

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040221\
 Data File : VN066474.D
 Acq On : 2 Apr 2021 17:51
 Operator : JC/MD
 Sample : M1886-03
 Misc : 5.98g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 RO-124027

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\82N032521W.M
 Title : SW846 8260

Signal : TIC: VN066474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.501	2143	2167	2181	rBV2	228652	590118	16.55%	2.981%
2	7.576	2181	2195	2217	rVB	401748	950145	26.64%	4.800%
3	7.788	2252	2274	2291	rBV4	17276	41149	1.15%	0.208%
4	7.941	2305	2331	2355	rBV2	261169	620040	17.39%	3.133%
5	8.121	2384	2398	2422	rVB2	39124	100596	2.82%	0.508%
6	8.354	2468	2485	2496	rBV3	34403	71005	1.99%	0.359%
7	8.507	2520	2542	2570	rBV	594257	1231412	34.53%	6.222%
8	8.915	2674	2694	2706	rBV3	19430	40056	1.12%	0.202%
9	9.006	2706	2728	2741	rVV6	31011	78346	2.20%	0.396%
10	9.446	2878	2892	2909	rVB2	30140	61178	1.72%	0.309%
11	9.585	2921	2944	2962	rBV4	38477	94779	2.66%	0.479%
12	9.660	2962	2972	2997	rVB4	22539	56770	1.59%	0.287%
13	9.805	3000	3026	3050	rBV4	21299	57911	1.62%	0.293%
14	10.025	3092	3108	3121	rBV	950042	1720854	48.25%	8.694%
15	10.089	3121	3132	3149	rVB	584356	1054087	29.56%	5.326%
16	10.221	3170	3181	3197	rVB2	56184	98420	2.76%	0.497%
17	10.371	3223	3237	3249	rVB5	26346	47826	1.34%	0.242%
18	10.467	3254	3273	3287	rBV6	20170	49638	1.39%	0.251%
19	10.567	3299	3310	3323	rVB6	26610	46953	1.32%	0.237%
20	10.819	3392	3404	3413	rVV9	17237	39056	1.10%	0.197%
21	10.889	3423	3430	3440	rVB3	29393	42508	1.19%	0.215%
22	10.945	3440	3451	3463	rVB3	36356	61605	1.73%	0.311%
23	11.146	3505	3526	3549	rVB7	85713	206475	5.79%	1.043%
24	11.243	3549	3562	3576	rBV2	51518	94538	2.65%	0.478%
25	11.347	3585	3601	3612	rBV	801676	1372964	38.50%	6.937%
26	11.406	3612	3623	3632	rVV	672643	1083734	30.39%	5.475%
27	11.452	3632	3640	3660	rVB	494660	841252	23.59%	4.250%
28	11.559	3660	3680	3703	rBV	1663219	3566461	100.00%	18.019%
29	11.889	3778	3803	3822	rBV2	509116	1166863	32.72%	5.895%
30	11.988	3832	3840	3848	rBV3	53506	74900	2.10%	0.378%
31	12.061	3859	3867	3874	rBV4	46492	67531	1.89%	0.341%
32	12.109	3875	3885	3905	rVB7	107845	223021	6.25%	1.127%
33	12.192	3907	3916	3925	rBV5	40396	60773	1.70%	0.307%
34	12.345	3961	3973	4001	rVB3	614595	1236016	34.66%	6.245%
35	12.600	4055	4068	4076	rBV	136291	252089	7.07%	1.274%
36	12.675	4087	4096	4127	rVB3	238141	555365	15.57%	2.806%

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Sampling : 1

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Peak Location: TOP

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Peak separation: 5

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Title : SW846 8260

37	12.905	4176	4182	4199	rVB6	59254	104998	2.94%	0.530%
38	12.983	4200	4211	4225	rBV	108173	188238	5.28%	0.951%
39	13.286	4311	4324	4363	rBV	694637	1395811	39.14%	7.052%
40	13.613	4436	4446	4469	rVB10	33847	83366	2.34%	0.421%
41	13.825	4518	4525	4537	rVB2	39150	63949	1.79%	0.323%

