

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061121\
 Data File : VN067291.D
 Acq On : 11 Jun 2021 16:18
 Operator : JC/MD
 Sample : M2674-02 10X
 Misc : 5.07g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TMR-DS-02-060921

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M

Title : SW846 8260

Signal : TIC: VN067291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.291	844	858	876	rBV	22439	56943	1.33%	0.223%
2	4.854	1042	1068	1107	rBV	573620	1814918	42.30%	7.116%
3	7.345	1979	1997	2016	rBV	36478	98253	2.29%	0.385%
4	7.844	2160	2183	2202	rBV3	101910	250363	5.84%	0.982%
5	8.021	2231	2249	2260	rBV	308104	736071	17.16%	2.886%
6	8.085	2261	2273	2302	rVB	586382	1323695	30.85%	5.190%
7	8.437	2386	2404	2428	rBV	383526	903477	21.06%	3.542%
8	8.968	2585	2602	2621	rBV	835742	1753039	40.86%	6.874%
9	9.764	2890	2899	2917	rVB3	107692	206115	4.80%	0.808%
10	10.443	3138	3152	3166	rBV	1298150	2447942	57.05%	9.598%
11	10.507	3167	3176	3199	rVB2	261964	505417	11.78%	1.982%
12	11.746	3625	3638	3654	rBV	1189509	2141852	49.92%	8.398%
13	11.846	3671	3675	3689	rVB	143103	201525	4.70%	0.790%
14	11.953	3705	3715	3738	rVB2	462624	973813	22.70%	3.818%
15	12.283	3829	3838	3852	rVB	263186	442176	10.31%	1.734%
16	12.733	3995	4006	4024	rVB	1097026	1923480	44.83%	7.542%
17	13.594	4319	4327	4338	rVB	218245	345099	8.04%	1.353%
18	13.675	4345	4357	4393	rVB5	1468338	4290624	100.00%	16.823%
19	14.514	4663	4670	4686	rVB6	229999	350612	8.17%	1.375%
20	14.815	4773	4782	4791	rBV7	194606	375796	8.76%	1.473%
21	15.088	4877	4884	4900	rVB3	156785	246840	5.75%	0.968%
22	15.587	5059	5070	5084	rVB	940366	1648847	38.43%	6.465%
