

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
 Data File : VX028735.D
 Acq On : 16 May 2022 16:42
 Operator : JC/MD
 Sample : N2862-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-9RR

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	692	706	718	rBV	166992	483345	6.40%	0.985%
2	5.556	718	733	751	rVB	263624	770204	10.21%	1.570%
3	5.958	788	799	814	rBV	184872	478570	6.34%	0.976%
4	6.763	922	931	942	rBV	431901	1025033	13.58%	2.090%
5	8.433	1191	1205	1210	rBV3	65612	139381	1.85%	0.284%
6	8.653	1235	1241	1248	rVB	915093	1430001	18.95%	2.916%
7	8.720	1248	1252	1257	rVB	82076	119783	1.59%	0.244%
8	8.958	1286	1291	1300	rVB	702314	1096731	14.53%	2.236%
9	9.049	1300	1306	1312	rBV	920332	1356642	17.98%	2.766%
10	9.458	1364	1373	1377	rBV	57190	94061	1.25%	0.192%
11	9.616	1394	1399	1404	rBV2	74851	119211	1.58%	0.243%
12	10.055	1466	1471	1481	rBV	974833	1323585	17.54%	2.699%
13	10.195	1490	1494	1496	rBV	91769	131733	1.75%	0.269%
14	10.299	1505	1511	1518	rVB	2409361	3292339	43.63%	6.713%
15	10.646	1562	1568	1577	rVB	5924381	7546790	100.00%	15.387%
16	10.963	1614	1620	1625	rBV	56341	78821	1.04%	0.161%
17	11.085	1634	1640	1645	rBV	792490	1062515	14.08%	2.166%
18	11.384	1681	1689	1696	rVV	1145420	1934142	25.63%	3.943%
19	11.451	1696	1700	1709	rVB	1364196	1629535	21.59%	3.322%
20	11.616	1721	1727	1734	rBV	2615180	3128460	41.45%	6.378%
21	11.756	1745	1750	1755	rVB	1852314	2278490	30.19%	4.645%
22	11.975	1780	1786	1789	rBV	147247	190387	2.52%	0.388%
23	12.024	1789	1794	1799	rVV	1123712	1384832	18.35%	2.823%
24	12.091	1799	1805	1813	rVV	3321394	3976416	52.69%	8.107%
25	12.244	1825	1830	1833	rBV2	829199	1115537	14.78%	2.274%
26	12.317	1838	1842	1849	rVB2	577540	781413	10.35%	1.593%
27	12.408	1849	1857	1862	rBV2	115253	167457	2.22%	0.341%
28	12.463	1862	1866	1872	rVB	260383	306333	4.06%	0.625%
29	12.530	1872	1877	1879	rBV	299805	379380	5.03%	0.773%
30	12.555	1879	1881	1886	rVB	368877	414281	5.49%	0.845%
31	12.616	1886	1891	1894	rBV	615547	712311	9.44%	1.452%
32	12.646	1894	1896	1900	rVV	117169	123757	1.64%	0.252%
33	12.701	1900	1905	1918	rVB2	906204	1270807	16.84%	2.591%
34	12.847	1924	1929	1934	rVB	386155	479739	6.36%	0.978%
35	12.920	1934	1941	1945	rBV	604371	772928	10.24%	1.576%
36	12.963	1945	1948	1954	rVB	652514	739591	9.80%	1.508%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

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

Peak separation: 5

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 Title : SW846 8260

37	13.042	1954	1961	1964	rBV3	78259	170566	2.26%	0.348%
38	13.170	1978	1982	1986	rVB	441275	526135	6.97%	1.073%
39	13.292	1997	2002	2007	rVB2	1829022	2323823	30.79%	4.738%
40	13.426	2019	2024	2030	rVB	238762	316573	4.19%	0.645%
41	13.506	2032	2037	2040	rBV2	59264	80977	1.07%	0.165%
42	13.542	2040	2043	2047	rVV	156265	227009	3.01%	0.463%
43	13.585	2047	2050	2055	rVV2	187693	308365	4.09%	0.629%
44	13.646	2055	2060	2061	rVV2	104647	164679	2.18%	0.336%
45	13.664	2061	2063	2068	rVB2	177407	215681	2.86%	0.440%
46	13.774	2075	2081	2089	rBV	870853	1109862	14.71%	2.263%
47	13.871	2091	2097	2102	rVB	160547	223379	2.96%	0.455%
48	14.213	2148	2153	2159	rBV	65807	110043	1.46%	0.224%
49	14.597	2211	2216	2219	rBV	140058	184072	2.44%	0.375%
50	14.640	2219	2223	2230	rVB	270375	362416	4.80%	0.739%
51	14.780	2241	2246	2253	rBV2	253704	389451	5.16%	0.794%

