

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
 Data File : VU042858.D
 Acq On : 31 Mar 2021 15:31
 Operator : SY/MD
 Sample : M1836-02
 Misc : 11.22g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 B1-10-12

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\82U032421W.M
 Title : SW846 8260

Signal : TIC: VU042858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.809	128	146	147	rBV9	4382	9077	1.28%	0.126%
2	1.960	187	193	211	rVB4	18991	44884	6.32%	0.624%
3	2.449	336	345	359	rVB2	6775	11220	1.58%	0.156%
4	3.221	568	585	595	rBV2	8647	23804	3.35%	0.331%
5	3.353	610	626	655	rVB5	62365	214193	30.16%	2.978%
6	4.526	975	991	992	rBV5	5821	8150	1.15%	0.113%
7	5.295	1215	1230	1243	rBV	107502	225375	31.73%	3.133%
8	5.378	1243	1256	1272	rVV	180107	373115	52.54%	5.187%
9	5.465	1274	1283	1293	rVB6	3486	7287	1.03%	0.101%
10	5.591	1312	1322	1335	rBB6	3772	7335	1.03%	0.102%
11	5.710	1343	1359	1369	rBV	123308	248770	35.03%	3.458%
12	5.777	1369	1380	1398	rVB	287860	575023	80.97%	7.994%
13	5.902	1407	1419	1435	rBV4	22802	50698	7.14%	0.705%
