Supplements to

Evaluating the accuracy of the QCEIMS approach for computational prediction of electron ionization mass spectra of purines and pyrimidines

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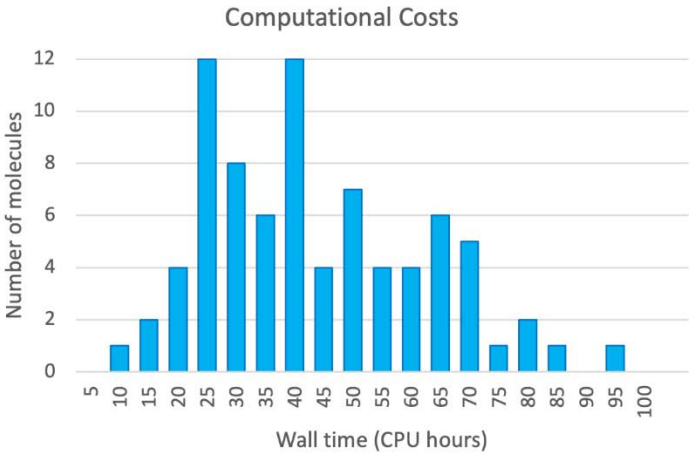
Supplement 1: Computational costs for QCEIMS prediction of 80 purines and pyrimidines.



Types of molecules	Num. of mols	Total time	Avg. time
Pyrimidines	14	468.90	33.49
Methylpurines	4	183.30	45.83
Amino/hydroxy-purines	5	185.19	37.04
Adenines	5	183.51	36.70
Xanthines	8	246.43	30.80
Hypoxanthines	3	94.64	31.55
Guanines	6	264.43	44.07
Lumazines	8	339.48	42.44
Quinazdine-diones	7	444.57	63.51
Reumycins	7	298.52	42.65
Pyridopyrimidines	13	583.61	54.02
others	7	259.47	37.07
		3292.59	41.16

Supplement 2: Exact masses, formulas, number of fragment ions ('peaks') in QCEIMS mass spectra and comparison to NIST17 targets with Wdot and cosine scores, and the matching rank when querying the overall NIST17 library.

	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
Group 1 Pyrimidines	2	126.042927	C5H4N2O2	Thymine	2,4(1H,3H)-Pyrimidinedione, 5-methyl- Thymin 2,4-Dihydroxy-5-methylpyrimidine 5-Methyluracil 5-Methyl-2,4-dioxypyrimidine 5-Methyl-2,4(1H,3H)-pyrimidinedione	62	963.1	750.3	1
	3	126.042927	C5H4N2O2	6-Methyluracil	2,4(1H,3H)-Pyrimidinedione, 6-methyl- 2(1H)-Pyrimidinone, 4-hydroxy-6-methyl- Pseudothymine Uracil, 6-methyl- 2,4-Dihydroxy-6-methylpyrimidine 2,4-Pyrimidinediol, 6-methyl- AWD 23-15 6-Methyl-1H-pyrimidine-2,4-dione 4-(6)-Methyluracil	62	978.94	916.9	1
	5	126.042927	C5H5N2O2	Uracil, 1-methyl-	1-Methyluracil 2,4(1H,3H)-Pyrimidinedione, 1-methyl- 1-Methyl-2,4(1H,3H)-pyrimidinedione #	54	925.32	586.1	7
	6	127.038177	C4H3N3O2	2,4(1H,3H)-Pyrimidinedione, 5-amino-	Uracil, 5-amino- 2,4-Dihydroxy-5-aminopyrimidine 5-Amino-2,4-dihydroxypyrimidine 5-Aminouracil 5-Amino-2,4(1H,3H)-pyrimidinedione #	51	983.56	909.6	2
	7	127.038177	C4H3N3O2	4-Amino-2,6-dihydroxypyrimidine	6-Amino-2,4-dihydroxypyrimidine 6-Aminouracil 4-Aminouracil 2,4(1H,3H)-Pyrimidinedione, 6-amino- Cytosine, 6-hydroxy- Uracil, 6-amino- 4-Amino-2,6-dihydroxylpyrimidine 4-Amino-2,6-dioxypyrimidine 4-Amino-2,6-pyrimidinediol	69	983.92	877.2	5
	8	130.017856	C4HFN2O2	5-Fluorouracil	2,4(1H,3H)-Pyrimidinedione, 5-fluoro- Fluorouracil Uracil, 5-fluoro- Efudex Fluoroplex Fluracil Fluril NSC 19893 Ro 2-9757	67	979.41	937.6	1
	16	140.058578	C6H7N2O2	2,4(1H,3H)-Pyrimidinedione, 3,6-dimethyl-	Uracil, 3,6-dimethyl- 3,6-Dimethyl-2,4(1H,3H)-pyrimidinedione 3,6-Dimethyluracil	22	168.5	718.9	1
	17	140.058578	C6H8N2O2	2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-	Uracil, 1,3-dimethyl- N,N'-Dimethyluracil N1,N3-Dimethyluracil 1,3-Dimethyluracil 2,4-Dihydroxy-1,3-dimethylpyrimidine 1,3-Dimethyl-2,4(1H,3H)-pyrimidinedione #	54	971.41	872.6	1
	18	140.058578	C6H6N2O2	2,4-Dihydroxy-5,6-dimethylpyrimidine	5,6-Dimethyluracil 2,4(1H,3H)-Pyrimidinedione, 5,6-dimethyl- Uracil, 5,6-dimethyl- 4,5-Dimethyluracil 5,6-Dimethyl-2,4(1H,3H)-pyrimidinedione #	74	944.6	896.3	1
	19	141.053826	C5H6N3O2	2,4(1H,3H)-Pyrimidinedione, 6-amino-1-methyl-	6-Amino-1-methyl-1H-pyrimidine-2,4-dione 6-Amino-1-methyl-2,4(1H,3H)-pyrimidinedione # 6-Amino-1-methyluracil	45	236.98	377.1	4
	41	154.074227	C7H10N2O2	2,4(1H,3H)-Pyrimidinedione, 1,3,5-trimethyl-	Uracil, 1,3,5-trimethyl- 1,3-Dimethylthymine 1,3,5-Trimethyl-2,4(1H,3H)-pyrimidinedione #	79	939.83	744.6	1

	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
	42	154.074227	C7H10N2O2	2,4(1H,3H)-Pyrimidinedione, 1,3,6-trimethyl-	Uracil, 1,3,6-trimethyl- 1,3,6-Trimethyl-2,4(1H,3H)-pyrimidinedione 1,3,6-Trimethyluracil	66	943.55	668.7	2
	43	155.069476	C6H9N3O2	6-Amino-1,3-dimethyluracil	4-Amino-1,3-dimethyl-2,6-dihydroxypyrimidine 4-Amino-1,3-dimethyluracil 2,4(1H,3H)-Pyrimidinedione, 6-amino-1,3-dimethyl- Uracil, 6-amino-1,3-dimethyl- 1,3-Dimethyl-6-amino-uracil 6-Amino-1,3-dimethyl-2,4(1H,3H)-pyrimidinedione #	59	955.28	763.2	1
	81	170.080376	C6H10N4O2	5,6-Diamino-1,3-dimethyluracil	2,4(1H,3H)-Pyrimidinedione, 5,6-diamino-1,3-dimethyl- Uracil, 5,6-diamino-1,3-dimethyl- 4,5-Diamino-1,3-dimethyluracil 5,6-Diamino-1,3-dimethyl-2,4(1H,3H)-pyrimidinedione #	127	958.09	586.5	48
Group 2 Methylpurines	1	120.043596	C5H3N4	9H-Purine	7H-Purine 1H-Purine Purine .beta.-Purine Isopurine 3,5,7-Triazaindole 6H-Imidazo[4,5-d]pyrimidine Imidazo(4,5-d)pyrimidine NSC 753	21	338.64	383.2	2
	9	134.059246	C6H5N4	1H-Purine, 2-methyl-	Purine, 2-methyl- 2-Methyl-9H-purine #	45	957.27	936.5	2
	10	134.059246	C6H5N4	1H-Purine, 6-methyl-	Purine, 6-methyl- 6-Methylpurine 6-Methyl-1H-purine 6-Methyl-9H-purine #	22	120.76	174.6	5
	11	134.059246	C6H5N4	1H-Purine, 8-methyl-	Purine, 8-methyl- 8-Methylpurine 8-Methyl-7H-purine #	53	950.07	757.3	4
Group 3 Amino/hydroxy-purines	13	135.054495	C5H4N5	2-Aminopurine	1H-Purin-2-amine Purine, 2-amino- SQ 22,451 SQ 22451 9H-Purin-2-amine #	35	139.71	219.6	1
	14	136.038510	C5H3N4O	2-Purinol	9H-Purin-2-ol #	69	874.17	843.8	15
	15	136.038510	C5H3N4O	1H-Purin-6-ol	Imidazo[5,4-d]pyrimidine, 6-hydroxy-	45	956.11	959.4	5
	22	145.038845	C6H2N5	1H-Purine-6-carbonitrile	6-Cyanopurine Purine-6-carbonitrile Purine, 6-cyano- 9H-Purine-6-carbonitrile #	9	73.029	98.2	1