23	15.673	5096	5102	5134	rVB6	312114	806077	18.79%	3.161%
24	16.617	5442	5454	5473	rVB2	698003	1661067	38.71%	6.513%

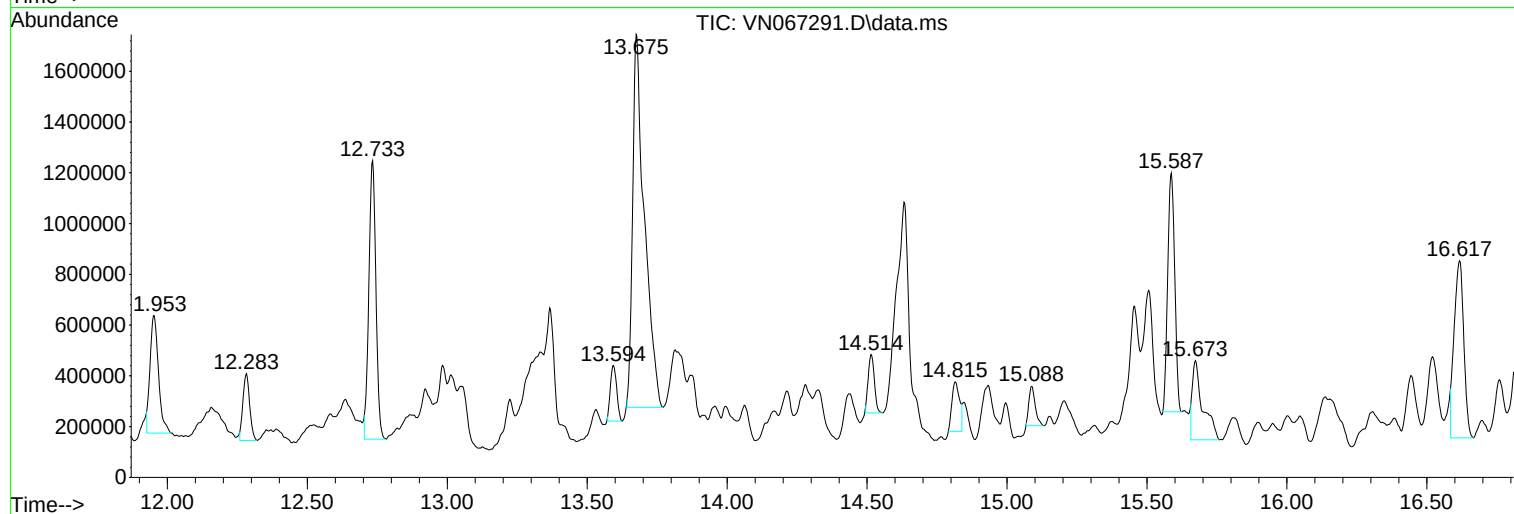
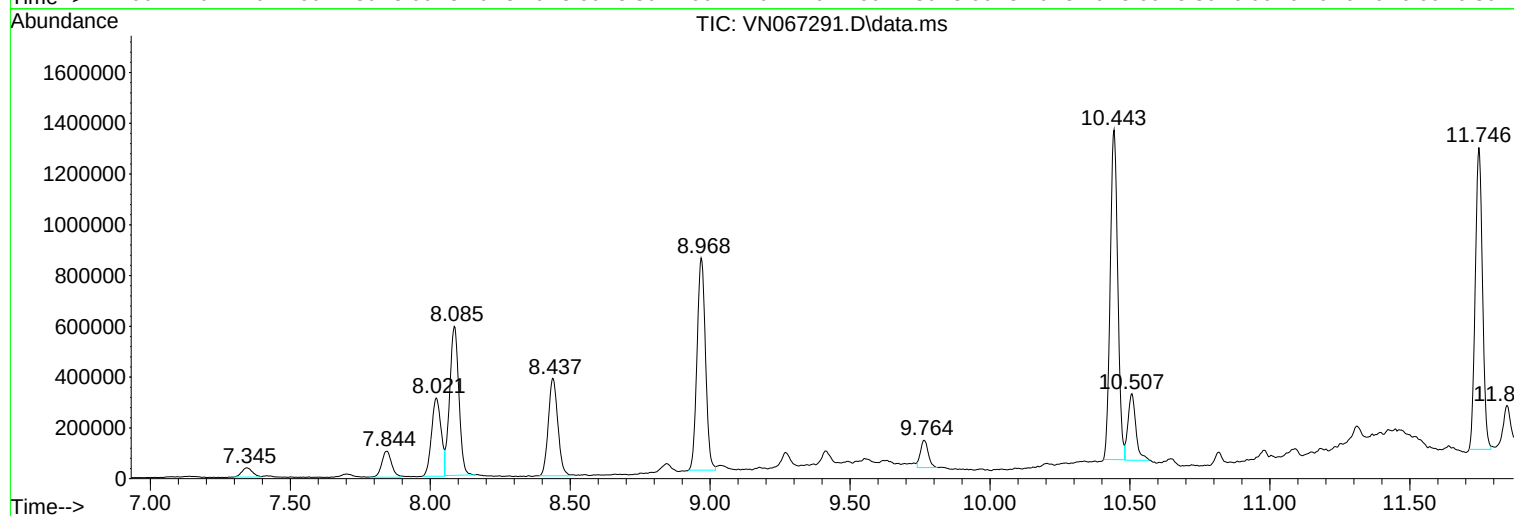
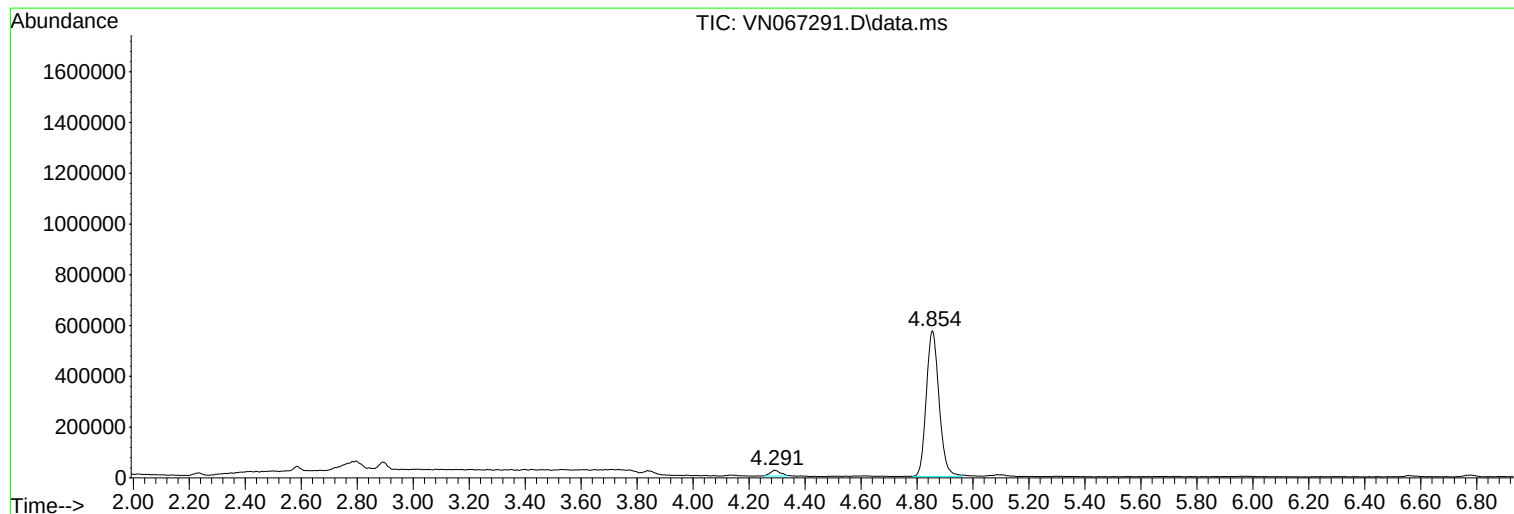
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Instrument :
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ClientSampleId :
TMR-DS-02-060921

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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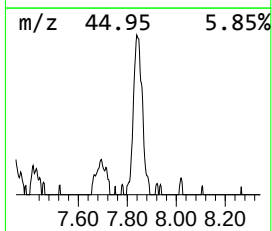
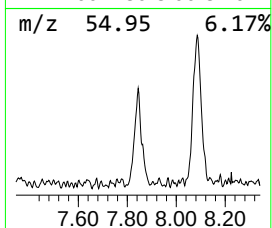
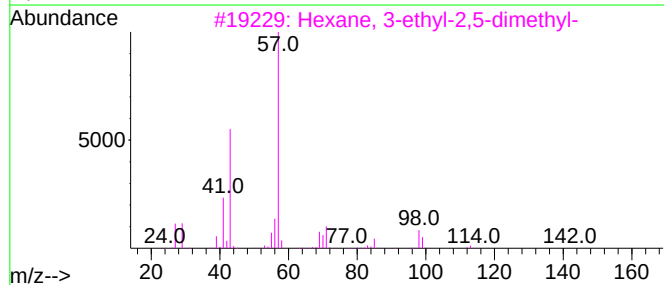
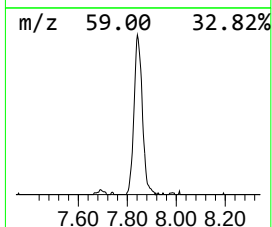
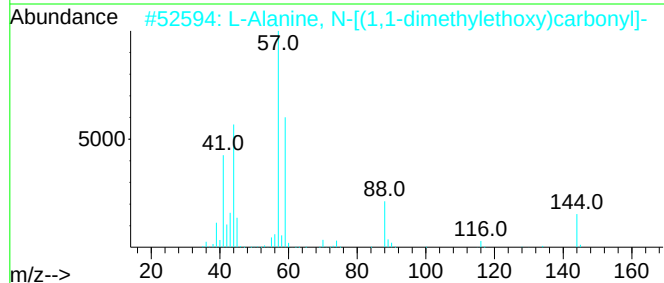
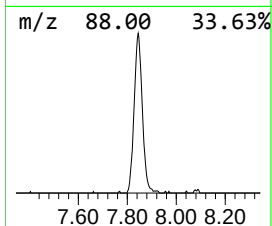
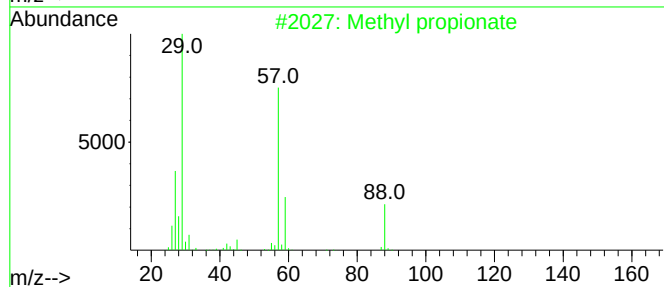