14	6.253	1513	1528	1548	rBV	253113	486767	68.54%	6.767%
15	6.767	1673	1688	1696	rBV6	4444	10900	1.53%	0.152%
16	7.259	1828	1841	1856	rVB2	19308	37058	5.22%	0.515%
17	7.388	1868	1881	1891	rBV4	20027	43914	6.18%	0.610%
18	7.661	1959	1966	1984	rVB5	3882	8265	1.16%	0.115%
19	7.844	2012	2023	2029	rBV3	5289	9929	1.40%	0.138%
20	7.906	2029	2042	2056	rVV	394485	682155	96.05%	9.483%
21	7.976	2056	2064	2075	rVB2	12434	20693	2.91%	0.288%
22	8.738	2286	2301	2314	rBV5	2639	8202	1.15%	0.114%
23	9.426	2499	2515	2532	rBV	360536	626437	88.21%	8.708%
24	9.578	2549	2562	2576	rBV	162099	267097	37.61%	3.713%
25	9.700	2587	2600	2611	rBV	85492	144300	20.32%	2.006%
26	10.108	2714	2727	2737	rBV2	27787	45616	6.42%	0.634%
27	10.494	2830	2847	2857	rBV2	18172	29064	4.09%	0.404%
28	10.645	2881	2894	2913	rVB	332298	556662	78.38%	7.738%
29	10.915	2960	2978	2992	rBV	69967	119942	16.89%	1.667%
30	11.008	2994	3007	3024	rBV	39160	87612	12.34%	1.218%
31	11.095	3025	3034	3051	rVB2	26151	45185	6.36%	0.628%
32	11.301	3085	3098	3109	rBV2	34877	53898	7.59%	0.749%
33	11.478	3139	3153	3167	rVB	93465	145764	20.52%	2.026%