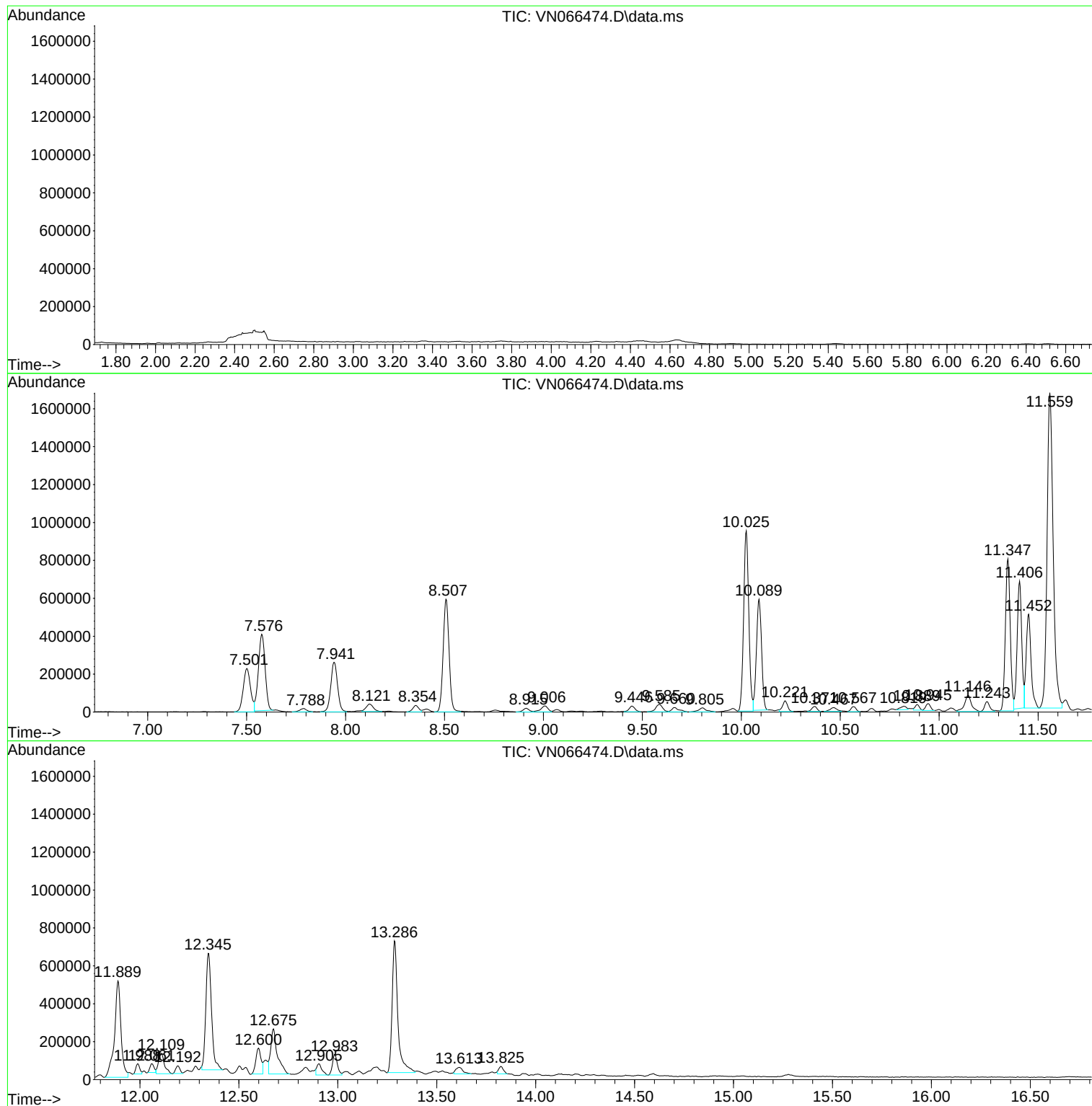
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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



