

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
 Data File : VX029640.D
 Acq On : 21 Jun 2022 04:59
 Operator : JC/MD
 Sample : N3354-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-48

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029640.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.294	26	34	43	rBV3	15967	56866	3.85%	0.398%
2	2.136	166	172	179	rVB	19791	33056	2.24%	0.231%
3	2.562	230	242	254	rBV3	8382	29947	2.03%	0.209%
4	2.867	286	292	301	rVB2	21849	44902	3.04%	0.314%
5	2.977	301	310	324	rVV	52313	143402	9.72%	1.003%
6	3.117	324	333	344	rVB	87104	200517	13.59%	1.402%
7	3.763	426	439	447	rBV4	25657	77621	5.26%	0.543%
8	4.306	516	528	540	rBV2	19653	55549	3.77%	0.388%
9	5.202	667	675	686	rVB4	7295	22851	1.55%	0.160%
10	5.391	693	706	715	rBV	147716	430337	29.17%	3.009%
11	5.556	724	733	751	rVB	270759	782420	53.03%	5.471%
12	5.958	788	799	811	rBV	157233	420474	28.50%	2.940%
13	6.202	830	839	845	rBV2	12304	36945	2.50%	0.258%
14	6.367	856	866	878	rVB2	5706	20007	1.36%	0.140%
15	6.763	922	931	943	rBV	413775	998585	67.68%	6.983%
16	6.848	943	945	958	rVB3	10903	25509	1.73%	0.178%
17	7.171	994	998	1006	rVB4	9197	20744	1.41%	0.145%
18	7.366	1021	1030	1039	rVB8	8082	24888	1.69%	0.174%
19	7.885	1104	1115	1122	rBB6	8146	28136	1.91%	0.197%
20	8.147	1145	1158	1163	rBV	23599	45422	3.08%	0.318%
21	8.427	1198	1204	1210	rBV2	16195	28962	1.96%	0.203%
22	8.506	1210	1217	1224	rVB3	23614	44394	3.01%	0.310%
23	8.653	1232	1241	1249	rBV	826969	1294898	87.77%	9.055%
24	8.958	1282	1291	1298	rBV	137557	215227	14.59%	1.505%
25	9.049	1298	1306	1313	rVV	152626	228243	15.47%	1.596%
26	9.165	1320	1325	1332	rVB	10671	16426	1.11%	0.115%
27	9.451	1364	1372	1375	rBV3	9725	21368	1.45%	0.149%
28	9.494	1375	1379	1386	rVB2	11233	20374	1.38%	0.142%
29	10.055	1461	1471	1481	rBV	816294	1111389	75.33%	7.772%
30	10.305	1506	1512	1517	rVB	18954	30284	2.05%	0.212%
31	10.409	1521	1529	1538	rVB6	12160	26337	1.79%	0.184%
32	10.963	1614	1620	1626	rBV	299005	366034	24.81%	2.560%
33	11.085	1634	1640	1646	rBV	610715	798671	54.13%	5.585%
34	11.305	1671	1676	1684	rBV	274002	333241	22.59%	2.330%
35	11.451	1696	1700	1707	rVB2	10004	15991	1.08%	0.112%
36	11.616	1722	1727	1735	rVB	43574	57512	3.90%	0.402%

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37	11.713	1735	1743	1747	rBV4	12401	20697	1.40%	0.145%
38	11.866	1762	1768	1770	rBV	26257	34770	2.36%	0.243%
39	11.890	1770	1772	1780	rVB	51118	60647	4.11%	0.424%
40	12.024	1789	1794	1805	rVB	779993	971913	65.88%	6.796%
41	12.177	1815	1819	1823	rBV	25829	33653	2.28%	0.235%
42	12.244	1823	1830	1836	rVV	1224581	1475343	100.00%	10.317%
43	12.317	1838	1842	1850	rVB2	30723	56057	3.80%	0.392%
44	12.408	1850	1857	1863	rBV	60955	80531	5.46%	0.563%
45	12.469	1863	1867	1872	rVB2	22052	33930	2.30%	0.237%
46	12.616	1886	1891	1894	rBV	228276	273835	18.56%	1.915%
47	12.646	1894	1896	1900	rVV	69457	78617	5.33%	0.550%
48	12.701	1900	1905	1912	rVV	453274	596078	40.40%	4.168%
49	12.841	1919	1928	1933	rVB	27546	40111	2.72%	0.280%
50	12.920	1934	1941	1946	rBV	358722	457469	31.01%	3.199%
51	12.963	1946	1948	1954	rVB3	11724	16206	1.10%	0.113%
52	13.030	1954	1959	1965	rVB3	21497	34031	2.31%	0.238%
53	13.097	1965	1970	1973	rBV	14568	20580	1.39%	0.144%
54	13.140	1973	1977	1979	rVV2	33202	41395	2.81%	0.289%
55	13.170	1979	1982	1992	rVB2	62181	95274	6.46%	0.666%
56	13.292	1997	2002	2007	rVB2	318259	415083	28.13%	2.903%
57	13.347	2007	2011	2014	rBV2	27945	33134	2.25%	0.232%
58	13.426	2020	2024	2029	rVB3	17438	25448	1.72%	0.178%
59	13.542	2039	2043	2047	rBV	44279	61113	4.14%	0.427%
60	13.579	2047	2049	2053	rVV2	40776	52790	3.58%	0.369%
61	13.621	2053	2056	2058	rVV	21258	28182	1.91%	0.197%
62	13.676	2061	2065	2070	rVB2	33864	62107	4.21%	0.434%
63	13.798	2080	2085	2089	rVB6	10262	17293	1.17%	0.121%
64	13.853	2090	2094	2099	rVV	59677	73928	5.01%	0.517%
65	13.926	2099	2106	2110	rVV	91716	119153	8.08%	0.833%
66	13.969	2110	2113	2118	rVB2	16077	21102	1.43%	0.148%
67	14.079	2126	2131	2133	rBV	26548	34647	2.35%	0.242%
68	14.103	2133	2135	2144	rVB2	17514	22245	1.51%	0.156%
69	14.213	2149	2153	2164	rVV2	15816	35450	2.40%	0.248%
70	14.323	2164	2171	2175	rVV	34118	50245	3.41%	0.351%
71	14.377	2176	2180	2186	rVB3	27969	42973	2.91%	0.301%
72	14.481	2192	2197	2203	rBV2	35649	50399	3.42%	0.352%
73	14.603	2211	2217	2220	rBV	26694	43365	2.94%	0.303%
74	14.676	2225	2229	2235	rVB5	8869	14866	1.01%	0.104%
75	14.780	2241	2246	2254	rBV	261413	350674	23.77%	2.452%
76	15.182	2305	2312	2317	rBV2	15208	25102	1.70%	0.176%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : SW846 8260

