

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110221\
 Data File : VU045506.D
 Acq On : 01 Nov 2021 22:45
 Operator : SY/MD
 Sample : M4438-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 FDR-20211101-WC-LM

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_U\Method\82U102821W.M
 Title : SW846 8260

Signal : TIC: VU045506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.700	105	112	134	rVB2	5857	13840	1.04%	0.168%
2	2.639	392	404	426	rVB	28686	58232	4.39%	0.708%
3	2.800	439	454	483	rBV2	16056	38910	2.93%	0.473%
4	4.456	954	969	989	rBV4	6527	19015	1.43%	0.231%
5	5.295	1212	1230	1243	rBV	189664	403629	30.40%	4.910%
6	5.379	1243	1256	1280	rVB	290525	602367	45.36%	7.327%
7	5.707	1343	1358	1372	rBV	227056	458104	34.50%	5.572%
8	6.253	1510	1528	1557	rBV	486680	924554	69.62%	11.246%
9	6.391	1558	1571	1594	rVB	63170	125182	9.43%	1.523%
10	7.903	2020	2041	2059	rBV	764472	1327937	100.00%	16.153%
11	8.170	2113	2124	2136	rBV	14241	25400	1.91%	0.309%
12	8.337	2166	2176	2194	rVB2	12227	19629	1.48%	0.239%
13	8.491	2214	2224	2235	rVB2	8693	14958	1.13%	0.182%
14	8.684	2274	2284	2295	rBV4	7952	13723	1.03%	0.167%
15	9.141	2416	2426	2441	rVB	19381	31454	2.37%	0.383%
16	9.420	2493	2513	2543	rVB	716117	1181915	89.00%	14.377%
17	9.645	2573	2583	2593	rVB2	22094	34823	2.62%	0.424%
18	10.359	2794	2805	2819	rBV5	8298	22017	1.66%	0.268%
19	10.539	2849	2861	2873	rBV4	7594	13884	1.05%	0.169%
20	10.636	2878	2891	2913	rVV	563652	905514	68.19%	11.015%
21	11.189	3055	3063	3074	rVB2	9454	14627	1.10%	0.178%
22	11.420	3121	3135	3145	rBV	150659	243286	18.32%	2.959%
23	11.745	3227	3236	3245	rVB2	25339	38871	2.93%	0.473%
24	11.816	3245	3258	3274	rBV	772177	1220492	91.91%	14.846%
25	12.240	3371	3390	3402	rBV2	20521	47593	3.58%	0.579%
26	12.687	3518	3529	3548	rVB	92048	148015	11.15%	1.800%
27	12.951	3600	3611	3622	rBV5	11166	23597	1.78%	0.287%
28	13.246	3693	3703	3718	rVB10	10191	26447	1.99%	0.322%
29	13.333	3721	3730	3741	rBV2	17073	28912	2.18%	0.352%
30	13.472	3766	3773	3790	rVB5	10722	20884	1.57%	0.254%
31	13.574	3793	3805	3815	rBV3	22359	47017	3.54%	0.572%
32	13.632	3816	3823	3834	rVV2	31616	51443	3.87%	0.626%
33	13.700	3837	3844	3854	rVB4	9857	15942	1.20%	0.194%
34	13.800	3863	3875	3883	rBV10	5991	14087	1.06%	0.171%
35	13.986	3928	3933	3944	rVB3	11775	15997	1.20%	0.195%
36	14.517	4091	4098	4109	rVB2	18264	28588	2.15%	0.348%

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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_U\Method\82U102821W.M
Title : SW846 8260

