

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
 Data File : VN072605.D
 Acq On : 24 May 2022 22:55
 Operator : JC\MD
 Sample : N2968-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-28

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\82N052422W.M
 Title : SW846 8260

Signal : TIC: VN072605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	36	45	50	rBV2	20379	37408	1.71%	0.414%
2	2.434	70	76	84	rVB	46079	71425	3.27%	0.790%
3	3.116	183	192	207	rVB2	49964	116245	5.32%	1.285%
4	3.510	251	259	271	rVB5	10024	30879	1.41%	0.341%
5	3.987	331	340	349	rBV4	8756	23152	1.06%	0.256%
6	5.181	533	543	559	rVB3	20671	74112	3.39%	0.819%
7	5.357	559	573	590	rBV2	124208	442290	20.26%	4.890%
8	5.604	604	615	629	rBV	58602	204780	9.38%	2.264%
9	6.487	750	765	777	rBV4	17798	61092	2.80%	0.675%
10	7.145	871	877	887	rVB4	15619	43993	2.02%	0.486%
11	8.016	1015	1025	1030	rBV	97787	232852	10.67%	2.575%
12	8.081	1030	1036	1045	rVV2	179327	409382	18.75%	4.526%
13	8.457	1087	1100	1109	rBV	882665	2183100	100.00%	24.137%
14	8.528	1109	1112	1118	rVB3	15281	25062	1.15%	0.277%
15	8.963	1175	1186	1201	rBV	280489	569387	26.08%	6.295%
16	10.192	1390	1395	1406	rVB2	13608	29285	1.34%	0.324%
17	10.439	1428	1437	1445	rBV	447374	825745	37.82%	9.130%
18	10.639	1460	1471	1477	rVB2	22372	40418	1.85%	0.447%
19	10.710	1477	1483	1491	rBV2	21989	38002	1.74%	0.420%
20	11.121	1549	1553	1564	rVB2	27451	52945	2.43%	0.585%
21	11.580	1625	1631	1638	rBV2	16688	30422	1.39%	0.336%
22	11.739	1650	1658	1669	rBV	607400	1051588	48.17%	11.627%
23	11.839	1669	1675	1684	rVB	36163	64529	2.96%	0.713%
24	11.951	1689	1694	1699	rBV	13435	23942	1.10%	0.265%
25	12.574	1793	1800	1807	rBV	37420	59866	2.74%	0.662%
26	12.727	1818	1826	1838	rBV	441631	722717	33.11%	7.991%
27	12.915	1852	1858	1865	rVB	41814	68700	3.15%	0.760%
28	13.357	1927	1933	1938	rVB3	13541	24187	1.11%	0.267%
29	13.668	1979	1986	2000	rBV	449783	815459	37.35%	9.016%
30	13.833	2007	2014	2016	rBV	25713	44486	2.04%	0.492%
31	13.868	2016	2020	2026	rVB	227746	373697	17.12%	4.132%
32	14.062	2047	2053	2059	rBV	19150	29466	1.35%	0.326%
33	14.210	2073	2078	2084	rBV	15883	25229	1.16%	0.279%
34	14.321	2092	2097	2104	rVB	50379	79337	3.63%	0.877%
35	14.533	2125	2133	2137	rBV2	25420	45554	2.09%	0.504%
36	14.927	2192	2200	2207	rVB3	17123	32286	1.48%	0.357%

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Instrument :
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ClientSampleId :
MW-28

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\82N052422W.M
Title : SW846 8260