	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
	69	167.044325	C5H4N5O2	2-Amino-6,8-dihydroxypurine	1H-Purine-6,8-dione, 2-amino-7,9-dihydro- 2-Amino-9H-purine-6,8-diol #	117	962.34	846.3	2
Group 4 Adenines	12	135.054495	C5H4N5	Adenine	GFFGJBXGBJISGV-UHFFFAOYSA-N	2	940.27	939.2	32
	25	149.070146	C6H7N5	6-Amino-3-methylpurine	FSASIHFSFGAIJM-UHFFFAOYSA-N	2	923.7	796.3	1
	26	149.070146	C6H7N5	7H-Purin-6-amine, 7-methyl-	HCGHYQLFMPXSDU-UHFFFAOYSA-N	2	820.27	560.2	2
	27	149.070146	C6H7N5	6-Amino-1-methylpurine	HPZMWTNATZPBIH-UHFFFAOYSA-N	2	932.23	907.8	4
	32	150.065394	C5H5N6	2,6-Diaminopurine	MSSXOMSJDRHRMC-UHFFFAOYSA-N	2	116.74	100.5	N/R
Group 5 Xanthines	37	152.033425	C5H3N4O2	Xanthine	1H-Purine-2,6-dione, 3,7-dihydro- Isoxanthine Pseudoxanthine Purine-2,6(1H,3H)-dione Xan Xanthic oxide Xanthin 1H-Purine-2,6-diol 2,6-Dioxo-1,2,3,6-tetrahydropurine	43	949	658.7	9
	39	153.028674	C4N5O2	8-Azaxanthine	1H-1,2,3-Triazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione v-Triazolo(4,5-d)pyrimidine-5,7-diol NSC 756 USAF cb-26 Xanthazol 1H-v-Triazolo(4,5-d)pyrimidine-5,7(4H,6H)-dione 2,6-Dioxy-8-azapurine	68	967.05	687.1	1
	66	166.049075	C6H4N4O2	2,6-Dihydroxy-7-methylpurine	7-Methylxanthine 1H-Purine-2,6-dione, 3,7-dihydro-7-methyl- Heteroxanthin Heteroxanthine Xanthine, 7-methyl- 7-Methylxanthin	31	943.54	913.7	1
	75	168.028340	C5N4O3	Uric acid	1H-Purine-2,6,8(3H)-trione, 7,9-dihydro- Lithic acid Purine-2,6,8(1H,3H,9H)-trione 1H-Purine-2,6,8-triol 2,6,8-Trioxopurine 2,6,8-Trioxypurine 7,9-Dihydro-1H-purine-2,6,8(3H)-trione 2,6,8-Trihydroxypurine 8-Hydroxyxanthine	139	786.88	457.4	6
	99	180.064726	C7H7N4O2	Theobromine	1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- Diurobromine Santheose SC 15090 Teobromin Theosalvose Theostene Thesal 3,7-Dimethylxanthine	49	949.83	762.8	1

	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
	100	180.064726	C7H7N4O2	Theophylline	1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl- Elixophyllin Elixophylline Lanophyllin Liquophylline Optiphyllin Parkophyllin Pseudotheophylline Solosin	48	953.5	732.5	1
	106	181.059975	C6H6N5O2	3H-N-Triazolo(4,5-d)pyrimidine-5,7(4H,6H)-dione, 3,6-dimethyl-	1,9-Dimethyl-8-azaxanthin 3,6-Dimethyl-3H-v-triazolo(4,5-d)pyrimidine-5,7(4H,6H)-dione	32	87.83	578.9	1
	132	195.075624	C7H9N5O2	3H-v-Triazolo(4,5-d)pyrimidine-5,7(4H,6H)-dione, 3,4,6-trimethyl-	1,3,9-Trimethyl-8-azaxanthin 3,4,6-Trimethyl-3H-v-triazolo(4,5-d)pyrimidine	38	254.35	515.5	2
Group 6 Hypoxanthines	28	150.054161	C6H5N4O	6H-Purin-6-one, 1,7-dihydro-7-methyl-	Hypoxanthine, 7-methyl- 7-Methylhypoxanthine 7-Methyl-6-hydroxypurine 7-Methyl-1,7-dihydro-6H-purin-6-one #	33	104.06	132.3	N/R
	31	150.054161	C6H5N4O	6H-Purin-6-one, 3,7-dihydro-3-methyl-	Hypoxanthine, 3-methyl- N3-Methylhypoxanthine 3-Methylhypoxanthine 3-Methyl-3,7-dihydro-6H-purin-6-one #	22	207.38	543.6	1
	52	164.069811	C7H8N4O	6H-Purin-6-one, 1,7-dihydro-1,7-dimethyl-	Hypoxanthine, 1,7-dimethyl- 1,7-Dimethylhypoxanthine 1,7-Dimethyl-1,7-dihydro-6H-purin-6-one #	75	891.87	870.3	1
Group 7 Guanines	35	151.049410	C5H3N5O	Guanine	6H-Purin-6-one, 2-amino-1,7-dihydro- C.I. Natural White 1 C.I. 75170 Dew Pearl Guanin Guanine enol Hypoxanthine, 2-amino- Mearlmaid Natural Pearl Essence	84	937.61	912.8	2
	53	165.065060	C6H6N5O	7-Methylguanine	6H-Purin-6-one, 2-amino-1,7-dihydro-7-methyl- Guanine, 7-methyl- N7-Methylguanine 2-Amino-7-methylhypoxanthine 2-Amino-1,7-dihydro-7-methyl-6H-purin-6-one 2-Amino-7-methyl-1,7-dihydro-6H-purin-6-one NSC 193444	38	127.23	381.7	2
	54	165.065060	C6H6N5O	6H-Purin-6-one, 2-amino-1,7-dihydro-1-methyl-	Guanine, 1-methyl- N1-Methylguanine 1-Methylguanine 2-Amino-1-methyl-1,7-dihydro-6H-purin-6-one #	30	166.66	423.5	1
	55	165.065060	C6H6N5O	2-Amino-6-hydroxy-9-methylpurine	9-Methylguanine 6H-Purin-6-one, 2-amino-1,9-dihydro-9-methyl- 2-Amino-9-methyl-1,9-dihydro-6H-purin-6-one #	100	937.71	940	1
	56	165.065060	C6H6N5O	6H-Purin-6-one, 2-amino-3,7-dihydro-3-methyl-	Guanine, 3-methyl- N3-Methylguanine 3-Methylguanine 2-Amino-3-methyl-3,7-dihydro-6H-purin-6-one #	48	230.74	518.6	1