34	11.822	3248	3260	3274	rBV	450288	710184	100.00%	9.873%
35	11.905	3274	3286	3294	rVV2	24980	38485	5.42%	0.535%
36	12.105	3332	3348	3365	rBV3	115013	196559	27.68%	2.732%

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37	12.195	3365	3376	3391	rVB4	29416	68442	9.64%	0.951%
38	12.317	3405	3414	3425	rBV8	5648	12089	1.70%	0.168%
39	12.385	3425	3435	3448	rVB	17385	26000	3.66%	0.361%
40	12.475	3452	3463	3468	rBV4	11629	18517	2.61%	0.257%
41	12.503	3468	3472	3481	rVV3	7766	10585	1.49%	0.147%
42	12.581	3483	3496	3504	rVV	57608	88529	12.47%	1.231%
43	12.622	3504	3509	3521	rVV4	10077	13626	1.92%	0.189%
44	12.693	3521	3531	3550	rVB2	26420	50092	7.05%	0.696%
45	12.983	3606	3621	3629	rBV	35866	55133	7.76%	0.766%
46	13.034	3629	3637	3648	rVB	16161	25021	3.52%	0.348%
47	13.114	3652	3662	3670	rBV5	4617	7879	1.11%	0.110%
48	13.301	3711	3720	3732	rVB	34319	52673	7.42%	0.732%
49	13.462	3747	3770	3784	rBV2	65921	124406	17.52%	1.729%
50	13.635	3815	3824	3836	rVB4	9231	14739	2.08%	0.205%
51	13.796	3865	3874	3881	rVV3	8298	12764	1.80%	0.177%