37	15.504	2287	2298	2304	rBV	20117	41504	1.90%	0.459%
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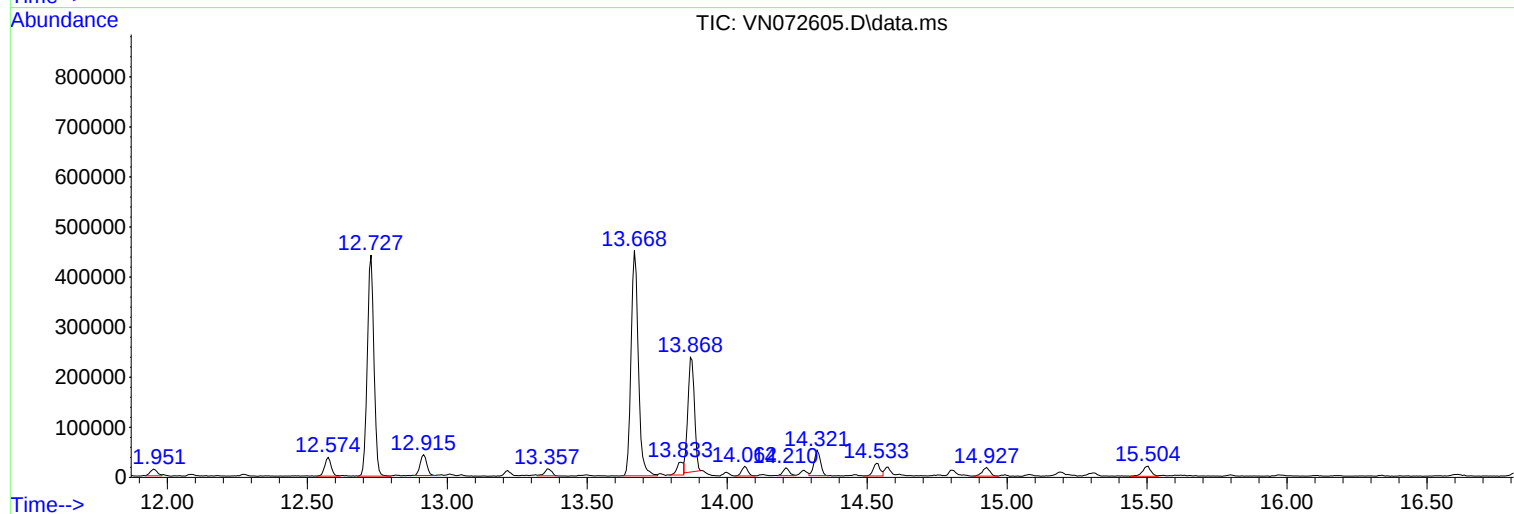
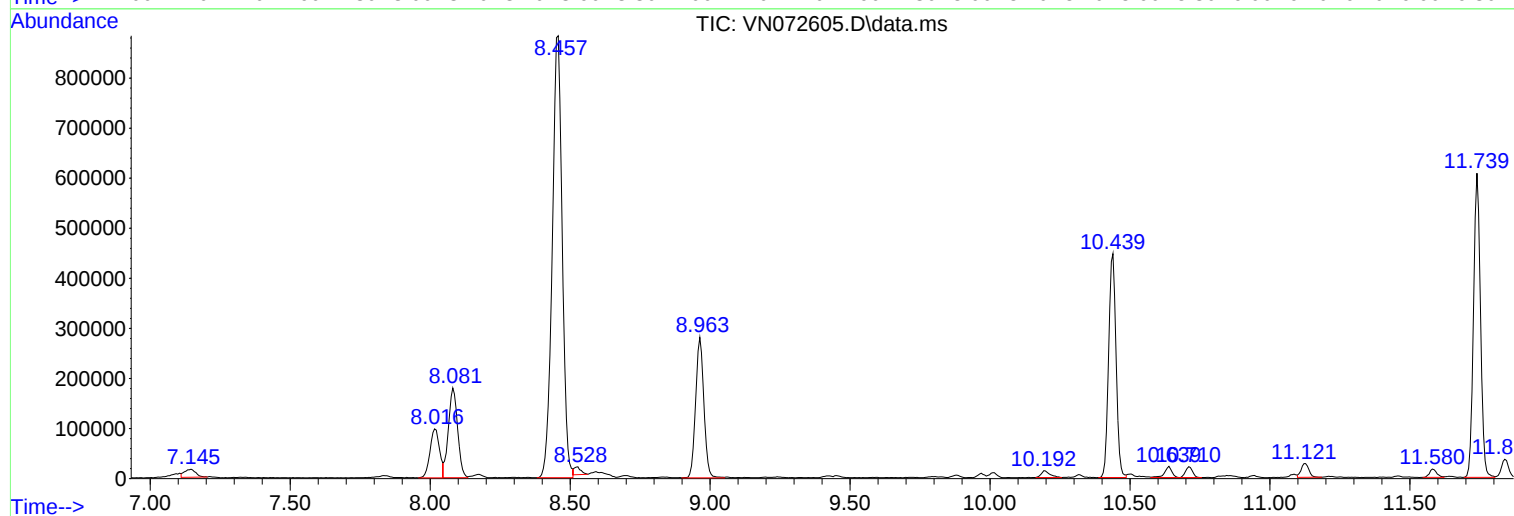