77	15.408	2345	2349	2354	rVB	15214	21503	1.46%	0.150%
78	15.615	2375	2383	2387	rVV3	21222	37452	2.54%	0.262%
79	15.810	2410	2415	2418	rVV	19977	32872	2.23%	0.230%
80	15.847	2418	2421	2425	rVB3	16551	23696	1.61%	0.166%
81	15.987	2438	2444	2453	rBV	33624	57307	3.88%	0.401%
82	16.328	2496	2500	2507	rVB2	10065	19493	1.32%	0.136%

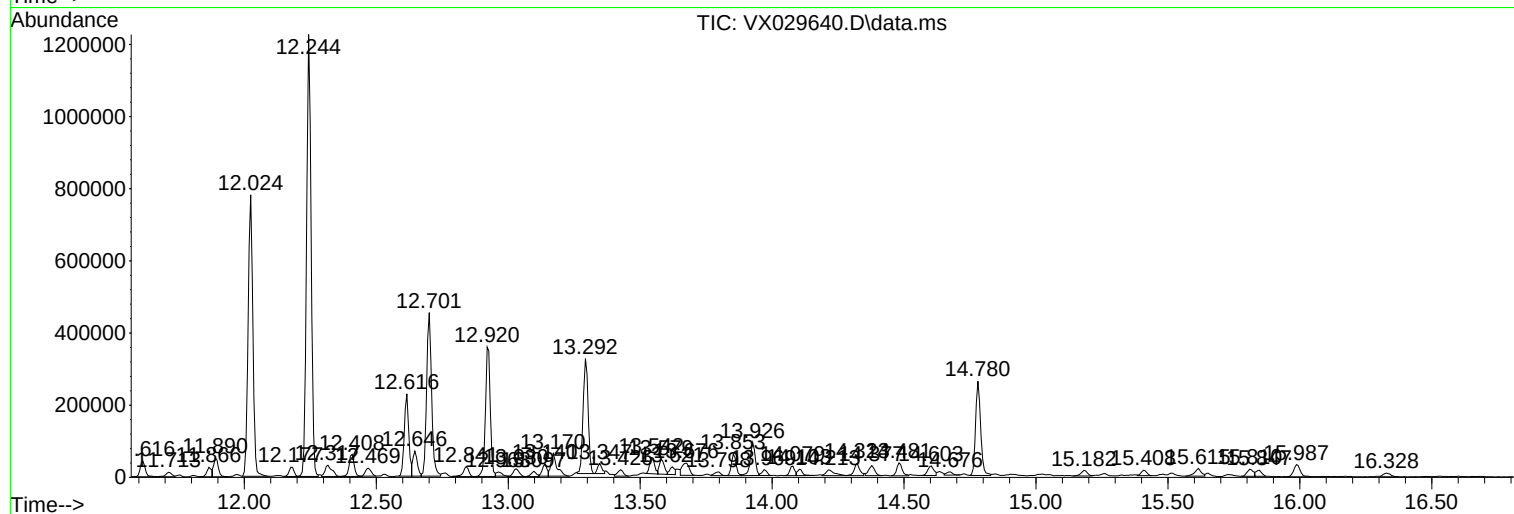
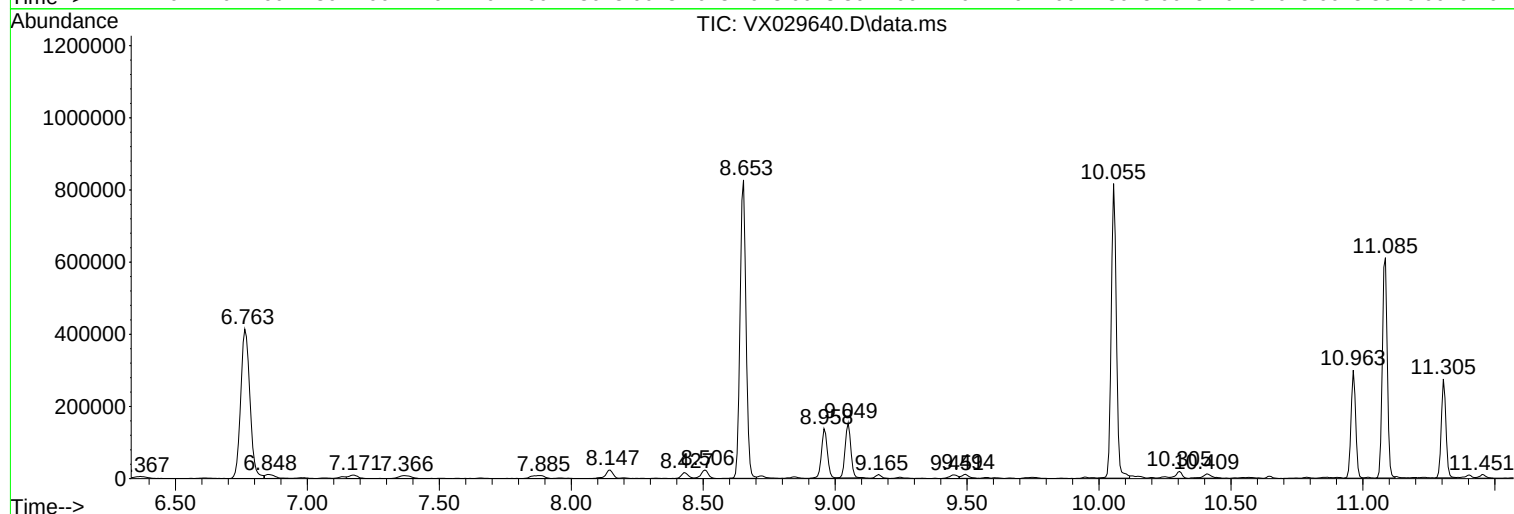
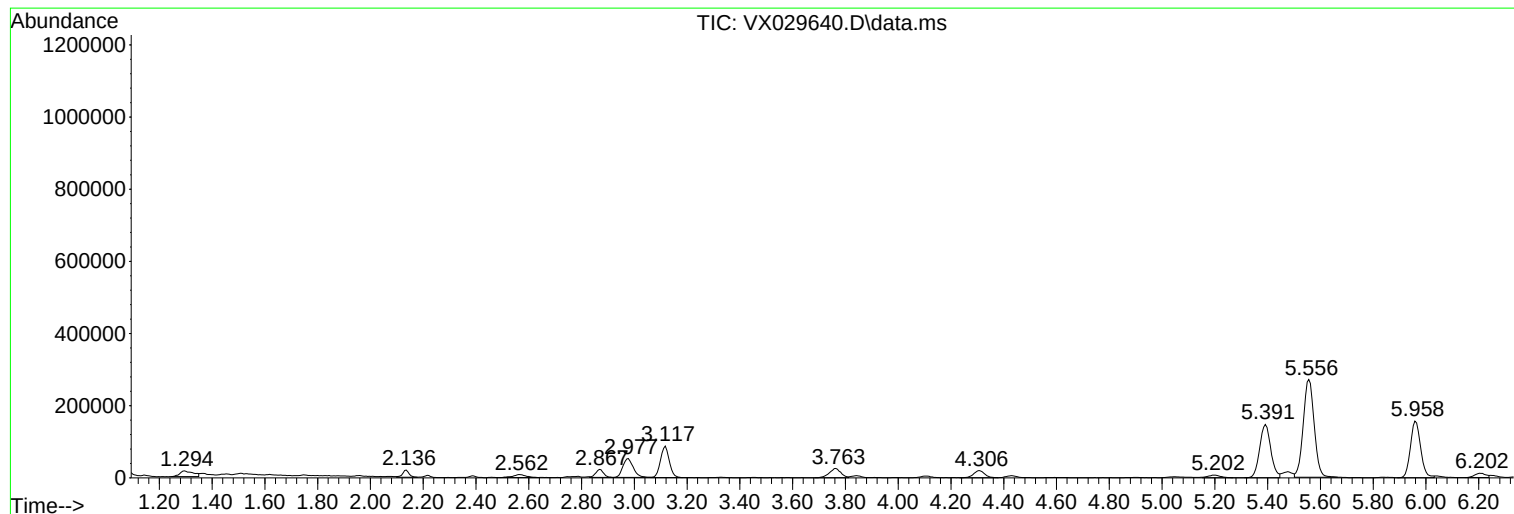
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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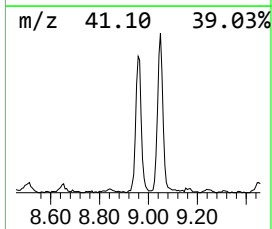
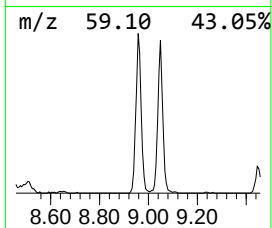