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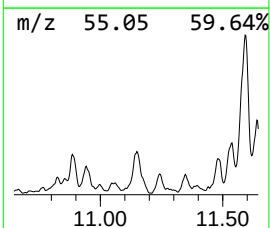
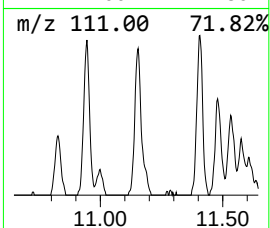
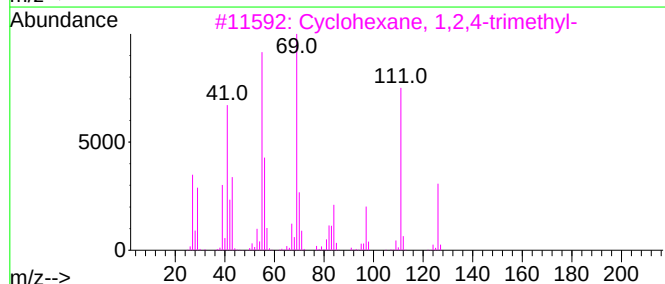
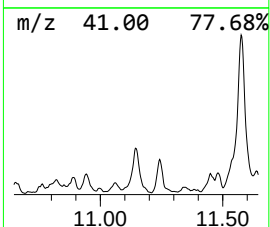
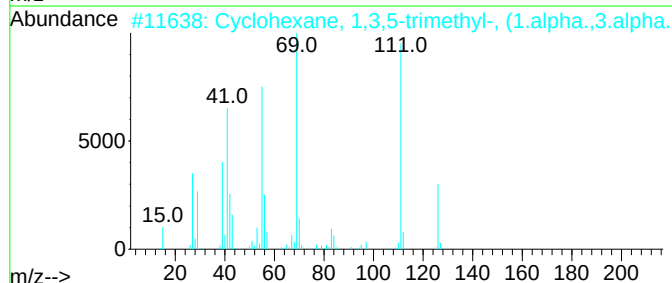
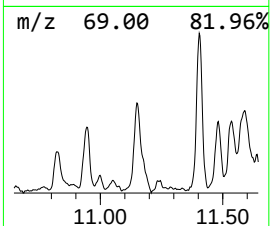
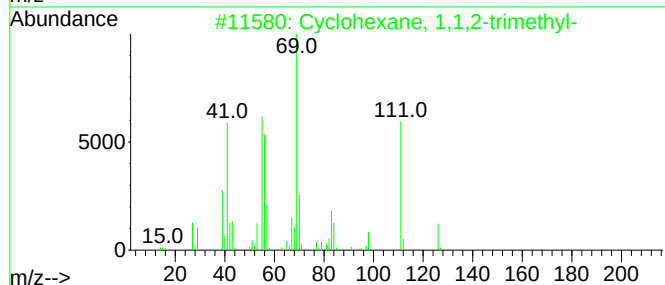
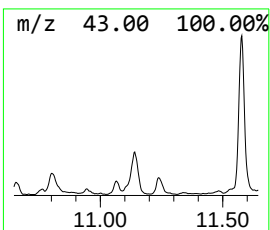
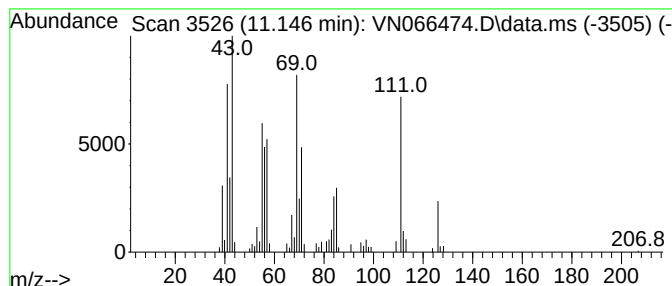
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,1,2-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	7.52 ug/l	206475	Chlorobenzene-d5	11.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	68
2			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	64
3			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	62
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	60
5			5-Methyl-1,3-cyclohexanedione	126	C7H10O2	004341-24-6	46



