

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
 Data File : VN076553.D
 Acq On : 06 Feb 2023 19:48
 Operator : JC\MD
 Sample : 01437-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31962

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\82N020623W.M
 Title : SW846 8260

Signal : TIC: VN076553.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.101	3	8	28	rVB	759876	1136789	10.43%	2.732%
2	2.336	40	48	60	rVB2	140624	224621	2.06%	0.540%
3	2.530	77	81	94	rVB	112165	223017	2.05%	0.536%
4	3.806	289	298	319	rBV	190795	535330	4.91%	1.286%
5	4.447	398	407	416	rBV	40875	122413	1.12%	0.294%
6	5.606	578	604	622	rBV2	574087	2005655	18.41%	4.819%
7	6.694	771	789	812	rBV	3207454	10896430	100.00%	26.184%
8	7.230	867	880	892	rBV	212469	611095	5.61%	1.468%
9	7.494	914	925	938	rVV	109613	293077	2.69%	0.704%
10	8.171	1030	1040	1045	rBV	424604	1018282	9.35%	2.447%
11	8.230	1045	1050	1067	rVB	832185	1920846	17.63%	4.616%
12	8.612	1095	1115	1122	rBV2	1211606	3496474	32.09%	8.402%
13	8.677	1122	1126	1139	rVB2	156299	340915	3.13%	0.819%
14	9.106	1190	1199	1214	rBV	1130833	2292399	21.04%	5.509%
15	10.571	1439	1448	1453	rBV	1636398	3032956	27.83%	7.288%
16	10.635	1453	1459	1472	rVV	1426761	2640614	24.23%	6.345%
17	11.870	1657	1669	1679	rBV	1451073	2597090	23.83%	6.241%
18	11.965	1679	1685	1695	rVB	143840	254831	2.34%	0.612%
19	12.070	1695	1703	1715	rVB	500593	970050	8.90%	2.331%
20	12.400	1746	1759	1774	rBV3	266898	596686	5.48%	1.434%
21	12.853	1827	1836	1848	rBV	1134758	1970916	18.09%	4.736%
22	13.341	1912	1919	1926	rVB3	80660	140016	1.28%	0.336%
23	13.482	1937	1943	1948	rBV2	93836	159797	1.47%	0.384%
24	13.794	1988	1996	2005	rBV	1408211	2472148	22.69%	5.940%
25	13.876	2005	2010	2020	rVB	200041	324617	2.98%	0.780%
26	14.176	2055	2061	2067	rBV	291210	481644	4.42%	1.157%
27	14.235	2067	2071	2084	rVB2	77651	142891	1.31%	0.343%
28	14.606	2123	2134	2141	rBV2	118191	233506	2.14%	0.561%
29	14.770	2157	2162	2171	rVB	91254	165789	1.52%	0.398%
30	15.053	2200	2210	2216	rBV3	58777	127077	1.17%	0.305%
31	15.641	2304	2310	2318	rVB	92188	187518	1.72%	0.451%