52	13.847	3881	3890	3904	rVB7	11969	21818	3.07%	0.303%
53	13.950	3916	3922	3939	rVB4	8119	16894	2.38%	0.235%
54	14.095	3954	3967	3987	rBV	174828	279756	39.39%	3.889%
55	14.497	4083	4092	4100	rVB	6626	9158	1.29%	0.127%
56	14.677	4139	4148	4160	rBV6	5648	11476	1.62%	0.160%
57	15.233	4310	4321	4334	rBV	40213	64991	9.15%	0.903%
58	15.420	4369	4379	4391	rBV3	21358	35269	4.97%	0.490%

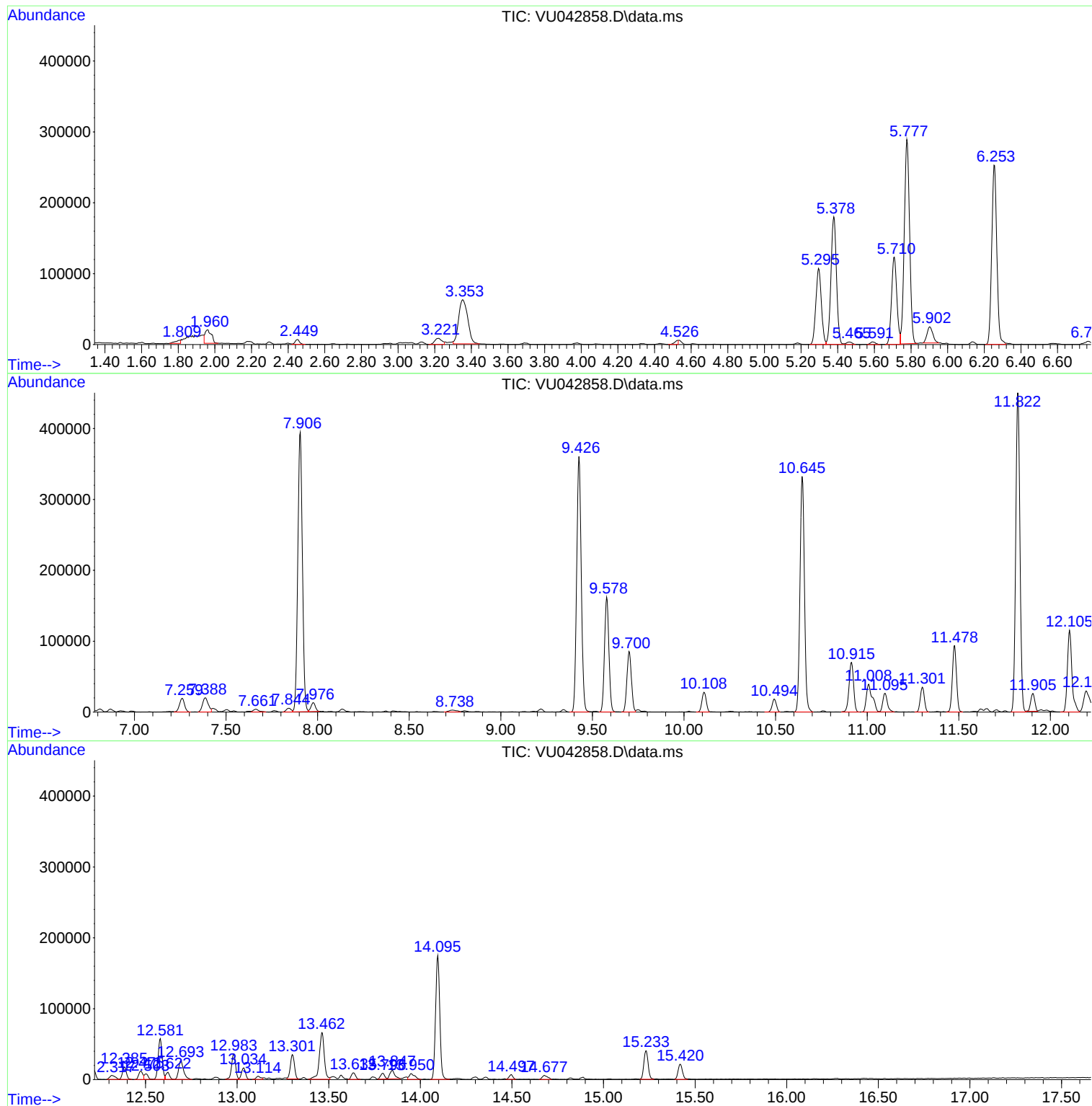
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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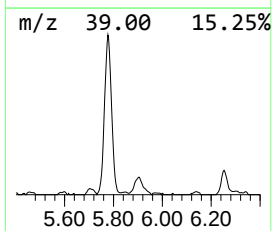
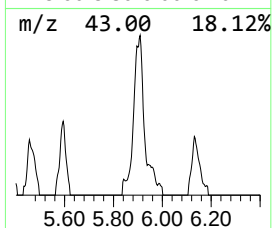
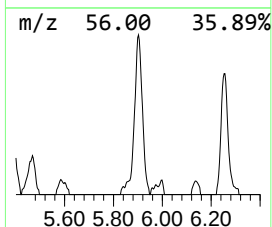
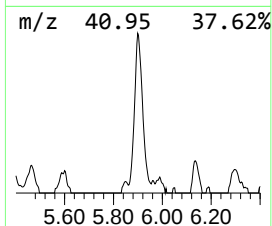
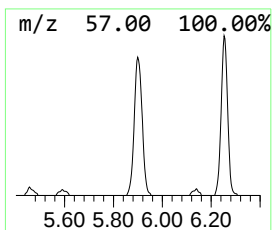
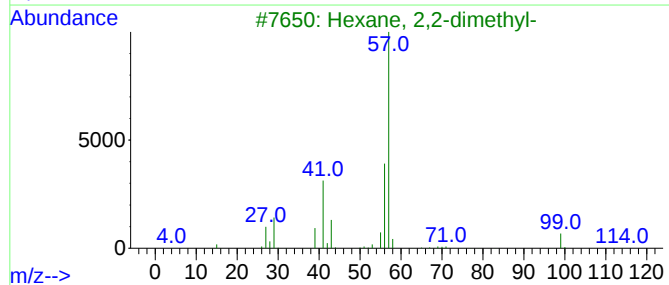
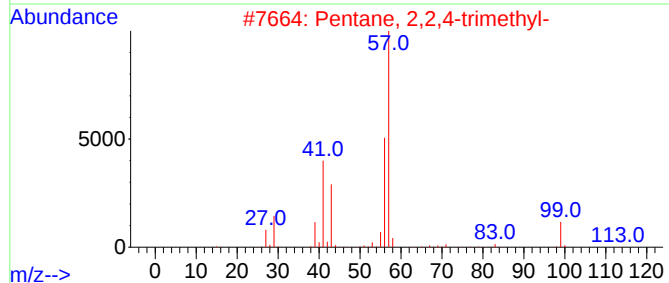
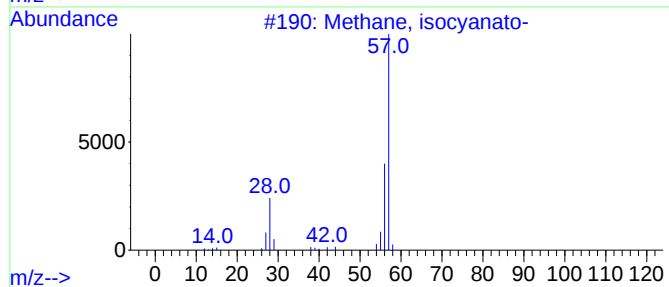
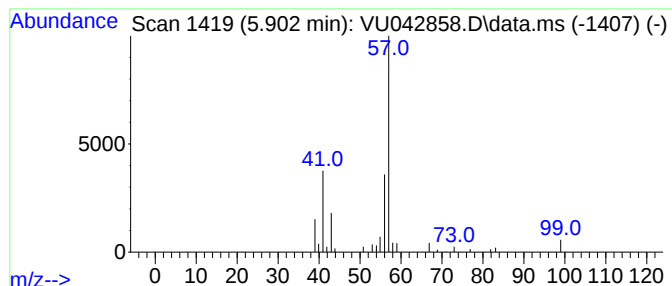
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 2 Methane, isocyanato- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	5.21 ug/l	50698	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, isocyanato-	57	C2H3NO	000624-83-9	50