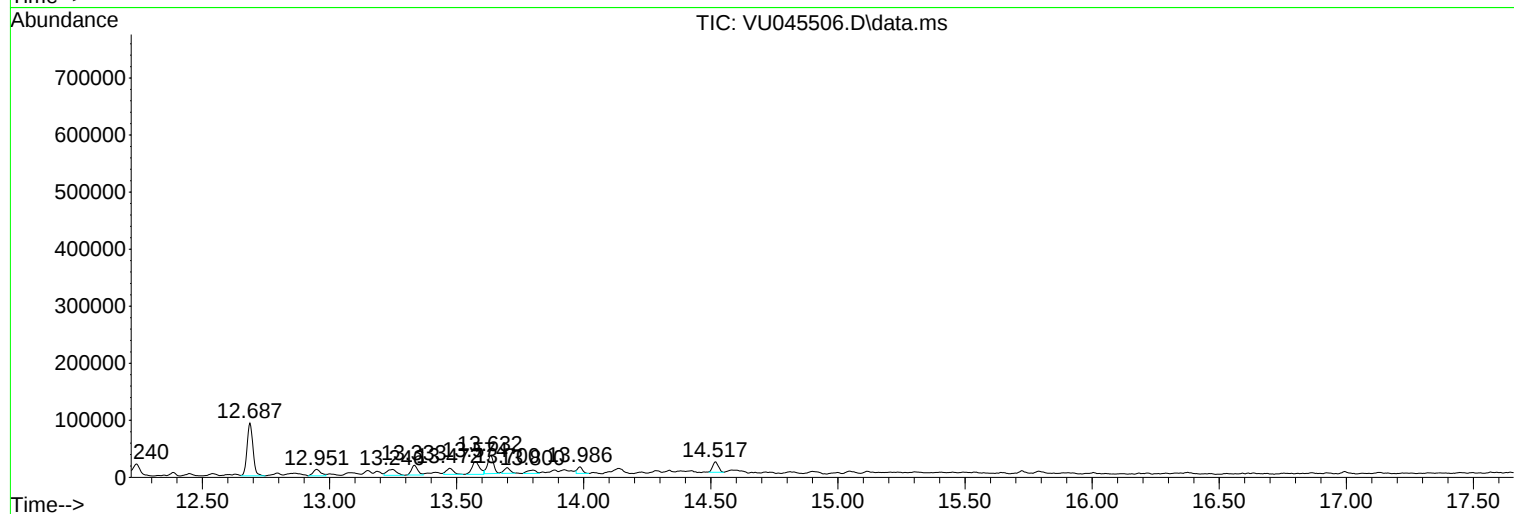
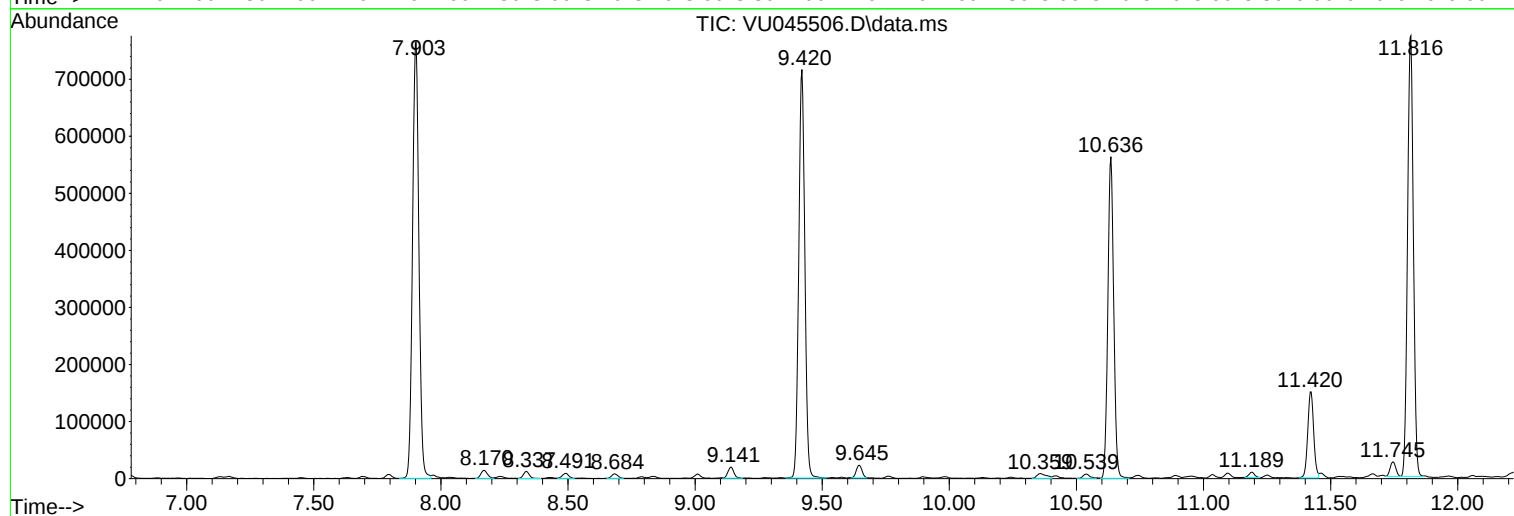