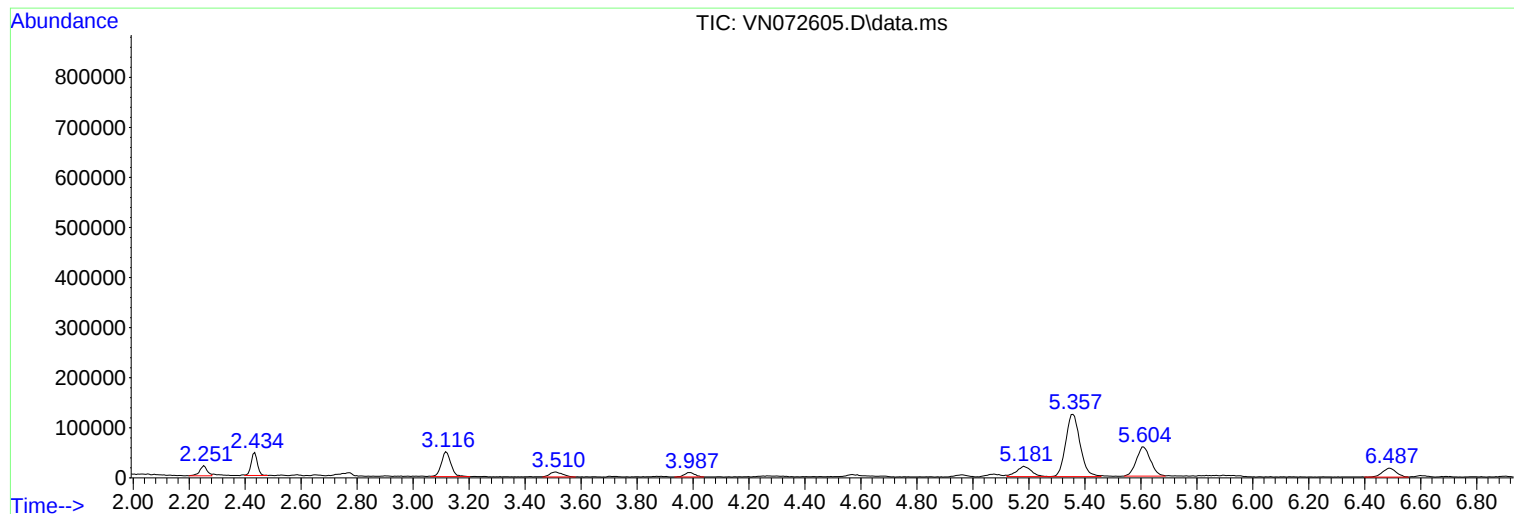
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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