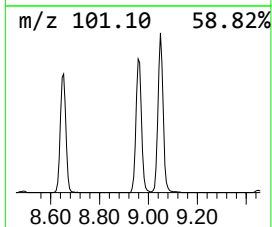
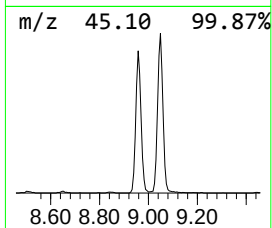
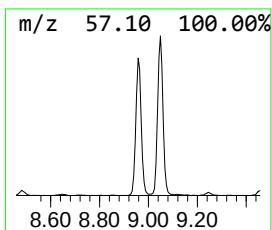
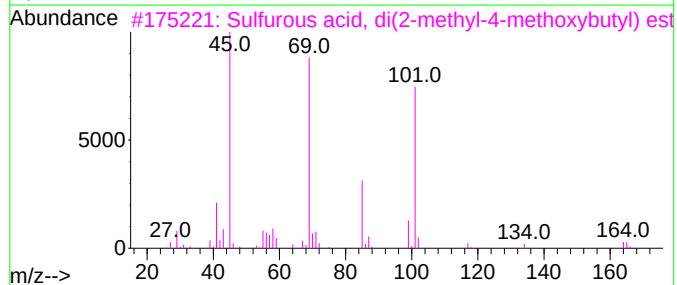
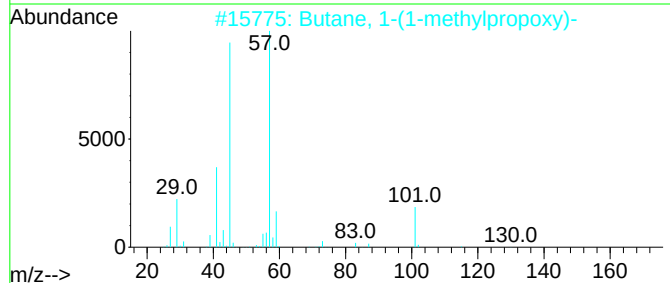
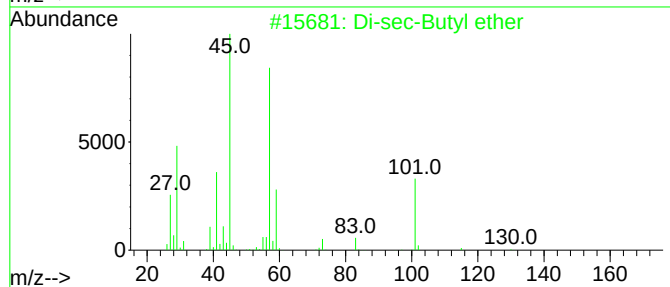
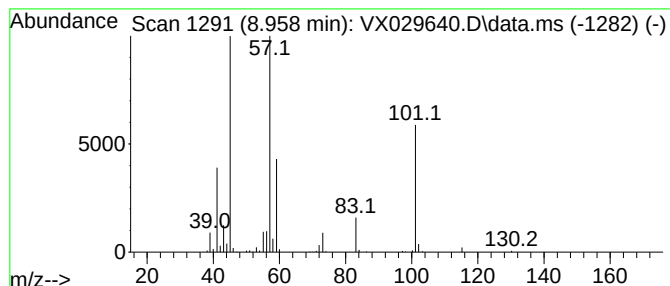
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Di-sec-Butyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	9.68 ug/l	215227	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			Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	47
4			2-t-Butyl-5-methyl[1,3]dioxolan...	158	C8H14O3	130930-47-1	42
5			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39