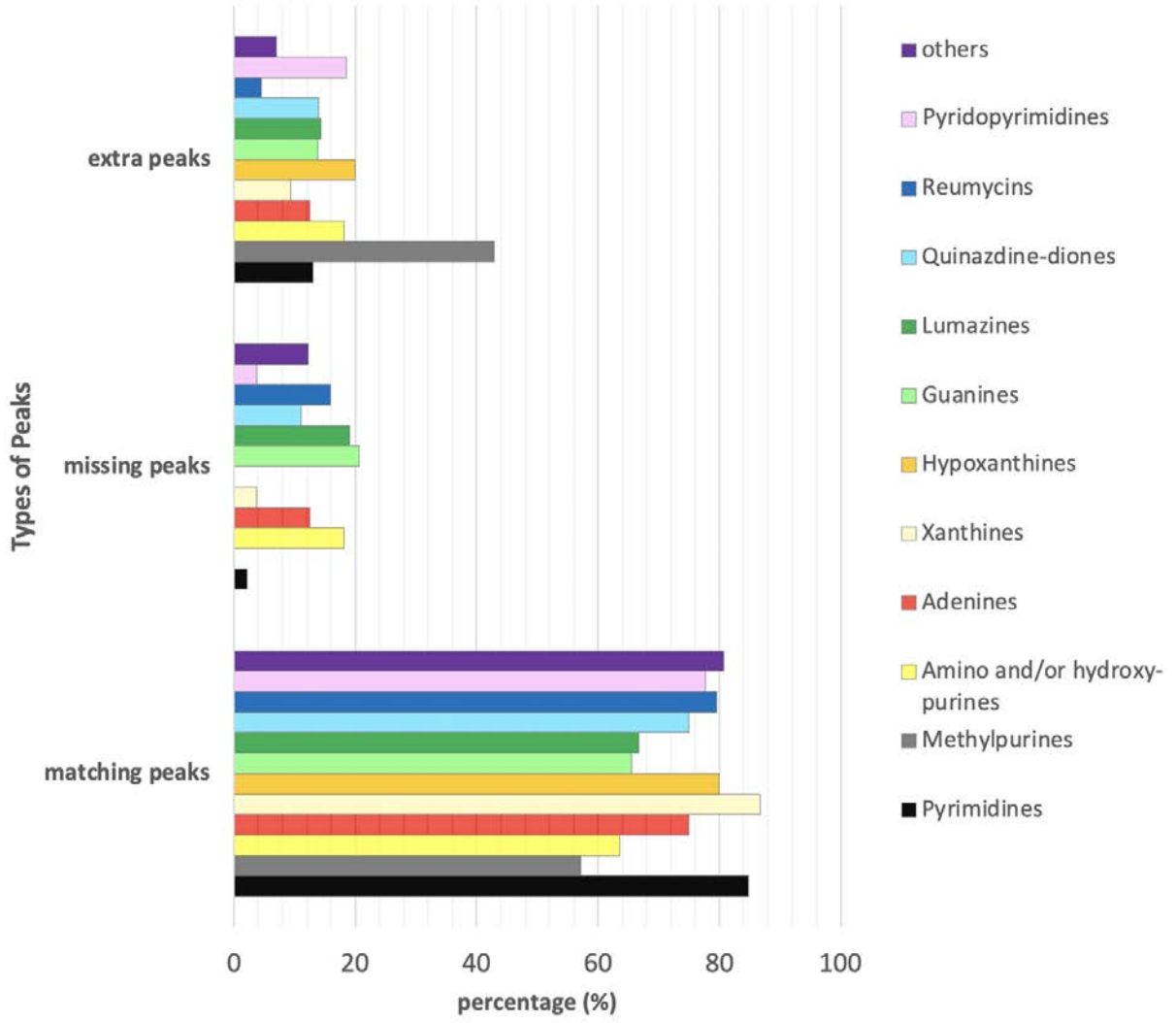
	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
	124	193.059975	C7H5N5O2	Acetamide, N-(6,7-dihydro-6-oxo-1H-purin-2-yl)-	N-2-Acetylguanine N-(6-Oxo-6,9-dihydro-1H-purin-2-yl)acetamide #	67	708.08	348.7	N/R
Group 8 Lumazines	51	164.033425	C6H2N4O2	Lumazine	2,4(1H,3H)-Pteridinedione 2,4(3H,8H)-Pteridinedione 2,4-Dihydroxypteridine 2,4-Pteridinediol Lumazin Pteridinedione, 2,4(1h,3h)-	92	951.94	896.2	1
	65	166.049075	C6H4N4O2	7,8-Dihydro-2,4(1H,3H)-pteridinedione		75	15.729	47.38	N/R
	88	178.049075	C7H5N4O2	2,4(1H,3H)-Pteridinedione, 8-methyl-	Lumazine, 8-methyl- 8-Methyl-2,4(3H,8H)-pteridinedione #	47	215.83	589.2	1
	91	178.049075	C7H4N4O2	2,4(1H,3H)-Pteridinedione, 6-methyl-	Lumazine, 6-methyl- 6-Methyl-2,4(1H,3H)-pteridinedione #	17	156.79	313.5	27
	95	180.028340	C6HN4O3	2,4,7(1H,3H,8H)-Pteridinetrione	Isoxantholumazine Lumazine, 7-hydroxy- Violapterin 2,4,7-Trihydroxypteridine 7-Hydroxylumazine 2,4,7-Pteridinetriol	83	909.86	615.5	8
	96	180.028340	C6HN4O3	2,4,6(3H)-Pteridinetrione, 1,5-dihydro-	Lumazine, 6-hydroxy- Pteridine-2,4,6-trione 2,4,6(1H,3H,5H)-Pteridinetrione 2,4,6-Pteridinetriol 2,4,6-Trihydroxypteridine 6-Hydroxylumazine 1,5-Dihydro-2,4,6(3H)-pteridinetrione #	23	52.832	135.5	N/R
	121	192.064726	C8H8N4O2	2,4(1H,3H)-Pteridinedione, 1,3-dimethyl-	Lumazine, 1,3-dimethyl- 1,3-Dimethyllumazine 1,3-Dimethylpteridine-2,4-dione N,N'-Dimethyllumazin 1,3-Dimethyl-2,4(1H,3H)-pteridinedione # N,N'-Dimethyllumazine	61	941.32	786.3	1
	128	194.043990	C7H3N4O3	2,4,7(1H,3H,8H)-Pteridinetrione, 6-methyl-	2,4,7-Pteridinetriol, 6-methyl- 2,4(1H,3H)-Pteridinedione, 7-hydroxy-6-methyl- 6-Methyl-2,4,7(1H,3H,8H)-quinazolinetrione #	46	818.57	533.3	N/R
	46	162.042928	C8H4N2O2	2,4(1H,3H)-Quinazolinedione	Benzouracil Benzoyleneurea Quinazoline-2,4-dione Quinazolinedione Urea, benzoylene- 1,2,3,4-Tetrahydroquinazoline-2,4-dione 2,4-Dihydroxyquinazoline (1H,3H)Quinazoline dione-2,4 2,4-Dioxotetrahydroquinazoline	75	953.38	846.8	9
	83	176.058578	C9H7N2O2	2,4(1H,3H)-Quinazolinedione, 3-methyl-	3-Methyl-2,4(1H,3H)-quinazolinedione	69	951.15	817.6	1

	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
Group 9 Quinazoline-diones	84	176.058578	C9H7N2O2	2,4(1H,3H)-Quinazolinedione, 1-methyl-	Glycosmicine 1-Methyl-2,4(1H,3H)-Quinazolinedione Methyl-1 (1H,3H)quinazolinedione-2,4	41	299.94	429.5	29
	86	177.053826	C8H6N3O2	3-Amino-1H-quinazoline-2,4-dione		60	233.5	298.9	N/R
	87	177.053826	C8H5N3O2	6-Amino-1H-quinazoline-2,4-dione		35	968.56	972.5	1
	115	190.074227	C10H10N2O2	1,3-Dimethyl-2,4(1H,3H)-quinazolinedione	2,4(1H,3H)-Quinazolinedione, 1,3-dimethyl- Dimethyl-1,3 (1H,3H)quinazolinedione-2,4 1,3-Dimethyl-1,2,3,4-tetrahydroquinazolin-2,4-dione	76	931.74	835.7	1
	120	192.053493	C9H8N2O3	2,4(1H,3H)-Quinazolinedione, 3-hydroxy-1-methyl-	3-Hydroxy-1-methyl-2,4(1H,3H)-quinazolinedione #	20	294.24	366	N/R
Group 10 Reumycins	92	179.044325	C6H4N5O2	Reumycin	Pyrimido(5,4-e)-as-triazine-5,7(6H,8H)-dione, 6-methyl- Reumitsin Rheumygin Pyrimido(5,4-e)-as-triazine-5,7(1H,6H)-dione, 6-methyl- BA 51-090492 6-Methylpyrimido(5,4-e)-as-triazine-5,7(1H,6H)-dione	32	534.26	451.3	30
	105	181.023589	C5HN5O3	Pyrimido[4,5-e][1,2,4]triazine-6,8(5H,7H)-dione, 3-hydroxy-		115	606.67	505.9	N/R
	123	193.059975	C7H7N5O2	5,7-Dimethylpyrimido[4,5-E]-1,2,4-triazine-6,8(5H,7H)-dione		30	920.23	954	1
	125	193.059975	C7H7N5O2	Fervenulin	Compd. 7215 Fervenuline FH-3582-A KC 1017 Planomycin Pyrimido(5,4-e)-as-triazine-5,7(6H,8H)-dione, 6,8-dimethyl- Pyrimido(5,4-e)-1,2,4-triazine-5,7(6H,8H)-dione, 6,8-dimethyl-	39	317.18	391.7	71
	126	193.059975	C7H7N5O2	Toxoflavin	Pyrimido(5,4-e)-as-triazine-5,7(1H,6H)-dione, 1,6-dimethyl- Pyrimido(5,4-e)-1,2,4-triazine-5,7(1H,6H)-dione, 1,6-dimethyl- Toxoflavine Xanthothricin Xanthotricin 1,6-Dimethyl-5,7-dioxo-1,5,6,7-tetrahydropyrimido(5,4-e)-as-triazine-	31	224.79	355.5	6
	133	195.075624	C7H8N5O2	Theophylline, 8-amino-	8-Aminoteofiliny 8-Aminotheophylline 1H-Purine-2,6-dione, 8-amino-3,7-dihydro-1,3-dimethyl- 7H-Purine-2,6(1H,3H)-dione, 8-amino-1,3-dimethyl- 8-Amino-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione #	134	971.05	825.9	1