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	45
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	45
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42



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Instrument :
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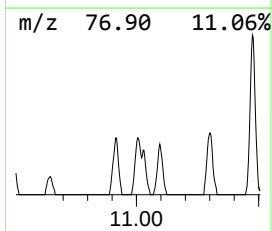
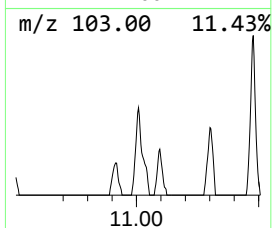
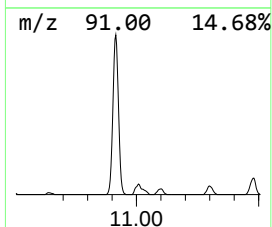
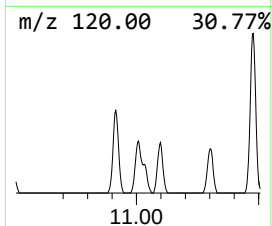
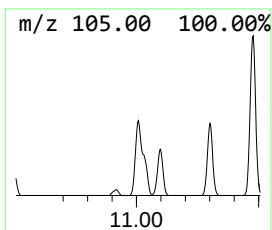
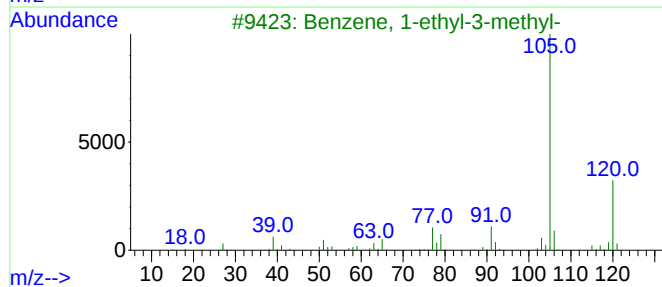
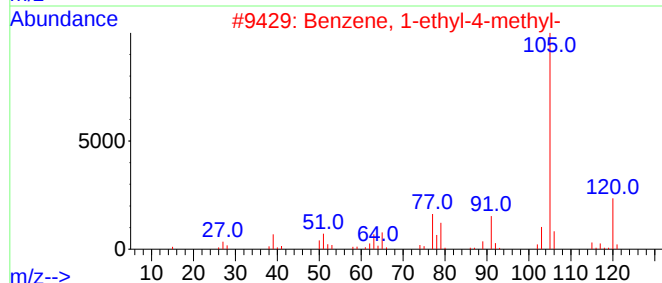
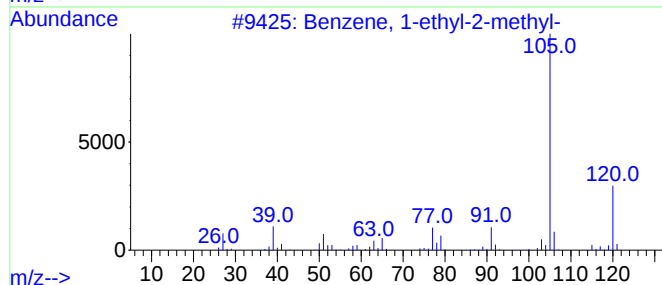
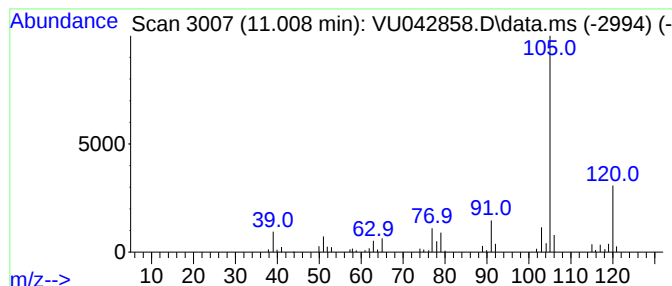
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.008	6.17 ug/l	87612	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	86



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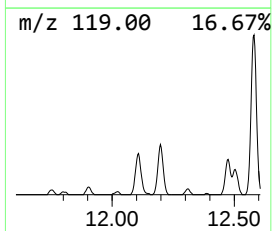
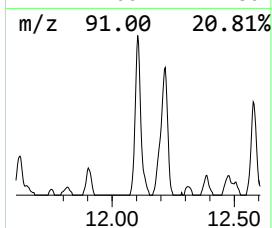
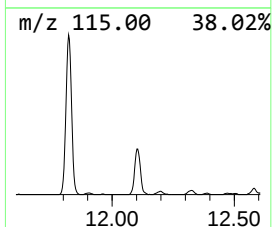
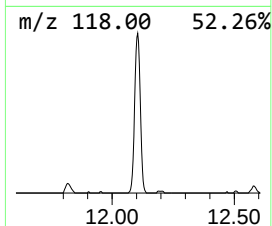
