

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
 Data File : VX039216.D
 Acq On : 14 Dec 2023 18:14
 Operator : JC/MD
 Sample : 05829-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-3

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_X\Method\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039216.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	20	26	42	rBV	24383	58489	3.40%	0.413%
2	5.098	646	658	667	rBV	23301	70636	4.10%	0.498%
3	5.385	693	705	716	rBV	85388	251339	14.60%	1.773%
4	5.550	722	732	749	rVB	129203	367180	21.32%	2.590%
5	5.952	789	798	809	rBV	98337	262617	15.25%	1.853%
6	6.757	921	930	953	rBV	230494	576576	33.48%	4.068%
7	8.647	1234	1240	1247	rBV	506689	782325	45.43%	5.519%
8	8.720	1247	1252	1264	rVB	183212	295407	17.15%	2.084%
9	10.055	1465	1471	1481	rBV	542423	773329	44.91%	5.456%
10	10.189	1488	1493	1504	rBV	729615	1001140	58.14%	7.063%
11	10.299	1504	1511	1522	rBV	1289933	1721999	100.00%	12.148%
12	10.640	1561	1567	1582	rVB	468981	603689	35.06%	4.259%
13	10.963	1615	1620	1627	rBV	48753	62941	3.66%	0.444%
14	11.079	1634	1639	1651	rBV	507554	631644	36.68%	4.456%
15	11.305	1670	1676	1682	rBV	100990	130219	7.56%	0.919%
16	11.378	1682	1688	1696	rVV	243571	470409	27.32%	3.319%
17	11.451	1696	1700	1708	rVB	233768	284448	16.52%	2.007%
18	11.609	1721	1726	1736	rVB	275916	347095	20.16%	2.449%
19	11.750	1744	1749	1756	rBV	1357811	1628788	94.59%	11.491%
20	12.018	1788	1793	1799	rBV	665311	842893	48.95%	5.947%
21	12.085	1799	1804	1810	rVB	406054	496458	28.83%	3.502%
22	12.243	1824	1830	1837	rBV	367382	516770	30.01%	3.646%
23	12.317	1837	1842	1852	rVB2	66510	97902	5.69%	0.691%
24	12.408	1852	1857	1862	rBV	51070	71458	4.15%	0.504%
25	12.463	1862	1866	1871	rVB	28434	37330	2.17%	0.263%
26	12.530	1871	1877	1879	rBV	66349	86375	5.02%	0.609%
27	12.554	1879	1881	1886	rVV	55579	58982	3.43%	0.416%
28	12.609	1886	1890	1894	rVV	88693	114386	6.64%	0.807%
29	12.646	1894	1896	1899	rVV	25533	25727	1.49%	0.182%
30	12.695	1899	1904	1913	rVB2	98089	138222	8.03%	0.975%
31	12.847	1923	1929	1935	rBV	32515	41553	2.41%	0.293%
32	12.920	1935	1941	1944	rVV	73042	89306	5.19%	0.630%
33	12.963	1944	1948	1953	rVB	89889	112762	6.55%	0.796%
34	13.164	1977	1981	1986	rVB	77647	92844	5.39%	0.655%
35	13.292	1997	2002	2007	rVV2	167194	214710	12.47%	1.515%
36	13.420	2019	2023	2030	rVB2	34361	46734	2.71%	0.330%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

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_X\Method\82X121323W.M

Title : SW846 8260

37	13.542	2039	2043	2046	rBV2	14151	18617	1.08%	0.131%
38	13.579	2046	2049	2055	rVV2	18039	33565	1.95%	0.237%
39	13.658	2055	2062	2069	rVB2	15451	35925	2.09%	0.253%
40	13.774	2075	2081	2088	rBV	402970	501432	29.12%	3.538%
41	13.865	2091	2096	2101	rVB	22685	30555	1.77%	0.216%
42	14.633	2218	2222	2232	rVB	59161	78308	4.55%	0.552%
43	14.780	2240	2246	2260	rVB	53781	71510	4.15%	0.504%

