

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV052720\
 Data File : VV016246.D
 Acq On : 27 May 2020 22:58
 Operator : SY/MD
 Sample : L2766-16
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BE4Z9

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR052620WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.222	36	41	47	rBV2	6722	6840	1.33%	0.175%
2	1.315	60	70	83	rVB2	48001	75364	14.69%	1.934%
3	1.399	89	96	106	rVB	16583	20717	4.04%	0.532%
4	1.582	145	153	163	rBV	35675	43573	8.49%	1.118%
5	2.126	312	322	334	rBV	66140	97659	19.03%	2.506%
6	2.209	335	348	374	rVB	33797	96630	18.83%	2.479%
7	2.753	487	517	561	rBV4	26591	184330	35.92%	4.729%
8	2.974	578	586	597	rVB6	3573	7251	1.41%	0.186%
9	3.190	645	653	669	rVB7	3072	7412	1.44%	0.190%
10	3.717	794	817	845	rBV2	190301	513154	100.00%	13.166%
11	3.936	872	885	906	rBV2	35222	116135	22.63%	2.980%
12	4.379	1008	1023	1049	rBV	51523	129185	25.17%	3.314%
13	4.704	1113	1124	1137	rVB6	2395	5567	1.08%	0.143%
14	5.074	1223	1239	1264	rBV3	119692	288248	56.17%	7.395%
15	5.643	1401	1416	1440	rBV	114845	234733	45.74%	6.022%
16	5.817	1460	1470	1482	rBV3	5614	13043	2.54%	0.335%
17	6.096	1542	1557	1583	rBV	68821	140103	27.30%	3.595%
18	6.563	1685	1702	1710	rBV	159586	323440	63.03%	8.298%
19	7.010	1830	1841	1863	rBV	32800	58570	11.41%	1.503%
20	7.338	1932	1943	1959	rBV	139573	243876	47.52%	6.257%
21	7.415	1959	1967	1979	rVB	7717	14679	2.86%	0.377%
22	7.646	2029	2039	2055	rBV2	19999	35346	6.89%	0.907%
23	8.116	2173	2185	2220	rBV	154220	300484	58.56%	7.709%
24	8.270	2225	2233	2247	rVB6	6232	12058	2.35%	0.309%
25	8.874	2409	2421	2447	rBV	173177	280243	54.61%	7.190%
26	9.833	2711	2719	2733	rBV3	5917	10050	1.96%	0.258%
27	9.919	2737	2746	2760	rVB	4261	7026	1.37%	0.180%
28	10.238	2834	2845	2857	rBV	49169	76935	14.99%	1.974%
29	10.501	2914	2927	2939	rBV4	2409	5399	1.05%	0.139%
30	11.270	3155	3166	3185	rVB	172195	274541	53.50%	7.044%
31	11.646	3273	3283	3300	rVB	133891	211074	41.13%	5.415%