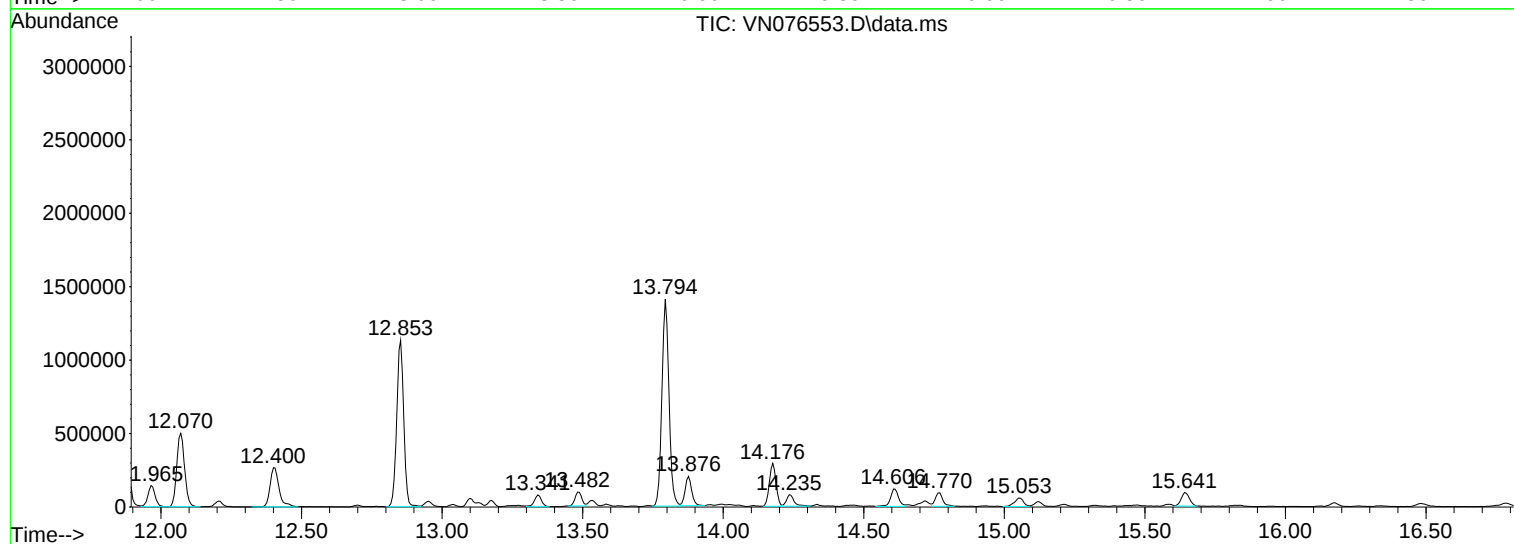
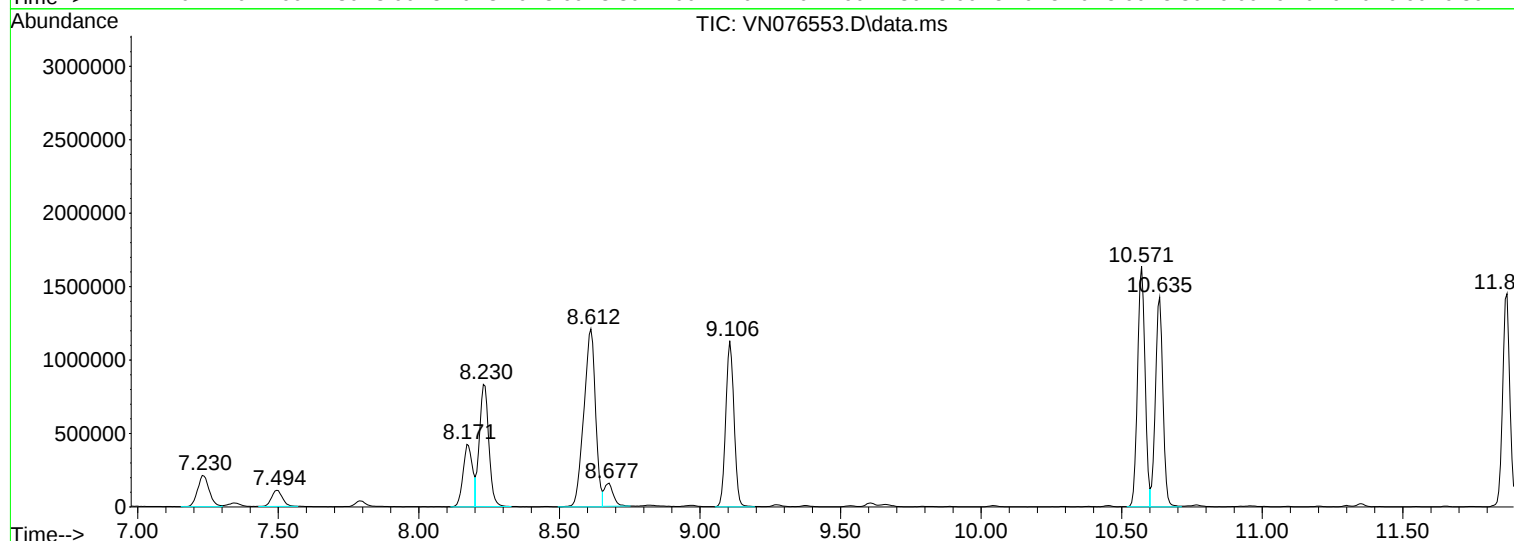
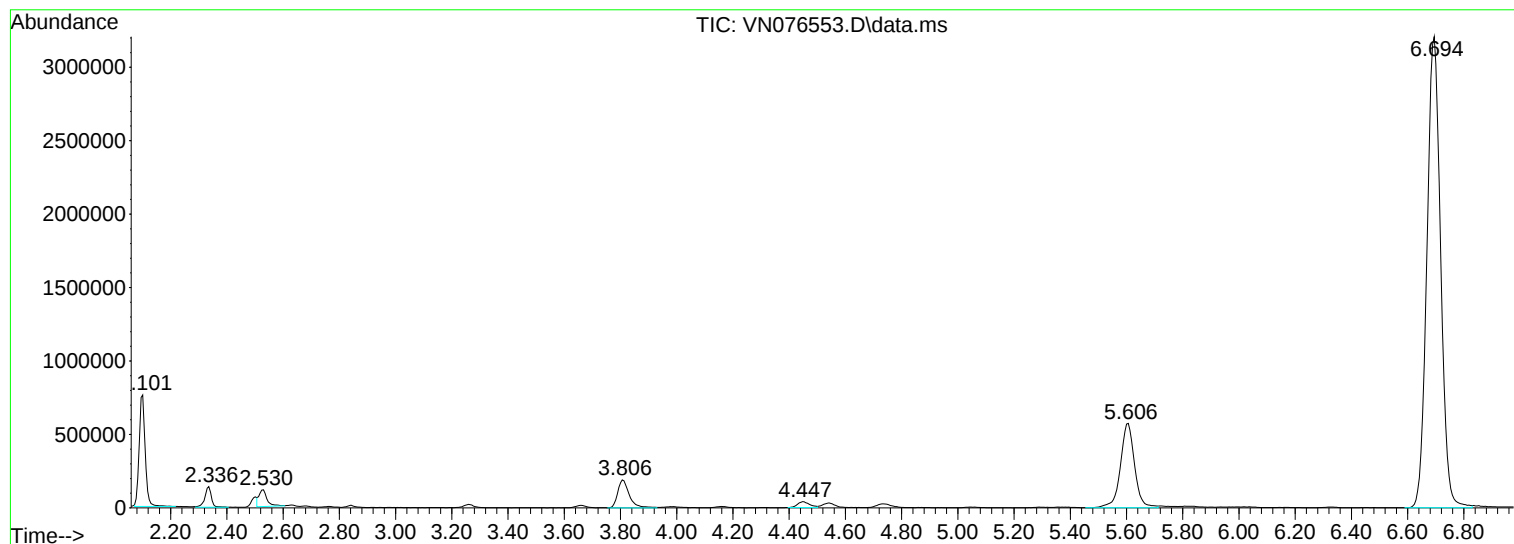
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Quant Title :