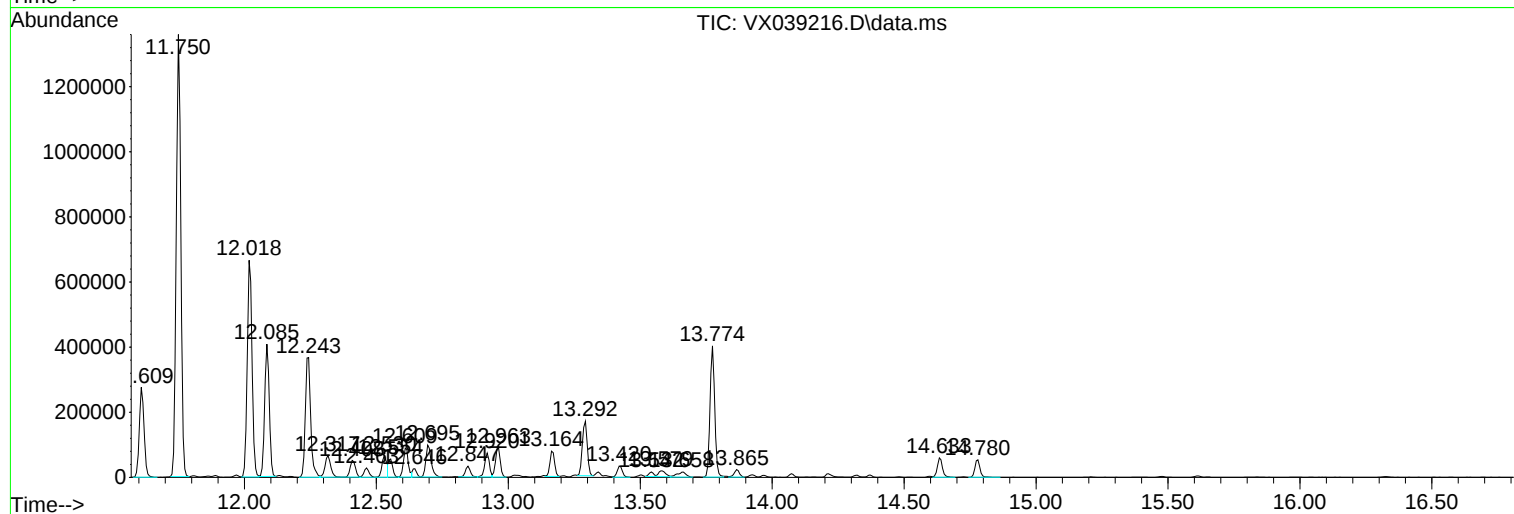
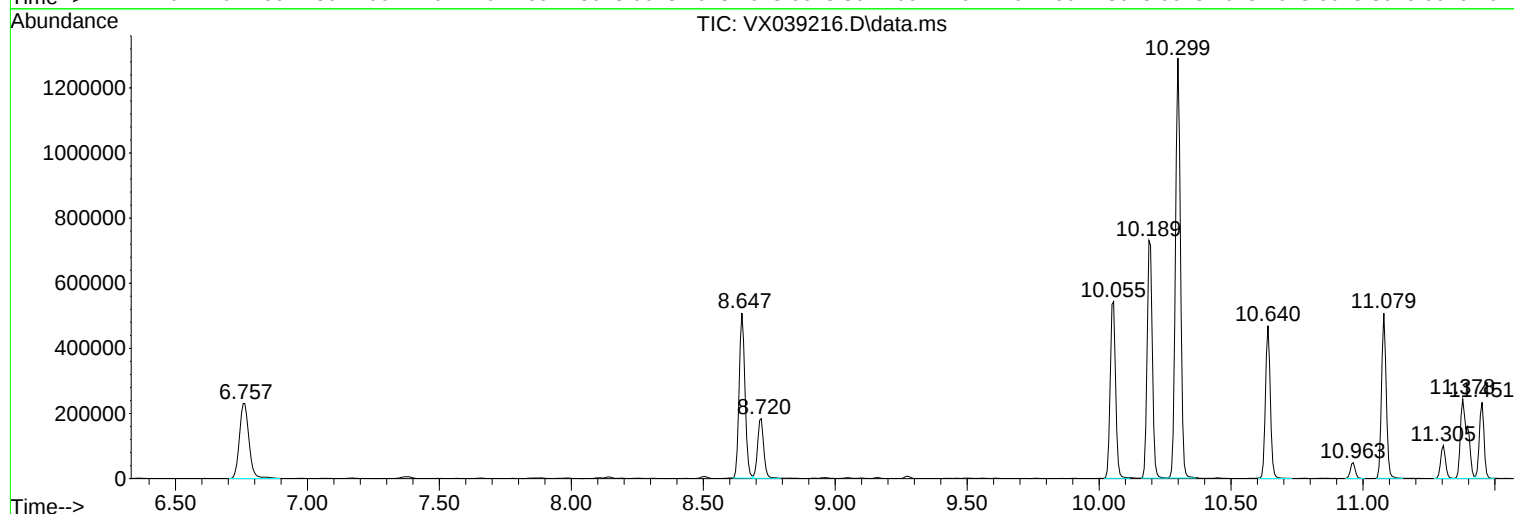
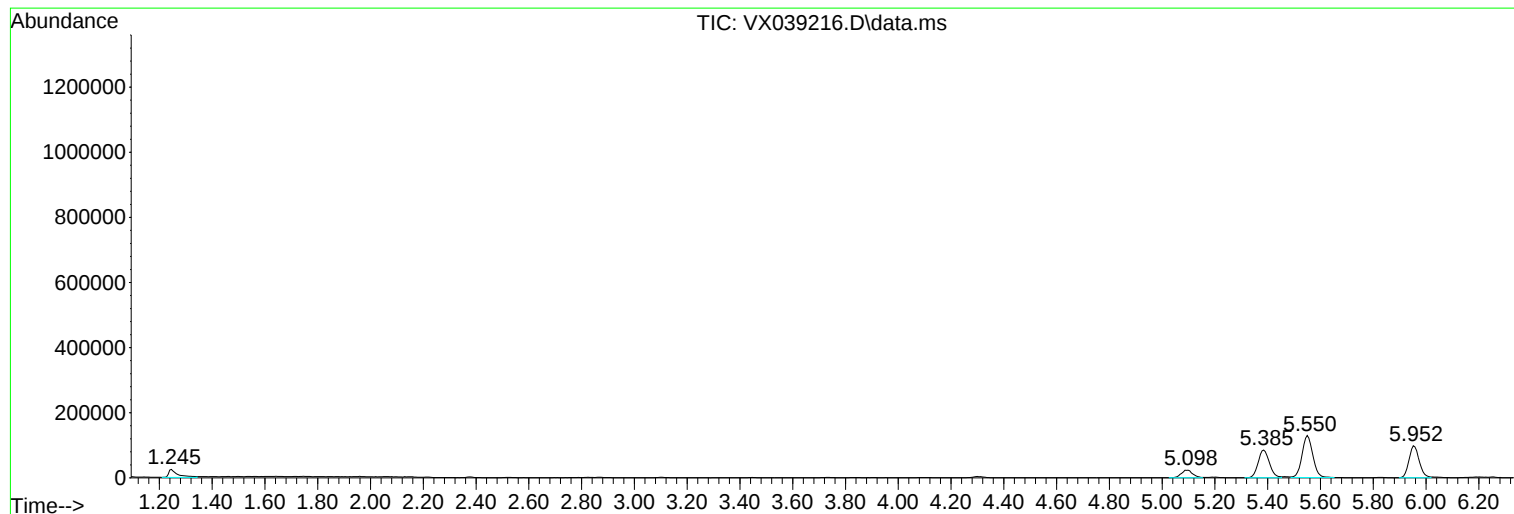
Sum of corrected areas: 14174594