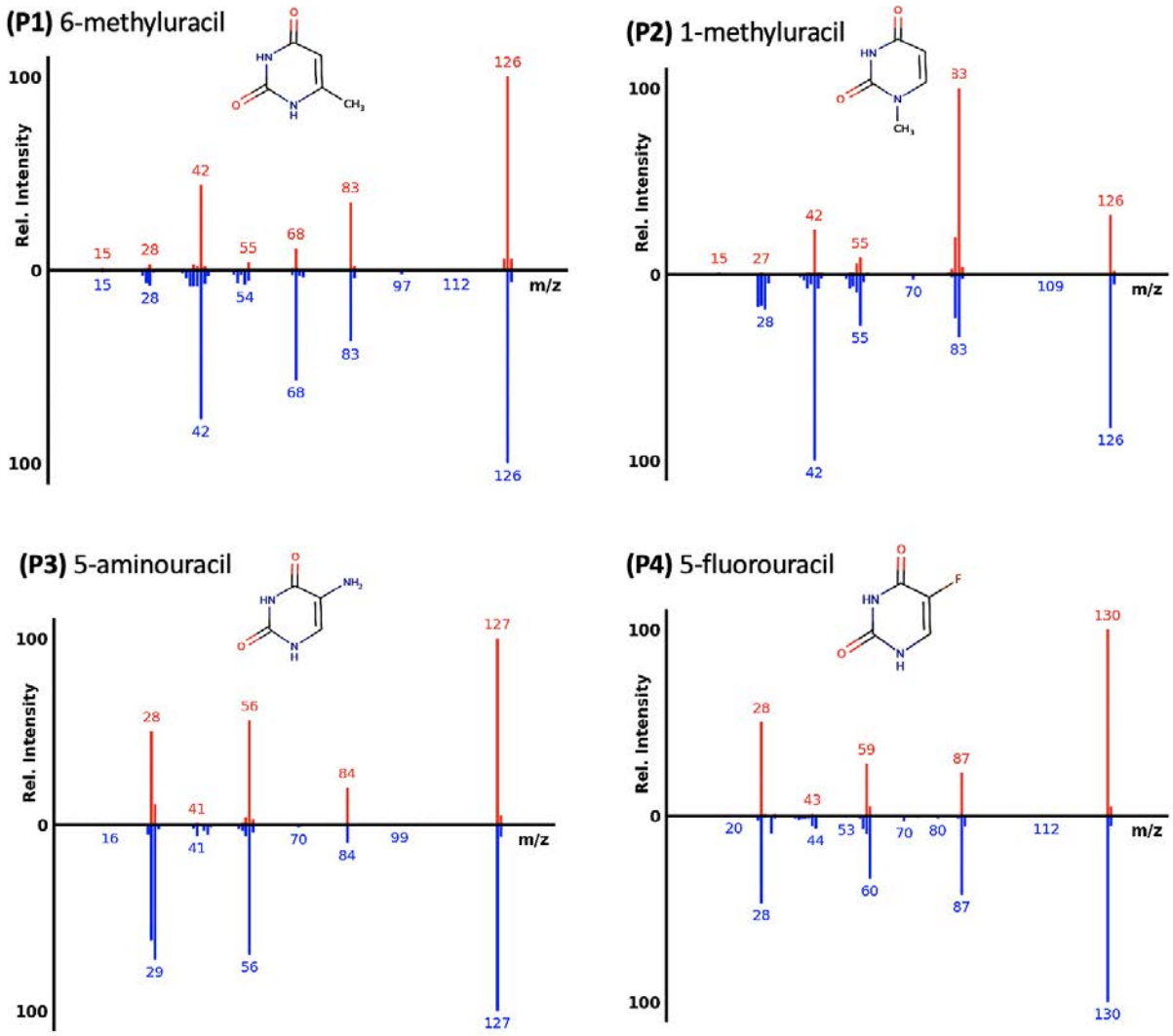
	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
Group 11 Pyridopyrimidines	47	163.038177	C7H3N3O2	Pyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione	Pyrido[3,2-d]pyrimidine-2,4-diol 2,4-Dihydroxypyrido[3,2-d]pyrimidine	24	249.32	761	1
	48	163.038177	C7H3N3O2	Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione		18	233.69	415.4	1
	50	163.038177	C7H3N3O2	Pyrido[4,3-d]pyrimidine-2,4(1H,3H)-dione	Pyrido[4,3-d]pyrimidin-4(3H)-one, 2-hydroxy-	37	939.71	757.7	11
	116	191.069476	C9H9N3O2	Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-	1,3-Dimethylpyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione #	28	169.72	295.1	N/R
	117	191.069476	C9H9N3O2	Pyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-	1,3-Dimethylpyrido[3,2-d]pyrimidine-2,4(1H,3H)-dione #	29	302.24	696	3
	118	191.069476	C9H9N3O2	Pyrido[3,4-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-	1,3-Dimethylpyrido[3,4-d]pyrimidine-2,4(1H,3H)-dione #	32	262.9	569.7	1
Group 12 Others	38	152.058578	C7H6N2O2	1H,3H,5H,6H,7H-Cyclopenta[d]pyrimidine-2,4-dione		64	935.12	842.9	N/R
	70	167.044325	C5H3N5O2	4-Methyl-3,4-dihydro-[1,2,3]triazolo[4,5-d]pyrimidine-5,7-dione		39	347.9	46.95	N/R
	74	168.017107	C6H2N2O4	1,5-Dihydrofuro[3,4-d]pyrimidine-2,4,7(3H)-trione		47	932.84	586.8	26
	80	170.007605	C4N4O4	1-Oxy-4H-[1,2,5]oxadiazolo[3,4-d]pyrimidine-5,7-dione		33	935.41	561.2	1

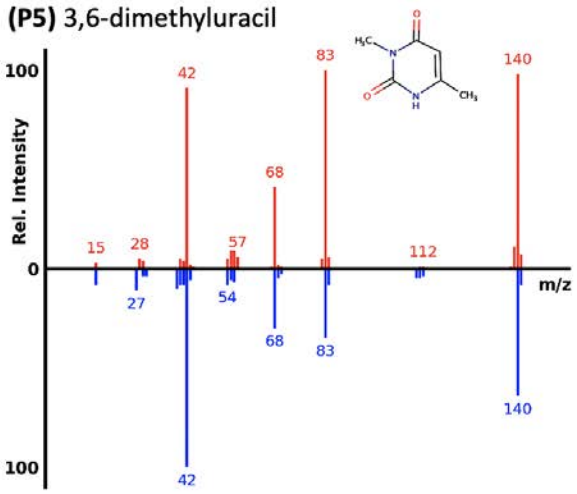
	Num	EXACT MASS	Formula	NAME	SYNONYMS	PEAK #'s	Wdot	cos	Rank
	93	179.069476	C8H8N3O2	1H-Pyrrolo(2,3-d)pyrimidine-2,4(3H,7H)-dione, 1,3-dimethyl-	1,3-Dimethyl-1H-pyrrolo(2,3-d)pyrimidine-2,4(3H,7H)-dione 1H-Pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione, 1,3-dimethyl- 1H-Pyrrolo[3,2-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl- 1H-Pyrrolo[3,2-d]pyrimidine-2,4(3H,5H)-dione, 1,3-dimethyl-	79	885.54	488.4	1
	122	192.064726	C8H6N4O2	1H-Pyrrolo[2,1-f]purine-2,4(3H,6H)-dione, 7,8-dihydro-		95	934.63	503.5	1
	146	207.075624	C8H9N5O2	Pyrimido[5,4-E][1,2,4]triazine-5,7(1H,6H)-dione, 1,3,6-trimethyl-		86	911.02	310.8	45

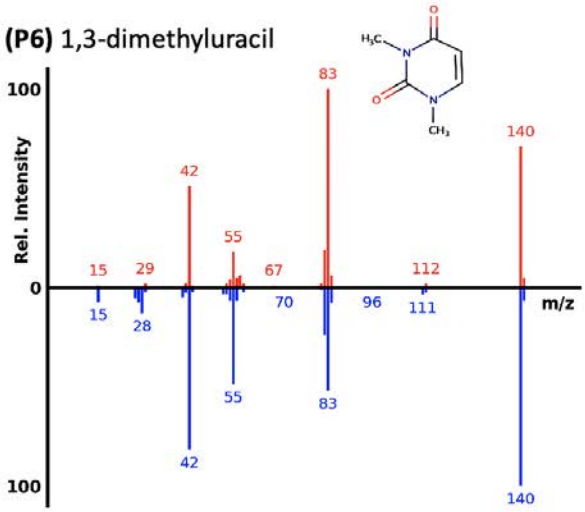
Supplement 3: The ability of QCEIMS to predict major fragment ions with abundance >20% of the base peak ion, distinguished by 12 subclasses of purines and pyrimidines. *Note*: Most major fragment ions were correctly predicted by QCEIMS for most structure subclasses. While QCEIMS predicted less than 20% of additional fragment ions not verified by experimental spectra, more than 40% extra fragment ions were predicted by QCEIMS of methylpurines.