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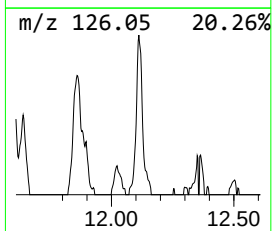
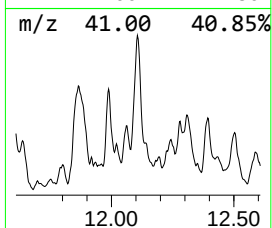
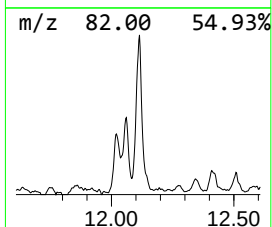
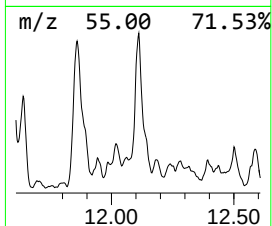
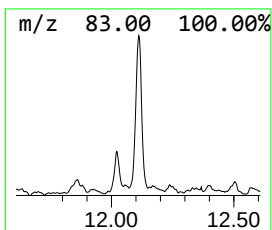
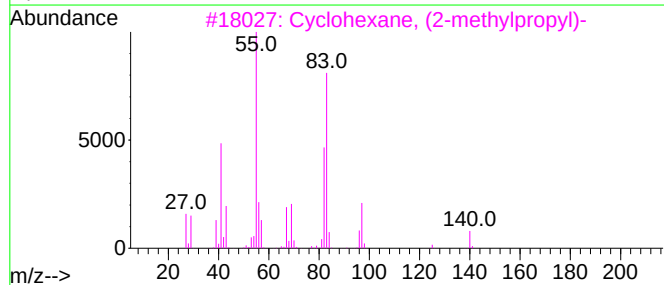
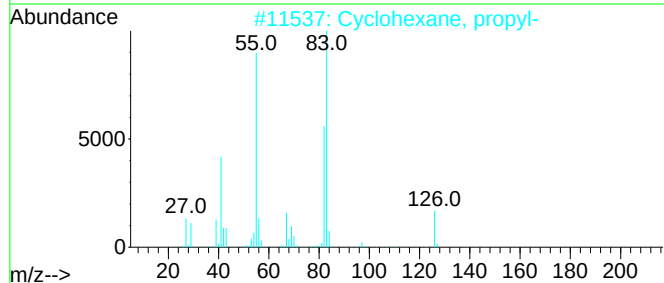
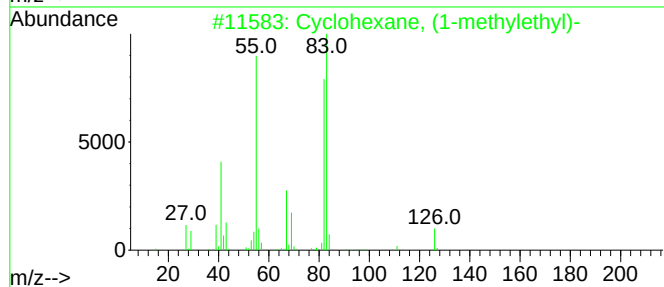
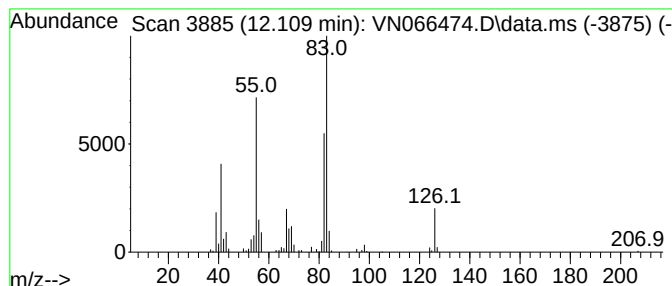
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, (1-methylethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.109	8.12 ug/l	223021	Chlorobenzene-d5	11.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	87
2			Cyclohexane, propyl-	126	C9H18	001678-92-8	87
3			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	64
4			Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
5			Cyclohexane, butyl-	140	C10H20	001678-93-9	64



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ALS Vial : 11 Sample Multiplier: 1