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Instrument :
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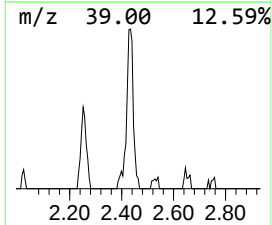
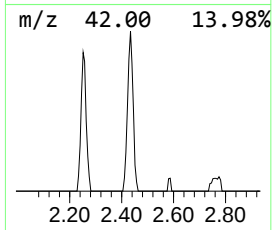
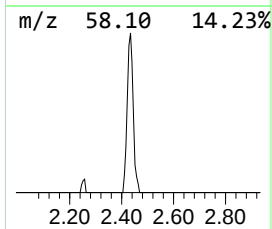
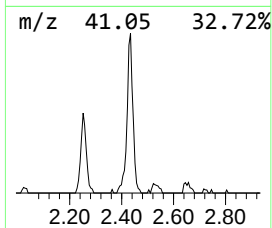
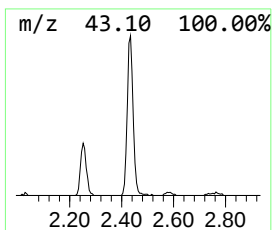
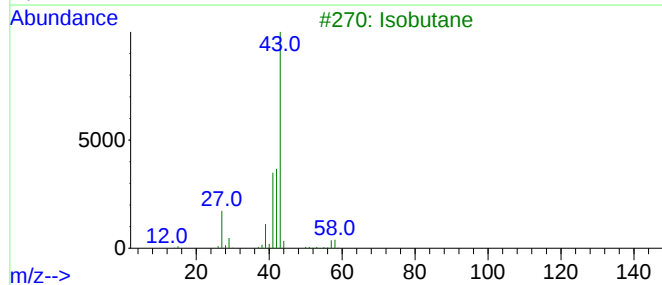
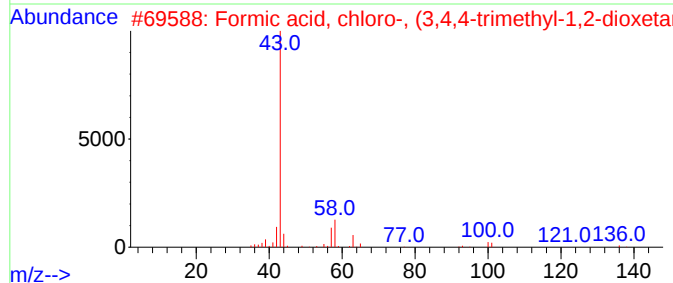
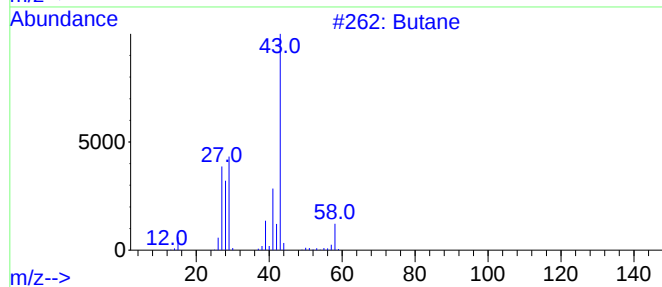
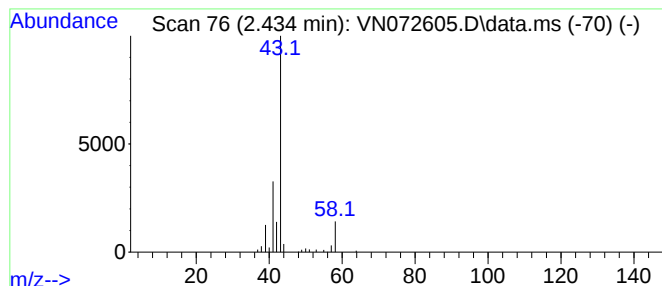
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	8.72 ug/l	71425	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	64
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Cyclobutylamine	71	C4H9N	002516-34-9	4