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

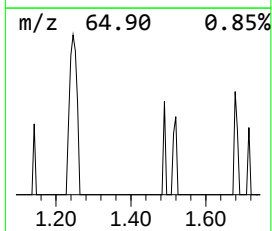
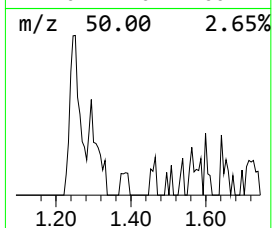
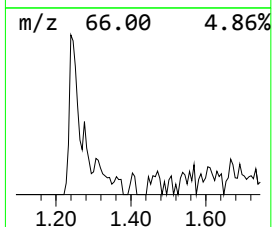
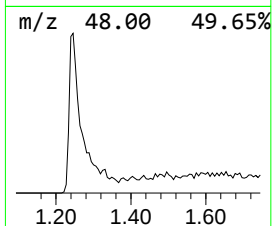
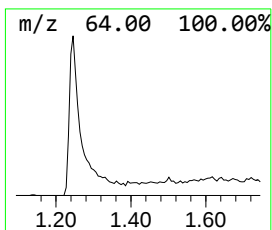
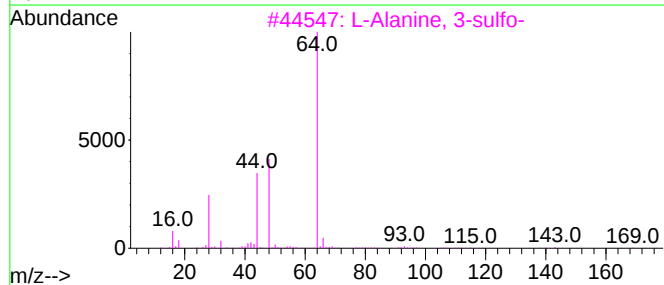
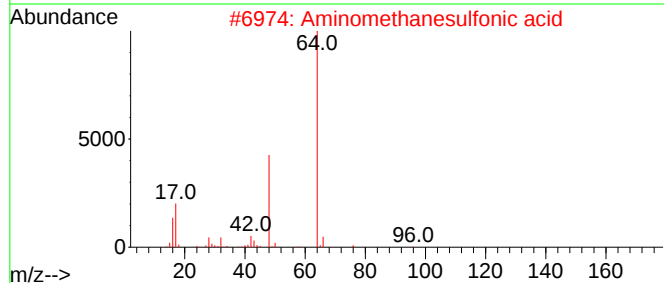
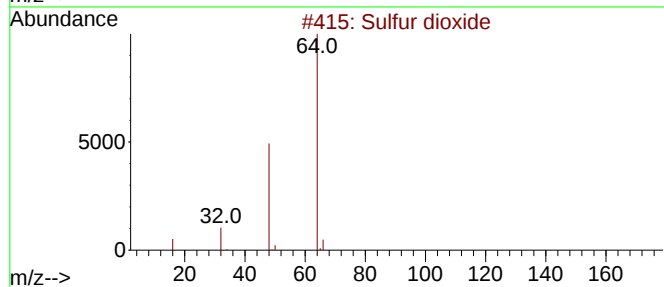
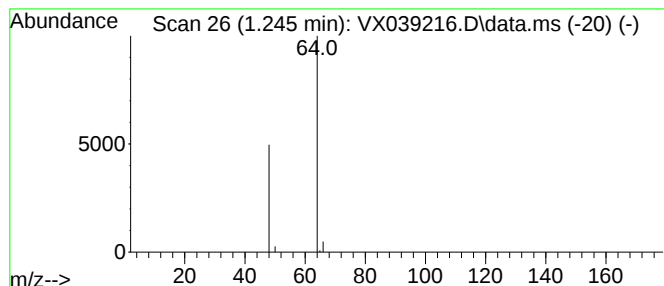
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.245	7.96 ug/l	58489	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

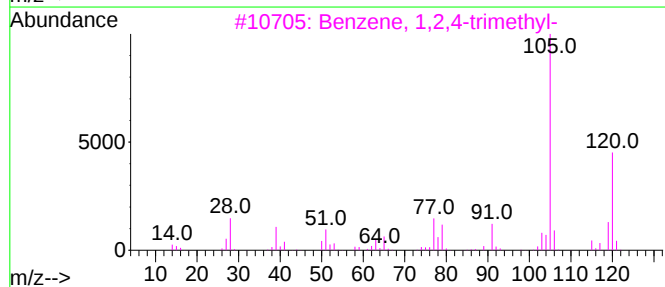
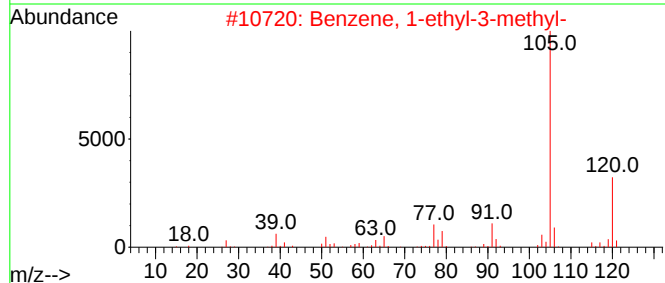
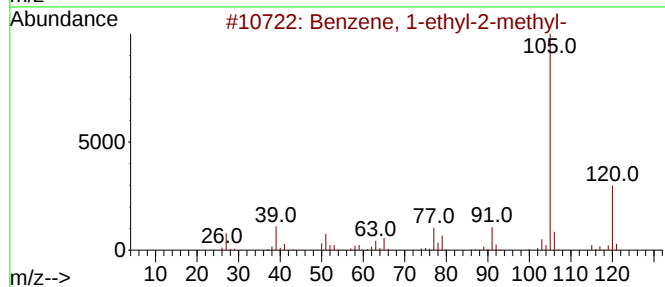
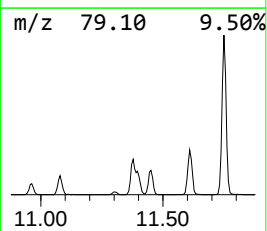
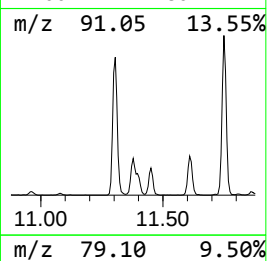
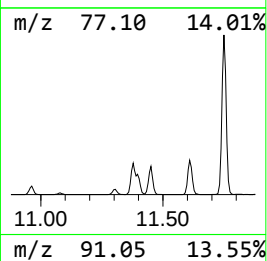
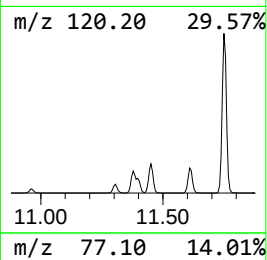
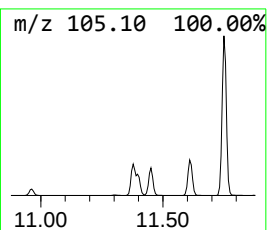
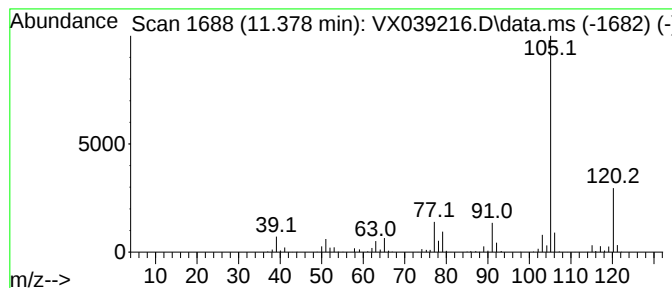
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	27.90 ug/l	470409	1,4-Dichlorobenzene-d4	12.018