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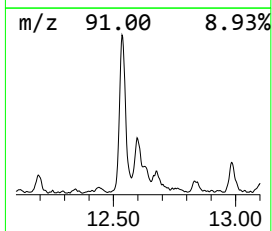
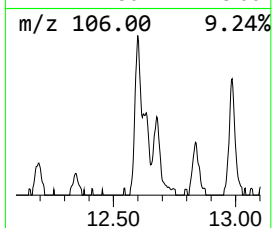
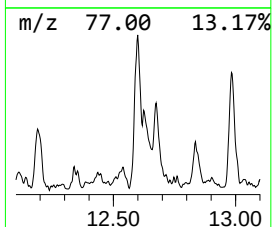
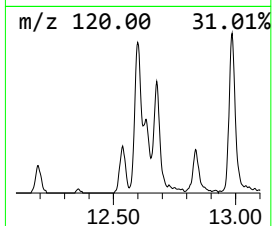
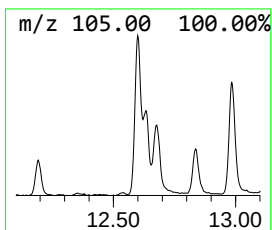
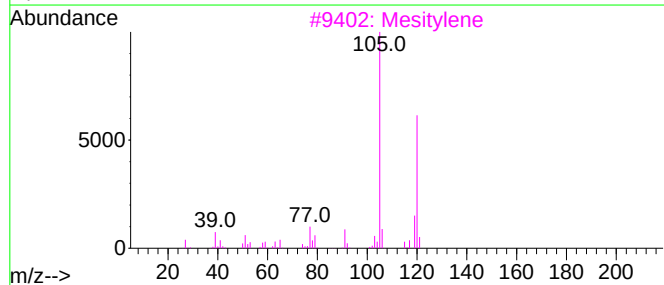
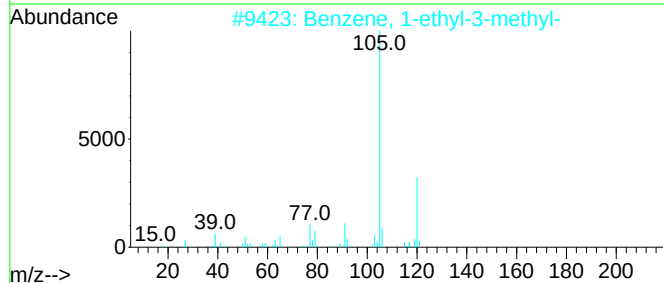
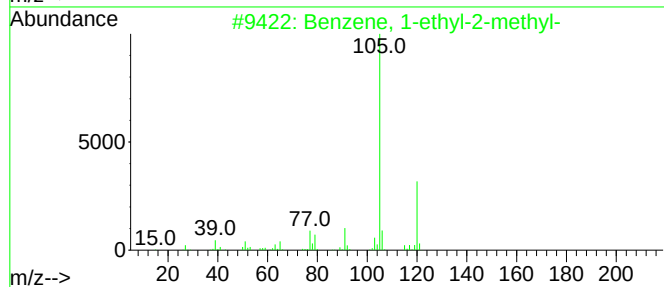
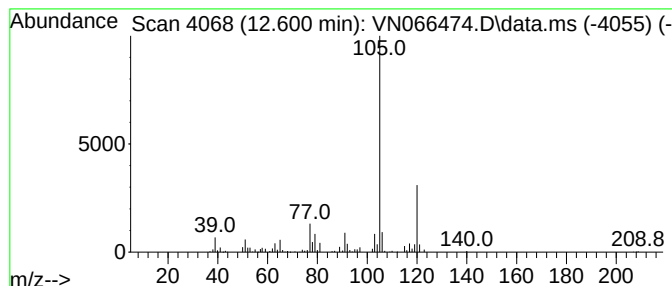
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.600	9.03 ug/l	252089	1,4-Dichlorobenzene-d4	13.289

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	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1,...	11.146	7.5	ug/l	206475	3	11.347	1372960	50.0
Cyclohexane, (1...	12.109	8.1	ug/l	223021	3	11.347	1372960	50.0
Benzene, 1-ethy...	12.600	9.0	ug/l	252089	4	13.289	1395810	50.0