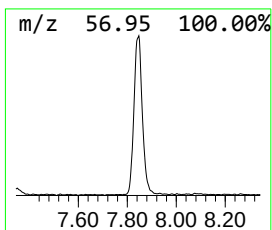
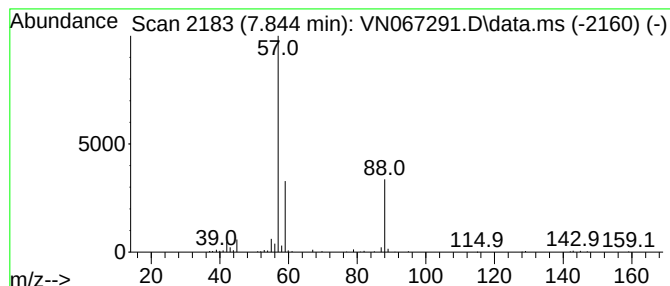
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methyl propionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.844	9.46 ug/l	250363	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl propionate	88	C4H8O2	000554-12-1	80
2			L-Alanine, N-[(1,1-dimethylethox...	189	C8H15NO4	015761-38-3	28
3			Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	9
4			Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9
5			Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	9



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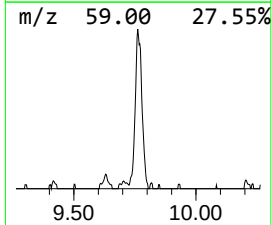
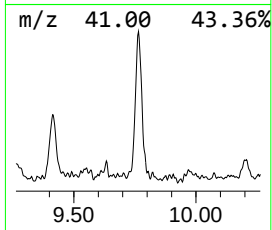
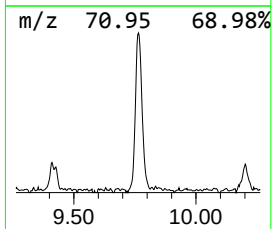
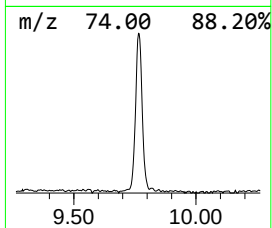