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			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

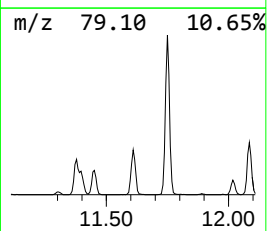
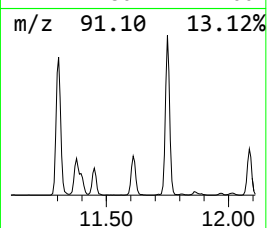
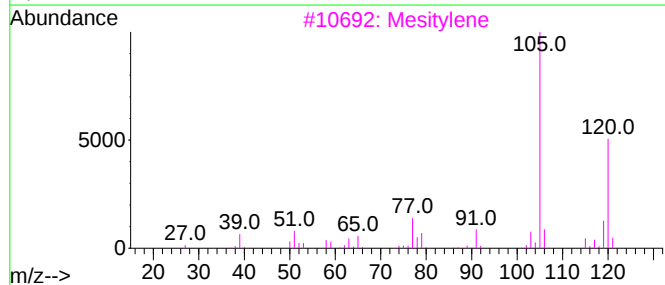
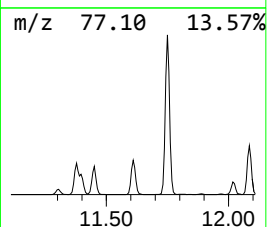
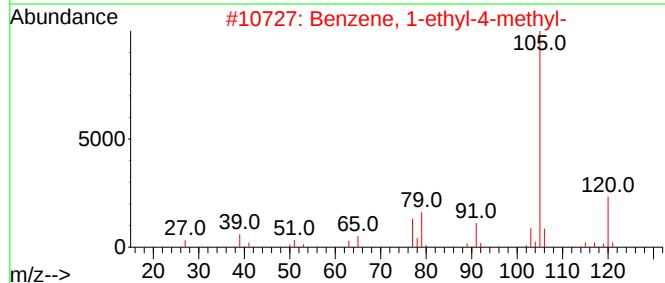
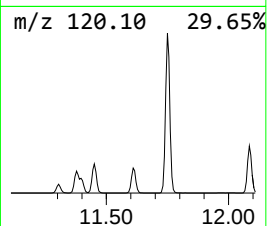
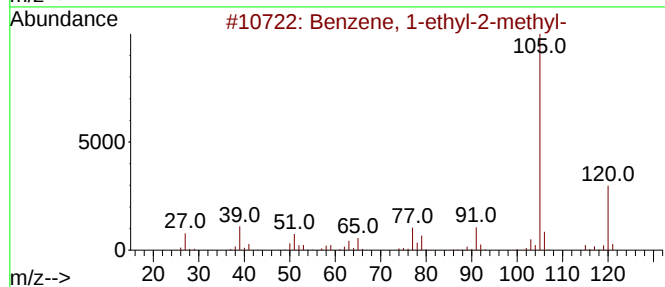
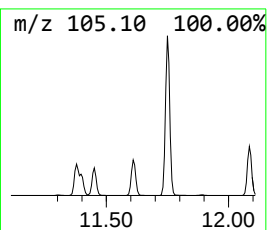
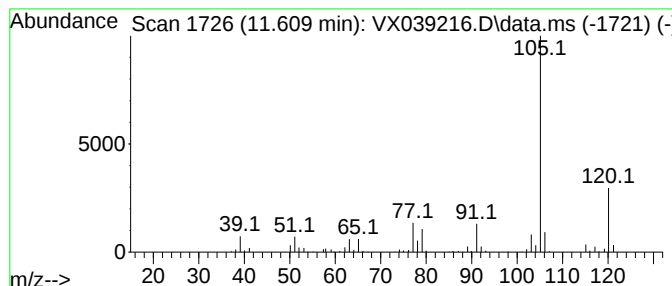
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.609	20.59 ug/l	347095	1,4-Dichlorobenzene-d4	12.018

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	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