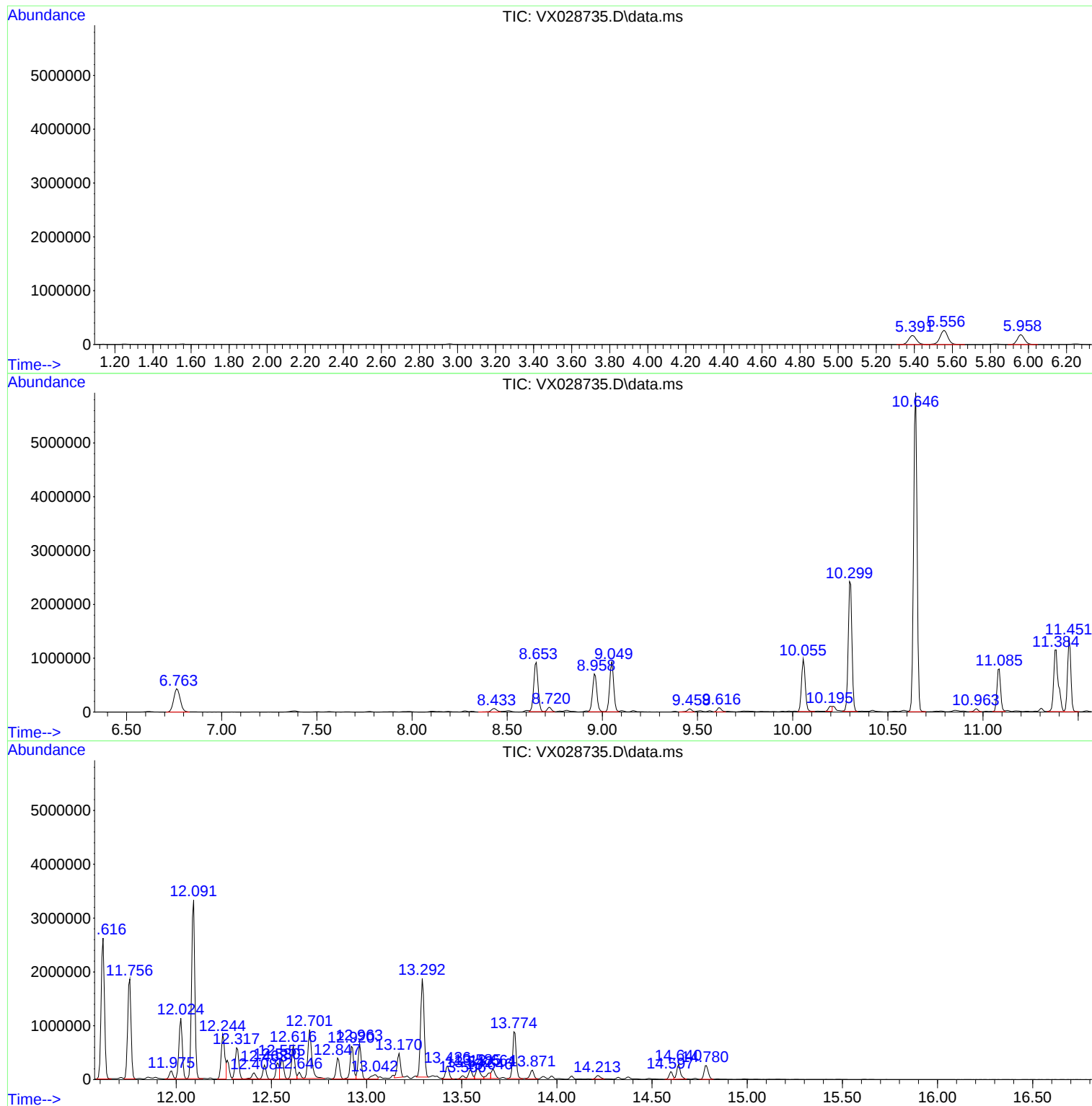
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

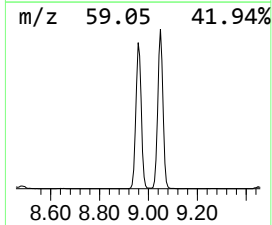
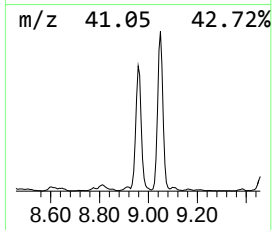
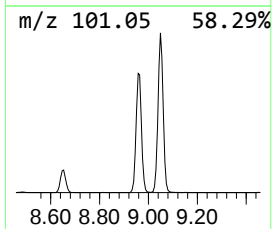
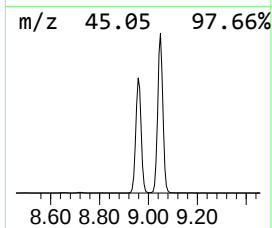
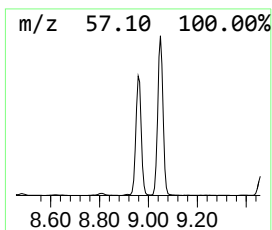
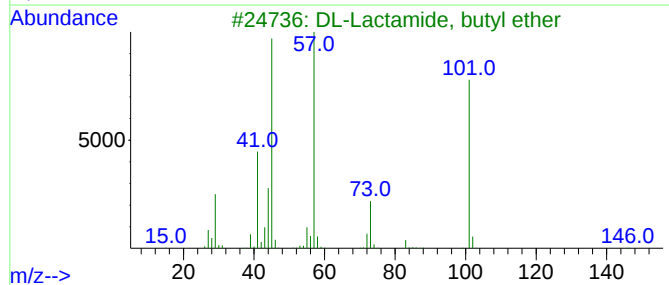
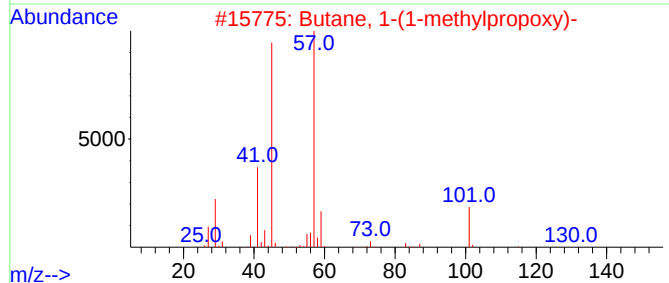
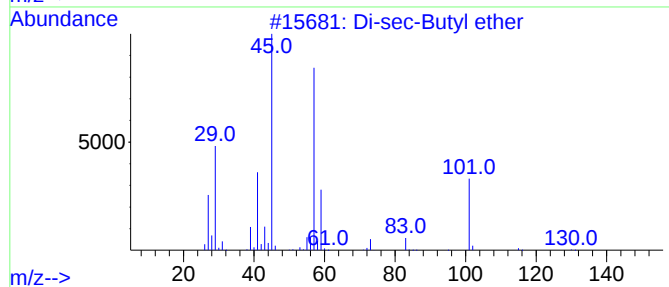
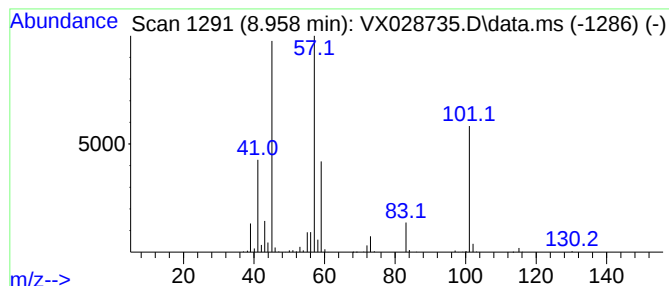
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Quant Title : SW846 8260

