

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
 Data File : VN070240.D
 Acq On : 20 Dec 2021 15:03
 Operator : JC/MD
 Sample : M5044-01
 Misc : 6.43g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-1-4.5

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070240.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	82	91	124	rVB5	56350	166015	1.09%	0.143%
2	5.044	1107	1139	1141	rBV4	58098	162038	1.06%	0.140%
3	5.581	1312	1339	1380	rVB4	64627	236690	1.55%	0.205%
4	7.131	1896	1917	1944	rVV5	85624	253543	1.66%	0.219%
5	8.016	2224	2247	2258	rBV2	902991	2217464	14.53%	1.916%
6	8.080	2259	2271	2290	rVV	1690647	3975547	26.04%	3.436%
7	8.163	2292	2302	2325	rVB4	105221	264278	1.73%	0.228%
8	8.284	2329	2347	2364	rBV2	68025	158428	1.04%	0.137%
9	8.434	2381	2403	2431	rBV2	1188727	2916974	19.11%	2.521%
10	8.606	2461	2467	2490	rVB2	87775	214113	1.40%	0.185%
11	8.963	2578	2600	2634	rBV	2760664	6021954	39.45%	5.205%
12	10.011	2981	2991	3005	rVB3	124593	244976	1.60%	0.212%
13	10.440	3133	3151	3162	rBV	4412549	8251125	54.05%	7.131%
14	10.505	3162	3175	3198	rVB	6364747	12029267	78.80%	10.397%
15	11.744	3620	3637	3657	rBV	4608114	8370428	54.83%	7.234%
16	11.843	3660	3674	3693	rVV	2216814	3782386	24.78%	3.269%
17	11.948	3697	3713	3749	rVV	7797618	15265237	100.00%	13.193%
18	12.278	3821	3836	3856	rBV	4054444	7057805	46.23%	6.100%
19	12.578	3937	3948	3961	rBV2	242500	418162	2.74%	0.361%
20	12.731	3988	4005	4027	rVB	4082874	7323021	47.97%	6.329%
21	12.919	4064	4075	4086	rBV	700946	1111749	7.28%	0.961%
22	12.983	4086	4099	4106	rBV	2542876	4292741	28.12%	3.710%
23	13.058	4119	4127	4146	rVB	1205926	1991824	13.05%	1.721%
24	13.219	4174	4187	4202	rBV	1207293	2080077	13.63%	1.798%
25	13.366	4229	4242	4273	rVB	5228835	8854469	58.00%	7.653%
26	13.672	4342	4356	4401	rVB2	4974000	11665672	76.42%	10.082%
27	13.839	4410	4418	4420	rBV2	160109	188545	1.24%	0.163%
28	13.873	4422	4431	4440	rVV3	804167	1355115	8.88%	1.171%
29	14.128	4517	4526	4532	rBV	318658	504781	3.31%	0.436%
30	14.214	4548	4558	4571	rBV	572989	910476	5.96%	0.787%
31	14.458	4642	4649	4661	rVB2	131718	191619	1.26%	0.166%
32	14.539	4670	4679	4685	rBV	293277	424218	2.78%	0.367%
33	14.579	4686	4694	4703	rVB	412262	600473	3.93%	0.519%
34	14.807	4771	4779	4790	rBV	226048	350184	2.29%	0.303%
35	14.925	4810	4823	4838	rBV3	410439	977270	6.40%	0.845%
36	15.504	5030	5039	5053	rVB2	476166	875704	5.74%	0.757%

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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_N\methods\82N120221W.M
Title : SW846 8260

