Korkola_Seminoma)	2.30E-04	0.203341554
InterPro	C-5 cytosine-specific DNA methylase	2.30E-04	0.079127168
InterPro	Aminoacyl-tRNA synthetase, class Ib	2.30E-04	0.079127168
InterPro	Generic methyltransferase	2.30E-04	0.079127168
InterPro	ATP:guanido phosphotransferase	2.30E-04	0.079127168
InterPro	E-class P450, CYP3A	2.30E-04	0.079127168
InterPro	Poly(ADP-ribose) polymerase, catalytic region	2.30E-04	0.079127168
InterPro	Poly(ADP-ribose) polymerase, regulatory region	2.30E-04	0.079127168
InterPro	Aromatic amino acid hydroxylase	2.30E-04	0.079127168
InterPro	Zn-finger-like, PHD finger	2.30E-04	0.079127168
Connectivity Map	CellLine Batch - description - Top 5% over-expressed in 25, MCF7 treated with acetylsalicylic acid (.0001 M) for 6 h (Lamb)	2.40E-04	0.720812442
InterPro	Aminoacyl-tRNA synthetase, class I	2.60E-04	5.41E-02
KEGG Pathway	Cysteine metabolism	2.70E-04	5.00E-03
Oncomine Clusters	Co-expressed across 54 Sarcoma samples (Detwiller_Sarcoma)	3.20E-04	2.03E-01
Oncomine Gene Expression Signatures	Normal Type - Top 1% over-expressed in Liver (Su)	3.50E-04	3.24E-01

GO Biological Process	protein amino acid glycosylation	3.50E-04	0.080328583
GO Biological Process	amino acid metabolism	3.50E-04	0.080328583
Connectivity Map	MCF Cells Treatment - Top 1% over-expressed in 504, MCF7 treated with 5253409 (.000017 M) for 6 h (Lamb)	3.50E-04	0.535540964
Oncomine Clusters	Co-expressed across 123 Normal samples (Shyamsundar_Normal)	3.80E-04	2.05E-01
KEGG Pathway	Taurine and hypotaurine metabolism	4.90E-04	0.008346354
KEGG Pathway	Urea cycle and metabolism of amino groups	5.10E-04	7.78E-03
Oncomine Clusters	Co-expressed across 27 Lymphoma samples (Storz_Lymphoma)	5.80E-04	2.90E-01
HPRD Interaction Sets	SUV39H1	6.90E-04	0.62888088
HPRD Interaction Sets	DNMT3L	6.90E-04	0.62888088
Chromosome Subregion	10q24	7.00E-04	0.221969167
Transfac TF Matrix - 1000bp	LEF-1	7.20E-04	0.260056043
Oncomine Gene Expression Signatures	Breast Ductal Carcinoma Docetaxol Response - Top 10% over-expressed in Resistant (Chang)	7.40E-04	0.518110232
KEGG Pathway	Selenoamino acid metabolism	7.80E-04	0.010978006
KEGG Pathway	Arginine and proline metabolism	8.10E-04	0.01047744
Connectivity Map	CellLine Batch - description - Top 1% over-expressed in 24, MCF7 treated with NU-1025 (.0001 M) for 6 h (Lamb)	8.10E-04	0.815410116
Oncomine Clusters	Co-expressed across 8 Breast samples (Poola_Breast)	8.10E-04	0.385349858
Oncomine Gene Expression Signatures	Acute Lymphoblastic Leukemia Genetic Features - Top 5% over-expressed in BCR-ABL positive (Kirschner-Schwabe)	8.10E-04	5.08E-01
Oncomine Gene Expression Signatures	Acute Myeloid Leukemia Karyotype - Top 5% under-expressed in 8 (Valk)	8.20E-04	0.459238728
Oncomine Clusters	Co-expressed across 60 Liver samples (Okada_Liver)	8.20E-04	0.378080678
Oncomine Gene Expression Signatures	Normal Type - Top 5% over-expressed in Liver (Su)	8.40E-04	0.428627835
Oncomine Clusters	Co-expressed across 9 Ovarian samples (Benetkiewicz_Ovarian_2)	9.10E-04	4.00E-01