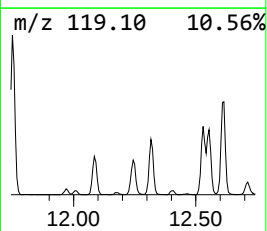
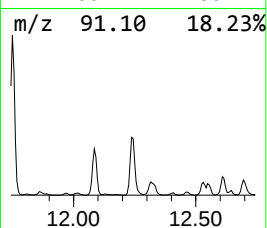
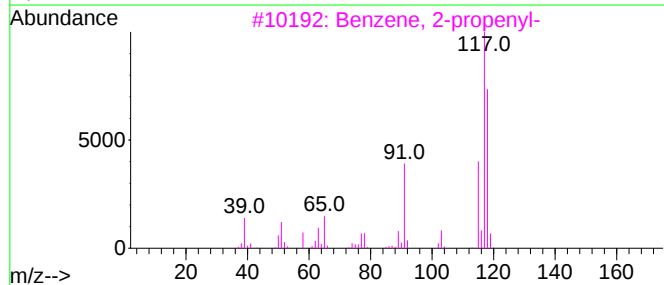
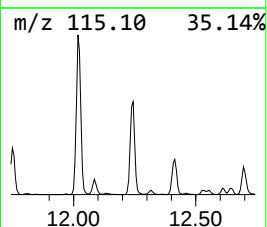
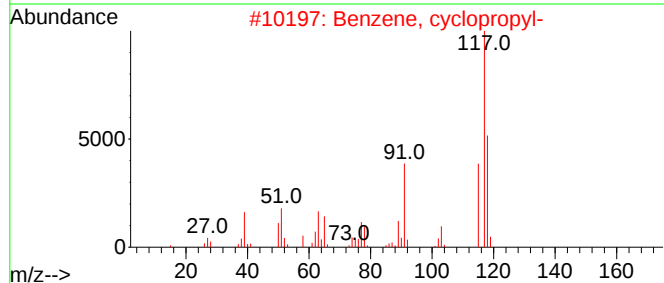
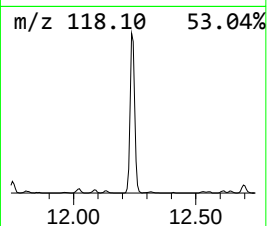
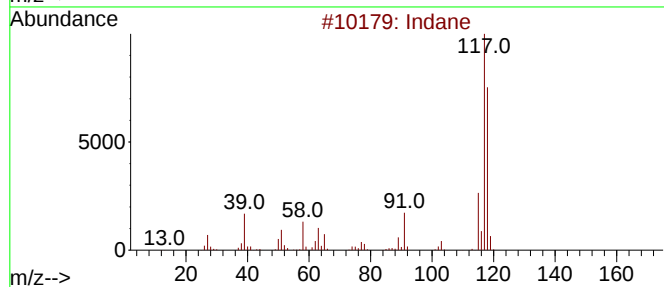
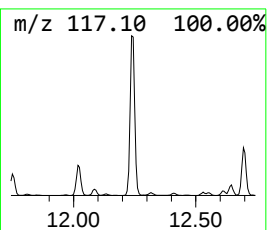
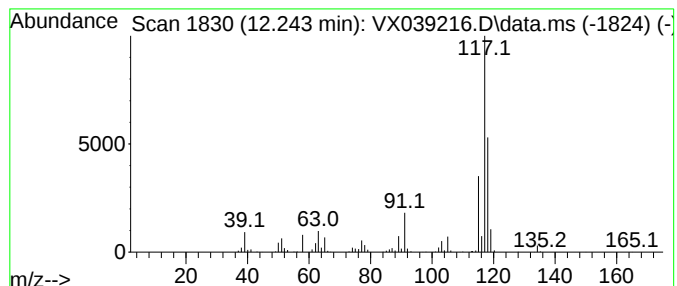
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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.
12.243	30.65 ug/l	516770	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4			Delatacyclene	118	C9H10	007785-10-6	58
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

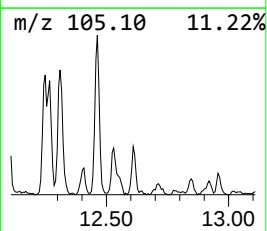
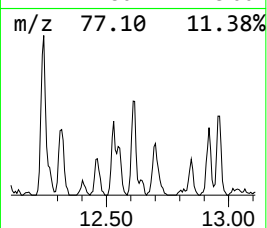
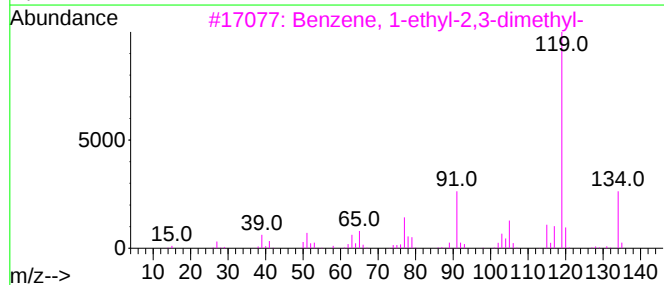
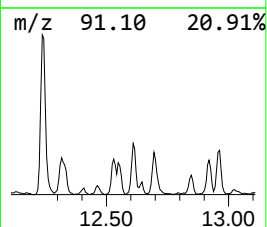
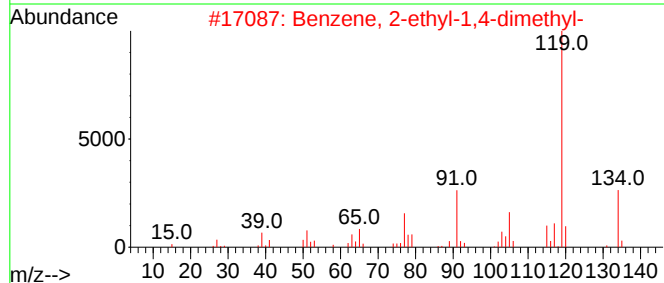
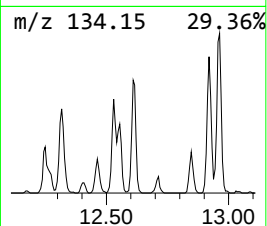
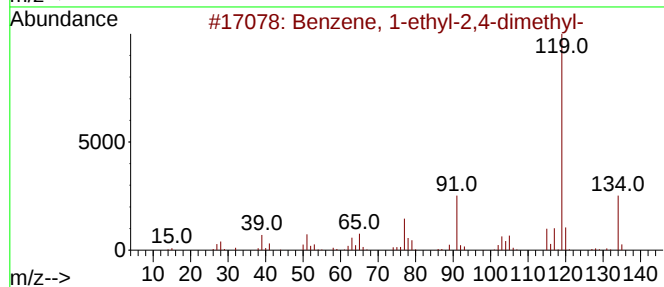
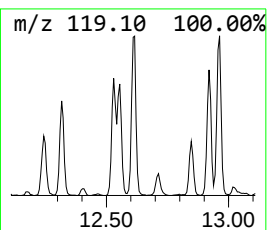
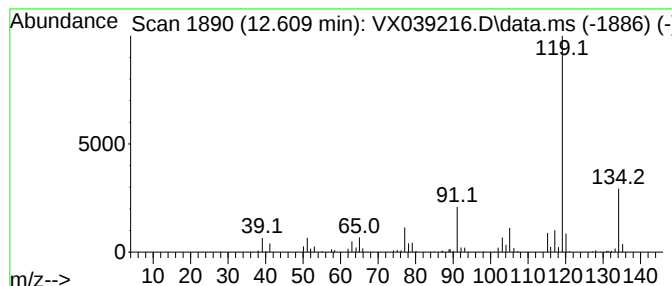
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.609	6.79 ug/l	114386	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