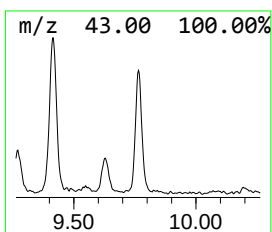
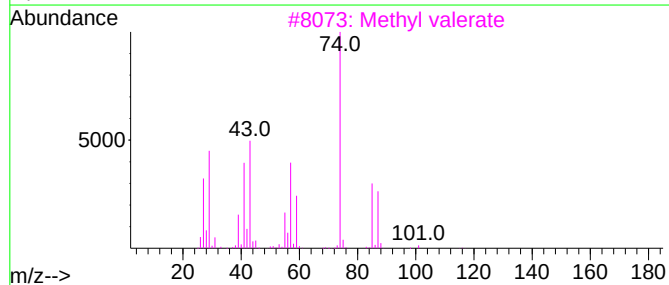
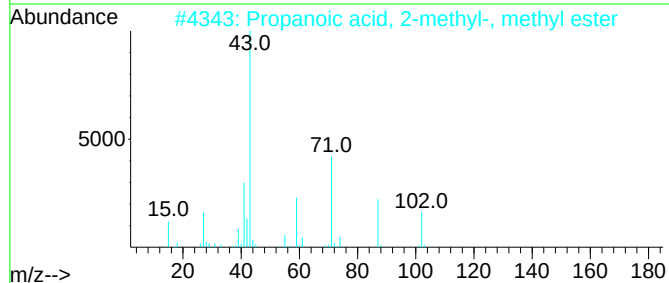
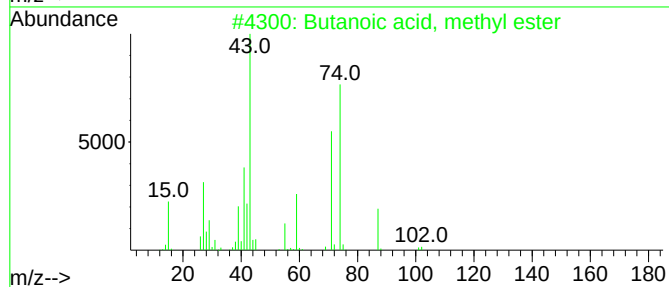
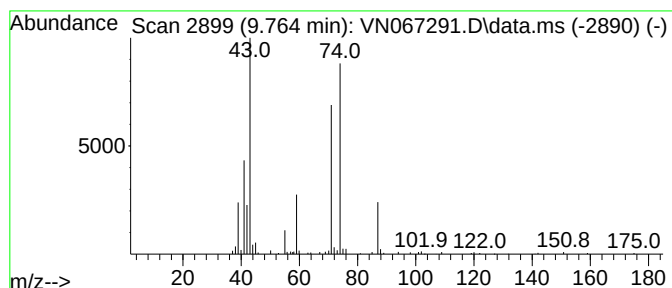
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.764	5.88 ug/l	206115	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	87
2	Propanoic acid, 2-methyl-, methy...	102	C5H10O2	000547-63-7	37
3	Methyl valerate	116	C6H12O2	000624-24-8	23
4	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	14
5	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	10



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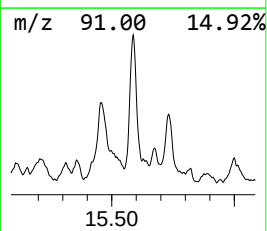
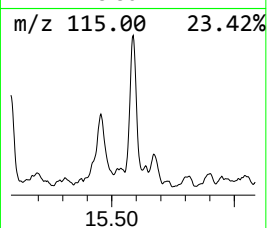
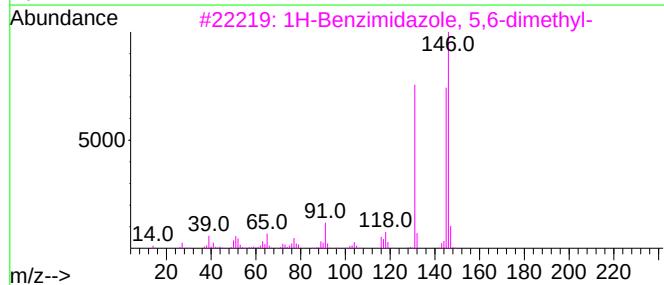
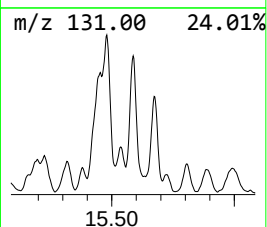
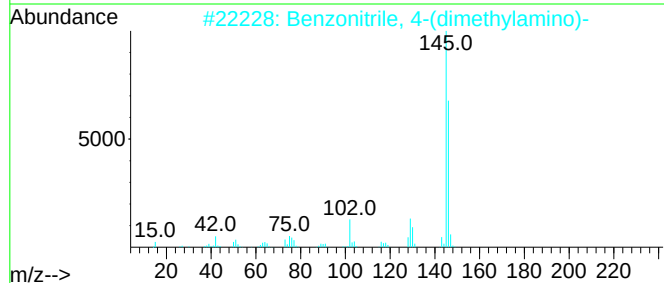