KEGG Pathway	Valine, leucine and isoleucine biosynthesis	9.20E-04	1.11E-02
GO Molecular Function	ligase activity	0.001	1.42E-01
Oncomine Clusters	Co-expressed across 20 CellLine samples (Irizarry_CellLine)	0.001	4.18E-01

Oncomine Clusters	Co-expressed across 60 Liver samples (Iizuka_Liver_2)	0.001	0.404281622
Oncomine Clusters	Co-expressed across 7 CellLine samples (Carson_CellLine)	0.001	4.04E-01
Oncomine Gene Expression Signatures	CellLine methotrexate - Top 10% under-expressed in indeterminate, resistant (Staunton)	0.001	0.485507652
Oncomine Gene Expression Signatures	Cancer Type - Top 10% under-expressed in Prostate Adenocarcinoma (Su)	0.001	4.92E-01
InterPro	AMP-dependent synthetase and ligase	0.001	0.247879434
GO Biological Process	aromatic amino acid family metabolism	0.001	0.240340733
Oncomine Gene Expression Signatures	head and neck squamous cell carcinoma Differentiation - Top 10% over-expressed in Poor (Chung)	0.001	0.491120675
Oncomine Gene Expression Signatures	Acute Lymphoblastic Leukemia Genetic Features - Top 10% over-expressed in BCR-ABL positive (Kirschner-Schwabe)	0.001	4.41E-01
Oncomine Gene Expression Signatures	Gastric Carcinoma Site - Top 10% over-expressed in Body (Leung)	0.001	4.50E-01
KEGG Pathway	Lysine degradation	0.002	0.017250199
Oncomine Gene Expression Signatures	Cancer Type - Top 20% under-expressed in Pancreatic Carcinoma (Uhlen)	0.002	4.56E-01
Oncomine Gene Expression Signatures	Cancer Type - v1 - Top 5% under-expressed in Breast Ductal Carcinoma (Bittner)	0.002	0.445717947
HPRD Interaction Sets	POR	0.002	1.131061392
Oncomine Gene Expression Signatures	Lung Cancer Type - Top 10% over-expressed in Lung Squamous Cell Carcinoma (Wigle)	0.002	4.36E-01
GO Biological Process	nucleoside metabolism	0.002	3.02E-01
Oncomine Clusters	Co-expressed across 79 Prostate samples (Glinsky_Prostate)	0.002	5.92E-01
Connectivity Map	CellLine Batch - description - Top 5% under-expressed in 109, SKMEL5 treated with benserazide (.00001 M) for 6 h (Lamb)	0.002	1.370133949
Oncomine Clusters	Co-expressed across 23 Ovarian samples (Gilks_Ovarian)	0.002	5.66E-01
Literature-defined Concepts	Downregulated genes in nasal polyps after glucocorticoid treatment	0.002	0.243768737
Oncomine Gene Expression Signatures	Normal Type - Top 1% over-expressed in Liver (Hsiao)	0.002	0.450894356
GO Molecular Function	DNA binding	0.002	0.25462993
Oncomine Gene Expression Signatures	Multi-Tissue Type - Top 1% under-expressed in lung cancer	0.002	4.69E-01

	(Uhlen)		
GO Biological Process	aspartyl-tRNA aminoacylation	0.002	0.322310681
GO Molecular Function	aspartate-tRNA ligase activity	0.002	2.57E-01
GO Biological Process	neurotransmitter biosynthesis	0.002	0.322310681
GO Biological Process	protein ubiquitination	0.002	0.322310681
GO Molecular Function	uridine kinase activity	0.002	2.57E-01
GO Molecular Function	beta-galactoside alpha-2,3-sialyltransferase activity	0.002	2.57E-01
Conserved Promoter Motif	CLUSTER_68__V$HSF1_01	0.002	0.365226308