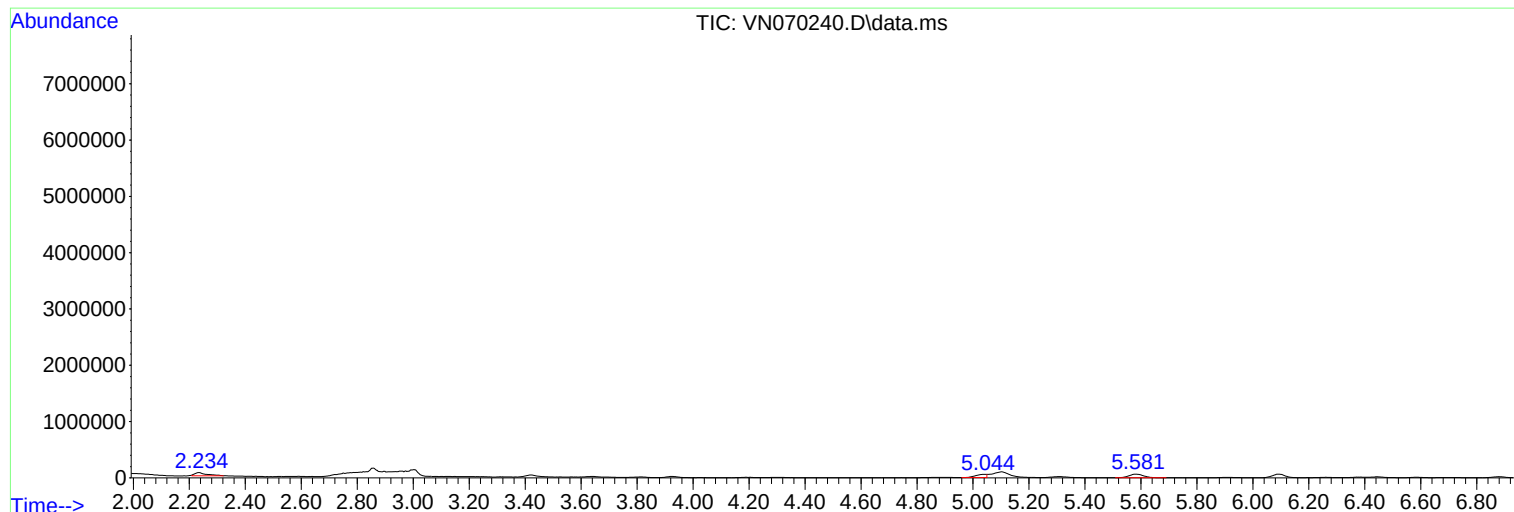
Sum of corrected areas: 115704368

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
DA-1-4.5

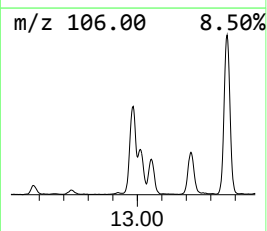
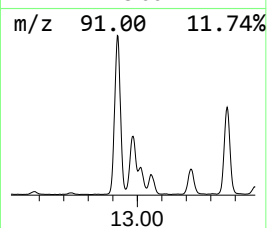
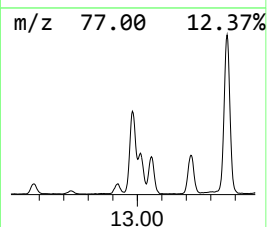
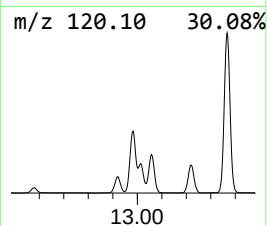
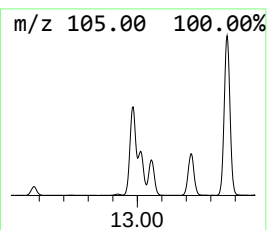
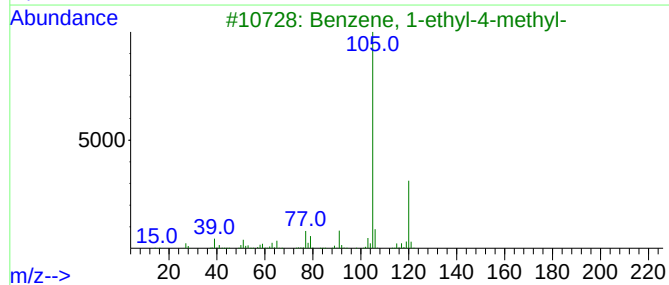
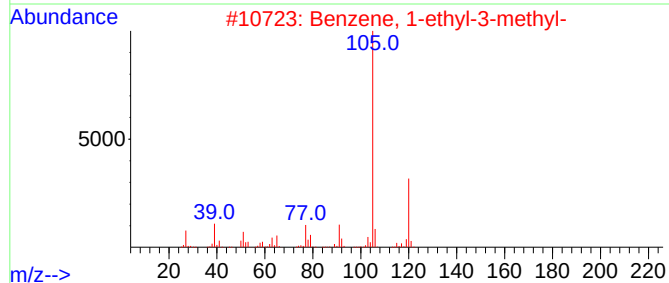
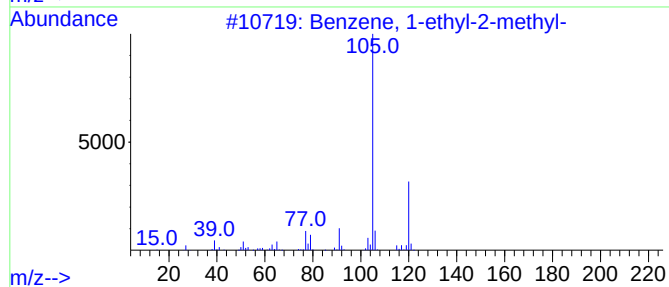
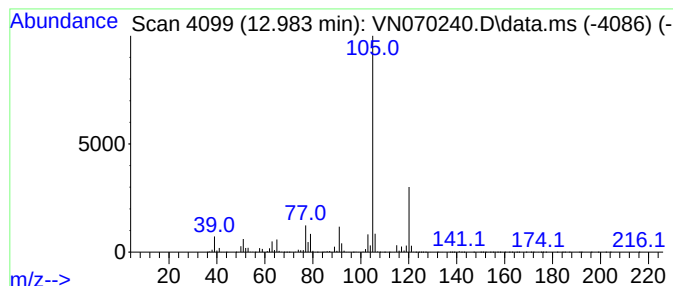
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	18.40 ug/l	4292740	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-1-4.5