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Operator : JC\MD
Sample : N2968-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

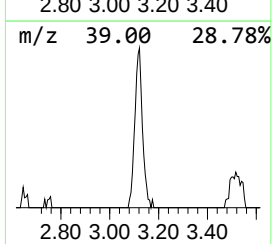
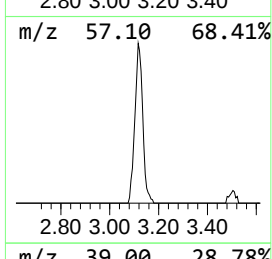
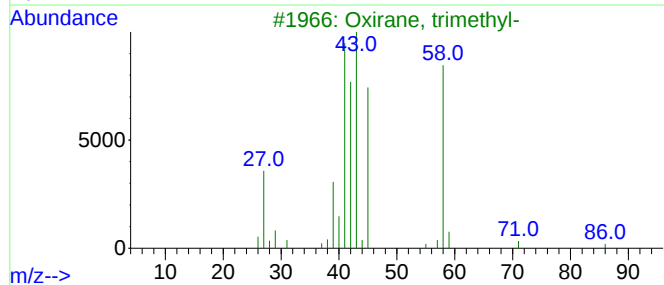
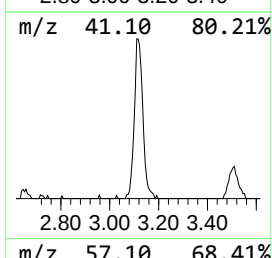
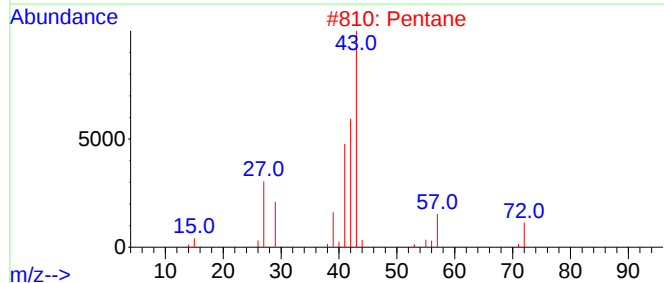
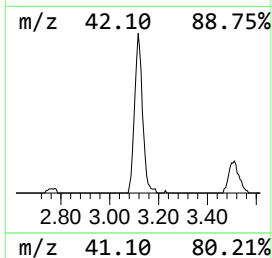
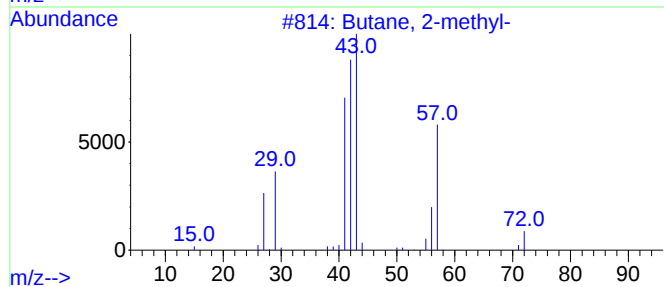
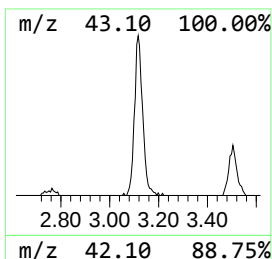
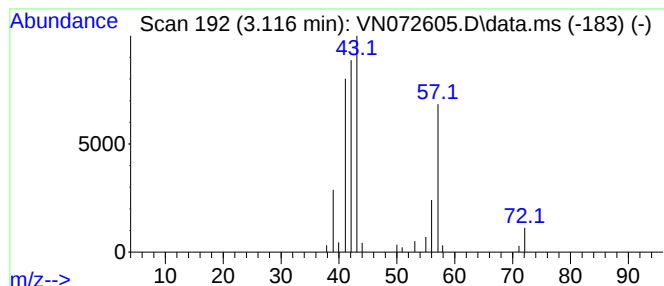
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	14.20 ug/l	116245	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	38
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
5			Oxirane, ethyl-	72	C4H8O	000106-88-7	9



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Data File : VN072605.D
Acq On : 24 May 2022 22:55
Operator : JC\MD
Sample : N2968-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