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

Peak Number 1 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	41.43 ug/l	1096730	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	45
4			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	42
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	37



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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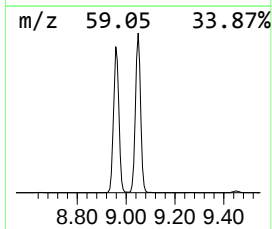
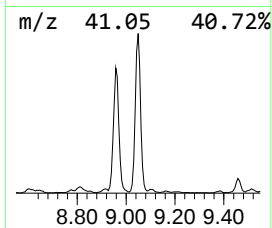
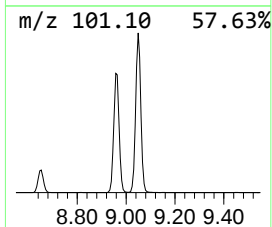
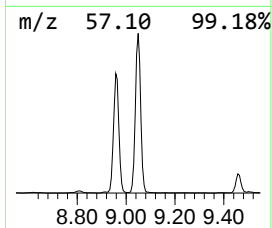
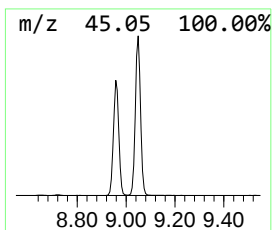
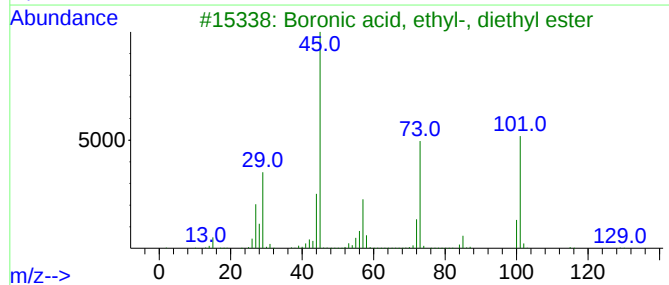
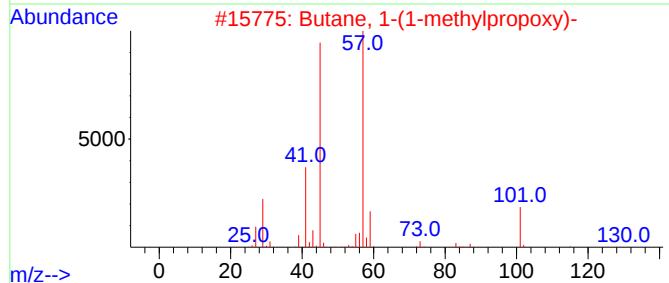
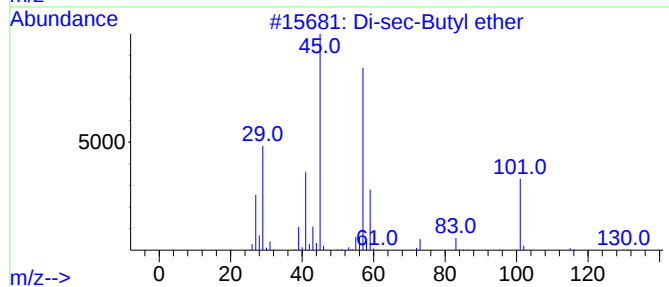
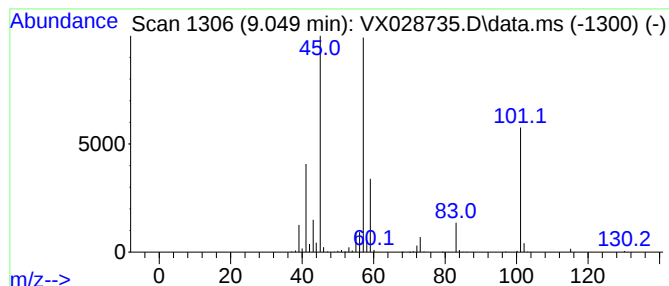
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 1-(1-methylpropoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	51.25 ug/l	1356640	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3			Boronic acid, ethyl-, diethyl ester	130	C6H15B02	053907-92-9	42
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
5			trans-2-Hexenyl lactate	172	C9H16O3	1000431-56-9	37



