CFM-ID - top-1 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	7	9	7	2	4	1	6	7	8	4	8	9	2	8	9	12	4	6	2	9	8	7	5	4	2	3	10	6
LC-MS²Struct	8	15	8	8	4	4	10	14	16	8	14	12	4	10	11	18	5	8	2	11	10	14	9	7	3	6	11	9
MS²+RT	7	9	7	3	4	1	7	8	7	4	8	8	2	8	8	18	3	6	3	9	8	8	4	4	2	4	15	6
MS²+logP	4	11	6	7	3	1	7	9	9	7	11	8	3	6	10	11	4	7	1	9	8	8	7	5	4	4	14	7
MS²+RO	9	11	6	4	4	4	7	6	8	5	12	12	3	8	9	18	4	8	1	10	9	11	5	6	3	5	12	7

Top-k acc. improvement (%p)

CFM-ID - top-20 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	36	53	39	50	31	36	35	41	49	38	47	53	39	50	41	82	44	45	30	54	50	45	46	49	36	36	72	44
LC-MS²Struct	40	58	48	61	40	48	49	48	58	43	56	61	48	56	45	84	49	51	32	61	57	55	51	54	41	45	75	51
MS²+RT	37	53	40	50	34	40	39	41	49	36	46	51	36	47	39	86	42	44	34	55	53	44	45	47	34	36	80	44
MS²+logP	33	51	42	52	31	33	35	44	48	39	47	53	32	49	40	82	47	44	27	55	49	49	46	47	33	37	59	43
MS²+RO	38	57	46	55	34	43	41	45	51	43	54	61	43	55	46	89	48	49	33	58	55	57	47	51	40	43	80	49

Top-k acc. improvement (%p)

MetFrag - top-1 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	12	10	5	5	3	4	12	12	15	4	8	5	7	5	5	10	7	7	3	10	8	6	7	4	3	2	3	7
LC-MS²Struct	20	20	9	8	9	7	17	28	27	11	18	13	12	12	11	28	12	11	15	22	15	13	14	8	8	5	6	14
MS²+RT	13	10	5	4	3	5	12	12	15	4	7	6	6	5	4	14	7	7	11	10	6	7	7	4	3	1	7	7
MS²+logP	11	11	5	4	3	3	13	14	15	7	8	8	13	7	6	10	6	8	3	12	9	9	9	4	3	3	3	8
MS²+RO	13	14	6	4	4	5	11	14	16	5	8	8	10	8	4	14	8	9	8	14	10	6	8	5	3	3	7	9

Top-k acc. improvement (%p)

MetFrag - top-20 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	52	55	43	35	31	30	33	57	62	50	59	59	57	55	47	82	54	51	37	57	44	42	51	50	34	34	50	47
LC-MS²Struct	54	65	52	51	39	42	56	74	74	58	68	67	67	61	62	90	60	58	45	71	56	55	60	61	50	47	64	58
MS²+RT	51	55	42	35	32	32	36	56	59	47	57	58	54	54	45	90	52	50	37	57	46	39	49	48	32	33	70	47
MS²+logP	51	59	43	38	30	30	33	62	68	50	59	53	54	55	44	82	55	52	35	58	43	42	58	52	39	38	43	48
MS²+RO	53	59	46	34	34	35	40	63	68	56	63	63	62	59	60	86	57	55	45	62	48	48	55	55	44	40	62	52

Top-k acc. improvement (%p)

SIRIUS - top-1 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	27	30	42	38	22	29	30	42	40	39	55	27	39	42	49	15	28	34	37	25	33	55	37	44	40	41	19	36
LC-MS²Struct	31	32	42	39	26	31	35	43	42	42	55	28	38	44	49	24	29	33	39	32	37	58	40	45	43	41	19	38
MS²+RT	27	31	40	37	21	27	32	41	38	38	54	24	37	40	47	16	27	34	37	26	33	53	35	42	38	39	23	35
MS²+logP	28	31	41	34	25	27	30	44	41	41	55	28	35	42	47	15	29	33	32	26	35	56	35	44	40	40	19	35
MS²+RO	29	31	42	38	24	29	31	42	43	42	57	28	39	41	47	21	29	33	38	28	35	56	37	46	43	42	19	37

Top-k acc. improvement (%p)

SIRIUS - top-20 accuracy

Scoring method	AC_003	AU_000	AU_002	AU_003	BML_000	BML_001	BS_000	EA_000	EA_001	EA_002	EA_003	EQ_001	EQ_003	EQ_004	EQ_006	LQB_000	LU_000	LU_001	NA_003	PR_000	PR_002	RP_001	SM_000	SM_001	UF_002	UF_003	UT_000	AVG.
Only-MS²	65	69	77	77	74	79	80	73	79	80	90	69	78	79	84	72	74	74	80	79	83	93	78	85	79	82	56	78
LC-MS²Struct	65	68	78	78	77	80	82	77	80	80	90	70	81	80	84	77	75	75	81	84	86	94	80	86	79	82	60	79
MS²+RT	63	68	75	75	72	76	78	71	77	77	88	65	74	75	80	82	71	72	79	78	81	89	74	80	75	79	62	75
MS²+logP	65	69	77	72	72	79	80	74	79	81	90	69	78	79	85	72	76	75	80	80	83	93	77	85	78	81	56	78
MS²+RO	65	70	79	79	76	81	82	75	79	81	90	70	80	79	85	73	75	75	82	82	85	93	80	86	79	83	57	79

Top-k acc. improvement (%p)