Oncomine Gene Expression Signatures	Head and Neck Squamous Cell Carcinoma Differentiation - Top 1% over-expressed in 3 (Cromer)	0.002	0.471233841
KEGG Pathway	Phenylalanine metabolism	0.002	0.023034851
Oncomine Clusters	Co-expressed across 85 Brain samples (Freije_Brain)	0.002	5.80E-01
Oncomine Clusters	Co-expressed across 24 CellLine samples (Robinson_CellLine)	0.002	5.80E-01
InterPro	FYVE/PHD zinc finger	0.002	0.426120985
InterPro	Aminotransferases class-I pyridoxal-phosphate-binding site	0.002	0.426120985
InterPro	OB-fold nucleic acid binding	0.002	0.426120985
InterPro	ValRS/IleRS editing	0.002	0.426120985
InterPro	WGR	0.002	0.426120985
InterPro	E-class P450, CYP2A	0.002	0.426120985
InterPro	Phosphoribulokinase/uridine kinase	0.002	0.426120985
InterPro	Acyl-CoA thioester hydrolase/bile acid-CoA amino acid N-acetyltransferase	0.002	0.426120985
InterPro	tRNA synthetase, class II (D, K and N)	0.002	0.426120985
InterPro	Uridine kinase	0.002	0.426120985
InterPro	Aspartyl-tRNA synthetase, class IIb	0.002	0.426120985
InterPro	Zn-finger, RING	0.002	0.426120985
InterPro	Amino acid-binding ACT	0.002	0.426120985
InterPro	Methyltransferase, NNMT/PNMT/TEMT	0.002	0.426120985
Oncomine Gene Expression Signatures	Bladder Type - Top 5% over-expressed in TCC (Blaveri)	0.002	4.92E-01
Oncomine Clusters	Co-expressed across 60 Bladder samples (Dyrskjot_Bladder_3)	0.002	5.86E-01

Connectivity Map	CellLine Batch - description - Top 1% over-expressed in 73, SKMEL5 treated with staurosporine (.00000001 M) for 6 h (Lamb)	0.002	1.468796451
Transfac TF Matrix - 1000bp	TGIF	0.002	0.439896229
GO Biological Process	protein amino acid ADP-ribosylation	0.002	3.00E-01
GO Molecular Function	NAD+ ADP-ribosyltransferase activity	0.002	0.254387046
Connectivity Map	CellLine Batch - description - Top 5% over-expressed in 71, SKMEL5 treated with indometacin (.0001 M) for 6 h (Lamb)	0.002	1.26E+00
Oncomine Gene Expression Signatures	Cancer Type 2 - Top 20% under-expressed in Pancreatic Carcinoma (Uhlen)	0.003	5.21E-01
Literature-defined Concepts	Differentially regulated genes between NSC 685989 sensitive and resistant cell lines, following exposure to the drug	0.003	0.276395957
Oncomine Gene Expression Signatures	Breast HER2 Status - Top 5% over-expressed in positive (Ma)	0.003	5.13E-01
KEGG Pathway	Novobiocin biosynthesis	0.003	2.58E-02
Oncomine Gene Expression Signatures	Acute Lymphoblastic Leukemia Treatment - Top 10% under-expressed in High-dose Methotrexate (Cheok)	0.003	5.36E-01
Oncomine Gene Expression Signatures	Breast Carcinoma p53 Mutation Type - Top 5% under-expressed in Stop Codon Point Mutation (Miller)	0.003	5.23E-01
Oncomine Clusters	Co-expressed across 60 Colon samples (Graudens_Colon)	0.003	0.64679695
Oncomine Gene Expression Signatures	Breast Lobular Carcinoma E-cadherin - Top 10% under-expressed in 3 (Zhao)	0.003	5.21E-01
Oncomine Gene Expression Signatures	Leukemia Daunorubicin Sensitivity - Top 10% over-expressed in Resistant (Holleman)	0.003	0.510326582
Oncomine Gene Expression Signatures	Ovarian Carcinoma Histologic Subtype - Top 5% under-expressed in Mucinous (Schwartz)	0.003	5.06E-01