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

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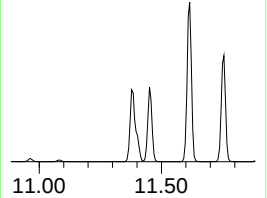
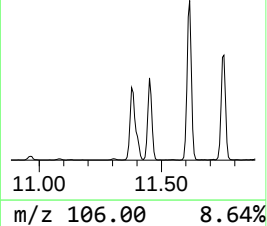
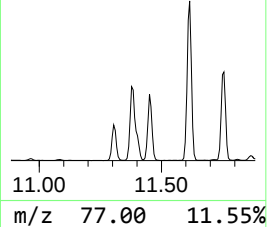
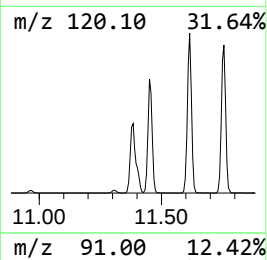
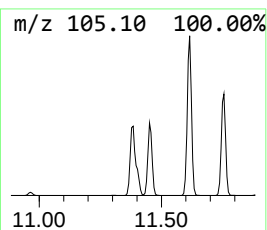
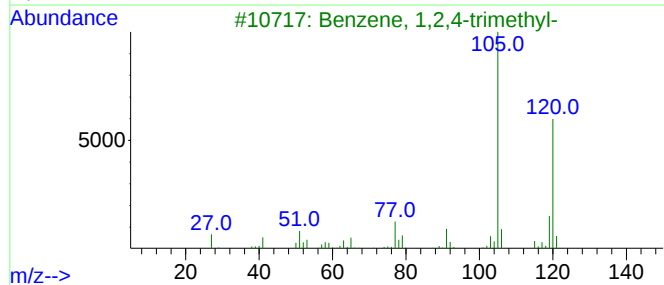
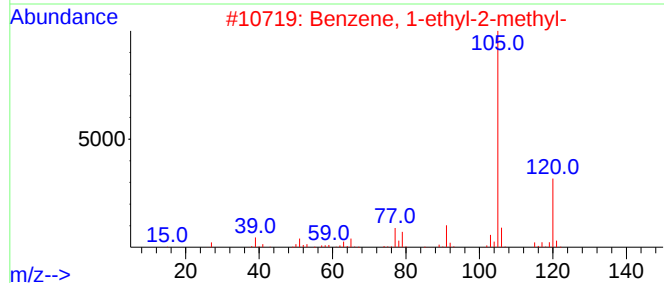
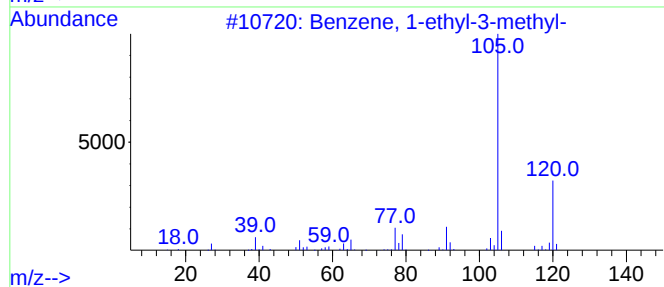
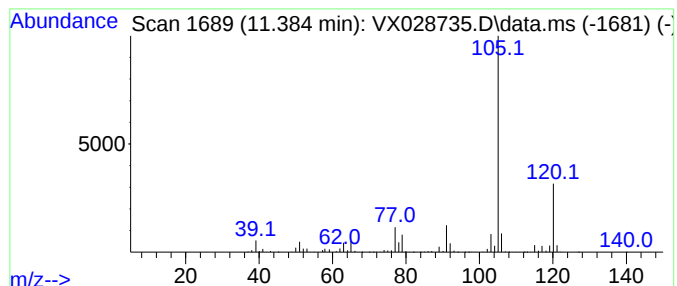
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	69.83 ug/l	1934140	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
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			Mesitylene	120	C9H12	000108-67-8	91



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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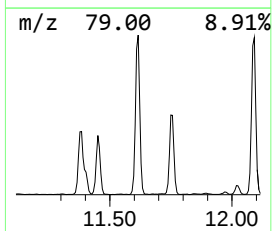
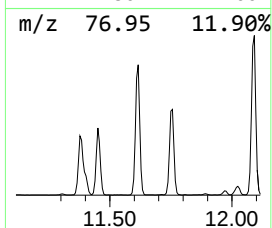
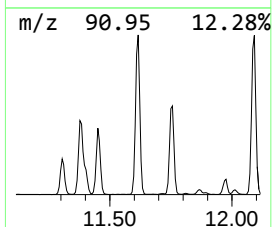
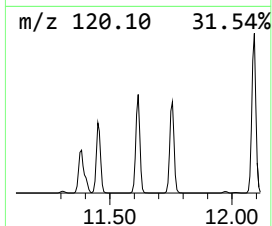
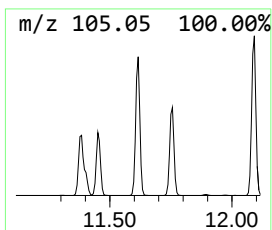
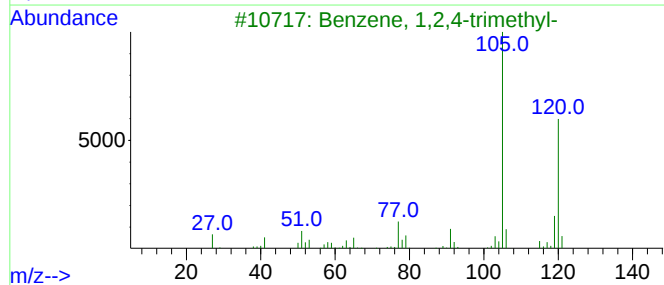
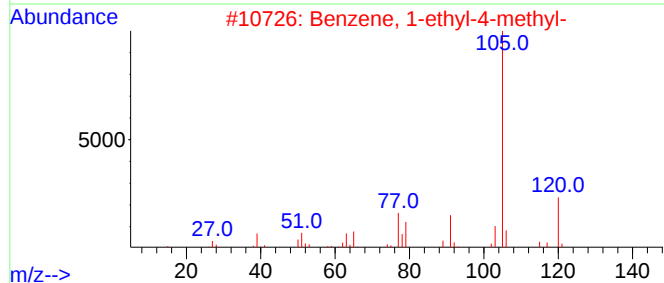
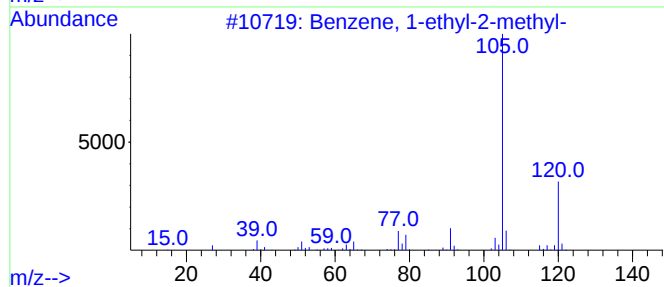
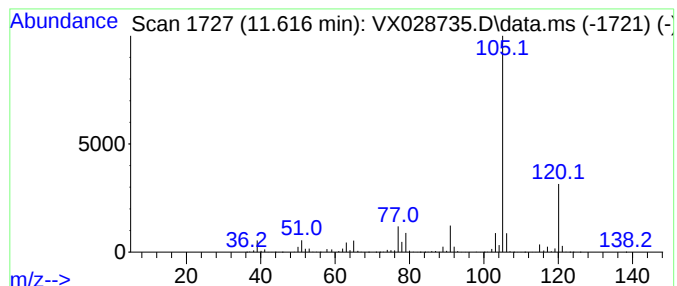
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	112.95 ug/l	3128460	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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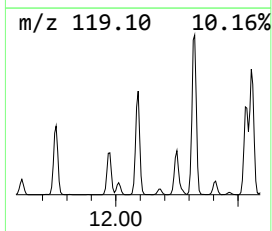
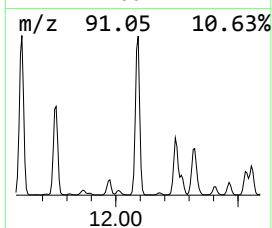
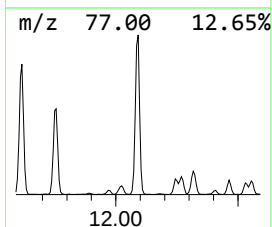
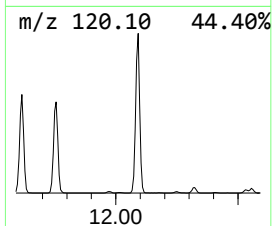
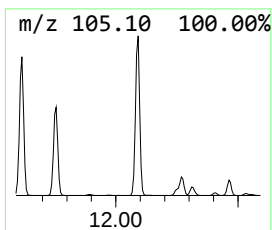
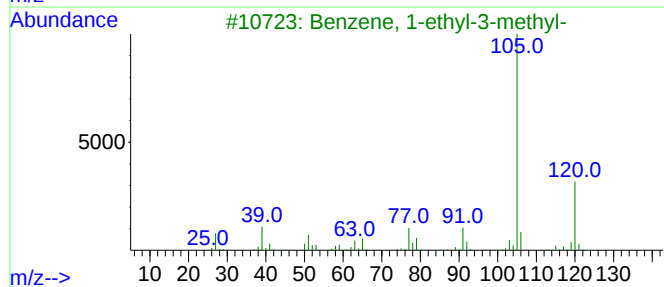
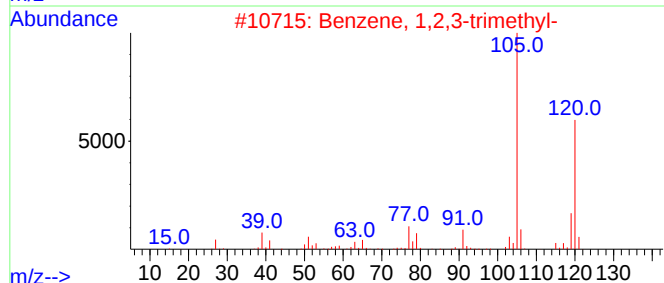
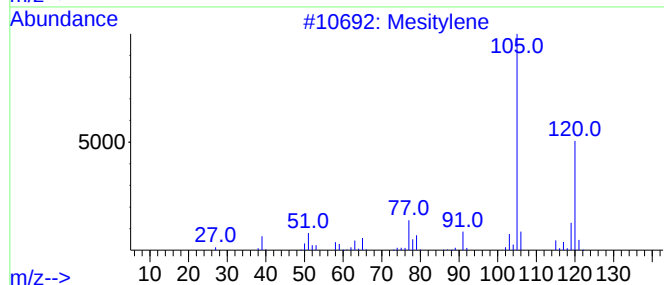
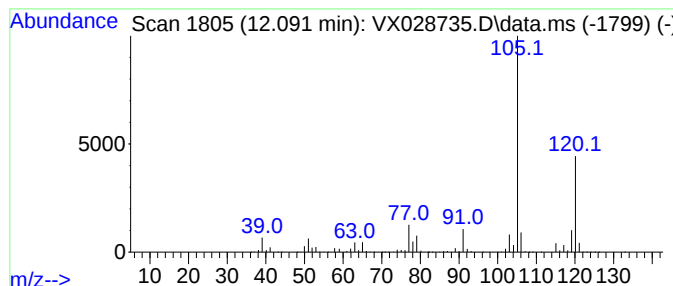
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	143.57 ug/l	3976420	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