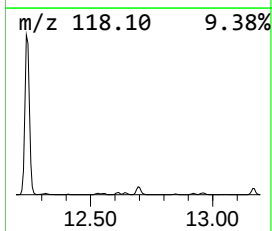
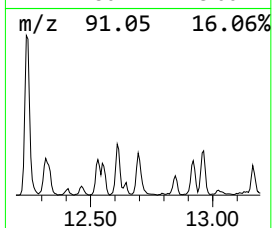
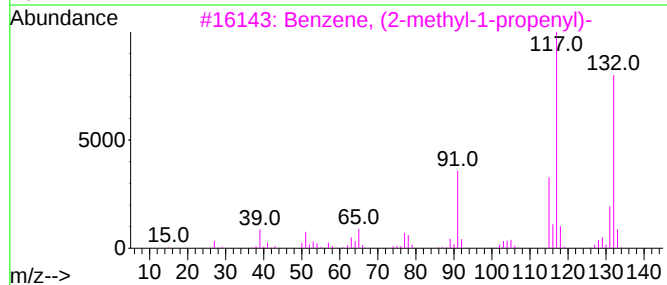
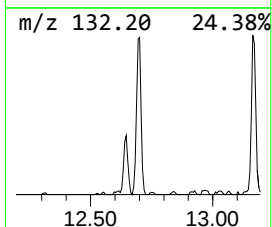
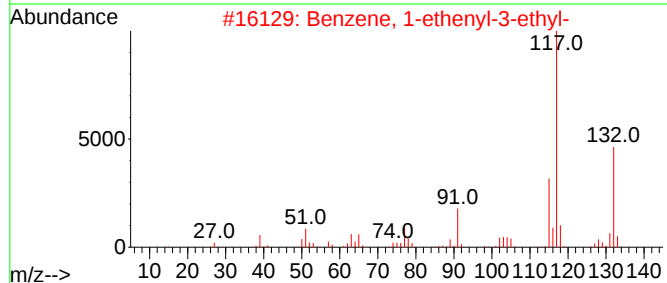
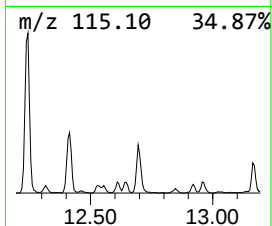
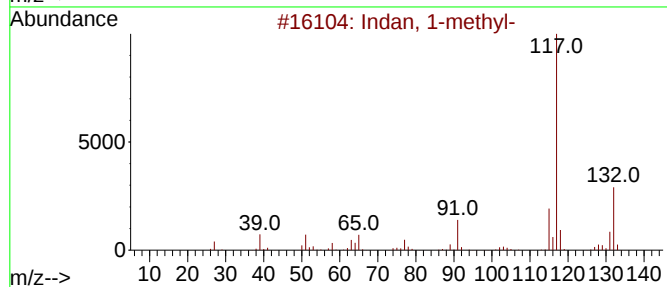
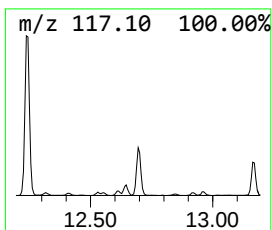
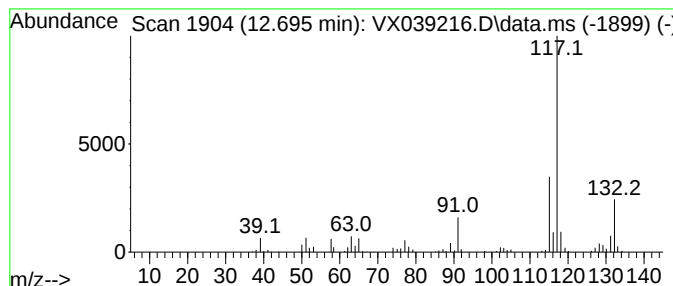
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	8.20 ug/l	138222	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