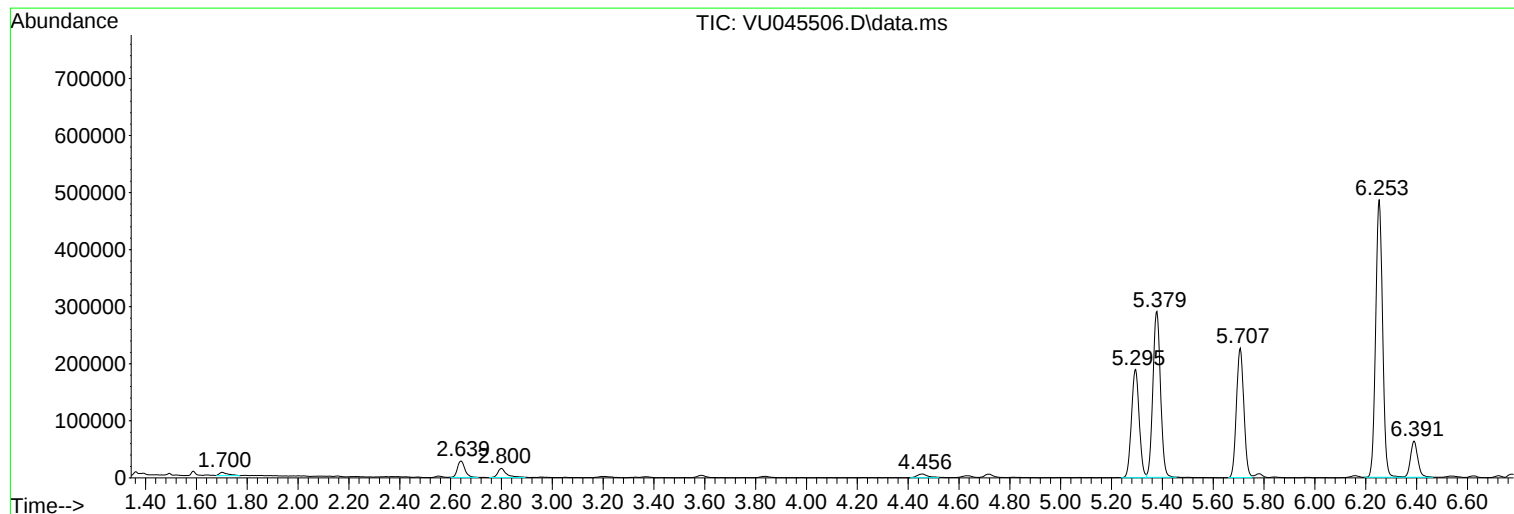
Sum of corrected areas: 8220885

