

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD041922\
 Data File : VD072628.D
 Acq On : 19 Apr 2022 16:47
 Operator : VA/SY
 Sample : N2445-01
 Misc : 5.05G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 282

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_D\Method\82D032922S.M
 Title : SW846 8260

Signal : TIC: VD072628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.156	377	380	390	rVB3	4496	10495	1.73%	0.268%
2	4.962	508	517	527	rBV6	6134	17842	2.94%	0.455%
3	5.173	543	553	554	rBV2	15139	26978	4.45%	0.689%
4	7.191	885	896	904	rBV	25803	71929	11.86%	1.836%
5	7.914	1007	1019	1024	rBV2	99346	255238	42.10%	6.514%
6	7.973	1024	1029	1042	rVB	125814	270708	44.65%	6.909%
7	8.326	1074	1089	1100	rVB2	144912	342608	56.51%	8.744%
8	8.861	1170	1180	1190	rBV	200687	400816	66.11%	10.229%
9	9.567	1293	1300	1308	rBV	29105	55643	9.18%	1.420%
10	10.332	1421	1430	1439	rBV	311957	563640	92.96%	14.385%
11	10.573	1465	1471	1479	rVB3	24475	43261	7.14%	1.104%
12	10.720	1490	1496	1504	rBV4	15509	29947	4.94%	0.764%
13	11.073	1550	1556	1564	rBV2	40186	70038	11.55%	1.787%
14	11.638	1644	1652	1665	rVB	343860	600048	98.97%	15.314%
15	12.620	1813	1819	1827	rBV	264723	444053	73.24%	11.333%
16	12.943	1870	1874	1879	rVB4	3902	7019	1.16%	0.179%
17	13.561	1972	1979	1986	rVB	365252	606319	100.00%	15.474%
18	13.761	2008	2013	2020	rBV3	12150	21812	3.60%	0.557%
19	15.385	2285	2289	2296	rVB4	9323	16317	2.69%	0.416%
20	16.484	2470	2476	2481	rVB8	9181	22565	3.72%	0.576%
21	16.679	2501	2509	2519	rBV5	16393	41034	6.77%	1.047%