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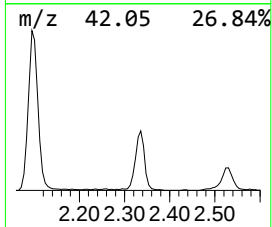
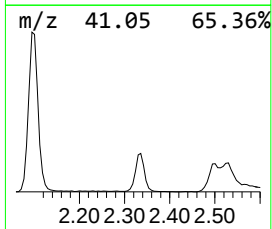
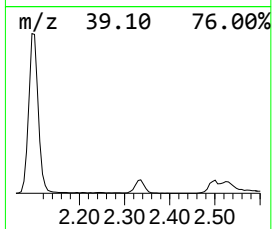
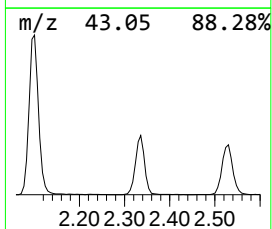
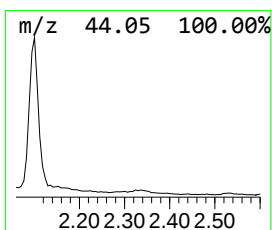
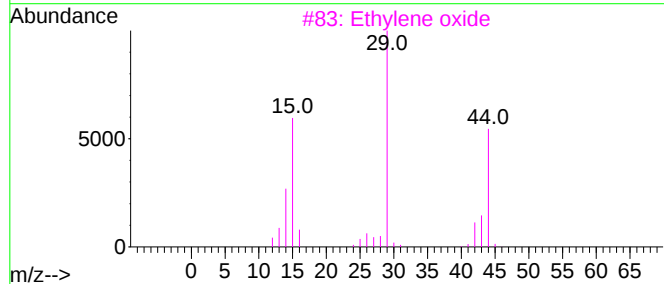
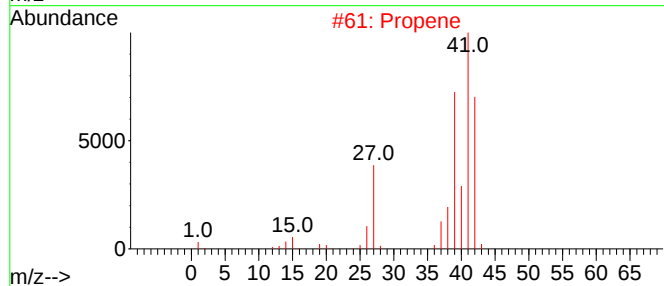
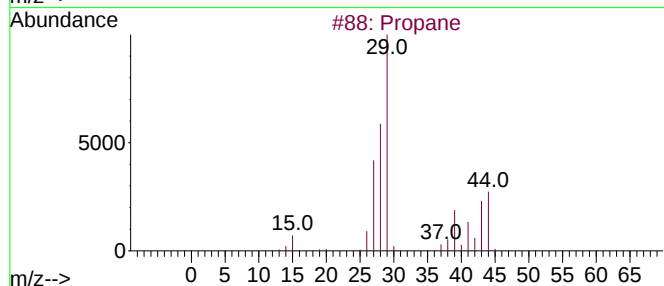
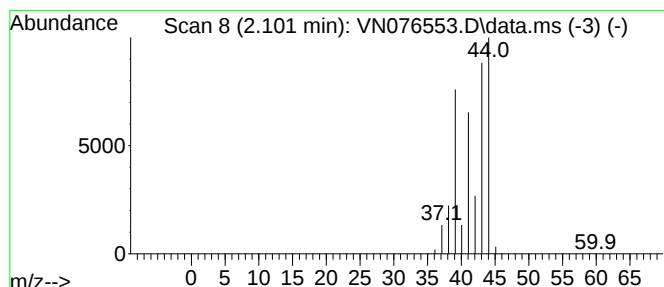
Quant Title :

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.101	29.59 ug/l	1136790	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane		44	C3H8	000074-98-6	90
2	Propene		42	C3H6	000115-07-1	9
3	Ethylene oxide		44	C2H4O	000075-21-8	5
4	Cyclopropene		40	C3H4	002781-85-3	2
5	Alanine		89	C3H7NO2	000056-41-7	2



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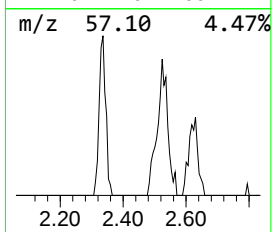
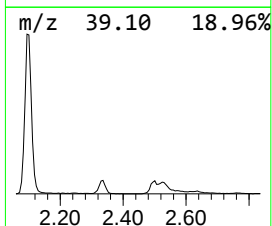
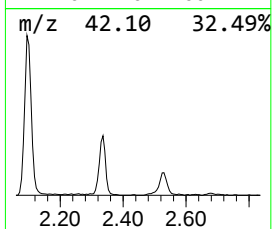
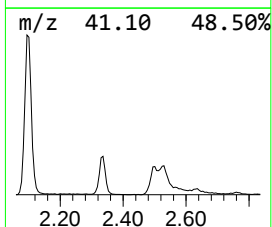
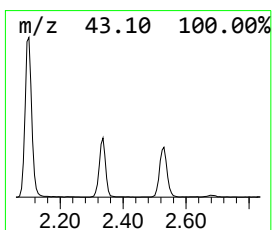
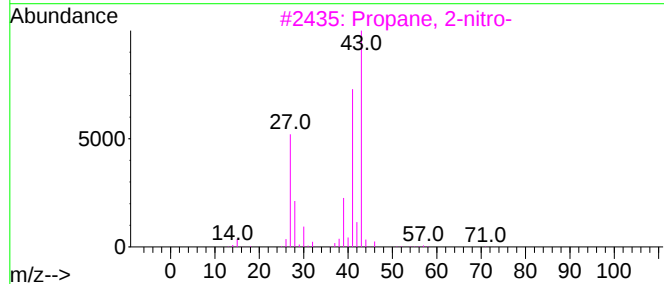
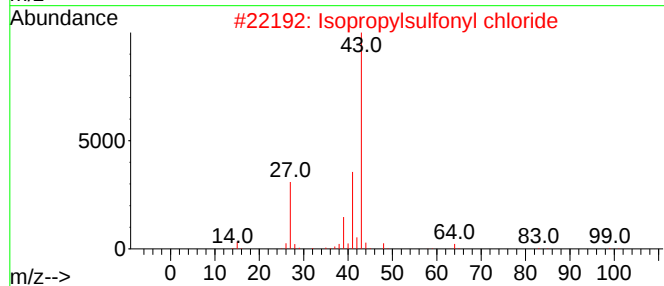
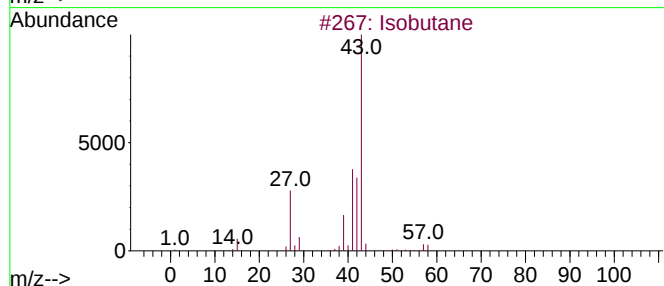
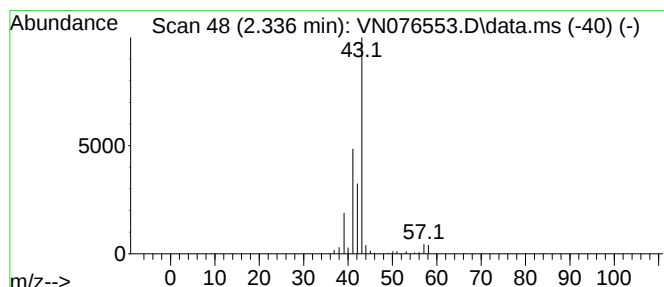
Quant Title :