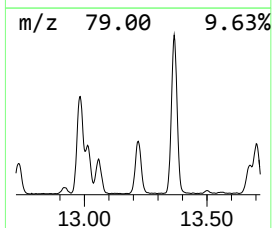
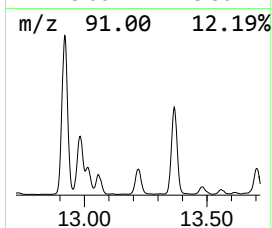
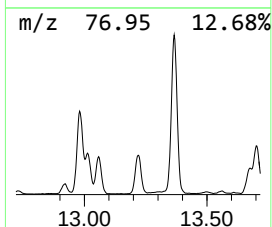
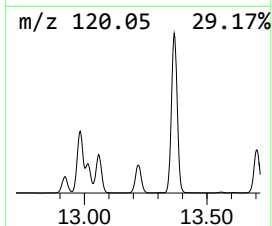
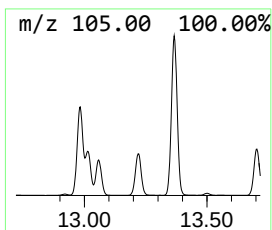
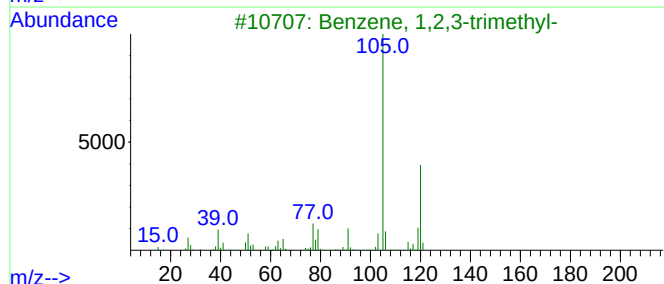
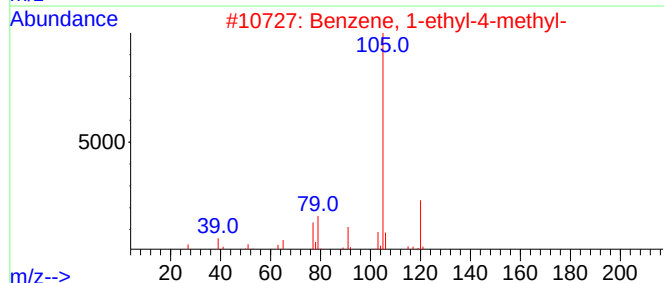
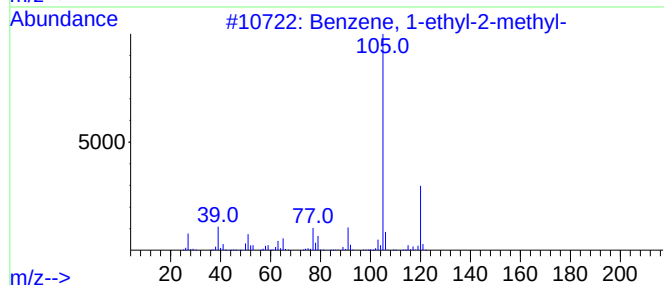
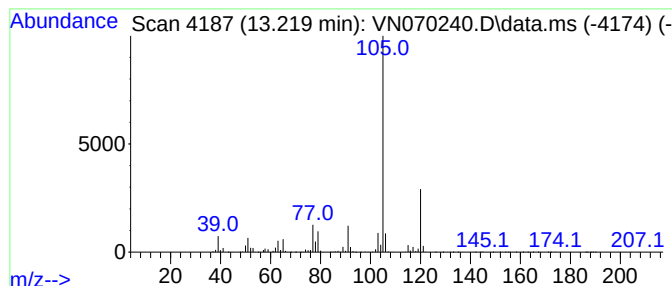
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	8.92 ug/l	2080080	1,4-Dichlorobenzene-d4	13.675