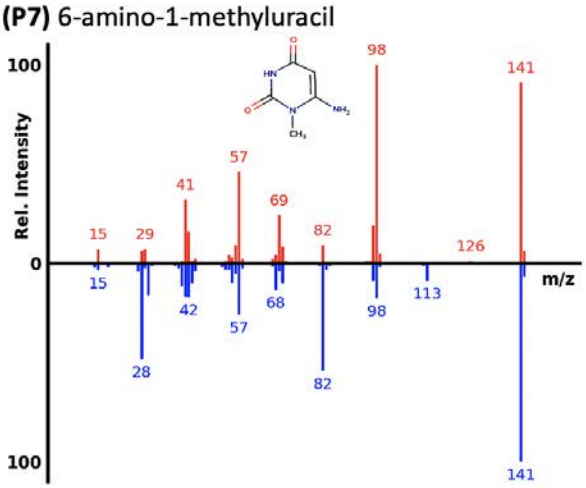


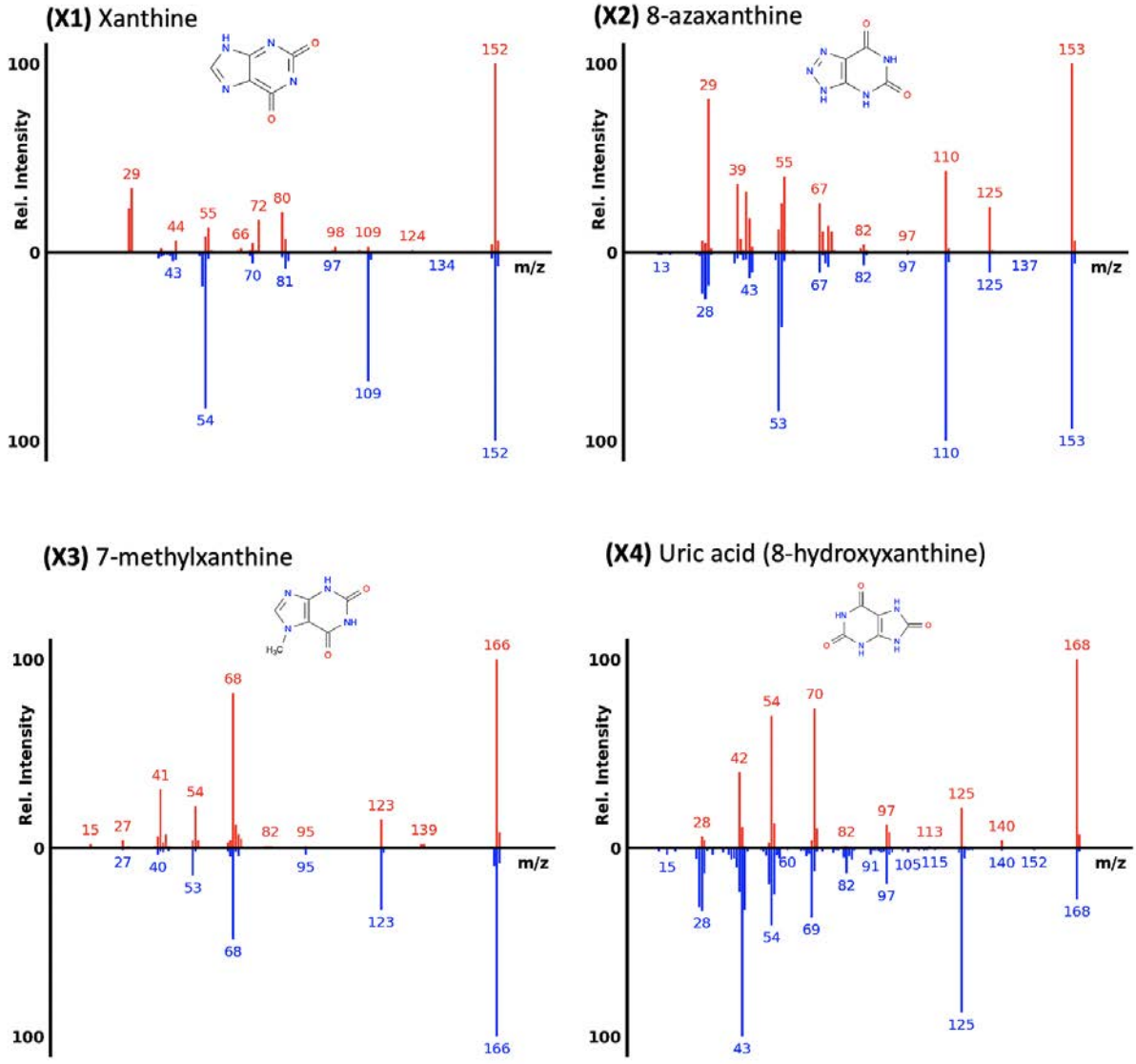
Supplement 4: 32 examples of QCEIMS predicted mass spectra (top) versus NIST17 experimental mass spectra (bottom) for purines and pyrimidines.



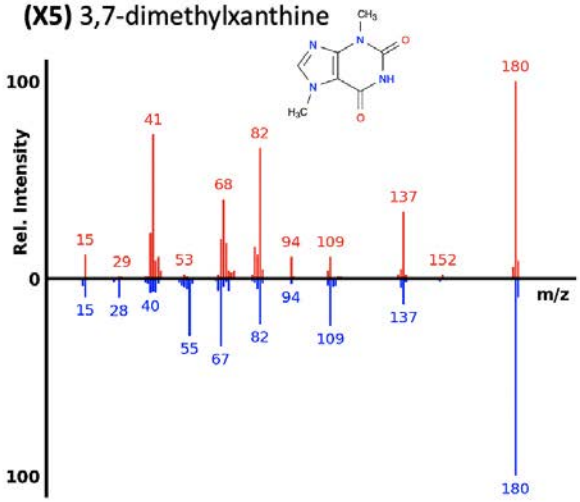

(P5) 3,6-dimethyluracil
Rel. Intensity
100
0
100
m/z
15
28
42
57
68
83
112
140
27
54
68
83
140
42


(P6) 1,3-dimethyluracil
Rel. Intensity
100
0
100
m/z
15
29
42
55
67
83
112
140
15
28
42
55
70
83
96
111
140

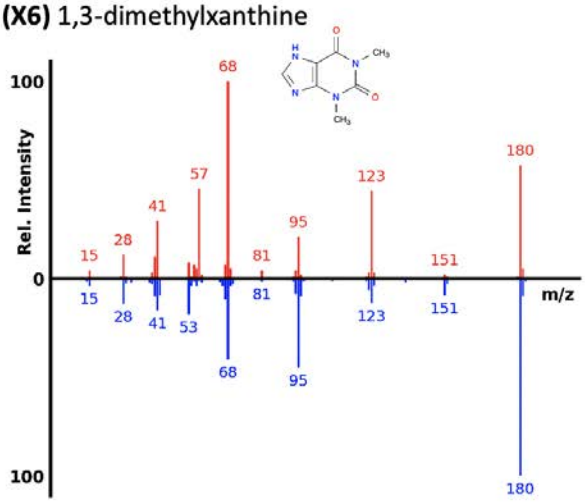

(P7) 6-amino-1-methyluracil
Rel. Intensity
100
0
100
m/z
15
29
41
57
69
82
98
126
141
15
28
42
57
68
82
98
113
141


(X1) Xanthine
100
Rel. Intensity
0
100
29
44
55
66
72
80
98
109
124
152
43
54
70
81
97
109
134
152
m/z
(X2) 8-azaxanthine
100
Rel. Intensity
0
100
29
39
55
67
82
97
110
125
153
13
28
43
53
67
82
97
110
125
137
153
m/z
(X3) 7-methylxanthine
100
Rel. Intensity
0
100
15
27
41
54
68
82
95
123
139
166
27
40
53
68
95
123
166
m/z
(X4) Uric acid (8-hydroxyxanthine)
100
Rel. Intensity
0
100
15
28
42
54
70
82
97
113
125
140
168
28
43
54
60
69
82
91
97
105
115
125
140
152
168
m/z