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U102821W.M
Quant Title : SW846 8260

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



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
FDR-20211101-WC-LM

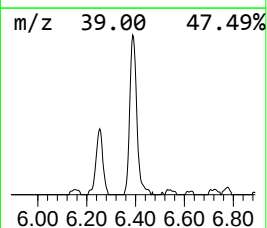
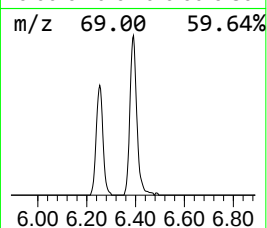
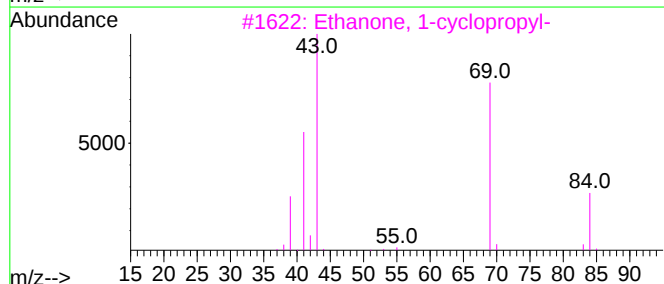
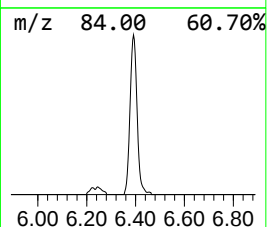
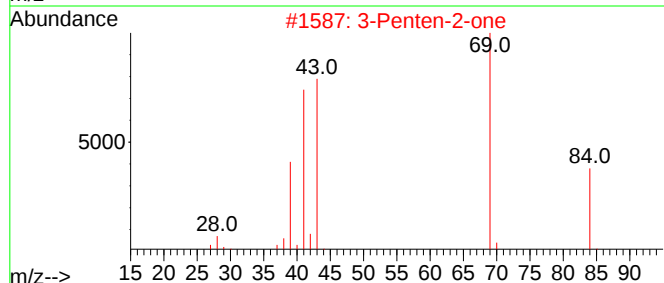
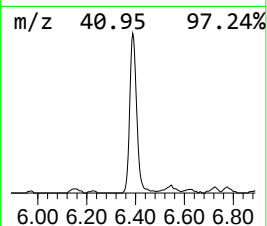
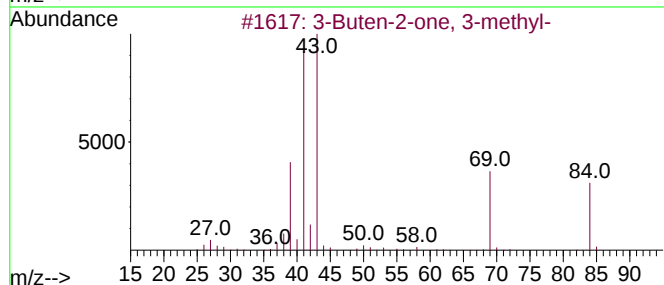
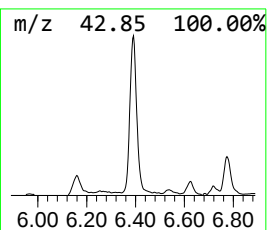
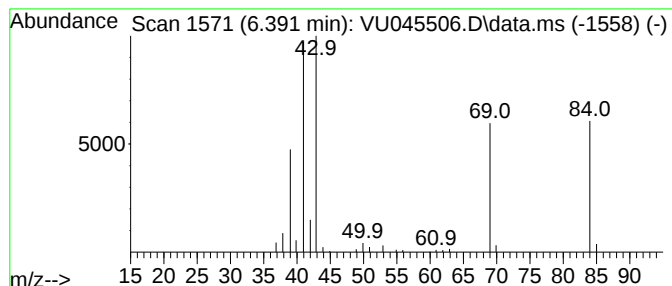
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U102821W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Buten-2-one, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.391	6.77 ug/l	125182	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2			3-Penten-2-one	84	C5H8O	000625-33-2	90
3			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	90
4			3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	47
5			2-Butanone, 4-hydroxy-3-(hydroxy...	132	C6H12O3	006868-97-9	42