32	12.260	3465	3474	3484	rBV7	3383	6270	1.22%	0.161%
33	13.527	3859	3868	3878	rBV2	17769	27756	5.41%	0.712%
34	13.778	3936	3946	3963	rVB2	19364	29976	5.84%	0.769%

LSC Area Percent Report

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_V\METHOD\SOMVTR052620WMA.M
Title : TRACE VOA SOM01.0

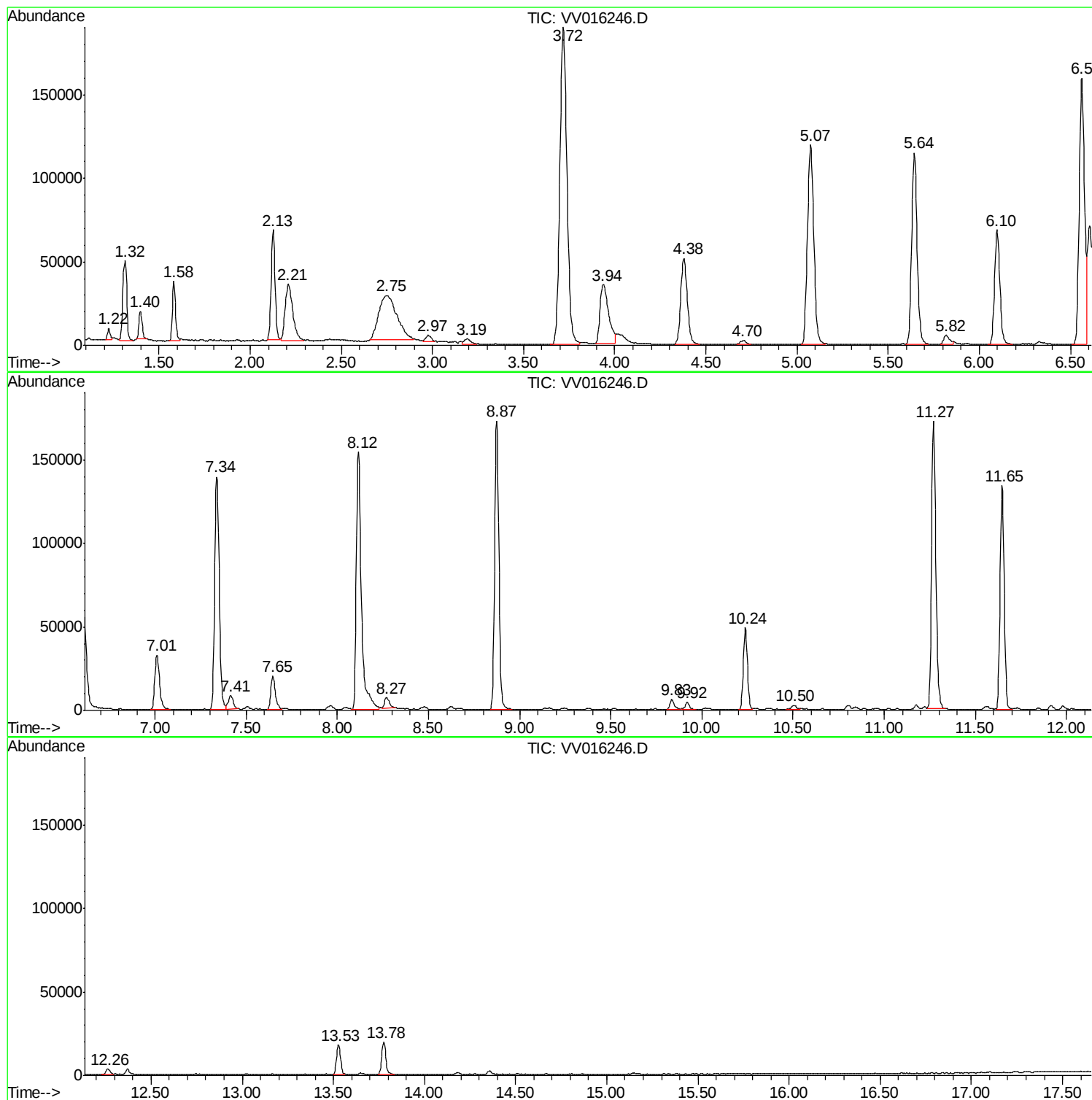
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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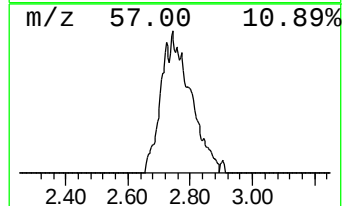
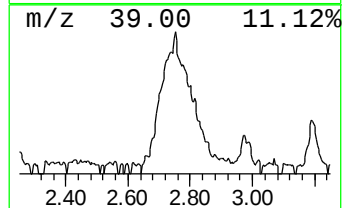
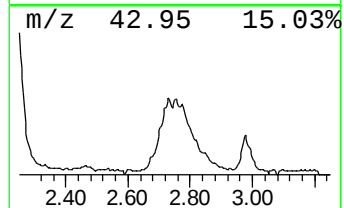
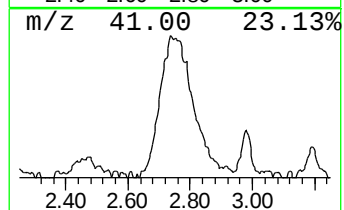
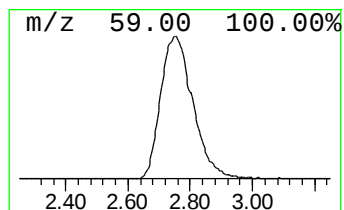
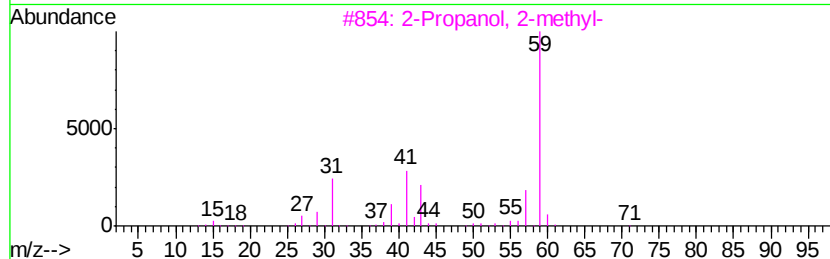
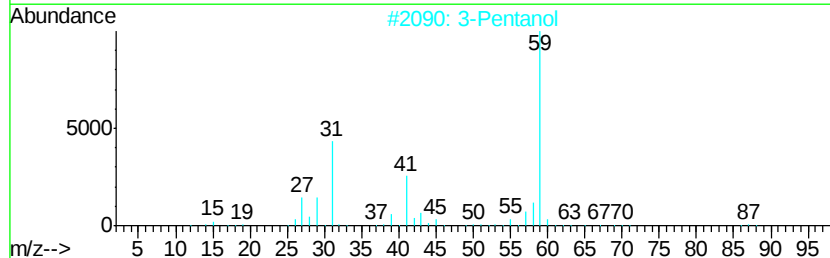
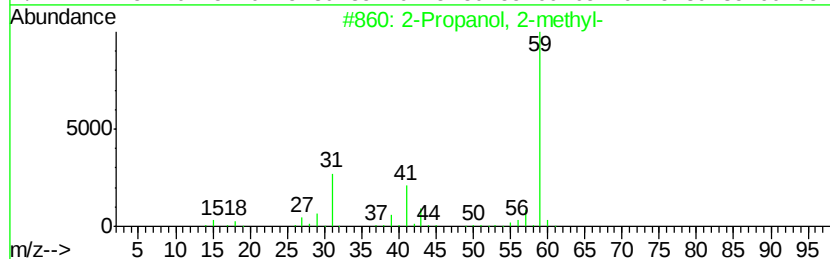
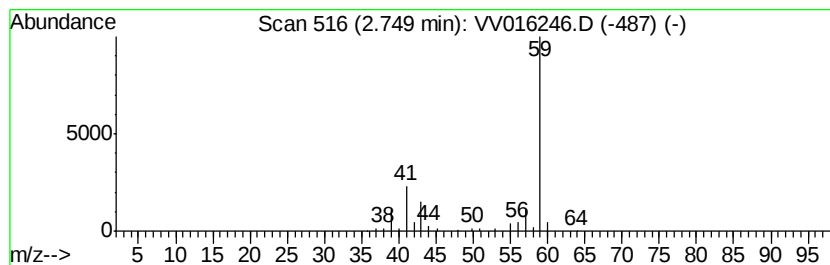
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR052620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.75	3.93 ug/L	184330	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