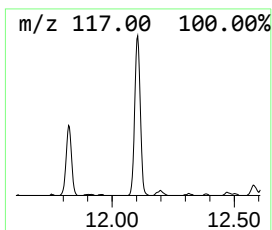
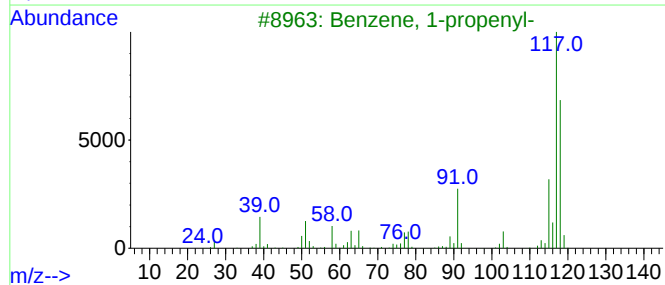
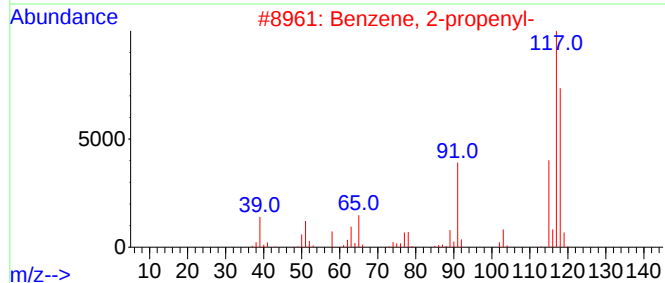
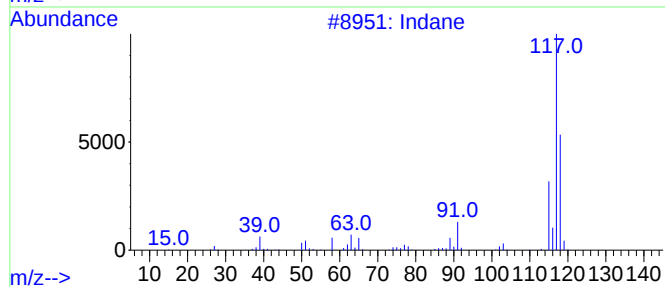
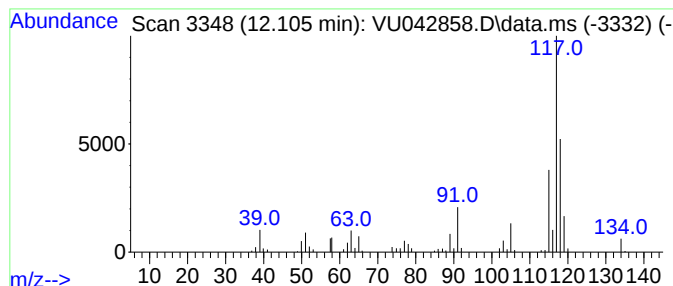
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	13.84 ug/l	196559	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	68
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Deltacyclene	118	C9H10	007785-10-6	58



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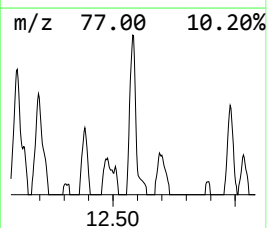
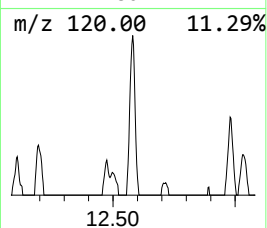
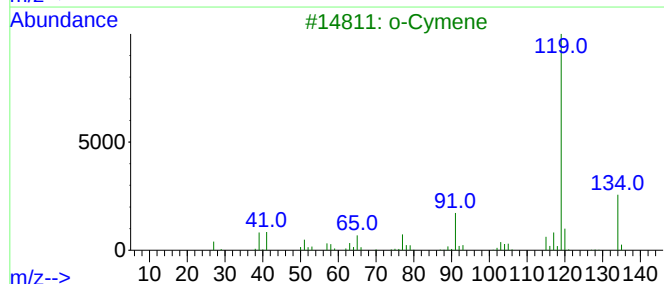
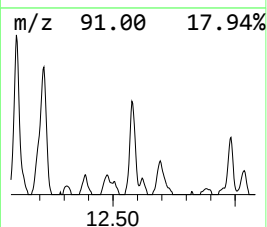
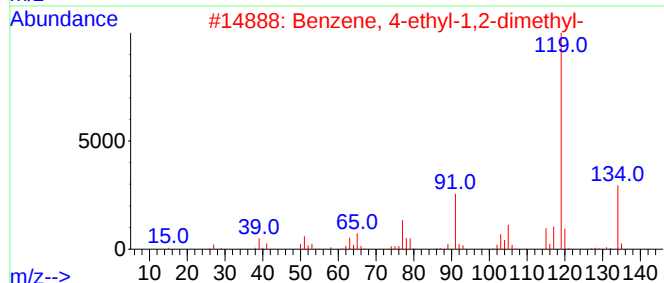
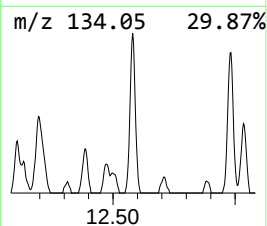
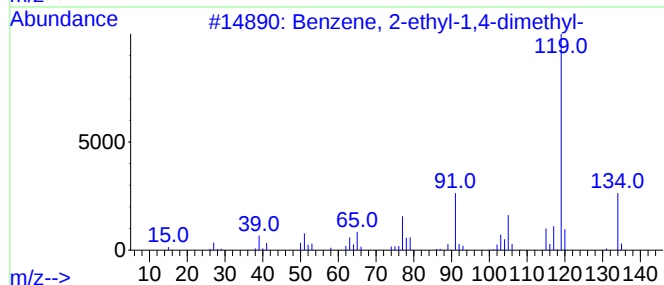
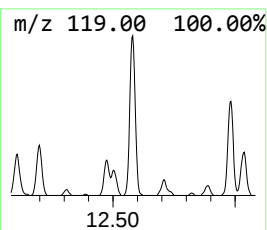
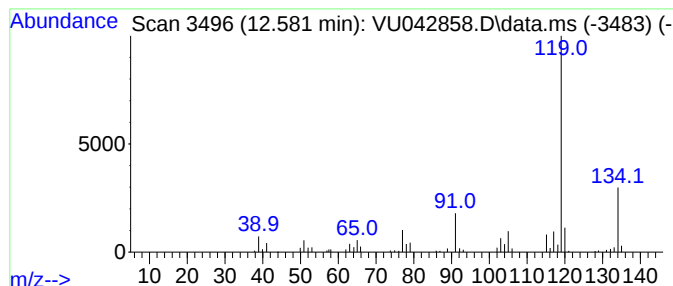
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.581	6.23 ug/l	88529	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



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B1-10-12

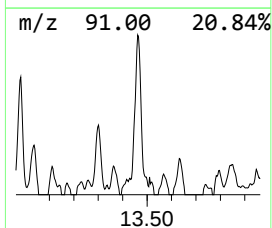