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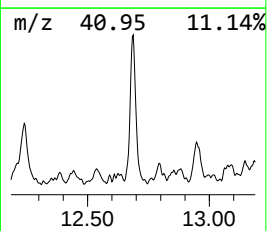
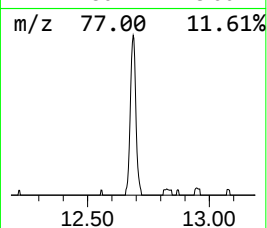
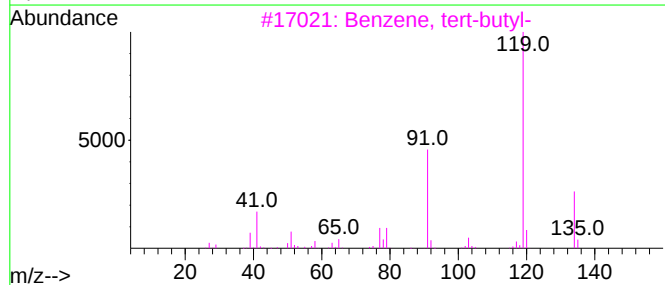
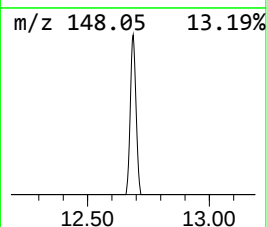
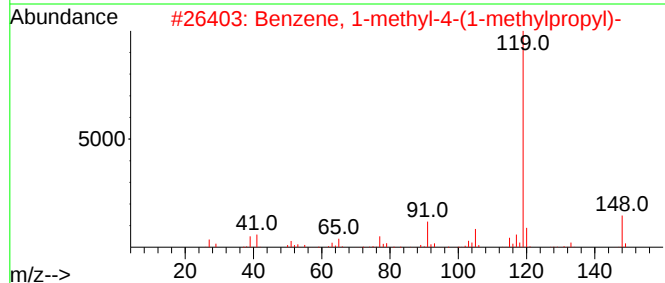
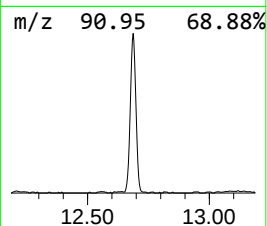
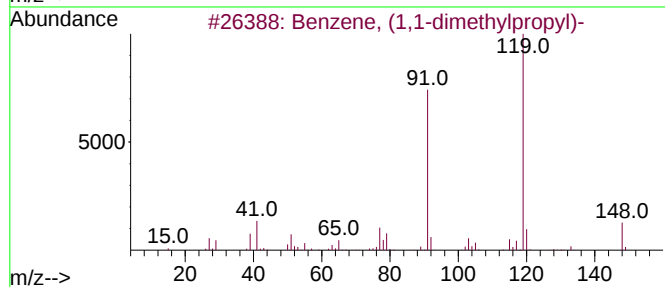
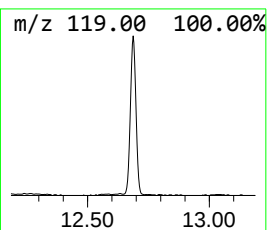
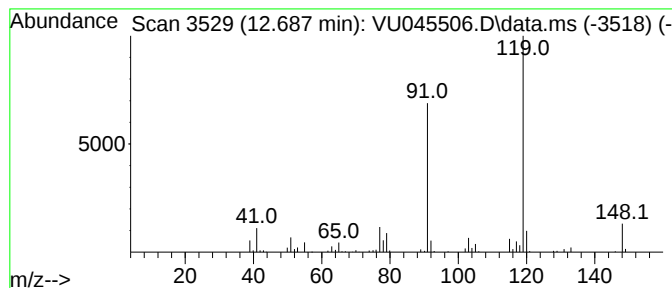
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzene, (1,1-dimethylpropyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.687	6.06 ug/l	148015	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	97
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	90
3			Benzene, tert-butyl-	134	C10H14	000098-06-6	86
4			Benzene, (1-ethylpropyl)-	148	C11H16	001196-58-3	80
5			Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	72



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-2-one, ...	6.391	6.8	ug/l	125182	2	6.253	924554	50.0
Benzene, (1,1-d...	12.687	6.1	ug/l	148015	4	11.816	1220490	50.0