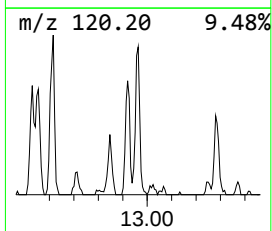
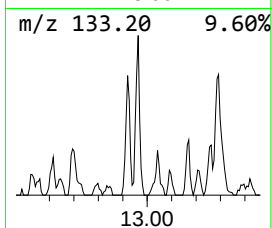
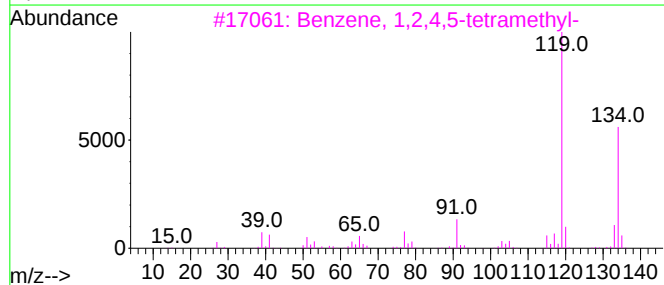
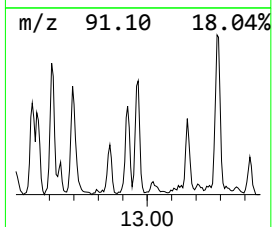
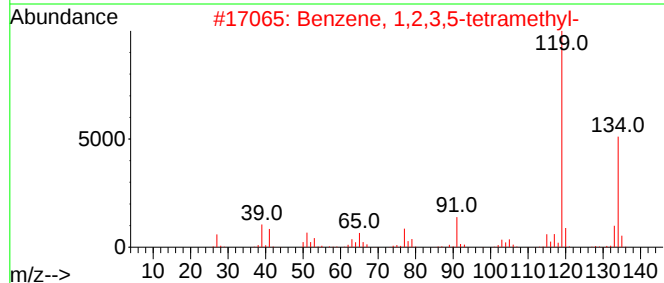
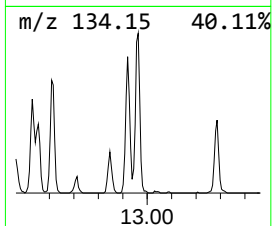
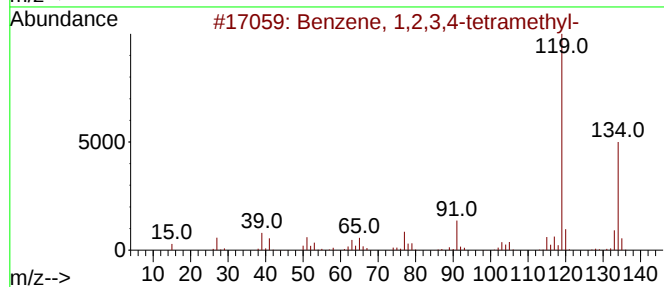
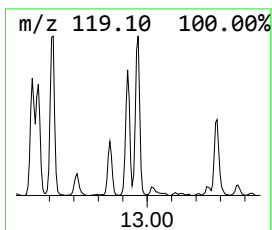
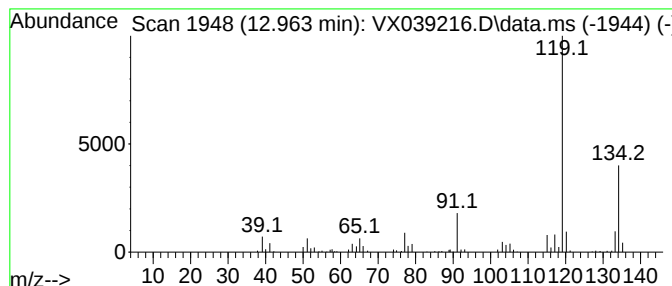
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	6.69 ug/l	112762	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

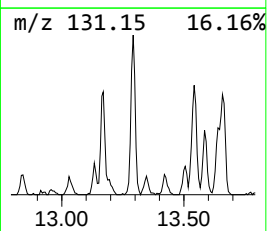
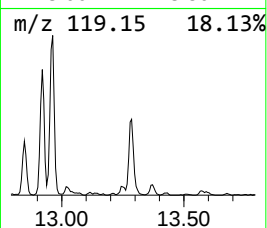
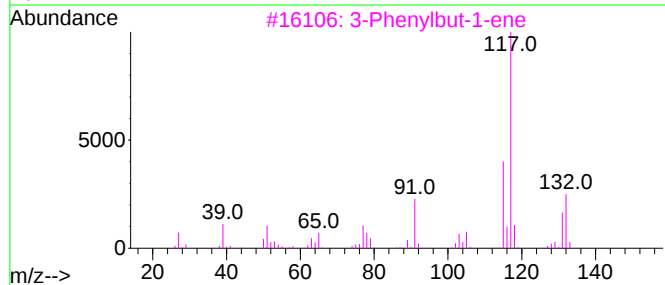
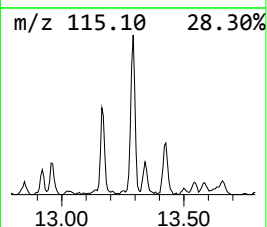
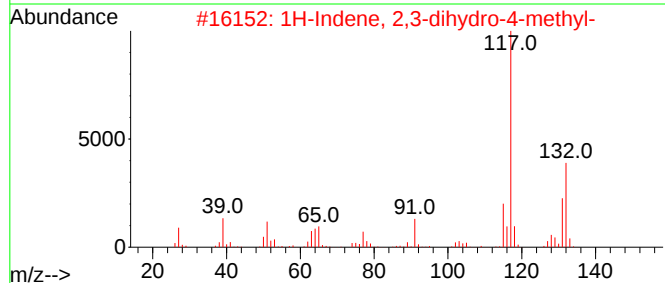
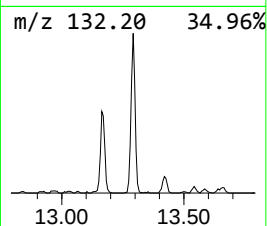
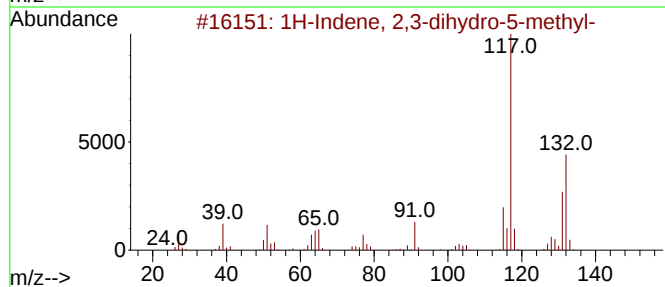
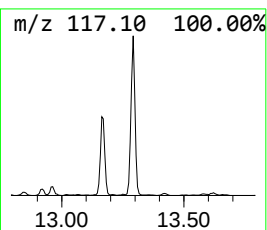
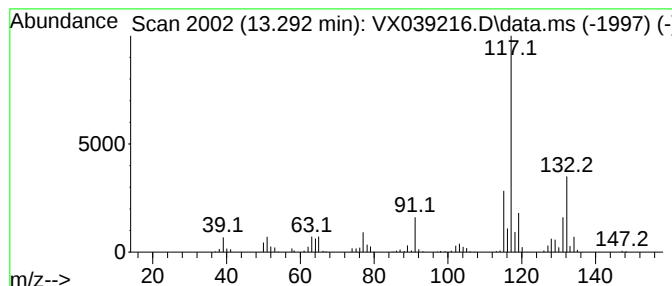
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	12.74 ug/l	214710	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
2		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