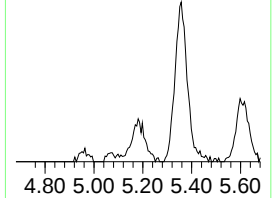
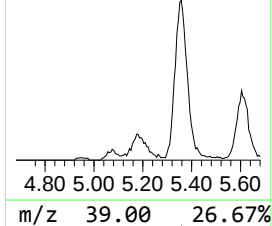
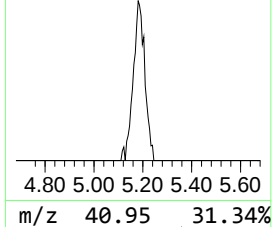
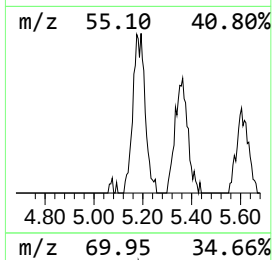
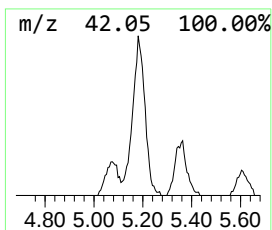
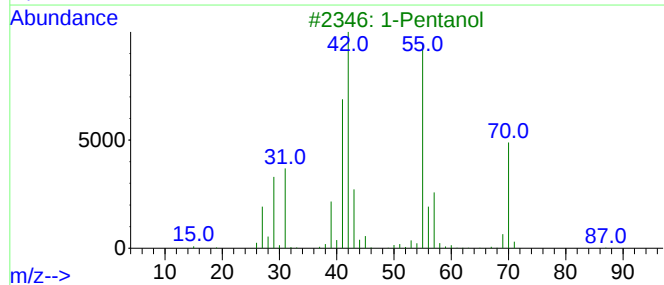
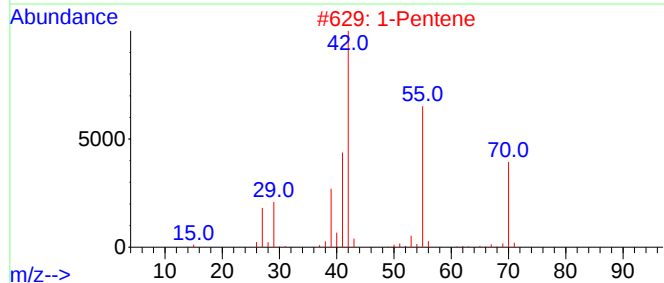
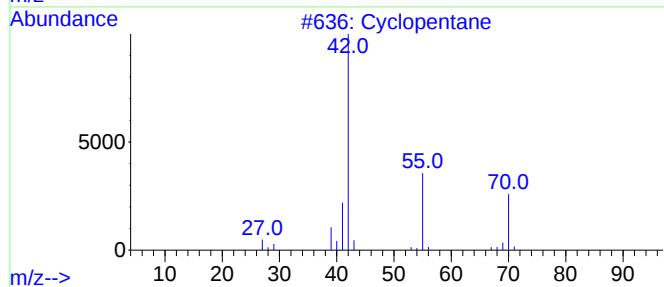
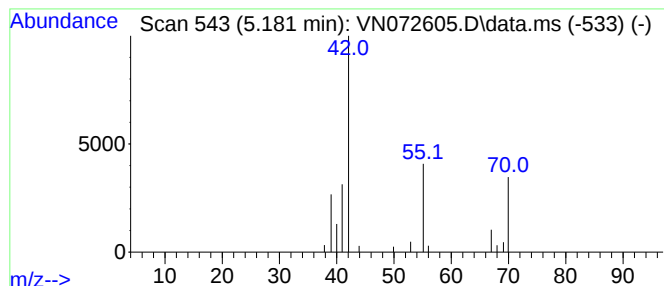
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	9.05 ug/l	74112	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	78
2			1-Pentene	70	C5H10	000109-67-1	64
3			1-Pentanol	88	C5H12O	000071-41-0	9
4			Cyclobutanone	70	C4H6O	001191-95-3	7
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	5



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Sample : N2968-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