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	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Mesitylene	120	C9H12	000108-67-8	91



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DA-1-4.5

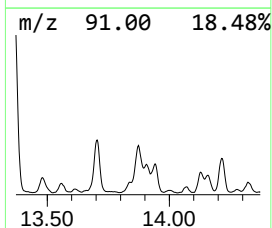
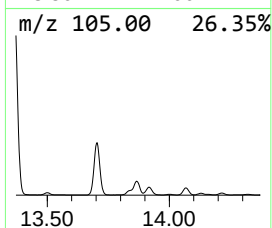
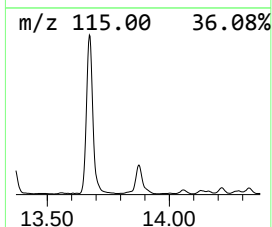
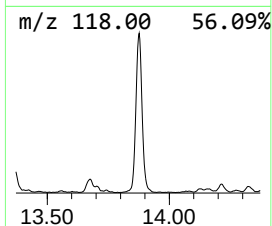
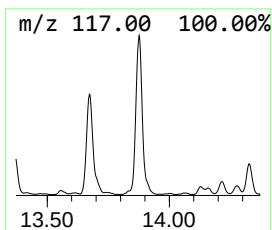
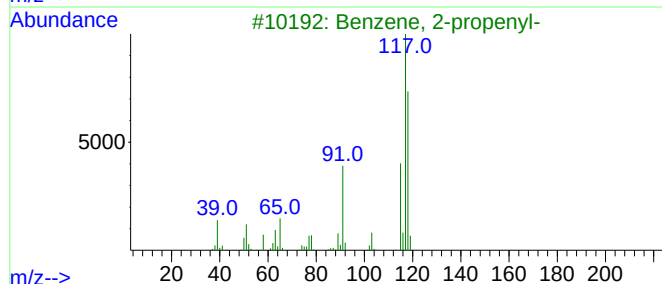
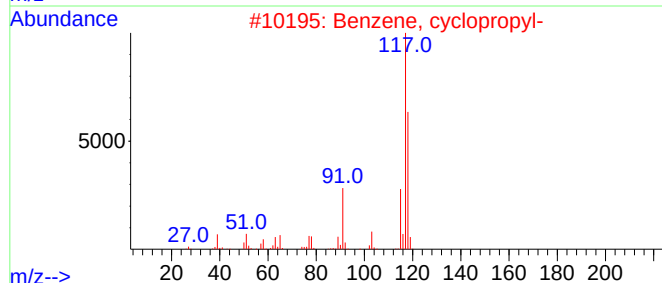
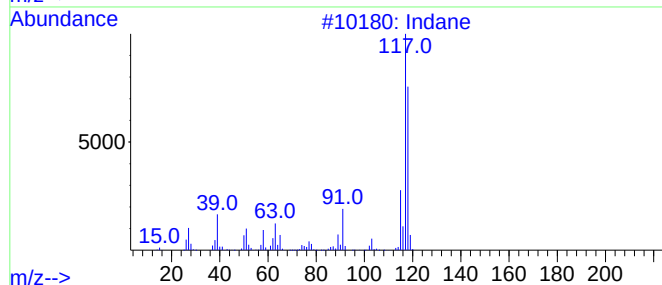
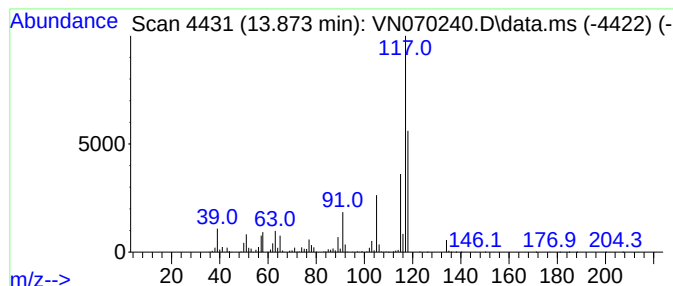
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	5.81 ug/l	1355120	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	92
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethy...	12.983	18.4	ug/l	4292740	4	13.675	11665700	50.0
Benzene, 1-ethy...	13.219	8.9	ug/l	2080080	4	13.675	11665700	50.0
Indane	13.873	5.8	ug/l	1355120	4	13.675	11665700	50.0