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.336	5.85 ug/l	224621	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	86
2		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3		Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4		Cyclobutylamine	71	C4H9N	002516-34-9	4
5		5-Methyloxazolidine	87	C4H9NO	058328-22-6	4



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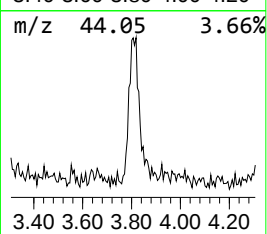
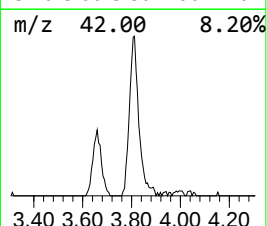
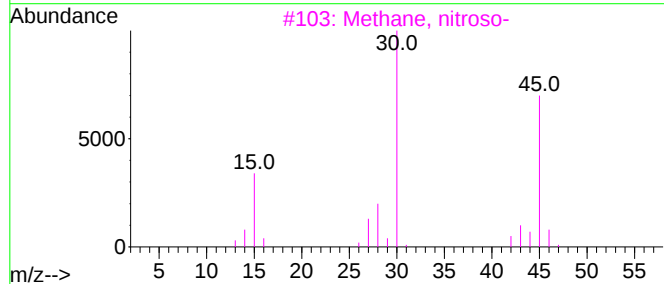
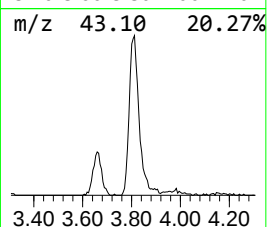
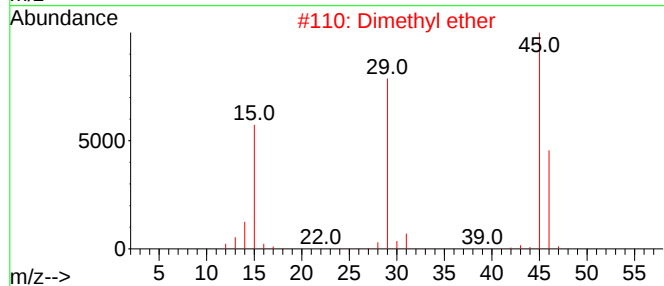
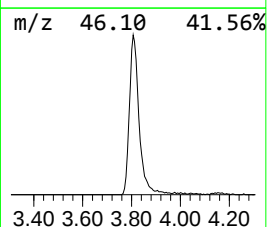
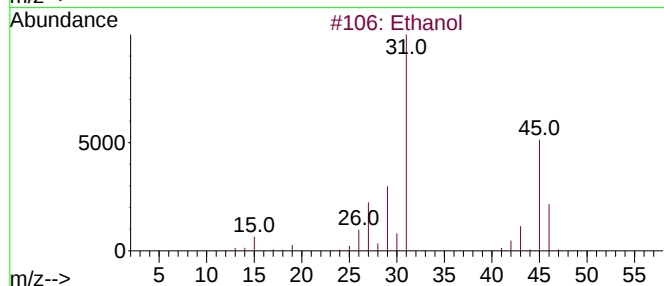
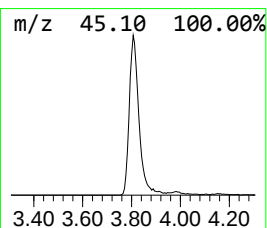
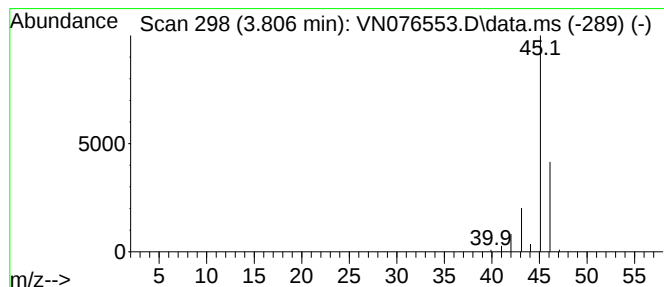
Quant Title :

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

Peak Number 4 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.806	13.93 ug/l	535330	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Oxalic acid			90	C2H2O4	000144-62-7	4
5	Formic acid			46	CH2O2	000064-18-6	4