GO Cellular Component	membrane	0.003	4.40E-01
Literature-defined Concepts	Differentially regulated genes between NSC 676916 sensitive and resistant cell lines, following exposure to the drug	0.003	0.289074972
Oncomine Gene Expression Signatures	Ovarian Adenocarcinoma CHTN Stage - Top 10% under-expressed in 4A (Welsh)	0.003	0.507441381
Connectivity Map	CellLine Batch - description - Top 5% over-expressed in 13, MCF7 treated with nordihydroguaiaretic acid (.000001 M) for 6 h (Lamb)	0.003	1.348077665

Oncomine Gene Expression Signatures	Diffuse Large B-Cell Lymphoma DLBCL Subgroup - Top 5% over-expressed in Activated B-Cell-like DLBCL (Rosenwald)	0.003	5.07E-01
KEGG Pathway	Stilbene, coumarine and lignin biosynthesis	0.003	3.00E-02
Oncomine Gene Expression Signatures	Pancreas Type - Top 5% over-expressed in Pancreatic Adenocarcinoma (Iacobuzio-Donahue)	0.003	5.00E-01
GO Molecular Function	iron ion binding	0.003	0.319851863
Oncomine Gene Expression Signatures	CellLine Cisplatin - Top 20% under-expressed in resistant (Staunton)	0.003	4.89E-01
Oncomine Gene Expression Signatures	Multi-Tissue Type - Top 20% under-expressed in prostate cancer (Uhlen)	0.003	4.86E-01
Connectivity Map	MCF Cells Treatment - Top 1% over-expressed in 504, MCF7 treated with 5230742 (.000017 M) for 6 h (Lamb)	0.003	1.250626134
Literature-defined Concepts	Up-regulated genes in fetal liver tissue compared to various other normal adult and fetal tissues	0.003	0.273062164
Oncomine Clusters	Co-expressed across 19 Adrenal samples (Giordano_Adrenal)	0.003	7.18E-01
Oncomine Gene Expression Signatures	Cancer Type 2 - Top 20% under-expressed in Urothelial Cancer (Uhlen)	0.003	4.86E-01
Oncomine Gene Expression Signatures	Ovarian Carcinoma Histology - Top 10% under-expressed in Mucinous Carcinoma (Bittner)	0.003	0.477331905
KEGG Pathway	Histidine metabolism	0.004	3.13E-02
Oncomine Gene Expression Signatures	Prostate Type - Top 10% over-expressed in Prostate Carcinoma (Luo)	0.004	4.85E-01
GO Biological Process	biosynthesis	0.004	0.410626982
Oncomine Gene Expression Signatures	Cancer Type - v1 - Top 1% under-expressed in Breast Ductal Carcinoma (Bittner)	0.004	0.48677182
Transfac TF Matrix - 1000bp	ARP-1	0.004	4.50E-01
Oncomine Gene Expression Signatures	CellLine methotrexate - Top 20% under-expressed in resistant (Staunton)	0.004	4.98E-01
Oncomine Gene Expression Signatures	Colon Type - Top 1% over-expressed in Colorectal Carcinoma Metastasis to Liver (Graudens)	0.004	4.87E-01
Oncomine Gene Expression Signatures	Lymphoid Type - Top 1% over-expressed in Cutaneous Diffuse Large B-Cell Lymphoma (Storz)	0.004	4.81E-01
Oncomine Gene Expression Signatures	Metastatic Prostate Cancer Site - Top 10% under-expressed in	0.004	0.481383508

	Bone (Dhanasekaran)		
Connectivity Map	CellLine Batch - description - Top 1% under-expressed in 44, HL60 treated with sodium phenylbutyrate (.001 M) for 6 h (Lamb)	0.004	1.37E+00
Oncomine Gene Expression Signatures	Acute Myeloid Leukemia Karyotype - Top 10% under-expressed in 8 (Valk)	0.004	4.75E-01