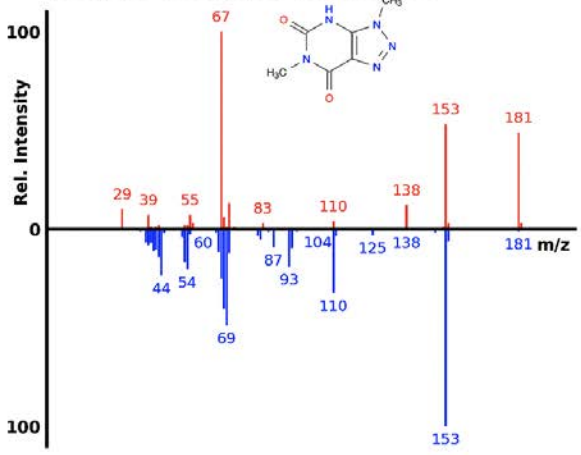
(X5) 3,7-dimethylxanthine



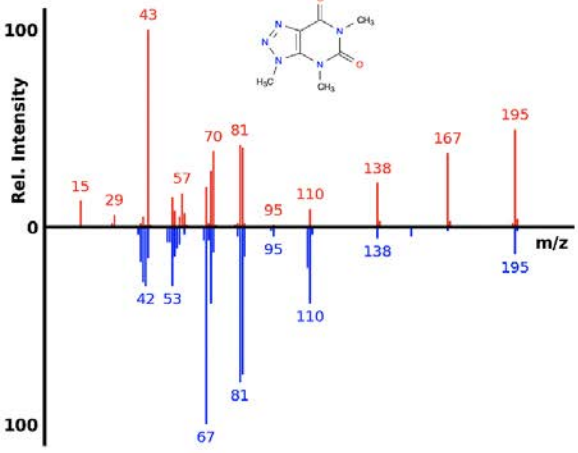
(X6) 1,3-dimethylxanthine

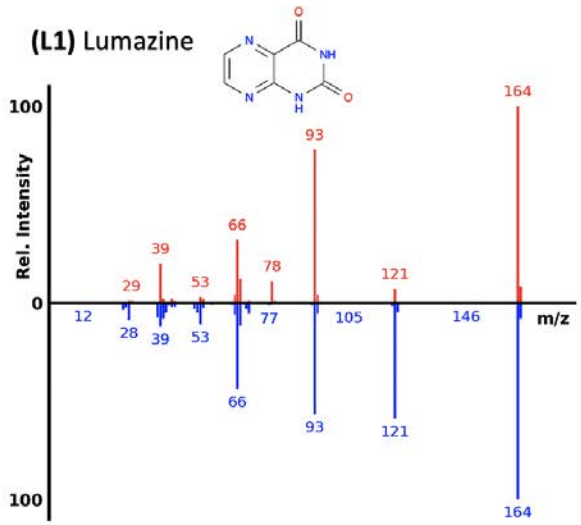


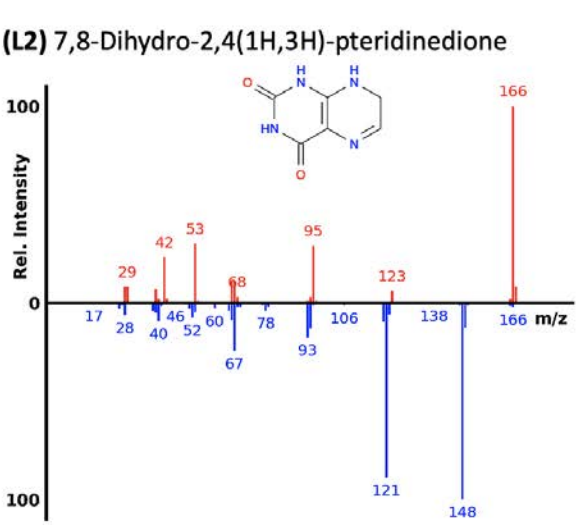
(X7) 1,9-dimethyl-8-azaxanthine

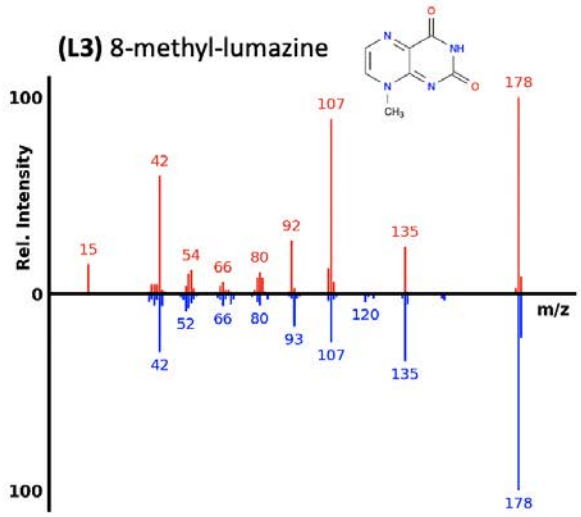


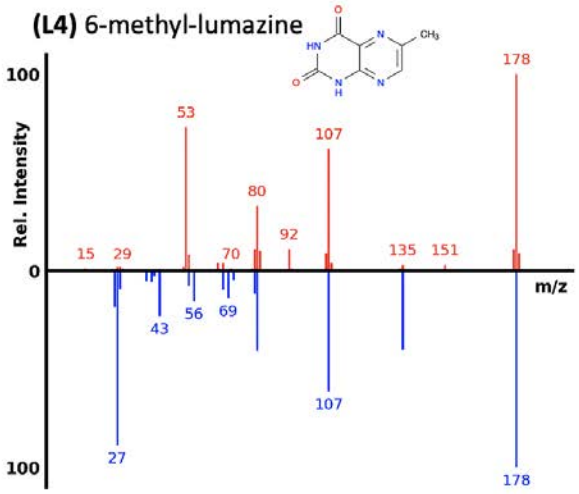
(X8) 1,3,9-trimethyl-8-azaxanthine

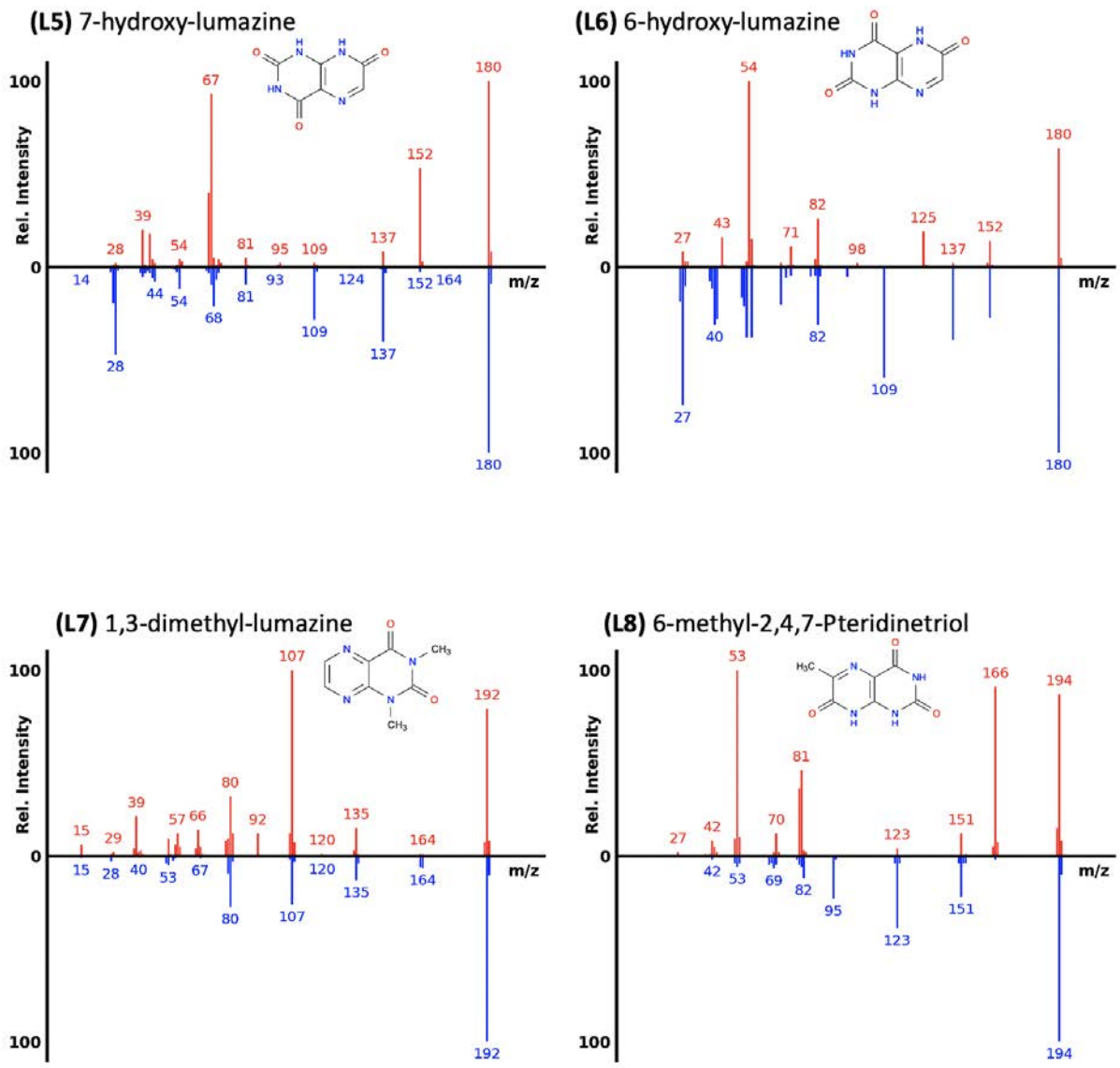



(L1) Lumazine
Rel. Intensity
100
0
100
m/z
164
93
66
39
29
53
78
121
12
28
39
53
66
77
93
105
121
146
164