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ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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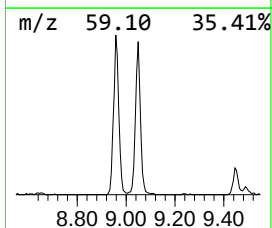
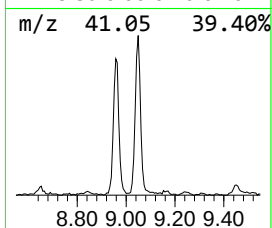
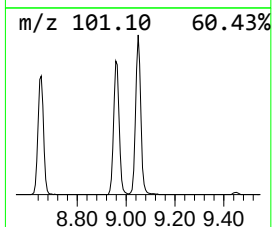
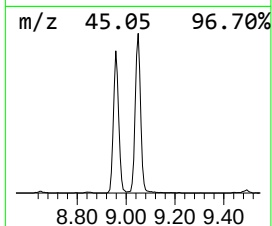
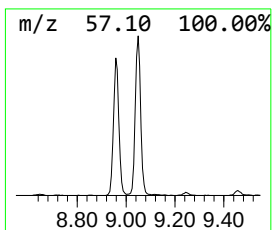
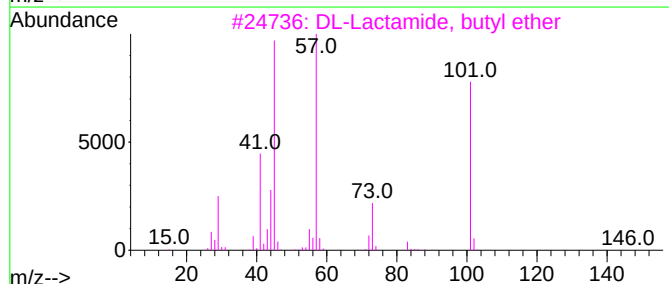
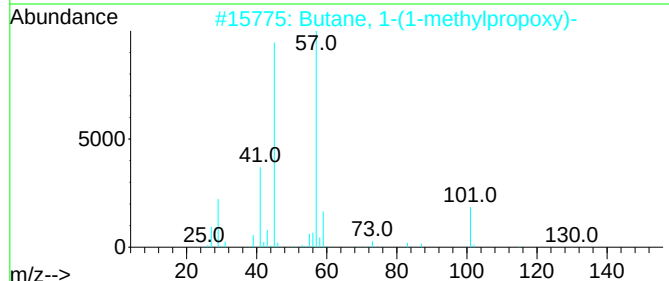
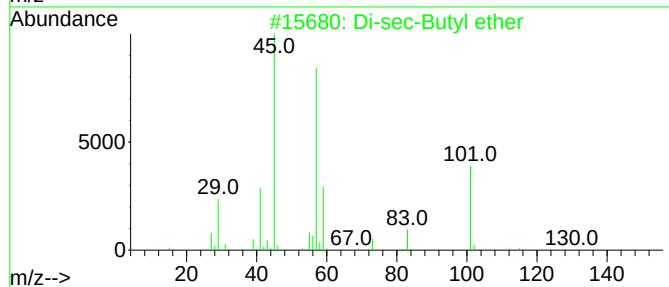
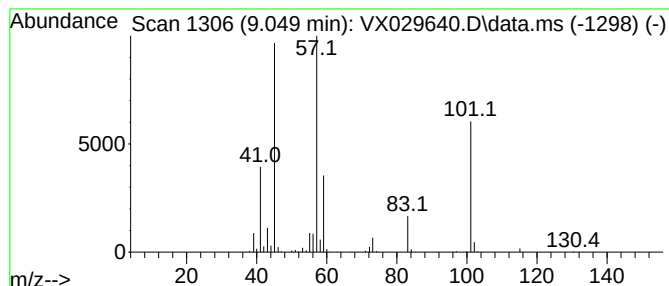
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 1-(1-methylpropoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	10.27 ug/l	228243	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			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
4			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	45
5			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	39



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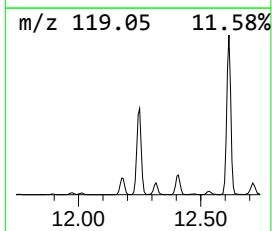
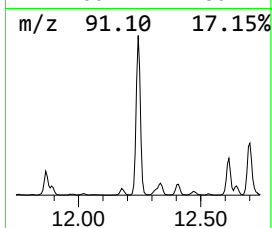
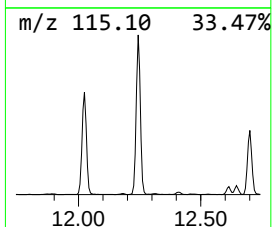
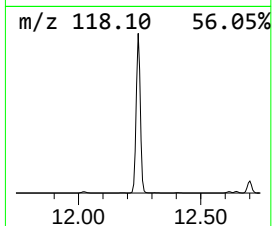
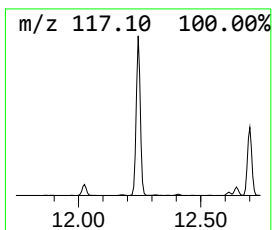
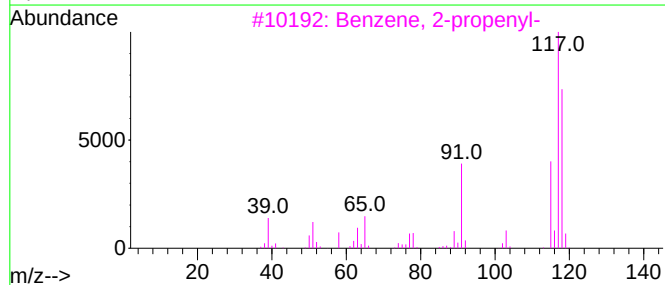
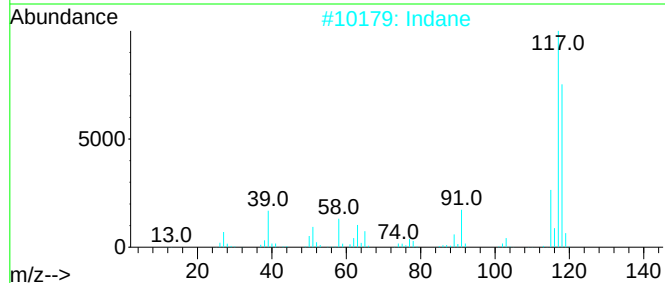
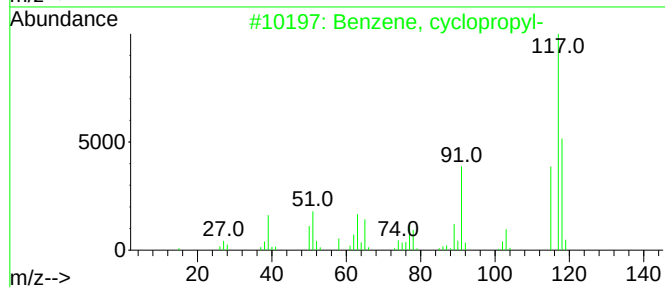
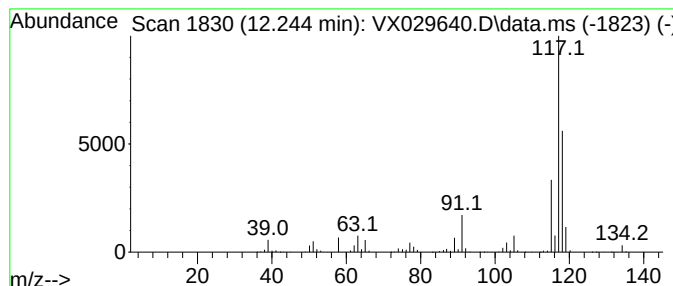
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	75.90 ug/l	1475340	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Deltacyclene	118	C9H10	007785-10-6	64