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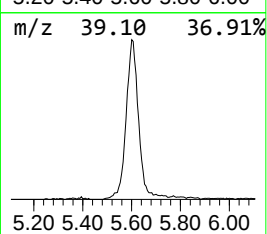
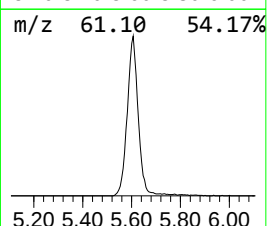
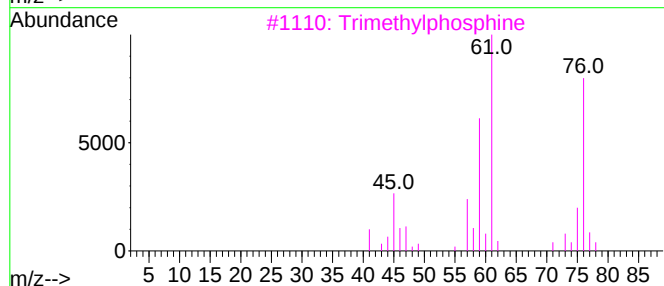
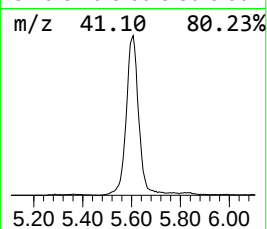
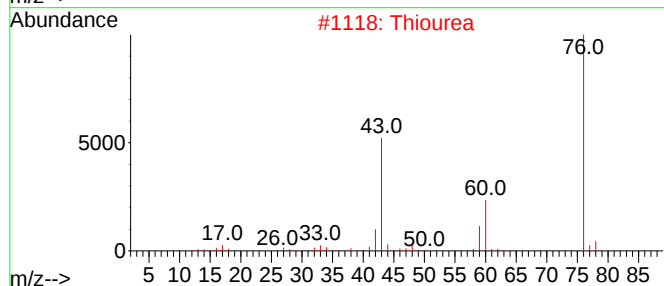
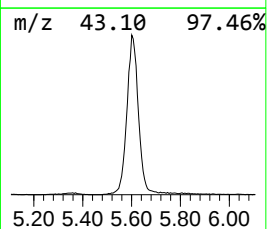
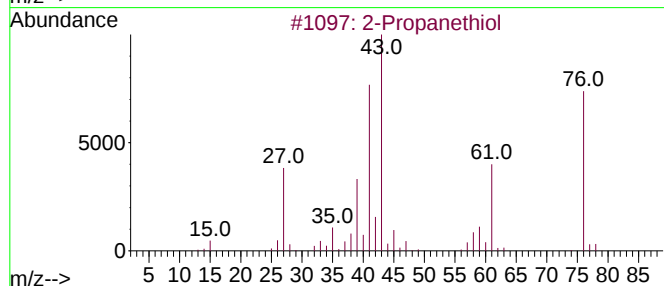
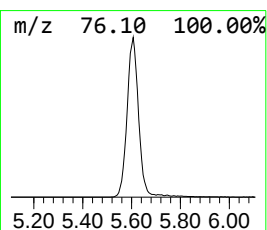
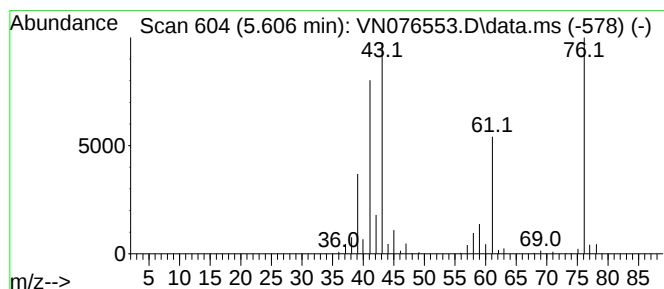
Quant Title :

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

Peak Number 5 2-Propanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.606	52.21 ug/l	2005660	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanethiol	76	C3H8S	000075-33-2	94
2		Thiourea	76	CH4N2S	000062-56-6	64
3		Trimethylphosphine	76	C3H9P	000594-09-2	64
4		Isopropyl phosphine	76	C3H9P	004538-29-8	64
5		Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9



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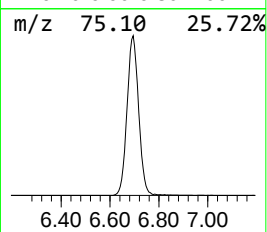
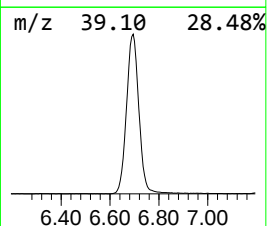
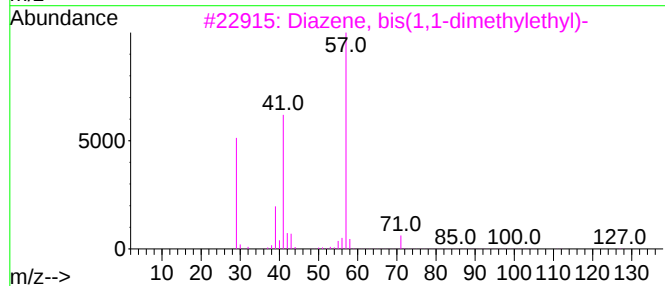
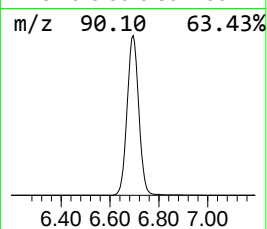
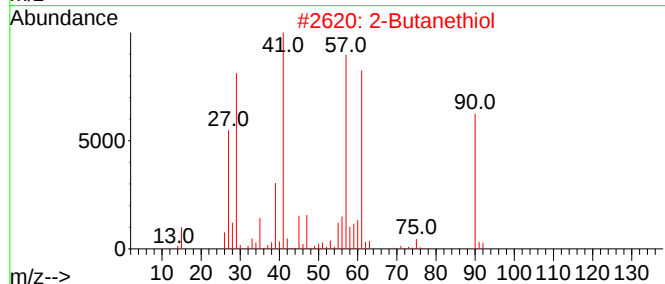
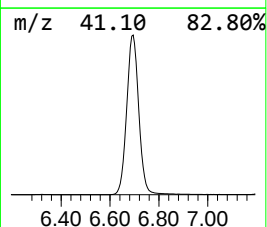
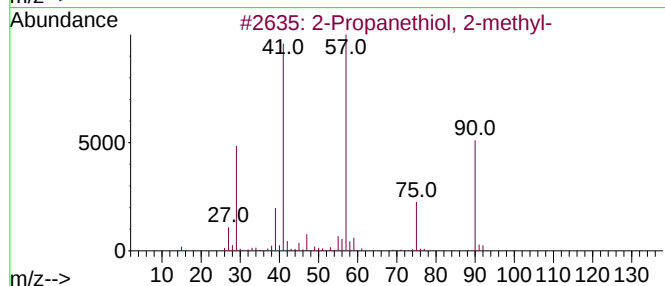
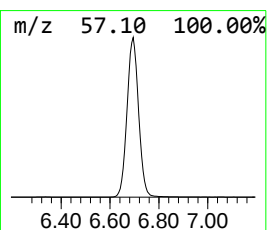
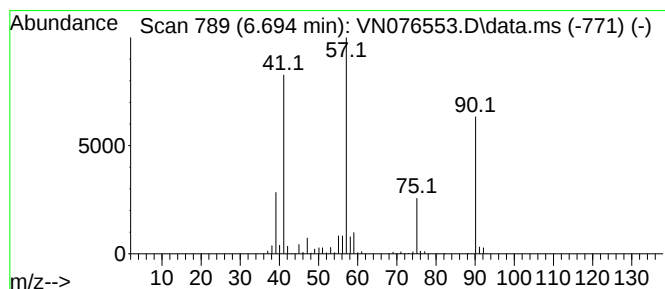
Quant Title :