Oncomine Gene Expression Signatures	Multi-Tissue Type - Top 20% under-expressed in breast cancer (Uhlen)	0.004	4.69E-01
Oncomine Gene Expression Signatures	Soft Tissue Cancer Type - Top 10% under-expressed in Soft Tissue Sarcoma (Segal)	0.004	0.461880615
Oncomine Gene Expression Signatures	Ovarian Carcinoma Histologic Subtype - Top 10% under-expressed in Mucinous (Schwartz)	0.004	4.53E-01
Oncomine Clusters	Co-expressed across 7 CellLine samples (Carson_CellLine)	0.004	8.73E-01
Connectivity Map	MCF Cells Treatment - Top 1% under-expressed in 502, MCF7 treated with trichostatin A (.000001 M) for 6 h (Lamb)	0.004	1.269887006
Chromosome Subregion	7q21	0.004	0.683671666
Oncomine Gene Expression Signatures	Normal Type - Top 5% under-expressed in Lung (Hsiao)	0.004	4.58E-01
Connectivity Map	CellLine Batch - description - Top 1% under-expressed in 2, MCF7 treated with phenyl biguanide (.00001 M) for 6 h (Lamb)	0.004	1.21E+00
InterPro	Aminoacyl-transfer RNA synthetase, class II	0.004	5.35E-01
GO Molecular Function	zinc ion binding	0.004	4.21E-01
Oncomine Gene Expression Signatures	Ovarian Histology - Top 10% under-expressed in Clear Cell (Lu)	0.004	4.66E-01
Oncomine Gene Expression Signatures	Leukemia Remission - day 33 - Top 1% under-expressed in No (Cario)	0.005	4.60E-01
Oncomine Gene Expression Signatures	Bladder Type - Top 10% over-expressed in TCC (Blaveri)	0.005	4.60E-01
Oncomine Clusters	Co-expressed across 17 Melanoma samples (Winnepenninckx_Melanoma_2)	0.005	9.11E-01
Oncomine Gene Expression Signatures	Breast Ductal Carcinoma Docetaxol Response - Top 5% over-expressed in Resistant (Chang)	0.005	4.63E-01
KEGG Pathway	beta-Alanine metabolism	0.005	0.039752937
Oncomine Gene Expression Signatures	Ovarian Type - Top 5% under-expressed in Clear cell Ovarian Carcinoma (Lu)	0.005	4.56E-01

Oncomine Gene Expression Signatures	Prostate Type - Top 5% over-expressed in Prostate Carcinoma (Luo)	0.005	4.50E-01
GO Cellular Component	cytosol	0.005	0.52366635
Literature-defined Concepts	Down-regulated genes in 3 primary human fibroblasts (S1, S2, S3), after gamma irradiation	0.005	3.51E-01
Literature-defined Concepts	Down-regulated genes in squamous cell lung cancer	0.005	0.324825274
GO Molecular Function	amino acid binding	0.005	4.47E-01
GO Cellular Component	ubiquitin ligase complex	0.005	0.433352922
Oncomine Gene Expression Signatures	Cancer Type - Top 10% under-expressed in Breast Carcinoma (Uhlen)	0.005	0.468443656
Oncomine Clusters	Co-expressed across 7 CellLine samples (Carson_CellLine)	0.005	8.73E-01
Oncomine Gene Expression Signatures	Cell Lines Cisplatin Sensitivity - Top 5% under-expressed in Resistant (Gyorffy)	0.005	0.459403346
Oncomine Gene Expression Signatures	Multi-Tissue Type - Top 20% under-expressed in urothelial cancer (Uhlen)	0.005	4.53E-01
HPRD Interaction Sets	PARP1	0.005	3.238532943
HPRD Interaction Sets	HDAC2	0.005	3.238532943
KEGG Pathway	Flavonoids, stilbene and lignin biosynthesis	0.005	4.31E-02