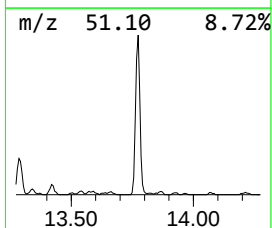
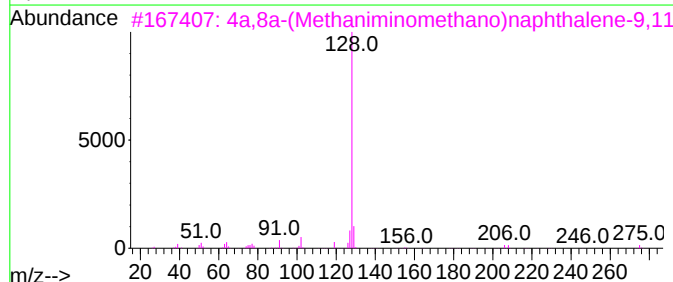
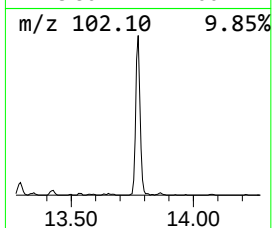
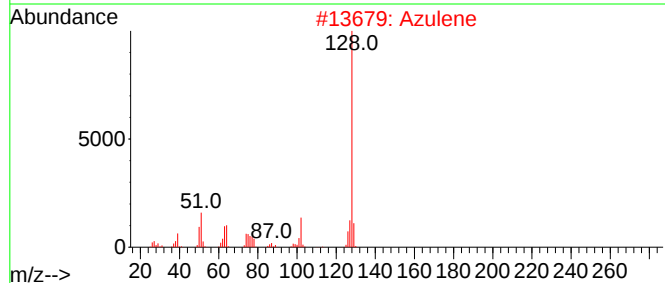
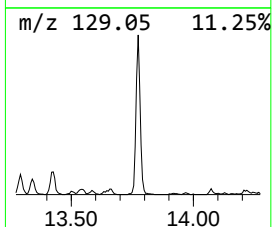
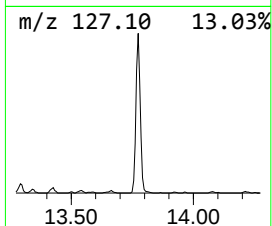
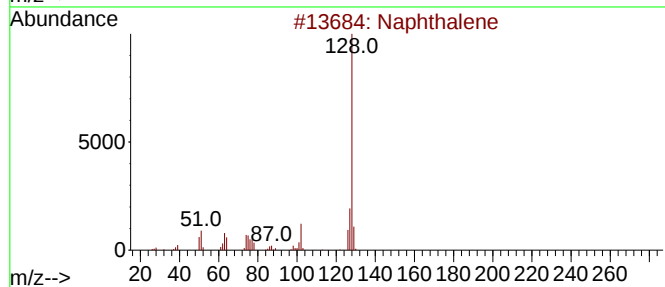
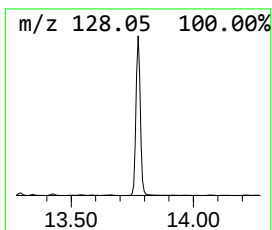
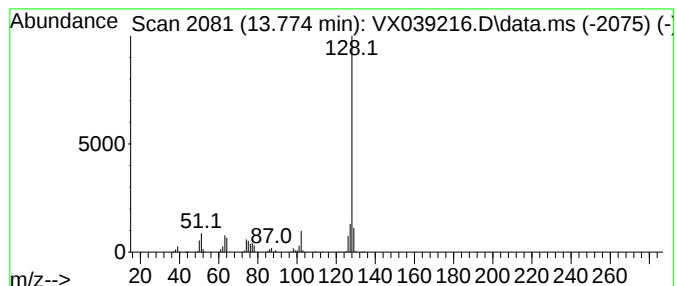
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	29.74 ug/l	501432	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	94
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	72
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121423\
Data File : VX039216.D
Acq On : 14 Dec 2023 18:14
Operator : JC/MD
Sample : 05829-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.245	8.0	ug/l	58489	1	5.550	367180	50.0
Benzene, 1-ethy...	11.378	27.9	ug/l	470409	4	12.018	842893	50.0
Benzene, 1-ethy...	11.609	20.6	ug/l	347095	4	12.018	842893	50.0
Indane	12.243	30.6	ug/l	516770	4	12.018	842893	50.0
Benzene, 1-ethy...	12.609	6.8	ug/l	114386	4	12.018	842893	50.0
Indan, 1-methyl-	12.695	8.2	ug/l	138222	4	12.018	842893	50.0
Benzene, 1,2,3,...	12.963	6.7	ug/l	112762	4	12.018	842893	50.0
1H-Indene, 2,3-...	13.292	12.7	ug/l	214710	4	12.018	842893	50.0
Azulene	13.774	29.7	ug/l	501432	4	12.018	842893	50.0