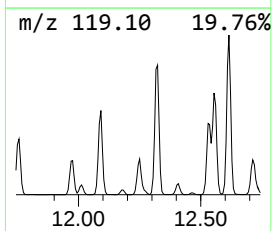
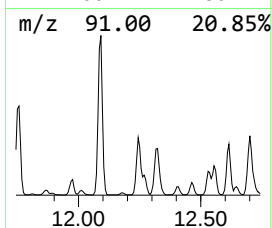
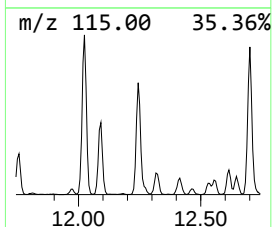
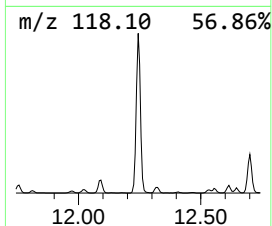
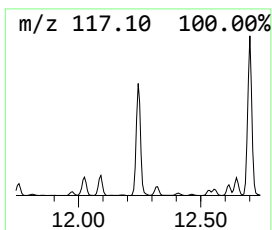
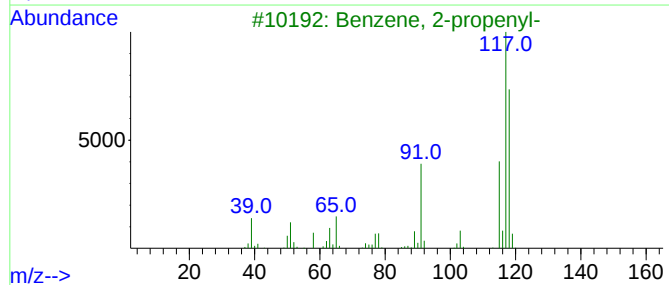
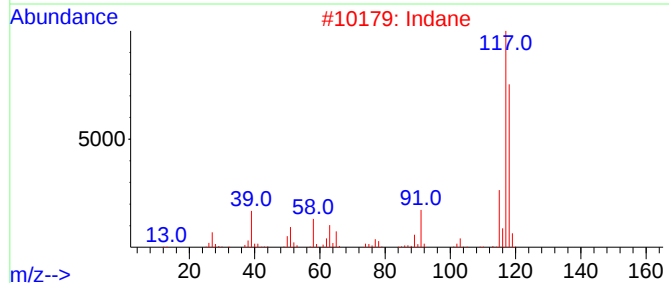
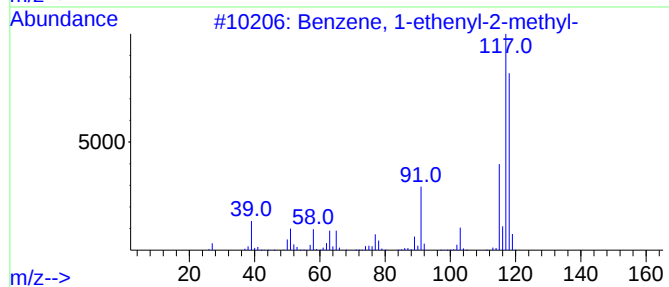
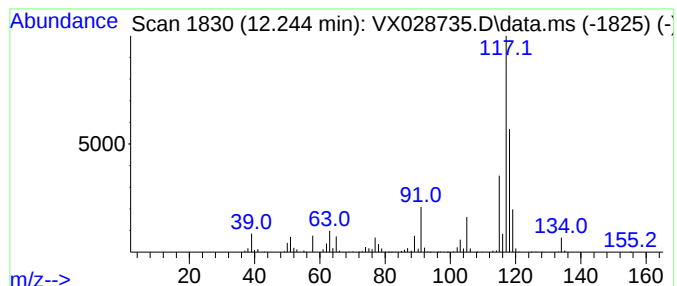
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	40.28 ug/l	1115540	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
2			Indane	118	C9H10	000496-11-7	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