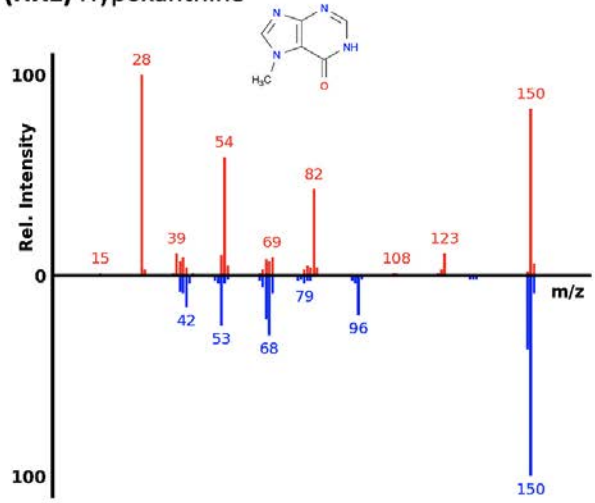

(L2) 7,8-Dihydro-2,4(1H,3H)-pteridinedione
Rel. Intensity
100
0
100
m/z
166
53
42
95
29
68
123
17
28
40
46
52
60
67
78
93
106
121
138
148
166


(L3) 8-methyl-lumazine
Rel. Intensity
100
0
100
m/z
178
107
42
92
135
15
54
66
80
42
52
66
80
93
107
120
135
178

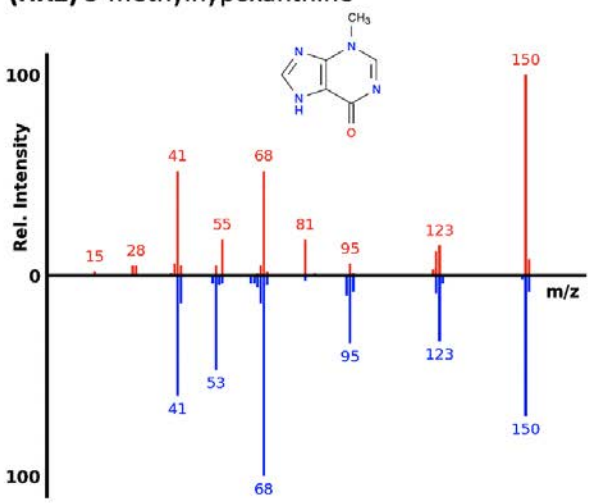

(L4) 6-methyl-lumazine
Rel. Intensity
100
0
100
m/z
178
53
107
80
92
15
29
70
135
151
27
43
56
69
107
178


(L5) 7-hydroxy-lumazine
(L6) 6-hydroxy-lumazine
(L7) 1,3-dimethyl-lumazine
(L8) 6-methyl-2,4,7-Pteridinetriol
Rel. Intensity
m/z
100
0