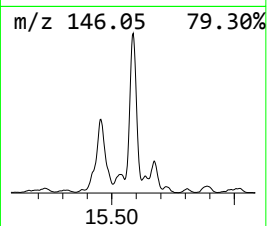
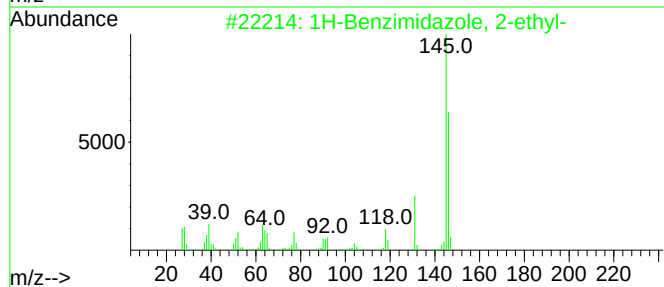
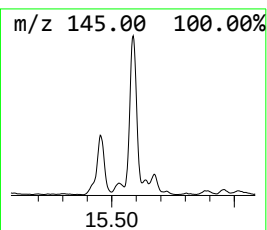
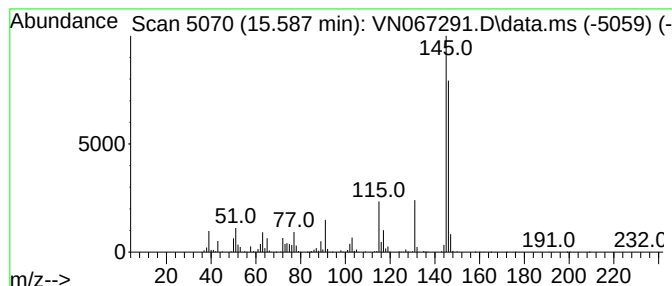
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Benzimidazole, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.587	19.21 ug/l	1648850	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	59
2			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
3			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	50
4			1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	49
5			2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	45



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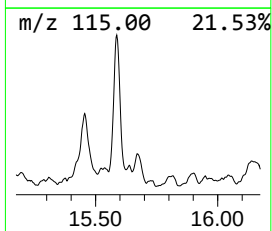
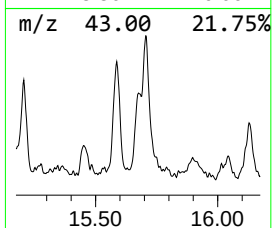
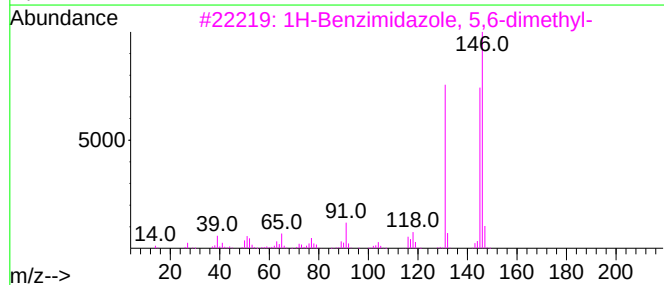