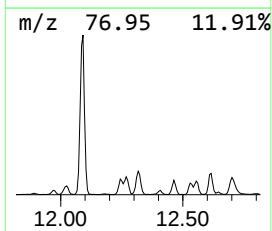
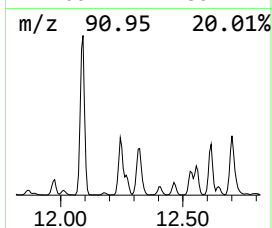
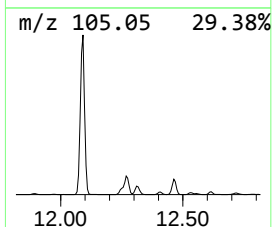
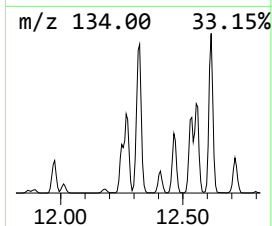
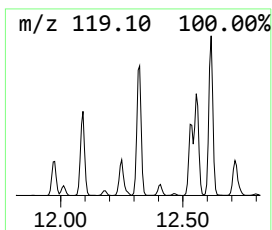
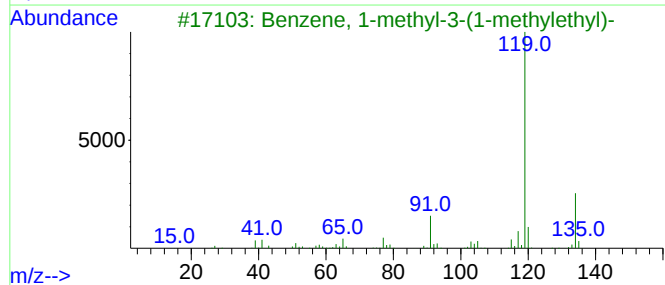
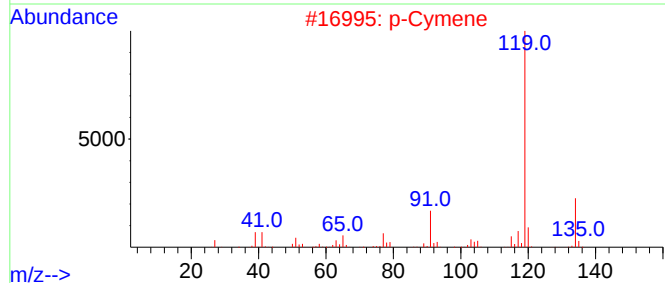
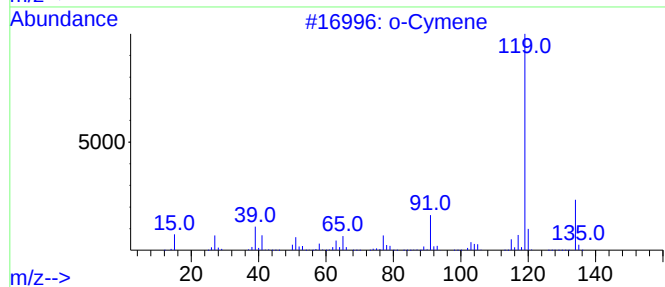
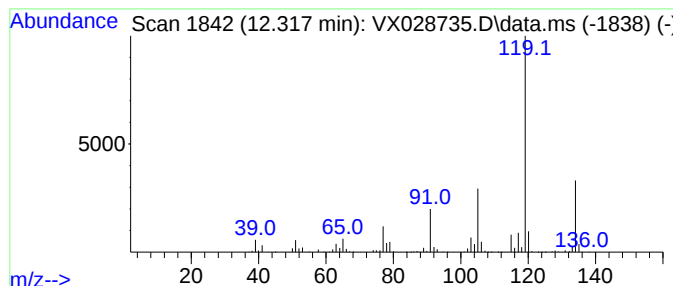
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.317	28.21 ug/l	781413	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			p-Cymene	134	C10H14	000099-87-6	95
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	94
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