2			3-Pentanol	88	C5H12O	000584-02-1	56
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	38
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9



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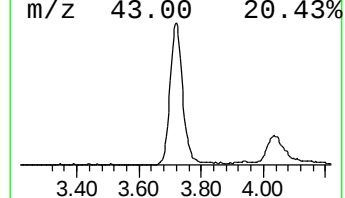
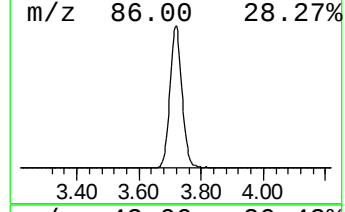
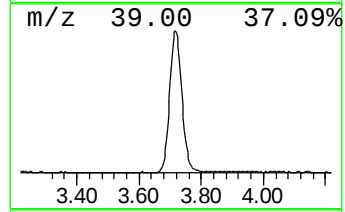
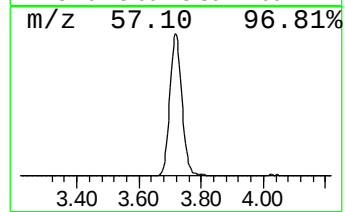
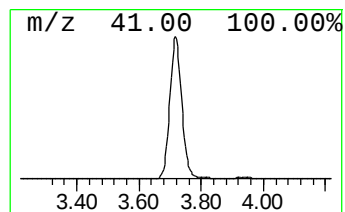
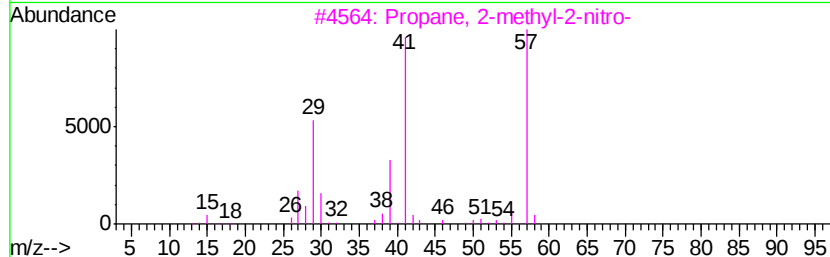
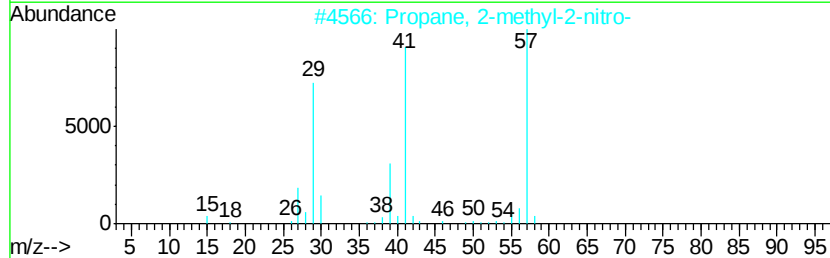
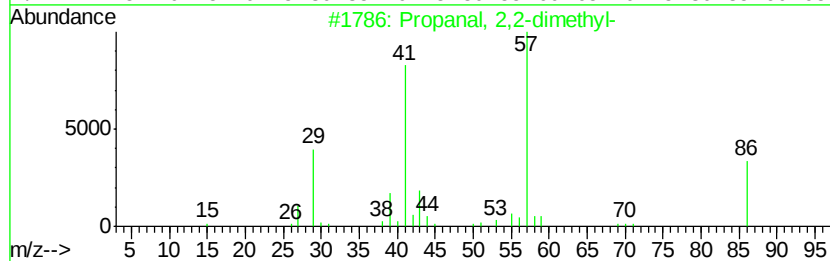
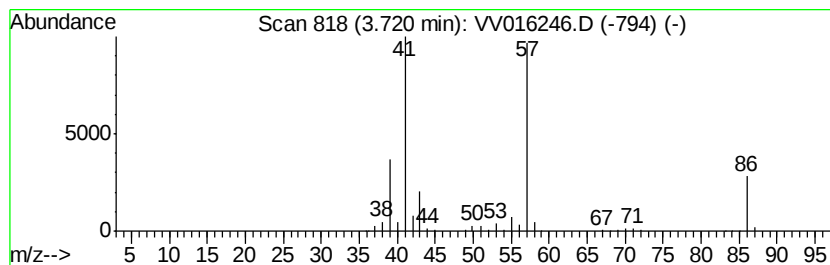
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR052620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	10.93 ug/L	513154	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	58
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	45
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40
5		3-Pentanone	86	C5H10O	000096-22-0	40



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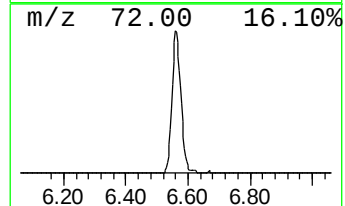