Oncomine Gene Expression Signatures	Lymphoma Type - Top 5% under-expressed in Follicular Lymphoma (Elenitoba-Johnson)	0.005	4.58E-01
KEGG Pathway	Keratan sulfate biosynthesis	0.005	4.17E-02
Literature-defined Concepts	Down-regulated genes in estrogen receptor alpha/beta heterodimer expressing U2OS osteosarcoma cell line, after 17beta-estradiol (E2) treatment	0.006	0.33573674
Oncomine Gene Expression Signatures	Bladder Type - Top 20% over-expressed in TCC (Blaveri)	0.006	4.68E-01
Oncomine Clusters	Co-expressed across 49 Breast samples (Farmer_Breast)	0.006	8.92E-01
Oncomine Clusters	Co-expressed across 28 Leukemia samples (Maia_Leukemia)	0.006	8.92E-01
Oncomine Clusters	Co-expressed across 72 CellLine samples (Baghdoyan_CellLine)	0.006	8.62E-01
Connectivity Map	MCF Cells Treatment - Top 1% over-expressed in 504, MCF7 treated with 5248896 (.000011 M) for 6 h (Lamb)	0.006	1.45E+00
Oncomine Gene Expression Signatures	Ovarian Type - Top 10% under-expressed in Clear cell Ovarian Carcinoma (Lu)	0.006	4.77E-01

Oncomine Gene Expression Signatures	Ovarian Type - Top 1% over-expressed in Endometriod Ovarian Carcinoma (Lu)	0.006	4.87E-01
Oncomine Gene Expression Signatures	Ovarian Histology - Top 1% over-expressed in Endometrioid (Lu)	0.006	4.87E-01
Transfac TF Matrix - 1000bp	1-Oct	0.006	0.540179617
Connectivity Map	CellLine Batch - description - Top 5% under-expressed in 45, ssMCF7 treated with trichostatin A (.0000001 M) for 6 h (Lamb)	0.006	1.40E+00
Oncomine Gene Expression Signatures	Cancer Type - Top 5% under-expressed in Colorectal Adenocarcinoma (Uhlen)	0.006	4.85E-01
Transfac TF Matrix - 1000bp	HFH-1	0.006	0.454647373
Oncomine Gene Expression Signatures	Cancer Type - v1 - Top 1% over-expressed in Rectal Adenocarcinoma (Bittner)	0.006	4.93E-01
Oncomine Clusters	Co-expressed across 24 Uterus samples (Quade_Uterus)	0.007	9.88E-01
Oncomine Gene Expression Signatures	Lung Cancer Type - Top 5% over-expressed in Lung Squamous Cell Carcinoma (Wigle)	0.007	5.40E-01
Oncomine Gene Expression Signatures	Cancer Type - Top 10% over-expressed in Hepatocellular Carcinoma (Su)	0.007	5.35E-01
Connectivity Map	CellLine Batch - description - Top 5% under-expressed in 44, HL60 treated with sodium phenylbutyrate (.001 M) for 6 h (Lamb)	0.007	1.53E+00
Literature-defined Concepts	Up-regulated genes in well-differentiated hepatocellular carcinoma compared to hepatocellular adenoma	0.007	3.95E-01
Oncomine Gene Expression Signatures	ER+ Breast Carcinoma AGTR1 Over-expression - Top 10% under-expressed in High (vandeVijver)	0.007	0.543796672
Oncomine Gene Expression Signatures	Lung Adenocarcinoma Primary/Metastasis - Top 5% under-expressed in Metastasis (Bhattacharjee)	0.007	5.41E-01
Literature-defined Concepts	Upregulated in Human Embryonic Stem Cells vs Differentiated Counterparts	0.007	0.38151934
Oncomine Gene Expression Signatures	Head and Neck Squamous Cell Carcinoma Stage - Top 5% over-expressed in IVB (Ginos)	0.008	5.54E-01
Oncomine Gene Expression Signatures	Normal Type - Top 5% under-expressed in Vulvar (Hsiao)	0.008	5.50E-01