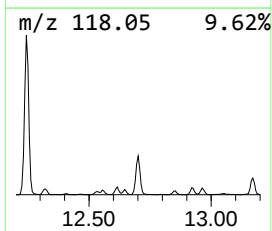
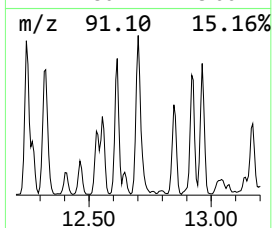
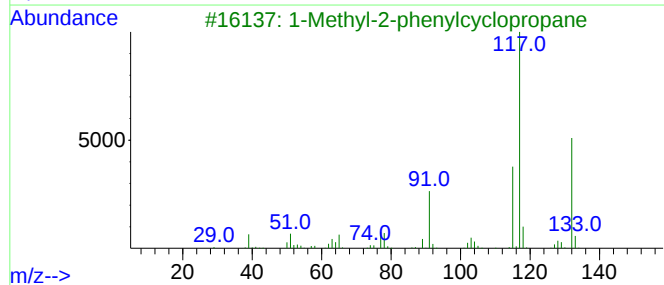
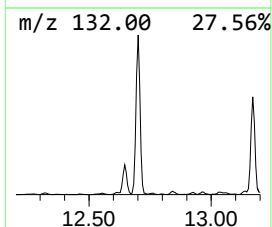
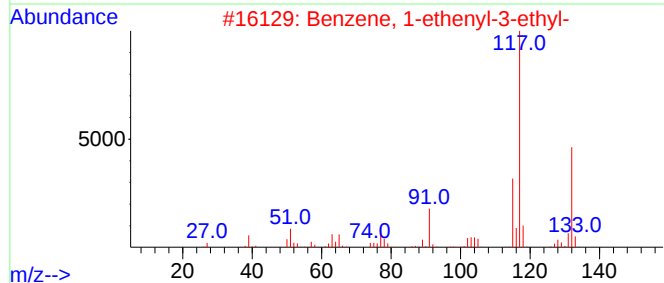
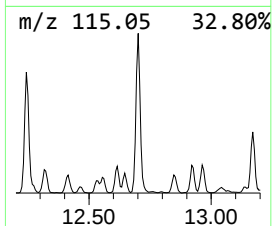
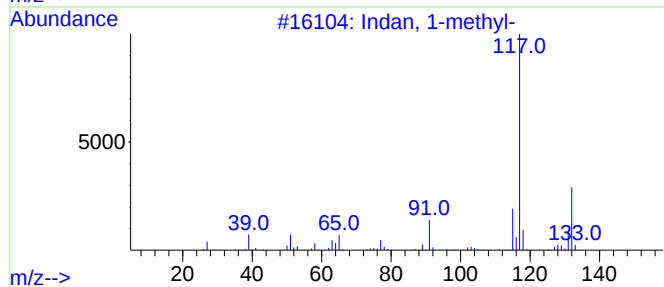
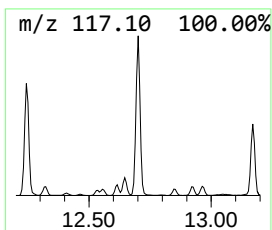
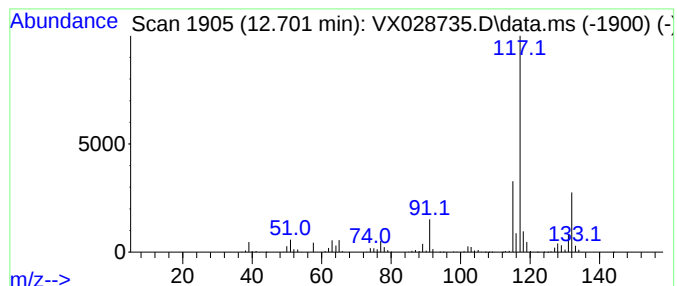
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Quant Title : SW846 8260

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

Peak Number 8 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	45.88 ug/l	1270810	1,4-Dichlorobenzene-d4	12.024

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	90
3		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

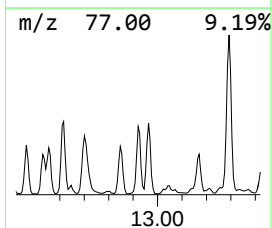
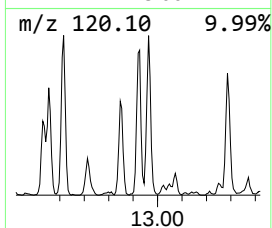
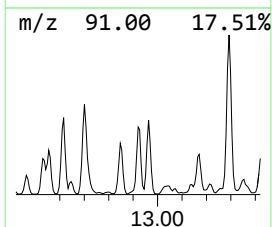
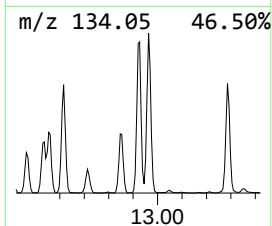
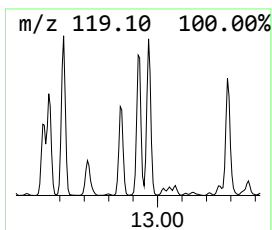
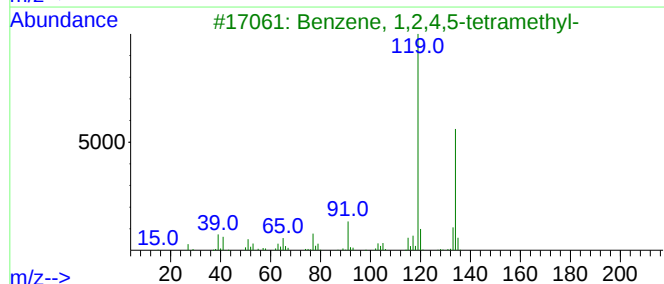
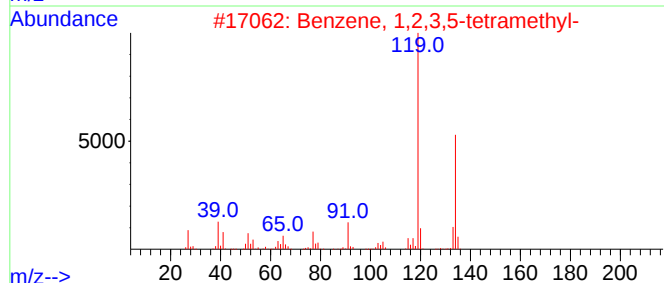
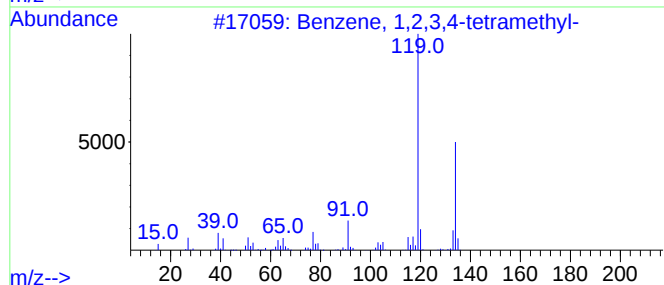
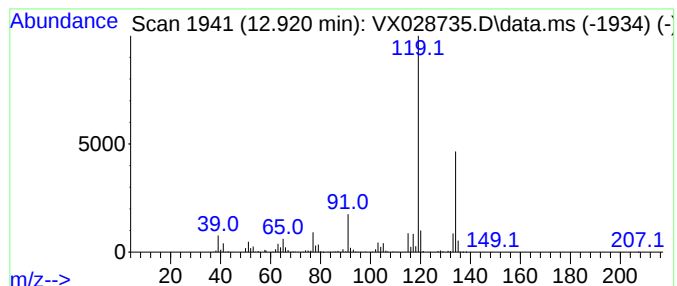
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	27.91 ug/l	772928	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