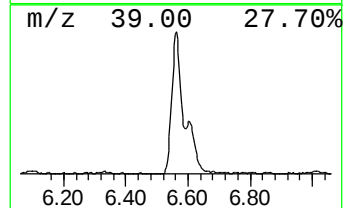
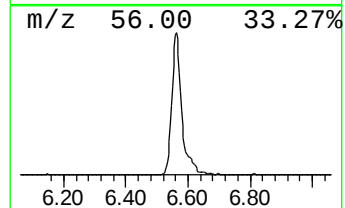
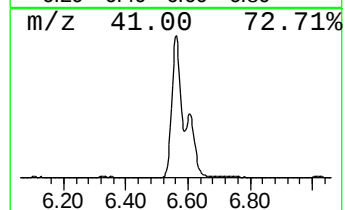
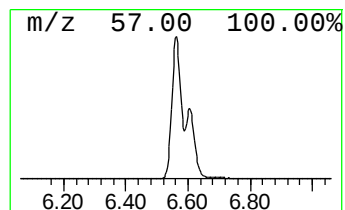
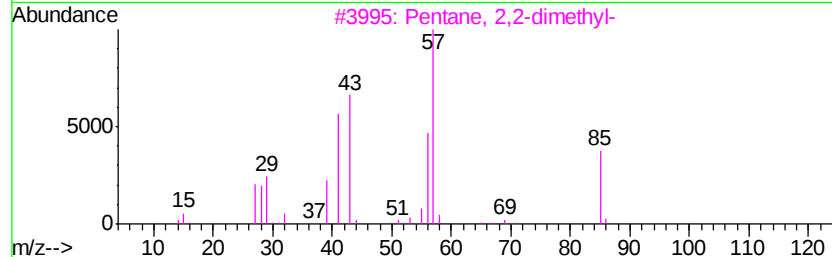
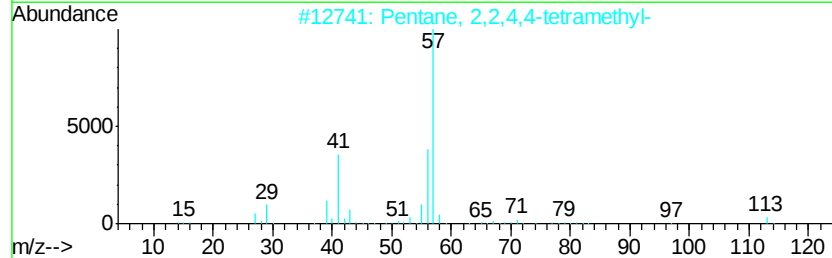
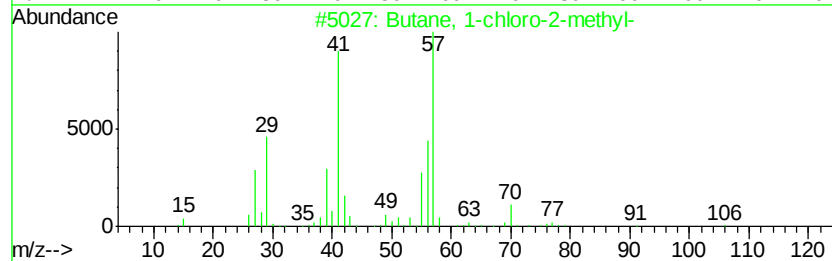
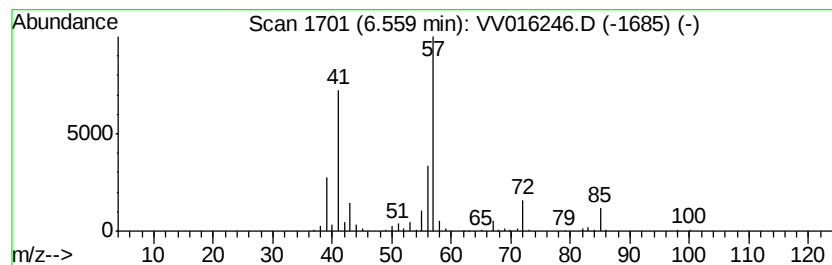
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 1-chloro-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	6.89 ug/L	323440	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	50
2		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	47
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	42
4		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	38
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38



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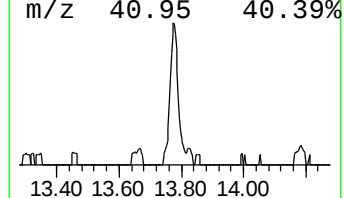
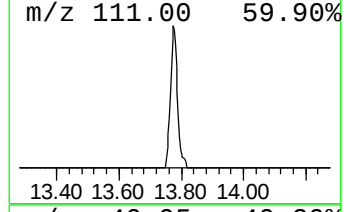
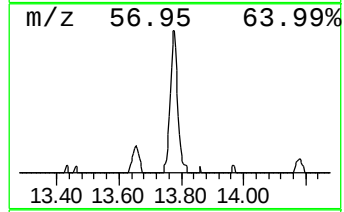
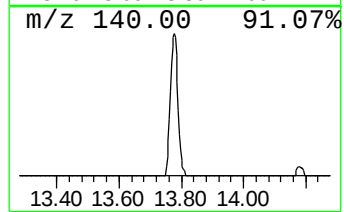