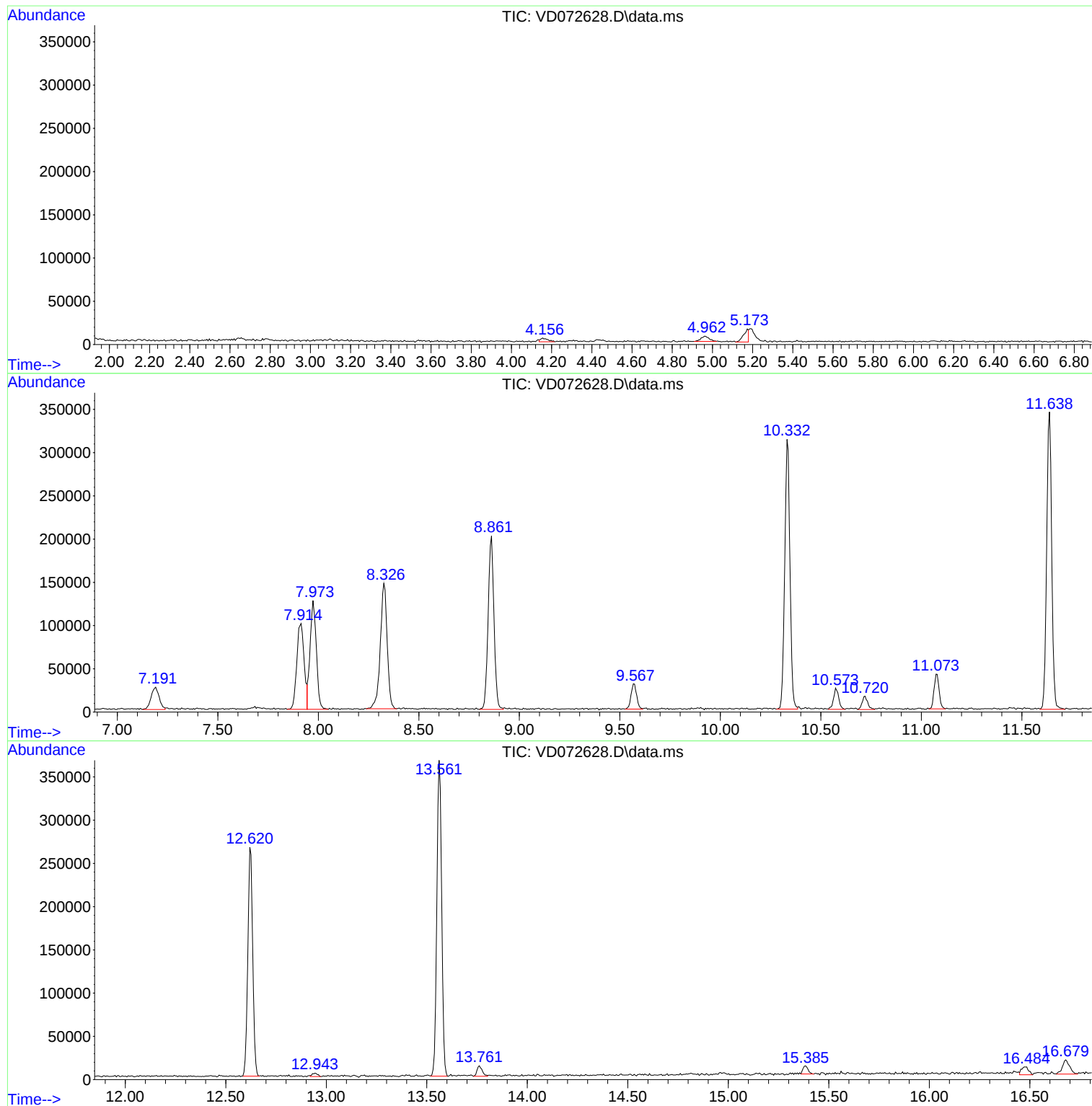
Sum of corrected areas: 3918310

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D032922S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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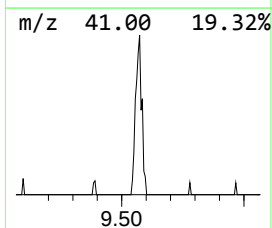
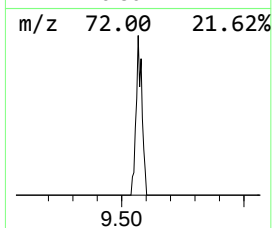
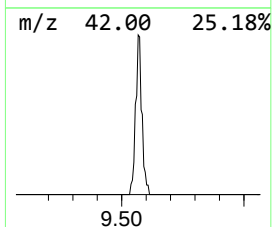
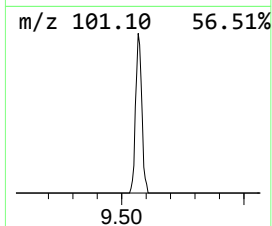
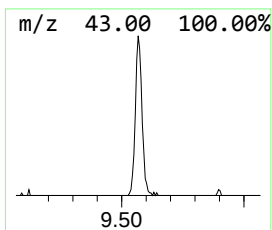
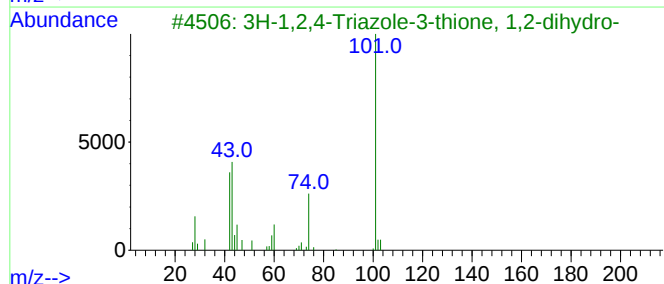
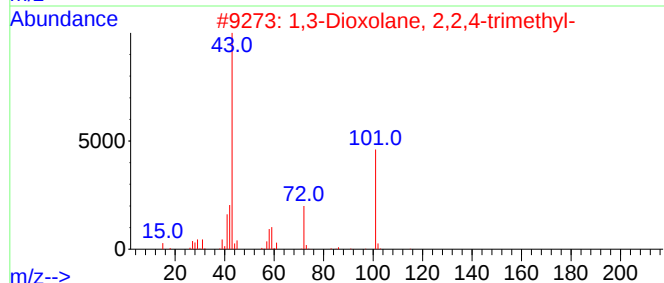
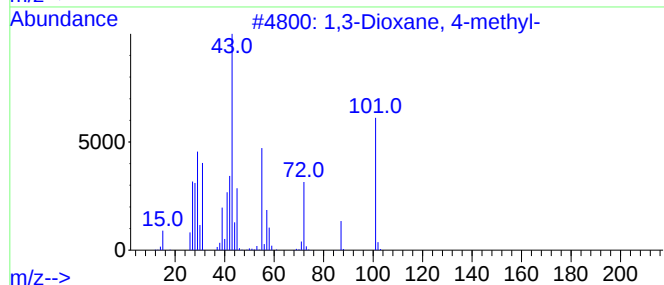
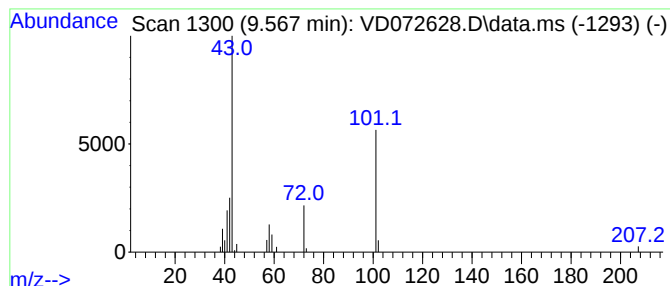
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D032922S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxane, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	6.94 ug/l	55643	1,4-Difluorobenzene	8.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	86
2			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	72
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	47
4			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	42
5			1,3-Dioxolane-2-acetic acid, 2,4-...	188	C9H16O4	090293-83-7	40