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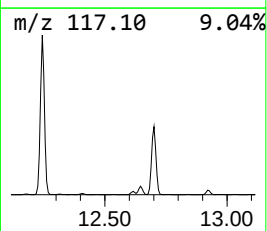
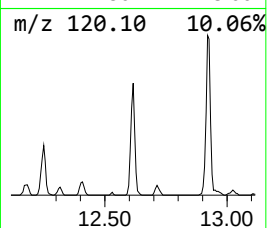
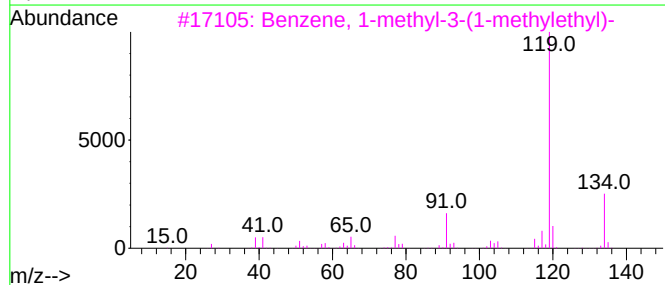
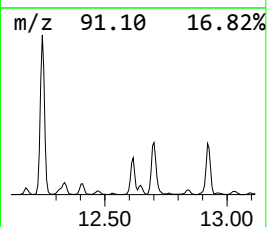
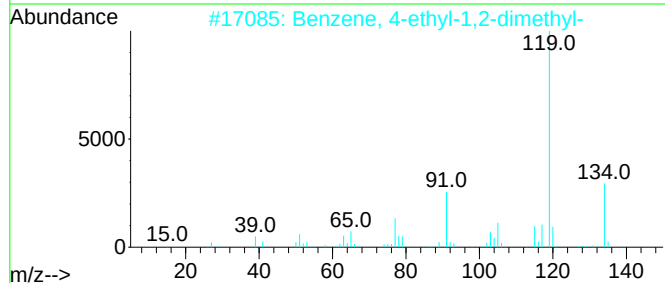
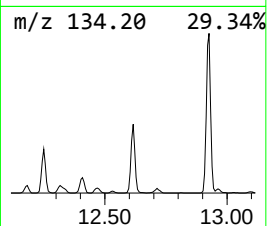
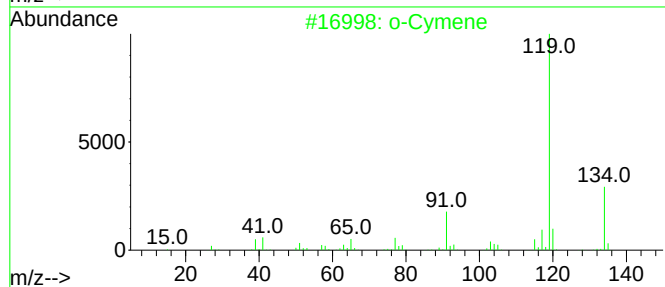
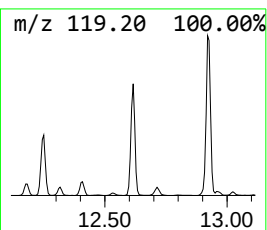
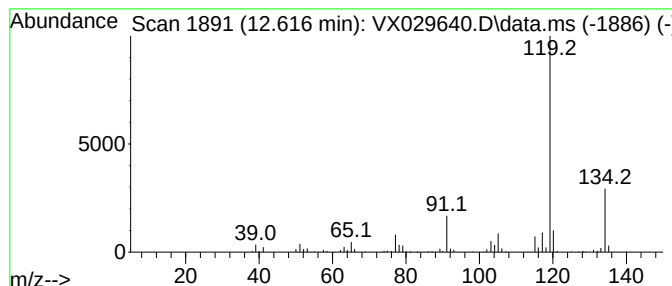
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Quant Title : SW846 8260

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

Peak Number 4 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	14.09 ug/l	273835	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