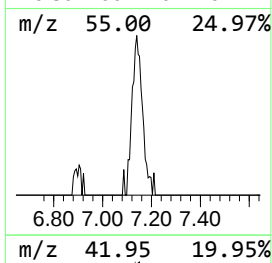
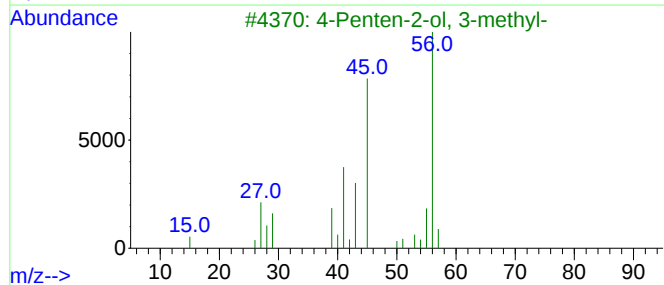
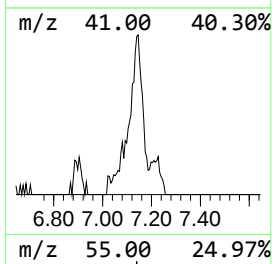
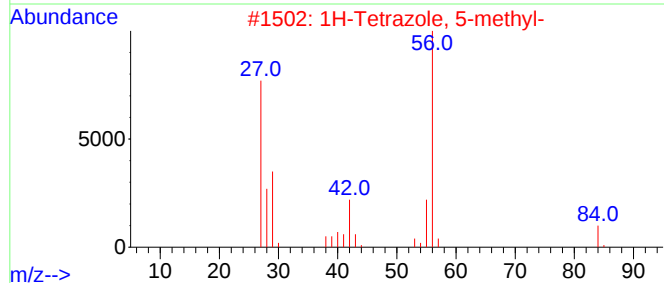
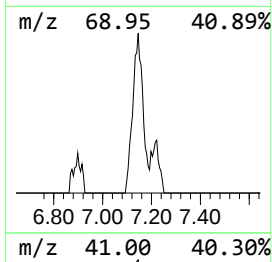
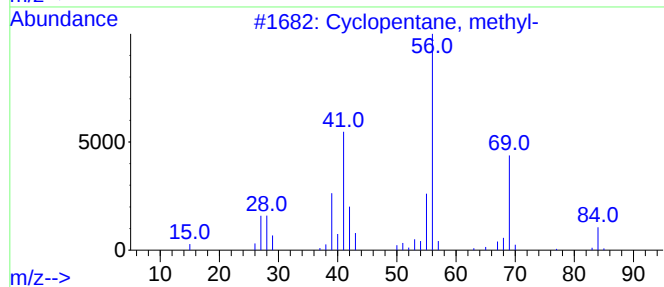
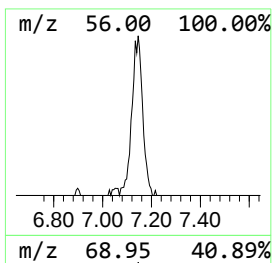
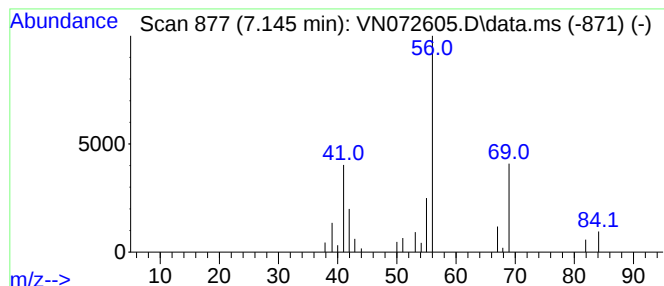
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	5.37 ug/l	43993	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	80
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3			4-Penten-2-ol, 3-methyl-	100	C6H12O	001569-59-1	33
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	9



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ALS Vial : 25 Sample Multiplier: 1