Oncomine Gene Expression Signatures	Lung Carcinoma 3 Year Survival - Top 5% over-expressed in	0.008	5.52E-01

	Dead (Bild)		
Oncomine Clusters	Co-expressed across 93 Bladder samples (Blaveri_Bladder_3)	0.008	1.06E+00
Oncomine Clusters	Co-expressed across 14 CellLine samples (Chen_CellLine_6)	0.008	1.07E+00
Literature-defined Concepts	Up-regulated genes in clear cell ovarian carcinomas compared with other histological types	0.008	3.76E-01
Literature-defined Concepts	Up-regulated genes in gastric cancer tissues	0.008	3.76E-01
Oncomine Gene Expression Signatures	Endocrine Syndrome - Top 5% under-expressed in MEN2B (Jain)	0.008	0.576133757
Oncomine Gene Expression Signatures	Breast Carcinoma p53 Mutation Status - Top 1% under-expressed in Mutated (Miller)	0.008	5.70E-01
Literature-defined Concepts	Up-regulated genes in adipocytes of obese Pima Indians	0.008	0.342529369
Transfac TF Matrix - 1000bp	HFH-8	0.008	5.04E-01
Oncomine Gene Expression Signatures	Breast Carcinoma Recurrence - 5 years - Top 10% under-expressed in Positive (Ma)	0.008	5.76E-01
Oncomine Gene Expression Signatures	Ovarian Histology - Top 5% under-expressed in Clear Cell (Lu)	0.008	5.70E-01
Oncomine Gene Expression Signatures	Liver Type - Top 1% under-expressed in Metastasis to Liver (Chen)	0.008	5.67E-01
Oncomine Gene Expression Signatures	Ductal Carcinoma in situ Progesterone Receptor Status - Top 10% under-expressed in positive (Ma)	0.009	5.73E-01
Oncomine Gene Expression Signatures	Bladder Type - Top 5% under-expressed in Superficial Transitional Cell Carcinoma, Invasive Transitional Cell Carcinoma (Dyrskjot)	0.009	6.00E-01
Oncomine Clusters	Co-expressed across 18 Brain samples (Dong_Brain)	0.009	1.13E+00
GO Molecular Function	peroxidase activity	0.009	8.20E-01
Oncomine Clusters	Co-expressed across 44 Renal samples (Higgins_Renal)	0.009	1.06E+00
Oncomine Clusters	Co-expressed across 7 CellLine samples (Carson_CellLine)	0.01	1.058904807
Oncomine Clusters	Co-expressed across 72 CellLine samples (Baghdoyan_CellLine)	0.01	1.05E+00
Literature-defined Concepts	Differentially regulated genes between NSC 696860 sensitive and resistant cell lines, following exposure to the drug	0.01	3.76E-01
Oncomine Clusters	Co-expressed across 28 Leukemia samples (Crossman_Leukemia)	0.01	1.06E+00
Oncomine Gene Expression Signatures	CellLine Vinblastine-newanalysis - Top 1% under-expressed in	0.01	0.630945671

	Resistant (Staunton)		
InterPro	Haem peroxidase	0.01	1.170969907
InterPro	Animal haem peroxidase	0.01	1.170969907
InterPro	Haem peroxidase, plant/fungal/bacterial	0.01	1.170969907
InterPro	Aminoacyl-tRNA synthetase, class Ia	0.01	1.170969907
Oncomine Gene Expression Signatures	Colon Type - Top 5% over-expressed in Colorectal Carcinoma Metastasis to Liver (Graudens)	0.01	6.26E-01
Oncomine Gene Expression Signatures	Renal Clear Cell Carcinoma Capsule Penetration - Top 5% under-expressed in positive (Lenburg)	0.01	6.20E-01
Oncomine Gene Expression Signatures	Bladder Grade - Top 5% over-expressed in High Grade (Dyrskjot)	0.01	6.15E-01