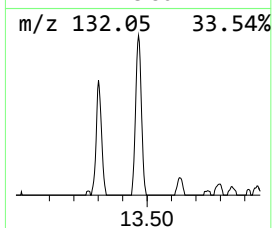
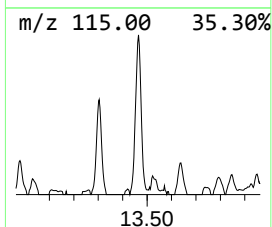
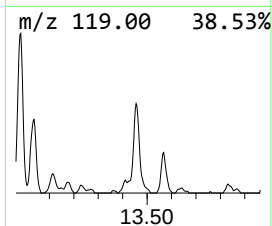
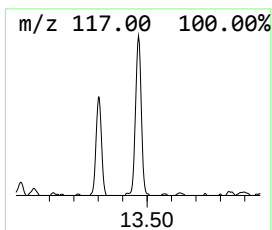
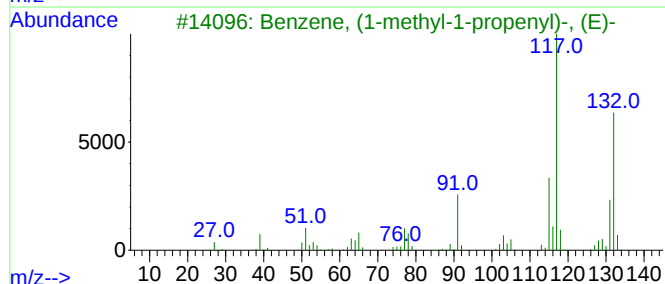
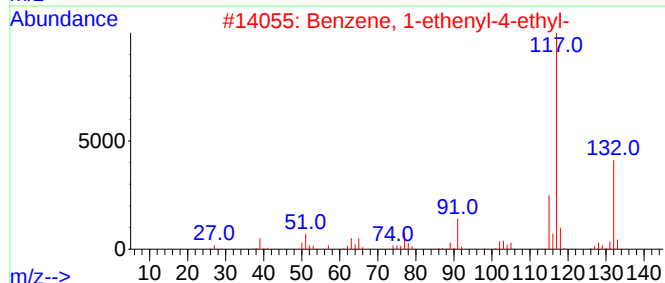
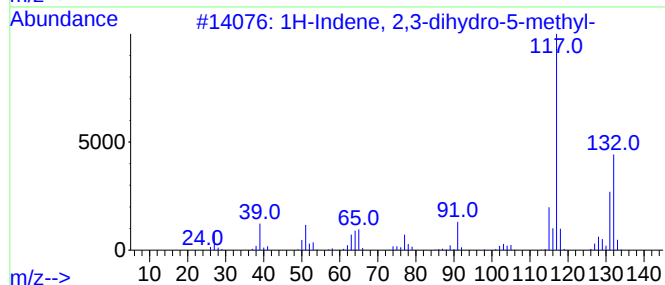
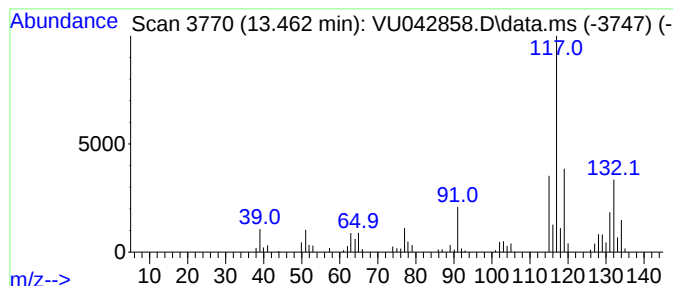
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.462	8.76 ug/l	124406	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
4			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	64
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042858.D
Acq On : 31 Mar 2021 15:31
Operator : SY/MD
Sample : M1836-02
Misc : 11.22g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B1-10-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methane, isocya...	5.902	5.2	ug/l	50698	2	6.256	486767	50.0
Benzene, 1-ethy...	11.008	6.2	ug/l	87612	4	11.822	710184	50.0
Indane	12.105	13.8	ug/l	196559	4	11.822	710184	50.0
Benzene, 2-ethy...	12.581	6.2	ug/l	88529	4	11.822	710184	50.0
1H-Indene, 2,3-...	13.462	8.8	ug/l	124406	4	11.822	710184	50.0