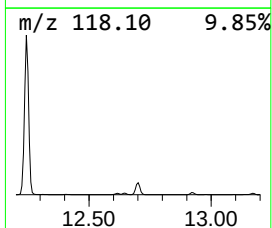
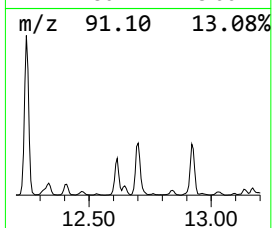
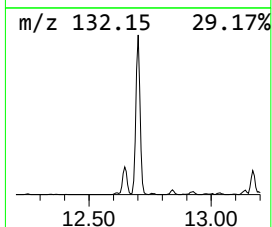
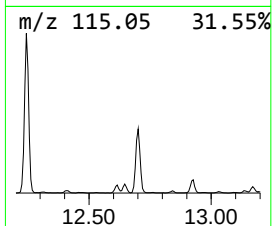
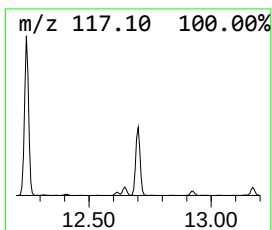
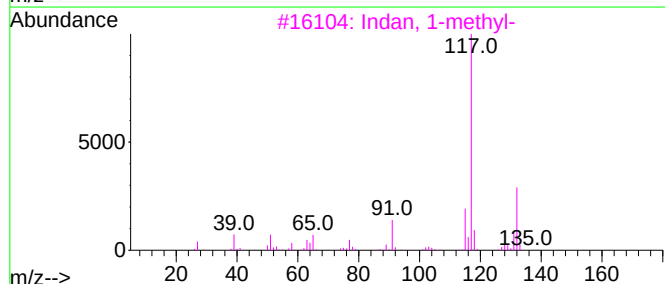
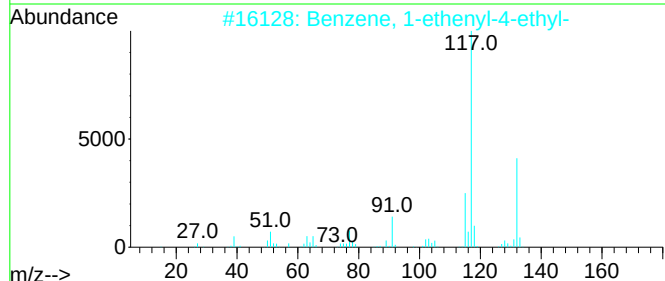
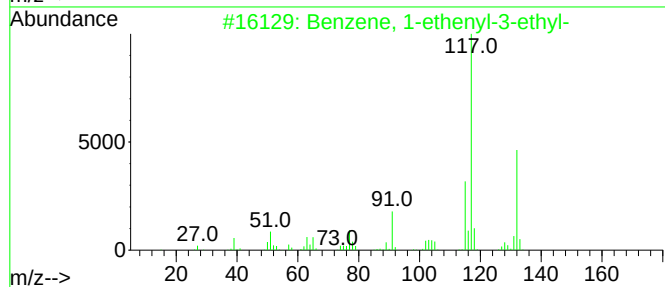
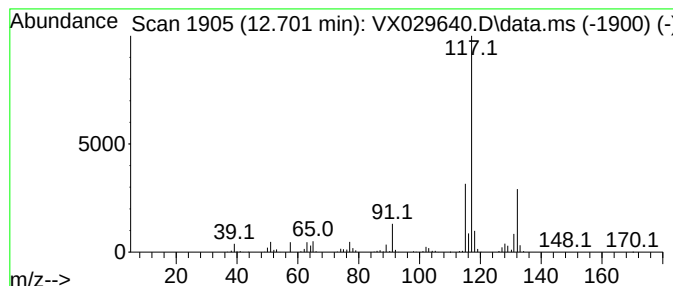
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	30.67 ug/l	596078	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	90
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

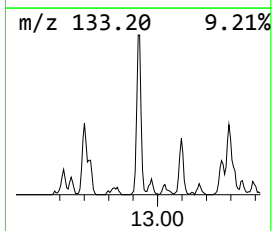
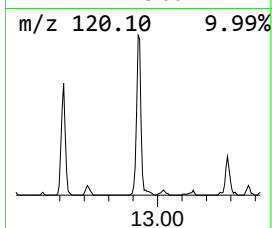
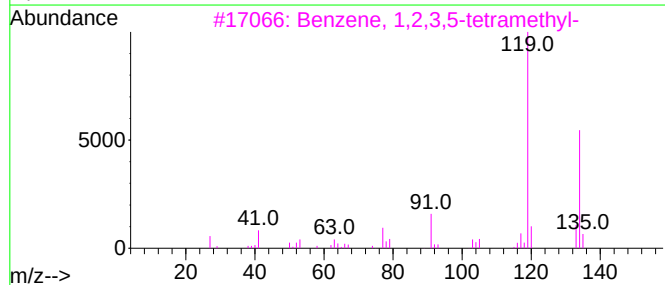
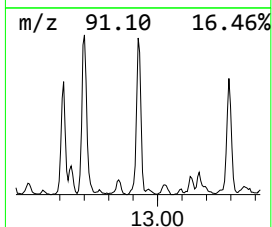
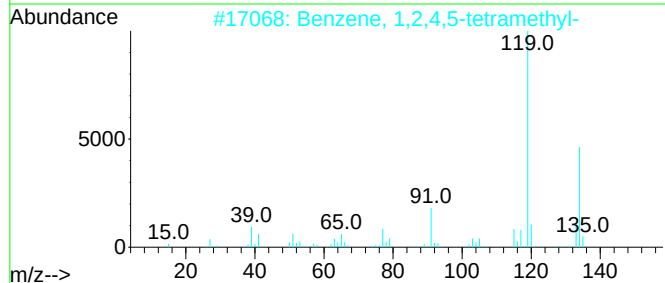
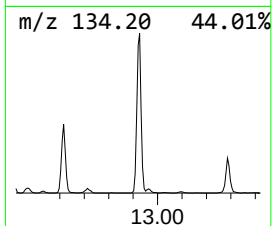
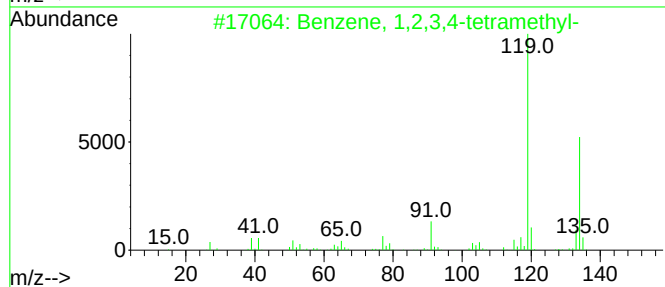
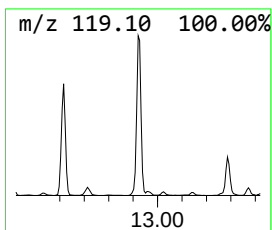
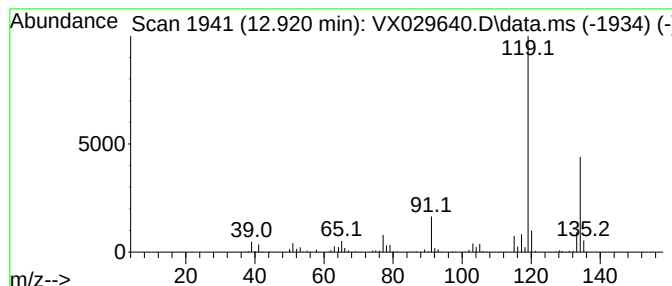
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	23.53 ug/l	457469	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, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