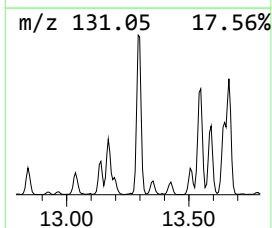
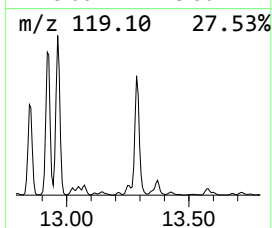
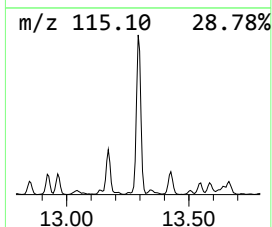
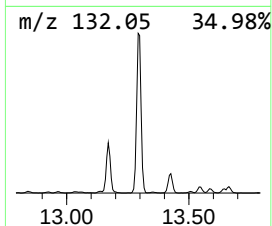
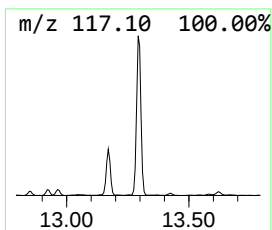
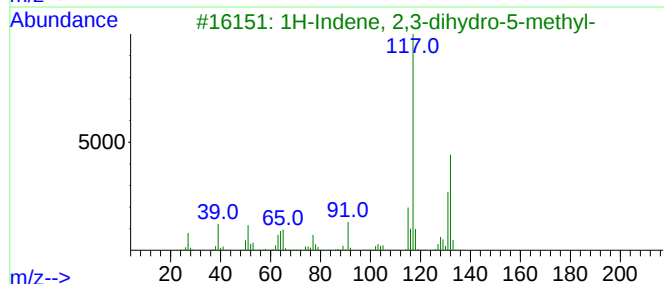
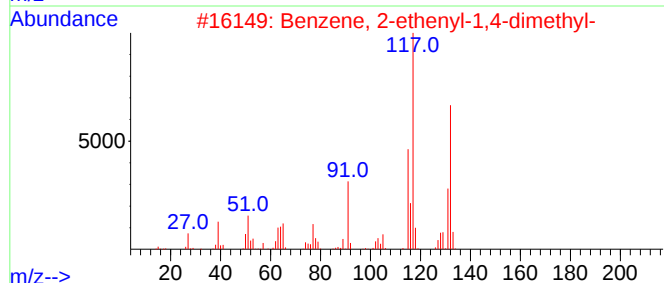
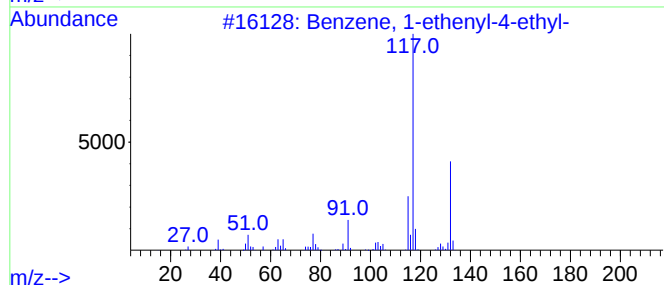
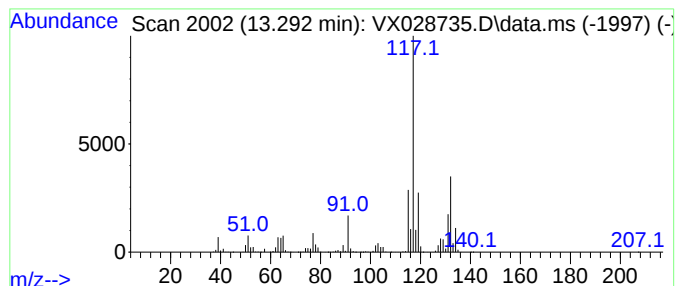
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	83.90 ug/l	2323820	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028735.D
Acq On : 16 May 2022 16:42
Operator : JC/MD
Sample : N2862-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-9RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
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Butane, 1-(1-me...	9.049	51.3	ug/l	1356640	3	10.055	1323590	50.0
Benzene, 1-ethy...	11.384	69.8	ug/l	1934140	4	12.024	1384830	50.0
Benzene, 1-ethy...	11.616	113.0	ug/l	3128460	4	12.024	1384830	50.0
Benzene, 1,2,3-...	12.091	143.6	ug/l	3976420	4	12.024	1384830	50.0
Benzene, 1-ethe...	12.244	40.3	ug/l	1115540	4	12.024	1384830	50.0
o-Cymene	12.317	28.2	ug/l	781413	4	12.024	1384830	50.0
Indan, 1-methyl-	12.701	45.9	ug/l	1270810	4	12.024	1384830	50.0
Benzene, 1,2,3,...	12.920	27.9	ug/l	772928	4	12.024	1384830	50.0
Benzene, 1-ethe...	13.292	83.9	ug/l	2323820	4	12.024	1384830	50.0