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TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.694	283.64 ug/l	10896400	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2		2-Butanethiol	90	C4H10S	000513-53-1	42
3		Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	14
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
5		Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	12



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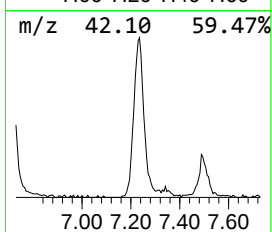
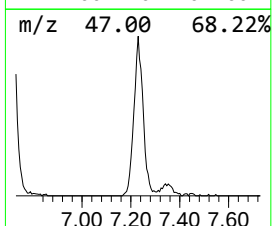
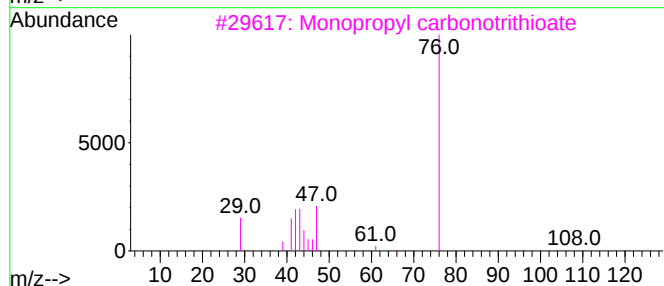
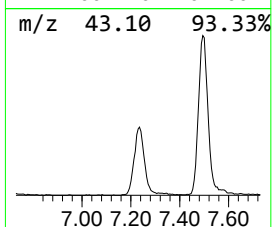
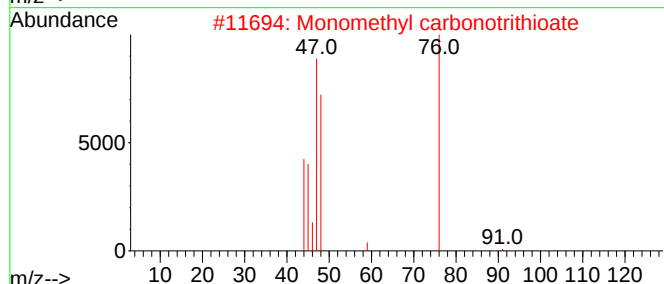
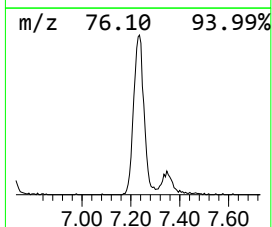
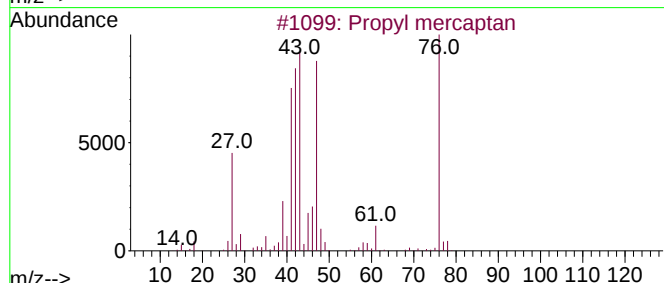
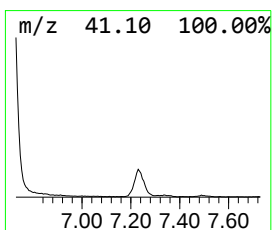
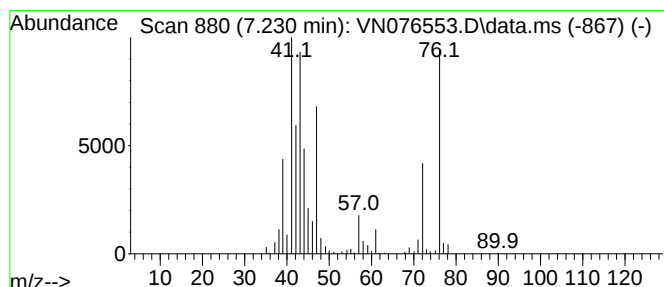
Quant Title :