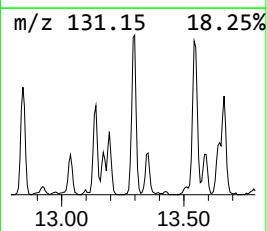
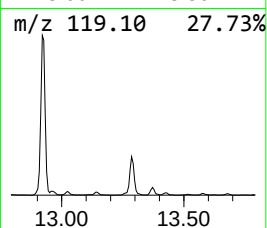
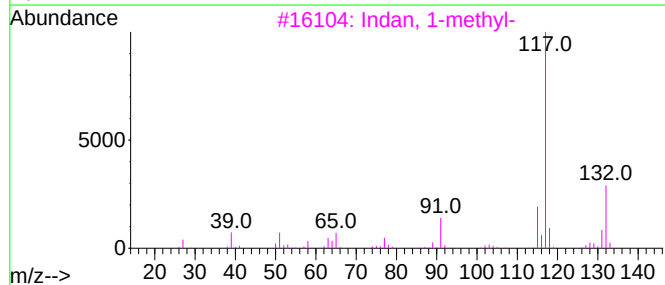
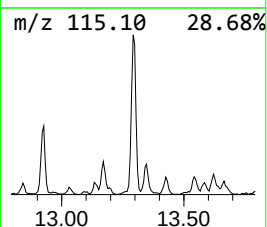
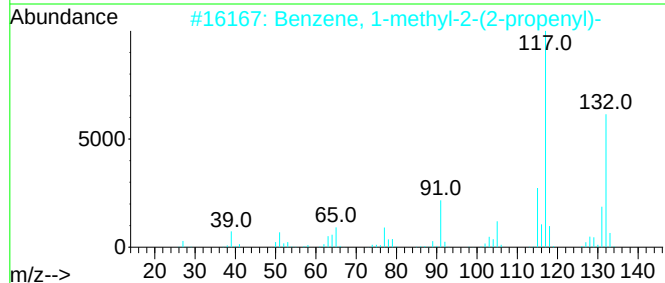
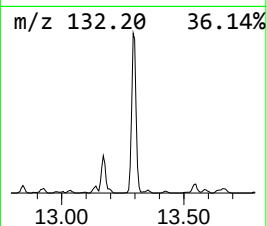
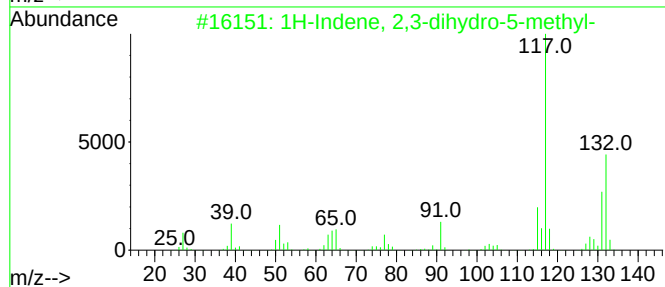
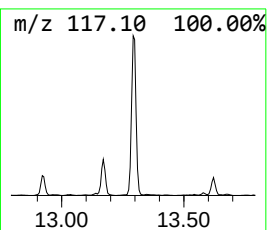
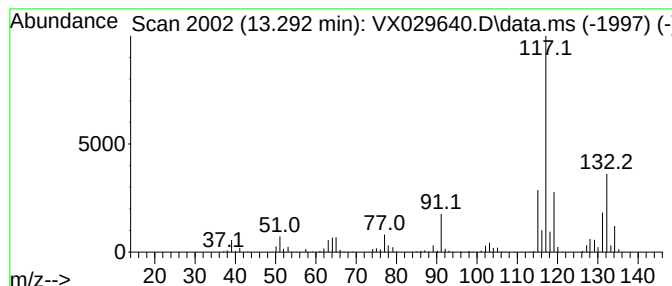
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	21.35 ug/l	415083	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
2		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
3		Indan, 1-methyl-	132	C10H12	000767-58-8	81
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

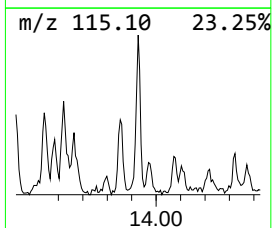
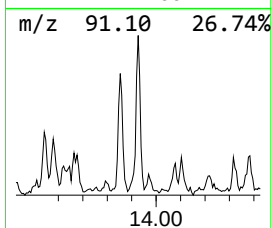
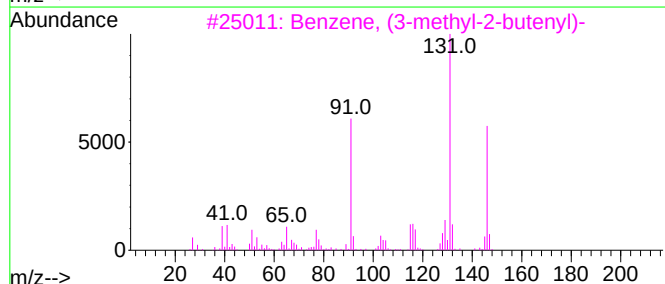
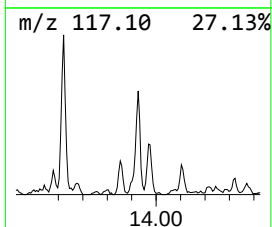
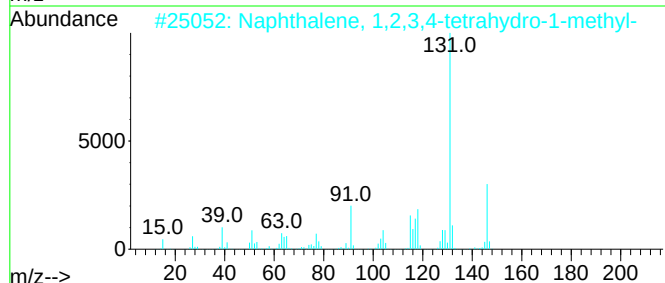
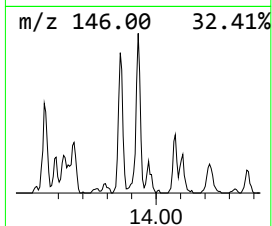
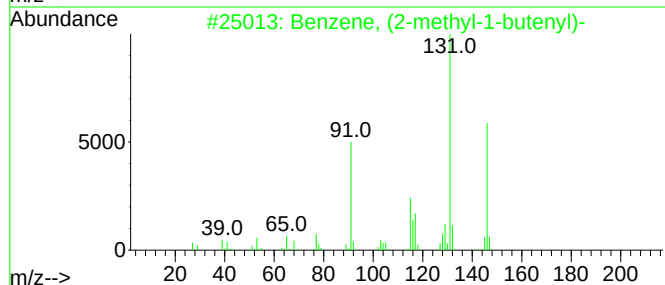
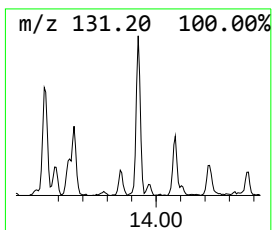
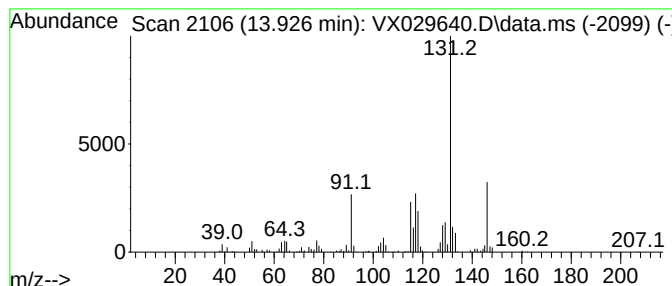
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	6.13 ug/l	119153	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	94
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	94
4			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