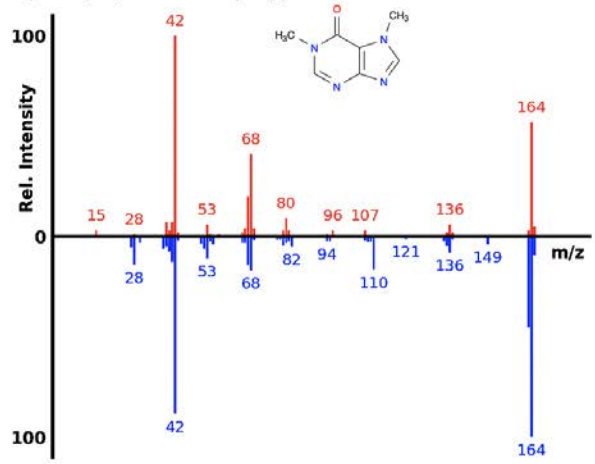
(HX1) Hypoxanthine

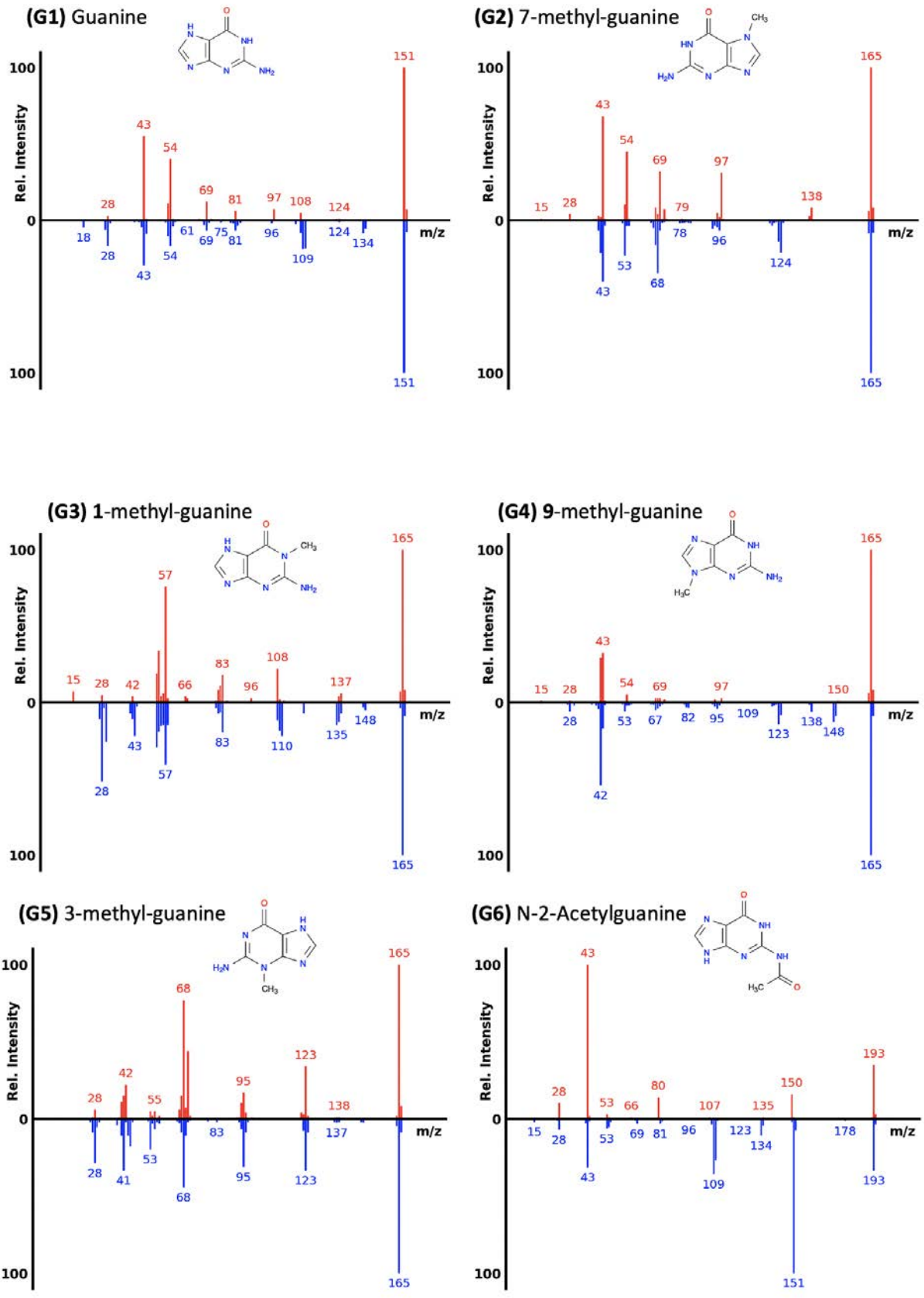


(HX2) 3-methylhypoxanthine



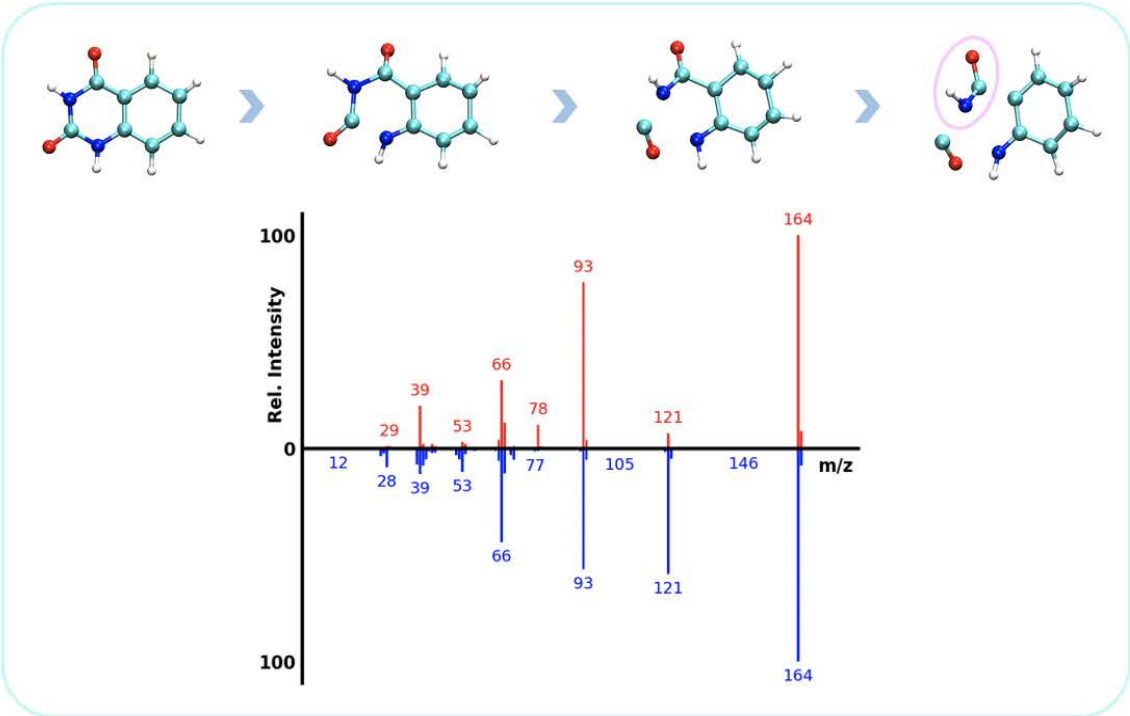
(HX3) 1,7-dimethylhypoxanthine



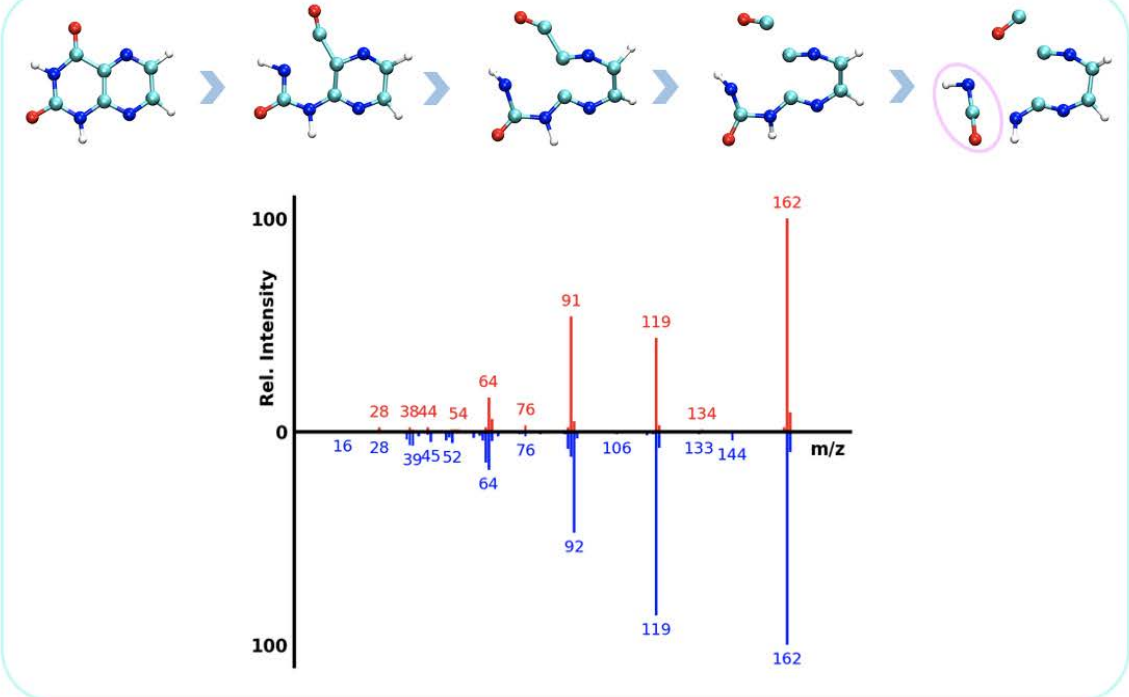

(G1) Guanine
Rel. Intensity
m/z
100
0
100
151
43
54
28
69
81
97
108
124
18
28
43
54
61
69
75
81
96
109
124
134
151
(G2) 7-methyl-guanine
Rel. Intensity
m/z
100
0
100
165
43
54
69
97
15
28
79
78
96
138
124
43
53
68
165
(G3) 1-methyl-guanine
Rel. Intensity
m/z
100
0
100
165
57
15
28
42
66
83
96
108
137
148
28
43
57
83
110
135
165
(G4) 9-methyl-guanine
Rel. Intensity
m/z
100
0
100
165
43
15
28
54
69
97
150
28
53
67
82
95
109
123
138
148
42
165
(G5) 3-methyl-guanine
Rel. Intensity
m/z
100
0
100
165
68
42
28
55
95
123
138
28
41
53
68
83
95
123
137
165
(G6) N-2-Acetylguanine
Rel. Intensity
m/z
100
0
100
193
43
28
53
80
66
107
150
135
15
28
43
53
69
81
96
109
123
134
151
178
193

Supplement 5 Analysis of QCEIMS trajectories marking the neutral loss of isocyanic acid (43 u, pink circle). (a) Benzouracil. (b) Lumazine.

(a)



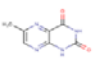
(b)

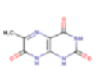
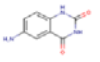
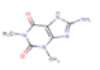


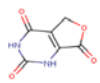
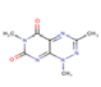
Supplement 6: List of molecular structures with the numbers of missing, matching, and extra ions generated by QCEIMS compared to NIST17 experimental mass spectra.

	Mol ID	Structure	# of matching peaks	# of missing peaks	# of extra peaks
Pyrimidines	2		12	7	1
	3		13	11	1
	5		14	7	0
	6		9	6	1
	7		10	12	0
	8		6	6	1
	16		16	4	6
	17		15	6	1
	18		14	13	1
	19		20	6	2
	41		19	6	1
	42		19	10	2
	43		16	7	1
	81		16	22	0
Methylpurines	1		8	4	5
	9		11	1	1
	10		9	6	5

	Mol ID	Structure	# of matching peaks	# of missing peaks	# of extra peaks
Methyl-purines	11		15	3	1
Amino/hydroxypurines	13		11	7	2
	14		11	13	1
	15		4	6	3
	22		4	0	6
	69		14	17	0
Adenines	12		8	7	1
	25		19	5	2
	26		24	3	1
	27		18	16	1
	32		7	4	5
Xanthines	37		10	5	5
	39		19	2	1
	66		11	2	3
	75		19	24	1
	99		24	6	4
	100		21	5	1

	Mol ID	Structure	# of matching peaks	# of missing peaks	# of extra peaks
Xanthines	106		18	5	10
	132		19	8	8
Hypoxanthines	28		14	7	8
	31		13	6	6
Guanines	52		21	13	2
	35		10	11	1
	53		13	9	6
	54		17	11	6
	55		10	15	0
	56		24	13	3
	124		7	8	1
Lumazines	51		15	8	1
	65		9	12	2
	88		23	9	4
	91		7	8	11
	95		20	5	1
	96		10	11	7

	Mol ID	Structure	# of matching peaks	# of missing peaks	# of extra peaks
Lumazines	121		12	2	1
	128		12	7	3
Quinazdine-dion	46		13	10	1
	83		10	1	2
	84		16	10	5
	86		21	12	2
	87		11	7	2
	115		14	1	1
	120		15	3	19
Reumycins	92		12	18	3
	105		14	13	2
	123		9	4	2
	125		17	20	3
	126		18	11	7
	133		24	7	3
	147		12	6	1
Others 1	47		13	8	4

	Mol ID	Structure	# of matching peaks	# of missing peaks	# of extra peaks
Others 1	48		12	3	3
	50		21	13	5
	116		19	7	16
	117		8	1	9
	118		21	9	6
Others 2	38		20	17	3
	70		6	3	5
	74		13	12	3
	80		11	7	3
	93		26	14	4
	122		18	7	3
	146		28	12	4
	Total		1162	663	269