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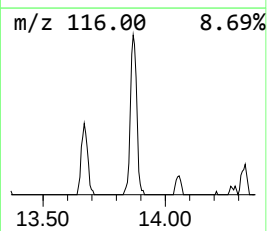
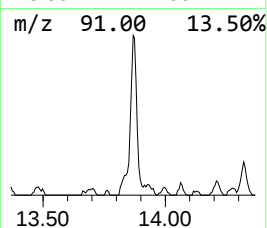
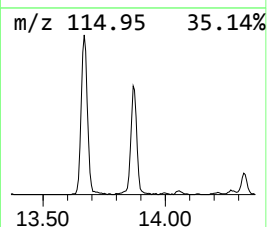
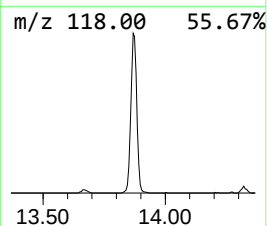
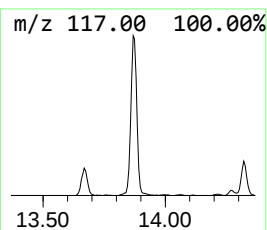
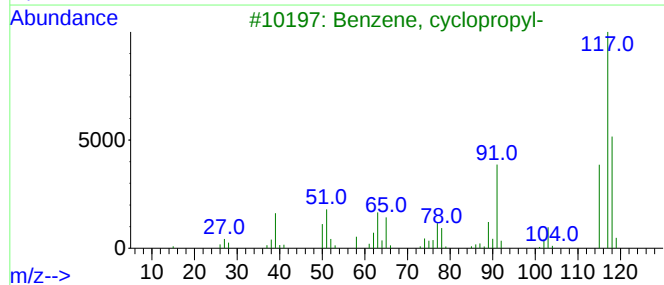
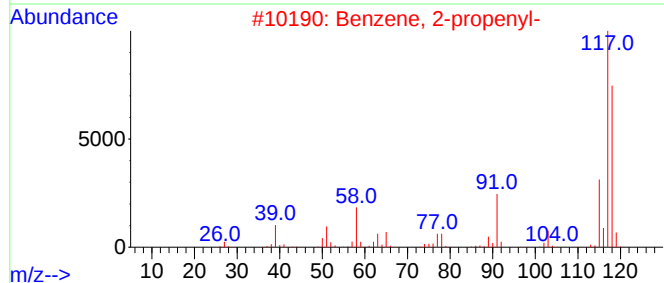
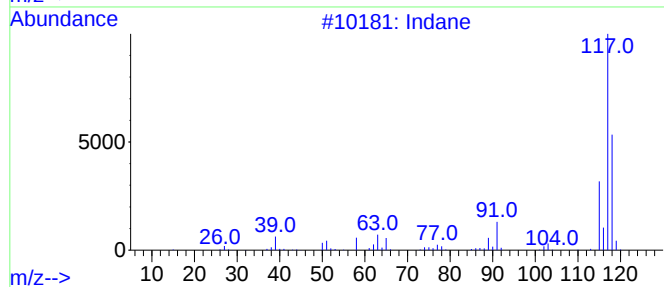
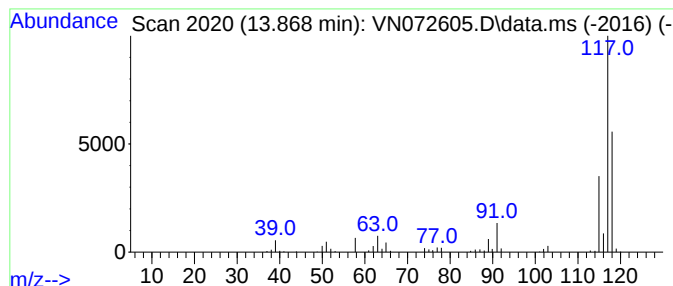
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	22.91 ug/l	373697	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052422\
Data File : VN072605.D
Acq On : 24 May 2022 22:55
Operator : JC\MD
Sample : N2968-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052422W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	2.434	8.7	ug/l	71425	1	8.081	409382	50.0
Butane, 2-methyl-	3.116	14.2	ug/l	116245	1	8.081	409382	50.0
Cyclopentane	5.181	9.1	ug/l	74112	1	8.081	409382	50.0
Cyclopentane, m...	7.145	5.4	ug/l	43993	1	8.081	409382	50.0
Indane	13.868	22.9	ug/l	373697	4	13.668	815459	50.0