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

Peak Number 7 Propyl mercaptan Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	15.91 ug/l	611095	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propyl mercaptan	76	C3H8S	000107-03-9	90
2		Monomethyl carbonotrithioate	124	C2H4S3	001113-26-4	36
3		Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	10
4		2-Propanethiol	76	C3H8S	000075-33-2	9
5		Thiourea	76	CH4N2S	000062-56-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076553.D
Acq On : 06 Feb 2023 19:48
Operator : JC\MD
Sample : 01437-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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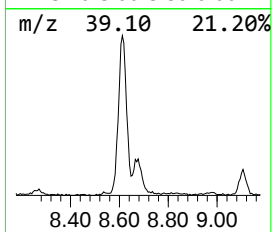
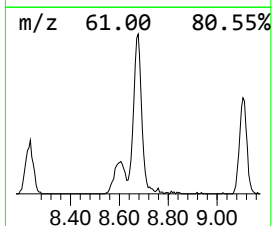
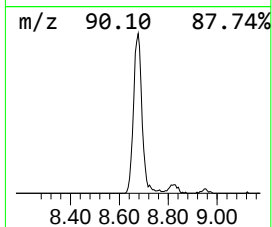
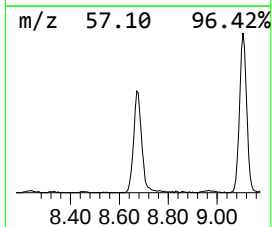
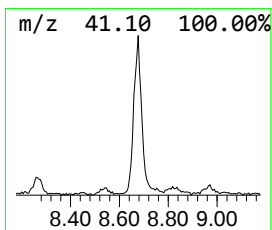
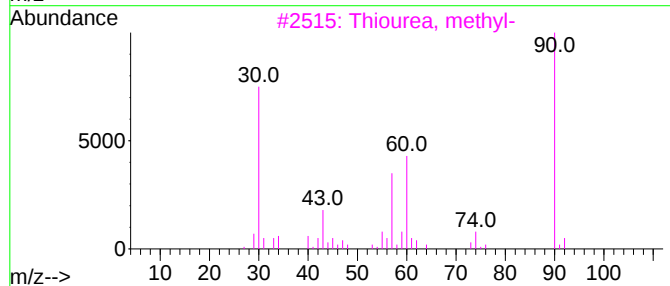
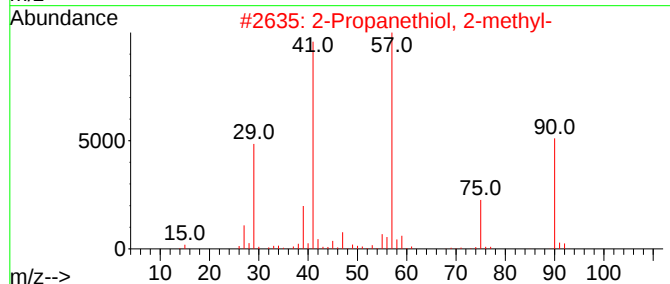
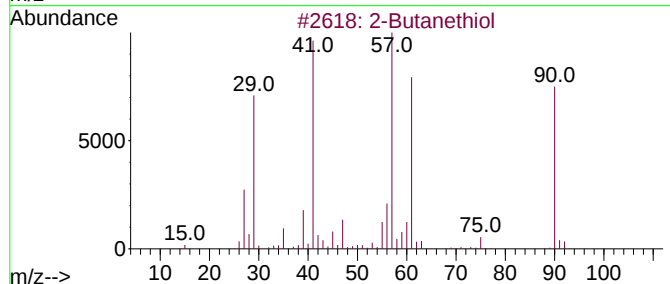
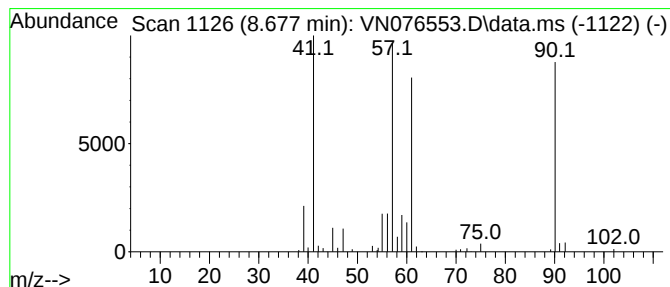
Quant Title :

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

Peak Number 8 2-Butanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.677	7.44 ug/l	340915	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanethiol	90	C4H10S	000513-53-1	91
2			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	59
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	36
4			Methane, nitro-	61	CH3NO2	000075-52-5	9
5			Hydroxylamine, TBDMS derivative	147	C6H17NOSi	041879-39-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076553.D
Acq On : 06 Feb 2023 19:48
Operator : JC\MD
Sample : 01437-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31962

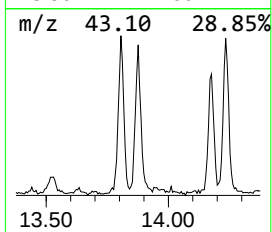
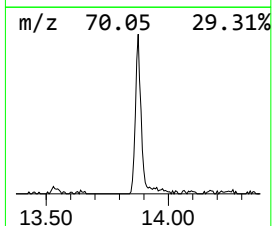
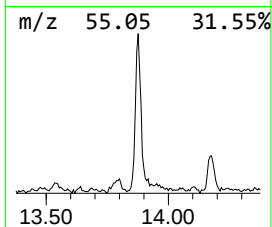
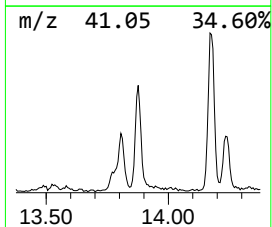
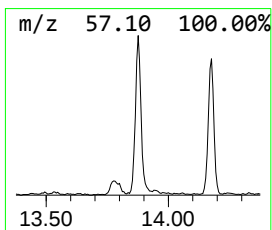
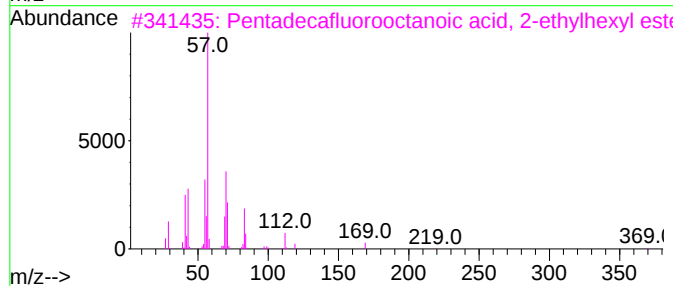
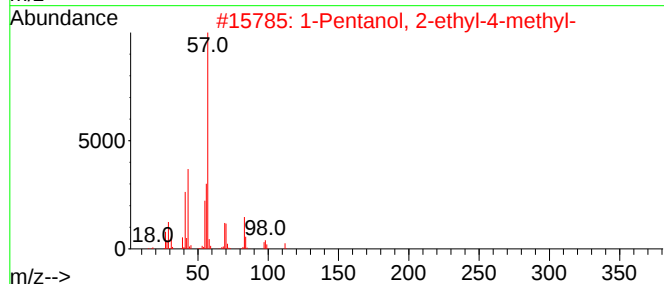
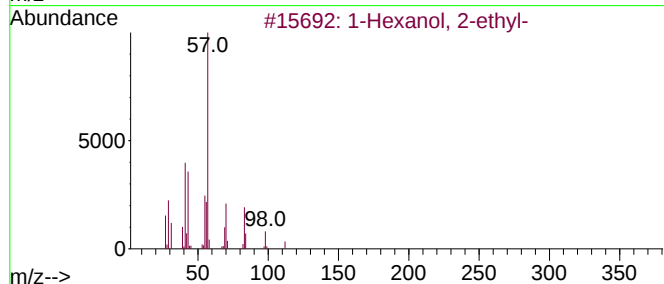
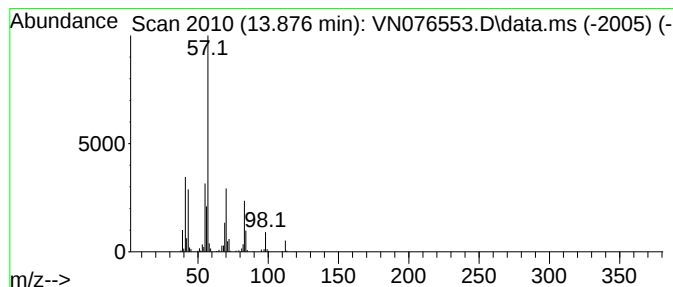
Quant Title :