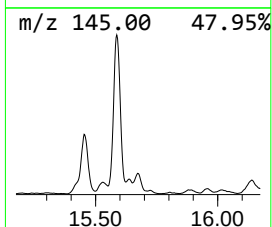
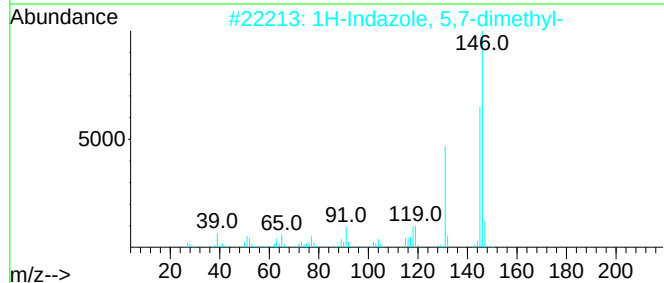
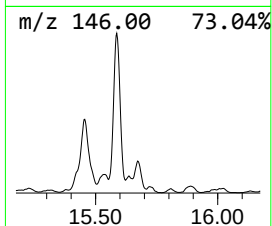
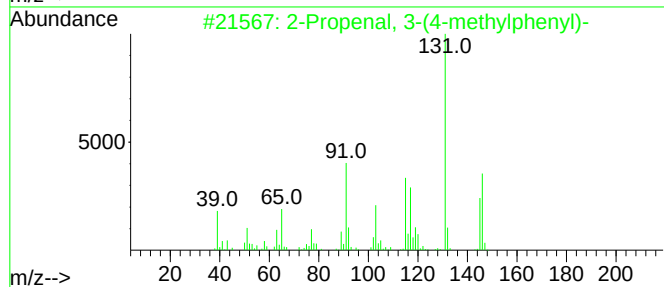
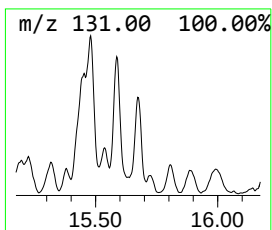
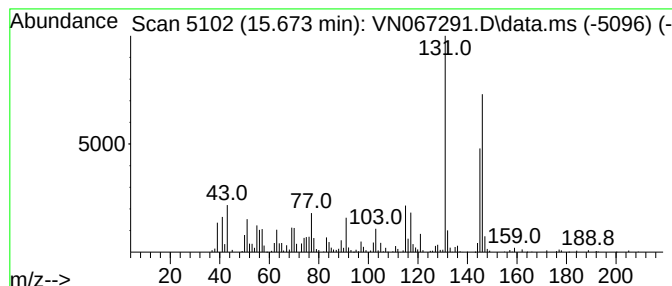
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Peak Number 4 2-Propenal, 3-(4-methylphen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.673	9.39 ug/l	806077	1,4-Dichlorobenzene-d4	13.677

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	91
2		1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	83
3		1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	74
4		Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	72
5		2-(2-Hydroxyphenyl)buta-1,3-diene	146	C10H10O	038865-47-3	64



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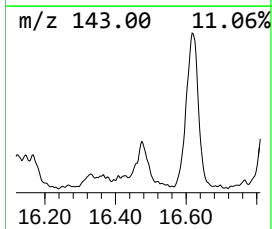