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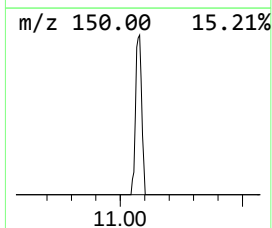
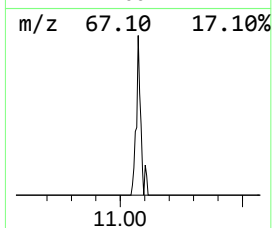
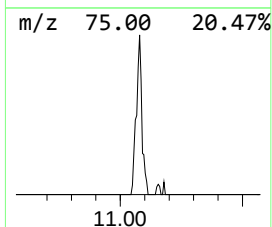
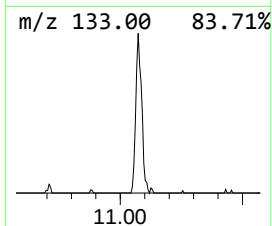
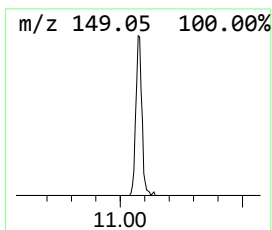
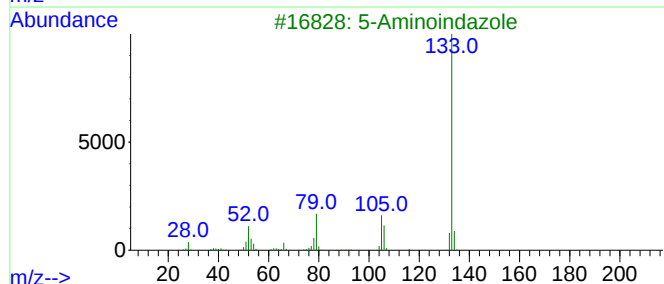
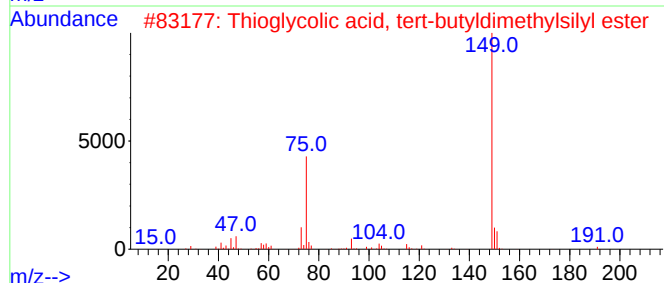
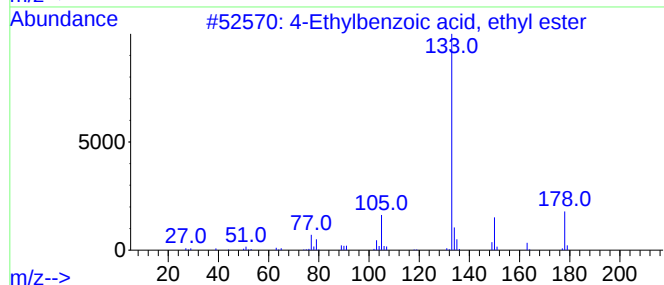
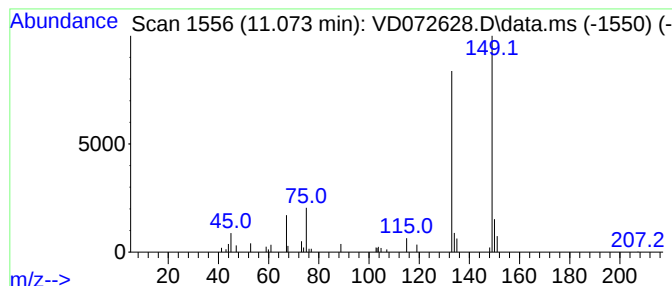
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Peak Number 3 4-Ethylbenzoic acid, ethyl ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	5.84 ug/l	70038	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzoic acid, ethyl ester	178	C11H14O2	036207-13-3	32
2			Thioglycolic acid, tert-butyldim...	206	C8H18O2SSi	1000476-01-2	32
3			5-Aminoindazole	133	C7H7N3	019335-11-6	22
4			4-Ethylbenzoic acid, 1-(cyclopen...	246	C16H22O2	1010293-32-2	17
5			4-Ethylbenzoic acid, 2-ethoxyeth...	222	C13H18O3	1000331-30-9	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Dioxane, 4-...	9.567	6.9	ug/l	55643	2	8.861	400816	50.0
4-Ethylbenzoic ...	11.073	5.8	ug/l	70038	3	11.638	600048	50.0