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	6.57 ug/l	324617	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076553.D
Acq On : 06 Feb 2023 19:48
Operator : JC\MD
Sample : 01437-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31962

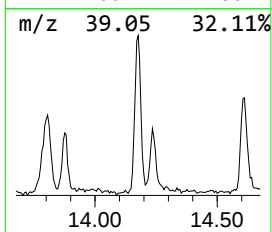
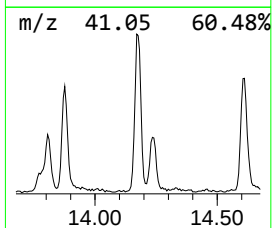
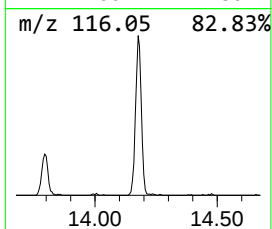
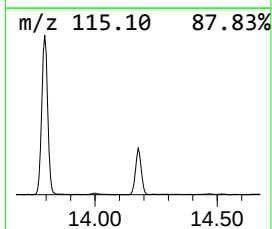
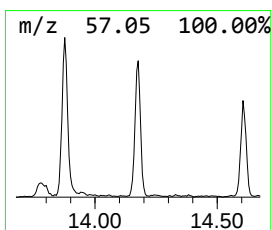
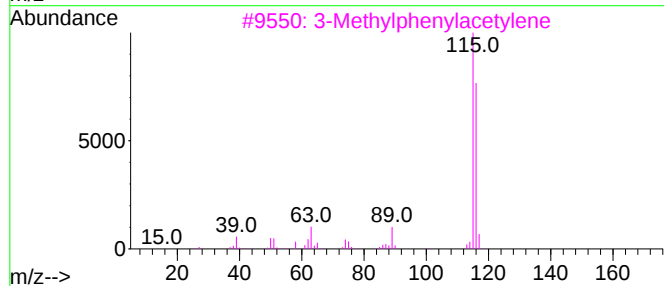
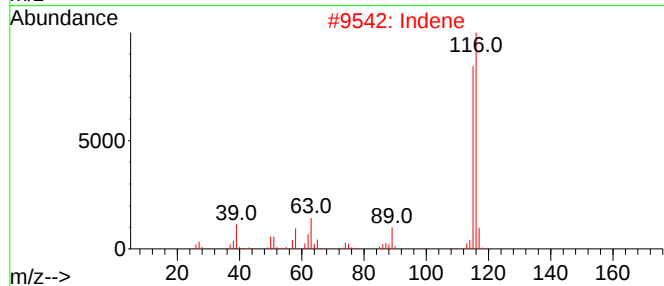
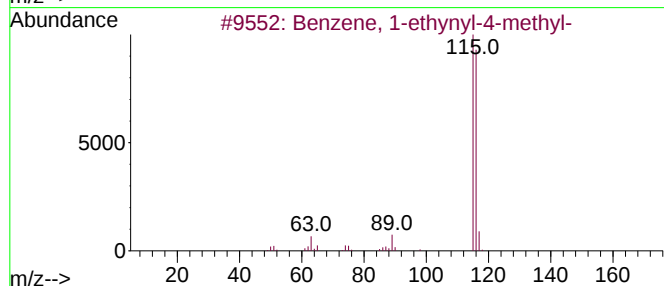
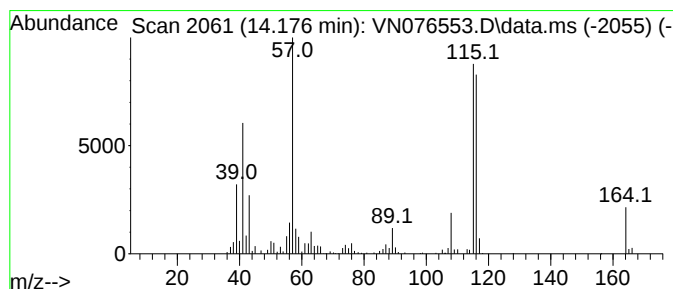
Quant Title :

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

Peak Number 10 Benzene, 1-ethynyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	9.74 ug/l	481644	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	76
2		Indene	116	C9H8	000095-13-6	76
3		3-Methylphenylacetylene	116	C9H8	000766-82-5	76
4		Benzene, 1-propynyl-	116	C9H8	000673-32-5	76
5		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020623\
Data File : VN076553.D
Acq On : 06 Feb 2023 19:48
Operator : JC\MD
Sample : 01437-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31962

Quant Title :

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	2.101	29.6	ug/l	1136790	1	8.230	1920850	50.0
Isobutane	2.336	5.8	ug/l	224621	1	8.230	1920850	50.0
Ethanol	3.806	13.9	ug/l	535330	1	8.230	1920850	50.0
2-Propanethiol	5.606	52.2	ug/l	2005660	1	8.230	1920850	50.0
2-Propanethiol,...	6.694	283.6	ug/l	10896400	1	8.230	1920850	50.0
Propyl mercaptan	7.230	15.9	ug/l	611095	1	8.230	1920850	50.0
2-Butanethiol	8.677	7.4	ug/l	340915	2	9.106	2292400	50.0
1-Hexanol, 2-et...	13.876	6.6	ug/l	324617	4	13.794	2472150	50.0
Benzene, 1-ethy...	14.176	9.7	ug/l	481644	4	13.794	2472150	50.0