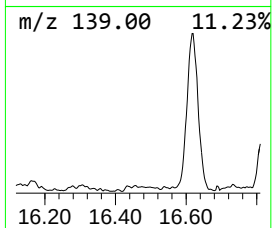
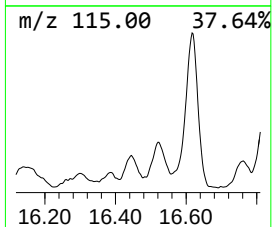
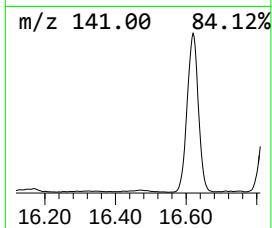
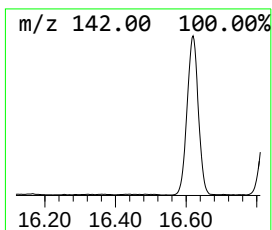
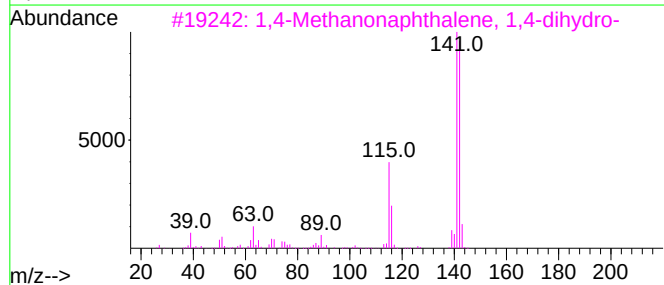
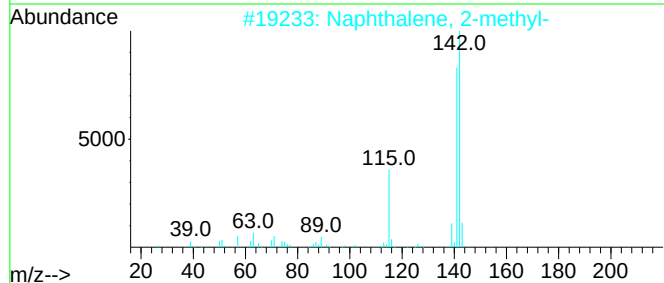
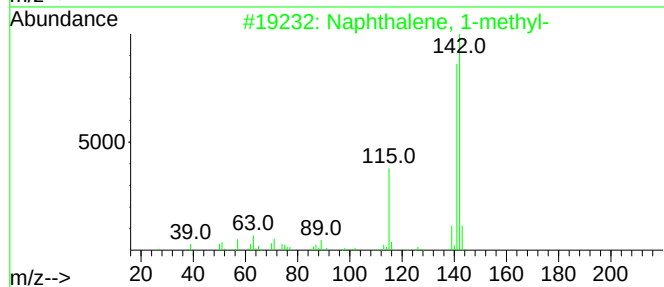
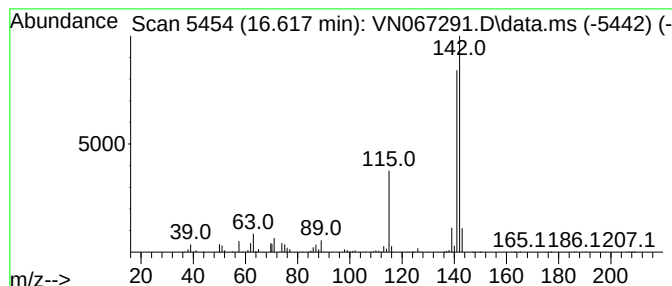
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.617	19.36 ug/l	1661070	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methyl propionate	7.844	9.5	ug/l	250363	1	8.085	1323700	50.0
Butanoic acid, ...	9.764	5.9	ug/l	206115	2	8.968	1753040	50.0
1H-Benzimidazol...	15.587	19.2	ug/l	1648850	4	13.677	4290620	50.0
2-Propenal, 3-(...	15.673	9.4	ug/l	806077	4	13.677	4290620	50.0
Naphthalene, 1-...	16.617	19.4	ug/l	1661070	4	13.677	4290620	50.0