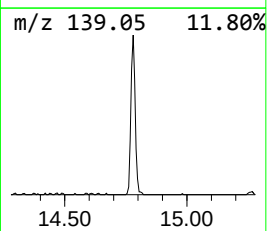
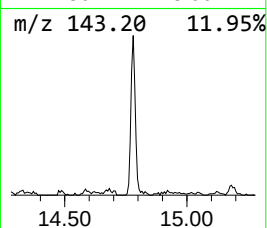
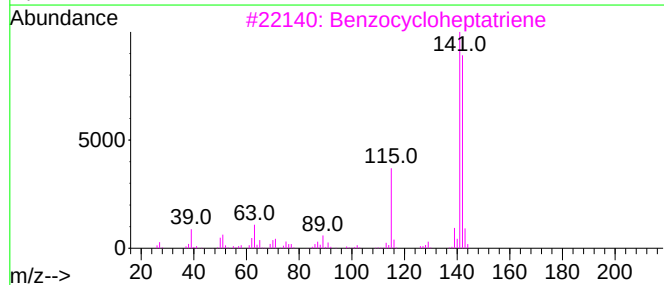
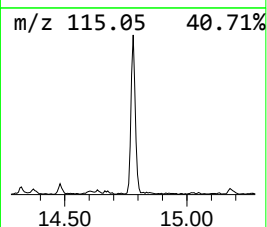
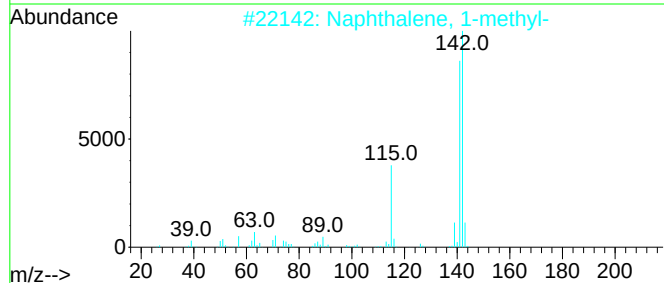
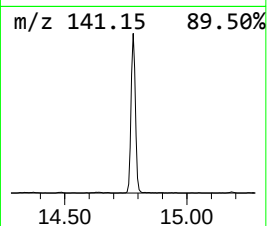
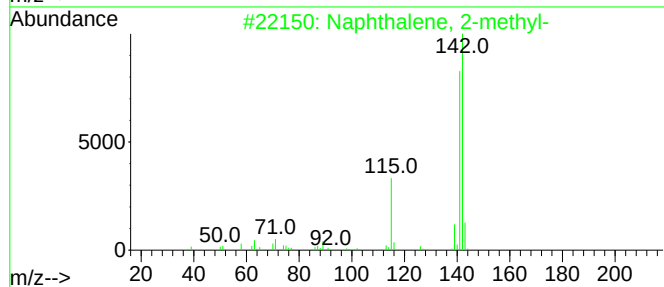
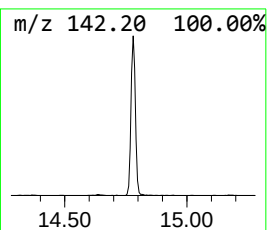
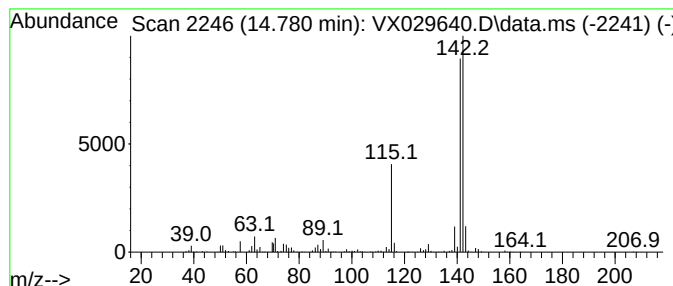
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Quant Title : SW846 8260

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

Peak Number 9 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	18.04 ug/l	350674	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029640.D
Acq On : 21 Jun 2022 04:59
Operator : JC/MD
Sample : N3354-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-48

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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	10.3	ug/l	228243	3	10.055	1111390	50.0
Benzene, cyclop...	12.244	75.9	ug/l	1475340	4	12.024	971913	50.0
o-Cymene	12.616	14.1	ug/l	273835	4	12.024	971913	50.0
Benzene, 1-ethe...	12.701	30.7	ug/l	596078	4	12.024	971913	50.0
Benzene, 1,2,3,...	12.920	23.5	ug/l	457469	4	12.024	971913	50.0
1H-Indene, 2,3-...	13.292	21.4	ug/l	415083	4	12.024	971913	50.0
Benzene, (2-met...	13.926	6.1	ug/l	119153	4	12.024	971913	50.0
Benzocyclohepta...	14.780	18.0	ug/l	350674	4	12.024	971913	50.0