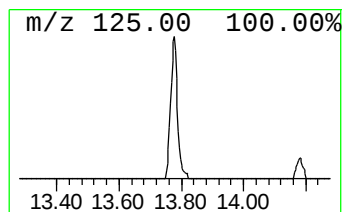
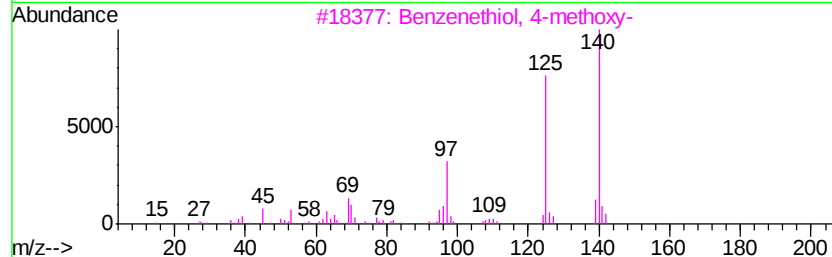
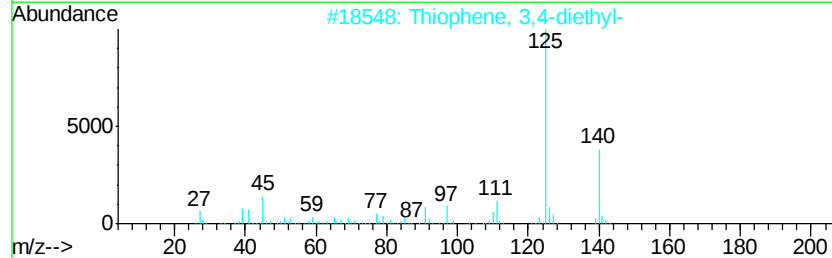
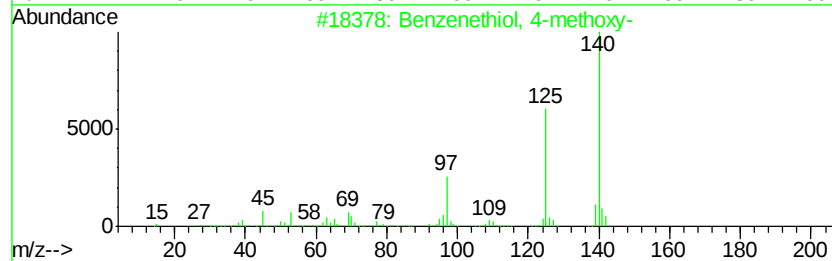
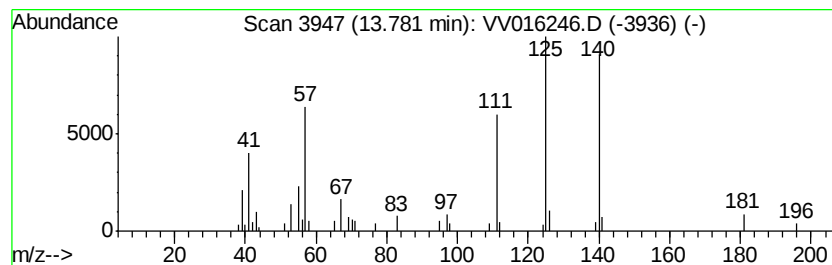
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenethiol, 4-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	0.55 ug/L	29976	1,4-Dichlorobenzene-d4	11.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	64
2			Thiophene, 3,4-diethyl-	140	C8H12S	035686-14-7	59
3			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59
4			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
5			1-Methoxy-6,6-dimethyl-cyclohex-...	140	C9H16O	073741-66-9	59



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Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-met...	2.75	3.9	ug/L	184330	1	5.64	234733	5.0
Propanal, 2,2-dim...	3.72	10.9	ug/L	513154	1	5.64	234733	5.0
Butane, 1-chloro-...	6.56	6.9	ug/L	323440	1	5.64	234733	5.0
Benzenethiol, 4-m...	13.78	0.6	ug/L	29976	3	11.27	274541	5.0